# SPECTRAL ANALYSIS OF 1-PARAMETER FAMILY NEWTON'S EQUIVALENT HAMILTONIAN WITH SQUARE WELL POTENTIALS

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Amornthep Tita

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# ABSTRACT


This thesis presents the aspect of alternative Hamiltonians, which are inequivalent to standard one (summation of kinetic and potential energy), yielding the same Newton's equation. These alternative Hamiltonians will be termed as *Newton-equivalent Hamiltonian (NEH)*. In this project a 1-parameter family Newton-equivalent Hamiltonians, which proposed by A.Degasperis and S.N.M. Ruijsenaars in 2001 [1], is studied. This 1-parameter family of NEH constructs from multiplicative case between variables $p$ and $x$ in 1-dimension. The property of NEH states that it recover to the standard Hamiltonian as a limit of parameter $c \to \infty$. Furthermore, in the context of quantum theory, the authors use canonical quantization to promote classical dynamical variables to quantum operators. Therefore, with appropriate ordering, a 1-parameter family Newton's equivalent quantum Hamiltonians (NEQH) is introduced. The parameter of NEQH is expressed in form of $\beta = 1/2mc$. These facts are already checked by Degasperis and Ruijsenaars in 2001 [1]. For our framework, by using NEQH to Schrödinger's equation, we analyzed the energy spectrum and the wavefunction of bound state with infinite quantum square well. Using continuity condition of wavefunction, we

found that the energy spectrum of system is a function of parameter $\beta$. In addition, we showed, in the limit case of parameter $\beta \to 0$, that the energy spectrum of NEQH will recover to standard case. Moreover, we also analyzed energy spectrum and wavefunction in bound state of finite square well with arbitrary deep well expressed as constant potential $V_0$. The energy spectrum of finite square well system is also depend on parameter $\beta$ for fixed any potential $V_0$. The exact solution of energy spectrum does not exist, because the equations for solving energy can be solved by graphical and numerical method. We obtained the energy spectrum for fixed any potential by using graphical method. Finally, we showed that, as the limit of $V_0 \to \infty$, the energy spectrum of finite square well will tent to infinite square well case.

# CHAPTER I

# INTRODUCTION

## 1.1 Background and motivation

In classical mechanical system motion of a particle, in one dimensional space, is described by the Newton's equation . For conservative system, potential $V(q)$ depend only on position $q$, the Newton's equation reads

$$m\ddot{q}(t) = -\frac{\partial V(q)}{\partial q}, \tag{1.1}$$

where $q$ is generalized coordinates, and $\ddot{q}$ is acceleration of a particle. Moreover, there exist frames of reference (inertial frame) which motion of a particle takes place. A reference frame on earth is a sufficient approximation to inertial frame. Integration (1.1) gives dynamics of a particle in time dependence coordinate $q(t)$ of a mass $m$ under influence $V(q)$. Obviously, the Newton's equation is a powerful tool to solve problems of motion. But, many problems in classical mechanics are easily analyzed by alternative methods. Such a method is contained in *Hamilton's principle*. This principle states that for every motion there is a well-defined function of coordinates $q$ and velocity $\dot{q}$ called Lagrangian $L$, such that the integral

$$S = \int_{t_1}^{t_2} L(q, \dot{q}, t)dt, \tag{1.2}$$

takes the extremum value. The requirement that $S$ satisfies Hamilton's principle gives second order differential equations which is called *Euler-Lagrange's equation*

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0. \tag{1.3}$$

For simple conservative system the Lagrangian, in this context is standard Lagrangian, has a simple form

$$L_E(q, \dot{q}) = \frac{1}{2}m\dot{q}^2 - V(q) = T - V, \tag{1.4}$$

where $T$ is the kinetic energy, and $V$ is their potential.

There is another method known as the Hamiltonian formulation. It describes the motion on a different perspective namely the motion is described in terms of first-order equations of motion. Moreover, these equations explain the behavior of the system in phase space whose coordinates are generalized coordinates $q$ and canonical momentum $p$. In general, the canonical momentum is not restricted to $m\dot{q}$, but it is introduced by the definition

$$p = \frac{\partial L(q, \dot{q}, t)}{\partial \dot{q}}. \tag{1.5}$$

The Hamiltonian $H(q, p, t)$ is generated by the Legendre transformation

$$H(q, p, t) = \dot{q}p - L(q, \dot{q}, t). \tag{1.6}$$

Hence, the requirement gives us Hamilton's canonical equations

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}. \tag{1.7}$$

Exactly, these two formulations lead the same Newton's equation (1.1). But, in 1887 a German Physicist name Hermann von Helmholtz investigated that the Lagrangian, which yield the same Newton equation, cannot be chosen uniquely [2, 3, 4]. In other words, we are able to find alternative Lagrangians apart form the standard one. This problem is known as " inverse problem of the calculus of variations ". According to the Euler-Lagrange's equation, the inverse problem studies a sufficient and necessary conditions for existence of an alternative Lagrangian yielding Newton's equation [5, 2].

Existence of alternative Lagrangians give rise alternative Hamiltonians, which not equal to standard one $H = p^2/2m + V(q)$, via Legendre transformation. However, another way to obtain alternative Hamiltonians yielding Newton's equation is that write down the Hamiltonian in form of Newton's equation

$$\frac{\partial^2 H}{\partial q \partial p}\frac{\partial H}{\partial p} - \frac{\partial^2 H}{\partial p^2}\frac{\partial H}{\partial q} = -\frac{1}{m}\frac{dV}{dq}. \tag{1.8}$$

An alternative Hamiltonians, which satisfy this equation (1.8), will be termed as "Newton's equivalent Hamiltonian (NEH)". Obviously, the standard Hamiltonian $H_E(q,p) = p^2/2m + V(q)$ is a solution of (1.8). But, solutions of (1.8) are not restricted to the standard one. This problem is firstly investigated by [6].

The example of NEH, as we show in Chapter II, is a 1-parameter family Newton equivalent Hamiltonians [1]. The potential of this NEH depend only on position. For a larger class of equations of motion with the force law depend on velocity and time, which called q-equivalence Hamiltonian, has been investigated in [7, 8].

In our framework, the multiplicative Hamiltonian which express in 1-parameter family yielding Newton's equation are studied. By using canonical quantization, with suitable ordering, the authors [1] introduced 1-parameter family Newton-equivalent Hamiltonians as quantum operator calling Newton-equivalent quantum Hamiltonians (NEQH). The multiplicative Lagrangian yielding Newton's equation was studied in detail by [9]. For the operators of q-equivalent Hamiltonian was studied by [10]. The 1-parameter family of Newton equivalent Hamiltonians in one dimensional Cartesian coordinate is expressed as

$$H_c(x,p) = 4mc^2 \cosh\left(\frac{p}{2mc}\right)\left(1 + \frac{V(x)}{2mc^2}\right)^{\frac{1}{2}} - 4mc^2, \tag{1.9}$$

where parameter $c \in (0, \infty)$. In limit of $c \to \infty$ this Hamiltonians will recover to standard Hamiltonian

$$\lim_{c\to\infty} H_c(x,p) = H_E(x,p). \tag{1.10}$$

In quantum mechanical system, we used canonical quantization to promote NEH as a function of quantum operator $\hat{x}$ and $\hat{p}$ satisfying the Heisenberg relation

$$[\hat{x}, \hat{p}] = i\hbar. \tag{1.11}$$

Then the NEH will become to quantum operator NEQH as

$$\begin{aligned}\hat{H}(\beta;\hat{x},\hat{p}) &= \frac{1}{2\beta^2 m}[(1+i\beta\sqrt{2mV(x)})^{1/2}\exp(-i\hbar\beta\frac{\partial}{\partial x})(1-i\beta\sqrt{2mV(x)})^{1/2} \\ &\quad +(1-i\beta\sqrt{2mV(x)})^{1/2}\exp(i\hbar\beta\frac{\partial}{\partial x})(1+i\beta\sqrt{2mV(x)})^{1/2}] - \frac{1}{\beta^2 m},\end{aligned} \tag{1.12}$$

where parameter $\beta = (2mc)^{-1}$ extend class of NEQH. We apply NEQH to Schrödinger's equation with infinite square well potential, and analyze discrete energy spectrum of this system for bound state. Finally we also analyze energy spectrum for finite square well system.

## 1.2 Objectives

We studied the 1-parameter family Newton equivalent Hamiltonians which proposed in paper *Newton-equivalent Hamiltonians for the Harmonic Oscillator* [1]. According to the paper, the authors presented discrete energy spectrum and wavefunction for Harmonic Oscillator system $V(x) = m\omega^2 x^2/2$. Thus, in our framework, we applied this 1-parameter family Newton's equivalent Hamiltonians to another systems i.e. infinite and finite square well potential. The aim of this thesis is to obtain discrete energy spectrum and wavefunction of both square well systems.

## 1.3 Frameworks

In chapter 1, we stated the introduction, motivation, objective, and frameworks of this thesis.

In chapter 2, we reviewed classical mechanical system which include topics of Lagrangian and Hamiltonian formulation, Legendre transformation, inverse problem, and canonical quantization. Moreover, we also mentioned 1-parameter family Newton's equivalent Hamiltonians in this chapter.

The review of standard Hamiltonian with infinite square well potential is mentioned in chapter 3. We exhibited the energy spectrum and wavefunction for this system.

In chapter 4, Energy spectrum and wavefunction of finite square well system with standard Hamiltonian are considered.

In chapter 5, we explained perturbation theory for non-degenerate system.

Result and discussion of NEQH of both infinite and finite square well are represented in chapter 6. We analyzed eigenvalue and eigenfunction of NEQH by using Schrödinger equation and discussed this energy spectrum in this chapter.

# CHAPTER II

# 1-PARAMETER FAMILY NEWTON'S EQUIVALENT HAMILTONIANS AND QUANTIZATION

As we have known for a long time. Newton's second law of motion gives a way to determine, how the motion of a particle change with arbitrary external force. The second law can be written as

$$\vec{F} = \frac{d\vec{p}}{dt} = m\vec{a}, \tag{2.1}$$

where momentum is defined as $\vec{p} = m\vec{v}$, and acceleration is $\vec{a} = d\vec{v}/dt$. Newton's second law (2.1) is powerful tool for solving problems in Cartesian coordinates, But it is difficult to change to different coordinate. To avoid this consideration new reformulations of classical mechanics, which called Lagrangian mechanics and Hamiltonian mechanics, are introduced. Such a methods are obtain in *Hamilton's principle* and the results are call *Euler-Lagrange's equation*. By using Legendre transformation, we obtain *Hamilton's equation*. The inverse problem mention about that Lagrangian is not unique. Idea of alternative Lagrangians and alternative Hamiltonians are arise. In this thesis, the 1-parameter family Newton's equivalent Hamiltonians are studied. Moreover, quantization of Hamiltonian are also studied.

## 2.1 Hamilton's principle and Euler-Lagrange's equation

Hamilton's principle is a formulation of the law of motion. It describes the motion of mechanical systems for which all forces are derivative of potential as a function of coordinates, velocities, and time. Hamilton's principle is considered more fundamental than Newton's equation. It can be stated as line integral or trajectory along configuration space from time $t_1$ to $t_2$ which is called "action" [11]

$$S(q(t)) = \int_{t_1}^{t_2} L(\dot{q}(t), q(t), t)dt, \tag{2.2}$$

where $L(\dot{q}, q, t)$ and $q(t)$ are the Lagrangian and generalized coordinates, respectively. The motion of system from time $t_1$ to the position at time $t_2$ in configuration space is actual path which has stationary value relative to neighboring paths. On the other hand, actual path is an extremum of action $S$ that is a function $q(t)$ gives the integral minimum (or maximum) value. This is based on a principle called *Hamilton's principle* or *least action principle.* In other words, in mathematical language, the Hamilton's principle states that the variation of action is zero

$$\delta S(q(t)) = \delta \int_{t_1}^{t_2} L(\dot{q}(t), q(t), t) dt = 0, \tag{2.3}$$

under the boundary condition, for fixed $t_1$ and $t_2$,

$$\delta q(t_1) = \delta q(t_2) = 0. \tag{2.4}$$

We require to find a particular path $q(t)$, for the action $S$ has a stationary value relative to some set of neighboring paths $\eta(t)$. A possible set of paths are given by

$$q(t, \alpha) = q(t, 0) + \alpha \eta(t), \tag{2.5}$$

where $q(t, 0)$ is the correct path, and $\alpha$ is infinitesimal parameter. Hence, the action is

$$S(\alpha) = \int_{t_1}^{t_2} L(\dot{q}(t, \alpha), q(t, \alpha), t) dt. \tag{2.6}$$

According to variation of action, we obtain

$$\delta S = \int_{t_1}^{t_2} \left( \frac{\partial L}{\partial q} \delta q + \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right) dt, \tag{2.7}$$

where $\delta q$ denote as $\partial q / \partial \alpha |_{\alpha=0} = \eta(t)$. Using integration by parts to the second term of (2.7) gives

$$\int_{t_1}^{t_2} \left( \frac{\partial L}{\partial \dot{q}} \delta \dot{q} \right) dt = \cancelto{0}{\left( \frac{\partial L}{\partial \dot{q}} \delta q \right) \Big|_{t_1}^{t_2}} - \int_{t_1}^{t_2} \left( \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \delta q \right) dt. \tag{2.8}$$

The first term of RHS vanishes at boundary. Thus, the equation (2.7) becomes

$$\delta S = \int_{t_1}^{t_2} \left( \frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right) \delta q dt. \tag{2.9}$$

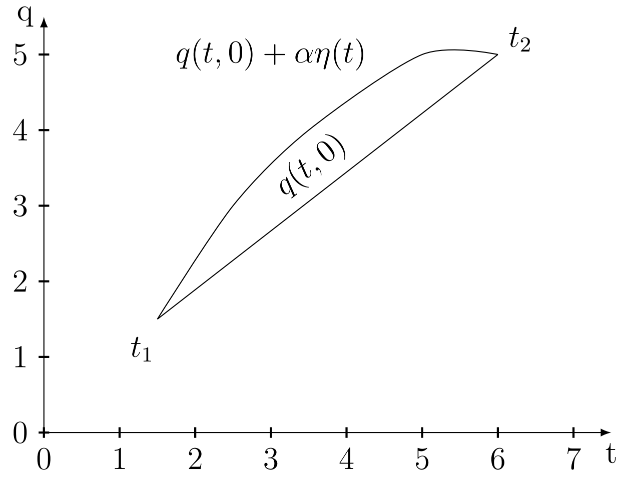


**Figure 1: The variation of a curve between fixed end points**

According to Hamilton's principle condition to obtain stationary point is $\delta S = 0$. Since $\delta q$ is arbitrary, therefore $S$ has stationary value where the equation

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0, \tag{2.10}$$

is valid. We obtain one degree of freedom Euler-Lagrange's equation (1.3) from Hamilton's principle [12, 13]. On the alternative structure of this theory, Hamiltonian $H = H(q, p, t)$ connect with Lagrangian $L = L(q, \dot{q}, t)$ via Legendre transformation.

## 2.2 Legendre transformation

Legendre transformation in classical mechanics is the procedure for changing Lagrangian to Hamiltonian corresponding to change the variables from $(q, \dot{q}, t)$ to $(q, p, t)$. The relationship between canonical momentum $p$ and $\dot{q}$ is $p = \partial L/\partial \dot{q}$. Therefore, the Hamiltonian $H(q, p, t)$ is generated by the Legendre transformation as[1]

$$H(q,p,t) = \dot{q}p - L(q,\dot{q},t). \tag{2.11}$$

Let us consider total differential of Lagrangian $L(q,\dot{q},t)$,

$$dL = \frac{\partial L}{\partial q}dq + \frac{\partial L}{\partial \dot{q}}d\dot{q} + \frac{\partial L}{\partial t}dt. \tag{2.12}$$

According to Euler-Lagrange's equation (1.3), by using canonical momentum $p = \partial L/\partial \dot{q}$, This gives

$$\dot{p} = \frac{\partial L}{\partial q}. \tag{2.13}$$

Hence, the total differential of Lagrangian $dL(q,\dot{q},t)$ becomes

$$dL = \dot{p}dq + pd\dot{q} + \frac{\partial L}{\partial t}dt. \tag{2.14}$$

Let us consider differential of (2.11) and substitute $dL(q,\dot{q},t)$. We obtain

$$\begin{aligned} dH &= \dot{q}dp + pd\dot{q} - dL(q,\dot{q},t), \\ &= \dot{q}dp + pd\dot{q} - \dot{p}dq - pd\dot{q} - \frac{\partial L}{\partial t}dt, \\ &= \dot{q}dp - \dot{p}dq - \frac{\partial L}{\partial t}dt. \end{aligned} \tag{2.15}$$

Comparing with total differential of Hamiltonian $H(q,p,t)$

$$dH = \frac{\partial H}{\partial q}dq + \frac{\partial H}{\partial p}dp + \frac{\partial H}{\partial t}dt, \tag{2.16}$$

we obtain the equations

$$\dot{q} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial q}, \qquad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}. \tag{2.17}$$

Since Hamiltonian is conserved, so the $3^{rd}$ equation of (2.17) vanish. Therefore, we get the Hamilton's equations (1.7) describing the motion in terms of first-order

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[1]Notice that the Hamiltonian (2.11) is only function of $(q,p,t)$. Let us consider derivative of $H$ with respect to $\dot{q}$,

$$\frac{dH(q,p,t)}{d\dot{q}} = p - \frac{dL(q,\dot{q},t)}{d\dot{q}} = 0,$$

where $p = dL(q,\dot{q},t)/d\dot{q}$. So, the Hamiltonian is not function of $\dot{q}$.

equation of motion. For simple conservative system, the Hamiltonian is automatically the total energy which express as summation of kinetic energy and potential energy, $H_E(q,p) = p^2/2m + V(q)$.

## 2.3 The inverse problem

Euler-Lagrange equation or Hamilton equations are lead to Newton equation where Lagrangian and Hamiltonian are function of $L = (1/2)m\dot{q}^2 - V(q)$ and $H = p^2/2m + V(q)$ respectively. But Helmholtz investigated that given equation of motion the Lagrangian cannot be chosen uniquely. It can be find alternative Lagrangians yielding Newton's equation which is knowns as "*the inverse problem of the calculus of variations*" [5]. The inverse problem identifies sufficient and necessary conditions for existence of alternative Lagrangian to admit a representation in Euler-Lagrange's equation. For classical mechanical system with one dimensional model, the paper [2] investigated that ambiguity in the choice of a Lagrangian always exist. Moreover, the inverse problem of phase space formulations lead to existence of an alternative Hamiltonian which connect to alternative Lagrangian via Legendre transformation.

In the context of alternative Hamiltonian yielding Newton's equation is constructed by representing acceleration $\ddot{q}$ as Poisson bracket of $\{\{q,H\},H\}$ with conservative potential [14]

$$\frac{\partial^2 H(q,p)}{\partial p \partial q}\frac{\partial H(p,q)}{\partial p} - \frac{\partial^2 H(p,q)}{\partial p^2}\frac{\partial H(q,p)}{\partial q} = -\frac{1}{m}\frac{dV(q)}{dq}. \tag{2.18}$$

Non-linear differential equation is obtained. Obviously, the standard Hamiltonian $H_E = p^2/2m + V(q)$ is a solution of (2.18). But, a solution of eq.(2.18) is not restricted to $H_E$. There are many solutions of $H$ which satisfy (2.18) to describe the same classical motions. To study quantum theory Hamiltonian will be quantized to quantum observable $\hat{H}$. Canonical quantization, which promotes a canonical variables $(q, p)$ to quantum observables $(\hat{q}, \hat{p})$, are studied.

## 2.4 Canonical quantization

*The correspondence principle* states that classical mechanics must be a limiting case of quantum mechanics. The important concepts in classical must reappear in quantum theory. The fundamental relation in quantum mechanics is commutation relation of an observable. Let $\hat{A}$ and $\hat{B}$ be observables. The commutation relation between $\hat{A}$ and $\hat{B}$ is

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}. \tag{2.19}$$

The observable in quantum mechanics associate with measurement of a system. In general, by effect of uncertainty principle, these two observable are not commute

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \neq 0. \tag{2.20}$$

According to correspondence principle, the structure of commutation relation in quantum mechanics is analog to Poisson bracket in classical mechanics. The method to promote classical mechanics to quantum one associated with Poisson bracket is called *canonical quantization*. The Poisson bracket (P.B.) of any two dynamical variables $u, v$ is given by

$$\{u, v\} = \frac{\partial u}{\partial q}\frac{\partial v}{\partial p} - \frac{\partial u}{\partial p}\frac{\partial v}{\partial q}, \tag{2.21}$$

where $u$ and $v$ are function of canonical coordinates and momentum. One of the properties of P.B. is

$$\{u, v_1 v_2\} = \{u, v_1\}v_2 + v_1\{u, v_2\}. \tag{2.22}$$

Let us introduce a quantum P.B. which be analog of classical mechanics. Assuming that dynamical variables are not commute. Evaluation of the P.B. $\{u_1 u_2, v_1 v_2\}$ in two different ways gives

$$\begin{aligned}\{u_1u_2, v_1v_2\} &= \{u_1, v_1v_2\}u_2 + u_1\{u_2, v_1v_2\}, \\ &= \{u_1, v_1\}v_2u_2 + v_1\{u_1, v_2\}u_2 + u_1\{u_2, v_1\}v_2 + u_1v_1\{u_2, v_2\},\end{aligned} \tag{2.23}$$

and

$$\begin{aligned}\{u_1u_2, v_1v_2\} &= \{u_1u_2, v_1\}v_2 + v_1\{u_1u_2, v_2\}, \\ &= \{u_1, v_1\}u_2v_2 + u_1\{u_2, v_1\}v_2 + v_1\{u_1, v_2\}u_2 + v_1u_1\{u_2, v_2\}.\end{aligned} \tag{2.24}$$

Equating these two solution, we get

$$\{u_1, v_1\}(u_2v_2 - v_2u_2) = (u_1v_1 - v_1u_1)\{u_2, v_2\}. \tag{2.25}$$

For the condition of quantum P.B. are not commute, and the condition of $u_1$ and $v_1$ are independently to $u_2$ and $v_2$. We get

$$\begin{aligned}u_1v_1 - v_1u_1 &= i\hbar\{u_1, v_1\}, \\ u_2v_2 - v_2u_2 &= i\hbar\{u_2, v_2\},\end{aligned} \tag{2.26}$$

where $\hbar$ neither depend on $u_1$ and $v_1$ nor $u_2$ and $v_2$ and should be a real (hermitian[2]). We require the Poisson bracket of any two real variables $u_1, u_2$ to be real. In general value of $u_1u_2$ is not real[3] and this fact also true for $v_1v_2$ [15]. For P.B. of two real variable to be real, coefficient "$i$" must appear in (2.26). Hence, we are led to

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[2]Hermitian operator is an operator which gives real eigenvalue

[3]If $\hat{A}$ and $\hat{B}$ are hermitian, hermitian conjugate of $(\hat{A}\hat{B})^\dagger$ gives eigenvalue not real. Let us consider

$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger = \hat{A}\hat{B} + [\hat{B}, \hat{A}],$$

in general $[\hat{B}, \hat{A}] \neq 0$, $\hat{A}\hat{B}$ is not hermitian.

following definition of the quantum P.B. (commutation relation) introduced by operator $\hat{u}$ and $\hat{v}$,

$$[\hat{u}, \hat{v}] = \hat{u}\hat{v} - \hat{v}\hat{u} = i\hbar\{u, v\}. \tag{2.27}$$

Let us consider the commutation relation involving the canonical momentum and generalized coordinates. For simplicity, we will consider in one dimensional Cartesian coordinate ($q = x$). Then (2.27) will become

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar\{x, p\} = i\hbar, \tag{2.28}$$

where the P.B. of $\{x, p\}$ is 1. According to Schrödinger's representation, $p$ and $x$ are promoted to quantum operator namely $\hat{x} = x$ $\hat{p} = -i\hbar\frac{\partial}{\partial x}$. The commutation relation (2.28) reads

$$\begin{aligned} [\hat{x}, \hat{p}]\psi(x) &= \hat{x}\hat{p}\psi(x) - \hat{p}\hat{x}\psi(x), \\ &= x(-i\hbar\frac{\partial\psi(x)}{\partial x}) - (-i\hbar\frac{\partial(x\psi(x))}{\partial x}), \\ &= -i\hbar x\frac{\partial\psi(x)}{\partial x} + i\hbar x\frac{\partial\psi(x)}{\partial x} + i\hbar\psi(x), \\ &= i\hbar\psi(x), \end{aligned} \tag{2.29}$$

where $\psi(x)$ is arbitrary function of $x$. Therefore, analog from classical theory to quantum one, we promote classical dynamical variables to quantum operators which satisfies the equation (2.28).

In the present day, we know that constructions of quantum systems without the classical analog are very difficult. Let us consider Dirac's statement [15, 16] "*classical mechanics must be limiting case of quantum mechanics.*" However, many papers exhibit that an alternative Hamiltonians give rise the canonically inequivalent structure of Poisson bracket. For this situation, noncanonical quantization are introduced for example in [17, 18].

One idea of noncanonical quantization was proposed by Wigner on the paper "*Do the equation of motion determine the quantum mechanical commuta-*

*tion relations?* [19]". Wigner notice that in suitable limit, which the alternative structure in quantum mechanics provide alternative structure available in classical mechanics? In other words, to describe in quantum framework, is it possible to show analog of alternative Hamiltonian? Wigner followed this idea and showed in [19] that compatibility with equation of motion, the quantum commutation relation are not unique. Wigner identified $H$ as the time evolution generator together with Newton's equation for harmonic oscillator. He analyzed the problem of quantum harmonic oscillator by set up the relation calling *Wigner's quantization*

$$\hat{v} = \frac{i}{\hbar}[\hat{H}, \hat{x}], \qquad -\omega^2 \hat{x} = \frac{i}{\hbar}[\hat{H}, \hat{v}], \qquad [\hat{x}, \hat{v}] = \frac{i\hbar}{m} F(\hat{H}), \tag{2.30}$$

where $F(\hat{H})$ is arbitrary function.

There are many papers to study system of inequivalent classical Hamiltonian by using noncanonical quantization. For example, the paper [20] studied about noncanonical one-dimensional harmonic oscillator. Paper [21] considered the quantization of Newton-equivalent Hamiltonians yielding the Newton's equation. From [22] studied about some of the algebraic structure that are compatible with the quantization of harmonic oscillator through its Newton equation. Inequivalent Hamiltonians exist for damped harmonic oscillator which make quantization of system ambiguous [23].

## 2.5 1-parameter family Newton's equivalent Hamiltonian

Let us consider the question: what are the other solutions of Hamiltonian yielding Newton's equation (1.1) with arbitrary force? To answer this question, let us consider Poisson bracket of velocity $\dot{x}$ in Cartesian coordinate [20],

$$\{\dot{x}, H\} = \ddot{x} = -\frac{1}{m}\frac{\partial V(x)}{\partial x}, \tag{2.31}$$

$$\frac{\partial \dot{x}}{\partial x}\frac{\partial H}{\partial p} - \frac{\partial \dot{x}}{\partial p}\frac{\partial H}{\partial x} = -\frac{1}{m}\frac{\partial V(x)}{\partial x}. \tag{2.32}$$

By using Hamilton's equation (1.7) the equation (2.32) reads

$$\frac{\partial^2 H}{\partial x \partial p}\frac{\partial H}{\partial p} - \frac{\partial^2 H}{\partial p^2}\frac{\partial H}{\partial x} + \frac{1}{m}\frac{\partial V(x)}{\partial x} = 0. \tag{2.33}$$

We obtain the non-linear differential equation. The standard Hamiltonian is a solution of (2.33) but a solution of (2.33) is not restricted to standard one. Let us consider another solution of equation (2.33) by using separation method in two cases i.e. additive case and multiplicative case, where $x$ and $p$ are independent variables.

In the first case, the Hamiltonian is additive:

$$H(x, p) = F(p) + G(x), \tag{2.34}$$

substituting (2.34) into (2.33) gives

$$-F''(p)G'(x) + \frac{1}{m}V'(x) = 0. \tag{2.35}$$

The function $p$ and $x$ are independent. So, the equation (2.35) is valid for

$$F''(p) = \frac{1}{m}\frac{V'(x)}{G'(x)} = 2A, \tag{2.36}$$

then

$$\begin{aligned} F''(p) &= 2A, \\ F'(p) &= 2Ap + B, \\ F(p) &= Ap^2 + Bp + C, \end{aligned} \tag{2.37}$$

where $A$ is arbitrary constant. We get $F(p)$ in the form of $Ap^2 + Bp + C$ with arbitrary constant $B$ and $C$. Therefore, $G(x)$ can be solved as follows

$$\begin{aligned} 2AG'(x) &= \frac{1}{m}V'(x), \\ \int G'(x)dx &= \int \frac{1}{2mA}V'(x)dx, \\ G(x) &= \frac{1}{2mA}V(x) + D. \end{aligned} \tag{2.38}$$

So, the solution (2.34) becomes

$$H(x,p) = Ap^2 + Bp + C + \frac{V(x)}{2mA} + D. \tag{2.39}$$

The solution (2.39) leads to the standard Hamiltonian $H_E(x,p)$ (1.7), for we choose the choice $A$, $B$,$C$, and $D$ as $A = 1/2m, B = C = D = 0$. This gives

$$H(x,p) = \frac{p^2}{2m} + V(x).$$

In the second case, let us consider the multiplicative case

$$H(x.p) = F(p)G(x). \tag{2.40}$$

Substituting (2.40) into (2.33) reads

$$\begin{aligned}
\frac{\partial^2(F(p)G(x))}{\partial x \partial p}\frac{\partial(F(p)G(x))}{\partial p} - \frac{\partial^2(F(p)G(x))}{\partial p^2}\frac{\partial(F(p)G(x))}{\partial x} + \frac{1}{m}\frac{\partial V(x)}{\partial x} &= 0, \\
\left(\frac{\partial G(x)F'(p)}{\partial x}\right)(G(x)F'(p)) - G(x)F''(p)F(p)G'(x) + \frac{1}{m}V'(x) &= 0, \\
G'(x)F'(p)^2G(x) - G(x)F(p)F''(p)G'(x) + \frac{1}{m}V'(x) &= 0.
\end{aligned}$$

Then (2.33) becomes

$$\left(F'(p)^2 - F''(p)F(p)\right)G'(x)G(x) + \frac{1}{m}V'(x) = 0. \tag{2.41}$$

This equation (2.41) is valid for term of nonlinear second order differential equation defined as $F'(p)^2 - F''(p)F(p) = -A$ where $A$ is constant. The solution of $F(p)$ can be solved as follows

$$\begin{aligned}
F'(p)^2 - F''(p)F(p) &= -A, \\
F'(p)^2 - F(p)\frac{dF'(p)}{dF}F'(p) &= -A, \\
F'(p)\left(F'(p) - F(p)\frac{dF'(p)}{dF}\right) &= -A, \\
F'(p) - F(p)\frac{dF'(p)}{dF} &= \frac{-A}{F'(p)}, \\
\left(F'(p) - F(p)\frac{dF'(p)}{dF}\right)\left(\frac{1}{F(p)^2}\right) &= \left(\frac{-A}{F'(p)}\right)\left(\frac{1}{F(p)^2}\right),
\end{aligned}$$

$$\begin{aligned}
\frac{d}{dF}\left(\frac{F'(p)}{F(p)}\right) &= \frac{A}{F'(p)/F(p)}\frac{1}{F(p)^3}, \\
\int\left(\frac{F'(p)}{F(p)}\right)d\left(\frac{F'(p)}{F(p)}\right) &= \int AF(p)^{-3}dF, \\
\left(\frac{F'(p)}{F(p)}\right)^2 &= -AF(p)^{-2}+C^2, \\
F'(p)^2 &= -A+C^2F(p)^2, \\
F'(p) &= \pm\sqrt{C^2F(p)^2-A},
\end{aligned}$$

setting $A=B^2$

$$\begin{aligned}
F'(p) &= \pm\sqrt{C^2F(p)^2-B^2}, \\
\int\frac{dF(p)}{\sqrt{C^2F(p)^2-B^2}} &= \pm\int dp, \\
\pm p &= \frac{1}{B}\int\frac{dF(p)}{\sqrt{\frac{C^2F(p)^2}{B^2}-1}}, \\
&= \frac{1}{B}\frac{B}{C}\int\frac{d(\frac{CF(p)}{B})}{\sqrt{(\frac{CF(p)}{B})^2-1}}, \\
&= \frac{1}{C}\int\frac{d(\frac{CF(p)}{B})}{\sqrt{(\frac{CF(p)}{B})^2-1}},
\end{aligned}$$

setting $\frac{CF(p)}{B}=\cosh\theta$

$$\pm p=\frac{1}{C}\int\frac{d(\cosh\theta)}{\sqrt{\cosh^2\theta-1}},$$

by using $\sinh^2\theta=\cosh^2\theta-1$,

$$\begin{aligned}
\pm Cp &= \int\frac{\sinh\theta d\theta}{\sinh\theta}, \\
\pm Cp &= \theta-D, \\
\theta &= \pm Cp+D, \\
\cosh^{-1}\left(\frac{CF(p)}{B}\right) &= \pm Cp+D, \\
\frac{CF(p)}{B} &= \cosh\left(\pm Cp+D\right),
\end{aligned}$$

using property of even function $\cosh(\pm\theta)=\cosh(\theta)$,

$$F(p) = \frac{B}{C}\cosh(Cp+D).$$

We define $\frac{B}{C} = c_1, C = c_2, D = c_3$, so the solution gives

$$F(p) = c_1 \cosh(c_2 p + c_3), \tag{2.42}$$

where $A = B^2 = c_1^2 c_2^2$. On the same way the negative of $A$, we get

$$F'(p) = \pm\sqrt{C^2 F(p)^2 - A},$$

setting $-A = B^2$,

$$\begin{aligned}
F'(p) &= \pm\sqrt{C^2 F(p)^2 + B^2}, \\
\int \frac{dF(p)}{\sqrt{C^2 F(p)^2 + B^2}} &= \pm \int dp, \\
\pm p &= \frac{1}{B} \int \frac{dF(p)}{\sqrt{\frac{C^2 F(p)^2}{B^2} + 1}}, \\
&= \frac{1}{B}\frac{B}{C} \int \frac{d(\frac{CF(p)}{B})}{\sqrt{(\frac{CF(p)}{B})^2 + 1}}, \\
&= \frac{1}{C} \int \frac{d(\frac{CF(p)}{B})}{\sqrt{(\frac{CF(p)}{B})^2 + 1}},
\end{aligned}$$

setting $\frac{CF(p)}{B} = \sinh\theta$,

$$\pm p = \frac{1}{C} \int \frac{d(\sinh\theta)}{\sqrt{\sinh^2\theta + 1}},$$

By using $\cosh^2\theta = \sinh^2\theta + 1$,

$$\begin{aligned}
\pm Cp &= \int \frac{\cosh\theta d\theta}{\cosh\theta}, \\
\pm Cp &= \theta - D, \\
\theta &= \pm Cp + D, \\
\sinh^{-1}\left(\frac{CF(p)}{B}\right) &= \pm Cp + D, \\
\frac{CF(p)}{B} &= \sinh\left(\pm Cp + D\right),
\end{aligned}$$

using property of odd function $\sinh(\pm\theta) = \pm\sinh(\theta)$,

$$F(p) = \pm\frac{B}{C}\sinh(Cp + D).$$

We define $\pm\frac{B}{C} = c_1, C = c_2, D = c_3$, so the solution gives

$$F(p) = c_1 \sinh(c_2 p + c_3), \tag{2.43}$$

where $A = -B^2 = -(\pm c_1 c_2)^2 = -c_1^2 c_2^2$. In either case, we deduce

$$\begin{aligned}
-AG(x)G'(x) + \frac{1}{m}V'(x) &= 0, \\
G'(x)G(x) &= \frac{1}{mA}V'(x), \\
\int G(x)dG(x) &= \frac{1}{mA}\int dV(x), \\
\frac{G^2(x)}{2} &= \frac{V(x)}{mA} + c_4, \\
G^2(x) &= \frac{2V(x)}{mA} + 2c_4,
\end{aligned}$$

$$G(x) = \left(\frac{2V(x)}{mA} + 2c_4\right)^{1/2}. \tag{2.44}$$

Assuming $V(x)$ is bounded below, we can select $A$ positive, and choose $c_4$ that the RHS (2.44) is positive. The analysis shows that the Hamiltonian express in form of

$$\begin{aligned}
H(x,p) &= F(p)G(x), \\
&= c_1 \cosh(c_2 p + c_3)\left(\frac{2V(x)}{mA} + 2c_4\right), \\
&= c_1 \cosh(c_2 p + c_3)\left(\frac{2V(x)}{mc_1^2 c_2^2} + 2c_4\right).
\end{aligned} \tag{2.45}$$

To construct (2.45) to 1-parameter family Hamiltonian, we choose $c_1 = 4mc^2, c_2 = 1/2mc^2, c_3 = 0, c_4 = 1/2$. Hence the solution, which proposed for the first time by [1], is expressed as

$$H_c(x,p) = 4mc^2 \cosh\left(\frac{p}{2mc}\right)\left(1 + \frac{V(x)}{2mc^2}\right)^{\frac{1}{2}}, \qquad c \in (0,\infty). \tag{2.46}$$

Notice that one of the Hamiltonians (fixed any $c$) needs to require

$$V(x) > -2mc^2, \tag{2.47}$$

for the Hamiltonians (2.46) to be real. For convenience to study later, we will redefine equation (2.46) by subtracting $4mc^2$

$$H_c(x,p) = 4mc^2 \cosh\left(\frac{p}{2mc}\right)\left(1+\frac{V(x)}{2mc^2}\right)^{\frac{1}{2}} - 4mc^2. \tag{2.48}$$

This alternative Hamiltonians give the Newton's equation. We can checked directly via (1.7)

$$\dot{x} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial x},$$

$$\begin{aligned} \dot{x} &= \frac{\partial}{\partial p}\left[4mc^2 \cosh\left(\frac{p}{2mc}\right)\left(1+\frac{V(x)}{2mc^2}\right)^{\frac{1}{2}} - 4mc^2\right], \\ &= 2c\sinh\left(\frac{p}{2mc}\right)\left(1+\frac{V(x)}{2mc^2}\right)^{\frac{1}{2}}, \end{aligned} \tag{2.49}$$

$$\begin{aligned} \dot{p} &= -\frac{\partial}{\partial x}\left[4mc^2 \cosh\left(\frac{p}{2mc}\right)\left(1+\frac{V(x)}{2mc^2}\right)^{\frac{1}{2}} - 4mc^2\right], \\ &= -\frac{dV(x)}{dx}\cosh\left(\frac{p}{2mc}\right)\left(1+\frac{V(x)}{2mc^2}\right)^{-\frac{1}{2}}. \end{aligned} \tag{2.50}$$

Taking time derivative to (2.49) and using $\dot{x}, \dot{p}$, we obtain

$$\begin{aligned} \ddot{x} &= \frac{\dot{p}}{m}\left(1+\frac{V(x)}{2mc^2}\right)^{1/2}\cosh\left(\frac{p}{2mc}\right) + \sinh\left(\frac{p}{2mc}\right)\left(1+\frac{V(x)}{2mc^2}\right)^{-1/2}\left(\frac{1}{2mc}\frac{dV(x)}{dx}\dot{x}\right), \\ &= -\frac{1}{m}\frac{dV(x)}{dx}\cosh\left(\frac{p}{2mc}\right)\left(1+\frac{V(x)}{2mc^2}\right)^{-1/2}\left(1+\frac{V(x)}{2mc^2}\right)^{1/2}\cosh\left(\frac{p}{2mc}\right) \\ &\quad +\sinh\left(\frac{p}{2mc}\right)\left(1+\frac{V(x)}{2mc^2}\right)^{-1/2}\left(\frac{1}{2mc}\frac{dV(x)}{dx}2c\sinh\left(\frac{p}{2mc}\right)\left(1+\frac{V(x)}{2mc^2}\right)^{1/2}\right), \\ &= -\frac{1}{m}\frac{dV(x)}{dx}\cosh^2\left(\frac{p}{2mc}\right) + \frac{1}{m}\frac{dV(x)}{dx}\sinh^2\left(\frac{p}{2mc}\right), \\ &= -\frac{1}{m}\frac{dV(x)}{dx}\left[\cosh^2\left(\frac{p}{2mc}\right) - \sinh^2\left(\frac{p}{2mc}\right)\right]. \end{aligned} \tag{2.51}$$

By using identity $\cosh^2(p/2mc) - \sinh^2(p/2mc) = 1$, we get the Newton's equation

$$m\ddot{x} = -\frac{dV(x)}{dx}.$$

We are able to conclude that the equation (2.48) is Newton-Equivalent Hamiltonians.

Moreover, the 1-parameter Newton's equivalent Hamiltonians (2.48) consist standard Hamiltonian $H_E = p^2/(2m) + V(x)$ as a limit case $c \to \infty$. By using Taylor expansion to $\cosh(x) = 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + ...$ and $(1+x)^n = 1 + nx + \frac{n(n-1)x^2}{2!} + ...$ to 1-parameter family (2.48), we have

$$\begin{aligned}
H_c(x,p) &= 4mc^2 \cosh\left(\frac{p}{2mc}\right)\left(1 + \frac{V(x)}{2mc^2}\right)^{\frac{1}{2}} - 4mc^2, \\
&= 4mc^2\left(1 + \frac{p^2}{2^2m^2c^2 2!} + \frac{p^4}{2^4m^4c^4 4!} + \cdots\right) \times \\
&\quad \left(1 + \frac{V(x)}{4mc^2} - \frac{V^2(x)}{16m^2c^4 2!} + \cdots\right) - 4mc^2, \\
&= 4mc^2 + V(x) + \frac{p^2}{2m} - \frac{V^2(x)}{8mc^2} + \frac{p^2V(x)}{8m^2c^2} - \frac{p^2V^2(x)}{32m^3c^4} \\
&\quad + \frac{p^4}{96m^3c^2} + \frac{p^4V(x)}{384m^4c^4} - \frac{p^4V^2(x)}{3072m^5c^6} + \cdots - 4mc^2, \\
&= \frac{p^2}{2m} + V(x) - \frac{V^2(x)}{8mc^2} + \frac{p^2V(x)}{8m^2c^2} - \frac{p^2V^2(x)}{32m^3c^4} + \frac{p^4}{96m^3c^2} \\
&\quad + \frac{p^4V(x)}{384m^4c^4} - \frac{p^4V^2(x)}{3072m^5c^6} + \cdots, \\
\lim_{c\to\infty}[H_c(x,p)] &= \frac{p^2}{2m} + V(x) = H_E(x,p). \qquad (2.52)
\end{aligned}$$

Now let us consider the quantum case of 1-parameter family Newton's equivalent Hamiltonian. By using the canonical quantization in one dimension, the dynamical variables are replaced by $p \to \hat{p} = i\hbar(\partial/\partial x)$ and $x \to \hat{x} = x$ to (2.48). The Hamiltonian (2.48) will become to quantum operator as

$$\hat{H}(\beta; \hat{x}, \hat{p}) = \frac{1}{\beta^2 m}\cosh(\beta\hat{p})(1 + 2m\beta^2 V(\hat{x}))^{1/2} - \frac{1}{\beta^2 m}. \qquad (2.53)$$

There are in fact many choices corresponding to alternative ordering. For example, the choice given by [1, 24] which insist in form self-adjoint and parity invariant

$$\begin{aligned}
\hat{H}(\beta; \hat{x}, \hat{p}) &= \frac{1}{2\beta^2 m}\Big[(1 + i\beta\sqrt{2mV(\hat{x})})^{1/2}\exp(-\beta\hat{p})(1 - i\beta\sqrt{2mV(\hat{x})})^{1/2} \\
&\quad + (1 - i\beta\sqrt{2mV(\hat{x})})^{1/2}\exp(\beta\hat{p})(1 + i\beta\sqrt{2mV(\hat{x})})^{1/2}\Big] - \frac{1}{\beta^2 m}.
\end{aligned} \qquad (2.54)$$

Substitution operator $\hat{x}, \hat{p}$ in Schrödinger picture the equation (2.54) reads

$$\begin{aligned}\hat{H}(\beta;\hat{x},\hat{p}) &= \frac{1}{2\beta^2 m}\Big[(1+i\beta\sqrt{2mV(x)})^{1/2}\exp(-i\hbar\beta\frac{\partial}{\partial x})(1-i\beta\sqrt{2mV(x)})^{1/2} \\ &\quad +(1-i\beta\sqrt{2mV(x)})^{1/2}\exp(i\hbar\beta\frac{\partial}{\partial x})(1+i\beta\sqrt{2mV(x)})^{1/2}\Big]-\frac{1}{\beta^2 m},\end{aligned} \tag{2.55}$$

where $\beta = (2mc)^{-1}$. The importance property of observable is Hermitian. Because the eigenvalue of an Hermitian operator correspond to a real physical quantity. Hence,we need to construct operator to hermitian. One idea to obtain hermitian operator is that present an operator in form adjoint operator. Let us consider inner product of operator $\hat{A}$ and adjoint of $\hat{A}^\dagger$,

$$\langle \hat{A}^\dagger \psi_l | \psi_n \rangle = \langle \psi_l | \hat{A} \psi_n \rangle. \tag{2.56}$$

Condition for hermitian operator [25] is

$$\langle \hat{A} \psi_l | \psi_n \rangle = \langle \psi_l | \hat{A} \psi_n \rangle. \tag{2.57}$$

The adjoint operator will become to hermitian operator, if equation

$$\hat{A}^\dagger = \hat{A}, \tag{2.58}$$

is true. A linear operator may equal its adjoint, and is then called self-adjoint operator. According to (2.55) the adjoint of NEQH is

$$\begin{aligned}\hat{H}^\dagger(\beta;\hat{x},\hat{p}) &= \frac{1}{2\beta^2 m}\Big[(1+i\beta\sqrt{2mV(\hat{x})})^{1/2}\exp(-\beta\hat{p})(1-i\beta\sqrt{2mV(\hat{x})})^{1/2} \\ &\quad +(1-i\beta\sqrt{2mV(\hat{x})})^{1/2}\exp(\beta\hat{p})(1+i\beta\sqrt{2mV(\hat{x})})^{1/2}\Big]^\dagger-\frac{1}{\beta^2 m}.\end{aligned} \tag{2.59}$$

By using Properties of adjoint operator

$$\begin{aligned}(\hat{A}\hat{B})^\dagger &= \hat{B}^\dagger \hat{A}^\dagger, \\ (\hat{A}+\hat{B})^\dagger &= \hat{A}^\dagger + \hat{B}^\dagger,\end{aligned}$$

the equation (2.59) becomes

$$\hat{H}^\dagger(\beta;\hat{x},\hat{p}) = \frac{1}{2\beta^2 m}\Big[(1+i\beta\sqrt{2mV(\hat{x^\dagger})})^{1/2}\exp(-\beta\hat{p^\dagger})(1-i\beta\sqrt{2mV(\hat{x^\dagger})})^{1/2} + (1-i\beta\sqrt{2mV(\hat{x^\dagger})})^{1/2}\exp(\beta\hat{p^\dagger})(1+i\beta\sqrt{2mV(\hat{x^\dagger})})^{1/2}\Big] - \frac{1}{\beta^2 m}. \tag{2.60}$$

The operator $\hat{x}$ and $\hat{p}$ are hermitian operator.[4] Hence, the equation (2.60) becomes

$$\begin{aligned}\hat{H}^\dagger(\beta;\hat{x},\hat{p}) &= \frac{1}{2\beta^2 m}\Big[(1+i\beta\sqrt{2mV(\hat{x})})^{1/2}\exp(-i\hbar\beta\frac{\partial}{\partial x})(1-i\beta\sqrt{2mV(\hat{x})})^{1/2} \\ &\quad + (1-i\beta\sqrt{2mV(\hat{x})})^{1/2}\exp(i\hbar\beta\frac{\partial}{\partial x})(1+i\beta\sqrt{2mV(\hat{x})})^{1/2}\Big] - \frac{1}{\beta^2 m} \\ &= H(\beta;\hat{x},\hat{p}).\end{aligned}$$

Clearly this NEQH operator is Hermitian operator.

[4]let us consider the hermitian conjugate of $\hat{x}$ and $\hat{p}$

$$\hat{x}^\dagger = \hat{x}$$

$$\hat{p}^\dagger = \left(-i\hbar\frac{d}{dx}\right)^\dagger = i\hbar\left(\frac{d}{dx}\right)^\dagger = i\hbar\left(-\frac{d}{dx}\right) = \hat{p}$$

where hermitian of $d/dx$ is $-d/dx$

# CHAPTER III

# QUANTUM INFINITE SQUARE WELL

The infinite square well potential restricts the motion of a particle between high (infinity) walls of width $L$. To find energy spectrum and wavefunction, let us consider the potential energy [26]

$$V(x) = \begin{cases} 0, & \text{if} \quad 0 \leq x \leq L \\ \infty, & \text{otherwise.} \end{cases} \tag{3.1}$$

This potential is illustrated in Figure 2.

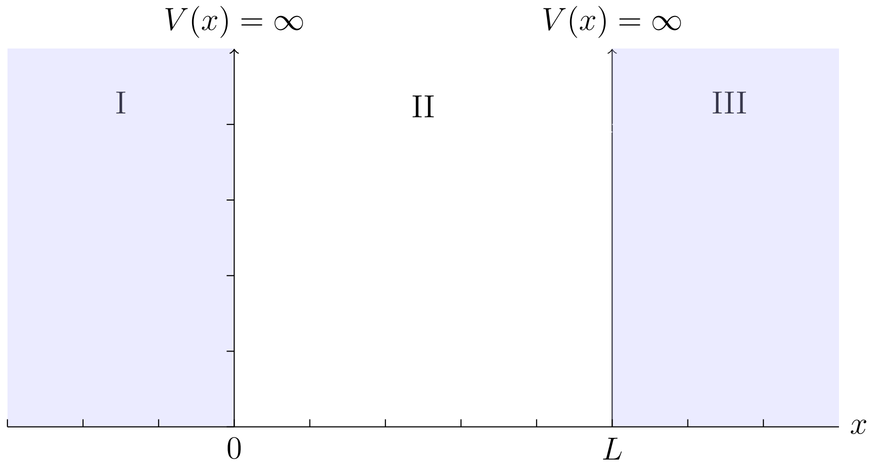


**Figure 2: 1-dimension infinite square well system**

Potential outside well is infinity $V(x) = \infty$. The probability of finding a particle outside the well is zero. Moreover wavefunction in this region, which must be continuous, vanish at the boundary namely $\psi(x) = 0$. Inside the well, the potential is zero $V(x) = 0$. Hence, a particle moving inside the well must be represented as a free particle. The time-independent Schrödinger's equation reads

$$\hat{H}\psi = E^S\psi, \tag{3.2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E^S\psi, \tag{3.3}$$

or

$$\frac{d^2\psi}{dx^2} = -k^2\psi, \qquad \text{where} \quad k \equiv \frac{\sqrt{2mE^S}}{\hbar}, \tag{3.4}$$

where $E^S$ is an energy which is generated by standard Hamiltonian. Let us consider the condition, where energy of a particle is positive $E^S \geq 0$. ($E^S < 0$ does not work because it has only trivial solution[5]). General solution of (3.4) can be solved as

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

By using characteristic equation,

$$\begin{aligned} p^2 + k^2 &= 0, \\ p^2 &= -k^2, \\ p &= \sqrt{-k^2}, \\ p &= \pm ik, \end{aligned}$$

the general solution of (3.4) reads

$$\psi(x) = c_1 e^{ikx} + c_2 e^{-ikx}. \tag{3.5}$$

By using the Euler relation $\exp(\pm ix) = \cos(x) \pm i\sin(x)$, we obtain

$$\begin{aligned} \psi(x) &= c_1(\cos(kx) + i\sin(kx)) + c_2(\cos(kx) - i\sin(kx)), \\ &= (ic_1 - ic_2)\sin kx + (c_1 + c_2)\cos kx, \\ &= A\sin kx + B\cos kx, \end{aligned} \tag{3.6}$$

where $A$ and $B$ are arbitrary constants.

Wavefunction represents a particle in the well, so the wavefunction must be continuous at the boundaries $x = 0$ and $x = L$. Wavefunction $\psi(x)$ must be

$$\psi(0) = \psi(L) = 0, \tag{3.7}$$

[5]There is no physically acceptable solution in this case

$$\psi(0) = A\mathrm{sin}0 + B\mathrm{cos}0 = B = 0, \tag{3.8}$$

and

$$\psi(L) = A\mathrm{sin}kL = 0, \tag{3.9}$$

where $A$ is arbitrary constant and $A \neq 0$. The equation (3.9) is valid for $\mathrm{sin}kL = 0$. This gives

$$k_n = \frac{n\pi}{L}, \qquad \text{with} \quad n = 1, 2, 3, \ldots \tag{3.10}$$

Hence the nontrivial solution of Schrödinger equation with boundary conditions is given by

$$\psi_n(x) = A\mathrm{sin}\left(\frac{n\pi x}{L}\right). \tag{3.11}$$

To guarantee that the particle are exactly found inside the well. Wavefunction satisfies

$$\int_0^L \psi^*(x)\psi(x)dx = 1. \tag{3.12}$$

The equation can be computed

$$\begin{aligned}
\int_0^L \psi^*(x)\psi(x)dx &= \int_0^L A^2\mathrm{sin}^2\left(\frac{n\pi x}{L}\right)dx, \\
&= \frac{A^2}{2}\int_0^L (1 - \cos\left(\frac{2n\pi x}{L}\right))dx, \\
&= \frac{A^2}{2}\left[x\Big|_0^L - \frac{L}{2n\pi}\mathrm{sin}\left(\frac{2n\pi x}{L}\right)\Big|_0^L\right], \\
&= \frac{A^2}{2}\left[L - \frac{L}{2n\pi}\mathrm{sin}\left(2n\pi\right)\right], \\
&= \frac{A^2 L}{2} = 1.
\end{aligned}$$

Therefore the arbitrary constant, which correspond to normalization condition, becomes

$$A = \sqrt{\frac{2}{L}}. \tag{3.13}$$

So, the normalized wavefunctions are expressed in the form

$$\psi_n(x) = \sqrt{\frac{2}{L}}\mathrm{sin}\left(\frac{n\pi x}{L}\right). \tag{3.14}$$

The energy is obtained by substituting (3.14) to the Schorödinger equation. This gives

$$\begin{aligned}
\hat{H}\psi(x) &= -\frac{\hbar^2}{2m}\sqrt{\frac{2}{L}}\frac{d^2}{dx^2}\sin\left(\frac{n\pi x}{L}\right), \\
&= -\frac{\hbar^2}{2m}\sqrt{\frac{2}{L}}\frac{L}{n\pi}\frac{d}{dx}\cos\left(\frac{n\pi x}{L}\right), \\
&= \frac{\hbar^2}{2m}\sqrt{\frac{2}{L}}\left(\frac{n\pi}{L}\right)^2\sin\left(\frac{n\pi x}{L}\right), \\
&= \frac{n^2\pi^2\hbar^2}{2mL^2}\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \\
&= \frac{n^2\pi^2\hbar^2}{2mL^2}\psi(x).
\end{aligned}$$

Hence, the energy spectrum of this system are expressed as

$$E_n^S = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2\pi^2\hbar^2}{8ma^2}, \qquad \text{where} \qquad a = L/2 \tag{3.15}$$

The illustration of wavefunction and energy of Infinite square well are given in Figure 3

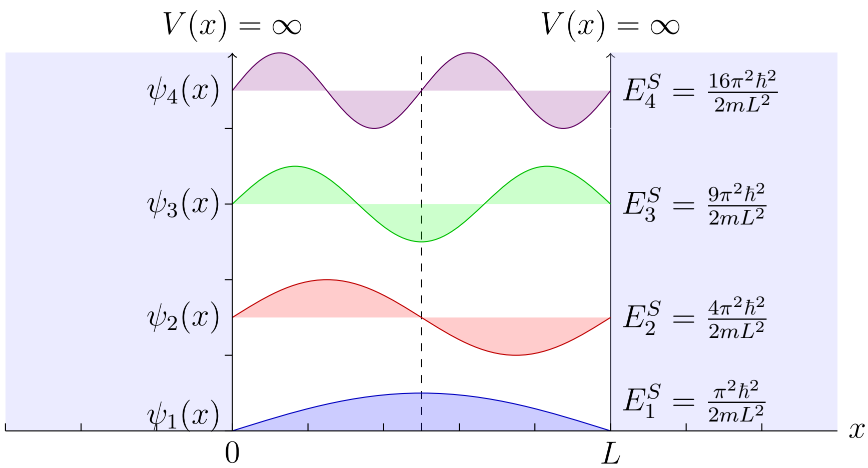


**Figure 3: Energy and wavefunction of infinite square well**

# CHAPTER IV

# QUANTUM FINITE SQUARE WELL

In this chapter, we mention the time-independent Schrödinger's equation in rectangular well potential system by following the text book [27]. The potential is expressed as

$$V(x) = \begin{cases} 0, & \text{if} \quad 0 < x < L \\ V_0, & \text{if} \quad x < 0, \quad x > L. \end{cases} \tag{4.1}$$

The potential is illustrated in Figure 4,

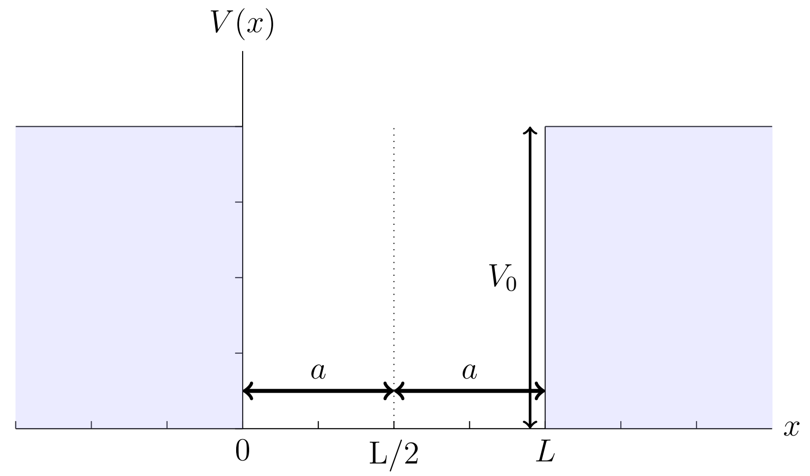


**Figure 4: 1-dimension finite square well system**

where $V_0$ and $L$ are depth and width of the well, respectively. If the energy of a particle is greater than potential $E > V_0$, the particle correspond to scattering problem which energy have a continuous spectrum. The case of energy less than potential $0 < E < V_0$[6], the energy spectrum will be discrete corresponding to a particle in bound state. The bound state of a particle is studied in our framework.

[6]The energy cannot less than the minimum value of the potential i.e. $E < 0$ because there is no physically acceptable solution of Schrödinger's equation.

The potential inside the well equals to zero $V_0 = 0$, then the time-independent Schrödinger's equation reads

$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{d^2\psi_{\rm II}(x)}{dx^2} &= E\psi_{\rm II}(x), \\
\frac{\hbar^2}{2m}\frac{d^2\psi_{\rm II}(x)}{dx^2} &= -E\psi_{\rm II}(x), \\
\frac{d^2\psi_{\rm II}(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi_{\rm II}(x) &= 0, \\
\frac{d^2\psi_{\rm II}(x)}{dx^2} + k^2\psi_{\rm II}(x) &= 0, \qquad k = \left[\frac{2mE}{\hbar^2}\right]^{1/2}. \qquad (4.2)
\end{aligned}$$

By using the characteristic equation, the Schrödinger's equation becomes

$$\begin{aligned}
p^2 + k^2 &= 0, \\
p &= \pm ik. \qquad (4.3)
\end{aligned}$$

Let us consider ansatz $\psi(x) = \exp(px)$, so the general solution of (4.2) reads

$$\psi_{\rm II}(x) = c_1 e^{ikx} + c_2 e^{-ikx}, \qquad (4.4)$$

where $\exp(i\alpha x)$ and $\exp(-i\alpha x)$ are linearly independent. Using Euler's identity,

$$e^{\pm i\theta} = \cos(\theta) \pm i\sin(\theta), \qquad (4.5)$$

the equation (4.4) gives

$$\begin{aligned}
\psi_{\rm II}(x) &= c_1\cos(kx) + c_1 i\sin(kx) + c_2\cos(kx) - c_2 i\cos(kx), \\
&= (c_1 + c_2)\cos(kx) + (c_1 i - c_2 i)\sin(kx), \\
&= A\cos(kx) + B\sin(kx), \quad 0 < x < L \qquad (4.6)
\end{aligned}$$

where the constant $A = c_1 + c_2$ and $B = c_1 i - c_2 i$.

In region outside the well the time-independent Schrödinger's equation can be written as

$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V_0\psi(x) &= E\psi(x), \\
-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+(V_0-E)\psi(x) &= 0, \\
\frac{d^2\psi(x)}{dx^2}-\frac{2m}{\hbar^2}(V_0-E)\psi(x) &= 0, \\
\frac{d^2\psi(x)}{dx^2}-\kappa^2\psi(x) &= 0, \quad \kappa=\left[\frac{2m}{\hbar^2}(V_0-E)\right]^{1/2}.
\end{aligned} \tag{4.7}$$

Using the characteristic equation, the Schrödinger's equation gives

$$\begin{aligned}
p^2-\kappa^2 &= 0, \\
p &= \pm\kappa.
\end{aligned} \tag{4.8}$$

Let us consider ansatz $\psi(x)=\exp(px)$, so the general solution reads

$$\psi(x)=Ce^{\kappa x}+De^{-\kappa x}. \tag{4.9}$$

We use the fact that wavefunction must be finite for all $x$, therefore as $x\to\pm\infty$ the wavefunction must be convergence. Let us consider the region III $x>L$, the first term of RHS of equation (4.9) will be divergence as $x\to\infty$. Therefore we must set the constant $C=0$, hence the solution (4.9) becomes

$$\psi_{\mathrm{III}}(x)=De^{-\kappa x}, \quad x>L. \tag{4.10}$$

In the same way as region III, the general solution in region I $x<0$ is expressed as

$$\psi_{\mathrm{I}}(x)=Fe^{\kappa x}+Ge^{-\kappa x}. \tag{4.11}$$

Due to the fact that wavefunction as $x\to-\infty$ must be finite, the second term of equation (4.11) will blows up. Therefore, to set constant $G=0$, the solution of (4.11) reads

$$\psi_{\mathrm{I}}(x)=Fe^{\kappa x}, \quad x<0. \tag{4.12}$$

Notice that $k$ and $\kappa$ obey the constraint

$$k^2+\kappa^2=\frac{2mE}{\hbar^2}+\frac{2m(V_0-E)}{\hbar^2}=\frac{2mV_0}{\hbar^2}. \tag{4.13}$$

Requirements of the boundary condition are that $\psi$ and $d\psi/dx$ must be continuous at $x = 0$ and $x = L$. At boundary $x = 0$, the conditions are $\psi_{\rm I}|_{x=0} = \psi_{\rm II}|_{x=0}$

$$\begin{aligned} \psi_{\rm I}|_{x=0} &= \psi_{\rm II}|_{x=0}, \\ Fe^0 &= A\cos(0) + B\sin(0), \\ F &= A, \end{aligned} \tag{4.14}$$

and $d\psi_{\rm I}/dx|_{x=0} = d\psi_{\rm II}/dx|_{x=0}$,

$$\begin{aligned} \frac{d\psi_{\rm I}}{dx}|_{x=0} &= \frac{d\psi_{\rm II}}{dx}|_{x=0}, \\ \kappa Ae^0 &= -Ak\sin(0) + Bk\cos(0), \\ \frac{\kappa}{k}A &= B. \end{aligned} \tag{4.15}$$

The other boundary conditions at $x = L$ are $\psi_{\rm II}|_{x=L} = \psi_{\rm III}|_{x=L}$ and $d\psi_{\rm II}/dx|_{x=L} = d\psi_{\rm III}/dx|_{x=L}$. First condition gives

$$\begin{aligned} \psi_{\rm II}|_{x=L} &= \psi_{\rm III}|_{x=L}, \\ A\cos(kL) + B\sin(kL) &= De^{-\kappa L}. \end{aligned} \tag{4.16}$$

The second condition gives

$$\begin{aligned} \frac{d\psi_{\rm II}}{dx}|_{x=L} &= \frac{d\psi_{\rm III}}{dx}|_{x=L}, \\ -Ak\sin(kL) + Bk\cos(kL) &= -\kappa De^{-\kappa L}. \end{aligned} \tag{4.17}$$

Substituting (4.16) into (4.17) gives

$$-Ak\sin(kL) + Bk\cos(kL) = -\kappa A\cos(kL) - \kappa B\sin(kL). \tag{4.18}$$

Substituting equation (4.14) and (4.15) into equation (4.18) gives

$$\begin{aligned} -Ak\sin(kL) + \frac{\kappa}{k}Ak\cos(kL) &= -\kappa A\cos(kL) - \kappa\frac{\kappa}{k}A\sin(kL), \\ -k\sin(kL) + \kappa\cos(kL) &= -\kappa\cos(kL) - \frac{\kappa^2}{k}\sin(kL), \\ -k^2\sin(kL) + k\kappa\cos(kL) &= -k\kappa\cos(kL) - \kappa^2\sin(kL), \\ \left(k^2 - \kappa^2\right)\sin(kL) - 2k\kappa\cos(kL) &= 0. \end{aligned} \tag{4.19}$$

The equation (4.19) is imaginary part of equation $(\kappa + ik)^2 e^{ikL}$. The proof of this relation expressed as

$$\begin{aligned}
\left(k^2 - \kappa^2\right)\sin(kL) - 2k\kappa\cos(kL) &= 0, \\
\mathrm{Im}[(\kappa^2 - k^2)\mathrm{cos}(kL) - 2k\kappa\mathrm{sin}(kL) + & \\
i\left((\kappa^2 - k^2)\mathrm{sin}(kL) + 2k\kappa\mathrm{cos}(kL)\right)] &= 0, \\
\mathrm{Im}(\kappa^2 + 2ik\kappa - k^2)(\mathrm{cos}(kL) + i\mathrm{sin}(kL)) &= 0, \\
\mathrm{Im}(\kappa + ik)^2 e^{ikL} &= 0. \qquad (4.20)
\end{aligned}$$

Hence, let us consider the equation (4.20)

$$\begin{aligned}
\mathrm{Im}\left(\kappa e^{ikL/2} + ike^{ikL/2}\right)^2 &= 0, \\
\mathrm{Im}\left(\kappa\mathrm{cos}(\frac{kL}{2}) + i\kappa\mathrm{sin}(\frac{kL}{2}) + ik\mathrm{cos}(\frac{kL}{2}) - k\mathrm{sin}(\frac{kL}{2})\right)^2 &= 0, \\
\mathrm{Im}\left(\kappa\mathrm{cos}(\frac{kL}{2}) - k\mathrm{sin}(\frac{kL}{2}) + i\left(\kappa\mathrm{sin}(\frac{kL}{2}) + k\mathrm{cos}(\frac{kL}{2})\right)\right)^2 &= 0.
\end{aligned}$$

Recalling $(x + iy)^2 = x^2 + 2ixy - y^2 = 0$ the imaginary part of (4.20) becomes

$$\begin{aligned}
2\left(\kappa\mathrm{sin}(\frac{kL}{2}) + k\mathrm{cos}(\frac{kL}{2})\right)\left(\kappa\mathrm{cos}(\frac{kL}{2}) - k\mathrm{sin}(\frac{kL}{2})\right) &= 0, \\
\left(\kappa + k\mathrm{cot}(\frac{kL}{2})\right)\left(\kappa\mathrm{cot}(\frac{kL}{2}) - k\right) &= 0. \qquad (4.21)
\end{aligned}$$

Two solution are obtained as follows

$$\kappa = -k\mathrm{cot}(\frac{kL}{2}) = -k\mathrm{cot}(ka), \qquad (4.22)$$

and

$$\kappa = k\mathrm{tan}(\frac{kL}{2}) = k\mathrm{tan}(ka), \qquad (4.23)$$

where $L/2 = a$ is a half width of the well[7]. The equation (4.22), (4.23), and constrain (4.13) can be solved graphically. First, let us define dimensionless quantities

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[7]All of these calculation will become easy, if we consider this system by using symmetry of square well

$x = ka$ and $y = \kappa a$ . So, the equations (4.22), (4.23) and (4.13) become

$$y = -x\cot(x), \tag{4.24}$$

$$y = x\tan(x), \tag{4.25}$$

$$x^2 + y^2 = \rho^2, \tag{4.26}$$

where $\rho = (mV_0L^2/2\hbar^2)^{1/2}$ is the dimensionless quantity to measure potential $V_0$. The plot of functions between $y = x\tan(x)$ and $x^2 + y^2 = \rho^2$ is expressed in Figure 5

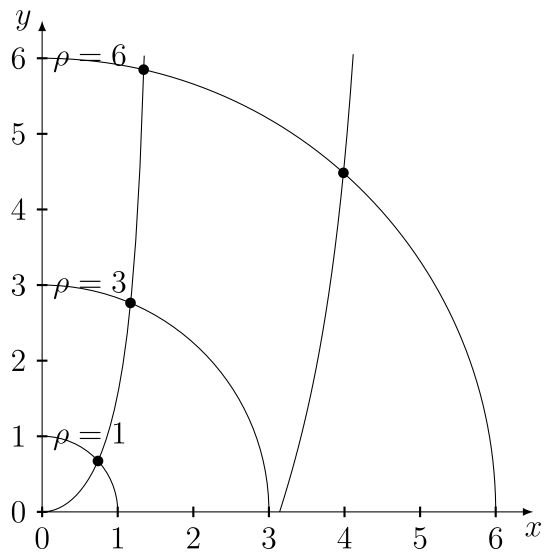



**Figure 5: Intersection points between $y = x\tan(x)$ and $x^2 + y^2 = \rho^2$**

Other plot between equation $y = -x\cot(x)$ and $x^2 + y^2 = \rho^2$ is showed in Figure 6

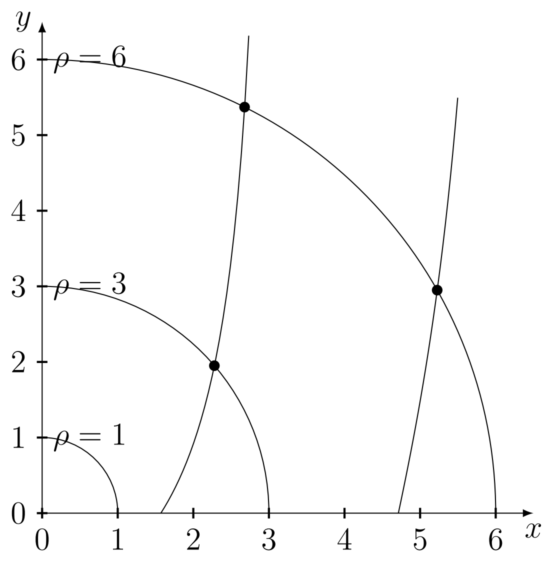



**Figure 6: Intersection points between** $y = -x\cot(x)$ **and** $x^2 + y^2 = \rho^2$

The energy level can be found by considering the intersection point between circle $x^2+y^2 = \rho^2$ and curves $y = x\tan(x)$ or $y = -x\cot(x)$. The intersection points are depend on the parameter $\rho$ which called " strength parameter " of potential [28]. For a fixed values of mass $m$ and fixed value of width $a$, the strength parameter $\rho$ depends only on potential. For example if the strength parameter $\rho$ increase ( in other words, potential increase ), the intersection points corresponding to solution appear successively (see Figure 5,6). We see from both figures 5,6 that $\rho = 1$, there is only one bound state, $\rho = 3$, there are two bound states, and $\rho = 6$, there are four bound states. The energy for each level can be obtained from equation $E_n = k_n^2\hbar^2/2m$, where $k_n = x_n/a$ relate to intersection point. For example, $\rho = 6$ give four bound state corresponding to intersection points as follows $x_1 = 1.34475, x_2 = 2.67878, x_3 = 3.98583, x_4 = 5.22596$. Thus the energy level, which expressed in dimensionless form, are showed in table 1.

Finally, let us consider the limiting case of finite square well namely $V_0 \to \infty$ (or $\rho \to \infty$). According to Figures 5, 6, the circle has radius $\rho \to \infty$. So the intersection points appear at infinity, and give infinite number of energy levels. It is

**Table 1: Energy level of finite square well for $\rho = 6$**

| n | intersection point ($x_n$) | dimensionless energy ($2mEa^2/\hbar^2 = x_n^2$) |
|---|---|---|
| 1 | 1.34475 | 1.80835 |
| 2 | 2.67878 | 7.17586 |
| 3 | 3.98583 | 15.88684 |
| 4 | 5.22596 | 27.31066 |

apparent that the roots ($x_n$) will be given by $x_n = k_n a = n\pi/2$ where $n = 1, 2, 3, ...$ is integer. Hence the energy spectrum become

$$\begin{aligned} x_n &= k_n a, \\ &= (\frac{2mE_n}{\hbar^2})^{1/2} a. \end{aligned}$$

Therefore, the intersection points satisfy $x_n = n\pi/2$. This gives

$$\begin{aligned} (\frac{2mE_n}{\hbar^2})^{1/2} a &= \frac{n\pi}{2}, \\ E_n &= \frac{n^2\pi^2\hbar^2}{8ma^2}. \qquad n = 1, 2, 3, ... \end{aligned}$$

The energy spectrum recover to infinite square well case.

# CHAPTER V

# NON-DEGENERATE PERTURBATION THEORY

## 5.1 General Formulation

The previous chapter, we have solved (standard) time-independent Schrödinger's equation for finite and infinite square well potentials:

$$H^0\psi_n^0 = E_n^0\psi_n^0, \tag{5.1}$$

where $H^0, \psi_n^0$ and $E_n^0$ are denoted as "unperturbed" Hamiltonian, wavefunction and energy respectively. Here a complete set of orthonormal eigenfunctions $\psi_n^0$ are given by

$$\langle\psi_n^0|\psi_m^0\rangle = \delta_{nm}. \tag{5.2}$$

Perturbation theory is a procedure for solving approximation of solution with known exact solutions of the unperturbed case. We would like to solve the new eigenfunctions and eigenvalues:

$$H\psi_n = E_n\psi_n. \tag{5.3}$$

We write the new Hamiltonian as

$$H = H^0 + lH' \tag{5.4}$$

where $H'$ is the perturbation Hamiltonian. The parameter $l$ has been introduced for convenience, and it will allow us to identify the different orders of the perturbative calculation. And later we will set parameter to 1. Writing $\psi_n$ and $E_n$ as power series in $l$, we obtain

$$\psi_n = \psi_n^0 + l\psi_n^1 + l^2\psi_n^2 + \cdots, \tag{5.5}$$

$$E_n = E_n^0 + lE_n^1 + l^2E_n^2 + \cdots, \tag{5.6}$$

where $E_n^1$, $E_n^2$ are the first-order and second-order corrections to eigenvalues respectively, and $\psi_n^1$, $\psi_n^2$ are the first-order and second-order corrections of eigenfunction respectively. Substituting equations (5.4), (5.5) and (5.6) into equation (5.3), we obtain

$$(H^0+lH')(\psi_n^0+l\psi_n^1+l^2\psi_n^2+\cdots) = (E_n^0+lE_n^1+l^2E_n^2+\cdots)(\psi_n^0+l\psi_n^1+l^2\psi_n^2+\cdots). \tag{5.7}$$

Collecting the powers of $l$, this gives

$$\begin{aligned} & H^0\psi_n^0 + l(H^0\psi_n^1 + H'\psi_n^0) + l^2(H^0\psi_n^2 + H'\psi_n^1) + \cdots \\ = \; & E_n^0\psi_n^0 + l(E_n^0\psi_n^1 + E_n^1\psi_n^0) + l^2(E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0) + \cdots . \end{aligned} \tag{5.8}$$

The lowest order of parameter ($l^0$) gives the unperturbed case $H^0\psi_n^0 = E_n^0\psi_n^0$. The first order ($l^1$) gives

$$H^0\psi_n^1 + H'\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0. \tag{5.9}$$

The second order ($l^2$) gives

$$H^0\psi_n^2 + H'\psi_n^1 = E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0. \tag{5.10}$$

### 5.2 First-Order Contribution

According to first order contribution, equation (5.9), taking the inner product to (5.9) with $\psi_n^0$ gives

$$\langle\psi_n^0|H^0|\psi_n^1\rangle + \langle\psi_n^0|H'|\psi_n^0\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle + E_n^1\langle\psi_n^0|\psi_n^0\rangle. \tag{5.11}$$

Using properties of orthonormal eigenfunction $\langle\psi_n^0|\psi_n^0\rangle = 1$, and Hermitian operator of unperturbed Hamiltonian $H^0$, the equation (5.11) becomes

$$\langle H^0\psi_n^0|\psi_n^1\rangle + \langle\psi_n^0|H'|\psi_n^0\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle + E_n^1\cancelto{1}{\langle\psi_n^0|\psi_n^0\rangle}, \tag{5.12}$$

$$\cancel{E_n^0\langle\psi_n^0|\psi_n^1\rangle} + \langle\psi_n^0|H'|\psi_n^0\rangle = \cancel{E_n^0\langle\psi_n^0|\psi_n^1\rangle} + E_n^1. \tag{5.13}$$

Hence, the first-order correction to the energy is expressed as

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle. \tag{5.14}$$

The energy of first-order correction is expectation value of perturbation Hamiltonian in unperturbed state.

The first-order correction to the wavefunction can be found by rewriting (5.9) as

$$(H^0 - E_n^0)\psi_n^1 = -(H' - E_n^1)\psi_n^0. \tag{5.15}$$

We know that the unperturbed wavefunctions constitute a complete set, so the first order wavefunction $\psi_n^1$ can be expressed as linear combination of unperturbed wavefunctions;

$$\psi_n^1 = \sum_{m \neq n} c_{nm}^1 \psi_m^0. \tag{5.16}$$

To find the coefficient $c_{nm}^1$, substituting equation (5.16) into (5.15) we have

$$\sum_{m \neq n} (H^0 - E_n^0) c_{nm}^1 \psi_m^0 = -(H' - E_n^1)\psi_n^0, \tag{5.17}$$

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_{nm}^1 \psi_m^0 = -(H' - E_n^1)\psi_n^0. \tag{5.18}$$

Taking inner product with $\psi_l^0$, we obtain

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_{nm}^1 \langle \psi_l^0 | \psi_m^0 \rangle = -\langle \psi_l^0 | (H' - E_n^1) | \psi_n^0 \rangle, \tag{5.19}$$

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_{nm}^1 \delta_{lm} = -\langle \psi_l^0 | H' | \psi_n^0 \rangle + E_n^1 \delta_{ln}. \tag{5.20}$$

It has two cases as follows, first $l = n$

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_{nm}^1 \delta_{nm} = -\langle \psi_n^0 | H' | \psi_n^0 \rangle + E_n^1 \delta_{nn}, \tag{5.21}$$

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle.$$

It recover to first-order correction to the energy (5.14). Second case, $l \neq n$, is

$$(E_l^0 - E_n^0) c_{nl}^1 = -\langle \psi_l^0 | H' | \psi_n^0 \rangle, \tag{5.22}$$

$$c_{nl}^1 = \frac{\langle \psi_l^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_l^0}, \tag{5.23}$$

or, changing index $l \to m$,

$$c_{nm}^1 = \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0}. \tag{5.24}$$

Therefore first-order correction to the wavefunction reads

$$\psi_n^1 = \sum_{m \neq n} c_{nm}^1 \psi_m^0 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0. \tag{5.25}$$

## 5.3 Second-order Contribution

Let us consider second-order correction. we take the inner product with $\psi_n^0$ to the equation (5.10):

$$\langle \psi_n^0 | H^0 | \psi_n^2 \rangle + \langle \psi_n^0 | H' | \psi_n^1 \rangle = E_n^0 \langle \psi_n^0 | \psi_n^2 \rangle + E_n^1 \langle \psi_n^0 | \psi_n^1 \rangle + E_n^2 \langle \psi_n^0 | \psi_n^0 \rangle. \tag{5.26}$$

By using the Hermiticity of $H^0$ and orthonormality of complete set, we obtain

$$\begin{aligned} \langle H^0 \psi_n^0 | \psi_n^2 \rangle + \langle \psi_n^0 | H' | \psi_n^1 \rangle &= E_n^0 \langle \psi_n^0 | \psi_n^2 \rangle + E_n^1 \langle \psi_n^0 | \psi_n^1 \rangle + E_n^2 \cancelto{1}{\langle \psi_n^0 | \psi_n^0 \rangle}, \\ \cancel{E_n^0 \langle \psi_n^0 | \psi_n^2 \rangle} + \langle \psi_n^0 | H' | \psi_n^1 \rangle &= \cancel{E_n^0 \langle \psi_n^0 | \psi_n^2 \rangle} + E_n^1 \langle \psi_n^0 | \psi_n^1 \rangle + E_n^2. \end{aligned} \tag{5.27}$$

We obtain a formula for $E_n^2$:

$$E_n^2 = \langle \psi_n^0 | H' | \psi_n^1 \rangle - E_n^1 \langle \psi_n^0 | \psi_n^1 \rangle, \tag{5.28}$$

but

$$\langle \psi_n^0 | \psi_n^1 \rangle = \sum_{m \neq n} c_{nm}^1 \langle \psi_n^0 | \psi_m^0 \rangle = \sum_{m \neq n} c_{nm}^1 \delta_{mn} = 0. \tag{5.29}$$

Therefore, the second-order correction to energy becomes

$$\begin{aligned} E_n^2 &= \langle \psi_n^0 | H' | \psi_n^1 \rangle = \sum_{m \neq n} c_{nm}^1 \langle \psi_n^0 | H' | \psi_m^0 \rangle, \\ &= \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle \langle \psi_n^0 | H' | \psi_m^0 \rangle}{E_n^0 - E_m^0}, \\ &= \sum_{m \neq n} \frac{|\langle \psi_m^0 | H' | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0}. \end{aligned} \tag{5.30}$$

This is the result of second-order correction to the energy.

To find the second-order correction to the wavefunction, let us rewrite equation (5.10) as

$$(H^0 - E_n^0)\psi_n^2 = -(H' - E_n^1)\psi_n^1 + E_n^2\psi_n^0. \tag{5.31}$$

Similarly to first-order correction, $\psi_n^2$ can be expressed as a linear combination of unperturbed wavefunction i.e.

$$\psi_n^2 = \sum_{m\neq n} c_{nm}^2 \psi_m^0. \tag{5.32}$$

By using the equation (5.16), (5.32) and unperturbed Schrödinger's equation (5.1) to the equation (5.31) gives

$$\sum_{m\neq n}(E_m^0 - E_n^0)c_{nm}^2\psi_m^0 = -\sum_{m\neq n}(H' - E_n^1)c_{nm}^1\psi_m^0 + E_0^2\psi_n^0. \tag{5.33}$$

Taking an inner product with $\psi_l^0$, we get

$$\begin{aligned}
\sum_{m\neq n}(E_m^0 - E_n^0)c_{nm}^2\langle\psi_l^0|\psi_m^0\rangle &= -\sum_{m\neq n} c_{nm}^1\langle\psi_l^0|(H' - E_n^1)|\psi_m^0\rangle + E_0^2\langle\psi_l^0|\psi_n^0\rangle, \\
\sum_{m\neq n}(E_m^0 - E_n^0)c_{nm}^2\delta_{lm} &= -\sum_{m\neq n} c_{nm}^1\langle\psi_l^0|H'|\psi_m^0\rangle + E_n^1\sum_{m\neq n} c_{nm}^1\delta_{lm} + E_0^2\delta_{ln}.
\end{aligned} \tag{5.34}$$

If $l = n$, LHS is zero and second term of RHS also zero. Hence, the equation (5.34) will recover to second-order correction to energy. For $l \neq n$, the last term of RHS is zero and the equation (5.34) will become

$$(E_l^0 - E_n^0)c_{nl}^2 = -\sum_{m\neq n} c_{nm}^1\langle\psi_l^0|H'|\psi_m^0\rangle + E_n^1 c_{nl}^1.$$

Using the first-order correction to the energy (5.14) and coefficient $c_{nm}^1$ (5.24), the coefficient $c_{nl}^2$ reads

$$\begin{aligned}
(E_l^0 - E_n^0)c_{nl}^2 &= -\sum_{m\neq n}\frac{\langle\psi_m^0|H'|\psi_n^0\rangle\langle\psi_l^0|H'|\psi_m^0\rangle}{E_n^0 - E_m^0} + \frac{\langle\psi_n^0|H'|\psi_n^0\rangle\langle\psi_l^0|H'|\psi_n^0\rangle}{E_n^0 - E_l^0}, \\
c_{nl}^2 &= \sum_{m\neq n}\frac{\langle\psi_m^0|H'|\psi_n^0\rangle\langle\psi_l^0|H'|\psi_m^0\rangle}{(E_n^0 - E_l^0)(E_n^0 - E_m^0)} - \frac{\langle\psi_n^0|H'|\psi_n^0\rangle\langle\psi_l^0|H'|\psi_n^0\rangle}{(E_n^0 - E_l^0)^2}.
\end{aligned} \tag{5.35}$$

Therefore the second-order correction to the wavefunction, by interchanging index $l \Leftrightarrow m$, is expressed as

$$\psi_n^2 = \sum_{m \neq n} \left[ \sum_{l \neq n} \frac{\langle \psi_l^0 | H' | \psi_n^0 \rangle \langle \psi_m^0 | H' | \psi_l^0 \rangle}{(E_n^0 - E_m^0)(E_n^0 - E_l^0)} - \frac{\langle \psi_n^0 | H' | \psi_n^0 \rangle \langle \psi_m^0 | H' | \psi_n^0 \rangle}{(E_n^0 - E_m^0)^2} \right] \psi_m^0. \qquad (5.36)$$

Summary, wavefunction and energy of new Hamiltonian (5.4) by consideration with perturbation theory are given by (5.6) and (5.5) where first-order corrections to the energy and wavefunction are (5.14) and (5.25) respectively, and second-order correction to the energy and wavefunction are (5.30) and (5.36) respectively. However, the perturbation theory gives us just an approximation value. Hence, if we obtain more higher-order than first or second one e.g. $E_n^0 + E_n^1 + E_n^2 + E_n^3 + ...$ the solution is quite close to the exact value $E_n$.

# CHAPTER VI

# RESULTS AND DISCUSSIONS

## 6.1 Newton's equivalent Hamiltonians with quantum infinite square well

As part of our work, we consider 1-parameter family Newton's equivalent Hamiltonians with infinite square well potential. Mathematical form is expressed as

$$V(x) = \begin{cases} 0, & \text{if} \quad 0 \leq x \leq L \\ \infty, & \text{otherwise.} \end{cases} \tag{6.1}$$

The potential is illustrated in Figure 7

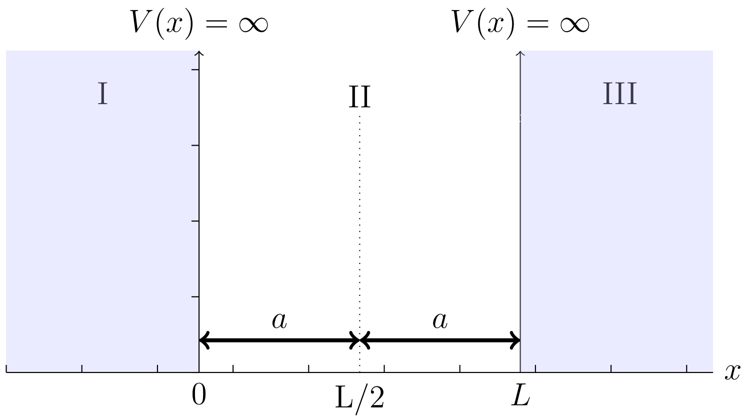



**Figure 7: Infinite square well system**

Inside the well, the NEQH is given by

$$\hat{H} = \frac{1}{2\beta^2 m}\left(e^{-i\hbar\beta\frac{\partial}{\partial x}} + e^{i\hbar\beta\frac{\partial}{\partial x}}\right) - \frac{1}{\beta^2 m}. \tag{6.2}$$

First, we want to check whether the NEQH (6.2) is a linear operator. The property of linear operator is given by

$$\hat{H}(a_1\psi_1 + a_2\psi_2) = a_1\hat{H}\psi_1 + a_2\hat{H}\psi_2.$$

Let us consider NEQH (6.2)

$$\begin{aligned}
\hat{H}(a_1\psi_1 + a_2\psi_2) &= \left[\frac{1}{2\beta^2 m}\left(e^{-i\hbar\beta\frac{\partial}{\partial x}} + e^{i\hbar\beta\frac{\partial}{\partial x}}\right) - \frac{1}{\beta^2 m}\right](a_1\psi_1 + a_2\psi_2), \\
&= \frac{1}{\beta^2 m}\left(a_1 e^{-i\hbar\beta\frac{\partial}{\partial x}}\psi_1 + a_2 e^{-i\hbar\beta\frac{\partial}{\partial x}}\psi_2 + a_1 e^{i\hbar\beta\frac{\partial}{\partial x}}\psi_1 + a_2 e^{i\hbar\beta\frac{\partial}{\partial x}}\psi_2\right) \\
&\quad -\frac{1}{\beta^2 m}(a_1\psi_1 + a_2\psi_2), \\
&= \frac{1}{2\beta^2 m}\left[a_1\left(e^{-i\hbar\beta\frac{\partial}{\partial x}} + e^{i\hbar\beta\frac{\partial}{\partial x}}\right)\psi_1 + a_2\left(e^{-i\hbar\beta\frac{\partial}{\partial x}} + e^{i\hbar\beta\frac{\partial}{\partial x}}\right)\psi_2\right] \\
&\quad -\frac{1}{\beta^2 m}(a_1\psi_1 + a_2\psi_2), \\
&= a_1\left[\frac{1}{2\beta^2 m}\left(e^{-i\hbar\beta\frac{\partial}{\partial x}} + e^{i\hbar\beta\frac{\partial}{\partial x}}\right) - \frac{1}{\beta^2 m}\right]\psi_1 \\
&\quad +a_2\left[\frac{1}{2\beta^2 m}\left(e^{-i\hbar\beta\frac{\partial}{\partial x}} + e^{i\hbar\beta\frac{\partial}{\partial x}}\right) - \frac{1}{\beta^2 m}\right]\psi_2, \\
&= a_1\hat{H}\psi_1 + a_2\hat{H}\psi_2. \qquad (6.3)
\end{aligned}$$

The NEQH agrees with property of linear operator, so the NEQH is linear operator.

The NEQH operating on a wavefunction $\psi(x)$ is given by

$$\hat{H}\psi(x) = \frac{1}{2\beta^2 m}\left(e^{-i\hbar\beta\frac{\partial}{\partial x}}\psi(x) + e^{i\hbar\beta\frac{\partial}{\partial x}}\psi(x)\right) - \frac{1}{\beta^2 m}\psi(x). \qquad (6.4)$$

Thus the Schrödinger equation will become a differential equation of infinite order

$$\begin{aligned}
\hat{H}\psi(x) &= E^N\psi(x), \\
\frac{1}{2\beta^2 m}\left(e^{-i\hbar\beta\frac{\partial}{\partial x}}\psi(x) + e^{i\hbar\beta\frac{\partial}{\partial x}}\psi(x)\right) - \frac{1}{\beta^2 m}\psi(x) &= E^N\psi(x). \qquad (6.5)
\end{aligned}$$

where $E^N$ is defined as energy of NEQH. Consider an ansatz

$$\psi(x) = e^{i\gamma x}, \qquad (6.6)$$

substituting (6.6) into (6.5) gives

$$\begin{aligned}
e^{i\gamma(x-i\hbar\beta)} + e^{i\gamma(x+i\hbar\beta)} &= (2\beta^2 m E^N + 2)e^{i\gamma x}, \\
\frac{\left(e^{\gamma\hbar\beta} + e^{-\gamma\hbar\beta}\right)}{2}\cancel{e^{i\gamma x}} &= (\beta^2 m E^N + 1)\cancel{e^{i\gamma x}}, \\
\cosh(\gamma\hbar\beta) &= 1 + \beta^2 m E^N. \qquad (6.7)
\end{aligned}$$

We have not assumed anything on $\gamma$. So let us write

$$\gamma = \gamma_R + i\gamma_I, \tag{6.8}$$

where $\gamma_R, \gamma_I \in \mathbb{R}$. Substituting (6.8) into (6.7) give

$$\cosh(\gamma_R\hbar\beta)\cos(\gamma_I\hbar\beta) + i\sinh(\gamma_R\hbar\beta)\sin(\gamma_I\hbar\beta) \;=\; 1 + \beta^2 mE^N. \tag{6.9}$$

By demanding that the imaginary part of the left-hand-side vanishes, we obtain the conditions

$$\sinh(\gamma_R\hbar\beta)\sin(\gamma_I\hbar\beta) = 0, \tag{6.10}$$

where solution is

$$\gamma_R = 0, \qquad \text{or} \qquad \gamma_I = \frac{n\pi}{\hbar\beta}. \tag{6.11}$$

Case 1: $\gamma_R = 0$. In this case, the equation (6.9) reduces to

$$\cos(\gamma_I\hbar\beta) = 1 + \beta^2 mE^N. \tag{6.12}$$

This case is only valid when

$$\frac{-2}{m\beta^2} \leq E^N \leq 0. \tag{6.13}$$

Case 2: $\gamma_I = \frac{n\pi}{\hbar\beta}$. In this case, the equation (6.9) reduces to

$$\cosh(\gamma_R\hbar\beta)(-1)^n = 1 + \beta^2 mE^N. \tag{6.14}$$

This is further separated into two subcases:

Case 2.1: $\gamma_I = \frac{n\pi}{\hbar\beta}$ with $n$ even, in this case equation (6.14) reads

$$\cosh(\gamma_R\hbar\beta) = 1 + \beta^2 mE^N. \tag{6.15}$$

This is valid for

$$E^N \geq 0. \tag{6.16}$$

Case 2.2: $\gamma_I = \frac{n\pi}{\hbar\beta}$ with n odd, in this case equation (6.14) becomes

$$\cosh(\gamma_R\hbar\beta) = -(1 + \beta^2 mE^N). \tag{6.17}$$

This is valid for

$$E^N \leq \frac{-2}{m\beta^2}. \tag{6.18}$$

According to analog classical mechanics, when a particle has energy E less than global minimum $V_{min}$ of potential, i.e. $E < V_{min}$, there is no physically acceptable solution in this case. Hence, cases 1 & 2.2 are invalid. For this, we only have case 2.1. This gives

$$\begin{aligned}
e^{\hbar\beta\gamma} + e^{-\hbar\beta\gamma} &= 2\beta^2 mE^N + 2, \\
e^{2\hbar\beta\gamma} + 1 &= 2mE^N\beta^2 e^{\hbar\beta\gamma} + 2e^{\hbar\beta\gamma}, \\
(e^{\hbar\beta\gamma})^2 - (2mE^N\beta^2 + 2)e^{\hbar\beta\gamma} + 1 &= 0, \\
e^{\hbar\beta\gamma} &= \frac{(2mE^N\beta^2 + 2) \pm \sqrt{(2mE^N\beta^2 + 2)^2 - 4}}{2}, \\
\ln e^{\hbar\beta\gamma} &= \ln\left((mE^N\beta^2 + 1) \pm \sqrt{(mE^N\beta^2 + 1)^2 - 1}\right), \\
\gamma_\pm &= \frac{1}{\hbar\beta}\ln\left((mE^N\beta^2 + 1) \pm \sqrt{(mE^N\beta^2 + 1)^2 - 1}\right).
\end{aligned} \tag{6.19}$$

The relationship between $\gamma_+$ and $\gamma_-$ of equation (6.19) is

$$\begin{aligned}
\gamma_- &= \frac{1}{\hbar\beta}\ln\left((mE^N\beta^2 + 1) - \sqrt{(mE^N\beta^2 + 1)^2 - 1}\right), \\
&= \frac{1}{\hbar\beta}\ln\Bigg[\left((mE^N\beta^2 + 1) - \sqrt{(mE^N\beta^2 + 1)^2 - 1}\right) \times \\
&\quad \frac{\left((mE^N\beta^2 + 1) + \sqrt{(mE^N\beta^2 + 1)^2 - 1}\right)}{\left((mE^N\beta^2 + 1) + \sqrt{(mE^N\beta^2 + 1)^2 - 1}\right)}\Bigg], \\
&= \frac{1}{\hbar\beta}\ln\left(\frac{(mE^N\beta^2 + 1)^2 - ((mE^N\beta^2 + 1)^2 - 1)}{(mE^N\beta^2 + 1) + \sqrt{(mE^N\beta^2 + 1)^2 - 1}}\right), \\
&= \frac{1}{\hbar\beta}\ln\left((mE^N\beta^2 + 1) + \sqrt{(mE^N\beta^2 + 1)^2 - 1}\right)^{-1}, \\
&= -\frac{1}{\hbar\beta}\ln\left((mE^N\beta^2 + 1) + \sqrt{(mE^N\beta^2 + 1)^2 - 1}\right), \\
&= -\gamma_+.
\end{aligned} \tag{6.20}$$

Recalling the ansatz (6.6), general solution to (6.5) is

$$\psi(x) = \sum_{k=-\infty}^{\infty} A_{k,+} e^{i(\gamma_+ + \frac{i\pi}{\hbar\beta}(2k))x} + \sum_{k=-\infty}^{\infty} A_{k,-} e^{i(\gamma_- + \frac{i\pi}{\hbar\beta}(2k))x}, \tag{6.21}$$

where $\gamma_+ = \frac{1}{\hbar\beta}\ln\left((mE^N\beta^2+1) + \sqrt{(mE^N\beta^2+1)^2-1}\right)$.

Let us consider a special solution $k=0$. The general solution (6.21) reduce to

$$\psi(x) = c_1 e^{i\gamma_+ x} + c_2 e^{i\gamma_- x}, \tag{6.22}$$

where $c_1 = A_{0,+}$ and $c_2 = A_{0_-}$ are arbitrary constants.

The continuity conditions at the boundaries $x=0$ and $x=L$ are given by

$$\psi(x=0) = 0; \qquad c_1 + c_2 = 0, \qquad c_2 = -c_1, \tag{6.23}$$

$$\psi(x=L) = 0; \qquad c_1 e^{i\gamma_+ L} + c_2 e^{i\gamma_- L} = 0. \tag{6.24}$$

Eq. (6.24) can be further simplified as follows

$$\begin{aligned} c_1 e^{i\gamma_+ L} - c_1 e^{i\gamma_- L} &= 0, \\ e^{i\gamma_+ L} - e^{i\gamma_- L} &= 0, \\ e^{i(\gamma_+ - \gamma_-)L} - 1 &= 0, \\ e^{i(\gamma_+ - \gamma_-)L} &= 1. \end{aligned} \tag{6.25}$$

Comparing equation (6.25) with Euler's equation $e^{i2n\pi} = \cos(2n\pi) \pm i\sin(2n\pi) = 1$ this gives

$$(\gamma_+ - \gamma_-)L = 2n\pi, \qquad n = 1, 2, 3, \ldots \tag{6.26}$$

According to relation (6.20) then the equation (6.26) becomes

$$\gamma_+ = \frac{n\pi}{L} = \frac{n\pi}{2a}, \qquad n = 1, 2, 3, \ldots \tag{6.27}$$

where *"a"* is defined as half width of the well, $L = 2a$. Hence the solution (6.22) with continuity conditions (6.23) reads

$$\psi(x) = c_1 \left(e^{i\left(\frac{n\pi}{2a}\right)x} - e^{-i\left(\frac{n\pi}{2a}\right)x}\right). \tag{6.28}$$

Using Euler's equation, $e^{\pm i\theta} = \cos\theta \pm i\sin\theta$, we obtain

$$\begin{aligned} \psi(x) &= c_1(\cos(\frac{n\pi x}{2a}) + i\sin(\frac{n\pi x}{2a}) - \cos(\frac{n\pi x}{2a}) + i\sin(\frac{n\pi x}{2a})), \\ &= A\sin(\frac{n\pi x}{2a}), \end{aligned} \tag{6.29}$$

where $A = 2ic_1$ is an arbitrary constant. According to normalization condition,

$$\int_0^{2a} dx\psi^*(x)\psi(x) = 1, \tag{6.30}$$

the constant $A$ becomes

$$\begin{aligned} \int_0^{2a} dx\left|A\right|^2\sin^2(\frac{n\pi x}{2a}) &= 1, \\ \frac{\left|A\right|^2}{2}\int_0^{2a} dx\left(1 - \cos(\frac{n\pi x}{a})\right) &= 1, \\ \frac{\left|A\right|^2}{2}\left(2a - \cancelto{0}{\frac{a}{n\pi}\sin(\frac{n\pi x}{a})\Big|_0^{2a}}\right) &= 1, \\ A &= \sqrt{\frac{1}{a}}. \end{aligned} \tag{6.31}$$

Therefore, normalized wavefunction of NEQH reads

$$\psi_n(x) = \sqrt{\frac{1}{a}}\sin(\frac{n\pi x}{2a}), \qquad n = 1, 2, 3, \ldots \tag{6.32}$$

To obtain the energy spectrum, substituting equation (6.32) into (6.4),

$$\begin{aligned} \hat{H}\psi(x) &= \left[\frac{1}{2\beta^2 m}\left(e^{-i\hbar\beta\frac{\partial}{\partial x}} + e^{i\hbar\beta\frac{\partial}{\partial x}}\right) - \frac{1}{\beta^2 m}\right]\left[\left(\sqrt{\frac{1}{a}}\sin(\frac{n\pi x}{2a})\right)\right], \\ &= \frac{1}{2\beta^2 m}\sqrt{\frac{1}{a}}\left(\sin(\frac{n\pi(x - i\hbar\beta)}{2a}) + \sin(\frac{n\pi(x + i\hbar\beta)}{2a})\right) \\ &\quad - \frac{1}{\beta^2 m}\left(\sqrt{\frac{1}{a}}\sin(\frac{n\pi x}{2a})\right), \\ &= \frac{1}{2\beta^2 m}\sqrt{\frac{1}{a}}\left(\sin(\frac{n\pi x}{2a})\cos(\frac{i\hbar\beta n\pi}{2a}) + \sin(\frac{n\pi x}{2a})\cos(\frac{i\hbar\beta n\pi}{2a})\right) \\ &\quad - \frac{1}{\beta^2 m}\left(\sqrt{\frac{1}{a}}\sin(\frac{n\pi x}{2a})\right), \\ &= \frac{1}{\beta^2 m}\cos(\frac{i\hbar\beta n\pi}{2a})\left(\sqrt{\frac{1}{a}}\sin(\frac{n\pi x}{2a})\right) - \frac{1}{\beta^2 m}\left(\sqrt{\frac{1}{a}}\sin(\frac{n\pi x}{2a})\right), \\ &= \left(\frac{1}{\beta^2 m}\cos(\frac{i\hbar\beta n\pi}{2a}) - \frac{1}{\beta^2 m}\right)\psi(x), \end{aligned} \tag{6.33}$$

and using the Schrödinger's equation, the energy of this system is given by

$$\begin{aligned}
\hat{H}\psi(x) &= E^N\psi(x), \\
\left(\frac{1}{\beta^2 m}\cos(\frac{i\hbar\beta n\pi}{2a}) - \frac{1}{\beta^2 m}\right)\psi(x) &= E_n^N\psi(x), \\
\left(\frac{1}{\beta^2 m}\cosh(\frac{\hbar\beta n\pi}{2a}) - \frac{1}{\beta^2 m}\right)\psi(x) &= E_n^N\psi(x).
\end{aligned} \tag{6.34}$$

Hence, the energy spectrum of this system becomes

$$E_n^N = \frac{1}{\beta^2 m}\cosh(\frac{\hbar\beta n\pi}{2a}) - \frac{1}{\beta^2 m}. \tag{6.35}$$

As we stated in previous chapter that as the suitable limit of parameter, the NEH will recover to standard Hamiltonian. For this, if we take limit $\beta \to 0$ to NEQH energy (6.35), we expect that the energy spectrum of (standard) infinite square well (3.15) is obtained. So, using Taylor's expansion to (6.35) and taking the limit of parameter $\beta \to 0$ , we obtain

$$\begin{aligned}
E_n^N &= \frac{1}{\beta^2 m}\left[1 + \frac{\hbar^2\beta^2 n^2\pi^2}{2(2a)^2} + \frac{\hbar^4\beta^4 n^4\pi^4}{4!(2a)^4} + ...\right] - \frac{1}{\beta^2 m}, \\
&= \frac{1}{\beta^2 m} + \frac{\hbar^2 n^2\pi^2}{2m(2a)^2} + \frac{\hbar^4\beta^2 n^4\pi^4}{4!m(2a)^4} + ... - \frac{1}{\beta^2 m}, \\
\lim_{\beta\to 0} E_n^N &= \frac{n^2\pi^2\hbar^2}{8ma^2} = E_n^S,
\end{aligned} \tag{6.36}$$

where $E_n^S$ is denoted as energy spectrum of standard case.

In contrast to classical case, the NEQH energy (6.35) is discrete. Recalling the standard infinite square well case, the energy has entirely discrete spectrum which consist infinite number of energy levels. Therefore, the result of NEQH energy also contains infinite number of energy levels similar to the standard case. However, difference between NEQH and standard case is that the NEQH is function of parameter $\beta$. Now we will evaluate effect of this parameter $\beta$ to the energy. Let us consider (6.35), and rewrite this equation in dimensionless quantities form,

$$E_n^d = \frac{1}{j^2}\cosh\left(\frac{jn\pi}{2}\right) - \frac{1}{j^2}, \tag{6.37}$$

where $E_n^d = ma^2 E_n^N/\hbar^2$ is dimensionless to measure energy, and $j = \hbar\beta/a$ is dimensionless to measure parameter $\beta$.

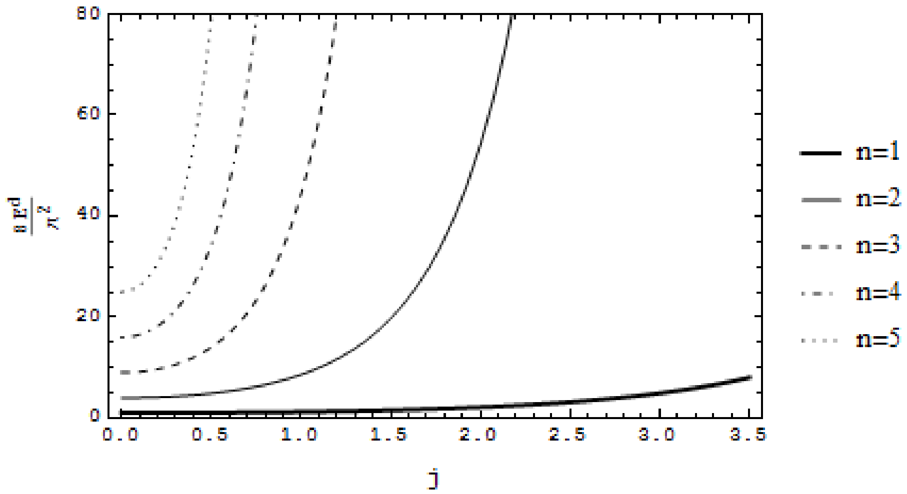



**Figure 8: Energy spectrum of NEQH with infinite square well**

For example, (dimensionless) energy plot for $n = 1, 2, 3, 4, 5$ with varying parameter $j$ is showed in Figure 8. According to this plot, NEQH energy is monotonically increasing i.e. energies of each levels are increase with respect to increasing of parameter $j$. Moreover, for the higher order of energy level for example n=5, it increases quicker than the lower one..

Taking limit $j \to 0$ to equation (6.37) gives

$$\lim_{j\to 0} E_n^d = \frac{n^2\pi^2}{8}. \tag{6.38}$$

NEQH energy recover to dimensionless form of standard energy (6.36). List of standard Hamiltonian energy levels (6.38) are shown in Table 2, and list of NEQH energy level with parameter $j$ are also presented in Table 3.

**Table 2: List of energy levels of standard Hamiltonian**

| n | energy level ($8E_n^d/\pi^2$) |
|---|---|
| 1 | 1 |
| 2 | 4 |
| 3 | 9 |
| 4 | 16 |
| 5 | 25 |
| 6 | 36 |
| $\vdots$ | $\vdots$ |

We have already shown that for small $j$, NEQH energy is close to standard energy. We also know that the NEQH energy is monotonically increase, so it can be expanded by series expansion. After that, we will consider higher order of energy spectrum by using perturbation in $j$ and compare with Taylor's expansion of NEQH energy. Now let us consider expansion of the NEQH (6.2)

$$\begin{aligned}
\hat{H}^N &= \frac{1}{2\beta^2 m}\left(\exp\left(-i\hbar\beta\frac{\partial}{\partial x}\right) + \exp\left(i\hbar\beta\frac{\partial}{\partial x}\right)\right) - \frac{1}{\beta^2 m}, \\
&= \frac{1}{\beta^2 m}\cos(\hbar\beta\frac{\partial}{\partial x}) - \frac{1}{\beta^2 m}, \\
&= \frac{1}{\beta^2 m}\left(1 - \frac{(\hbar\beta\frac{\partial}{\partial x})^2}{2!} + \frac{(\hbar\beta\frac{\partial}{\partial x})^4}{4!} - \frac{(\hbar\beta\frac{\partial}{\partial x})^6}{6!} + \frac{(\hbar\beta\frac{\partial}{\partial x})^8}{8!} - ...\right) - \frac{1}{\beta^2 m}, \\
&= \frac{1}{\beta^2 m} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{\hbar^4\beta^2}{4!m}\frac{\partial^4}{\partial x^4} - \frac{\hbar^6\beta^4}{6!m}\frac{\partial^6}{\partial x^6} + \frac{\hbar^8\beta^6}{8!m}\frac{\partial^8}{\partial x^8} - ... - \frac{1}{\beta^2 m}, \\
&= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{\hbar^4\beta^2}{24m}\frac{\partial^4}{\partial x^4} - \frac{\hbar^6\beta^4}{6!m}\frac{\partial^6}{\partial x^6} + \frac{\hbar^8\beta^6}{8!m}\frac{\partial^8}{\partial x^8} - ..., \\
&= H^0 + H^1 + H^2 + H^3 + \cdots . \qquad (6.39)
\end{aligned}$$

Therefore, zero-order perturbation Hamiltonian (standard Hamiltonian) gives

$$H^0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}. \qquad (6.40)$$

**Table 3: List of NEQH energy levels with varying parameter $j$**

| **n** | $j = 0$ | $j = 0.01$ | $j = 0.11$ | $j = 0.21$ | $j = 0.31$ | $j = 0.41$ | $j = 0.51$ | $j = 0.61$ | $j = 0.71$ | $j = 0.81$ | $j = 0.91$ | $\cdots$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1.000026 | 1.00249 | 1.0091 | 1.01992 | 1.03505 | 1.05464 | 1.07889 | 1.10805 | 1.1424 | 1.1823 | $\cdots$ |
| 2 | 4 | 4.00033 | 4.03997 | 4.1472 | 4.32632 | 4.58453 | 4.93237 | 5.38426 | 5.9593 | 6.68233 | 7.58534 | $\cdots$ |
| 3 | 9 | 9.00167 | 9.20334 | 9.75888 | 10.7188 | 12.1723 | 14.2578 | 17.1808 | 21.239 | 26.8653 | 34.6772 | $\cdots$ |
| 4 | 16 | 16.0053 | 16.6471 | 18.4603 | 21.7434 | 27.0558 | 35.3427 | 48.1535 | 68.0091 | 99.0173 | 147.905 | $\cdots$ |
| 5 | 25 | 25.0129 | 26.5942 | 31.2069 | 40.0663 | 55.6245 | 82.458 | 128.983 | 210.725 | 356.576 | 620.797 | $\cdots$ |
| 6 | 36 | 36.0267 | 39.3422 | 49.3984 | 70.1186 | 110.143 | 187.493 | 339.733 | 646.08 | 1275.86 | 2595.74 | $\cdots$ |
| 7 | 49 | 49.0494 | 55.2726 | 75.0321 | 119.168 | 214.017 | 421.54 | 889.164 | 1974.08 | 4557.00 | 10843.7 | $\cdots$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | |

First-order perturbation Hamiltonian gives

$$H^1 = \frac{\hbar^4\beta^2}{24m}\frac{\partial^4}{\partial x^4}. \tag{6.41}$$

Second-order perturbation Hamiltonian gives

$$H^2 = -\frac{\hbar^6\beta^4}{6!m}\frac{\partial^6}{\partial x^6}. \tag{6.42}$$

Recalling the perturbation theory, the first-order perturbation energy is expressed by equation (5.14). This gives

$$\begin{aligned}
E_n^1 &= \langle\psi_n^0|H^1|\psi_n^0\rangle, \\
&= \int_0^{2a}\sqrt{\frac{1}{a}}\sin(\frac{n\pi x}{2a})\frac{\hbar^4\beta^2}{24m}\left(\frac{\partial^4}{\partial x^4}\sqrt{\frac{1}{a}}\sin(\frac{n\pi x}{2a})\right)dx, \\
&= \frac{1}{a}\frac{\hbar^4\beta^2}{24m}\int_0^{2a}\sin(\frac{n\pi x}{2a})\frac{\partial^4}{\partial x^4}\sin(\frac{n\pi x}{2a})dx, \\
&= \frac{1}{a}\frac{\hbar^4\beta^2}{24m}\left(\frac{n\pi}{2a}\right)^4\int_0^{2a}\sin^2(\frac{n\pi x}{2a})dx, \\
&= \frac{1}{a}\frac{\hbar^4\beta^2}{24m}\left(\frac{n\pi}{2a}\right)^4\left(\frac{2a}{2}\right), \\
&= \frac{n^4\hbar^4\beta^2\pi^4}{384ma^4}.
\end{aligned} \tag{6.43}$$

Hence, first-order correction to the energy is

$$E_n^1 = \frac{n^4\hbar^4\beta^2\pi^4}{384ma^4}. \tag{6.44}$$

Expanding NEQH energy gives

$$\begin{aligned}
E_n^N &= \frac{1}{\beta^2 m}\cosh\left(\frac{\hbar\beta n\pi}{2a}\right) - \frac{1}{\beta^2 m}, \\
&= \frac{1}{\beta^2 m}\left[1+\frac{1}{2}\left(\frac{\hbar\beta n\pi}{2a}\right)^2+\frac{1}{4!}\left(\frac{\hbar\beta n\pi}{2a}\right)^4+\frac{1}{6!}\left(\frac{\hbar\beta n\pi}{2a}\right)^6+\cdot\right]-\frac{1}{\beta^2 m}, \\
&= \frac{1}{\beta^2 m}+\frac{n^2\hbar^2\pi^2}{2m(2a)^2}+\frac{n^4\hbar^4\beta^2\pi^4}{24m(2a)^4}+\frac{n^6\hbar^6\beta^4\pi^6}{6!m(2a)^6}+\cdots-\frac{1}{\beta^2 m.}, \\
&= \frac{n^2\hbar^2\pi^2}{8ma^2}+\frac{n^4\hbar^4\beta^2\pi^4}{384ma^4}+\frac{n^6\hbar^6\beta^4\pi^6}{6!m(2a)^6}+\cdots, \\
&= E_n^0+E_n^1+E_n^2+\cdots,
\end{aligned} \tag{6.45}$$

where $E_n^0$ and $E_n^1$ are zero-order energy (unperturbed energy) and first-order energy. Notice that the first-order correction to the energy (6.44) and first-order of expanding NEQH energy (6.45) are equivalent.

According to perturbation of wavefunction, notice that the wavefunctions of standard (3.14) and NEQH (6.32) are the same value. In the sense, these wavefunctions are not perturbed in parameter $\beta$. Hence, we expect that perturbation wavefunctions is zero. Now The expansion of perturbed wavefunctions are given by,

$$\psi_n = \psi_n^0 + \psi_n^1 + \cdots , \tag{6.46}$$

where $\psi_n^0$ are unperturbed wavefunctions and $\psi_n^1$ are fist-order perturbed wavefunctions. The first-order correction to wavefunction is expressed by equation (5.25)

$$\psi_n^1 = \sum_{r\neq n} \frac{\langle \psi_r^0 | H^1 | \psi_n^0 | \rangle}{(E_n^0 - E_r^0)} \psi_r^0.$$

We have

$$\begin{aligned} H^1|\psi_n^0\rangle &= \frac{\hbar^4\beta^2}{24m}\frac{\partial^4}{\partial x^4}\sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right), & (6.47)\\ &= \frac{\hbar^4\beta^2}{24m}\sqrt{\frac{1}{a}}\left(\frac{n\pi}{2a}\right)^4\sin\left(\frac{n\pi x}{2a}\right), & (6.48)\end{aligned}$$

then

$$\begin{aligned} \psi_n^1 &= \sum_{r\neq n} \frac{\int_0^{2a}\sqrt{\frac{1}{a}}\sin(\frac{r\pi x}{2a})\frac{\hbar^4\beta^2}{24m}\sqrt{\frac{1}{a}}\left(\frac{n\pi}{2a}\right)^4\sin(\frac{n\pi x}{2a})dx}{\frac{\hbar^2\pi^2}{2mL^2}(n^2-r^2)}\psi_r^0, \\ &= \frac{n^4\pi^2\hbar^2\beta^2}{48a^3}\sum_{r\neq n}\frac{\int_0^{2a}\sin(\frac{r\pi x}{2a})\sin(\frac{n\pi x}{2a})dx}{r^2-n^2}\psi_r^0, \\ &= \frac{n^4\pi^2\hbar^2\beta^2}{24a^3}\sum_{r\neq n}\frac{an\overbrace{\sin(r\pi)}^{0}\cos(n\pi) - ar\cos(r\pi)\overbrace{\sin(n\pi)}^{0}}{r^2-n^2}\sqrt{\frac{1}{a}}\sin\left(\frac{r\pi x}{2a}\right), \\ &= 0. & (6.49)\end{aligned}$$

The first-order correction to the wavefunction is zero. Therefore the NEQH wavefunctions reads

$$\psi_n = \psi_n^0 + \psi_n^1 = \sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right). \tag{6.50}$$

It satisfies what we expect.

For the case of second-order correction we need to modify formula (5.30) which add second-order term to Hamiltonian namely

$$H = H^0 + lH^1 + l^2H^2. \tag{6.51}$$

Wavefunction and energy can be expressed in power series as

$$\begin{aligned} \psi_n &= \psi^0 + l\psi^1 + l^2\psi^2 + \cdots , \\ E_n &= E_n^0 + lE_0^1 + l^2E_n^2 + \cdots . \end{aligned}$$

Substituting into Schrödinger's equation, $H\psi_n = E_n\psi_n$, the second-order ($l^2$) is given by

$$H^0\psi_n^2 + H^1\psi_n^1 + H^2\psi_n^0 = E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0. \tag{6.52}$$

Taking inner product $\psi_n^0$, we obtain

$$\langle\psi_n^0|H^0|\psi_n^2\rangle + \langle\psi_n^0|H^1|\psi_n^1\rangle + \langle\psi_n^0|H^2|\psi_n^0\rangle = E_n^0\langle\psi_n^0|\psi_n^2\rangle + E_n^1\langle\psi_n^0|\psi_n^1\rangle + E_n^2\langle\psi_n^0|\psi_n^0\rangle. \tag{6.53}$$

For the Hermiticity of $H^0$ the first term of left-hand-side of the equation (6.53) reads

$$\langle\psi_n^0|H^0|\psi_n^2\rangle = \langle H^0\psi_n^0|\psi_n^2\rangle = E_n^0\langle\psi_n^0|\psi_n^2\rangle, \tag{6.54}$$

and cancel out to the first term of right-hand-side. Hence the equation (6.53) becomes

$$\langle\psi_n^0|H^1|\psi_n^1\rangle + \langle\psi_n^0|H^2|\psi_n^0\rangle = E_n^1\langle\psi_n^0|\psi_n^1\rangle + E_n^2. \tag{6.55}$$

Writing $\psi_n^1$ with linear combination of $\psi_n^0$ and substituting into equation (6.55) gives

$$\sum_{m\neq n} c_{nm}^1\langle\psi_n^0|H^1|\psi_m^0\rangle + \langle\psi_n^0|H^2|\psi_n^0\rangle = E_n^1\sum_{m\neq n}\langle\psi_n^0|\psi_m^0\rangle + E_n^2. \tag{6.56}$$

Using orthonormality of wavefunction the first term of right-hand-side of equation (6.56) is zero, and using equation (5.24) the second-order correction to energy is expressed as

$$E_n^2 = \sum_{m\neq n} \frac{\langle\psi_m^0|H^1|\psi_n^0\rangle\langle\psi_n^0|H^1|\psi_m^0\rangle}{E_n^0 - E_m^0} + \langle\psi_n^0|H^2|\psi_n^0\rangle,$$
$$= \sum_{m\neq n} \frac{|\langle\psi_n^0|H^1|\psi_m^0\rangle|^2}{E_n^0 - E_m^0} + \langle\psi_n^0|H^2|\psi_n^0\rangle. \quad (6.57)$$

Substituting equation (6.41), (6.42) into equation (6.57) the second-order correction to the energy is then given by

$$E_n^2 = \sum_{r\neq n} \frac{\left|\left\langle\sqrt{\tfrac{1}{a}}\sin\left(\tfrac{n\pi x}{2a}\right)\middle|\tfrac{\hbar^4\beta^2}{24m}\tfrac{\partial^4}{\partial x^4}\sqrt{\tfrac{1}{a}}\sin\left(\tfrac{r\pi x}{2a}\right)\right\rangle\right|^2}{\frac{\hbar^2\pi^2(n^2-r^2)}{8ma^2}} + \langle\psi_n^0|H^2|\psi_n^0\rangle,$$
$$= \sum_{r\neq n} \frac{\left|\tfrac{1}{a}\tfrac{\hbar^4\beta^2}{24m}\left\langle\sin\left(\tfrac{n\pi x}{2a}\right)\middle|\tfrac{\partial^4}{\partial x^4}\sin\left(\tfrac{r\pi x}{2a}\right)\right\rangle\right|^2}{\frac{\hbar^2\pi^2(n^2-r^2)}{8ma^2}} + \langle\psi_n^0|H^2|\psi_n^0\rangle,$$
$$= \sum_{r\neq n} \frac{\left|\tfrac{1}{a}\tfrac{\hbar^4\beta^2}{24m}\left(\tfrac{n\pi}{2a}\right)^4\int_0^{2a}\sin\left(\frac{n\pi x}{2a}\right)\sin\left(\frac{r\pi x}{2a}\right)dx\right|^2}{\frac{\hbar^2\pi^2(n^2-r^2)}{8ma^2}} + \langle\psi_n^0|H^2|\psi_n^0\rangle,$$
$$= \sum_{r\neq n} \frac{\left|\tfrac{1}{a}\tfrac{\hbar^4\beta^2}{24m}\left(\tfrac{n\pi}{2a}\right)^4\left[an\cancelto{0}{\sin(r\pi)}\cos(n\pi) - ar\cos(r\pi)\cancelto{0}{\sin(n\pi)}\right]\right|^2}{\frac{\hbar^2\pi^2(n^2-r^2)}{8ma^2}} + \langle\psi_n^0|H^2|\psi_n^0\rangle,$$
(6.58)

$$E_n^2 = \langle\psi_n^0|H^2|\psi_n^0\rangle = \left\langle\sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right)\middle|\frac{-\hbar^6\beta^4}{6!m}\frac{\partial^6}{\partial x^6}\sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right)\right\rangle,$$
$$= -\frac{1}{a}\frac{\hbar^6\beta^4}{6!m}\left(\frac{n\pi}{2a}\right)^6\left[-\cancelto{a}{\int_0^{2a}\sin^2\left(\frac{n\pi x}{2a}\right)dx}\right],$$
$$= \frac{n^6\pi^6\hbar^6\beta^4}{6!m(2a)^6}. \quad (6.59)$$

This energy $E_n^2$ agrees with the second-order energy which expand by Talor's expansion (6.45).

Second-order correction to the wavefunction can be found. By rewriting equation (6.52) and taking inner product with $\psi_l^0$, we obtain

$$\begin{aligned}
(H^0 - E_n^0)\psi_n^2 &= -(H^1 - E_n^1)\psi_n^1 - (H^2 - E_n^2)\psi_n^0, \\
\langle\psi_l^0|(H^0 - E_n^0)|\psi_n^2\rangle &= -\langle\psi_l^0|(H^1 - E_n^1)|\psi_n^1\rangle - \langle\psi_l^0|(H^2 - E_n^2)|\psi_n^0\rangle, \\
\sum_{m\neq n}(E_m^0 - E_n^0)c_{nm}^2\langle\psi_l^0|\psi_m^0\rangle &= -\sum_{m\neq n} c_{nm}^1\langle\psi_l^0|H^1|\psi_m^0\rangle + E_n^1\sum_{m\neq n} c_{nm}^1\langle\psi_l^0|\psi_m^0\rangle, \\
&\quad -\langle\psi_l^0|H^2|\psi_n^0\rangle + E_n^2\langle\psi_l^0|\psi_n^0\rangle. \qquad (6.60)
\end{aligned}$$

If $l = n$, the equation (6.60) recover to second-order correction to energy. The second case, if $l \neq n$, the last equation of right-hand-side of (6.60) is zero, then the equation (6.60) becomes

$$\begin{aligned}
(E_l^0 - E_n^0)c_{nl}^2 &= -\sum_{m\neq n} c_{nm}^1\langle\psi_l^0|H^1|\psi_m^0\rangle + E_n^1 c_{nl}^1 - \langle\psi_l^0|H^2|\psi_n^0\rangle, \\
&= -\sum_{m\neq n}\frac{\langle\psi_m^0|H^1|\psi_n^0\rangle\langle\psi_l^0|H^1|\psi_m^0\rangle}{E_n^0 - E_m^0} + \frac{\langle\psi_n^0|H^1|\psi_n^0\rangle\langle\psi_l^0|H^1|\psi_n^0\rangle}{E_n^0 - E_l^0} \\
&\quad -\langle\psi_l^0|H^2|\psi_n^0\rangle, \qquad (6.61)
\end{aligned}$$

$$c_{nl}^2 = \sum_{m\neq n}\frac{\langle\psi_m^0|H^1|\psi_n^0\rangle\langle\psi_l^0|H^1|\psi_m^0\rangle}{(E_n^0 - E_l^0)(E_n^0 - E_m^0)} - \frac{\langle\psi_n^0|H^1|\psi_n^0\rangle\langle\psi_l^0|H^1|\psi_n^0\rangle}{(E_n^0 - E_l^0)^2} + \frac{\langle\psi_l^0|H^2|\psi_n^0\rangle}{E_n^0 - E_l^0}. \quad (6.62)$$

Hence second-order correction to wavefunctions, by interchanging index $l \Leftrightarrow m$, is expressed as

$$\psi_n^2 = \sum_{m\neq n}\left[\sum_{l\neq n}\frac{\langle\psi_l^0|H^1|\psi_n^0\rangle\langle\psi_m^0|H^1|\psi_l^0\rangle}{(E_n^0 - E_m^0)(E_n^0 - E_l^0)} - \frac{\langle\psi_n^0|H^1|\psi_n^0\rangle\langle\psi_m^0|H^1|\psi_n^0\rangle}{(E_n^0 - E_m^0)^2} + \frac{\langle\psi_m^0|H^2|\psi_n^0\rangle}{E_n^0 - E_m^0}\right]\psi_m^0. \quad (6.63)$$

To obtain second-order correction to wavefunction, let us consider the equation (6.63) by using (6.41) and (6.42). This gives

$$\psi_n^2 = \sum_{m\neq n}\left[\underbrace{\sum_{l\neq n}\frac{\langle\psi_l^0|H^1|\psi_n^0\rangle\langle\psi_m^0|H^1|\psi_l^0\rangle}{(E_n^0 - E_m^0)(E_n^0 - E_l^0)}}_{1} - \underbrace{\frac{\langle\psi_n^0|H^1|\psi_n^0\rangle\langle\psi_m^0|H^1|\psi_n^0\rangle}{(E_n^0 - E_m^0)^2}}_{2} + \underbrace{\frac{\langle\psi_m^0|H^2|\psi_n^0\rangle}{E_n^0 - E_m^0}}_{3}\right]\psi_m^0. \quad (6.64)$$

The first term gives

$$
\begin{aligned}
&\sum_{l\neq n}\frac{\langle\psi_l^0|H^1|\psi_n^0\rangle\langle\psi_m^0|H^1|\psi_l^0\rangle}{(E_n^0-E_m^0)(E_n^0-E_l^0)}\\
=\;&\sum_{l\neq n}\frac{\left[\int_0^{2a}\sqrt{\frac{1}{a}}\sin\left(\frac{l\pi x}{2a}\right)\frac{\hbar^4\beta^2}{24m}\frac{\partial^4}{\partial x^4}\sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right)dx\right]\left[\int_0^{2a}\sqrt{\frac{1}{a}}\sin\left(\frac{m\pi x}{2a}\right)\frac{\hbar^4\beta^2}{24m}\frac{\partial^4}{\partial x^4}\sqrt{\frac{1}{a}}\sin\left(\frac{l\pi x}{2a}\right)dx\right]}{(E_n^0-E_m^0)(E_n^0-E_l^0)},\\
=\;&\sum_{l\neq n}\frac{\left[\frac{1}{a}\frac{\hbar^4\beta^2}{24m}\left(\frac{n\pi}{2a}\right)^4\int_0^{2a}\sin\left(\frac{l\pi x}{2a}\right)\sin\left(\frac{n\pi x}{2a}\right)dx\right]\left[\frac{1}{a}\frac{\hbar^4\beta^2}{24m}\left(\frac{l\pi}{2a}\right)^4\int_0^{2a}\sin\left(\frac{m\pi x}{2a}\right)\sin\left(\frac{l\pi x}{2a}\right)dx\right]}{(E_n^0-E_m^0)(E_n^0-E_l^0)},\\
=\;&\sum_{l\neq n}\left[\frac{1}{a}\frac{\hbar^4\beta^2}{24m}\left(\frac{n\pi}{2a}\right)^4\left(al\cancelto{0}{\sin(n\pi)}\cos(l\pi)-an\cos(n\pi)\cancelto{0}{\sin(l\pi)}\right)\right]\\
&\times\left[\frac{1}{a}\frac{\hbar^4\beta^2}{24m}\left(\frac{l\pi}{2a}\right)^4\left(am\cancelto{0}{\sin(l\pi)}\cos(m\pi)-al\cos(l\pi)\cancelto{0}{\sin(m\pi)}\right)\right]\Bigg/(E_n^0-E_m^0)(E_n^0-E_l^0),\\
=\;&0.
\end{aligned}
$$

The second term gives

$$
\begin{aligned}
&\frac{\langle\psi_n^0|H^1|\psi_n^0\rangle\langle\psi_m^0|H^1|\psi_n^0\rangle}{(E_n^0-E_m^0)^2}\\
=\;&\frac{\left[\int_0^{2a}\sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right)\frac{\hbar^4\beta^2}{24m}\frac{\partial^4}{\partial x^4}\sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right)dx\right]\left[\int_0^{2a}\sqrt{\frac{1}{a}}\sin\left(\frac{m\pi x}{2a}\right)\frac{\hbar^4\beta^2}{24m}\frac{\partial^4}{\partial x^4}\sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right)dx\right]}{(E_n^0-E_m^0)^2},\\
=\;&\frac{\left[\frac{1}{a}\frac{\hbar^4\beta^2}{24m}\left(\frac{n\pi}{2a}\right)^4\cancelto{a}{\int_0^{2a}\sin^2\left(\frac{n\pi x}{2a}\right)dx}\right]\left[\frac{1}{a}\frac{\hbar^4\beta^2}{24m}\left(\frac{n\pi}{2a}\right)^4\int_0^{2a}\sin\left(\frac{m\pi x}{2a}\right)\sin\left(\frac{n\pi x}{2a}\right)dx\right]}{(E_n^0-E_m^0)^2},\\
=\;&\frac{\left[\frac{\hbar^4\beta^2}{24m}\left(\frac{n\pi}{2a}\right)^4\right]\left[\frac{1}{a}\frac{\hbar^4\beta^2}{24m}\left(\frac{n\pi}{2a}\right)^4\left(am\cancelto{0}{\sin(n\pi)}\cos(m\pi)-an\cos(n\pi)\cancelto{0}{\sin(m\pi)}\right)\right]}{(E_n^0-E_m^0)^2},\\
=\;&0.
\end{aligned}
$$

The third term gives

$$
\begin{aligned}
&\frac{\langle\psi_m^0|H^2|\psi_n^0\rangle}{E_n^0 - E_m^0} \\
&= \frac{\int_0^{2a}\sqrt{\frac{1}{a}}\sin\left(\frac{m\pi x}{2a}\right)\left[-\frac{\hbar^6\beta^6}{6!m}\frac{\partial^6}{\partial x^6}\sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right)\right]dx}{E_n^0 - E_m^0}, \\
&= \frac{\left[-\frac{1}{a}\frac{\hbar^6\beta^6}{6!m}\left(\frac{n\pi}{2a}\right)^6\right]\left[-\int_0^{2a}\sin\left(\frac{m\pi x}{2a}\right)\sin\left(\frac{n\pi x}{2a}\right)dx\right]}{E_n^0 - E_m^0}, \\
&= \frac{\left[\frac{1}{a}\frac{\hbar^6\beta^6}{6!m}\left(\frac{n\pi}{2a}\right)^6\right]\left[\left(am\cancelto{0}{\sin(n\pi)}\cos(m\pi) - an\cos(n\pi)\cancelto{0}{\sin(m\pi)}\right)\right]}{E_n^0 - E_m^0}, \\
&= 0.
\end{aligned}
$$

The first, second, and third terms of equation (6.64) are zero. Hence, the second-order correction to wavefunction is

$$\psi_n^2 = 0. \tag{6.65}$$

The first- and second- order correction to the wavefucntons are zero, thus the wavefunctions is then given by

$$\psi_n = \psi_n^0 + \psi_n^1 + \psi_n^2 = \sqrt{\frac{1}{a}}\sin\left(\frac{n\pi x}{2a}\right). \tag{6.66}$$

### 6.2 Newton's equivalent Hamiltonians with quantum finite square well

Next physical system, which we apply NEQH, is finite square well potential:

$$V(x) = \begin{cases} 0, & \text{if} \quad 0 \leq x \leq L \\ V_0, & \text{if} \quad x < 0, \quad x > L. \end{cases} \tag{6.67}$$

The illustration of this potential is expressed in Figure 9.

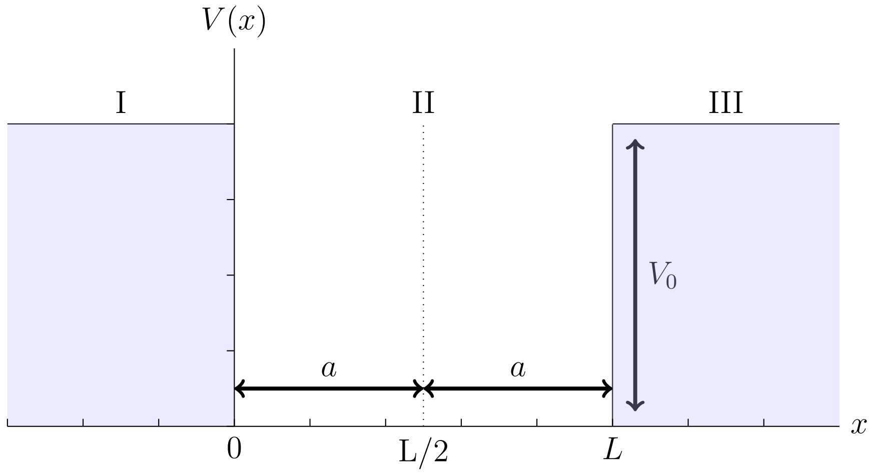



**Figure 9: Finite square well system**

The difference between this system and infinite square well is that this system has two cases of energy. First, energy of a particle has greater than potential, $E^N > V_0$. This case is called scattering case. Second case is bound state, and the energy of a particle has less than potential, $E^N < V_0$. As part of our work, we interested in case of bound state, and showed the occurrence of quantized energy with Schrödinger's equation.

Let us follow the standard method of solving finite square well potential by first studying the three regions separately.

$$\begin{aligned} &\text{Region I} && x < 0, \\ &\text{Region II} && 0 < x < L, \\ &\text{Region III} && x > L. \end{aligned} \tag{6.68}$$

In region II ($0 < x < L$), the potential is zero, $V(x) = 0$. The NEQH (2.55) becomes

$$\hat{H} = \frac{1}{2\beta^2 m}\left(e^{-i\hbar\beta\frac{\partial}{\partial x}} + e^{i\hbar\beta\frac{\partial}{\partial x}}\right) - \frac{1}{\beta^2 m}.$$

Time independent Schrödinger's equation gives same solution as infinite square well. Therefore the solution reads

$$\psi_{\text{II}} = B\cos(\gamma_+ x) + C\sin(\gamma_+ x), \tag{6.69}$$

where $\gamma_+ = (1/\hbar\beta)\ln\left(m\beta^2 E^N + 1 + \sqrt{(m\beta^2 E^N + 1)^2 - 1}\right)$. In order to obtain energy spectrum, substituting this wavefunction (6.69) into NEQH Schrödinger equation gives

$$E^N = \frac{1}{\beta^2 m}\cosh(\hbar\beta\gamma_+) - \frac{1}{\beta^2 m}. \tag{6.70}$$

In region I, $x < 0$, the potential $V(x)$ is a constant, denoted as $V(x) = V_0$. The Hamiltonian operator (2.55) becomes

$$\begin{aligned} \hat{H} &= \frac{1}{2\beta^2 m}\left[(1 + i\beta\sqrt{2mV_0})^{1/2} e^{-i\hbar\beta\frac{\partial}{\partial x}}(1 - i\beta\sqrt{2mV_0})^{1/2} + (i \to -i)\right] - \frac{1}{\beta^2 m}, \\ &= \frac{1}{2\beta^2 m}\left[(1 - i^2 2\beta^2 m V_0)^{1/2} e^{-i\hbar\beta\frac{\partial}{\partial x}} + (i \to -i)\right] - \frac{1}{\beta^2 m}, \\ &= \frac{1}{2\beta^2 m}\left[(1 + 2\beta^2 m V_0)^{1/2} e^{-i\hbar\beta\frac{\partial}{\partial x}} + (1 + 2\beta^2 m V_0)^{1/2} e^{i\hbar\beta\frac{\partial}{\partial x}}\right] - \frac{1}{\beta^2 m}, \\ &= \frac{\sqrt{1 + 2\beta^2 m V_0}}{2\beta^2 m}\left[e^{-i\hbar\beta\frac{\partial}{\partial x}} + e^{i\hbar\beta\frac{\partial}{\partial x}}\right] - \frac{1}{\beta^2 m}. \end{aligned} \tag{6.71}$$

Time independent Schrödinger's equation then reads

$$\frac{\sqrt{1 + 2m\beta^2 V_0}}{2\beta^2 m}\left(e^{-i\hbar\beta\frac{\partial}{\partial x}} + e^{i\hbar\beta\frac{\partial}{\partial x}}\right)\psi(x) - \frac{1}{\beta^2 m}\psi(x) = E^N\psi(x). \tag{6.72}$$

This is simply a homogeneous ordinary differential equation. Therefore, let us consider an ansatz $\psi(x) = e^{ilx}$, where $l \in \mathbb{C}$. This gives

$$\sqrt{1+2m\beta^2 V_0}\cosh(l\hbar\beta) = 1 + m\beta^2 E^N. \tag{6.73}$$

By writing $l$ in terms of its real and imaginary part as $l = l_R + il_I$, we obtain

$$\begin{aligned} \cosh(l_R\hbar\beta + il_I\hbar\beta) &= \frac{1+m\beta^2 E^N}{\sqrt{1+2m\beta^2 V_0}}, \\ \cosh(l_R\hbar\beta)\cos(l_I\hbar\beta) + i\sinh(l_R\hbar\beta)\sin(l_I\hbar\beta) &= \frac{1+m\beta^2 E^N}{\sqrt{1+2m\beta^2 V_0}}. \end{aligned} \tag{6.74}$$

By demanding that the imaginary part of the left-hand-side vanishes, we obtain the conditions

$$l_R = 0, \qquad \textit{or} \qquad l_I = \frac{n\pi}{\hbar\beta}. \tag{6.75}$$

That is, there are two main cases to consider.

<u>Case1</u>: $l_R = 0$. In this case, the equation (6.74) reduces to

$$\cos(l_I\hbar\beta) = \frac{1+m\beta^2 E^N}{\sqrt{1+2m\beta^2 V_0}}. \tag{6.76}$$

Solution of this equation reads

$$l_I = \pm\frac{1}{\hbar\beta}\cos^{-1}\left(\frac{1+m\beta^2 E^N}{\sqrt{1+2m\beta^2 V_0}}\right) + \frac{2k\pi}{\hbar\beta}, \tag{6.77}$$

This case is valid for

$$\frac{-\sqrt{1+2m\beta^2 V_0}-1}{m\beta^2} \leq E^N \leq \frac{\sqrt{1+2m\beta^2 V_0}-1}{m\beta^2}. \tag{6.78}$$

<u>Case2</u>: $l_I = n\pi/\hbar\beta$. In this case, the equation (6.74) reduce to

$$\cosh(\hbar\beta l_R)(-1)^n = \frac{1+m\beta^2 E^N}{\sqrt{1+2m\beta^2 V_0}}. \tag{6.79}$$

This is further separated into two subcases:

<u>Case2.1</u>: $l_I = n\pi/\hbar\beta$ with $n$ even. In this case

$$\cosh(\hbar\beta l_R) = \frac{1+m\beta^2 E^N}{\sqrt{1+2m\beta^2 V_0}}. \tag{6.80}$$

Solution of this equation reads

$$l_R = \pm\frac{1}{\hbar\beta}\ln\left(\frac{1+m\beta^2E^N+\sqrt{(1+m\beta^2E^N)^2}-(1+2m\beta^2V_0)}{\sqrt{1+2m\beta^2V_0}}\right). \tag{6.81}$$

It is valid for

$$E^N \geq \frac{\sqrt{1+2m\beta^2V_0}-1}{m\beta^2}. \tag{6.82}$$

Case2.2:$l_I = n\pi/\hbar\beta$ with $n$ odd. In this case,

$$\cosh(\hbar\beta l_R) = -\frac{1+m\beta^2E^N}{\sqrt{1+2m\beta^2V_0}}. \tag{6.83}$$

Solution of this equation reads

$$l_R = \pm\frac{1}{\hbar\beta}\ln\left(\frac{-(1+m\beta^2E^N)+\sqrt{(1+m\beta^2E^N)^2-(1+2m\beta^2V_0)}}{\sqrt{1+2m\beta^2V_0}}\right). \tag{6.84}$$

It is valid for

$$E^N \leq \frac{-\sqrt{1+2m\beta^2V_0}-1}{m\beta^2}. \tag{6.85}$$

In principle, in order to solve the time independent Schrödinger's equation (6.72), one starts from giving the value of $E^N$. Then in each region, one determines the range into which this value of $E^N$ falls. This gives the corresponding case to be considered. We are interested in bound states. So let us first consider the value of $E^N$ such that in Region I&III, Case 1 is applied. This gives

$$0 \leq E^N \leq \frac{\sqrt{1+2m\beta^2V_0}-1}{m\beta^2}. \tag{6.86}$$

We consider this case because it will reduce in the limit $\beta \to 0$ to finite square well in standard quantum mechanics. Now, The solution of wavefunction in Region I is given by

$$\psi_{\mathrm{I}}(x) = \sum_{k=-\infty}^{\infty}(A_{k,-}e^{-l_{I0}x}+A_{k,+}e^{l_{I0}x})e^{\frac{2\pi kx}{\hbar\beta}}, \tag{6.87}$$

where

$$l_{I0} = \frac{1}{\hbar\beta}\cos^{-1}\left(\frac{1+m\beta^2E^N}{\sqrt{1+2m\beta^2V_0}}\right). \tag{6.88}$$

It can be seen that there are infinite many arbitrary constants $A_{k,\pm}$. So, we restrict ourself by considering only special case $k = 0$. The equation (6.87) reduces to

$$\psi_{\mathrm{I}} = A_{0,-}e^{-l_{I0}x} + A_{0,+}e^{l_{I0}x}. \tag{6.89}$$

By demanding $\psi_{\mathrm{I}}(x) \to 0$ as $x \to -\infty$, we obtain

$$\psi_{\mathrm{I}} = Ae^{l_{I0}x}, \tag{6.90}$$

where $A_{0,-} = A$ is arbitrary constant. In order to obtain energy spectrum for Region II, substituting wavefunction (6.90) into Schrödinger equation gives

$$E^N = \frac{\sqrt{1+2\beta^2 mV_0}}{\beta^2 m}\cos(\hbar\beta l_{I0}) - \frac{1}{\beta^2 m}. \tag{6.91}$$

The analysis in Region III can be done in similar way except that the condition $\psi_{\mathrm{III}} \to 0$ as $x \to \infty$ has to be imposed. This gives

$$\psi_{\mathrm{III}} = De^{-l_{I0}x}. \tag{6.92}$$

The energy spectrum in this Region is also the same as Region I. Now we have summary three equations of wavefunction in three region i.e.

$$\begin{aligned}
\psi_{\mathrm{I}} &= Ae^{l_{I0}x}, \\
\psi_{\mathrm{II}} &= B\cos(\gamma_+ x) + C\sin(\gamma_+ x), \\
\psi_{\mathrm{III}} &= De^{-l_{I0}x},
\end{aligned}$$

where $l_{I0} = (1/\hbar\beta)\cos^{-1}\left((m\beta^2 E^N + 1)/\sqrt{1+2m\beta^2 V_0}\right)$,
and $\gamma_+ = (1/\hbar\beta)\ln\left((m\beta^2 E^N + 1) + \sqrt{(m\beta^2 E^N+1)^2 - 1}\right)$.

At the boundaries at $x = 0$ and $x = L$ has to satisfy continuity conditions as follows. 1.) $\psi$ is always continuous, and 2.) $d\psi/dx$ is continuous. In this case the first boundary condition at $x = 0$ tell us

$$\psi_{\mathrm{I}}|_{x=0} = \psi_{\mathrm{II}}|_{x=0}, \tag{6.93}$$

$$\begin{aligned} Ae^{l_{I0}(0)} &= B\cos(\gamma_+(0)) + C\sin(\gamma_+(0)), \\ A &= B, \end{aligned} \tag{6.94}$$

and second boundary gives

$$\frac{d\psi_{\mathrm{I}}}{dx}\Big|_{x=0} = \frac{d\psi_{\mathrm{II}}}{dx}\Big|_{x=0}, \tag{6.95}$$

$$\begin{aligned} l_{I0}Ae^{l_{I0}x}|_{x=0} &= -B\gamma_+\sin(\gamma_+x)|_{x=0} + C\gamma_+\cos(\gamma_+x)|_{x=0}, \\ l_{I0}A &= C\gamma_+, \\ C &= \frac{l_{I0}}{\gamma_+}A. \end{aligned} \tag{6.96}$$

At the boundary $x = L$ is given by

$$\psi_{\mathrm{II}}\big|_{x=L} = \psi_{\mathrm{III}}\big|_{x=L}, \tag{6.97}$$

$$B\cos(\gamma_+L) + C\sin(\gamma_+L) = De^{-l_{I0}L}, \tag{6.98}$$

and

$$\frac{d\psi_{\mathrm{II}}}{dx}\Big|_{x=L} = \frac{d\psi_{\mathrm{III}}}{dx}\Big|_{x=L}, \tag{6.99}$$

$$\begin{aligned} -B\gamma_+\sin(\gamma_+x)|_{x=L} + C\gamma_+\cos(\gamma_+x)|_{x=L} &= -l_{I0}De^{-l_{I0}x}|_{x=L}, \\ -B\gamma_+\sin(\gamma_+L) + C\gamma_+\cos(\gamma_+L) &= -l_{I0}De^{-l_{I0}L}. \end{aligned} \tag{6.100}$$

Substituting equation (6.98) into (6.100) and using equation (6.94), (6.96) gives

$$\begin{aligned} -B\gamma_+\sin(\gamma_+L) + C\gamma_+\cos(\gamma_+L) &= -l_{I0}\left(B\cos(\gamma_+L) + C\sin(\gamma_+L)\right), \\ -A\gamma_+\sin(\gamma_+L) + \left(\frac{l_{I0}}{\gamma_+}\right)A\gamma_+\cos(\gamma_+L) &= -l_{I0}\left(A\cos(\gamma_+L) + \left(\frac{l_{I0}}{\gamma_+}\right)A\sin(\gamma_+L)\right), \\ -\gamma_+\sin(\gamma_+L) + \left(\frac{l_{I0}}{\gamma_+}\right)\gamma_+\cos(\gamma_+L) &= -l_{I0}\cos(\gamma_+L) - l_{I0}\left(\frac{l_{I0}}{\gamma_+}\right)\sin(\gamma_+L), \\ \gamma_+^2\sin(\gamma_+L) - l_{I0}^2\sin(\gamma_+L) &= 2l_{I0}\gamma_+\cos(\gamma_+L), \\ \left(\gamma_+^2 - l_{I0}^2\right)\sin(\gamma_+L) &= 2l_{I0}\gamma_+\cos(\gamma_+L). \end{aligned} \tag{6.101}$$

This solution (6.101) comes from imaginary part of equation $\text{Im}(l_{I0}+i\gamma_+)^2 e^{i\gamma_+ L} = 0$.

Proof:

$$\begin{aligned}
\text{Im}(l_{I0}+i\gamma_+)^2 e^{i\gamma_+ L} &= \text{Im}(l_{I0}^2 + 2il_{I0}\gamma_+ - \gamma_+^2)(\cos(\gamma_+ L) + i\sin(\gamma_+ L)), \\
&= \text{Im}\Big[(l_{I0}^2 - \gamma_+^2)c\cos(\gamma_+ L) - 2\gamma_+ l_{I0}\sin(\gamma_+ L) \\
&\quad i((l_{I0}^2 - \gamma_+)\sin(\gamma_+ L) + 2\gamma_+ l_{I0}\cos(\gamma_+ L))\Big], \\
&= (l_{I0}^2 - \gamma_+)\sin(\gamma_+ L) + 2\gamma_+ l_{I0}\cos(\gamma_+ L), \qquad (6.102)
\end{aligned}$$

when, $\text{Im}(l_{I0}+i\gamma_+)^2 e^{i\gamma_+ L} = 0$,

$$\begin{aligned}
(l_{I0}^2 - \gamma_+)\sin(\gamma_+ L) + 2\gamma_+ l_{I0}\cos(\gamma_+ L) &= 0, \\
(\gamma_+^2 - l_{I0}^2)\sin(\gamma_+ L) &= 2\gamma_+ l_{I0}\cos(\gamma_+ L). \qquad (6.103)
\end{aligned}$$

Hence, the solution agree with (6.101). Now let us consider imaginary part of equation $(l_{I0}+i\gamma_+)^2 e^{i\gamma_+ L} = 0$,

$$\begin{aligned}
\text{Im}(l_{I0}+i\gamma_+)^2 e^{i\gamma_+ L} &= 0, \\
\text{Im}(l_{I0}e^{i\gamma_+\frac{L}{2}} + i\gamma_+ e^{i\gamma_+\frac{L}{2}})^2 &= 0, \\
\text{Im}\left[l_{I0}\left(\cos(\gamma_+\frac{L}{2}) + i\sin(\gamma_+\frac{L}{2})\right) + i\gamma_+\left(\cos(\gamma_+\frac{L}{2}) + i\sin(\gamma_+\frac{L}{2})\right)\right]^2 &= 0, \\
\text{Im}\left[l_{I0}\cos(\gamma_+\frac{L}{2}) + il_{I0}\sin(\gamma_+\frac{L}{2}) + i\gamma_+\cos(\gamma_+\frac{L}{2}) - \gamma_+\sin(\gamma_+\frac{L}{2})\right]^2 &= 0, \\
\text{Im}\left[\underbrace{l_{I0}\cos(\gamma_+\frac{L}{2}) - \gamma_+\sin(\gamma_+\frac{L}{2})}_{x} + \underbrace{i\left(l_{I0}\sin(\gamma_+\frac{L}{2}) + \gamma_+\cos(\gamma_+\frac{L}{2})\right)}_{iy}\right]^2 &= 0,
\end{aligned}$$

consider in square bracket

$$\begin{aligned}
(x+iy)^2 &= x^2 + i2xy - y^2, \\
\text{Im}(x+iy)^2 &= 2xy,
\end{aligned}$$

so the imaginary part is given by

$$2\left(l_{I0}\cos(\gamma_+\frac{L}{2}) - \gamma_+\sin(\gamma_+\frac{L}{2})\right)\left(l_{I0}\sin(\gamma_+\frac{L}{2}) + \gamma_+\cos(\gamma_+\frac{L}{2})\right) = 0. \qquad (6.104)$$

The equation (6.104) is valid, when two solutions exist as follows

$$
\begin{aligned}
l_{I0}\cos(\gamma_+\frac{L}{2}) &= \gamma_+\sin(\gamma_+\frac{L}{2}), && (6.105)\\
l_{I0}\sin(\gamma_+\frac{L}{2}) &= -\gamma_+\cos(\gamma_+\frac{L}{2}), && (6.106)
\end{aligned}
$$

or

$$
\begin{aligned}
l_{I0} &= \gamma_+\tan\left(\frac{\gamma_+ L}{2}\right) = \gamma_+\tan(\gamma_+ a), && (6.107)\\
l_{I0} &= -\gamma_+\cot\left(\frac{\gamma_+ L}{2}\right) = -\gamma_+\cot(\gamma_+ a), && (6.108)
\end{aligned}
$$

where $L/2 = a$.

Substituting equation for $\gamma_+$ and $l_{I0}$, this equation determines the values of energy $E^N$. Let us consider equation

$$
\begin{aligned}
l_{I0} &= \frac{1}{\hbar\beta}\cos^{-1}\left(\frac{m\beta^2E^N+1}{\sqrt{1+2m\beta^2V_0}}\right),\\
\cos(\hbar\beta l_{I0}) &= \frac{m\beta^2E^N+1}{\sqrt{1+2m\beta^2V_0}},\\
m\beta^2E^N+1 &= \cos(\hbar\beta l_{I0})\sqrt{1+2m\beta^2V_0}. && (6.109)
\end{aligned}
$$

And equation

$$
\gamma_+ = \frac{1}{\hbar\beta}\ln\left((m\beta^2E^N+1)+\sqrt{(m\beta^2E^N+1)^2-1}\right),
$$

by using relation

$$
\cosh^{-1}(x) = \ln(x+\sqrt{(x^2-1)}), \tag{6.110}
$$

this equation becomes

$$
\begin{aligned}
\hbar\beta\gamma_+ &= \cosh^{-1}(m\beta^2E^N+1),\\
m\beta^2E^N+1 &= \cosh(\gamma_+\hbar\beta). && (6.111)
\end{aligned}
$$

Equating the equation (6.109) and (6.111) gives

$$
\begin{aligned}
\cosh(\gamma_+\hbar\beta) &= \cos(\hbar\beta l_{I0})\sqrt{1+2m\beta^2V_0},\\
l_{I0} &= \frac{1}{\hbar\beta}\cos^{-1}\left(\frac{\cosh(\gamma_+\hbar\beta)}{\sqrt{1+2m\beta^2V_0}}\right). && (6.112)
\end{aligned}
$$

Conclusion, these equation, (6.107), (6.108) and (6.112) can be solved by graphically. By plotting these equation on the same grid, and looking for intersection points.

Let us rewrite these equation, (6.107), (6.108) and (6.112) as dimensionless quantities. But, there are a many dimensionless quantities to choose. First, let us consider expansion of NEQH with $V(x) = V_0$,

$$\begin{aligned}
\hat{H} &= \frac{1}{2\beta^2 m}(1+2\beta^2 mV_0)^{1/2}\left(e^{-i\hbar\beta\frac{\partial}{\partial x}} + e^{i\hbar\beta\frac{\partial}{\partial x}}\right) - \frac{1}{\beta^2 m}, \\
&= \frac{1}{2\beta^2 m}(1+2\beta^2 mV_0)^{1/2}\Big(1 + (-i\hbar\beta\frac{\partial}{\partial x}) + (-\frac{i}{2}\hbar\beta\frac{\partial}{\partial x})^2 + 1 + (\frac{i}{2}\hbar\beta\frac{\partial}{\partial x}) \\
&\quad +(i\hbar\beta\frac{\partial}{\partial x})^2 + O(\beta^3)\Big) - \frac{1}{\beta^2 m}, \\
&= \frac{1}{2\beta^2 m}(1+2\beta^2 mV_0)^{1/2}\left(2 - \hbar^2\beta^2\frac{\partial^2}{\partial x^2} + O(\beta^3)\right) - \frac{1}{\beta^2 m}, \\
&= \frac{1}{2m\beta^2}\left(2 - \hbar^2\beta^2\frac{\partial^2}{\partial x^2} + 2\beta^2 mV_0 + O(\beta^3)\right) - \frac{1}{\beta^2 m}, \\
&= \frac{1}{m\beta^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0 + O(\beta) - \frac{1}{\beta^2 m}, \\
&= \hat{H}^S + O(\beta), \qquad (6.113)
\end{aligned}$$

where $\hat{H}^S$ is standard Hamiltonian. Therefore, substituting(6.113) into Schrödinger equation gives

$$E^N = E^S + O(\beta). \qquad (6.114)$$

Further, let us consider expansion of $\gamma_+$ which using relation (6.114)

$$\begin{aligned}
\gamma_+ &= \frac{1}{\hbar\beta}\ln\left((m\beta^2 E^N + 1) + \sqrt{(m\beta^2 E^N + 1)^2 - 1}\right), \\
&= \frac{1}{\hbar\beta}\ln\left((m\beta^2 E^N + 1) + \sqrt{(m\beta^2 E^N)(m\beta^2 E^N + 2)}\right), \\
&= \frac{1}{\hbar\beta}\ln\Big[1 + m\beta^2 E^S + O(\beta^3) + \\
&\quad \sqrt{\left(m\beta^2 E^S + O(\beta^3)\right)\left(2 + m\beta^2 E^S + O(\beta^3)\right)}\Big],
\end{aligned}$$

$$\begin{aligned}
\gamma_+ &= \frac{1}{\hbar\beta}\ln\left(1 + m\beta^2 E^S + O(\beta^3) + \sqrt{2m\beta^2 E^S + O(\beta^3)}\right), \\
&= \frac{1}{\hbar\beta}\ln\left(1 + m\beta^2 E^S + O(\beta^3) + (2m\beta^2 E^S)^{1/2}\sqrt{1 + O(\beta)}\right), \\
&= \frac{1}{\hbar\beta}\ln\left(1 + m\beta^2 E^S + O(\beta^3) + (2m\beta^2 E^S)^{1/2}\left(1 + O(\beta)\right)\right), \\
&= \frac{1}{\hbar\beta}\ln\left(1 + (2m\beta^2 E^S)^{1/2} + O(\beta^2)\right), \\
&= \frac{1}{\hbar\beta}\left((2m\beta^2 E^S)^{1/2} + O(\beta^2)\right), \\
&= \frac{\sqrt{2mE^S}}{\hbar} + O(\beta), \\
&= k + O(\beta). \qquad (6.115)
\end{aligned}$$

The wavenumber $\gamma_+$ can be expanded in standard wavenumber $k$ and term of parameter $\beta$. As limit of $\beta \to 0$, $\gamma_+$ will recover to standard case $k$. According to standard finite square well [26] dimensionless quantity is defined as $ka$, so analog to the standard case, we will define dimensionless quantities in this system as "$\gamma_+ a$".

Next, let us consider expansion of $l$

$$l_{I0} = \frac{1}{\hbar\beta}\cos^{-1}\left(\frac{m\beta^2 E^N + 1}{\sqrt{1 + 2m\beta^2 V_0}}\right).$$

Rewriting this equation and using equation (6.114), we obtain

$$\begin{aligned}
\cos(l_{I0}\hbar\beta) &= \frac{(m\beta^2 E^N + 1)}{\sqrt{1 + 2m\beta^2 V_0}}, \\
&= \frac{m\beta^2(E^S + O(\beta)) + 1}{\sqrt{1 + 2m\beta^2 V_0}}, \\
&= \frac{1 + m\beta^2 E^S + O(\beta^3)}{\sqrt{1 + 2m\beta^2 V_0}}, \qquad (6.116)
\end{aligned}$$

Using Taylor's expansion to the left-hand-side of equation (6.116) gives

$$\cos(l_{I0}\hbar\beta) = 1 - \frac{(l_{I0}\hbar\beta)^2}{2!} + O(\beta^4). \qquad (6.117)$$

Taylor's expansion to the right-hand-side of equation (6.116) gives

$$\begin{aligned}
\frac{1 + m\beta^2 E^S + O(\beta^3)}{(1 + 2m\beta^2 V_0)^{1/2}} &= \left[1 + m\beta^2 E^S + O(\beta^3)\right]\left[1 - \frac{1}{2}(2m\beta^2 V_0) + O(\beta^4)\right], \\
&= 1 - m\beta^2 V_0 + m\beta^2 E^S + O(\beta^3). \qquad (6.118)
\end{aligned}$$

Equating left-hand-side and right-hand-side, we obtain

$$\begin{aligned}
1-\frac{(l_{I0}\hbar\beta)^2}{2!}+O(\beta^4) &= 1-m\beta^2V_0+m\beta^2E^S+O(\beta^3),\\
-m\beta^2V_0+m\beta^2E^S+O(\beta^3) &= -\frac{1}{2}l_{I0}^2\hbar^2\beta^2,\\
l_{I0}^2 &= \frac{2m}{\hbar^2}(V_0-E^S)+O(\beta),\\
l_{I0} &= \sqrt{\frac{2m}{\hbar^2}(V_0-E^S)+O(\beta)},\\
&= \left(\sqrt{\frac{2m}{\hbar^2}(V_0-E^S)}\right)\Big(1+O(\beta)\Big),\\
&= \sqrt{\frac{2m}{\hbar^2}(V_0-E^S)}+O(\beta),\\
&= \kappa+O(\beta). \qquad (6.119)
\end{aligned}$$

We obtain $l_{I0}$ in the expression of standard $\kappa$ and parameter $\beta$. As limit of $\beta \to 0$, $l_{I0}$ will recover to standard $\kappa$. Dimensionless quantities of standard quantum for wavenumber outside the well is "$\kappa a$" [26] so, analog to standard case the dimensionless quantities for $l_{I0}$ is "$l_{I0}a$".

Therefore, dimensionless quantities of equation (6.107), (6.108) and (6.112) become

$$\begin{aligned}
\underbrace{l_{I0}a}_{y} &= \underbrace{\gamma_+a}_{x}\tan(\underbrace{\gamma_+a}_{x}),\\
y &= x\tan(x). \qquad (6.120)
\end{aligned}$$

Equivalent to the equation (6.108) we get

$$y = -x\cot(x), \qquad (6.121)$$

where $y = l_{I0}a$, $x = \gamma_+a$ are represent dimensionless to measure size of the square well. According to (6.112) the dimensionless quantities of this equation reads

$$\begin{aligned}
\frac{\hbar\beta}{a}y &= \cos^{-1}\left(\frac{\cosh(\frac{\hbar\beta}{a}x)}{\sqrt{1+\left(\frac{2ma^2V_0}{\hbar^2}\right)\left(\frac{\hbar^2\beta^2}{a^2}\right)}}\right),\\
y &= \frac{1}{j}\cos^{-1}\left(\frac{\cosh(jx)}{\sqrt{1+z^2j^2}}\right), \qquad (6.122)
\end{aligned}$$

where $j = \hbar\beta/a$ presents dimensionless to measure of parameter $\beta$, and $z = (2ma^2V_0/\hbar^2)^{1/2}$ is dimensionless to measure potential. Hence, we have three equations to determine energy

$$\begin{aligned} y &= x\tan(x), \\ y &= -x\cot(x), \\ y &= \frac{1}{j}\cos^{-1}\left(\frac{\cosh(jx)}{\sqrt{1+z^2j^2}}\right), \end{aligned} \tag{6.123}$$

these equations can be solve graphically. However, we are not solving these equations simultaneously. We only need intersection points between two equation [8] namely between (6.120) and (6.122), and between (6.121) and (6.122) which showed in Figure 10.

The energy spectrum can be obtained by rewriting equation (6.70) in dimensionless quantity. This gives

$$E_n^d = \frac{1}{j^2}\cosh(x_n j) - \frac{1}{j^2}, \tag{6.124}$$

where $E_n^d = ma^2E_n^N/\hbar^2$ is dimensionless to measure energy and $x_n$ is intersection points. To obtain the energy spectrum, we find out the intersection points $x_n$. And using these intersection points to equation (6.124) to obtain the energy. For example, Figure 10 express intersection points between curve of equations (6.123) for fixed $z = 5$ and $j = 0.0001$.

[8] As we consider symmetry of square well. The equation (6.120) and (6.121) come from the boundary conditions for odd function and even function. So, we need intersection points from both functions.

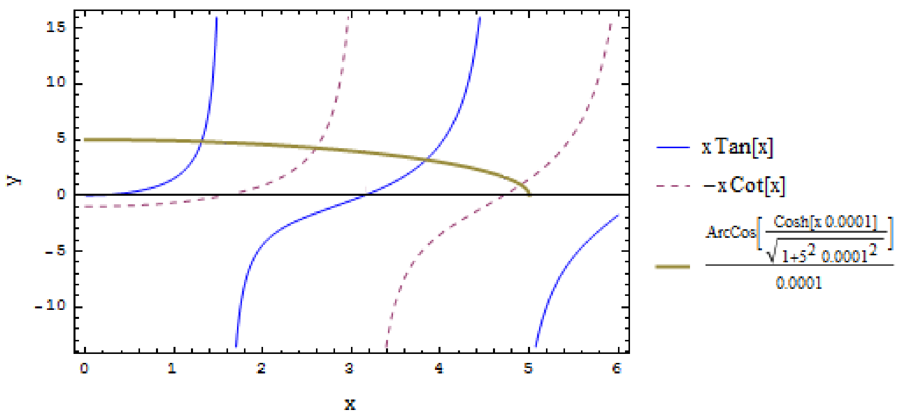



**Figure 10: Intersection points for $j = 0.0001$ and $z = 5$**

According to Figure 10, we have four intersection points. It is corresponding to four energy levels which represented in Table 4.

**Table 4: Intersection points and energy levels for $j = 0.0001$,$z = 5$**

| n | intersection point($x_n$) | energy($8E_n^d/\pi^2$) |
|---|---|---|
| 1 | 1.30644 | 0.691734 |
| 2 | 2.59574 | 2.73075 |
| 3 | 3.83747 | 5.96829 |
| 4 | 4.9063 | 9.75591 |

The energy spectrum of NEQH with finite square well is depend on both potential $z$ and parameter $j$.

In the first case, we consider in fixed the potential $z$, and vary only parameter $j$. The results are showed in Table 5,6,7, and the illustrations are expressed in Figure 11, 12, 13.

**Table 5: First energy level of $z = 5, z = 10, z = 30, z = 50$**

| **parameter,** $j$ | **energy,** $z = 5$ | **energy,** $z = 10$ | **energy,** $z = 30$ | **energy,** $z = 50$ |
|---|---|---|---|---|
| 0.0001 | 0.853393 | 1.01895 | 1.15536 | 1.18579 |
| 0.001 | 0.853391 | 1.01895 | 1.15534 | 1.18575 |
| 0.01 | 0.853169 | 1.01835 | 1.1532 | 1.18217 |
| 0.1 | 0.832842 | 0.971913 | 1.05971 | 1.07416 |
| 0.3 | 0.732041 | 0.815339 | 0.865075 | 0.874127 |
| 0.5 | 0.634472 | 0.693669 | 0.7305 | 0.737512 |
| 0.7 | 0.557518 | 0.604356 | 0.634431 | 0.640291 |
| 0.9 | 0.497726 | 0.537205 | 0.563147 | 0.568275 |
| 1.1 | 0.450606 | 0.485282 | 0.508481 | 0.513116 |
| 1.3 | 0.412772 | 0.444122 | 0.465407 | 0.469695 |
| 1.5 | 0.381846 | 0.410796 | 0.430702 | 0.43474 |
| 1.7 | 0.356158 | 0.383328 | 0.402219 | 0.406075 |
| 1.9 | 0.334522 | 0.360342 | 0.378481 | 0.382203 |
| 2.1 | 0.316073 | 0.340859 | 0.358438 | 0.362064 |
| 2.3 | 0.300174 | 0.324161 | 0.341328 | 0.344886 |
| 2.5 | 0.286342 | 0.309712 | 0.326583 | 0.330097 |
| 2.7 | 0.27421 | 0.297106 | 0.313773 | 0.31726 |
| 2.9 | 0.263489 | 0.286025 | 0.302566 | 0.306042 |
| 3.1 | 0.253952 | 0.276224 | 0.2927 | 0.296178 |
| 3.3 | 0.24542 | 0.267503 | 0.28397 | 0.28746 |
| 3.5 | 0.237744 | 0.259704 | 0.276208 | 0.279721 |
| 3.7 | 0.230806 | 0.252698 | 0.269279 | 0.272824 |
| 3.9 | 0.224507 | 0.246379 | 0.263072 | 0.266657 |
| 4.1 | 0.218765 | 0.240657 | 0.257495 | 0.261126 |
| 4.3 | 0.213511 | 0.235459 | 0.252471 | 0.256155 |
| 4.5 | 0.208686 | 0.230722 | 0.247934 | 0.251678 |
| 4.7 | 0.204243 | 0.226394 | 0.24383 | 0.247639 |
| 4.9 | 0.200137 | 0.222429 | 0.240111 | 0.243992 |

| **parameter,** $j$ | **energy,** $z = 5$ | **energy,** $z = 10$ | **energy,** $z = 30$ | **energy,** $z = 50$ |
|---|---|---|---|---|
| 5.1 | 0.196333 | 0.218788 | 0.236738 | 0.240695 |
| 5.3 | 0.1928 | 0.215438 | 0.233675 | 0.237714 |
| 5.5 | 0.18951 | 0.212349 | 0.230893 | 0.235018 |
| 5.7 | 0.186439 | 0.209496 | 0.228364 | 0.23258 |
| 5.9 | 0.183567 | 0.206856 | 0.226065 | 0.230378 |
| 6.1 | 0.180874 | 0.20441 | 0.223976 | 0.228391 |
| 6.3 | 0.178345 | 0.20214 | 0.22208 | 0.2266 |
| 6.5 | 0.175966 | 0.200031 | 0.220359 | 0.22499 |
| 6.7 | 0.173722 | 0.198068 | 0.2188 | 0.223546 |
| 6.9 | 0.171603 | 0.196241 | 0.21739 | 0.222256 |
| 7.1 | 0.169599 | 0.194536 | 0.216118 | 0.221108 |
| 7.3 | 0.1677 | 0.192946 | 0.214973 | 0.220093 |
| 9 | 0.154816 | 0.18294 | 0.209276 | 0.215683 |
| 11 | 0.144411 | 0.176259 | 0.208742 | 0.217126 |
| 13 | 0.13676 | 0.172419 | 0.212061 | 0.222967 |
| 15 | 0.130646 | 0.17 | 0.217639 | 0.231654 |
| 17 | 0.125448 | 0.168248 | 0.224517 | 0.242255 |
| 19 | 0.120836 | 0.166745 | 0.232057 | 0.254127 |
| 21 | 0.116624 | 0.165262 | 0.239803 | 0.266782 |
| 23 | 0.112708 | 0.16368 | 0.247423 | 0.279824 |
| 25 | 0.109027 | 0.161945 | 0.254673 | 0.292919 |
| 27 | 0.105543 | 0.160041 | 0.261379 | 0.305789 |

**Table 6: Second energy level of $z = 5, z = 10, z = 30, z = 50$**

| **parameter,** $j$ | **energy,** $z = 5$ | **energy,** $z = 10$ | **energy,** $z = 30$ | **energy,** $z = 50$ |
|---|---|---|---|---|
| 0.0001 | 3.36893 | 4.06793 | 4.62105 | 4.74306 |
| 0.001 | 3.36892 | 4.06575 | 4.61268 | 4.74291 |
| 0.01 | 3.3682 | 3.901 | 4.26442 | 4.72889 |
| 0.1 | 3.30268 | 3.41857 | 3.65538 | 4.32355 |
| 0.3 | 3.00989 | 3.14742 | 3.36851 | 3.69816 |
| 0.5 | 2.78628 | 3.0361 | 3.27589 | 3.41061 |
| 0.7 | 2.663 | 3.03067 | 3.31375 | 3.32311 |
| 0.9 | 2.60886 | 3.10005 | 3.45264 | 3.37108 |
| 1.1 | 2.5957 | 3.22458 | 3.67969 | 3.52606 |
| 1.3 | 2.59889 | 3.3886 | 3.99026 | 3.77727 |
| 1.5 | 2.59169 | 3.57548 | 4.38353 | 4.12344 |
| 1.7 | 2.53699 | 3.76316 | 4.85957 | 4.56869 |
| 1.9 | | 3.91824 | 5.41656 | 5.12015 |
| 2.1 | | 3.98419 | 6.04768 | 5.78593 |
| 2.3 | | | 6.73677 | 6.5728 |
| 2.5 | | | 7.4522 | 7.48317 |
| 2.7 | | | 8.1366 | 8.51074 |
| 2.9 | | | 8.68681 | 9.63416 |
| 3.1 | | | 8.89817 | 10.8073 |
| 3.3 | | | | 11.9432 |
| 3.5 | | | | 12.8817 |
| 3.7 | | | | 13.2985 |

**Table 7: Third energy level of $z = 5, z = 10, z = 30, z = 50$**

| parameter, $j$ | energy, $z = 5$ | energy, $z = 10$ | energy, $z = 30$ | energy, $z = 50$ |
|---|---|---|---|---|
| 0.0001 | 7.36307 | 9.12113 | 10.3959 | 10.6715 |
| 0.001 | 7.36192 | 9.11703 | 10.3781 | 10.6712 |
| 0.01 | 7.26173 | 8.82324 | 9.69101 | 10.6407 |
| 0.1 | 6.89667 | 8.2665 | 8.97586 | 9.8292 |
| 0.3 | 6.58142 | 8.4859 | 9.42814 | 9.10119 |
| 0.5 | | 9.21159 | 10.7835 | 9.60307 |
| 0.7 | | 9.79026 | 13.0286 | 11.0799 |
| 0.9 | | | 16.1763 | 13.5926 |
| 1.1 | | | 19.8056 | 17.3423 |
| 1.3 | | | | 22.4886 |
| 1.5 | | | | 28.5426 |

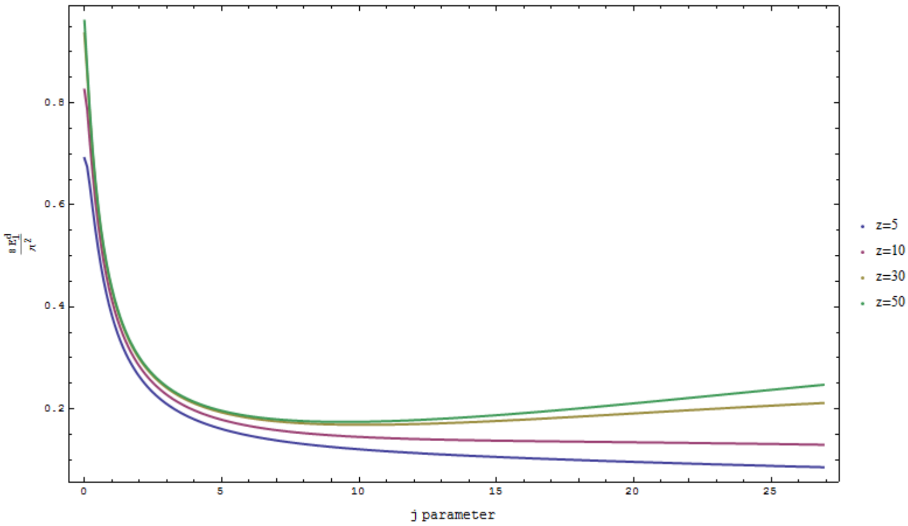



**Figure 11: First energy level of $z = 5, z = 10, z = 30, z = 50$**

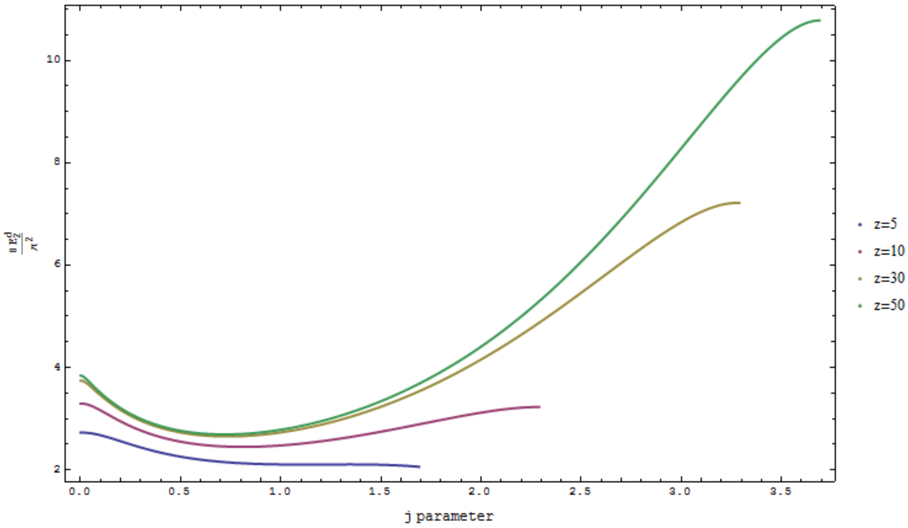



**Figure 12: Second energy level of** $z = 5, z = 10, z = 30, z = 50$

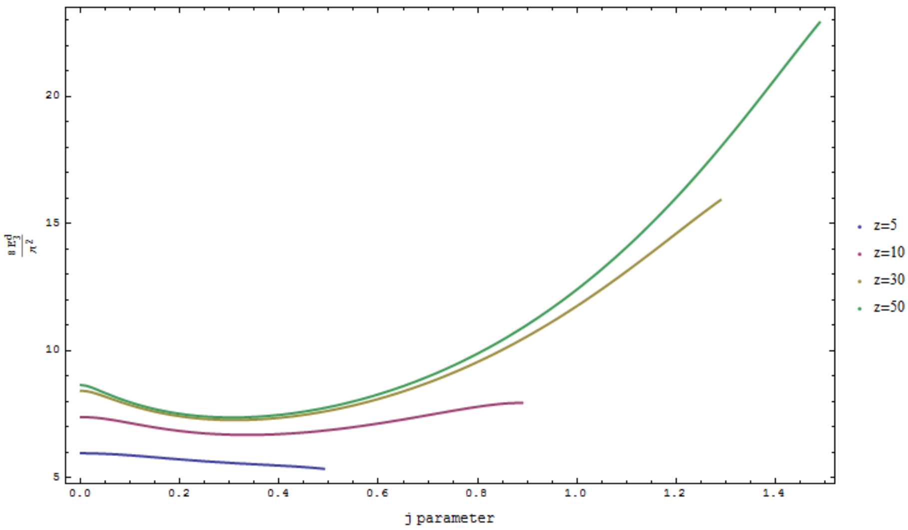



**Figure 13: Third energy level of** $z = 5, z = 10, z = 30, z = 50$

Figure 11 exhibits the first energy levels of potential $z = 5, 10, 30, 50$. Similarly for Figure 12 and 13 show the second energy levels and third one for each potential respectively. According to the plots, the energy is increased corresponding to increasing of the potential. But, if parameter $j$ increase, it is interesting because the energies for each energy levels decrease at the beginning, and then there increase. Moreover, The energy of higher potential is increases quicker than the lower one. For increasing of parameter $j$ till some value, the energy levels for each potentials are disappear except the first level. It is mean that, the energy of NEQH alway exist at least one state, and number of energy levels are decrease while parameter $j$ increase.

Recalling the NEQH energy of infinite square well, it will recover to standard energy at the limit parameter $j \to 0$. Therefore we will expect that the NEQH energy of finite square well is recover to the standard energy at limit parameter $j \to 0$. Table 8 shows the energy of standard finite square well for $z = 5$ and Table 9,10,11,12 show the NEQH energy of finite square well for $z = 5$ and parameter $j = 0.01, 0.1, 0.3, 0.5$ respectively. According to the Table, as parameter $j \to 0$ the NEQH energy will close to standard case.

**Table 8: Energy level of standard finite square well** $z = 5$

| **n** | **intersection point**$(x_n)$ | **energy**$(8E_n^d/\pi^2)$ |
|---|---|---|
| 1 | 1.30644 | 0.691734 |
| 2 | 2.59574 | 2.73075 |
| 3 | 3.83747 | 5.96829 |
| 4 | 4.9063 | 9.75591 |

**Table 9: Energy level of NEQH** $j = 0.01$ **and** $z = 5$

| **n** | **intersection point**$(x_n)$ | **energy**$(8E_n^d/\pi^2)$ |
|---|---|---|
| 1 | 1.30626 | 0.691553 |
| 2 | 2.59538 | 2.73016 |
| 3 | 3.83693 | 5.96735 |
| 4 | 4.90522 | 9.75357 |

**Table 10: Energy levels of NEQH $j = 0.1$ and $z = 5$**

| n | intersection point($x_n$) | energy($8E_n^d/\pi^2$) |
|---|---|---|
| 1 | 1.28972 | 0.675077 |
| 2 | 2.56307 | 2.67705 |
| 3 | 3.78827 | 5.88614 |
| 4 | 4.79463 | 9.49672 |

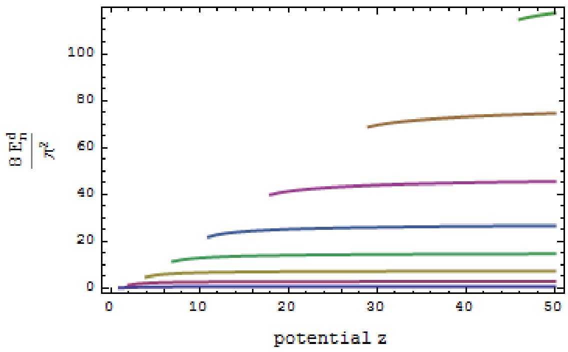
**Table 11: Energy levels of NEQH $j = 0.3$ and $z = 5$**

| n | intersection point($x_n$) | energy($8E_n^d/\pi^2$) |
|---|---|---|
| 1 | 1.20345 | 0.59337 |
| 2 | 2.40126 | 2.43972 |
| 3 | 3.54456 | 5.59023 |

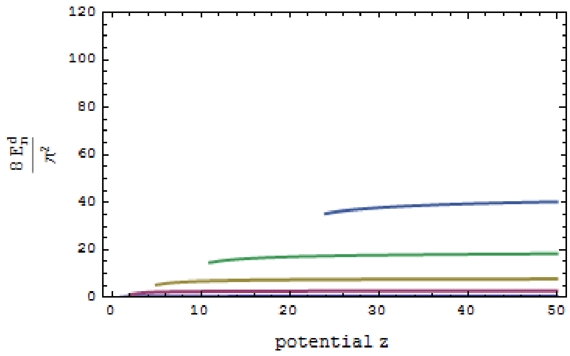
**Table 12: Energy levels of NEQH $j = 0.5$ and $z = 5$**

| n | intersection point($x_n$) | energy($8E_n^d/\pi^2$) |
|---|---|---|
| 1 | 1.11209 | 0.514283 |
| 2 | 2.24147 | 2.25848 |
| 3 | 3.25629 | 5.3347 |

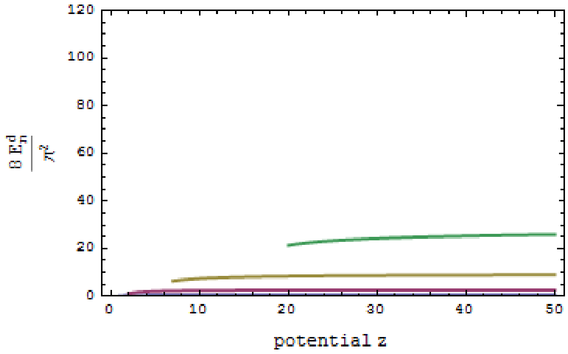
Next, let us consider in second case for fixed parameter $j$, and vary only potential $z$. Then, the plots for fixed $j = 0.01, 0.1, 0.3, 0.5, 0.7$, and $j = 1$ as follows in Figure 14. According to the plots, the number of energy level increase for increasing of potential. But, for parameter $j$ increase, the number of energy levels are decrease. Now, as the potential close to infinity, we expect that the energy will



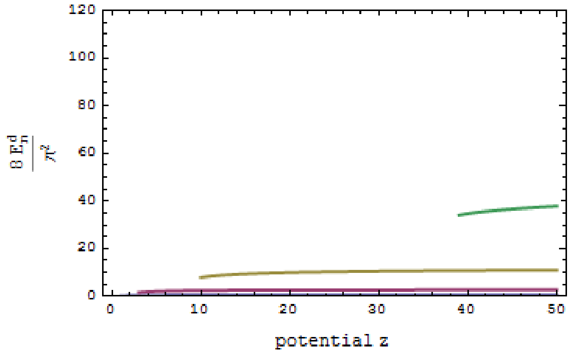

**(a)** $j = 0.3$



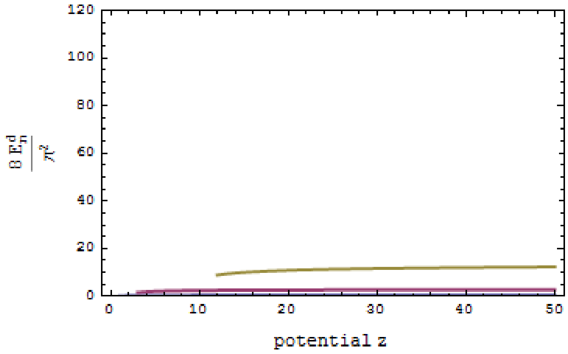

**(b)** $j = 0.5$



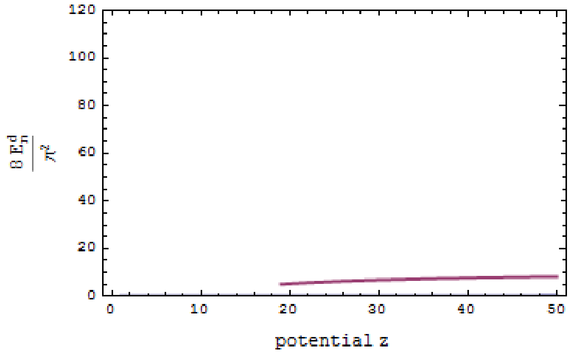

**(c)** $j = 0.7$




**(d)** $j = 0.9$




**(e)** $j = 1$




**(f)** $j = 3$

**Figure 14: Energy levels with varying potential**

close to standard infinite square well case as limit parameter $j \to 0$. Figure 15 and Table 13 exhibit first and second energy levels of $j = 0.0001$ for any potential, $z = 0$ to $z = 50$. We will see that the energy tented to energy of standard infinite square well which showed in Table 2.

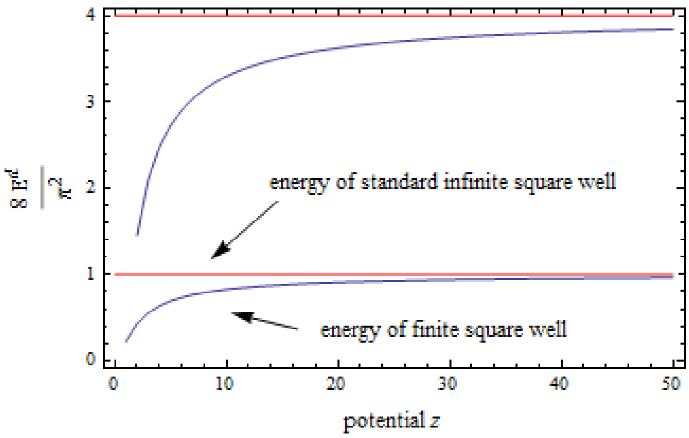



**Figure 15: Plot of first and second energy levels of finite square well energy and infinite square well**

**Table 13: First and second energy levels of** $j = 0.0001$

| potential z | first level ($8E_1^d/\pi^2$) | second level ($8E_2^d/\pi^2$) | potential z | first level ($8E_1^d/\pi^2$) | second level ($8E_2^d/\pi^2$) |
|---|---|---|---|---|---|
| 1 | 0.221386 | - | 26 | 0.927259 | 3.70857 |
| 2 | 0.429855 | 1.45615 | 27 | 0.929812 | 3.71883 |
| 3 | 0.554909 | 2.10473 | 28 | 0.932192 | 3.72839 |
| 4 | 0.635644 | 2.48177 | 29 | 0.934416 | 3.73732 |
| 5 | 0.691734 | 2.73075 | 30 | 0.936498 | 3.74568 |
| 6 | 0.732899 | 2.90827 | 31 | 0.938453 | 3.75353 |
| 7 | 0.764377 | 3.04158 | 32 | 0.94029 | 3.7609 |
| 8 | 0.789221 | 3.14552 | 33 | 0.942022 | 3.76785 |
| 9 | 0.809327 | 3.22891 | 34 | 0.943655 | 3.7744 |
| 10 | 0.825931 | 3.29734 | 35 | 0.945199 | 3.7806 |
| 11 | 0.839875 | 3.35453 | 36 | 0.946661 | 3.78646 |
| 12 | 0.85175 | 3.40306 | 37 | 0.948046 | 3.79201 |
| 13 | 0.861985 | 3.44476 | 38 | 0.949362 | 3.79729 |
| 14 | 0.870898 | 3.48098 | 39 | 0.950613 | 3.8023 |
| 15 | 0.878729 | 3.51275 | 40 | 0.951803 | 3.80707 |
| 16 | 0.885664 | 3.54085 | 41 | 0.952937 | 3.81162 |
| 17 | 0.891849 | 3.56586 | 42 | 0.954019 | 3.81596 |
| 18 | 0.897399 | 3.58829 | 43 | 0.955052 | 3.8201 |
| 19 | 0.902407 | 3.6085 | 44 | 0.95604 | 3.82406 |
| 20 | 0.906949 | 3.62682 | 45 | 0.956986 | 3.82785 |
| 21 | 0.911086 | 3.64349 | 46 | 0.957892 | 3.83148 |
| 22 | 0.914872 | 3.65874 | 47 | 0.95876 | 3.83495 |
| 23 | 0.918348 | 3.67273 | 48 | 0.959593 | 3.83829 |
| 24 | 0.921551 | 3.68562 | 49 | 0.960393 | 3.8415 |
| 25 | 0.924513 | 3.69753 | 50 | 0.961163 | 3.84458 |

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# BIOGRAPHY

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