Introduction to Quantum Mechanics
Unit 2. Time Independent Schroedinger Equation

A. Stationary States

1. Time Independent Schroedinger Equation

(i) Separation of variables on Schroedinger equation:

Let \( \Psi(x, t) = \psi(x)\varphi(t) \)

Substitute this into the Schrödinger equation:

\[
\frac{\hbar}{i} \frac{\partial}{\partial t} \Psi(x, t) = -\frac{\hbar^2}{2m} \Psi(x, t) + V\Psi(x, t) \Rightarrow \frac{\hbar}{i} \frac{\partial}{\partial t} \psi(x)\varphi(t) = \frac{\hbar^2}{2m} \psi(x)\varphi(t) + V\psi(x)\varphi(t)
\]

\[
\Rightarrow \frac{\hbar}{i} \frac{\partial}{\partial t} \psi(x)\varphi(t) = \varphi(t) \left[ \frac{\hbar^2}{2m} \psi(x) + V\psi(x) \right]
\]

\[
\Rightarrow \frac{\hbar}{i} \frac{\partial}{\partial t} \psi(x)\varphi(t) = \varphi(t) \left[ \frac{\hbar^2}{2m} \psi(x) + V\psi(x) \right]
\]

L.H.S. is a function of \( t \) only and R.H.S. is a function of \( x \), so they can only equal to a constant \( E \).

Now Schrödinger becomes two equations:

- L.H.S. \( \Rightarrow \frac{\hbar}{i} \frac{\partial}{\partial t} \varphi(t) = E\varphi(t) \)
- R.H.S. \( \Rightarrow -\frac{\hbar^2}{2m} \psi(x) + V\psi(x) = E\psi(x) \), or simply \( \hat{H}\psi(x) = E\psi(x) \)

(ii) The first equation is readily soluble.

Let \( \varphi(t) = e^{\Omega t} \)

\[
\frac{\hbar}{i} \frac{\partial}{\partial t} \varphi(t) = E\varphi(t) \Rightarrow i\hbar e^{\Omega t} = Ee^{\Omega t} \Rightarrow \Omega = \frac{E}{\hbar}
\]

Therefore, \( \varphi(t) = e^{-i\Omega t} \) where \( \omega = \frac{E}{\hbar} \)

(iii) Therefore, the general solution of the Schroedinger equation must be in the form

\[
\Psi(x, t) = \psi(x)e^{-i\omega t}
\]

where \( \omega = \frac{E}{\hbar} \) and \( E \) and \( \psi(x) \) are determined by the time independent Schrodinger equation:

\[
-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V\psi(x) = E\psi(x)
\]

2. Properties of the Stationary States \( \psi(x) \)
(i) Suppose we find all solutions of the time independent Schrödinger equation and label them as \( n \), i.e. \( H\psi_n(x) = E_n\psi_n(x) \). In here, for simplicity, we assume \( n \) is discrete (i.e. these solutions are countable one by one). In reality, \( n \) can be continuous and \( E \) will be a continuous variable in that case.

(ii) Note that since \( H\psi_n(x) = E_n\psi_n(x) \), \( \psi_n(x) \) is an eigenfunction of the Hamiltonian.

(iii) Since \( H \) is Hermitian, all the solution of the time independent Schrödinger equation form an orthonormal basis, and let us call this basis \( E \). So that this time, for the same linear space, there are three bases we know well. They are \( X \), \( P \), and \( E \). Unlike linear momentum, the basis are always formed by eigenstates (in \( x \)-representation):

\[
\frac{1}{\sqrt{2\pi}} e^{i\frac{Ex}{\hbar}}
\]

The basis \( E \) depend on the potential and are solution of the equation:

\[
-\frac{\hbar^2}{2m} \psi_n''(x) + V(x)\psi_n(x) = E_n\psi_n(x)
\]

(iv) Solving above equation to determine \( \psi_n(x) \) is the same as diagonalizing the Hamiltonian \( H \).

(v) Any linear combination of \( \psi_n \) with the time factor is a solution of the original time dependent Schrödinger equation, i.e.:

\[
| \Psi > = a_1\psi_1 e^{-i\omega_1 t} + a_2\psi_2 e^{-i\omega_2 t} + \cdots + a_N e^{-i\omega_N t} \psi_N
\]

is a solution of the original time dependent Schrödinger equation, even though

\[
a_1\psi_1 + a_2\psi_2 + \cdots + a_N\psi_N
\]

it is NOT an eigenstate of the Hamiltonian.

If

\[
| \Psi > = a_1\psi_1 e^{-i\omega_1 t} + a_2\psi_2 e^{-i\omega_2 t} + \cdots + a_N e^{-i\omega_N t} \psi_N
\]

\[

\therefore H| \Psi > = a_1E_1\psi_1 e^{-i\omega_1 t} + a_2E_2\psi_2 e^{-i\omega_2 t} + \cdots + a_N E_N \psi_N e^{-i\omega_N t}
\]

\[

i\hbar \frac{\partial}{\partial t} | \Psi > = i\hbar \left[ (-i\omega_1 a_1\psi_1 e^{-i\omega_1 t}) + (-i\omega_2 a_2\psi_2 e^{-i\omega_2 t}) + \cdots + (-i\omega_N a_N \psi_N e^{-i\omega_N t}) \right]
\]

\[
= \left[ \hbar \omega_1 a_1\psi_1 e^{-i\omega_1 t} + \hbar \omega_2 a_2\psi_2 e^{-i\omega_2 t} + \cdots + \hbar \omega_N a_N \psi_N e^{-i\omega_N t} \right]
\]

\[
= a_1E_1\psi_1 e^{-i\omega_1 t} + a_2E_2\psi_2 e^{-i\omega_2 t} + \cdots + a_N E_N \psi_N e^{-i\omega_N t}
\]

\[
\therefore i\hbar \frac{\partial}{\partial t} | \Psi > = H| \Psi >
\]

(vi) Eigenstates of \( H \) (or \( \psi_n(x) \)) will evolve with time as

\[
\psi_n(x, t) = \psi_n(x) e^{-i\omega_n t}
\]

Note that ONLY \( \psi_n(x) \) vary with time in this simple harmonic form. They are also called stationary state, because its probability density is independent of time:

\[
P(x, t) = \psi_n^*(x, t)\psi_n(x, t) = \psi_n^*(x) e^{i\omega_n t} \psi_n(x) e^{-i\omega_n t} = \psi_n^*(x)\psi_n(x)
\]
Any other arbitrary state function will depend on time in a more complex way:

$$|\Psi\rangle = a_1\psi_1 e^{-i\omega_1 t} + a_2\psi_2 e^{-i\omega_2 t} + \cdots + a_N e^{-i\omega_N t}$$

and the probability density will NOT be a constant of time.

(vii) Above show why the diagonalization of the Hamiltonian is so important. We know exactly how these stationary states vary with time. Now, given any arbitrary wave function at t=0 (i.e. $\Psi(x,0)$), we will know how it will evolve with time if we can express it as a linear combination of $\psi_n$ at t=0:

$$\Psi(x,t) = a_1\psi_1(x,t) + a_2\psi_2(x,t) + \cdots + a_N\psi_N(x,t)$$

$$= a_1\psi_1(x)e^{-i\omega_1 t} + a_2\psi_2(x)e^{-i\omega_2 t} + \cdots + a_N\psi_N(x)e^{-i\omega_N t}$$

(viii) How to determine $a_1$, $a_2$, ..., $a_N$? Do not forget that a Hermitian H will ensure an orthonormal basis $E$, in other words, $\langle \psi_n | \psi_m \rangle = \delta_{nm}$.

$$|\Psi(0)\rangle = a_1 |\psi_1(0)\rangle + a_2 |\psi_2(0)\rangle + \cdots + a_N |\psi_N(0)\rangle = \sum a_i |\psi_i(0)\rangle$$

$$\Rightarrow \langle \psi_j(0) | \Psi(0) \rangle = \sum \langle \psi_j(0) |\psi_i(0)\rangle a_i = \sum a_i \delta_{ij} = a_j$$

i.e. $a_j = \langle \psi_j(0) | \Psi(0) \rangle$

or in continuous case,

$$a_j = \int \psi_j^*(x,0) \Psi(x,0) dx$$

B. Particle in a box

1. General solution

(i) Consider potential

$$V(x) = \begin{cases} 0 & 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}$$

This is the case when a particle is trapped in the box $0 \leq x \leq a$. 
(ii) By insight, we should know that $\psi_n(x) = 0$ for $x \leq 0$ and $x \geq a$. $\psi_n(x)$ is continuous at $x = 0$ and $x = a$, but $\psi_n'(x)$ is NOT continuous at these two points because $V$ is infinity at these two points.

(iii) By insight from standing waves, we should be able to write down the solution directly:

$$\psi_n(x) = \begin{cases} A \sin kx & 0 \leq x \leq a \\ 0 & x \leq 0 \text{ or } x \geq a \end{cases}$$

$$\psi_n(x) = 0 \Rightarrow k_n = \frac{n\pi}{a} \quad (n = 1, 2, 3, \ldots) \quad \text{(why not 0 or negative?)}$$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

(iv) Together with the time dependent part, the energy eigenvectors are:

$$\psi_n(x, t) = \begin{cases} Ae^{-i\omega_n t} \sin kx & 0 \leq x \leq a \\ 0 & x \leq 0 \text{ or } x \geq a \end{cases}$$

$$\omega_n = \frac{E_n}{\hbar} = \frac{n^2 \pi^2 \hbar}{2ma^2}$$

(v) By insight, we know the integration (why?)

$$\int_{\text{box}} \sin^2 k_n x \, dx = \int_{\text{box}} \cos^2 k_n x \, dx = \frac{a}{2}$$

and $$\int_{\text{box}} \sin k_n x \cos k_n x \, dx = 0$$

This immediate gives

$$A^2 \cdot \frac{a}{2} = 1 \Rightarrow A = \frac{\sqrt{2}}{a}$$

(vi) At this point we know all the eigenvectors in basis $E$ for a particle in a box. Since $\mathcal{H}$ is a Hermitian operator, these vectors are orthonormal.

(vii) All eigenvectors in basis $E$ satisfy boundary condition $\psi_n(a) = \psi_n(0) = 0$. Any state vector $|\Psi>\text{ can be expressed as linear combination of } \psi_n$ and this will ensure $|\Psi>$ also satisfy the boundary condition $\Psi(a) = \Psi(0) = 0$. 
(viii) For any state function $|\Psi\rangle$, we can easily express it as a linear combination of $\psi_n$ at any time (say, $t=0$) because of the orthonormal property of basis $E$:

$$\Psi(x,0) = a_1 \psi_1(x,0) + a_2 \psi_2(x,0) + \cdots + a_N \psi_N(x,0) = \sum a_i \psi_i(x,0)$$

$$\Rightarrow \langle \psi_j(x,0)|\Psi(x,0)\rangle = \sum a_i \langle \psi_j(x,0)|\psi_i(x,0)\rangle = \sum a_i \langle \psi_j(x,0)|\psi_j(x)\rangle = \sum a_i \delta_{ij} = a_j$$

*i.e.* $a_j = \langle \psi_j(x,0)|\Psi(x,0)\rangle$

Or in continuous case,

$$a_j = \int \psi_j^*(x,0)\Psi(x,0)dx = \frac{\sqrt{2}}{a} \int \sin k_n x \Psi(x,0)dx$$

(ix) And now we can calculate how the wave function evolves over time:

$$\Psi(x,t) = a_1 \psi_1(x,t) + a_2 \psi_2(x,t) + \cdots + a_N \psi_N(x,t)$$

$$= a_1 \psi_1(x,0)e^{-i\omega t} + a_2 \psi_2(x,0)e^{-i\omega t} + \cdots + a_N \psi_N(x,0)e^{-i\omega t}$$

$$= \sum a_i \psi_i(x,0)e^{-i\omega t}$$

$$= \sum \left[ \frac{\sqrt{2}}{a} \int \sin k_n x' \Psi(x',0)dx' \right] \left[ \frac{\sqrt{2}}{a} \sin k_n x x'e^{-i\omega t} \right]$$

$$= \frac{2}{a} \sum \int \sin k_n x' \Psi(x',0)dx' \sin k_n x x'e^{-i\omega t}$$

(x) The following are constant of time, or “stationary”, or time independent:

(a) Expectation of energy $\langle E \rangle$

(b) Probability density of the energy eigenstates $|\psi_n(x,t)|^2$. For this reason, the Hamiltonian eigenstates are also known as stationary states.

(c) Energy eigenvalues $E_n$.

(d) Operator (e.g., H and p) and their corresponding eigenvalues (Schroedinger picture).

The following are NOT constant of time:

(a) Eigenstates $|\psi_n\rangle$ of the Hamiltonian or energy (don’t forget the $e^{-i\omega t}$ factor in it).

(b) Any state vector $|\Psi\rangle$

(c) $\langle x \rangle$ (it oscillates!)

(d) $\langle p \rangle$

and so on.
A particle of mass \( m \) is confined to a one-dimensional region \( 0 \leq x \leq a \) with the potential

\[
V(x) = \begin{cases} 
\infty & x < 0 \\
0 & 0 < x < a \\
\infty & x > 0 
\end{cases}
\]

At \( t=0 \) its normalized wave function is

\[
\Psi(x, t = 0) = \sqrt{\frac{8}{5a}} \left[ 1 + \cos \left( \frac{\pi x}{a} \right) \right] \sin \left( \frac{\pi x}{a} \right)
\]

The Schrödinger eigenfunctions and eigenvalues for the above potential are given as

\[
\Psi_n = \sqrt{\frac{2}{\pi}} \sin \left( \frac{n\pi x}{a} \right) \quad ; \quad E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}
\]

(a) What is the wave function at a later time \( t = t_0 \)?

\[
\Psi(x, t) = \frac{2}{\sqrt{5}} \Psi_1 e^{i(E_1/\hbar)t} + \frac{1}{\sqrt{5}} \Psi_2 e^{-i(E_2/\hbar)t}
\]

\[
= \frac{2}{\sqrt{5}} \left[ \sqrt{\frac{8}{5a}} \sin \left( \frac{\pi x}{a} \right) \exp \left( -i \frac{\pi^2 \hbar t}{2ma^2} \right) \right] + \frac{1}{\sqrt{5}} \left[ \sqrt{\frac{8}{5a}} \sin \left( \frac{2\pi x}{a} \right) \exp \left( -i \frac{3\pi^2 \hbar t}{2ma^2} \right) \right]
\]

or

\[
\Psi(x, t) = \sqrt{\frac{8}{5a}} \left[ 1 + \cos \left( \frac{\pi x}{a} \right) \right] \exp \left( -i \frac{3\pi^2 \hbar t}{2ma^2} \right) \sin \left( \frac{\pi x}{a} \right)
\]
(b) What is the average energy of the system at \( t = 0 \) and at \( t = t_0 \)?

\[
\Psi(x, t) = \frac{2}{\sqrt{5}} \psi_1 e^{-i(E_1/\hbar) t} + \frac{1}{\sqrt{5}} \psi_2 e^{-i(E_2/\hbar) t} 
\]

\[
\langle E \rangle = \int \left[ \frac{2}{\sqrt{5}} \psi_1^* e^{i(E_1/\hbar) t} + \frac{1}{\sqrt{5}} \psi_2^* e^{i(E_2/\hbar) t} \right] \hat{H} \left[ \frac{2}{\sqrt{5}} \psi_1 e^{-i(E_1/\hbar) t} + \frac{1}{\sqrt{5}} \psi_2 e^{-i(E_2/\hbar) t} \right] dx 
\]

\[
= \int \left[ \frac{2}{\sqrt{5}} \psi_1^* e^{i(E_1/\hbar) t} + \frac{1}{\sqrt{5}} \psi_2^* e^{i(E_2/\hbar) t} \right] \left[ \frac{2E_1}{\sqrt{5}} \psi_1 e^{-i(E_1/\hbar) t} + \frac{E_2}{\sqrt{5}} \psi_2 e^{-i(E_2/\hbar) t} \right] dx 
\]

\[
= \frac{4}{5} E_1 + \frac{1}{5} E_2 
\]

\[
= \frac{4 \pi^2 \hbar^2}{5 2ma^2} = \frac{4 \pi^2 \hbar^2}{5 ma^2} 
\]

This is a constant of motion and has the same value of \( t = 0 \) and \( t = t_0 \).

(c) What is the probability that the particle is found in the left half of the box (i.e., in the region \( 0 \leq x \leq a/2 \)) at \( t = t_0 \)?

\[
P(0 \leq x \leq a/2) = \int_0^{a/2} |\Psi(x, t_0)|^2 dx 
\]

\[
= \int_0^{a/2} \left[ \frac{8}{5a} \sin \left( \frac{\pi x}{a} \right) \exp \left( -\frac{i \pi^2 \hbar t_0}{2ma^2} \right) + \frac{2}{\sqrt{5a}} \sin \left( \frac{2\pi x}{a} \right) \exp \left( \frac{-i 2 \pi^2 \hbar t_0}{ma^2} \right) \right]^2 dx 
\]

\[
= \int_0^{a/2} \left[ \frac{8}{5a} \sin \left( \frac{\pi x}{a} \right) \right]^2 + \left[ \frac{2}{\sqrt{5a}} \sin \left( \frac{2\pi x}{a} \right) \right]^2 dx 
\]

\[
+ \int_0^{a/2} \frac{8}{5a} \sin \left( \frac{\pi x}{a} \right) \frac{2}{\sqrt{5a}} \sin \left( \frac{2\pi x}{a} \right) \cos \frac{3 \pi^2 \hbar t_0}{2ma^2} dx 
\]

\[
= \frac{8}{5a} \int_0^{a/2} \left[ \frac{1}{2} - \frac{1}{2} \cos \left( \frac{2\pi x}{a} \right) \right] dx + \frac{2}{5a} \int_0^{a/2} \left[ \frac{1}{2} - \frac{1}{2} \cos \left( \frac{4\pi x}{a} \right) \right] dx 
\]

\[
+ \frac{4}{5a} \cos \left( \frac{3 \pi^2 \hbar t_0}{2ma^2} \right) \int_0^{a/2} \cos \left( \frac{\pi x}{a} \right) - \cos \left( \frac{3 \pi x}{a} \right) \cos \left( \frac{3 \pi x}{a} \right) dx 
\]

\[
= \frac{8}{5a} \left( \frac{a}{4} \right) + \frac{2}{5a} \left( \frac{a}{4} \right) + \frac{4}{5a} \cos \left( \frac{3 \pi^2 \hbar t_0}{2ma^2} \right) \left\{ \cos \left( \frac{\pi x}{a} \right) - \cos \left( \frac{3 \pi x}{a} \right) \right\} dx 
\]

\[
= \frac{1}{2} + \frac{4}{5a} \cos \left( \frac{3 \pi^2 \hbar t_0}{2ma^2} \right) \left\{ \frac{a}{\pi} \sin \left( \frac{\pi x}{a} \right) \right\} - \frac{a}{3\pi} \sin \left( \frac{3 \pi x}{a} \right) \right\} dx 
\]
C. Harmonic oscillator – Hermite polynomials

(i) The harmonic potential is \( V(x) = \frac{kx^2}{2} \). Substitute this into the Schrödinger equation:

\[
-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + \frac{1}{2} kx^2 \psi(x) = E \psi(x)
\]

(ii) Importance of Harmonic oscillators: Locally all equilibrium potential always look like this:

Any potential like this can be approximated locally with an open upward parabola. In other words, a simple harmonic oscillator potential is the first order approximation of equilibrium potential. That is the reason why we can approximate between atoms in a crystal with springs:
(iii) Insight: From our previous knowledge, we should know that the energy eigenvalues are:

\[ E_n = (n + \frac{1}{2})\hbar \omega \]

where the angular frequency \( \omega \) is defined in the classical way:

\[ \omega = \sqrt{\frac{k}{m}} \]

Schroedinger equation becomes

\[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + \frac{1}{2} m \omega^2 x^2 \psi(x) = E \psi(x)\]

(iv) Simplifying the Schroedinger equation:

\[-\hbar^2 \frac{d^2}{2m} \psi(x) + \frac{1}{2} m \omega^2 x^2 \psi(x) = E \psi(x) \Rightarrow - \frac{d^2}{dx^2} \psi(x) + \frac{m \omega^2}{\hbar^2} x^2 \psi(x) = \frac{2m}{\hbar^2} E \psi(x)\]

\[ \Rightarrow - \frac{m \omega}{\hbar} \frac{d}{dx^2} \psi(x) + \frac{m \omega}{\hbar} x^2 \psi(x) = \frac{2m}{\hbar^2} E \psi(x)\]

\[ \Rightarrow - \frac{d^2}{d\left(\sqrt{\frac{m \omega}{\hbar}} x\right)^2} \psi(x) + \left(\sqrt{\frac{m \omega}{\hbar}} x\right)^2 \psi(x) = \frac{2}{\hbar \omega} E \psi(x)\]

Let \( \xi = \sqrt{\frac{m \omega}{\hbar}} x \), and \( K = \frac{2}{\hbar \omega} E \), Schroedinger equation becomes:

\[- \frac{d^2}{d\xi^2} \psi(x) + \xi^2 \psi(x) = K \psi(x)\]

(v) Solution at large \( x \).

At large \( x \) (or \( \xi \)), above Schroedinger equation becomes
- $\frac{d^2}{d\xi^2} \psi(x) + \xi^2 \psi(x) = 0 \Rightarrow \psi(x) \to e^{\frac{\xi^2}{2}}$ as $\xi \to \pm \infty$

Convergence of $\psi(x) \Rightarrow \psi(x) \to e^{\frac{\xi^2}{2}}$ as $\xi \to \pm \infty$

(vi) Complete solution

The complete solution of the Schroedinger equation has to be in the form

$$\psi(\xi) = A \, H(\xi) \, e^{\frac{-\xi^2}{2}}$$

Where $H(x)$ is some polynomials which can be solved by series method (see p. 52-54 of textbook). We will not try to do the solution here. Instead, we will focus on some important properties of $H(x)$ here.

(vii) Since series solution is involved here, we know that $H(x)$ is a polynomial. By convergence of $\psi(x)$, we know $H(x)$ should be finite in the highest order of $x$. We can use this to label $H(x)$. For example, the highest order of $x$ in $H_n(x)$ is $x_n$. This requirement will "force" $E$ (or $K$) to taking discrete values $E_n$ only. As expected,

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

i.e.

$$- \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_n(x) + \frac{1}{2} m \omega^2 x^2 \psi_n(x) = E_n \psi_n(x) = (n + \frac{1}{2}) \hbar \omega \psi_n(x)$$

(viii) $H_n(x)$ is known as the Hermite polynomials and all the coefficients are real. i.e. $H^*(x) = H(x)$.

(viii) Insight: Since the Hamiltonian is Hermitian, All $\psi_n(x)$ must be complete and orthonormal.

$$\int_{-\infty}^{\infty} \psi_n(x) \psi_m(x) dx = \delta_{nm} \text{ or } \int_{-\infty}^{\infty} A^2 H_n(\frac{m\omega}{\hbar} x) H_m(\frac{m\omega}{\hbar} x) e^{\frac{m^2 \omega^2}{\hbar^2}} dx = \delta_{nm}$$

Attention: Hermite polynomials itself are not orthogonal, but $\psi_n$’s are.

(ix) Integration remarks:

Integration involving $\psi_n(x)$ and power of $x$ can be readily calculated using the following relationship (for generality we start our limit of integration from $0$ instead of $-\infty$):
Define $I_n = \int_{-\infty}^{\infty} x^n e^{-\alpha x^2} \, dx$

Note that $d(x^{n-1}e^{-\alpha x^2}) = -2\alpha x^n e^{-\alpha x^2} + (n-1)x^{n-2}e^{-\alpha x^2} \Rightarrow x^n e^{-\alpha x^2} = \frac{1}{-2\alpha} d(x^{n-1}e^{-\alpha x^2}) + \frac{(n-1)}{2\alpha} x^{n-2}e^{-\alpha x^2}$

$\therefore I_n = \int_{-\infty}^{\infty} x^n e^{-\alpha x^2} \, dx = \left[ \frac{1}{-2\alpha} (x^{n-1}e^{-\alpha x^2}) \right]_{-\infty}^{\infty} = \frac{(n-1)}{2\alpha} \int_{-\infty}^{\infty} x^{n-2}e^{-\alpha x^2} \, dx = \frac{(n-1)}{2\alpha} I_{n-2}$

At the end, we need to know $I_0$ and $I_1$:

$I_1 = \int_{0}^{\infty} xe^{-\alpha x^2} \, dx = \frac{1}{2} \int_{0}^{\infty} e^{-\alpha u} \, du \quad (u=x^2)$

$= \left[ -\frac{1}{2\alpha} e^{-\alpha u} \right]_{0}^{\infty} = \frac{1}{2\alpha}$

$I_0^2 = \int_{0}^{\infty} e^{-\alpha x^2} \, dx \int_{0}^{\infty} e^{-\alpha y^2} \, dy = \int_{0}^{\infty} e^{-\alpha R^2} \, dR \int_{0}^{2\pi} d\theta = 2\pi I_1 = \frac{\pi}{\alpha} \Rightarrow I_0 = \sqrt{\frac{\pi}{\alpha}}$

(ix) The normalization constant can be calculated as:

$$A_n = \left( \frac{m\omega}{\pi \hbar} \right)^{\frac{1}{2}} \cdot \frac{1}{\sqrt{2^n n!}}$$

Unlike particle in a box, different eigenfunction has different normalization constant.

(x) Hermite polynomials can be generated by the following triangles:
(xi) If we denote \((n,m)\) as the coefficient of \(\xi^m\) in Hermite polynomials \(H_n\). Above construction comes from the recurrence relation:

\[
\frac{dH_n}{d\xi} = 2nH_{n-1}(\xi) \Rightarrow m(n,m) = 2n(n-1, m-1)
\]

\[
H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi) \Rightarrow (n+1, m) = 2(n, m-1) - 2(n-1, m)
\]

In specific, denote \(y=(n,m), z=(n+1,m+1),\) and \(x=(n-1,m+1)\) with the following relative position in the triangle:

\[
\begin{array}{ccc}
\circ & \circ & \circ \\
x & & n-1 \\
\circ & & n \\
y & & \\
\circ & \circ & n+1 \\
z & m & m+1 \\
\end{array}
\]
Above recurring relations imply:

\[ m(n, m) = 2(n - 1, m - 1) \Rightarrow (m + 1)(n + 1, m + 1) = 2(n + 1)(n, m) \]

\[ \Rightarrow (m + 1)z = 2(n + 1)y \quad \text{(1)} \]

\[ (n + 1, m) = 2(n, m - 1) - 2n(n - 1, m) \Rightarrow (n + 1, m + 1) = 2(n, m) - 2n(n - 1, m + 1) \]

\[ \Rightarrow z = 2y - 2nx \quad \text{(2)} \]

Substitute (2) into (1):

\[ (m + 1)z = 2(n + 1) \left( \frac{z + 2nx}{2} \right) \Rightarrow (m + 1)z = (n + 1)z + 2n(n + 1)x \]

\[ \Rightarrow z = \frac{2n(n + 1)}{m - n} x \]

We just keep on using this equation to construct the element two rows directly below. The last two elements in a row cannot be done by this way (because there is nothing above!), just add a zero (the second last element) and 2 times the last element of the previous row.

(xii) Some properties of Hermit polynomials (hence \( \psi_n \)):

a. If \( n \) is even:
   \( H_n \) is in all even power of \( x \), and hence \( H_n \) and \( \psi_n \) are even in \( x \) (\( \psi_n(x) = \psi_n(-x) \)).
   If \( n \) is odd:
   \( H_n \) is in all odd power of \( x \), and hence \( H_n \) and \( \psi_n \) are odd in \( x \) (\( \psi_n(x) = -\psi_n(-x) \)).

b. Starting from a positive highest order term \( a_nx^n \), The sign within a Hermite polynomial alternates.

c. Coefficient of \( x_n \) in \( H_n = 2 \times \) Coefficient of \( x_{n-1} \) in \( H_{n-1} \).

d. All coefficients are even numbers. The only exception is the “1” in \( H_0=1 \).

e. The complete wave function of a simple harmonic oscillator is:

\[
\psi_n(x) = \left( \frac{m_0}{\hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2} \quad \text{with } \xi = \sqrt{\frac{m_0}{\hbar}} x
\]

Energy eigenvalue of \( \psi_n(x) \) is \( E_n = (n + \frac{1}{2})\hbar\omega \)

\( \psi_n \) form a complete orthonomal set. Any function of \( x \) satisfying boundary conditions \( f(\infty) = f(-\infty) = 0 \) can be expressed as a linear combination of \( \psi_n \).

f. For a wavefunction in polynomial form:
We just need to express it as linear combination of \( \psi_1, \psi_2, \ldots \) up to \( \psi_n \). Eigenfunction of order larger than \( n \) will not contribute to the combination because they will give power of \( x \) with order larger than \( n \).

(xiii) For example:

Let us construct \( f(x) = \psi_0 + \frac{1}{\sqrt{2}} \psi_1 + \sqrt{2} \psi_2 \)

\[
= \left( \frac{m \omega}{\hbar \pi} \right)^{\frac{1}{4}} (1) e^{-\xi^2/2} + \frac{1}{\sqrt{2}} \left( \frac{m \omega}{\hbar \pi} \right)^{\frac{1}{4}} (2 \xi) e^{-\xi^2/2} + \sqrt{2} \left( \frac{m \omega}{\hbar \pi} \right)^{\frac{1}{4}} \frac{1}{\sqrt{8}} (4 \xi^2 - 2) e^{-\xi^2/2}
\]

\[
= \left( \frac{m \omega}{\hbar \pi} \right)^{\frac{1}{4}} (1) e^{-\xi^2/2} + \left( \frac{m \omega}{\hbar \pi} \right)^{\frac{1}{4}} (\xi) e^{-\xi^2/2} + \left( \frac{m \omega}{\hbar \pi} \right)^{\frac{1}{4}} (2 \xi^2 - 1) e^{-\xi^2/2}
\]

\[
= \left( \frac{m \omega}{\hbar \pi} \right)^{\frac{1}{4}} (2 \xi^2 + \xi) e^{-\xi^2/2}
\]
Here is how thing work:

\[
\int_{-\infty}^{\infty} H_0^*(x)f(x)dx = \int_{-\infty}^{\infty} \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} e^{-\xi^2/2} \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} (2\xi^2 + \xi)e^{-\xi^2/2}dx \\
= \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\xi^2} 2\xi^2 \sqrt{\frac{\hbar}{m\omega}} d\xi \\
= \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} \xi^2 e^{-\xi^2} d\xi \\
= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\xi^2} d\xi \\
= \frac{1}{\sqrt{\pi}} \sqrt{\pi} = 1
\]

\[
\int_{-\infty}^{\infty} H_1^*(x)f(x)dx = \int_{-\infty}^{\infty} \left[ \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^2 \cdot 2!}} (2\xi)e^{-\xi^2/2} \right] \left(\frac{m\omega}{\hbar}\pi\right)^{\frac{1}{4}} (2\xi^2 + \xi)e^{-\xi^2/2}dx \\
= \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\xi^2} \sqrt{\frac{\hbar}{m\omega}} d\xi \\
= \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} \xi^2 e^{-\xi^2} d\xi \\
= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \xi^2 e^{-\xi^2} d\xi \\
= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\pi}{2}} = \frac{1}{\sqrt{2}}
\]

\[
\int_{-\infty}^{\infty} H_2^*(x)f(x)dx = \int_{-\infty}^{\infty} \left[ \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^2 \cdot 2!}} (4\xi^2 - 2)e^{-\xi^2/2} \right] \left(\frac{m\omega}{\hbar}\pi\right)^{\frac{1}{4}} (2\xi^2 + \xi)e^{-\xi^2/2}dx \\
= \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\xi^2} \frac{1}{\sqrt{8}} (8\xi^4 - 4\xi^2) \sqrt{\frac{\hbar}{m\omega}} d\xi \\
= \frac{2}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (2\xi^4 - \xi^2) e^{-\xi^2} d\xi \\
= \frac{2}{\sqrt{2\pi}} \left[ 2 \cdot \frac{3 \cdot 1}{2 \cdot 2} - \frac{1}{2} \right] \sqrt{\pi} \\
= \frac{2}{\sqrt{2}} = \sqrt{2}
\]
D. Simple Harmonic Oscillator - Ladder operator.

(ii) (iii) When this happen, we can always write the operator in expression of ladder operators.

(iv) For simplicity, let us consider operator Z, with eigenvectors $|\psi_0\rangle$, $|\psi_1\rangle$, $|\psi_2\rangle$, … and corresponding eigenvalues $B$, $A+B$, $A+2B$, …… In its own (Z) representation, operator Z is simply the matrix

$$
Z = \begin{pmatrix}
nA + B & 0 & \cdots & 0 \\
\vdots & 2A + B & \vdots & \vdots \\
0 & \vdots & \ddots & 0 \\
0 & 0 & \cdots & A + B
\end{pmatrix}
$$

(iv) Ladder operators are formed by step up and step down operators. Definition of step up operator $a^+$ (in Z-representation):

$$
a^+ = \begin{pmatrix}
0 & \sqrt{f(n-1)} & 0 & 0 & 0 \\
0 & \ddots & \ddots & \ddots & 0 \\
0 & 0 & 0 & \sqrt{f(2)} & 0 \\
0 & 0 & 0 & 0 & \sqrt{f(1)} \\
0 & 0 & 0 & 0 & 0
\end{pmatrix}
$$

Where $f(i)$ is some functional form of index $i$. Under this definition, for finite cases, we can assume the “boundary values” $f(n)=f(0)=0$ (since they are not used). The self adjoint of $a^+$ is known as the step down operator:

$$
a = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
\sqrt{f(n-1)} & \ddots & 0 & 0 & 0 \\
0 & \ddots & \ddots & \ddots & 0 \\
0 & 0 & \sqrt{f(2)} & \ddots & 0 \\
0 & 0 & 0 & \sqrt{f(1)} & 0
\end{pmatrix}
$$
From these we have:

\[
a^+ a = \begin{pmatrix}
0 & \sqrt{f(n-1)} & 0 & 0 & 0 \\
0 & \ddots & \ddots & 0 & 0 \\
0 & 0 & \sqrt{f(2)} & 0 & 0 \\
0 & 0 & 0 & \sqrt{f(1)} & 0 \\
0 & 0 & 0 & 0 & 0
\end{pmatrix} \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & \sqrt{f(n-1)} & \ddots & 0 & 0 \\
0 & 0 & \sqrt{f(2)} & 0 & 0 \\
0 & 0 & 0 & \sqrt{f(1)} & 0 \\
0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

\[
= \begin{pmatrix}
(f(n-1)) & 0 & 0 & 0 & 0 \\
0 & \ddots & \ddots & 0 & 0 \\
0 & 0 & f(2) & 0 & 0 \\
0 & 0 & 0 & f(1) & 0 \\
0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

Similarly,

\[
a a^+ = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & f(n-1) & 0 & 0 & 0 \\
0 & 0 & \ddots & \ddots & 0 \\
0 & 0 & 0 & f(2) & 0 \\
0 & 0 & 0 & 0 & f(1)
\end{pmatrix}
\]

(v) Meaning of step up and step down operators:

\[
a^+ |\psi_i\rangle = \begin{pmatrix}
0 & \sqrt{f(n-1)} & 0 & 0 & 0 \\
0 & \ddots & \ddots & 0 & 0 \\
0 & 0 & \sqrt{f(2)} & 0 & 0 \\
0 & 0 & 0 & \sqrt{f(1)} & 0 \\
0 & 0 & 0 & 0 & 0
\end{pmatrix} \begin{pmatrix}
0 \\
0 \\
1 \\
0 \\
0
\end{pmatrix} = \sqrt{f(i)} |\psi_{i+1}\rangle
\]

\[
a^+ |\psi_{\text{max}}\rangle = 0
\]

\[
a |\psi_i\rangle = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & \sqrt{f(n-1)} & \ddots & 0 & 0 \\
0 & 0 & \sqrt{f(2)} & 0 & 0 \\
0 & 0 & 0 & \sqrt{f(1)} & 0 \\
0 & 0 & 0 & 0 & 0
\end{pmatrix} \begin{pmatrix}
0 \\
0 \\
1 \\
0 \\
0
\end{pmatrix} = \sqrt{f(i-1)} |\psi_{i-1}\rangle
\]

\[
a^+ |\psi_{\text{min}}\rangle = 0
\]
(vi) \( a^+ \) and \( a \) are not Hermitian. They are just a mathematical tool!

(vii) \( a^+a \) and \( aa^+ \) are diagonal matrices. From this we know ladder operators have to satisfy the general condition: 
\[ [Z, a^+a] = [Z, aa^+] = 0, \]
where \( a \) and \( a^+ \) are ladder operators correspond to operator \( Z \).

(viii) \( a^+ \) and \( a \) do not commute:
\[
a^+a = \begin{pmatrix}
    f(n-1) & 0 & 0 & 0 & 0 \\
    0 & \ddots & 0 & 0 & 0 \\
    0 & 0 & f(2) & 0 & 0 \\
    0 & 0 & 0 & f(1) & 0 \\
    0 & 0 & 0 & 0 & 0
\end{pmatrix} \quad ; \quad aa^+ = \begin{pmatrix}
    0 & 0 & 0 & 0 & 0 \\
    f(n-1) & 0 & 0 & 0 & 0 \\
    0 & \ddots & 0 & 0 & 0 \\
    0 & 0 & f(2) & 0 & 0 \\
    0 & 0 & 0 & f(1) & 0 \\
    0 & 0 & 0 & 0 & f(0) - f(1)
\end{pmatrix}
\]
(Note that \( f(n) = f(0) = 0 \)).

(ix) \([Z, a^+]\) or \([Z, a]\) provides a recurrence relationship:
\[
Za^+ = \begin{pmatrix}
    Z_n & 0 & 0 & 0 & 0 \\
    0 & \ddots & 0 & 0 & 0 \\
    0 & 0 & Z_3 & 0 & 0 \\
    0 & 0 & Z_2 & 0 & 0 \\
    0 & 0 & Z_1 & 0 & 0 \\
\end{pmatrix} \begin{pmatrix}
    0 & 0 & \sqrt{f(n-1)} & 0 & 0 \\
    0 & \ddots & 0 & 0 & 0 \\
    0 & 0 & 0 & \sqrt{f(2)} & 0 \\
    0 & 0 & 0 & 0 & \sqrt{f(1)} \\
    0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}
\]
\[
= \begin{pmatrix}
    0 & Z_n \sqrt{f(n-1)} & 0 & 0 & 0 \\
    0 & 0 & Z_3 \sqrt{f(n-2)} & 0 & 0 \\
    0 & 0 & 0 & Z_2 \sqrt{f(1)} & 0 \\
    0 & 0 & 0 & 0 & Z_1 \sqrt{f(0)} \\
    0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}
\]
So far the formulation is quite general. We do not even put any requirement on the explicit form of f(i). To make use of the above recurrence relationship, we need to know \([Z, a^+]\) explicitly. Note that \([Z, a^+]\) itself looks like a step up operator.

For example, let us consider the simplest situations under which the ladder operators are most effectively used:

We require \(Z\) to have eigenvalues in the form \(A+B, 2A+B, 3A+B, \ldots, nA+B\) and so on, where \(A\) and \(B\) are some constants. We can use \(n\) to label the corresponding eigenvector of the operator \((n=1,2,\ldots,n\) in this case).

Examples of these operators are the z-component of angular momentum, number operator in second quantization, and of course, the Hamiltonian of the simple harmonic oscillator. In the case of simple harmonic Hamiltonian, \(A=nh\omega\) and \(B=\hbar\omega/2\).

Now \(Z|\psi_j\rangle=jA+B|\psi_j\rangle\), we can calculate \([Z, a^+]\) explicitly:

\[
[Z, a^+]|\psi_j\rangle = [Za^* - a^*Z]|\psi_j\rangle = Za^*|\psi_j\rangle - a^*Z|\psi_j\rangle = Z\sqrt{f(j)}|\psi_{j+1}\rangle - a^*(jA+B)|\psi_j\rangle = [(j+1)A+B]\sqrt{f(j)}|\psi_{j+1}\rangle - \sqrt{f(j)}(jA+B)|\psi_{j+1}\rangle = \sqrt{f(j)}A|\psi_{j+1}\rangle = (Aa^* |\psi_j\rangle)
\]
Put this result into our recurrence relationship:

\[ [Z, a^+] |ψ_i⟩ = \sqrt{f(i)} A |ψ_{i+1}⟩ \quad \text{and} \quad [Z, a^+] |ψ_{i+1}⟩ = (Z_{i+1} - Z_i) \sqrt{f(i)} |ψ_{i+1}⟩ \]

\[ \therefore \sqrt{f(i)} A |ψ_{i+1}⟩ = (Z_{i+1} - Z_i) \sqrt{f(i)} |ψ_{i+1}⟩ \quad ⇒ \quad Z_{i+1} = Z_i + A \]

(xi) Above looks obvious, because we are working in Z-representation itself! In a real problem, Z is posted in another representation and we have no idea what are its eigenvalues and eigenvectors. In situation like this, we will follow the above procedure in the given representation:

(a) In the given representation, construct step up or step down operators by investigating operators satisfying the commutation relation \([Z, a^+ a] = 0\). Show that it is a proper ladder operators by showing

\[ a^+ |ψ_i⟩ = \sqrt{f(i)} |ψ_{i+1}⟩ \quad \text{and} \quad a |ψ_i⟩ = \sqrt{f(i-1)} |ψ_{i-1}⟩ \]

It is useful to know \(f(i)\).

(b) Once we know \(a^+\) and \(a\), we can construct \([Z, a^+]\) (or \([Z, a]\)). If it is one of the simple case of eigenvalues with equal separation, \([Z,a]\) will be proportional to \(a^+\) and the “proportional constant” will be equal to the equal increment \(A\) in eigenvalues (as we have shown above).

(c) We can then plug \([Z, a^+]\) into the recurrence relationship

\[ [Z, a^+] |ψ_i⟩ = (Z_{i+1} - Z_i) \sqrt{f(i)} |ψ_{i+1}⟩ \]

to get a relationship between \(Z_{i+1}\) and \(Z_i\).

(d) If \(Z\) is infinite dimension and have no upper AND lower bounds, we need to know some eigenvalues of \(Z\) to begin with. If \(Z\) has upper or lower bounds, we can determine the limiting eigenvalues (at least in most simple cases) by writing \(Z\) in terms of \(a\) and \(a^+\), and make use of the equation \(a^+ |ψ_{\text{max}}⟩ = 0\) and \(a |ψ_{\text{min}}⟩ = 0\).

(xii) Now a practical case for simple harmonic oscillator. From our previous knowledge we know that it is a simple case with consecutive eigenvalues differ by \(\hbar \omega\).

Step 1 (the most difficult) is to construct \(a\) and \(a^+\) in x-representation. In x-representation, the Hamiltonian is

\[ H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 \]

If we can “factorize” \(H\) in the form \((Ax+iBp)(Ax-iBp)\) where \(A\) and \(B\) are some real constants, then one factor is the complex conjugate of the other and it just looks like \(a^+ a\) (or \(aa^+\) which we do not know at this point) and \(H\) must commute with it (since they are equal!). So we now work out the algebra:
= A^2x^2 + B^2p^2 - iAB[x, p]
= A^2x^2 + B^2p^2 + iABh

So if we set A = \[\frac{1}{\sqrt{2}} m \omega^2\] and B = \[\frac{1}{\sqrt{2}m}\] and AB = \[\frac{1}{2}\] \omega

H = \[\frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2\] = \[\left(\frac{m \omega^2}{2} x + i \sqrt{\frac{1}{2m}} p\right)\left(\frac{m \omega^2}{2} x - i \sqrt{\frac{1}{2m}} p\right)\] - \[\frac{1}{2}\] h\omega

At this point we can suspect a (or a^+)= \[\left(\frac{m \omega^2}{2} x + i \sqrt{\frac{1}{2m}} p\right)\]
and a^+ (or a) = \[\left(\frac{m \omega^2}{2} x - i \sqrt{\frac{1}{2m}} p\right)\]

With this notation, we know [a^+, a] = \[\left(\frac{m \omega^2}{2} x - i \sqrt{\frac{1}{2m}} p\right)\left(\frac{m \omega^2}{2} x + i \sqrt{\frac{1}{2m}} p\right)\] = \[2\left(i \omega x p - \frac{i \omega}{2} p x\right)\] = i\omega[x, p] = -h\omega

Also: H = aa^+ - \[\frac{1}{2}\] h\omega = a^+ a + \[\frac{1}{2}\] h\omega

The plan is slightly off from the original because of the constant term \[\frac{1}{2}\] h\omega, but it is just a constant and hence aa^+ (or a^+a) still commute with H in accordance to the original plan.

Now let us calculate Ha^+ |\psi_n\rangle to make sure a^+ is really a step up (not step down) operator:

Ha^+ |\psi_n\rangle = (a^+ a + \[\frac{1}{2}\] h\omega) a^+ |\psi_n\rangle = (a^+ aa^+ + \[\frac{1}{2}\] h\omega a^+) |\psi_n\rangle
= a^+ \left(aa^+ + \[\frac{1}{2}\] h\omega\right) |\psi_n\rangle
= a^+ \left(aa^+ + h\omega - \[\frac{1}{2}\] h\omega\right) |\psi_n\rangle
= a^+ (H + h\omega) |\psi_n\rangle
= (E_n + h\omega) a^+ |\psi_n\rangle

In other words, a^+ |\psi_n\rangle is also an eigenvector of H with eigenvalue E_n + h\omega and hence a^+ is a "step down" operator. Similar argument can be applied to step down (a) operator.
Since we now know that $a^+$ and $a$ are step up and step down operators, above relationship provide us a recurrence relationship to calculate $E_{n+1}$ from $E_n$:

$$H a^+ |\psi_n> = (E_n + \hbar \omega) a^+ |\psi_n> \Rightarrow E_{n+1} = E_n + \hbar \omega$$

as expected.

(xii) However, there are two things we have to address before the problem is solved:

(a) We need to know $E_0$!
(b) We know that $a^+ |\psi_n>$ is $(f_i) |\psi_{n+1}>$, but what is in that factor $(f_i)$? (i.e. what is $f(i)$?)

To answer the first question, we need to work on the ground state with the fact that $a|\psi_0>=0$.

$$H = aa^+ - \frac{1}{2} \hbar \omega = a^+ a + \frac{1}{2} \hbar \omega$$

$$\therefore H |\psi_0> = (a^+ a + \frac{1}{2} \hbar \omega) |\psi_0> = 0 + \frac{1}{2} \hbar \omega |\psi_0>$$

Therefore, $E_0 = \frac{1}{2} \hbar \omega$.

$$E_{n+1} = E_n + \hbar \omega \Rightarrow E_1 = \frac{1}{2} \hbar \omega + \hbar \omega = \frac{3}{2} \hbar \omega \ldots \ldots \ E_{n+1} = n \hbar \omega + \frac{1}{2} \hbar \omega$$

To answer the second question, let $a^+ |\psi_i> = \sqrt{f_i} |\psi_{i+1}>$:

$$\therefore f_i <\psi_{i+1} |\psi_i> = <\psi_i |aa^+ |\psi_i> = 1$$

but $H = aa^+ - \frac{1}{2} \hbar \omega \Rightarrow aa^+ = H + \frac{1}{2} \hbar \omega$

$$\therefore aa^+ |\psi_i> = (H + \frac{1}{2} \hbar \omega) |\psi_i> = (i + \frac{1}{2} \hbar \omega) |\psi_i> = (i+1) \hbar \omega |\psi_i>$$

$$\therefore f_i = (i+1) \hbar \omega \Rightarrow \sqrt{f_i} = \sqrt{(i+1) \hbar \omega}$$

or $a^+ |\psi_i> = \sqrt{(i+1) \hbar \omega} |\psi_{i+1}>$

Similarly, by replacing the $i$ in the coefficient with $i-1$, $a |\psi_i> = \sqrt{i \hbar \omega} |\psi_{i-1}>$
(i) We know that any wavefunction has to be continuous. The second derivative in the Schrödinger equation cannot be calculated at points where the wavefunction is not continuous.

\[
\Psi(x) = \int \Psi(x) \, dx.
\]

(ii) For the first derivative of the wavefunction, integrate the Schrödinger equation:

\[
-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) + V(x) \Psi(x) = E \Psi(x) \Rightarrow -\frac{\hbar^2}{2m} \frac{d}{dx} \left[ \frac{d}{dx} \Psi(x) \right]_{x=\pm \epsilon} + \int_{-\epsilon}^{\epsilon} V(x) \Psi(x) \, dx = E \int_{-\epsilon}^{\epsilon} \Psi(x) \, dx
\]

\[
\Rightarrow -\frac{\hbar^2}{2m} \left[ \frac{d}{dx} \Psi(x) \right]_{x=\pm \epsilon} = 0 \quad \text{(i.e. } \frac{d}{dx} \Psi(x) \text{ is continuous)}
\]

if \( V(x) \) is continuous so that \( \int_{-\epsilon}^{\epsilon} V(x) \Psi(x) \, dx = 0 \).

(iii) The first derivative of the wavefunction does not need to be continuous at points where \( V(x) \) is infinite. At points where \( V(x) \) is infinite,

\[
\int_{-\epsilon}^{\epsilon} V(x) \Psi(x) \, dx \neq 0
\]

Example is particle in a box:

\[
\begin{bmatrix}
0 & 0 & \sqrt{3}\hbar \omega & 0 & 0 \\
0 & 0 & 0 & \sqrt{2}\hbar \omega & 0 \\
0 & 0 & 0 & 0 & \sqrt{\hbar \omega} \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

E. Delta function potential

Wavefunction is not continuous at these two points.
(iv) Consider a delta function potential at $x=0$:

$$V(x) = -\alpha \delta(x)$$

(v) We should now know that the first derivative of the wavefunction will not be continuous at $x=0$. Instead, at $x=0$:

$$\begin{align*}
-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) - \alpha \delta(x) \Psi(x) &= E \Psi(x) \\
\Rightarrow -\frac{\hbar^2}{2m} \left[ \frac{d}{dx} \Psi(x) \right]^{+\varepsilon}_{-\varepsilon} + \int_{-\varepsilon}^{+\varepsilon} \alpha \delta(x) \Psi(x) dx &= E \int_{-\varepsilon}^{+\varepsilon} \Psi(x) dx \\
\Rightarrow -\frac{\hbar^2}{2m} \left[ \frac{d}{dx} \Psi(x) \right]^{+\varepsilon}_{-\varepsilon} &= \alpha \Psi(0) \\
\Rightarrow \Psi'(+\varepsilon) - \Psi'(-\varepsilon) &= -\frac{2m\alpha}{\hbar^2} \Psi(0)
\end{align*}$$

(vi) We can now solve the Schroedinger equation with the above boundary conditions. First consider the bound state situation:

At any point $x \neq 0$, $V(x) = 0$:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) = E \Psi(x) \Rightarrow -\frac{d^2}{dx^2} \Psi(x) = -\frac{2mE}{\hbar^2} \Psi(x)$$

Case 1. Bound state ($E < 0$)

$$\frac{d^2}{dx^2} \Psi(x) = \kappa^2 \Psi(x) \quad \text{where} \quad \kappa^2 = -\frac{2mE}{\hbar^2}$$

$$\Rightarrow \Psi(x) = Ae^{\kappa x} + Be^{-\kappa x}$$

For $\Psi(x)$ to be integrable:

$$\Psi(x) = \begin{cases} 
\Psi_1(x) = Ce^{\kappa x} & x < 0 \\
\Psi_2(x) = De^{-\kappa x} & x > 0
\end{cases}$$
\[ \Psi \text{ is continuous at } x = 0 \Rightarrow \Psi_1(0) = \Psi_2(0) \Rightarrow C = D \]

\[ \therefore \Psi(x) = \begin{cases} 
\Psi_1(x) = Ce^{\kappa x} & x < 0 \\
\Psi_2(x) = Ce^{-\kappa x} & x > 0 
\end{cases} \]

C is determined by normalization:

\[ \int_{-\infty}^{\infty} |\Psi(x)|^2 \, dx = 1 \Rightarrow \int_{-\infty}^{0} |Ce^{\kappa x}|^2 \, dx + \int_{0}^{\infty} |Ce^{-\kappa x}|^2 \, dx = 1 \]

\[ \Rightarrow 2\int_{0}^{\infty} C^2 e^{-2\kappa x} \, dx = 1 \]

\[ \Rightarrow 2C^2 \left[ -\frac{1}{2\kappa} e^{-2\kappa x} \right]_{0}^{\infty} = 1 \]

\[ \Rightarrow \frac{C^2}{\kappa} = 1 \Rightarrow C = \sqrt{\kappa} \]

\[ \therefore \Psi(x) = \begin{cases} 
\Psi_1(x) = \sqrt{\kappa} e^{\kappa x} & x < 0 \\
\Psi_2(x) = \sqrt{\kappa} e^{-\kappa x} & x > 0 
\end{cases} \]

Now \( \kappa \) cannot take any value because of the boundary condition:

\[ \Psi'(x) = \begin{cases} 
\Psi_1'(x) = \sqrt{\kappa} k e^{\kappa x} & x < 0 \\
\Psi_2'(x) = -\sqrt{\kappa} k e^{-\kappa x} & x > 0 
\end{cases} \]

\[ \Psi'(+) - \Psi'(-) = -\frac{2m\alpha}{\hbar^2} \Psi(0) \Rightarrow (\sqrt{\kappa} k) - (-\sqrt{\kappa} k) = -\frac{2m\alpha}{\hbar^2} \sqrt{\kappa} \]

\[ \Rightarrow \kappa = -\frac{m\alpha}{\hbar^2} \sqrt{\kappa} \]

(vii) There is only one bound state for delta function potential, no matter what is the value of \( \alpha \). In other word, there is only one eigenfunction with \( E < 0 \) in the Hilbert space that can satisfy the boundary conditions required by the delta function potential.
\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) = E\Psi(x) \Rightarrow -\frac{\hbar^2}{2m} \kappa^2 \Psi(x) = E\Psi(x) \]
\[ \Rightarrow E = -\frac{\hbar^2}{2m} \kappa^2 \]
\[ \Rightarrow E = -\frac{\hbar^2}{2m} \frac{m^2 \alpha^2}{\hbar^4} \]
\[ \Rightarrow E = -\frac{m \alpha^2}{2\hbar^2} \]

This is the energy of the bound state. As expected, the energy is negative.

(ix) Now consider the continuous case \((E > 0)\).

At any point \(x \neq 0\), \(V(x) = 0\):
\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) = E\Psi(x) \Rightarrow \frac{d^2}{dx^2} \Psi(x) = -\frac{2mE}{\hbar^2} \Psi(x) \]

Case 2. Scattering states \((E > 0)\)
\[ \frac{d^2}{dx^2} \Psi(x) = -k^2 \Psi(x) \quad \text{where} \quad k^2 = \frac{2mE}{\hbar^2} \]
\[ \Rightarrow \Psi(x) = Ae^{ikx} + Be^{-ikx} \]
\[ \Rightarrow \Psi(x) = \begin{cases} 
\Psi_I(x) = Ae^{ikx} + Be^{-ikx} & x < 0 \\
\Psi_II(x) = Fe^{ikx} + Ge^{-ikx} & x > 0 
\end{cases} \]
Continuity at \(x = 0\):
\(\Psi_I(0) = \Psi_II(0) \Rightarrow A + B = F + G\)
Now consider the discontinuity of \(\Psi'(x)\) at \(x = 0\):
\[ \Psi'(x) = \begin{cases} 
\Psi'_I(x) = Ai e^{ikx} - Bi e^{-ikx} & x < 0 \\
\Psi'_II(x) = Fi e^{ikx} - Gi e^{-ikx} & x > 0 
\end{cases} \]
\[ \Psi'(x^+) - \Psi'(x^-) = -\frac{2m\alpha}{\hbar^2} \Psi(0) \Rightarrow (Fik - Gik) - (Aik - Bik) = -\frac{2m\alpha}{\hbar^2} (A + B) \]
\[ \Rightarrow F - G = A \left(1 - \frac{2m\alpha}{i\hbar^2} \right) - B \left(1 + \frac{2m\alpha}{i\hbar^2} \right) \]
\[ \Rightarrow F - G = A \left(1 + \frac{i2m\alpha}{\hbar^2} \right) - B \left(1 - \frac{i2m\alpha}{\hbar^2} \right) \]
\[ \Rightarrow F - G = A(1 + 2i\beta) - B(1 - 2i\beta) \quad \text{where} \quad \beta = \frac{m\alpha}{\hbar^2} \]
(x) There are two boundary conditions for the coefficients to follow, and then there is one normalization condition. There are a total of four undetermined coefficients, so we have the freedom to assign one arbitrarily.

(xi) There are four components involved in the above solution. Physical meaning of these components:

\[
\begin{align*}
A e^{i\kappa x} & \quad \longrightarrow \quad Fe^{i\kappa x} \\
B e^{-i\kappa x} & \quad \longleftrightarrow \quad Ge^{-i\kappa x}
\end{align*}
\]

(xii) In here, we can assume the wave is incoming to the potential from the left and “arbitrarily” choose \( G = 0 \). Under this assumption:

\[ A + B = F \]

\[ F = A(1 + 2i\beta) - B(1 - 2i\beta) \]

\[
F = \frac{A}{1 - i\beta}, \quad \text{where} \quad \beta = \frac{m\alpha}{kh^2}
\]

Solving for \( F \):

\[ (1 - 2i\beta)F + F = (1 - 2i\beta)A + A(1 + 2i\beta) \Rightarrow 2(1 - i\beta)F = 2A \]

\[ \Rightarrow F = \frac{A}{1 - i\beta} \quad \text{(or} \quad \frac{1 + i\beta}{1 + \beta^2}A) \]

\[ A + B = A(1 + 2i\beta) - B(1 - 2i\beta) \Rightarrow 2B(1 - i\beta) = 2i\beta A \]

\[ \Rightarrow 2B(1 - i\beta) = \frac{i\beta}{(1 - i\beta)}A \quad \text{(or} \quad \frac{\beta^2 + i\beta}{1 + \beta^2}A) \]

(xiii) The reflection and transmission coefficients are defined as:

\[ R = \frac{B^2}{A^2} = \left| \frac{i\beta}{(1 - i\beta)} \right|^2 = \frac{\beta^2}{1 + \beta^2} = \frac{1}{1 + \frac{1}{\beta^2}} = \frac{1}{1 + \left( \frac{kh^2}{m\alpha} \right)^2} = \frac{1}{1 + \frac{k^2\hbar^4}{m^2\alpha^2}} = \frac{1}{1 + \frac{2E\hbar^2}{m\alpha^2}} \]

\[ T = \frac{F^2}{A^2} = \left| \frac{1}{1 - i\beta} \right|^2 = \frac{1}{1 + \beta^2} = \frac{1}{1 + \left( \frac{m\alpha}{kh^2} \right)^2} = \frac{1}{1 + \frac{m\alpha^2}{2E\hbar^2}} \]
Notes: (a) \( R+T=1 \)
(b) \( R \) and \( T \) depends on \( E \). The higher the energy, the smaller the \( R \) and the larger the \( T \). Does it make sense?

(xiv) We can define Transfer matrix \( M \) in relating the coefficients at right (\( F, G \)) to that at left (\( A, B \)):
\[
\begin{pmatrix} F \\ G \end{pmatrix} = M \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}
\]
In the case of delta potential:
\[
M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = \begin{pmatrix} 1+i\beta & i\beta \\ -i\beta & 1-i\beta \end{pmatrix}
\]
Properties of \( M \) for symmetric potential:
(a) \( \det(M)=1 \)
(b) \( M_{11}=M_{22}^* \)
(c) \( M_{12}=-M_{12}^* \) (i.e. pure impurity) = \( -M_{21}=M_{21}^* \) (i.e. \( M_{12} \) and \( M_{21} \) are conjugate of each other).

(xv) It is more appropriate to define another scattering matrix \( S \) as:
\[
\begin{pmatrix} B \\ F \end{pmatrix} = S \begin{pmatrix} A \\ G \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} A \\ G \end{pmatrix}
\]
This relates the outgoing waves (\( B \) and \( F \) after scattering) from the potential to the incoming waves (\( A \) and \( G \)).
In the case of delta potential:
\[
S = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} i\beta & 1 \\ 1-i\beta & 1+i\beta \\ 1 & 1-i\beta \\ 1-i\beta & 1+i\beta \end{pmatrix}
\]
Properties of \( S \) for symmetric potential:
(a) \( S^*S=1 \)
(b) \( S_{11}=S_{22} \)
(c) \( S_{12}=S_{12} \)

F. Finite square well

(i) \[
\begin{array}{c}
\begin{pmatrix} \text{I} \\ \text{II} \\ \text{III} \end{pmatrix}
\end{array}
\]
\[ V(x) = \begin{cases} -V_0 & -a < x < a \\ 0 & |x| > a \end{cases} \]

Note that the potential is symmetric in this problem. This introduces special properties to the energy eigen functions.

(ii) For symmetric potential \( V(x) = V(-x) \):

\[
-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) + V(x)\Psi(x) = E\Psi(x) \Rightarrow \quad -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(-x) + V(-x)\Psi(-x) = E\Psi(-x)
\]

\[
\Rightarrow -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(-x) + V(x)\Psi(-x) = E\Psi(-x)
\]

\( \because \) Both \( \Psi(x) \) and \( \Psi(-x) \) are solutions of the original Schrödinger equation of the same eigenvalue \( E \).

Case 1. Non-degenerate case: There is only one linear independent eigenfunction for eigenvalue \( E \).

\( \Psi(x) \) and \( \Psi(-x) \) must be linearly dependent of each other.

Let \( \Psi(-x) = \varepsilon \Psi(x) \)

Changing the sign of \( x \) \( \Rightarrow \) \( \Psi(x) = \varepsilon \Psi(-x) \)

\( \therefore \) \( \Psi(-x) = \varepsilon^2 \Psi(-x) \Rightarrow \varepsilon^2 = 1 \Rightarrow \varepsilon = \pm 1 \)

\( \Psi(x) \) is either even \( (\varepsilon = +1) \) or odd \( (\varepsilon = -1) \) function. This is a direct consequence of a symmetric potential.

Case 2. Degenerate case: There are more than one linear independent eigenfunction for eigenvalue \( E \).

Suppose \( \Psi_1(x) \) and \( \Psi_2(x) \) are two linearly independent solutions for the same eigenvalue \( E \).

These two may not be even or odd functions of \( x \). However, we can construct

\[ \Psi_+ (x) = \frac{1}{2} [\Psi_1 (x) + \Psi_2 (x)] \text{ and } \Psi_- (x) = \frac{1}{2} [\Psi_1 (x) - \Psi_2 (x)] \]

It is clear that

(i) \( \Psi_+ (x) \) and \( \Psi_- (x) \) are eigenfunctions with the same eigenvalue \( E \).

(ii) \( \Psi_+ (x) \) and \( \Psi_- (x) \) are linearly independent of each other.

(iii) \( \Psi_+ (x) \) is even and \( \Psi_- (x) \) is odd.

In summary:

If the potential is symmetric such that \( V(x) = V(-x) \), then the solution of the time independent Schrödinger equation must be even or odd for non-degenerate case, and can be even or odd for degenerate case.

(iii) Case 1 – bound state \( E < 0 \)
For $|x| > a$, $V(x) = 0$:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) = E\Psi(x) \Rightarrow \frac{d^2}{dx^2} \Psi(x) = -\frac{2mE}{\hbar^2} \Psi(x)$$

$$\Rightarrow \frac{d^2}{dx^2} \Psi(x) = \kappa^2 \Psi(x)$$

where $\kappa^2 = -\frac{2mE}{\hbar^2}$

$$\Rightarrow \Psi(x) = Ae^{\kappa x} + Be^{-\kappa x}$$

For $\Psi(x)$ to be integrable:

$$\Psi(x) = \begin{cases} \Psi_1(x) = Ae^{\kappa x} & x < -a \\ \Psi_2(x) = Be^{-\kappa x} & x > -a \end{cases}$$

[Since we know that $\Psi(-x) = \pm \Psi(x)$, hence $B = \pm A$]

For $-a < x < a$, $V(x) = -V_0$:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) - V_0 \Psi(x) = E\Psi(x) \Rightarrow \frac{d^2}{dx^2} \Psi(x) = -\frac{2m}{\hbar^2} (E + V_0) \Psi(x)$$

$$\Rightarrow \frac{d^2}{dx^2} \Psi(x) = -\ell^2 \Psi(x)$$

where $\ell = \sqrt{\frac{2m}{\hbar^2} (E + V_0)}$

We can either write the solution as

$$\Psi_1(x) = C e^{i\ell x} + D e^{-i\ell x}$$

or

$$\Psi_1(x) = C \cos \ell x + D \sin \ell x$$

Since we know that $\Psi(-x) = \pm \Psi(x)$, hence $\Psi_1(x)$ can only be $C \cos \ell x$ (even) or $D \sin \ell x$ (odd).

(iv) **Even solution**

$$\Psi_1(x) = A e^{\kappa x}$$

$$\Psi_2(x) = C \cos \ell x$$

$$\Psi_3(x) = A e^{-\kappa x}$$

Because the symmetric properties are included in the above solution, we just need to consider the boundary conditions at either $x = a$ or $x = -a$.

Continuity of $\Psi(x)$ at $x = a \Rightarrow A e^{\kappa a} = C \cos \ell a$ \hspace{1cm} (1)

Continuity of $\Psi'(x)$ at $x = a \Rightarrow -A \kappa e^{\kappa a} = -C \ell \sin \ell a$ \hspace{1cm} (2)

(2)/(1) $\Rightarrow \kappa = \ell \tan \ell a$

Let $\ell a = z \Rightarrow \sqrt{\frac{2m}{\hbar^2} (E + V_0)} a = z$ and $z_0 = \sqrt{\frac{2m}{\hbar^2} V_0} a$ (Note that $E$ is "inside" $z$)
\[ \kappa = \sqrt{\frac{-2m}{\hbar^2}} E = \sqrt{\left(\frac{z_0}{a}\right)^2 - \left(\frac{z}{a}\right)^2} = \frac{1}{a} \sqrt{z_0^2 - z^2} \]

\[ \kappa = \ell \tan \ell a \Rightarrow \frac{1}{a} \sqrt{z_0^2 - z^2} = \frac{z}{a} \tan z \Rightarrow \tan z = \sqrt{\left(\frac{z_0}{z}\right)^2} - 1 \]

This can be solved graphically:

(v) \text{ Odd solution }

\[ \Psi_1(x) = -A e^{\kappa x} \]
\[ \Psi_{\Pi}(x) = C \sin \ell x \]
\[ \Psi_{\text{III}}(x) = A e^{-\kappa x} \]

Continuity of \( \Psi_1(x) \) at \( x = a \) \( \Rightarrow \) \( A e^{-\kappa a} = C \sin \ell a \) \hspace{1cm} -(1)

Continuity of \( \Psi_1'(x) \) at \( x = a \) \( \Rightarrow \) \( -A \kappa e^{-\kappa a} = C \ell \cos \ell a \) \hspace{1cm} -(2)

(2)/(4) \( \Rightarrow \kappa = -\ell \cot \ell a \)

Let \( \ell a = z \Rightarrow \sqrt{\frac{2m}{\hbar^2}} (E + V_0) a = z \) and \( z_0 = \sqrt{\frac{2m}{\hbar^2}} V_0 a \) \hspace{1cm} (Note that E is "inside" z)

\[ \therefore \kappa = \sqrt{\frac{-2m}{\hbar^2}} E = \sqrt{\left(\frac{z_0}{a}\right)^2 - \left(\frac{z}{a}\right)^2} = \frac{1}{a} \sqrt{z_0^2 - z^2} \]

\[ \kappa = -\ell \cot \ell a \Rightarrow \frac{1}{a} \sqrt{z_0^2 - z^2} = \frac{z}{a} \cot z \Rightarrow \cot z = -\sqrt{\left(\frac{z_0}{z}\right)^2} - 1 \]

This can be solved graphically:
(iv) From these graphs, we can see:

(a) As $z_0$ (i.e. $V_0$) is increased, the red curve will be pulled taller and wider at the same time.
(b) The number of bound states depends on the value of $z_0$ (i.e. $V_0$). The deeper the well (i.e. larger $V_0$), the more bound states are there.
(c) For very shallow well (i.e. small $z_0$ when $z_0 < \pi/2$), there will be only one bound state. However, no matter how shallow is the will, there will be at least one bound state. As $z_0 \to 0$ (i.e. $V_0 \to 0$), there is still one bound state with $E \to 0$.
(d) As $z_0 \to \infty$ (i.e. $V_0 \to \infty$), the well become infinite.

Even solution:

$$\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1} \Rightarrow \tan z = \frac{z_0}{z} \quad \text{(large } z_0 \text{)}$$

$$\Rightarrow z \approx \frac{n\pi}{2} \quad \text{(odd } n \text{)}$$

Odd solution:

$$\cot z = -\sqrt{\left(\frac{z_0}{z}\right)^2 - 1} \Rightarrow \cot z = -\frac{z_0}{z} \quad \text{(large } z_0 \text{)}$$

$$\Rightarrow \cot z \approx m\pi$$

$$\Rightarrow z \approx \frac{n\pi}{2} \quad \text{(even } n \text{)}$$
\[ z = \sqrt{\frac{2m}{\hbar^2}(E + V_0)} \quad a \Rightarrow \frac{2m}{\hbar^2}(E + V_0) \approx \frac{n^2 \pi^2}{(2a)^2} \]

\[ \Rightarrow E \approx \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2} - V_0 \]

This is the same as our previous results on infinite square well of width 2a:
(a) \( n \) takes odd integers for even solution, even integers for odd solution.
(b) The energy value is pressed down by an amount of \( V_0 \) as expected.

(vi) Case 2 – continuous state \( E > 0 \)

Solution for \( \Psi(x) \):

\[ \Psi(x) = \begin{cases} 
\Psi_1(x) = Ae^{ikx} + Be^{-ikx} & x < -a \\
\Psi_2(x) = Ce^{i\xi x} + De^{-i\xi x} & -a < x < a \\
\Psi_3(x) = Fe^{ikx} + Ge^{-ikx} & x > a
\end{cases} \]

where \( \ell = \sqrt{\frac{2m}{\hbar^2}(E + V_0)} \) and \( k = \sqrt{\frac{2m}{\hbar^2}E} \)

\[ \Psi_1'(-a) = \Psi_2(-a) \Rightarrow Ce^{-i\xi a} + De^{-i\ell a} = Ae^{-ika} + Be^{ika} \quad - - (1) \]

\[ \Psi_1'(-a) = \Psi_2'(-a) \Rightarrow Ci\ell e^{-i\xi a} - Di\ell e^{-i\ell a} = Ai\ell e^{-ika} - Bi\ell e^{ika} \quad - - (2) \]

(1) \( \times i\ell + (2) \Rightarrow 2Ci\ell e^{-i\xi a} = Ai(k + \ell)e^{-ika} + Bi(\ell - k)e^{ika} \]

\[ \Rightarrow C = \frac{1}{2} A(1 + \frac{k}{\ell})e^{i(k+\ell)a} + \frac{1}{2} B(1 - \frac{k}{\ell})e^{i(k+\ell)a} \quad - - (3) \]

(1) \( \times i\ell - (2) \Rightarrow 2Di\ell e^{-i\xi a} = Ai(\ell - k)e^{-ika} + Bi(\ell + k)e^{ika} \]

\[ \Rightarrow D = \frac{1}{2} A(1 - \frac{k}{\ell})e^{-i(k+\ell)a} + \frac{1}{2} B(1 + \frac{k}{\ell})e^{-i(k+\ell)a} \quad - - (4) \]

(3) and (4) \( \Rightarrow \begin{pmatrix} C \\ D \end{pmatrix} = \frac{1}{2} \begin{pmatrix} (1 + \frac{k}{\ell})e^{i(k+\ell)a} & (1 - \frac{k}{\ell})e^{i(k+\ell)a} \\ (1 - \frac{k}{\ell})e^{-i(k+\ell)a} & (1 + \frac{k}{\ell})e^{-i(k+\ell)a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \quad - - (5) \]

Now consider continuity conditions at \( x = a \):

\[ \Psi_2(a) = \Psi_3(a) \Rightarrow Fe^{ika} + Ge^{-ika} = Ce^{i\xi a} + De^{-i\ell a} \quad - - (6) \]

\[ \Psi_2'(a) = \Psi_3'(a) \Rightarrow Ci\ell e^{ika} - Di\ell e^{-ika} = Ci\ell e^{i\xi a} - Di\ell e^{-i\ell a} \quad - - (7) \]

(6) \( \times ik + (7) \Rightarrow 2Fi\ell e^{ika} = Ci(k + \ell)e^{i\xi a} + Di(k - \ell)e^{-i\ell a} \]

\[ \Rightarrow F = \frac{1}{2} C(1 + \frac{\ell}{k})e^{i(\ell + k)a} + \frac{1}{2} D(1 - \frac{\ell}{k})e^{-i(\ell + k)a} \quad - - (8) \]

(6) \( \times ik - (7) \Rightarrow 2Gike^{-ika} = Ci(k - \ell)e^{i\xi a} + Di(k + \ell)e^{-i\ell a} \]

\[ \Rightarrow G = \frac{1}{2} C(1 - \frac{\ell}{k})e^{i(\ell - k)a} + \frac{1}{2} D(1 + \frac{\ell}{k})e^{-i(\ell - k)a} \quad - - (9) \]

(8) and (9) \( \Rightarrow \begin{pmatrix} F \\ G \end{pmatrix} = \frac{1}{2} \begin{pmatrix} (1 + \frac{\ell}{k})e^{i(\ell + k)a} & (1 - \frac{\ell}{k})e^{-i(\ell + k)a} \\ (1 - \frac{\ell}{k})e^{i(\ell - k)a} & (1 + \frac{\ell}{k})e^{-i(\ell - k)a} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \quad - - (10) \]
(5) & (10) \[ \begin{pmatrix} F \\ G \end{pmatrix} = M \begin{pmatrix} A \\ B \end{pmatrix} \]

\[
M = \frac{1}{2} \begin{pmatrix} (1 + \frac{\ell}{k})e^{i(\ell-k)a} & (1 - \frac{\ell}{k})e^{-i(\ell-k)a} \\ (1 - \frac{\ell}{k})e^{i(\ell+k)a} & (1 + \frac{\ell}{k})e^{-i(\ell+k)a} \end{pmatrix} \cdot \frac{1}{2} \begin{pmatrix} (1 + \frac{k}{\ell})e^{i(\ell-k)a} & (1 - \frac{k}{\ell})e^{-i(\ell-k)a} \\ (1 - \frac{k}{\ell})e^{-i(\ell+k)a} & (1 + \frac{k}{\ell})e^{i(\ell+k)a} \end{pmatrix}
\]

\[
= \frac{1}{4} \begin{pmatrix} (1 + \frac{\ell}{k})(1 + \frac{k}{\ell})e^{2i(\ell-k)a} + (1 - \frac{\ell}{k})(1 - \frac{k}{\ell})e^{-2i(\ell-k)a} & (1 + \frac{\ell}{k})(1 - \frac{k}{\ell})e^{2i(\ell+k)a} + (1 - \frac{\ell}{k})(1 + \frac{k}{\ell})e^{-2i(\ell+k)a} \\ (1 - \frac{\ell}{k})(1 + \frac{k}{\ell})e^{2i(\ell+k)a} + (1 + \frac{\ell}{k})(1 - \frac{k}{\ell})e^{-2i(\ell+k)a} & (1 + \frac{\ell}{k})(1 - \frac{k}{\ell})e^{2i(\ell-k)a} + (1 - \frac{\ell}{k})(1 + \frac{k}{\ell})e^{-2i(\ell-k)a} \end{pmatrix}
\]

Let \( \eta = \frac{\ell}{k} + \frac{k}{\ell} \) and \( \epsilon = \frac{k}{\ell} - \frac{\ell}{k} \)

\[
M = \frac{1}{4} \begin{pmatrix} (2 + \eta)e^{2i(\ell-k)a} + (2 - \eta)e^{-2i(\ell-k)a} & -\epsilon e^{2i\ell a} + \epsilon e^{-2i\ell a} \\ \epsilon e^{-2i\ell a} - \epsilon e^{2i\ell a} & (2 - \eta)e^{2i(\ell+k)a} + (2 + \eta)e^{-2i(\ell+k)a} \end{pmatrix}
\]

\[
= \begin{pmatrix} \cos 2\ell a + \frac{\eta}{2}\sin 2\ell a \ e^{-2ka} & -\frac{i\epsilon}{2}\sin 2\ell a \\ \frac{i\epsilon}{2}\sin 2\ell a & \cos 2\ell a - \frac{\eta}{2}\sin 2\ell a \ e^{2ka} \end{pmatrix}
\]

Note this satisfy the following properties of M:

(a) \( \det(M) = 1 \)
(b) \( M_{11} = M_{22}^* \)
(c) \( M_{12} = -M_{12}^* \) (i.e. pure impurity) = - \( M_{21} = M_{21}^* \) (i.e. \( M_{12} \) and \( M_{21} \) are conjugate of each other).

\( R \) and \( T \) can be determined from \( M \) by putting \( G = 0 \):

\[
F = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \Rightarrow \begin{cases} F = M_{11}A + M_{12}B \\ M_{12}A + M_{22}B = 0 \end{cases}
\]

\( M_{21}A + M_{22}B = 0 \) \Rightarrow \( \frac{B}{A} = -\frac{M_{21}}{M_{22}} \)

\[
R = \left| \frac{B}{A} \right|^2 = \left| \frac{M_{21}}{M_{22}} \right|^2
\]

\[
F = M_{11}A + M_{12}B \Rightarrow \frac{F}{A} = M_{11} + M_{12} \frac{B}{A}
\]

\[
\Rightarrow \frac{F}{A} = M_{11} - M_{12} \frac{M_{21}}{M_{22}}
\]
\[ \therefore T = \left| \frac{F}{A} \right|^2 = \left| M_{11} - M_{12} \frac{M_{21}}{M_{22}} \right|^2 \]

Now plug in the details:

\[
R = \left| \frac{M_{21}}{M_{22}} \right|^2 = \left( \frac{i\varepsilon}{2} \frac{\sin 2\ell a}{\cos 2\ell a - i\frac{\eta}{2} \sin 2\ell a} \right)^2 \frac{\varepsilon^2 \sin^2 2\ell a}{4 \cos^2 2\ell a + \eta^2 \sin^2 2\ell a}
\]

\[
T = \left| M_{11} - M_{12} \frac{M_{21}}{M_{22}} \right|^2 = \left( \frac{\cos 2\ell a + i\frac{\eta}{2} \sin 2\ell a}{\cos 2\ell a - i\frac{\eta}{2} \sin 2\ell a} \right)^2 \frac{i\varepsilon}{2} \frac{\sin 2\ell a}{\cos^2 2\ell a + \frac{\eta^2}{4} \sin^2 2\ell a}
\]

Note that \( \eta = \frac{\ell}{k} + \frac{k}{\ell} \) and \( \varepsilon = \frac{k}{\ell} - \frac{\ell}{k} \Rightarrow \eta^2 - \varepsilon^2 = 4 \)

\[
\therefore T = \frac{\left( \cos^2 2\ell a + \sin^2 2\ell a \right)^2}{\cos^2 2\ell a + \frac{\eta^2}{4} \sin^2 2\ell a} = \frac{1}{\cos^2 2\ell a + \frac{\eta^2}{4} \sin^2 2\ell a} = \frac{4}{4 \cos^2 2\ell a + (4 + \varepsilon^2) \sin^2 2\ell a} = \frac{1}{1 + \varepsilon^2 \sin^2 2\ell a}
\]

\[
T + R = \frac{4}{4 \cos^2 2\ell a + \eta^2 \sin^2 2\ell a} + \frac{\varepsilon^2 \sin^2 2\ell a}{4 \cos^2 2\ell a + \eta^2 \sin^2 2\ell a}
\]

\[
= \frac{4 + \varepsilon^2 \sin^2 2\ell a}{4 \cos^2 2\ell a + \eta^2 \sin^2 2\ell a}
\]

\[
= \frac{4 + \left( \frac{\eta^2}{4} - 4 \right) \sin^2 2\ell a}{4 \cos^2 2\ell a + \eta^2 \sin^2 2\ell a}
\]

\[
= \frac{4 \cos^2 2\ell a + \eta^2 \sin^2 2\ell a}{4 \cos^2 2\ell a + \eta^2 \sin^2 2\ell a} = 1
\]
Scattering matrix can be derived as follow:

\[
\begin{pmatrix}
F \\
G
\end{pmatrix}
= 
\begin{pmatrix}
M_{11} & M_{12} \\
M_{21} & M_{22}
\end{pmatrix}
\begin{pmatrix}
A \\
B
\end{pmatrix}
\]

\[F = M_{11}A + M_{12}B \quad ---(1)\]

\[G = M_{21}A + M_{22}B \quad ---(2)\]

Write B and F in terms of A and G:

\[B = \frac{M_{21}}{M_{22}} A + \frac{1}{M_{22}} G \quad ---(2)\]

Substitute this into (1):

\[F = M_{11}A + M_{12}B = M_{11}A + M_{12}\left(\frac{M_{21}}{M_{22}} A + \frac{1}{M_{22}} G\right)\]

\[= \frac{M_{11}M_{22} - M_{12}M_{21}}{M_{22}} A + \frac{M_{12}}{M_{22}} G\]

\[= \frac{\text{det}(M)}{M_{22}} A + \frac{M_{12}}{M_{22}} G\]

\[= \frac{1}{M_{22}} A + \frac{M_{12}}{M_{22}} G \quad \text{(det}(M) = 1)\]

\[B = \begin{pmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{pmatrix}
\begin{pmatrix}
A \\
G
\end{pmatrix}\]

\[
\begin{pmatrix} F \\ B \end{pmatrix} = \begin{pmatrix}
S_{11} & S_{12} \\
S_{21} & S_{22}
\end{pmatrix}
\begin{pmatrix}
A \\
G
\end{pmatrix}
\]

Now plug in the details:

\[S = \begin{pmatrix}
\frac{M_{11}}{M_{22}} & \frac{1}{M_{22}} \\
\frac{1}{M_{22}} & \frac{M_{22}}{M_{22}}
\end{pmatrix}
= \frac{\epsilon^{-2\lambda a}}{\cos 2\lambda a - i \frac{\eta}{2} \sin 2\lambda a}
\begin{pmatrix}
\frac{i\epsilon}{2} \sin 2\lambda a & 1 \\
-\frac{i\epsilon}{2} \sin 2\lambda a & 1
\end{pmatrix}\]
(vii) Now look at

\[ T = \frac{1}{1 + \varepsilon^2 \sin^2 2\ell a} \]

T oscillates with \( a \), with a maximum when

\[ 2\ell a = n\pi \quad \text{ (n = integers)} \]

\( \ell \) is effectively the wave number of the wave within the well, let \( \ell = \frac{2\pi}{\lambda} \)

\[ \therefore 2\frac{2\pi}{\lambda} a = n\pi \Rightarrow n\lambda = 4a. \]

This corresponds to a constructive interference with a path difference of 4a.

- \( T \) is also energy dependence. When energy is small, there is a higher chance for the particle to get trapped by the well and less chance to be transmitted.