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Eigenvalues of the $\mu x^2 + \lambda x^{2m}$ interaction

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Abstract. The even and odd parity eigenvalues for the bounded potential $\mu x^2 + \lambda x^{2m}$ with both positive and negative values of μ and $m = 2, 3, 4, 5, 6$ are obtained by the method of series solution for any positive value of the coupling constant λ. When μ is negative the lower order eigenvalues are closely bunched in pairs in the low-λ regime ($\lambda \ll 1$). The results agree well with existing results.

Keywords. Bounded potential; series solution; double-well oscillator; bunched spectrum.

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1. Introduction

The problem of quantum anharmonic oscillator is of much interest from the analytical and numerical points of view due to its important applications in molecular physics (Bell 1945; Chan *et al* 1960; Chan and Stelman 1963; Moore and Pimental 1964; Reid 1970). The eigenvalues of the anharmonic oscillator of type $\mu x^2 + \lambda x^{2m}$ have been calculated by many authors using perturbation theory (Bender and Wu 1969), variational techniques (Bazley and Fox 1961; Bozzole *et al* 1982), logarithmic perturbation expansion (Aharonov and Au 1979; Au *et al* 1983; Dolgov *et al* 1980), WKB techniques (Bender *et al* 1977; Kesarwani and Varshni 1980; Seetharaman *et al* 1982), approximate canonical transformation (Halpern 1973), convergent perturbation theory (Turbiner 1981), the Hill determinant method (Biswas *et al* 1971, 1973), the scaled characteristic infinite determinant method (Banerjee *et al* 1978; Banerjee 1978) and the series approach with a convergent x-factor in the wave-function (Killingbeck 1981; Ginsburg 1982).

Bender and Wu (1969) have extensively investigated the problem using the perturbation series in terms of the parameter λ and have shown that the series is divergent for all λ though each term of the series is finite. The Borel-Padé methods (Simon 1970; Graffi and Greechi 1978, Loeffel *et al* 1970) have been used to recover finite results for the energy correction. A variational method has been formulated (Chan *et al* 1964) for calculating the energy levels of the quartic anharmonic oscillator quite accurately by using the pure quartic oscillator representation. It is also shown that the quartic oscillator representation yields significantly better energies than the conventional harmonic oscillator representation even for moderate quartic anharmonicities. The logarithmic perturbation expansion which is used to study the λx^4 anharmonic oscillator yields excellent results for the ground state of the oscillator. The method is, however, not very accurate for the excited state energy eigenvalues due

to introduction of cut-offs in the numerical integrations. The energy eigenvalues of the pure quartic and quartic anharmonic oscillators are also obtained in a semi-empirical manner (Hioe and Montroll 1975; Hioe *et al* 1978, Mathews *et al* 1981) using the extended WKB formula. Using the same formalism the eigenvalue problem of the general $\mu x^2 + \lambda x^{2m}$ anharmonic oscillator has been discussed by Hioe *et al* (1976). The Hill determinant method (Biswas *et al* 1971, 1973) produces eigenvalues to a high degree of accuracy for $m \leqslant 4$ and $\lambda \leqslant 100$. The Hill determinant method becomes unreliable for higher values of m and λ due to large truncation error in the numerical computation of the problem (Biswas *et al* 1973). Very accurate eigenvalues have been obtained by the scaled characteristic infinite determinant method (Banerjee 1978) in all regimes of the quantum number n and the anharmonicity constant λ. Recently Banerjee and Bhattacharjee (1984) have developed a scaled Hill determinant technique and an equivalent harmonic oscillator model for the eigenvalues of the potential $V(x) = \pm x^2 + \lambda x^4$ for all values of the coupling parameter λ. They have also given analytic expressions for the eigenvalues of the problem. Most of the previous calculations of the eigenvalues of λx^{2m} anharmonic oscillators are suitable for $m \leqslant 4$. This paper is concerned with the determination of the energy levels of λx^{2m} anharmonic oscillators for any arbitrary positive integer values of m.

Auluck and Kothari (1945) considered the problem of a bounded linear harmonic oscillator and showed that the effect of enclosing the oscillator in a box is to displace the energy levels of the oscillator towards higher energies. The energy eigenvalues of the unbounded oscillator may be obtained by this method by gradually increasing the dimension of confinement of the oscillator. It seems that this simple and accurate method for the evaluation of the energy eigenvalues of the Schrödinger equation associated with a confining potential has not been used extensively. Recently the pure oscillators confined in a box have been studied (Barakat and Rosner 1981; Chaudhuri and Mukherjee 1983) by the method of convergent power series, 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. This finite box method is applied here to the interaction $V(x) = \mu x^2 + \lambda x^{2m}$ with both positive and negative values of μ and positive λ. In § 2 we describe this method for the unbunched spectrum of the anharmonic oscillator. In § 3 we discuss the problem of double-well oscillators $\mu x^2 + \lambda x^{2m}$ when μ is negative. Double-minimum potential with $m = 2$ has been employed by Snyder and Ibers (1962), Somorjai and Hornig (1962) in their discussions of the O . . . H . . . O hydrogen bond in hydrogen-bonded solids. The characteristic feature of the eigenvalue spectrum of the double-well oscillator is that the lower eigenvalues are closely bunched in pairs if the two wells are sufficiently separated (Gildener and Patrascioiu 1977; Polyakov 1977; Banerjee and Bhatnagar 1978). Our method of finite box approximation is applicable for all double-minimum potentials of type $\mu x^2 + \lambda x^{2m}$, with $\mu < 0$, $\lambda > 0$ and $m = 2, 3, 4, \ldots$. In the regime of low λ it is found that the separation between the pairs of energy levels increases with increasing m for a fixed value of λ.

2. Power-series solutions for energy eigenvalues

We have to solve the eigenvalue equation

$$H(\mu, \lambda)\psi(x) = E\psi(x), \tag{1}$$

where the Hamiltonian $H(\mu, \lambda)$ is given by

$$H(\mu, \lambda) = -\mathrm{d}^2/\mathrm{d}x^2 + \mu x^2 + \lambda x^{2m}, \quad m = 1,2,3,\ldots. \tag{2}$$

It should be noted that the Hamiltonian has the following scale transformation property

$$H(\mu,\lambda) = \lambda^{1/(m+1)} H(\mu\lambda^{-2/(m+1)}, 1), \tag{3}$$

so that

$$H(\mu, \lambda) \xrightarrow[\lambda \to \infty]{} \lambda^{1/(m+1)} H(0, 1)\ldots, \tag{4}$$

where $H(0, 1)$ is the Hamiltonian for the pure x^{2m} oscillator. Due to the scale transformation property (4) it is easy to find the eigenvalues of $H(\mu, \lambda)$ for large λ if the eigenvalues of $H(0, 1)$ are known.

Equation (1) with the Hamiltonian (2) can be written as

$$[-\mathrm{d}^2/\mathrm{d}y^2 + \mu' y^2 + y^{2m}]\psi(y) = E'\psi(y), \tag{5}$$

where

$$y = x\lambda^{1/(2m+2)}, \tag{6a}$$

$$\mu' = \mu\lambda^{-2/(m+1)}, \tag{6b}$$

$$E' = E\lambda^{-1/(m+1)}. \tag{6c}$$

The main problem of solving (5) by the method of series solution about $y = 0$ is that the point at infinity is an irregular singular point of the differential equation so that the boundary condition $\psi(y) \to 0$ as $|y| \to \infty$ cannot be imposed on it. We put infinitely high potentials at $y = \pm L$ so that the boundary conditions become $\psi(\pm L) = 0$ which do not pose any problem for the series solution of (5). We make the change of variable $u = y/L$ so that the boundary conditions become $\psi(u = \pm 1) = 0$ and (5) is transformed to

$$[\mathrm{d}^2/\mathrm{d}u^2 + \varepsilon - au^2 - bu^{2m}]\psi(u) = 0, \tag{7}$$

where $\varepsilon = E'L^2$, $a = \mu' L^4$ and $b = L^{2m+2}$. It is clear from (7) that $u = 0$ is an ordinary point of (7). Therefore (7) admits a convergent series solution valid in the region $|u| < \infty$

$$\psi(u) = \sum_{n=0}^{\infty} A_n u^{2n+v}, \tag{8}$$

where $v = 0$ for the even parity solution and $v = 1$ for that of odd parity. Substituting (8) into (7) we obtain the following recurrence relation

$$\begin{aligned}&(2n+v+2)(2n+v+1)A_{n+1} + \varepsilon A_n \\ &- aA_{n-1} - bA_{n-m} = 0, \quad n \geqslant 0,\end{aligned} \tag{9}$$

with $A_{-1} = A_{-2} = \ldots = A_{-m} = 0$.

We find from (9) that

$$|A_{n+1}/A_n| \to 0(n^{-2/(m+1)}) \text{ as } n \to \infty$$

which shows that the series ΣA_n is convergent for all m.

The zeros of the function

$$\psi(u = 1) = \sum_{n=0}^{\infty} A_n \tag{10}$$

in terms of the parameter E' gives the eigenvalues of the bounded potential $\mu' y^2 + y^{2m}$. We calculate the first four eigenvalues E' for $L = 2, 3, m = 2, 3, 4, 5, 6, \mu = -1, 0, 1$ and $\lambda = 0.1, 1, 10, 100$ and 1000. Using (6c) we evaluate the corresponding eigenvalues E of the bounded potential $\mu x^2 + \lambda x^{2m}$. These values are presented in tables 1–4 and the results for $L = 3$ are also compared with the eigenvalues of the unbounded oscillators for $m = 2, 3, 4$. The agreement is excellent. It is clear from table 4 that when $m \geqslant 5$ the eigenvalues remain almost unchanged (up to five decimal places) for $L = 2$ and 3 where the potentials are made infinitely high. This is because for $m \geqslant 5$ the potential function $\mu' y^2 + y^{2m}$ becomes effectively infinite at $y = 2$ in comparison with its values around

Table 1. The first four eigenvalues of the bounded potential $\mu x^2 + \lambda x^4$ with $L = 2, 3$ and those of the unbounded ($L \to \infty$) oscillator (Chan and Stelman 1963, for $\mu = 0$ and Banerjee 1978, for $\mu = 1$)

μ	λ	$L = 2$	$L = 3$	Unbounded oscillator $L \to \infty$
−1	1	0·68685	0·65765	
		2·98474	2·83454	
		6·66473	6·16392	
		11·32304	10·03873	
0	1	1·07262	1·06036	1·060362
		3·88241	3·79967	3·799657
		7·78371	7·45570	7·455702
		12·58357	11·64477	11·64475
1	0·1	1·06549	1·06529	1·065286
		3·30979	3·30687	3·306872
		5·76847	5·74789	5·747959
		8·43847	8·35268	8·352678
1	1	1·39783	1·39235	1·392352
		4·69501	4·64881	4·648813
		8·86798	8·65505	8·655050
		13·83598	13·15681	13·156804
1	10	2·47127	2·44917	2·449174
		8·75619	8·59900	8·599003
		17·28009	16·63593	16·635921
		27·69409	25·80632	25·806276
1	100	5·05415	4·99942	4·999418
		18·20428	17·83019	17·830192
		36·36630	34·87400	34·873984
		58·67881	54·38541	54·385291
1	1000	10·76135	10·63977	10·639789
		38·91029	38·08661	38·086833
		77·94745	74·68124	74·681404
		125·96151	116·60345	116·603199

Table 2. The first four eigenvalues of the bounded potential $\mu x^2 + \lambda x^6$ with $L = 2, 3$ and those of the unbounded ($L \to \infty$) oscillator (Turbiner 1981, for $\mu = 0$ and Banerjee 1978, for $\mu = 1$)

μ	λ	$L = 2$	$L = 3$	Unbounded Oscillator $L \to \infty$
−1	1	0·81788	0·81663	
		3·60137	3·59496	
		8.18270	8·15927	
		13·93643	13·86437	
0	1	1·14531	1·14480	1·144802
		4·34279	4·33860	4·338599
		9·09011	9·07308	
		14·99095	14·93517	
1	0·1	1·10915	1·10909	1·109087
		3·59665	3·59604	3·596037
		6·64776	6·64439	6·644392
		10·25142	10·23787	10·237874
1	1	1·43599	1·43562	1·435625
		5·03613	5·03340	5·033396
		9·97884	9·96662	9·966622
		16·03240	15·98944	15·989441
1	10	2·20671	2·20572	2·205723
		8·12135	8·11484	8·114843
		16·66847	16·64121	16·641218
		27·24647	27·15508	27·155086
1	100	3·71897	3·71697	3·716975
		13·95889	13·94621	13·946207
		29·02940	28·97729	28·977294
		47·73692	47·56498	47·564985
1	1000	6·49604	6·49235	6·492350
		24·54855	24·52531	24·525316
		51·27722	51·18248	51·182480
		84·48669	84·17559	84·175584

$y = 0$. The eigenvalues of the interaction $\mu' y^2 + y^{2m}$ with $m \geqslant 7$ can also be obtained by this method by confining the oscillator in the region $|y| \leqslant 2$. For large m the region of confinement of the potential can be reduced further.

3. Two-well oscillator

We apply the method described in §2 for the two-well potential $-x^2 + \lambda x^{2m}$ in the small-λ regime. In table 5 we tabulate the first four eigenvalues of the bounded potential $-x^2 + \lambda x^{2m}$ for $L = 3, 4$, $m = 2, 3, 4$ and $\lambda = 0.1, 0.01$. Our values for $m = 2$ are also compared with the exact eigenvalues obtained by Banerjee and Bhatnagar (1978) for the unbounded ($L \to \infty$) oscillator. The agreement is quite good. It is found that in the present scheme the eigenvalues of the oscillator $-x^2 + \lambda x^8$ is reliable only up to the

Table 3. The first four eigenvalues of the bounded potential $\mu x^2 + \lambda x^8$ with $L = 2$, 3 and those of the unbounded ($L \to \infty$) oscillator (Turbiner 1981, for $\mu = 0$ and Banerjee 1978, for $\mu = 1$).

μ	λ	$L = 2$	$L = 3$	Unbounded oscillator $L \to \infty$
−1	1	0·93529	0·93528	
		4·11350	4·11347	
		9·49022	9·49009	
		16·49203	16·49163	
0	1	1·22582	1·22582	1·225820
		4·75590	4·75587	4·755875
		10·24502	10·24495	
		17·34341	17·34309	
1	0·1	1·16897	1·16897	1·168970
		3·93973	3·93972	3·939721
		7·63998	7·63995	7·639948
		12·28129	12·28117	12·281168
1	1	1·49102	1·49102	1·491020
		5·36880	5·36878	5·368779
		10·99382	10·99374	10·993737
		18·19137	18·19110	18·191100
1	10	2·11455	2·11454	2·114545
		7·92972	7·92968	7·929683
		16·71117	16·71102	16·711022
		28·02322	28·02275	28·022750
1	100	3·18867	3·18866	3·188654
		12·19509	12·19502	12·195022
		26·03370	26·03346	26·033458
		43·90290	43·90211	43·902113
1	1000	4·94951	4·94949	4·949487
		19·09092	19·09081	19·090814
		40·97504	40·97480	40·974800
		69·25881	69·25754	69·257538

third decimal place for $L = 4$ due to large truncation error in the numerical computation of the problem.

4. Discussion

The present scheme of finite box approximation is very simple and accurate. The advantage of the method is that the eigenvalues are obtained from a single equation for both positive and negative values of μ so long as λ is positive. For the double-well oscillator the lower order eigenvalues are closely bunched in pairs in the low-λ regime ($\lambda \ll 1$). The splittings between these pairs of energy levels is dependent on the separation distance between the two minima of the walls, which is given by

$$2(1/m\lambda)^{1/2m-2}.$$

Table 4. The first four eigenvalues of the bounded potential $\mu x^2 + \lambda x^{2m}$ with $m = 5$, 6 and $L = 2$, 3.

		$m = 5$		$m = 6$	
μ	λ	$L = 2$	$L = 3$	$L = 2$	$L = 3$
−1	1	1·03206	1·03206	1·11370	1·11370
		4·51533	4·51533	4·84470	4·84470
		10·48698	10·48698	11·28131	11·28131
		18·45464	18·45464	19·99988	19·99988
0	1	1·29884	1·29884	1·36376	1·36376
		5·09788	5·09788	5·38694	5·38694
		11·15382	11·15382	11·89301	11·89301
		19·18881	19·18881	20·66163	20·66163
1	0·1	1·23389	1·23389	1·29783	1·29783
		4·28034	4·28034	4·59708	4·59708
		8·57323	8·57323	9·40825	9·40825
		14·15050	14·15050	15·79185	15·79185
1	1	1·54626	1·54626	1·59799	1·59799
		5·65934	5·65934	5·91265	5·91265
		11·81997	11·81997	12·50471	12·50471
		19·92310	19·92310	21·32474	21·32474
1	10	2·07830	2·07830	2·06610	2·06610
		7·86893	7·86893	7·86629	7·86629
		16·82630	16·82630	16·96565	16·96565
		28·66562	28·66562	29·18628	29·18628
1	100	2·91644	2·91644	2·75718	2·75718
		11·24741	11·24741	10·67593	10·67593
		24·34068	24·34068	23·27876	23·27876
		41·68189	41·68189	40·23461	40·23461
1	1000	4·18816	4·18816	3·74829	3·74829
		16·30139	16·30139	14·65010	14·65010
		35·48390	35·48390	32·13344	32·13344
		60·91256	60·91256	55·67588	55·67588

The lower eigenvalues are closely bunched in pairs if the two wells are sufficiently separated.

The zeros of the function ΣA_n (equation (10)) in terms of the energy parameter give us the energy levels of the oscillator. The lowest root will correspond to the ground state energy level and the excited levels will be given by the sequence of higher roots. Therefore the present method is not suitable when the quantum number n becomes large. In the regime of large n one has to apply some other technique such as WKB approximation which is good when n is large.

The present technique can be applied to three-dimensional anharmonic oscillators of type $\mu r^2 + \lambda r^{2m}$. We put an infinite potential barrier at $r = L$ so that the radial wavefunction vanishes at the spherical boundary. Since the power series is convergent in the region $r \leqslant L$ there is no problem in imposing the boundary condition $R(L) = 0$. It may be mentioned that this method of confining the potential in a spherical box yields

Table 5. The first four eigenvalues of the bounded two-well potential $-x^2+\lambda x^{2m}$ for $L=3, 4$, $m=2, 3, 4$ and $\lambda=0{\cdot}1$ and $0{\cdot}01$ and those of the unbounded ($L\to\infty$) oscillator (Banerjee and Bhatnagar 1978, for $m=2$).

m	λ	$L=3$	$L=4$	Unbounded oscillator $L\to\infty$
	0·1	−1·26520	−1·26549	−1·265493
		−1·15268	−1·15310	−1·153059
		0·51046	0·50949	0·509489
		1·54665	1·54355	1·543546
2	0·01	−18·92230	−23·53593	−23·595951
		−18·92168	−23·53558	−23·595951
		−13·85340	−20·57250	−20·829806
		−13·85326	−20·56742	−20·829806
	0·1	−0·04424	−0·04424	
		1·00631	1·00630	
		3·45704	3·45704	
		6·46792	6·46791	
3	0·01	−2·05525	−2·05526	
		−2·01123	−2·01124	
		0·22121	0·22118	
		1·17735	1·17724	
	0·1	0·27540	0·275	
		1·94425	1·944	
		5·26573	5·266	
		9·59068	9·591	
4	0·01	−0·50993	−0·510	
		0·04861	0·049	
		2·21815	2·218	
		4·75948	4·759	

excellent results for the low lying states of the linear plus Coulomb potential (Chaudhuri 1984).

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