

Energy Eigenvalues of Quantum Anharmonic Oscillators: Exact Expression for the Pure λx^{2m} Oscillators and a Simple Expression for $x^2 + \lambda x^{2m}$ Oscillators

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Abstract

We propose an exact expression for the energy eigenvalues of the pure λx^{2m} quantum anharmonic oscillators. The only information needed for the purpose is $K_0^{(m,n)}$, which is the first term of strong-coupling expansion for oscillator with potential λx^{2m} for the n^{th} excited state. We then propose simple expression for the eigenvalues of the $x^2 + \lambda x^{2m}$ oscillators which reproduce both the ground state and excited states energies of these oscillators with a fairly good accuracy. The present formula is found to better reproduce the energy eigenvalues than those calculated by earlier authors.

Keywords: Anharmonic Oscillator, Quartic, sextic and Octic Oscillators, Weak and strong coupling expansion.

1. Introduction

A large number of articles have already been written on quantum anharmonic oscillators with no sign yet of waning interest. Though it is almost impossible to give even a partial list, we mention only a few [1-6]. One of the basic reasons for this active interest is that the anharmonic oscillators serve as a rather simple model for understanding the non-trivial features of a large number of complicated problems in different branches of physics like reproducing the molecular spectra or understanding the Higg's mechanism. It is not an easy problem to solve the one dimensional Schrodinger equation with potential $x^2 + \lambda x^{2m}$ or λx^{2m} where λ is the coupling parameter. A number of numerical techniques have been developed to obtain the energy eigenvalues of such oscillators [7-9].

The purpose of this article is to present an extremely simple formula which exactly reproduces the energy levels of the oscillator with potential λx^{2m} and fairly accurately reproduces the energies of the $x^2 + \lambda x^{2m}$ oscillators for the ground state as well as the excited states. It may be mentioned that Bhattacharya et. al. [10] proposed a simple prescription for obtaining the ground state energy of the anharmonic oscillators and subsequently Dasgupta et. al. [1] generalised the scheme to obtain both the ground state and excited state energies of the oscillators. The results obtained by present scheme are found to be much better.

Table 1. Some energy eigenvalues $e^{(m,n)}$ for the quartic, sextic and dectic anharmonic oscillators obtained from equations (6), and (7) are placed in the first row. The values reported by Meißner and Steinborn [11] are referred to as the exact values, are placed in the second row. The numbers within bracket in the first row are those predicted by the formula given in reference [1].

λ	0.2	10	100
$e^{(2,0)}$ <i>exact</i>	1.115 (1.103) 1.118293	2.446 (2.430) 2.449174	4.998 (4.989) 4.999418
$e^{(2,5)}$ <i>exact</i>	15.829 (15.612) 15.799534	46.742 (46.638) 46.729081	99.038 (98.989) 99.032837
$e^{(2,10)}$ <i>exact</i>	34.764 (34.35) 34.703815	109.795 (109.63) 109.772571	233.966 (233.89) 233.966226
$e^{(3,0)}$ <i>exact</i>	1.1626 (1.127) 1.173889	2.1973 (2.162) 2.205723	3.7119 (3.690) 3.716975
$e^{(3,5)}$ <i>exact</i>	21.617 (21.19) 21.559198	52.859 (52.69) 52.849513	93.060 (92.98) 93.073891
$e^{(3,10)}$ <i>exact</i>	54.271 (53.63) 54.306663	137.86 (137.59) 138.185314	243.85 (243.70) 244.478368
$e^{(4,0)}$ <i>exact</i>	1.223 (1.163) 1.241028	2.102 (2.051) 2.114545	3.180 (3.145) 3.188654
$e^{(4,5)}$ <i>exact</i>	27.193 (26.709) 27.121781	56.944 (56.71) 56.898990	89.610 (89.45) 89.569749
$e^{(4,10)}$ <i>exact</i>	74.034 (73.373) 73.954525	158.601 (158.28) 158.599178	250.532 (250.33) 250.575192

2. Energy Eigenvalues of Anharmonic Oscillators

2.1 Pure Anharmonic Oscillator

Using a suitably chosen set of units, the Hamiltonian for the harmonic oscillator is $H_0 = p^2 + \frac{1}{2}m\omega^2x^2$ which has the eigenvalues $(2n + 1)$. It is a dimensionless quantity and corresponding energy is $(2n + 1)\frac{\hbar\omega}{2}$. The Schrodinger equation for the pure λx^{2m} anharmonic oscillator is given by

$$-\frac{d^2\Psi}{dx^2} + \lambda x^{2m}\Psi = e_p^{(m,n)}(\lambda)\Psi \quad (1)$$

Here we use the subscript p to emphasize that e_p is the eigenvalue of the pure λx^{2m} oscillator. Here λ and x are dimensionless quantity. Replacing x by αx and choosing $\alpha = \lambda^{-1/(2m+2)}$, the above equation can be reduced to

$$-\frac{d^2\Psi}{dx^2} + x^{2m}\Psi = \lambda^{-1/(m+1)}e_p^{(m,n)}(\lambda)\Psi \quad (2)$$

Equation (2) implies $e_p^{(m,n)}(\lambda) = \lambda^{1/(m+1)}e_p^{(m,n)}(1)$. This relation is true for any λ [4]. It is well known [6] that for the Schrodinger equation with potential $x^2 + \lambda x^{2m}$ one can develop the following strong coupling expansion.

$$e^{(m,n)}(\lambda) = (2n + 1)\lambda^{\frac{1}{m+1}}\sum_{j=0}^{\infty}K_j^{(m,n)}\lambda^{-2j/(m+1)} \quad (3)$$

For very large λ , the x^2 term in the Hamiltonian of the $x^2 + \lambda x^{2m}$ oscillator is negligible and the Hamiltonian reduces to that of the pure λx^{2m} oscillator. Hence in the limit $\lambda \rightarrow \infty$, we can write

$$e_p^{(m,n)}(\lambda) = (2n + 1)\lambda^{\frac{1}{m+1}}K_0^{(m,n)} \quad (4)$$

$K_0^{(m,n)}$ is the first term of the strong coupling expansion. We can thus conclude that $e_p^{(m,n)}(1) = (2n + 1)K_0^{(m,n)}$ and $e_p^{(m,0)}(1) = K_0^{(m,0)}$.

The equation (4) gives the exact expression for the eigenvalue of the pure λx^{2m} oscillator. For $m = 1$ it reproduces the eigenvalues $(2n + 1)\sqrt{\lambda}$ (with $K_0^{(1,n)} = 1$ for all n) corresponding to those of the harmonic oscillator as expected.

For $m = 2, 3, 4, 5$, $K_0^{(m,0)}$ has been calculated by different authors [12, 13]. For the quartic oscillator $K_0^{(2,n)}$ has been calculated by Skala et al [12] for $n = 2, \dots, 10$. Dasgupta et al [1] also estimated some of the values for $K_0^{(m,n)}$ and also provided expressions for $K_0^{(m,n)}$ for $m = 2, 3, 4$ as functions of n and a global approximation for $K_0^{(m,0)}$. Jafarpour and Afshar [14] calculated energy eigenvalues for some specific values of λ of the Hamiltonian $(\frac{1}{2})p^2 + \lambda x^{2m}$ for $m = 2, 3, 4$ and 5. For $\lambda = 1$, they obtained $e^{(2,0)} = 0.66798625916$, $e^{(3,0)} = 0.6807036117$, and $e^{(4,0)} = 0.70404885$. To obtain the eigenvalues for the Hamiltonian $p^2 + \lambda x^{2m}$ we must multiply these values by $\lambda^{\frac{m}{2m+1}}$ and these values agree with $K_0^{(m,0)}$ to the last decimal places. The values of $e^{(m,n)}(\lambda)$ reported in reference [14] are also exactly reproduced.

2.2 New expression for the energy eigenvalues of $x^2 + \lambda x^{2m}$ oscillators

We now proceed to find the energy eigenvalues for the potential $x^2 + \lambda x^{2m}$. We know the eigenvalues for the harmonic oscillator exactly and it is evident for our previous discussion that we also know the eigenvalues for the pure λx^{2m} oscillator. We rewrite the Hamiltonian $H = p^2 + x^2 + \lambda x^{2m}$ as follows.

$$H = H_1 + H_2$$

$$H = \left(\frac{1}{f}p^2 + x^2\right) + \left(\frac{f-1}{f}p^2 + \lambda x^{2m}\right) \quad (5)$$

Where f is some real positive number greater than 1. If the eigenfunctions of H, H_1 and H_2 are identical, then the sum of the eigenvalues e_1 and e_2 of H_1 and H_2 respectively will be strictly equal to the eigenvalue e of H . We find that the eigenfunctions of H, H_1 and H_2 for the quartic anharmonic oscillator at $\lambda = 1$ and these are not widely different and we assume the same to be true for other oscillators at different coupling parameters as well. If we assume that the eigenvalue of H is the sum of the eigenvalues of H_1 and H_2 , then we can write

$$e^{(m,n)}(\lambda) = (2n + 1) \left[\frac{1}{\sqrt{f}} + K_0^{(m,n)} \lambda^{\frac{1}{m+1}} \frac{1}{\left(\frac{f}{f-1}\right)^{\frac{m}{m+1}}} \right] \quad (6)$$

Choice of value of $f \rightarrow$

We chose that value of f for which the eigenvalue is maximum which is obtained by differentiating the eigenvalue with respect to f and equating to zero and this gives the equation

$$f^{m-1}(f-1)^2 = \left[\frac{2m}{m+1} K_0^{(m,n)} \lambda^{\frac{1}{m+1}} \right]^{2(m+1)} \quad (7)$$

Thus f is a function of m, n and λ and we write $f(m, n, \lambda)$ and for the quartic and sextic oscillators the equation can be solved. For the quartic oscillator one has to solve a cubic equation and two of the roots are complex and we consider the real positive root for $f(2, n, \lambda)$. For the sextic oscillator the expression is simple and we choose the positive root. For the octic oscillator $f(4, n, \lambda)$ can be obtained by numerically solving the equation.

Table 1 displays some energy eigenvalues for the quartic, sextic and octic oscillators for ground as well as some excited states for different coupling parameters and the agreement is good enough.

3. Conclusion

In conclusion, we like to comment that the simple formula given by equation (4) exactly reproduces the energy eigenvalues of the pure λx^{2m} oscillator. Moreover, the simple formula given by equation (6) reproduces the energy values of $x^2 + \lambda x^{2m}$ oscillator with surprising accuracy. If one knows $K_0^{(m,n)}$, then one can obtain the eigenvalues of $x^2 + \lambda x^{2m}$ oscillator for any m and n and for any coupling parameter. One great advantage of the present scheme is that, unlike in the case of systematics [1], it has the possibility of being extended to the case of polynomial potentials like $c_1 x^2 + c_2 x^4 + c_3 x^6 + \dots$ and can be helpful in studying double well potential as well.

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