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The eigenvalues of the bounded λx^{2m} oscillators

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Abstract. The even- and odd-parity eigenvalues of the bounded pure λx^{2m} oscillators are obtained as the roots of two equations derived explicitly.

The unbounded anharmonic oscillators have been studied by a number of authors (Banerjee *et al* 1978, Bender and Wu 1969, Loeffel *et al* 1970, Fung *et al* 1978, Drummond 1981) using different perturbative techniques. Different non-perturbative techniques have also been applied by a number of authors (Biswas *et al* 1971, 1973, Halpern 1973, Singh *et al* 1978, Bozzolo *et al* 1982, Killingbeck 1978, Austin and Killingbeck 1982). The perturbation series in terms of the coupling constant has its domain of applicability and most of the non-perturbative calculations require very elaborate computations for the energy eigenvalues. The method described by Killingbeck (1978) is, however, quite simple for obtaining the perturbation series for the energy without any calculation of the perturbed wavefunctions. 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. The anharmonic oscillator problem is of much interest from the analytical, as well as the numerical, point of view due to its important physical applications. Bell (1945) studied the pure quartic oscillator in connection with the mode of plane rings of atoms. The knowledge of the exact eigenvalues of pure quartic anharmonic oscillators is of particular interest in molecular physics (Chan and Stellman 1963, Reid 1970). Recently Barakat and Rosner (1981) studied the pure x^4 oscillator bounded by infinite potentials at $x = \pm L$ and showed that the lower-order eigenvalues tend rapidly to the values of the unbounded oscillator as L is made larger.

The purpose of this paper is to study the eigenvalues of the pure λx^{2m} oscillators bounded by infinitely high potentials at $x = \pm L$. We have to solve the eigenvalue equation

$$[(\mathrm{d}^2/\mathrm{d}x^2) + E - \lambda x^{2m}]\psi(x) = 0, \qquad m = 1, 2, 3, \ldots, \tag{1}$$

subject to the boundary conditions $\psi(\pm L) = 0$. First of all we make the change of variable $y = x/L$ so that (1) is transformed to the equation

$$[(\mathrm{d}^2/\mathrm{d}y^2) + \varepsilon - by^{2m}]\psi(y) = 0 \tag{2}$$

with the boundary conditions $\psi(y = \pm 1) = 0$, $\varepsilon = EL^2$ and $b = \lambda L^{2m+2}$.

The symmetry of equation (2) implies that $\psi(y)$ has even and odd power series

$$\psi^{e}(y)=\sum_{n=0}^{\infty} A_{2n}y^{2n}, \tag{3}$$

$$\psi^{o}(y)=\sum_{n=0}^{\infty} A_{2n+1}y^{2n+1}, \tag{4}$$

where the superscripts e and o refer to the even- and odd-parity solutions. It should be noted that the replacement of n by $n+\frac{1}{2}$ in the even-series solution reproduces the odd-series solution. The coefficients A_{2n} and A_{2n+1} satisfy a set of recursion relations. We put $A_0=A_1=1$ and apply the recursion relations repeatedly to evaluate

$$f^{e}(\varepsilon)=\sum_{n=0}^{\infty} A_{2n}, \qquad f^{o}(\varepsilon)=\sum_{n=0}^{\infty} A_{2n+1}.$$

Collecting the terms of same order of b we finally obtain

$$f^{e}(\varepsilon)=\cos\sqrt{\varepsilon}+\sum_{k=1}^{\infty} b^{k}\sum_{n=0}^{\infty}(-1)^{n}C^{e}_{nk}\varepsilon^{n}, \tag{5}$$

$$f^{o}(\varepsilon)=\frac{\sin\sqrt{\varepsilon}}{\sqrt{\varepsilon}}+\sum_{k=1}^{\infty} b^{k}\sum_{n=0}^{\infty}(-1)^{n}C^{o}_{nk}\varepsilon^{n}, \tag{6}$$

where the coefficients $C^{e,o}_{nK}$ are given by

$$C^{e,o}_{01}=[(2m+2+v)(2m+1+v)]^{-1},$$

$$C^{e,o}_{n1}=[(2m+2n+2+v)(2m+2n+1+v)]^{-1}[C^{e,o}_{n-1\,1}+((2n+v)!)^{-1}], \qquad n\geqslant 1,$$

$$C^{e,o}_{0K}=\frac{C^{e,o}_{0K-1}}{(2Km+2K+v)(2Km+2K-1+v)}, \qquad K\geqslant 2,$$

$$C^{e,o}_{nK}=\frac{C^{e,o}_{nK-1}+C^{e,o}_{n-1K}}{(2Km+2K+2n+v)(2Km+2K+2n-1+v)}, \qquad n\geqslant 1, K\geqslant 2,$$

with $v=0$ for the even series and $v=1$ for the odd series. Equations (5) and (6) may be written as

$$f^{e}(\varepsilon)=\cos\sqrt{\varepsilon}+\sum_{n=0}^{\infty}(-1)^{n}\alpha^{e}_{n}\varepsilon^{n}, \tag{7}$$

$$f^{o}(\varepsilon)=\frac{\sin\sqrt{\varepsilon}}{\sqrt{\varepsilon}}+\sum_{n=0}^{\infty}(-1)^{n}\alpha^{o}_{n}\varepsilon^{n}, \tag{8}$$

where

$$\alpha^{e,o}_{n}=\sum_{k=1}^{\infty} b^{K}C^{e,o}_{nK}.$$

The zeros of the functions $f^{e,o}(\varepsilon)$ give us the eigenvalues of the even- and odd-parity solutions. In these equations the coefficients of successive powers of ε alternate in sign when λ is positive, showing that there are no real negative eigenvalues. It should also be noted that for a particular value of m the coefficients $C^{e,o}_{nK}$ decrease very fast with both n and K, so that in finding the roots only a few terms are to be considered. When $b<1$ the perturbation series in terms of b or the coupling constant λ may be obtained from (5) and (6) by retaining terms up to certain orders in b. When the oscillator is confined to a very small region of space the eigenvalues may be found from the zeros of $\cos\sqrt{\varepsilon}$ and $(\sin\sqrt{\varepsilon})/\sqrt{\varepsilon}$:

$$E_n^e = (n+\tfrac{1}{2})^2\pi^2/L^2, \qquad n = 0, 1, 2, \ldots, \tag{9}$$

$$E_n^o = n^2\pi^2/L^2, \qquad n = 1, 2, 3, \ldots. \tag{10}$$

Equations (9) and (10) show that the oscillator energy increases rapidly with the decrease in the dimension of the confinement of the oscillator when b is very small.

Equations (7) and (8) are suitable for numerical evaluation of the eigenvalues of the bounded oscillators for any values of λ and L, and integer values of m. Since no approximation is made in deriving the equations and the explicit expressions of the functions $f^{e,o}(\varepsilon)$ are given, one may compute the eigenvalues to a high degree of accuracy by considering a large number of terms of the infinite series. We may find the eigenvalues of the unbounded oscillators as observed by Barakat and Rosner (1981) by gradually making L large. In table 1 we tabulate the first four eigenvalues of confined λx^{2m} oscillators with $\lambda = 1$, $m = 1, 2, 3, 4, 5$ and $L = 1, 2, 3, 4$. We find from the table that when m is large the lower-order eigenvalues remain almost unchanged for $L = 2, 3$ and 4 where the potentials are made infinitely high. This is because for large m the potential function x^{2m} becomes effectively infinite at $x = 2$ in comparison to its values around $x = 0$. Our values for $m = 2$ with large L may be compared with the first four eigenvalues for the unbounded oscillator as given by Chan and Stellman (1963): 1.060 362, 3.799 657, 7.455 702, 11.644 75. The exact eigenvalues for the unbounded oscillator for $m = 1$ (the harmonic oscillator problem) are given by $E_n = (2n+1)$, $n = 0, 1, 2, \ldots$. Thus we find that the lower-order eigenvalues tend rapidly to the values of the unbounded oscillators as L is made larger.

The method described here is applicable to any form of bounded potentials having no singularity for finite values of x. The potential function can be expressed as a Taylor series about $x = 0$ and then the series solution is applicable to the problem.

Table 1. First four eigenvalues of confined λx^{2m} oscillators with $\lambda = 1$, $m = 1, 2, 3, 4, 5$ and $L = 1, 2, 3, 4$.

m \ L	1	2	3	4	m \ L	1	2	3	4
1	2.597	1.075	1.001	1.000	4	2.477	1.226	1.226	1.226
	10.151	3.530	3.012	3.000		9.901	4.756	4.756	4.756
	22.518	6.800	5.082	5.000		22.261	10.245	10.245	10.245
	39.799	11.169	7.328	7.000		39.551	17.343	17.343	17.343
2	2.508	1.073	1.060	1.060	5	2.473	1.296	1.296	1.296
	9.983	3.882	3.800	3.800		9.889	5.098	5.098	5.098
	22.364	7.784	7.456	7.456		22.242	11.154	11.154	11.154
	39.654	12.584	11.645	11.645		39.528	19.189	19.189	19.189
3	2.485	1.145	1.145	1.145					
	9.926	4.343	4.339	4.339					
	22.296	9.090	9.073	9.073					
	39.588	14.991	14.935	14.935					

One should be cautious in applying the series method for the unbounded oscillator. The method fails even for the harmonic oscillator problem. It is easy to show that the Hill determinant method (Biswas *et al* 1971, 1973, Chaudhuri 1983) fails completely for the harmonic oscillator problem if the exponential x term is not factored out from the wavefunction. For the unbounded oscillator the main problem of solving the differential equation (1) by the method of series solution about $x=0$ is that the point at infinity is an irregular singular point of the differential equation so that the boundary conditions $\lim_{x\to\pm\infty}\psi(x)=0$ cannot be imposed on it. For the bounded oscillator problem the boundary conditions are $\psi(\pm L)=0$, and since the series solutions are valid for all finite values of x there is no problem in imposing the boundary conditions. For the unbounded eigenvalue problem one has to find a proper convergence factor for the wavefunction (Ginsburg 1982, Killingbeck 1981). The convergence factor is not required for the evaluation of the energy eigenvalues of the bounded potential problem by the infinite series method. It is always better to start with the bounded eigenvalue problem where the series solution is applicable and then make the dimension of the confinement of the oscillator gradually large. By this method the eigenvalues of anharmonic oscillators can be found easily.

It should be mentioned here that our finite box method is similar to the power series method based on the renormalisation approach (Killingbeck 1981, Austin and Killingbeck 1982). Equations (5) and (6) are suitable for numerical evaluation of the eigenvalues for small negative values of λ. The limit $\lambda\to 0$ does not give rise to any problem in our case, whereas Rayleigh–Schrödinger perturbation theory is sometimes not applicable (Khare 1981) in the case of anharmonic oscillators for $\lambda<0$. However, the problem of stabilisation effect (Hazi and Taylor 1970) may set in for negative λ as in the renormalisation series approach. This point is still under investigation.

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