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RESEARCH ARTICLE

Investigating Single Quantum Anharmonic Oscillator with Perturbation Theory

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ABSTRACT

In this article, for pedagogical purposes we have discussed the application of nondegenerate perturbation theory up to the third order to compute energy eigenvalues and wave functions for the quantum anharmonic oscillator. Energy levels of a single quartic oscillator for λ values in range of 0.1-1 are given. Perturbed and non-perturbed wave functions of the levels up to the fourth excited level are compared. Ground, first and second excited energy levels are also calculated by applying finite differences method and, results are compared with the ones obtained via perturbation theory. It is found that perturbation theory gives comparable results only for a small λ parameter and for the ground state. The quartic term in the Hamiltonian of the anharmonic oscillator leads to a more effective confinement of the particle which is deduced from the plots of wavefunctions and probability distributions. Meanwhile, the number of zero crossing nodes of the wavefunctions increases as the energy level increases, which is an expected result for both the harmonic and anharmonic oscillator.

Keywords: anharmonic oscillators; perturbation theory; quantum oscillator

1. INTRODUCTION

The quantum anharmonic oscillator has been analytically studied in the literature by Bender & Wu (1969, 1973). In their articles published in 1969, they examined the anharmonic oscillator defined by the following differential equation,

$$\left(-\frac{d^2}{dx^2}+\frac{1}{4}x^2+\frac{1}{4}\lambda x^4\right)\phi(x)=E(\lambda)\phi(x). \tag{1}$$

They also investigated the boundary conditions for this oscillator. Using the Wentzel–Kramers–Brillouin (WKB) approximation method, they discovered that there are an infinite number of branch points as a function of λ^α in the limit as λ approaches 0. In an article published in 1973, they further studied the Rayleigh-Schrödinger expansions of energy eigenvalues for high-order perturbations of the anharmonic oscillator.

In a famous classical problem book of quantum mechanics Flügge (1999), cubic ($\lambda_1 x^3$) and quartic ($\lambda_2 x^4$) perturbations are added to the quantum harmonic oscillator's Hamiltonian and energy levels of the anharmonic oscillator are calculated by a perturbation method in first and second-order approximation.

Turbiner (1981) proposed a new iteration procedure for the solution of a Schrödinger equation with arbitrary local potential. With this method, both eigenvalues and eigenfunctions are represented as a convergent series. Potentials $x^n (n = 2, 3, 4)$ type and $m^2g^2 + gx^4$ in one-dimensional space are considered as examples.

In another article of Turbiner (2005), quantum anharmonic oscillator was given by the following Schrödinger equation

$$-\frac{d^2\psi}{dx^2}+m^2x^2\psi+gx^4\psi=E(m^2,g)\psi, \tag{2}$$

which was solved by logarithmic derivation of the eigenfunction approximation. As a result of his approach, the $y(x)$ function has no singularities at real values of x and shows asymptotic behavior as $\lim_{|x|\to\infty}$. He defined the simplest interpolation of $y(x)$ between $x = 0$ and $x = \infty$ as

$$y_0 = ax + b\sqrt{g}x|x|. \tag{3}$$

Subsequently, first, second, and third corrections to the energy for different a, b, c, m^2 values, and the first correction to the wave function for $m^2 = -1$ and $g = 2$ were evaluated.

In a further study, Turbiner & del Valle (2021) studied in the framework of perturbation theory with the logarithmic derivation of the wave function for the potential

$$V = x^2 + g^2x^4. \tag{4}$$

They used Riccati-Bloch equation for perturbation theory in g^2 in x-space and generalized Bloch equation for semiclassical expansion in the power of $\hbar$ for energy in (gx)-space. Then they showed the Riccati-Bloch equation and generalized Bloch

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equations yield the same expansion in powers of λ for the energy. The eigenfunctions were expressed in terms of interpolation parameters A, B. These parameters are dependent on the n, p quantum numbers. Variational energy was determined for $n = 0, 1, 2$, $p = 0, 1$ and $g^2 = 0.1, 1, 10, 20, 100$, with plots of the parameters A and B presented. As summarized above quantum anharmonic oscillator is still an interesting topic and also finds applications in mathematical physics such as in Gaudreau et al. (2013, 2015).

In this study, primarily for pedagogical purposes the energy levels of the quantum anharmonic oscillator and the corresponding wave functions have been obtained using non-degenerate perturbation theory up to the third order.

2. PERTURBATION THEORY

When a system's energy undergoes an external disturbance i.e., when an effect that changes the system's energy is applied, the Hamiltonian of the system changes. For a non-perturbed system, the Hamiltonian of the system satisfies the time-independent Schrödinger equation,

$$H\psi_n = E_n\psi_n. \tag{5}$$

For a perturbed system, the Hamiltonian is written within the framework of perturbation theory as

$$H = H^{(0)} + \lambda H'. \tag{6}$$

Here, the parameter λ is a number between 0 and 1. In this equation, $H^{(0)}$ represents the unperturbed Hamiltonian, and H' represents the perturbation term. In the framework of perturbation theory, the wave function ψ_n and the energies E_n are expanded in powers of λ as follows

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \lambda^3 E_n^{(3)} + \ldots, \tag{7}$$

$$\psi_n = \psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \lambda^3\psi_n^{(3)} + \ldots. \tag{8}$$

Here, $\psi_n^{(1)}$ represents the first-order correction to the eigenfunction representing n^{th} level and $E_n^{(1)}$ represents the first-order correction to the n^{th} energy eigenvalue. Similar expressions hold for higher-order corrections.

In general, when solving physics problems across various fields, it is often sufficient to compute terms up to the second order in these series, including the second-degree terms.

2.1. Perturbation Terms for Energy

The first-order energy correction is the expectation value of the perturbed term that is calculated by using the unperturbed wave functions.

$$E_n^{(1)} = \langle\psi_n^{(0)}|\ H'\ |\psi_n^{(0)}\rangle. \tag{9}$$

The second-order energy correction is calculated as

$$E_n^{(2)} = \sum_{m\neq n} \frac{|\langle\psi_m^{(0)}|\ H'\ |\psi_n^{(0)}\rangle|^2}{E_n^{(0)} - E_m^{(0)}}. \tag{10}$$

This formula involves a sum over all states m that is different from the state n. The matrix element $\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle$ is calculated again by using the wave functions of the unperturbed harmonic oscillator. For the third-order energy correction, a more complicated expression is used.

$$E_n^{(3)} = \sum_{k_2\neq n}\sum_{k_3\neq n} \frac{\langle\psi_n^{(0)}|\ H'\ |\psi_{k_3}^{(0)}\rangle\langle\psi_{k_3}^{(0)}|\ H'\ |\psi_{k_2}^{(0)}\rangle\langle\psi_{k_2}^{(0)}|\ H'\ |\psi_n^{(0)}\rangle}{(E_n^{(0)} - E_{k_2}^{(0)})(E_n^{(0)} - E_{k_3}^{(0)})}$$
$$- \langle\psi_n^{(0)}|\ H'\ |\psi_n^{(0)}\rangle \sum_{k_3\neq n} \frac{|\langle\psi_n^{(0)}|\ H'\ |\psi_{k_3}^{(0)}\rangle|^2}{(E_n^{(0)} - E_{k_3}^{(0)})^2}. \tag{11}$$

2.2. Perturbation Terms for Wave Function

The first-order wave function correction is given by

$$|\psi_n^{(1)}\rangle = \sum_{k_1\neq n} \frac{\langle\psi_{k_1}^{(0)}|\ H'\ |\psi_n^{(0)}\rangle}{E_n^{(0)} - E_{k_1}^{(0)}} |\psi_{k_1}^{(0)}\rangle. \tag{12}$$

This equation involves a sum over all states k_1 that are different from the state n. The matrix element $\langle\psi_{k_1}^{(0)}|H'|\psi_n^{(0)}\rangle$ is computed using the wave functions of the unperturbed harmonic oscillator. The second and third-order corrections are more complicated as the following[1],

$$|\psi_n^{(2)}\rangle = \sum_{k_1\neq n}\sum_{k_2\neq n} \left(\frac{\langle\psi_{k_1}^{(0)}|\ H'\ |\psi_{k_2}^{(0)}\rangle\langle\psi_{k_2}^{(0)}|\ H'\ |\psi_n^{(0)}\rangle}{(E_n^{(0)} - E_{k_1}^{(0)})(E_n^{(0)} - E_{k_2}^{(0)})} \right.$$
$$\left. - \frac{\langle\psi_n^{(0)}|\ H'\ |\psi_n^{(0)}\rangle\langle\psi_{k_1}^{(0)}|\ H'\ |\psi_n^{(0)}}{(E_n^{(0)} - E_{k_1}^{(0)})^2} \right) |\psi_{k_1}^{(0)}\rangle$$
$$- \frac{1}{2} \sum_{k_1\neq n} \frac{\langle\psi_n^{(0)}|\ H'\ |\psi_{k_1}^{(0)}\rangle\langle\psi_{k_1}^{(0)}|\ H'\ |\psi_n^{(0)}\rangle}{(E_{k_1}^{(0)} - E_n^{(0)})^2} |\psi_n^{(0)}\rangle, \tag{13}$$

[1] https://en.wikipedia.org/wiki/Perturbation_theory_(quantum_mechanics)

$$
\begin{aligned}
|\psi_n^{(3)}\rangle = \sum_{k_1\neq n}\sum_{k_2\neq n}\sum_{k_3\neq n}\Bigg[& \\
& -\frac{\langle\psi_{k_1}^{(0)}|\ H'\ |\psi_{k_2}^{(0)}\rangle\langle\psi_{k_2}^{(0)}|\ H'\ |\psi_{k_3}^{(0)}\rangle\langle\psi_{k_3}^{(0)}|\ H'\ |\psi_n^{(0)}\rangle}{(E_{k_1}^{(0)}-E_n^{(0)})(E_n^{(0)}-E_{k_2}^{(0)})(E_n^{(0)}-E_{k_3}^{(0)})} \\
& +\frac{\langle\psi_n^{(0)}|\ H'\ |\psi_n^{(0)}\rangle\langle\psi_{k_1}^{(0)}|\ H'\ |\psi_{k_2}^{(0)}\rangle\langle\psi_{k_2}^{(0)}|\ H'\ |\psi_n^{(0)}\rangle}{(E_{k_1}^{(0)}-E_n^{(0)})(E_n^{(0)}-E_{k_2}^{(0)})} \\
& (\frac{1}{E_n^{(0)}-E_{k_1}^{(0)}}+\frac{1}{E_n^{(0)}-E_{k_2}^{(0)}})-\frac{|\langle\psi_n^{(0)}|\ H'\ |\psi_n^{(0)}\rangle|^2\langle\psi_{k_1}^{(0)}|\ H'\ |\psi_n^{(0)}\rangle}{(E_{k_1}^{(0)}-E_n^{(0)})^3} \\
& +\frac{|\langle\psi_n^{(0)}|\ H'\ |\psi_{k_2}^{(0)}\rangle|^2\langle\psi_{k_1}^{(0)}|\ H'\ |\psi_n^{(0)}\rangle}{(E_{k_1}^{(0)}-E_n^{(0)})(E_n^{(0)}-E_{k_2}^{(0)})} \\
& (\frac{1}{E_n^{(0)}-E_{k_1}^{(0)}}+\frac{1}{2(E_n^{(0)}-E_{k_2}^{(0)})})\Bigg]|\psi_{k_1}^{(0)}\rangle+\sum_{k_1\neq n}\sum_{k_2\neq n}\Bigg[\\
& -\frac{\langle\psi_n^{(0)}|\ H'\ |\psi_{k_2}^{(0)}\rangle\langle\psi_{k_2}^{(0)}|\ H'\ |\psi_{k_1}^{(0)}\rangle\langle\psi_{k_1}^{(0)}|\ H'\ |\psi_n^{(0)}\rangle}{2(E_n^{(0)}-E_{k_2}^{(0)})^2(E_n^{(0)}-E_{k_1}^{(0)})} \\
& +\frac{\langle\psi_{k_2}^{(0)}|\ H'\ |\psi_n^{(0)}\rangle\langle\psi_{k_1}^{(0)}|\ H'\ |\psi_{k_2}^{(0)}\rangle\langle\psi_n^{(0)}|\ H'\ |\psi_{k_1}^{(0)}\rangle}{2(E_n^{(0)}-E_{k_2}^{(0)})^2(E_n^{(0)}-E_{k_1}^{(0)})} \\
& +\frac{|\langle\psi_n^{(0)}|\ H'\ |\psi_{k_1}^{(0)}\rangle|^2\langle\psi_n^{(0)}|\ H'\ |\psi_n^{(0)}\rangle}{(E_n^{(0)}-E_{k_1}^{(0)})^3}\Bigg]|\psi_n^{(0)}\rangle.
\end{aligned}
\tag{14}
$$

3. THE QUANTUM ANHARMONIC OSCILLATOR

In one dimension the Hamiltonian for the quantum anharmonic oscillator is given as

$$H = \frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2+\lambda x^4, \tag{15}$$

where H includes an additional term to the quantum harmonic oscillator proportional to x^4. The energy levels of quantum harmonic oscillator are determined by

$$E_n^{(0)} = \left(n+\frac{1}{2}\right)\hbar\omega, \tag{16}$$

where n is the quantum number, which can take on integer values, including zero. The wave function for the n^{th} state is expressed as

$$\psi_n(x) = A_n a_+^n \psi_0(x), \tag{17}$$

where, A_n is a normalization constant, a_+ is the raising operator and $\psi_0(x)$ is the ground state wave function. In our work, we first calculated perturbation terms by using algebraic methods of the quantum harmonic oscillator. Afterwards, the obtained ket states were replaced with normalized analytical functions of the quantum harmonic oscillator.

In the algebraic formalism of the quantum harmonic oscillator, the following operators are used. Momentum and position operators, respectively

$$p = \frac{\hbar}{i}\frac{d}{dx}, \quad x = \sqrt{\frac{\hbar}{2m\omega}}(a_+ + a_-), \tag{18}$$

and x^2 operator,

$$x^2 = \frac{\hbar}{2m\omega}[a_+^2 + a_+a_- + a_-a_+ + a_-^2], \tag{19}$$

also raising (creation) and lowering (annihilation) operators are given as

$$a_+ = \frac{1}{\sqrt{2\hbar m\omega}}(-ip + m\omega x), \tag{20}$$

$$a_- = \frac{1}{\sqrt{2\hbar m\omega}}(+ip + m\omega x). \tag{21}$$

If we apply the raising and lowering operators to the n^{th} ket state, we would obtain the following results.

$$a_+|n\rangle = \sqrt{n+1}|n+1\rangle, \tag{22}$$

$$a_-|n\rangle = \sqrt{n}|n-1\rangle. \tag{23}$$

For the quantum anharmonic oscillator, the perturbation term depending on the 4^{th} power of x will be written in terms of raising and lowering operators as the following

$$H' = \frac{\hbar^2\left(a+a^\dagger\right)^4}{4m^2\omega^2}. \tag{24}$$

3.1. Energy Corrections

The perturbation energy for the anharmonic oscillator is calculated using the perturbation theory formulas presented in Section 2.1. The terms of the series expansion of the n^{th} energy level of the quantum anharmonic oscillator are calculated as follows,

$$E_n^{(1)} = \frac{3\hbar^2\left(2n^2+2n+1\right)}{4m^2\omega^2}, \tag{25}$$

$$E_n^{(2)} = -\frac{\hbar^3\left(34n^3+51n^2+59n+21\right)}{8m^4\omega^5}, \tag{26}$$

$$E_n^{(3)} = \frac{3\hbar^4\left(125n^4+250n^3+472n^2+347n+111\right)}{16m^6\omega^8}. \tag{27}$$

As anticipated, $E_n^{(1)}$, $E_n^{(2)}$, and $E_n^{(3)}$ terms are proportional to $\hbar^2$, $\hbar^3$ and $\hbar^4$ whereas the unperturbed energy $E_n^{(0)}$ is proportional to $\hbar$.

The total energy expression is calculated as the series expansion given by Equation 7. Energy values calculated for the ground and first two excited states for λ values ranging from 0.1 to 1 are given in Table 1. When compared to Hioe et al. (1978)'s work, our power series expansion-based perturbation theory calculations only give similar results for small perturbation parameter λ and low-energy states. It might be useful here to compare perturbation theory calculations with numerical results obtained by the finite differences method (FDM) as

Table 1. Energy levels of a single quartic oscillator for various λ values.

	Perturbation Method NumPy, SciPy, SymPy			Finite Differences Method Mathematica			Finite Differences Method SciPy, NumPy, finndif		
λ	E_0	E_1	E_2	E_0	E_1	E_2	E_0	E_1	E_2
0.1	0.5696	1.9134	3.9612	0.5591	1.7694	3.1383	0.5590	1.7688	3.1366
0.2	0.7115	3.3825	11.415	0.6024	1.9504	3.5359	0.6023	1.9497	3.5336
0.3	1.0507	7.3753	32.390	0.6380	2.0945	3.8443	0.6378	2.0936	3.8415
0.4	1.7120	15.360	74.416	0.6687	2.2167	4.1022	0.6686	2.2157	4.0990
0.5	2.8203	28.805	145.02	0.6961	2.3242	4.3268	0.6960	2.3231	4.3232
0.6	4.5005	49.178	251.74	0.7210	2.4208	4.5274	0.7208	2.4195	4.5233
0.7	6.8774	77.947	402.10	0.7439	2.5090	4.7095	0.7437	2.5076	4.7051
0.8	10.076	116.58	603.63	0.7651	2.5904	4.8770	0.7649	2.5890	4.8723
0.9	14.221	166.55	863.86	0.7850	2.6663	5.0326	0.7848	2.6648	5.0275
1.0	19.438	229.31	1190.3	0.8037	2.7376	5.1783	0.8035	2.7359	5.1728

presented in Table 1. In FDM, the second derivative operator $\frac{d^2}{dx^2}$ is replaced with finite differences and expressed as a tridiagonal matrix. Moreover, the potential operator is a diagonal matrix and summation with the tridiagonal matrix leads to the spatial discretization of the Schrödinger equation on a grid. The related mathematica code xslittlegras[2] which calculates energy eigenvalues and corresponding wave functions, is provided in the Supplementary section. FDM gives almost the same results as given in Table 4 in Hioe et al. (1978)'s work. Another implementation of FDM is done by using SciPy, NumPy, and findiff Python libraries Mathcube[3] and the obtained results are listed in Table 1.

3.2. Wave Function Corrections

Using perturbation theory, the terms of the series expansion of the wave function corresponding to the n^{th} energy level of the quantum anharmonic oscillator were calculated as follows,

$$
\begin{aligned}
|\psi_n^{(1)}\rangle = \frac{\hbar}{16m^2\omega^3}\Bigg(&\left[\sqrt{n(n-3)(n-2)(n-1)}|n-4\rangle\right] \\
&+\left[(8n-4)\sqrt{n(n-1)}|n-2\rangle\right] \\
&-\left[(8n+12)\sqrt{n^2+3n+2}|n+2\rangle\right] \\
&-\left[\sqrt{n^4+10n^3+35n^2+50n+24}|n+4\rangle\right]\Bigg),
\end{aligned}
\tag{28}
$$

the second and third-order corrections to wave function $\psi_n^{(2)}$ is computed as mentioned in Section 2.2. Second-order correction to wave function is found as

$$
\begin{aligned}
|\psi_n^{(2)}\rangle = \frac{\hbar^2}{256m^4\omega^6}\Bigg(&\left(32n^{\frac{5}{2}}-144n^{\frac{3}{2}}+112\sqrt{n}\right) \\
&\sqrt{n-3}\sqrt{n-2}\sqrt{n-1}\,|n-4\rangle \\
&+\left(-8n^{\frac{7}{2}}-516n^{\frac{5}{2}}+428n^{\frac{3}{2}}-264\sqrt{n}\right)\sqrt{n-1}\,|n-2\rangle \\
&-\left(65n^4+130n^3+487n^2+422n+156\right)|n\rangle \\
&+\left(-8n^3+492n^2+1436n+1200\right)\sqrt{n^2+3n+2}\,|n+2\rangle \\
&+\left(32n^2+208n+288\right)\sqrt{n^4+10n^3+35n^2+50n+24}|n+4\rangle\Bigg),
\end{aligned}
\tag{29}
$$

and third-order correction to wave function is found as

$$
\begin{aligned}
|\psi_n^{(3)}\rangle = \frac{\hbar^3}{512m^6\omega^9}\Bigg(&\Bigg(-4n^{\frac{9}{2}}-406n^{\frac{7}{2}}+2062n^{\frac{5}{2}}-2576n^{\frac{3}{2}} \\
&+1359\sqrt{n}+2\hbar^2\omega^2\left(-17n^{\frac{9}{2}}-34n^{\frac{7}{2}}-139n^{\frac{5}{2}}-122n^{\frac{3}{2}}-48\sqrt{n}\right)\Bigg) \\
&\left(\sqrt{n-3}\sqrt{n-2}\sqrt{n-1}\right)|n-4\rangle+\Bigg(30n^{\frac{11}{2}} \\
&+325n^{\frac{9}{2}}+6124n^{\frac{7}{2}}-5941n^{\frac{5}{2}}+8582n^{\frac{3}{2}}-2040\sqrt{n} \\
&+2\hbar^2\omega^2\left(-136n^{\frac{11}{2}}-204n^{\frac{9}{2}}-976n^{\frac{7}{2}}-420n^{\frac{5}{2}}+104n^{\frac{3}{2}}+192\sqrt{n}\right)\Bigg) \\
&\left(\sqrt{n-1}\right)|n-2\rangle+\Bigg(1068n^5+2670n^4+13776n^3 \\
&+17994n^2+14748n+4464\Bigg)|n\rangle+\Bigg(-30n^5+175n^4-5124n^3 \\
&-22663n^2-37686n-22392 \\
&+2\hbar^2\omega^2\left(136n^5+476n^4+150n^3+2644n^2+1848n+576\right)\Bigg) \\
&\left(\sqrt{n^2+3n+2}\right)|n+2\rangle+\Bigg(4n^4-390n^3-3256n^2-7902n \\
&-6399+2\hbar^2\omega^2\left(17n^4+34n^3+139n^2+122n+48\right)\Bigg) \\
&\left(\sqrt{n^4+10n^3+35n^2+50n+24}\right)|n+4\rangle\Bigg).
\end{aligned}
\tag{30}
$$

[2] https://mathematica.stackexchange.com/questions/32293/find-eigen-energies-of-time-independent-schr%C3%B6dinger-equation

[3] https://medium.com/@mathcube7/two-lines-of-python-to-solve-the-schr%C3%B6dinger-equation-2bced55c2a0e

Table 2. Zeros of wave functions for various λ values (only positive x and $x = 0$ points are listed).

λ	ψ_0	ψ_1	ψ_2	ψ_3	ψ_4
0.1	2.275	0, 2.146	0.738, 2.354	0, 1.373, 2.749	0.867, 1.903, 3.243
0.2	1.581	0, 1.805	0.884, 2.226	0, 0.302, 1.432, 2.682	0.101, 0.906, 1.911, 3.179
0.3	1.369	0, 1.753	0.908, 2.208	0, 0.331, 1.430, 2.666	0.101, 0.900, 1.897, 3.150
0.4	1.294	0, 1.739	0.910, 2.201	0, 0.330, 1.425, 2.659	0.095, 0.895, 1.889, 3.136
0.5	1.263	0, 1.733	0.910, 2.198	0, 0.326, 1.422, 2.654	0.090, 0.892, 1.883, 3.128
0.6	1.249	0, 1.730	0.908, 2.195	0, 0.323, 1.419, 2.651	0.086, 0.890, 1.880, 3.122
0.7	1.242	0, 1.728	0.907, 2.193	0, 0.317, 1.417, 2.648	0.081, 0.888, 1.877, 3.199
0.8	1.237	0, 1.727	0.906, 2.192	0, 0.317, 1.416, 2.647	0.079, 0.887, 1.875, 3.116
0.9	1.235	0, 1.726	0.905, 2.191	0, 0.315, 1.415, 2.645	0.076, 0.886, 1.874, 3.114
1.0	1.233	0, 1.725	0.904, 2.190	0, 0.313, 1.414, 2.644	0.074, 0.885, 1.873, 3.112

In each correction term kets are replaced with normalized wave functions of quantum harmonic oscillator. In the following, we presented constituent terms of the wave function for the ground and first excited states where $\hbar, m, \omega$ selected as 1. Terms of the ground state wave function are

$$\begin{aligned}
\psi_0^{(0)}(x) &= \frac{e^{-\frac{x^2}{2}}}{\sqrt[4]{\pi}}, \\
\psi_0^{(1)}(x) &= \frac{\left(-4x^4 - 12x^2 + 9\right) e^{-\frac{x^2}{2}}}{16\sqrt[4]{\pi}}, \\
\psi_0^{(2)}(x) &= \frac{3 \cdot \left(96x^4 - 88x^2 - 41\right) e^{-\frac{x^2}{2}}}{64\sqrt[4]{\pi}}, \\
\psi_0^{(3)}(x) &= \frac{3\left(-8404x^4 + 11052x^2 + 2265\right) e^{-\frac{x^2}{2}}}{512\sqrt[4]{\pi}},
\end{aligned} \tag{31}$$

and terms of the first excited state wave function are

$$\begin{aligned}
\psi_1^{(0)}(x) &= \frac{\sqrt{2}xe^{-\frac{x^2}{2}}}{\sqrt[4]{\pi}}, \\
\psi_1^{(1)}(x) &= \frac{\sqrt{2}x\left(-4x^4 - 20x^2 + 45\right) e^{-\frac{x^2}{2}}}{16\sqrt[4]{\pi}}, \\
\psi_1^{(2)}(x) &= \frac{3\sqrt{2}x\left(176x^4 - 360x^2 - 225\right) e^{-\frac{x^2}{2}}}{64\sqrt[4]{\pi}}, \\
\psi_1^{(3)}(x) &= \frac{3\sqrt{2}x\left(-22964x^4 + 65940x^2 + 5445\right) e^{-\frac{x^2}{2}}}{512\sqrt[4]{\pi}}.
\end{aligned} \tag{32}$$

The total wave function is calculated by using Equation 8. Care must be taken to ensure that the total wave function obtained by perturbation expansion must be checked for normalization. In this work, for each level n, the wave function is checked and normalized numerically. In Figure 1, total normalized wave functions belonging to quantum anharmonic and harmonic oscillators are presented. As seen from the plots, oscillations in the wave functions of the anharmonic oscillator are not well-periodic. Moreover, one and two additional peaks occur in the wave functions and probability distributions for odd and even parity solutions, respectively.

In Table 2, for the wave functions representing the ground and the first four excited states plotted in Figure 1, the numerical values of the x positions of the nodes are listed for λ values between 0.1 and 1. As expected, odd-numbered states are anti-symmetric, and even-numbered states are symmetric with respect to the origin. Therefore in Table 2, only positive roots and the $x = 0$ point intersections are listed. The number of intersections with the x-axis increases as the quantum state number increases, as expected. More interestingly, with the increase of the λ perturbation parameter, spreading of the peaks of the wave functions along the x-axis decreases.

As an example for the excited state with $n = 10$ and perturbation parameter $\lambda = 0.1$, probability distributions of quantum harmonic and anharmonic oscillators are given in Figure 2. If one compares the two probability distributions, it can be deduced that, due to the quartic term in the Hamiltonian, the localization range of the particle in one dimension decreases in the anharmonic oscillator case compared to the harmonic oscillator.

4. CONCLUSION

In this article we have computed the energy and wave function corrections for the quantum anharmonic oscillator up to the third order by using non-degenerate perturbation theory. Consistent energy values with the literature are found only for small perturbation parameters and low quantum levels. The x^4 term in the Hamiltonian leads to an increase in the intensity of confinement, which facilitates the localization of a particle.

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Conflict of Interest: Authors declared no conflict of interest.
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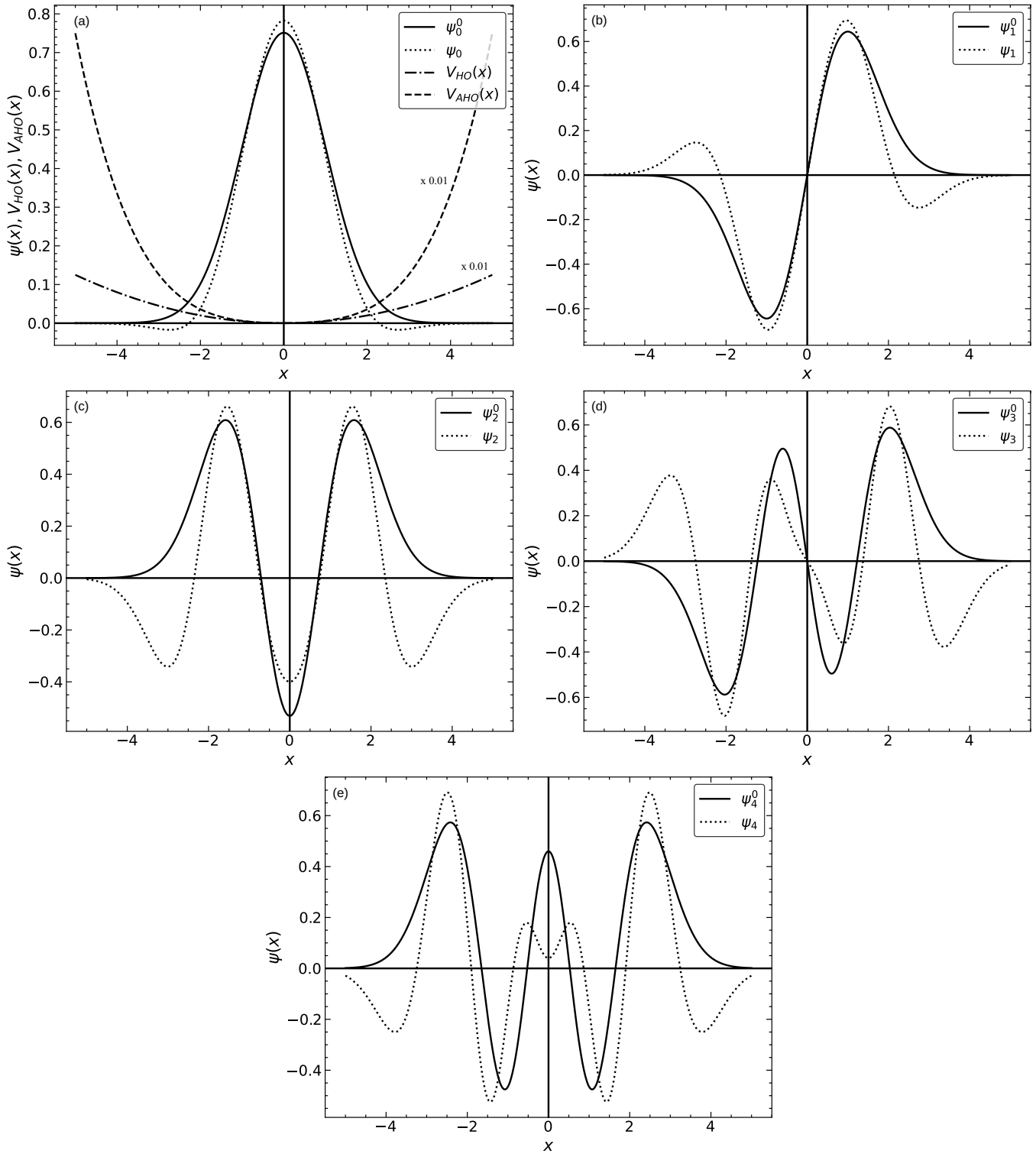

Figure 1. Wave functions of harmonic (solid) and quartic anharmonic (dotted) oscillator with $\lambda = 0.1$. In (a) harmonic and quartic potentials with $\lambda = 0.1$ are also plotted.

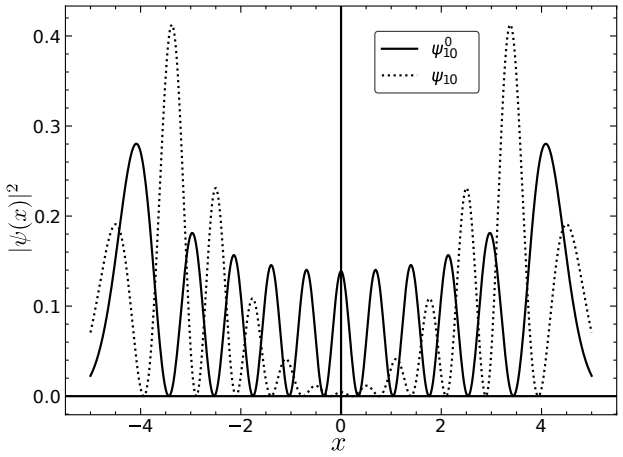

Figure 2. Probability distribution of quantum harmonic (solid) and quartic anharmonic (dotted) oscillator for quantum level $n = 10$ and $\lambda = 0.1$.

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[4] https://www.wolfram.com/mathematica/new-in-13/

SUPPLEMENTARY

Codes that are used in calculating energy eigenvalues for anharmonic quantum oscillator are listed below.

Mathematica

```
ClearAll["Global‘*"];
TISE1D[U_Function, {xmin_, xmax_}, N0Grid_ : 101,
  BoundaryCondition_String : "zero"] :=
 Module[{dx = (xmax - xmin)/(N0Grid -
1), Hmtx, Tmtx, Vmtx},
  Tmtx = -(1/(2 (dx)^2))
    SparseArray[{{i_, i_} -> -2, {i_, j_} /; Abs[i -
j] == 1 -> 1},
     {N0Grid, N0Grid}];
  Vmtx = DiagonalMatrix[U /@ Range[xmin, xmax, dx]];
  Hmtx = Tmtx + Vmtx;
  If[BoundaryCondition == "periodic",
   Hmtx[[1, -1]] = Hmtx[[-1, 1]] = -(1/(2 (dx)^2));];
  Sort[Transpose@Eigensystem[Hmtx],
  (#1[[1]] < #2[[1]]) &]]
TableForm[Table[V1[x_] = 1/2. x^2 + \[Lambda] x^4 ;
  Flatten[{\[Lambda],
    Transpose[
      Round[TISE1D[Function[{x}, V1[x]], {-
10, 10}, 1000], 0.0001]][[
     1, 1 ;; 3]]}],
  {\[Lambda], 0.1, 1, 0.1}],
 TableHeadings -> {None, {"\[Lambda]",
    "\!\(\*SubscriptBox[\(E\), \(0\)]\)",
    "\!\(\*SubscriptBox[\(E\), \(1\)]\)",
    "\!\(\*SubscriptBox[\(E\), \(2\)]\)",
    "\!\(\*SubscriptBox[\(E\), \(3\)]\)"}},
 TableAlignments -> Center]
```

Python

```
    import numpy as np
    from scipy.sparse import diags
    from scipy.sparse.linalg import eigs
    from findiff import FinDiff
    l_E = np.array([])
    il=0.1
    V = {"V2":lambda x:1/2*x**2,
         "V4":lambda x:1/2*x**2 + il*x**4}["V4"]
    for il in np.arange(0.1, 1.1 ,0.1):
        x = np.linspace(-5, 5, 200)
        energies, states = eigs(
            -0.5 * FinDiff(0, x[1]-
x[0], 2).matrix(x.shape) +
            diags(V(x)),
            k=3, which='SR')
        energies = np.insert(energies, [0], il)
        l_E = np.append(l_E, energies)
    l_E = np.round(l_E.real, 4).reshape((10,4))
    print("\tl\t E0\t\t E1\t\t E2\n", l_E)
```