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Modified Hill determinant approach to the eigenvalues of the anharmonic oscillator

R N CHAUDHURI and M MONDAL

Department of Physics, Visva-Bharati University, Santiniketan 731 235, India

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Abstract. The unperturbed Hamiltonian of quantum anharmonic oscillator is modified by introducing a simple variational scale parameter. A suitable choice of this parameter makes the eigenvalues rapidly convergent for small size of the determinant in the method of infinite Hill determinant. Simple analytic expressions for the eigenvalues are obtained by matrix diagonalization method.

Keywords. Anharmonic oscillator; variational parameter; Hill determinant; matrix diagonalization.

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1. Introduction

The problem of quantum anharmonic oscillators is of much interest due to its important applications in molecular physics and quantum field theory (Itzykson and Zuber 1980; Boyd 1978; Chang 1975). The energy level perturbation calculation (Bender and Wu 1969) of the $\mu x^2 + \lambda x^4$ anharmonic oscillator gives rise to a divergent series in terms of the parameter λ. The Borel–Padé methods have been used to get finite results for the energy correction (Graffi and Greechi 1978). The energy eigenvalues of the pure quartic and quartic anharmonic oscillators are obtained in a semi-empirical manner (Hioe and Montroll 1975) using the extended WKB formula. The Hill determinant method (Biswas *et al* 1971) produces the eigenvalues of high accuracy for any arbitrary values of the coupling constant λ. Accurate eigenvalues have been obtained for the potential $V(x) = \pm x^2 + \lambda x^4$ by the scaled Hill determinant technique and an equivalent harmonic oscillator model (Banerjee 1978; Banerjee and Bhattacharya 1984): Richardson and Blankenbecler (1979) have computed accurate energy eigenvalues by making a suitable guess for the $\langle x^N \rangle$ for large N in any particular state and using hypervirial theorem to compute $\langle x^N \rangle$ for lower N's. Accurate energy levels of the generalized quantum anharmonic oscillators are obtained by Taseli and Demiralp (1988) by introducing integration-free Wronskian approach. Tight upper and lower bounds for the energy eigenvalues of one-dimensional anharmonic oscillators are obtained by Fernández *et al* (1989) by a method based on a rational functional approximation for the series expansion of the solution of the Riccati equation for the logarithmic derivative of the wave function. Recently eigenvalues and matrix elements of anharmonic oscillators in N-dimensional space were determined to a high accuracy by applying an elegant method (Bhargava *et al*

1989a, b) for determining the eigenvalues and eigenvectors of real symmetric para-p diagonal matrices. In this method the matrix is broken up into many blocks and algebraic operations including inversions are performed on these blocks.

Although different non-perturbative techniques produce the eigenenergies of the anharmonic oscillators to high accuracy, some kind of perturbation theory is in use for a long time. Hsue and Chern (1984) developed an elegant method to determine the accurate energy eigenvalues for the anharmonic oscillator using coherent state ansatz. Recently Patnaik (1986) developed a perturbation theory for an anharmonic oscillator by suitable modification of the results of Hsue and Chern (1984). The anharmonic oscillators confined in a box have been studied by convergent power series (Chaudhuri and Mukherjee 1984, 1985) and it has been shown that the lower order eigenvalues tend rapidly to the values of the unbounded oscillator as the box is made of larger length.

The linearization technique of random phase approximation (Rowe 1970) has been applied by Ullah (1985) to obtain a modified perturbation series. Feranchuk and Komarov (1982) solved the anharmonic oscillator problem using variational plus perturbation procedure. Here we solve the same problem by simply adding and subtracting a harmonic term to the Hamiltonian and thus modifying the unperturbed Hamiltonian to a slightly different form. By varying the coupling of this harmonic term we obtain a simple accurate expression for the ground state energy of the anharmonic oscillator $\mu x^2 + \lambda x^4$, which is analogous to that obtained by Hsue and Chern (1984) using coherent state ansatz.

Killingbeck (1981) introduced a variational parameter in the exponential convergence factor of the wave function of the anharmonic oscillator and showed by the process of computation that the Hill determinant method of Biswas *et al* (1971) without the variational parameter improved remarkably when the parameter was properly adjusted. Here we have given an analytic expression for the proper choice of this parameter and have obtained eigenvalues quite accurately with a determinant of small size.

Following the method of Hsue and Chern (1984) we construct the matrix element $H_{mn} = \langle m|H|n\rangle$ of the Hamiltonian H and diagonalize the truncated matrix for $m, n, \leqslant N$. By diagonalizing a 5×5 matrix we obtain analytic expressions for the ground state and two excited states of the anharmonic oscillators, which give remarkably good results.

2. Formulation

The Hamiltonian of the anharmonic oscillator

$$H = -(\mathrm{d}^2/\mathrm{d}x^2) + \mu x^2 + \lambda x^4, \quad \lambda > 0 \tag{1}$$

is modified by adding and subtracting the harmonic term βx^2 to it which is then expressed in terms of creation and annihilation operators.

$$H = (a^\dagger a + \tfrac{1}{2})\omega + \frac{\lambda}{\omega^2}(a^\dagger + a)^4 - \frac{\beta}{\omega}(a^\dagger + a)^2 \tag{2}$$

where

$$\omega = 2(\mu + \beta)^{\frac{1}{2}}. \tag{3}$$

By using the commutation $[a, a^\dagger] = 1$ we express H in the following form

$$H = E_0 + a^\dagger a\left(\omega + \frac{12\lambda}{\omega^2} - \frac{2\beta}{\omega}\right) + (a^{\dagger 2} + a^2)\left(\frac{6\lambda}{\omega^2} - \frac{\beta}{\omega}\right)$$
$$+ \frac{\lambda}{\omega^2}(a^{\dagger 4} + 4a^{\dagger 3}a + 6a^{\dagger 2}a^2 + 4a^\dagger a^3 + a^4) \qquad (4)$$

where

$$E_0 = \tfrac{1}{4}\omega + 3\lambda/\omega^2 + \mu/\omega. \qquad (5)$$

The parameter β or ω is fixed by variational principle so that the energy E_0 acquires its minimum value. This yields

$$\omega^3 - 4\mu\omega - 24\lambda = 0 \qquad (6)$$

which can be solved easily by Cardon's method. Equation (5) gives the energy eigenvalues of the ground state with errors less than 2% for the entire range of λ values.

It may be noticed that (6) also guarantees that the coefficients of a^2 and $a^{\dagger 2}$ in $H(4)$ are zero, which also sets the matrix element of H between ψ_0 and ψ_2 to zero. This procedure has been adopted in nuclear physics (Nesbet 1955) for a long time to find the most effective Hamiltonian. The Hamiltonian (2) now takes the form

$$H = H_0 + H' \qquad (7)$$

with

$$H_0 = E_0 + \omega a^\dagger a + \frac{6\lambda}{\omega^2}a^{\dagger 2}a^2 \qquad (8)$$

$$H' = \frac{\lambda}{\omega^2}(a^{\dagger 4} + 4a^{\dagger 3}a + 4a^\dagger a^3 + a^4). \qquad (9)$$

According to Patnaik (1986) perturbation theory is applicable to the Hamiltonian (7) with H_0 as the unperturbed Hamiltonian and H' as the perturbation term.

3. Hill determinant approach

If we expand the wave function ψ in terms of the orthonormal basis vectors $|m\rangle$ as

$$\psi = \sum_{m=0}^{\infty} A_m|m\rangle \qquad (10)$$

and use the equation $H\psi = E\psi$, we get the following recurrence relations satisfied by A_m

$$P_m A_{m-4} + Q_m A_{m-2} + R_m A_m + S_m A_{m+2} + T_m A_{m+4} = 0 \qquad (11)$$

where

$$P_m = \frac{\lambda}{\omega^2}[m(m-1)(m-2)(m-3)]^{\frac{1}{2}} \qquad (12a)$$

$$Q_m = \frac{4\lambda}{\omega^2}(m-2)[m(m-1)]^{\frac{1}{2}} \qquad (12b)$$

$$R_m = \frac{\omega}{4} + \frac{3\lambda}{\omega^2} + \frac{\mu}{\omega} + m\omega + \frac{6\lambda}{\omega^2} m(m-1) - E \tag{12c}$$

$$S_m = \frac{4\lambda}{\omega^2} m[(m+2)(m+1)]^{\frac{1}{2}} \tag{12d}$$

$$T_m = \frac{\lambda}{\omega^2} [(m+1)(m+2)(m+3)(m+4)]^{\frac{1}{2}}. \tag{12e}$$

The eigenvalue condition of Hill determinant for large n is

$$\text{Det } D_n = 0 \tag{13}$$

with

$$D_n = \begin{pmatrix} R_\nu & S_\nu & T_\nu & 0 & 0 & \cdots \\ Q_{2+\nu} & R_{2+\nu} & S_{2+\nu} & T_{2+\nu} & 0 & \cdots \\ P_{4+\nu} & Q_{4+\nu} & R_{4+\nu} & S_{4+\nu} & T_{4+\nu} & \cdots \\ 0 & P_{6+\nu} & Q_{6+\nu} & R_{6+\nu} & S_{6+\nu} & \cdots \\ 0 & 0 & P_{8+\nu} & Q_{8+\nu} & R_{8+\nu} & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \\ \cdot & \cdot & \cdot & \cdot & \cdot & \end{pmatrix} \tag{14}$$

where $\nu = 0$ for even-parity eigenvalues and $\nu = 1$ for those of odd-parity. The zeros of Det D_n as a function of the parameter E give the energy eigenvalues of the problem.

4. Matrix diagonalization and approximate eigenvalues

Considering the total Hamiltonian H we construct a 5×5 matrix H_{mn} whose elements are $H_{mn} = \langle m|H|n\rangle$ and compute the eigenvalues from the vanishing of the secular determinant

$$\text{Det}(H_{mn} - EI) = 0. \tag{15}$$

The non-vanishing matrix elements of H are

$$\langle n|H|n\rangle = \varepsilon_n = E_0 + n\omega + \frac{6\lambda}{\omega^2} n(n-1) \tag{16}$$

$$\langle n-2|H|n\rangle = \langle n|H|n-2\rangle = \frac{4\lambda}{\omega^2}(n-2)[n(n-1)]^{\frac{1}{2}} \tag{17}$$

$$\langle n-4|H|n\rangle = \langle n|H|n-4\rangle = \frac{\lambda}{\omega^2}[n(n-1)(n-2)(n-3)]^{\frac{1}{2}}. \tag{18}$$

We assume that $E_n - \varepsilon_n = \delta_n$ is a small correction term so that we may neglect the δ_n^2 and higher order terms. We obtain the following simple expression for the correction terms of the ground state and the first two excited states

$$\delta_0 = -\frac{6\lambda^2(\omega^9 + 18\lambda\omega^6 + 40\lambda^2\omega^3 - 192\lambda^3)}{\omega^2(\omega^{12} + 36\lambda\omega^9 + 257\lambda^2\omega^6 - 780\lambda^3\omega^3 - 720\lambda^4)} \tag{19}$$

$$\delta_1 = -\frac{48\lambda^2(\omega^9 + 36\lambda\omega^6 + 40\lambda^2\omega^3 + 96\lambda^3)}{\omega^2(\omega^{12} + 54\lambda\omega^9 + 672\lambda^2\omega^6 + 1200\lambda^3\omega^3 + 2880\lambda^4)} \tag{20}$$

$$\delta_2 = -\frac{384\lambda^2(\omega^9 + 42\lambda\omega^6 + 600\lambda^2\omega^3 + 2304\lambda^3)}{\omega^2(\omega^{12} + 72\lambda\omega^9 + 2058\lambda^2\omega^6 + 32040\lambda^3\omega^3 + 171072\lambda^4)} \tag{21}$$

5. Results and discussion

In table 1 we present the first four eigenvalues of the $\mu x^2 + \lambda x^4$ anharmonic oscillator as obtained by the modified Hill determinant method for $\mu = 1$, $\lambda = 100$ and $\mu = 0$, $\lambda = 1$ and compare our results with the exact values. We have shown in parentheses the roots of the Hill determinant without the variational parameter ($\beta = 0$ or $\omega = 2$). We also consider the double-well oscillators of type $-x^2 + \lambda x^4$ and compare our eigenvalues in table 2 with the exact values. We find that our calculation converges quickly to give stable roots for small size of the determinant. Biswas *et al* (1971) obtained the ground state of the $x^2 + \lambda x^4$ oscillator for $\lambda = 1$ with 100×100 determinant and for $\lambda = 10$ with 240×240 determinant without the variational scale parameter. We achieve the same order of accuracy with a determinant of order 15.

Table 1. Comparison of the first four eigenvalues of the potential $\mu x^2 + \lambda x^4$ obtained by the method of modified Hill determinant with the exact values (Banerjee 1978, for $\mu = 1$; Fernandez *et al* 1989 for $\mu = 0$). The roots of the Hill determinant for $\beta = 0$ are given in the parentheses for $\mu = 1$ and $\lambda = 100$.

		Modified Hill determinant method with determinant of size			
μ	λ	5×5	9×9	15×15	Exact
1	100	4·999 800	4·999 419	4·999 418	4·999 418
		(8·084 645)	(5·284 808)	(5·020 073)	
		17·830 643	17·830 194	17·830 193	17·830 192
		(44·731 982)	(22·964 396)	(18·164 436)	
		34·920 733	34·874 124	34·873 985	34·873 984
		(190·147 547)	(72·236 102)	(40·687 879)	
		54·509 913	54·385 763	54·385 292	54·385 292
		(440·514 468)	(165·533 068)	(79·872 450)	
0	1	1·060 450	1·060 362	1·060 362	1·060 362
		3·799 775	3·799 673	3·799 673	3·799 673
		7·466 340	7·455 731	7·455 698	7·455 698
		11·672 588	11·644 854	11·644 746	11·644 746

Table 2. Comparison of the first four eigenenergies of the double-well oscillator $-x^2 + 0{\cdot}1x^4$ obtained by the method of modified Hill determinant with the exact values (Banerjee and Bhatnagar 1978).

Modified Hill determinant method with determinant of size			
11 × 11	35 × 35	40 × 40	Exact
−1·264252	−1·265492	−1·265492	−1·265493
−1·149333	−1·153058	−1·153058	−1·153059
0·517939	0·509489	0·509489	0·509489
1·559178	1·543547	1·543547	1·543546

This simple procedure is a significant improvement over the original method of Biswas *et al* (1971). Moreover, the original Hill determinant method of Biswas *et al* (1971) is not applicable for non-positive values of μ. Our method yields excellent results for pure quartic oscillator ($\mu = 0$) and double-well oscillator ($\mu < 0$).

In §4 we have obtained approximate eigenvalues $\varepsilon_n + \delta_n$ for the first three eigenvalues of the anharmonic oscillator $\mu x^2 + \lambda x^4$ by diagonalizing a matrix of order five. This gives errors of 0·24% for the ground state, 0·77% for the first excited state and 1·40% for the second excited state for $\mu = 1$ and $\lambda = 1000$. The errors decrease for lower values of λ. When $\lambda \to \infty$, $\omega = (24\lambda)^{1/3}$, the ground state energy $\varepsilon_0 + \delta_0 = 1{\cdot}063\lambda^{1/3}$ which is in good agreement with the exact value of $1{\cdot}060\lambda^{1/3}$ obtained by Hioe and Montroll (1975) in a complicated manner using Bergman representation. Diagonalization of the 5 × 5 matrix yields only five diagonal elements of which lower order eigenvalues are accurate. For higher order eigenvalues one has to find the zeros of the Hill determinant (eq. 13) numerically. Equations (16), (19)–(21) give the analytic expressions for the first three eigenvalues for all values of the coupling constant. We compute the first ten eigenvalues of the $x^2 + \lambda x^4$ oscillator by the modified Hill determinant method and represent them graphically in figure 1. It appears from the graph that the eigenvalues form a family of almost parallel lines on log scales.

The method discussed here is very general and can be applied to any general anharmonic oscillator problem. Recently we have shown that this method removes the difficulties encountered by others with the sextic oscillator (Chaudhuri and Mondal 1989). We mention here that the expectation values $\langle x^{2m} \rangle$ can be calculated approximately by this method for the general anharmonic oscillator problem. If a potential term αx^{2m} is added to the Hamiltonian the energy change according to the first order perturbation theory is

$$\Delta E = \alpha \langle x^{2m} \rangle,$$

where α is sufficiently small so that the first order perturbation result is quite accurate. We can calculate E and ΔE and hence $\langle x^{2m} \rangle$ by the application of modified Hill determinant method. The application of modified Hill determinant method to the general anharmonic oscillator and computation of $\langle x^{2m} \rangle$ in any particular state will be discussed elsewhere.

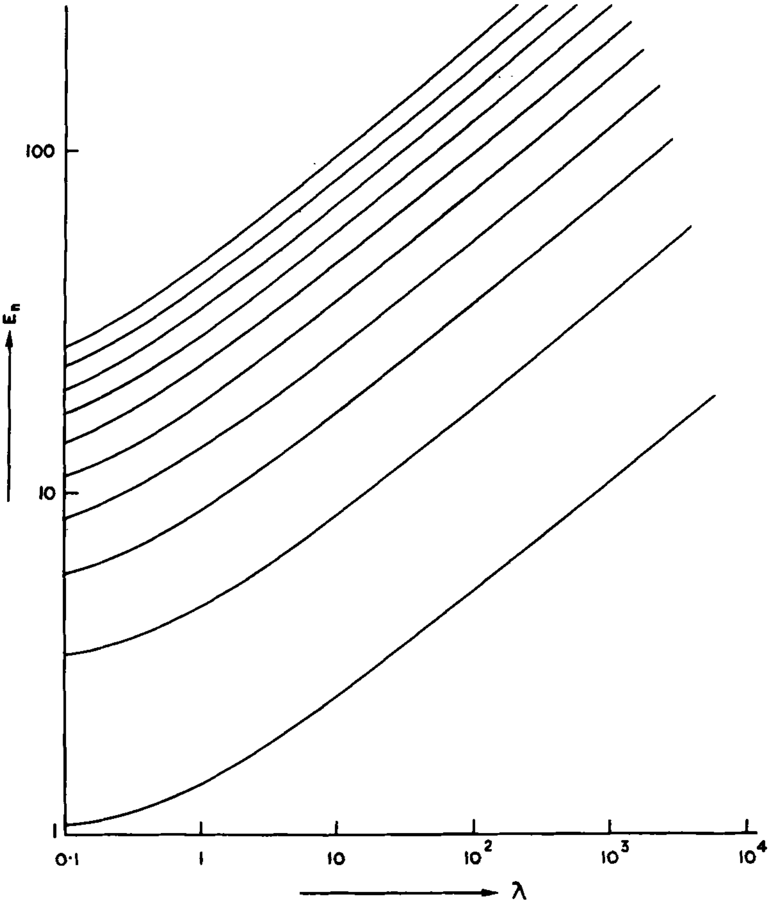

Figure 1. The first ten eigenenergies E_n of the oscillator $x^2 + \lambda x^4$ are plotted against the anharmonic coupling λ.

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