

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

V T A BHARGAVA, P M MATHEWS\* and M SEETHARAMAN\*\*

Department of Physics, Madras Christian College, Tambaram, Madras 600059, India

\*Harvard Smithsonian Centre for Astrophysics, Cambridge, MA 02138, USA

\*\*Department of Theoretical Physics, University of Madras, Guindy Campus, Madras 600025, India

MS received 26 July 1988

**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.

PACS No. 03.65

### 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  $N \rightarrow \infty$  one recovers the eigenvalues. Their matrix is specifically non-

---

\*On leave of absence from the Department of Theoretical Physics, University of Madras, Madras 600025, India.

\*\*To whom correspondence should be addressed.

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

$$H = \mathbf{p}^2/2m + \frac{1}{2}mw^2r^2 + \lambda r^4 \quad (1)$$

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

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

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  $k$ th 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  $k$ th level, we rewrite the Hamiltonian as

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

The 'renormalized' frequency  $w_0$  is so chosen that the expectation value of  $H$  in the  $k$ th 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

$$v = w/w_0 \quad \text{and} \quad \rho^2 = 2\lambda\hbar/m^2w^3 \quad (3a)$$

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

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

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  $a = 0.895\ 647\ 259$   $b = -0.125\ 020$   $c = -0.85$   $e = -0.1$ . The expectation value of  $H$  in the  $k$ th state  $|k, l\rangle$  of the harmonic oscillator with  $w_0$  determined from the above is given by

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

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

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

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

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

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  $\varepsilon_{kl}$ . Then, by definition,

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

Our task therefore is to determine that the eigenvalue  $\varepsilon$  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  $k$ th



in units of  $\hbar\omega_0$ . (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  $p$ .

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

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

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

$$Q'_i = \begin{pmatrix} q_{s+2i-1} & l_{s+2i-1} \\ l_{s+2i-1} & q_{s+2i} \end{pmatrix}, \quad (12)$$

$$U'_i = \begin{pmatrix} p_{s+2i-1} & l_{s+2i} \\ 0 & p_{s+2i} \end{pmatrix}. \quad (13)$$

### 3. Computation of $\varepsilon_{kl}$

The remaining task is to compute  $\varepsilon_{kl}$ , 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)

$$\varepsilon = f(\varepsilon), \quad (14a)$$

where

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

with

$$\sigma(\varepsilon) = \phi(\varepsilon)\beta\chi(\varepsilon) \quad (14c)$$

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



multiply the number obtained for  $E_{kl}$  obtained as above (in  $\hbar\omega_0$  units) by  $1/\nu$  in order to convert to  $\hbar\omega$  units. The tabulated results are all of course in units of  $\hbar\omega$ .

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 | $4 \times 10^1$ |
| 1   | 1   | 0.646 290 599 986 387 | $1 \times 10^1$ |
| 2   | 0   | 0.108 824 355 768 198 | $0 \times 10^2$ |
|     | 2   | 0.103 906 272 955 037 | $8 \times 10^2$ |
| 5   | 1   | 0.259 691 635 685 670 | $1 \times 10^2$ |
|     | 3   | 0.253 133 789 941 425 | $1 \times 10^2$ |
|     | 5   | 0.240 331 661 934 708 | $4 \times 10^2$ |
| 10  | 0   | 0.567 798 591 256 604 | $1 \times 10^2$ |
|     | 2   | 0.565 506 297 037 042 | $2 \times 10^2$ |
|     | 4   | 0.558 667 656 239 447 | $8 \times 10^2$ |
|     | 6   | 0.547 392 009 847 857 | $0 \times 10^2$ |
|     | 8   | 0.531 845 576 281 474 | $7 \times 10^2$ |
|     | 10  | 0.512 232 949 617 362 | $5 \times 10^2$ |
| 500 | 0   | 0.873 714 850 331 599 | $9 \times 10^4$ |
|     | 100 | 0.868 858 853 774 934 | $6 \times 10^4$ |
|     | 200 | 0.854 407 245 481 313 | $5 \times 10^4$ |
|     | 300 | 0.830 686 757 884 318 | $1 \times 10^4$ |
|     | 400 | 0.798 177 713 735 053 | $5 \times 10^4$ |
|     | 500 | 0.757 445 991 396 957 | $9 \times 10^4$ |

**Table 2.** Three-dimensional quartic anharmonic oscillator.

| $k$ | $l$ | $2E_{kl}$             |                 |
|-----|-----|-----------------------|-----------------|
| 0   | 0   | 0.464 881 270 421 207 | $7 \times 10^1$ |
| 1   | 1   | 0.838 034 253 010 158 | $4 \times 10^1$ |
| 2   | 0   | 0.131 568 038 980 498 | $7 \times 10^2$ |
|     | 2   | 0.124 855 560 509 998 | $6 \times 10^2$ |
| 5   | 1   | 0.286 777 321 755 446 | $9 \times 10^2$ |
|     | 3   | 0.278 984 177 600 082 | $5 \times 10^2$ |
|     | 5   | 0.265 289 175 581 239 | $2 \times 10^2$ |
| 10  | 0   | 0.601 295 229 591 577 | $6 \times 10^2$ |
|     | 2   | 0.597 951 856 023 007 | $6 \times 10^2$ |
|     | 4   | 0.590 200 252 145 363 | $0 \times 10^2$ |
|     | 6   | 0.578 153 165 006 542 | $5 \times 10^2$ |
|     | 8   | 0.561 971 823 628 909 | $6 \times 10^2$ |
|     | 10  | 0.541 849 846 104 544 | $2 \times 10^2$ |
| 500 | 0   | 0.874 874 719 432 883 | $5 \times 10^4$ |
|     | 100 | 0.869 973 480 821 741 | $4 \times 10^4$ |
|     | 200 | 0.855 483 846 575 847 | $9 \times 10^4$ |
|     | 300 | 0.831 732 675 434 741 | $5 \times 10^4$ |
|     | 400 | 0.799 199 814 785 757 | $9 \times 10^4$ |
|     | 500 | 0.758 450 305 163 626 | $6 \times 10^4$ |

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

| $k$ | $d = 1$                 |     |     |     |                         |     |     |     | $d = 3$                 |     |     |     |                         |     |     |    |
|-----|-------------------------|-----|-----|-----|-------------------------|-----|-----|-----|-------------------------|-----|-----|-----|-------------------------|-----|-----|----|
|     | $\langle x^2 \rangle_k$ |     |     |     | $\langle x^4 \rangle_k$ |     |     |     | $\langle r^2 \rangle_k$ |     |     |     | $\langle r^4 \rangle_k$ |     |     |    |
| 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).

| $(k, k')$ | $d = 1$                  |     |     |     |                            |     |     |     | $d = 3$                        |     |     |     |                                  |     |     |    |
|-----------|--------------------------|-----|-----|-----|----------------------------|-----|-----|-----|--------------------------------|-----|-----|-----|----------------------------------|-----|-----|----|
|           | $\langle k x k' \rangle$ |     |     |     | $\langle k x^3 k' \rangle$ |     |     |     | $\langle k, 0 r k', 1 \rangle$ |     |     |     | $\langle k, 0 r^3 k', 1 \rangle$ |     |     |    |
| (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 | $6 \times 10^1$ |
| 1   | 1   | 0.714     | 992 | 860 | 143 | 855 | $0 \times 10^1$ |
| 3   | 1   | 0.191     | 867 | 174 | 220 | 680 | $8 \times 10^2$ |
|     | 3   | 0.173     | 872 | 078 | 074 | 601 | $8 \times 10^2$ |
| 5   | 1   | 0.346     | 174 | 140 | 053 | 972 | $8 \times 10^2$ |
|     | 3   | 0.331     | 490 | 551 | 728 | 027 | $4 \times 10^2$ |
|     | 5   | 0.300     | 188 | 806 | 321 | 731 | $4 \times 10^2$ |
| 50  | 0   | 0.829     | 060 | 129 | 057 | 987 | $9 \times 10^3$ |
|     | 20  | 0.753     | 939 | 539 | 423 | 519 | $3 \times 10^3$ |
|     | 50  | 0.652     | 205 | 431 | 120 | 790 | $6 \times 10^3$ |
| 500 | 0   | 0.254     | 131 | 685 | 870 | 129 | $3 \times 10^5$ |
|     | 200 | 0.247     | 174 | 715 | 334 | 645 | $2 \times 10^5$ |
|     | 500 | 0.197     | 191 | 328 | 911 | 524 | $0 \times 10^5$ |

#### 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 | $6 \times 10^1$ |
| 1   | 1   | 0.945 553 527 684 122 | $9 \times 10^1$ |
| 3   | 1   | 0.225 039 357 759 694 | $8 \times 10^2$ |
|     | 3   | 0.203 386 103 330 132 | $5 \times 10^2$ |
| 5   | 1   | 0.387 053 868 023 440 | $6 \times 10^2$ |
|     | 3   | 0.369 201 929 676 158 | $1 \times 10^2$ |
|     | 5   | 0.335 032 553 666 928 | $2 \times 10^2$ |
| 50  | 0   | 0.841 225 182 040 561 | $9 \times 10^3$ |
|     | 20  | 0.764 642 675 743 970 | $4 \times 10^3$ |
|     | 50  | 0.661 692 230 608 347 | $6 \times 10^3$ |
| 500 | 0   | 0.254 512 038 367 464 | $4 \times 10^5$ |
|     | 200 | 0.247 517 254 044 689 | $8 \times 10^5$ |
|     | 500 | 0.197 486 186 403 443 | $8 \times 10^5$ |

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.

### Acknowledgement

Two of us (VTAB and MS) are thankful to Dr Sekhar Raghavan for help in numerical computation.

### References

- Banerjee K, Bhatnagar S P, Choudhary V and Kanwal S S 1978 *Proc. R. Soc. London* **A360** 575  
 Bhargava V T A 1982 *Studies on the quantum anharmonic oscillators in  $d \leq 3$  dimensions* Ph.D. Thesis  
 Bhargava V T A, Mathews P M and Seetharaman M 1989 *Pramana - J. Phys.* **32** 99  
 Biswas S N, Datta K, Saxena R P, Srivastava P K and Varma V S 1971 *Phys. Rev.* **D4** 3617  
 Mathews P M, Seetharaman M, Sekhar Raghavan and Bhargava V T A 1981a *Phys. Lett.* **A83** 118  
 Mathews P M, Seetharaman M, Sekhar Raghavan and Bhargava V T A 1981b *Pramana - J. Phys.* **17**:121  
 Richardson J L and Blankenbecler R 1979 *Phys. Rev.* **D19** 496