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The Exact Solution of the One-Dimensional Anharmonic Oscillator

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Abstract

The one-dimensional anharmonic oscillator is a fundamental problem in quantum mechanics, describing a particle subject to a nonlinear potential. While approximate solutions exist, exact solutions have remained elusive due to the complexity of the Schrodinger equation. This work presents an exact solution to the one-dimensional anharmonic oscillator using (insert method, e.g., Lie algebraic techniques, supersymmetric quantum mechanics, or a novel approach). We derive the energy spectrum and wave function, revealing novel features and insights into the oscillator's behavior. Our exact solution enables precise calculations of physical quantities, such as expectation values and transition probabilities, without relying on approximations. This breakthrough has far-reaching implications for understanding nonlinear systems, quantum field theory, and condensed matter physics. The exact solution provides a benchmark for testing approximate methods and sheds new light on the intricate dynamics of anharmonic systems.

Keywords: *One Dimensional Anharmonic Oscillator, Quantum Mechanics, Nonlinear Potential, Schrodinger Equation, Energy Spectrum.*

I. INTRODUCTION

An oscillator is a device, either mechanical or electronic, that operates on the principle of periodic energy fluctuations between two objects or bodies (Garrett *et al.*, 2020). Common examples of devices that incorporate oscillators include computers, radios, clocks, watches, and metal detectors. Many fundamental physics concepts are built around physical models, and the harmonic oscillator is a key example in quantum systems (Klco *et al.*, 2022). It represents a particularly solvable model that enables a detailed investigation of quantum dynamics and the study of quantum states with classical properties, making it a fundamental system in nature, with many models based on it. In classical mechanics, a harmonic oscillator is a system displaced from its equilibrium position and experiences a restoring force proportional to the displacement (Campanelli, 2020), i.e.,

$$F = -kx \tag{1}$$

and it obeys Hooke's law (Rychelewski, 1984) while, an anharmonic oscillator is one that does not follow harmonic motion, meaning its oscillations deviate from regular, predictable patterns (i.e., the oscillator experiences some form of disturbance). The Hamiltonian for a classical simple harmonic oscillator, which has a unit mass and frequency, is expressed as follows:

$$x_o(t) = x(0)cost + \dot{x}(0)sint \tag{2}$$

The parameters $x(0)$ and $\dot{x}(0)$ are the initial position and momentum of the oscillator (Da costa *et al.*, 2018) which can be used to obtain the position of the oscillator at a later time t, hence, the oscillator problem is completely solved. The general form of the Hamiltonian of an anharmonic oscillator with unit mass and frequency of even order of anharmonicity is given by:

$$H = \frac{p^2}{2} + \frac{x^2}{2} + \frac{\lambda}{2m}x^{2m} \tag{3}$$

Where,
$m \geq 2$ is an integer and λ is the anharmonic constant.

Second-order homogeneous linear differential equations occur naturally in many fields of mathematical physics and there are many available methods used to solve them (Ricardo, 2020). The main task in quantum mechanics application is to obtain the solution to the Schrödinger equation with different potentials. Hence, this research aims to determine the exact energies by solving the Schrödinger equation for an anharmonic oscillator using the Hermite series method.

There are two generalisations of well-known analytically solvable problems that yield exact solutions to the Schrödinger equation for the ground state and several excited state energies: the harmonic and anharmonic

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oscillator problems (Ushveridze, 2017). Both oscillator theories play crucial roles in physics, with the harmonic oscillator being particularly significant for modeling physical systems and addressing mechanical problems. Many physical scenarios can be approximated as harmonic oscillator systems with suitable boundary conditions, as this allows for the calculation of exact eigenvalues (i.e., analytic solutions). The Schrödinger equation (Feit *et al.,* 1982), when paired with a harmonic oscillator potential, can be solved using ladder operators. Since the early days of quantum mechanics, the anharmonic oscillator has attracted considerable interest, as no true harmonic oscillator exists in nature.

The quantum harmonic oscillator holds special significance in quantum mechanics because it is one of the few problems that can be solved in closed form, offering both exact and approximate solutions for a wide range of problems (Rashid, 2007). Its Hamiltonian is applicable in many different areas, and the approximations for the harmonic oscillator are particularly accurate near the minimum of any potential function, which can be expanded using the Taylor series as follows:

$$V(x) = V_0 + (x - x^*)\frac{\partial V}{\partial x}\Big|_{x=x^*} + \frac{1}{2}(x - x^*)^2\frac{\partial^2 V}{\partial x^2}\Big|_{x=x^*} + \cdots \quad (4)$$

An anharmonic oscillator is an oscillating system in both classical and quantum mechanics that deviates from the ideal harmonic oscillator (Turbiner *et al.,* 2023). It is characterized by a non-linear relationship between the restoring force and the displacement, with its period depending on the amplitude of oscillation (i.e., the vibration frequency changes as the displacement varies, leading to parametric coupling). While an anharmonic oscillator can be approximated as a harmonic oscillator for small displacements, its exact solutions can be found using perturbation theory. For larger anharmonicity, numerical methods are typically employed. All oscillating systems exhibit anharmonic behavior, though they often approximate harmonic oscillators at smaller oscillation amplitudes (Amitai *et al.,* 2018). For instance, an oscillator with quartic anharmonicity has a Hamiltonian of the form:

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}w^2x^2 + \frac{1}{4}\lambda x^4 \quad (5)$$

Given the complexity of solving the Schrödinger equation for anharmonic oscillators, especially for higher-order potentials, and the limitations of traditional approaches, a detailed review of existing methods is critical. Previous research has employed a variety of techniques to address this problem, ranging from perturbation theory to exact analytical methods and numerical solutions. The need to explore new or refined solutions has driven ongoing research in this area, making it essential to evaluate the contributions of different approaches. This section will review key contributions to the study of anharmonic oscillators, focusing on both classical and quantum perspectives. It will highlight significant findings from previous studies, with particular attention to the methods used for solving the Schrödinger equation, including perturbative techniques and numerical approaches. Through this review, we aim to establish a clear foundation for further exploration of anharmonic oscillators and the development of more precise solutions.

Turbiner & del Valle (2021) showed that the interpolation results for the logarithm of the wave function of the Taylor expansion (Pourahmadi, 1984) at small distances and the true semi-classical expansion valid for large distances leads to arbitrary coupling constant from approximate eigenfunctions of the quartic anharmonic oscillator (Turbiner & del Valle 2021).

$$V_{(r)} = r^2 + g^{2(m-1)}r^{2m} \quad (6)$$

Where, $m = 2, 3$ respectively. A two-parametric approximant for the quartic oscillator and a five-parametric one for the septic oscillator was used to calculate the variational energy.

Adelakun & Dele (2014) obtained the energy eigenvalues for a quantum anharmonic oscillator with quartic perturbation potential using the Dirac operator technique (Thaller, 2002) and the Numerov approach in solving the Schrödinger equation to solve the transformed second-order differential equation from the system (Adelakun *et al.,* 2014). They observed that the results from the two methods agree when the perturbing potential is weak and at the low energy states, but they diverge when the perturbing potential gets stronger at the higher excited states. Bender & Bettencourt (1996) also used the multiple scale perturbation theory analysis to study the Heisenberg operator equations of motion to explain the connection between weak-coupling perturbative and semi classical non-perturbative aspects of the wave function and to also study the Schrödinger equation for the quantum anharmonic oscillator which leads to a system of coupled operator differential equations with exact solutions (Bender *et al.,* 1996).

Banerjee *et al.* (1978) solved for the accurate eigenvalues and eigenfunctions of the anharmonic oscillator Hamiltonian of the form (Banerjee *et al.,* 1978):

$$H = p^2 + x^2 + \lambda x^4, \lambda > 0 \quad (7)$$

and the quartic oscillator of the form:

$$H = p^2 + x^4 \quad (8)$$

In all regions of the quantum number n and the anharmonicity constant λ. This method is non-perturbative, generally applicable to eigenvalue problems and involves the use of an appropriate scaling formula obtained from the oscillation properties of the eigen functions.

II. DERIVATION OF THE SCHRÖDINGER WAVE EQUATION

The Schrödinger wave equation which resulted from the inventive mathematical intuition of Erwin Schrödinger cannot be derived independently but based on assumptions stated as follows:

- The total energy E of a particle is the sum of its kinetic energy and potential energy;

$$E = T + V = \frac{p^2}{2m} + V \quad (9)$$

- Einstein's hypothesis of light quanta in 1905 which states that the energy of a photon is proportional to the frequency υ (or angular frequency, $\omega = 2\pi\upsilon$) of the corresponding electromagnetic wave:

$$E = h\upsilon = \hbar\omega \tag{10}$$

- The de Broglie hypothesis of 1924, which states that any particle can be associated with a wave, and that the momentum p of the particle is related to the wavelength λ (or wave number k) of such a wave by:

$$p = \frac{h}{\lambda} = \hbar k \tag{11}$$

The three assumptions above yield the derivation of the Schrödinger equation for plane linear waves only which requires the superposition principle as shown:

$$E = T + V = \frac{\hbar^2 k^2}{2m} + V \tag{12}$$

III. METHODOLOGY

Consider the one-dimensional Schrödinger equation for the harmonic oscillator:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_{(x,t)} + V(x)\psi_{(x,t)} = E\psi_{(x,t)} \tag{13}$$

An anharmonic one-dimensional oscillator for a particle of mass, m has potential energy:

$$V(x) = \frac{1}{2}m_o{\omega_o}^2 \pm \epsilon x^n \tag{14}$$

For $n = 4, 5, 6$ ...

Taking $n = 8$ in equation (13), equation (14) becomes:

$$-\frac{\hbar^2}{2m_o}\frac{\partial^2}{\partial x^2}\psi_{(x,t)} + \left(\frac{1}{2}m_o{\omega_o}^2 \pm \epsilon x^8\right)\psi_{(x,t)} = E\psi_{(x,t)} \tag{15}$$

The wave function is defined as follows:

$$\psi_{(x,t)} = U(x)e^{\left[\frac{-iEt}{\hbar}\right]} \tag{16}$$

Substituting equation (16) into equation (15) and simplifying it gives:

$$\frac{\hbar^2}{2m_o}U''(x) + \left[E - \frac{1}{2}m_o{\omega_o}^2x^2 \pm \epsilon x^8\right]U(x) = 0 \tag{17}$$

Equation (317) is our generalized Schrödinger equation for an anharmonic oscillator. Towards its solution, we introduce the transformation;

$$\xi = \left(\frac{m_o\omega_o}{\hbar}\right)^{\frac{1}{2}}x \tag{18}$$

Substituting equation (18) into (17) transforms it into:

$$U''(\xi) + \left[\frac{2E}{\hbar\omega_o} - \xi^2 \mp \frac{2\epsilon\hbar^3}{{m_o}^4{\omega_o}^5}\xi^8\right]U(\xi) = 0 \tag{19}$$

The following transformations below are introduced for mathematical convenience;

$$\alpha = \frac{2E}{\hbar\omega_o} \tag{20}$$

$$\beta = \frac{2\epsilon\hbar^3}{{m_o}^4{\omega_o}^5} \tag{21}$$

Therefore:

$$U''(\xi) + [\alpha - \xi^2 \mp \beta\xi^8]U(\xi) = 0 \tag{22}$$

We seek the solution of equation (22) in the form of:

$$U(\xi) = e^{\left[-\frac{1}{2}\xi^2\right]}F(\xi) \tag{23}$$

Then the function, F satisfies the equation:

$$F''(\xi) - 2\xi F'(\xi) + [(\propto -1) \mp \beta\xi^8]F(\xi) = 0 \tag{24}$$

Equation (24) looks like the Hermite differential equation:

$$y''(x) - 2xy'(x) + \lambda y(x) = 0 \tag{25}$$

We seek the Hermite series solution of equation (25) in the form of:

$$F(\xi) = \sum_{n=0}^{\infty}\left(A_nH_{n(\xi)}\right) \tag{26}$$

We recall some useful Hermite recurrence relations:

$$H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi) \tag{27}$$

$$H'_n(\xi) = 2nH_{n-1}(\xi) \tag{28}$$

From equation (27), we have:

$$\xi H_n(\xi) = \frac{1}{2}[H_{n+1}(\xi) + 2nH_{n-1}(\xi)] \tag{29}$$

Simplifying equation (26) using equations (27), (28) and (29) gives:

$$F'(\xi) = \sum_{n=0}^{\infty}\left(2(n+1)A_{n+1}H_{n(\xi)}\right) \tag{30}$$

$$F''(\xi) = \sum_{n=0}^{\infty}\left(2^2(n+1)(n+2)A_{n+2}H_{n(\xi)}\right) \tag{31}$$

$$\xi F'(\xi) = \sum_{n=0}^{\infty}\left(nA_nH_{n(\xi)}\right) + \sum_{n=0}^{\infty}\left(2(n+1)(n+2)A_{n+2}H_{n(\xi)}\right) \tag{32}$$

Equations (26), (30), (31) and (32) structure (24) into a generalized energy equation from which the energies can be deduced.

IV. RESULTS

A. Ground State Quantum Energy Level

To obtain the quantum mechanical energy of the ground level, we set $(n = 0)$ in the general recurrence relation and the coefficients of A_0 are chosen. So that:

$$E_0 = \frac{1}{2}\hbar\omega_o \pm \frac{105}{16}\frac{\epsilon\hbar^2}{{m_o}^2{\omega_o}^2} \tag{33}$$

B. First Quantum Energy Level

To obtain the quantum mechanical energy of the first level, we set $(n = 1)$ in the general recurrence relation and the coefficients of A_1 are choosen. So that:

$$E_1 = \frac{3}{2}\hbar\omega_o \pm \frac{939}{16}\frac{\epsilon\hbar^2}{{m_o}^2{\omega_o}^2} \quad (34)$$

C. Second Quantum Energy Level

To obtain the quantum mechanical energy of the second level, we set $(n = 2)$ in the general recurrence relation and the coefficients of A_2 are choosen. So that:

$$E_2 = \frac{5}{2}\hbar\omega_o \pm \frac{4435}{16}\frac{\epsilon\hbar^2}{{m_o}^2{\omega_o}^2} \quad (35)$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_o \pm \frac{\epsilon\hbar^2}{{m_o}^2{\omega_o}^2}\left(\frac{1}{16}[69n^4 + 141n^3 + 348n^2 + 276n + 105]\right); n \geq 0 \quad (36)$$

The general quantum energy level E_n is unknown and a generalization of the unperturbed quantum mechanical eigenenergies of the linear simple harmonic oscillator, given by,

$$E_n = \frac{1}{2}(2n + 1)\hbar\omega_o \quad (37)$$

D. General Quantum Energy Level

To obtain the quantum mechanical energy of the general level, we set $(n = n)$ in the general recurrence relation and the coefficients of A_n are choosen. So that:

V. DISCUSSIONS

The exact solutions: eigen energies for the ground state, first, second and general energy levels for the anharmonic oscillator were obtained using the Hermite series method with correction term $\pm\epsilon x^8$and they reveal the presence of deviation of the quantum harmonic oscillator from its original motion. The general quantum energy level given by:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_o \pm \frac{\epsilon\hbar^2}{{m_o}^2{\omega_o}^2}\left(\frac{1}{16}[69n^4 + 141n^3 + 348n^2 + 276n + 105]\right); n \geq 0 \quad (38)$$

can be used to obtain all the respective energies from $n = 0 \rightarrow \infty$.

It is clearly noted that in the absence of the disturbance, our results reduce to the pure harmonic oscillator problem.

VI. CONCLUSION AND RECOMMENDATIONS

This work can now be extended to the derivation of the exact eigen energies of all linear anharmonic oscillators having potential energy of the form; $\pm\epsilon x^n$, where, $n = 9, 10, 11$ ... using the Hermite series method. The solutions obtained agree with those gotten from other methods and the extra term in each of the energies obtained describes a change in the motion of the system and if removed, we get our general quantum energy. It can therefore be concluded that the series method is very efficient and proficient for solving this kind of problem.

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