The Hypervirial-Padé Summation Method Applied to the Anharmonic Oscillator

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Abstract. The energy eigenvalues of the anharmonic oscillator characterized by the cubic potential for various eigenstates are determined within the framework of the hypervirial-Padé summation method. For this purpose the $E[3,3]$ and $E[3,4]$ Padé approximants are formed to the energy perturbation series and given the energy eigenvalues up to fourth order in terms of the anharmonicity parameter $\lambda$.

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1. Introduction

There has been a great deal of interest in the analytical and numerical investigation of the one-dimensional anharmonic oscillator. They are of interest because of their importance in molecular vibrations[1] as well as in solid state physics[2, 3]. On the other hand, the anharmonic oscillators with cubic and/or quartic potentials can serve as a testing ground for the various methods based on perturbative and nonperturbative approaches such as a group-theoretical approach[4], the multiple scale technique[5], Hill determinant method[6, 7] and supersymmetric approaches[8].

In the past few decades, the hypervirial-Padé summation method are applied to various kind of potentials[9], e.g. the hydrogen atom with perturbation $\alpha r$[10], the quartic anharmonic oscillator within hypervirial JWKB method[11], the gaussian potential[12] and the screened Coulomb potential[13]. In addition, the hypervirial relations and the Hellman-Feynman theorems are applied to anharmonic oscillators[14]. However, the energy perturbation series of the anharmonic oscillator diverges asymptotically for the perturbation parameter, so one can use the Padé summation method to recover finite results for the energy series[16]. In this note, we would like to apply the hypervirial-Padé summation method to the case of the anharmonic oscillator with the potential

$$V(x) = \frac{1}{2} \omega^2 x^2 + \frac{1}{2} \lambda x^2 + \lambda^2 x^3,$$  

(1)

In this potential we take the cubic term as a perturbation term, but with this term we also have a quartic perturbation term. We pointed out that the present method can be applied to the system described by this potential and gives the numerical results which are in agreement with those of Ref.[17]. In Section 2, we present the formulation of the method for the case given by Eq.(1) and a relation between the energy and the expectation values of $x$ with various powers. With this relation and the help of the Hellman-Feynman theorems we find an equation which is related the energy series coefficients to the coefficients of the power series of $\langle x^N \rangle$ and obtain recurrence relations in powers of $\lambda$. In Section 3, we give the formula for the energy levels up to fourth order in $\lambda$. We also evaluate the $E[3,3]$ and $E[3,4]$ Padé approximants to the energy series and list the numerical results of the energy eigenvalues for the ground and first five excited energy states in Tables. Then we present the conclusion in Section 4.

2. Mathematical Formulation

The Hamiltonian for the anharmonic oscillators described by Eq.(1) is given by

$$H = -\frac{1}{2} \frac{d^2}{dx^2} + V(x),$$

(2)

where the anharmonic potential considered in this note in terms of the perturbation parameter $\lambda$ is taken to be

$$V(x) = \frac{1}{2} \omega^2 x^2 + \frac{1}{2} \lambda x^2 + \lambda^2 x^3,$$


Here, we use the units \( m = \hbar = 1 \). By applying the Hellman-Feynman theorems, one obtains the following relations between the energy and the expectation values \( \langle x^N \rangle \) [14]:

\[
E \langle x^N \rangle = (\lambda + \omega^2) \frac{N + 2}{2(N + 1)} \langle x^{N+2} \rangle + \lambda^2 \frac{2N + 5}{2(N + 1)} \langle x^{N+3} \rangle - \frac{1}{8} N(N - 1) \langle x^{N-2} \rangle ,
\]

(3)

One can assume that the energy \( E_n \) and the expectation values \( \langle x^N \rangle \) can be expanded in power series of \( \lambda \) as

\[
E_n = \sum_{k=0}^{\infty} E_n^{(k)} \lambda^k ,
\]

(4)

\[
\langle x^N \rangle = \sum_{k=0}^{\infty} A_N^{(k)} \lambda^k ,
\]

(5)

where the energy of the unperturbed \( n \)th state is

\[
E_n^{(0)} = \omega \left( n + \frac{1}{2} \right) ,
\]

(6)

From the normalization condition that \( \langle x^0 \rangle = \langle 1 \rangle = 1 \) [14], one has

\[
A_0^{(k)} = \delta_{k0} ,
\]

(7)

The energy coefficients \( E_n^{(k)} \) are related to the coefficients \( A_N^{(k)} \) through the use of the Hellman-Feynman theorem [9]. From the Hellman-Feynman theorem

\[
\langle \frac{\partial V}{\partial \lambda} \rangle = \frac{\partial E}{\partial \lambda} = \langle \frac{\partial H}{\partial \lambda} \rangle ,
\]

(8)

one can find

\[
E_n^{(k+1)} = \frac{1}{2(k + 1)} A_2^{(k)} + \frac{2}{k + 1} A_3^{(k-1)} \quad k \geq 1 ,
\]

(9)

By equating the coefficients of various powers of \( \lambda \) on both sides of Eq.(3) with equations (4),(5) and (9), we can calculate the energy coefficients \( E_n^{(k)} \) in a hierarchical manner [14, 15]. For example, we find, from the coefficients of \( \lambda^0, \lambda^1, \lambda^2 \) the following relations

\[
A_N^{(0)} = \frac{1}{E_n^{(0)}} \left[ \frac{N + 2}{2(N + 1)} \omega^2 A_N^{(0)} - \frac{1}{8} N(N - 1) A_N^{(0)} \right] ,
\]

(10)

\[
A_N^{(1)} = \frac{1}{E_n^{(0)}} \left[ \frac{N + 2}{2(N + 1)} \omega^2 A_N^{(1)} + \frac{N + 2}{2(N + 1)} A_N^{(0)} - \frac{1}{8} N(N - 1) A_N^{(0)} \right] - E_n^{(1)} A_N^{(0)} ,
\]

(11)

\[
A_N^{(2)} = \frac{1}{E_n^{(0)}} \left[ \frac{N + 2}{2(N + 1)} \omega^2 A_N^{(2)} + \frac{N + 2}{2(N + 1)} A_N^{(1)} + \frac{2N + 5}{2(N + 1)} A_N^{(0)} - \frac{1}{8} N(N - 1) A_N^{(2)} - E_n^{(1)} A_N^{(1)} - E_n^{(2)} A_N^{(0)} \right] ,
\]

(12)

From the above relations one can calculate the energy coefficients \( E_n^{(k)} \) from the knowledge of \( A_N^{(m)} \) and \( E_n^{(m)} \) in a hierarchical manner.
3. The Results

The energy $E_n$ so obtained of the anharmonic oscillator given by Eq.(1) to the fourth order in $\lambda$ is given by

$$
E_n[4] = \omega(n + \frac{1}{2}) + \frac{\lambda}{2\omega}(n + \frac{1}{2}) - \frac{\lambda^2}{8\omega^3}(n + \frac{1}{2}) - \frac{\lambda^3}{\omega^4}\left[\frac{5}{96\omega}(2n + 1) \right. \\
+ \frac{2}{3}(4n^2 + 4n + 1) \left. \right] + \frac{\lambda^4}{4\omega^4}\left[\frac{25}{96\omega^3}(n + \frac{1}{2}) + \frac{23}{12\omega^2}(4n^2 + 4n + 1) \right. \\
+ \frac{7}{2}(2n^2 + 2n + 1) \left. \right] + \ldots,
$$

(13)

The energy series given by (4) is a divergent-asymptotic series, therefore one can use the Padé approximants to calculate the energy eigenvalues\[16]. The $[N,M]$ Padé approximant to (4) is given by

$$
E[N, M] = E_n^{(0)}(1 + \lambda p_1 + \lambda^2 p_2 + \ldots + \lambda^M p_M) \frac{1}{1 + \lambda q_1 + \lambda^2 q_2 + \ldots + \lambda^N q_N},
$$

$$
= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots + \lambda^{N+M} E_n^{(N+M)},
$$

(14)

where the coefficients $p_i(i = 1, \ldots, M)$ and $q_j(j = 1, \ldots, N)$ in this equation can be calculated from the knowledge of the energy coefficients $E_n^{(m)}$ up to the order of $\lambda^{N+M}$.

| $n$ | $\lambda$ | $E[4]$  | $E[3, 3]$ | $E[3, 4]$  |
|-----|-----------|---------|-----------|-----------|
| 0   | 0.005     | 0.501248| 0.501248  | 0.501248  |
|     | 0.01      | 0.502493| 0.502493  | 0.502493  |
|     | 0.05      | 0.512252| 0.512252  | 0.512249  |
|     | 0.1       | 0.523620| 0.523634  | 0.523590  |
| 1   | 0.005     | 1.503740| 1.503740  | 1.503740  |
|     | 0.01      | 1.507480| 1.507480  | 1.507480  |
|     | 0.05      | 1.536260| 1.536260  | 1.536240  |
|     | 0.1       | 1.566970| 1.567010  | 1.566660  |

Table 1. Energy eigenvalues as functions of the parameter $\lambda$ for the $n = 0$ and $n = 1$ states.

The numerical results are given in Tables 1, 2 and 3. In the calculations we have the quadratic term in the potential as one of the perturbation terms. In view of this, the energy eigenvalues of the anharmonic oscillator are evaluated for different values of the anharmonicity parameter $\lambda$ for the eigenstates $n = 0$ to 5. In the Tables, we also list the energy eigenvalues $E[4]$ which are correct to the fourth order of $\lambda$.

4. Conclusion

Using the hypervirial relations (Eq.(3)), we have calculated the energy coefficients $E_n^{(k)}$ of the anharmonic oscillator with the potential given by Eq.(1) in a hierarchical
The energy series is asymptotically divergent. We have then evaluated the Padé approximants $E_{[3,3]}$ and $E_{[3,4]}$ to the energy series. The results for the potential without of the cubic term are in agreement with those of Ref.[17]. Therefore, we conclude that the hypervirial-Padé summation method can be used to determine the energy eigenvalues of the anharmonic potential given by Eq.(1).

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