Chapter 3: Solving the Time-Independent Schrödinger Equation (TISE) for Some One-dimensional Systems

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TISE for One-dimensional Systems

- A one-dimensional (1D) system is one in which the particle is confined to move only in one spatial dimension
- Conventionally, we take that dimension to be the x axis
- Thus, for a general 1D system, the Schrödinger Equation will be of the form

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t), \tag{1}$$

where $V(x,t)$ is a general 1D time-dependent potential to which the particle is exposed

TISE in 1D...

- However, at present we want to restrict ourselves to time-independent problems for which the potential is of the form $V = V(x)$
- We know from the previous chapter that for the time-independent potentials, the problem reduces to time-independent Schrödinger equation (TISE)

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

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

- Let us first discuss a few important points related to the TISE

TISE in 1D: Important Assumptions

- We will assume that $\psi(x)$ is continuous everywhere in space
- This is a postulate, because there is no mathematical guarantee that the solutions of the TISE are continuous
- The regions in which $V(x) = \infty$, $\psi(x) = 0$, or else the TISE will be divergent in those regions
- We will also show an important result that the first derivative of $\psi(x)$, i.e., $\dfrac{d\psi}{dx}$ will be continuous across a finite discontinuity of $V(x)$
- We prove this important result next

Continuity of the first-derivative of the wave function

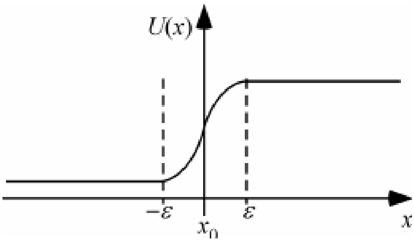
- Let us assume that $V(x)$ is discontinuous at $x = x_0$
- But, everywhere the potential is finite
- We assume that

$$\lim_{\varepsilon \to 0} V(x_0 - \varepsilon) = V(x_0^-) = V_1$$
$$\lim_{\varepsilon \to 0} V(x_0 + \varepsilon) = V(x_0^+) = V_2,$$

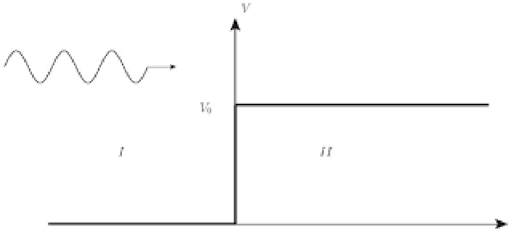
with $V_1 \neq V_2 \neq \infty$

1D discontinuous potential

- An example of a finite discontinuous potential in the limit $\varepsilon \to 0$



- When limit $\varepsilon \to 0$ is taken, the potential looks like



1D Discontinuous potentials...

- There can be more complicated potentials such as square well, finite barrier, etc.
- Let us integrate the TISE for this potential with a discontinuity at $x = x_0$ in the region $x \in (x_0 - \varepsilon, x_0 + \varepsilon)$

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon} \left(-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) \right) dx = E \int_{x_0-\varepsilon}^{x_0+\varepsilon} \psi(x) dx$$

$$\left. \frac{d\psi(x)}{dx} \right|_{x_0+\varepsilon} - \left. \frac{d\psi(x)}{dx} \right|_{x_0-\varepsilon} = \frac{2m}{\hbar^2} \int_{x_0-\varepsilon}^{x_0+\varepsilon} (V - E)\psi(x) dx$$

1D discontinuous potential...

- As long as $V(x)$ is bounded in the range of integration

$$\lim_{\varepsilon \to 0} \frac{2m}{\hbar^2} \left| \int_{x_0-\varepsilon}^{x_0+\varepsilon} (V-E)\psi(x)dx \right| \leq \lim_{\varepsilon \to 0} \frac{2m}{\hbar^2} |(2\varepsilon)(V_{max}-E)\psi_{max}| \to 0$$

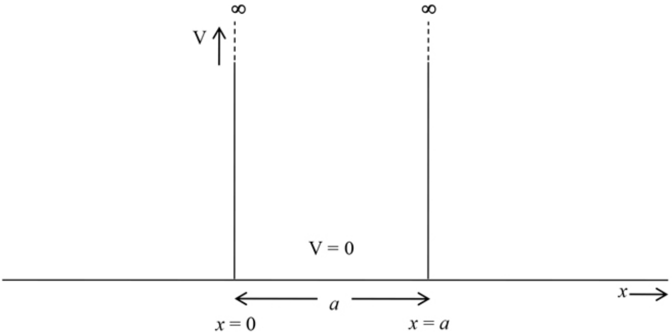
- This means that $\lim_{\varepsilon \to 0} \frac{2m}{\hbar^2} \int_{x_0-\varepsilon}^{x_0+\varepsilon} (V-E)\psi(x)dx = 0$, implying that $\frac{d\psi(x)}{dx}$ is continuous across x_0

$$\left.\frac{d\psi(x)}{dx}\right|_{x_0^+} = \left.\frac{d\psi(x)}{dx}\right|_{x_0^-} \tag{3}$$

- Next, we solve the 1D-TISE for potentials that are discontinuous, starting with the case of particle in a box

Particle in a 1D Box

- Let us consider a particle exposed to the potential shown in the picture below



- Above $V(x) = \infty$, for $x \leq 0$ and $x \geq a$, and $V(x) = 0$ for $0 < x < a$
- Therefore, $\psi(x) = 0$, $x \leq 0$ and $x \geq a$

Particle in a box...

- For $0 < x < a$, the particle satisfies the free-particle TDSE

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

where $k = \sqrt{\frac{2mE}{\hbar^2}}$.

- Clearly, the most general solution is

$$\psi(x) = A\sin kx + B\cos kx \tag{4}$$

- But this solution must satisfy the boundary conditions on the wave function

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

Particle in a box...

- On imposing $\psi(x=0)=0$ on Eq. 4, we have

$$B=0$$

- While, on imposing $\psi(x=a)=0$ on Eq. 4, we obtain

$$\begin{aligned} A\sin ka &= 0 \\ \implies ka &= n\pi \\ \implies k \equiv k_n &= \frac{n\pi}{a} \end{aligned} \tag{5}$$

  above $n=1,2,3,4,\ldots$

- Now the eigenfunctions are

$$\psi_n(x) = A_n \sin\frac{n\pi x}{a},$$

  where A_n is the normalization constant we will determine shortly

Particle in a box...

- Using $k = \sqrt{\frac{2mE}{\hbar^2}}$, we immediately get the energy eigenvalues

$$k_n = \sqrt{\frac{2mE_n}{\hbar^2}} = \frac{n\pi}{a}$$

$$\implies E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \tag{6}$$

- Next, we normalize the eigenfunctions to determine A_ns

$$\int_{-\infty}^{\infty} \psi_n^2(x)dx = A_n^2 \int_0^a \sin^2 \frac{n\pi x}{a} dx = 1$$

$$\implies \frac{A_n^2}{2} \int_0^a \left(1 - \cos \frac{2n\pi x}{a}\right) dx = 1$$

$$\frac{A_n^2}{2} a = 1$$

$$\implies A_n = \sqrt{\frac{2}{a}}$$

Particle in a box...

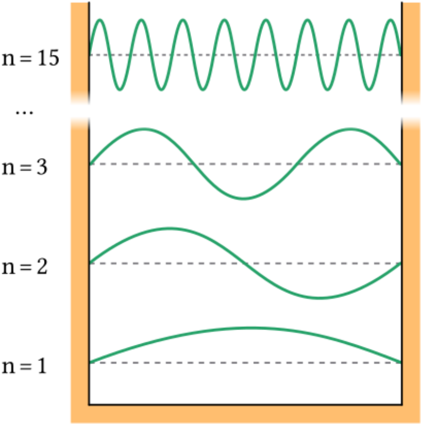
- Thus, our final expression for the energy eigenvalues, and the normalized energy eigenfunctions is

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$
$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a},$$

  for $n = 1, 2, 3, 4, \ldots$.
- The reason $n = 0$ is excluded because the wave function $\psi_{n=0}(x) = 0$.
- Clearly, the lowest-energy state, i.e., the ground state of the system corresponds to $n = 1$
- While all higher values of n, i.e., $n = 2, 3, 4, \ldots$ correspond to the excited states of the system

Particle in a box

- Plots of a few wave functions are given in the figure below



- Note that boundary conditions $\psi_n(0) = \psi_n(a) = 0$ are satisfied for all n

Particle in a box...

- Also note that the number of nodes in $\psi_n(x)$ in the interior region $(0 < x < a)$ is $n-1$
- What if the box is two dimensional, i.e., $V(x,y) = 0$ for $0 < x < a$ and $0 < y < b$, and infinite everywhere else
- Or three dimensional with $V(x,y,z) = 0$ for $0 < x < a$, $0 < y < b$, and $0 < z < c$, and infinite everywhere else
- Both the problems can be easily solved using the method of separation of variables
- The results for the 2D case are

$$E_{n_1,n_2} = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2}\right)$$

$$\psi_{n_1,n_2}(x,y) = \sqrt{\frac{4}{ab}}\sin\frac{n_1\pi x}{a}\sin\frac{n_2\pi y}{b}.$$

Particle in a box...

- And for the 3D case, we obtain

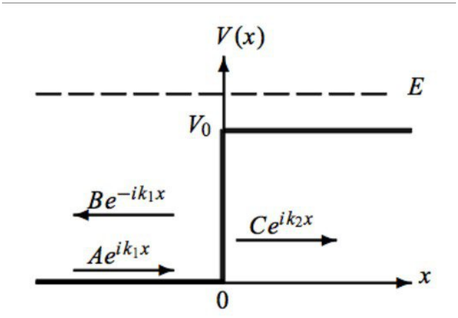
$$E_{n_1,n_2,n_3} = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2}\right)$$

$$\psi_{n_1,n_2,n_3}(x,y,z) = \sqrt{\frac{8}{abc}}\sin\frac{n_1\pi x}{a}\sin\frac{n_2\pi y}{b}\sin\frac{n_3\pi z}{c}.$$

- Next, we consider the problem of a particle exposed to a step potential

The case of a Step Potential

- Let us consider a particle exposed to a step potential



- This potential is given by

$$
\begin{aligned}
V(x) &= 0 \quad \text{for } x \leq 0 \\
V(x) &= V_0 \quad \text{for } x \geq 0
\end{aligned}
$$

- Clearly, the potential has a finite discontinuity at $x = 0$
- Therefore, the wave function and its first derivative will be continuous at $x = 0$

1D step potential...

- Let us call region $x \leq 0$ region I and $x \geq 0$ as region II
- Clearly, in region I, TISE will be that of a free particle $(V(x) = 0)$, therefore, its solutions will be

$$\psi_I(x) = Ae^{ik_1 x} + Be^{-ik_1 x}, \tag{7}$$

  where $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$, where E is the energy of the incident particle
- Clearly, the first term on the RHS of Eq. 7 denotes the incident wave, and the second one the reflected wave as also shown in the figure

1D step potential...

- In region II, the TISE is

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}(x)}{dx^2} + V_0\psi_{II}(x) &= E\psi_{II}(x) \\
\implies \frac{d^2\psi_{II}(x)}{dx^2} + k_2^2\psi_{II}(x) &= 0 \\
\text{where } k_2 &= \sqrt{\frac{2m(E-V_0)}{\hbar^2}} \qquad (8)
\end{aligned}
$$

- Thus, the possible solution in region II is

$$\psi_{II}(x) = Ce^{ik_2 x}, \qquad (9)$$

  which denotes the transmitted wave traveling to the right
- In region II, there is no possibility of a left moving wave

1D step potential...

- What are the quantities of interest which we should calculate
- They are the transmission coefficient T and reflection coefficient R defined as

$$
\begin{aligned}
T &= \frac{k_2|C|^2}{k_1|A|^2} \\
R &= \frac{|B|^2}{|A|^2},
\end{aligned}
\tag{10}
$$

  where k_1 and k_2 must be real.
- These coefficients, respectively, quantify the probabilities of transmission or reflection of a particle at the step
- In order to compute R and T, we need A, B, and C
- How do we compute those?

1D step potential

- To determine A, B, and C, we use the continuity conditions on $\psi(x)$ and $\psi'(x) = \dfrac{d\psi}{dx}$, at $x = 0$
- This means

$$\begin{aligned}\psi_I(0) &= \psi_{II}(0)\\ \psi_I'(0) &= \psi_{II}'(0)\end{aligned}$$

- Using Eqs. 7 and 9, and using the fact that $\dfrac{de^{\pm ikx}}{dx} = \pm ike^{\pm ikx}$, we obtain

$$\begin{aligned}A + B &= C\\ ik_1(A - B) &= ik_2 C\end{aligned} \tag{11}$$

1D Step potential...

- Here we will only consider the cases when $E > 0$, so that $k_1 = \sqrt{\dfrac{2mE}{\hbar^2}}$ is always real
- There are two possibilities regarding the value of the eigenenergy E of the particle: (a) case I $E > V_0$, and (b) case II, $E < V_0$
- For case I, clearly, $k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ is real, which we solve next

1D Step Potential, Case I: $E > V_0$

- We can easily solve Eqs. 11 to obtain

$$A = \frac{1}{2}\left(1 + \frac{k_2}{k_1}\right) C$$
$$B = \frac{1}{2}\left(1 - \frac{k_2}{k_1}\right) C$$

- From these equations we immediately get the reflection and transmission coefficients

$$\begin{aligned} R &= \frac{|B|^2}{|A|^2} = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \\ T &= \frac{k_2 |C|^2}{k_1 |A|^2} = \frac{4k_1^2 k_2}{k_1 (k_1 + k_2)^2} = \frac{4 k_1 k_2}{(k_1 + k_2)^2} \end{aligned} \tag{12}$$

- Easy to verify that $R + T = 1$, as expected

1D step potential, case I...

- How does our quantum mechanical result compare with the classical one
- If we compute the transmission probability for classical waves, we will obtain complete transmission
- That is

$$R = 0$$
$$T = 1$$

- However, from Eqs.12 it is obvious that we will obtain that result in quantum mechanics only for the trivial case when $k_1 = k_2$, that is no potential barrier
- Thus quantum mechanical result predicting both $R > 0$ and $T < 1$ is quite remarkable!

- It is obvious that for this case, the only difference as compared to the previous case is the nature of the solution in region II ($x > 0$), because

$$k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} = \pm i\rho$$

where

$$\rho = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} > 0 \text{ and real}$$

1D step potential, case II...

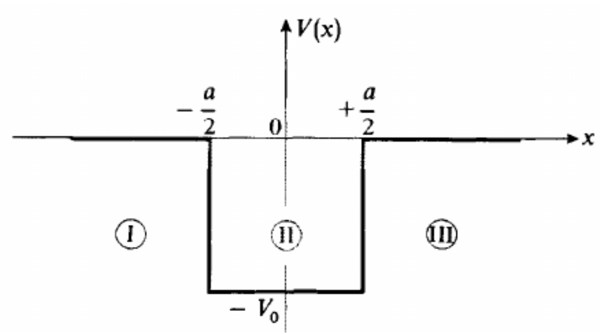
- With this, the most general wave function in region II will be of the form
$$\psi_{II}(x) = Ce^{-\rho x} + De^{\rho x}$$
- But $\lim_{x\to\infty} e^{\rho x} \to \infty$, therefore, for the normalizability of the wave function in region II, $D = 0$, leading to
$$\psi_{II}(x) = Ce^{-\rho x}$$
- Note that $\psi_{II}(x)$ is a decaying function of x, and not a wave-like function
- This implies that the probability of finding the particle in region II will decay exponentially with the distance inside the barrier
- Because $\mathrm{Re}(k_2) = 0$, we immediately get the expected results from Eqs. 12
$$R = 1$$
$$T = 0$$

1D step potential, case II...

- This result is in full agreement with classical mechanics
- Because if a particle were to penetrate region II, for the fixed E its kinetic energy will become negative, leading to an imaginary speed!
- Therefore, region II is classically strictly forbidden!
- In quantum mechanics, it is not strictly forbidden, but the probability of a particle being there falls off rapidly with the increasing penetration depth.
- Next, we discuss the case of a particle in a finite potential well

A particle in a finite potential well

- Let us consider a potential shown below



- This potential can be written as

$$
\begin{aligned}
V(x) &= 0 \text{ for } -\infty \leq x \leq -a/2 \\
V(x) &= -V_0 \text{ for } -a/2 \leq x \leq a/2 \\
V(x) &= 0 \text{ for } a/2 \leq x \leq \infty
\end{aligned}
$$

Finite potential well...

- Clearly, this potential has two finite discontinuities at $x = \pm\frac{a}{2}$
- Therefore, in order to solve this problem, we will have to apply boundary conditions at both these points
- We consider the case of when particle has the energy E in the range $0 \geq E \geq -V_0$
- In such a case, a classical particle will be completely bound inside the well
- That is it will not be able to escape the well
- Let us see what happens when the problem is solved quantum mechanically

Finite potential well...

- In regions I ($x \leq -a/2$) and III ($x \geq a/2$) the particle is a free particle, however, with $E < 0$.
- Taking $E = -|E|$, in regions I and II, the value of k is

$$k = \sqrt{\frac{-2m|E|}{\hbar^2}} = \pm i\rho$$

$$\text{with } \rho = \sqrt{\frac{2m|E|}{\hbar^2}}$$

- Therefore, in those regions wave functions will be of the form

$$\psi_I(x) = Ae^{\rho x} + Be^{-\rho x}$$
$$\psi_{III}(x) = Fe^{\rho x} + Ee^{-\rho x}$$

- However, $e^{-\rho x}$ term is unbounded in region I, as $x \to -\infty$
- And $e^{\rho x}$ term is unbounded in region III, as $x \to \infty$

- Therefore, to have bounded wave function, we must set $B = F = 0$, to yield the final forms in I and III

$$\psi_I(x) = Ae^{\rho x}$$
$$\psi_{III}(x) = De^{-\rho x}$$

- In region II, the TISE is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}(x)}{dx^2} - V_0\psi_{II}(x) = -|E|\psi_{II}(x)$$
$$\Longrightarrow \frac{d^2\psi_{II}(x)}{dx^2} + k^2\psi_{II}(x) = 0,$$

where

$$k = \sqrt{\frac{2m(V_0 - |E|)}{\hbar^2}} \tag{13}$$

Finite Potential well...

- Because $V_0 > |E|$, clearly k will be real, leading to oscillatory solutions in regions II

$$\psi_{II}(x) = Be^{ikx} + Ce^{-ikx}$$

- Finally, putting the expressions of the wave function in all the three regions

$$\begin{aligned}\psi_I(x) &= Ae^{\rho x}\\ \psi_{II}(x) &= Be^{ikx} + Ce^{-ikx}\\ \psi_{III}(x) &= De^{-\rho x}\end{aligned} \tag{14}$$

- Unknown coefficients A, B, C, and D are determined from the four continuity equations

$$\begin{aligned}\psi_I(-a/2) &= \psi_{II}(-a/2)\\ \psi_I'(-a/2) &= \psi_{II}'(-a/2)\\ \psi_{II}(a/2) &= \psi_{III}(a/2)\\ \psi_{II}'(a/2) &= \psi_{III}'(a/2)\end{aligned}$$

Finite Potential well...

- Boundary conditions at $x = -a/2$ are

$$Ae^{-\rho a/2} = Be^{-ika/2} + Ce^{ika/2}$$
$$\rho Ae^{-\rho a/2} = ik(Be^{-ika/2} - Ce^{ika/2})$$

- which lead to

$$B = \frac{1}{2}\left(1 - i\frac{\rho}{k}\right) e^{(ika-\rho a)/2} A \tag{15}$$
$$C = \frac{1}{2}\left(1 + i\frac{\rho}{k}\right) e^{-(ika+\rho a)/2} A \tag{16}$$

- Boundary conditions at $x = a/2$ are

$$Be^{ika/2} + Ce^{-ika/2} = De^{-\rho a/2}$$
$$ik(Be^{ika/2} - Ce^{-ika/2}) = -\rho De^{-\rho a/2}$$

Finite Potential well...

- which can be solved as

$$B = \frac{1}{2}\left(1 + i\frac{\rho}{k}\right) e^{-(ika+\rho a)/2} D \tag{17}$$

$$C = \frac{1}{2}\left(1 - i\frac{\rho}{k}\right) e^{(ika-\rho a)/2} D \tag{18}$$

- On dividing Eq. 17 by 15, we get

$$\frac{k + i\rho}{k - i\rho} e^{-ika} \frac{D}{A} = 1$$

$$\implies \frac{D}{A} = \frac{k - i\rho}{k + i\rho} e^{ika} \tag{19}$$

- Similarly, by dividing 18 by 16, we have

$$\frac{D}{A} = \frac{k + i\rho}{k - i\rho} e^{-ika} \tag{20}$$

- Equating Eqs. 19 and 20, we get the quantization condition

$$\left(\frac{k+i\rho}{k-i\rho}\right)^2 = e^{2ika}$$
$$\implies \frac{k+i\rho}{k-i\rho} = \pm e^{ika} \tag{21}$$

- We will consider both the cases of Eq. 21 one by one. Let us start with

$$\frac{k+i\rho}{k-i\rho} = e^{ika}$$
$$\implies k+i\rho = ke^{ika} - i\rho e^{ika}$$
$$\implies \frac{\rho}{k} = \frac{(e^{ika}-1)}{i(e^{ika}+1)} = \frac{(e^{ika/2}-e^{-ika/2})}{i(e^{ika/2}+e^{-ika/2})}$$
$$\implies \frac{\rho}{k} = \tan\left(\frac{ka}{2}\right) \tag{22}$$

Finite well potential...

- Let us define

$$k_0 = \sqrt{\frac{2mV_0}{\hbar^2}} = \sqrt{k^2 + \rho^2} \tag{23}$$

- Using Eqs. 22 and 23, we have

$$\begin{aligned} \sec^2\left(\frac{ka}{2}\right) &= 1 + \tan^2\left(\frac{ka}{2}\right) \\ &= 1 + \frac{\rho^2}{k^2} = \frac{k_0^2}{k^2} \end{aligned}$$

- Which can be written as

$$\begin{cases} \left|\cos\left(\frac{ka}{2}\right)\right| = \frac{k}{k_0} \\ \tan\left(\frac{ka}{2}\right) > 0 \end{cases} \tag{24}$$

Finite well potential...

- Now we consider the second possibility, i.e., Eq. 21 with the negative sign on the RHS

$$
\begin{aligned}
\frac{k+i\rho}{k-i\rho} &= -e^{ika} \\
\implies k+i\rho &= -ke^{ika} + i\rho e^{ika} \\
\implies \frac{\rho}{k} &= \frac{(e^{ika}+1)}{i(e^{ika}-1)} = \frac{(e^{ika/2}+e^{-ika/2})}{i(e^{ika/2}-e^{-ika/2})} \\
\implies \frac{\rho}{k} &= -\cot\left(\frac{ka}{2}\right)
\end{aligned}
\tag{25}
$$

- This leads to the condition

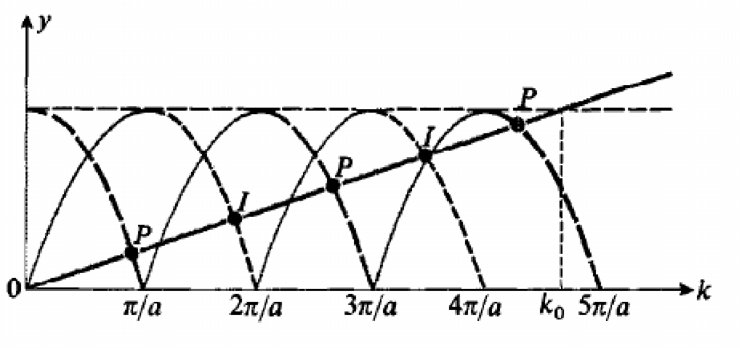
$$
\begin{cases}
\left|\sin\left(\frac{ka}{2}\right)\right| = \frac{k}{k_0} \\
\tan\left(\frac{ka}{2}\right) < 0
\end{cases}
\tag{26}
$$

Finite well potential...

- We recall that for the case of particle-in-a-box, analytical solutions for its energy eigenvalues were available
- However, in the present case, that is not possible
- One has to obtain numerical or graphical solutions of Eqs. 24 and 26 to obtain the k values, corresponding to which the eigenenergies $-|E|$, can be determined.
- Next, we try to obtain the graphical solutions of Eqs. 24 and 26
- For the purpose, we plot $\left|\cos\left(\frac{ka}{2}\right)\right|$, $\left|\sin\left(\frac{ka}{2}\right)\right|$, and $\dfrac{k}{k_0}$ as functions of k in the same plot
- The points of intersection of the curves will be the k values corresponding to various energy eigenvalues

Finite well potential...

- These are shown in the figure below



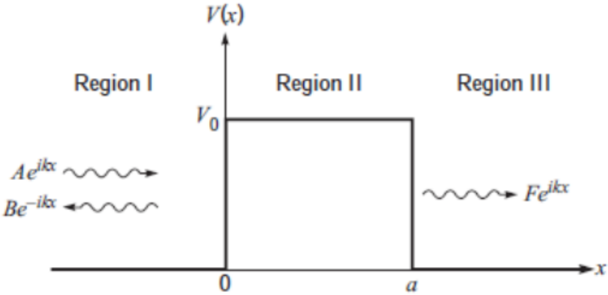
- Points labeled P are solutions of Eq. 24, while those labeled I are solutions of Eq. 26
- Note that the allowed values of k satisfy $0 \leq k \leq k_0$
- The above plot is for a chosen value of V_0 for which five bound states are possible

Finite well potential...

- If we increase the depth of the well V_0, more bound solutions will be possible
- Because for larger values of V_0, k_0 will be larger leading to more intersection points of the curves $\left|\cos\left(\frac{ka}{2}\right)\right|, \left|\sin\left(\frac{ka}{2}\right)\right|$ and $\dfrac{k}{k_0}$
- Next, we consider the case of a finite potential barrier

One-dimensional Potential Barrier of Finite Width

- Here we consider a potential barrier of a finite height V_0 and width a as shown



- We can write this potential as

$$V(x) = 0 \text{ for } -\infty \leq x \leq 0$$
$$V(x) = V_0 \text{ for } 0 \leq x \leq a$$
$$V(x) = 0 \text{ for } a \leq x \leq \infty$$

Finite potential barrier...

- This potential also has two finite discontinuities in the potential at $x = 0$ and $x = a$
- If the wave functions in regions I ($x \leq 0$), II ($0 \leq x \leq a$), and III ($x \geq a$) are $\psi_I(x)$, $\psi_{II}(x)$, and $\psi_{III}(x)$, respectively
- The continuity conditions on the wave function and its first derivative will be

$$\psi_I(0) = \psi_{II}(0)$$
$$\psi_I'(0) = \psi_{II}'(0)$$
$$\psi_{II}(a) = \psi_{III}(a)$$
$$\psi_{II}'(a) = \psi_{III}'(a)$$

Finite potential barrier...

- In regions I and III, the particle is a free particle. Assuming that it is incident from the left, we have

$$\begin{aligned} \psi_I(x) &= Ae^{ikx} + Be^{-ikx} \\ \psi_{III}(x) &= Fe^{ikx}, \end{aligned} \tag{27}$$

where $k = \sqrt{\dfrac{2mE}{\hbar^2}}$

- The wave function in region II, $\psi_{II}(x)$, depends on whether the energy E of the incident particle is larger than the height of the barrier ($E > V_0$) or smaller ($E < V_0$)

Finite potential barrier...

- Let us first consider when $E > V_0$, in which case $\psi_{II}(x)$ will be of the oscillatory form

$$\psi_{II}(x) = Ce^{ik'x} + De^{-ik'x}, \tag{28}$$

where $k' = \sqrt{\dfrac{2m(E - V_0)}{\hbar^2}}$

- Continuity conditions on $\psi(x)$ and $\psi'(x)$ at $x = 0$ yield

$$\begin{aligned} A + B &= C + D \\ ik(A - B) &= ik'(C - D) \end{aligned} \tag{29}$$

- While the continuity conditions at $x = a$ are

$$\begin{aligned} Ce^{ik'a} + De^{-ik'a} &= Fe^{ika} \\ ik'(Ce^{ik'a} - De^{-ik'a}) &= ikFe^{ika} \end{aligned} \tag{30}$$

Finite potential barrier...

- Eqs. 29 yield

$$A = \frac{C}{2}\left(1+\frac{k'}{k}\right) + \frac{D}{2}\left(1-\frac{k'}{k}\right)$$
$$B = \frac{C}{2}\left(1-\frac{k'}{k}\right) + \frac{D}{2}\left(1+\frac{k'}{k}\right) \tag{31}$$

- While from Eqs. 30, we obtain

$$C = \frac{F}{2}\left(1+\frac{k}{k'}\right) e^{i(k-k')a}$$
$$D = \frac{F}{2}\left(1-\frac{k}{k'}\right) e^{i(k+k')a} \tag{32}$$

Finite potential barrier...

- On substituting Eqs. 32 in 31, we have

$$A = \frac{F}{4}\left(1+\frac{k'}{k}\right)\left(1+\frac{k}{k'}\right)e^{i(k-k')a} + \frac{F}{4}\left(1-\frac{k'}{k}\right)\left(1-\frac{k}{k'}\right)e^{i(k+k')a}$$

and

$$B = \frac{F}{4}\left(1-\frac{k'}{k}\right)\left(1+\frac{k}{k'}\right)e^{i(k-k')a} + \frac{F}{4}\left(1+\frac{k'}{k}\right)\left(1-\frac{k}{k'}\right)e^{i(k+k')a}$$

Finite potential barrier...

- These equations can be simplified to

$$A = \frac{Fe^{ika}}{2}\left\{2\cos k'a - i\left(\frac{k'}{k}+\frac{k}{k'}\right)\sin k'a\right\} \tag{33}$$

- And

$$B = i\frac{Fe^{ika}}{2}\left(\frac{k'}{k}-\frac{k}{k'}\right)\sin k'a \tag{34}$$

- The transmission coefficient is

$$T = \frac{|F|^2}{|A|^2} = \frac{4}{\left\{4\cos^2 k'a + \left(\frac{k'}{k}+\frac{k}{k'}\right)^2 \sin^2 k'a\right\}}$$

Finite potential barrier...

- Using $\cos^2 k'a = 1 - \sin^2 k'a$, we obtain

$$T = \frac{4}{\left\{4 + \left(\left(\frac{k'}{k} + \frac{k}{k'}\right)^2 - 4\right)\sin^2 k'a\right\}}$$
$$= \frac{4}{\left\{4 + \left(\frac{k'}{k} - \frac{k}{k'}\right)^2 \sin^2 k'a\right\}}$$

- Which simplifies to

$$T = \frac{4k'^2k^2}{\left\{4k'^2k^2 + (k^2 - k'^2)^2 \sin^2 k'a\right\}}. \qquad (35)$$

- Using the expressions for k and k', we have

$$k^2 - k'^2 = \frac{2mE}{\hbar^2} - \frac{2m(E - V_0)}{\hbar^2} = \frac{2mV_0}{\hbar^2}$$

Finite potential barrier...

- On substituting these in Eq. 35, we obtain

$$T = \frac{4E(E - V_0)}{4E(E - V_0) + V_0^2 \sin^2 \sqrt{2m(E - V_0)}a/\hbar} \tag{36}$$

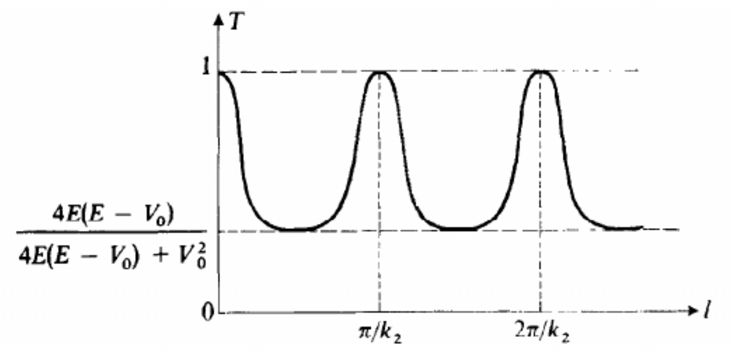
- And the reflection coefficient R will be

$$R = 1 - T = \frac{V_0^2 \sin^2 k'a}{4E(E - V_0) + V_0^2 \sin^2 k'a}$$

- We can verify that we will get the same result if we compute it as $R = \dfrac{|B|^2}{|A|^2}$, using the expressions of A and B derived in Eqs. 33 and 34.

Finite potential barrier...

- Let us look at the plot of the transmission coefficient of Eq. 36 as a function of barrier width a. In the figure k' and a are denoted as k_2 and l, respectively.



- We note that T shows resonances (maxima) for $k'a = n\pi$

Finite potential barrier...

- Using $k' = 2\pi/\lambda'$, where λ' is the de Broglie wavelength inside the barrier, we obtain the condition of resonances to be

$$a = n\left(\frac{\lambda'}{2}\right)$$

- That is, we get the resonances, when the barrier width is a multiple of half de Broglie wavelength
- Which is nothing but the condition for formation of standing de Broglie waves inside the barrier!
- Next, we consider the case when $E < V_0$, which leads to the amazing phenomenon of quantum mechanical tunneling.

Finite potential barrier with $E < V_0$: Tunneling

- The only difference as compared to the previous case is in the nature of wave function in region II, which is classically forbidden because there $E < V_0$
- Therefore

$$k' = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} = i\sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = i\rho \qquad (37)$$

- We can obtain $\psi_{II}(x)$ by substituting Eq. 37 in Eq. 28, which is now of exponential type

$$\psi_{II}(x) = Ce^{-\rho x} + De^{\rho x} \qquad (38)$$

- However, we need not repeat all the previous steps to obtain the reflection/transmission coefficients.
- All we need to do is substitute $k' = i\rho$ in the earlier expressions, and using in Eq. 36

$$\sin(k'a) = \sin(i\rho a) = \frac{e^{-\rho a} - e^{\rho a}}{2i} = i\sinh\rho a,$$

Tunneling...

- We obtain the expression for the transmission coefficient for the present case to be

$$T = \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \sinh^2 \sqrt{2m(V_0 - E)}a/\hbar} \tag{39}$$

- An important special case is $\rho a \gg 1$
- For this

$$\sinh^2 \sqrt{2m(V_0 - E)}a/\hbar \approx \frac{1}{4} e^{2\sqrt{2m(V_0 - E)}a/\hbar}$$

- Leading to

$$T \approx \frac{16E(V_0 - E)}{V_0^2} e^{-2\sqrt{2m(V_0 - E)}a/\hbar}$$

- Clearly, T is large when $a \leq \frac{\hbar}{\sqrt{2m(V_0 - E)}} = \frac{1.96}{\sqrt{V_0 - E}}$Å for electrons

Tunneling...

- Clearly, if we take $V_0 = 2$ eV and $E = 1$ eV, for electrons the width of the barrier for large tunneling condition will be 1.96 Å.
- For these value $T = 0.78$, i.e., 78% of the electrons will be able to tunnel through
- This is quite amazing because in classical mechanics tunneling is forbidden
- Fine example of a tunneling based device is a Josephson junction
- Next, we solve the TISE of 1D simple harmonic oscillator (1D-SHO).

One-dimensional Simple Harmonic Oscillator

- The study of simple harmonic oscillator (SHO) occupies an important place in classical mechanics (CM).
- It serves as an important model system which illustrates several important concepts in CM
- In quantum mechanics also the SHO enjoys a similar status.
- The microscopic behavior of several systems much as molecules, solids, and quantum dots can be described using a quantum mechanical harmonic oscillator model.
- For molecules and solids, the vibrational dynamics can be described reasonably well using an oscillator model
- For quantum dots, energy levels of electrons can be described using this model.

1D SHO

- The energy of a classical SHO is conserved, and given by (in 1D)

$$E = T + V = \frac{p^2}{2m} + \frac{1}{2}kx^2, \tag{40}$$

above $T = \frac{p^2}{2m}$ denotes the kinetic energy of a particle of mass m, while $V = \frac{1}{2}kx^2$ is its potential energy.

- Therefore, using the rules of quantization in the r-represenation

$$p \to -i\hbar\nabla \equiv -i\hbar\frac{d}{dx} \quad \text{for a 1D system}$$

$$E \to H$$

- Now

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 = \frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)^2 + \frac{1}{2}kx^2 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2$$

1D-SHO...

- Because potential $V = \frac{1}{2}kx^2$ is time independent, we will solve the TISE of this system given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}kx^2\psi = E\psi \qquad (41)$$

- Using the relation $\omega = \sqrt{\frac{k}{m}} \Rightarrow k = m\omega^2$, we rewrite the previous equation as

$$\frac{d^2\psi}{dx^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2}x^2\right)\psi = 0 \qquad (42)$$

- We can check that the quantity $\sqrt{\frac{\hbar}{m\omega}}$ has the dimensions of length
- So we define a dimensionless length variable $\tilde{x}$ as

$$\tilde{x} = \sqrt{\frac{m\omega}{\hbar}}x \qquad (43)$$

- Denoting the normalization integral by $\langle\psi|\psi\rangle$, we have

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = 1 \tag{44}$$

- From this equation it is obvious that $\psi(x)$ has the dimensions of length$^{-1/2}$
- Therefore, we define a dimensionless wave function $\tilde{\psi}(\tilde{x})$, expressed in terms of $\tilde{x}$ as

$$\tilde{\psi}(\tilde{x}) = \left(\frac{\hbar}{m\omega}\right)^{1/4} \psi(x = \tilde{x}) \tag{45}$$

- So that

$$\langle\psi \mid \psi\rangle = 1 \Rightarrow \langle\tilde{\psi} \mid \tilde{\psi}\rangle = \int_{-\infty}^{\infty} \tilde{\psi}^*(\tilde{x})\tilde{\psi}(\tilde{x})d\tilde{x} = 1$$

- Next, we transform the TISE (Eq. 42) to express it in terms of $\tilde{x}$ and $\tilde{\psi}(\tilde{x})$.

- By substituting the following in Eq. 42

$$\frac{d}{dx} = \frac{d\tilde{x}}{dx}\frac{d}{d\tilde{x}} = \sqrt{\frac{m\omega}{\hbar}}\frac{d}{d\tilde{x}}$$

$$\Rightarrow \quad \frac{d^2}{dx^2} = \frac{m\omega}{\hbar}\frac{d^2}{d\tilde{x}^2}$$

- We obtain

$$\left(\frac{m\omega}{\hbar}\right) \times \left(\frac{m\omega}{\hbar}\right)^{1/4} \frac{d^2\tilde{\psi}}{d\tilde{x}^2} + \left(\frac{2mE}{\hbar^2} - \frac{m\omega}{\hbar}\tilde{x}^2\right)\left(\frac{m\omega}{\hbar}\right)^{1/4}\tilde{\psi} = 0$$

$$\Rightarrow \left(\frac{m\omega}{\hbar}\right)^{5/4}\left\{\frac{d^2\tilde{\psi}}{d\tilde{x}^2} + \left(\frac{2E}{\hbar\omega} - \tilde{x}^2\right)\tilde{\psi}\right\} = 0$$

Dimensionless TISE of 1D-SHO

- Since $\hbar\omega$ has the units of energy, we define a dimensionless energy

$$\tilde{E} = \frac{E}{\hbar\omega}$$

to finally obtain the TISE of 1D-SHO in terms of the dimensionless quantities

$$\frac{d^2\tilde{\psi}}{d\tilde{x}^2} + \left(2\tilde{E} - \tilde{x}^2\right)\tilde{\psi} = 0 \tag{46}$$

- In the asymptotic limit $\tilde{x} \to \pm\infty$, one can neglect $\tilde{E}$ term above to yield

$$\frac{d^2\tilde{\psi}}{d\tilde{x}^2} - \tilde{x}^2\tilde{\psi} = 0$$

which has the solutions

$$\lim_{x\to\infty} \tilde{\psi}(\tilde{x}) \longrightarrow e^{\pm\tilde{x}^2/2}$$

- But $\lim_{x\to\infty}\tilde{\psi}(\tilde{x}) = e^{\tilde{x}^2/2} \to \infty$, making it unnormalizable. Therefore, we reject it.
- We, instead try the solution of the form

$$\tilde{\psi}(\tilde{x}) = e^{-\tilde{x}^2/2} H(\tilde{x}), \tag{47}$$

where $H(\tilde{x})$ is an unknown function to be determined

- Since

$$\frac{d\tilde{\psi}}{d\tilde{x}} = \left\{ -\tilde{x}e^{-\tilde{x}^2/2} H(\tilde{x}) + e^{-\tilde{x}^2/2} H'(\tilde{x}) \right\},$$

- we obtain

$$\frac{d^2\tilde{\psi}}{d\tilde{x}^2} = \Big\{ -e^{-\tilde{x}^2/2} H(\tilde{x}) + \tilde{x}^2 e^{-\tilde{x}^2/2} H(\tilde{x}) - \tilde{x}e^{-\tilde{x}^2/2} H'(\tilde{x})$$
$$-\tilde{x}e^{-\tilde{x}^2/2} \dot{H}'(\tilde{x}) + e^{-\tilde{x}^2/2} \dot{H}''(\tilde{x}) \Big\}$$

1D-SHO: Hermite Differential Equation

- On substituting these in Eq. 46, we have

$$e^{-\tilde{x}^2/2}\left\{\frac{d^2H}{d\tilde{x}^2}-2\tilde{x}\frac{dH}{d\tilde{x}}+(2\tilde{E}-1)H\right\}=0$$

- Finally, we obtain the differential equation satisfied by $H(\tilde{x})$

$$\frac{d^2H}{d\tilde{x}^2}-2\tilde{x}\frac{dH}{d\tilde{x}}+(2\tilde{E}-1)H=0 \tag{48}$$

- This second-order linear differential equation is nothing but the famous Hermite differential equation of mathematics written as

$$\frac{d^2y}{dx^2}-2x\frac{dy}{dx}+\lambda y=0, \tag{49}$$

which admits several solutions.

1D-SHO: Hermite Polynomials

- One can solve it using the power-series expansion approach in which we plug in the solution of the form

$$H(\tilde{x}) = \sum_{m=0}^{\infty} a_m x^{m+\alpha} \tag{50}$$

  in Eq. 48, and obtain the expressions for a_m and α
- But, we are not interested in infinite series solutions for $H(\tilde{x})$ because it will lead to unnormalizable $\tilde{\psi}(\tilde{x})$ when plugged into Eq. 47.
- This problem can be solved by requiring that Eq. 50 terminates for some value of m, leading to a polynomial form for $H(\tilde{x})$

Hermite Polynomials

- It can be shown that the polynomial form for $H(\tilde{x})$ is obtained if the following condition is satisfied

$$2\tilde{E} - 1 = 2n, \text{ with } \; n = 0, 1, 2, 3, \ldots$$
$$\tilde{E} \equiv \tilde{E}_n = \left(n + \frac{1}{2}\right), \text{ with } \; n = 0, 1, 2, 3, \ldots$$

- Using the fact that $E = \tilde{E}\hbar\omega$, we obtain the famous expression for the energy eigenvalues of 1D-SHO

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega. \tag{51}$$

- And the corresponding polynomials $H(\tilde{x}) \equiv H_n(\tilde{x})$, are given by the expression

$$H_n(x) = n! \sum_{m=0}^{[n/2]} \frac{(-1)^m (2x)^{n-2m}}{(n-2m)!m!}, \tag{52}$$

where

$$\begin{aligned} \left[\frac{n}{2}\right] &= \frac{n}{2} \text{ for even } n \\ \left[\frac{n}{2}\right] &= \frac{n-1}{2} \text{ for odd } n \end{aligned} \tag{53}$$

- The polynomials $H_n(x)$ defined by equations above are called Hermite polynomials
- Noteworthy point is that $H_n(x)$ is a polynomial of degree n, i.e., the highest power of x in it will be n

1D-SHO: wave function

- Easy to verify that for even (odd) values of n, $H_n(x)$ is an even (odd) function of x

$$H_n(-x) = (-1)^n H_n(x)$$

- For a few values of n, we list the $H_n(x)$ below

$$\begin{aligned}
H_0(x) &= 1 \\
H_1(x) &= 2x \\
H_2(x) &= 4x^2 - 2 \\
H_3(x) &= 8x^3 - 12x \\
H_4(x) &= 16x^4 - 48x^2 + 12
\end{aligned}$$

1D-SHO: Wave function...

- The wave function $\tilde{\psi}(\tilde{x})$ of Eq. 47 acquires the form

$$\tilde{\psi}_n(\tilde{x}) = C_n e^{-\tilde{x}^2/2} H_n(\tilde{x})$$

where C_n's are determined by the normalization condition

$$\langle \tilde{\psi}_n | \tilde{\psi}_n \rangle = \int_{-\infty}^{\infty} \tilde{\psi}_n^*(\tilde{x}) \tilde{\psi}_n(\tilde{x}) d\tilde{x} = |C_n|^2 \int_{-\infty}^{\infty} e^{-\tilde{x}^2} H_n^2(\tilde{x}) d\tilde{x} = 1$$

- Using the orthonormality of the Hermite polynomials

$$\int_{-\infty}^{\infty} e^{-\tilde{x}^2} H_n(\tilde{x}) H_m(\tilde{x}) d\tilde{x} = 2^n \sqrt{\pi} n! \delta_{nm}$$

and the phase choice that C_n's are real, we obtain

$$C_n = \frac{1}{2^{n/2} \sqrt{n!} \pi^{1/4}}$$

leading to

$$\tilde{\psi}_n(\tilde{x}) = \frac{1}{2^{n/2} \sqrt{n!} \pi^{1/h}} e^{-\tilde{x}^2/2} H_n(\tilde{x})$$

1D-SHO: Wave function

- Finally, using Eqs. 43 and 45, we can obtain the expression for $\psi_n(x)$.
- Thus, the eigenvalues and eigenvectors of the TISE for 1D-SHO are

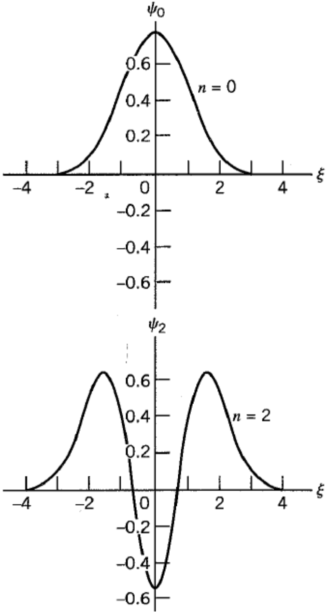
$$\begin{aligned} E_n &= \left(n + \frac{1}{2}\right)\hbar\omega \\ \psi_n(x) &= 2^{-n/2}(n!)^{-1/2}\left(\frac{m\omega}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) \end{aligned} \tag{54}$$

- Note that ψ_n's are completely real, and form an orthonormal basis set

$$\langle \psi_n \mid \psi_m \rangle = \int_{-\infty}^{\infty} \psi_n^*(x)\psi_m(x)dx = \delta_{nm}.$$

Plots of wave functions of 1D-SHO

- Plots of $\psi_n(\tilde{x})$, for $n = 0, 1, 2$, and 3. In the plot ξ denotes $\tilde{x}$



SHO in 2D and 3D

- Next, the question arises, what are the solutions for the TISE for the SHOs in higher dimensions, i.e., 2D and 3D
- The TISE for the most general SHO in 2D will be

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y)}{\partial x^2}+\frac{\partial^2\psi(x,y)}{\partial y^2}\right)+\frac{1}{2}m\left(\omega_x^2x^2+\omega_y^2y^2\right)\psi(x,y) = E^{(2)}\psi(x,y) \tag{55}$$

- And in 3D

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi(x,y,z)}{\partial x^2}+\frac{\partial^2\psi(x,y,z)}{\partial y^2}+\frac{\partial^2\psi(x,y,z)}{\partial z^2}\right) + \frac{1}{2}m\left(\omega_x^2x^2+\omega_y^2y^2+\omega_z^2z^2\right)\psi(x,y,z) = E^{(3)}\psi(x,y,z) \tag{56}$$

- How do we solve the TISE in 2D and 3D?
- From Eqs. 55 and 56 it is obvious that they are uncoupled in variables x, y, and z.
- Therefore, the method of separation of variables should work.
- And it indeed does, leading to the solutions for the 2D and 3D cases, respectively

$$\begin{aligned} E^{(2)}_{n_x,n_y} &= \left(n_x + \frac{1}{2}\right)\hbar\omega_x + \left(n_y + \frac{1}{2}\right)\hbar\omega_y \\ \psi_{n_x,n_y}(x,y) &= \psi_{n_x}(x,\omega_x)\psi_{n_y}(y,\omega_y) \\ &\text{where } n_x, n_y = 0,1,2,3,\ldots \end{aligned} \tag{57}$$

$$\begin{aligned} E^{(3)}_{n_x,n_y,n_z} &= \left(n_x + \frac{1}{2}\right)\hbar\omega_x + \left(n_y + \frac{1}{2}\right)\hbar\omega_y + \left(n_z + \frac{1}{2}\right)\hbar\omega_z \\ \psi_{n_x,n_y,n_z}(x,y,z) &= \psi_{n_x}(x,\omega_x)\psi_{n_y}(y,\omega_y)\psi_{n_z}(z,\omega_z) \\ &\text{where } n_x, n_y, n_z = 0,1,2,3,\ldots \end{aligned} \tag{58}$$

- Above, the wave functions corresponding to various dimensions are defined as

$$\psi_{n_x}(x,\omega_x) = 2^{-n_x/2}(n_x!)^{-1/2}\left(\frac{m\omega_x}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega_x}{2\hbar}x^2} H_{n_x}\left(\sqrt{\frac{m\omega_x}{\hbar}}x\right)$$

$$\psi_{n_y}(y,\omega_y) = 2^{-n_y/2}(n_y!)^{-1/2}\left(\frac{m\omega_y}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega_y}{2\hbar}y^2} H_{n_y}\left(\sqrt{\frac{m\omega_y}{\hbar}}y\right)$$

$$\psi_{n_z}(z,\omega_z) = 2^{-n_z/2}(n_z!)^{-1/2}\left(\frac{m\omega_z}{\hbar\pi}\right)^{1/4} e^{-\frac{m\omega_z}{2\hbar}z^2} H_{n_z}\left(\sqrt{\frac{m\omega_z}{\hbar}}z\right)$$

Symmetry and Degeneracy

- So far we have considered the general cases of 2D and 3D SHO's assuming $\omega_x \neq \omega_y \neq \omega_z$.
- In such cases the oscillators are said to be anisotropic
- Let us consider a 2D isotropic SHO, satisfying $\omega_x = \omega_y = \omega_0$
- Isotropic 2D SHO is also called a circular SHO, because of the circular symmetry obvious in its potential energy

$$V(x, y) = \frac{1}{2} m\omega_0^2 \left(x^2 + y^2\right)$$

- If we use plane polar coordinates (r, θ), and substitute $x = r\cos\theta$ and $y = r\sin\theta$, above

$$V(x, y) = V(r) = \frac{1}{2} m\omega_0^2 r^2$$

The Circular SHO

- Actually, we can solve the TISE of a 2D circular oscillator also using the plane polar coordinates, leading to the same solution
- However, for now let us consider the eigenenergies of this oscillator which can be written as

$$E^{(2)}_{n_x,n_y} = \left(n_x + \frac{1}{2}\right)\hbar\omega_0 + \left(n_y + \frac{1}{2}\right)\hbar\omega_0 = (n_x + n_y + 1)\hbar\omega_0$$

- These energy levels are highly degenerate as is obvious from the following table

Degeneracies of a circular SHO

- Recall that in quantum mechanics, when there are several eigenvectors corresponding to a given eigenvalue, it is said to be degenerate
- The degeneracy table for the first three energy levels of the circular SHO is given below

Sr. #	n_x	n_y	$E^{(2)}_{n_x,n_y}$	Degeneracy	
1	0	0	$\hbar\omega_0$	1	
2	1	0	$2\hbar\omega_0$	—	
3	0	1	$2\hbar\omega_0$	2	
4	2	0	$3\hbar\omega_0$	—	
5	1	1	$3\hbar\omega_0$	—	
6	0	2	$3\hbar\omega_0$	3	

- It is obvious that the level with energy eigenvalue $n\hbar\omega$ will be n-fold degenerate

Symmetries and Degeneracies

- One can similarly perform a degeneracy analysis for the 3D isotropic SHO, also called the spherical SHO
- For an anisotropic oscillator in any dimension there will be no degeneracies
- While for circular and spherical oscillators levels are degenerate, why?
- For a particle in a square box ($a = b$) or a cubic box ($a = b = c$), similar degeneracies will be found. But, why?
- Actually, there is a deep connection between the symmetries and degeneracies.
- Systems which are symmetric will always exhibit degeneracies
- However, a deeper study of this topic is outside the scope of this course