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Determination of eigenvalues of real symmetric para-p diagonal matrices

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Abstract. A method is presented for an accurate numerical determination of eigenvalues of real symmetric para-p diagonal matrices. The method takes advantage of the band structure to break up the matrix into $p \times p$ blocks and performing algebraic operations including inversions on these blocks only, no matter what the size of the matrix is. The eigenvalues are determined independently one at a time. Thus any error in the determination of one eigenvalue does not affect the other eigenvalues. The method is ideally suited for the Schrödinger eigen value problem of the anharmonic potentials, which is taken up in the following paper.

Keywords. Eigenvalues; real symmetric para-p diagonal matrices.

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1. Introduction

The Schrödinger energy eigenvalue problem for a given potential $V(r)$ can be converted to a matrix eigenvalue problem by expanding the energy eigenstate in a suitable set of basis functions. For polynomial potentials, the resulting Hamiltonian matrix will be of a band type with non-zero elements only along the main diagonal and a set of p sub-diagonals above and below. In this paper, we present a method to calculate any one eigenvalue at a time of such a matrix to an arbitrary accuracy numerically. The method involves taking advantage of the band structure to break up the matrix into $p \times p$ blocks and performing algebraic operations including inversions on these blocks only, no matter what the size of the matrix is. One obtains an implicit equation for the energy eigenvalue which can be solved iteratively, starting with a suitable initial value. Unlike in conventional diagonalization procedures (Carnahan *et al* 1969) which seek to determine all the eigenvalues simultaneously, the present method picks on one eigenvalue at a time and the accuracy with which this can be determined is independent of the other eigenvalues and thus it avoids errors being carried over from the determination of one eigenvalue to another. To our knowledge, the present method

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does not seem to have appeared in the literature on matrix theory before. The method is ideally suited for solving numerically the Schrödinger eigenvalue problem of the anharmonic oscillators. In the present paper, we outline the method, and in the following one, apply it to various types of anharmonic oscillators (AHO) to determine their energy eigenvalues and other physical observables. The method has uniform applicability for the various anharmonicities, quantum levels, oscillator dimensions, nature of the AHO interaction (quartic, sextic etc.) and, in each case, is capable of yielding any desired accuracy for the eigenvalues, limited only by the computer tolerance. For the quartic AHO for instance, the first several eigenvalues can be determined to a fifteen figure accuracy by our method by considering matrices of dimension 20 or so. For large quantum levels, the dimension of the matrix needed for the same accuracy is far smaller than the level number.

2. The method

Let

$$H\psi(\mathbf{x}) = E\psi(\mathbf{x}), \quad H = (\mathbf{p}^2/2m) + V(r) \tag{1}$$

be the bound-state eigenvalue equation for a particle moving in a potential $V(r)$. Expanding ψ in a suitable real orthonormal basis set of functions $\phi(x)$ as

$$\psi(x) = \sum C_m \phi_m(x),$$

$$\langle m|n\rangle \equiv \int \phi_m(x)\phi_n(x)\,\mathrm{d}x = \delta_{mn}, \tag{2}$$

the above equation (1) can be converted to the form

$$\sum_m (H_{nm} - E\delta_{nm})C_m = 0$$

with

$$H_{nm} = \langle n|H|m\rangle. \tag{3}$$

Note that H is a real symmetric matrix. Suppose, to determine a particular eigenvalue E_k, we have chosen a basis such that H_{kk} closely approximates E_k, then, we can write,

$$E_k = H_{kk} + \varepsilon_k. \tag{4}$$

On using this, (3) can be cast in the form

$$\mathbf{H}c = \varepsilon_k c, \tag{5a}$$

where

$$\mathbf{H}_{nm} = H_{nm} - H_{kk}\delta_{nm} \tag{5b}$$

and c is a column matrix.

We observe that the kth diagonal element of $\mathbf{H}$ is now zero. Our method is ideally suited to determine ε_k, which, by its very definition, is expected to be small, for a given kth level whose energy we seek to determine. In the following paper we show how the splitting of E as in (4) can be done for the AHOs. Let us now take up the determination of ε_k for the matrix $\mathbf{H}$.

The real symmetric matrix H can be written in the block form as

$$H = \begin{pmatrix} A & x & B \\ \tilde{x} & o & \tilde{y} \\ \tilde{B} & y & C \end{pmatrix}, \tag{6}$$

where A and C are symmetric matrices, x and y are one-column matrices and B a rectangular matrix. Let us write the eigenvector c of $\mathbf{H}$ in the form $(v, 1, w)^{\sim}$. Equation (5) can be reduced to the following:

$$v = [(A - \varepsilon I) - B(C - \varepsilon I)^{-1}\tilde{B}]^{-1}[B(C - \varepsilon I)^{-1}y - x], \tag{7a}$$

$$w = [(C - \varepsilon I) - \tilde{B}(A - \varepsilon I)^{-1}B]^{-1}[\tilde{B}(A - \varepsilon I)^{-1}x - y] \tag{7b}$$

and

$$\varepsilon = \tilde{x}v + \tilde{y}w. \tag{8}$$

(For ease of notation we have dropped the subscript on ε.) Since both v and w are functions ε, equation (8) determines ε implicitly. By standard iterative techniques, the solution of (8) can be found.

The main task before us is the repeated inversion of the matrices of the dimension of A and C. For a para-p-diagonal matrix having non-zero elements only along the main diagonal and p sub-diagonals above and below, this task can be reduced to one of dealing with only p-dimensional matrices, no matter how large the dimensions of A and C are. In fact, this is the pivotal point in our analysis. For the quartic AHO, p is two, and hence, inversions of only two-dimensional matrices are involved. To demonstrate this, we proceed as follows:

Because $\mathbf{H}$ is para-p-diagonal, the non-vanishing elements of x are its lowermost p elements, and of y its uppermost p elements. Also the non-zero block of B is a $p \times p$ block confined to the bottom left hand corner:

$$x = \begin{pmatrix} 0 \\ x_u \end{pmatrix}; \quad y = \begin{pmatrix} y_u \\ 0 \end{pmatrix}; \quad B = \begin{pmatrix} 0 & 0 \\ \beta & 0 \end{pmatrix}, \tag{9}$$

β is a $p \times p$ matrix and x_u and y_u are column matrices with p elements. For convenience, let us partition $(A - \varepsilon I)^{-1}$ and $(C - \varepsilon I)^{-1}$ as follows:

$$(A - \varepsilon I)^{-1} = \begin{pmatrix} \chi & Y \\ \tilde{Y} & \phi \end{pmatrix}, \quad (c - \varepsilon I)^{-1} = \begin{pmatrix} \chi' & \tilde{Y}' \\ Y' & \phi' \end{pmatrix}. \tag{10}$$

The ϕ and χ' are taken to be p-dimensional square matrices. Substituting this form in (7), the expressions for v and w can be written as:

$$v = \begin{pmatrix} Y[1 + \beta\chi'\tilde{\beta}(1 - \phi\beta\chi'\tilde{\beta})^{-1}\phi](\beta\chi' y_u - x_u) \\ (1 - \phi\beta\chi'\tilde{\beta})^{-1}\phi(\beta\chi' y_u - x_u) \end{pmatrix}, \tag{11}$$

$$w = \begin{pmatrix} (1 - \chi'\tilde{\beta}\phi\beta)^{-1}\chi'(\tilde{\beta}\phi x_u - y_u) \\ y'[\tilde{\beta}\phi\beta(1 - \chi'\tilde{\beta}\phi\beta)^{-1}\chi' + 1](\tilde{\beta}\phi x_u - y_u) \end{pmatrix}. \tag{12}$$

The point to note is that the lower block of v and the upper block of w are

p-dimensional. Consequently ε of (8) takes the form:

$$\begin{aligned}\varepsilon &= \tilde{x}v + \tilde{y}w = (0\tilde{x}_u)v + (\tilde{y}_u 0)w \\ &= \tilde{x}_u(1 - \phi\beta\chi'\tilde{\beta})^{-1}\phi(\beta\chi' y_u - x_u) \\ &\quad + \tilde{y}_u(1 - \chi'\beta\phi\beta)^{-1}\chi'(\tilde{\beta}\phi x_u - y_u). \end{aligned} \tag{13}$$

The important point to notice in this equation is that it involves only one p-dimensional block, ϕ of $(A - \varepsilon I)^{-1}$ and another p-dimensional block, χ' of $(C - \varepsilon I)^{-1}$ besides the explicitly known p-component columns x_u, y_u and the p-dimensional matrix β. To be more specific, as far as the determination of the eigenvalue is concerned, one does not need to know the full matrices but only a small p-dimensional sub-block of each. If the eigenvector is also required, one needs in addition, Y and Y' i.e., the last p columns of $(A - \varepsilon I)^{-1}$ and the first p columns of $(C - \varepsilon I)^{-1}$ which is still a far less onerous task than computing all of $(A - \varepsilon I)^{-1}$ and $(C - \varepsilon I)^{-1}$. The remaining task is to find the ϕ and χ'. Let us write $(A - \varepsilon I)$ as

$$\begin{pmatrix} R & S \\ \tilde{S} & T \end{pmatrix},$$

where T is a $p \times p$ matrix. Then

$$Y = -R^{-1}S\phi, \tag{14}$$

$$\phi = (T - \tilde{S}R^{-1}S)^{-1}, \tag{15}$$

$$\tilde{Y} = -T^{-1}\tilde{S}\chi, \tag{16}$$

and

$$\chi = (R - ST^{-1}\tilde{S})^{-1}. \tag{17}$$

What is effected in the above steps in a conversion of the problem of inverting a matrix M of dimension d say, into one of inverting smaller matrices of dimensions p and $(d - p)$ where p is the dimension of T (and hence $(d - p)$ is that of R). This can be made the first step of a recursive algorithm in a rather obvious way. What one needs to do is the following. Replacing R, S, T by R_1, S_1, T_1 and partitioning R_1 in the same way as $(A - \varepsilon I)$ was partitioned, as

$$\begin{pmatrix} R_2 & S_2 \\ \tilde{S}_2 & T_2 \end{pmatrix}$$

and more generally

$$R_{i-1} = \begin{pmatrix} R_i & S_i \\ \tilde{S}_i & T_i \end{pmatrix}, \tag{18}$$

where each T_i is square, of the same dimension p as T_1 and R_i is also square, with

dimension less than that of R_{i-1} by p. Thus $(A-\varepsilon I)$ itself would finally appear as

$$(A-\varepsilon I)=\begin{pmatrix} T_L & & & S_2 & \\ & \ddots & & & S_1 \\ & & \tilde{S}_2 & T_2 & \\ & & \tilde{S}_1 & & T_1 \end{pmatrix} \tag{19}$$

wherein all the diagonal blocks T_i are of dimension p except for the last one at the top left hand corner which has dimension $\leqslant p$. Now if we put

$$S_i=\underbrace{\begin{pmatrix} 0 \\ U_i \end{pmatrix}}_{p \text{ columns}}\Big\}\ p \text{ rows.} \tag{20}$$

Equation (15) becomes

$$\phi_i=(T_i-\tilde{U}_i\phi_{i+1}U_i)^{-1} \tag{21}$$

with

$$\phi_L=T_L^{-1} \quad \text{and} \quad \phi_1=\phi. \tag{22}$$

More explicitly

$$\phi\equiv\phi_1=(T_1-\tilde{U}_1(T_2-\tilde{U}_2(\cdots)^{-1}U_2)^{-1}U_1)^{-1} \tag{23a}$$

In a similar manner

$$Y=Y_1=\begin{pmatrix} \cdots\cdots\cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ -\phi_4U_3\phi_3U_2\phi_2U_1\phi_1 \\ \phi_3U_2\phi_2U_1\phi_1 \\ -\phi_2U_1\phi_1 \end{pmatrix}. \tag{23b}$$

So, the procedure outlined above yields the last p columns, namely, $\begin{pmatrix} Y \\ \phi \end{pmatrix}$ in the inverse of any para-p-diagonal matrix. This is just what we need in the case of $(A-\varepsilon I)^{-1}$, in the process of determining the eigenvalues and eigenvector of the para-p-diagonal matrix H. As regards the matrix $(C-\varepsilon I)^{-1}$, we need the first p columns, but these can be obtained by a slight (and rather obvious) modification of what we have done above. We observe that

$$\chi'\equiv\chi_1'=(R_1'-\tilde{U}_1'(R_2'-\tilde{U}_2'(\cdots)^{-1}U_2')^{-1}U_1')^{-1}, \tag{24a}$$

and

$$Y' \equiv Y'_1 = \begin{pmatrix} -\chi'_2 U'_1 \chi'_1 \\ \chi'_3 U'_2 \chi'_2 U'_1 \chi'_1 \\ -\chi'_4 U'_3 \chi'_3 U'_2 \chi'_2 U'_1 \chi'_1 \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \end{pmatrix} \tag{24b}$$

The way to computing eigenvalues and eigenvectors of a para-diagonal matrix H is now clear. We first rewrite the implicit equation (13) for the eigenvalue in a compressed notation as

$$\varepsilon = \tilde{x}_u(1 - \sigma\tilde{\beta})^{-1}(\sigma y_u - \phi x_u) + \tilde{y}_u(1 - \tilde{\sigma}\beta)^{-1}(\tilde{\sigma} x_u - \chi' y_u), \tag{25}$$

where we have introduced

$$\sigma = \phi\beta\chi \equiv \phi\beta\chi'. \tag{26}$$

Since ϕ and χ' are submatrices of $(A - \varepsilon I)^{-1}$ and $(C - \varepsilon I)^{-1}$, they are both functions of ε, making the right hand member of (25) a function of ε, say $f(\varepsilon)$. This completes the task of finding the eigenvalues and eigenvectors of a para-p-diagonal matrix. The implicit energy equation

$$\varepsilon = f(\varepsilon)$$

can be solved by any one of the several well-known methods till a desired convergence of ε is reached.

Table 1. Variation of eigenvalue with matrix dimension.

L, L'	Correction
20	−7·028 552 006 574
22	−1·140 324 181 899
24	−0·074 823 434 509
26	−0·002 302 407 417
28	−0·000 157 881 484
30	−0·000 125 054 634
32	−0·000 124 769 068
34	−0·000 124 767 563
35	−0·000 124 767 558
36	−0·000 124 767 558

Note: The matrix dimension is $M = 2(L + L') + 1$ for the above (where L, L' denote the number of 2×2 blocks above and below the 'central' element) so that we find that convergence of energy to 15 places occurs at $M = 141$. The convergence of ε to 12 decimals only is needed to give E to the required accuracy. The converged value of energy is $E = 8748{\cdot}747\ 194\ 328\ 835$.

3. Discussion

Our method is, in some sense, an expansion of a determinant around a particular diagonal element. In the context of the quantum mechanical eigenvalue problem C is essentially an infinite-dimensional matrix, but A is finite though may be large. For the lower levels the dimension of A may not be exactly a multiple of p. In such cases, one can either augment the less than p-dimensional part to p dimensions by adding suitable 1's along the main diagonal or one can simply use the inverse of these matrices directly in the rest of the calculation. The eigenvalues computed converge quite rapidly. In table 1 we demonstrate for the 3-dimensional AHO, defined by

$$H = p^2 + r^2 + r^4,$$

the rate of convergence of ε for $k = 500$ and $l = 0$ with the dimensions of A and C. The converged ε yields the energy eigenvalue correct to 15-figure accuracy. The details of our calculations for the various AHOs will be presented in the following paper in this issue.

Reference

Carnahan B, Luther H A and Wilkies James O 1969 *Applied numerical methods* (New York: John Wiley).