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Energy eigenvalues of quartic oscillators in $d \le 3$ dimensions

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Abstract. We present a simple approximate analytical expression for the energy eigenvalues $E^{(d)}$ of the pure quartic oscillator in $d \leq 3$ dimensions. The formula reproduces with high accuracy the results from accurate numerical computations reported in the literature. The eigenvalue $E_{n,l}^{(d)}$ for given *n* is seen to decrease as *l* increases contrary to the prediction of the Quigg-Rosner formula (for d = 3) which is incorrect in this respect. We also give a generalisation (from the pure quartic to the quartic anharmonic oscillator) of our formula, good for any *d*. This formula involves four parameters (one less in the pure quartic case) of which all but one are obtainable by consideration of the WKB limit; the values of all the parameters are independent of the dimension *d*.

1. Introduction

The literature available on higher-dimensional anharmonic oscillators is rather limited, when compared with that available for the one-dimensional system. Exhaustive numerical tables as well as many analytical formulae (with limited domains of validity) have been reported in the literature for the energy spectra associated with anharmonic potentials $V = \omega^2 x^2 + \lambda x^{2\alpha}$ in one dimension, both for the case $\omega \neq 0$ and $\omega = 0^{\dagger}$ (Bazley and Fox 1961, Chan and Stelman 1963, Biswas et al 1971, 1973, Lakshmanan and Prabhakaran 1973, Hioe and Montroll 1975, Hioe et al 1976, 1978, Banerjee et al 1978, Banerjee 1978, Ginsburg and Montroll 1978, Caswell 1979, Richardson and Blankenbecler 1979, Halliday and Suranyi 1980, Killingbeck 1981, Mathews et al 1981). Bell et al (1970a, b, see also Lu and Nigam 1969) have computed numerically the first 100 energy levels of the two- and three-dimensional quartic oscillators $(V = \lambda (\mathbf{r} \cdot \mathbf{r})^2)$ by diagonalising large dimensional matrices of order 800. More recently Pasupathy and Singh (1980), Quigg and Rosner (1979) and Lakshmanan and Kaliappan (1980) have derived approximate formulae for the three-dimensional quartic or quartic anharmonic oscillator (a system of interest in charmonium physics) via WKB or phase integral techniques. While Pasupathy and Singh's WKB results are for s waves, and are therefore equivalent to results for the one-dimensional system, the generalisation of the s-wave result to l > 0 by Quigg and Rosner is incorrect. (Their claim that for large but fixed n, the energy will depend only on n + l but not on n and l separately is at variance with the formula given in this paper as well as the numerical results known for the system.) Lakshmanan and Kaliappan have adopted the semiclassical Bohr-Sommerfeld quantisation scheme and as such their analytical formula is expected to be

⁺ The literature on the one-dimensional oscillator is so vast that what we have given is only a selective sample over the years in which a variety of methods has been used to obtain results.

satisfactory only in the large-n regime. Since no numerical results have been given by them, there is no information on the degree of accuracy of their formula. However for two- and three-dimensional oscillators a single analytical formula which is capable of yielding the energy values with a high degree of accuracy for all values of the quantum numbers has so far been lacking. It is our aim in this paper to present a simple and accurate formula for the energy levels $E_{n,l}^{(d)}$ of the pure quartic oscillator ($V = (\mathbf{r} \cdot \mathbf{r})^2$) in $d \leq 3$ dimensions. It reproduces with considerable accuracy the numerically computed values reported by earlier workers, for all values of level number n and the angular momentum quantum number l. To our knowledge no such formula has so far been published in the literature. We wish to emphasise that we consider the formula as an end in itself. No great profundity is involved in its derivation, but that does not detract in any way from its utility as a means of estimating $E_{n,l}^{(d)}$ quickly for any desired n, l and d. This estimate could be very useful as a starting point in various types of numerical schemes intended for calculation of eigenvalues to arbitrary accuracy. It is in the same spirit that we also write down, towards the end of the paper, a formula for the energy levels of the quartic anharmonic oscillator $(V = \frac{1}{2}m\omega^2 \mathbf{r} \cdot \mathbf{r} + \lambda (\mathbf{r} \cdot \mathbf{r})^2)$ in d dimensions. This generalises the expression of the d = 1 case presented in a recent note by Mathews et al (1981).

The approximate expression that we give below for the energy eigenvalue $E_{n,l}^{(d)}(\lambda)$ of the Hamiltonian

$$H^{(d)} = \frac{1}{2m} \boldsymbol{p} \cdot \boldsymbol{p} + \frac{1}{2}m\omega^2 \boldsymbol{r} \cdot \boldsymbol{r} + \lambda \left(\boldsymbol{r} \cdot \boldsymbol{r}\right)^2$$
$$H^{(d)} |\psi\rangle = E^{(d)} |\psi\rangle$$

(where r and $p = -i\nabla$ are position and momentum operators in d(=1, 2, 3) dimensions) is nothing but the expectation value of $H^{(d)}$, calculated with respect to the basis states of a 'renormalised harmonic oscillator'. The details of how to choose the renormalised frequency $\omega_0(n, l, \lambda)$ so as to make the expectation value quite close to the actual energy will be discussed in the next section. We may also mention here that the work of Banerjee and co-workers (1978) for the one-dimensional oscillator also rests on the use of renormalised basis states, but their aim is not to obtain a simple analytic formula for E_n but to compute E_n numerically to high accuracy[‡].

2. Energy values of the pure quartic oscillators

The Hamiltonian for a particle moving in a quartic potential

$$V = \lambda \left(\boldsymbol{r} \cdot \boldsymbol{r} \right)^2 \tag{1}$$

(where $r = (r_1, r_2, ..., r_d)$ and d = (1, 2 or 3)) is given by \ddagger

$$H^{(d)} = \frac{1}{2m} \mathbf{p} \cdot \mathbf{p} + \lambda \left(\mathbf{r} \cdot \mathbf{r} \right)^2.$$
⁽²⁾

 \dagger Killingbeck (1981) has developed a perturbation series method for the one-dimensional AHO using a renormalised harmonic oscillator basis states, but his perturbation series is expected to be divergent. The divergent Rayleigh-Schrödinger series is known to be summable by the method of Pade approximants (Loeffel *et al* 1969), and one of the referees has stated that Austin and Killingbeck have found similar Padé summability for Killingbeck's renormalised perturbation series.

[‡] The results for the potential $V = \frac{1}{2}m\omega^2 \mathbf{r} \cdot \mathbf{r} + \lambda (\mathbf{r} \cdot \mathbf{r})^2$ will be mentioned at the end.

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A scaling argument shows readily that the eigenvalues of (2) are $(\lambda \hbar^4/m^2)^{1/3}$ times those of $\frac{1}{2}\mathbf{p} \cdot \mathbf{p} + (\mathbf{r} \cdot \mathbf{r})^2$ and we can therefore assume without loss of generality that $m = \lambda = \hbar = 1$. We consider now the matrix representation of $H^{(d)}$ in a harmonic oscillator basis which diagonalises

$$H_0^{(d)} = \frac{1}{2} \mathbf{p} \cdot \mathbf{p} + \frac{1}{2} \omega_0^2 \mathbf{r} \cdot \mathbf{r}$$
(3)

where ω_0 is a renormalised frequency. The non-vanishing matrix elements of $H^{(d)}$ are easily determined (Bell 1970):

$$\langle n, l | H^{(d)} | n, l \rangle \equiv H_{nn}$$

= { $\frac{1}{2}(n + \frac{1}{2}d) + \frac{1}{4}\omega_0^{-3}[6n(n+d) - 2l(l+d-2) + d(d+2)]\}\omega_0$ (4a)
 $\langle n, l | H^{(d)} | n+2, l \rangle = \langle n+2, l | H^{(d)} | n, l \rangle \equiv H_{n,n+2}$

$$= [(n-l+2)(n+l+d)]^{1/2} [\frac{1}{4} - \omega_0^{-3}(n+\frac{1}{2}d+1)] \omega_0$$
(4b)

$$\langle n, l | H^{(d)} | n+4, l \rangle = \langle n+4, l | H^{(d)} | n, l \rangle \equiv H_{n,n+4}$$

= $\frac{1}{4}\omega_0^{-2} [(n-l+2)(n-l+4)(n+l+d)(n+l+d+2)]^{1/2}$ (4c)

where n = 0, 1, 2, ... and for given n, l takes values[†] n, n-2, n-4, ..., 1 or 0. The frequency ω_0 is arbitrary and, as yet, undetermined. For a given n and l, we wish to choose ω_0 in such a way that the diagonal element (4a) closely approximates the actual eigenvalue $E_{n,l}^{(d)}$. The fairly obvious idea that this may become possible if we make the matrix elements immediately close to H_{nn} (namely $H_{n\pm 2,n}$ and $H_{n,n\pm 2}$) as small as possible leads to the condition

$$\omega_0^3 = 4(n + \frac{1}{2}d). \tag{5}$$

We shall see that with slight modifications of this equation (dictated by what is known about the asymptotic—large-n—limit of E_n and other considerations) the energy eigenvalues with quite high accuracy are obtained from (4a):

$$E_{n,l}^{(d)} \simeq H_{nn} = \{\frac{1}{2}(n+\frac{1}{2}d) + \frac{1}{4}\omega_0^{-3}[6n(n+d) - 2l(l+d-2) + d(d+2)]\}\omega_0.$$
(6)

2.1 Refinement in the choice of ω_0

(i) One-dimensional case (d = 1). In the large-n limit, equations (5) and (6) yield, to the two leading orders in $(n + \frac{1}{2})$,

$$E \simeq 1.389(n + \frac{1}{2})^{4/3} \left(1 + \frac{3}{28(n + \frac{1}{2})^2} \right).$$
⁽⁷⁾

Equation (7) has the same form as the two leading terms in the asymptotic WKB expression (Hioe and Montroll 1975, Pasupathy and Singh 1980). In the latter,

$$E^{(WKB)} \simeq C(n+\frac{1}{2})^{4/3} \left(1+\frac{\delta}{(n+\frac{1}{2})^2}+\ldots\right)$$

where $C = 3^{4/3} \pi^2 [\Gamma(\frac{1}{4})]^{-8/3} = 1.3765074$ and $\delta = 1/9\pi = 0.0354$. The values in (7) namely 1.389 and 3/28 are not very far from the corresponding WKB ones. It is readily seen that adjustment of these coefficients can be accomplished by modifying the

[†] For d = 2, the angular momentum is actually $\pm l$ but the energy is degenerate with respect to the sign. Clearly l = 0 for the one-dimensional oscillator. PM Mathews, M Seetharaman and S Raghavan

defining equation for ω_0 to

$$\omega_0^3 = \frac{4(n + \frac{1}{2}d)}{a + c/(n + \frac{1}{2}d)^2}.$$
(8)

The large-*n* limit of E of equation (6) then retains the same form as (7) but with the two leading coefficients modified to

$$\frac{1}{2}(4/a)^{1/3}(1+\frac{3}{4}a) \tag{9}$$

and

$$c\left(-\frac{1}{3a}+\frac{3}{4+3a}\right)+\frac{3a}{4(4+3a)}$$
(10)

respectively.

Note that only a is involved in the leading coefficient, and that the second coefficient involves c linearly. By requiring (9) and (10) to have the WKB values we find the values needed for a and c to be

$$a = 0.895\ 647\ 259\tag{11}$$

$$c = -0.85.$$
 (12)

The energies now calculated from (6) and (8) are given in table 1, and as can be seen, they are in good agreement with numerical results of Banerjee *et al* (1978) not only in the region of large *n* but over the entire range of *n* values. It may be mentioned here that in a recent note by us (Mathews *et al* 1981) a more general formula applicable to anharmonic oscillators in one dimension $(V = \frac{1}{2}m\omega^2 x^2 + \lambda x^4)$ was presented. It involves, besides the same *a* and *c* as above, one more parameter *b*. The generalisation of that formula to *d* dimensions is given in equations (15) and (16) below.

(ii) d = 3. It is well known that the s-wave levels in a spherically symmetric potential are the same as the odd-parity levels of the one-dimensional system with the

Table 1. Energy levels of the pure quartic oscillator in one dimension.

n	Energy $E_{n,0}^{(1)}$
0	0.675
	(68)
2	4.700
	(697)
4	10.244 92
	(31)
6	16.712 1
	(19)
8	23.890 1
	(0 0)
10	31.659 54
	(46)
20	77.236 11
	(08)
48	243.467 364
	(38)

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same potential. More precisely $E_{n,0}^{(3)} = E_{n+1}^{(1)}$. Consequently the WKB limit has the same form as in the one-dimensional case and hence also the same values of the parameters aand c in ω_0 (equation (8)). One sees from the expression (6) that $E_{n,l}^{(3)}$ decreases as lincreases (for fixed n), through a term proportional to l(l+1). While this is found to take care of the l dependence very well for large n, small deviations from the available numerical results appear when n is small. An empirical modification, consisting of a change in the defining equation of ω_0 to

$$\omega_0^3 = \frac{4(n + \frac{1}{2}d)}{a + [c + el(l + d - 2)]/(n + \frac{1}{2}d)^2}$$
(13)

with e = -0.1 almost wipes out even these discrepancies, reducing the residual error to less than 1% at the worst (which occurs for small n). The form (13) is chosen in order

n l	0	2	4	6	8
0	1.490				
	(77)				
2	6.001 6	5.671			
	(3 4)	(24)			
4	11.801 4	11.545	10.82		
	(24)	(35)	(76)		
6	18.458 05	18.249 3	17.640	16.68	
	(82)	(54)	(16)	(60)	
8	25.791 17	25.613 2	25.088	24.240	23.12
	(79)	(15)	(76)	(01)	(01)
10	33.693 8	33.537 4	33.073	32.316	31.292
	(4 3)	(66)	(67)	(295)	(33)
20	79.763 7	79.661 5	79.355 84	78.849 3	78.146
	(4 1)	(17)	(19)	(63)	(38)
48	246.823 10	246.764 9	246.590 41	246.299 89	245.893 797
	(26)	(51)	(64)	(300 07)	(12)
	1	3	5	7	9
1	3,424			······	
	(398)				
3	8.704 2	8.15			
	(04)	(09)			
5	14.978 6	14.526	13.671		
	(78)	(09)	(01)		
7	21.999 662	21.6187	20.880	19.83	
	(00)	(13)	(50)	(74)	
9	29.634 71	29.304	28.654	27.71	26.52
	(88)	(00)	(38)	(67)	(40)
11	39.798 09	37.503 6	36.923	36.071	34.972
	(35)	(15)	(13)	(42)	(02)
21	84.841 9	84.643 92	84.249 5	83.662	82.885
	(2 2)	(86)	(8 2)	(57)	(74)
49	253.547 47	253.432 66	253.203 20	252.859 45	252.401 93
	(65)	(87)	(43)	(57)	(59)

Table 2. Energy levels $E_{n,l}^{(2)}$ of the pure quartic oscillator in two dimensions.

$\sum I$					
n	0	2	4	6	8
0	2.41				
	(39)				
2	7.3357	6.879			
	(70)	(30)			
4	13.379 69	13.019	12.22		
	(34)	(05)	(16)		
6	20.221 0	19.922	19.225	18.24	
	(0 9)	(16)	(18)	(15)	
8	27.706 49	27.449 1	26.859	25.963	24.80
	(39)	(59)	(45)	(19)	(69)
10	35.740 380	31.512 9	34.988 4	34.182	33.12
	(12)	(10)	(02)	(57)	(06)
20	82.299 370	82.148 51	81.7977	81.249 8	80.51
	(45)	(23)	(6.5)	(5 9)	(50)
48	250.183 369	250.096 671	249.894 504	249,577 179	249.145 2
	(51)	(79)	(45)	(38)	(4.8)
	1	3	5	7	9
1	4.51			****	
	(48)				
3	10.108	9.458			
	(00)	(01)			
5	16.602	16.067	15.16		
	(00)	(46)	(08)		
7	23.797 6	23.341	22.546	21.46	
	(62)	(32)	(08)	(36)	
9	31.578 86	31.1790	30.474	29.490	28.26
	(08)	(36)	(55)	(36)	(14)
11	39.869 49	39.512	38.877	37.982	36.85
	(01)	(09)	(65)	(49)	(77)
21	87.392 96	87.149 3	86.712 6	86.086 1	85.275
	(87)	(88)	(06)	(0.5)	(62)
49	256.916 238	256.773 69	256.517 316	256.147 50	255.664 80
	(20)	(74)	(38)	(37)	(15

Table 3. The energy levels $E_{n,l}^{(3)}$ of the pure quartic oscillator in three dimensions.

that the asymptotic expression (for large n) should have the same form as with old definition of ω_0 , except for the necessary small changes in the values of the numerical coefficients appearing in the leading two orders. The values of $E_{n,l}^{(3)}$ calculated from (6) with ω_0 , a, c and e given by (13), (11) and (12) are tabulated (table 3) and found to be in good agreement over the entire range of n and l for which accurate numerical values are available from earlier works[†].

(iii) d = 2. The common formula equations (6) and (13) applicable to d = 1 and d = 3 was itself found to be very accurate for d = 2 also, with the parameters a, c and e having the same values as in (11) and (12). The results are given in table 2.

[†] One of the referees has intimated that according to unpublished calculations by Killingbeck based on the renormalised perturbation series, the results of Bell *et al* (1970b) in the case d = 3 are slightly in error (in the last one or two decimal places given) for n > 20.

3. Discussion

The results for different n, l in the three cases d = 1, 2 and 3 are presented in tables 1, 2 and 3. 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.

A few observations on our results are in order. Firstly, the estimation of the ground-state and the first-excited-state energy values is not as good as for higher levels. The reason is basically that, while for other values of $n(n \ge 2)$ 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 n = 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 $H_{n,n}$ to take account of the off-diagonal elements very close to H_{00} or H_{11} as the case may be[†]. Secondly, as we have seen above, for given n we have adopted a renormalised frequency $\omega_0(n)$ by equation (13) and the *n*th diagonal element H_{nn} of the Hamiltonian matrix in the basis of *this* renormalised ω_0 then closely approximates the actual energy E_n . The merit of our prescription for choosing $\omega_0(n)$ is that the smallest eigenvalue ε_n of the matrix $\mathcal{H} = H - H_{nn}I$ (where I is a unit matrix) turns out to be close to zero thereby showing that the off-diagonal elements of H around H_{nn} (in the basis of $\omega_0(n)$) contribute only a small correction to H_{nn} . In table 4 we exhibit for a typical case, n = 45, l=9 the values of ε_n when \mathcal{H} is truncated to be a $(2M+1)\times(2M+1)$ matrix with elements

$$\mathcal{H}_{ij} = H_{2i-n,2j-n} - H_{nn\delta_{ij}} \qquad (i, j = n - M, \ldots, n + M).$$

We observe from table 4 that as M increases the value of ε_n stabilises, and the corrected energy $H_{nn} + \varepsilon_n$ coincides with the Bell *et al* (1970b) value[‡]. Thirdly, for both two- and three-dimensional oscillators, the energy will decrease with l (for fixed n). The formula given by Quigg and Rosner for the WKB regime depends only on n + l, and as such, for fixed n, predicts an increase of E which is incorrect (cf the table of $E_{n,l}$ computed by Bell *et al*).

М	ε_n	$E_{45,9} + \varepsilon_n$
2	-0.160 332	228.662 062
3	-0.822 558	227.999 836
5	-0.066 226	228.756 168
8	-0.000 192	228.822 202
10	-0.000 960	228.821 434
12	-0.000 988	228.821 406
15	-0.000 997	228.821 397
		(228.821 395)

Table 4. Residual correction to the eigenvalue with n = 45, l = 9. $\mathscr{E}_{45,9} = E_{45,9} + \varepsilon_n = 228.822394 + \varepsilon_n$.

⁺ What is shown against n = 0 in the tables is not $H_{00}^{(d)}$ but the lower of the eigenvalues of the matrix $\begin{pmatrix} H_{00}^{(d)} & H_{02}^{(d)} \\ H_{20}^{(d)} & H_{22}^{(d)} \end{pmatrix}$ in a representation with ω_0 given by (13) with a - 1 = c = e = 0. For n = 1 also the effect of the

nearest off-diagonal elements $H_{13}^{(d)}$, $H_{31}^{(d)}$ has been taken into account in a similar fashion.

[‡] A powerful algorithm for estimating ε numerically to a high accuracy (one part in 10¹⁵) has been developed by one of us (PMM) the details of which will be published separately.

Finally we give below an expression for the eigenvalues $E_{n,l}^{(d)}$ of the anharmonic oscillator Hamiltonian in $d \leq 3$ dimensions.

$$H = p^{2}/2m + \frac{1}{2}m\omega^{2}r \cdot r + \lambda (r \cdot r)^{2}$$
⁽¹⁴⁾

$$E_{n,l}^{(d)} = \{\frac{1}{2}\nu^{-1}(n+\frac{1}{2}d)(1+\nu^2) + \frac{1}{8}\rho^2\nu^2[6n(n+d) - 2l(l+d-2) + d(d+2)]\}\hbar\omega$$
(15)

where $\rho^2 = 2\lambda \hbar/m^2 \omega^3$ and $\nu = \omega/\omega_0$ is the solution lying between 0 and 1 of the algebraic equation

$$(2n+d)\rho^{2}\nu^{3} = (1-\nu^{2})\left(1+(a-1)(1-\nu^{2})+b\nu^{2}+\frac{c+el(l+d-2)}{(n+\frac{1}{2}d)^{2}}\right)$$
(16)

where the values of the constants a, c and e are the same as in equations (11) and (12) and

$$b = -0.125\ 020.$$

This value of b was found necessary in order that in the WKB limit, the coefficient of the next to the leading term in λ of the energy (namely 0.268 055 $\lambda^{-1/3}(n+\frac{1}{2})^{2/3}$) is also reproduced correctly by (15).

The special case of this formula with d = 1 was first proposed by Mathews *et al* (1981) who demonstrated its accuracy over the entire domain of n and λ values. Also as $\omega \to 0$ (for any d) equations (15) and (16) do go over into the equations (6) and (13) of the pure quartic case which were considered in detail in this paper. In view of the experience with both these special cases ($d = 1, \omega$ arbitrary; $\omega \to 0, d = 1, 2, 3$) it is to be expected that the formula (15) will yield results of the same kind of accuracy also for d = 2, 3 with $\omega \neq 0$. We do not present any numerical results for these anharmonic oscillators, however, as no independently computed values are available in the literature for comparison purposes.

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Note added in proof. The n of Quigg and Rosner is the radial quantum number n_r and is related to our n as $n = 2n_r + l$. The Quigg-Rosner levels with different sets of values of n_r and l but with a fixed n are therefore degenerate in energy. The l-dependent term in our formula (6) removes this degeneracy. The l-dependence of the Quigg-Rosner formula is spurious in the same sense as that of the formula for the hydrogen atom would be if it were written in terms of the radial quantum number as constant/ $(n_r + l + 1)^2$.

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