Solution of Quantum Anharmonic Oscillator with Quartic Perturbation

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Abstract

This study was designed to obtain the energy eigenvalues for a Quantum Anharmonic Oscillator with Quartic Perturbation Potential. Two independent methods, the Dirac operator technique and the Numerov approach in solving Schrodinger equation, were used to solve the second order differential equation obtained from this system. An iterative procedure was carried out using the fourth order Runge-Kutta method on the transformed second order differential equation in line with the Numerov equation. The results showed that the normalized eigenvalues obtained from the Dirac operator technique, when compared with eigenvalues obtained from the use of the Fourth order Runge-Kutta method within the Numerov approach agreed closely when the convergence in the perturbing potential is weak, but the set of results diverges only at high excitation states. For the results from the two approaches to be closely compatible at high excitation states, the choice of Zeta axis was made to satisfy the boundary conditions $-1 < \zeta < +1$.

Keywords: QQAHO, Hamiltonian, Perturbation, Dirac Operation Technique, Numerov Approach, Zeta (ζ), Runge - Kutta Method and Eigenvalues.

1. Introduction.

One of the sources of progress of the sciences depends on the study of the same problem from different point of view based on different mathematical formalism. This why this study is focused on obtaining a set of energy eigenvalues from two independent mathematical methods, the Dirac operator technique and Fourth order Runge-Kutta method within the Numerov approach in solving Schrodinger equation for purpose of establishing a simple but robust method for solving Quantum Anharmonic Oscillator with Quartic Perturbation Potential. Determination of energy eigenvalues of the Schrodinger equation via asymptotic iteration method (AIM) has been widely applied to establish energy eigenvalues of the Schrodinger type equations [1], [2], arising from the development of fast computers simulations. Although the AIM formalism is very efficient to obtain eigenvalues of the Schrodinger equation, it requires tedious calculations in order to determine wave functions of systems which are not exactly solvable and thus the calculation of wave function involving a large number of terms will lose its simplicity and accuracy [3]. Much of the problems encountered in giving solutions to quantum anharmonic oscillator with quartic perturbation potential were first noticed with the Rayleigh-Schrodinger perturbation series for the simple system of the quartic anharmonic oscillator whose eigenvalues diverged even for small values of the coupling constants [4], [5]. The quantum solution for anharmonic oscillator with quartic perturbation is very useful in $\varphi 4$ field (the scalar field which interacts with itself through the interaction $\lambda \varphi 4$) theory and in the studies of quantum statistical properties of radiation field interacting with a cubic nonlinearity leading to a *quartic interaction* [7], [8]. A single mode of the radiation field

interacting with an optical fiber of cubic nonlinearity gives rise to the model of a quartic oscillator. Beyond the present system which form the focus of this study, the quantum anharmonic oscillator with sextic, octic, and the general one – perturbation term, λx^m, has been studied more recently, each with a diverse associated shortcomings [9], [10], [11].

In this study, the two methods used to obtain the energy eigenvalues for the system under consideration are classified under two mathematical formalisms. The Dirac operator technique is termed as the eigenvalues problem which takes care of the time development of wave functions in the Schrödinger concept, and Fourth order Runge-Kutta method within the Numerov approach is an directly used to get the time development of the operators within the Heisenberg frame-work.

This paper is organized as follows after the brief introduction in section 1. We solve the time independent Schrodinger equation in section 2 using the Dirac operation technique. In section 3 a detailed process of solution for quantum anharmonic oscillator with quartic perturbation potential using Numerov approach is presented. In section 4, the computational procedures and results are presented while section 5 contains the discussion of the results and conclusion.

The Quantum Anharmonic Oscillator with Quartic Perturbation Potential is respectively captioned in the Hamiltonian and Schrödinger equation for the Dirac technique as

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 + \frac{1}{2}k^/ x^4 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad \ldots (1)$$

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + \frac{1}{2}kx^2\Psi(x) + \frac{1}{2}k^/ x^4\Psi(x) = E\Psi(x) \ldots\ldots\ldots\ldots\ldots\ldots \quad .(2)$$

By setting $\zeta = \frac{x}{a}$, $E = \frac{\hbar w}{2\in}$ and $\frac{d^2}{d\zeta^2} = \frac{1}{a^2}\frac{d^2}{d\zeta^2}$, equation (2) can be written as

$$\frac{\hbar}{2m}\left(\frac{1}{a^2}\right)\left(\frac{d^2}{d\zeta^2}\right)\Psi(\zeta) + \frac{1}{2}m\omega^2\zeta^2\Psi(\zeta) + \frac{1}{2}k^/\zeta^4\Psi(\zeta) = \hbar\omega\varepsilon\Psi(\zeta) \ldots\ldots\ldots\ldots.. (3)$$

This transformation is necessary so that the Fourth order Runge-Kutta method within the Numerov approach in solving Schrodinger equation can be applied.

3. Solution of Time Independent Schrodinger Equation using Dirac Operator Technique

Two main operators, $\hat{a}$ is the lowering or annihilation operator and $\hat{a}^+$ is the raising or creation operator, necessary to specify the relation between the position and the momentum are defied as follows.

$$\hat{a} = \beta/\sqrt{2}[x + p/m\omega] \ldots\ldots\ldots\ldots\ldots (4) \quad \hat{a} = \beta/\sqrt{2}[x - ip/m\omega] \ldots\ldots\ldots \quad \ldots (5)$$

where x = position operator, m = mass of the particle, p = linear momentum operator ω = angular frequency.

The relationship coined from the parameters shown above is

$$\beta = \sqrt{mw}/\hbar \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (6)$$

where $\hbar = h/2\pi$.

The number operator is defined as

$$N = \hat{a}^+\hat{a} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (7)$$

The Hamiltonian of the harmonic oscillator in relation to the operator defined in equation (5) are given as

$$H = \hbar\omega(\hat{a}^+\hat{a} + \tfrac{1}{2}) \ldots\ldots\ldots\ldots\ldots.. (8) \text{ and } H = \hbar\omega(\hat{a}^+\hat{a} - \tfrac{1}{2}) \ldots\ldots\ldots\ldots\ldots \quad .(9)$$

The wave function of the harmonic oscillator, written as Ψ_n for the n state, $|n\rangle$, is properly defined such that the product of $\hat{a}^+\hat{a}$ satisfies

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle \dots\dots\dots\dots\dots\dots \text{(10)}, \quad \hat{a}^{+}|n\rangle = \sqrt{n}|n+1\rangle \dots\dots\dots\dots\dots\dots\text{(11)}$$

The Hamiltonian as expressed in equation (1) can be expressed as

$$\hat{H} = \hat{H}_0 + \lambda\hat{H}_1 \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \text{(12)}$$

where $\hat{H}_0$ =Unperturbed Hamiltonian, represented by $\hat{H}_O = \dfrac{p^2}{2m} + \dfrac{1}{2}kx^2$, $\hat{H}_1$ = Hamiltonian for the quartic

perturbation given as $\frac{1}{2}K' x^4$ and λ = perturbation coefficient.

The Schrodinger equation for the system under consideration and properly defined in terms of lowering, or annihilation operator $\hat{a}$ and $\hat{a}^+$ is the raising or creation operator, is give as

$$\hat{H}_o \Psi_n^o = E_n^o + E_n^{(1)} \dots\dots\dots\dots\dots\dots\dots\dots\dots \dots \text{(13)}$$

In Dirac notation, equation (11) becomes

$$\hat{H} = \langle n|\hat{H}|n\rangle = \langle n|\hat{H}_0|n\rangle + \lambda\langle n|\hat{H}_1|n\rangle \dots\dots\dots\dots\dots\dots \text{(14)}$$

where $\hat{H}_O = \hbar\omega(\hat{a}^+\hat{a})$, $E_n^{(o)} = \hbar\omega\left(n + \dfrac{1}{2}\right)$

The energy function is then given as $E_n^{(n)} = \lambda\langle n|\dot{x}^4|n\rangle \dots\dots\dots\dots\dots\dots \text{(15)}$

If $\dot{x} = \dfrac{\sqrt{2}}{\sqrt{2\beta^4}}(\hat{a} + \hat{a}^+)$, then the results of equation (15) is

$$E_n = \frac{1}{2}\left(\frac{K'}{4\beta^4}\right)\left[6n^2 + 6n + 3\right] \dots\dots\dots\dots\dots\dots \dots \text{(16)}$$

Factorizing, we have that

$$E_n = \frac{3K'}{8\beta^4}\left[2n^2 + 2n + 1\right] \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \text{(17)}.$$

From equation (6), we get that $\beta^4 = (m\omega/\hbar)^2$ then the energy equation (17) is finally given as

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) + \frac{3\hbar^2}{8m^2\omega^2}K'\left[2n^2 + 2n + 1\right]\dots\dots\dots\dots\dots \text{(18)}$$

With the following normalization units: $m = 1.0$, $\hbar = 1.0$, $w = 1.0$ and $K' = 0.01$ and the various values denoted by $n = 0, 1, 2, 3\dots\dots$, the various energy levels can be obtained. The values of the energy levels from the ground state to excited states are put together in table 1.0.

4. Computation of Eigenvalues using Numerov Approach

Numerov method was designed to solve numerical second order differential equations of the form

$$\frac{d^2 y}{dx^2} = F(x, y) \dots\dots\dots\dots\dots\dots\dots \text{(19)}$$

The values for equation (18) are determined using both the Predictor and Corrector iterative expressions respectively given as

Predictor $\qquad Y_{k+1} = 2Y_{k-1} + \dfrac{h}{12}\big[10F_k + F_{k-1}\big]$ ………..………………… (20)

Corrector $\qquad Y_{k+1} = 2Y_{k-1} + \dfrac{h}{12}\big[10F_{k+1} + F_k + F_{k-1}\big]$………………………….….. (21)

In this study, Schrodinger Equation for Quartic Perturbation in its transformed form, as expressed in equation (3) is reduced to the form of equation (19) so that the iterative procedures in equations (20) and (21) can be used effectively to obtain the solution to the Schrodinger Equation for Quartic Perturbation in equation (2).

By a simple transformation technique, equation (3) reduces to

$$\left[\frac{d^2}{d\zeta^2} - \zeta^2 - 2\lambda\zeta^4\right]\psi(\zeta) = -\varepsilon\psi(\zeta) \qquad \text{……………………………….....} \qquad (22)$$

where λ is an adjustable parameter. On expansion, we have that

$$\frac{d^2\Psi(\zeta)}{d\zeta^2} = (\zeta^2 - \varepsilon + 2\lambda\zeta^4)\Psi(\zeta) \qquad \text{…………….……………………..…} \qquad .. (23)$$

The solution to equation (23) using the predictor equation yields

$$\Psi(\zeta) = 10(\zeta^2 - \varepsilon_N + 2\lambda\zeta^4)\Psi_{N,K} + (\zeta^2 - \varepsilon_N + 2\lambda\zeta^4)\Psi_{N,K-1} \text{……………….} \qquad .. (24)$$

Applying the corrector equation (21) yields

$$\Psi_{N,K+1} = 2\Psi_{N,K} - \Psi_{N,K-1} + \frac{\hbar^2}{12}\big[F_{K+1} + 10F_k + F_{k-1}\big] \text{……………………..…….} \qquad ... (25)$$

where $N = 1,2,3,4\ldots$

Thus the expression to iterated becomes

$$\Psi_{N,K+1} = 2\Psi_{N,K} - \Psi_{N,K-1} + \frac{\hbar^2}{12}\big[10(\zeta^2 - \varepsilon_N + 2\lambda\zeta^4)\Psi_{N,K} + (\zeta^2 - \varepsilon_N + 2\lambda\zeta^4)\Psi_{N,K-1}\big] \text{…. (26)}$$

The results generated from these two approaches are tabulated in table 1.0.

5. Results and Discussion

The calculated values for the eigenvalues from the two methods are put together in table 1.0. The eigenvalues obtained by Dirac Operator Techniques are in the first column. The second column contains the eigenvalues obtained by Numerov Approach. The Normalized Eigen values from Numerov on Dirac Operation Techniques are put together in column three and the percent difference are compiled in column four for the various energy levels computed in this study. The normalized eigenvalues from the Numerov approach compared well with the eigenvalues obtained by Dirac Operator Techniques as shown by the percentage difference in the values obtained from these two methods for each of the energy levels. The convergence shown in the results presented in the table is made possible by the choice of Zeta, (ζ). The choice of Zeta axis which satisfies the related convergence of the two results are found to be within the boundary conditions $-1 < \zeta < +1$. The results show a consistence increase in the values of the normalized eigenvalues as n increases for each state regardless of the change in the value of Zeta. Also, the

percentage differences between the two results at the ground, first and second energy state levels are less than 1%.

6. Conclusion

Numerov and Dirac operation techniques have been used to calculate the ground energy state and the first nine eigenvalues energy states for an anharmonic oscillator potential with the quartic perturbation potential. The percentage differences for the nine states are less than 1% when the results from the two methods are compared. It was observed that results from these two methods agree when the perturbing potential is weak and particularly at the low energy states. As the perturbing potential gets stronger at the higher excited states, the results from the Dirac operator techniques start to diverge from those obtained from the numerical schemes. The methods used in this study provide a simple technique for solving anharmonic oscillator potential with the quartic perturbation potential and of higher perturbation potential, because the mathematical method can easily be solved using simple computer simulations.

Table 1.0. Values of the Eigen values obtained from the Dirac operator techniques and from the Numerov iteration method.

Energy Level	Eigenvalues obtained by Dirac Operator Techniques	Eigenvalues obtained by Numerov Approach	Eigenvalues by Numerov Normalized on Dirac Operation Technique	Percent Difference
Ground State	0.50375	2.91500	0.4028349	0.2505%
First Excited State	1.51875	10.99000	1.5281498	0.0062%
Second Excited State	2.54875	24.99000	3.4534630	0.2619%
Third Excited State	3.59375	32.51414	4.4932520	0.2002%
Fourth Excited State	4.65375	34.42000	4.7566306	0.0216%
Fifth Excited State	5.72875	42.71000	5.9022572	0.0294%
Sixth Excited State	6.81875	50.72500	7.0098805	0.0273%
Seventh Excited State	7.92375	58.43500	8.0753547	0.0188%
Eighth Excited State	8.68125	64.21400	8.8739767	0.0217%
Ninth Excited State	9.72625	72.35000	9.9983214	0.0272%

where Normalized constant $k = \dfrac{1.51875}{10.9900} = 0.1381938$

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