QM-I Lecture Notes-Part III

Potential Problems – Mostly Bound States

A Course of Lectures Planned to Be Given at IIT Bhubaneswar[1]

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Lesson 1

Piece wise Continuous Potentials

§1 Particle in a box

The energy levels of a particle in one dimensional infinite well

$$V(x) = \begin{cases} 0, & 0 \le x \le L \\ \infty & \text{outside} \end{cases} \tag{1.1}$$

can be found by solving the Schrödinger equation for $0 \le x \le L$, where the particle is like a free particle and the solution is given by

$$u(x) = A \sin kx + B \cos kx, \qquad k^2 = \frac{2mE}{\hbar^2}. \tag{1.2}$$

Out side the box, the potential is infinity and the solution vanishes:

$$u(x) = 0, \qquad \text{if } x < 0, \text{ or } x > L. \tag{1.3}$$

The boundary conditions to be imposed on the solution are

$$u(0) = u(L) = 0, \tag{1.4}$$

and no restriction on the derivatives at the boundary points $x = 0, x = L$. This gives

$$u(0) = 0 \quad \Rightarrow \quad B = 0, \tag{1.5}$$

$$u(L) = 0 \quad \Rightarrow \quad \sin kL = 0. \tag{1.6}$$

The solutions of this equation are $k_n = n\pi/L, n = 1, 2, \ldots$. The energy levels are given by

$$E_n = \frac{\hbar^2 k_n^2}{2m}, = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \tag{1.7}$$

and the corresponding wave functions are

$$u_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & 0 \le x \le L \\ 0 & x < 0 \text{ or } x > L. \end{cases} \tag{1.8}$$

and n takes all positive integral values.*It should be noted that for $k = 0$ the solution vanishes identically and therefore $n = 0$ is unacceptable.*

§2 Square well

We shall discuss the energy spectrum for a square well potential shown in figure below. Within the range of the well, it is an attractive, and constant, potential. With suitable reference for potential energy, the potential can be chosen to be 0 inside the well. It is again a constant outside the range of the potential well. We have chosen $V_0 > 0$ to denote the value of the potential outside the well. We shall now obtain the solution for energy levels of a square well potential in one dimension.

The square well potential is given by

$$V(x) = \begin{cases} 0 & 0 \le x \le L \\ V_0 & \text{outside} \end{cases}$$

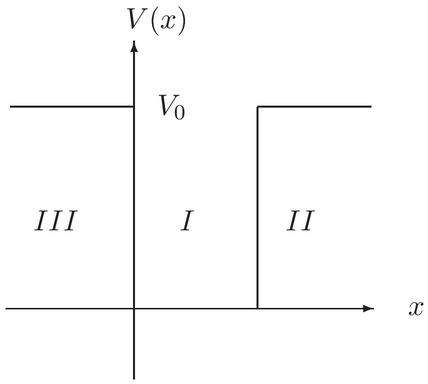

Fig. 1

Since the potential has different expressions for different values of x, the Schrödinger equation is solved in the three regions (i) $x < 0$ (ii) $0 \le x \le L$ and (iii) $x > L$ separately. Also the two ranges of energy $0 < E < V_0$ and $E > V_0$ will be considered separately.

Bound states

The bound states correspond to $0 < E < V_0$. For the bound states one must insist that $\psi(x) \to 0$ at large distances, because $|\psi|^2 dx$ represents probability of particle being found between x and $x + dx$. Thus in the limit $x \to \pm\infty$, we must have $\lim \psi(x) \to 0$. The solutions will be obtained in the three regions I,II, and III separately. Besides vanishing of the solution at infinity, we shall impose the requiremnet of continuity on the solution for the eigenfunctions and their derivatives.

Region I: The Schrödinger equation is

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

or

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

where $k^2 = 2mE/\hbar^2$ and most general solution is

$$\psi_I(x) = A\sin kx + B\cos kx$$

Region II: When $x > L$, $V(x) = V_0$ and the Schrödinger equation takes the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + (V_0 - E)\psi = 0$$

or

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(V_0 - E)\psi = 0$$

Denoting $\frac{2m}{\hbar^2}(V_0 - E) = \alpha^2$, where α is real the most general solution for $x < 0$ is

$$\psi_{II} = Ce^{\alpha x} + De^{-\alpha x}$$

Region III The solution for $x < 0$, will have the same form as in the region II.

$$\psi_{III} = Fe^{\alpha x} + Ge^{-\alpha x}$$

Boundary conditions at infinity

For the bound states the wave function must vanish for large distances.

(i) We want that $\psi_{III}(x)$ should $\to 0$ as $x \to -\infty$.
$\therefore G = 0$

(ii) Also $\psi_{II}(x)$ should $\to 0$ as $x \to \infty$

$\therefore \quad C = 0$

Continuity Conditions Next we require that the wave function and its derivative be continuous at $x = 0$ and $x = L$.

(i) Continuity conditions for the solution and its derivative at $x = 0$ give

$$\psi_{III}(x)|_{x=0} = \psi_I(x)|_{x=0} \tag{1.9}$$
$$\psi'_{III}(x)|_{x=0} = \psi'_I(x)|_{x=0} \tag{1.10}$$

writing out these and using $G = 0$ gives

$$F = B \tag{1.11}$$
$$\alpha F = kA \tag{1.12}$$

which implies

$$B = kA/\alpha \tag{1.13}$$

(ii) Continuity conditions for the derivative at $x = L$ give

$$\psi_I(x)|_{x=L} = \psi_{II}(x)|_{x=L} \tag{1.14}$$
$$\psi'_I(x)|_{x=L} = \psi'_{II}(x)|_{x=L} \tag{1.15}$$

These equations imply

$$A\sin kL + B\cos kL = De^{-\alpha L} \tag{1.16}$$
$$kA\cos kL - kB\sin kL = -D\alpha e^{-\alpha L} \tag{1.17}$$

We use Eq.(13) to eliminate B in favour of A, next using Eq.(16) and ((17)) we get two equations for A and D. These two equations can be written in form of a matrix

$$\begin{bmatrix} \sin kL + \frac{k}{\alpha}\cos kL & -e^{-\alpha L} \\ k\cos kL - \frac{k^2}{\alpha}\sin kL & \alpha e^{-\alpha L} \end{bmatrix} \begin{bmatrix} A \\ D \end{bmatrix} = 0$$

These equations have a non trivial solution only when the determinant of the matrix on left hand side is zero. This requirement gives a condition on the allowed values of energy and can be cast in the forms

$$\alpha(\sin kL + \frac{k}{\alpha}\cos kL) + (k\cos kL - \frac{k^2}{\alpha}\sin kL) = 0 \tag{1.18}$$
$$(k^2 - \alpha^2)\sin kL - 2k\alpha\cos kL = 0. \tag{1.19}$$

i.e.

$$\tan kL = \frac{2k\alpha}{k^2 - \alpha^2} \equiv \tan 2\theta, \tag{1.20}$$

where θ is defined by $\tan\theta = \alpha/k$, it is now easy to see that bound state energy eigenvalue must satisfy

$$k\tan kL/2 = \alpha, \qquad \text{or} \qquad k\cot kL/2 = -\alpha \tag{1.21}$$

Energy E appears in the above quantization condition through k and α and can be determined graphically.

§3 Dirac Delta Function Potential

§4 Harmonic oscillator

We shall now outline the steps for deriving energy levels and wave functions for harmonic oscillator in the coordinate representation. The eigenvalue equation

$$H\psi = E\psi$$

for the harmonic oscillator becomes the following differential equation in coordinate representation

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 q^2\right)\psi(q) = E\psi(q) \tag{1.22}$$

The main steps in solution of the eigenvalue problem in coordinate representation are as follows.

1. In terms of dimensionless variables $\xi = \alpha q$, $\lambda = 2E/\hbar\omega$, where $\alpha^2 = m\omega/\hbar$, the Schrödinger equation (1) becomes

$$\frac{d^2\psi}{d\xi^2} + (\lambda - \xi^2)\psi = 0 \ .$$

2. It can be seen that for *large* ξ solutions to the differential equation behave as a polynomial times $e^{\pm\xi^2/2}$.

3. Define $H(\xi)$ by means of the equation

$$\psi(\xi) = H(\xi)e^{-\xi^2/2}$$

then $H(\xi)$ satisfies equation.

$$H'' - 2\xi H' + (\lambda - 1)H = 0 \ . \tag{1.23}$$

4. The above equation is well known Hermite equation and can be solved by the method of series solution. To solve the Hermite equation we write a series expansion

$$H(\xi) = \xi^c(a_o + a_1\xi + a_2\xi^2 + \cdots) \tag{1.24}$$

The series (3) is substituted in (1), and coefficient of each power of ξ coming from the L.H.S. of (2) must be set equal to zero. This gives value of c

$$c(c-1) = 0 \quad \Rightarrow c = 0, 1$$

and recurrence relations for the coefficients an

$$a_{n+2} = \frac{2n + 2c + 1 - \lambda}{(n+c+1)(n+c+2)}\, a_n \ . \tag{1.25}$$

5. *For* $c = 0$ all the even coefficients are determined in terms of a_o and all the odd coefficients are proportional to a_1, and a_o and a_1 are arbitrary. Thus one gets

$$H(\xi) = a_1 y_1(\xi) + a_2 y_2(\xi) \tag{1.26}$$

For $c = 1$ the solution for $H(\xi)$ is proportional to $y_2(\xi)$ and is already contained in (5). Hence this case, $c = 1$, need not be considered separately.

Note the eqn.(2) is a second order differential equation and the most general solution is a linear combination of two independent solutions $y_1(\xi)$ and $y_2(\xi)$.

6. Next we must explore large ξ behaviour of (5). The relation (4) for large n takes the form

$$\frac{a_{n+2}}{a_n} \sim \frac{2}{n} \ .$$

which coincides with the ratio of the expansion coefficients, in the series for $\exp(\xi^2)$

$$\exp(\xi^2) = \sum \frac{\xi^{2n}}{n!}$$

Thus the two solutions $y_1(\xi)$ and $y_2(\xi)$ behave like $\exp(\xi^2)$ for large ξ and

$$\begin{aligned} \psi(\xi) &= H(\xi) e^{\xi^2/2} && (1.27) \\ \xi\to\infty &\sim e^{\xi^2} \times e^{-\xi^2/2} = e^{\xi^2/2} && (1.28) \end{aligned}$$

This behaviour of $\psi(\xi)$ for large ξ makes the solution unacceptable because $\psi(\xi)$ would not be square integrable.

7. The only way one can get a square integrable solution for $\psi(q)$ is that the solution $H(\xi)$ must reduce to a polynomial. If $H(\xi)$ is to contain a maximum power n then we must demand the following conditions.

   (i) $a_{n+2} = 0$
   $\Rightarrow 2n + 2c + 1 - \lambda = 0$
   $\lambda = 2n + 1$
   and

   (ii) $a_1 = 0$ if $n =$ even
   $a_o = 0$ if $n =$ odd.

8. The condition $\lambda = (2n + 1)$ is equivalent to the energy quantization

$$E = (n + \frac{1}{2})\hbar\omega \ .$$

The wave functions are obtained by using conditions, as in (i) and (ii) above, and the recurrence relations to solve for the coefficients a_n. The resulting solutions for H_n are Hermite polynomials and the normalized eigenfunctions are given by

$$\psi_n(q) = \left(\frac{\alpha}{\sqrt{\pi}\; 2^n n!}\right)^{1/2} H_n(\alpha q) \exp(-\alpha^2 q^2/2)$$

These coincide with the wave functions obtained from operator methods $\frac{1}{n!}(a^\dagger)^n \phi_0(q)$.

Lesson 2

Reflection and Transmission

§1 Defining Reflection and Transmission Coefficients

The reflection and transmission coefficients for a particle through a potential will be defined in terms of large distance asymptotic properties of the solutions of the Schrödinger equation. We shall, therefore, consider the motion of a particle in a one dimensional potential $V(x)$. We assume that the potential is such that it approaches a constant value V_1 as $x \to -\infty$ and a constant value V_2 as $x \to +\infty$.

$$\lim_{x\to-\infty} = V_1, \qquad \lim_{x\to+\infty} = V_2. \tag{2.1}$$

The motion of the particle from $-\infty$ to $+\infty$ is possible only when energy E of the particle is greater than both E_1 and E_2. We assume this to be the case. The Schrödinger equation for the particle is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x). \tag{2.2}$$

We look for behaviour of solutions as $x \to -\infty$, so replace $V(x)$ with V_1 and solve the resulting equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_1\psi(x) = E\psi(x). \tag{2.3}$$

or

$$\frac{d^2\psi}{dx^2} + \frac{2m(E-V_1)}{\hbar^2}\psi(x) = 0. \tag{2.4}$$

Defining k_1 by

$$k_1 = \sqrt{\frac{2m(E-V_1)}{\hbar^2}} \tag{2.5}$$

we get, for $x \to -\infty$,

$$\frac{d^2\psi}{dx^2} + k_1^2\psi(x) = 0. \tag{2.6}$$

Therefore we have

$$\psi(x) \to Ae^{ik_1x} + Be^{-ik_1x} \tag{2.7}$$

as $x \to -\infty$. Similarly, the most general form of the solution for large $x \to \infty$ is

$$\psi(x) \to Ce^{ik_2x} + De^{-ik_2x} \tag{2.8}$$

where

$$k_2 = \sqrt{\frac{2m(E - V_2)}{\hbar^2}}. \tag{2.9}$$

The four constants A, B, C, D are not arbitrary and have two relations to satisfy. Hence two parameters remain undetermined and there will be two linearly independent solutions for energy $E > V_1, V_2$.

The physical interpretation of the wave function for the problem of reflection and transmission, requires a suitable additional boundary condition that will restrict further the parameters. We will have only one (linearly independent) solution from which the reflection and transmission coefficients can be determined.

Let us now turn to analysis of scattering experiment. We consider a beam of particles incident on a target whose effect will be modelled by the potential $V(x)$ satisfying conditions (29). A part of the beam will get reflected and a part will will be transmitted. If the beam is incident from the left, (from $= -\infty$), we shall have only transmitted beam on the right of the target. A part of the incident beam will get reflected and will be travelling to the left. Also the transmitted beam will be travelling to the right.

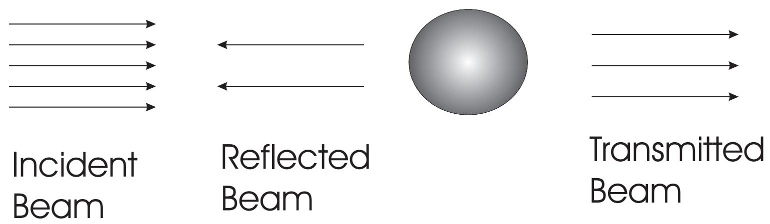

Fig. 5

Thus to the left of the target, we have superposition of plane waves travelling to the left and to the right, but on the right, as $x \to \infty$, we have wave travelling in the positive x

direction only.This experimental situation will be described by a wave function satisfying the following asymptotic behaviour for large distances.

$$\psi(x) \stackrel{x\to-\infty}{\longrightarrow} A\exp(ik_1x) + B\exp(-ik_1x) \tag{2.10}$$

$$\psi(x) \stackrel{x\to+\infty}{\longrightarrow} C\exp(ik_2x). \tag{2.11}$$

i.e. we should look for solutions of the Schrödinger equation satisfying (38) and (39) ($D = 0$ in $Eq.$(36).

The physical interpretation of the coefficients A, B, C in the wave function is obtained by computing the current density

$$j(x) = \frac{\hbar}{2im}\left[\psi^*(x)\frac{d}{dx}\psi(x) - \psi(x)\frac{d}{dx}\psi^*(x)\right] \tag{2.12}$$

for large distances. We have

$$\begin{aligned} &\text{as } x\to-\infty, \quad j \to (|A|^2 - |B|^2)\times\left(\frac{\hbar k_1}{m}\right) \\ &\text{as } x\to+\infty \quad j\to |C|^2\left(\frac{\hbar k_2}{m}\right) \end{aligned} \tag{2.13}$$

In the region $x\to-\infty$ we have a superposition of waves travelling to the right and to the left with fluxes $|A|^2\times\frac{\hbar k_1}{m}$ and $|B|^2\times\frac{\hbar k_1}{m}$ respectively. In the region $x\to+\infty$ we have a wave travelling to the right with flux $|C|^2\frac{\hbar k_2}{m}$. Hence we are led to define the reflection and transmission coefficients as

$$T = \frac{\text{Flux for the transmitted beam}}{\text{Incident flux}} = \left|\frac{C}{A}\right|^2\frac{k_2}{k_1} \tag{2.14}$$

$$R = \frac{\text{Flux for the reflected beam}}{\text{Incident flux}} = \left|\frac{B}{A}\right|^2. \tag{2.15}$$

We will now show that the conservation of probability holds for a real local potential and that it implies

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0 \tag{2.16}$$

$$\rho(\vec{r},t) = |\psi(x)|^2, \quad \vec{j}(\vec{r},t) = \frac{\hbar}{2im}\Big(\psi^*(\vec{r},t)\nabla\psi(\vec{r},t) - \psi(\vec{r},t)\nabla\psi^*(\vec{r},t)\Big). \tag{2.17}$$

For one dimensional problems, $\vec{j}$ has only one component and

$$j(x) = \frac{\hbar}{2im}\Big(\psi^*(x)\frac{d}{dx}\psi(x) - \psi(x)\frac{d}{dx}\psi^*(x)\Big). \tag{2.18}$$

As $\psi(x,t)$ is corresponds to a definite energy E, its time dependence is given by

$$\psi(x,t) = e^{-iEt/hbar}\psi(x,0), \tag{2.19}$$

and hence the probability density

$$\rho = |\psi(x,0)|^2 \tag{2.20}$$

is independent of time and $\frac{d\rho}{dt} = 0$. Thus for a stationary state in one dimension $Eq.$(44) implies that

$$\frac{dj}{dx} \Rightarrow j(x) = \text{constant}, \tag{2.21}$$

Thus $j(x)$ is independent of x and

$$j(+\infty) = j(-\infty) \tag{2.22}$$

Using $Eq.$(41) we get

$$\frac{\hbar k_1}{m}(|A|^2 - |A|^2) = \frac{\hbar k_2}{m}|C|^2. \tag{2.23}$$

Divide by $\frac{\hbar k_1}{m}|A|^2$ to get

$$1 - \left|\frac{B}{A}\right|^2 = \frac{k_2}{k_2}|C|^2 \Rightarrow 1 - R = T \tag{2.24}$$

Thus as a consequence of probability conservation we get the result that the transmission and reflection coefficients must add to unity, *i.e.* nothing is lost in transmission.

§2 Reflection and Transmission Through a Square Barrier

We wish to compute the reflection and transmission coefficients for a beam incident on a target represented by a square barrier. The potential is assumed to be of the form

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & 0 \le x \le L \\ 0, & x > L \end{cases}. \tag{2.25}$$

where $V_0 > 0$.

Solve eigenvalue problem

We assume $0 < E < V_0$ and write the solutions in the three regions R_I, R_{II}, R_{III}

$$R_I = \{x|x < 0\}, \qquad R_{II} = \{x|0 \le x \le L\}, \qquad R_{III} = \{x|x > L\}.$$

as

$$\begin{aligned}
\psi_{\text{I}}(x) &= A\exp(ikx) + B\exp(-ikx) && (2.26)\\
\psi_{\text{II}}(x) &= C\exp(\alpha x) + B\exp(-\alpha x) && (2.27)\\
\psi_{\text{III}}(x) &= F\exp(ikx) + G\exp(-ikx) && (2.28)
\end{aligned}$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \qquad \alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}. \tag{2.29}$$

Now we ask what boundary conditions and matching conditions are to be imposed on the solution of the Schrödinger equation to fix the unknown constants. The wave function and its derivative must be continuous at $x = 0$ and at $x = L$.

Apart from above general requirements, a boundary condition specific to the problem of finding the reflection and transmission coefficients is to be imposed. Let us assume that the incident beam is coming from the left. In general some particles will be reflected and some will be transmitted. Thus we should expect particles travelling both ways, to the left and to the right in region R_{I}, but in R_{III} there are only transmitted particles travelling to the right. Thus the solution in R_{III} should have only $\exp(ikx)$ term and we must set $G = 0$.

Setting $G = 0$ and requiring continuity of wave function and its derivative at $x = 0$ and at $x = L$ gives

$$\begin{array}{ll}
\underline{x=0} & A + B = C + D \\
 & ik(A - B) = \alpha(C - D) \\
\underline{x=L} & C\exp(\alpha L) + D\exp(-\alpha L) = F\exp(ikL) \\
 & i\alpha C\exp(\alpha L) - i\alpha D\exp(-\alpha L) = ikF\exp(ikL)
\end{array} \tag{2.30}$$

Solving these equations for F/A we get the transmission amplitude as

$$S(E) = \frac{F}{A} = \frac{2i\alpha k}{2i\alpha k\cosh\alpha L + (k^2 - L^2)\sinh\alpha L} \tag{2.31}$$

and the transmission coefficient is

$$T = |S(E)|^2 = \left[1 + \frac{\sinh^2\alpha L}{4(E/V_0)(1 - E/V_0)}\right]^2 \tag{2.32}$$

A classical particle with energy $E < V_0$ cannot cross the barrier. However, quantum mechanically there is nonzero probability that the particle will be transmitted and we say that the particle 'tunnels through the barrier'. For $E \approx V_0, \alpha \approx 0$, and one has

$$T(E) \to \left(1 + \frac{mV_0L^2}{2\hbar^2}\right)^{-1}. \tag{2.33}$$

For an opaque barrier $\alpha L >> 1$ the transmission coefficient is given by

$$T(V_0) \approx \left(\frac{16E(E - V_0)}{V_0^2}\right) \exp(-2\alpha L). \tag{2.34}$$

Lesson 3

Harmonic Oscillator

We shall now outline the steps for deriving energy levels and wave functions for harmonic oscillator in the coordinate representation. The eigenvalue equation

$$H\psi = E\psi$$

for the harmonic oscillator becomes the following differential equation in coordinate representation

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 q^2\right)\psi(q) = E\psi(q) \tag{3.1}$$

The main steps in solution of the eigenvalue problem in coordinate representation are as follows.

1. In terms of dimensionless variables $\xi = \alpha q$, $\lambda = 2E/\hbar\omega$, where $\alpha^2 = m\omega/\hbar$, the Schrödinger equation (1) becomes

$$\frac{d^2\psi}{d\xi^2} + (\lambda - \xi^2)\psi = 0 \ .$$

2. It can be seen that for *large* ξ solutions to the differential equation behave as a polynomial times $e^{\pm\xi^2/2}$.

3. Define $H(\xi)$ by means of the equation

$$\psi(\xi) = H(\xi)e^{-\xi^2/2}$$

   then $H(\xi)$ satisfies equation.

$$H'' - 2\xi H' + (\lambda - 1)H = 0 \ . \tag{3.2}$$

4. The above equation is well known Hermite equation and can be solved by the method of series solution. To solve the Hermite equation we write a series expansion

$$H(\xi) = \xi^c(a_o + a_1\xi + a_2\xi^2 + \cdots) \tag{3.3}$$

The series (3) is substituted in (1), and coefficient of each power of ξ coming from the L.H.S. of (2) must be set equal to zero. This gives value of c

$$c(c-1) = 0 \quad \Rightarrow c = 0, 1$$

and recurrence relations for the coefficients an

$$a_{n+2} = \frac{2n + 2c + 1 - \lambda}{(n + c + 1)(n + c + 2)}\, a_n \quad . \tag{3.4}$$

5. *For* $c = 0$ all the even coefficients are determined in terms of a_o and all the odd coefficients are proportional to a_1, and a_o and a_1 are arbitrary. Thus one gets

$$H(\xi) = a_1 y_1(\xi) + a_2 y_2(\xi) \tag{3.5}$$

For $c = 1$ the solution for $H(\xi)$ is proportional to $y_2(\xi)$ and is already contained in (5). Hence this case, $c = 1$, need not be considered separately.

Note the eqn.(2) is a second order differential equation and the most general solution is a linear combination of two independent solutions $y_1(\xi)$ and $y_2(\xi)$.

6. Next we must explore large ξ behaviour of (5). The relation (4) for large n takes the form

$$\frac{a_{n+2}}{a_n} \sim \frac{2}{n} \quad .$$

which coincides with the ratio of the expansion coefficients, in the series for $\exp(\xi^2)$

$$\exp(\xi^2) = \sum \frac{\xi^{2n}}{n!}$$

Thus the two solutions $y_1(\xi)$ and $y_2(\xi)$ behave like $\exp(\xi^2)$ for large ξ and

$$\begin{aligned} \psi(\xi) &= H(\xi)e^{\xi^2/2} && (3.6)\\ {}_{\xi\to\infty} &\sim e^{\xi^2} \times e^{-\xi^2/2} = e^{\xi^2/2} && (3.7) \end{aligned}$$

This behaviour of $\psi(\xi)$ for large ξ makes the solution unacceptable because $\psi(\xi)$ would not be square integrable.

7. The only way one can get a square integrable solution for $\psi(q)$ is that the solution $H(\xi)$ must reduce to a polynomial. If $H(\xi)$ is to contain a maximum power n then we must demand the following conditions.

(i) $a_{n+2} = 0$
$\Rightarrow 2n + 2c + 1 - \lambda = 0$
$\lambda = 2n + 1$
and

(ii) $a_1 = 0$ if $n =$ even
$a_o = 0$ if $n =$ odd.

8. The condition $\lambda = (2n + 1)$ is equivalent to the energy quantization

$$E = (n + \frac{1}{2})\hbar\omega \ .$$

The wave functions are obtained by using conditions, as in (i) and (ii) above, and the recurrence relations to solve for the coefficients a_n. The resulting solutions for H_n are Hermite polynomials and the normalized eigenfunctions are given by

$$\psi_n(q) = \left(\frac{\alpha}{\sqrt{\pi}\ 2^n n!} \right)^{1/2} H_n(\alpha q) \exp(-\alpha^2 q^2/2)$$

These coincide with the wave functions obtained from operator methods $\frac{1}{n!}(a^\dagger)^n \phi_0(q)$.

Lesson 4

General Properties of Motion In One Dimension

1. *Bound state eigenvalues are non-degenerate :*

   Proof: We shall show that if for a given bound state energy eigenvalue E there are two eigenfunctions ψ_1 and ψ_2, the two solutions must be proportional. Thus we have Eqs(70) and (71)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} + V\psi_1 = E\psi_1 \tag{4.1}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V\psi_2 = E\psi_2 \tag{4.2}$$

   Multiply 70 by ψ_2 and 71 by ψ_1 and subtract to get

$$-\frac{\hbar^2}{2m}\left(\psi_2\frac{d^2\psi_1}{dx^2} - \psi_1\frac{d^2\psi_2}{dx^2}\right) = 0 \tag{4.3}$$

$$\text{or} \qquad \frac{d}{dx}\left(\psi_2\frac{d\psi_1}{dx} - \psi_1\frac{d\psi_2}{dx}\right) = 0 \tag{4.4}$$

   Integrating we get

$$\left(\psi_2\frac{d\psi_1}{dx} - \psi_1\frac{d\psi_2}{dx}\right) = \text{const.}\ , C$$

   The constant C can be fixed by evaluating the left hand side at $x = \infty$. As $x \to \pm\infty$, $\psi_1 \to 0$, $\psi_2 \to 0$ for bound states

   $\therefore \quad C = 0$

   Thus we get

$$\psi_2\frac{d\psi_1}{dx} - \psi_1\frac{d\psi_2}{dx} = 0 \tag{4.5}$$

$$\text{or} \qquad \frac{1}{\psi_1}\frac{d\psi_1}{dx} - \frac{1}{\psi_2}\frac{d\psi_2}{dx} = 0 \tag{4.6}$$

Integrating we get

$$\begin{aligned} \ln\psi_1 - \ln\psi_2 &= \text{const.},\ K && (4.7)\\ \text{or} \qquad \ln(\psi_2/\psi_1) &= \ln K && (4.8)\\ \text{or} \qquad \psi_2 &= K\psi_1 && (4.9) \end{aligned}$$

$\therefore$ ψ_1 and ψ_2 are linearly dependent. Hence the bound state eigenvalues in one dimension are *non degenerate*. An exception to this result is particle in twin, (or more) boxes described by the potential

$$V(x) = \begin{cases} 0 & 0 \le x \le L \\ 0 & 2L \le x \le 3L \\ \infty & \text{otherwise} \end{cases}$$

For this potential each energy eigenvalue has two linearly independent solutions.

2. *Behaviour of the energy eigenfunctions for large distances* Consider the motion of a particle in one dimension in a potential $V(x)$ such that

   a) $V(x)$ has a minimum value V_{min}

   b) as $x \to +\infty$ $V(x) \to V_+$

   c) as $x \to -\infty$ $V(x) \to V_-$

   Then the large distance behaviour of the corresponding energy eigenfunction is as follows.

   a) The energy eigenfunction for $E < V_o$ is exponentially damped

$$\psi_E(x) \longrightarrow \exp(-\alpha_1 x) \qquad \text{as} \qquad x \to \infty \tag{4.10}$$

$$\psi_E(x) \longrightarrow \exp(\alpha_2 x) \qquad \text{as} \qquad x \to -\infty \tag{4.11}$$

   where $\alpha_1 = \sqrt{\frac{2m(V_- E)}{\hbar^2}}$, $\alpha_2 = \sqrt{\frac{2m(V_+ - E)}{\hbar^2}}$

   b) For $E > V_o$, the solution behaves like plane waves (i.e., it is oscillatory) at large distances. As $x \to \infty$

$$\psi(x) \to \begin{cases} A\cos k_1 x + B\sin k_1 x \\ \text{or} \\ Ae^{ik_1 x} + Be^{-ik_1 x} \qquad\qquad k_1 = \sqrt{2m(E - V_+)}\hbar^2 \end{cases} \tag{4.12}$$

   and as $x \to -\infty$ we get

$$\psi(x) \to \begin{cases} A\cos k_2 x + B\sin k_2 x \\ \text{or} \\ Ae^{ik_2 x} + Be^{-ik_2 x} \qquad\qquad k_2 = \frac{\sqrt{2m(E-V_-)}}{\hbar^2} \end{cases}$$

3. *Nature and degeneracy of energy eigenvalues*
   The nature of energy eigenvalues, discrete or continuous, degenerate or non-degenerate, is generally given by the following rules. It may be added that the rules give us an idea what to expect for given potential and that exceptions to some of these rules below are known to exist.

   - It can be proved that the energy eigenvalues must be greater than or equal to V_{min}.
   - Bound states exist for energy greater than V_{min} and but below both V_+ and V_-. The corresponding energy eigenvalues are discrete and nondegenerate.
   - For E between V_+, V_-, the eigenvalues are continuous and non-degenerate.
   - For E greater than both V_+ and V_-, the energies are continuous and doubly degenerate.

   You may check validity of these rules for the potential problems for which you have seen exact solutions such as square well, harmonic oscillator and other potentials .

4. *Minimum bound state energy*
   If the potential function has a minimum at x_o with a value V_{min}. In classical mechanics, a state with zero momentum, $p = 0$, and $x = x_o$ can exist and the energy will be V_{min}. In QM x and p cannot have sharp values simultaneously, and for the lowest bound state the energy will, in general, be greater than V_{min}. The ground state energy can be estimated using the uncertainty principle. We shall illustrate this by means of the harmonic oscillator.

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

   $V_{min} = 0$ classically $x = 0$, $p = 0$, $E = 0$ is a possible state. Quantum mechanically, the values of x and p will have some uncertainties Δx and Δp which are subject to the uncertainty relation $\Delta p \Delta x \simeq \hbar$. Taking the averages of x^2 and p^2 of the order of $(\Delta x)^2$ and $(\Delta p)^2$, respectively, and using $\Delta p \approx \frac{\hbar}{\Delta x}$, we have

   $$\begin{aligned} < KE > &\approx \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{2m(\Delta x)^2} && (4.13)\\ < V(x) > &\approx \frac{1}{2}m\omega^2(\Delta x)^2 && (4.14)\\ E &\approx \frac{\hbar^2}{2m}\left(\frac{1}{\Delta x}\right)^2 + \frac{1}{2}m\omega^2(\Delta x)^2 && (4.15)\end{aligned}$$

Minimizing E w.r.t. Δx we get

$$\begin{aligned}
\frac{\hbar^2}{2m}\left(\frac{-2}{(\Delta x)^3}\right)+\frac{1}{2}m\omega^2 2(\Delta x) &= 0 && (4.16)\\
(\Delta x)^4 &= \frac{\hbar^2}{2m}\times\frac{2m}{m\omega^2} && (4.17)\\
(\Delta x)^2 &= \frac{\hbar}{m\omega} && (4.18)\\
E &\approx \frac{\hbar^2}{2m}\frac{m\omega}{\hbar}+\frac{1}{2}m\omega^2\frac{\hbar^2}{m\omega} && (4.19)\\
&= \hbar\omega && (4.20)
\end{aligned}$$

If we had used $\Delta p\Delta x \geq \hbar/2$ we would have obtained

$$E_{min} = \frac{\hbar\omega}{2}$$

which matches with the exact ground state energy of the harmonic oscillator. In general this argent can be used to get a quick estimate of the ground state energy for a given potential.

5. *Parity*

If the potential is an even function of x,*i.e.*, $V(-x) = V(x)$, the parity operator commutes with the Hamiltonian.

$$\hat{P}\hat{H} - \hat{H}\hat{P} = 0 \qquad (4.21)$$

If $u_E(x)$ is an eigenfunction of energy with eigenvalue E, $v(x) = Pu(x) = u(-x)$ is also an eigenfunction of Hamiltonian with the same eigenvalue E. This is easily seen by applying $\hat{H}$ on $v(x)$.

$$\begin{aligned}
\hat{H}v(x) &= \hat{H}\hat{P}u(x) && (4.22)\\
&= \hat{P}\hat{H}u(x) && (4.23)\\
&= E\hat{P}u(x) && (4.24)\\
&= Ev(x) && (4.25)
\end{aligned}$$

Now there are two possibilities.

(a) When the eigenvalue is non-degenerate there is only one linearly independent eigenfunction and $u(x)$ and $v(x)$ must be proportional. There must exist a constant c such that

$$u(x) = cv(x) \qquad (4.26)$$

Noting the relation $v(x) = u(-x)$, we have

$$u(x) = cu(-x) \qquad (4.27)$$

Making a replacement $x \to -x$ in this equation implies

$$u(-x) = cu(x) \tag{4.28}$$

Now Eq.(95) and Eq.(96) imply that $c^2 = 1$ and hence $c = \pm 1$. This gives $u(x) = \pm u(-x)$ and $u(x)$ must be an eigenfunction of parity.

(b) In the first case when $u(x)$ and $v(x)$ are linearly independent, v(x) is a new solution of the eigenvalue problem. This happens if and only if the energy is degenerate. This is the case for example for a symmetric square well for positive energies. If form the combinations $w_1(x), w_2(x)$ defined by

$$\begin{aligned} w_1(x) &= u(x) + v(x) = u(x) + u(-x) & (4.29)\\ w_2(x) &= u(x) - v(x) = u(x) - u(-x) & (4.30) \end{aligned}$$

and these will be eigenfunctions of parity.

Similar comments, though differing in details, will apply for any operator which commutes with Hamiltonian of the system.

6. *Tunnelling through a barrier*

Consider an example of a particle is initially confined to a box whose walls can be represented by a potential barrier of finite height V_0. For example considering a one dimensional box having walls represented by a potential of height V_0. Let the potential inside and outside box be zero.

If the energy of the particle is less than barrier height V_0, classicallythe particle will always remain confined to the box. Similarly for the two potentials shown in Fig. 2 and Fig. 3 bounded motion is possible for a classical particle for energies between V_1 and V_2 if the particle is on the left of the maximum at $x = b$, it cannot cross the barrier at x=b when $E < V_2$.

However, in quantum mechanics, the bound state energies for both the potentials in Fig. 2 and in Fig. 3, do not correspond to this range $V_1 < E < V_2$. For potential of Fig. 2 there are no bound states at all. For all energies $E > V_0$ the energies are continuous and particle has a non zero wave function at ∞. For the potential of Fig.3 bound states energy must lie betwee0 and V_2. This happens because quantum mechanically a particle can cross a barrier even if it has energy less than the barrier height. Exactly in a similar fashion, a classical particle incident from the right $(x > b)$ within$E < V_2$ cannot reach the region $x < b$, whereas a quantum particle can.

This phenomenon is known as barrier penetration or tunnelling. earliest know example of tunnelling phenomenon is α decay.

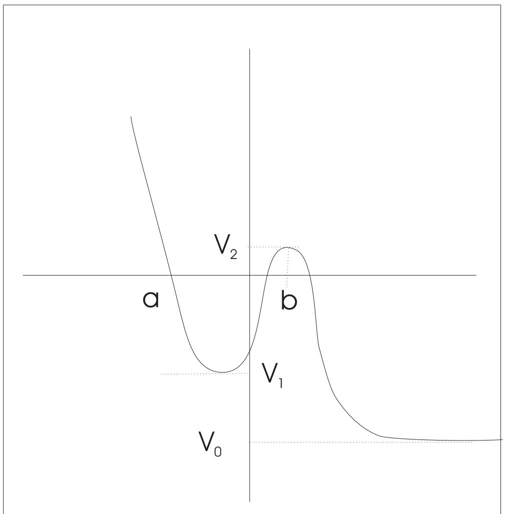

Fig 2

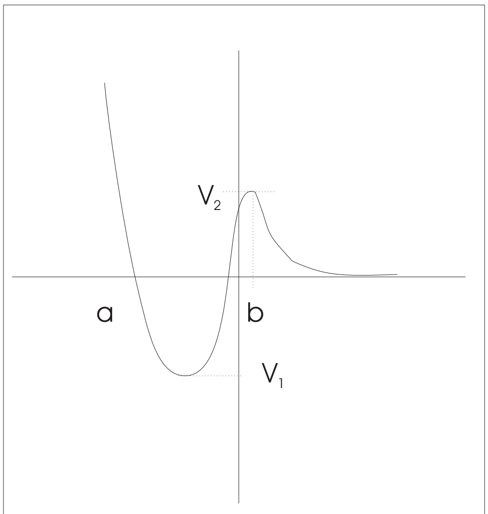

Fig 3

7. *Periodic potentials, Energy bands* Let $V(x)$ be a periodic potential with period L

$$V(x+L) = V(x) \ .$$

The energy eigenvalues has bands of allowed energies and forbidden energies and the energy level diagram is schematically shown in Fig. 4.

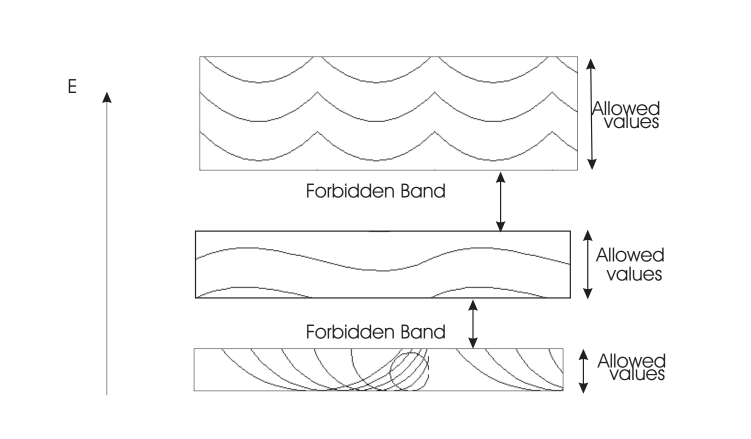

Fig 4 Bands in Energy Level Diagram of a Periodic Potential