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On the energy spectra of one-dimensional anharmonic oscillators

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Abstract. In this paper we present explicit and simple analytical formulae for the energy eigenvalues $E_n(\lambda)$ of one-dimensional anharmonic oscillators characterized by the potentials $\frac{1}{2}m\omega^2x^2 + \lambda x^{2\alpha}$ with $\alpha = 2$, 3 and 4. A simple intuitive criterion supplemented by the requirement of correct asymptotic behaviour, has been employed in arriving at the formulae. Our energy values over a wide range of n and λ are in good agreement with the numerical values computed by earlier workers through very elaborate techniques. To our knowledge this is the first time that formulae of such wide validity have been given. The results for pure power oscillators are trivially obtained by going over to the $\omega \to 0$ limit. Approximate analytic expressions for the low order even moments of x are also given.

Keywords. Anharmonic oscillator; renormalized frequency; energy eigenvalue moments;

1. Introduction

The study of quantum anharmonic oscillators (AHO) has received considerable attention in the literature because of their many applications and their importance as simplified models for nonlinear fields. The main quantities of interest have been the energy eigenvalues E_n, moments of x^2, x^4... in various eigenstates and the matrix elements of x, x^2, x^3,... between eigenstates of oscillators having Hamiltonians of the general form

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 + \lambda x^{2\alpha},$$

for $\alpha = 2, 3, 4, \ldots$ For accurate numerical computation of the energy levels the ordinary (Rayleigh-Schrödinger) perturbation procedure is of no direct use. The reason is that $E_n(\lambda)$ is not analytic in λ at $\lambda = 0$ and the perturbation series is strongly divergent. The nature of the nonanalytic behaviour has been studied in detail by Bender and Wu (1969), Simon (1970) and Loeffel *et al* (1969). Several kinds of procedures have been suggested and employed during the past few years for numerical computations of $E_n(\lambda)$. These include* the Borel summation of the (strongly diver-

*The literature on this subject is so vast that it is next to impossible to quote every important paper. What we have included is only a sample based on personal taste and references to other techniques can be traced from these.

gent) perturbation series with the aid of Padè approximants (Graffi *et al* 1970 for $\alpha = 2$)*, the use of a WKB approximation carried to arbitrary order (Bender *et al* 1977) which however also yields only an asymptotic series though the nearest approach to the exact values is quite close, Hill determinant techniques (Biswas *et al* 1971, 1973) a method of continued fractions (Graffi and Grecchi 1975; Singh *et al* 1978), variational methods (Bazley and Fox 1961; Graffi and Grecchi 1973) and a variety of other methods of a more specialized nature (Lakshmanan and Prabhakaran 1973; Mathews and Govindarajan 1977; Ginzburg and Montroll 1978; Richardson and Blankenbecler 1979; Behera and Khare 1980; Magyari 1981). A variety of other methods have also been devised by various workers, to obtain approximate analytical formulae which give $E_n(\lambda)$ directly or indirectly and to compute $E_n(\lambda)$ numerically to high accuracy. Montroll and co-workers (Hioe and Montroll 1975; Hioe *et al* 1976, 1978) have succeeded in presenting a number of such formulae which are accurate in different domains of n and λ. There is no way of deciding however as to which of the formulae is the most accurate in a transition region between two such domains. The numerical computations presented by them cover the relatively low lying levels, for values of λ ranging from very small to very large. They have noted that accuracy is hardest to obtain when n is small and λ is very large. The most extensive tabulation of numerical values of $E_n(\lambda)$ computed with high accuracy is due to Banerjee and co-workers (Banerjee *et al* 1978; Banerjee 1978). They present $E_n(\lambda)$ for both n and λ varying from very small to very high values, for the quartic ($\alpha = 2$), sextic ($\alpha = 3$) and octic ($\alpha = 4$) oscillators. However, a single analytical formula for a given α which is capable of yielding $E_n(\lambda)$ with high accuracy for all n and λ has so far been lacking. In a recent note (Mathews *et al* 1981) we have briefly presented such a formula. In this paper we describe the derivation of the formula in more detail and extend it to the sextic and octic oscillators ($\alpha = 3, 4$). The predictions of our simple formulae are accurate** as can be seen from a comparison with the tabulations of values available in the literature.

The essence of our method is the determination of a 'renormalized' frequency $\omega_0(n, \lambda)$ such that $E_n(\lambda)$ is very closely approximated by $\langle n | H | n \rangle$ where $| n \rangle$ is defined in relation to the renormalized harmonic oscillator.

$$H_0 | n \rangle = (n + \tfrac{1}{2}) \hbar\omega_0 | n \rangle, \; 2m \; H_0 = p^2 + \frac{1}{2} m\omega_0^2 x^2.$$

The details as to how $\omega_0(n, \lambda)$ is determined for $\alpha = 2$, 3 and 4 are given in the succeeding sections. It may be mentioned here that the work of Banerjee and co-workers also rests on the use of a matrix representation for H in the basis of a renormalized harmonic oscillator†, but their aim is not to obtain a simple analytic formula for

*The recent work of Caswell (1979) employs a renormalized perturbation series which is useful for all n and λ.

**This makes it possible to use the formula with confidence for accurate estimation of $E_n(\lambda)$ for any desired n and λ for which tabulated values are not available.

†Killingbeck (1981) has recently suggested the case of a perturbation treatment with a renormalized frequency for the unperturbed Hamiltonian. The perturbation series is however expected to be divergent. Halliday and Suranyi (1980) have developed a convergent perturbation series wherein the unperturbed part is taken to be square of the HO Hamiltonian with a renormalized frequency.

$E_n(\lambda)$ but to compute $E_n(\lambda)$ numerically to a high degree of accuracy (1 in 10^{15}) employing the Hill determinant method (used earlier by Biswas and co-workers without 'renormalization'). The freedom to split H into unperturbed and perturbation parts in any manner has also been used in the early work of Chan *et al* (1964) who evaluated the low lying energy eigenvalues and also some moments and matrix elements of x.

The plan of the paper is as follows: In the next section we take up the quartic AHO ($\alpha = 2$; $\omega \neq 0$) and obtain an (approximate) expression for its energy eigenvalues. Approximate expressions for x^2 and x^4 moments are also obtained using the Feynman-Hellmann theorem. Results for the pure quartic oscillator ($\alpha = 2$; $\omega = 0$) are shown to follow from the anharmonic case on letting $\omega \rightarrow 0$. Sections 3 and 4 are devoted to sextic ($\alpha = 3$) and octic ($\alpha = 4$) potentials. The last section is devoted to a discussion of our results.

2. The quartic anharmonic oscillator

The Hamiltonian for the one-dimensional quartic AHO is given by

$$H = \frac{p^2}{2m} + \frac{1}{2} m\, \omega^2 x^2 + \lambda x^4, \quad (\lambda > 0). \tag{1}$$

We consider the matrix representation of H in a basis which diagonalizes

$$H_0 \equiv \frac{p^2}{2m} + \frac{1}{2} m\, \omega_0^2 x^2, \tag{2}$$

where the 'renormalized' frequency ω_0 is a free parameter and we shall choose it in a well-defined way. The matrix elements of H in the basis defined by the eigenstates of H_0 are easily determined to be the following (Mathews and Venkatesan 1976):

$$\langle n|H|n\rangle \equiv H_{nn} = \frac{\hbar\,\omega_0}{2}\left[\left(n+\frac{1}{2}\right)(1+\nu^2) + \frac{3}{2}\rho^2\nu^3\left\{\left(n+\frac{1}{2}\right)^2 + \frac{1}{4}\right\}\right], \tag{3a}$$

$$\langle n+2|H|n\rangle = \langle n|H|n+2\rangle \equiv H_{n,\, n+2}$$

$$= \hbar\,\omega_0\left[-\frac{1}{4}(1-\nu^2) + \frac{1}{2}\rho^2\nu^3\left(n+\frac{3}{2}\right)\right]\{(n+2)(n+1)\}^{1/2}, \tag{3b}$$

$$\langle n+4|H|n\rangle = \langle n|H|n+4\rangle \equiv H_{n,\, n+4}$$

$$= \hbar\,\omega_0\left(\frac{\rho^2\nu^3}{8}\right)[(n+4)(n+3)(n+2)(n+1)]^{1/2}. \tag{3c}$$

All other matrix elements of H are zero. In the above equation ν is a positive quantity defined by

$$\nu = \omega/\omega_0, \tag{4}$$

and $$\rho^2 = 2\lambda\hbar/m^2\,\omega^3, \tag{5}$$

is a non-dimensional parameter characterizing the relative strengths of the quartic and quadratic terms in the potential. It is clear that the exact eigenvalues $E_n(\lambda)$ of the matrix H (with elements H_{nm}) will be independent of the value of ω_0. We can therefore use this freedom to our advantage and choose ω_0 adapted to any particular level n and λ such that the diagonal element H_{nn} of H (in the HO basis of such ω_0) closely approximates E_n. We choose ω_0 so as to make the matrix elements immediately close to H_{nn} (*viz.* $H_{n\pm2,\,n}$ and $H_{n,\,n\pm2}$) as small as possible. This gives the following equation to determine ν:

$$\rho^2\,\nu^3 = (1-\nu^2)/2\,(n+\tfrac{1}{2}). \tag{6}$$

With the value of ν determined, the (approximate) value for the nth energy level of the AHO is to be calculated from (3a):

$$E_n \simeq H_{nn} = \frac{1}{2\nu}\,[(n+\tfrac{1}{2})(1+\nu^2) + \tfrac{3}{2}\rho^2\nu^3\{(n+\tfrac{1}{2})^2+\tfrac{1}{4}\}]\,\hbar\,\omega. \tag{7}$$

We may note that for given n and ρ^2, equation (6) admits only one positive root and it lies between zero and unity. Making use of the known WKB – large n and λ – results, the equation for ν can be further refined as indicated below.

When $(n+\frac{1}{2})\,\rho^2$ is very large, the solution of (6) can be written as

$$\nu \sim [2\,\rho^2\,(n+\tfrac{1}{2})]^{-1/3}\,\{1-\tfrac{1}{3}\,[2\,\rho^2\,(n+\tfrac{1}{2})]^{-2/3}+\ldots\}. \tag{8}$$

On substituting this in (7), E_n becomes*

$$E_n \sim \lambda^{1/3}\left[1{\cdot}389\,(n+\tfrac{1}{2})^{4/3}\left\{1+\frac{3}{28\,(n+\frac{1}{2})^2}\right\} + 0{\cdot}262\,(n+\tfrac{1}{2})^{2/3}\,\lambda^{-2/3}+\ldots\right]. \tag{9}$$

Let us compare this with the known WKB expression** (Hioe and Montroll 1975; Pasupathy and Singh 1980);

$$E_n^{WKB} \sim \lambda^{1/3}\left[1{\cdot}37651\,(n+\tfrac{1}{2})^{4/3}\left\{1+\frac{1}{9\,\pi\,(n+\frac{1}{2})^2}\right\} + 0{\cdot}26805\,(n+\tfrac{1}{2})^{2/3}\,\lambda^{-2/3}+\ldots\right]. \tag{10}$$

*For ease of writing we have set $\hbar = m = \omega = 1$ in (9) and (10). Fuller expressions are given in the Appendix.

**We collect the necessary WKB results in the Appendix and show how the constants a, b and c (equation 12) are determined in terms of the WKB coefficients.

We find that our expression (7) for E gives the same power dependence on n and λ as in (10) but with slightly different coefficients. A little reflection shows that by a modification of the defining equation for ν, the coefficients in the various terms in the large $(n + \frac{1}{2})\,\rho^2$ limit of (7) can be made to coincide with those in the WKB expression. The modified form is

$$\rho^2 \nu^3 = \frac{(1-\nu^2)}{2\,(n+\frac{1}{2})}\left[1 + (a-1)\,(1-\nu^2) + b\,\nu^2 + \frac{c}{(n+\frac{1}{2})^2}\right]. \tag{11}$$

The role of the parameters a, b and c in determining the various coefficients may be seen from equations (A7) and (A8) of the Appendix. From these equations we find that the values needed for a, b and c, in order that the asymptotic form should coincide with the WKB limit are

$$\begin{aligned} a &= 0{\cdot}895647, \\ b &= -\,0{\cdot}125, \\ c &= -\,0{\cdot}85. \end{aligned} \tag{12}$$

We note incidentally that for all ρ^2 and $n \geqslant 2$ the above equation for ν still admits a positive root lying between zero and unity and it deviates only slightly from the corresponding solution of (6).*

Equation (7) with ν determined from (11) and (12) constitutes our result for the quartic anharmonic oscillator. The E_n are readily calculated, the value of ν in each case being obtained by numerical solution of the quartic algebraic equation (11). The results obtained are displayed in table 1. As can be seen from the results, our expression reproduces the energy values with a remarkably high degree of accuracy for all n and λ, though only the limit of large $(n + \frac{1}{2})\,\rho^2$ was used in determining the parameters (12). Only the last one or two digits in the tabulated values differ from the corresponding digits (shown in brackets below each number) of the accurate values obtained by earlier workers through very elaborate computations.

Table 1. Energy eigenvalues of quartic anharmonic and pure quartic oscillators.

	Anharmonic oscillator $2E_n/\hbar\omega$			Pure quartic oscillator
n \ ρ^2	0·0001	1·0	10000·0	$E_n \Big/ \left(\frac{2\lambda\hbar^4}{m^2}\right)^{1/3}$
2	5.000 974 6	8.663	160.81	7.461
	(4 6)	(55)	(69)	(56)
5	11.004 571 40	23·2998	457.677	21.238 94
	(36)	(74)	(65)	(37)
10	21.016 550	53·450	1082.891	50·256 38
	(30)	(49)	(89)	(25)
100	202.494 10	1035.544 35	21997·240 49	1020.990 00
	(08)	(18)	(27)	(89 99)
1000	2134·252	21932·783 86	471075.928 46	21865·262 120
	(43)	(71)	(38)	(18)
0	1.000 074 988	1·397 8	23.09	1·071
	(7)	(2 4)	(22.86)	(60)
1	3.000 374 91	4·670	82·57	3·831
	(0)	(49)	(81·90)	(00)

*n=0 and n=1 are special cases and the results for them will be separately indicated below.

A comment on the values given against $n = 0$ and $n = 1$ may be in order. The estimation of $E_0(\lambda)$ and $E_1(\lambda)$ by our formula was not found to be quite so good as for $n \geqslant 2$, especially when λ is large. The reason is basically that while for other values of n, the effects of the off-diagonal elements $H_{mm'}$ with $m+m' < 2n$ are largely counterbalanced by those with $m + m' > 2n$, for $n = 0$ and 1 there is an imbalance because no non-vanishing $H_{mm'}$ with $m + m' < 2n$ exist. The obvious remedy is to add a correction to H_{nn} to take account of the off-diagonal elements very close to H_{00} or H_{11} as the case may be. What is shown against $n = 0$ in table 1 is therefore not H_{00} but the lower of the eigenvalues of the matrix

$$\begin{pmatrix} H_{00} & H_{02} \\ H_{20} & H_{22} \end{pmatrix}$$

in a representation with ν taken as the relevant solution of (11) with $a - 1 = b = c = 0$. For $n = 1$ also the effect of the nearest off-diagonal elements H_{13} and H_{31} has been taken into account in a similar manner.*

2.1 *Pure quartic oscillator*

Results for the pure quartic oscillator ($\omega = 0$) are trivially obtained from our above given expressions, by noting that as $\omega \to 0$, ν also goes to zero such that

$$\omega/\nu = \omega_0 \neq 0 \text{ and } \rho^2\, \nu^3 = \frac{2\lambda\hbar}{m^2\omega_0^3} \neq 0.$$

The explicit expression for the energy value of the quartic oscillator is found to be the following:

$$E_n = \frac{\Delta}{4}\left\{\left(n+\frac{1}{2}\right) + \frac{12}{\Delta^3}\left[\left(n+\frac{1}{2}\right)^2 + \frac{1}{4}\right]\right\}\left(\frac{2\lambda\hbar^4}{m^2}\right)^{1/3}, \tag{13a}$$

with
$$\Delta^3 = \frac{16(n+\frac{1}{2})}{a + c/(n+\frac{1}{2})^2}. \tag{13b}$$

Note that here Δ is given explicitly, unlike ν of the anharmonic case which had to be found as the solution of an algebraic equation. This simple formula (13) reproduces with great accuracy the energy values of the quartic oscillator computed by Banerjee and co-workers (table 1).

2.2 *The even moments of x*

For the Hamiltonian (1); the Feynman-Hellmann theorem (Quigg and Rosner 1979) states that

$$\tfrac{1}{2}m^2 \langle x^2\rangle_n = \partial\mathscr{E}_n/\partial\omega^2, \tag{14a}$$

and
$$\langle x^4\rangle_n = \partial\mathscr{E}_n/\partial\lambda, \tag{14b}$$

*A similar procedure has been adopted for getting the energy values for the $n = 0$ and $n = 1$ levels of all the other oscillators considered in the rest of the paper.

where the expectation values on the left side are with respect to the exact eigenstate of H with exact eigenvalue $\mathscr{E}_n$. As we have seen above, our approximate expression E_n for the energy is quite close to $\mathscr{E}_n$. Therefore we can derive (approximate) expressions for $\langle x^2\rangle_n$ and $\langle x^4\rangle_n$ by replacing $\mathscr{E}_n$ on the r.h.s. of (14) by E_n itself. Explicitly

$$\langle x^2\rangle_n \simeq \frac{2}{m^2}\frac{\partial E_n}{\partial\omega^2} = \frac{h\nu}{m\omega}\left\{\left(n+\frac{1}{2}\right)+\rho^2\nu^3\left[\frac{(n+\frac{1}{2})^2}{a'+b'\nu^2}-\frac{3}{2}\left(\left(n+\frac{1}{2}\right)^2+\frac{1}{4}\right)\right]\right.$$
$$\left.\left[\frac{b'-a'-2b'\nu^2}{(n+\frac{1}{2})\rho^2\nu^3-2a'-(b'-a')\nu^2}\right]\right\}, \tag{15a}$$

and

$$\langle x^4\rangle_n \simeq \frac{\partial E_n}{\partial\lambda} = \frac{2\hbar^2}{m^2}\frac{(\nu)^2}{\omega^2}\left\{\frac{3}{4}\left[\left(n+\frac{1}{2}\right)^2+\frac{1}{4}\right]-2\left(n+\frac{1}{2}\right)\rho^2\nu^3\right.$$
$$\left.\frac{[\frac{3}{2}((n+\frac{1}{2})^2+\frac{1}{4})-(n+\frac{1}{2})^2/a'+b'\nu^2]}{3a'+(b'-a')\nu^2+b'\nu^4}\right\}, \tag{15b}$$

where $\quad a' = a + c/(n+\frac{1}{2})^2$ and $b' = 1 - a + b, \quad$ (16)

and ν is the relevant solution of (11). Once $\langle x^2\rangle_n$ and $\langle x^4\rangle_n$ are determined, all the higher even moments, $\langle x^{2s}\rangle_n$ can be computed by making use of the moment recursion relations (Banerjee 1977; Richardson and Blankenbecler 1979).

Results for the pure quartic oscillator ($\omega\to 0$) are particularly simple and we find in this limit that (15) reduces to

$$\langle x^2\rangle_n \simeq \left(\frac{4h^2}{m\lambda}\right)^{1/3}\frac{1}{\Delta}\left\{\left(n+\frac{1}{2}\right)+\frac{\Delta^3(a'-b')}{48(n+\frac{1}{2})}\left[\left(n+\frac{1}{2}\right)-\frac{24}{\Delta^3}\right.\right.$$
$$\left.\left.\left(\left(n+\frac{1}{2}\right)^2+\frac{1}{4}\right)\right]\right\}. \tag{16a}$$

$$\langle x^4\rangle_n \simeq E_n/3\lambda, \tag{16b}$$

with E_n and Δ given by (13). The values of $\langle x^2\rangle_n$ obtained from (16a) are given in table 2 and they compare very favourably with the accurate values of Banerjee *et al* (1978). From the moment recursion relations one can deduce that $\langle x^4\rangle_n = \mathscr{E}_n/3\lambda$. Therefore our values of $\langle x^4\rangle_n$ given by (16b) have the same accuracy as the energy values themselves.

3. The sextic anharmonic oscillator

Since the procedure for obtaining energy expressions for the sextic (and octic) oscillators is similar to the one adopted above for the quartic potential, we will keep the details to the unavoidable minimum.

Table 2. Values of $\langle x^2\rangle_n$ for the pure quartic oscillator.

n	$(2\lambda m/\hbar^2)^{1/3}\,\langle x^2\rangle_n$
2	1·249 5 (4 7)
3	1·562 (58)
5	2·107 4 (5 0)
7	2·590 (88)
9	3·031 2 (0 0)
0	0·348 (62)
1	0·889 (901)

The Hamiltonian for the sextic AHO is given by

$$H=\frac{p^2}{2m}+\tfrac{1}{2}\,m\,\omega^2\,x^2+\lambda\,x^6,\ (\lambda>0). \tag{17}$$

As before we approximate the eigenvalue E_n of H by the expectation value H_{nn} of H in a HO basis corresponding to a renormalized frequency ω_0, which is so chosen that the off-diagonal elements adjacent to H_{nn} are made small. This requires that $\nu\equiv\omega/\omega_0$ be a solution of the equation

$$\rho^2\,\nu^4=\frac{4}{15}\,\frac{(1-\nu^2)}{(n+\frac{1}{2})^2+\frac{7}{4}}. \tag{18}$$

The energy is then to be computed from

$$E_n\sim H_{nn}=\frac{(n+\frac{1}{2})}{2\nu}\left[(1+\nu^2)+\frac{5}{2}\,\rho^2\,\nu^4\left\{(n+\tfrac{1}{2})^2+\frac{5}{4}\right\}\right]\hbar\omega, \tag{19}$$

where $\rho^2=2\lambda\hbar^2/m^3\omega^4.$ (20)

It is easily seen that for all n and λ, (18) admits a positive solution lying between 0 and unity. As in the previous section, the equation for ν has to be slightly modified in order to yield the WKB limit with correct coefficients. The modified equation for ν is found to be

$$\rho^2\,\nu^4=\frac{4}{15}\,\frac{(1-\nu^2)}{[(n+\frac{1}{2})^2+\frac{7}{4}]}\left[1+(a-1)\,(1-\nu^2)+b\nu^2+\frac{c}{(n+\frac{1}{2})^2}\right], \tag{21}$$

with $a=0{\cdot}831488755$, $b=-0{\cdot}213865$, and $c=-1{\cdot}349$. (22)

It is very interesting to note that in contrast to the quartic case – the above equation for ν is quadratic in ν^2 and hence we can solve for ν analytically. The values obtained for E_n from (19) and (21) (table 2) are found to be quite close to the values given in the extensive tables of Banerjee *et al*.

3.1 *Pure sextic limit*

The results for this case are obtained as limiting values of $\omega \to 0$ in (19) and (21). We note that this implies $\nu \to 0$ such that

$$\rho^2 \nu^4 = \rho^2\omega^4/\omega_0^4 \to 2\lambda\hbar^2/m^2\omega_0^4.$$

On using this we get the following explicit expression for E_n:

$$E_n = \tfrac{1}{2}(n+\tfrac{1}{2})\,\Delta\left[1+\frac{5}{2\Delta^4}\left\{(n+\tfrac{1}{2})^2+\frac{5}{4}\right\}\right](2\lambda\hbar^6/m^3)^{1/4}, \tag{23a}$$

where $$\Delta^4 = 15\left\{(n+\tfrac{1}{2})^2+7/4\right\}/4\left\{a+c/(n+\tfrac{1}{2})^2\right\}. \tag{23b}$$

The results obtained from this expression for E are shown in table 3*.

4. The octic anharmonic oscillator

The expectation value H_{nn} of the octic AHO Hamiltonian

$$H = \frac{p^2}{2m}+\frac{1}{2}m\,\omega^2x^2+\lambda x^8, \quad (\lambda > 0), \tag{24}$$

Table 3. Energy eigenvalues of the sextic anharmonic and pure sextic oscillators.

	Anharmonic oscillator $2E_n/\hbar\omega$			Pure sextic oscillator
n \ ρ^2	0·000 1	1·0	10000·0	$2E_n/(2\lambda\hbar^6/m^3)^{1/4}$
2	5·004 668 0 (4 7)	10·04 (9·97)	91·56 (90·82)	9·15
5	11·042 642 (09)	30·639 (23)	293·22 (13)	29·308
10	21·278 1 (7 8)	78·963 (58)	771·474 (57)	77·129
100	283·340 (23)	2287·793 74 (57)	22821·750 0 (49 9)	2282·118 23
1000	7346·850 (38)	71700·060 51 (49)	716823·285 171 (70)	71682·149 4
0	1·000 187 34 (23)	1·481 (36)	12·18 (11·48)	1·215
1	3·001 310 (09)	5·15 (03)	44·98 (43·46)	4·49

*Accurate numerical tables for the energy values do not seem to be available for pure sextic (and octic) potentials, for comparison purposes. But in view of the excellent agreement seen in the anharmonic case for high ρ^2 (*i.e.* with the sextic potential predominating) it can safely be presumed that our results have accuracies of the *same* order also in the pure sextic (and octic) case.

in the state $| n \rangle$ of the HO with a renormalized frequency ω_0 is given by

$$E_n \simeq H_{nn} = \frac{1}{2\nu}\left[(n+\tfrac{1}{2})(1+\nu^2) + \frac{35}{8}\rho^2 \nu^5 \left\{(n+\tfrac{1}{2})^4 + \frac{7}{2}(n+\tfrac{1}{2})^2 + \frac{9}{16}\right\}\right]\hbar\omega, \tag{25}$$

where $\rho^2 = 2\lambda\, \hbar^3/m^4\omega^5.$ (26)

The parameter $\nu \equiv \omega/\omega_0$ is the solution lying between 0 and unity of the following equation:

$$\rho^2\nu^5 = (1-\nu^2)/7(n+\tfrac{1}{2})\left[(n+\tfrac{1}{2})^2 + \frac{23}{4}\right]. \tag{27}$$

The WKB coefficients for this potential are correctly reproduced if we modify the equation for ν as

$$\rho^2\nu^5 = \frac{(1-\nu^2)\left[1+(a-1)(1-\nu^2)+b\nu^2+\dfrac{c}{(n+\frac{1}{2})^2}\right]}{7(n+\frac{1}{2})\left[(n+\frac{1}{2})^2+\dfrac{23}{4}\right]}, \tag{28}$$

where the constants a, b and c have values

$$a = 0{\cdot}787\ 128\ 845,\ b = -0{\cdot}277\ 492 \text{ and } c = -1{\cdot}609. \tag{29}$$

4.1 *Pure octic potential*

In the limit of $\omega \to 0$ the above results simplify to give the following explicit expression for the energy

$$E_n = \frac{\Delta}{2}\left[(n+\tfrac{1}{2}) + \frac{35}{8\Delta^5}\left\{(n+\tfrac{1}{2})^4 + \frac{7}{2}(n+\tfrac{1}{2})^2 + \frac{9}{16}\right\}\right]\left(\frac{2\lambda\hbar^8}{m^4}\right)^{1/5}, \tag{30a}$$

with

$$\Delta^5 = 7(n+\tfrac{1}{2})\left[(n+\tfrac{1}{2})^2+\frac{23}{4}\right]\Big/\left[a+\frac{c}{(n+\frac{1}{2})^2}\right]. \tag{30b}$$

The results obtained from (22) and (27) for several n and λ are shown in table 4.

5. Discussion

The simple analytical formulae presented in this paper reproduce the energy eigenvalues of the anharmonic oscillators (both for $\omega \neq 0$ and $\omega = 0$) for all n and λ quite well. Physical observables like the moments are also given satisfactorily by our

Table 4. Energy eigenvalues of the octic anharmonic and pure octic oscillators.

	Anharmonic oscillator $2E_n/\hbar\omega$			Pure octic oscillator
n \ ρ^2	0·000 1	1·0	10000·0	$2E_n/(2\lambda\hbar^8/m^4)^{1/5}$
2	5·025 83 (40)	11·25 (10·99)	66·48 (64·76)	10·52
5	11·362 (56)	36·588 (09)	224·56 (14)	35·564
10	23·744 (29)	100·879 (57)	628·42 (32)	99·564
100	605·184 (79)	3693·329 0 (8 7)	23283·471 91 (40)	3690·100 5
1000	23167·125 85 (10)	145860·545 64 (56)	920268·034 1 (3 6)	145852·450 91
0	1·000 653 (46)	1·56 (49)	8·57 (7·78)	1·35
1	3·005 82 (73)	5·65 (37)	32·28 (30·11)	5·16

Table 5 Residual correction to the pure quartic oscillator eigenvalue with $n = 49$

$\mathscr{E}_{49} = E_{49} + \epsilon_n = 397{\cdot}141\ 342 + \epsilon_n$

M	ϵ_n	$E_{49} + \epsilon_n$
2	−0·304 058	396·837 284
4	−0·250 690	396·890 652
7	−0·001 154	397·140 188
12	−0·000 012	397·141 330
14	−0·000 015	397·141 327
15	−0·000 015	397.141 327

Banerjee *et al*'s (1978) value: 397·141 327

expressions. It is interesting to note that the criterion adopted for determining the renormalized frequency is the same for all anharmonic potentials (quartic, sextic, etc.) A merit of our prescription for determining the value of $\omega_0(n, \lambda)$ for a given n and λ is the following: Let us suppose that for a given λ we wish to calculate the eigenvalue of the nth level of the AHO Hamiltonian to arbitrary accuracy. Our approximate expression E_n for this eigenvalue is (as pointed out in the text) just the nth diagonal element of the matrix whose elements H_{mn} are all calculated in the basis of the HO with the renormalized frequency $\omega_0(n, \lambda)$. Since E_n is quite close to the actual energy, the residual correction $\epsilon_n = (\mathscr{E}_n - E_n)$ will be quite small and much less than the level spacing ($|\mathscr{E}_{n+1} - \mathscr{E}_n|$). The value of ϵ_n can be estimated quite accurately by taking into account more and more elements of the matrix around H_{nn}. A systematic procedure for doing this has been developed by one of us (PMM) whose details will be published separately. For a typical value of $n = 49$ of the pure quartic oscillator ($\omega = 0$) we show in table 5 the numerical correction ϵ_n which is the smallest eigenvalue of the matrix $\mathscr{H} = H - H_{nn} I$, when $\mathscr{H}$ is truncated to be a $(2M + 1) \times (2M + 1)$

matrix whose central element is H_{nn}. The convergence rate is quite rapid and the accuracy obtainable is limited only by the computer tolerance (1 in 10^{15}). Finally we wish to observe that our method (for obtaining approximate energy values) can be extended to higher dimensional oscillators as well (Mathews *et al* 1981a).

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Appendix

We collect here the WKB results for the one-dimensional AHOs and then outline how the parameters a, b and c of the text are determined from the WKB coefficients.

The WKB expression for the energy of the general AHO Hamiltonian is given by

$$E_n^{(\mathrm{WKB})} = \left(\frac{\lambda \hbar^{2\alpha}}{m^\alpha}\right)^{\frac{1}{\alpha+1}} \left[x_\alpha \left\{ (n+\tfrac{1}{2}) + \frac{\delta_\alpha}{(n+\tfrac{1}{2})} \right\}^{\frac{2\alpha}{1+\alpha}} + y_\alpha \frac{(n+\tfrac{1}{2})^{\frac{2}{\alpha+1}}}{\lambda} \left(\frac{m\,\omega}{\hbar}\right)^2 \left(\frac{\hbar^2}{m}\right)^{\frac{2}{\alpha+1}} + \dots \right], \tag{A2}$$

where

$$x_\alpha = 2^{\left(\frac{\alpha-2}{\alpha+1}\right)} \left[\frac{\pi(\alpha+1)\,\Gamma(1/\alpha)}{\Gamma^2(1/2\alpha)}\right]^{\frac{2\alpha}{\alpha+1}}, \tag{A3}$$

and

$$y_\alpha = 2^{\left(\frac{2-\alpha}{1+\alpha}\right)} \left[\frac{\pi(\alpha+1)\,\Gamma(1/\alpha)}{\Gamma^2(1/2\alpha)}\right]^{\frac{2}{\alpha+1}} \frac{\Gamma(1/\alpha)\,\Gamma^2(3/2\alpha)}{\Gamma(3/\alpha)\,\Gamma^2(1/2\alpha)}. \tag{A4}$$

For the quartic AHO, Hioe and Montroll (1975) have estimated δ_2 to have a value of $\sim 0{\cdot}02650$. In a recent paper Pasupathy and Virendra Singh (1980) have obtained an analytic expression for the first two terms of the WKB series for pure $x^{2\alpha}$ potentials. More precisely, Pasupathy and Singh's result is for s-waves of the three-dimensional potential $V = \lambda r^k$, but as is well-known, the results for three-dimensional s-waves of such potentials and odd parity levels of the corresponding one-dimensional system are the same. For large n, it hardly matters whether n is even or odd. Their result gives

$$\delta_\alpha = \frac{(2\alpha-1)}{12\pi(\alpha+1)} \cot(\pi/2\alpha). \tag{A5}$$

For $\alpha = 2$, the above expression gives $\delta_2 = 1/12\pi = 0{\cdot}02652$ in agreement with Hioe and Montroll's value.

We shall now indicate how we have obtained the value of a, b and c (equation (12)) for the quartic anharmonic oscillator. For large n and λ, equation (11) gives the following value for ν

$$\nu \simeq [a/2\rho^2 (n+\tfrac{1}{2})]^{1/3} \left\{1 + \frac{1-2a+b}{3} [2\rho^2 (n+\tfrac{1}{2})]^{-2/3} + \dots\right\}. \tag{A6}$$

Substituting this in (7) , we obtain

$$E_n \simeq \left(\frac{\lambda \hbar^4}{m^2}\right)^{1/3} \left[A\,(n+\tfrac{1}{2})^{4/3} \left\{1 + \frac{C}{(n+\tfrac{1}{2})^2}\right\} + B\,(n+\tfrac{1}{2})^{2/3}\,\lambda^{-2/3} \left(\frac{m\omega}{\hbar}\right)^2 \left(\frac{\hbar^2}{m}\right)^{2/3} + \dots\right], \tag{A7}$$

with $$A = \frac{1}{2}\left(\frac{4}{a}\right)^{1/3}\left(1+\frac{3a}{4}\right)$$

$$B = \frac{1}{2}\left(\frac{a}{4}\right)^{1/3}\left\{1 + (1+b-2a)\left(\frac{1}{2} - \frac{1}{3a}\right)\right\} \tag{A8}$$

$$C = c\left(-\frac{1}{3a} + \frac{3}{(4+3a)}\right) + \frac{3a}{4(4+3a)}$$

Comparing (A7) and (A8) with (A2) and (A3) we obtain a, b and c in terms of the WKB coefficients. Using the values of the latter the parameters are determined to have values as given in (12). In a similar manner, the parameters of the sextic and octic AHOs have also been obtained. Incidentally we may point out that the leading WKB coefficient of the sextic AHO in equation (A2) *viz* x_3, has a value 1·34683 and not 1·346760 as given by Hioe *et al* (1976).

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