College of Science
Department of Physics
Fourth Class
Lecture 6

Quantum Mechanics

2023-2024

Lecture 6: An introduction to some Hamiltonian

Preparation

Assist. prof. Alaa Abdul Hakeim

3.5 An introduction to some Hamiltonian

In this unit we shall introduce the energy operators "Hamiltonian", corresponding to several of the problem which we wish to solve in latter units.

3.5.1 A Free particle

Classical mechanics tell us that a free particle will either be at rest or moving with a constant momentum (p)

V(x,y,z)= const.

And

$$F_x = -\frac{\partial V}{\partial x} = F_y = -\frac{\partial V}{\partial y} = F_z = -\frac{\partial V}{\partial z} = zero$$

The total energy is constant, and the Hamiltonian is

$\hat{H}$ = K.E operator + P.E operator

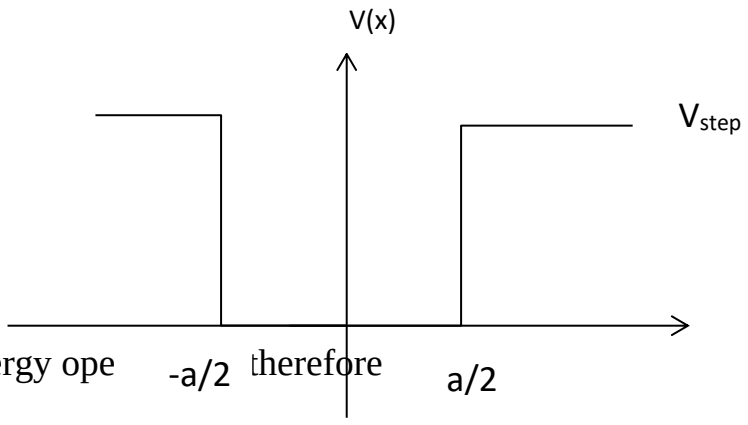
$$= \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + V(x,y,z)$$

$$= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + const.$$

$$= -\frac{\hbar^2}{2m}\nabla^2 + const.$$

3.5.2 A particle in a rectangular potential well

Such a model when generalized to three dimensions, might very well describe a molecule trapped inside a box or even a free electron inside a piece of metal.



The potential energy ope therefore

$$V(x) = \begin{cases} 0 & \frac{-a}{2} < x < \frac{a}{2} \\ V_{step} & x < \frac{-a}{2} \ , x > \frac{a}{2} \end{cases}$$

$$\therefore \ \hat{\mathrm{H}}_{pot.well} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

3.5.3 A Harmonic Oscillator

The H.O. can be used to describe a broad class of problems in which a particle executes small vibrations about some equilibrium position. atomic vibrations in solids. At the position of equilibrium V(x) must be a minimum, and we allow this minimum to define both the zero of potential and the origin of coordinates. Furthermore, the relation between the potential energy and the displacement from equilibrium for a simple harmonic oscillator is usually written as

$$V(x) = \frac{1}{2}kx^2$$

Where k is the force constant, i.e.

$$F = -\frac{\partial V}{\partial x} = -kx$$

Where $k = m\omega^2$

$$\mathrm{V(x)} = \frac{1}{2}m\omega^2x^2$$

Where the force constant has been rewritten in terms of the particle mass and its classical angular frequency ω, and the potential energy curve therefore looks like Fig 4.1 and the energy operator of H.O. is

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2x^2$$

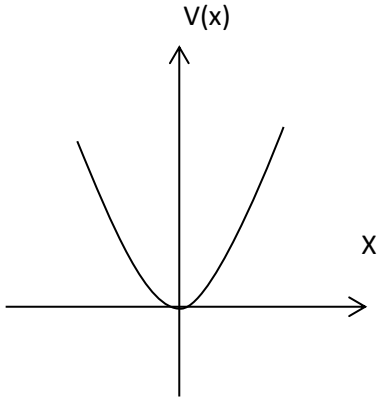


Fig 4.1

3.5.4 One particle in the Coulomb field of another

This forms the beginning of a discussion of the hydrogen atom. The Coulomb field of a point charge is isotropic and the potential energy between equal and opposite charges at (x_1,y_1,z_1)and (x_2,y_2,z_2) is

$$V(x_1, - - - -, z_2) = \frac{-e^2}{\sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2}}$$

In addition the K.E has two terms in these cases, i.e.one for each particle .

Thus, the wave mechanical energy operator is

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2m_1}\nabla_1{}^2 - \frac{\hbar^2}{2m_2}\nabla_2{}^2 - \frac{e^2}{\sqrt{(x_2-x_1)^2+(y_2-y_1)^2+(z_2-z_1)^2}}$$

3.6 Eigen functions

3.6.1 The normalization of eigen function

Normalization of eigen function can be achieved by evaluating

$$\int_{-\infty}^{\infty} \emptyset^*(x)\emptyset(x)dx = A$$

And writing the new normalized function

$$\Psi(x) = \frac{1}{\sqrt{A}}\emptyset(x)$$

Such that

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

$$\int_{-\infty}^{\infty} \frac{1}{\sqrt{A}}\emptyset^*(x)\frac{1}{\sqrt{A}}\emptyset(x)dx = 1$$

$$\int_{-\infty}^{\infty} \emptyset^*(x)\emptyset(x)dx = A$$

For normalized state function the expression for the expectation value (see unit 3 postulate 4) of repeated observation $\hat{A}$ takes on the slightly simpler form

$$\bar{a} = \frac{\int_{-\infty}^{\infty} \Psi^*(x)\hat{A}\,\Psi(x)dx}{\int_{-\infty}^{\infty} \Psi^*(x)\,\Psi(x)dx}$$

$$\therefore \boxed{\langle \hat{A} \rangle = \bar{a} = \int_{-\infty}^{\infty} \Psi^*(x)\hat{A}\,\Psi(x)dx}$$

As

$\boxed{\int_{-\infty}^{\infty} \Psi^*(x)\Psi(x)dx = 1}$ = normalization condition

Applying this formula to the special case $\hat{A} = \hat{x}$

We get the expectation value of position

$$\langle \hat{x} \rangle = \bar{x} = \int_{-\infty}^{\infty} \Psi^*(x)\hat{x}\,\Psi(x)dx$$

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

The most direct physical interpretation of the state function is that

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

Its modulus square determines the probability density of the particle in space

$$\boxed{|\Psi(x)|^2 = \left|\sqrt{\Psi^2(x)}\right|^2 = \Psi^2(x)}$$

Example:

Normalize the wave function $\Psi(\emptyset) = Ce^{im\emptyset}$ when m is const. and ($0 \leq \emptyset \leq 2\pi$).

Solution

$$\int \Psi^*(\emptyset)\Psi(\emptyset)d\emptyset = 1$$

$$\int_0^{2\pi} C^* e^{-im\emptyset} C e^{im\emptyset} d\emptyset = 1$$

$$|C|^2 \int_0^{2\pi} d\emptyset = 1$$

$$|C|^2[2\pi - 0] = 1$$

$$|C|^2 = \frac{1}{2\pi} \rightarrow |C| = \frac{1}{\sqrt{2\pi}}$$

$\therefore \Psi(\emptyset) = \frac{1}{\sqrt{2\pi}} e^{im\emptyset}$

3.6.2 Orthogonality of eigen functions

If $\boxed{\int_{-\infty}^{\infty} \Psi^*(x)\Psi(x)dx = 1}$ normalization

What would be the value of a similar integral over the different eigen function $\Psi_m(x)$ & $\Psi_n(x)$

$$\int_{-\infty}^{\infty} \Psi_m^*(x)\Psi_n(x)dx = \begin{cases} 0 & m \neq n \ orthogonal \\ 1 & m = n \ normalize \end{cases}$$