

# Determination of the Exact Eigenvalues and Eigenfunctions of a Class of Quantum Anharmonic Oscillators With Polynomial Potential Functions

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## Abstract

We determine the exact eigenvalues and eigenfunctions of a class of quantum anharmonic oscillator using a novel non perturbative approach. Our method which has already been applied to quantum harmonic oscillator incorporates the Gram Schmidt Orthogonalization process to generate separate even and odd eigenfunction sequences. For concreteness, we study a specific instance of a quantum anharmonic oscillator having a polynomial potential of order six. The general class of quantum anharmonic oscillators considered here are those characterized by certain polynomial functions with terms of even power.

**Keywords:** quantization, anharmonic Oscillator, exact solution

## 1. Introduction

The restoring force of the classical linear Harmonic Oscillator is directly proportional to the displacement from the origin. Thus, the governing equation is given by the following linear differential equation:

$$m\ddot{x} + c_0x = 0. \quad (1)$$

Integrating the above equation, we obtain the corresponding energy equation

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

In accordance with quantum theory, the time - independent Schrödinger Equation of the Linear Harmonic Oscillator is prescribed as

$$E_n\Phi_n = -\frac{\hbar^2}{2m} \frac{d^2\Phi_n}{dx^2} + \frac{1}{2}m\omega^2x^2\Phi_n. \quad (3)$$

Here,  $c_0 = m\omega^2$  and  $p, m, \hbar, \omega$  have their usual meanings, and  $E_n$  is an Eigenvalue of the Hamiltonian operator  $H$  with corresponding eigenfunction  $\Phi_n$ . The above equation is obtained by the principle of correspondence which is given by the associations:  $\hat{H} \rightarrow \frac{i\hbar\partial}{\partial t}$ ,  $\hat{p} \rightarrow -\frac{i\hbar\partial}{\partial x}$ ,  $\hat{x} \rightarrow x$ .

We shall, in this paper, without loss of generality, use the standardized units such that  $\omega = \hbar = m = 1$  (Joachain & Bransden, 2000).

For our purposes, the classical anharmonic oscillators being nonlinear, will however be characterized as having a restoring force which has a polynomial dependence on the displacement. This leads to an energy equation of the normal form

$$E = \frac{\hat{p}^2}{2m} + \frac{1}{2}c_0x^2 + c_1x^3 + \dots + c_Nx^N \quad (4)$$

where  $N > 2$  and  $c_0, c_1, \dots, c_N$  are real constants.

In accordance again, with the correspondence principle, we have that, the quantum anharmonic oscillator has a time independent Schrödinger equation given by

$$E_m \Phi_m = -\frac{\hbar^2}{2m} \frac{d^2 \Phi_m}{dx^2} + \left( \frac{1}{2} c_0 x^2 + c_1 x^3 + \dots + c_N x^N \right) \Phi_m \tag{5}$$

where  $E_n$  is the eigenvalue of the Hamiltonian operator and  $\Phi_n$  is the corresponding eigenfunction.

Existing studies, hitherto, of the quantum anharmonic oscillator having been restricted to perturbation theoretic and semi-classical methods have consequently produced only approximate solutions in respect of energy eigenvalues and the eigenfunctions. Close form exact solutions have thus, been virtually unavailable (Ghatak, 2012; Biswas, 1999).

Boxi (2017) noted that “...since non-linear second order ordinary differential equation has, in general, no analytic solution, an approximation method is usually applied to tackle the problem.” Nonetheless, in this paper, we seek precisely to provide a non - perturbative method for the determination of a closed form exact eigenvalues and the corresponding eigenfunctions for a specific class of quantum anharmonic oscillators. The basis of the method used here is an extension of a framework used by Oduro and Odoom (2021), which entailed the application of Gram - Schmidt Orthogonalization process to an alternative study of the Quantum Harmonic oscillator.

In this vein, using the solutions of an appropriate linear differential equation of Second Order, we recover the Schrödinger Equation together with its eigenvalues and corresponding eigenfunctions of a specified class of Quantum Anharmonic Oscillators. The applications of quantum anharmonic oscillators abound practically in most areas of modern physics including molecular, condensed matter, high energy physics as well as, more recently Quantum Computing (Cao, Betzholz, Zhang, and Cai, 2017) and Quantum Finance (Wolf, 2021; Schaden, 2002).

The paper has the following structure: In section two, we provide a short review of perturbation theory, applying it to obtain the first order energy correction of a specified quantum anharmonic oscillator. In section three, we present some propositions and a Lemma in respect of the development of our method. In the sections that follow, we implement the proposed method in terms of some specific computations which comprise even and odd cases of eigenfunctions.

## 2. An Existing Perturbation Method

We briefly present here an exposition of the Ladder Operator perturbation method and apply it to quantum anharmonic oscillator with fourth order polynomial potential function.

According Griffiths (2016), “...*Perturbation Theory is a systematic procedure for obtaining approximate solutions to the perturbed problem by building on the known exact solutions to the unperturbed case*”.

We may write the new Hamiltonian as the sum of two terms:

$$\hat{H} = \hat{H}^0 + \lambda \hat{H}' \tag{6}$$

where  $\hat{H}$  is the Hamiltonian,  $\hat{H}^0$  is the unperturbed Hamiltonian and  $\hat{H}'$  is the perturbation.

The eigenvalue problem that we intends to solve is given by

$$\hat{H} \phi_n = \lambda \phi_n. \tag{7}$$

Writing  $\phi_n$  and  $E_n$  as power series in  $\lambda$ , we have

$$\phi_n = \phi_n^0 + \lambda \phi_n^1 + \lambda^2 \phi_n^2 + \dots \tag{8}$$

$$\hat{E}_n = E_n^0 + \lambda \hat{E}_n^1 + \lambda^2 \hat{E}_n^2 + \dots \tag{9}$$

Here  $E_m^1$  is the first - order correction to the  $n^{th}$  eigenvalue, and  $\phi_m^1$  is the first - order correction to the  $m^{th}$  eigenfunction;  $E_m^2$  and  $\phi_m^2$  are the second - order corrections, and so on.

Putting (6), (8) and (9) into equation (7), and properly simplifying it, we get

$$E_m^1 = \langle \phi_m^0 | \hat{H}' | \phi_m^0 \rangle \tag{10}$$

and

$$\phi_m^1 = \sum_{m \neq n} \frac{\langle \phi_m^0 | \hat{H}' | \phi_n^0 \rangle}{(E_n^0 - \hat{E}_m^0)} \tag{11}$$

$E_n^1$  and  $\phi_n^1$  are respectively the first - order correction of the energy eigenvalue and the eigenfunction.

## 2.1 Computations of the Eigenvalues of a Quantum Anharmonic Oscillator Using the Ladder Operator Method

### 2.1.1 Ladder Operator Method

It is always commodious to introduce a dimensionless complex operator known as the Ladder Operators when solving the Schrödinger equation such that

$$a^\dagger = \frac{x - i\hat{p}}{\sqrt{2}}. \tag{12}$$

The Adjoint of  $a^\dagger$  which is  $\bar{a}$  will be given by

$$a = \frac{x + i\hat{p}}{\sqrt{2}}. \tag{13}$$

By adding equations (12) and (13), we get  $x$ , such that

$$x = \frac{1}{\sqrt{2}}(a^\dagger + a). \tag{14}$$

We must first and foremost note that when a ket vector acts on the raising(creation) and lowering (annihilation) operators, the final results are given respectively as

$$a^\dagger |n\rangle = \sqrt{(n+1)} |n+1\rangle \tag{15}$$

$$a |n\rangle = \sqrt{n} |n-1\rangle. \tag{16}$$

(Clark, 2011).

Consider the Hamiltonian of a quantum anharmonic oscillator which can be written as

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}c_0x^2 + c_1x^3 + c_2x^4. \tag{17}$$

Comparing (17) to equation (6), we have

$$\hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2}c_0x^2 \tag{18}$$

which is the unperturbed Hamiltonian of the linear harmonic oscillator and

$$\hat{H}' = c_1x^3 + c_2x^4 \tag{19}$$

which is also the perturbed Hamiltonian representing the anharmonic term, where  $c_1$  and  $c_2$  are the perturbed terms. Such anharmonic corrections occur in the studies such as vibrational spectra of molecules.

Considering Equation (19), and making use of equation (10), we can solve for the first - order correction to the energy eigenvalue of the  $m$ th state  $E_m^{(1)}$ , which is given by

$$E_m^{(1)} = c_1 (x^3)_{mm} + c_2 (x^4)_{mm} \tag{20}$$

$$E_m^{(1)} = \int_{-\infty}^{+\infty} (c_1x^3 + c_2x^4) |\Phi_m^{(0)}(x)|^2 dx. \tag{21}$$

We must take note that  $x^3$  is an odd function of  $x$ . As a result, the diagonal matrix element  $(x^3)_{mm}$  vanishes, and the term  $c_1x^3$  does not contribute to the energy  $E_m^{(1)}$ . That is

$$\langle m | x^3 | m \rangle = 0$$

This means that the first energy correction  $E_m^{(1)}$  reduces to

$$E_m^{(1)} = (x^4)_{mm} = \langle m | x^4 | m \rangle \tag{22}$$

We can find  $x^4$  from equation (22) as

$$x^4 = \left(\frac{1}{\sqrt{2}}\right)^2 [(a^\dagger + a)(a^\dagger + a)(a^\dagger + a)(a^\dagger + a)]. \tag{23}$$

After going through rigorous calculation, and making use of equation (10), we have the First - Order Correction to the energy eigenvalue of the quantum anharmonic oscillator given by

$$E_m^{(1)} = \frac{3c_2}{8} [2m^2 + 2m + 1]. \tag{24}$$

But the unperturbed energy levels  $E_m^{(0)}$  is also given by

$$E_m^{(0)} = \left(m + \frac{1}{2}\right). \tag{25}$$

Therefore, the total energy  $E_m$  of the quantum anharmonic oscillator is given by

$$E_m = E_m^{(0)} + E_m^{(1)} \tag{26}$$

Substituting (24) and (25) into equation (26), we get the total energy  $E_m$  as

$$E_m = \left(m + \frac{1}{2}\right) + \frac{3c_2}{8} [2m^2 + 2m + 1]. \tag{27}$$

Putting  $m = 0, 1, 2, 3, 4, 5$  and  $c_2 = \frac{1}{6}$  into equation (27), we have the ground state and the next four excited states energy eigenvalues given by

$$E_0^{(1)} = 0.5625; \hat{E}_1^{(1)} = 1.8125; E_2^{(1)} = 3.3125; E_3^{(1)} = 5.0625; E_4^{(1)} = 7.0625; E_5^{(1)} = 9.3125$$

The foregoing computations by means of the Ladder operator perturbation method have yielded only approximate eigenvalues of a particular quantum anharmonic oscillator. However, in the next section, we present a non-perturbative determination of the exact eigenvalues and eigenfunctions of a class of quantum anharmonic oscillators.

### 3. Results and Discussion

As in Oduro and Odoom (2021), the idea behind the next proposition reflects the symmetry of an anharmonic oscillator with respect to a displacement from the origin. Thus, the most basic **smooth function** having this symmetry beyond the function  $e^{-\frac{x^2}{2}}$  would be  $e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}$ . In accordance with Born’s rule, the probability density is a product of a conjugate pair of functions. Thus, the appropriate pair of linearly independent functions would be  $e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}$  and  $xe^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}$  in order to ensure a non - vanishing Wronskian, and for these functions to be solutions of a second order differential equation while being candidate wave functions compatible with Born’s Rule as in Spiegel,(1976).

#### 3.1 Theoretical Results

Following the notation of Oduro and Odoom, (2021), we have:

##### 3.1.1 Proposition 1

The set of functions

$$U_n = x^n e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)} \tag{28}$$

where  $n = 0, 1, 2, \dots$ , constitutes a solution to the second order differential equation

$$\frac{d^2 U_n}{dx^2} = n(n - 1)x^{-2}U_n - (2n + 1) U_n - \frac{n}{3}x^2U_n + \left(\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6\right) U_n. \tag{29}$$

#### Proof

We apply Leibniz Theorem to equation (28). We will let  $U_n = uv$  and substitute the results into the Leibniz expansion  $\frac{d^2 U_n}{dx^2} = \frac{d^2 u}{dx^2}v + 2\frac{du}{dx}\frac{dv}{dx} + u\frac{d^2 v}{dx^2}$  so as to generate equation (29).

#### Example

Inserting  $n = 0$  into equation (29), we obtain:

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\left(\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6\right)\right]U_0(x) = \frac{1}{2}U_0(x). \tag{30}$$

**Remark 1**

Equations (30) is a Schrödinger equation of quantum anharmonic oscillator of the form

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} f(x) \right] U_0(x) = \lambda_0 U_0(x) \tag{31}$$

where the potential  $f(x) = \left(\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6\right)$  with an eigenvalue  $\lambda = \frac{1}{2}$ , and its corresponding eigenfunction  $U_0(x) = e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}$ .

Note that the  $U_0$  is the ground state of a Quantum Anharmonic Oscillator. The corresponding energy eigenvalue is the zero point energy.

However, for  $n \geq 1$ , we failed to obtain the eigenvalue problem and therefore we are not able to recover the Schrödinger Equation from equation (31) at this point.

For instance, for  $n = 1$  and  $n = 2$  we have the respective equations as

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} \left( \frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right] U_1(x) = \frac{3}{2}U_1(x) + \frac{1}{6}U_3(x) \tag{32}$$

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} \left( \frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right] U_2(x) = \frac{5}{2}U_2(x) + \frac{1}{3}U_4(x) - U_0(x). \tag{33}$$

3.1.2 Lemma 1

Let  $P$  be Hermitian operator acting on an inner product Space  $H$  and also let  $PV = \lambda V + \epsilon$  where  $V, \epsilon$  are vectors in  $H$ ,  $V \perp \epsilon$  and  $\lambda$  is an eigenvalue of  $P$ . Then, there exists a Hermitian Operator  $P'$  on  $H$  such that  $P'V = \lambda V$ .

**Proof**

Let  $PV = \lambda V + \epsilon$  where  $P$  is a Hermitian operator on the inner product space  $H$ , and  $V \perp \epsilon$ . Now, if  $\lambda$  is an eigenvalue of  $P$ , then the above expression should be in conformity with the unique expansion given by the Spectral decomposition theorem (Hoffman and Kunze, 1971):

$$PV_m = \lambda_m V_m + \sum_{k \neq m} \lambda_k V_k, \tag{34}$$

where we have put  $\lambda = \lambda_m$  and  $V = V_m$ , so that

$$\epsilon = \sum_{k \neq m} \lambda_k V_k.$$

Indeed, according to the spectral decomposition theorem,  $P$  may be expanded as

$$P = \sum_k \lambda_k P_k \equiv \sum_k P|_{span V_k}, \tag{35}$$

where the  $P_k$  are the projection operators and  $P_k V_k = V_k$  with the  $Ker(P_k) = (span P_k)^\perp$  (Orthogonal Complement). Thus,

$$P|_{span V_k} V_k = \lambda_k V_k.$$

In particular,

$$P|_{span V_m} V_m = \lambda_m V_m. \tag{36}$$

Therefore,  $P'$  exists and is given by

$$P' = P|_{span V_m}.$$

It is clear that  $P'$  may be computed by orthogonal projection as follows:

$$\begin{aligned} \langle V_m | (P' V_m) \rangle |V_m\rangle &= \lambda_m \langle V_m | V_m \rangle |V_m\rangle + \sum_{k \neq m} \lambda_k \langle V_m | V_k \rangle |V_m\rangle \\ &= \lambda_m |V_m\rangle + 0 \end{aligned} \tag{37}$$

since  $\langle V_m | V_k \rangle = 0$  for all  $(k \neq m)$  and  $\langle V_m | V_m \rangle = 1$  wlog, Therefore,

$$P|_{span V} = \lambda V.$$

Hence

$$P' = P|_{\text{span}V} \tag{38}$$

so that

$$P'V = \lambda V. \tag{39}$$

### 3.1.3 Proposition 2

The family of functions  $\{V_m(x)\}$  satisfies the equation

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + f(x)\right] V_m(x) = \left(m + \frac{1}{2} + \frac{m}{6} \alpha_m\right) V_m(x) + \frac{m}{6} V_{m+2} + \frac{m}{6} \sum_{k=0,1}^{m-2} \beta_k V_k(x), \tag{40}$$

where

$$V_m = U_m - \sum_{k=0,1}^{m-2} \frac{\langle U_m, V_k \rangle}{\langle V_k, V_k \rangle} V_k, \tag{41}$$

$$\alpha_m = \frac{\langle U_{m+2}, V_m \rangle}{\langle V_m, V_m \rangle}, \tag{42}$$

$$\beta_k = \frac{\langle U_{m+2}, V_k \rangle}{\langle V_k, V_k \rangle}, \tag{43}$$

and  $\{U_m\}$  constitute solutions to equation (29).

### Proof

Equation (29) can be written as

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + f(x)\right] U_m(x) = \left(m + \frac{1}{2}\right) U_m(x) + \frac{m}{6} U_{m+2} + m(m-1)x^{-2}U_m. \tag{44}$$

Following Oduro and Odoom (2021), we may carry out a change of basis ( $U_m \mapsto V_m$ ) using Gram Schmidt orthogonalization process initialized by  $U_0 = V_0$  and  $U_1 = V_1$ .

Equation (44) then becomes

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + f(x)\right] V_m(x) = \left(m + \frac{1}{2}\right) V_m(x) + \frac{m}{6} U_{m+2}. \tag{45}$$

Equation (45) is a Schrödinger equation plus an “extra potential term”  $\frac{m}{6} U_{m+2}$  on the RHS. We may eliminate the extra potential term as follows: (still in the context of transforming  $U_m \mapsto V_m$ ),

$$U_{m+2} = \frac{\langle U_{m+2}, V_m \rangle}{\langle V_m, V_m \rangle} V_m + \sum_{k=0,1}^{m-2} \frac{\langle U_{m+2}, V_k \rangle}{\langle V_k, V_k \rangle} V_k + V_{m+2} \tag{46}$$

where

$$\alpha_m = \frac{\langle U_{m+2}, V_m \rangle}{\langle V_m, V_m \rangle} V_m,$$

and

$$\beta_k = \frac{\langle U_{m+2}, V_k \rangle}{\langle V_k, V_k \rangle} V_k.$$

Substituting (46) into equation (45), we have

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + f(x)\right] V_m(x) = \left\{ \left(m + \frac{1}{2}\right) + \frac{m}{6} \alpha_m \right\} V_m(x) + \frac{m}{6} \left\{ V_{m+2} + \sum_{k=0,1}^{m-2} \beta_k V_k(x) \right\}. \tag{47}$$

as required, where  $k \neq m$ .

### Remark 2

In the notation of Lemma 1, equation (47) is of the form

$$PV = \lambda V + \epsilon \tag{48}$$

where  $\lambda = \left\{ \left( m + \frac{1}{2} \right) + \frac{m}{6} \alpha_m \right\}$  and  $\epsilon = \frac{m}{6} V_{m+2} + \frac{m}{6} \sum_{k=0,1}^{m-2} \beta_k V_k(x)$ , since  $\lambda$  is the eigenvalue of the Hermitian operator  $\left[ -\frac{1}{2} \frac{d^2}{dx^2} + f(x) \right]$  and  $V_m \perp \frac{m}{6} \left( V_{m+2} + \sum_{k=0,1}^{m-2} \beta_k V_k(x) \right)$ . Therefore, in accordance to Lemma 1, equation (47) can be written as

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + f(x) \right]_{\text{span} V_m} V_m(x) = \left\{ \left( m + \frac{1}{2} \right) + \frac{m}{6} \alpha_m \right\} V_m(x). \tag{49}$$

### 3.1.4 Proposition 3

Let a class of polynomial potential function  $f(x)$  be given by

$$f(x) = (g'(x))^2 + g''(x) + C \tag{50}$$

where  $g(x)$  is a polynomial of order  $2p$  given by

$$g(x) = \sum_{j=1}^p \kappa_j x^{2j} \tag{51}$$

where  $\kappa_j$  and  $C$  are real numbers. Then, the quantum anharmonic oscillator with potential  $f(x)$  has an eigenfunctions given by

$$V_m = U_m - \sum_{k=0,1}^{m-2} \frac{\langle U_m, g_k \rangle}{\langle V_k, V_k \rangle} V_k \tag{52}$$

where  $U_n = x^n e^{-g(x)}$  and  $k = 0, 2, 4$  for even numbers and  $k = 1, 3, 5$  for odd numbers.

(The choice of  $\kappa_j$  should be consistent with the existence of inner product in the Hilbert space). **Proof**

The proof of this proposition is almost identical to Proposition 2 above and involves a change of basis by the Gram Schmidt orthogonalization process as well as elimination of “extra potential term.”

#### Remark 3

So far, the instance of the general class of quantum anharmonic oscillators with polynomial functions which have been elaborated here were in respect of the case  $p = 2$  and  $\kappa_1 = \frac{1}{2!}, \kappa_2 = \frac{1}{4!}$ .

Therefore,  $\lambda_m = \left\{ \left( m + \frac{1}{2} \right) + \frac{m}{6} \alpha_m \right\}$  and  $g(x) = \left( \frac{x^2}{2!} + \frac{x^4}{4!} \right)$  so that  $U_m = x^m e^{-\left( \frac{x^2}{2} + \frac{x^4}{24} \right)}$ .

### 3.2 Specific Computations of the Eigenfunctions of the Quantum Anharmonic Oscillator

#### 3.2.1 Even Eigenfunctions for $m \geq 2$

In order to get the eigenvalue problem, we need to apply Gram Schmidt Orthogonalization process to the trial solutions for  $m \geq 2$  to compute the eigenfunctions.

For convenience, **we want to find**  $V_2$ .

We now start by setting  $n = 0$ , into equation (28) to yield

$$V_0 = U_0 = e^{-\left( \frac{x^2}{2} + \frac{x^4}{24} \right)}. \tag{53}$$

For  $n = 2$ , we again have

$$U_2 = x^2 e^{-\left( \frac{x^2}{2} + \frac{x^4}{24} \right)}. \tag{54}$$

By applying Gram Schmidt process to the trial solutions (53) and (54), we obtain

$$V_2 = x^2 e^{-\left( \frac{x^2}{2} + \frac{x^4}{24} \right)} - \frac{\left\langle x^2 e^{-\left( \frac{x^2}{2} + \frac{x^4}{24} \right)}, e^{-\left( \frac{x^2}{2} + \frac{x^4}{24} \right)} \right\rangle}{\left\langle e^{-\left( \frac{x^2}{2} + \frac{x^4}{24} \right)}, e^{-\left( \frac{x^2}{2} + \frac{x^4}{24} \right)} \right\rangle} e^{-\left( \frac{x^2}{2} + \frac{x^4}{24} \right)}. \tag{55}$$

Equation (55) is expanded as

$$V_2 = x^2 e^{-\left( \frac{x^2}{2} + \frac{x^4}{24} \right)} - \frac{\int_{-\infty}^{+\infty} x^2 e^{-\left( x^2 + \frac{x^4}{12} \right)} dx}{\int_{-\infty}^{+\infty} e^{-\left( x^2 + \frac{x^4}{12} \right)} dx} e^{-\left( \frac{x^2}{2} + \frac{x^4}{24} \right)}. \tag{56}$$

Equation (56) may be simplified as

$$V_2 = \left( x^2 - 0.419262 \right) e^{-\left( \frac{x^2}{2} + \frac{x^4}{24} \right)}. \tag{57}$$

Similarly, we want to generate  $V_4$  as we substitute  $V_0, V_2, U_2$ , and  $U_4$  into the Gram Schmidt equation. This gives us

$$V_4 = x^4 e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)} - \frac{\left\langle x^4 e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}, e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)} \right\rangle}{\left\langle e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}, e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)} \right\rangle} e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)} - \frac{\left\langle x^4 e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}, (x^2 - 0.419262) e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)} \right\rangle}{\left\langle (x^2 - 0.419262) e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}, (x^2 - 0.419262) e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)} \right\rangle} (x^2 - 0.419262) e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}. \tag{58}$$

Equation (58) is further simplified as

$$V_4 = \left(x^4 - 2.15752x^2 + 0.57839\right) e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}. \tag{59}$$

Therefore, the Orthogonal Basis  $\{V_0, V_2, V_4\}$  are written as

$$\left\{1, (x^2 - 0.419262), (x^4 - 2.15752x^2 + 0.57839)\right\} e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}. \tag{60}$$

Equation (60) replaces the original trial solution basis  $\{U_0, U_2, U_4\}$ . Thus, equation (60) gives the orthogonal bases corresponding to even trial functions which were orthogonalized.

### 3.2.2 Eigenvalues Corresponding to Even Eigenfunctions for $V_2$ and $V_4$

We want to find the eigenvalue corresponding to the eigenfunction  $V_2$ .

Substituting  $m = 2$  into equation (47), we get

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \frac{1}{2} \left(-\frac{1}{2} x^2 + \frac{1}{3} x^4 + \frac{1}{36} x^6\right)\right] V_2(x) = \left(\frac{5}{2} + \frac{1}{3} \alpha_2\right) V_2 + \frac{1}{3} V_4 + \frac{1}{2} V_0(x). \tag{61}$$

According to equation (42)  $\alpha_2$  is given by

$$\alpha_2 = \frac{\langle U_4, V_2 \rangle}{\langle V_2, V_2 \rangle} V_2. \tag{62}$$

Substituting the expansions of  $U_4$  and  $V_2$  into equation (62), we have

$$\alpha_2 = 2.15752.$$

If we put  $\alpha_2$  into equation (43) and simplify, we have

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \frac{1}{2} \left(-\frac{1}{2} x^2 + \frac{1}{3} x^4 + \frac{1}{36} x^6\right)\right] V_2(x) = 3.22V_2 + \frac{1}{3} V_4 + \frac{1}{30} V_0(x). \tag{63}$$

Comparing (63) to equation (49), and in accordance to Lemma 1, we can conclude that equation (63) can finally be written as

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \frac{1}{2} \left(-\frac{1}{2} x^2 + \frac{1}{3} x^4 + \frac{1}{36} x^6\right)\right]_{spanV_2} V_2(x) = 3.22V_2(x) \tag{64}$$

which is now an eigenvalue problem.

Similarly, for  $V_4$ , putting  $m=4$  into equation (47), we have

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + \frac{1}{2} \left(-\frac{1}{2} x^2 + \frac{1}{3} x^4 + \frac{1}{36} x^6\right)\right] V_4(x) = \left(\frac{9}{2} + \frac{2}{3} \alpha_4\right) V_4 + \frac{2}{3} \{\beta_0 V_0(x) + \beta_2 V_2 + V_6\}. \tag{65}$$

Solving for  $\alpha_4$  which is given by

$$\alpha_4 = \frac{\langle U_6, V_4 \rangle}{\langle V_4, V_4 \rangle} V_4 = 4.8864V_4. \tag{66}$$

From equation (43), we can similarly calculate  $\beta_0$  and  $\beta_2$  as follows:

$$\beta_0 = \frac{\langle U_4, V_0 \rangle}{\langle V_0, V_0 \rangle} = 0.4844$$



and

$$\beta_2 = \frac{\langle U_4, V_2 \rangle}{\langle V_2, V_2 \rangle} = 2.15753$$

Substituting  $\alpha_4, \beta_0$  and  $\beta_2$  into equation (47) we have

$$\begin{aligned} & \left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{1}{2} \left( -\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right] V_4(x) \\ & = 7.776V_4 + \frac{2}{3} \{0.844V_0(x) + 2.1575V_2 + V_6\}. \end{aligned} \tag{67}$$

In accordance to Lemma 1, equation (67) becomes

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{1}{2} \left( -\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right] V_4 = 7.776V_4. \tag{68}$$

Equations (64) and (68) are the eigenvalue equations for the quantum anharmonic Oscillator representing the eigenfunctions  $V_2$  and  $V_4$  respectively.

### 3.2.3 Computations of the Odd Eigenfunctions of the Quantum Anharmonic Oscillator for $m \geq 1$

Similarly, we want to consider the Proposition 1 given above and start by setting  $n = 1$  and  $n = 3$  into equation (28) and this gives us

$$V_1 = U_1 = xe^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)} \tag{69}$$

and

$$U_3 = x^3e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)} \tag{70}$$

Substituting  $V_1$  and  $U_3$  into the Gram Schmidt equation (41) and proceed as the even case, we get

$$V_3 = x^3e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)} - \frac{\int_{-\infty}^{+\infty} x^4e^{-\left(x^2 + \frac{x^4}{12}\right)} dx}{\int_{-\infty}^{+\infty} x^2e^{-\left(x^2 + \frac{x^4}{12}\right)} dx} xe^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)} \tag{71}$$

which simplifies to

$$V_3 = \left(x^3 - 1.1554x\right)e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}. \tag{72}$$

**We can go through the same process to generate  $V_5$  as**

$$V_5 = \left(x^5 - 3.39397x^3 + 1.8572x\right)e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}. \tag{73}$$

The Orthogonal Basis are

$$\left\{x, \left(x^3 - 1.1554x\right), \left(x^5 - 3.39397x^3 + 1.8572x\right)\right\}e^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}. \tag{74}$$

### 3.2.4 Eigenvalues Corresponding to Odd Eigenfunctions for $V_1, V_3$ and $V_5$

From equation (28), we have  $V_1$  given by

$$V_1 = U_1 = xe^{-\left(\frac{x^2}{2} + \frac{x^4}{24}\right)}.$$

To find the eigenvalue of  $V_1$ , we will put  $m = 1$  into equation (47) given by

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{1}{2} \left( -\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right] V_1(x) = \left(\frac{3}{2} + \frac{1}{6}\alpha_1\right) V_1 + \frac{1}{6}V_3(x) \tag{75}$$

Solving for  $\alpha_1$  gives

$$\alpha_1 = \frac{\langle U_3, V_1 \rangle}{\langle V_1, V_1 \rangle} V_1 = \frac{6}{5}V_1 \tag{76}$$

Substituting  $\alpha_1$  into equation (47) we have

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{1}{2} \left( -\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right] V_1(x) = 1.667V_1 + \frac{1}{6}V_3 \tag{77}$$

where  $\epsilon = \frac{1}{6}V_3 = 0$ , and in accordance with equation (49), then equation (77) reduces to

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{1}{2} \left( -\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right]_{spanV_1} V_1(x) = 1.667V_1(x). \tag{78}$$

**We also want to find the eigenvalue of  $V_3$**  as we consider Equation (47) and substitute  $m = 3$ . This is given by

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{1}{2} \left( -\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right] V_3(x) = \left( \frac{7}{2} + \frac{1}{2}\alpha_3 \right) V_3 + \frac{1}{2}V_5 + \frac{1}{20}V_1(x). \tag{79}$$

Solving for  $\alpha_3$  gives

$$\alpha_3 = \frac{\langle U_5, V_3 \rangle}{\langle V_3, V_3 \rangle} V_3 = 3.23V_3. \tag{80}$$

Substituting  $\alpha_3$  into equation (79) we have

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{1}{2} \left( -\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right] V_3(x) = 5.115V_3 + \frac{1}{2}V_5 + \frac{1}{20}V_1(x) \tag{81}$$

Equation (81) reduces to

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{1}{2} \left( -\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right]_{spanV_3} V_3(x) = 5.115V_3(x). \tag{82}$$

**We want to consider the eigenfunction  $V_5$**  as we find the general equation from Equation (47) written as

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{1}{2} \left( -\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right] V_5(x) = \left( \frac{11}{2} + \frac{5}{6}\alpha_5 \right) V_5 + \frac{5}{6}V_7 + \frac{9}{5}V_3(x) + \frac{21}{15}V_1 \tag{83}$$

Solving for  $\alpha_5$  gives

$$\alpha_5 = \frac{\langle U_7, V_5 \rangle}{\langle V_5, V_5 \rangle} V_5 = 6.53738V_5. \tag{84}$$

Substituting  $\alpha_5$  into equation (83) we have

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{1}{2} \left( -\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right] V_5(x) = 10.94V_5 + \frac{5}{6}V_7 + \frac{3183}{75}V_3 + \frac{27757}{750}V_1, \tag{85}$$

where  $\epsilon = \frac{5}{6}V_7 + \frac{3183}{75}V_3 + \frac{27757}{750}V_1 = 0$ , then equation (85) finally reduces to

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{1}{2} \left( -\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6 \right) \right]_{spanV_5} V_5(x) = 10.94V_5(x). \tag{86}$$

Table 1. A summary of the first six Energy Eigenstates Obtained from Perturbative and Non - Perturbative Methods

Energy Eigenvalues, $\lambda_m$	Perturbative Method	Non - Perturbative Method
0	0.5625	0.500
1	1.8125	1.667
2	3.3125	3.230
3	5.0625	5.115
4	7.0625	7.758
5	9.3125	10.940

The results of calculations done in section 1 using perturbative approach appears to be of the same order of magnitude as done using the Non - perturbative approach as summarized in table 1 above.

From table 2, the polynomials associated with the eigenfunctions for both harmonic and anharmonic oscillators are distinct but of the same order. It is observed that the eigenfunctions of the quantum anharmonic oscillator considered here constitute a kind of generalization of the Hermite functions.

Table 2. Comparison of the Eigenfunctions of the Quantum Harmonic Oscillator with the Quantum Anharmonic Oscillator under consideration

$m$	Quantum Harmonic Oscillator, $V_m$	Quantum Anhrmonic Oscillator, $V_m$
0	$e^{-\frac{x^2}{2}}$	$e^{-(\frac{x^2}{2} + \frac{x^4}{24})}$
1	$xe^{-\frac{x^2}{2}}$	$xe^{-(\frac{x^2}{2} + \frac{x^4}{24})}$
2	$(x^2 - \frac{1}{2})e^{-\frac{x^2}{2}}$	$(x^2 - \frac{2}{5})e^{-(\frac{x^2}{2} + \frac{x^4}{24})}$
3	$(x^3 - \frac{6}{5}x)e^{-\frac{x^2}{2}}$	$(x^3 - \frac{3}{2}x)e^{-(\frac{x^2}{2} + \frac{x^4}{24})}$
4	$(x^4 - 3x^2 + \frac{3}{4})e^{-\frac{x^2}{2}}$	$(x^4 - 2x^2 + \frac{3}{5})e^{-(\frac{x^2}{2} + \frac{x^4}{24})}$
5	$(x^5 - 5x^3 + \frac{15}{4}x)e^{-\frac{x^2}{2}}$	$(x^5 - \frac{17}{5}x^3 + \frac{19}{10}x)e^{-(\frac{x^2}{2} + \frac{x^4}{24})}$

#### 4. Conclusion

Starting with an appropriate family of solutions to a relevant second order linear differential equation, we have, by means of Gram Schmidt orthogonalization process, been able to recover the Schrödinger Equation for a particular case of a quantum anharmonic oscillator having potential function given by  $f_1(x) = \frac{1}{2}(-\frac{1}{2}x^2 + \frac{1}{3}x^4 + \frac{1}{36}x^6)$ , together with the eigenvalues  $\lambda_m = [(m + \frac{1}{2}) + \frac{m}{6}]$  and eigenfunctions  $V_m = e^{-(\frac{x^2}{2} + \frac{x^4}{24})} - \sum_{k=0,1}^{m-2} \frac{\langle U_m, V_k \rangle}{\langle V_k, V_k \rangle} V_k$ . Specific calculations have been performed to obtain these results for cases  $m = 0, 1, 2, 3, 4, 5$  pertaining to the ground state and the excited states. A comparison with results obtained elsewhere by the use of perturbation methods indicate that our results are of the same order of magnitude. We have also shown that the method developed here is in general applicable to a specified class of anharmonic oscillators characterized by certain polynomial potential functions with terms of even powers. In a subsequent paper, we shall study a class of quantum anharmonic oscillator with transcendental potential functions.

#### References

Adesso, G., Franco, R. L., & Parigi, V. (2018). Foundations of quantum mechanics and their impact on contemporary society. *Philosophical transactions. Series A, Mathematical, physical, and engineering sciences*, 376(2123), 20180112. <https://doi.org/10.1098/rsta.2018.0112>

Biswas, T. (1999). *Quantum Mechanics - Concepts and Applications*. University of New York Press, New York.

Bransden, B., & Joachain, C. J. (2000). *Quantum Mechanics*. Pearson Education Limited, Asia, 51 - 124, 2nd Edition.

Boxi, L. (2017, December, 1st.) The WKB approximation <https://www.thphys.uni-heidelberg.de>

Cao, P., Betzholz, R., Zhang, S., & Cai, J. (2021) Entangling Distant Solid-State spins via Thermal Phonons. *Physical Review B: Covering Condensed Matter and Material Physics*. doi:10.1103/PhysRevB. 96.245418.

Clark, A. (2011). A closed form solution for quantum oscillator perturbations using Lie algebras. *Journal of Physical Mathematics*. Vol. 3 Article ID P101201. <https://doi.org/10.4303/jpm/P101201>

Ghatak, A., & Lokanathan, S. (2012). *Quantum Mechanics: Theory and Applications*. (5th ed.). Trinity Press, India.

Griffiths, D. J. (2016). *Introduction to Quantum Mechanics*. Prentice Hall, Upper-Saddle River, New Jersey.

Hoffman, K., & Kunze, R. (1971). *Linear Algebra*. (2nd Ed.). Prentice - Hall, Inc., Englewood Cliffs, New Jersey.

Oduro, F. T., & Odoom, A. (2021). A New Framework for the Determination of the Eigenvalues and Eigenfunctions of the Quantum Harmonic Oscillator. *Journal of Mathematics Research*, 136. <https://doi.org/10.5539/jmr.v13n6p20>

Schaden, M. (2002). Quantum Finance. *Physica A: Statistical Mechanics and its Applications*. [http://dx.doi.org/10.1016/50378-4371\(02\)01200-1](http://dx.doi.org/10.1016/50378-4371(02)01200-1)

Seymour, L. & Lipson, M. L. (2004). *Outline of Theory and Problems of Linear Algebra, 3/e*. The McGraw - Hill Companies, New York.

Spiegel, R. M. (1976). *Schaum's Outline of Theory and Problems of Advanced Mathematics for Engineering and Scientists*. Schaum's Outline Series McGraw - Hill Companies, New York.

Wolf, R. (2021). *Quantum Computing: Lecture Notes*. University of Amsterdam.  
Retrieved from <http://www.shoup.net/papers/dbounds>.

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