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# Exactly Solvable Problems in Quantum Mechanics

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## Abstract

Some of the problems in quantum mechanics can be exactly solved without any approximation. Some of the exactly solvable problems are discussed in this chapter. Broadly there are two main approaches to solve such problems. They are (i) based on the solution of the Schrödinger equation and (ii) based on operators. The normalized eigen function, eigen values, and the physical significance of some of the selected problems are discussed.

**Keywords:** exactly solvable, Schrödinger equation, eigen function, eigen values

## 1. Potential well

The potential well is the region where the particle is confined in a small region. In general, the potential of the confined region is lower than the surroundings (**Figure 1**) [1, 2].

The potential of the system is defined as

$$V = \begin{cases} 0, & -L < x < L \\ \infty, & \text{Otherwise} \end{cases}$$

The one dimensional Schrödinger equation in Cartesian coordinate is given as

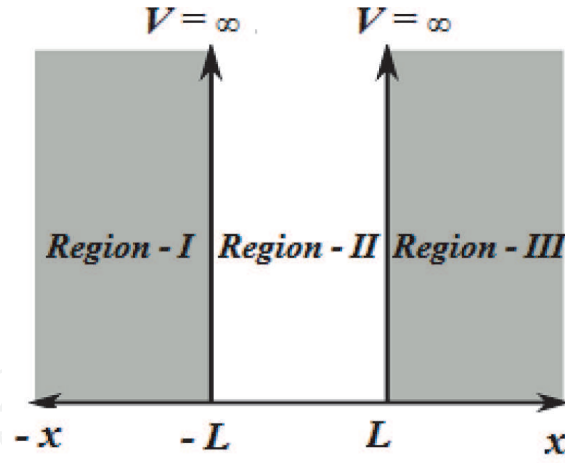
$$\frac{-\hbar^2}{2m} \Psi'' + V\Psi = E\Psi \Rightarrow \Psi'' + \frac{2m}{\hbar^2} (E - V)\Psi = 0 \quad (1)$$

In the infinite potential well, the confined particle is present in the well region (Region-II) for an infinitely long time. So the solution of the Schrödinger equation in the Region-II and Region-III can be omitted for our discussion right now. The Schrödinger equation in the Region-II is written as

$$\begin{aligned} \Psi'' + \frac{2m}{\hbar^2} (E)\Psi &= 0 \\ \Psi'' + \alpha^2 \Psi &= 0, \text{ where } \alpha^2 = \frac{2mE}{\hbar^2} \end{aligned} \quad (2)$$

The solution of the Eq. (2) is

$$\Psi = A_1 \sin \alpha x + A_2 \cos \alpha x \quad (3)$$



**Figure 1.**  
Infinite potential well.

At  $x = -L$ , and at  $x = L$ , the wave function vanishes since the potential is infinite. Hence, At  $x = -L$ ,

$$-A_1 \sin \alpha L + A_2 \cos \alpha L = 0 \quad (4)$$

Similarly, at  $x = L$

$$A_1 \sin \alpha L + A_2 \cos \alpha L = 0 \quad (5)$$

The addition and subtraction of these equations give two different solutions.

- i.  $2A_2 \cos \alpha L = 0 \Rightarrow \cos \alpha L = 0 \Rightarrow \alpha L = n\pi/2 \Rightarrow \alpha^2 = n^2\pi^2/4L^2; n = 1, 3, 5, \dots$   
 Since  $\alpha^2 = \frac{2mE}{\hbar^2}$ ,  $\frac{2mE}{\hbar^2} = n^2\pi^2/4L^2$ , the energy eigen value is found as

$$E = n^2\pi^2\hbar^2/8mL^2 \quad (6)$$

The eigen function is  $\Psi = A_1 \cos \alpha x$

$$= A_1 \cos (n\pi x/2L)$$

According to the normalization condition,

$$\int_{-L}^L \Psi^* \Psi dx = 0 \Rightarrow A_1 = L^{-1/2}$$

Hence the normalized eigen function for  $n = 1, 3, 5, \dots$  is

$$\Psi = L^{-1/2} \cos (n\pi x/2L) \quad (7)$$

- ii.  $2A_1 \sin \alpha L = 0 \Rightarrow \sin \alpha L = 0 \Rightarrow \alpha L = n\pi/2 \Rightarrow \alpha^2 = n^2\pi^2/4L^2; n = 2, 4, 6, \dots$   
 For this case,  $n = 2, 4, 6, \dots$ , the corresponding energy eigen value is

$$E = n^2\pi^2\hbar^2/8mL^2 \quad (8)$$

The eigen function is  $\Psi = A_2 \cos \alpha x$  and the normalized eigen function is

$$\Psi = L^{-1/2} \sin (n\pi x/2L) \quad (9)$$

In Summary, the eigen value is  $E = n^2 \pi^2 \hbar^2 / 8mL^2$  for all positive integer values of “n.” The normalized eigen functions are

$$\Psi = \begin{cases} L^{-1/2} \cos (n\pi x/2L), n = 1, 3, 5, \dots \\ L^{-1/2} \sin (n\pi x/2L), n = 2, 4, 6, \dots \end{cases} \quad (10)$$

The integer “n” is the quantum number and it denotes the discrete energy states in the quantum well. We can extract some physical information from the eigen solutions.

- The minimum energy state can be calculated by setting  $n = 1$ , which corresponds to the ground state. The ground state energy is

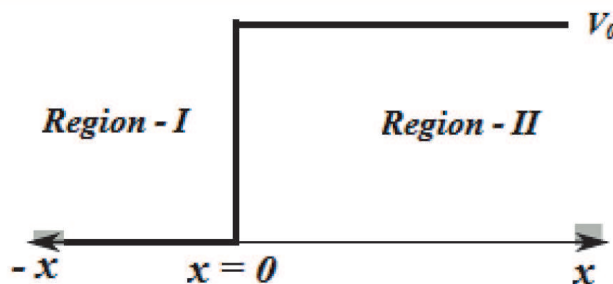
$$E_1 = \pi^2 \hbar^2 / 8mL^2 \quad (11)$$

This is known as zero-point energy in the case of the potential well. The excited state energies are  $E_2 = 4\pi^2 \hbar^2 / 8mL^2$ ,  $E_3 = 9\pi^2 \hbar^2 / 8mL^2$ ,  $E_4 = 16\pi^2 \hbar^2 / 8mL^2$ , and so on. In general,  $E_n = n^2 \times E_1$ .

- The energy difference between the successive states is simply the difference between the energy eigen value of the corresponding state. For example,  $\Delta E_{12} = E_2 - E_1 = 3E_1$  and  $\Delta E_{23} = E_3 - E_2 = 5E_1$ . Hence the energy difference between any two successive states is not the same.
- Though the eigen functions for odd and even values of “n” are different, the energy eigen value remains the same.
- If the potential well is chosen in the limit  $0 < x < 2L$  (width of the well is  $2L$ ), the energy eigen value is the same as given in Eqs.(6) and (8). But if the limit is chosen as  $0 < x < L$  (width of the well is  $L$ ), the for all positive integers of “n,” the eigen function is  $\Psi = (2/L)^{1/2} \sin (n\pi x/L)$  and the energy eigen function is  $E = n^2 \pi^2 \hbar^2 / 2mL^2$ .

## 2. Step potential

Step potential is a problem that has two different finite potentials [3]. Classically, the tunneling probability is 1 when the energy of the particle is greater than the height of the barrier. But the result is not true based on wave mechanics (**Figure 2**).



**Figure 2.**  
Step potential.

The potential of the system

$$V = \begin{cases} 0, & -\infty < x < 0 \\ V_0, & 0 \leq x < \infty \end{cases}$$

The Schrödinger equation in the Region-I and Region-II is given, respectively as,

$$\Psi'' + \frac{2m}{\hbar^2}(E)\Psi = 0 \quad (12)$$

$$\Psi'' + \frac{2m}{\hbar^2}(E - V)\Psi = 0 \quad (13)$$

Case (i): when  $E < V_0$ , the solutions of the Schrödinger equations in the Region-I and Region-II, respectively, are given as

$$\Psi_1 = A_1 \exp(i\alpha x) + B_1 \exp(-i\alpha x) \quad (14)$$

$$\Psi_2 = A_2 \exp(-\beta x) + B_2 \exp(\beta x)$$

where  $\alpha^2 = \frac{2mE}{\hbar^2}$  and  $\beta^2 = \frac{2m(E-V_0)}{\hbar^2}$ . Here,  $B_2 \exp(\beta x)$  represents the exponentially increasing wave along the x-direction. The wave function  $\Psi_2$  must be finite as  $x \rightarrow \infty$ . This is possible only by setting  $B_2 = 0$ . Hence the eigen function in the Region-II is

$$\Psi_2 = A_2 \exp(-\beta x) \quad (15)$$

According to admissibility conditions of wave functions, at  $x = 0$ ,  $\Psi_1 = \Psi_2$  and  $\Psi'_1 = \Psi'_2$ . It gives us

$$A_1 + B_1 = A_2 \quad (16)$$

$$A_1 - B_1 = i\left(\frac{\beta}{\alpha}\right)A_2 \quad (17)$$

From these two equations,

$$A_2 = \left(\frac{2\alpha}{\alpha + i\beta}\right)A_1$$

$$B_1 = \left(\frac{\alpha - i\beta}{\alpha + i\beta}\right)A_1$$

The reflection coefficient R is given as

$$R = \frac{|B_1|^2}{|A_1|^2} = \left|\frac{\alpha - i\beta}{\alpha + i\beta}\right|^2 = 1 \quad (18)$$

It is interesting to note that all the particles that encounter the step potential are reflected back. This is due to the fact that the width of the step potential is infinite. The number of particles in the process is conserved, which leads that  $T = 0$ , since  $T + R = 1$ .

Case (ii): when  $E > V_0$ , the solutions are given as

$$\Psi_1 = A_1 \exp(i\alpha x) + B_1 \exp(-i\alpha x)$$

$$\Psi_2 = A_2 \exp(i\beta x) + B_2 \exp(-i\beta x)$$

where  $\beta^2 = \frac{2m(E-V_0)}{\hbar^2}$ . As  $x \rightarrow \infty$ , the wave function  $\Psi_2$  must be finite. Hence  $\Psi_2 = A_2 \exp(i\beta x)$  by setting  $B_2 = 0$ . According to the boundary conditions at  $x = 0$ ,

$$A_1 + B_1 = A_2 \quad (19)$$

$$A_1 - B_1 = \left(\frac{\beta}{\alpha}\right) A_2 \quad (20)$$

From these equations,

$$A_2 = \left(\frac{2\alpha}{\alpha + \beta}\right) A_1$$

$$B_1 = \left(\frac{\alpha - \beta}{\alpha + \beta}\right) A_1$$

The reflection coefficient  $R$  and the transmission coefficient  $T$ , respectively, are given as

$$R = \frac{|B_1|^2}{|A_1|^2} = \left(\frac{\alpha - \beta}{\alpha + \beta}\right)^2 \quad (21)$$

$$T = \frac{|A_2|^2}{|A_1|^2} = \frac{4\alpha\beta}{(\alpha + \beta)^2} \quad (22)$$

From these easily one can show that

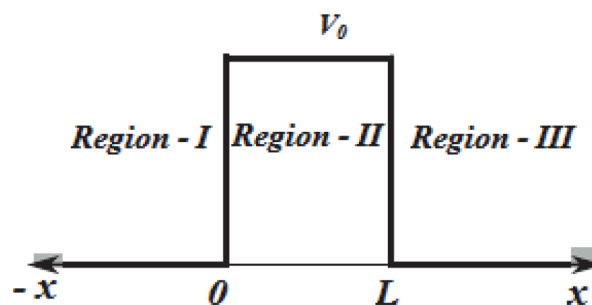
$$T + R = \frac{4\alpha\beta}{(\alpha + \beta)^2} + \left(\frac{\alpha - \beta}{\alpha + \beta}\right)^2 = 1 \quad (23)$$

The results again indicate that the total number of particles which encounters the step potential is conserved.

### 3. Potential barrier

This problem clearly explains the wave-mechanical tunneling [3, 4]. The potential of the system is given as (**Figure 3**)

$$V = \begin{cases} V_0, & 0 < x < L \\ 0, & \text{Otherwise} \end{cases}$$



**Figure 3.**  
Potential barrier.

In the Region-I, the Schrödinger equation is  $\Psi'' + \alpha^2\Psi = 0$ . The wave function in this region is given as

$$\Psi_1 = A_1 \exp(i\alpha x) + B_1 \exp(-i\alpha x) \text{ where } \alpha^2 = \frac{2mE}{\hbar^2} \quad (24)$$

In Region-II, if  $E < V_0$ , the Schrödinger equation is  $\Psi'' - \beta^2\Psi = 0$ . The solution of the equation is given as

$$\Psi_2 = A_2 \exp(\beta x) + B_2 \exp(-\beta x) \text{ where } \beta^2 = \frac{2m(E - V_0)}{\hbar^2} \quad (25)$$

The Schrödinger equation in the Region-III is  $\Psi'' + \alpha^2\Psi = 0$ . The corresponding solution is  $\Psi_3 = A_3 \exp(i\alpha x) + B_3 \exp(-i\alpha x)$ . But in the Region-III, the waves can travel only along positive x-direction and there is no particle coming from the right,  $B_3 = 0$ . Hence

$$\Psi_3 = A_3 \exp(i\alpha x) \quad (26)$$

At  $x = 0$ ,  $\Psi_1 = \Psi_2$  and  $\Psi'_1 = \Psi'_2$ . These give us two equations

$$A_1 + B_1 = A_2 + B_2 \quad (27)$$

$$A_1 - B_1 = \left(\frac{\beta}{i\alpha}\right)(A_2 - B_2) \quad (28)$$

At  $x = L$ ,  $\Psi_2 = \Psi_3$  and  $\Psi'_2 = \Psi'_3$ . These conditions give us another two equations

$$A_2 \exp(\beta L) + B_2 \exp(-\beta L) = A_3 \exp(i\alpha L) \quad (29)$$

$$A_2 \exp(\beta L) - B_2 \exp(-\beta L) = A_3 \left(\frac{i\alpha}{\beta}\right) \exp(i\alpha L) \quad (30)$$

Solving the equations from (27) to (30), one can find the coefficients in the equations. The reflection coefficient is R is found as

$$R = \frac{|B_1|^2}{|A_1|^2} = \left[ \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\beta L) \right] \left[ 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\beta L) \right]^{-1} \quad (31)$$

The transmission coefficient T is found as

$$T = \frac{|A_2|^2}{|A_1|^2} = \left[ 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\beta L) \right]^{-1} \quad (32)$$

From Eqs. (31) and (32), one can show that  $T + R = 1$ . The following are the conclusions obtained from the above mathematical analysis.

- When  $E < V_0$ , though the energy of the incident particles is less than the height of the barrier, the particle can tunnel into the barrier region. This is in contrast to the laws of classical physics. This is known as the tunnel effect.
- As  $V_0 \rightarrow \infty$ , the transmission coefficient is zero. Hence the tunneling is not possible only when  $V_0 \rightarrow \infty$ .

- When the length of the barrier is an integral multiple of  $\pi/\beta$ , there is no reflection from the barrier. This is termed as resonance scattering.
- The tunneling probability depends on the height and width of the barrier.
- Later, Kronig and Penney extended this idea to explain the motion of a charge carrier in a periodic potential which is nothing but the one-dimensional lattices.

#### 4. Delta potential

The Dirac delta potential is infinitesimally narrow potential only at some point (generally at the origin, for convenience) [3]. The potential of the system

$$V = \begin{cases} -\lambda\delta(x), & x = 0 \\ 0, & \text{Otherwise} \end{cases}$$

Here  $\lambda$  is the positive constant, which is the strength of the delta potential. Here, we confine ourselves only to the bound states, hence  $E < 0$  (**Figure 4**).

The Schrödinger equation is

$$\Psi'' + \frac{2m}{\hbar^2} (E - V)\Psi = 0 \Rightarrow \Psi'' + \frac{2m}{\hbar^2} (E + \lambda\delta(x))\Psi = 0 \quad (33)$$

The solution of the Schrödinger equation is given as

$$\text{Region - I : } \Psi_1 = A_1 \exp(\beta x) \quad (34)$$

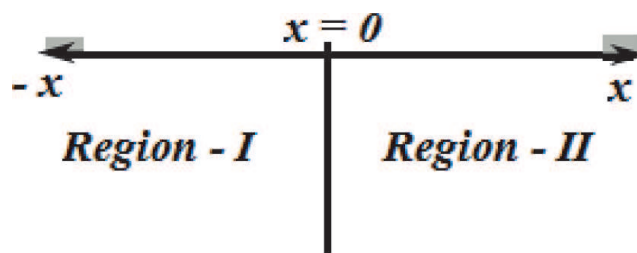
$$\text{Region - II : } \Psi_2 = A_2 \exp(-\beta x) \quad (35)$$

where  $\beta^2 = \frac{-2mE}{\hbar^2}$ . At  $x = 0$ ,  $\Psi_1 = \Psi_2$ . So the coefficients  $A_1$  and  $A_2$  are equal. But  $\Psi'_1 \neq \Psi'_2$ , since the first derivative causes the discontinuity. The first derivatives are related by the following equation

$$\Psi'_2 - \Psi'_1 = -\frac{2m\lambda}{\hbar^2} \quad (36)$$

This gives us

$$\beta = \frac{m\lambda}{\hbar^2} \quad (37)$$



**Figure 4.**  
Dirac delta potential.



Equating the value of  $\beta$  gives the energy eigen value as

$$E = -\frac{m\lambda^2}{2\hbar^2} \quad (38)$$

The energy eigen value expression does not have any integer like in the case of the potential well. Hence there is only one bound state which is available for a particular value of “m.”

The eigen function can be evaluated as follows: The eigen function is always continuous. At  $x = 0$  gives us  $A_1 = A_2 = A$ . Hence the eigen function is

$$\Psi = A \exp(\beta|x|)$$

To normalize  $\Psi$ ,

$$\int_{-\infty}^{\infty} |\Psi|^2 dx = 1 \Rightarrow 2 \int_0^{\infty} |\Psi|^2 dx = 1$$

This gives us  $A = \sqrt{\beta} = \frac{\sqrt{m\lambda}}{\hbar}$ .

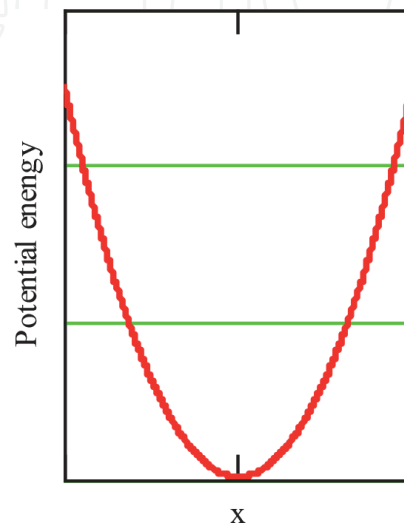
## 5. Linear harmonic oscillator

Simple harmonic oscillator, damped harmonic oscillator, and force harmonic oscillator are the few famous problems in classical physics. But if one looks into the atomic world, the atoms are vibrating even at 0 K. Such atomic oscillations need the tool of quantum physics to understand its nature. In all the previous examples, the potential is constant in any particular region. But in this case, the potential is a function of the position coordinate “x.”

### 5.1 Schrodinger method

The potential of the linear harmonic oscillator as a function of “x” is given as (Figure 5) [4–6]:

$$V = \frac{m\omega^2 x^2}{2} \quad (39)$$



**Figure 5.**  
Potential energy of the linear harmonic oscillator.

The time-independent Schrödinger equation is given as

$$\Psi'' + \frac{2m}{\hbar^2} \left( E - \frac{m\omega^2 x^2}{2} \right) \Psi = 0 \quad (40)$$

The potential is not constant since it is a function of “x”; Eq. (40) cannot solve directly as the previous problems. Let

$$\alpha = \left( \frac{m\omega}{\hbar} \right)^{1/2} x \text{ and } \beta = \frac{2E}{\hbar\omega}.$$

Using the new constant  $\beta$  and the variable  $\alpha$ , the Schrödinger equation has the form

$$\frac{d^2\Psi}{d\alpha^2} + (\beta - \alpha^2)\Psi = 0 \quad (41)$$

The asymptotic Schrödinger equation ( $\alpha \rightarrow \infty$ ) is given as

$$\frac{d^2\Psi}{d\alpha^2} - \alpha^2\Psi = 0 \quad (42)$$

The general solution of the equation is  $\exp(\pm\alpha^2/2)$ . As  $\alpha \rightarrow \infty$ ,  $\exp(+\alpha^2/2)$  becomes infinite, hence it cannot be a solution. So the only possible solution is  $\exp(-\alpha^2/2)$ . Based on the asymptotic solution, the general solution of Eq. (42) is given as

$$\Psi = H_n(\alpha) \exp(-\alpha^2/2)$$

The normalized eigen function is

$$\Psi = \left[ \left( \frac{m\omega}{\hbar\pi} \right)^{1/2} \left( \frac{1}{2^n \times n!} \right) \right]^{1/2} H_n(\alpha) \exp(-\alpha^2/2) \quad (43)$$

The solution given in Eq. (43) is valid if the condition  $2n + 1 - \frac{2E}{\hbar\omega} = 0$  holds. This gives the energy eigen value as

$$E = \left( n + \frac{1}{2} \right) \hbar\omega \quad (44)$$

The important results are given as follows:

- The integer  $n = 0$  represents the ground state,  $n = 1$  represents the first excited state, and so on. The ground state energy of the linear harmonic oscillator is  $E = \hbar\omega/2$ . This minimum energy is known as ground state energy.
- The ground state normalized eigen function is

$$\Psi_0(x) = \left( \frac{m\omega}{\hbar\pi} \right)^{1/4} \exp\left(-\frac{m\omega x^2}{2\hbar}\right) \quad (45)$$

- The energy difference between any two successive levels is  $\hbar\omega$ . Hence the energy difference between any two successive levels is constant. But this is not true in the case of real oscillators.

## 5.2 Operator method

The operator method is also one of the convenient methods to solve the exactly solvable problem as well as approximation methods in quantum mechanics [5]. The Hamiltonian of the linear harmonic oscillator is given as,

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \quad (46)$$

Let us define the operator “a,” lowering operator, in such a way that

$$a = (2m\omega\hbar)^{-1/2}(m\omega x + ip) \quad (47)$$

and the corresponding Hermitian adjoint, raising operator, is

$$a^+ = (2m\omega\hbar)^{-1/2}(m\omega x - ip) \quad (48)$$

$$\begin{aligned} a^+ a &= (2m\omega\hbar)^{-1}(m\omega x - ip)(m\omega x + ip) \\ &= (2m\omega\hbar)^{-1}(m^2\omega^2 x^2 + p^2 + im\omega xp - im\omega px) \\ &= (2m\omega\hbar)^{-1}(m^2\omega^2 x^2 + p^2 + im\omega[x, p]) \end{aligned} \quad (49)$$

Here,  $[x, p]$  represents the commutation between the operators  $x$  and  $p$ .  $[x, p] = i$  and Eq. (49) becomes

$$\begin{aligned} a^+ a &= (2m\omega\hbar)^{-1}(m^2\omega^2 x^2 + p^2 - m\omega\hbar) \\ &= \frac{1}{\omega\hbar} \left( \frac{1}{2}m\omega^2 x^2 + \frac{p^2}{2m} \right) - \frac{1}{2} \\ &= \frac{H}{\hbar\omega} - \frac{1}{2} \end{aligned} \quad (50)$$

In the same way, one can find the  $aa^+$  and it is given as

$$aa^+ = \frac{H}{\hbar\omega} + \frac{1}{2} \quad (51)$$

Adding Eqs. (50) and (51) gives us the Hamiltonian in terms of the operators.

$$H = \frac{\hbar\omega}{2}(aa^+ + a^+a) \quad (52)$$

Subtracting Eq. (50) from (51) gives,  $aa^+ - a^+a = 1$ . This can be simplified as

$$[a, a^+] = 1 \quad (53)$$

The Hamiltonian  $H$  acts on any state  $|n\rangle$  that gives the eigen value  $E_n$  times the same state  $|n\rangle$ , that is,  $H|n\rangle = E_n|n\rangle$ .

The expectation value of  $a^+a$  is

$$\begin{aligned}\langle a^+a \rangle &\equiv \langle n|a^+a|n \rangle = \langle n|\frac{H}{\hbar\omega} - \frac{1}{2}|n \rangle \\ &= \frac{1}{\hbar\omega} \langle n|H|n \rangle - \langle n|\frac{1}{2}|n \rangle \\ &= \frac{1}{\hbar\omega} E_n \langle n|n \rangle - \frac{1}{2} = \frac{E_n}{\hbar\omega} - \frac{1}{2}\end{aligned}\quad (54)$$

Let us consider the ground state  $|0\rangle$ .

$$\langle 0|a^+a|0 \rangle = \frac{E_0}{\hbar\omega} - \frac{1}{2}$$

Since  $a|0\rangle = 0$ ,  $\langle 0|a^+a|0 \rangle = 0$ . Thus,

$$\frac{E_0}{\hbar\omega} - \frac{1}{2} = 0 \Rightarrow E_0 = \frac{\hbar\omega}{2}\quad (55)$$

Similarly, the energy of the first excited state is found as follows:

$$\begin{aligned}\langle 1|a^+a|1 \rangle &= \frac{E_1}{\hbar\omega} - \frac{1}{2} \\ \sqrt{1}\langle 1|a^+|0 \rangle &= \frac{E_1}{\hbar\omega} - \frac{1}{2} \\ \sqrt{1}\cdot\sqrt{1}\langle 1|1 \rangle &= \frac{E_1}{\hbar\omega} - \frac{1}{2} \\ 1 &= \frac{E_1}{\hbar\omega} - \frac{1}{2} \Rightarrow E_1 = \frac{3}{2}\hbar\omega\end{aligned}\quad (56)$$

In the same way,  $E_2 = 5\hbar\omega/2$ ,  $E_3 = 7\hbar\omega/2$ , and so on. Hence, one can generalize the result as

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega\quad (57)$$

The uncertainties in position and momentum, respectively, are given as

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}\quad (58)$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}\quad (59)$$

In order to evaluate the uncertainties  $\langle x^2 \rangle$ ,  $\langle x \rangle^2$ ,  $\langle p^2 \rangle$ , and  $\langle p \rangle^2$  have to be evaluated. From Eqs. (47) and (48) the position and momentum operators are found as

$$x = \left(\frac{\hbar}{2m\omega}\right)^{1/2} (a + a^+)\quad (60)$$

$$p = \left(\frac{m\omega\hbar}{2}\right)^{1/2} \left(\frac{a - a^+}{i}\right)\quad (61)$$

a. The expectation value of 'x' is given as,

$$\begin{aligned}
 \langle x \rangle &\equiv \langle n|x|n \rangle = \left( \frac{\hbar}{2m\omega} \right)^{1/2} \langle n|(a + a^+)|n \rangle \\
 &= \left( \frac{\hbar}{2m\omega} \right)^{1/2} (\langle n|a|n \rangle + \langle n|a^+|n \rangle) \\
 &= \left( \frac{\hbar}{2m\omega} \right)^{1/2} (\sqrt{n} \langle n|n-1 \rangle + \sqrt{n+1} \langle n|n+1 \rangle)
 \end{aligned}$$

Since the states  $n-1, n, n+1$  are orthogonal to each other,  $\langle n|n-1 \rangle = 0$  and  $\langle n|n+1 \rangle = 0$ . So  $\langle x \rangle = 0$ . The expectation value of the position in any state is zero.

b. The expectation value of momentum is

$$\langle p \rangle \equiv \langle n|p|n \rangle = \left( \frac{m\omega\hbar}{2} \right)^{1/2} \left( \frac{1}{i} \right) \langle n|a - a^+|n \rangle \Rightarrow \langle p \rangle = 0.$$

Not only position, the expectation value of momentum in any state is also zero.

c.

$$\begin{aligned}
 \langle x^2 \rangle &\equiv \langle n|x^2|n \rangle = \frac{\hbar}{2m\omega} \langle n|(a + a^+)(a + a^+)|n \rangle \\
 &= \frac{\hbar}{2m\omega} \langle n|(a^2 + a^{+2} + aa^+ + a^+a)|n \rangle \\
 &= \frac{\hbar}{2m\omega} (\langle n|a^2|n \rangle + \langle n|a^{+2}|n \rangle + \langle n|aa^+|n \rangle + \langle n|a^+a|n \rangle) \\
 &= \frac{\hbar}{2m\omega} (\sqrt{n}\sqrt{n-1} \langle n|n-2 \rangle + \sqrt{n+1}\sqrt{n+2} \langle n|n+2 \rangle + (n+1) \langle n|n \rangle + n \langle n|n \rangle) \\
 &= \frac{\hbar}{2m\omega} (2n+1)
 \end{aligned}$$

d.

$$\begin{aligned}
 \langle p^2 \rangle &\equiv \langle n|p^2|n \rangle = -\left( \frac{m\omega\hbar}{2} \right) \langle n|(a - a^+)(a - a^+)|n \rangle \\
 &= -\left( \frac{m\omega\hbar}{2} \right) (\langle n|a^2|n \rangle + \langle n|a^{+2}|n \rangle - \langle n|aa^+|n \rangle - \langle n|a^+a|n \rangle) \\
 &= -\left( \frac{m\omega\hbar}{2} \right) (\sqrt{n}\sqrt{n-1} \langle n|n-2 \rangle + \sqrt{n+1}\sqrt{n+2} \langle n|n+2 \rangle - (n+1) \langle n|n \rangle - n \langle n|n \rangle) \\
 &= \left( \frac{m\omega\hbar}{2} \right) (2n+1)
 \end{aligned}$$

From Eq. (58) and (59), the uncertainty in position and momentum, respectively are given as,

$$\Delta x = \left( \frac{\hbar}{2m\omega} (2n+1) \right)^{1/2} \quad (62)$$

$$\Delta p = \left( \left( \frac{m\omega\hbar}{2} \right) (2n+1) \right)^{1/2} \quad (63)$$

$$\Delta x \cdot \Delta p = \frac{\hbar}{2} (2n+1) \quad (64)$$

## 6. Conclusions

- The minimum uncertainty state is the ground state. In this state,  $\Delta x = \left( \frac{\hbar}{2m\omega} \right)^{1/2}$  and  $\Delta p = \left( \frac{m\omega}{2} \right)^{1/2}$ .
- Hence the minimum uncertainty product is  $\Delta x \cdot \Delta p = \frac{\hbar}{2}$ . Since the other states have higher uncertainty than the ground state, the general uncertainty is  $\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$ . This is the mathematical representation of Heisenberg's uncertainty relation.
- Since  $\Psi_0(x)$  corresponds to the low energy state, a  $\Psi_0(x) = 0$ . This gives us the ground state eigen function. This can be done as follows:

$$a \Psi_0(x) = 0$$

$$(2m\omega\hbar)^{-1/2} (m\omega x + ip) \Psi_0(x) = 0$$

$$\left( \left( \frac{m\omega}{2\hbar} \right)^{1/2} x + i \frac{(-i\hbar\partial/\partial x)}{(2m\omega\hbar)^{1/2}} \right) \Psi_0(x) = 0$$

$$\frac{\hbar}{m\omega} \frac{\partial \Psi_0(x)}{\partial x} = -x \Psi_0(x)$$

$$\frac{d \Psi_0(x)}{\Psi_0(x)} = -\frac{m\omega x}{\hbar} dx$$

Integrating the above equation gives,

$$\ln \Psi_0(x) = -\frac{m\omega}{\hbar} \left( \frac{x^2}{2} \right) + \ln A$$

$$\Psi_0(x) = A \exp \left( -\frac{m\omega x^2}{2\hbar} \right)$$

The normalized eigen function is given as

$$\Psi_0(x) = \left( \frac{m\omega}{\hbar\pi} \right)^{1/4} \exp \left( -\frac{m\omega x^2}{2\hbar} \right)$$

One can see that this result is identical to Eq. (45).

- The other eigen states can be evaluated using the equation,  
 $\Psi_n(x) = ((a^+)^n / \sqrt{n!}) \Psi_0(x)$ .

## 7. Particle in a 3D box

The confinement of a particle in a three-dimensional potential is discussed in this section [4, 6]. The potential is defined as (**Figure 6**)

$$V = \begin{cases} 0, & 0 \leq x < a; 0 \leq y < b; 0 \leq z < c \\ \infty, & \text{Otherwise} \end{cases}$$

The three dimensional time-independent Schrödinger equation is given as

$$\nabla^2 \Psi(x, y, z) - \frac{2m}{\hbar^2} V \Psi(x, y, z) = -E \Psi(x, y, z) \quad (65)$$

Let the eigen function  $\Psi(x, y, z)$  is taken as the product of  $\Psi_x(x)$ ,  $\Psi_y(y)$  and  $\Psi_z(z)$  according to the technique of separation of variables. i.e.,  $\Psi(x, y, z) = \Psi_x(x)\Psi_y(y)\Psi_z(z)$ .

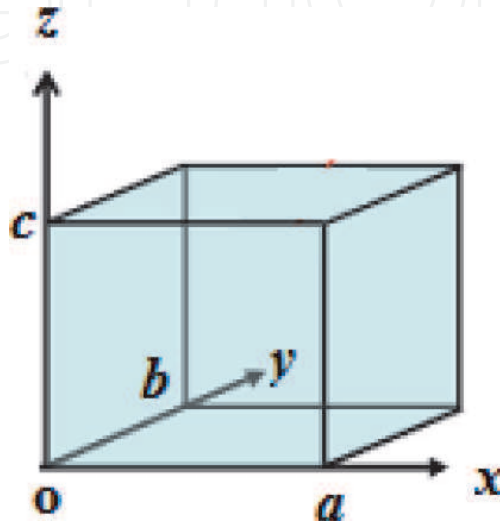
$$\begin{aligned} \Psi_y(y)\Psi_z(z) \frac{d^2 \Psi_x(x)}{dx^2} + \Psi_x(x)\Psi_z(z) \frac{d^2 \Psi_y(y)}{dy^2} + \Psi_x(x)\Psi_y(y) \frac{d^2 \Psi_z(z)}{dz^2} - \frac{2m}{\hbar^2} V \Psi(x, y, z) \\ = -\frac{2m}{\hbar^2} E \Psi(x, y, z) \end{aligned}$$

Divide the above equation by  $\Psi(x, y, z)$  gives us

$$\frac{1}{\Psi_x(x)} \frac{d^2 \Psi_x(x)}{dx^2} + \frac{1}{\Psi_y(y)} \frac{d^2 \Psi_y(y)}{dy^2} + \frac{1}{\Psi_z(z)} \frac{d^2 \Psi_z(z)}{dz^2} = -\frac{2m}{\hbar^2} E \quad (66)$$

Now we can boldly write  $E$  as  $E_x(x) + E_y(y) + E_z(z)$

$$\frac{1}{\Psi_x(x)} \frac{d^2 \Psi_x(x)}{dx^2} + \frac{1}{\Psi_y(y)} \frac{d^2 \Psi_y(y)}{dy^2} + \frac{1}{\Psi_z(z)} \frac{d^2 \Psi_z(z)}{dz^2} = -\frac{2m}{\hbar^2} (E_x(x) + E_y(y) + E_z(z)) \quad (67)$$



**Figure 6.**  
Three-dimensional potential box.

Now the equation can be separated as follows:

$$\frac{d^2\Psi_x(x)}{dx^2} + \frac{2m}{\hbar^2} E_x(x) \Psi_x(x) = 0$$

$$\frac{d^2\Psi_y(y)}{dy^2} + \frac{2m}{\hbar^2} E_y(y) \Psi_y(y) = 0$$

$$\frac{d^2\Psi_z(z)}{dz^2} + \frac{2m}{\hbar^2} E_z(z) \Psi_z(z) = 0$$

The normalized eigen function  $\Psi_x(x)$  is given as

$$\Psi_x(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n_x\pi x}{a}\right)$$

In the same way,  $\Psi_y(y)$  and  $\Psi_z(z)$  are given as

$$\Psi_y(y) = \left(\frac{2}{b}\right)^{1/2} \sin\left(\frac{n_y\pi y}{b}\right)$$

$$\Psi_z(z) = \left(\frac{2}{c}\right)^{1/2} \sin\left(\frac{n_z\pi z}{c}\right)$$

Hence, the eigen function  $\Psi(x, y, z)$  is given as

$$\Psi(x, y, z) = \Psi_x(x) \Psi_y(y) \Psi_z(z) = \left(\frac{8}{abc}\right)^{1/2} \sin\left(\frac{n_x\pi x}{a}\right) \sin\left(\frac{n_y\pi y}{b}\right) \sin\left(\frac{n_z\pi z}{c}\right) \quad (68)$$

The energy given values are given as

$$E_x(x) = \frac{n_x^2 \pi^2 \hbar^2}{2ma^2}$$

$$E_y(y) = \frac{n_y^2 \pi^2 \hbar^2}{2mb^2}$$

$$E_z(z) = \frac{n_z^2 \pi^2 \hbar^2}{2mc^2}$$

The total energy  $E$  is

$$E = E_x(x) + E_y(y) + E_z(z) = \frac{\pi^2 \hbar^2}{2m} \left( \frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right) \quad (69)$$

Some of the results are summarized here:

- In a cubical potential box,  $a = b = c$ , then the energy eigen value becomes,

$$E = \frac{\pi^2 \hbar^2}{2ma^2} (n_x^2 + n_y^2 + n_z^2).$$



- The minimum energy that corresponds to the ground state is  $E_1 = \frac{3\pi^2\hbar^2}{2ma^2}$ . Here  $n_x = n_y = n_z = 1$ .
- Different states with different quantum numbers may have the same energy. This phenomenon is known as degeneracy. For example, the states (i)  $n_x = 2; n_y = n_z = 1$ , (ii)  $n_y = 2; n_x = n_z = 1$ ; and (iii)  $n_z = 2; n_x = n_y = 1$  have the same energy of  $E = \frac{6\pi^2\hbar^2}{ma^2}$ . So we can say that the energy  $\frac{6\pi^2\hbar^2}{ma^2}$  has a 3-fold degenerate.
- The states (111), (222), (333), (444), ... has no degeneracy.
- In this problem, the state may have zero-fold degeneracy, 3-fold degeneracy or 6-fold degeneracy.

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