FORTRAN IV PROGRAMS FOR THE EXTRACTION OF POTENTIAL WELL PARAMETERS FROM
THE ENERGY DEPENDENCE OF TOTAL ELASTIC SCATTERING CROSS SECTIONS

R. A. LaBudde

TECHNICAL NOTES
PRELIMINARY - NOT FOR PUBLICATION

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FORTRAN IV PROGRAMS FOR THE EXTRACTION OF POTENTIAL WELL PARAMETERS FROM
THE ENERGY DEPENDENCE OF TOTAL ELASTIC SCATTERING CROSS SECTIONS

by

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PREFACE

An attempt has been made to keep the programs as subroutine oriented as possible. Usually only the main programs are directly concerned with the problem of total cross sections. In particular the subroutines POLFIT (IV.A), BILINR (V.B), GASS59/MAXLIK (VI.D), SYMQR (VI.E), MATIN (VI.F), STUDNT (VI.G), DINTERP (VII.E), DIFTAB (VII.F), FORDIF (VII.G), EPSALG (VII.H), REGFAL (VII.I), AND ADSIMP (VII.J), are completely general, and are concerned only with the problems of numerical analysis and statistics. Each subroutine is independently documented.
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I. DISCUSSION

The total cross section $Q(v)$, where $v$ is the relative velocity, is assumed to be a sum of two components: $Q_{SLL}(v)$, dependent upon the long-range force constant $C_6$, and $\Delta Q_g(v)$, an oscillatory term due to the presence of glory extrema

$$Q(v) = Q_{SLL}(v) + \Delta Q_g(v) \quad (I-1)$$

where

$$Q_{SLL}(v) \simeq 8.083 \left( \frac{C_6}{\hbar v} \right)^{2/5} \quad (I-2a)$$

$$\Delta Q_g(v) \simeq \frac{4\pi^{3/2}}{k^2} \frac{L_g}{(-\eta_m'')^{1/2}} \sin \left( 2\eta_m - \frac{3\pi}{4} \right) \quad (I-2b)$$

where $k = \mu v / \hbar$ is the wavenumber, $L_g$ is value of the orbital quantum number $l$ corresponding to $\eta_m$, a maximum in the phase shift, and $\eta_m''$ is the second-derivative of $\eta_m$ with respect to $l$ evaluated at $L_g$.

It can be shown that by expanding about the high-velocity limit, (2b) may be written

$$\Delta Q_g(v) = (2\pi r_m)^{3/2} g_0 \left( \frac{\hbar v}{\epsilon} \right)^{1/2} \left[ 1 + \frac{H_1 \epsilon}{E} + \frac{H_2 \epsilon^2}{E^2} + \ldots \right] \sin \phi \quad (I-3)$$

where $E = \frac{1}{2} \mu v^2$ is the energy,

$$\phi = -\frac{3\pi}{4} + 4 \frac{\epsilon r_m}{\hbar v} \left( a_1 + \frac{A_1 \epsilon}{E} + \frac{A_2 \epsilon^2}{E^2} + \ldots \right) \quad (I-4)$$

and \( r_m \) is the position of the minimum of (of depth \( \varepsilon \)) the potential. The constants \( g_0 \), \( a_1 \) are related to the curvature of the potential well at \( r = r_m \), and the constants \( H_1 \), \( H_2 \), \( A_1 \), \( A_2 \), \( A_3 \), \( A_4 \), were found to be to a good approximation independent of the curvature, \( \varepsilon \), and \( r_m \), and of the form of the potential. Furthermore, for the energy range \( 1 \leq E^* \leq 100 \), where \( E^* = E/\varepsilon \) is the reduced energy, it was found only the terms \( H_1 \) and \( A_1 \), \( A_2 \), \( A_3 \) and \( A_4 \) were required.

For a Lennard-Jones 12-6 potential, i.e.,

\[
\mathcal{V}(r) = \varepsilon \left[ \left( \frac{r_m}{r} \right)^{12} - 2 \left( \frac{r_m}{r} \right)^{6} \right]
\]

the values of the constants are:

\[
\begin{align*}
g_0 &= 0.186299 \quad \text{(I-5a)} \\
H_1 &= 3.267 \pm 0.80 \quad \text{(I-5b)} \\
a_1 &= 0.4215587 \quad \text{(I-5c)} \\
A_1 &= -0.1655 \pm 0.0016 \quad \text{(I-5d)} \\
A_2 &= 0.1057 \pm 0.0160 \quad \text{(I-5e)} \\
A_3 &= -0.0544 \pm 0.0160 \quad \text{(I-5f)} \\
A_4 &= 0.0139 \pm 0.0084 \quad \text{(I-5g)}
\end{align*}
\]

In terms of free parameters, (1) may be rewritten

\[
\mathcal{Q}(\nu) = Y_1 \nu^{-2/5} + Y_2 \nu^{\nu_2} \left( 1 + \frac{H_1 \varepsilon}{E} \right) \sin \phi \quad \text{(I-6)}
\]

and

\[
\phi = -\frac{3\pi}{4} + \frac{Y_3}{\nu} + \frac{Y_4}{\nu E} \left( A_1 + \frac{A_2 \varepsilon}{E} + \frac{A_3 \varepsilon^2}{E^2} + \frac{A_4 \varepsilon^3}{E^3} \right) \quad \text{(I-7)}
\]
It has been shown previously that when the $r^{-8}$ term in the potential begins to affect the cross section, it may be accounted for by replacing $Q_{\text{SSL}}(v)$ in (1) by $Q_{\text{SSL}}(v) + 2\pi/3 \beta$, where $\beta = C_8/C_6$.

It is clear from the form of (I-6) that $Q(v)$ has an oscillatory component. The condition for extrema in $Q$ is that $\sin \phi = \pm 1$, which can be shown to lead to:

$$\left( N - \frac{3}{\beta} \right) v_g^2 = \frac{2 2 \alpha r_m}{\hbar} \left( a_1 + \frac{A_1 \varepsilon}{E} + \frac{A_2 \varepsilon^2}{E^2} + \frac{A_3 \varepsilon^3}{E^3} + \frac{A_4 \varepsilon^4}{E^4} \right)$$

where the maxima and minima in $Q(v)$ are indexed by $N(v_g)$ in the order they occur, i.e., $N = 1$ corresponds to the first maximum, $N = 1.5$ corresponds to the first minimum, $N = 2$ is the second maximum, etc. The quantities $v_g$ are the associated values of $v$ at the extrema.
II. **UNITS**

All of the results and programs below assume the following system of units:

- **Mass**: \( M = 10^{-24} \text{ g} = 1 \text{ ppg} \) (picopicogram)
- **Length**: \( L = 10^{-8} \text{ cm} = 1 \text{ Å (Ångström)} \)
- **Time**: \( T = 10^{-13} \text{ sec} = 1 \text{ dps (decipicosecond)} \)

In this system,

- \( 1 \text{ amu} = 1.660531 \text{ ppg} \)
- \( 1 \text{ a.u.} = 0.52917715 \text{ Å} \)
- \( 1 \text{ Km/sec} = 1 \text{ Å/dps} \)
- \( 1 \text{ eV} = 160.21917 \text{ cpe} \)
- \( 1 \text{ Kcal/mole} = 6.94793 \text{ cpe} \)

\[ h = 6.626196 \text{ cpe-dps} \]
\[ \hbar = 1.0545919 \text{ cpe-dps} \]
\[ kT = 1.380622 \text{ cpe} @ T = 100^\circ \text{K} \]
The purpose of the main program XSECT is to calculate total cross sections $Q(v)$ by means of (I-6)-(I-8). The assumption is made that $H_1$ and $A_1, A_2, A_3, A_4$ are those for the L-J (12-6) potential given in (I-5).

The first card of the data set contains (18A4) 72 columns of title information, which is reproduced at the top of the output.

The second card of the data specifies $N, \mu, \epsilon, A_1, B_0, C_1, C_6,$ in that order, according to the format (I5, 6F10.4, E15.6), where:

- $N$ - No. of velocities for which $Q(v)$ is to be calculated
- $\mu$ - $u$ (reduced mass)
- $\epsilon$ - $\varepsilon$
- $B_0, C_1$ - $b_o$ and $c_1$ are related to the leading terms in the expansion in powers of $1/\varepsilon$ of $L_L$ and $\eta_m$ respectively.
- Since the only quantity required is $g_0 = b_o / c_1^{1/2}$, $b_o$ may be set equal to $g_0$ and $c_1$ to 1.
- $C_6 = C_6$ the long-range force constant.

The succeeding cards of the data contain the velocities $V(I), I = 1, \ldots, N$, for which the $Q(v)$ are to be calculated, according to the format (8F10.4).

The output of the program is a table of the values of $V(I), QSLL, DELQ, Q$, and $QF$ for $I = 1, \ldots, N$, where
\[ \text{QSSL} = Q_{SLL}(v) \]
\[ \text{DELQ} = \Delta Q_g(v) \]
\[ Q = Q(v) = Q_{SLL}(v) + \Delta Q_g(v) \]
\[ QF = \frac{\Delta Q_g(v)}{Q_{SLL}(v)} \]
PROGRAM TO GENERATE RAPID CROSS SECTIONS

REAL MU, KF
DIMENSION V(200), A(4), TITLE(18)
DATA A/-0.155, 0.1057, 0.0544, 0.0139, M1/3.267, M4/...,
DATA PI/3.14159265, HCROSS/1.05459197/
6 100 READ (5,5) (TITLE(I), I=1,18)
7 5 FORMAT (18A4)
8 6 FORMAT (1H1,10X,18A4)
10 10 FORMAT (I5,6F10.4,E15.6)
WRITE (5,6) (TITLE(I), I=1,18)
WRITE (6,4) (I5,6F10.4)
READ (5,30) (V(I), I=1,N)
D1 = C6/HCROSS
D2 = 2.*PI*RM/A0
D3 = 4.*RM/HCROSS
D4 = 2.*PI*RM/HCROSS/EPS*C1!
WRITE (6,40) (I5,6F10.4)
READ (5,30) NV(1,1) = I+N
QSLL = 8.083*(D1/V(I))*C.4
ETR = 0.5*MU*V(I)*V(I)
Z = EPS/ETR
PHI = -0.75*PI + D3*EPS*A1 + Z*(A(2) + Z*(A(3) + Z*
1 A(4))/V(I))
DELQ = D2*SINT(D4*V(I)*I + M1*Z)*SINT(PHI)
Q = QSLL + DELQ
GO TO 100
END

END OF COMPILATION: NO DIAGNOSTICS.

COMPILED BY FOR-V S7E6 ON 06 SEP 71 AT 17:41:11.

USED: CODE(1) 000270; DATA(0) 000515

IND OF COMPILATION:

COMPILATION TIME: 0.653 SEC.
I/O REQUESTS: 50
I/O WORDS TRANSFERED: 57470
IV. PHASHT

The purpose of this program is to produce a fit of the experimental variable \( Y = (N - \frac{3}{8})v_N \) to the model

\[
Y = I + \left( \frac{S_1}{E} \right) + \left( \frac{S_2}{E^2} \right) + \cdots \tag{IV-1}
\]

where, after regression, the following ansatz is made:

\[
I = \frac{2a_1 \varepsilon r_m}{\pi h} \quad \text{and} \quad S_i = 2 \frac{\varepsilon^{i+1} r_m}{\pi h} A_i, \quad i = 1, 2, \ldots \tag{IV-2}
\]

which leads to

\[
a_1 \varepsilon r_m = \frac{\pi h}{2} I
\]

\[
\varepsilon^2 r_m = \frac{\pi h}{2} \frac{S_1}{A_1}
\]

\[
\varepsilon = \frac{A_1 S_2}{A_2 S_1} \tag{IV-3}
\]

Values of \( \varepsilon^2 r_m \) and \( \varepsilon \) are calculated from (IV-2) assuming \( A_1, A_2, A_3, A_4 \) are given by (I-5). "ERROR" denotes 95% confidence interval halfwidths. The confidence intervals were calculated using first-order propagation of error,** and took the error in \( A_1, A_2, A_3, A_4 \) into account.

** I.e., if \( y = f(x_1, x_2) \), then

\[
\sigma_y^2 \approx \left( \frac{\partial f}{\partial x_1} \right)^2 \sigma_{x_1}^2 + 2 \left( \frac{\partial f}{\partial x_1} \right) \left( \frac{\partial f}{\partial x_2} \right) \text{cov}(x_1, x_2) + \left( \frac{\partial f}{\partial x_2} \right)^2 \sigma_{x_2}^2
\]
Input to the program is as follows:

Card 1: title information in columns 1-72 (18A4)

Card 2: NOB, IWGHT, MU (2I5, F10.4)

Card 3 (or more): V(I), I = 1, ..., NOB (8F10.4)

Card 4 (or more): INDEX(I), I = 1, ..., NOB (8F10.4)

where

NOB - number of observed extrema

IWGHT - if 0 data has assumed constant absolute error. If 1, data is assumed to have constant relative error.

MU = \mu \text{ (reduced mass)}

V(I) - extrema velocity \( v_N \) for I-th extremum

INDEX(I) - extrema index \( N \) for I-th extremum
REAL INDEX (30), M
DIMENSION X(30), Y(30), V(30), A(19), C(19), E(19), K(5, 5), TITLE(10)
DATA A/0.921559, 1.0/0.013797
1/ERA/0.998564, 1/ERA/0.91932/27
9 0 C HEAD IN EXPERIMENT TITLE
10 0 C READ IN NO. OF DATA POINTS, NOB, WEIGHT SWITCH (WGHT IF 0 ABSOLUT
11 0 C ERROR AND W(1) = 1. IF 1, RELATIVE ERROR AND W(1) = 1/(1+0.21)
12 0 C AND REDUCED MASS M;
13 0 C NOTE ... IF V IN UNITS OF KM/SEC AND M IN 1.E-24 GRAM, THEN UNIT
14 0 C OF ENERGY WILL BE 1.E-14 ERGS; (NOTE THAT CONS HAS UNITS OF ACTIO
15 0 C ... I
16 0 C READ (5, 30) (V(1), I = 1; NOB)
17 0 C READ (5, 30) (INDEX(1), I = 1; NOB)
18 0 C WRITE (6, 20) NOB, WGHT, M;
19 0 C WRITE (6, 20) NOB, WGHT, M;
20 0 C FORMAT (100, 10X, "NO. OF OBSERVATIONS ": 10/11X, "WEIGHTING SWIT
21 0 C IN ": 10/11X, "REDUCED MASS": 10/11X, "ERROR": 10/11X)
22 0 C READ IN EXTREMA VELOCITIES AND EXTREMA INDICES
23 0 C READ (5, 30) (V(I), I = 1; NOB)
24 0 C READ (5, 30) (INDEX(I), I = 1; NOB)
25 0 C WRITE (6, 90) NOB,)
26 0 C WRITE (6, 90) NOB,)
27 0 C FORMAT ("///5X, "NO. ": 8X, "V*: 8X, "INDEX": 11X, "X*: 11X, "Y#
28 0 C 11X, "X": 11X, "Y#
29 0 C FORMAT (11X, "INDEX": 11X, "X*: 11X, "Y#
30 0 C DO 500 I = 1, NOB
31 0 C ETR = 0.5*M*V(I)*V(I)
32 0 C X(I) = 1./ETR
33 0 C Y(I) = (INDEX(I) - 0.375)*V(I)
34 0 C WI = 1.0
35 0 C IF (WGHT < EQ. 1) W(I) = 1./(Y(I)+Y(I))
36 0 C WRITE (6, 50) 1, V(I), ETR, INDEX(I), X(I), Y(I)
37 0 C FORMAT (15, 8E15.5)
38 0 C CALL POLFIT (X, Y, M, NOB, C, E, R, NOEG, SIG)
39 0 C WRITE (6, 60) NOEG, SIG
40 0 C FORMAT ("///10X, "POLYNOMIAL OF DEGREE*: 15*: DETERMINED": 10X, "MMS A
41 0 C (SIDEOE + ...E15.5/11X, "TERM", 15, 13)CDEPPJCIENT", 10X, "ERROR": 5X.50
42 0 C 21H=1/7)
43 0 C 11H = NOEG = 1
44 0 C DO 400 I = 1, 11H
45 0 C J = I-1
46 0 C WRITE (6, 70) J, C(J)
47 0 C FORMAT (15, 6E15.5/11X, "TERM", 15, 13)CDEPPJCIENT", 10X, "ERROR": 5X.50
48 0 C AER = CONS0C(I)
49 0 C EE = CONS0C(I)
50 0 C EPSRM = AER/A1
51 0 C EE2 = EE/A1
52 0 C WRITE (6, 80) AER, EE, EPSRM, EE2
53 0 C FORMAT ("///10X, "AER", "EE", "EPSRM", "EE2", "ERROR": 12.5, 2X", "ERROR": 12.5, 2X")
54 0 C IRM FROM A1 = 0.921559; 12.5, 2X", "ERROR": 12.5, 2X")
244 53* IF (NDEG .EQ. 0) GO TO 100
246 54* EER = CONS*E(2)/A(1)
247 55* EE = ABS(CONS*E(2)/A(1))
250 56* EPS = EER/EPSRM
251 57* EE2 = EPS*SQRT(R(1,1)/C(1)*2 + R(2,2)/C(2)*2 - 2*R(1,2)/C(1)*C(2))
251 58* (21) + ERA1
252 59* WRITE (6,85) EER,EE,EPS,EE2
260 61* 1 FROM A1 =0.421559,...,E12.5,2X,(ERROR = E12.5,10)
261 62* IF (NDEG .EQ. 1) GO TO 100
263 63* EPS = CONS*A(1)/(C(2)*A(2))
264 64* EE = EPS*SQRT(R(2,2)/C(2)*2 + R(3,3)/C(3)*2 - 2*R(2,3)/C(2)*C(3))
264 65* (C(3)) + ERA1A2
265 66* WRITE (6,90) EPS,EE
271 67* 90 FORMAT (/10X,E12.5,2X,(ERROR = E12.5,10)
272 68* GO TO 100
273 69* END

END OF Compilation: NO DIAGNOSTICS.

Compilation Time: 0.959 sec.
I/O Requests: 61
I/O Words Transferred: 61198
A. POLFIT

This subroutine fits a polynomial

\[ p(x) = \sum_{k=0}^{M} a_k x^k \]

to a set of \( N \) data points \((x_i, y_i)\), \( 1 \leq i \leq N \), by weighted forward regression. The criterion used to determine \( a_0, a_1, \ldots, a_M \) is the minimization of the approximate variance of fit \( s^2 \):

\[ s^2 = \frac{1}{N-M-1} \sum_{i=1}^{N} w_i (y_i - p(x_i))^2 \]

where \( w_i \) is the weight assigned to the i-th data point (if the variance of the i-th data point is \( \sigma_i^2 \), then \( w_i \propto 1/\sigma_i^2 \)).

The mechanics of the fit are performed by use of calculated orthogonal polynomials:

\[ p(x) = \sum_{k=0}^{M} a_k P_k(x) \]

where the \( P_k \)'s satisfy \( P_0(x) = 1 \) and

\[ P_{k+1}(x) = (x - u_k) P_k(x) - v_k P_{k-1}(x) \]

\[ \sum_{i=1}^{N} w_i P_k(x_i) P_j(x_i) = \delta_{kj} D_k \]

The fit is continued until all terms whose contributions to the variance \( s^2 \) are significant at the 90\% level (F-test) have been added.
CALL POLFIT (X, Y, W, N, C, E, R, M, SIG)

Input:
X(I) - abscissa $x_i$ of the I-th data point
Y(I) - ordinate $y_i$ of the I-th data point
W(I) - weight $w_i$ of the I-th data point
N - no. of data points

Output:
C(I) - $C_{i-1}$, coefficient of $x^{i-1}$ in final polynomial
E(I) - 95% confidence interval halfwidth of C(I), i.e., $t \sigma_i$
R(I,J) - covariance of C(I) and C(J) multiplied by $t^2$, i.e., $t^2 \text{cov}(I,J)$
M - degree of final fitted polynomial
SIG - $S$, standard error of fit where $t$ is the critical value of the student-t statistic for $\alpha = .05$ (Equal-Tails) and $N-M-1$ degrees of freedom.

NOTE: Because of dimensioning, the program in its given form is limited to $N \leq 21$ and $M \leq 4.$
SUBROUTINE POLFIT (X,Y,W,N,C,E,M,SIG)
FITS A POLYNOMIAL OF DEGREE M (DETERMINED BY ROUTINE) TO A SET OF
N POINTS (X(I),Y(I)) I=1,...,N.

W(I) IS THE WEIGHT ASSIGNED TO POINT I. E.G. FOR ASSUMED CONSTANT
ABSOLUTE ERROR, W(I) = 1., AND FOR ASSUMED CONSTANT PERCENTAGE
ERROR, W(I) = 1./XY(Y(I)*Y(I)).

THE POLYNOMIAL IS GIVEN BY P(X) = C(1) + ... C(M+1)*X^M
E(I) IS THE 95 PERCENT CONFIDENCE INTERVAL HALFWIDTH OF C(I)
R(I,J) IS THE COVARIANCE BETWEEN C(I) AND C(J), MULTIPLIED BY THE
SQUARE OF THE CRITICAL VALUE OF THE STUDENT T STATISTIC
THE DEGREE IS INCREASED UNTIL ALL TERMS SIGNIFICANT AT THE 90
PERCENT LEVEL HAVE BEEN INCLUDED.

THE POLYNOMIAL IS DETERMINED USING THE METHOD OF ORTHOGONAL
POLYNOMIALS.
AT EXIT FROM THE ROUTINE M WILL BE THE DETERMINED DEGREE OF THE
POLYNOMIAL AND SIG WILL CONTAIN THE RMS RESIDUAL OF THE FIT.

DOUBLE PRECISION U,V,A,B,VY,AYY,WAYY,SYN,T,WORK,P1,P2,SYM1,SYM2,
SUM1,SUM2, SUM3,SUM4.

DIMENSION X(1),Y(1),W(1),C(1),E(1),U(5),V(5),A(5),B(5),V(5),
R(5,5),F90(25),T95(25).
EQUIVALENCE (VY,B(1,5)) , (T, B(1,4)) , (WAYY,B(1,3)) , (SYN,B(2,5)).

DATA V(Y)/0. DO/:
DO 200 I = 1,4
100
data 1
DO 100 J = 1,11
225
data 100
data 100
SUM1 = 0.DO
SUM2 = 0.DO
SUM3 = 0.DO

VY = 0.DO
DO 300.I = 1,N
T = W(I)

SUM1 = SUM1 + T
SUM2 = SUM2 + T*X(I)
T = T*Y(I)
SUM3 = SUM3 + T
VY = VY + T*Y(I)
AY(1) = SUM3/SUM1

D(1) = SUM1
U(I) = SUM2/SUM1
B(2,1) = - U(I)
AYY = 0.DO
2001 69* 700  
2002 70*  
2003 71*  
2004 72*  
2005 73*  
2006 800  
2007 74*  
2008 75*  
2009 76*  
2010 77*  
2011 78*  
2012 79*  
2013 80*  
2014 81*  
2015 82*  
2016 83*  
2017 84*  
2018 900  
2019 85*  
2020 86*  
2021 87*  
2022 88*  
2023 1100  
2024 89*  
2025 90*  
2026 91*  
2027 92*  
2028 93*  
2029 94*  
2030 95*  
2031 96*  
2032 97*  
2033 98*  
2034 99*  
2035 100*  
2036 101*  
2037 102*  
2038 103*  
2039 104*  
2040 105*  
2041 106*  
2042 107*  
2043 108*  
2044 109*  
2045 110*  

VY = VY - A(1)*A(1)*D(1)  
I = I + 1  
IF (I * GT. 5) GO TO 1100  
II = I - 1  
SUM1 = 0.00  
SUM2 = 0.00  
SUM3 = 0.00  
SUM4 = 0.00  
DO 800 J = 1, N  
P1 = 1.00  
P2 = 0.00  
WORK = X(J)  
DO 700 K = 1, II  
T = (WORK - U(IK))*P1 - V(K)*P2  
P2 = P1  
T = W(J)*P1  
SUM1 = SUM1 + T*P1*WORK  
SUM2 = SUM2 + T*P2*WORK  
SUM3 = SUM3 + T*P1  
SUM4 = SUM4 + T*Y(J)  
D(I) = SUM3  
U(I) = SUM1/SUM3  
V(I) = SUM2/D(I1)  
A(I) = SUM4/SUM3  
WAYY = A(1)*A(1) *D(1)  
AYY = AYY + WAYY  
IF (I*EQ.2) GO TO 1000  
B(I+1) = -U(I)*B(I,1) - V(I)*B(I-2,1)  
DO 900 J = 2, II  
B(I,J) = B(I,J-1) - U(I)*B(I,J) - V(I)*B(I-2,J)  
SYN = DABS(VY - AYY)/IDF  
FP = WAYY/SYN  
IF (FP * GT. F90(1DF)) GO TO 500  
MM = I-1  
M = MM-1  
AYY = AYY - WAYY  
IDF = N-MM  
SYN = DABS(VY - AYY)/IDF  
DO 1600 K = 1, MM  
T = 0.00  
DO 1500 J = K, MM  
T = T + A(J)*B(J,K)  
C(K) = T  
COEF = SYN*T95*(1DF)*2  
DO 2000 K = 1, MM  
DO 1900 J = K, MM  
T = 0.00  
DO 1800 L = J, MM  
T = T + B(L,K)*B(L,J)/D(L)  
R(K,J) = T*COEF  
R(J,K) = K(K,J)  
E(K) = SQRT(R(K,K))  
SIG = SQRT(SYN)  
RETURN
300 110• END

END OF COMPILATION:  NO DIAGNOSTICS.

COMPILATION TIME:  1.526 SEC.
I/O REQUESTS:  66
I/O WORDS TRANSFERED:  62865
B. **EXAMPLES**

Four example calculations are given.

   IWGHT = 1 (assumed constant relative error), so the rms residual $S$ for the fit is an estimate of the coefficient of variation of the data. The value $S = 0.31\%$ is compatible with known experimental precision.

Examples 2-4 are based upon the synthetic data calculated from (IV-1) with $I, S_1, S_2, S_3, S_4$, given by (IV-2), with $\varepsilon = 8 \text{ cpe}, r_m = 4 \text{ Å}$, $a_1 = 0.421559$. I.e.,

$$\hat{Y}_i = I + \frac{S_1}{E_i} + \frac{S_2}{E_i^2} + \frac{S_3}{E_i^3} + \frac{S_4}{E_i^4} \quad (1 \leq i \leq 13)$$

and $Y_i = \hat{Y}_i (1 + \delta)$ where $\delta$ is a normal distributed random variable with mean 0 and variance $\sigma^2$. In each case IWGHT = 1, so the calculated value of $S$ should approximate $\sigma$.

2. $Y = \hat{Y}$, i.e., $\sigma = 0$. Calculated $S = 0.0098\%$.

3. $\sigma = 0.5\%$. Calculated $S = 0.55\%$.

4. $\sigma = 0.25\%$. Calculated $S = 0.18\%$. 
DATA OF U. BUCK, K. A. KOHLER, AND H. PAULY; Z. PHYSIK 244, 180 (1971)

NO. OF OBSERVATIONS: 13
WEIGHTING SWITCH: 1
REDUCED MASS: 342.99+02

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POLYNOMIAL OF DEGREE 3 DETERMINED
RMS RESIDUAL: 31262+02

TERM | COEFFICIENT | ERROR
-----|-------------|-----
| 0   | 11338+02    | 15915+00 |
| 1   | -55601+02   | 1417+02  |
| 2   | 52421+03    | 34821+03 |
| 3   | -22900+04   | 25523+04 |

A1*EPS*RMS = 18782+02 (ERROR = 26364+00)
EPS*RMS FROM A1 = 0.421559 ••• 44553+02 (ERROR = 62538+00)
EPS*EPS*RMS = 55653+03 (ERROR = 14030+03)
EPS FROM A1 = 0.421559 ••• 12492+02 (ERROR = 29827+01)
EPS = 14762+02 (ERROR = 42864+01)
### TEST DATA

**EPS = 8.**  **RM = 4.**  **NO ERROR.**

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### Polynomial of Degree 4 Determined

RMS Residual: **97530-04**

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### EPS from A1

EPS_EPM: **13490+02** (ERROR = **17097-01**)  
EPS_EPM FROM A1 = 0.421559  **32000+02** (ERROR = **40556-01**)  
EPS_EPM: **25600+03** (ERROR = **96126-01**)  
EPS FROM A1 = 0.421559  **80000+01** (ERROR = **30107-00**)  
EPS = **79998+01** (ERROR = **16387+01**)
### TEST DATA

**EPS = 8, RM = 4, SIGMA = 0.005**

**NO. OF OBSERVATIONS ... 13**
**WEIGHTING SWITCH ... 1**
**REDUCED MASS ... 300000+02**

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**POLYNOMIAL OF DEGREE 3 DETERMINED**

**RMS RESIDUAL ... 54587-02**

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A1*EPS*RM = 13979+02 (ERROR = 38967+00)
EPS*RM FROM A1 = 0.421559 (ERROR = 33161+02)

EPS = 15858+02 (ERROR = 51957+01)
TEST DATA --- EPS = 8. --- RM = 4. --- SIGMA = 0.0025

NO. OF OBSERVATIONS • • • 13
WEIGHTING SWITCH • • • 1
REDUCED MASS • • • 0.300000+02

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POLYNOMIAL OF DEGREE 3 DETERMINED
RMS RESIDUAL • • • 0.18440+02

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A1 EPS*RM = 13571+02 (ERROR = 11158+00)
EPS*RM FROM A1 = 0.421559+01 + 32192+02 (ERROR = 31212+00)

EPS*EPS*RM = 28646+03 (ERROR = 53236+02)
EPS FROM A1 = 0.421559+01 + 88986+01 (ERROR = 15719+01)

EPS = 10101+02 (ERROR = 37969+01)
This main program produces a fit of the experimental variable

\[ Y = (N - \frac{3}{8}) v N \]

to the model

\[ Y = \frac{c_1}{E} + \frac{c_2}{E} \left( A_1 + \frac{A_2 c_2}{E} + \frac{A_3 c_3}{E^2} + \frac{A_4 c_3^2}{E^3} \right) \]  \hspace{1cm} (V-1)

where, after regression the following ansatz is made:

\[ c_1 = 2 a_1 \epsilon m / \pi^2 \; ; \; c_2 = 2 \epsilon^2 m / \pi \; ; \; c_3 = \epsilon \]  \hspace{1cm} (V-2)

which lead to

\[ a_1 \epsilon m = \frac{\pi \epsilon m^2}{2} c_1 \]

\[ \epsilon^2 m = \frac{\pi \epsilon m}{2} c_2 \]

\[ \epsilon = c_3 \]  \hspace{1cm} (V-3)

The details of the fitting procedure are described in V.A (FIT).

The description of the input and output is the same as in Section IV.
REAL INDEX (30), MU

DIMENSION E(30), Y(30), W(30), V(30), TITLE(18)

DATA 41/0.421559/

READ (5,10) TITLE(1), I=1, 18

FORMAT (18A4)

WRITE (6,6) (TITLE(I), I=1, 18)

FORMAT (16H1, 10X, 18A4)

C READ IN NO. OF DATA POINTS NOB, WEIGHT SWITCH IWGHT (IF 0 ABSOLUTE
C ERROR AND W(I) = 1. IF 1, RELATIVE ERROR AND W(I) = 1/Y(I)**2)

C AND REDUCED MASS MU

C NOTE ... IF V IN UNITS OF KM/SEC AND MU IN 1. E-24 GRAM, THEN UNITS
C OF ENERGY WILL BE 1. E-14 ERGS. (NOTE THAT CONS HAS UNITS OF ACTION

C I. E-27 ERG-SEC)

READ (5,10) NOB, IWGHT, MU

WRITE (6,20) NOB, IWGHT, MU

FORMAT (10D10.4)

READ IN EXTREMA VELOCITIES AND EXTREMA INDICES

READ (5,30) (V(I), I=1, NOB)

READ (5,30) (INDEX(I), I=1, NOB)

FORMAT (8F10.4)

WRITE (6,40)

FORMAT (1//5X,'NO.', 8X, 'V', 15X, 'ETR', 11X, 'INDEX', 11X,'Y'/6X, 601

DO 500 I = 1, NOB

E(I) = 0.5*MU*V(I)**2

Y(I) = (INDEX(I) - 0.375)*V(I)

IF (IWGHT*EQ. 1) W(I) = 1.

WRITE (6,50) I, V(I), Y(I), INDEX(I), V(I)

FORMAT (3X, 15F10.4)

SIG = FIT (E, Y, W, NOB, AIERM, ERAER, E2R, ERE2R, EPS, EREPS, RM, ERM)

WRITE (6,60) SIG

WRITE (6,70) RMS RESIDUAL OF FIT ..., E12.5/)

EPSRM = AIERM/1

EE = ERAER/AI

WRITE (6,80) AIERM, ERAER, EPSRM, EE

FORMAT (10X, AI*EPSRM = 'E12.5,2X, (ERROR = 'E12.5,**1)/10X, EPS*

IRM FROM AI = 0.421559 ***, 'E12.5,2X, (ERROR = 'E12.5,**1)

EPS2 = E2R/EPSRM

EE = EPS2*SQRT ( (ERE2R/E2R)**2 + (EE/EPSRM)**2 )

WRITE (6,85) E2R, ERE2R, EPS2, EE

FORMAT (1/10X, EPS*EPSRM = 'E12.5,2X, (ERROR = 'E12.5,**1)/10X, EPS*

I FROM AI = 0.421559 ***, 'E12.5,2X, (LOWER BOUND ON ERROR = 'E12.5,

GO TO 100
END OF COMPIlATION: NO DIAGNOSTICS.

COMPILATION TIME: 0.731 SEC.

I/O REQUESTS: 51
I/O WORDS TRANSFERED: 55235
This subprogram performs the mechanics of the fit of (V-1), given data \( E(I), Y(I), W(I) \), for \( I = 1, \ldots, N \), where \( W(I) \) is the weight of the \( I \)-th data point. Initial estimates of \( c_2 \) and \( c_3 \) (80 and 5, resp.) are iteratively refined by bilinear regression of the first-order expansion

\[
Y_i \approx c_1 \left( \frac{\partial Y}{\partial c_2} \right) \frac{c_2}{c_2, c_3} + \left( \frac{\partial Y}{\partial c_3} \right) \frac{c_3}{c_2, c_3} \tag{V-4}
\]

where

\[
\frac{\partial Y}{\partial c_2} = \frac{1}{E} \left( A_1 + A_2 \frac{c_3}{E} + A_3 \frac{c_3^2}{E^2} + A_4 \frac{c_3^3}{E^3} \right) \tag{V-5}
\]

\[
\frac{\partial Y}{\partial c_3} = \frac{c_2}{E^2} \left( A_2 + \frac{2 A_3 c_3}{E} + \frac{3 A_4 c_3^2}{E^2} \right)
\]

The iteration is continued until the rms residual converges to 1%.

\[
Z = \text{FIT}(E, Y, W, N, \text{AIERM, ERAEM, E2R, ERE2R, EPS, EREPS, RM, ERRM})
\]

returns \( Z = S \) the rms residual and

\[
\text{AIERM} = a_1 \epsilon r_m, \quad \text{E2R} = \epsilon^2 r_m, \quad \text{EPS} = \epsilon, \quad \text{and}
\]

\( \text{ERAEM, ERE2R, ERRM} \), the resp. 95% confidence interval halfwidths of these quantities.
FUNCTION FIT (E,Y,W,N,ALFM,ERAER,E2R,ERE2R,EPSEPERS,ERM,ERR)

C PERFORMS ITERATIVE FITTING OF EXTREMA VALUES ...

C E(I) = TRANSLATIONAL ENERGY OF POINT I

C Y(I) = (N-0.375)*V(I) --- EXTREMA ORDI NATE

DIMENSION E(I),Y(I),W(I),X(30,2),C(3),ER(4),AS(4)

DATA A/-0.15,-0.15,0.15,0.15/2.

C NOTE - CONS = PI*HCRROSS/2.

EPS = 5.
E2R = 80.
SIGP = 0.

KOUNT = 0

KOUNT = KOUNT + 1

IF (KOUNT .GT. 10) GO TO 400

DO 200 I = 1,N

X(I,1) = (A(I) + EPS *(A(2) + EPS *(A(3) + EPS *A(4)/E(1)))/E(I))/E(I)

200 X(I,2) = E2R *(A(2) + EPS *(2.*AS(3) + 3.*EPS *A(4)/E(1))/E(I))

1. (E(1) + E(I))

SIG = BILINR (X,Y,W,N,C,ER,RHO,30)

EPS = EPS + C(3)
E2R = C(2)
DEL = SIG - SIGP

SIGP = SIG

IF (ABS(DEL) .GT. 0.01*SIG) GO TO 100

AIFMM = CONS*(C(1)

ERAER = CONS*ER(I)
E2R = CONS*E2R
ERE2R = CONS*ER(2)

EPSEPERS = ER(3)
RM = E2R/(EPS*EPS)

ERRM = RM * SQRT( 4.*EPSEPERS/EPS)*2 + (ERE2R/E2R)**2 - 4.*RHO*EREPSE

1.*ERE2R/(EPS*E2R )

FIT = SIG

RETURN

400 WRITE (6,10)

10 FORMAT (/10X, '*****FAILURE TO CONVERGE IN 10 ITERATIONS*****')

GO TO 300

END OF COMPILATION: NO DIAGNOSTICS.

COMPILATION TIME: 0.644 SEC

I/O REQUESTS: 50

I/O WORDS TRANSFERRED: 54973
B. BILINR

Performs a weighted bilinear regression of the model
\[ \hat{Y}_i = \mathcal{C}_1 + \mathcal{C}_2 X_{i1} + \mathcal{C}_3 X_{i2} \]

\[ Z = \text{BILINR} \left( X, Y, W, N, C, E, \text{RHO, NDIM} \right) \]

Input:
- \( X(I,1) \) - \( X_{i1} \), I-th value of first variable
- \( X(I,2) \) - \( X_{i2} \), I-th value of second variable
- \( Y(I), W(I) \) - ordinate and weight of I-th data pt.
- \( N \) - No. of data
- \( \text{NDIM} \) - row dimension of \( X \)

Output:
- \( C(J) \) - \( c_j \), J-th parameter
- \( E(J) \) - 95% confidence interval half width of \( C(J) \)
- \( \text{RHO} \) - \( r_{23} \) correlation coefficient between \( c_2 \) and \( c_3 \)
- \( Z = S \) rms residual of fit, calculated from

\[ S^2 = \frac{1}{N-3} \sum_{i=1}^{N} w_i \left( Y_i - \hat{Y}_i \right)^2 \]
53* SIG2 = 0.0D0
54* SUMY = 0.0D0
55* DO 200 I = 1,N
56* T = Y(I) - C(1) - C(2) * X(I) - C(3) * X(I+NDIM)
57* SIG2 = SIG2 + W(I) * T * T
58* 200 SUMY = SUMY + W(I) * T
59* C(1) = C(1) + SUMY/SUMW
60* IDF = N-3
61* SIG2 = SIG2/IDF
62* BILINE = DSORT(SIG2)
63* T = T95(IDF)*BILINE
64* E(2) = T*DSORT(A11)
65* E(1) = T*DSORT(A22)
66* E(3) = T*DSORT(A22)
67* IDF = N-3
68* RHO = A21/DSORT(A11*A22)
69* RETURN
70* END

END OF COMPIATION: NO DIAGNOSTICS.

COMPILATION TIME: 1.094 SEC.
I/O REQUESTS: 58
I/O WORDS TRANSFERED: 58883
C. **EXAMPLES**

The four examples are the same as described in IV-B.

1. Note that $s = 0.31\%$
2. $s = 0.12 \times 10^{-5} \%$ (true 0%)
3. $s = 0.66\%$ (true 0.5%)
4. $s = 0.21\%$ (true 0.25%)
DATA OF U. BUCK, K. A. KÖHLER, AND H. PAULY • Z. PHYSIK 244 180 (1971)

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RMS RESIDUAL OF FIT ... 0.30755-02

A1*EPS®RM = 1.18748+02 (ERROR = 0.13757+00 )
EPS®RM FROM A1 = 0.4421559 ... 0.44747+02 (ERROR = 0.32633+00 )

EPS*EPS®RM = 0.56106+03 (ERROR = 0.57075+02 )
EPS FROM A1 = 0.421559 ... 1.2615+02 (LOWER BOUND ON ERROR = 0.12867+01 )

EPS = 1.1831+02 (ERROR = 0.24142+01 )
RM = 0.15522+01 (ERROR = 0.26027+00 )
**TEST DATA -- NEW TERMS -- NO ERROR -- EPS = 0. -- RM = 4.**

**NO. OF OBSERVATIONS:** 13  
**WEIGHTING SWITCH:** 1  
**REDUCED MASS:** 300000.02

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**RMS RESIDUAL OF FIT:** 1.2267-07

**AI*EPS*RM:** 1.3490-02  (ERROR = 59740.06)
**EPS*RM FROM AI:** 0.421559  (ERROR = 1.471-05)

**EPS*EPS*RM:** 2.5600-03  (ERROR = 2.1102-03)
**EPS FROM AI:** 0.421559  (ERROR = 80000.01)  (LOWER BOUND ON ERROR = 66039.05)

**EPS:** 80000.01  (ERROR = 15783.04)
**RM:** 40000.01  (ERROR = 12538.04)
### TEST DATA

**EPS = 8, RM = 4, SIGMA = 0.005**

**NO. OF OBSERVATIONS:** 13  
**WEIGHTING SWITCH:** 1  
**REDUCED MASS:** 300000.02

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**RMS RESIDUAL OF FIT:** 66103-02

**A1 * EPS*RM = 13653+02**  
**ERROR = 32379+00**

**EPS*RM FROM A1 = 421559**  
**ERROR = 76808+00**

**EPS*EPS*RM = 30311+03**  
**ERROR = 12063+03**

**EPS FROM A1 = 421559**  
**ERROR = 93591+01**  
**LOWER BOUND ON ERROR = 37312+01**

**EPS = 98608+01**  
**ERROR = 79641+01**

**RM = 31173+01**  
**ERROR = 38182+01**
## Test Data

### No. of Observations

13

### Weighting Switch

1

### Reduced Mass

\( \frac{300000}{0.02} \)

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### RMS Residual of Fit

\( 20544+02 \)

### A1 * EPS * RM

\( 13495+02 \) (ERROR = \( 98363+01 \))

### EPS * RM FROM A1

\( 0.421559 \) (ERROR = \( 0.23333+00 \))

### EPS * EPS * RM

\( 25410+03 \) (ERROR = \( 34287+02 \))

### EPS FROM A1

\( 0.421559 \) (LOWER BOUND ON ERROR = \( 0.10726+01 \))

### EPS

\( 77712+01 \) (ERROR = \( 25466+01 \))

### RM

\( 42075+01 \) (ERROR = \( 21990+01 \))
VI. QFIT

This main program directs a weighted nonlinear regression of the model

\[ \hat{Q}(\nu) = Y_1 \nu^{-2/5} + Y_2 \nu^{Y_2} \left[ 1 + \frac{H_1 Y_5}{E} \right] \sin \phi \]  

(VI-1)

where

\[ \phi = -\frac{3\pi}{4} + \frac{Y_3}{\nu} + \frac{Y_4}{\nu E} \left( A_1 + A_2 Y_5 + \frac{A_3 Y_5^2}{E^2} + \frac{A_4 Y_5^3}{E^3} \right) \]  

(VI-2)

and after regression the ansatz \( Y_5 = \epsilon \) and (I-8) is made, leading to

\[
\begin{align*}
C_6 &= \frac{\hbar}{2} (Y_1 / 8.083)^{5/2} \\
\gamma_m &= \frac{\hbar Y_4}{4 Y_5^2} \\
\alpha_1 &= Y_3 Y_5 / Y_4 \\
q_0 &= Y_5^{+1/2} Y_2 / \hbar^2 (\pi Y_4 / 2)^{3/2} \\
\epsilon &= Y_5 
\end{align*}
\]  

(VI-3)

The regression is automatically repeated with initial values for \( Y_1 - Y_5 \) being the values obtained from the first regression, and a new adjustable parameter \( Y_6 \) being added to the model:

\[ \hat{Q}(\nu) = Y_1 \nu^{-2/5} + Y_2 \nu^{Y_2} \left[ 1 + \frac{H_1 Y_5}{E} \right] \sin \phi + Y_6 \]  

(VI-4)
After regression the ansatz

\[ \gamma_6 = \frac{2\pi}{3} \frac{c_8}{c_6} \]  

is made, leading to

\[ c_8 = \frac{3h}{2\pi} \gamma_6 \left( \frac{\gamma_1}{8.083} \right)^{5/2} \]

The required input is of the following form:

CARD 1: Title information (18A4)
CARD 2: N, MU, EPS, RM, A1, GO, C6, IWGHT (I5,5F10.4,E15.6,15)
CARD 3 (or more): V(I), I = 1, ..., N (8F10.4)
CARD 4 (or more): Q(I), I = 1, ..., N (8F10.4)

where

N - Number of velocities at which cross sections are given
MU - \( \mu \), reduced mass of the system
EPS, RM, A1, GO, C6 - initial estimates for \( \varepsilon, r_m, a_1, g_o, C_6 \)
IWGHT - if 0 data are assumed to have constant absolute error; if 1, constant relative error
V(I) - the I-th velocity observation
Q(I) - the I-th cross section observation.

If the scale of the Q's is not known, \( C_6, c_8 \) and \( g_o \) will be found finally to contain the same factor, but no other parameters will be affected.
Output of the program includes the values of $\nu_1, \ldots, \nu_6$ with error intervals (denoted parameters 1-6), and the correlation matrix of the errors of $\nu_1, \ldots, \nu_6$. 

A CONSISTENT SET OF UNITS FOR THIS PROGRAM IS ...

AND KM/SEC FOR VELOCITY.

REAL MU

DOUBLER PRECISION R(36),X,PAR,ER,F(200),FZ(200),BUP(6),BLOW(6)

DIMENSION X(200),Q(200),W(200),PAR(6),ER(6)

COMMON V(200),E(200)

DATA BLOW/6*0.00/0.62/0.62/5*0.62/2*0.10/2*0.10/ 0

EXTERNAL XSECT,DXSECT

READ (5,10) (Q(I),I=1,18)

WRITE (5,20) (Q(I),I=1,18)

FORMAT (1H1,10X,18A4)

FORMAT (I5,5F10.4,E15.6)

FORMAT (I5,5F10.4,E15.6)

READ (5,30) N,MU,EPS,RM,A1,GO,C6,IGWHT

IF IGWHT = 0, ASSUMED CONSTANT ERROR. IF IGWHT = 1, ASSUMED
CONSTANT RELATIVE ERROR.

FOR A LENNARD-JONES 12-6 POTENTIAL--A1= -0.421559, B0= -0.186299

CRUDE INITIAL ESTIMATES FOR EPS AND RM MIGHT BE 5. AND 4. RESP.

FORMAT (I5,5F10.4,E15.6)

WRITE (5,35) N,MU,EPS,RM,A1,GO,C6,IGWHT

WRITE (5,35) N,MU,EPS,RM,A1,GO,C6,IGWHT

CALL TRYAL (PAR,C6,A1,GO,EPS,LM)

CALL GASS59 (XSECT,DXSECT,N,W,G,5,PAR,BUP,BLOW,1,D-3.1,D-3.1,D-6

CALL FINAL (PAR,ER)

GO TO 100

END OF compilation:

NO DIAGNOSTICS.

COMPILATION TIME: 0.664 SEC.

I/O REQUESTS: 51

I/O WORDS TRANSFERED: 55129
A. **TRIAL**

This subprogram converts initial estimates for $\varepsilon$, $r_m$, $a_1$, $g_0$ and $C_6$ into initial estimates for $\gamma_1$, ..., $\gamma_6$ (denoted by PAR(1) ... PAR(6)).

CALL TRIAL (PAR, C6, A1, GO, EPS, RM)

Input:

- $C_6$ - long-range $C_6$
- $A1$ - $a_1$ (I-5c)
- $GO$ - $g_0$ (I-5a)
- $EPS$ - $\varepsilon$
- $RM$ - $r_m$

Output:

- $\text{PAR}(1) = \gamma_1$ (I-8)
- $\text{PAR}(2) = \gamma_2$ (I-8)
- $\text{PAR}(6) = \gamma_6$ (VI-8)
<table>
<thead>
<tr>
<th>Line</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>SUBROUTINE TRIAL (PAR,C6,A1,GO <em>EPS</em>RM)</td>
</tr>
<tr>
<td>2</td>
<td>DOUBLE PRECISION PAR</td>
</tr>
<tr>
<td>3</td>
<td>DIMENSION PAR(1)</td>
</tr>
<tr>
<td>4</td>
<td>DATA HCROSS/1.0545919/,PI/3.14159265/</td>
</tr>
<tr>
<td>5</td>
<td>PAR(1) = 8.083*(C6/HCROSS)**0.4</td>
</tr>
<tr>
<td>6</td>
<td>PAR(2) = (2.<em>PI</em>RM)*GO <em>SQR((2.<em>PI</em>RM</em>HCROSS)/EPS)</td>
</tr>
<tr>
<td>7</td>
<td>PAR(3) = EPS</td>
</tr>
<tr>
<td>8</td>
<td>PAR(4) = 4.<em>RM</em>EPS/HCROSS</td>
</tr>
<tr>
<td>9</td>
<td>PAR(5) = EPS*PAR(4)</td>
</tr>
<tr>
<td>10</td>
<td>PAR(4) = A1*PAR(4)</td>
</tr>
<tr>
<td>11</td>
<td>PAR(6) = 0.</td>
</tr>
<tr>
<td>12</td>
<td>RETURN</td>
</tr>
<tr>
<td>13</td>
<td>END</td>
</tr>
</tbody>
</table>

END OF COMPILATION: NO DIAGNOSTICS.

COMPILATION TIME: 0.395 SEC.
I/O REQUESTS: 49
I/O WORDS TRANSFERRED: 52841
B. FINAL

This subprogram takes the final values of $\gamma_1, \ldots, \gamma_6$ and their errors, and outputs values and errors for $\epsilon, a_1, r_m, C_6, g_0$, $a_1\varepsilon r_m$, $\varepsilon^2 r_m$, $\beta$, and $C_8$.

CALL FINAL (NP, PAR, ERR, R)

where:

NP - no. of parameters of fit (5 or 6)

PAR(I) - $\gamma_i$, 1 $\leq$ I $\leq$ NP

ERR(I) - 95% confidence interval halfwidth for PAR(I)

R(I,J) - correlation coefficient $r_{ij}$ between PAR(I) and PAR(J), stored as an NPxNP matrix.
C. XSECT/DXSECT

Subprogram which calculates \( Q(v) \) given \( \gamma_1, \ldots, \gamma_6 \) by means of (I-6) (XSECT), or \( \partial Q(v) / \partial \gamma_i, 1 \leq i \leq 6 \) (DXSECT).

1. CALL XSECT (PAR, F, NOB, NP)
   
   Input:
   
   \( \text{PAR}(I) - \gamma_i \quad 1 \leq I \leq \text{NP} \)
   
   NOB - No. of velocities \( v \)
   
   NP - No. of parameters \( \gamma_i \) (= 5 or 6)
   
   Output:
   
   \( F(I) - Q(v) \) for \( I \)-th velocity

2. CALL DXSECT (PAR, F, NOB, NP)
   
   Input:
   
   \( \text{PAR}(I), \text{NOB}, \text{NP} \) - as above
   
   Output:
   
   \( F(I,J) - (\text{NOB} \times \text{NP} \text{ matrix}) \partial Q(v) / \partial \gamma_j \) for \( I \)-th velocity
SUBROUTINE XSECT (PAR,F,NOB,NP)
C SUBROUTINE WHICH CALCULATES CROSS SECTIONS GIVEN VALUES
C OF THE FOLLOWING PARAMETERS ...
C
PAR(1) = 8.083*(IC6/HCROSS)**0.4
C
PAR(2) = 2.*PI*RM*60*SQRT(2.*PI*RM*HCROSS/EPS)
C
PAR(3) = EPS
C
PAR(4) = 4.*A1*EPS*RM/HCROSS
C
PAR(5) = 4.*EPS*PS*RM/HCROSS
C
PAR(6) = 2.*PI*C8/(IC6*3.)
C
DOUBLE PRECISION PAR,F,A,H,PHI,Z
C
DIMENSION PAR(1),F(1),A(4)
C
COMMON V(200),E(200)
C
DATA A/-0.1655D0,0.1057D0,-0.5440D-1,0.1390D-1/
C
DATA H/3.2670D0,-PI75/2.3551944900/
C
DO 100 I = 1,NOB
200 F(I) = PAR(1)/V(I)**0.4 + PAR(2)*DSQRT(V(I))**0.4 + 1.*DO/PI75*(A1*EPS*RM/HCROSS)**0.4
C
100 Z = PAR(3)/E(I)
C
C ENTRY POINT WHICH RETURNS MATRIX OF DERIVATIVES OF MODEL WITH
C RESPECT TO PARAMETERS
C
DO 500 I = 1,NOB
C
SUM = (A(1) + Z*A(2) + Z*(A(3) + Z*A(4)))/E(I)
C
PHI = -PI75*(PAR(4) + PAR(5)*(A(1) + Z*(A(2) + Z*(A(3) + Z*A(4)))))/E(I)
C
SPHI = DSIN(PHI)
C
C PHI = DCOS(PHI)
C
ROOTV = SQRT(V(I))
C
TERM = 1.DO + H1*Z
C
PROD = ROOTV*TERM
C
F(I+NBO) = PROD*SPHI
C
F(I+2*NBO) = PAR(2)*ROOTV*(TERM*SPHI*PAR(5)*(A(2) + Z*(A(3) + Z*A(4))))
C
1.3*Z*A(4))*/E(I)**V(I)** + H1*SPHI)/E(I)
C
PROD = PROD*PAR(2)*SPHI
C
F(I+3*NBO) = PROD/E(I)
C
IF (NP, .EQ., 6) F(I+5*NBO) = 1.DO
C
500 F(I+NBO) = PROD*SUM/V(I)
C
RETURN
C
END
C

END OF COMPILATION: NO DIAGNOSTICS.

COMPILATION TIME: 0.978 SEC.
I/O REQUESTS: 59
I/O WORDS TRANSFERRED: 57954
This subprogram performs general nonlinear regression of \( N \) observations \( Y(I) \), with weights \( W(I) \), to the model

\[
\hat{Y} = \hat{Y} (\theta_1, \ldots, \theta_n)
\]

This program is a reworked version of a program of the same name of the Univ. Wis. Computing Center.

1. CALL GASS59(IO, YMU, DYMU, NOB, W, Y, NP, TH, BUP, BLOW, EPS1, EPS2, EPS3, MAXIT, D, E, F, R, DELZ)

INPUT: IO – I/O parameter. If 0, no printing is done. If 1, only last iteration is printed. If 2, all printing is performed.

CALL YMU (TH, F, NOB, NP) - stores \( \hat{Y}(I) \) in \( F(I) \) \( 1 \leq I \leq NOB \)

CALL DYMU (TH, DELZ, NOB, NP) - Stores \( \partial Y(I)/\partial \theta_j \) in \( DELZ(I,J) \)

\( 1 \leq I \leq NOB, 1 \leq J \leq NP \).

NOB – No. of observations

\( Y(I) \) – I-th observed value

NP – n, No. of parameters \( \theta_1, \ldots \theta_n \)

TH(J) – J-th parameter value \( \theta_j \). Initially should be set to an estimate of \( \theta_j \).

BUP(J), BLOW(J) – Bounds set upon the allowable values of TH(J):

\( BLOW(J) \leq TH(J) \leq BUP(J) \).

EPS1 – Stopping criterion for relative change in the sum of squared residuals (SSR) per iteration.

EPS2 – Stopping criterion for relative change in each parameter per iteration.
EPS3 - Stopping criterion for relative change in SSR from initial SSR.

MAXIT - Maximum allowed number of iterations (e.g. 20)

F,R - work vectors of size NOB

DELZ - work space of size NOB X NP

OUTPUT: TH(I) - determined value of \( \theta_i \)

\[ D(I,J) - (NP \times NP \text{ matrix}) \text{ determined value of correlation between } \theta_i \text{ and } \theta_j \]

E(I) - determined 95% confidence interval halfwidth for \( \theta_i \)

2. CALL MAXLIK (IO, YMU, DYMU, NOB, W, Y, NP, TH, D, E, F, R, DELZ)

The iterative fitting of the \( \theta \) vector is done between entry points GASS59 and MAXLIK; from entry point MAXLIK onwards, the statistics of the fit are determined. A call to MAXLIK calculates the statistics for the given \( \theta \) vector, but does not determine the \( \theta \) vector by means of a fit.
SUBROUTINE GASS59 (IO,YMU,DYMU,NOB,W,Y,NP,TH,BUP,BLOW,EPS1,EPS2,EPS3,MAXIT,D,E,F,R,DELZ)

IMPLICIT DOUBLE PRECISION (A-H,O-Z)

REAL Y,W . . .

REAL STUDNT - ~ '

DIMENSION Y(1),W(1),TH(1),BUP(1),BLOW(1),D(1),E(1),F(1),R(1),DELZ(1)

DATA FLAM/I=0-2*/FNU/I=0-1/

NP50 = NP*NP

IF (IO .EQ. 0) GO TO 50
WRITE (6,1) NOB,NP
WRITE (6,2) I5X , 'INITIAL PARAMETER VALUES', I5X, 'UPPER-BOUND', 9X, 'PARAMETERS IN THE MODEL'
WRITE (5,200) (I,BLOY(I),TH(I),BUP(I),I=1,NP)
ITER = 1
SSQ = 0.D0
CALL YMU(TH,F,NOB,NP)
DO 100 I = 1,NOB
R(I) = Y(I) - F(I)
100 SSQ = SSQ + W(I)*R(I)*R(I)
KOUNT = 1
SUMD = 0.D0
DO 500 K = 1,N
SSQ84 = SSQ
IF (SSQ .LT. 1.D-50) RETURN

GAS = GA*DSQRT(SSQ/SSQ84)/FNU
SSQ84 = SSQ
INTCNT = 0
CALL DYMU(TH,DELZ,NOB,NP)
NI = - NOB
DO 650 I = 1,NP
NI = NI + NOB
II = (I-1)*NP
IJ = I - NP
NJ = - NOB
650 DO 550 J = 1,I
NJ = NJ + NOB
IJ = IJ + NP
JI = II + J
SUMD = 0.D0
550 DO 500 K = 1,N
SUMD = SUMD + DELZ(INI*K)*DELZ(NJ*K)*W(K)
500 D(JI) = SUMD

FORMAT (//'ENTRY TO GASS59'//I0X,'FIT TO',I8,3X,'OBSERVATIONS'//I0X
'THERE-ARE',I8,3X,'PARAMETERS IN THE MODEL'/)
WRITE (6,3) I5X, 'INITIAL SUM OF SQUARES', D20.10
IF (SSQ .LT. 1.D-50) RETURN

CONTINUE
WRITE (6,4) I5X, 'AT ITERATION', I5X, 'CUMULATIVE NO. FUNCTION CALLS'
1 MADE',II0)

FUNCTION CALLS

IF (IO .GE. 2) WRITE (6,4) ITER,KOUNT
<table>
<thead>
<tr>
<th>Line</th>
<th>Code</th>
</tr>
</thead>
<tbody>
<tr>
<td>53</td>
<td>D(IJ) = SUMO</td>
</tr>
<tr>
<td>54</td>
<td>Q(I) = 0.00</td>
</tr>
<tr>
<td>55</td>
<td>DO 600 K = 1, N0B</td>
</tr>
<tr>
<td>56</td>
<td>G(I) = G(I) + W(K) * DELZ(NI+K) * R(K)</td>
</tr>
<tr>
<td>57</td>
<td>II = I * I</td>
</tr>
<tr>
<td>58</td>
<td>IF (DI(I) + LT. 1.D-50) DII(I) = 1.D-50</td>
</tr>
<tr>
<td>59</td>
<td>E(I) = D9RT1(DI(I))</td>
</tr>
<tr>
<td>60</td>
<td>NI = - NP</td>
</tr>
<tr>
<td>61</td>
<td>DO 710 I = 1, NP</td>
</tr>
<tr>
<td>62</td>
<td>NI = NI * NP</td>
</tr>
<tr>
<td>63</td>
<td>IJ = I - NP</td>
</tr>
<tr>
<td>64</td>
<td>WTS(I) = 0.00</td>
</tr>
<tr>
<td>65</td>
<td>DO 710 J = 1 + I</td>
</tr>
<tr>
<td>66</td>
<td>IJ = IJ + NP</td>
</tr>
<tr>
<td>67</td>
<td>JI = NI + J</td>
</tr>
<tr>
<td>68</td>
<td>TEMP = D(IJ)</td>
</tr>
<tr>
<td>69</td>
<td>A(IJ) = TEMP</td>
</tr>
<tr>
<td>70</td>
<td>A(IJ) = TEMP</td>
</tr>
<tr>
<td>71</td>
<td>CALL SYMQR(A<em>NP</em>NP*NP+DELZ)</td>
</tr>
<tr>
<td>72</td>
<td>NI = - NP</td>
</tr>
<tr>
<td>73</td>
<td>DO 730 I = 1, NP</td>
</tr>
<tr>
<td>74</td>
<td>NI = NI * NP</td>
</tr>
<tr>
<td>75</td>
<td>DO 730 J = 1, NP</td>
</tr>
<tr>
<td>76</td>
<td>JI = NI * J</td>
</tr>
<tr>
<td>77</td>
<td>WTS(J) = WTS(I) + DABS(DELZ+JII)*P(I)</td>
</tr>
<tr>
<td>78</td>
<td>MASTER = 1</td>
</tr>
<tr>
<td>79</td>
<td>DPROD = 1.00</td>
</tr>
<tr>
<td>80</td>
<td>NI = - NP</td>
</tr>
<tr>
<td>81</td>
<td>DO 770 I = 1, NP</td>
</tr>
<tr>
<td>82</td>
<td>NI = NI * NP</td>
</tr>
<tr>
<td>83</td>
<td>IF (WTS(I) + GT. WTS(MASTER)) MASTER = I</td>
</tr>
<tr>
<td>84</td>
<td>DPROD = DPROD*D(NI+I)**(I./NP)</td>
</tr>
<tr>
<td>85</td>
<td>IJ = I - NP</td>
</tr>
<tr>
<td>86</td>
<td>DO 770 J = 1 + I</td>
</tr>
<tr>
<td>87</td>
<td>IJ = IJ + NP</td>
</tr>
<tr>
<td>88</td>
<td>JI = NI + J</td>
</tr>
<tr>
<td>89</td>
<td>A(IJ) = D(IJ)/E(I)E(JI)</td>
</tr>
<tr>
<td>90</td>
<td>A(IJ) = A(IJ)</td>
</tr>
<tr>
<td>91</td>
<td>IF (DPROD + LT. 1.D-50) DPROD = 1.D-50</td>
</tr>
<tr>
<td>92</td>
<td>WTSMS1 = WTS(MASTER)</td>
</tr>
<tr>
<td>93</td>
<td>DO 780 I = 1, NP</td>
</tr>
<tr>
<td>94</td>
<td>II = (I-I)*NP + I</td>
</tr>
<tr>
<td>95</td>
<td>P(I) = 0(I)/E(I)</td>
</tr>
<tr>
<td>96</td>
<td>PHI(I) = P(I)</td>
</tr>
<tr>
<td>97</td>
<td>IF (DABS(WTS(I)) + LT. 1.D-50) WTS(I) = 1.D-50</td>
</tr>
<tr>
<td>98</td>
<td>WTS(I) = WTSMS1/WTS(I)</td>
</tr>
<tr>
<td>99</td>
<td>A(I) = A(I) + GA*WTS(I)*DPROD/DIII</td>
</tr>
<tr>
<td>100</td>
<td>CALL MATIN(A<em>NP</em>P1<em>DET</em>PIVRAT)</td>
</tr>
<tr>
<td>101</td>
<td>IF (PIVRAT + LT. 1.D-16) GO TO 990</td>
</tr>
<tr>
<td>102</td>
<td>STEP = 1.00</td>
</tr>
<tr>
<td>103</td>
<td>SUM1 = 0.00</td>
</tr>
<tr>
<td>104</td>
<td>SUM2 = 0.00</td>
</tr>
<tr>
<td>105</td>
<td>SUM3 = 0.00</td>
</tr>
<tr>
<td>106</td>
<td>DO 790 I = 1, NP</td>
</tr>
<tr>
<td>107</td>
<td>SUM1 = P(I)*PHI(I) + SUM1</td>
</tr>
<tr>
<td>108</td>
<td>SUM2 = SUM2 + P(I)*P(I)</td>
</tr>
<tr>
<td>109</td>
<td>SUM3 = SUM3 + PHI(I)*PHI(I)</td>
</tr>
</tbody>
</table>
**X•DIAGNOSTIC•** THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.

110* 790 PHI(I) = P(I)
111* TEMP = SUM1/DSORT(SUM2*SUM3)
112* IF (DABS(TMP) .GT. 1.00) TEMP = 1.00
113* TEMP = 57.29578D0*DACOS(TMP)
114* IF (IO .LT. 2) GO TO 800
115* WRITE (6,6) DET+PIVRAT+TEMP
116* 6 FORMAT (/9X,'DETERMINANT.'+D20.10,'9X,'RATIO OF PIVOTS.'+D20.10/)
117* 19X,'ANGLE IN SCALED COORDINATES.'+F10.5)
118* 800 DO 810 I = 1,NP
119* 810 P(I) = PHI(I)*STEP/E(I)
120* ISW = 0
121* DO 820 I = 1,NP
122* TBI(I) = TH(I) + P(I)
123* 820 IF (TB(I) .GT. BUP(I) .OR. TB(I) .LT. BLOW(I)) ISW = 1
124* IF (IO .LT. 2) GO TO 830
125* WRITE (6,7)
126* 7 FORMAT (/9X,'TEST POINT PARAMETER VALUES')
127* WRITE (6,211) (TB(I),I = 1,NP)
128* 830 IF (ISW .EQ. 1) GO TO 860
129* SUMB = 0.00
130* CALL YMU(TB,F,NOB,NP)
131* KOUNT = KOUNT + 1
132* DO 840 I = 1,NP
133* R(I) = Y(I)-F(I)
134* 840 SUMB = SUMB + R(I)*R(I)
135* IF (IO .LT. 1) WRITE (6,8) SUMB
136* 8 FORMAT (/9X,'TEST POINT SUM OF SQUARES.'+D20.10/)
137* 850 IF (SUMB .LE. (1.00+EPS1)*SSQ) GO TO 890
138* 860 IF (TEMP .GT. 3.01 .AND. GA .GT. 1.0-50) GO TO 880
139* 870 STEP = 0.500*STEP
140* INTCNT = INTCNT + 1
141* IF (INTCNT .GE. 36) GO TO 990
142* GO TO 800
143* 880 GA = GA*FNU
144* INTCNT = INTCNT + 1
145* IF (INTCNT .GE. 36) GO TO 980
146* GO TO 760
147* 890 DO 900 I = 1,NP
148* 900 THII1 = TB(I)
149* SSG = SUMB
150* IF (IO .GE. 2) WRITE (6,10) GA
151* 10 FORMAT (/9X,'AT THE END OF THE REGRESSION; GAMMA IS.'+D20.10/)
152* IF (Eps3 .LT. 0.00) GO TO 920
153* DO 910 I = 1,NP
154* IF (DABS(P(I)) .GT. DABS(TH(I)*EPS2)) GO TO 920
155* 910 CONTINUE
156* WRITE (6,11) EPS2
157* 11 FORMAT (/'ITERATION STOPS ... RELATIVE CHANGE IN EACH PARAMETER I
158* 15 LESS THAN.'+D20.10/)
159* 920 DO 999 I = 1,NP
160* 930 IF (STEP .NE. 1.00) GO TO 970
280*   E(I) = TEMP*TFACTR
281*   2500 IF (I0 .NE. O) WRITE (6,2001) I+10(I)+10*TEMP*E(I)
282*   3000 IF (I0 .EQ. O .OR. PIVMAT .LT. 1.D-12) RETURN
283*   DC 3100 I = 1*NP
284*   II = (I-1)*NP + I
285*   3100 Q(I) = A(II)
286*   CALL SYMQR (A, NP, NP, P, DELZ)
287*   NI = - NP
288*   DO 3200 I = 1*NP
289*   NI = NI + NP
290*   AI(II) = Q(I)
291*   IJ = I - NP
292*   DO 3200 J = 1*NP
293*   IJ = IJ + NP
294*   3200 A(IJ) = A(NI+J)
295*   WRITE (6,2003)
296*   2003 FORMAT (/9X,'EIGENVALUES OF MOMENT MATRIX-FINAL ANALYSIS'/)
297*   WRITE (6,2011) (P(I), I=1*NP)
298*   RETURN
299*   END

END OF COMPILATION: 1 DIAGNOSTICS.

COMPILATION TIME: 4.829 SEC.
I/O REQUESTS: 124
I/O WORDS TRANSFERED: 94557
E. **SYMQR**

This program is a reworked version of a Univ. of Wis. Computing Center routine of the same name which computes the eigenvalues and eigenvectors of a $N \times N$ symmetric matrix $A$ by means of the Q-R method.

CALL SYMQR (A, N, NDIM, EIG, VEC)

INPUT:  
- $A$ - matrix of which eigenset is to be found. (Only the lower triangle of $A$ is used)
- $N$ - size of $A$
- $NDIM$ - dimensioned size of $A$

OUTPUT:  
- $EIG(I)$ - $I$-th largest eigenvalue of $A$
- $VEC(J,I)$ - ($NDIM \times N$ matrix) - $J$-th component of eigenvector $I$. 
SUBROUTINE SYMQR (A, N, NDIM, EIG, VEC)
USES THE QR ALGORITHM ON SYMMETRIC MATRIX A TO OBTAIN EIGENVALUES
NOTE THAT ONLY LOWER TRIANGLE OF A IS USED (AND DESTROYED)
EIG = VECTOR OF EIGENVALUES IN DESCENDING ORDER
VEC = MATRIX OF EIGENVECTORS IN ORDER OF EIGENVALUES
IND = ERROR RETURN INDICATOR
IF A NORMAL, SUM OF EIGENVALUES NOT TRACE
IF 2 SUM OF SQUARED EIG NOT EQUAL TO NORM
IF 3 BOTH OF ERRORS
DIMENSION A(N), GAMMA(50), BETA(50), BETASQ(50), EIG(1), W(49), VEC(1)
EQUIVALENCE (IPOSV(1), GAMMA(1)), (IPOS(1), BETA(1)), (ORDER(1), BETASQ)
IND = 0
IF (N .EQ. 0) GO TO 560
N1 = N - 1
N2 = N - 2
ENORM = 0.00
TRACE = 0.00
NJ = - NDIM
DO 110 J = 1, N
NJ = NJ + NDIM
JJ = NJ + J
DO 100 I = 1, N
IJ = NJ + 1
ENORM = ENORM + A(IJ)**2
TRACE = TRACE + A(JJ)
100 ENORM = ENORM + 0.50*A(JJ)**2
ENORM = ENORM + ENORM
GAMMA(1) = A(1)
IF (N2) 280, 270, 120
NRN = - NDIM
DO 260 NR = 1, N2
NRN = NRN + NDIM
ISUB = NRN + NR + 1
B = A(ISUB)
S = 0.00
DO 130 I = NR, N2
S = S + A(NRN + I + 2)**2
A(ISUB) = S**0.50
IF (S .LE. 0.00) GO TO 250
S = S + B**2
SGN = 1.00
IF (B .GE. 0.00) GO TO 160
SGN = -1.00
DO 160 SQRTS = D SQRT(S)
D = 0.50*SGN/SQRTS
TEMP = SQRTS(0.50 + B**2)
WIN(R) = TEMP
A(ISUB) = TEMP
D = D/TEMP
250
260
270
280
120
B = 'SGN*SQRTS
DO 170 I = NR+N2
TEMP = D*A(NRN + I + 2)
W(I+1) = TEMP
170 A(NRN + I + 2) = TEMP
WTAW = D*DO
DO 220 I = NR+N1
SUM = O*DO
DO 180 J = NR+1
I J = J*NDIM + I + 1
180 SUM = SUM + A(IJ)*W(J)
I I = I + 1
IF (N1 *LT* II) GO TO 210
190 DO 230 J = II+1
I J = I*NDIM + J + 1
230 SUM = SUM + A(IJ)*W(J)
210 P(1) = SUM
220 WTAW = WTAW + SUM*W(I)
DO 230 I = NR+N1
Q(I) = P(I) - WTAW*W(1)
DO 240 J = NR+N1
QJ = Q(J)
WJ = W(J)
DO 240 I = J*N1
IJ = J*NDIM + I + 1
240 A(IJ) = A(IJ) - 2*DO*(W(I)*QJ + WJ*Q(I))
250 BETA(NR) = B
BETASQ(NR) = B*B
GAMMA(NR+1) = A(IJ+NDIM)
260 IJ = N2*NDIM + N
B = A(IJ)
BETA(N-1) = B
BETASQ(N-1) = B*B
GAMMA(N) = A(IJ + NDIM)
280 BETASQ(N) = O*DO
DO 300 I = 1,N
DO 290 J = 1,N
IJ = I*J + NDIM
DO 300 VEC(IJ) = O*DO
IJ = (I-1)*NDIM + 1
300 VEC(IJ) = I*DO
M = N
SUM = O*DO
NPAS = 1
GO TO 400
310 SUM = SUM + SHIFT
COSA = I*DO
G = GAMMA(I) - SHIFT
PP = G
PBP = PP*PP + BETASQ(I)
PBR = DSQRT(PBP)
NJ = NDIM
DO 370 J = 1,N
NJ = NJ + NDIM
COSAP = COSA
*DIAGNOSTIC* THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.
109* IF (PPBS .NE. 0.0) GO TO 320
110* SINA = 0.0
111* SINA2 = 0.0
112* COSA = 1.0
113* GO TO 350
114* 320  SINA = BETA(J)/PPBR
115* SINA2 = BETASQ(J)/PPBS
116* COSA = PP/PPBR
117* NT = J + NPAS
118* IF (NT .GT. N) NT = N
119* 330  DO 340 I = 1,NT
120* IJ = NJ + I
121* TEMP = COSA * VEC(IJ) + SINA * VEC(IJ + NDIM)
122* VEC(IJ + NDIM) = -SINA * VEC(IJ) + COSA * VEC(IJ + NDIM)
123* 340  VEC(IJ) = TEMP
124* 350  DIA = GAMMA(J+1) - SHIFT
125*  U = SINA2 * (G + DIA)
126*  GAMMA(J) = G + U
127*  G = DIA - U
128*  PP = DIA * COSA - SINA * COSA * BETA(J)
129*  IF (J .NE. M) GO TO 360
130*  BETA(J) = SINA * PP
131*  BETASQ(J) = SINA2 * PP * PP
132*  GO TO 380
133* 360  PPBS = PP * PP + BETASQ(J+1)
134*  PPBR = DSQRT(PPBS)
135*  BETA(J) = SINA * PPBR
136* 370  BETASQ(J) = SINA2 * PPBS
137* 380  GAMMA(M+1) = G
138*  NPAS = NPAS + 1
139*  IF (BETASQ(M) .GT. 1.0 - 2) GO TO 390
140* 390  EIG(M+1) = GAMMA(M+1) + SUM
141* 400  BETA(M) = 0.0
142* 410  BETASQ(M) = 0.0
143* 420  M = M - 1
144*  IF (M .EQ. 0) GO TO 430
145*  IF (BETASQ(M) .LE. 1.0 - 2) GO TO 390
146* 410  A2 = GAMMA(M+1)
147*  R2 = U + DDU * A2
148*  R1 = U + DDU * GAMMA(M)
149*  R12 = R1 + R2
150*  DIF = R1 - R2
151*  TEMP = DSQRT(DIF * DIF + BETASQ(M))
152*  R1 = R12 + TEMP
153*  R2 = R12 - TEMP
154*  DIF = DABS(A2 - R1) - DABS(A2 - R2)
155*  IF (DIF .LT. 0.0) GO TO 420
156*  SHIFT = -R2
157*  GO TO 310
158* 420  SHIFT = R1
159*  GO TO 310
160* 430  EIG(1) = GAMMA(1) + SUM
161*  DO 440 J = 1,N
162*  IPOSV(J) = J
163* 440  IORD(J) = J
164* 440  M = N
GO TO 470
450 DO 460 J = 1, M
166* IF (EIG(J) .GE. EIG(J+1)) GO TO 460
169* TEMP = EIG(J)
170* EIG(J) = EIG(J+1)
171* EIG(J+1) = TEMP
172* ITEMP = IORD(J)
173* IORD(J) = IORD(J+1)
174* IORD(J+1) = ITEMP
460 CONTINUE
176* 470 M = M - 1
177* IF (M .NE. 0) GO TO 450
178* IF (N1 .EQ. O) GO TO 500
179* NL = - NDIM
180* DO 490 L = 1, N1
181* NL = NL + NDIM
182* NV = IORD(L)
183* NP = IPOLS(NV)
184* IF (NP .EQ. L) GO TO 490
185* LV = IPOLS(L)
186* IPOLS(NP) = LV
187* IPOLS(LV) = NP
188* NNP = (NP + 1) * NDIM
189* DO 480 I = 1, N
190* IL = NL + I
191* INP = NNP + I
192* TEMP = VEC(IL)
193* VEC(IL) = VEC(INP)
480 VEC(INP) = TEMP
490 CONTINUE
500 ESUM = 0.0D0
501 ESSQ = 0.0D0
198* DO 550 NRR = 1, N
199* K = N1
200* 510 K = K - 1
201* IF (K .LE. 0) GO TO 540
202* SUM = 0.0D0
203* DO 520 I = K, N1
204* IL = (NRR - 1) * NDIM + I + 1
205* IJ = (K - 1) * NDIM + I + 1
206* 520 SUM = SUM + VEC(IL) * A(IJ)
207* SUM = SUM + SUM
208* DO 530 I = K, N1
209* IL = (NRR - 1) * NDIM + I + 1
210* IJ = (K - 1) * NDIM + I + 1
211* 530 VEC(IL) = VEC(IL) + SUM * A(IJ)
212* GO TO 510
540 ESUM = ESUM + EIG(NRR)
549 550 ESSQ = ESSQ + EIG(NRR) * 2
215* TEMP = DABS(128.0D0 * TRACE)
*DIAGNOSTIC* THE TEST FOR EQUALITY BETWEEN NON-INTGERS MAY NOT BE MEANINGFUL.
216* IF (DABS(TRACE - ESUM) + TEMP) = TEMP * NE. 0.0D0) IND = IND + 1
217* TEMP = 256.0D0 * ENORM
*DIAGNOSTIC* THE TEST FOR EQUALITY BETWEEN NON-INTGERS MAY NOT BE MEANINGFUL.
218* IF (DABS(ENORM - ESSQ) + TEMP) = TEMP * NE. 0.0D0) IND = IND + 2
219* IF (IND .NE. 0) WRITE (6, 86) IND
220* 86 FORMAT (*D0*, PROBABLE ERROR IN SYMPR. INDICATOR=\,1,5)
END OF COMPILATION: 3 DIAGNOSTICS.

COMPILATION TIME: 3.176 SEC.
I/O REQUESTS: 92
I/O WORDS TRANSFERRED: 79676

SYMQR
018A-09/08-10143
F. MATIN

Program which solves the set of equations $AX = B$, and inverts $A$, by means of Gaussian elimination with no pivoting.

CALL MATIN (A, N, B, NB, DET, PIVRAT)

where:

$A$ - $N \times N$ matrix of equations (replaced by $A^{-1}$).

$N$ - size of $A$

$B$ - $N \times NB$ matrix of right-hand side of equations (replaced by solution matrix $X$)

$NB$ - no. of different right-hand sides (if 0, $B$ is ignored by routine)

$DET$ - returned determinant of $A$

$PIVRAT$ - set to ratio of minimum to maximum pivots ($-\log_{10} PIVRAT$ is approx. no. of decimal figures lost in the computations).
FORTRAN subroutine MATIN

YCL 030 compiled by FOR-V S601 on 09 Aug 70 at 18:34:36.

0101 1* SUBROUTINE MATIN (A,N,B,NB,DET,PIVRAT)
0103 2* IMPLICIT DOUBLE PRECISION (A-H,O-Z)
0104 3* DIMENSION A(I),B(N)
0105 4* AL = AABS(A(I))
0106 5* AU = AL
0107 6* DET = 1.0D0
0110 7* NK = -N
0111 8* DO 1000 K = 1,N
0114 9* NK = NK + N
0115 10* KK = NK + K
0116 11* PIVOT = A(KK)
0117 12* PIVRAT = DABS(PIVOT)
0120 13* IF (AL.GT.PIVRAT) AL = PIVRAT
0122 14* IF (AU.LT.PIVRAT) AU = PIVRAT
0124 15* DET = DET*PIVOT
0125 16* IF (PIVRAT.LT.1.D-50) PIVOT = 1.D-50
0127 17* A(KK) = 1.D0
0130 16* PIVOT = 1.D0/PIVOT
0131 19* KI = K - N
0132 20* DO 1000 I = 1,N
0135 21* KI = KI + N
0136 22* 100 A(KI) = A(KI) *PIVOT
0138 23* IF (NB.LEQ.0) GO TO 100
0142 24* KI = K - N
0143 25* DO 300 I = 1,NB
0146 26* KI = KI + N
0147 27* 200 B(KI) = B(KI) *PIVOT
0151 28* 300 DO 1000 J = 1,N
0154 29* IF (J.EQ.K) GO TO 1000
0156 30* JK = NK + J
0157 31* T = A(JK)
0158 32* A(KI) = 0.D0
0161 33* JT = J - N
0162 34* KI = K - N
0163 35* DO 400 I = 1,N
0166 36* JI = JI + N
0167 37* KI = KI + N
0168 38* 400 A(JI) = A(JI) - A(KI)*T
0170 39* IF (NB.EQ.0) GO TO 1000
0172 39* JT = J - N
0174 40* KI = K - N
0176 42* DO 500 I = 1,NB
0179 43* JI = JI + N
0182 44* KI = KI + N
0182 45* 500 RIJI = BIJI - B(KI)*T
0185 46* 1000 CONTINUE
0187 47* PIVRAT = AL/AU
0188 48* RETURN
0190 49* END

END OF COMPILATION: NO DIAGNOSTICS.
G. STUDNT

This function returns the value of the student-t statistic for IDF degrees of freedom at the 95% level. (Equal-Tails).

\[ T = \text{STUDNT} (\text{IDF}) \]
FUNCTION STUDNT (IDF)
C RETURNS 95 PERCENT STUDENT-T VALUE FOR IDF DEG. OF FREEDOM
DIMENSION T(29)
DATA T/12.706,4.303,3.182,2.776,2.571,2.447,2.365,2.306,2.262,2.228,2.201,2.179,2.160,2.145,2.131,2.120,2.110,2.101,2.093,2.086,2.080,2.071,2.069,2.064,2.060,2.056,2.052,2.048,2.045/
IF (IDF .LT. 60) GO TO 100
STUONT = 1.960 + 2.4/IDF
50 RETURN
100 IF (IDF .LT. 30) GO TO 200
STUONT = 1.958 + 2.52/IDF
200 IF (IDF .LE. 0) GO TO 300
STUONT = T(IDF)
300 STUONT = 1.E+30
GO TO 50
END
END OF COMPILATION: NO DIAGNOSTICS.

COMPILATION TIME: 0.282 SEC.
I/O REQUESTS: 46
I/O WORDS TRANSFERED: 56744
H. EXAMPLES

The example is 48 cross sections \( Q(v) \) for \( 1 < E^* < 40 \) generated by means of XSECT (see Sect. II) from a L-J \((12,6)\) potential with

\[ \varepsilon = 13.3 \text{ cpe}, \quad r_m = 4.92 \AA \text{ (intended to mimic Li-Hg)}, \quad \mu = 9.69925 \text{ ppg.}, \]

\[ g_0 = 0.186299, \quad a_1 = 0.421559, \quad C_6 = 0.378 \times 10^6 \text{ cpe}^{-6}. \quad (\sigma = 0.25\%) \]

1. True value of \( \gamma_5 = 0 \)

(a) \( NP = 5 \) (No \( C_8 \))

(1) Note that the correlation between \( \gamma_1(C_6) \) and the other parameters is small.

(2) The "STANDARD ERROR OF ESTIMATE" is 0.262%, which is compatible with the precision of the calculated \( Q(v)'s. \)

(b) \( NP = 6 \) (\( C_8 \) assumed present)

(1) STANDARD ERROR OF ESTIMATE IS 0.259%, no change from \( NP = 5 \), indicating \( \gamma_6 \) is not necessary to the fit.

(2) The correlation between \( \gamma_1 \) and \( \gamma_6 \) is high. (-0.98)

(3) The determined value of \( C_8 \) is not significantly different from zero.

(4) The precision of \( C_6 \) has decreased markedly.

2. True value of \( \gamma_5 = 2 \)

(a) \( NP = 5 \) (\( C_8 \) assumed zero)

(1) STANDARD ERROR OF ESTIMATE = 0.388% (larger than before)

(2) Precision of \( C_6 \) is lower than before.

(b) \( NP = 6 \) (\( C_8 \) assumed present)

(1) STANDARD ERROR OF ESTIMATE = 0.260%, lowered from \( NP = 5 \).
(2) $C_8$ is found to be significantly greater than zero.

(3) $C_6$ still has comparatively low precision.

It is to be noted that the presence of $C_8$, either real or imagined, results in an uncertainty in the value of $C_6$. 
**TEST RUN ON O-DRIEN G'S -- FAST CROSS SECTION GENERATOR**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>No of Data Points</td>
<td>48</td>
</tr>
<tr>
<td>Reduced Mass</td>
<td>0.969925 * 10^01</td>
</tr>
<tr>
<td>Initial EPS</td>
<td>0.140000 * 10^02</td>
</tr>
<tr>
<td>Initial RM</td>
<td>0.470000 * 10^01</td>
</tr>
<tr>
<td>Initial A1</td>
<td>0.440000 * 10^00</td>
</tr>
<tr>
<td>Initial G0</td>
<td>0.190000 * 10^00</td>
</tr>
<tr>
<td>Initial C6</td>
<td>0.378000 * 10^06</td>
</tr>
<tr>
<td>Weighting Switch</td>
<td>1</td>
</tr>
</tbody>
</table>

**Fit with 5 Parameters (No C8)**
ENTRY TO GASS59

FIT TO 48 OBSERVATIONS
THERE ARE 5 PARAMETERS IN THE MODEL

INITIAL PARAMETER VALUES

<table>
<thead>
<tr>
<th>LOWER BOUND</th>
<th>PARAMETER VALUE</th>
<th>UPPER BOUND</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>.0000000000E+00</td>
<td>.1346960506E+04</td>
</tr>
<tr>
<td>2</td>
<td>.0000000000E+00</td>
<td>.8358514457E+01</td>
</tr>
<tr>
<td>3</td>
<td>.0000000000E+00</td>
<td>.1400000000E+02</td>
</tr>
<tr>
<td>4</td>
<td>.0000000000E+00</td>
<td>.1093139943E+03</td>
</tr>
<tr>
<td>5</td>
<td>.0000000000E+00</td>
<td>.3494053018E+04</td>
</tr>
</tbody>
</table>

INITIAL SUM OF SQUARES 6924430832.E01

ITERATION STOPS ... RELATIVE CHANGE IN EACH PARAMETER IS LESS THAN 1000000000.E-02

CORRELATION MATRIX
<table>
<thead>
<tr>
<th>ROW</th>
<th>1</th>
<th>1.000000</th>
</tr>
</thead>
<tbody>
<tr>
<td>ROW 2</td>
<td>-1.25735</td>
<td>1.000000</td>
</tr>
<tr>
<td>ROW 3</td>
<td>-1.19972</td>
<td>-0.785788</td>
</tr>
<tr>
<td>ROW 4</td>
<td>0.069570</td>
<td>-0.619235</td>
</tr>
<tr>
<td>ROW 5</td>
<td>-0.101764</td>
<td>-0.763495</td>
</tr>
</tbody>
</table>

**Determinant** \( \frac{4639324922}{-0.22} \)

**Ratio of Pivots** \( \frac{1051003265}{-0.65} \)

**Sum of S squared residuals** \( 2956066462 - 0.03 \)

**Mean square residuals** \( 0.6874573157 - 0.05 \) (for 43 degrees of freedom)

**Standard error of estimate** \( 2621940725 - 0.02 \)

**Critical student-t value** \( 2.017 \)

**Sum of weights** \( 0.7377959458 - 0.04 \)

<table>
<thead>
<tr>
<th>No.</th>
<th>Parameter value</th>
<th>Standard error</th>
<th>Confid. band half-width</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.1346493596 + 0.004</td>
<td>0.515192449 + 0.000</td>
<td>0.1040863953 + 0.001</td>
</tr>
<tr>
<td>2</td>
<td>0.8849899637 + 0.001</td>
<td>0.187534427 + 0.000</td>
<td>0.3781827452 + 0.000</td>
</tr>
<tr>
<td>3</td>
<td>0.1399192168 + 0.002</td>
<td>0.5074537144 + 0.000</td>
<td>0.1023333511 + 0.001</td>
</tr>
<tr>
<td>4</td>
<td>0.1047705400 + 0.003</td>
<td>0.1596391954 + 0.000</td>
<td>0.3219291408 + 0.000</td>
</tr>
<tr>
<td>5</td>
<td>0.3369161074 + 0.004</td>
<td>0.5615948134 + 0.002</td>
<td>0.1334358660 + 0.003</td>
</tr>
</tbody>
</table>

**Eigenvalues of moment matrix—final analysis**

- \( \frac{6864768359}{0.02} \)
- \( \frac{5771285384}{0.03} \)
- \( \frac{2862986311}{0.03} \)
- \( \frac{2605084319}{0.04} \)
- \( \frac{1576656418}{0.00} \)
<table>
<thead>
<tr>
<th>TERM</th>
<th>VALUE</th>
<th>95 PERCENT HALFWIDTH</th>
</tr>
</thead>
<tbody>
<tr>
<td>C6</td>
<td>377715×10^6</td>
<td>729954×10^3</td>
</tr>
<tr>
<td>G0</td>
<td>211935×10^0</td>
<td>627958×10^1</td>
</tr>
<tr>
<td>EPS</td>
<td>139949×10^2</td>
<td>102333×10^1</td>
</tr>
<tr>
<td>A1</td>
<td>435199×10^0</td>
<td>363346×10^1</td>
</tr>
<tr>
<td>RM</td>
<td>453529×10^0</td>
<td>687149×10^0</td>
</tr>
<tr>
<td>A1<em>EPS</em>RM</td>
<td>276225×10^2</td>
<td>848760×10^1</td>
</tr>
<tr>
<td>RM<em>EPS</em>2</td>
<td>888272×10^3</td>
<td>351800×10^2</td>
</tr>
</tbody>
</table>

**FIT WITH 6 PARAMETERS (WITH C8)**
ENTRY TO GASS59

FIT TO 48 OBSERVATIONS
THERE ARE 6 PARAMETERS IN THE MODEL

INITIAL PARAMETER VALUES

<table>
<thead>
<tr>
<th>LOWER BOUND</th>
<th>PARAMETER VALUE</th>
<th>UPPER BOUND</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1.00000000E+00</td>
<td>1.34649359E+04</td>
<td>1.00000000E+09</td>
</tr>
<tr>
<td>-1.00000000E+00</td>
<td>8.84989963E+01</td>
<td>1.00000000E+03</td>
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INITIAL SUM OF SQUARES .2956066462-CC3

ITERATION STOPS ... RELATIVE CHANGE IN EACH PARAMETER IS LESS THAN .1000000000-002

CORRELATION MATRIX

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<thead>
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<td>ROW 6</td>
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<td>-1.36736</td>
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DETERMINANT .1298484915-027 RATIO OF PIVOTS .1049823447-005

SUM OF SQ. RESIDUALS .2827158327-003 MEAN SQ. RESIDUALS .6731329349-005 (FOR 42 DEGREES OF FREEDOM) STANDARD ERROR OF ESTIMATE .2594490555-002 CRITICAL STUDENT-T VALUE 2.013 SUM OF WEIGHTS .737959458-004
<table>
<thead>
<tr>
<th>No.</th>
<th>Parameter</th>
<th>Value</th>
<th>Standard Error</th>
<th>Config. Band Half-Width</th>
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Eigenvalues of moment matrix—final analysis

- 5837116884-002
- 5765694688-003
- 2864523427-003
- 9792655089-004
- 7620278987-00

<table>
<thead>
<tr>
<th>Term</th>
<th>Value</th>
<th>95 Percent Halfwidth</th>
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<tr>
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<tr>
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<td>RM</td>
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<tr>
<td>A1<em>EPS</em>RM</td>
<td>.275243+02</td>
<td>.849153+01</td>
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<tr>
<td>RM*EPS**2</td>
<td>.888520+03</td>
<td>.351628+02</td>
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<tr>
<td>BETA</td>
<td>.101129+01</td>
<td>.148513+01</td>
</tr>
<tr>
<td>C8</td>
<td>.379520+06</td>
<td>.561013+06</td>
</tr>
</tbody>
</table>
TEST RUN ON O'BRIEN 0.5 --- WITH C8 = C6

NO OF DATA POINTS 48
REDUCED MASS 969925×10-1
INITIAL EPS 140000×102
INITIAL RM 470000×101
INITIAL A1 440000×100
INITIAL G0 190000×100
INITIAL C6 378000×106
WEIGHTING SWITCH 1

FIT WITH 5 PARAMETERS (NO C8)
ENTRY TO GASS59

FIT TO 48 OBSERVATIONS
THERE ARE 5 PARAMETERS IN THE MODEL

INITIAL PARAMETER VALUES

<table>
<thead>
<tr>
<th>LOWER BOUND</th>
<th>PARAMETER VALUE</th>
<th>UPPER BOUND</th>
</tr>
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<tbody>
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</table>

INITIAL SUM OF SQUARES .6949308972-001

ITERATION STEPS ... RELATIVE CHANGE IN SUM OF SQUARES IS LESS THAN .100000000-002

CORRELATION MATRIX

<p>| ROW 1 | 1.000000 |
| ROW 2 | -.125949  | 1.000000 |
| ROW 3 | -.120120  | -.785519  | 1.000000 |
| ROW 4 | .596945   | -.619105  | .774527  | 1.000000 |
| ROW 5 | .101897   | -.763207  | .964780  | .903471  | 1.000000 |</p>
<table>
<thead>
<tr>
<th>No.</th>
<th>Parameter Value</th>
<th>Standard Error</th>
<th>Confid. Band Half-Width</th>
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Eigenvalues of Moment Matrix-Final Analysis

-6840167958-002  5749404385-003  2851315924-003  2592519684-004  1561022854-000
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<tr>
<th>TERM</th>
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<tr>
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<td>RM</td>
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<tr>
<td>RM<em>EPS</em>2</td>
<td>889104+03</td>
<td>522576+02</td>
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</tbody>
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FIT WITH 6 PARAMETERS (WITH C8)
ENTRY TO GASS59

"IT TO 48 OBSERVATIONS
THERE ARE 6 PARAMETERS IN THE MODEL

INITIAL PARAMETER VALUES

<table>
<thead>
<tr>
<th>LOWER BOUND</th>
<th>PARAMETER VALUE</th>
<th>UPPER BOUND</th>
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INITIAL SUM OF SQUARES .6485054621-CC3

ITERATION STOPS ... RELATIVE CHANGE IN SUM OF SQUARES IS LESS THAN .100000000-002

CORRELATION MATRIX

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DETERMINANT .1264424246-027

SUM OF S.G. RESIDUALS .2834185229-003
MEAN S.G. RESIDUALS .6748060070-005 (FOR 42 DEGREES OF FREEDOM)
STANDARD ERROR OF ESTIMATE .2597702845-002 CRITICAL STUDENT-T VALUE 2.019
SUM OF WEIGHTS .7339488055-004
## Eigenvalues of Moment Matrix - Final Analysis

<table>
<thead>
<tr>
<th>No.</th>
<th>Parameter Value</th>
<th>Standard Error</th>
<th>Confid. Band Half-Width</th>
</tr>
</thead>
<tbody>
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<tr>
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</tr>
<tr>
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<tr>
<td>4</td>
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<tr>
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</tbody>
</table>

## EIGENVALUES OF MOMENT MATRIX - FINAL ANALYSIS

**TERM** | **VALUE** | **95 PERCENT HALFWIDTH**
-----------|-----------|-------------------------|
C6         | 3.75267+06 | 3.62412+04             |
G0         | 2.11948*00  | 7.22491-01             |
EPS        | 1.40107*02  | 1.02261+1              |
A1         | 4.35184*00  | 4.39069-01             |
RM         | 4.53693*01  | 8.38421+00             |
A1*EPS*RM  | 2.76261+02  | 8.52789-01             |
RM*EPS**2  | 8.89422*03  | 3.53809+02             |
BETA       | 1.97094*01  | 1.49093*01             |
C8         | 7.39608*06  | 5.66678*06             |
VII. JWKB

This main program computes JWKB phase shifts \( \eta_l(E) \) for given reduced energies \( E^* = E/e \) and values of the orbital quantum number \( l \) such that \( b^* = (l + \frac{1}{2})/k \alpha \) is a multiple of 0.05 (For details of the calculation of \( \eta_l \), see function PHASHT).

The total cross section is given by

\[
Q(E) = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \eta_l \tag{VII-1}
\]

Letting

\[
\delta q_l = b \sin^2 \eta_l \tag{VII-2}
\]

and

\[
q_L = \sum_{l=0}^{L} \delta q_l \tag{VII-3}
\]

Since \( Q = \frac{8\pi}{k} q_\infty \), the program computes \( Q \) by means of

\[
Q = \frac{8\pi}{k} \left( q_L + \Delta q_L \right) \tag{VII-4}
\]

where \( L \) is a value large enough so that \( \Delta q_L = q_\infty - q_L \) can be estimated accurately.

Values of \( \delta q_L \) are calculated at every 0.05 in \( b^* \) until one of the following is true:

1. \( b^* > 2 \) and \( \delta Q = \frac{8\pi}{k} \delta q_L < 0.1 \ \text{\AA}^2/b \) (This condition forces the remaining cross section \( \Delta Q \) to be less than 0.05 \( \text{\AA}^2 \)).
(2) The Jeffreys-Born long-range phase shift \( \eta^J_B = \frac{3\pi}{16 \, \kappa \nu \beta} < 2 \)
and agrees with \( \eta^J_B \) to within 0.01 radians for 3 successive values of \( \ell \).

When either condition is satisfied, this value of \( \ell \) is taken as \( L \).

The intermediate values of \( \eta^J_B \) are then calculated by interpolation (DNTERP)*. The remaining cross section \( \Delta Q = \frac{8\pi}{\kappa} \Delta Q_L \) is

* The program could be improved by replacement of DNTERP with a continued-fraction interpolation program, since the limiting form of \( \eta^J_B \) is

\[ \alpha \frac{1}{\beta} \]

estimated two different ways:

\[ \Delta Q_L = \frac{\eta^J_B}{\eta^J_B} \int_L^\infty b \sin^2 \eta^J_B \, d\ell \quad (QJBVAL) \quad (VII-5) \]

(The factor of \( \eta^J_B/\eta^J_B \) is to correct for the discrepancy between \( \eta^J_B \) and \( \eta^J_B \))

\[ q(\ell) = \lim_{\ell \to \infty} q(\ell) \quad \text{is obtained by means of the } \varepsilon\text{-algorithm (EPSALC).} \]

Finally, the apparent \( C_6 \) constant \( C^\text{app}_6 \) is calculated by means of:

\[ C^\text{app}_6 = \frac{\kappa^2 b}{\mu} \left( \frac{Q}{8.083} \right)^{5/2} \quad (VII-6) \]

**INPUT:**

Card 1: Title (20A4)
Card 2: NE, MU (I5, F10.4)
Card 3: (ELIST(I), I = 1,NE) (10F8.0)
where:

NE - No. of energies (in reduced units) for which cross sections are to be calculated

MU - reduced mass of system in ppg.

ELIST(I) - I-th energy in reduced units

NOTE: In addition, a user defined function POTIN/POT is required (q.v.)

OUTPUT: The values of $E$, $C_6$, and $\sigma$ (zero of potential) are in reduced units. The quantities EUNIT = $e$ and RUNIT = $a$ are the reducing units of energy and distance returned by POTIN (q.v.): they should be of the order of $e$ and $r_m$, respectively.

For $\ell$ corresponding to every 0.05 in $b = \left( \ell + \frac{1}{2} \right)/A$, the following are outputted:

- $L = \ell$
- $B = b^*$
- $Y_0 = y_o = 1/r_o$
- $R_0 = r_o$ the outer most zero of $1-b^2/r^2 - V(r)/E$ (in reduced units)
- $\eta_{\ell}$
- $\eta_{\ell,JB}$ (in reduced units)
- $\delta_{\ell}$
- IER - Error return from determination of turning point. If = 0, normal convergence. If $\neq 0$ turning point is incorrect (see REGFAL)
- ISW - Error return from determination of $\eta_{\ell}$. If = 0, normal convergence. If $\neq 0$, did not converge (see PHASHT).
A table of the above quantities is printed out, the units being those obtained treating EUNIT and RUNIT as dimensional units.

Finally, the ϵ-algorithm sequence of diagonal convergents (EPSVEC(I), I = 1,M) are printed out, M being the number of applications of the algorithm, and the convergents for $q_{\infty}$ appearing at every other element (the first such appearance being the one used). The following are then printed out:

- **T**: Execution time in seconds
- **CROSS**: $Q_{L} = \frac{B}{R} q_{L} (A^2)$
- **Q**: $q_{L}$
- **QJB**: $Q_{L} + \Delta Q_{JB}$ from eq. (VII-5) (A)$^2$
- **C6APP**: $C_{app,JB} (cpe-A^2)$
- **ND**: highest degree used in interpolation (see DIFTAB)

and finally,

- **CROSS**: $Q = \frac{Q_{\infty}}{R}$
- **EPSVEC(J)**: $q_{\infty}$
- **C6APP**: $C_{app}$

**NOTE**: Values of $q_{\infty}$ outputted are in reduced units.

**REMARKS**: (1) A user-defined potential function POTIN/POT is required (q.v.)

(2) EUNIT and RUNIT are treated as dimensional units except for actual cross sections which are in A$^2$.

(3) The subroutines TIMSET (in line 54) and TIMGET (in line 93) are specific to the UWCC Univac 1108, and set and read an internal clock. These functions are not necessary for execution of the program. Line 54 may be deleted and line 93 replaced with "600 CONTINUE"
(4) The convergence tolerances for the calculation of $\eta^J$, convergence to $\eta^E$, and determination of the turning point, are given by EPS (absolute), TOLJB (relative/absolute), TOLYO (relative), in line 8.

(5) The phase shift calculations generally terminate at $b^* < 3^{02}$ and give a cross section which has limits of error $\pm 5A^2$. 
*05 / 3/ 72-01153112 (10) JWKB

1. C PROGRAM WHICH COMPUTES JWKB PHASE SHIFTS AND TOTAL CROSS SECTIONS
2. C A CONSISTENT SET OF UNITS FOR THIS PROGRAM ARE
3. C ANGSTROMS, PICOPICOMETERS, AND DECIPICISECONDS (GIVING CENTIPEDEERGS
4. C AS THE UNIT OF ENERGY)
5. C REAL MU
6. C DIMENSION ELIST(200), ETAB(200), DIF(2000), EPSVE(200)
7. C COMMON B,RO,E X
8. C DATA EPS/0.005/, TOLJB/0.01/, TOLYO/1.E-5/
9. C DATA PI2/1.57079633/, HX2/1.1216294/
10. C EXTERNAL VEFF
11. C WRITE (6,2) TOLYO, EPS, TOLJB
12. C FORMAT (1H1, 1S, "ENTRY TO JWKB/DINTERP ", //5X, "TOLERANCE FOR YO (REL
13. C LATIVELY)", E12.5/5X, "TOLERANCE FOR ETA (ABS) ", E12.5/5X, "TOLERANCE F0
14. 2R JB LIMIT", E12.5)
15. C READ IN TITLE OF EXPERIMENT
16. C READ (5,3) (DIF(I), I=1,20)
17. C FORMAT (20A4)
18. C WRITE (6,5), (DIF(I), I=1,20)
19. C FORMAT (1H1, 1O, 2A4)
20. C READ IN NO. OF ENERGIES NE AND REDUCED MASS MU
21. C READ (5,6) NE,MU
22. C FORMAT (15,F10.4)
23. C READ IN LIST OF ENERGIES
24. C READ (5,7) (ELIST(I), I=1,NE)
25. C FORMAT (10F8.0)
27. C C6 SHOULD BE VALUE OF LONG-RANGE C6 IN REDUCED UNITS, THE
28. C SCALE OF WHICH ARE GIVEN IN EUNIT(ENERGY) AND RUNIT (LENGTH)
29. C SIGMA = POTIN(C6+EUNIT, RUNIT)
30. C SIGINV = 1./SIGMA
31. C SIGIN2 = 2.*SIGINV
32. C CONSJB = 0.1875*PI2*C6
33. C ECONS = 2.*MU*EUNIT/HX2
34. C WRITE (6,9), MU, C6, SIGMA, EUNIT, RUNIT
35. C FORMAT (//5X, "PHASE SHIFTS AND CROSS SECTIONS FOR REDUCED MASS",
37. 2S, "UNITS OF ENERGY AND LENGTH", E14.6)
38. C DO 1000 J = 1, NE
39. C E = ELIST(J)
40. C WAVE = SQRT(E+ECONS)
41. C A = WAVE*RUNIT
42. C CJB = CONSJB*A/A
43. C COEF = 16.*PI2*RUNIT/WAVE
44. C WRITE (6,10), E, WAVE, A
45. C FORMAT (//5X, "ENERGY", F10.5, "WAVE NO.", E15.6, "5X", "A=WAVE*RUNIT"
46. C 1, E14.6//5X, "FOLLOWING TABLE IN REDUCED UNITS EUNIT, RUNIT")
47. C WRITE (6,15)
49. C 9X, "DELQ", 7X, "IER", 3X, "ISW", 5X, 100(1H)1)
50. C IJB = 0
51. C CALCULATE PHASE SHIFTS AT EVERY 0.05 IN REDUCED IMPACT PARAMETER
52. C LSTEP = A/20.
53. C IF (LSTEP .LT. 1.) LSTEP = 1
54. C CALL Timset(0.)
55. C DO 500 LL = 1,200
56  NETA = LL
57  L = LSTEP*(LL=1)
58  B = (L+0.5)/A
59  IF-(B *GT_SIGMA)-GO TO 100
60  XL = SIGINV
61  XU = SIGINV
62  GO TO 200
63  XL = 1/B
64  XU = SIGINV
65  C FIND TURNING POINT YO = 1/RO
66  C IER = 0, NORMAL. IF NOT 0, ERROR IN ROOT (SEE REGFAL)
67  200 CALL REGFAL(XL, XU, X, XEFF, TOL, YO, 5, 20, IER)
68  RO = 1/X
69  C CALCULATE PHASE SHIFT FROM
70  C ISW = 0, NORMAL. IF NOT 0, THEN DID NOT CONVERGE TO EPS ACCURACY
71  TOL = EPS/A
72  ETAJB = CJ/A/B**5
73  IF (ETAJB *LT-1.) TOL = ETAJB*TOL
74  ETATAB(LL) = A*PHASHT(TOL, 9, ISW)
75  DEIQ = B*(SIN(ETATAB(LL))^2)
76  WRITE (6, 20) L, B, X, RO, ETATAB(LL), ETAJB, DEIQ, IER, ISW
77  20 FORMAT (10X, 15, 3F10, 6, 3E14, 6, 216)
78  IF (COEF *DEIQ *GT* 0.1 *OR* B *LT+2.) GO TO 400
79  WRITE (6, 22)
80  22 FORMAT (/5X, 'REM A I N I NG CROSS SECTION IS LESS THAN 0.05 SQ ANG')
81  GO TO 600
82  400 TOL = TOA JB
83  IF (ETAJB *LT-1.) TOL = ETAJB*TOL
84  IF (ABS(ETATAB(LL) = ETAJB *LT TOL ) IJB = IJB + 1
85  IF (IJB, LT-1 *OR* ETAJB *GT-2.) GO TO 600
86  WRITE (6, 23) IJB
87  23 FORMAT (/5X, 'AFTER ', 18, 5X, 'ASYMPTOTIC PHASE SHIFTS, ETAJB IS LESS
88  THAN 1')
89  GO TO 600
90  500 CONTINUE
91  WRITE (6, 25)
92  25 FORMAT (10X, 'MORE THAN 200 PARTIAL WAVES ARE REQUIRED')
93  600 T = TIMGET(0)
94  ND = 10
95  CALL DFTAB(ETATAB, NETA, DIF, ND, EPS)
96  NMAX = LSTEP*(NETA=1) + 1
97  BSTEP = LSTEP/A
98  BO = 0.5/A
99  M = 0
100  IEPS = 0
101  Q = 0
102  DO 700 LL = 1, NMAX
103  L = LL + 1
104  B = (L+0.5)/A
105  TOL = EPS
106  ETAJB = CJ/B**5
107  IF (ETAJB *LT-1.) TOL = ETAJB*TOL
108  ETA = DINTERP(B, BO, BSTEP, ETATAB, NETA, DIF, ND, TOL)
109  DEIQ = B*(SIN(ETA))**2
110  Q = Q + DEIQ
111  IF (LL + LE, NMAX = 20 *OR* IEPS, EQ, 1) GO TO 700
112  CALL EPSALG(Q, M, EPSVEC)
J = 2 + 2*(M/2) = M

IF (M .LE. 2) GO TO 700

IF (ABS(EPSVEC(J) = EPSVEC(J+2)) .GT. 0.1) GO TO 700

IEPS = 1

WRITE (6,21) (EPSVEC(K),K=1,M)

FORMAT (/5X,'EPSILON ALGORITHM CONVERGES.../(5X,1DF11.4))

GO TO 800

700 CONTINUE

B = B + 1./A

QJB = Q + ETA*QJB*VAL(CJB,B)/ETAJB

CROSJB = COEF*QJB

CROSS = COEF*Q

C6APP = HX2*WAVE*(CROSJB/8.083)**2*5/MU

WRITE (6,30)T,CROSS,Q,CROSJB,QJB,C6APP,ND

FORMAT (/5X,'TIME (SEC) ',F10.3,'10X','CROSS SECTION AT LAST PHASE S 2NG)',F10.2,'10X','QB EXTRAPOLATD CROSS SECTION (SQ A',F10.3,'10X','C6 APARENT',E15.6,'10X','HIGHEST OR

3DER.DIFERENCE USED IN INTERPOLATION',F18.5)

IF (M .EQ. 0) GO TO 1000

CROSS = COEF*EPSVEC(J)

C6APP = HX2*WAVE*(CROSS/8.083)**2*5/MU

WRITE (6,40)CROSS,EPSVEC(J),C6APP

FORMAT (10X,'EPSILON ALGORITHM CROSS SECTION',F10.2,'10X','QB',F10.3,'10X','C6 APARENT',E14.6)

1000 CONTINUE

STOP

END

ND OF COMPILATION: NO DIAGNOSTICS.
A. PHASHT

This function computes the value of the JWKB phase shift \( \eta_l \) for given \( E \) and \( b = (k + \frac{1}{2})/k \), to a given absolute tolerance, by means of the formulae

\[
\eta_l = \eta_1 + \eta_2 \quad (b > r_0)
\]
\[
\eta_l = \frac{\pi}{2} b - r_0 - \int_{0}^{y_0} \frac{1 - F_{y_2}}{y_2} \, dy \quad (b \leq r_0)
\]

(VII-7)

where \( V(r) \) is the potential, \( r_0 \) is the largest positive zero of \( F(r) \)

\[
F(r) = 1 - \frac{b^2}{r^2} - \frac{V(r)}{E}
\]

and \( y = 1/r \) (\( y_o = 1/r_o \)). The quantities \( \eta_1 \) and \( \eta_2 \) are given by

\[
\eta_1 = \int_{1/b}^{y_0} \frac{F_{\sqrt{2}}}{y_2} \, dy
\]
\[
\eta_2 = \int_{0}^{1/b} \frac{F_{\sqrt{2}} - \sqrt{1 - b^2 y^2}}{y^2} \, dy
\]

(VII-8)

The integrals are performed by function ADSIMP (q.v.)

CALL: ETA = PHASHT (EPS, NITER, ISW)

INPUT: EPS - Absolute error tolerance for integrals in Eq. (VII-7,8)
NITER - \( 2^{\text{NITER}} \) is the maximum number of points which may be used in the integrations.
OUTPUT: ISW = 0, Normal convergence of integrations; if ≠ 0, integrals did not converge (see ADSIMP)

PHASHT - value of \( \eta_2 (b, E) \)

NOTE: Values of \( B(b), R_0(r_o), \) and \( Y_0(y_o) \) are obtained through the COMMON statement of line 10.
M PHASHT

9=05/31/72=01153117 (.0) PHASHT
1. FUNCTION PHASHT (EPS, NITER, ISW)
2. C FINDS VALUE OF JWKB PHASE SHIFT FOR IMPACT PARAMETER B, TURNING
3. C POINT RO, EPS IS ABS ERROR CRITERION, 2*NITER IS MAX NO. OF
4. C POINTS WHICH MAY BE USED IN INTEGRATION (NITER/.LE. 9)
5. C IF ISW .NE. 0, FAILED TO CONVERGE TO ACCURACY EPS
6. C NOTE. REQUIRES FUNCTIONS F, F2, F3, WHICH FOR Y = 1/R RETURN
7. C F(Y) = (1-SQRT((1-(B*Y)**2 - V(R)/E)))/(Y*Y)
8. C F2(Y) = SQRT((1-(B*Y)**2-V(R)/E))/(Y*Y)
9. C F3(Y) = SQRT((1-(B*Y)**2-V(R)/E)*SQRT(1-(B*Y)**2))/((Y*Y)
10. COMMON B, R0, E, Y0
11. DATA PI2/1, 57079633/
12. EXTERNAL F, F2, F3
13. LIMIT = 2*NITER
14. IF (B .LE. R0) GO TO 100
15. BINV = 1/B
16. TOL = .05*EPS
17. ETA1 = ADSIMP(BINV, Y0, F2, TOL, LIMIT, ISW1)
18. ETA2 = ADSIMP(.0, BINV, F3, TOL, LIMIT, ISW2)
19. ISW = ISW1 * ISW2
20. PHASHT = ETA1 + ETA2
21. RETURN
22. 100 PHASHT = PI2*B - RO = ADSIMP(.0, Y0, F, EPS, LIMIT, ISW)
23. RETURN
24. END

END OF Compilation: NO DIAGNOSTICS.
B. \texttt{VEFF/F/F2/F3}

Four entry-point function which returns values of
\begin{align*}
\text{VEFF}(y) &= 1 - b \frac{2}{y^2} - \frac{V(r)}{E} \\
F(y) &= (1 - \sqrt{\text{VEFF}})/y^2 \\
F2(y) &= \sqrt{\text{VEFF}}/y^2 \\
F3(y) &= (\sqrt{\text{VEFF}} - \sqrt{1 - b \frac{2}{y^2}})/y^2
\end{align*}

where $y = 1/r$, and $b$ and $E$ are obtained via the \texttt{COMMON} statement of line 2.

\texttt{CALLS} \quad Z = \text{VEFF}(X) \\
Z = F(X) \\
Z = F2(X) \\
Z = F3(X)

\texttt{ARGUMENT:} \quad X = y
FUNCTION VEFF(X)
COMMON B,R0,E,Y
U = B*X
VEFF = 1.0 - U*U - POT(1.0/X)/E
RETURN
ENTRY F(X)
IF (X LT 1.0E3) GO TO 200
U2 = X*X
V = POT(1.0/X)/E
WORK = B*B*U2 + V
IF (WORK LT 0.01) GO TO 100
IF (WORK GT 0.999999 AND WORK LT 1.001) WORK = 0.999999
VEFF = SQRT(WORK)/U2
RETURN
100 VEFF = 0.5*(B*B+V/U2)*1.0 + 0.25*WORK*(1.0 + 0.5*WORK))
RETURN
200 VEFF = 0.5*B*B
ENTRY F2(X)
U = B*X
WORK = 1.0 - U*U - POT(1.0/X)/E
IF (WORK LT 0.01) GO TO 300
VEFF = SQRT(WORK)/(X*X)
RETURN
ENTRY F3(X)
IF (X LT 1.0E3) GO TO 400
U2 = X*X
BB = B*B
DODA = BB + POT(1.0/X)/(U2*E)
WORK = U2*DODA
IF (WORK LT 0.01) GO TO 300
VEFF = (SQRT(ABS(1.0*WORK)) - SQRT(ABS(1.0*BB*U2)))/U2
RETURN
300 WORK = DODA*DODA
V = BB*BB
VEFF = 0.5*(BB*V/DODA) - 0.125*U2*(V*WORK) - 0.5*U2*(BB*V*WORK)
DODA)
RETURN
400 VEFF = 0.5
RETURN
END

ND OF Compilation! NO DIAGNOSTICS.
C. POTIN/POT

This function is a user-defined routine which returns values of potential constants (POTIN) and values of $V(r)$ (POT)

1. POTIN

CALL: SIGMA = POTIN (C6,EUNIT, RUNIT)

OUTPUT: C6 - values of $C_6$ in reduced units EUNIT = e and RUNIT = a

EUNIT - e dimensional unit in cpe of energy (of order $\varepsilon$)

RUNIT - a dimensional unit in Å of distance (of order $r_m$ or $\sigma$)

POTIN - returns value of $\sigma$ ($V(\sigma) = 0$) in units of RUNIT

2. POT

CALL: V = POT(R)

INPUT: R = r in reduced units

OUTPUT: POT - $V(r)$ in reduced units
3. **SAMPLE PROGRAM**

The program listing is of a function which reads in a pointwise potential (EUNIT = ε and RUNIT = r). The value of V(r) is calculated by quadratic interpolation

\[
V(r) \approx V + Ar + Br^2
\]  

(VII-9)

where A(I) and B(I) are calculated by the routine. Extrapolation to low r is done by extrapolation of the closest quadratic, extrapolation to large r is done by

\[
V(r) \approx -\frac{C_6}{r^6} - \frac{C_8}{r^8}
\]  

(VII-10)

where \( C_8 = C_6 \) is calculated from the last data point and \( C_6 \).

**INPUT:** Card 1: NOB (I5)
Card 2: EPS, RM, C6, SIGMA (10F8.3)
Card 3ff: (X(I), V(I), I = 1,NOB) (10F8.3)

where

- NOB - no. of points
- EPS - \( \varepsilon \) (cpe)
- RM - \( r_m \) (Å)
- C6 - \( C_6 \) (reduced units)
- SIGMA - \( \sigma \) (reduced units)
- X(I) - I-th value of \( r \) (reduced units)
- V(I) - I-th value of V (reduced units)
REMARKS: (1) $C_8$ is calculated from $C_8 = - r^8 V - r^6 C_6$ for $r = X(NOGR)$, $V = V(NOGR)$

(2) It is not necessary that $EPS = \epsilon$ and $RM = r_m$, but any scale factors may be used.
FUNCTION POTIN(C6CONS,EPS,RM)
DIMENSION X(50),V(50),A(50),B(50)
READ (5,10) NOB
10 FORMAT (15)
READ (5,20) EPS, RM, C6, SIGMA
C6CONS = C6
FORMAT (10F8.3)
READ (5,20) (X(I),V(I),I=1,NOB)
R2 = X(NOB)*X(NOB)
R6 = R2*R2*R2
C8 = (V(NOB)*R6 + C6)
R2 = R2*R2*R2
R6 = R2*R2*R2
TEST = R6*(R2*C8 + C6)/V(NOB=1)
NN = NOB = 1
DO 90 90 = 2, NN
H1 = X(I) = X(I=1)
H2 = X(I+1) = X(I)
HH = X(I+1) = X(I)
D12 = V=1 = V(I=1)
D23 = V(I+1) = V(I)
H12 = H1/H2
A(I) = (HI2*D23 + D12/H12)/HH
B(I) = (HI2*D23 - D12)/(HI*HH)
90 NN = (NOB+1)/2
RUP = X(NOB)
POTIN = SIGMA
RETURN
ENTRY POT(R)
IF (R < GT RUP) GO TO 500
I = NN
100 IF (R < GT X(I)) GO TO 200
I = (I+1)/2
IF (I < GT I) GO TO 100
I = 2
GO TO 400
200 I = I + 1
IF (I < EQ NOB) GO TO 300
IF (R< X(I)) 400, 400, 200
300 I = NOB = 1
400 HH = R = X(I)
POTIN = V(I) + HH*(A(I) + HH*B(I))
RETURN
500 R2 = I/(R*E)
R6 = R2*R2*R2
POTIN = R6*(R2*C8+C6)
RETURN
END
D. **QJBVAL**

Function which computes \( \int_{b}^{\infty} b' \sin^2 \eta_{l}^{JB} dB' \) where the integral is done by expansion of \( \sin^2 \) and 
\[
\eta_{l}^{JB} = \frac{3\pi}{32} \frac{C_6 A}{E_{6.5}}
\]

**CALL:** \( Q = QJBVAL \) (CJB,B)

**INPUT:**
- CJB - \( 3\pi AC_6/32E \)
- B - b

**OUTPUT:** \( QJBVAL = \int_{b}^{\infty} b' \sin^2 \eta_{l}^{JB} dB' \)

**REMARKS:** The value returned is correct to more than 3 significant figures for values of B for which \( \eta_{l}^{JB} \leq 2 \).
FUNCTION QJBVAL(CJB,B)
C PERFORMS INTEGRAL FROM B TO INFINITY OF B*(SIN ETAJB)**2
C WHERE ETAJB IS J-B PHASE SHIFT FOR LONG-RANGE C6:
C ETAJB = CJB/B**5 + CJB*3*PI*C6/(32*E).
DIMENSION S(10)
DATA S/1.,0.33333333,0.04444444,0.31796031E-2,0.19109347E-3,
1 = 4.2755597E-5,0.93968345E-7,0.15661391E-8,0.20472406E-10/.
2 = 2.1549902E-12/.
QJBVAL = 0.
T = B*B.
Z = CJB/(T*T).
Z = Z*Z.
T = Z/T.
DODA = 1.
DO 500 I = 1,10
DELA = S(I)*DODA/(10*I+2).
QJBVAL = QJBVAL + DELQ.
IF (ABS(DELA) LT 1.E-3) QJBVAL GO TO 600.
500 DODA = DODA*T.
600 QJBVAL = Z*QJBVAL.
RETURN.
END.
E. **DNTERP**

This function performs finite difference interpolation based on a difference table constructed by DIFTAB (q.v.) The appropriate formula (Forward, Backward, or Stirling's central difference) is used with maximum order such that:

1. The order is less than or equal to the size of the difference table.
2. The size of the next term to be added is less than the propagated error.

CALL: VALUE = DNTERP (X, XO, H, N, D, ND, EPS)

ARGUMENTS:
- X - abscissa of interpolant
- XO - left-most abscissa of data
- H - stepsize of data
- Y(I) - I-th ordinate of data
- D - difference table from DIFTAB (q.v.)
- ND - highest-order difference available in D (returned by DIFTAB, q.v.)
- EPS - estimate of the absolute error of a Y(I)

OUTPUT: DNTERP - value of interpolated ordinate corresponding to X.

REMARK: The program extrapolates beyond the range of the data by means of the nearest forward/backwards difference polynomial. (This could be improved by extrapolating the difference table.)
I DINTERP

FUNCTION DINTERP(X, XO, H, Y, N, D, ND, EPS)

C PERFORMS DIFFERENCE INTERPOLATION UP TO ORDER ND

C D = DIFFERENCE TABLE FROM DIFTAB

C EPS = ESTIMATE OF ABSOLUTE ERROR IN Y'S

DIMENSION Y(I), D(I)

M = 0

DODA = 1.

TOL = EPS

THETA = (X - XO)/H

I = THETA + 0.5

IF (I LT 0) I = 0

IF (I GE N) I = N - 1

THETA = THETA + 1

I = I + 1

DINTERP = Y(I)

IF (I GTH N - ND) GO TO 2000

IF (I LT ND) GO TO 1000

USE STIRLING'S CENTRAL DIFFERENCE FORMULA

DO 200 J = 1, ND

TOL = 2. * TOL

L = J/2

K = M + 1

IF (ABS(D(K)) LE TOL) GO TO 500

DODA = DODA/J

IF (2*L NE J) GO TO 300

TERM = THETA * DODA

DODA = DODA * (THETA - L)

GO TO 350

300 DODA = DODA * (THETA + L)

DINTERP = DINTERP + 0.5 * DODA * (D(K) + D(K+1))

GO TO 400

350 DINTERP = DINTERP + TERM * D(K)

400 M = M + N - J

500 RETURN

C USE NEWTON'S FORWARD DIFFERENCE FORMULA

1000 DO 1500 J = 1, ND

TOL = 2. * TOL

K = M + 1

IF (ABS(D(K)) LE TOL) GO TO 1600

DODA = DODA * (THETA - J+1)/J

DINTERP = DINTERP + DODA * D(K)

1500 M = M + N - J

1600 RETURN

C USE NEWTON'S BACKWARDS DIFFERENCE FORMULA

2000 DO 2500 J = 1, ND

TOL = 2. * TOL

K = M + 1

IF (ABS(D(K)) LE TOL) GO TO 2600

DODA = DODA * (THETA + J-1)/J

DINTERP = DINTERP + DODA * D(K)

2500 M = M + N - J

2600 RETURN

END

END OF COMPILATION! NO DIAGNOSTICS.
F. DIFTAB

This program constructs a finite difference table from N equally-spaced data points, with ordinates \( y_i \) (\( 1 \leq i \leq N \)). Successively higher order differences are computed until no element of the current column in the difference table is larger than the propagated error.

CALL DIFTAB (Y, N, D, ND, EPS)

INPUT:  
Y(I) - \( y_i \)  I-th ordinate  
N - no. data points  
EPS - estimate of absolute errors in Y(I)

OUTPUT:  
D - difference table stored in packed-mode: i.e., the first-order differences are in D(1) ... D(N-1), the second-order differences in D(N) ... D(2N-2), etc.  
ND - set to highest-order difference calculated.
SUBROUTINE DIFTAB(N,N,D,ND,EPS)
CALCULATES DIFFERENCE TABLE OF Y(1),...,Y(N).
NOTE: D MUST BE DIMENSIONED AT LEAST ND*(N-1).
ND: UPON ENTRY, MAX. ORDER DIFFERENCE TO BE CALCULATED UPON
RETURN IS ACTUAL HIGHEST ORDER.
EPS: ABSOLUTE ERROR ESTIMATE OF Y'S TO STOP DIFFERENCES.
DIMENSION Y(1),D(1)
MAXD = ND
ERRLVL = 2.0*EPS
M = N
T = FORDIF(Y,M,D)
ND = 1
K = 1
100 IF (ND .GE. MAXD OR M .LE. 1 OR T .LE. ERRLVL) GO TO 200
ND = ND + 1
ERRLVL = 2.0*ERRLVL
J = K + M
T = FORDIF(D(K),M,D,1)
K = J
GO TO 100
200 RETURN
END
G. FORDIF

Function which calculates the vector of forward-differences corresponding to a vector of ordinates.

CALL: DMAX = FORDIF (Y, N, D)

INPUT:  Y(I) - I-th ordinate
         N - No. of data

OUTPUT: D(I) - I-th forward difference, Y(I+1) - Y(I)
        FORDIF - max|D(I)| 1 ≤ I ≤ N-1
FORDIF
05/31/72=01:53:121 (.0) FORDIF

1. FUNCTION FORDIF(Y,N,D)
2. C CALCULATES FORWARD DIFFERENCES D(I) = Y(I+1) - Y(I)
3. C RETURNS VALUE OF MAXIMUM DIFFERENCE
4. DIMENSION Y(1),D(1)
5. N = N + 1
6. T = 0
7. DO 100 I = 1,N
8. D(1) = Y(I+1) - Y(I)
9. 100 IF (T .LT. ABS(D(I))) T = ABS(D(I))
10. FORDIF = T
11. RETURN
12. END

END OF COMPILATION: NO DIAGNOSTICS.
Subroutine which extrapolates a sequence of partial sums to a limit by means of the ε-algorithm. Only the diagonal of the matrix of convergents is stored.

* See P. Wynn, "Five Lectures on the Numerical Application of Continued Fractions", Orientation Lecture Series No. 5, Mathematics Research Center, University of Wisconsin, Madison, Wisconsin, 53706.

The algorithm is as follows to find the limit of a sequence of partial sums $S_m (m = 0, 1, 2, ...)$:

$$
\begin{align*}
\varepsilon_{-1}^{(m)} &= 0 \quad (m = 1, 2, ...) \\
\varepsilon_0^{(m)} &= S_m \quad (m = 0, 1, 2, ...) \\
\varepsilon_{r+1}^{(m)} &= \varepsilon_{r-1}^{(m)} + 1/(\varepsilon_r^{(m+1)} - \varepsilon_r^{(m)}) \quad (r = 1, 2, ...)
\end{align*}
$$

The $\varepsilon_{2r}^{(m)}$ are improved estimates of the limit.

CALL EPSALG (S, M, X)

INPUT: S – current value of partial sum

M – Number of times EPSALG has been called previously for this series

OUTPUT: M – will be replaced by M + 1

X(1) ... X(M) – will contain the ε-diagonal of convergents.
REMARKS: The approximations to the limit of the series will be in every other \( X(i) \). The best value for the limit will be found in \( X(1) \) if \( M \) is odd or \( X(2) \) if \( M \) is even.
SUBROUTINE EPSALG(S,M,X)

C_EXTRAPOLATES_SUM_OF_SERIES_S_BY_EPSILON_ALGORITHM
C_S_IS_VALUE_OF_CURRENT_PARTIAL_SUM_AT_EXIT_M_IS_LENGTH_OF
C_THE_EPSILON_DIAGONAL_X(1).....X(M).
C_BEST_ESTIMATE_OF_SUM_IS_IN_X(J), WHERE J = 2*MOD(M,2)
DIMENSION X(M)
K = M
M = M + 1
X(M) = 0
10 A1 = S
100 IF (K LE 0) GO TO 200
12 A0 = X(K+1) + 1.0/(A1*X(K))
13 X(K+1) = A1
14 A1 = A0
15 K = K + 1
16 GO TO 100
200 X(1) = A1
18 RETURN
19 END

NO_DIAGNOSTICS_
I. **REGFAL**

This subroutine finds a root of the equation $F(x) = 0$, given an interval which contains the root, by a strategy using regula falsi and the method of bisection. Barring multiple roots or excessive rounding-error, the routine guarantees convergence. The algorithm proceeds as follows:

1. Bisect the original interval until a sign change is found. (If none is found, error return.)

2. Apply regula falsi (secant method) until convergence is attained.
   
   (a) If the change in interval length at any step is less than 10% of the previous interval length, apply the method of bisection once.
   
   (b) If convergence is not attained, or the root is lost, error return.

CALL REGFAL (XL, XU, X, F, EPS, LIM1, LIM2, IER)

**INPUT:**

XL, XU - Endpoints of an interval containing the root

F - name of function which stores the value of $F(x)$ in $y$ in the call $y = F(x)$

EPS - relative error criterion for root. Termination occurs when relative change in root is less than EPS or the root itself is less than EPS

LIM1 - Limit on number of applications of bisection to find a sign change; if LIM1 = 0, Step (1) above is skipped

LIM2 - limit on number of applications of regula falsi in step (2)
OUTPUT: X - estimate of root

IER - 0 Normal

1 No root or a multiple root in interval (to tolerance EPS)
2 No sign change found with LIM1 iterations
3 No convergence to EPS tolerance with LIM2 iterations
4 Root was lost in regula falsi iterations (no longer a sign change)

REMARK: The convergence testing could be improved slightly by adding

line 12.5  \( HO = EPS*H \)

and replacing line 50 with

\[
\text{IF (ABS(DELX) . LT . HO) GO TO 1000}
\]
REGFAL

05/31/72 01.153124 (,0) REGFAL

1 SUBROUTINE REGFAL (XL,XU,X,F,EPS,LIM1,LIM2,IER)

2 FINDS ROOT OF THE EQTN F(X) = 0 IN INTERVAL (XL,XU)

3 BY METHOD OF REGULA FALSI (GUARANTEED CONVERGENCE)

4 EPS = RELATIVE ERROR TOLERANCE FOR ROOT

5 LIM1 = ALLOWABLE ITER. TO FIND SIGN CHANGE IN AN INTERVAL

6 LIM2 = ALLOWABLE ITERATIONS TO FIND ROOT

7 IER = 0, NORMAL: = 1 NO OR MULT ROOT TO TOLERANCE EPS: = 2 NO

8 SIGN CHANGE WITH LIM1 ITERATIONS: = 3 NO CONVERGENCE WITH LIM2 IT

9 C = 4, LOST ROOT IN REG. FALSI ITERATIONS

10 FA = F(XL)

11 X = XL

12 H = XU - XL

13 IF (LIM1 = EQ. 0) GO TO 300

14 J = 1

15 HH = EPS*H

16 DO 200 1 = 1,LIM1

17 IF (H * LE* HH) GO TO 250

18 X = XL

19 DO 100 K = 1,J

20 FB = F(X*H)

21 IF (FA*FB * LE* 0) GO TO 350

22 100 X = X + H

23 H = 0.5*H

24 200 J = 2*J

25 IER = 2

26 RETURN

27 250 IER = 1

28 RETURN

29 300 FB = F(X*H)

30 350 A = X

31 B = X + H

32 FA = F(A)

33 HH = ABS(H)

34 XP = A

35 DO 800 1 = 1,LIM2

36 X = A = FA*H/(FB*FA)

37 J = 1

38 400 FX = F(X)

39 IF (FX*FA ) 500,1000,600

40 500 FB = FX

41 B = X

42 GO TO 700

43 600 FA = FX

44 A = X

45 IF (FA*FB * GT* 0) GO TO 900

46 700 H = B - A

47 IF (J = EQ. 2) GO TO 800

48 DELX = X - XP

49 XP = X

50 IF (ABS(DELX) * LT* EPS*ABS(X) * OR* ABS(X) * LT* EPS) GO TO 1000

51 IF (ABS(H) * LT* 0.9*HH) GO TO 800

52 X = 0.5*(A+B)

53 J = 2

54 GO TO 400

55 800 HH = ABS(H)
IER = 3
RETURN
IER = 4
RETURN
IER = 0
RETURN
END

ND OF COMPIATION!

NO DIAGNOSTICS.
This function returns the value of the integral
\[ \int_{x_L}^{x_U} F(x) \, dx \]
obtained by means of adaptive application of Simpson's rule. The program is a slightly modified version of Alg. 182, Comm. ACM 6, 315 (1963).

CALL: VALUE = ADSIMP (XL, XU, F, ERRTOL, MAX, IER)

INPUT: XL, XU - Endpoints of the interval of integration

F - name of function which stores the value of the integrand in Y from the call Y = F(X)

ERRTOL - Error bound on absolute error of the integral

MAX - maximum number of integration points which may be used

OUTPUT: IER - if 0, normal convergence. If \# 0, then more than MAX points are needed for convergence.

ADSIMP - Returned value of integral

REMARK: All of the dimensions in lines 6-8 could be safely reduced to 15. (which necessitates a 15 in line 41)
FUNCTION ADSIMP(XL,XU,F,ERRTOL,M) IER

INTEGRATES F(X) FROM XL TO XU BY ADAPTIVE SIMPSONS RULE

ERRTOL = ALLOWABLE ABSOLUTE ERROR TOLERANCE

MAX = LIMIT ON NO. FUNCTION CALLS

IF IER *NE* 0 MORE THAN MAX POINTS ARE REQUIRED

DIMENSION DX(30), EPSP(30), X2(30), X3(30), F2(30), F3(30), F4(30)

IFMP(30), FB(30), EST2(30), EST3(30), PVAL(30,3)

INTEGER RTRN(30)

EPS = ERRTOL

A = XL

B = XU

LVL = 0

EST = 1.0

DA = B - A

FA = F(A)

FM = 4.0*F(A+B)/3.0

FB = F(B)

KOUNT = 3

LVL = LVL + 1

DX(LVL) = 0.333333333333333333

SX = DX(LVL)*0.16666666666666666

F1 = 4.0*F(A+B)/3.0*DX(LVL)

X2(LVL) = A + DX(LVL)

F2(LVL) = F(X2(LVL))

X3(LVL) = X2(LVL) + DX(LVL)

F3(LVL) = F(X3(LVL))

EPSP(LVL) = EPS

F4(LVL) = 4.0*F(X3(LVL) + 0.5*DX(LVL))/3.0

FMP(LVL) = FM

EST1 = SX*(FA + F1 + F2(LVL))

FBP(LVL) = FB

EST2(LVL) = SX*(F2(LVL) + F3(LVL)) + FM

EST3(LVL) = SX*(F3(LVL) + F4(LVL)) + FB

SUM = EST1 + EST2(LVL) + EST3(LVL)

KOUNT = KOUNT + 4

IF (ABS(SUM) + EPS*(EPSP(LVL)) < 1) GO TO 500

LVL = LVL + 1

1 = RTRN(LVL)

PVAL(LVL,1) = SUM

GO TO 600

IF (LVL <= 30 OR KOUNT <= MAX) GO TO 400

RTRN(LVL) = 1

FM = F1

FB = F2(LVL)

EST = EST1

550 DA = DX(LVL)

EPS = 0.5*EPSP(LVL)

GO TO 100

600 RTRN(LVL) = 2

FA = F2(LVL)

FM = FMP(LVL)

FB = F3(LVL)

EST = EST2(LVL)

A = X2(LVL)

GO TO 550
56.    700  RTRN (LVL) = 3
57.    FA = F3(LVL)
58.    FM = F4(LVL)
59.    FB = FBP(LVL)
60.    EST = EST3(LVL)
61.    A = X3(LVL)
62.    GO TO 550
63.    800  SUM = PVAL(LVL,1) + PVAL(LVL,2) + PVAL(LVL,3)
64.    IF (LVL GT 1) GO TO 400
65.    ADSIMP = SUM
66.    IER = 0
67.    IF (KOUNT GT MAX) IER = 1
68.    RETURN
69.    END
K. SAMPLE OUTPUT

The problem shown is for the Na-Hg system with the pointwise potential taken from U. Buck and H. Pauly, J. Chem. Phys. 54, 1929 (1971).

The units of energy and length were \( \epsilon = 8.79 \text{ cpe} \) and \( r_m = 4.72 \text{ Å} \), resp. The output shown is for \( E^* = 1.65 \).

NOTES: (1) The last partial wave calculated was at \( l = 455, (b^* = 3) \), when \( \delta Q < 0.1 \text{ Å}^2/b \).

(2) The convergents of the \( \epsilon \)-algorithm after 5 extrapolations were:

\[ 175.4996 \text{ (best), } 175.4999, 175.0902. \]

(3) The calculation took 6 seconds on an Univac 1108 (1.5 \( \mu \)s add time).

Since every seventh \( \eta_2 \) was calculated, without interpolation the execution would have taken 40 seconds.

(4) The \( \epsilon \)-algorithm extrapolated cross section was \( 696.6 \text{ Å}^2 \), with \( C_6^{\text{app}} = 0.6690 \times 10^5 \text{ cpe} \cdot \text{Å}^6 \).
ENTRY TO JWKB/DINTERP

TOLERANCE FOR Yo (RELATIVE)  \times 10^00000000.2
TOLERANCE FOR ETA (ABS)  \times 50000000.002
TOLERANCE FOR JB LIMIT  \times 100000000.001

BUCK=PAULY NA=HG 45-POINT INTERPOLATED POTENTIAL

PHASE SHIFTS AND CROSS SECTIONS FOR REDUCED MASS  \times 34251302
LONG-RANGE C6  \times 50000000.00
ZERO OF POTENTIAL  \times 81084000.00
UNITS OF ENERGY AND LENGTH  \times 87900000.01 \times 47200000.01
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**MAINTAINING CROSS SECTION IS LESS THAN 0.05 SQ ANG**

**E (SEC) 5.937**

**CROSS SECTION AT LAST PHASE SHIFT 696.92**

**JB EXTRAPOLATED CROSS SECTION (SQ ANG) 696.51**

**C6 APPARENT 668939**

**HIGHEST ORDER DIFFERENCE USED IN INTERPOLATION 10**

**EPSILON ALGORITHM CROSS SECTION 696.55**

**Q 175.090**

**QJB 175.490**

**Q 175.500**

**C6 APPARENT 669031+05**