Note on an alternate method for the computation of rotational energy levels of rigid asymmetric top molecules

By Eric L. Jones*

This note briefly describes a technique for the solution of the general eigenvalue problem and its application to a recent publication on the computation of rotational energy levels. Whereas the previous method involved computation of the eigenvalues of the pertinent tridiagonal arrays via a four-stage, double-precision process combining three iteration techniques, it is demonstrated that similar results may be obtained through the single stage procedure of this note using only single-precision arithmetic.

Recently, a method was given for the computation of reduced energy levels of rigid asymmetric top molecules (Rachman, 1965). This procedure involved the expansion of a secular determinant of a tridiagonal submatrix yielding a polynomial in the eigenvalue parameter. This polynomial, after a necessary scaling to prevent overflow, was then solved using a combination of Muller's, *regula falsi*, and dichotomy procedures. The paper pointed out the presence of rounding and convergence problems which require that his procedure be carried out in double-precision. It is the purpose of this note to call attention to the existence (Barlow and Jones, 1966) of a method for the solution of general eigenvalue problems which is readily used for the special case here. The example given by Rachman has been solved and presented here to demonstrate the effectiveness of the method.

Method

The problem presented by Rachman is one of the class of ordinary eigenvalue problems of the form

$(A - I\lambda)\vec{x} = O$, where A is a nonsymmetric matrix, I the identity matrix, and λ is the eigenvalue parameter. This is a special case of the general eigenvalue problem

$$H(\lambda)\vec{x} = O,$$

where H is an array in which λ may appear in any or all of the elements. Eigenvalues, values of λ such that nonvanishing solutions $\vec{x}$ exist, are solutions of

$$F(\lambda) = |H(\lambda)| = 0; \quad (1)$$

hence any method for solving for zeros of functions may be applied using for functional values the computed determinant values for each selected λ.

It has been found (Barlow and Jones, 1965) that a quite successful general method for solution of problems given by (1) is obtained by considering λ to be a complex variable and applying the recursive formula

$$\delta^{(N+1)} = \delta^{(N)} \frac{F(z^{(N)})}{F(z^{(N)}) - F(z^{(N-1)})}, \quad (2)$$

where

$$\delta^{(N)} = z^{(N)} - z^{(N-1)}.$$

This recursion, formally the extension of the secant method to the complex plane (the complex extension is especially advantageous when a real equation possesses complex roots), has superlinear convergence properties in addition to retaining the original accuracy of the undisturbed array. Additional information including convergence, accelerating procedures for multiple roots, removal of effects of previously found zeros and numerical details are given in the aforementioned paper.

Table 1

Energy levels for $J = 25$ submatrix 0^+

ENERGY LEVEL	RACHMAN (IN KMHZ)	PRESENT METHOD (IN KMHZ)
$25_{1 \cdot 25}$	590·78784	590·78851
$25_{3 \cdot 23}$	670·95029	670·95061
$25_{5 \cdot 21}$	737·23383	737·23380
$25_{7 \cdot 19}$	796·13159	796·13142
$25_{9 \cdot 17}$	868·91611	868·91595
$25_{11 \cdot 15}$	962·60090	962·60081
$25_{13 \cdot 13}$	1,076·40023	1,076·40014
$25_{15 \cdot 11}$	1,209·82522	1,209·82517
$25_{17 \cdot 9}$	1,362·66840	1,362·66836
$25_{19 \cdot 7}$	1,534·82845	1,534·82844
$25_{21 \cdot 5}$	1,726·25069	1,726·25069
$25_{23 \cdot 3}$	1,936·90344	1,936·90342
$25_{25 \cdot 1}$	2,166·76724	2,166·76725
REDUCED LEVEL TRACE 2,904·62087	2,904·62070	2,904·62086

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Discussion and results

Several points should now be made in connection with the problem in question. First, the reduction of the determinantal equation to an explicit polynomial is not necessary and, indeed, leads to a more ill-conditioned problem by the reduction to a fewer number of coefficients (from the array to the polynomial), and introduces possible inaccuracy problems. Scaling problems, magnified by a data-condensation process, may be handled easily in the original array if, in fact, such difficulties exist initially. Although the computations for the results below were computed using complex arithmetic (in an existing IBM 7044 computer program), the same results could have been obtained for this case with real variables since no complex conjugate roots are present to establish symmetry problems in applying the real secant method. The values of the determinant were obtained using elimination methods, again due to the usage of a general-purpose program, whereas the

inclusion of an initial reduction for Hyman's method is helpful in solving ordinary eigenvalue problems with this method (note, however, that this initial reduction also reduces the number of coefficients for the problem).

Using this method the following results are obtained and appended to Rachman's table for the parameters and matrix given in his paper.

The data in the last column of **Table 1** were computed in single-precision arithmetic (36 bits, 27 for mantissa) with no preconditioning nor scaling of the array. Total computation time was approximately 30 seconds on the IBM 7044. It should be noted that the trace (as Rachman points out, not a sufficient accuracy test) as calculated here is in excellent agreement with the true value; we also add that the nine-digit numbers given in the table were obtained in converting eight-digit reduced eigenvalues to the tabled values, and the ninth digit is retained only to aid in immediate comparison to previous data.

References

BARLOW, JR., C. A., and JONES, E. L. (1966). "A Method for the Solution of a Nonlinear Equation and for Solution of the General Eigenvalue Problem," *J. Assoc. Comp. Mach.*, Vol. 13, p. 135.

RACHMAN, A. (1965). "Computation of Rotational Energy Levels of Rigid Asymmetric Top Molecules," *The Computer Journal*, Vol. 8, p. 147.

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To the Editor,
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Timetabling and scheduling problems

Sir,

Some of the difficulties associated with computer application to general class timetables and scheduling are well known, and more aspects have recently appeared in an airline study which support Elizabeth Barraclough's comments (this *Journal*, Vol. 8, p. 136) that the choice for a best method for compiling timetables seems to lie between a theoretical and a manual method. The need she mentions for some parameters of the input data related to the "degree of success" of the timetable is also supported. Apart from this the study has a cautionary bearing on the type of linear programming analysis used by Dr. R. E. Miller (*Domestic Airline Efficiency—An Application of Linear Programming*, M.I.T. Press 1963).

In a scheduling and timetabling study made for the recent introduction of Boeing 727 aircraft into Australian domestic airlines it was required to schedule initially two 727 aircraft (and later three), between five capital cities in Australia daily under the following conditions:

   (i) Transcontinental flight Sydney–Perth via Adelaide preferably daily;

   (ii) Daily return Sydney–Brisbane, Sydney–Adelaide;

   (iii) No positioning (empty) flights allowed and one aircraft to end at Sydney and one at Melbourne each evening;

   (iv) First flights to be between Melbourne and Sydney and not earlier than 7.45 a.m.;

   (v) No flights later than 9.00 p.m. and allowance made for time differences coast to coast;

   (vi) Allowance for ground time at airports;

   (vii) Allowance for all routing patterns and possible connecting flights of the 727 aircraft to achieve the specified inter-capital service;

   (viii) What effect of time for some alternate daylight servicing of aircraft;

   (ix) Maximum flights between the major business centres Melbourne and Sydney;

   (x) Annual flying hour usage for each aircraft to be a maximum up to 3,750 hours.

Manual trial and error methods were started by experienced airline operations staff while the computer method was developed. In the latter, a binary notation of routing was used using a series of binary δ's which finally allowed 16 routing possibilities to be designated by variables which had to be either zero or unity.

The single case of δ_1 will illustrate the method which led into integer programming formulation to cover routing possibilities in the timetabling problem:

$\delta_1 = 1$ designated a return flight Sydney–Brisbane prior to Sydney–Adelaide (direct or via Melbourne depending on δ_2)

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