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Anharmonic oscillators in higher dimension: Accurate energy eigenvalues and matrix elements

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Abstract. Energy eigenvalues and matrix elements of various anharmonic oscillators are determined to a high accuracy by applying a method for determining the eigenvalues and eigenvectors of real symmetric para-p diagonal matrices (described in the preceding paper). Our results for the 2- and 3-dimensional oscillators are new and complement similar accurate results for the one dimensional oscillators available in the literature.

Keywords. Anharmonic oscillators; energy eigenvalues; matrix elements.

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1. Introduction

As an application of the method presented by us in the preceding paper, we consider here the determination of the energy values and other physical observables of various anharmonic oscillators (AHO), in one or higher dimensions. There is a vast literature on AHOs and a critical analysis of these may be found in the work of Bhargava (1982). As we are interested in computing the energies and other observables of the AHOs to a very high accuracy, we deem it necessary to discuss only those methods in the literature that sought to obtain highly accurate results and compare them with our method. The method of Hill determinant by Biswas *et al* (1971) and its improvisation by Banerjee *et al* (1978) and the moment method of Richardson and Blankenbecler (1979) are therefore the ones upon which we shall now comment.

The work of Biswas *et al* was the first to claim arbitrary accuracy for the energy values. In their technique, the Schrödinger equation is converted into a matrix eigenvalue equation by expanding the energy functions as $\psi = \exp(-x^2/2)\sum_m c_m x^m$. The resulting infinite determinant is evaluated by truncation (to a $N \times N$ matrix) and in the limit of $N \to \infty$ one recovers the eigenvalues. Their matrix is specifically non-

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symmetrical and therefore the appearance of spurious complex or unphysical energy eigenvalues at the intermediate stages of the calculation could not be ruled out. Also, the dimension of the matrix needed to yield a particular energy level is very much larger compared to the level number itself. In contrast, our method is based on symmetric matrices and hence at no stage do complex values ever appear. The dimension of the matrix needed is also much less than the level number. Typically, in our case a matrix dimension of about 25 is enough to secure a 15-figure accuracy to all low-lying levels and this dimension increases to about 140 for the 500th level for the same accuracy. The method of Banerjee *et al* is a significant improvement over the method of Biswas *et al* but our above remarks hold for this method as well. Both Biswas *et al* and Banerjee *et al* deal extensively with the one-dimensional oscillators. In contrast, we focus on higher dimensions. Regarding the method of Richardson and Blankenbecler, one computes energies by starting with asymptotic expressions for the diagonal moments of x^N with large N and uses, the hypervirial theorem to compute x^N for lower N's down to zero. The lowermost moment is related to the energy in a simple manner. This is essentially a trial and error method. To get the various energy levels one has to make a suitable guess for the $\langle x^N \rangle$ for large N in any particular eigenstate. For instance, one has to start with $N = 10^4$ to get a 9-figure accuracy of the lowest level for a quartic oscillator. Further, the method was typically designed for a one-dimensional problem and its extension to higher dimensions and the resulting efficiency are not fully investigated. In contrast, our method is applicable to any AHO in higher dimensions as well.

We shall illustrate our method by computing the eigenvalues and matrix elements for the Hamiltonian

$$H = \mathbf{p}^2/2m + \tfrac{1}{2}mw^2r^2 + \lambda r^4 \tag{1}$$

in 1, 2 or 3 dimensions. Since the analysis is similar, only results for the case

$$H = \mathbf{p}^2/2m + \tfrac{1}{2}mw^2r^2 + \lambda r^6$$

will be given at the end.

2. Basis, matrix elements and the approximate energy level formula

We wish to determine the energy levels and matrix elements of H in (1). Let $E_{k,l}$ be the energy eigenvalue of the kth level with an orbital angular momentum l. Since l is a good quantum number, H has non-vanishing matrix elements only between states of the same l. To choose a basis set of states for this kth level, we rewrite the Hamiltnonian as

$$H = \mathbf{p}^2/2m + \tfrac{1}{2}mw_0^2r^2 + \tfrac{1}{2}m(w^2 - w_0^2)r^2 + \lambda r^4. \tag{2}$$

The 'renormalized' frequency w_0 is so chosen that the expectation value of H in the kth state of the harmonic oscillator with frequency w_0 provides a good approximation to $E_{k,l}$. In an earlier paper, we have discussed how this must be done (Mathews *et al* (1981a, b)). To recall, define

$$\nu = w/w_0 \quad \text{and} \quad \rho^2 = 2\lambda\hbar/m^2w^3 \tag{3a}$$

and choose v to be the root between 0 and 1 of the equation

$$(2k+d)\rho^2 v^3 = (1-v^2)\left[1+(a-1)(1-v^2)+bv^2+\frac{c+el(l+d-2)}{\left(k+\frac{d}{2}\right)^2}\right], \quad (3b)$$

where d is the dimension of the space ($d = 1, 2, 3$). The constants a, b, c and e are independent of d and their values are $a = 0{\cdot}895\ 647\ 259$ $b = -0{\cdot}125\ 020$ $c = -0{\cdot}85$ $e = -0{\cdot}1$. The expectation value of H in the kth state $|k, l\rangle$ of the harmonic oscillator with w_0 determined from the above is given by

$$H_{kl,kl} = \langle kl|H|kl\rangle = \tfrac{1}{2}(1+v^2)\left(k+\frac{d}{2}\right) + \tfrac{1}{8}\rho^2 v^3\{6k(k+d) - 2l(l+d-2) + d(d+2)\}. \quad (4)$$

The expectation value of H given in (4) then provides a good approximation to the kth energy level of (1). In the basis of harmonic oscillator states with frequency w_0, the non-vanishing elements of H are given by

$$H_{nl,nl} = \left[\tfrac{1}{2}(1+v^2)\left(n+\frac{d}{2}\right) + \tfrac{1}{8}\rho^2 v^3(6n(n+d) - 2l(l+d-2) + d(d+2))\right], \quad (5a)$$

$$H_{nl,n+2l} = H_{n+2l,nl} = \left[-\tfrac{1}{4}(1-v^2) + \tfrac{1}{2}\rho^2 v^3\left(n+\frac{d}{2}+1\right)\right] \times [(n-l+2)\cdot(n+l+d)]^{\frac{1}{2}}, \quad (5b)$$

$$H_{nl,n+4l} = H_{n+4l,nl} = \tfrac{1}{8}\rho^2 v^3[(n-l+2)(n-l+4) \times (n+l+d)(n+l+d+2)]^{\frac{1}{2}}, \quad (5c)$$

in $\hbar w_0$ units. The formula (4) will be the starting approximation for applying our method described in the preceding paper (Bhargava *et al* 1989) to determine the energy levels quite accurately. We observe at the outset that the angular momentum and parity are good quantum numbers and therefore the Hamiltonian matrix can be separated into a direct sum of submatrices $H^{(l)}$ pertaining to a particular l and parity. Because the diagonal element associated with the quantum number k of the Hamiltonian H^l in the representation chosen by us is very close to the corresponding eigenvalue, the matrix $\mathbf{H}^l = (H^l - H_{kl,kl}I)$ will have a very small value for its eigenvalue labelled by this particular k. Let this eigenvalue be ε_{kl}. Then, by definition,

$$E_{kl} = H_{kl,kl} + \varepsilon_{kl}. \quad (6)$$

Our task therefore is to determine that the eigenvalue ε of $\mathbf{H}^l$ which is very close to zero.

The matrix $\mathbf{H}^l$ is symmetric and para-2-diagonal and by construction the kth

diagonal element of this is zero. Therefore $\mathbf{H}^l$ can be put in the partitioned form

$$\mathbf{H}^l = \begin{pmatrix} A & x & B \\ \tilde{x} & 0 & \tilde{y} \\ \tilde{B} & y & C \end{pmatrix}$$

which we have dealt with in the preceding paper. More explicitly,

$$\mathbf{H}^l = \begin{pmatrix} \ddots & \ddots & & & & & & \\ \ddots & P_3 & U_2 & & & & & \\ & \tilde{U}_2 & P_2 & U_1 & & & & \\ & & \tilde{U}_1 & P_1 & x_u & \beta & & \\ & & & \tilde{x}u & 0 & \tilde{y}_u & & \\ & & & \tilde{\beta} & y_u & Q_1' & \tilde{U}_1' & \\ & & & & & U_1' & Q_2' & \tilde{U}_2' \ddots \\ & & & & & & U_2' & Q_3' \ddots \\ & & & & & & \ddots & \ddots \end{pmatrix} \tag{7}$$

where the P_i, Q_i', U_i, U_i', β are all 2×2 blocks and x_u and y_u are 2×1 columns. All elements outside these blocks are zero. We observe that the labels of adjacent rows or columns of the matrix differ by 2. By a relabelling, this can be made 1 as follows:

Let us define for even n

$$n = 2r - 2, \quad (r = 1, 2, 3, \ldots)$$

$$k = 2s - 2, \quad (s = \text{some fixed positive integer}).$$

With this correspondence between n and r, we replace

$$\mathbf{H}^l_{nn} \to q_r,$$

$$\mathbf{H}^l_{nn+2} \to l_r,$$

$$H^l_{nn+4} \to p_r$$

and the explicit expressions for the q_s', l's and p's are follows:

$$q_r = (r - s)\left[(1 + v^2) + 3\rho^2 v^3 \left(r + s + \frac{d}{2} - 2 \right) \right], \tag{8a}$$

$$l_r = \left[-\tfrac{1}{2}(1 - v^2) + 2\rho^2 v^3 \left(r + \frac{d}{4} - \frac{1}{2} \right) \right] \times [(r - l/2)(r + l/2 + d/2 - 1)]^{\frac{1}{2}}, \tag{8b}$$

$$p_r = \tfrac{1}{2}\rho^2 v^3 [(r - l/2)(r - l/2 + 1)(r + l/2 + d/2 - 1)(r + l/2 + d/2)]^{\frac{1}{2}} \tag{8c}$$

in units of $\hbar w_0$. (For the odd-parity levels, similar change of indices can be made).

In the notation of the preceding paper, the various blocks in the partitioned form of $\mathbf{H}^l$ may now be written in terms of q, l and p.

$$x_u = \begin{pmatrix} p_{s-2} \\ l_{s-1} \end{pmatrix}; \quad y_u = \begin{pmatrix} l_s \\ p_s \end{pmatrix}; \quad \beta = \begin{pmatrix} 0 & 0 \\ p_{s-1} & 0 \end{pmatrix}, \tag{9}$$

$$P_i = \begin{pmatrix} q_{s-2i} & l_{s-2i} \\ l_{s-2i} & q_{s-2i+1} \end{pmatrix}, \tag{10}$$

$$U_i = \begin{pmatrix} p_{s-2i-2} & 0 \\ l_{s-2i-1} & p_{s-2i-1} \end{pmatrix}, \tag{11}$$

$$Q_i' = \begin{pmatrix} q_{s+2i-1} & l_{s+2i-1} \\ l_{s+2i-1} & q_{s+2i} \end{pmatrix}, \tag{12}$$

$$U_i' = \begin{pmatrix} p_{s+2i-1} & l_{s+2i} \\ 0 & p_{s+2i} \end{pmatrix}. \tag{13}$$

3. Computation of ε_{kl}

The remaining task is to compute ε_{kl}, the eigenvalue close to zero of the matrix $\mathbf{H}^l$. It will be recalled—see (6)—that this is the residual to be added to H_{klkl} in order to obtain the energy eigenvalue E_{kl}. This is done by applying the theory of § 2 of our previous paper to the matrix $\mathbf{H}^l$ of (7) but $\mathbf{H}^l$, which is an infinite dimensional matrix, must first be truncated. Suppose we truncate $\mathbf{H}^l$ in such a way that the block at the top left hand corner is P_L, and the last one at the bottom right hand corner is $Q_{L'}'$, i.e., $2L$ rows above (and columns to the left of) the 'central' element are retained as well as $2L'$ rows below (and columns to the right of) the central element. As L and L' are both increased the eigenvalues of the truncated matrix would approach those of the full matrix $\mathbf{H}^l$.

For the truncated matrix we have to set up and solve the equation (§ 2 of previous paper)

$$\varepsilon = f(\varepsilon), \tag{14a}$$

where

$$f(\varepsilon) = \tilde{x}_u[1 - \sigma(\varepsilon)\tilde{\beta}]^{-1}[\sigma(\varepsilon)y_u - \phi(\varepsilon)x_u] + \tilde{y}_u[1 - \tilde{\sigma}(\varepsilon)\beta]^{-1}[\tilde{\sigma}(\varepsilon)x_u - \chi(\varepsilon)y_u] \tag{14b}$$

with

$$\sigma(\varepsilon) = \phi(\varepsilon)\beta\chi(\varepsilon) \tag{14c}$$

$\phi(\varepsilon)$ being the 2×2 block at the bottom right hand corner of $(A - \varepsilon I)^{-1}$ and $\chi(\varepsilon)$ the top left hand corner block (2×2) of $(C - \varepsilon I)^{-1}$. The matrices $(A - \varepsilon I)$ and $(C - \varepsilon I)$ for the

current problem are

$$(A-\varepsilon I)=\begin{pmatrix} T_L & U_{L-1} & & & & \\ \tilde{U}_{L-1} & T_{L-1} & \ddots & & & \\ & \ddots & \ddots & U_2 & & \\ & & & \tilde{U}_2 & T_2 & U_1 \\ & & & & \tilde{U}_1 & T_1 \end{pmatrix} \tag{15a}$$

with (15b)

$$T_i = P_i - \varepsilon I$$

and

$$(C-\varepsilon I)=\begin{pmatrix} R'_1 & \tilde{U}'_1 & & & & \\ U'_1 & R'_2 & \tilde{U}'_2 & & & \\ & U'_2 & \ddots & \ddots & & \\ & & \ddots & R'_{L'-1} & \tilde{U}_{L'-1} & \\ & & & U'_{L'-1} & R'_L & \end{pmatrix} \tag{16a}$$

with

$$R'_i = Q'_i - \varepsilon I \tag{16b}$$

x_u, y_u, β, P_i, U_i, Q'_i and U'_i are defined in (9) to (11). To compute $\phi(\varepsilon)$ for any particular ε we start with $\phi_L = T_L^{-1}$ and use the recurrence relation $\phi_i = (T_i - \tilde{U}_i \phi_{i+1} U_i)^{-1}$ repeatedly till we get ϕ_1 which is by definition $\phi(\varepsilon)$. Similarly, we compute $\chi(\varepsilon) \equiv \chi_1$ by starting with $\chi_{L'} = (R'_{L'})^{-1}$ and using the recurrence relation $\chi_i = (R'_i - \tilde{U}'_i \chi'_{i+1} U_i)^{-1}$ Having determined both ϕ and χ, one is able to compute $\sigma(\varepsilon)$ and finally $f(\varepsilon)$.

In our computation we have used the iterative Newton-Raphson process

$$\varepsilon_{i+1} = \varepsilon_i - F(\varepsilon_i)/[F'(\varepsilon_i)], \tag{17}$$

where $F(\varepsilon) \equiv \varepsilon - f(\varepsilon)$. Actually instead of $F'(\varepsilon_i)$, the slope of the tangent at ε_i, the slope of a chord at ε_i, namely $[F(\varepsilon_i + \delta_i) - F(\varepsilon_i)]/\delta_i$ was used with δ_i chosen as a small fraction of $(\varepsilon_i - \varepsilon_{i-1})$. The starting value of ε was taken as $\varepsilon_0 = 0$ (since the root we are seeking is the one near zero) and δ_0 was taken as about one thousandth of the level spacing at the energy level of interest. For large k, the dominant dependence of E_k on k is as $(k+\frac{1}{2})^{4/3}$, from which the level spacing $\sim \partial E_k/\partial k$ comes out to be $3E_k/4k \approx 3H_{kk}/4k$. It was satisfactory to take $\delta_0 = H_{kk}/1000k$ for all k except $k=0$. (For $k=0$, we have used $k+1$ instead of k in slope determination). The iteration was continued till $(\varepsilon_{i+1} - \varepsilon_i)/\varepsilon_i$ became less than 10^{-15}. The converged value, which is the eigenvalue ε_{kl} of $\mathbf{H}^l$, added to H_{klkl} then gave the eigenvalue E_{kl} sought. The value of H_{klkl} was itself calculated from (5a), the value of v occurring therein being obtained by the numerical solution of (3). Recalling that the matrix elements have been given in units of $\hbar w_0$, one has to

multiply the number obtained for E_{kl} obtained as above (in $\hbar w_0$ units) by $1/v$ in order to convert to $\hbar w$ units. The tabulated results are all of course in units of $\hbar w$.

The computations were all done on the IBM 370 computer system at IIT, Madras. Tables 1 and 2 show the results obtained for the quartic AHOs in 2- and 3-dimensions for a typical value $\rho^2 = 1$ (equivalent to $\lambda_{\text{Banerjee}} = 2 \times \lambda_{\text{Montroll}} = 1$) of the degree of anharmonicity.

Table 1. Two-dimensional quartic anharmonic oscillator.

k	l	$2E_{kl}$	
0	0	0·295 205 009 196 287	4×10^1
1	1	0·646 290 599 986 387	1×10^1
2	0	0·108 824 355 768 198	0×10^2
	2	0·103 906 272 955 037	8×10^2
5	1	0·259 691 635 685 670	1×10^2
	3	0·253 133 789 941 425	1×10^2
	5	0·240 331 661 934 708	4×10^2
10	0	0·567 798 591 256 604	1×10^2
	2	0·565 506 297 037 042	2×10^2
	4	0·558 667 656 239 447	8×10^2
	6	0·547 392 009 847 857	0×10^2
	8	0·531 845 576 281 474	7×10^2
	10	0·512 232 949 617 362	5×10^2
500	0	0·873 714 850 331 599	9×10^4
	100	0·868 858 853 774 934	6×10^4
	200	0·854 407 245 481 313	5×10^4
	300	0·830 686 757 884 318	1×10^4
	400	0·798 177 713 735 053	5×10^4
	500	0·757 445 991 396 957	9×10^4

Table 2. Three-dimensional quartic anharmonic oscillator.

k	l	$2E_{kl}$	
0	0	0·464 881 270 421 207	7×10^1
1	1	0·838 034 253 010 158	4×10^1
2	0	0·131 568 038 980 498	7×10^2
	2	0·124 855 560 509 998	6×10^2
5	1	0·286 777 321 755 446	9×10^2
	3	0·278 984 177 600 082	5×10^2
	5	0·265 289 175 581 239	2×10^2
10	0	0·601 295 229 591 577	6×10^2
	2	0·597 951 856 023 007	6×10^2
	4	0·590 200 252 145 363	0×10^2
	6	0·578 153 165 006 542	5×10^2
	8	0·561 971 823 628 909	6×10^2
	10	0·541 849 846 104 544	2×10^2
500	0	0·874 874 719 432 883	5×10^4
	100	0·869 973 480 821 741	4×10^4
	200	0·855 483 846 575 847	9×10^4
	300	0·831 732 675 434 741	5×10^4
	400	0·799 199 814 785 757	9×10^4
	500	0·758 450 305 163 626	6×10^4

Table 3. Diagonal moments ($d = 1$ and 3).

	$d=1$		$d=3$	
k	$\langle x^2\rangle_k$	$\langle x^4\rangle_k$	$\langle r^2\rangle_k$	$\langle r^4\rangle_k$
0	0·305 813 650 718	0·260 241 446 698	0·801 250 595 541	1·015 437 171 04
1	0·801 250 595 541	1·015 437 171 04	1·214 551 385 74	1·983 746 586 20
4	1·750 939 501 76	4·851 892 810 93	2·014 067 745 28	6·423 101 986 89
5	2·014 067 745 28	6·423 101 986 89	2·280 362 022 97	8·039 002 709 87
8	2·721 984 850 99	11·748 805 460 0	2·938 362 108 80	13·696 095 096 0
9	2·938 362 108 80	13·696 095 096 0	3·157 627 830 13	15·671 952 878 9
49	9·013 375 232 60	129·391 415 659	9·137 001 247 51	132·912 815 791
50	9·135 599 169 31	132·928 354 982	9·257 019 170 45	136·489 257 660

Table 4. Matrix elements ($d = 1$ and 3).

	$d=1$		$d=3$	
(k, k')	$\langle k\|x\|k'\rangle$	$\langle k\|x^3\|k'\rangle$	$\langle k,0\|r\|k',1\rangle$	$\langle k,0\|r^3\|k',1\rangle$
(0, 1)	−0·552 565 959 314	−0·456 180 404 562	−0·894 531 209 969	−1·109 701 170 41
(4, 5)	−0·970 612 527 510	−2·845 882 579 49	−1·133 864 353 35	−3·535 889 127 36
(8, 9)	−1·189 039 213 30	−5·257 173 256 06	−1·305 501 445 01	−5·960 803 769 52
(49, 50)	2·128 094 609 90	30·281 934 134 3	2·116 776 818 03	30·779 760 079 8

Table 5. Two-dimensional sextic anharmonic oscillator.

k	l	$2E_{kl}$	
0	0	0·312 193 547 424 642	6×10^1
1	1	0·714 992 860 143 855	0×10^1
3	1	0·191 867 174 220 680	8×10^2
	3	0·173 872 078 074 601	8×10^2
5	1	0·346 174 140 053 972	8×10^2
	3	0·331 490 551 728 027	4×10^2
	5	0·300 188 806 321 731	4×10^2
50	0	0·829 060 129 057 987	9×10^3
	20	0·753 939 539 423 519	3×10^3
	50	0·652 205 431 120 790	6×10^3
500	0	0·254 131 685 870 129	3×10^5
	200	0·247 174 715 334 645	2×10^5
	500	0·197 191 328 911 524	0×10^5

4. Discussion

As indicated earlier, the method yields not only the eigenvalue but also the eigenvector of the given level. While computing the matrix elements of H, one has to take into account the fact that the matrix elements of x, for instance, connects states of different l

Table 6. Three-dimensional sextic anharmonic oscillator.

k	l	$2E_{kl}$	
0	0	0·503 339 593 772 026	6×10^1
1	1	0·945 553 527 684 122	9×10^1
3	1	0·225 039 357 759 694	8×10^2
	3	0·203 386 103 330 132	5×10^2
5	1	0·387 053 868 023 440	6×10^2
	3	0·369 201 929 676 158	1×10^2
	5	0·335 032 553 666 928	2×10^2
50	0	0·841 225 182 040 561	9×10^3
	20	0·764 642 675 743 970	4×10^3
	50	0·661 692 230 608 347	6×10^3
500	0	0·254 512 038 367 464	4×10^5
	200	0·247 517 254 044 689	8×10^5
	500	0·197 486 186 403 443	8×10^5

and n. Since the harmonic oscillator frequency w_0 depends on n and l we will be calculating matrix elements in non-orthogonal basis set of functions. To avoid such complications, we have chosen an oscillator basis with frequency midway between the given nl and $n'l'$ and computed the required numbers. It is well known that between a given pair of states if one calculates the energy levels and the matrix elements of low powers of x, the matrix elements of high powers of x can be computed by hypervirial relations. In tables 3 and 4, we present the moments and the matrix elements for the 1- and 3-dimensional AHOs between some typical pair of levels. Finally, we may mention that the method can be extended in a straightforward manner to higher anharmonicities. For instance, in the case of the sextic AHO $H = \frac{1}{2}(\mathbf{p}^2 + r^2 + r^6)$, one has to deal with para-3-diagonal matrices but they do not introduce any additional complication. In tables 5 and 6, we present the energy eigenvalues for this case.

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