

AN INVESTIGATION OF RELATIONSHIPS BETWEEN  
THE USUAL QUANTUM HARMONIC OSCILLATOR  
AND ITS ONE-PARAMETER FAMILY VERSION



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## ABSTRACT

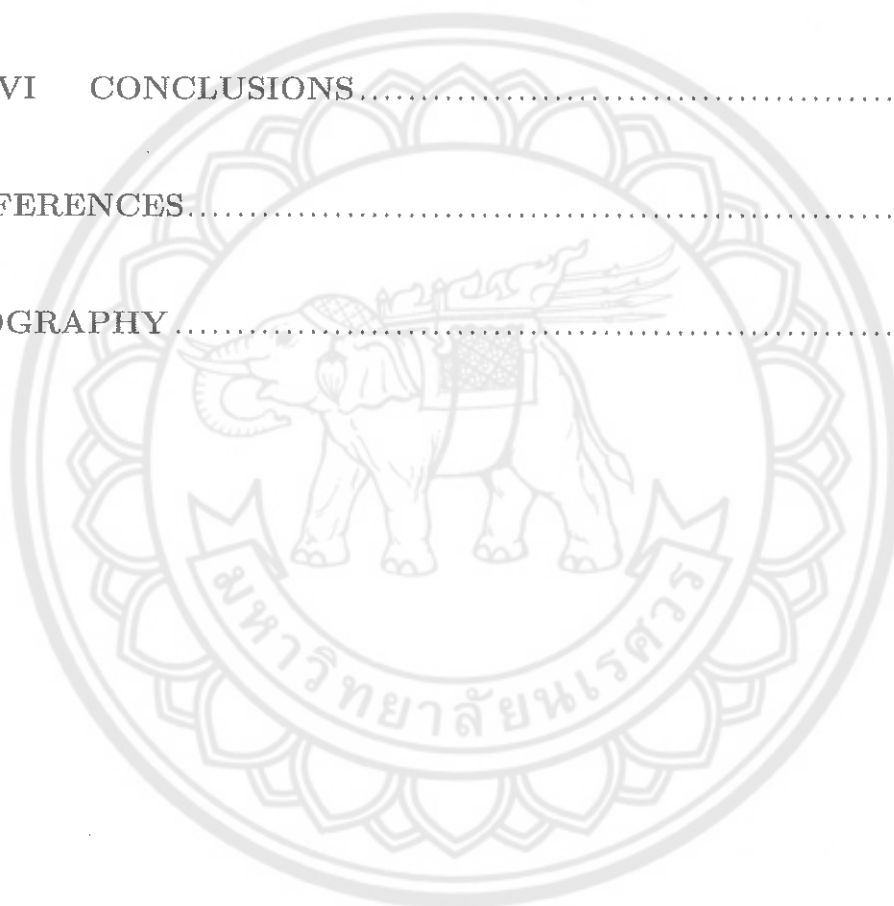
Newton-equivalent Hamiltonians are Hamiltonians whose classical dynamics agree with those from the standard Hamiltonian. In this work, we in particular are interested in its prescription for quantum harmonic oscillator. A modified perturbation theory is used to evaluate energy spectra and wavefunctions of this Hamiltonian. The energy spectra we obtain seem to agree with those of the standard Hamiltonian. We also study this Hamiltonian with additional term  $\alpha x^4$  to obtain the Newton-equivalent anharmonic oscillator Hamiltonian. Its spectrum depend on the one-parameter family ( $\beta$ ).

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# CHAPTER I

## INTRODUCTION

### 1.1 Background and motivation

We first review quantization, which is the process to obtain quantum theory from classical theory. There are two approaches which are canonical and non-canonical approach. For more extensive review, see for example [1]. Canonical quantization consists of Poisson bracket, such as  $\{x, p\} = 1$ , which has definition in canonical coordinates.

In their one-dimensional version, the canonical commutation relation, is given by

$$[\hat{x}, \hat{p}] = i\hbar. \quad (1.1)$$

Then one will consider the simple but important example: the harmonic oscillator with the classical Hamiltonian given by

$$H_E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2. \quad (1.2)$$

Promoting it to quantum case, one will obtain the quantum Hamiltonian

$$\hat{H}_E = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 \hat{x}^2. \quad (1.3)$$

Besides the Hamiltonian composed by kinetic energy and potential energy eq.(1.2), which has a separable dependence on  $x$  and  $p$ , one has the form in multiplicative case written as

$$H(x, p) = F(p)G(x), \quad (1.4)$$

which is given by

$$H_c(x, p) = 4mc^2 p \cosh\left(\frac{p}{2mc}\right) \left(1 + \frac{V(x)}{2mc^2}\right)^{1/2}; \quad c \in (0, \infty). \quad (1.5)$$

This one-parameter Hamiltonian as a limit case is  $H_E(x, p)$

$$\lim_{c \rightarrow \infty} (H_c(x, p) - 4mc^2) = H_E(x, p). \quad (1.6)$$

In quantum case, there are ordering problem, but we in particular are interested in the form chosen by [2] which is based on physical insight of [3]. The Hamiltonian is given by

$$\hat{H}_\beta \equiv \frac{1}{2\beta^2 m} \left( (1 + i\beta m \omega \hat{x})^{1/2} \exp(-i\hbar\beta \partial_x) (1 - i\beta m \omega \hat{x})^{1/2} + (i \rightarrow -i) \right), \quad (1.7)$$

where  $\beta = (2mc)^{-1}$ .

Then we will discuss about another approach which is noncanonical approach. An important example of noncanonical approach is noncommutative geometry (NCG) which is an approach or a model to explain quantum spacetime. Another important example is Wigner's idea [4], [5], [6]. It is not based on phase space variables but based on configuration space variables. The algebraic relation for  $\hat{x}$ ,  $\hat{v} = d\hat{x}/dt$  and  $\hat{H}$  is given by

$$\hat{v} = \frac{i}{\hbar} [\hat{H}, \hat{x}], \quad -\omega^2 \hat{x} = \frac{i}{\hbar} [\hat{H}, \hat{v}], \quad [\hat{x}, \hat{v}] = \frac{i\hbar}{m} F(\hat{H}), \quad (1.8)$$

where the last commutator is a consequence of the Jacobi identity, and  $F(\hat{H})$  is an arbitrary function, [7], [8], [9]. In the usual quantum harmonic oscillator  $F(\hat{H}) = 1$ , but in the case of one-parameter family Hamiltonian (1.7),  $F(\hat{H})$  is given by

$$F(\hat{H}) = \hat{H}/4mc^2. \quad (1.9)$$

However, there are other alternative Hamiltonians [10], [11], [12], [13] which lead to the same Newton equation of motion. The investigation of Newton-equivalent Hamiltonian was presented in [14], and in the bihamiltonian description of physical system [15].

In this work, perturbation theory is considered in order to study the quantum Hamiltonian (1.7).  $\hat{H}_\beta$  is treated as the perturbed Hamiltonian of the standard

unperturbed Hamiltonian (1.3). Then we find energy spectra and eigenfunctions of this Hamiltonian. For simplicity, we consider a Hamiltonian

$$\hat{H} = \hat{H}^0 + \lambda \hat{H}^1 + \lambda^2 \hat{H}^2 + \dots \quad (1.10)$$

to obtain the first and second-order correction to the  $n^{th}$  eigenvalue of the Newton-equivalent Hamiltonian  $(E_n^1, E_n^2)$ . We therefore obtain the energy spectra. In addition, we also add the potential term  $(\alpha x^4)$  into  $\hat{H}(\beta)$  to obtain the appropriately perturbed Hamiltonian of  $\hat{H}(\beta)$ . This gives the Newton-equivalent anharmonic oscillator (NEAHO) Hamiltonian  $(\hat{H}(\beta, \alpha))$ . We define the Hamiltonian in pattern of the factorised Hamiltonian [16], [17] which is simple factorised form in discrete quantum mechanics [18], [19].

Finally, we find the first and second-order correction to the  $n^{th}$  eigenvalue of the Newton-equivalent anharmonic oscillator Hamiltonian  $(E_{An}^1, E_{An}^2)$  and obtain the energy spectra.

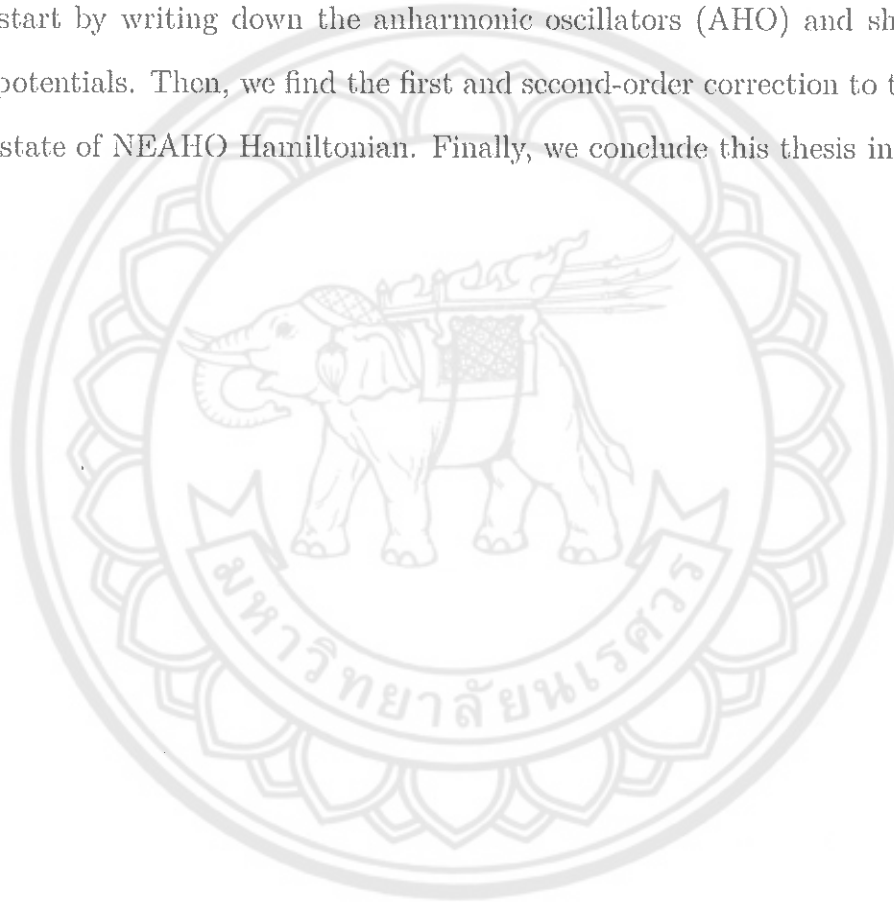
## 1.2 Objectives

In this work, we review the one-parameter family Hamiltonian of quantum hamornic oscillator obtained by [2]. Then, we study perturbation theory for finding energy spectra and wavefunctions of the Newton-equivalent Hamiltonian  $(\hat{H}(\beta))$ . Moreover, we study NEAHO Hamiltonian  $(\hat{H}_A(\beta, \alpha))$  and also find its energy spectra.

## 1.3 Frameworks

Firstly, in chapter 1, we show background and motivation of this thesis. We review the one-parameter family Hamiltonian of quantum hamornic oscillator and its quantum case in chapter 2. Then, in chapter 3, we study quantum harmonic oscillator, in which the energy spectra and wavefunctions is obtained. In chapter

4, we write down perturbation theory in the form which will be suitable to our study. We start from reviewing the standard perturbation theory, then discuss the case where the Hamiltonian is expressed as a polynomial of one parameter. Next, we consider perturbation theory of Newton-equivalent Hamiltonian to find the first and second-order correction to the energy in any state. In chapter 5, we use the perturbation theory in the form discussed in chapter 4 to study NEAHO. We start by writing down the anharmonic oscillators (AHO) and show graph of the potentials. Then, we find the first and second-order correction to the energy in any state of NEAHO Hamiltonian. Finally, we conclude this thesis in chapter 6.



## CHAPTER II

### ALTERNATIVE HAMILTONIANS

In this chapter we will review part of the Newton-equivalent Hamiltonians for the harmonic oscillator [2] which gives a one-parameter family of Hamiltonians whose classical version satisfy Newton equation for usual simple harmonic oscillator. One obtains the Hamiltonian which can be applied in the perturbation theory (Chapter 4).

#### 2.1 The one-parameter family of Newton-equivalent Hamiltonian

The first of all one knows that the motion of a classical mechanical system with one degree of freedom is given by the Newton equation. The integration of its equation provides the time dependence of the coordinate  $x(t)$  of a particle of mass  $m$  in the potential  $V(x)$

$$m\ddot{x} + \frac{d}{dx}V(x) = 0. \quad (2.1)$$

In the Newton equation, one considers the second derivative of  $x$  in term of the Hamiltonian by using Hamilton equation

$$\dot{x} = \frac{\partial H(x, p)}{\partial p}, \quad \dot{p} = -\frac{\partial H(x, p)}{\partial x}. \quad (2.2)$$

One obtains

$$\begin{aligned} \ddot{x} &= \frac{d}{dt} \left( \frac{\partial H}{\partial p} \right) \\ &= \frac{\partial}{\partial x} \left( \frac{\partial H}{\partial p} \right) \frac{dx}{dt} + \frac{\partial}{\partial p} \left( \frac{\partial H}{\partial p} \right) \frac{dp}{dt} \\ &= \frac{\partial}{\partial x} \left( \frac{\partial H}{\partial p} \right) \left( \frac{\partial H}{\partial p} \right) + \frac{\partial}{\partial p} \left( \frac{\partial H}{\partial p} \right) \left( -\frac{\partial H}{\partial x} \right), \end{aligned} \quad (2.3)$$

therefore

$$\ddot{x} = \frac{\partial^2 H}{\partial x \partial p} \frac{\partial H}{\partial p} - \frac{\partial^2 H}{\partial p^2} \frac{\partial H}{\partial x}. \quad (2.4)$$

One substitutes this second derivative into eq.(2.1), one will obtain the Newton equation in term of the Hamiltonian

$$\frac{\partial^2 H}{\partial x \partial p} \frac{\partial H}{\partial p} - \frac{\partial^2 H}{\partial p^2} \frac{\partial H}{\partial x} + \frac{1}{m} \frac{\partial V(x)}{\partial x} = 0. \quad (2.5)$$

However,  $H$  has as a separable dependence on  $x$  and  $p$ , one studies two cases. The first case is the additive case which is  $H(x, p) = F(p) + G(x)$ , and the second case is the multiplicative case which is  $H(x, p) = F(p)G(x)$ .

In the first case  $H(x, p) = F(p) + G(x)$ , eq.(2.5) is rewritten as

$$-F''(p)G'(x) + \frac{1}{m}V'(x) = 0. \quad (2.6)$$

Then, one obtains

$$F''(p) = \frac{V'(x)}{mG'(x)} = 2A, \quad (2.7)$$

where  $A$  is an arbitrary constant, then one obtains  $F(p)$  by integrating twice, which gives

$$F(p) = Ap^2 + Bp + C \quad (2.8)$$

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

One obtains  $G(x)$  from the second equality of eq.(2.7) by integrating once,

$$G(x) = \frac{1}{2mA}V(x) + D \quad (2.9)$$

therefore, from  $H(x, p) = F(p) + G(x)$  one gains

$$H(x, p) = Ap^2 + Bp + C + \frac{V(x)}{2mA} + D. \quad (2.10)$$

To compare this Hamiltonian equation with the well-known Hamiltonian, one chooses  $A = 1/2m$ ,  $B = C = D = 0$ , hence, one obtains Hamiltonian of harmonic potential system

$$H(x, p) = \frac{p^2}{2m} + V(x). \quad (2.11)$$

One substitutes this Hamiltonian into Hamilton equation (2.2) to obtain Newton equation.

Next, considering the second case  $H(x, p) = F(p)G(x)$ , one substitutes this Hamiltonian into eq.(2.5). One obtains

$$(F'(p)^2 - F(p)F''(p)) G(x)G'(x) + \frac{1}{m}V'(x) = 0. \quad (2.12)$$

One obtains the nonlinear second-order differential equation  $F'(p)^2 - F(p)F''(p) = -A$ , which is to be solved for  $F(p)$ . For positive A this second order ordinary differential equation (ODE) is solved by  $F(p) = c_1 \cosh(c_2 p + c_3)$  with  $c_1^2 c_2^2 = A$ , and for negative A by  $F(p) = c_1 \sinh(c_2 p + c_3)$  with  $c_1^2 c_2^2 = -A$ . Then, one will find  $G(x)$  from

$$\begin{aligned} -AG(x)G'(x) + \frac{1}{m}V'(x) &= 0 \\ G(x) &= \left( \frac{2V(x)}{mA} + D \right)^{1/2}. \end{aligned} \quad (2.13)$$

Hence, one obtains

$$\begin{aligned} H(x, p) &= F(p)G(x) \\ &= c_1 \cosh(c_2 p + c_3) \left( \frac{2V(x)}{mA} + D \right)^{1/2} \\ &= c_1 \cosh(c_2 p + c_3) \left( \frac{2V(x)}{mc_1^2 c_2^2} + D \right)^{1/2}. \end{aligned} \quad (2.14)$$

One chooses  $c_1 = 4mc^2$ ,  $c_2 = \frac{1}{2mc}$ ,  $c_3 = 0$  and  $D = 1$ . Finally, one obtains the Hamiltonian in the one-parameter family

$$H_c(x, p) = 4mc^2 \cosh\left(\frac{p}{2mc}\right) \left(1 + \frac{V(x)}{2mc^2}\right)^{1/2}. \quad (2.15)$$

The one-parameter family includes  $H_E(x, p)$  as limit case

$$\lim_{c \rightarrow \infty} (H_c(x, p) - 4mc^2) = H_E(x, p), \quad (2.16)$$

where  $\cosh(x) = 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \dots$  and  $(1+x)^n = 1 + nx + \frac{n(n-1)x^2}{2!} + \dots$

## 2.2 The quantum case

One got the one-parameter family Hamiltonians in harmonic oscillator system, then one defines the parameter  $\beta$

$$\beta = (2mc)^{-1}. \quad (2.17)$$

Therefore, Newton-equivalent Hamiltonians is given by

$$H_c = H(\beta; x, p) = \frac{1}{\beta^2 m} \cosh(\beta p) (1 + \beta^2 m^2 \omega^2 x^2)^{1/2}. \quad (2.18)$$

In one-parameter family: there is ordering problem in quantization, but we in particular are interested in the form chosen by [2] which is based on physical insight of [3]. The Hamiltonian is given by the canonical quantization prescription  $p \rightarrow \hat{p} = -i\hbar\partial_x$ ,  $x \rightarrow \hat{x}$ , one obtains the Newton-equivalent Hamiltonian in the form

$$\hat{H}(\beta) \equiv \frac{1}{2\beta^2 m} \left( (1 + i\beta m \omega \hat{x})^{1/2} \exp(-i\hbar\beta\partial_x) (1 - i\beta m \omega \hat{x})^{1/2} + (i \rightarrow -i) \right). \quad (2.19)$$

Then, we will take this Hamiltonian into perturbation theory in chapter 4.



## CHAPTER III

### QUANTUM HARMONIC OSCILLATOR

The quantum harmonic oscillator is rather natural system directly inspired by the classical harmonic oscillator. In the one-dimensional motion of a particle of mass  $m$  which is attracted to a fixed centre by a force  $F$  proportional to displacement  $x$  from that centre. One chooses its origin as the centre of force. Thus, the restoring force is given by  $F = -kx$ , where  $k$  is the force constant. The corresponding potential energy is given by

$$V(x) = \frac{1}{2}kx^2. \quad (3.1)$$

One then obtains the Hamiltonian operator of quantum harmonic oscillator which given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 \quad (3.2)$$

where  $\omega$  is the angular frequency of the harmonic oscillator ( $\omega = \sqrt{\frac{k}{m}}$ ),  $\hat{p}$  is the momentum operator ( $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ ), and  $\hat{x}$  is the position operator ( $\hat{x} = x$ ). Then, substituting the Hamiltonian operator in the time-independent Schrödinger equation, one obtains

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2 \psi(x) = E\psi(x). \quad (3.3)$$

The wavefunction  $\psi(x)$  should be single-valued, continuous, differentiable and finite everywhere. For this, it is convenient to make use of dimensionless quantities. More explicitly, one defines  $y \equiv \left(\frac{m\omega}{\hbar}\right)^{1/2} x$  and using this variable, the differential equation (3.3) can be written as

$$\left( \frac{d^2}{dy^2} - y^2 + \lambda \right) \psi(y) = 0 \quad (3.4)$$

where

$$\lambda = \frac{2E}{\hbar\omega}. \quad (3.5)$$

If one know the constant  $\lambda$ , one then know the energy  $E$ . For large values of  $y$ , the constant  $\lambda$  can be ignored as compared to  $y^2$ . So eq.(3.4) can be approximated as

$$\frac{d^2}{dy^2}\psi(y) \approx y^2\psi(y), \quad (3.6)$$

which has the approximate solution

$$\psi(y) \approx Ae^{-y^2/2} + Be^{y^2/2}. \quad (3.7)$$

The wavefunction  $\psi(y)$  has to be bounded everywhere but the expression  $e^{y^2/2}$  blows up as  $|x| \rightarrow \infty$ . Therefore one sets coefficient  $B$  equal to 0. Consequently, the satisfactory asymptotic solution of the wave equation is

$$\psi(y) \approx Ae^{-y^2/2}. \quad (3.8)$$

It is then reasonable to assume that the correct solution of the wave equation (3.4) is

$$\psi(y) = f(y)e^{-y^2/2}, \quad (3.9)$$

where  $f(y)$  is a power series expansion in  $y$ . Substituting this solution into eq.(3.4), one obtains the differential equation for the function  $f(y)$

$$f''(y) - 2yf'(y) + (\lambda - 1)f(y) = 0. \quad (3.10)$$

Then one expands  $f(y)$  by using a power series expansion

$$f(y) = \sum_{j=0}^{\infty} a_j y^j. \quad (3.11)$$

Differentiating the series, one obtains

$$f'(y) = \sum_{j=0}^{\infty} j a_j y^{j-1}, \quad (3.12)$$

and

$$f''(y) = \sum_{j=0}^{\infty} (j+1)(j+2)a_{j+2}y^j. \quad (3.13)$$

Substituting these series in eq.(3.10), one obtains

$$\sum_{j=0}^{\infty} ((j+1)(j+2)a_{j+2} - 2ja_j + (\lambda-1)a_j)y^j = 0. \quad (3.14)$$

Then, one finds that the equation will be satisfied only if the coefficients of individual powers of  $y$  vanish,

$$(j+1)(j+2)a_{j+2} - 2ja_j + (\lambda-1)a_j = 0, \quad (3.15)$$

and one obtains a recursion relation between the coefficients which can be written as

$$a_{j+2} = \frac{(2j+1-\lambda)}{(j+1)(j+2)}a_j. \quad (3.16)$$

It is found that all of the coefficients can be expressed in terms of  $a_0$  and  $a_1$ . If  $a_0$  is set equal to zero, the series will contain only odd powers of  $y$ . On the other hand, if  $a_1$  is zero, the series will contain only even powers of  $y$ .

### 3.1 Energy levels

For large  $j$ , the recursion relation eq.(3.16) gives

$$\frac{a_{j+2}}{a_j} \approx \frac{2}{j}. \quad (3.17)$$

Then, the series  $f(y)$  behaves as  $e^{y^2}$ , since that

$$e^{y^2} = \sum_{n=0}^{\infty} \frac{(y^2)^n}{n!} = \sum_{j \in \text{even}} \frac{y^j}{(j/2)!}. \quad (3.18)$$

This series has coefficients  $b_j = \frac{1}{(j/2)!}$  for even  $j$ , one then show that

$$\frac{b_{j+2}}{b_j} = \frac{(j/2)!}{((j+2)/2)!} \approx \frac{2}{j}. \quad (3.19)$$

One obtains the wavefunction eq.(3.9) which behaves as  $e^{y^2/2}$ . This is not acceptable and so the power series of the normalizable solutions must terminate after a finite number of terms ( $n$ ), such that  $a_{n+2} = 0$ . From eq.(3.16) and eq.(3.5), one obtains

$$\lambda = \frac{2E}{\hbar\omega} = 2n + 1. \quad (3.20)$$

This leads to the energy levels for the quantum harmonic oscillator which is given by

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega, \quad \text{for } n = 0, 1, 2, \dots, \quad (3.21)$$

where  $n$  is the quantum number of the harmonic oscillator. Consequently, the energies are quantized and the energy levels are evenly spaced.

### 3.2 Wavefunctions

In the wavefunction eq.(3.9),  $f(y)$  will be a polynomial of degree  $n$  in  $y$ . So the correct solution is given by

$$\psi_n(y) = A_n e^{-y^2/2} f(y) = A_n e^{-y^2/2} T_n(y), \quad (3.22)$$

where  $A_n$  is the normalization constant to be determined and  $T_n(y)$  is the (physicists') Hermite polynomials

$$T_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n} e^{-y^2}, \quad n = 0, 1, 2, \dots \quad (3.23)$$

It satisfies the differential equation

$$T_n''(y) - 2yT_n'(y) + 2nT_n(y) = 0, \quad (3.24)$$

and the orthogonality relation

$$\int_{-\infty}^{\infty} e^{-y^2} T_n(y) T_k(y) dy = \begin{cases} 0 & ; n \neq k \\ \sqrt{\pi} 2^n n! & ; n = k. \end{cases} \quad (3.25)$$

Then we show the (physicists') Hermite polynomials of  $n = 0, 1, \dots, 6$  in Table 1.

If the wavefunctions  $\psi_n(y)$  are normalized such that

$$\int_{-\infty}^{\infty} \psi_n^*(x) \psi_k(x) dx = \delta_{n,k}, \quad (3.26)$$

where  $y \equiv \left(\frac{m\omega}{\hbar}\right)^{1/2} x$ , then the normalized function  $\psi_n(x)$  is given by the wavefunctions

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} T_n(y) e^{-y^2/2}, \quad n = 0, 1, 2, \dots \quad (3.27)$$

Table 1: List of the (physicists') Hermite polynomials

$n$	$T_n(y)$
0	1
1	$2y$
2	$4y^2 - 2$
3	$8y^3 - 12y$
4	$16y^4 - 48y^2 + 12$
5	$32y^5 - 160y^3 + 120y$
6	$64y^6 - 480y^4 + 720y^2 - 120$

## CHAPTER IV

### PERTURBATION THEORY

Perturbation theory is the theory in quantum mechanics. It is used in order to approximate energy spectra and wavefunctions of some complicated systems that cannot be solved exactly. In later chapter, we will use this theory to analyse Newton-equivalent Hamiltonian.

#### 4.1 Extensions of time-independent non-degenerate perturbation theory

##### 4.1.1 Standard perturbation theory

As a first step we will consider the time-independent Schrödinger equation which is given by

$$H\psi_n = E_n\psi_n, \quad (4.1)$$

where  $n$  is a discrete label of state. From this chapter to the last chapter, we will ignore the hat symbol ( $\hat{\phantom{x}}$ ) that placed on top of variables for simplicity. Then, we consider a Hamiltonian of the form

$$H = H^0 + \lambda H^1, \quad (4.2)$$

where, one refers to  $H^0$  as the unperturbed Hamiltonian,  $H^1$  as the perturbation Hamiltonian and  $\lambda$  as a small parameter.  $H^0$  is the Hamiltonian that satisfies

$$H^0\psi_n^0 = E_n^0\psi_n^0, \quad (4.3)$$

where the unperturbed energy  $E_n^0$  and the unperturbed wavefunction  $\psi_n^0$  are those of simple harmonic oscillator in eq.(3.21) and eq.(3.27) respectively. In addition, eigenenergies ( $E_n$ ) and eigenfunctions ( $\psi_n$ ) can be written in series of  $\lambda$

$$\psi_n = \psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \cdots, \quad (4.4)$$

and

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots \quad (4.5)$$

Then one substitutes eq.(4.2), eq.(4.4) and (4.5) into eq.(4.1), one obtains

$$(H^0 + \lambda H^1)(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots) = (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots)(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots) \quad (4.6)$$

and writes them in term of power of  $\lambda$

$$\lambda^0 : H^0 \psi_n^0 = E_n^0 \psi_n^0 \quad (4.7)$$

$$\lambda^1 : H^0 \psi_n^1 + H^1 \psi_n^0 = E_n^0 \psi_n^1 + E_n^1 \psi_n^0 \quad (4.8)$$

$$\lambda^2 : H^0 \psi_n^2 + H^1 \psi_n^1 = E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^2 \psi_n^0 \quad (4.9)$$

:

Next, Let us find the first-order correction to the  $n^{th}$  eigenvalue ( $E_n^1$ ). Taking the inner product of eq.(4.8) with  $\psi_n^0$ , one obtains

$$\langle \psi_n^0 | H^0 | \psi_n^1 \rangle + \langle \psi_n^0 | H^1 | \psi_n^0 \rangle = E_n^0 \langle \psi_n^0 | \psi_n^1 \rangle + E_n^1 \langle \psi_n^0 | \psi_n^0 \rangle \quad (4.10)$$

which gives

$$E_n^1 = \langle \psi_n^0 | H^1 | \psi_n^0 \rangle. \quad (4.11)$$

Then let us consider the first-order correction in the  $n^{th}$  eigenfunction ( $\psi_n^1$ ). One defines

$$\psi_n^1 = \sum_{m \neq n}^{\infty} c_m^{(n)} \psi_m^0 \quad (4.12)$$

and substitutes it into eq.(4.8), one obtains

$$\sum_{m \neq n}^{\infty} c_m^{(n)} (H^0 - E_n^0) \psi_m^0 = -(H^1 - E_n^1) \psi_n^0. \quad (4.13)$$

Taking the inner product of eq.(4.13) with  $\psi_l^0$ , one obtains

$$\sum_{m \neq n}^{\infty} c_m^{(n)} (E_m^0 - E_n^0) \langle \psi_l^0 | \psi_m^0 \rangle = -\langle \psi_l^0 | H^1 | \psi_n^0 \rangle + E_n^1 \langle \psi_l^0 | \psi_n^0 \rangle. \quad (4.14)$$

One considers in two cases

$$l = n \quad ; \quad E_n^1 = \langle \psi_n^0 | H^1 | \psi_n^0 \rangle \quad (4.15)$$

$$l \neq n \quad ; \quad c_l^{(n)}(E_l^0 - E_n^0) = -\langle \psi_l^0 | H^1 | \psi_n^0 \rangle, \quad (4.16)$$

which gives

$$c_l^{(n)} = \frac{\langle \psi_l^0 | H^1 | \psi_n^0 \rangle}{E_n^0 - E_l^0}. \quad (4.17)$$

Therefore, eq.(4.12) can be rewritten as

$$\psi_n^1 = \sum_{m \neq n}^{\infty} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0. \quad (4.18)$$

Next, Let us find the second-order correction to the  $n^{th}$  eigenvalue ( $E_n^2$ ). Taking the inner product of eq.(4.9) with  $\psi_n^0$ , one obtains

$$\langle \psi_n^0 | H^0 | \psi_n^2 \rangle + \langle \psi_n^0 | H^1 | \psi_n^1 \rangle = E_n^0 \langle \psi_n^0 | \psi_n^2 \rangle + E_n^1 \langle \psi_n^0 | \psi_n^1 \rangle + E_n^2 \langle \psi_n^0 | \psi_n^0 \rangle \quad (4.19)$$

which gives

$$E_n^2 = \sum_{m \neq n}^{\infty} \frac{|\langle \psi_m^0 | H^1 | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0}. \quad (4.20)$$

Then let us consider the second-order correction in the  $n^{th}$  eigenfunction ( $\psi_n^2$ ). One defines

$$\psi_n^2 = \sum_{p \neq n}^{\infty} d_p^{(n)} \psi_p^0 \quad (4.21)$$

and substitutes it into eq.(4.9), one obtains

$$\sum_{p \neq n}^{\infty} d_p^{(n)} (H^0 - E_n^0) \psi_p^0 = -(H^1 - E_n^1) \psi_n^1 + E_n^2 \psi_n^0. \quad (4.22)$$

Taking the inner product of eq.(4.22) with  $\psi_l^0$ , one obtains

$$\begin{aligned} \sum_{p \neq n}^{\infty} d_p^{(n)} (E_p^0 - E_n^0) \langle \psi_l^0 | \psi_p^0 \rangle &= E_n^1 \sum_{m \neq n}^{\infty} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle}{E_n^0 - E_m^0} \langle \psi_l^0 | \psi_m^0 \rangle + E_n^2 \langle \psi_l^0 | \psi_n^0 \rangle \\ &\quad - \sum_{m \neq n}^{\infty} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle}{E_n^0 - E_m^0} \langle \psi_l^0 | H^1 | \psi_m^0 \rangle. \end{aligned} \quad (4.23)$$



One considers in two cases

$$l = n \quad ; \quad E_n^2 = \sum_{m \neq n}^{\infty} \frac{|\langle \psi_m^0 | H^1 | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0} \quad (4.24)$$

$$l \neq n \quad ; \quad d_l^{(n)}(E_l^0 - E_n^0) = \frac{\langle \psi_n^0 | H^1 | \psi_n^0 \rangle \langle \psi_l^0 | H^1 | \psi_n^0 \rangle}{E_n^0 - E_l^0} - \sum_{m \neq n}^{\infty} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle \langle \psi_l^0 | H^1 | \psi_m^0 \rangle}{E_n^0 - E_m^0}, \quad (4.25)$$

which gives

$$d_l^{(n)} = - \sum_{m \neq n}^{\infty} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle \langle \psi_l^0 | H^1 | \psi_m^0 \rangle}{(E_l^0 - E_n^0)(E_n^0 - E_m^0)} - \frac{\langle \psi_n^0 | H^1 | \psi_n^0 \rangle \langle \psi_l^0 | H^1 | \psi_n^0 \rangle}{(E_l^0 - E_n^0)^2}. \quad (4.26)$$

Therefore, eq.(4.21) can be rewritten as

$$\psi_n^2 = - \sum_{p \neq n}^{\infty} \sum_{m \neq n}^{\infty} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle \langle \psi_p^0 | H^1 | \psi_m^0 \rangle \psi_p^0}{(E_p^0 - E_n^0)(E_n^0 - E_m^0)} - \sum_{p \neq n}^{\infty} \frac{\langle \psi_n^0 | H^1 | \psi_n^0 \rangle \langle \psi_p^0 | H^1 | \psi_n^0 \rangle \psi_p^0}{(E_p^0 - E_n^0)^2}. \quad (4.27)$$

#### 4.1.2 Perturbation theory for one-parameter Hamiltonian

In our case, we consider the one-parameter Hamiltonian of the form

$$H = H^0 + \lambda H^1 + \lambda^2 H^2 + \dots, \quad (4.28)$$

Then the next steps are similar to the standard perturbation theory, we substitute eq.(4.28), eq. (4.5) and (4.4) into eq.(4.1). We obtain

$$\begin{aligned} (H^0 + \lambda H^1 + \lambda^2 H^2 + \dots)(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots) \\ = (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots)(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots), \end{aligned} \quad (4.29)$$

then

$$\lambda^0 : \quad H^0 \psi_n^0 = E_n^0 \psi_n^0 \quad (4.30)$$

$$\lambda^1 : \quad H^0 \psi_n^1 + H^1 \psi_n^0 = E_n^0 \psi_n^1 + E_n^1 \psi_n^0 \quad (4.31)$$

$$\lambda^2 : \quad H^0 \psi_n^2 + H^1 \psi_n^1 + H^2 \psi_n^0 = E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^2 \psi_n^0. \quad (4.32)$$

:

The first-order correction to the  $n^{th}$  eigenvalue and eigenfunction are given by

$$E_n^1 = \langle \psi_n^0 | H^1 | \psi_n^0 \rangle, \quad (4.33)$$

and

$$\psi_n^1 = \sum_{m \neq n}^{\infty} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0. \quad (4.34)$$

Next, let us find the second-order correction to the  $n^{th}$  eigenvalue ( $E_n^2$ ). Taking the inner product with  $\psi_n^0$  into eq.(4.32), we obtain

$$\langle \psi_n^0 | H^0 | \psi_n^2 \rangle + \langle \psi_n^0 | H^1 | \psi_n^1 \rangle + \langle \psi_n^0 | H^2 | \psi_n^0 \rangle = E_n^0 \langle \psi_n^0 | \psi_n^2 \rangle + E_n^1 \langle \psi_n^0 | \psi_n^1 \rangle + E_n^2 \langle \psi_n^0 | \psi_n^0 \rangle, \quad (4.35)$$

which gives

$$E_n^2 = \sum_{m \neq n}^{\infty} \frac{|\langle \psi_m^0 | H^1 | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0} + \langle \psi_n^0 | H^2 | \psi_n^0 \rangle. \quad (4.36)$$

Then let us consider the second-order correction in the  $n^{th}$  eigenfunction ( $\psi_n^2$ ). We define

$$\psi_n^2 = \sum_{p \neq n}^{\infty} c_p^{(n)} \psi_p^0 \quad (4.37)$$

and substitutes it into eq.(4.32).

$$\sum_{p \neq n}^{\infty} c_p^{(n)} (H^0 - E_n^0) \psi_p^0 = -(H^1 - E_n^1) \psi_n^1 - (H^2 - E_n^2) \psi_n^0. \quad (4.38)$$

Taking the inner product of eq.(4.38) with  $\psi_l^0$ , we obtain

$$\begin{aligned} \sum_{p \neq n}^{\infty} c_p^{(n)} (E_p^0 - E_n^0) \langle \psi_l^0 | \psi_p^0 \rangle &= E_n^1 \sum_{m \neq n}^{\infty} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle}{E_n^0 - E_m^0} \langle \psi_l^0 | \psi_m^0 \rangle \\ &\quad - \sum_{m \neq n}^{\infty} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle}{E_n^0 - E_m^0} \langle \psi_l^0 | H^1 | \psi_m^0 \rangle \\ &\quad - \langle \psi_l^0 | H^2 | \psi_n^0 \rangle + E_n^2 \langle \psi_l^0 | \psi_n^0 \rangle. \end{aligned} \quad (4.39)$$

We consider in two cases

$$\begin{aligned}
 l = n; \quad E_n^2 &= \sum_{m \neq n}^{\infty} \frac{|\langle \psi_m^0 | H^1 | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0} + \langle \psi_n^0 | H^2 | \psi_n^0 \rangle \\
 l \neq n; \quad c_l^{(n)}(E_l^0 - E_n^0) &= \frac{\langle \psi_n^0 | H^1 | \psi_n^0 \rangle \langle \psi_l^0 | H^1 | \psi_n^0 \rangle}{E_n^0 - E_l^0} \\
 &\quad - \sum_{m \neq n}^{\infty} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle \langle \psi_l^0 | H^1 | \psi_m^0 \rangle}{E_n^0 - E_m^0} \\
 &\quad - \langle \psi_l^0 | H^2 | \psi_n^0 \rangle
 \end{aligned} \tag{4.40}$$

which gives

$$\begin{aligned}
 c_l^{(n)} &= - \sum_{m \neq n}^{\infty} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle \langle \psi_l^0 | H^1 | \psi_m^0 \rangle}{(E_l^0 - E_n^0)(E_n^0 - E_m^0)} - \frac{\langle \psi_n^0 | H^1 | \psi_n^0 \rangle \langle \psi_l^0 | H^1 | \psi_n^0 \rangle}{(E_l^0 - E_n^0)^2} \\
 &\quad - \frac{\langle \psi_l^0 | H^2 | \psi_n^0 \rangle}{E_l^0 - E_n^0}.
 \end{aligned} \tag{4.41}$$

Therefore, eq.(4.37) can be rewritten as

$$\begin{aligned}
 \psi_n^2 &= - \sum_{p \neq n}^{\infty} \sum_{m \neq n}^{\infty} \frac{\langle \psi_m^0 | H^1 | \psi_n^0 \rangle \langle \psi_p^0 | H^1 | \psi_m^0 \rangle \psi_p^0}{(E_p^0 - E_n^0)(E_n^0 - E_m^0)} - \sum_{p \neq n}^{\infty} \frac{\langle \psi_n^0 | H^1 | \psi_n^0 \rangle \langle \psi_p^0 | H^1 | \psi_n^0 \rangle \psi_p^0}{(E_p^0 - E_n^0)^2} \\
 &\quad - \sum_{p \neq n}^{\infty} \frac{\langle \psi_p^0 | H^2 | \psi_n^0 \rangle \psi_p^0}{E_p^0 - E_n^0}.
 \end{aligned} \tag{4.42}$$

## 4.2 Perturbation theory of Newton-equivalent Hamiltonian

We got the energy and the eigenfunction in the first-order correction. Then, we will expand the Hamiltonian ( $H(\beta)$ ) to determine the perturbation Hamiltonian ( $H^1$ ). From our one-parameter family of Newton-equivalent Hamiltonian,

$$H(\beta) \equiv \frac{1}{2\beta^2 m} \left( (1 + i\beta m \omega x)^{1/2} \exp(-i\hbar\beta\partial_x) (1 - i\beta m \omega x)^{1/2} + (i \rightarrow -i) \right), \tag{4.43}$$

it is convenient to make use of dimensionless quantities. More explicitly, we define

$$y \equiv \left( \frac{m\omega}{\hbar} \right)^{1/2} x. \tag{4.44}$$

Then, eq.(4.43) can be rewritten as

$$\begin{aligned}
 H(\beta) &= \frac{1}{2\beta^2 m} \left( (1 + i\beta m\omega \left(\frac{\hbar}{m\omega}\right)^{1/2} y)^{1/2} \exp(-i\hbar\beta \left(\frac{m\omega}{\hbar}\right)^{1/2} \partial_y) \right. \\
 &\quad \left. (1 - i\beta m\omega \left(\frac{\hbar}{m\omega}\right)^{1/2} y)^{1/2} + (i \rightarrow -i) \right) \\
 &= \frac{1}{2\beta^2 m} \left( (1 + i\beta(m\omega\hbar)^{1/2} y)^{1/2} \exp(-i\beta(m\omega\hbar)^{1/2} \partial_y) \right. \\
 &\quad \left. (1 - i\beta(m\omega\hbar)^{1/2} y)^{1/2} + (i \rightarrow -i) \right).
 \end{aligned} \tag{4.45}$$

In the calculation, we use the property of exponential function of  $\partial_y$  to shift  $f(y)$  to  $f(y \pm a)$

$$\exp(\pm a \partial_y) f(y) = f(y \pm a), \tag{4.46}$$

therefore, the Hamiltonian becomes

$$\begin{aligned}
 H(\beta) &= \frac{1}{2\beta^2 m} \left( (1 + i\beta(m\omega\hbar)^{1/2} y)^{1/2} (1 - i\beta(m\omega\hbar)^{1/2} (y - i\beta(m\omega\hbar)^{1/2}))^{1/2} \right. \\
 &\quad \left. \exp(-i\beta(m\omega\hbar)^{1/2} \partial_y) + (i \rightarrow -i) \right).
 \end{aligned} \tag{4.47}$$

Using series expansion, we obtain

$$\begin{aligned}
 H(\beta) &= \frac{1}{m\beta^2} + \left( -\frac{1}{2} + \frac{y^2}{2} - \frac{\partial_y^2}{2} \right) \omega\hbar \\
 &\quad + \left( -\frac{1}{8} + \frac{y^2}{4} - \frac{y^4}{8} - \frac{y\partial_y}{2} - \frac{y^2\partial_y^2}{4} + \frac{\partial_y^2}{4} + \frac{\partial_y^4}{24} \right) m\beta^2\omega^2\hbar^2 \\
 &\quad + \left( -\frac{1}{16} + \frac{5y^2}{16} - \frac{3y^4}{16} + \frac{y^6}{16} - \frac{y\partial_y}{4} + \frac{y\partial_y^3}{12} - \frac{y^2\partial_y^2}{8} + \frac{y^2\partial_y^4}{48} \right. \\
 &\quad \left. + \frac{y^3\partial_y}{4} + \frac{y^4\partial_y^2}{16} + \frac{\partial_y^2}{16} - \frac{\partial_y^4}{48} - \frac{\partial_y^6}{720} \right) m^2\beta^4\omega^3\hbar^3 + O(\beta^6).
 \end{aligned} \tag{4.48}$$

From our Hamiltonian in series of  $\lambda$  in eq.(4.28), we therefore obtain

$$\begin{aligned}
 H^0 &= \left( \frac{y^2}{2} - \frac{\partial_y^2}{2} \right) \omega\hbar, \\
 H^1 &= \left( -\frac{1}{8} + \frac{y^2}{4} - \frac{y^4}{8} - \frac{y\partial_y}{2} - \frac{y^2\partial_y^2}{4} + \frac{\partial_y^2}{4} + \frac{\partial_y^4}{24} \right) m\beta^2\omega^2\hbar^2, \\
 H^2 &= \left( -\frac{1}{16} + \frac{5y^2}{16} - \frac{3y^4}{16} + \frac{y^6}{16} - \frac{y\partial_y}{4} + \frac{y\partial_y^3}{12} - \frac{y^2\partial_y^2}{8} + \frac{y^2\partial_y^4}{48} + \frac{y^3\partial_y}{4} \right. \\
 &\quad \left. + \frac{y^4\partial_y^2}{16} + \frac{\partial_y^2}{16} - \frac{\partial_y^4}{48} - \frac{\partial_y^6}{720} \right) m^2\beta^4\omega^3\hbar^3.
 \end{aligned} \tag{4.49}$$

We discard  $\beta^{-2}(1/m)$  and  $-\omega\hbar/2$  which are constants. Their only effect is to increase all the energy spectra with the same amount. This is not physically relevant as we only care about difference of energy between different levels. Then we will check that our unperturbed Hamiltonian ( $H^0$ ) is equal to the simple harmonic oscillator ( $H_E$ )

$$\begin{aligned} H^0 &= \left( \frac{y^2}{2} - \frac{\partial_y^2}{2} \right) \omega\hbar \\ &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \end{aligned} \quad (4.50)$$

this will make sure that the unperturbed Hamiltonian is indeed simple harmonic oscillator ( $H_E$ ).

Then we consider the first-order correction to the ground state eigenvalue using eq.(4.33), we obtain

$$E_0^1 = \langle \psi_0^0 | H^1 | \psi_0^0 \rangle = \int \psi_0^{0*} H^1 \psi_0^0 dx. \quad (4.51)$$

Let us calculate the perturbation Hamiltonian acting on unperturbed ground state wavefunction

$$\psi_0^0 = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-y^2/2}. \quad (4.52)$$

This gives

$$\begin{aligned} H^1 \psi_0^0 &= \frac{1}{24} m\omega^2 \hbar^2 (-3(-1+y^2)^2 - 6(-1+y^2)\partial_y^2 - 12y\partial_y + \partial_y^4) \beta^2 \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-y^2/2} \\ &= \frac{m(\beta\omega\hbar)^2}{2} \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-y^2/2} \left( -\frac{1}{24} T_4 \right). \end{aligned} \quad (4.53)$$

Hence, the first-order correction to the ground state energy is given by

$$\begin{aligned} E_0^1 &= \langle \psi_0^0 | H^1 | \psi_0^0 \rangle \\ &= \int_{-\infty}^{\infty} dy \left( \frac{\hbar}{m\omega} \right)^{1/2} \psi_0^{0*} H^1 \psi_0^0 \\ &= \left( \frac{m(\beta\omega\hbar)^2}{\pi^{1/2}} \right) \left( -\frac{1}{48} \right) \int_{-\infty}^{\infty} dy e^{-y^2} T_4 T_0 \\ &= 0 \end{aligned} \quad (4.54)$$

where we used the property of the Hermite polynomials (3.25). By direct calculations, we obtain

$$H^1 T_0 e^{-y^2/2} = \left( -\frac{m(\beta\omega\hbar)^2}{48} \right) T_4 e^{-y^2/2}, \quad (4.55)$$

$$H^1 T_1 e^{-y^2/2} = m(\beta\omega\hbar)^2 \left( -\frac{1}{12} T_3 - \frac{1}{48} T_5 \right) e^{-y^2/2}. \quad (4.56)$$

Therefore, we can define

$$H^1 T_n(y) e^{-y^2/2} = \sum_{\eta=0}^{\infty} a_{n,\eta} T_{\eta} e^{-y^2/2} \quad (4.57)$$

where  $a_{n,\eta}$  are constants. We have calculated  $a_{n,\eta}$  for  $n = 0, 1, \dots, 40$  and  $\eta = 0, 1, \dots, 44$ . In Table 2, we show the list of  $a_{n,\eta}$  where  $n = 0, 1, \dots, 7$  and  $\eta = 0, 1, \dots, 10$ . By using eq.(4.57), we obtain the first-order perturbation Hamiltonian acting on the unperturbed ground state wavefunction ( $H^1 \psi_n^0$ ) in order to calculate the energy spectra and the wavefunctions.

Moreover, by direct calculations we obtain

$$H^2 T_0 e^{-y^2/2} = m^2 \beta^4 \omega^3 \hbar^3 \left( \frac{1}{24} T_0 + \frac{1}{16} T_2 + \frac{1}{64} T_4 + \frac{13}{5760} T_6 \right) e^{-y^2/2}, \quad (4.58)$$

$$H^2 T_1 e^{-y^2/2} = m^2 \beta^4 \omega^3 \hbar^3 \left( \frac{7}{24} T_1 + \frac{3}{16} T_3 + \frac{29}{960} T_5 + \frac{13}{5760} T_7 \right) e^{-y^2/2}. \quad (4.59)$$

Therefore, we can define

$$H^2 T_n(y) e^{-y^2/2} = \sum_{\eta=0}^{\infty} b_{n,\eta} T_{\eta} e^{-y^2/2}, \quad (4.60)$$

where  $b_{n,\eta}$  are constants. We have calculated  $b_{n,\eta}$  for  $n = 0, 1, \dots, 40$  and  $\eta = 0, 1, \dots, 46$ . In Table 3, we show list of  $b_{n,\eta}$  where  $n = 0, 1, \dots, 6$  and  $\eta = 0, 1, \dots, 10$ . By using eq.(4.60), we obtain the first-order perturbation Hamiltonian acting on the unperturbed ground state wavefunction ( $H^1 \psi_n^0$ ) in order to calculate the energy spectra and the wavefunctions.

Table 2: List of  $a_{n,\eta}$ 

$\eta \backslash n$	0	1	2	3	4	5	6	7	...
0	0	0	0	0	$-8\tilde{\beta}$	0	0	0	...
1	0	0	0	$-2\tilde{\beta}$	0	$-40\tilde{\beta}$	0	0	...
2	0	0	0	0	$-8\tilde{\beta}$	0	$-120\tilde{\beta}$	0	...
3	0	$-\frac{1}{12}\tilde{\beta}$	0	0	0	$-20\tilde{\beta}$	0	$-280\tilde{\beta}$	...
4	$-\frac{1}{48}\tilde{\beta}$	0	$-\frac{1}{6}\tilde{\beta}$	0	0	0	$-40\tilde{\beta}$	0	...
5	0	$-\frac{1}{48}\tilde{\beta}$	0	$-\frac{1}{4}\tilde{\beta}$	0	0	0	$-70\tilde{\beta}$	...
6	0	0	$-\frac{1}{48}\tilde{\beta}$	0	$-\frac{1}{3}\tilde{\beta}$	0	0	0	...
7	0	0	0	$-\frac{1}{48}\tilde{\beta}$	0	$-\frac{5}{12}\tilde{\beta}$	0	0	...
8	0	0	0	0	$-\frac{1}{48}\tilde{\beta}$	0	$-\frac{1}{2}\tilde{\beta}$	0	...
9	0	0	0	0	0	$-\frac{1}{48}\tilde{\beta}$	0	$-\frac{7}{12}\tilde{\beta}$	...
10	0	0	0	0	0	0	$-\frac{1}{48}\tilde{\beta}$	0	...
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	

where  $\tilde{\beta} = m\beta^2\omega^2\hbar^2$ ,  $n = 0, 1, 2, \dots, 7$  and  $\eta = 0, 1, 2, \dots, 10$

Next, let us find the first-order correction to the  $n^{th}$  eigenvalue ( $E_n^1$ ), in similar method to  $E_0^1$ , using eq.(4.33) and eq.(4.57), let us consider

$$\langle \psi_l^0 | H^1 | \psi_n^0 \rangle = \int dy \left( \frac{\hbar}{m\omega} \right)^{1/2} \psi_l^{0*} (H^1) \psi_n^0. \quad (4.61)$$

Table 3: List of  $b_{n,\eta}$ 

$\eta \backslash n$	0	1	2	3	4	5	6	...
0	$\frac{1}{24}\tilde{\beta}_1$	0	$\frac{1}{2}\tilde{\beta}_1$	0	$6\tilde{\beta}_1$	0	$104\tilde{\beta}_1$	...
1	0	$\frac{7}{24}\tilde{\beta}_1$	0	$\frac{9}{2}\tilde{\beta}_1$	0	$58\tilde{\beta}_1$	0	...
2	$\frac{1}{16}\tilde{\beta}_1$	0	$\frac{31}{24}\tilde{\beta}_1$	0	$20\tilde{\beta}_1$	0	$258\tilde{\beta}_1$	...
3	0	$\frac{3}{16}\tilde{\beta}_1$	0	$\frac{31}{8}\tilde{\beta}_1$	0	$60\tilde{\beta}_1$	0	...
4	$\frac{1}{64}\tilde{\beta}_1$	0	$\frac{5}{12}\tilde{\beta}_1$	0	$\frac{71}{8}\tilde{\beta}_1$	0	$\frac{285}{2}\tilde{\beta}_1$	...
5	0	$\frac{29}{960}\tilde{\beta}_1$	0	$\frac{3}{4}\tilde{\beta}_1$	0	$\frac{137}{8}\tilde{\beta}_1$	0	...
6	$\frac{13}{5760}\tilde{\beta}_1$	0	$\frac{43}{960}\tilde{\beta}_1$	0	$\frac{19}{16}\tilde{\beta}_1$	0	$\frac{707}{24}\tilde{\beta}_1$	...
7	0	$\frac{13}{5760}\tilde{\beta}_1$	0	$\frac{19}{320}\tilde{\beta}_1$	0	$\frac{83}{48}\tilde{\beta}_1$	0	...
8	0	0	$\frac{13}{5760}\tilde{\beta}_1$	0	$\frac{71}{960}\tilde{\beta}_1$	0	$\frac{19}{8}\tilde{\beta}_1$	...
9	0	0	0	$\frac{13}{5760}\tilde{\beta}_1$	0	$\frac{17}{192}\tilde{\beta}_1$	0	...
10	0	0	0	0	$\frac{13}{5760}\tilde{\beta}_1$	0	$\frac{33}{320}\tilde{\beta}_1$	...
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	

where  $\tilde{\beta}_1 = m^2 \beta^4 \omega^3 \hbar^3$ ,  $n = 0, 1, 2, \dots, 6$  and  $\eta = 0, 1, 2, \dots, 10$

Therefore, we obtain

$$\begin{aligned}
\langle \psi_l^0 | H^1 | \psi_n^0 \rangle &= \frac{1}{(2^{l+n} l! n! \pi)^{1/2}} \sum_{\eta=0}^{\infty} a_{n,\eta} \int e^{-y^2} T_l(y) T_\eta(y) dy \\
&= \frac{1}{(2^{l+n} l! n! \pi)^{1/2}} \sum_{\eta=0}^{\infty} a_{n,\eta} (\sqrt{\pi} 2^\eta \eta! \delta_{nl}) \\
&= \frac{a_{n,l} (\sqrt{\pi} 2^l l!)}{(2^{l+n} l! n! \pi)^{1/2}} \\
&= a_{n,l} \left( \frac{2^l l!}{2^n n!} \right)^{1/2}.
\end{aligned} \tag{4.62}$$

The first-order correction to the  $n^{th}$  eigenvalue following eq.(4.62) and Table 2 is



given by

$$\begin{aligned}
 E_n^1 &= \langle \psi_n^0 | H^1 | \psi_n^0 \rangle \\
 &= a_{n,n} \\
 &= 0,
 \end{aligned} \tag{4.63}$$

where  $n = 0, 1, 2, \dots, 40$ .

Next, let us consider  $\psi_n^1$ , using eq.(4.34), we obtain

$$\psi_n^1 = \sum_{k \neq n}^{\infty} \frac{\langle \psi_k^0 | H^1 | \psi_n^0 \rangle}{E_n^0 - E_k^0} \psi_k^0. \tag{4.64}$$

Then we calculate them by using eq.(3.21), eq.(3.27) and eq.(4.62), we finally obtain

$$\psi_n^1 = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} \frac{1}{\sqrt{2^n n!}} \sum_{k \neq n}^{\infty} \frac{a_{n,k}}{(n-k)\hbar\omega} T_k(y) e^{-y^2/2}. \tag{4.65}$$

Then, let us find the second-order correction to the  $n^{th}$  eigenvalue ( $E_n^2$ ). In eq.(4.36), let us first consider

$$\begin{aligned}
 |\langle \psi_k^0 | H^1 | \psi_n^0 \rangle|^2 &= \langle \psi_k^0 | H^1 | \psi_n^0 \rangle \langle \psi_k^0 | H^1 | \psi_n^0 \rangle^* \\
 &= \langle \psi_k^0 | H^1 | \psi_n^0 \rangle \langle \psi_n^0 | H^1 | \psi_k^0 \rangle.
 \end{aligned} \tag{4.66}$$

Using eq.(4.62), we obtain

$$|\langle \psi_k^0 | H^1 | \psi_n^0 \rangle|^2 = a_{n,k} a_{k,n}. \tag{4.67}$$

Then, let us consider the second term of eq.(4.36) by using eq.(4.60), we obtain

$$\langle \psi_l^0 | H^2 | \psi_n^0 \rangle = b_{n,l} \left( \frac{2^l l!}{2^n n!} \right)^{1/2}, \tag{4.68}$$

so

$$\langle \psi_n^0 | H^2 | \psi_n^0 \rangle = b_{n,n}. \tag{4.69}$$

Therefore, we rewrite eq.(4.36) which calculated from Table 2 and Table 3, is given

by

$$\begin{aligned}
 E_n^2 &= \sum_{k \neq n}^{\infty} \frac{|\langle \psi_k^0 | H^1 | \psi_n^0 \rangle|^2}{E_n^0 - E_k^0} + \langle \psi_n^0 | H^2 | \psi_n^0 \rangle \\
 &= \sum_{k \neq n}^{\infty} \frac{a_{n,k} a_{k,n}}{(n-k)\hbar\omega} + b_{n,n} \\
 &= 0,
 \end{aligned} \tag{4.70}$$

where  $n = 0, 1, 2, \dots, 40$ .

It can be concluded that the result agree with that of the paper [2], namely the energy spectra do not depend on  $\beta$ . Higher values of  $n$  can also be checked, and we expect that the expression remains true for these cases. Although we do not have an explicit proof that this is indeed valid for any given  $n$ , the result should be sufficient to convince that perturbative calculation is working as expected. Let us then proceed to perturbatively analyse Newton-equivalent Hamiltonians for anharmonic oscillator.

## CHAPTER V

### NEWTON-EQUIVALENT ANHARMONIC OSCILLATOR HAMILTONIAN

#### 5.1 Anharmonic Oscillator

Anharmonic oscillators (AHO) is an oscillator that does not oscillating in harmonic motion. It can be approximated to harmonic oscillator. Perturbation theory is usually applied to AHO with small anharmonicity. For a large anharmonicity, we have to use other numerical techniques in calculation. The usual anharmonic oscillator potential is given by

$$V(x) = \frac{1}{2}m\omega^2x^2 + \alpha x^4. \quad (5.1)$$

For this, it is convenient to make use of dimensionless quantities. More explicitly, we define two new variables

$$\tilde{V}(y) = \frac{V(y)}{\hbar\omega}, \quad \tilde{\alpha} = \frac{\hbar}{m^2\omega^3}\alpha. \quad (5.2)$$

Eq.(5.1) can be rewritten as

$$\tilde{V}(y) = \frac{y^2}{2} + \tilde{\alpha}y^4. \quad (5.3)$$

Figure 1 shows graph of  $\tilde{V}(y)$  for  $\tilde{\alpha}$  lower than 0, Figure 2 shows  $\tilde{V}(y)$  for  $\tilde{\alpha}$  equal to 0 and Figure 3 shows  $\tilde{V}(y)$  for  $\tilde{\alpha}$  greater than 0.

Let us consider AHO Hamiltonian ( $H_a$ ) which is given by

$$H_a = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 + \alpha x^4. \quad (5.4)$$

Perturbation theory is used to find energy spectra and wavefunctions. The unperturbed Hamiltonian  $H^0$  is usual harmonic oscillator Hamiltonian and the pertur-

Figure 1: Graph of  $\tilde{V}(y)$  where  $\tilde{\alpha} < 0$

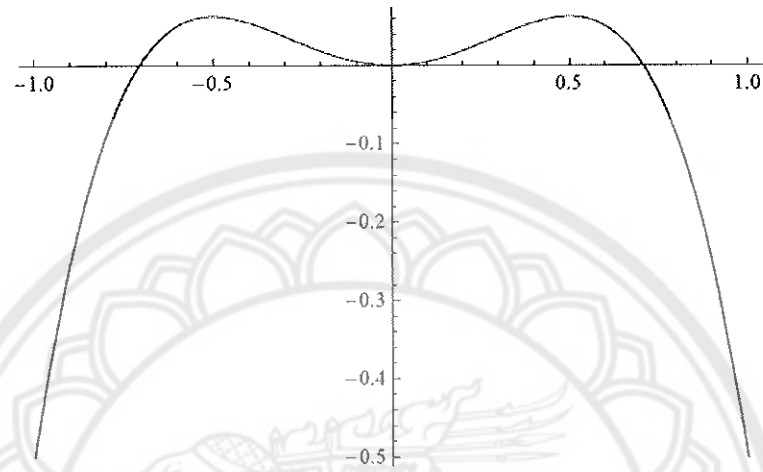


Figure 2: Graph of  $\tilde{V}(y)$  where  $\tilde{\alpha} = 0$

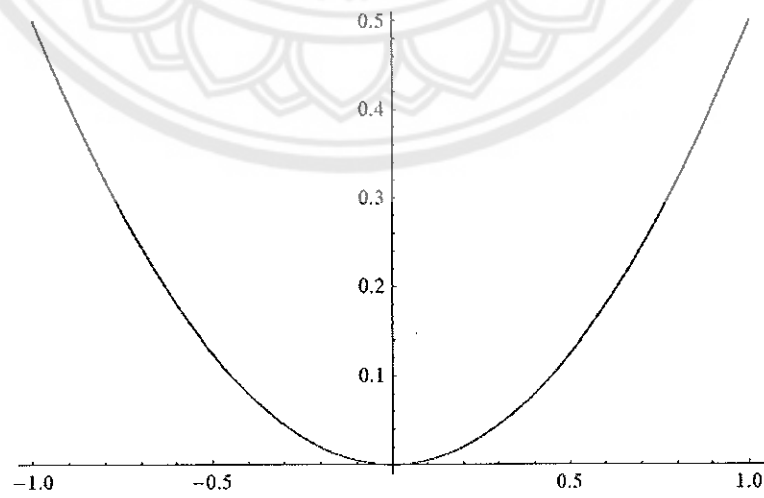
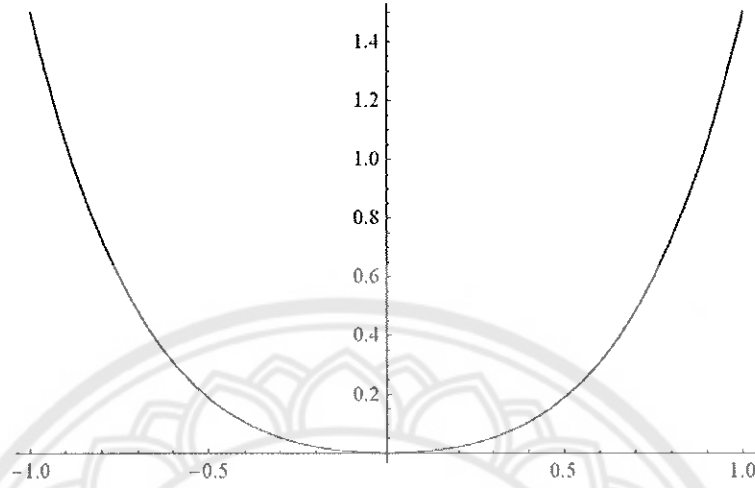


Figure 3: Graph of  $\tilde{V}(y)$  where  $\tilde{\alpha} > 0$ 

bation Hamiltonian  $H^1$  equal to  $\alpha x^4$ . So by using eq.(4.33), we obtain

$$\begin{aligned}
 E_n^1 &= \langle \psi_n^0 | H^1 | \psi_n^0 \rangle \\
 &= \int_{-\infty}^{\infty} dy \left( \frac{\hbar}{m\omega} \right)^{1/2} \psi_n^0 H^1 \psi_n^0 \\
 &= \frac{3(2n^2 + 2n + 1)}{4} \frac{\alpha \hbar^2}{m^2 \omega^2}.
 \end{aligned} \tag{5.5}$$

By using eq.(3.21), we obtain energy spectra of usual anharmonic oscillator Hamiltonian

$$E_n = \left( n + \frac{1}{2} \right) \hbar \omega + \frac{3(2n^2 + 2n + 1)}{4} \frac{\alpha \hbar^2}{m^2 \omega^2} + \dots \tag{5.6}$$

where  $n = 0, 1, 2, \dots$

## 5.2 NEAHO

Let us now discuss Hamiltonian for Newton-equivalent anharmonic oscillator (NEAHO). Back to chapter 2, eq.(2.19), the Newton-equivalent Hamiltonian for simple harmonic oscillator was considered. In order to obtain the Hamiltonian for NEAHO ( $H_A$ ), one needs to add the potential term  $\alpha x^4$  into this Hamiltonian. Let us consider

$$(1 + i\beta m \omega x)^{1/2} (1 - i\beta m \omega x)^{1/2} = (1 + 2\beta^2 m V(x))^{1/2}, \tag{5.7}$$

where  $V(x) = \frac{1}{2}m\omega^2x^2$ . Then we add term  $\alpha x^4$  into the potential  $V(x)$  and obtain

$$(1 + i(\beta^2 m^2 \omega^2 x^2 + 2\beta^2 m \alpha x^4)^{1/2})^{1/2} (1 - i(\beta^2 m^2 \omega^2 x^2 + 2\beta^2 m \alpha x^4)^{1/2})^{1/2}. \quad (5.8)$$

We substitute this term into  $H(\beta)$  eq.(2.19), namely replacing  $(1 + i\beta m\omega x)^{1/2}$  by  $(1 + i(\beta^2 m^2 \omega^2 x^2 + 2\beta^2 m \alpha x^4)^{1/2})^{1/2}$  and  $(1 - i\beta m\omega x)^{1/2}$  by  $(1 - i(\beta^2 m^2 \omega^2 x^2 + 2\beta^2 m \alpha x^4)^{1/2})^{1/2}$ . Therefore, Hamiltonian for Newton-equivalent anharmonic oscillator (NEAHO) can be written as

$$H_A = \frac{1}{2\beta^2 m} \left( (1 + i\beta \sqrt{2mV(x)})^{1/2} \exp(-i\hbar\beta\partial_x) (1 - i\beta \sqrt{2mV(x)})^{1/2} + (i \rightarrow -i) \right), \quad (5.9)$$

where

$$V(x) = \frac{1}{2}m\omega^2x^2 + \alpha x^4. \quad (5.10)$$

The Hamiltonian follow the pattern similar to that of the factorised Hamiltonian [16], [17], which is simple factorised form in discrete quantum mechanics [18], [19]

$$H = \sqrt{A(x)}e^{\gamma p} \sqrt{A^*(x)} + \sqrt{A^*(x)}e^{-\gamma p} \sqrt{A(x)} - A(x) - A^*(x), \quad (5.11)$$

where

$$\begin{aligned} A(x) &= 1 + i(\beta^2 m^2 \omega^2 x^2 + 2\beta^2 m \alpha x^4)^{1/2} \\ A^*(x) &= 1 - i(\beta^2 m^2 \omega^2 x^2 + 2\beta^2 m \alpha x^4)^{1/2} \\ \gamma &= \beta \\ p &= -i\hbar\partial_x. \end{aligned} \quad (5.12)$$

However, our Hamiltonian does not have the last two terms  $(-A(x), -A^*(x))$ . We would like to know the pattern of this two terms. Therefore, we obtain Hamiltonian

which added of the constant  $1/\beta^2 m$  into  $H_A(\beta)$

$$\begin{aligned}
 H_A(\beta) &= \frac{1}{2\beta^2 m} \left( (1 + i(\beta^2 m^2 \omega^2 x^2 + 2\beta^2 m \alpha x^4)^{1/2})^{1/2} \exp(-i\hbar\beta\partial_x) \right. \\
 &\quad \left. (1 - i(\beta^2 m^2 \omega^2 x^2 + 2\beta^2 m \alpha x^4)^{1/2})^{1/2} + (i \rightarrow -i) + 2 \right) \\
 &= \frac{1}{2\beta^2 m} \left( (1 + i(\beta^2 m^2 \omega^2 x^2 + 2\beta^2 m \alpha x^4)^{1/2})^{1/2} (1 - i(\beta^2 m^2 \omega^2 (x - i\hbar\beta)^2 \right. \\
 &\quad \left. + 2\beta^2 m \alpha (x - i\hbar\beta)^4)^{1/2})^{1/2} \exp(-i\hbar\beta\partial_x) + (i \rightarrow -i) + 2 \right).
 \end{aligned} \tag{5.13}$$

The difference of this Hamiltonian eq.(5.13) and eq.(5.9) is just the constant  $1/\beta^2 m$ . It does not effect to the Hamiltonian. We therefore use this Hamiltonian eq.(5.13) to evaluate the energy spectra and wavefunction.

### 5.3 Perturbation theory of NEAHO

In perturbation theory, we obtain the Hamiltonian, eigenenergies and eigenfunctions in series of  $\kappa$

$$H_A = H_A^0 + \kappa H_A^1 + \kappa^2 H_A^2 + \cdots, \tag{5.14}$$

$$\psi_{An} = \psi_{An}^0 + \kappa \psi_{An}^1 + \kappa^2 \psi_{An}^2 + \cdots, \tag{5.15}$$

$$E_{An} = E_{An}^0 + \kappa E_{An}^1 + \kappa^2 E_{An}^2 + \cdots, \tag{5.16}$$

where  $\kappa$  is a bookkeeping parameter which will be set equal to 1 in the end of the calculation. Using eq.(4.4) and eq.(4.28), we define

$$H_A^0 = H^0 + \lambda H^1 + \cdots, \tag{5.17}$$

$$\psi_{An}^0 = \psi_n^0 + \lambda \psi_n^1 + \cdots. \tag{5.18}$$

In addition,  $H_A^0$  is the Hamiltonian that satisfies the equation

$$H_A^0 \psi_{An}^0 = E_{An}^0 \psi_{An}^0. \tag{5.19}$$

By using eq.(4.33) and eq.(4.36), we obtain

$$E_{An}^1 = \langle \psi_{An}^0 | H_A^1 | \psi_{An}^0 \rangle, \quad (5.20)$$

$$E_{An}^2 = \sum_{l \neq n}^{\infty} \frac{|\langle \psi_{Al}^0 | H_A^1 | \psi_{An}^0 \rangle|^2}{E_{An}^0 - E_{Al}^0} + \langle \psi_{An}^0 | H_A^2 | \psi_{An}^0 \rangle. \quad (5.21)$$

Then we consider  $H_A$  by using Taylor series expansion in dimensionless quantities, we obtain

$$\begin{aligned} H_A^0 &= \left( \frac{y^2}{2} - \frac{\partial_y^2}{2} \right) \omega \hbar + \left( -\frac{1}{8} + \frac{y^2}{4} - \frac{y^4}{8} - \frac{y \partial_y}{2} + \frac{\partial_y^2}{4} - \frac{y^2 \partial_y^2}{4} + \frac{\partial_y^4}{24} \right) m \beta^2 \omega^2 \hbar^2, \\ H_A^1 &= \left( \left( -\frac{3y^2}{2} + y^4 \right) \frac{\hbar^2}{m^2 \omega^2} \right. \\ &\quad \left. + \left( \frac{1}{2} - \frac{9y^2}{4} + \frac{5y^4}{4} - \frac{y^6}{2} + \frac{3y \partial_y}{2} - 2y^3 \partial_y + \frac{3y^2 \partial_y^2}{4} - \frac{y^4 \partial_y^2}{2} \right) \frac{\beta^2 \hbar^3}{m \omega} \right) \alpha, \\ H_A^2 &= \left( \left( \frac{5y^4}{4} \right) \frac{\hbar^3}{m^4 \omega^5} + \left( -\frac{5y^2}{2} + \frac{7y^6}{8} - \frac{y^8}{2} - \frac{5y^3 \partial_y}{2} + \frac{y^4}{2} - \frac{5y^4 \partial_y^2}{8} \right) \frac{\beta^2 \hbar^4}{m^3 \omega^4} \right) \alpha^2. \end{aligned} \quad (5.22)$$

Next, we follow the calculation similar to the case of NEAHO Hamiltonian. We then consider

$$\begin{aligned} H_A^1 \psi_0^0 &= \left( \frac{m \omega}{\pi \hbar} \right)^{1/4} \left( -\frac{1}{4} \frac{\beta^2 \hbar^3}{m \omega} T_0 + \left( \frac{3}{8} \frac{\hbar^2}{m^2 \omega^2} - \frac{9}{16} \frac{\beta^2 \hbar^3}{m \omega} \right) T_2 \right. \\ &\quad \left. + \left( \frac{1}{16} \frac{\hbar^2}{m^2 \omega^2} - \frac{3}{16} \frac{\beta^2 \hbar^3}{m \omega} \right) T_4 - \frac{1}{64} T_6 \right) e^{-y^2/2}, \\ H_A^1 T_1(y) e^{-y^2/2} &= \left( -\frac{1}{4} \frac{\beta^2 \hbar^3}{m \omega} T_0 + \left( \frac{3}{8} \frac{\hbar^2}{m^2 \omega^2} - \frac{9}{16} \frac{\beta^2 \hbar^3}{m \omega} \right) T_2 \right. \\ &\quad \left. + \left( \frac{1}{16} \frac{\hbar^2}{m^2 \omega^2} - \frac{3}{16} \frac{\beta^2 \hbar^3}{m \omega} \right) T_4 - \frac{1}{64} T_6 \right) e^{-y^2/2}, \end{aligned} \quad (5.23)$$

and similar to  $H_A^1 T_2(y) e^{-y^2/2}$ ,  $H_A^1 T_3(y) e^{-y^2/2}$  and so on, we therefore define NEAHO Hamiltonian, acting on  $T_n(y) e^{-y^2/2}$  is given by

$$H_A^1 T_n(y) e^{-y^2/2} = \sum_{\eta=0}^{\infty} c_{n,\eta} T_{\eta} e^{-y^2/2}, \quad (5.24)$$

where  $c_{n,\eta}$  are constants. We have calculated  $c_{n,\eta}$  for  $n = 0, 1, \dots, 40$  and  $\eta = 0, 1, \dots, 46$ . In Table 4, we show list of  $c_{n,\eta}$  where  $n = 0, 1, \dots, 4$  and  $\eta = 0, 1, \dots, 10$ .



Table 4: List of  $c_{n,\eta}$ 

$\eta \backslash n$	0	1	2	3	4	...
0	$-\frac{1}{4}\tilde{\beta}_2$	0	$3\tilde{h} - \frac{9}{2}\tilde{\beta}_2$	0	$24\tilde{h} - 72\tilde{\beta}_2$	...
1	0	$\frac{3}{2}\tilde{h} - \frac{5}{2}\tilde{\beta}_2$	0	$21\tilde{h} - \frac{81}{2}\tilde{\beta}_2$	0	...
2	$\frac{3}{8}\tilde{h} - \frac{9}{16}\tilde{\beta}_2$	0	$6\tilde{h} - \frac{43}{4}\tilde{\beta}_2$	0	$66\tilde{h} - 177\tilde{\beta}_2$	...
3	0	$\frac{7}{8}\tilde{h} - \frac{27}{16}\tilde{\beta}_2$	0	$\frac{27}{2}\tilde{h} - 31\tilde{\beta}_2$	0	...
4	$\frac{1}{16}\tilde{h} - \frac{3}{16}\tilde{\beta}_2$	0	$\frac{11}{8}\tilde{h} - \frac{59}{16}\tilde{\beta}_2$	0	$24\tilde{h} - \frac{277}{4}\tilde{\beta}_2$	...
5	0	$\frac{1}{16}\tilde{h} - \frac{5}{16}\tilde{\beta}_2$	0	$\frac{15}{8}\tilde{h} - \frac{105}{16}\tilde{\beta}_2$	0	...
6	$-\frac{1}{64}\tilde{\beta}_2$	0	$\frac{1}{16}\tilde{h} - \frac{7}{16}\tilde{\beta}_2$	0	$\frac{19}{8}\tilde{h} - \frac{165}{16}\tilde{\beta}_2$	...
7	0	$-\frac{1}{64}\tilde{\beta}_2$	0	$\frac{1}{16}\tilde{h} - \frac{9}{16}\tilde{\beta}_2$	0	...
8	0	0	$-\frac{1}{64}\tilde{\beta}_2$	0	$\frac{1}{16}\tilde{h} - \frac{11}{16}\tilde{\beta}_2$	...
9	0	0	0	$-\frac{1}{64}\tilde{\beta}_2$	0	...
10	0	0	0	0	$-\frac{1}{64}\tilde{\beta}_2$	...
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	

where  $\tilde{\beta}_2 = \frac{\beta^2 h^3}{m\omega}$ ,  $\tilde{h} = \frac{h^2}{m^2\omega^2}$ ,  $n = 0, 1, 2, \dots, 4$  and  $\eta = 0, 1, 2, \dots, 10$

Table 5: List of  $d_{n,\eta}$ 

$\eta \backslash n$	0	1	2	3	...
0	$\frac{15}{16}\tilde{h}_1 - \frac{43}{32}\tilde{\beta}_3$	0	$\frac{15}{2}\tilde{h}_1 - \frac{241}{8}\tilde{\beta}_3$	0	...
1	0	$\frac{75}{16}\tilde{h}_1 - \frac{495}{32}\tilde{\beta}_3$	0	$\frac{75}{2}\tilde{h}_1 - \frac{2535}{8}\tilde{\beta}_3$	...
2	$\frac{15}{16}\tilde{h}_1 - \frac{241}{64}\tilde{\beta}_3$	0	$\frac{195}{16}\tilde{h}_1 - \frac{2699}{32}\tilde{\beta}_3$	0	...
3	0	$\frac{25}{16}\tilde{h}_1 - \frac{845}{64}\tilde{\beta}_3$	0	$\frac{375}{16}\tilde{h}_1 - \frac{9535}{32}\tilde{\beta}_3$	...
4	$\frac{5}{64}\tilde{h}_1 - \frac{83}{64}\tilde{\beta}_3$	0	$\frac{35}{16}\tilde{h}_1 - \frac{2179}{64}\tilde{\beta}_3$	0	...
5	0	$\frac{5}{64}\tilde{h}_1 - \frac{159}{64}\tilde{\beta}_3$	0	$\frac{45}{16}\tilde{h}_1 - \frac{4579}{64}\tilde{\beta}_3$	...
6	$-\frac{27}{256}\tilde{\beta}_3$	0	$\frac{5}{64}\tilde{h}_1 - \frac{263}{64}\tilde{\beta}_3$	0	...
7	0	$-\frac{35}{256}\tilde{\beta}_3$	0	$\frac{5}{64}\tilde{h}_1 - \frac{395}{64}\tilde{\beta}_3$	...
8	$-\frac{1}{512}\tilde{\beta}_3$	0	$-\frac{43}{256}\tilde{\beta}_3$	0	...
9	0	$-\frac{1}{512}\tilde{\beta}_3$	0	$-\frac{51}{256}\tilde{\beta}_3$	...
10	0	0	$-\frac{1}{512}\tilde{\beta}_3$	0	...
11	0	0	0	$-\frac{1}{512}\tilde{\beta}_3$	...
12	0	0	0	0	...
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

where  $\tilde{\beta}_3 = \frac{\beta^2 \hbar^4}{m^3 \omega^4}$ ,  $\tilde{h}_1 = \frac{\hbar^3}{m^4 \omega^5}$ ,  $n = 0, 1, 2, \dots, 3$  and  $\eta = 0, 1, 2, \dots, 12$

In a similar way to eq.(4.57), eq.(4.60) and eq.(5.24), let us define

$$H_A^2 T_n(y) e^{-y^2/2} = \sum_{\eta=0}^{\infty} d_{n,\eta} T_\eta e^{-y^2/2}. \quad (5.25)$$

We have calculated  $d_{n,\eta}$  for  $n = 0, 1, \dots, 40$  and  $\eta = 0, 1, \dots, 48$ . In Table 5, we show list of  $d_{n,\eta}$  where  $n = 0, 1, \dots, 3$  and  $\eta = 0, 1, \dots, 12$ .

Next, let us find the first-order correction to the  $n^{th}$  eigenvalue of the

Newton-equivalent anharmonic oscillator Hamiltonian ( $E_{An}^1$ ). We obtain

$$\begin{aligned}
 E_{An}^1 &= \langle \psi_{An}^0 | H_A^1 | \psi_{An}^0 \rangle \\
 &= \langle \psi_n^0 + \lambda \psi_n^1 + \dots | H_A^1 | \psi_n^0 + \lambda \psi_n^1 + \dots \rangle \\
 &= \langle \psi_n^0 | H_A^1 | \psi_n^0 \rangle + \langle \psi_n^0 | H_A^1 | \psi_n^1 \rangle + \langle \psi_n^1 | H_A^1 | \psi_n^0 \rangle + \dots
 \end{aligned} \tag{5.26}$$

where using  $\psi_n^0$  and  $\psi_n^1$  in eq.(3.27) and eq.(4.65) respectively. We consider  $E_{An}^1$  up to order  $\beta^2$  and  $a_{n,k}$  in  $\psi_n^1$  was written in term of  $\beta^2$ . So we consider just only the first three terms in eq.(5.26). Let us start from  $\langle \psi_l^0 | H_A^1 | \psi_n^1 \rangle$

$$\begin{aligned}
 \langle \psi_l^0 | H_A^1 | \psi_n^1 \rangle &= \int dy \left( \frac{\hbar}{m\omega} \right)^{1/2} \psi_l^{0*}(H_A^1) \psi_n^1 \\
 &= \frac{1}{(2^{l+n} l! n! \pi)^{1/2}} \sum_{k \neq n}^{\infty} \frac{a_{n,k}}{(n-k) \hbar \omega} \int dy T_l(y) e^{-y^2/2} (H_A^1) T_k(y) e^{-y^2/2},
 \end{aligned} \tag{5.27}$$

where in eq.(5.24)  $H_A^1 T_k(y) e^{-y^2/2} = \sum_{\zeta=0}^{\infty} c_{k,\zeta} T_{\zeta} e^{-y^2/2}$ ,  $c_{k,\zeta}$  are constants. We obtain

$$\begin{aligned}
 \langle \psi_l^0 | H_A^1 | \psi_n^1 \rangle &= \frac{1}{(2^{l+n} l! n! \pi)^{1/2}} \sum_{k \neq n}^{\infty} \frac{a_{n,k}}{(n-k) \hbar \omega} \sum_{\zeta=0}^{\infty} c_{k,\zeta} \int dy e^{-y^2} T_l(y) T_{\zeta}(y) \\
 &= \frac{1}{(2^{l+n} l! n! \pi)^{1/2}} \sum_{k \neq n}^{\infty} \frac{a_{n,k}}{(n-k) \hbar \omega} \sum_{\zeta=0}^{\infty} c_{k,\zeta} (\sqrt{\pi} 2^{\zeta} \zeta! \delta_{\zeta l}) \\
 &= \frac{1}{(2^{l+n} l! n! \pi)^{1/2}} \sum_{k \neq n}^{\infty} \frac{a_{n,k}}{(n-k) \hbar \omega} c_{k,l} (\sqrt{\pi} 2^l l!),
 \end{aligned} \tag{5.28}$$

therefore,

$$\langle \psi_l^0 | H_A^1 | \psi_n^1 \rangle = \sum_{k \neq n}^{\infty} \frac{a_{n,k} c_{k,l}}{(n-k) \hbar \omega} \left( \frac{2^l l!}{2^n n!} \right)^{1/2}. \tag{5.29}$$

Since  $\langle \psi_l^0 | H_A^1 | \psi_n^1 \rangle = \langle \psi_l^0 | H_A^1 | \psi_n^1 \rangle^* = \langle \psi_n^1 | H_A^1 | \psi_l^0 \rangle$ , so from eq.(5.26), we obtain

$$E_{An}^1 = \langle \psi_n^0 | H_A^1 | \psi_n^0 \rangle + 2 \langle \psi_n^0 | H_A^1 | \psi_n^1 \rangle. \tag{5.30}$$

Next, let us consider  $\langle \psi_n^0 | H_A^1 | \psi_n^0 \rangle$  which is the same calculation as  $\langle \psi_l^0 | H_A^1 | \psi_n^0 \rangle$  from eq.(4.62), using eq.(5.24), we obtain

$$\langle \psi_l^0 | H_A^1 | \psi_n^0 \rangle = c_{n,l} \left( \frac{2^l l!}{2^n n!} \right)^{1/2}. \tag{5.31}$$

Then we substitute eq.(5.29) and eq.(5.31) into eq.(5.30). Therefore,  $E_{An}^1$  is written as

$$E_{An}^1 = c_{n,n} + 2 \sum_{k \neq n}^{\infty} \frac{a_{n,k} c_{k,n}}{(n-k)\hbar\omega}. \quad (5.32)$$

In Table 2 and Table 4, we finally obtain  $E_{An}^1$  in term of  $\beta$

$$E_{An}^1 = \left( \left( 0, \frac{3}{2}, 6, \frac{27}{2}, \dots \right) \frac{\hbar^2}{m^2\omega^2} + \left( 0, \frac{1}{2}, 4, \frac{27}{2}, \dots \right) \frac{\beta^2 \hbar^3}{m\omega} + O(\beta^4) \right) \alpha \quad (5.33)$$

where  $n = 0, 1, 2, 3, \dots, 40$ .

Next, let us find the second-order correction to the  $n^{th}$  eigenvalue of the Newton-equivalent anharmonic oscillator Hamiltonian ( $E_{An}^2$ ), we knew that

$$E_{An}^2 = \sum_{l \neq n}^{\infty} \frac{|\langle \psi_{Al}^0 | H_A^1 | \psi_{An}^0 \rangle|^2}{E_{An}^0 - E_{Al}^0} + \langle \psi_{An}^0 | H_A^2 | \psi_{An}^0 \rangle. \quad (5.34)$$

Let us first consider

$$\begin{aligned} |\langle \psi_{Al}^0 | H_A^1 | \psi_{An}^0 \rangle|^2 &= \langle \psi_{Al}^0 | H_A^1 | \psi_{An}^0 \rangle \langle \psi_{Al}^0 | H_A^1 | \psi_{An}^0 \rangle^* \\ &= \langle \psi_{Al}^0 | H_A^1 | \psi_{An}^0 \rangle \langle \psi_{An}^0 | H_A^1 | \psi_{Al}^0 \rangle \\ &= \langle \psi_l^0 + \psi_l^1 | H_A^1 | \psi_n^0 + \psi_n^1 \rangle \langle \psi_n^0 + \psi_n^1 | H_A^1 | \psi_l^0 + \psi_l^1 \rangle, \end{aligned} \quad (5.35)$$

and we consider  $E_{An}^2$  up to order  $\beta^2$ , therefore eq.(5.35) leave only three terms

$$\begin{aligned} |\langle \psi_{Al}^0 | H_A^1 | \psi_{An}^0 \rangle|^2 &= \langle \psi_l^0 | H_A^1 | \psi_n^0 \rangle \langle \psi_n^0 | H_A^1 | \psi_l^0 \rangle \\ &\quad + 2 \langle \psi_l^0 | H_A^1 | \psi_n^0 \rangle \langle \psi_n^0 | H_A^1 | \psi_l^1 \rangle \\ &\quad + 2 \langle \psi_l^0 | H_A^1 | \psi_n^0 \rangle \langle \psi_l^1 | H_A^1 | \psi_n^1 \rangle. \end{aligned} \quad (5.36)$$

Then substitute eq.(5.29) and eq.(5.31) into eq.(5.36), we obtain

$$|\langle \psi_{Al}^0 | H_A^1 | \psi_{An}^0 \rangle|^2 = c_{n,l} c_{l,n} + 2 \sum_{k \neq n}^{\infty} \frac{a_{l,k} c_{k,n} c_{n,l}}{(l-k)\hbar\omega} + 2 \sum_{k \neq n}^{\infty} \frac{a_{n,k} c_{k,l} c_{l,n}}{(n-k)\hbar\omega}. \quad (5.37)$$

Next we consider the second term of eq.(5.34) that similar method to  $E_{An}^1$  in eq.(5.32), using eq.(5.25), we obtain  $\langle \psi_{An}^0 | H_A^2 | \psi_{An}^0 \rangle$

$$\langle \psi_{An}^0 | H_A^2 | \psi_{An}^0 \rangle = d_{n,n} + 2 \sum_{k \neq n}^{\infty} \frac{a_{n,k} d_{k,n}}{(n-k)\hbar\omega}. \quad (5.38)$$

Therefore, the second-order correction to the  $n^{th}$  eigenvalue of the Newton-equivalent anharmonic oscillator Hamiltonian are

$$\begin{aligned}
 E_{An}^2 &= \sum_{l \neq n}^{\infty} \frac{|\langle \psi_{Al}^0 | H_A^1 | \psi_{An}^0 \rangle|^2}{E_{An}^0 - E_{Al}^0} + \langle \psi_{An}^0 | H_A^2 | \psi_{An}^0 \rangle \\
 &= \sum_{l \neq n}^{\infty} \frac{1}{(n-l)\hbar\omega} \left( c_{n,l} c_{l,n} + 2 \sum_{k \neq n}^{\infty} \frac{a_{l,k} c_{k,n} c_{n,l}}{(l-k)\hbar\omega} + 2 \sum_{k \neq n}^{\infty} \frac{a_{n,k} c_{k,l} c_{l,n}}{(n-k)\hbar\omega} \right) \\
 &\quad + d_{n,n} + 2 \sum_{k \neq n}^{\infty} \frac{a_{n,k} d_{k,n}}{(n-k)\hbar\omega}.
 \end{aligned} \tag{5.39}$$

Follow the Table 2, 4 and 5, we can calculate the spectra

$$\begin{aligned}
 E_{An}^2 &= \left( \left( 0, -\frac{51}{8}, -\frac{153}{4}, -\frac{969}{8}, \dots \right) \frac{\hbar^3}{m^4 \omega^5} \right. \\
 &\quad \left. + \left( 0, -6, -\frac{231}{4}, -\frac{513}{2}, \dots \right) \frac{\beta^2 \hbar^4}{m^3 \omega^4} + O(\beta^4) \right) \alpha^2,
 \end{aligned} \tag{5.40}$$

where  $n = 0, 1, \dots, 40$ .

In addition, in eq.(5.19), we obtain  $E_{An}^0$  equal to  $4\left(n + \frac{1}{2}\right)\hbar\omega$ . By using eq.(5.33), eq.(5.40), and  $E_{An}^0$ , we finally obtain the energy spectra

$$\begin{aligned}
 E_{An} &= E_{An}^0 + \kappa E_{An}^1 + \kappa^2 E_{An}^2 \\
 &= (2, 6, 10, 14, \dots) \hbar\omega \\
 &\quad + \left( \left( 0, \frac{3}{2}, 6, \frac{27}{2}, \dots \right) \frac{\hbar^2}{m^2 \omega^2} + \left( 0, \frac{1}{2}, 4, \frac{27}{2}, \dots \right) \frac{\beta^2 \hbar^3}{m \omega} + O(\beta^4) \right) \alpha \\
 &\quad + \left( \left( 0, -\frac{51}{8}, -\frac{153}{4}, -\frac{969}{8}, \dots \right) \frac{\hbar^3}{m^4 \omega^5} \right. \\
 &\quad \left. + \left( 0, -6, -\frac{231}{4}, -\frac{513}{2}, \dots \right) \frac{\beta^2 \hbar^4}{m^3 \omega^4} + O(\beta^4) \right) \alpha^2
 \end{aligned} \tag{5.41}$$

where  $n = 0, 1, \dots, 40$  and we set  $\kappa = \lambda = 1$ .

Higher values of  $n$  can also be checked, and we expect that the expression remains equal to term of  $\beta$ .

## CHAPTER VI

### CONCLUSIONS

Newton-equivalent Hamiltonian in quantum case is considered. Because of its complication we therefore find its energy spectra by using perturbation theory. We also use the (physicists') Hermite polynomials ( $T_n(y)$ ) to evaluate the energy spectra. In perturbation theory, we use modified Hamiltonian  $H = H^0 + \lambda H^1 + \lambda^2 H^2 + \dots$  to obtain the first and second-order correction to the  $n^{th}$  eigenvalue of the Newton-equivalent Hamiltonian ( $E_n^1, E_n^2$ ).  $E_n^1$  equal to 0 and  $E_n^2$  also equal to 0 for  $n = 0, 1, 2, \dots, 40$ . However, they do not depend on the one-parameter family ( $\beta$ ). Therefore, the energy spectra equal to  $E_n = (n + \frac{1}{2}) \hbar \omega$  where  $n = 0, 1, 2, \dots, 40$ , which agree with those of the standard Hamiltonian. In anharmonic oscillator Hamiltonian, we add potential term ( $\alpha x^4$ ) into the Newton-equivalent Hamiltonian in pattern of the factorised Hamiltonian [16], [17] which is simple factorised form in discrete quantum mechanics [18], [19]. Finally, we obtain the first and second-order correction to the  $n^{th}$  eigenvalue of the Newton-equivalent anharmonic oscillator Hamiltonian ( $E_{An}^1, E_{An}^2$ ) written in term of  $\beta$ .

So as a future work, one may wish to proceed by using the perturbation theory to analyse more complicated NEAHO Hamiltonians, for example those whose potentials are of the form

$$V(x) = \frac{1}{2} m \omega^2 x^2 + \alpha_1 x^4 + \alpha_2 x^6 + \alpha_3 x^8 + \dots \quad (6.1)$$

Eigenenergies and wavefunctions for NEAHO corresponding to this potential can be obtained by using perturbation theory.

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