

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 λ .

Key Words: Anharmonic oscillator, Schrodinger equation, hypervirial theorems, Padé summation method.

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 to the understanding of molecular vibrations [1] and in other areas of 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].

To obtain the energy eigenvalues of the Hamiltonians which are not exactly solvable, one has to use approximate schemes, one of which is, for example, the Rayleigh-Schrodinger perturbation method. In this method, as is well-known, the energy is written as an infinite power series of the perturbation parameter. In the present paper, instead of that, the power series of the energy of the anharmonic oscillator is written using the hypervirial relations (HVR) and Hellman-Feynman theorems (HFT). To use the HVR and HFT, the energy and the expectation value of the position coordinate is taken as a power series of the perturbation parameter λ . With the help of the HVR and HFT it becomes possible to find an expression which is related the energy series coefficients to the coefficients of the expectation value series of the position coordinate. The hypervirial relations and the Hellman-Feynman theorems are applied to anharmonic oscillators [9]. However, the energy perturbation series is an asymptotically divergent series for the perturbation parameter. One of the methods to recover a finite results for the energy series is the Padé summation method [10]. Consequently, the combination of the Padé summation method with the preceding theorems and relations can be used to find the energy eigenvalues of the systems which have different potentials. In the past few decades, the hypervirial-Padé summation method are applied to various kinds of potentials [11], e.g. the hydrogen atom with perturbation αr [12], the quartic anharmonic oscillator within hypervirial JWKB method [13], the

*This note is dedicated to my father T. Arda.

gaussian potential [14] and the screened Coulomb potential [16]. In this note, we apply the hypervirial-Padé summation method to the case of the anharmonic oscillator with the potential

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

In this potential we take the cubic term as a perturbation term; but with this term we also have a quadratic perturbation term. We pointed out that the present method can be applied to the system described by this potential and give the numerical results which are in agreement with those of Ref.[17]. In Section 2, we present the formulation of the method for the above potential 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 λ . In Section 3, we give the formula for the energy levels up to fourth order in λ . Before this equation we have calculated the first and second order corrections to the energy as an example. 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. The Theory

The Hamiltonian for the anharmonic oscillators described by the preceding potential is given by

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

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

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

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 $\langle x^N \rangle$ [9]

$$\begin{aligned} E \langle x^N \rangle &= (\lambda + \omega^2) \frac{N+2}{2(N+1)} \langle x^{N+2} \rangle + \lambda^2 \frac{2N+5}{2(N+1)} \langle x^{N+3} \rangle \\ &\quad - \frac{1}{8} N(N-1) \langle x^{N-2} \rangle, \end{aligned} \quad (3)$$

One can assume that the energy E_n and the expectation values $\langle x^N \rangle$ can be expanded in a power series of λ as

$$E_n = \sum_{k=0}^{\infty} E_n^{(k)} \lambda^k, \quad (4)$$

$$\langle x^N \rangle = \sum_{k=0}^{\infty} A_N^{(k)} \lambda^k, \quad (5)$$

where the energy of the unperturbed n th state is

$$E_n^{(0)} = \omega \left(n + \frac{1}{2} \right). \quad (6)$$

From the normalization condition that $\langle x^0 \rangle = \langle 1 \rangle = 1$ [9], one has

$$A_0^{(k)} = \delta_{k0}. \quad (7)$$

The energy coefficients $E_n^{(k)}$ are related to the coefficients $A_N^{(k)}$ through the use of the Hellman-Feynman theorem[11]. From the Hellman-Feynman theorem

$$\left\langle \frac{\partial V}{\partial \lambda} \right\rangle = \frac{\partial E}{\partial \lambda} = \left\langle \frac{\partial H}{\partial \lambda} \right\rangle, \quad (8)$$

one can find

$$E_n^{(k+1)} = \frac{1}{2(k+1)} A_2^{(k)} + \frac{2}{k+1} A_3^{(k-1)}. \quad (9)$$

By equating the coefficients of various powers of λ 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 [9, 15]. For example, we find, from the coefficients of $\lambda^0, \lambda^1, \lambda^2$ the following relations:

$$A_N^{(0)} = \frac{1}{E_n^{(0)}} \left[\frac{N+2}{2(N+1)} \omega^2 A_{N+2}^{(0)} - \frac{1}{8} N(N-1) A_{N-2}^{(0)} \right], \quad (10)$$

$$A_N^{(1)} = \frac{1}{E_n^{(0)}} \left[\frac{N+2}{2(N+1)} \omega^2 A_{N+2}^{(1)} + \frac{N+2}{2(N+1)} A_{N+2}^{(0)} - \frac{1}{8} N(N-1) A_{N-2}^{(1)} - E_n^{(1)} A_N^{(0)} \right], \quad (11)$$

$$A_N^{(2)} = \frac{1}{E_n^{(0)}} \left[\frac{N+2}{2(N+1)} \omega^2 A_{N+2}^{(2)} + \frac{N+2}{2(N+1)} A_{N+2}^{(1)} + \frac{2N+5}{2(N+1)} A_{N+3}^{(0)} - \frac{1}{8} N(N-1) A_{N-2}^{(2)} - E_n^{(1)} A_N^{(1)} - E_n^{(2)} A_N^{(0)} \right]. \quad (12)$$

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 Numerical Results

Now we want to calculate the expressions for the some coefficients in the series given by Eq. (4); for this purpose we use Eq. (9). From the equation, we obtain for $E_n^{(1)}$ and $E_n^{(2)}$, for example,

$$E_n^{(1)} = \frac{1}{2} A_2^{(0)}, \quad (13)$$

$$E_n^{(2)} = \frac{1}{4} A_2^{(1)} + A_3^{(0)}. \quad (14)$$

To obtain the first order correction to the energy we need to know the coefficient $A_2^{(0)}$; thus with the help of Eq. (10) one can obtain

$$E_n^{(1)} = \frac{1}{2\omega^2} E_n^{(0)}. \quad (15)$$

After that one can find $A_2^{(1)}$ from Eq. (11) with the knowledge of $E_n^{(1)}$ and the coefficient $A_3^{(0)}$ from Eq. (10). The energy E_n so obtained of the anharmonic oscillator given by Eq. (2) to the fourth order in λ is

given by

$$\begin{aligned}
 E_n[4] &= \frac{\omega}{2}(2n+1) + \frac{\lambda}{4\omega}(2n+1) - \frac{\lambda^2}{16\omega^3}(2n+1) - \frac{\lambda^3}{\omega^4} \left[\frac{5}{96\omega}(2n+1) \right. \\
 &+ \left. \frac{2}{3}(4n^2+4n+1) \right] + \frac{\lambda^4}{4\omega^4} \left[\frac{25}{96\omega^3} \left(n + \frac{1}{2} \right) + \frac{23}{12\omega^2}(4n^2+4n+1) \right. \\
 &+ \left. \frac{7}{2}(2n^2+2n+1) \right] + \dots
 \end{aligned}
 \tag{16}$$

The energy series given by (4) is a divergent-asymptotic series; therefore one can use the Padé approximants to calculate the energy eigenvalues[10]. The [N, M] Padé approximant to (4) is given by

$$\begin{aligned}
 E[N, M] &= E_n^{(0)} \frac{1 + \lambda p_1 + \lambda^2 p_2 + \dots + \lambda^M p_M}{1 + \lambda q_1 + \lambda^2 q_2 + \dots + \lambda^N q_N}, \\
 &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots + \lambda^{N+M} E_n^{(N+M)},
 \end{aligned}
 \tag{17}$$

where the coefficients $p_i (i = 1, \dots, M)$ and $q_j (j = 1, \dots, N)$ in this equation can be calculated from the knowledge of the energy coefficients $E_n^{(m)}$ up to the order of λ^{N+M} . According to these equation to find the coefficients p_i and q_j one has to know the energy up to the order of $(M + N)$. To calculate the coefficients, one has to expand the denominator of the E[N,M] Padé approximant to the Taylor series in terms of λ and than by equating the coefficients of various powers of λ on both sides one has a system of linear equations with $(M+N)$ unknowns. In this note we have solved two different systems of linear equations corresponding to the E[3, 3] and E[3, 4] Padé approximants. In the present work, we have used Mathematica to do the calculations and the numerical analysis.

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

n	λ	$E[4]$	$E[3, 3]$	$E[3, 4]$
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

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 λ 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 λ .

Table 2. Energy eigenvalues as functions of the parameter λ for the $n = 2$ and $n = 3$ states.

n	λ	$E[4]$	$E[3, 3]$	$E[3, 4]$
2	0.005	2.506240	2.506240	2.506240
	0.01	2.512450	2.512450	2.512450
	0.05	2.559610	2.559610	2.559530
	0.1	2.605020	2.605080	2.604100
3	0.005	3.508730	3.508730	3.508730
	0.01	3.517420	3.517420	3.517420
	0.05	3.582290	3.582290	3.582120
	0.1	3.637780	3.637800	3.635920

Table 3. Energy eigenvalues as functions of the parameter λ for the $n = 4$ and $n = 5$ states.

n	λ	$E[4]$	$E[3, 3]$	$E[3, 4]$
4	0.005	4.511230	4.511230	4.511230
	0.01	4.522390	4.522390	4.522390
	0.05	4.604310	4.604310	4.604000
	0.1	4.665230	4.665130	4.662200
5	0.005	5.513720	5.513720	5.513720
	0.01	5.527350	5.527350	5.525180
	0.05	5.625660	5.625670	5.378930
	0.1	5.687380	5.687040	4.284910

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. (2) in a hierarchical manner. 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 perturbative part of the present potential has two terms: one of them is a quadratic term, and the other is cubic. If we ignore the cubic term in the potential and we take only the quadratic term as a perturbation, the results obtained for this 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. (2).

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