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On the $\mu x^2 + \lambda x^4 + \eta x^6$ interaction

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Abstract. A class of exact even and odd parity solutions of the Schrödinger equation for the interaction $\mu x^2 + \lambda x^4 + \eta x^6$, $\eta > 0$ is obtained in the form (polynomial) ×(exponential) when μ , λ and η satisfy some specific relations. In the general case the eigenvalues of the bounded potential problem are found by the method of series solution for any value of η . We have also shown that the analytic continued fraction method does not always lead to the correct results.

1. Introduction

The problem of the quantum anharmonic oscillator has been the subject of much discussion (Banerjee et al 1978, Bender and Wu 1969, Loeffel et al 1970, Fung et al 1978, Drummond 1981, Biswas et al 1971, 1973, Halpern 1973, Bozzolo et al 1982, Killingbeck 1978, Austin and Killingbeck 1982, Hioe and Montrol 1975, Hioe et al 1978), both from the analytical and the numerical point of view, because of its importance in quantum field theory (Boyd 1978) and molecular physics (Chan and Stellman 1963, Reid 1970). The energy levels perturbation calculation (Bender and Wu 1969) of the λx^4 anharmonic oscillator gives rise to a divergent series in terms of the parameter λ . The Borel-Padé methods (Simon 1970, Graffi et al 1970, Graffi and Greechi 1978, Loeffel et al 1970) have been used to obtain finite results for the energy correction. The eigenvalues of the anharmonic oscillators of type ηx^{2m} have been calculated by Biswas et al (1971, 1973) using the Hill determinant method. Some other approximation procedures to the anharmonic oscillator problem are WKB techniques (Lu et al 1973, Seetharaman et al 1982, Bender et al 1977), approximate canonical transformation (Halpern 1973), convergent perturbation theory (Turbiner 1981), variational techniques (Bozzolo et al 1982, Bazley and Fox 1961) and logarithmic perturbation expansion (Dolgov et al 1980, Aharonov and Au 1979, Au 1980, Au et al 1983).

The doubly anharmonic oscillator of the type

$$V(x) = \mu x^2 + \lambda x^4 + \eta x^6, \qquad \eta > 0 \tag{1}$$

is of great interest in scalar field theory (Aragao de Carvalho 1977, Sobelman 1979). Sobelman uses double series perturbation expansions for both the eigenfunction and the eigenvalue in terms of the two coupling constants λ and η . These series converge for $\lambda > 0$, $\eta > 0$ and for $\lambda < 0$, $\mu > \lambda/4\eta$. Flessas (1979) and Flessas and Das (1980) have presented exact solutions, valid for positive and negative λ , of the Schrödinger equation for the doubly anharmonic oscillator. Recently Flessas (1981) has obtained

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solutions with an essentially different form from (polynomial) × (exponential). These are valid if two relations between μ , λ and η hold whence $\lambda < 0$ follows. Khare (1981) has shown that Rayleigh-Schrödinger perturbation theory may not be applicable for the potential when $\lambda < 0$.

The problem of the doubly anharmonic oscillator (1) has been studied extensively by Singh *et al* (1978) using the theory of continued fractions (Wall 1948). They have shown that the energy eigenvalues of the oscillator occur as poles in the energy plane of an infinite continued fraction, which is defined as the Green function for the problem. In this paper we have shown that the analytic continued fraction method, or equivalently the Hill determinant method, may lead to incorrect results for some values of the coupling constants. We have systematically studied the exact even and odd parity solutions in the form of products of exponential and polynomial functions of x. For the existence of these types of solutions it is necessary that μ , λ and η are related. We describe this method in § 2 and point out the drawbacks of the Hill determinant method.

Recently the anharmonic oscillators of type ηx^{2m} , bounded by infinite potentials at $x = \pm L$, have been studied (Chaudhuri and Mukherjee 1983, 1984, Barakat and Rosner 1981) by the series solution method and it has been shown that the lower-order eigenvalues tend rapidly to the values of the unbounded oscillator as L is made larger. In § 3 we describe the finite box approximation for the potential V(x) given by (1), with positive η and positive or negative μ and λ . In § 4 we discuss the scale transformation property of the Hamiltonian which can be used to find the eigenvalues for arbitrarily large positive values of η .

2. Exact solution to the Schrödinger equation

The Schrödinger equation

$$(-d^{2}/dx^{2} + V(x))\psi(x) = E\psi(x)$$
(2)

with the potential V(x) given by (1) is transformed to the following form

$$\frac{d^2\phi}{dx^2} + 2(-\alpha x^3 + \beta x)\frac{d\phi}{dx} + [(\beta^2 - 3\alpha - \mu)x^2 + (E + \beta)]\phi = 0$$
(3)

by making the substitution

$$\psi(x) = \exp(-\frac{1}{4}\alpha x^4 + \frac{1}{2}\beta x^2)\phi(x)$$
(4)

where

$$\alpha = \sqrt{\eta} > 0, \qquad \beta = -\frac{1}{2}\lambda/\sqrt{\eta}.$$

It is clear from (3) that x = 0 is an ordinary point and $x = \infty$ is an irregular singular point of this differential equation. Therefore equation (3) admits a convergent series solution

$$\phi(x) = \sum_{n=0}^{\infty} A_n x^{2n+\nu}$$
(5)

valid in the region $|x| < \infty$. In (5) we set $\nu = 0$ for the even parity solutions and $\nu = 1$

for the odd parity solutions. The coefficients A_n satisfy the difference equation

$$(2n+2+\nu)(2n+1+\nu)A_{n+1} + [E+\beta(4n+1+2\nu)]A_n + [\beta^2 - \mu - (4n-1+2\nu)\alpha]A_{n-1} = 0, \qquad n \ge 0$$
(6)

with $A_{-1} = 0$. By repeated application of this equation we can express all the coefficients in terms of A_0

$$A_n = (-1)^n D_n A_0 / (2n + \nu)! \tag{7}$$

where D_n is an $n \times n$ determiant:

$$D_{n} = \begin{vmatrix} b_{11} & b_{12} & 0 & \dots \\ b_{21} & b_{22} & b_{23} & \dots \\ \vdots & \vdots & \ddots & \\ & & & & b_{nn} \end{vmatrix}.$$
(8)

The non-zero tridiagonal matrix elements b_{ij} of equation (8) are given by

$$b_{i\,i} = E + (4i - 3 + 2\nu)\beta \tag{9a}$$

$$b_{i,i+1} = (2i+\nu)(2i-1+\nu) \tag{9b}$$

$$b_{i_{i-1}} = \beta^2 - \mu - (4i - 5 + 2\nu)\alpha \tag{9c}$$

with $i = 1, 2, 3, ..., D_n$ as $n \to \infty$ is the Hill determinant. The necessary and sufficient condition for solving (6) is that non-trivial A_n exist, and for this the infinite Hill determinant must vanish. The D_n satisfy the following difference equation

$$D_{n} = [E + (4n - 3 + 2\nu)\beta]D_{n-1}$$
$$- [\beta^{2} - \mu - (4n - 5 + 2\nu)\alpha](2n - 2 + \nu)(2n - 3 + \nu)D_{n-2}.$$
(10)

According to Singh *et al* (1978) the zeros of D_n in the energy parameter E determine the energy eigenvalues of the problem when $n \to \infty$. Firstly one notes that the ratio $|D_n/D_{n-1}| \to O(n^{3/2})$ for large n and therefore D_n forms a divergent sequence. It is impossible to numerically evaluate D_n for very large n using the Hill determinant method, this being one of its serious drawbacks. If we put $\mu > 0$ and $\beta = 0$ or $\lambda = 0$ in (10) we find that

$$D_1 = E,$$
 $D_2 = E^2 + [\mu + (3+2\nu)\alpha](2+\nu)(1+\nu)$

and all higher-order determinants are positive for positive values of E. Thus D_n will never vanish for any positive value of E. But the potential $\mu x^2 + \eta x^6$ with both μ and $\eta > 0$ goes to $+\infty$ as $|x| \to \infty$ and therefore the eigen-energy should go to $+\infty$. It is well known that all the eigenvalues are positive for this problem. Thus the Hill determinant method of Singh *et al* (1978) has only a limited domain of applicability in the plane of couplings.

It has been pointed out (Flessas 1982, Chaudhuri 1983, Masson 1983) that all the eigenvalues determined by the Hill determinant method should not be allowed since the boundary condition $\psi(x) \rightarrow 0$ as $|x| \rightarrow \infty$ is not incorporated into the method. Since $x = \infty$ is an irregular singular point of the differential equation the series (5) may not be valid at $x = \pm \infty$ and therefore the boundary conditions at $x = \pm \infty$ may not be satisfied by the wavefunction. The boundary conditions are satisfied when the series

(5) terminates. From (6) it is clear that when $A_n = 0$ and

$$\beta^2 - \mu - (4n - 1 + 2\nu)\alpha = 0 \tag{11}$$

 $A_{n+1} = A_{n+2} = ... = 0$ and $\phi(x)$ will reduce to a polynomial. Equation (11) gives us the relation between μ , λ and η that should be satisfied for polynomial solution of $\phi(x)$. The condition for A_n to vanish is $D_n = 0$ (from (7)) which gives *n* number of eigenvalues. Under the condition (11) the infinite Hill determinant reduces to

$$\begin{vmatrix} A & C \\ 0 & B \end{vmatrix} = |A||B|$$
(12)

where $|A| = D_n$ is an $n \times n$ determinant and B is a determinant of infinite order

$$|B| = \begin{vmatrix} b_{n+1 \ n+1} & b_{n+1 \ n+2} & 0 & \dots \\ b_{n+2 \ n+1} & b_{n+2 \ n+2} & b_{n+2 \ n+3 \dots} & \dots \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ \end{vmatrix} .$$
(13)

We obtain *n* eigen-energies and well behaved eigenfunctions from the vanishing of |A| or D_n . This immediately raises the question of what happens to the remaining eigenvalues as there must be an infinite number of solutions. Singh *et al* (1978) conjectured that the remaining solutions are obtained from the zeros of the infinite determinant *B*. We would like to show that this conjecture may lead to incorrect results.

When $b_{n+1n} = 0$ or the condition (11) is satisfied, the *n* eigenvalues are obtained from the vanishing of D_n (8) and the eigenfunctions (apart from the exponential x factor) are given by

$$\phi(x) = \sum_{m=0}^{n-1} A_m x^{2m+\nu}$$
(14)

with A_m as obtained from (7). If B_r is the first $r \times r$ determinant of B then we have in the general case (11)

$$B_{r} = \{E + [4(n+r) - 3 + 2\nu]\beta\}B_{r-1} + 4(r-1)(2n+2r-2+\nu)(2n+2r-n+\nu)\alpha B_{r-2}$$
(15)

with $B_0 = 1$ and $B_1 = E + (4n + 1 + 2\nu)\beta$.

If $\beta > 0$ all the determinants B_1 , B_2 are positive when E > 0. But the potential (1) has an infinite number of discrete eigenvalues, most of which are positive (Powell and Crasemann 1953). Thus the conjecture of Singh *et al* is not correct for negative λ . The correct eigenvalues may be obtained by an analytic continuation of the continued fraction, accomplished with the aid of modified approximants (Masson 1983). The condition of wavefunction normalisation should be imposed (Chaudhuri 1983) as well as the eigenvalue condition.

3. Series solution

As in our previous two papers (Chaudhuri and Mukherjee 1983, 1984) we put infinitely high potentials at $x = \pm L$ so that the boundary conditions become $\psi(\pm L) = 0$, which do not pose any problem for the series solution of equation (2). We make the change of variable y = x/L and write the wavefunction $\psi(y)$ as convergent even and odd

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power series:

$$\psi(y) = \sum_{n=0}^{\infty} A_n y^{2n+\nu}.$$
 (16)

Substituting (16) into (2) we obtain the following recurrence relation satisfied by A_n

$$(2n+\nu)(2n+\nu-1)A_n + \varepsilon A_{n-1} - aA_{n-2} - bA_{n-3} - cA_{n-4} = 0, \qquad n \ge 1$$
(17)
with

with

$$\varepsilon = EL^2,$$
 $a = \mu L^4,$ $b = \lambda L^6,$
 $c = \eta L^8,$ $A_{-1} = A_{-2} = A_{-3} = 0.$

If $|A_n/A_{n-1}| \to O(n^{\delta})$ as $n \to \infty$, we find from (17) that $\delta = -\frac{1}{2}$ which shows that A_n forms a convergent sequence. The zeros of the functions

$$\psi(y=1) = \sum_{n=0}^{\infty} A_n \tag{18}$$

with $\nu = 0$ and 1, give us the eigenvalues of the even and odd parity solutions. In table 1 the first four eigenvalues of the confined $(\mu x^2 + \lambda x^4 + \eta x^6)$ oscillator are shown, with $\eta = 1, \mu, \lambda = -2, 0, 2$ and L = 1, 2, 3. Our values for L = 3 are also compared with the eigenvalues for the unbounded oscillators available in the literature. It is found that agreement is excellent.

4. Large η behaviour of the eigenvalues

The Hamiltonian

$$H(\mu, \lambda, \eta) = -d^2/dx^2 + \mu x^2 + \lambda x^4 + \eta x^6$$
(19)

has the following scale transformation property

$$H(\mu, \lambda, \eta) = \eta^{1/4} H(\mu \eta^{-1/2}, \lambda \eta^{-3/4}, 1)$$
(20)

so that

$$H(\mu, \lambda, \eta) \xrightarrow[\eta \to \infty]{} \eta^{1/4} H(0, 0, 1)$$
(21)

where H(0, 0, 1) is the Hamiltonian for the pure x^6 oscillator. The eigenvalues of the pure x^{2m} oscillator have already been discussed (Chaudhuri and Mukherjee 1983). Due to the scale transformation property (21) it is easy to find the eigenvalues of $H(\mu, \lambda, \eta)$ for large η if the eigenvalues of H(0, 0, 1) are known.

Equation (2) can be written as

$$(-d^2/du^2 + \mu'\mu^2 + \lambda'u^4 + u^6)\psi = E'\psi$$
(22)

where

$$u = x\eta^{1/8} \tag{23a}$$

$$\mu' = \mu \eta^{-1/2} \tag{23b}$$

$$\lambda' = \lambda \eta^{-3/4} \tag{23c}$$

$$E' = E\eta^{-1/4}.$$
 (23*d*)

μ	λ	<i>L</i> = 1	L = 2	<i>L</i> = 3	Unbounded oscillator $(L \rightarrow \infty)$
-2.0	-2.0	2.1326	-0.9160	-1.0000	-1†
		9.1226	0.0060	-0.1537	
		21.3697	3.8978	3.6281	
		38.5977	8.5944	8.0150	
	0.0	2.2203	0.4424	0.4401	
		9.3553	2.8060	2.7960	
		21.6763	7.2632	7.2312	
		38.9476	12.8723	12.7785	
	2.0	2.3053	1.0002	1.0000	1+
		9.5882	4.3739	4.3730	
		21.9945	9.7477	9.7436	
		39.2967	16.2767	16.2618	
0.0	-2.0	2.4025	0.4040	0.3853	
		9.6966	2.2397	2.1741	
		21.9718	5.8919	5.7310	
		39.2367	10.9284	10.6341	
	0.0	2.4852	1.1455	1.1448	1.144 802‡
		9.9256	4.3428	4.3386	4.338 60‡
		22.2959	9.0879	9.0730	
		39.5877	14.9910	14.9350	
0.0	2.0	2.5656	1.5291	1.5291	
		10.1504	5.6057	5.6053	
		22.6101	11.3210	11.3188	
		39.9387	18.1704	18.1509	
2.0	-2.0	2.6626	1.2455	1.2410	
		10.2614	4.0915	4.0788	
		22.6022	8.0091	7.9008	
		39.8782	13.1866	13.1302	
2.0	0.0	2.7408	1.6974	1.6972	1.697§
		10.4846	5.6868	5.6850	
		22.9175	10.8453	10.8366	10.836§
		40.2303	17.0692	17.0235	
	2.0	2.8168	1.9792	1.9790	
		10.7040	6.7235	6.7220	
		23.2300	12.8272	12.8261	
		40.5830	19.9861	19.9792	

Table 1. The first four eigenvalues for the bounded potential $\mu x^2 + \lambda x^4 + \eta x^6$ with $\eta = 1$, μ , $\lambda = -2$, 0, 2 and L = 1, 2, 3 and those of the unbounded $(L \rightarrow \infty)$ oscillator.

 $D_1 = 0$ (equation (12)).

‡ Turbiner (1981).

§ Biswas et al (1973).

It is clear from (23) that μ' , λ' and E' decrease with increasing η and therefore for finding the energy eigenvalues of the interaction (1) it will be convenient to use equation (22) when $\eta > 1$.

In table 2 we present the eigenvalues $E_n(\mu, \lambda, \eta)$ of the Hamiltonian $H(\mu, \lambda, \eta)$ when η is large for L = 3, and compare with the asymptotic $(\eta \to \infty)$ values given by $\eta^{1/4}E_n(0, 0, 1)$. We also compute the percentage error involved in using the asymptotic formula in the eigenvalues of the Hamiltonian $H(\mu, \lambda, \eta)$. It is found that the error is given empirically by $A_n\eta^m$ where $m \approx -0.5$ and A_n decreases with increasing *n*.

Table 2. The first four eigenvalues of the potential $x^2 + \eta x^6$ for large values of η : A, the bounded potential (L=3); B, the asymptotic $(\eta \to \infty)$ values; C, the unbounded oscillator (Biswas *et al* 1973).

	The present calculation for $L = 3$	Unbounded oscillator $L \rightarrow \infty$	$\eta^{1/4} E_n(0,0,1)$	$\frac{A-B}{A} \times 100$
η			<i>D</i>	
10	2.2057	2.205 72	2.0358	7.703
	8.1148		7.7152	4.924
	16.6412	16.641 21	16.1344	3.045
	27.1551		26.5589	2.196
10 ²	3.7170	3.71697	3.6202	2.604
	13.9462		13.7199	1.623
	28.9772		28.6916	0.986
	47.5650		47.2291	0.706
10 ³	6.4924		6.4377	0.843
	24.5253		24.3977	0.520
	51.1825		51.0217	0.314
	84.1756		83.9866	0.225
104	11.4788		11.4480	0.268
	43.4578		43.3860	0.165
	90.8213		90.7308	0.100
	149.4579		149.3517	0.071
10 ⁵	20.3751		20.3577	0.085
	77.1928		77.1524	0.052
	161.3957		161.3447	0.032
	265.6488		265.5890	0.023
106	36.2116		36.2017	0.027
	137.2212		137.1985	0.017
	286.9447		286.9159	0.010
	472.3251		472.2914	0.007
107	64.3824		64.3768	0.009
	243.9901		243.9774	0.005
	510.2331		510.2167	0.003
	839.8852		839.8661	0.002

5. Conclusion

The advantage of our method of finite box approximation is that the eigenvalues are obtained from a single equation for both positive and negative values of μ and λ as long as η is positive. When $\mu = \lambda = -2$ and $\eta = 1$ the condition (11) is satisfied for n = 1 and $\nu = 0$ (even parity solution). The corresponding exact eigenvalue is $E = -\beta = -1$ which can be compared with the value obtained by the series method (table 1). We have shown in § 2 that the Hill determinant method of Singh *et al* (1978) produces no positive eigenvalue under this condition. However, we find in § 3 that the first excited even parity eigenvalue is 3.6281 which clearly shows that the conjecture of Singh *et al* is not correct for this case.

The Hill determinant method of Biswas *et al* (1973) produces the eigenvalues of $x^2 + \eta x^6$ oscillator to a high degree of accuracy when $\eta \le 100$. The method, however, becomes unreliable for $\eta > 100$ because of the large truncation error in the numerical

computation. The method described here is simple and accurate for numerical evaluation of the eigenvalues of the anharmonic oscillator for any value, however large, of the coupling constants.

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