Free Particle

Quantum mechanics for some simple system

يمكن استخدام طرق ميكانيك الكم لبعض الانظمة البسيطة ويمكن ان تحل بمعادلة Schrodinger فتكون تعابير لدالة الموجة

(Energy and wave function $\Psi_{(x)}$ النظام وطاقته)

1-Free Particle Problem

An object of mass (m) in direction (x) of constant potential energy V (x) .

H^ = T + V

$= -i\,\mathbf{h}^2/2m\,\partial^2/\partial^2x + V(x)$

$H\Psi = E\Psi$ Schrodinger equation

$-i\,\mathbf{h}^2/2m\,\partial^2/\partial^2x\,\Psi_{(x)} = E\,\Psi_{(x)}$ ....x $-2m/\mathbf{h}^2$

$\partial^2/\partial^2x\,\Psi_{(x)} = -2m/\mathbf{h}^2\,E\,\Psi_{(x)}$

Suppose that $2mE/h^2 = k^2$ ....$E = \mathbf{h}^2 k^2/2m$, $\mathbf{h} = h/2\pi$

One dimension $i = \sqrt{-1}$, $i^2 = -1$

$$\Psi_{(x)} = A\,e^{-ikx} + B\,e^{ikx}$$

by using [Euler law]

$e^{\pm i\alpha} = \cos\alpha \pm I\sin\alpha$ .... $\alpha = kx$

$\Psi_{(x)} = A(\cos kx + I\sin kx) + B(\cos kx - I\sin kx)$

$= A\cos kx + A\,I\sin kx + B\cos kx - B\,I\sin kx$

$= (A+B)\cos kx + (A-B)\,i\sin kx$

$\Psi_{(x)} = C\cos kx + D\,i\sin kx$

k constant طاقة الجسيم الحر غير مكممة

1-inside box

Boundary condition

1- $V(x) = 0$				
2- $0 < x < a$				
3 -$\Psi(0)=0$,	$\Psi(a) =0$,	$x=0$,	$x= a$	

Ex1/ prove an object in box a quantized ?

$\Psi_{(x)} = C \cos kx + D\, i \sin kx$

$\Psi_{(x)} = \Psi_{(0)} = C \cos k(0) + D\, i \sin k(0)$

$0=C x 1 + \text{zero}$ ……..$\sin 0= 0$, $\cos 0= 1$

$0=C$

لكي يكون مجموع الحدين zero يجب ان تكون قيمة الثابت C مساوية الى zero لذلك يلغى الحد $0=C \cos kx$

$\Psi_{(x)} = D\, i \sin kx$

$\Psi_{(x)} = \Psi_{(a)} = D\, i \sin ka$

$ka = n\pi$ ………$k = n\pi/a$, $n=1,2,3$ ……

$E=\mathbf{h}^2 k^2 /2m = h^2 n^2 \pi^2/4\pi^2 a^2/2m = n^2 h^2 / 8ma^2 =E$

$\mathbf{E= n^2 h^2 / 8ma^2}$ Energy of an object in box quantity

2- outside box

Boundary condition

1- $V(x) = \infty$
2- $0 > x > a$
3 -$\Psi(x)=0$

$H\hat{} = T + V$

$= -i\, \mathbf{h}^2 / 2m\, \partial^2/\partial^2 x + V(x)$

$H\, \Psi_{(x)} = E\ \Psi_{(x)}$ Schrodinger equation

$(-i\, \mathbf{h}^2 / 2m\, \partial^2/\partial^2 x + V_{(x)})\Psi_{(x)} = E\ \Psi_{(x)}$

$-i\, \mathbf{h}^2 / 2m\, \partial^2/\partial^2 x\ \Psi_{(x)} + V_{(x)}\Psi_{(x)} = E\, \Psi_{(x)}$

$V(x) = \infty$

$-i\, \mathbf{h}^2 / 2m\, \partial^2/\partial^2 x\ \Psi_{(x)} + \infty\Psi_{(x)} = E\, \Psi_{(x)}$

$\Psi_{(x)} = E\, \Psi_{(x)} + i\, \mathbf{h}^2 / 2m\, \partial^2/\partial^2 x \Psi_{(x)} / \infty \cong 0$

$\Psi_{(x)} = 0$

Impossible finding of an object position

Ex2/ Determine the constant D for the wave function of an object in a potential box if that $\Psi_{(x)} = D\sin kx \quad or \quad D\sin \frac{n\pi x}{a}$

$\mathrm{Sin}^2 kx = 1/2\ (1-\cos 2kx)$

$\int \Psi^* \Psi\, \partial x = 1$

$\int D \sin kx\ D \sin kx = 1$

$D^2 \int \sin^2 kx\ \partial x = 1$

$\sin^2 kx = 1/2\ (1-\cos 2kx)$

$D^2 \int 1/2\ (1-\cos 2kx)\ \partial x = 1$

$D^2/2(1\text{-}\cos 2kx)\,\partial x = 1$ …….$D^2/2\,[x\text{-}\ 1/2k\ \mathrm{Sin}\ 2kx\,] = 1$

$D^2/2\,[\,a - 1/2k\ \mathrm{Sin}\ 2k\,(a)] = 1$ ………. $k = n\pi/a$

$D^2/2\,[\,a\text{-}\ a/2n\pi\ \mathrm{Sin}\ 2n\pi/a\,] = 1$

$D^2/2\ a = 1$ ………$D^2 = 2/a$ …….$D = (2/a)^{1/2}$

………………………………………

الفروقات في المستويات الطاقية لنظام مثالي تتزايد بارتفاع المستوى الطاقي

n=1	$E = n^2h^2/8ma^2$	$E = h^2/8ma^2$
n=2	$E = 4h^2/8ma^2$	$E = h^2/2ma^2$
n=3	$E = 9\,h^2/8ma^2$	$E = 1.12\,h^2/ma^2$
a=bond length , m= mass of electron , $h = 6.62\times10^{-34}$ J.s		

Probability of finding an object if $\Psi(x) = D\,e^{\pm kx}$

$P = \int \Psi^*\Psi\,\partial t = \int D^2 e^{kx} e^{-kx}\,\partial x = \int D^2\,\partial x$

$D^2\,[x]$ …….$D^2\,(a\text{-}0) = D^2\,a$

$P = aD^2$ (constant)

لا يمكن ايجاد جسيم حر في كل المواقع لان الاحتمالية ثابت الطاقة مكممة

If cubic dimension for an object in potential box

a=b=c

$$\Psi_{(x,y,z)} = \left(\frac{2}{a}\right)^{3/2} \sin\frac{n\pi x}{a}\,\sin\frac{n\pi y}{a}\,\sin\frac{n\pi z}{a}$$

$\Psi(a) \ddagger \Psi(y) \ddagger \Psi(z)$

$$E\,(x, y, z) = \frac{h^2}{8ma^2}\left(n_x{}^2 + n_y{}^2 + n_z{}^2\right) \quad \ldots\ldots n = 1$$

Three and two dimension for an object in potential box

Inside box	Outside
$0 \leq x \leq a$	$0 > x > a$
$0 \leq y \leq b$	$0 > y > b$
$0 \leq z \leq c$	$0 > z > c$

V (x)= 0	V (x)= ∞

$$\hat{H} = -\mathbf{h}^2 / 2m\,(\partial^2/\partial^2x + \partial^2/\partial^2y + \partial^2/\partial^2z)$$

$$\nabla^{-2}{}_{(x,y,z)} = (\partial^2/\partial^2x + \partial^2/\partial^2y + \partial^2/\partial^2z)$$

$$\hat{H} = -\mathbf{h}^2/2m\,\nabla^{-2}{}_{(x,y,z)}$$

Schrodinger equation of three dimension

$-h^2/2m\,\nabla^{-2}\Psi_{(x,y,z)} = E_{(x,y,z)}\,\Psi_{(x,y,z)}$
$\Psi_{(x,y,z)} = \left(\frac{8}{abc}\right)^{1/2} \sin\frac{n\pi x}{a}\,\sin\frac{n\pi y}{b}\,\sin\frac{n\pi z}{c}$
$E_{(x,y,z)} = \frac{h^2}{8m}\left(\frac{n_x{}^2}{a^2} + \frac{n_y{}^2}{b^2} + \frac{n_z{}^2}{c^2}\right)$

Ex3/ Determine the wave function $\Psi_{(2,1,1)}$ and energy for an object in a potential box ?

Sol/ $\Psi_{(2,1,1)} = \left(\frac{8}{abc}\right)^{1/2} \sin\frac{n\pi x}{a}\,\sin\frac{n\pi y}{b}\,\sin\frac{n\pi z}{c}$

$$= \left(\frac{8}{abc}\right)^{1/2} \sin\frac{2\pi}{a}\,\sin\frac{\pi}{b}\,\sin\frac{\pi}{c}$$

$$E_{(2,1,1)} = \frac{h^2}{8m}\left(\frac{n_x{}^2}{a^2} + \frac{n_y{}^2}{b^2} + \frac{n_z{}^2}{c^2}\right)$$

$$E_{(2,1,1)} = \frac{h^2}{8m}\left(\frac{2^2}{a^2} + \frac{1^2}{b^2} + \frac{1^2}{c^2}\right)$$

Homework EX4/ Determine the wave function $\Psi_{(1,2,1)}$ and energy for an object in a potential box ?