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THE IBM SHARE PROGRAM D2 NU SCHR 1072 FOR SOLUTION OF THE SCHÖDINGER RADIAL EQUATION, BY J. W. COOLEY: NECESSARY AND USEFUL MODIFICATIONS FOR ITS USE ON AN IBM 7090

R. N. Zare and J. K. Cashion

July 1963
ERRATA

TO: All recipients of UCRL-10881
FROM: Technical Information Division

Please make the following corrections on subject report.

Page 18

1. Card "MOD 5" should be changed to read

   899 FORMAT(36H DIFFERENCE EQUATION TECHNIQUE FAILS) MOD 5

2. Insert between cards "MOD 5 and MOD 6" the following card

   SCHR = 1.

MOD 5.5
The IBM SHARE Program D2 NU SCHR 1072 for Solution of the Schrödinger Radial Equation, by J. W. Cooley; Necessary and Useful Modifications for Its Use on an IBM 7090.

R. N. Zare and J. K. Cashion

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Introduction

An efficient method for solving the radial Schrödinger equation numerically has been proposed recently by Cooley. He has contributed a Fortran program embodying his procedure to the IBM SHARE project, D2 NU SCHR 1072. The authors of the present report have found his program extremely useful as a means of generating eigenvalues and eigenfunctions for diatomic molecule calculations. The program was written for an IBM 704 and must be modified slightly in order to be compatible with an IBM 7090. (The same modifications are necessary for its use on the 709 or 7094.) The principal purpose of this report is to make this information available to 7090 users.

A few modifications and additions which the authors have found useful also will be described. These in no way derogate from Cooley's skill as a programmer. On the contrary his program can be recommended not only for its utility but also as an excellent example of the efficient use of Fortran coupled with a clarity of presentation which makes it easy for others to adapt his work to their own particular needs.

Tests of the accuracy of this procedure when up to 200 intervals are used in the integration have been given by Cooley. Additional information on its use with up to 2000 intervals has been given elsewhere by one of (J.K.C.). Other applications in which this program has been very useful to us include a study of vibration-rotation interaction (J.K.C.) and a calculation.
of the intensity distribution in the iodine fluorescence spectrum based on Rydberg-Klein-Rees potentials (R.N.Z.⁴).

The Numerical Method

The following is taken largely from Cooley's summary of the method as given in the SHARE distribution description of this program. To facilitate comparison with the listing of the symbolic deck given in Appendix B, variable names employed in the program are also used in the following equations.

The program calculates the eigenvalue $E$ and the normalized eigenfunction $S$ of the second-order differential equation

$$\frac{d^2S}{dr^2} = (V - E)S$$  \hspace{1cm} (1)

where $V$ is a given numerical potential function.

It is customary to separate the Schrödinger equation for a diatomic molecule into its radial and angular parts and express its solution in the form

$$\psi(r, \theta, \varphi) = R(r) \Theta(\theta) \Phi(\varphi).$$  \hspace{1cm} (2)

Eq. (1) is equivalent to the radial Schrödinger equation when length and energy are expressed in dimensionless units. Its solution $S(r)$ is equal to $r$ times $R(r)$. $S(r)$ provides a more convenient computational form since the product of any two functions $S$ will include the volume element of integration. Hence, the expectation value for any quantity $F$ is given by

$$[F] = \int R F_{op} R \cdot r^2 dr = \int S F_{op} S dr$$  \hspace{1cm} (3)
If length is measured in units of Bohr radii, \( a_0 = 0.529172 \, \text{Å} \), the energies \( V \) and \( E \) must be expressed in a dimensionless unit equivalent to \( \hbar N_0 / 8\pi^2 c a_0^2 \mu_A \) wave numbers, where \( N_0 \) is Avagadro's number (physical scale) and \( \mu_A \) is the reduced mass in Aston units. The numerical value of this factor is \( 60.2198 / \mu_A \). Hence to convert eigenvalues generated by this program to the more familiar units of cm\(^{-1}\), multiply them by this factor. Note that the Aston unit of reduced mass is based on the physical scale of atomic weight, i.e., \( \mu_A = m_1 m_2 / (m_1 + m_2) \) where \( m_1 \) and \( m_2 \) are the atomic weights of atoms relative to \( O^{16} = 16 \). Herzberg's\(^5\) table 39 is a convenient source for \( \mu_A \) values.

Regarding the potential \( V(r) \) two things should be noted. First, its zero is taken at the dissociation limit. Therefore a Morse potential, for example, must be generated from the relation

\[
V(r) = D_e [1 - e^{-\beta (r-r_e)}]^2 - D_e
\]

where the dissociation energy \( D_e \) is a positive quantity.

Secondly, \( V(r) \) is an effective potential which may include a rotational term, \( [J(J+1) - \Lambda]/r^2 \), where \( J \) is the rotational quantum number and \( \Lambda \) is the quantum number for the \( z \)-component of electronic angular momentum. Since this term is inherently positive its addition to the potential for the rotationless state always raises the potential.

Initially, a non-normalized solution \( P(r) \) for Eq. (1) is calculated from the integration formula

\[
-Y_{i-1} + 2Y_i - Y_{i+1} + \hbar^2 (V_i - E) P_i = 0
\]
where

\[ P_1 = P(r_1) \]

\[ V_1 = \frac{1}{2} \left( h^2/12 \right) (v_i - E) \]

\[ V_i = V(r_i) \]

\[ h = r_{i+1} - r_i. \]

The error associated with the use of Eq. (5) as a predictor is \( \frac{h^6}{240} P_1 \).

Starting with the boundary values

\[ P_n = 10^{-30} \]  \hspace{1cm} (7)

\[ P_{n-1} = P_n \cdot \exp \left[ r_n (V_n - E)^{1/2} - r_{n-1} (V_{n-1} - E)^{1/2} \right] \]  \hspace{1cm} (8)

and a trial value of \( E \), Eq. (5) is used to integrate inward, giving \( P_{n-2}, P_{n-3}, \ldots, P_m \), where \( m \) is selected as the first point for which \( |P_m| < |P_{m+1}| \). [Eq. (8) is based on the WKB approximation.] Then, \( P_i \) is replaced by \( P_i/P_m \) for \( i = m, m+1, \ldots, n \).

Starting with the boundary values

\[ P_0 = 0, \ P_1 = 10^{-20} \]

Eq. (5) is used to integrate outwards, giving \( P_2, \ldots, P_m \), after which \( P_1 \) is replaced by \( P_1/P_m \) for \( i = 1, 2, \ldots, m \). This yields a trial solution satisfying Eq. (5) at all points except \( r_m \), the crossing-point for the outward and inward curves. A correction to \( E \) is calculated by applying the Newton-Raphson method to the calculation of the zeros of the function
\[ F(E) = h^{-2}(-Y_{m-1} + 2Y_m - Y_{m+1}) + (V_m - E)P_m \]  

which is a measure of the amount by which the \( m \)th equation of Eq. (2) is not satisfied. The derivative of Eq. (9) is

\[ F'(E) = -\sum_{i=1}^{n} P_i^2 \]  

The correction to \( E \), by the Newton-Raphson method, is

\[ DE = -\frac{F(E)}{F'(E)}. \]  

After adding this correction to \( E \) to obtain a new trial eigenvalue the process is repeated until \( DE \leq \epsilon \). When convergence is achieved, the normalized solution is calculated,

\[ S_i = P_i / \left( h \sum_{j=1}^{n} P_j^2 \right)^{1/2}, \quad i=1,2,\ldots,n. \]  

**Necessary Modifications**

The SHARE distribution includes the main program NU SCHR either in the form of 177 Fortran source program cards or as 43 relocatable binary cards. In addition binary cards labelled NU EMFT, 1-4 and NU LRT, 1-6 are also supplied. For 7090 use, discard all ten of these binary cards. Replace them with the FAP deck for subroutine EMFT which is listed in Appendix A. When compiled this subroutine will be contained on four binary cards.

**Useful Modifications**

Appendix B contains a listing of one Fortran source deck used by the authors. Frequently a particular application will
require recompilation with an altered DIMENSION statement, probably the inclusion of a COMMON card and perhaps some modification of output control or formats. The changes to be described below were either found to be generally useful or were made to remedy failures of the subroutine in particular applications. All symbolic cards which have been modified are labelled MOD 1 to 20; those labelled SCHRO004 to 176 are unaltered from the original SHARE distribution.

MOD 2 - The Call Statement

The variables which must be supplied are

NI,NS: Output control parameters whose function is explained in the comment cards SCHRO004-007.

RMAX,RMIN: Specify the range of r. RMIN ≤ r ≤ RMAX.

V,S: Singly-dimensional arrays containing respectively the numerical potential and the solution, on exit. The source program must contain these in a DIMENSION statement.

N: The number of equally-spaced intervals used in the integration. The length of each interval is h=(RMAX-RMIN)/N.

KV: the number of nodes in the solution. See comments on this below.

EO: Upon entry, EO is the first trial eigenvalue provided to SCHR by the user's program. EO must be a negative number. At exit time it is replaced by the E calculated on the last iteration. (Note: the second symbol in this variable name is a zero, not the letter 0.)
EPS: The convergence criterion is \( E' - E \leq \text{EPS} \) where \( E' = E + \Delta E \). One may use \( \text{EPS} = 0 \), except in rare circumstances where the magnitude of the solution \( E \) is extremely small relative to the \( V_i \)'s.

MAXIT: Is the maximum number of the iterations to be performed. It might be noted that frequently the iteration procedure will not satisfy a zero epsilon test. For eigenfunctions with an odd number of nodes especially it can oscillate between two values differing by only 1 unit in the last figure. Hence, considerable time can be wasted by making MAXIT unnecessarily large. In most cases this could be prevented by making \( \epsilon = 2 \times 10^{-8} \) \( E_{\text{trial}} \). A convenient way of doing this would be to insert the following statement near the beginning of the subroutine, following MOD 2, say,

\[
\text{EPS} = 2.0 - 8 \times \text{EO}
\]

Cooley has written this subroutine as a FUNCTION with the following purpose in view. At exit time, \( \text{SCHR} = 0 \) if convergence has been achieved in MAXIT iterations or 1 less. Otherwise, \( \text{SCHR} = 1 \) and EO and S are the results for MAXIT iterations. Therefore, if one wants to test for convergence one should write in the source program

\[
\text{IF [SCHR(...)]} \text{ N1, N2, N3.}
\]

When not testing for convergence, one may write

\[
\text{CALL SCHR (...)}.\]
MOD 3 - The Range of Integration

Cooley's published application of his program was to the \( \text{H}_2^+ \) molecule-ion. The values of its eigenfunctions at \( r = 0 \) are in the range of \( 10^{-25} \). For most molecules the values at \( r = 0 \) are much smaller than \( 10^{-39} \), which produces a machine zero on the 7090. Hence the use of \( r = 0 \) as a lower bound needlessly extends the range of the integration. Values of \( \text{RMIN} = r_e - 2 \) and \( \text{RMAX} = r_e + 5 \) (in atomic units) will give a satisfactory range for molecules having \( \omega_e/\omega_e \cdot x_e \approx 50 \). The larger this ratio, the more the range may be reduced. It is well to print the eigenvalues at the two extremes in order to be sure that they are sufficiently small.

MOD 4-6 - Trial Eigenvalue too High

It can happen that an iteration will result in a large correction to the trial eigenvalue and place the new trial eigenvalue beyond the range of bound states. Cooley's provision for this was to replace such a trial value by the third last potential value, \( V(N-2) \), and then continue with the next iteration. Our experience was that when such a failure occurred resumption of the iteration through this artifice never led to the eigenvalue which was being sought originally. Hence we preferred to terminate the procedure with a print-out to indicate the source of the failure.

MOD 7-11 - Test for Crossing Point

Cooley used three separate tests for terminating the inward integration: a decrease in the eigenfunction, an increase in
the potential, and, if neither of these tests did it before
the value \( r_2 \) was reached, it was made the crossing-point. We
have removed the test on the potential for the following reason.
In deriving some RKR-type potentials various interpolation
schemes were used. In some cases it was found that small local
irregularities could be introduced, especially near the
classical turning points or near the extremities of the potential
where various approximate forms were joined on to the RKR
segment. If the inward integration is terminated very far away
from the maximum of the eigenfunction, the efficiency of the
iteration procedure is greatly reduced and may result in
failure of the program. It is necessary to retain the IF(M-2)
test, for if the eigenfunction test were never satisfied a
tight loop would result. The number of cases in which termin-
ation was effected by this test were very few, and all were
associated with potentials generated in part by interpolation.
The detailed reasons for failure in these cases were never
ascertained but were thought to be closely related to the small
irregularities arising from unsatisfactory interpolation
procedures. The print-out of the crossing-point (MOD 8-11)
was made principally to investigate the difficulties encountered
in these instances.

**MOD 12-15 - Node-Count**

Frequently the normalized solutions will have values smaller
in magnitude than \( 10^{-39} \) near either end of the integration. On
the 7090 underflow will occur producing a zero, but one which

...
The modifications made here prevent an oscillation in the signs of these zeros from being counted as a node. In connection with the node-count we might point out a danger in specifying by a number rather than by a variable any parameter in a CALL statement. If the parameter is changed by the subroutine its new value will be used in any subsequent Fortran statements employing that parameter. If one used the statement CALL SCHR (..., ..., 5, ...) where 5 specified KV, errors could easily result if the node-count actually differed from 5. For instance, if 6 nodes were counted a later program statement J = J+5 would be executed as J = J+6. (A number used for E0 in the CALL will be altered on exit.) In this program the input KV is never used so there is no point to specifying it numerically anyway.

MOD 16-19 - Print Control

This modification is included merely as an example of an additional output option controlled by the parameter NS. With NS = 10 and NI > 9 only the node-count and eigenvalues are printed. It should be noted that MOD 17 and MOD 4 are not under the control of NI, nor have we included the option of on-line printing for these output statements. While it is most unlikely that a 7090 user would ever be printing results on line, the option provided by Cooley has not been removed from this deck. It is useful since some monitor systems interpret the PRINT command as WRITE OUTPUT TAPE 3. Where this is the case the user would have to replace cards MOD 4 and 17 by corresponding PRINT
statements, but could use Cooley's output formats by setting the appropriate control parameter equal to zero.

A Numerical Example

For the convenience of anyone wishing to check out a program which uses SCHR, we provide the following test case. Using the input parameters $N = 1000$, $R_{\text{MAX}} = 7.5$ and $R_{\text{MIN}} = 0.5$ generate an array of $r$ values in which

$$R(1) = R_{\text{MIN}} + H$$

where

$$H = (R_{\text{MAX}} - R_{\text{MIN}})/N$$

and

$$R(J) = R(J - 1) + H, \quad J = 2, N$$

Use these values to generate the Morse potential, Eq. (4), with the parameters $D_e = 605.559$, $r_e = 2.40873$ and $\beta = 0.988879$. [Note that the value of $V(R_{\text{MIN}})$ is not used. $V(1) = V(R_{\text{MIN}} + H)$.] Call SCHR after specifying the trial eigenvalue $E_0 = -581.46902$. On exit print out the values of $R(300)$, $V(300)$, $S(300)$ and $E_0$. A program intended for generating vibrational-rotational eigenfunctions will include provision for altering the rotation-less potential to the one appropriate for any $J$ state. Use it to provide the $V$ array for $J = 20$, change $E_0$ to $-508.62023$, call SCHR and then make the same print-outs as before. The values which should be obtained are given in Table I.

The first trial eigenvalues given in the text above were calculated from equations which may be found in reference 2. For purposes of this test there should be no need to specify them beyond two figures unless the value of MAXIT is very small.
Table 1. Morse Eigenvalues for the \( J=0 \) and \( J=20 \) rotational states of HCl. Values of the potentials and the eigenfunctions at \( r=2.5999998 \) atomic units are also given.

<table>
<thead>
<tr>
<th></th>
<th>( J=0 )</th>
<th>( J=20 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E )</td>
<td>-581.46913</td>
<td>-511.65467</td>
</tr>
<tr>
<td>( V(r) )</td>
<td>-587.57499</td>
<td>-525.44473</td>
</tr>
<tr>
<td>( S(r) )</td>
<td>1.1936730</td>
<td>1.4065177</td>
</tr>
</tbody>
</table>

For the sake of completeness the potentials and eigenfunctions obtained in the test are shown in Figures 1 and 2.

Finally, it might be noted that appendices A and B are photographic reproductions of the machine listings of the two decks. These decks were compiled and employed in a test program which used every statement with the exception of the on-line print commands. No errors were detected.
References

4. R. N. Zare, to be published.
Captions for Figures

1. Morse potentials for HCl with $J = 0$ and $J = 20$.

2. Ground state eigenfunctions for the potentials shown in Fig. 1.
Fig. 1.

Fig. 2.
APPENDIX A

REM NU EFM, EFM AND LFM FOR FORTRAN 2
REM
ENTRY EFM
ENTRY EFMT

LFM OCT 476000000004
TTR 1+4

EFMT CLA 1+4
STA SETN+1
CLA TTR
TXT EFM+1,4,-1

EFM CLA HPR
STO OVER+2
OCT 476000000002

SET CLA X
STO 8
TTR 1+4
TTR ANALY

ANALY SXD SAVEX+1
LXD 0+1
TTR **+1,1
TTR MQO

SAVEX PZE
TTR ACMO
TTR AC
TTR MQ

ZERO PZE
TTR ACMQO
TTR ACO
TTR RETRN

ACMQ CLA ZERO
TTR MQO

MQ LDQ ZERO
RETRN LXD SAVEX+1
STO SAVEX
CLA 0
STA *+,2
CLA SAVEX
TTR **

ACMQO ORA MAX
MQO STO SAVEA
LLS 0
LDQ MAX
LRG 0
TTR OVER+1

ACO ORA MAX
OVER STO SAVEA
CLA 0
HPR 63

SAVEA PZE
THREE PZE 0+0+3
TTR TTR SETN
HPR HPR 63

EFMT 02
EFMT 03
EFMT 16
EFMT 17
EFMT 18
EFMT 19
EFMT 20
EFMT 21
EFMT 22
EFMT 23
EFMT 24
EFMT 25
EFMT 26
EFMT 27
EFMT 28
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EFMT 51
EFMT 52
EFMT 53
EFMT 54
EFMT 55
EFMT 56
EFMT 57
EFMT 58
EFMT 59
EFMT 60
EFMT 61
EFMT 62
EFMT 63
EFMT 64
EFMT 65
EFMT 66
SETN  ANA  THREE
STO -
TTR OVER+3
MAX  OCT  777777777777
END

EFMT 67
EFMT 68
EFMT 69
EFMT 70
EFMT 71
APPENDIX B

C MODIFIED SYMBOLIC DECK FOR COOLEYS D2 NU SCHR 1072
C
C FUNCTION SCHR(N1,NS,RMAX,RMIN,V,N,KV,EO,EPS,MAXIT,S)
C
C
C N1=0 PRINT ITER ON-LINE
C N1=1,...,9 PRINT OFF-LINE TAPE NI
C N1=OTHERWISE, DONT PRINT
C NS, SAME EXCEPT FOR SOLUTIONS
C DIMENSION S(500),V(500),P(500),Y(3)
C
C IF(N1)6,2,1
1 IF(N1-10)4,6,6
2 PRINT 3
3 GO TO 6

3 FORMAT(70H0 ITER E F(E) DF(E)

4 WRITE OUTPUT TAPE NI,3
6 CALL EFMT(K)
H = (RMAX-RMIN)/FLOAT(N)
H2=H**2
HV=H2/12
E=EO
TEST = = -1.
DE=0.

C START ITER LOOP
C
C 12 DO 171 IT=1,MAXIT
C 171 ••••• START INWARD INTEGRATION
C
C 30 P(N)=1.E-30
32 GN=V(N)-E
34 GI=V(N-1)-E
C 35 WRITE OUTPUT TAPE 3, 899
C 36 FORMAT(WIDTH,30W,4.15)
C MOD 5
C 899 FORMAT(WIDTH,30W,4.15)
C MOD 6
C RETURN
C
C 37 PCNl=1.E-30
38 GN=VCNl-E
39 GI=VIN-11-E
C 40 WRITE OUTPUT TAPE 3, 899
C 41 FORMAT(WIDTH,30W,4.15)
C MOD 6
C RETURN
C
C 41 WRITE OUTPUT TAPE 3, 899
C 42 FORMAT(WIDTH,30W,4.15)
C MOD 6
C RETURN
C
C 44 M=N-2
46 Y(3)=Y(2)+((Y(2)-Y)+H2*GI*P(M+1))
48 GI=V(M)-E
50 P(M)=Y(3)/(1.-HV*GI)
C 51 WRITE OUTPUT TAPE 3, 899
C 52 FORMAT(WIDTH,30W,4.15)
C MOD 6
C RETURN
C
C 53 WRITE OUTPUT TAPE 3, 899
C 54 FORMAT(WIDTH,30W,4.15)
C MOD 6
C RETURN
C
C 55 DO 56 J=M1,N
56 P(J)=P(J)/PM
58 Y=Y/PM
60 Y(2)=Y(2)/PM
62 Y(3)=Y(3)/PM
64 GI= V(M+1) - E
C
GO TO 46

C *******TEST FOR CROSSING PT
70 IF(ABSF(P(M)) - ABSF(P(M+1)) < 90, 90, 72
72 IF(M-2)/90, 90, 81
81 Y= Y(2)
82 Y(2) = Y(3)
84 M=M+1
86 GO TO 46

C 90 PM=P(M)
92 MSAVE = M
94 YIN=Y(2)/PM
96 DO 96 J=M,N
98 P(J) = P(J)/PM

C 100 P(1) = 1*E-20
102 Y=0.
104 GI=V-E
106 Y(2) = (1 - HV*GI)*P
108 DO 132 I=2,M
110 Y(3) = Y(2) + ((Y(2)-Y)+H2*GI*P(I-1))
112 GI=V(I)-E
114 P(I) = Y(3)/(1 - HV*GI)

C 116 IF(K)118,130,118
118 K=0
120 I1=I-1
122 PM=P(11)
124 DO 120 J=1,I1
126 Y= Y/P M
128 Y(2)=Y(2)/PM
130 Y(3)=Y(3)/PM
132 GI=V(I)-E
134 IF(K)135,149,135
135 YOUT=Y/PM
136 YM=Y(3)/PM
138 DO 140 J=1,M
140 P(J) = P(J)/PM

C 142 DF=0.
144 DO 146 J=1,N
146 DF=DF-P(J)**2
148 F=(-YOUT-YIN+2.*YM)/(H2+(V(M)-E))
150 DOLD=DF
152 IF(K)149,150,149
154 F=9.9999999E+29
156 DF=-F
DE=ABS(F*0.0001*E)
GO TO 152
150 DE=-F/DF
152 IF(NI)164,158,154
154 IF(NI-10)162,164,164
156 FORMAT(1HO I4,2X 1PE16.7, 5X 31H THE CROSSING POINT OCCURS AT I4)
158 PRINT 156,IT,E,F,DF,DE
GO TO 164
160 WRITE OUTPUT TAPE NI, 156, IT,E,F,DF,DE,MSAVE
162 EOLD = E
E=E+DE
164 TEST=MAX(ABS(F(DOLD)-ABS(F(DE)),TEST)
166 IF(TEST171,170,170
170 IF(ABS(F-EOLD) - EPS ) 172,172,171
171 CONTINUE
SCHR=1,
GO TO 173
C ******CONVERGED-COUNT NODES
172 SCHR=0.
173 KV=0
174 NL=N-2
176 IF(P(J)+J178,177,177
177 IF(P(J-1))180,192,192
178 IF(P(J-1))192,270,184
C POS. NODE
180 IF(P(J+1))192,182,182
182 IF(P(J-2))190,192,192
C NEG. NODE
184 IF(P(J+1))186,192,192
186 IF(P(J-2))190,190,190
C IGNORE FALSE NODE DUE TO UNDERFLOW
270 IF(P(J+1))280,192,192
280 IF(P(J-2))192,192,192
190 KV=KV+1
192 CONTINUE
C ******NORMALIZE
200 SN=SQRTF(-H*DF)
202 DO 204 J=1,N
204 S(J)=P(J)/SN
C ******PRINT SOLUTION
206 IF(NS)236,210,208
208 IF(NS-10)210,236,236
210 DO 234 JF=1,N,300
212 IF(NS)236,216,218
214 FORMAT(47H1SCHR- SOLUTION OF RADIAL SCHR.EQUATION FOR V= I3, 7H
X E= 1PE15.7 /20HO 1 S(I) 5120H 1 S(I) )
216 PRINT 214,KV,E
GO TO 220
218 WRITE OUTPUT TAPE NS,214,KV,E
220 JL=XMINOF(JF+49,N)
222 DO 234 J=JF,JL
224 IL=XMINOF(J+250,N)
226 IF(NS)236,230,232
228 FORMAT(6(15,1PE15.7))
230 PRINT 228,(I,S(I)),I=J,IL,50
GO TO 234
232 WRITE OUTPUT TAPE NS,228,(I,S(I)),I=J,IL,50
234 CONTINUE
236  E0=E
     IF(NS-10)250,KV,E

875  WRITE OUTPUT TAPE 3.

876  FORMAT(54H0 SOLUTION OF THE RADIAL SCHRODINGER EQUATION FOR V =
     1 13,8H  E = 1PE15.7)

250  RETURN

     FREQUENCY 52(0,1,0)*70(0,0,1)*72(0,0,1)*94(100)*55(50)*108(100)*11
     X 6(0,1,0)*138(100)*144(200)*152(1,0,0)*154(0,1,1)*202(200)

  END
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