QM-13 Lecture Notes

One Dimensional Potential Problems

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Contents

§1 Intoduction

Solving the eigenvalue problem for the Hamiltonian gives the allowed values of energies of a system. Working within the Schrödinger representation, the eigenvalues and eigenfunctions for a particle in box, square well, delta function potential and the harmonic oscillator will be obtained. In the Schrödinger representation the Hamiltonian operator, for a particle in one dimension, is

$$H = \frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x), \tag{1}$$

and the eigenfunctions are obtained by solving the Schrödinger equation

$$Hu(x) = Eu(x) \tag{2}$$

$$\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} + V(x)u(x) = Eu(x). \tag{3}$$

Let us talk about the requirements that must be imposed on $u(x)$, so that the solution may be acceptable. When the potential is a continuous function of x, the differential equation Eq.(3) requires the second derivative must exist and hence that $u(x)$ and its first derivative $u'(x)$ must be continuous. The same requirement holds for the potentials, such as square well, which are piecewise continuous with a finite jump at the discontinuity. *For more singular potentials, the correct requirements on the solution and the its derivative will be found either from the Schrödinger equation directly, or by regarding the potential as a limiting case of suitable potential.* I will go through this exercise for infinite well and the Dirac delta function potential.

Additional physical requirements on acceptable wave functions follow from the fact that the absolute square $|u(x)|^2$ has the interpretation of being probability density. For motion in one dimension, in order that the position probability for every interval may be finite, the solution $u(x)$ must be less singular than $|x - a|^{-1/2}$ for all x. Moreover, for bound state solutions, the probability density, $|u(x)|^2$ must approach zero as $x \to \infty$. This means that the solution must go to zero faster than $x^{-1/2}$ for large distances. An exception will be made for continuous energy solutions which describe scattering from a potential. For the scattering problems when the potential is a finite range, I will follow a common, though not rigorous, practise to accept solutions which behave like free particle (plane waves in one dimension) at large distances. This is consistent with the physical picture for scattering that the particles behave like free particle at large distances.

We summarise a few important rules about the nature of solutions of the Schrödinger equation. Thought there are exceptions to these rules, they are valid for the cases of interest in our lectures. Let V_m denote the absolute minimum of the potential $V(x)$, *i.e.* $V_m \leq V(x), \forall x$. Denoting the asymptotic values of the potential $V(x)$ as $x \to \pm infty$ by $V_\pm$, it should be noted that

1. Energy must must be greater than the minimum value V_m.

2. If the bound states exist, their energies are quantized and must be less than both $V_\pm$, in addition to being greater than V_m.

3. For energies greater than V_-, or greater than V_+, bound state solutions can not be found and there in no quantisation of energy.

A detailed discussion of nature and properties of solutions will be taken up in a later lecture.

§2   Piecewise Continuous Potentials

§1   Particle in a box

The energy levels of a particle in one dimensional infinite well

$$V(x) = \begin{cases} 0, & 0 \leq x \leq L \\ \infty & \text{outside} \end{cases} \tag{4}$$

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

$$u(x) = A\sin kx + B\cos kx, \qquad k^2 = \frac{2mE}{\hbar^2}. \tag{5}$$

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

$$u(x) = 0, \qquad \text{if } x < 0, \text{ or } x > L. \tag{6}$$

The boundary conditions to be imposed on the solution are

$$u(0) = u(L) = 0, \tag{7}$$

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

$$u(0) = 0 \quad \Rightarrow \quad B = 0, \tag{8}$$
$$u(L) = 0 \quad \Rightarrow \quad \sin kL = 0. \tag{9}$$

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

$$E_n = \frac{\hbar^2 k_n^2}{2m}, = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \tag{10}$$

and the corresponding wave functions are

$$u_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) & 0 \le x \le L \\ 0 & x < 0 \text{ or } x > L. \end{cases} \tag{11}$$

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

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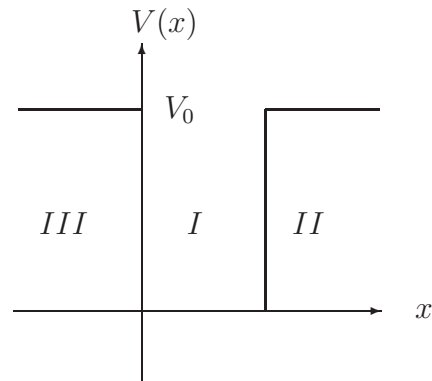

Fig. 1

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 $x \to \infty$

  $\therefore\ \ C = 0$

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

$$\psi_{III}(x)|_{x=0} = \psi_I(x)|_{x=0} \tag{12}$$
$$\psi'_{III}(x)|_{x=0} = \psi'_I(x)|_{x=0} \tag{13}$$

writing out these and using $G = 0$ gives

$$F = B \tag{14}$$
$$\alpha F = kA \tag{15}$$

which implies

$$B = kA/\alpha \tag{16}$$

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

$$\psi_I(x)|_{x=L} = \psi_{II}(x)|_{x=L} \tag{17}$$
$$\psi'_I(x)|_{x=L} = \psi'_{II}(x)|_{x=L} \tag{18}$$

These equations imply

$$A \sin kL + B \cos kL = D e^{-\alpha L} \tag{19}$$
$$kA \cos kL - kB \sin kL = -D\alpha e^{-\alpha L} \tag{20}$$

We use Eq.(16) to eliminate B in favour of A, next using Eq.(19) and ((20)) 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

$$\alpha(\sin kL + \frac{k}{\alpha} \cos kL) + (k \cos kL - \frac{k^2}{\alpha} \sin kL) = 0 \tag{21}$$
$$(k^2 - \alpha^2) \sin kL - 2k\alpha \cos kL = 0. \tag{22}$$

i.e.

$$\tan kL = \frac{2k\alpha}{k^2 - \alpha^2} \equiv \tan 2\theta, \tag{23}$$

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

$$k \tan kL/2 = \alpha, \qquad \text{or} \qquad k \cot kL/2 = -\alpha \tag{24}$$

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

§3   Delta function potential

We will use the following three methods for obtaining the solutions to the energy eigenvalue problem for the Dirac δ function potential

$$V(x) = -g\delta(x) \tag{25}$$

where $g > 0$ is a constant. The three methods are

1. Dirac delta function potential as a limit of square well potential.

2. Solution of the eigenvalue problem by direct integration of the Schrödinger equation.

3. Solution of the eigenvalue problem in momentum space.

For $E > 0$ the eigenvalues will be seen to be continuous and doubly degenerate. The bound state exists only for $E < 0$. It will be shown that there is only one bound state with energy level given by $E = -|E|$,

$$|E| = \frac{mg^2}{\hbar^2}. \tag{26}$$

§1 δ function potential as limit of square well

To solve the δ function potential problem,

$$V(x) = -g\delta(x), \quad g > 0, \tag{27}$$

we consider it to be a limiting case of a square well potential of the form

$$V(x) = \begin{cases} 0, & \text{if } |x| > a, \\ -V_0 & \text{if } |x| < a. \end{cases}$$

When the strength of the potential $V_0 \to \infty$ and the range $a \to 0$ in such a way that the area under the potential energy curve remains constant $V_0 a \equiv g$,

$$\int_0^a V(x)\,dx = -2V_0 a. \tag{28}$$

we would get

$$\lim V(x) = -g\delta(x). \tag{29}$$

The solution of the square well is well known and we have the energy eigenfunction given by

$$u(x) = \begin{cases} u_1(x) = A\sin kx + B\cos kx & \text{if } -a < x < a, \\ u_2(x) = C\exp(-\alpha x), & \text{if } x > a, \\ u_3(x) = D\exp(-\alpha x), & \text{if } x < -a. \end{cases} \tag{30}$$

where

$$k^2 = \frac{2m(V_0 - |E|)}{\hbar^2}, \qquad \alpha^2 = \frac{2m|E|}{\hbar^2} \tag{31}$$

Since the bound state energy is expected to turn out to be negative, we have written $E = -|E|$. The boundary conditions, that the wave function and its derivative must be continuous at $x = \pm a$, give the result that the energy eigenvalue must satisfy one of the following two conditions.

$$k\tan ka = \alpha, \quad \text{or} \quad k\cot ka = -\alpha. \tag{32}$$

In order to consider limit $V_0 \to \infty, a \to 0$ with $g = 2V_0 a$ held fixed, we substitute $V_0 = g/2a$ and consider limit $a \to 0$. In this limit assuming $|E|$ to remain finite, we can substitute

$$k^2 = \frac{2m(V_0 - |E|)}{\hbar^2} \sim \frac{2mV_0}{\hbar^2} \sim \frac{mg}{\hbar^2 a}. \tag{33}$$

Therefore

$$ka \sim \sqrt{\frac{mga}{\hbar^2}}, \tag{34}$$

and the condition $k\tan ka = \alpha$ becomes

$$\sqrt{\frac{mg}{\hbar^2 a}} \tan\left(\sqrt{\frac{mga}{\hbar^2}}\right) = \sqrt{\frac{2m|E|}{\hbar^2}} \tag{35}$$

$$\sqrt{\frac{mg}{\hbar^2}} \frac{1}{\sqrt{a}} \tan\left(\sqrt{\frac{mga}{\hbar^2}}\right) = \sqrt{\frac{2m|E|}{\hbar^2}}. \tag{36}$$

We use the value $\lim_{x\to 0}\left(\dfrac{\tan \lambda x}{x}\right) = \lambda$, with $x \sim \sqrt{a}$ we get

$$\lim_{a\to 0} \frac{1}{\sqrt{a}} \tan\left(\sqrt{\frac{mg}{\hbar^2}}\sqrt{a}\right) = \sqrt{\frac{mg}{\hbar^2}}. \tag{37}$$

Using this in the left hand side of (36) we get the bound state condition

$$\frac{mg}{\hbar^2} = \sqrt{\frac{2m|E|}{\hbar^2}} \tag{38}$$

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Hence we have the bound state energy given by

$$E = -|E| = -\frac{mg^2}{2\hbar^2}. \tag{39}$$

It can be shown that there are no other solutions for the energy eigenvalues.

§2 Direct integration of the Schrödinger equation

We integrate the Schrödinger equation to derive boundary condition on the derivative of the eigenfunction at $x = 0$. We rewrite the Schrödinger equation for the delta function potential

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} - g\delta(x)u(x) = Eu(x) \tag{40}$$

in the form

$$\frac{d^2u(x)}{dx^2} + \frac{2mg}{\hbar^2}\delta(x)u(x) = \frac{2mE}{\hbar^2}u(x). \tag{41}$$

We want to solve for the bound state energy, hence E is negative and we set $E = -|E|$ and rewrite the Schrödinger equation as

$$\frac{d^2u(x)}{dx^2} + \frac{2mg}{\hbar^2}u(x) - \alpha^2 u(x) = 0, \tag{42}$$

where $\alpha^2 = \frac{2m|E|}{\hbar^2}$.

Since $\delta(x)$ is zero for $x \neq 0$, the Schrödinger equation for $x < 0$ and $x > 0$, both, takes the form

$$\frac{d^2u(x)}{dx^2} - \alpha^2 u(x) = 0 \tag{43}$$

which has two independent solutions $e^{\alpha x}$ and $e^{-\alpha x}$ and we write the most general solution as

$$u(x) = \begin{cases} u_1(x) = A\exp(\alpha x) + B\exp(-\alpha x) & x < 0 \\ u_2(x) = C\exp(\alpha x) + D\exp(-\alpha x) & x > 0 \end{cases} \tag{44}$$

Taking the boundary condition $u(x) \to 0$ as $x \to \pm\infty$ we get $B = C = 0$ and the solution for the eigenfunction becomes

$$u(x) = \begin{cases} u_1(x) = A\exp(\alpha x) & x < 0 \\ u_2(x) = D\exp(-\alpha x) & x > 0 \end{cases} \tag{45}$$

Demanding that the wave function be continuous at $x = 0$ ($u_1(0) = u_2(0)$) gives $D = A$ and we get

$$u(x) = \begin{cases} u_1(x) = A\exp(\alpha x) & x < 0 \\ u_2(x) = A\exp(-\alpha x) & x > 0 \end{cases} \tag{46}$$

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We integrate the Schrödinger equation, Eq.(42), from $-\epsilon$ to ϵ and take the limit $\epsilon \to 0$.

$$\int_{-\epsilon}^{\epsilon} \frac{d^2u}{dx^2}\,dx + \frac{mg}{\hbar^2}\int_{-\epsilon}^{\epsilon}\delta(x)u(x)\,dx - \alpha^2\int_{-\epsilon}^{\epsilon}u(x)\,dx = 0. \tag{47}$$

$$\text{or}\quad \left.\frac{du}{dx}\right|_{-\epsilon}^{\epsilon} + \frac{2mg}{\hbar^2}u(0) - \alpha^2\int_{-\epsilon}^{\epsilon}u(x)\,dx = 0. \tag{48}$$

The solution $u(x)$ is continuous at $x = 0$, hence in the limit $\epsilon \to 0$ the region of integration shrinks to zero and the last terms vanishes and we get the boundary condition on the first derivative at $x = 0$ as

$$\boxed{\left.\frac{du_2}{dx}\right|_{x=\epsilon} - \left.\frac{du_1}{dx}\right|_{x=-\epsilon} + \frac{2mg}{\hbar^2}u(0) = 0.} \tag{49}$$

Now using the explicit solution, Eq.(46), we get

$$u(0) = u_1(0) = u_2(0) = A \tag{50}$$

and

$$\left.\frac{du}{dx}\right|_{x=\epsilon} = \left.\frac{du_2}{dx}\right|_{x=\epsilon} = -A\alpha e^{-\alpha\epsilon}, \tag{51}$$

$$\left.\frac{du}{dx}\right|_{x=-\epsilon} = \left.\frac{du_1}{dx}\right|_{x=-\epsilon} = A\alpha e^{-\alpha\epsilon}. \tag{52}$$

The boundary condition, Eq.(49), in the limit $\epsilon \to 0$ becomes

$$-A\alpha e^{-\alpha\epsilon} - A\alpha e^{\alpha\epsilon} + \frac{2mg}{\hbar^2}A = 0 \tag{53}$$

$$\frac{2mg}{\hbar^2} = 2\alpha \Rightarrow \frac{m^2g^2}{\hbar^4} = \alpha^2 = \frac{2m|E|}{\hbar^2}. \tag{54}$$

Thus we get the bound state energy as

$$|E| = \frac{mg^2}{\hbar^2} \implies E = -|E| = -\frac{mg^2}{\hbar^2}. \tag{55}$$

The final form of the energy eigenfunction

$$u(x) = A\exp(-\alpha|x|), \tag{56}$$

after normalization

$$\int_{-\infty}^{\infty}|u(x)|^2\,dx = 1 \Rightarrow 2\int_0^{\infty}|A|^2\exp(-2\alpha x)\,dx = 1, \tag{57}$$

is given by

$$u(x) = \alpha^{-1/2}e^{-\alpha|x|}, \qquad \alpha = \frac{2mg}{\hbar^2}. \tag{58}$$

and the corresponding energy is given by Eq.(55).

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§3   Solution in Momentum Space

The Schrodinger equation for Dirac delta function potential is

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} - g\delta(x)u(x) = Eu(x) \tag{59}$$

Noting that $\delta(x)f(x) = \delta(x)f(0)$, for a continuous function $f(x)$ we rewrite the Schrödinger equation as

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2} - g\delta(x)u(0) = Eu(x) \tag{60}$$

Next the solution in coordinate space, $u(x)$, is related to the momentum space solution by

$$u(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\tilde{u}(k)\,dk, \tag{61}$$

also the Dirac delta function has the Fourier representation

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\,dk. \tag{62}$$

Substituting (61), (62) in Eq.(60) we get

$$k^2\tilde{u}(k) - \frac{2mg}{\hbar^2}u(0) = \frac{2mE}{\hbar^2}\tilde{u}(k). \tag{63}$$

Solving for momentum space wave function $\tilde{u}(k)$, (with $E = -|E|$) we get

$$\tilde{u}(k) = \frac{2mgu(0)}{\hbar^2 k^2 + 2m|E|} \tag{64}$$

and the solution $u(x)$ becomes

$$u(x) = \frac{2mgu(0)}{2\pi}\int \frac{e^{ikx}}{\hbar^2 k^2 + 2m|E|}\,dk, \tag{65}$$

$$= \frac{mgu(0)}{\alpha\hbar^2}e^{-\alpha|x|}. \tag{66}$$

where use has been made of

$$\int_{-\infty}^{\infty} \frac{e^{ikx}}{k^2 + a^2}\,dk = \frac{\pi}{a}e^{-k|x|}, \tag{67}$$

a result which can be proved by the method of contour integration. Setting $x = 0$ Eq.(66), and remembering the $u(0) \neq 0$ we get

$$\frac{mg}{\alpha^2} = 1 \Rightarrow |E| = \frac{mg^2}{\hbar^2}. \tag{68}$$

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and

$$u(x) = u(0)e^{-\alpha|x|}. \tag{69}$$

The unknown constant $u(0)$ is to be fixed by normalization

$$\int_{-\infty}^{\infty} |u(x)|^2 \, dx = 1 \implies \alpha|u(0)|^2 = 1. \tag{70}$$

The final expressions for the bound state eigenfunction and energy are given by

$$\boxed{E = -\frac{mg^2}{\hbar^2}, \qquad u(x) = \alpha^{-1/2} e^{-\alpha|x|}.} \tag{71}$$

§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

$$\left(\frac{-\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 q^2 \right) \psi(q) = E\psi(q) \tag{72}$$

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.

$$H'' - 2\xi H' + (\lambda - 1)H = 0 \ . \tag{73}$$

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

$$H(\xi) = \xi^c(a_o + a_1\xi + a_2\xi^2 + \cdots) \tag{74}$$

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

$$a_{n+2} = \frac{2n + 2c + 1 - \lambda}{(n+c+1)(n+c+2)} a_n \ . \tag{75}$$

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

$$H(\xi) = a_1 y_1(\xi) + a_2 y_2(\xi) \tag{76}$$

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

$$\psi(\xi) = H(\xi)e^{\xi^2/2} \tag{77}$$
$$\xi \to \infty \sim e^{\xi^2} \times e^{-\xi^2/2} = e^{\xi^2/2} \tag{78}$$

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 $\frac{1}{n!}(a^\dagger)^n \phi_0(q)$.

§5 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 (79) and (80)

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_1}{dx^2} + V\psi_1 \ = \ E\psi_1 \tag{79}$$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_2}{dx^2} + V\psi_2 \ = \ E\psi_2 \tag{80}$$

Multiply (79) by ψ_2 and (80) by ψ_1 and subtract to get

$$-\frac{\hbar^2}{2m}\left(\psi_2\frac{d^2\psi_1}{dx^2} - \psi_1\frac{d^2\psi_2}{dx^2}\right) = 0 \tag{81}$$

$$\text{or} \qquad \frac{d}{dx}\left(\psi_2\frac{d\psi_1}{dx} - \psi_1\frac{d\psi_2}{dx}\right) = 0 \tag{82}$$

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

$$\psi_2\frac{d\psi_1}{dx} - \psi_1\frac{d\psi_2}{dx} = 0 \tag{83}$$

$$\text{or} \qquad \frac{1}{\psi_1}\frac{d\psi_1}{dx} - \frac{1}{\psi_2}\frac{d\psi_2}{dx} = 0 \tag{84}$$

Integrating we get

$$\ln\psi_1 - \ln\psi_2 = \text{const., } K \tag{85}$$

$$\text{or} \qquad \ln(\psi_2/\psi_1) = \ln K \tag{86}$$

$$\text{or} \qquad \psi_2 = K\psi_1 \tag{87}$$

$\therefore$ 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 $x \to -\infty \quad V(x) \to V_-$

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

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

$$\psi_E(x) \longrightarrow \exp(-\alpha_1 x) \qquad \text{as} \qquad x \to \infty \tag{88}$$

$$\psi_E(x) \longrightarrow \exp(\alpha_2 x) \qquad \text{as} \qquad x \to -\infty \tag{89}$$

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

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

$$\psi(x) \to \begin{cases} A \cos k_1 x + B \sin k_1 x \\ \text{or} \\ A e^{ik_1 x} + B e^{-ik_1 x} \qquad k_1 = \sqrt{2m(E - V_+)} \hbar^2 \end{cases} \tag{90}$$

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

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

§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

$$< KE > \quad \approx \quad \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{2m(\Delta x)^2} \tag{91}$$

$$< V(x) > \quad \approx \quad \frac{1}{2}m\omega^2(\Delta x)^2 \tag{92}$$

$$E \quad \approx \quad \frac{\hbar^2}{2m}\left(\frac{1}{\Delta x}\right)^2 + \frac{1}{2}m\omega^2(\Delta x)^2 \tag{93}$$

Minimizing E w.r.t. Δx we get

$$\frac{\hbar^2}{2m}\left(\frac{-2}{(\Delta x)^3}\right) + \frac{1}{2}m\omega^2 2(\Delta x) \quad = \quad 0 \tag{94}$$

$$(\Delta x)^4 \quad = \quad \frac{\hbar^2}{2m} \times \frac{2m}{m\omega^2} \tag{95}$$

$$(\Delta x)^2 \quad = \quad \frac{\hbar}{m\omega} \tag{96}$$

$$E \quad \approx \quad \frac{\hbar^2}{2m}\frac{m\omega}{\hbar} + \frac{1}{2}m\omega^2\frac{\hbar^2}{m\omega} \tag{97}$$

$$= \quad \hbar\omega \tag{98}$$

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.

$$\hat{P}\hat{H} - \hat{H}\hat{P} = 0 \qquad (99)$$

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 $v(x)$.

$$
\begin{aligned}
\hat{H}v(x) &= \hat{H}\hat{P}u(x) & (100) \\
&= \hat{P}\hat{H}u(x) & (101) \\
&= E\hat{P}u(x) & (102) \\
&= Ev(x) & (103)
\end{aligned}
$$

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

$$u(x) = cv(x) \qquad (104)$$

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

$$u(x) = cu(-x) \qquad (105)$$

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

$$u(-x) = cu(x) \qquad (106)$$

Now Eq.(104) and Eq.(105) 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

$$
\begin{aligned}
w_1(x) &= u(x) + v(x) = u(x) + u(-x) & (107) \\
w_2(x) &= u(x) - v(x) = u(x) - u(-x) & (108)
\end{aligned}
$$

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.
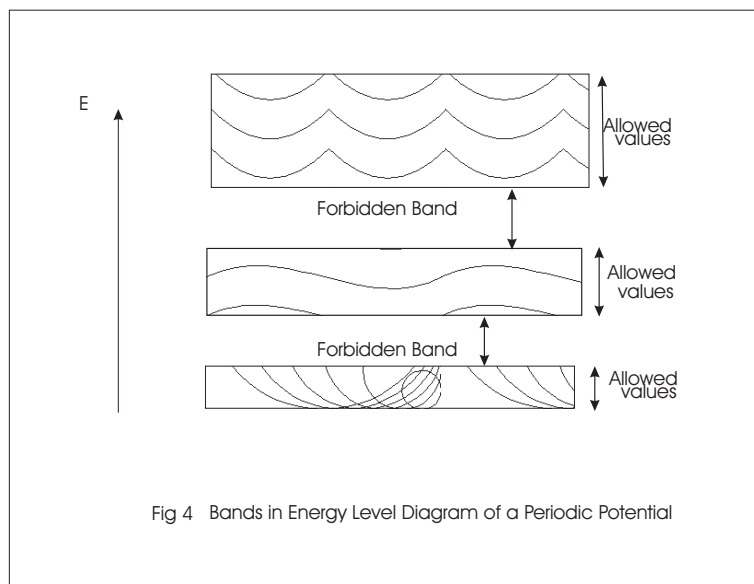

Fig 2

Fig 3
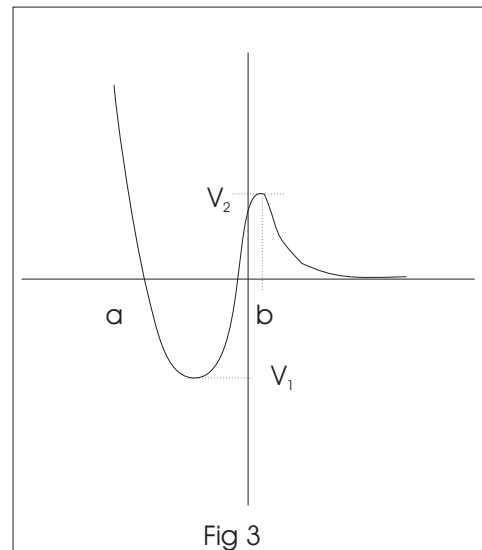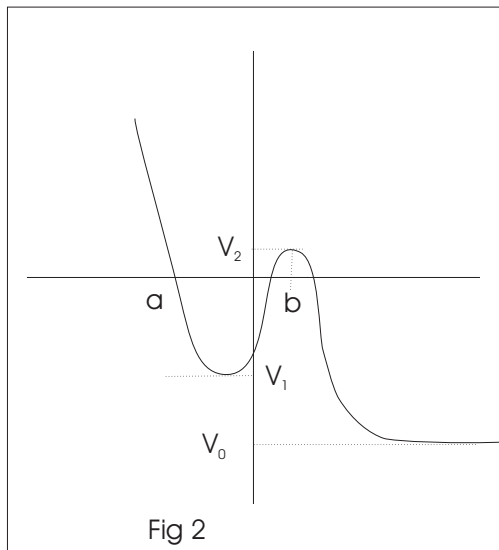
§7 *Periodic potentials, Energy bands*

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