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1. Supplement
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The Karlsruhe Code MODINA for Model Independent Analysis of Elastic Scattering of Spinless Particles

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Abstract

The Karlsruhe code MODINA (KfK 3063, published November 1980) has been extended in particular with respect to new approximations in the folding models and to the calculation of errors in the Fourier-Bessel potentials. The corresponding subroutines replacing previous ones are compiled in this first supplement.

The listings of the fit-routine-package FITEX missing in the first publication of MODINA are also included now.

Der Karlsruher Code MODINA zur modellunabhängigen Analyse der elastischen Streuung spinloser Teilchen mit dem optischen Modell

1. Supplement

Der Karlsruher Code MODINA (erstmals publiziert im November 1980, KfK 3063) wurde im Hinblick auf neue Näherungen in den Faltungsmodellen und hinsichtlich der Fehlerrechnungen in den Fourier-Bessel-Potentialen erweitert. Die entsprechenden Subroutinen sind in diesem ersten Supplement zusammengestellt.

Die Listen des Fit-Routine-Paketes FITEX, die in der ersten Publikation von MODINA fehlten, sind ebenfalls aufgeführt.

1. Introduction

In the present first supplement to the program description of the code MODINA [1] new options and models are introduced and the corresponding FORTRAN-listings are compiled. Since there is no general change in the structure of the input and in the output of the code only the few changes in the handling of the program are explained in the following. Hence, the present report has to be used in close connection with KfK 3063 to the pages of which is directly referred.

2. to 4. as in the first edition

5. Input Description

5.1.2.1 Options

CARD 2 (FORMAT 8I5)

		further comments on page	
FOLDED COULOMB POTENTIAL	1	22	1st edition
REAL POTENTIAL	4	19	" "
TARGET DENSITY (FOLDING)	0	26	" "
IMAGINARY POTENTIAL	1	19	" "
CONSERVE VOLUME-INTEGRAL	0	21	" "
RELATIVISTIC KINEMATICS	0		
NORMALIZATION VEFF (FOLDING)	0	3	1st suppl.
CONSTRAINTS	0	3+5	" "

5.4. Folding Models

Systematic studies [2] of different forms of a Local Density Approximation (LDA) in density dependent αN-interactions showed that the previously used form (eq. 5.4.2) is not the best choice. Therefore, eq. 5.4.2 should be replaced by the following ex-

pression

rev. (5.4.2)
$$V_{PN}(\vec{r}) = -\lambda \cdot f(|\vec{r}-\vec{r}'|) \cdot$$
$$\{[1-m\gamma\ \rho_m^{2/3}(\vec{r}')] \cdot [1-(1-m)\gamma\ \rho_m^{2/3}(\vec{r})]\}$$

where the term in the curly brackets considers the new form ("mixed") of the LDA [2].

5.4.1 Effective interaction

The analytic integration of eq. 5.4.1 is no longer used. For any formfactor $f(\vec{x})$ (which may be defined by the user in SUBROUTINE FXV) a numerical integration is furtheron used. Therefore, the folding model blocks POGA, POGAFB, POAR, and POARFB may be replaced by the blocks POGYNA and POGYNAFB, where the latter is valid for the Fourier-Bessel option (FB) in the densities (see below).

The form factor f(x) (eq. 5.4.3) of the effective interaction coded now in POGYNA and POGYNAFB is a Gaussian plus Yukawa interaction [3].

rev. (5.4.3)
$$f(x) = V_G \cdot \exp(-x^2/a_G^2) + V_Y \cdot \exp(-x/a_Y)/(x/a_Y)$$

The corresponding subroutines are contained in the module POGYNA which has to be included in front of MODINA. The options for this folding models are

```
_INCLUDE_LØAD(POGYNA)
```

REAL POTENTIAL	= 7			
TARGET DENSITY (FOLDING)	= 1	OR	2	(see 5.4.2)
IMAGINARY POTENTIAL	= 1	OR	2	(see 5.3.1)

The number of parameters for POGYNA is NP = 28

The parameters of the interaction are

P(4)	= λ	=	1.		
P(5)	= a_G	=	2.009	fm	
P(6)	= γ	=	1.645	fm^2	
P(14)	= V_G	=	20.6	MeV	
P(15)	= m	=	0.2		
P(18)	= R_V	=	8.0	fm	Cut-off radius of f(x)
P(19)	= V_Y	=	111.	MeV	
P(20)	= a_Y	=	0.85	fm	
P(21)	= R_ρ	=	10	fm	Cut-off radius of densities

The given values are suitable for elastic α-particle scattering from medium weight nuclei at E_α = 104 MeV [2,3].

When using the folding model POGYNA the parameters of the form-factor in most cases may not be varied during the fit. Hence, f(x) is usually computed only once at the beginning of the job, in order to save computing time. If one, however, wishes to vary parameters of f(x) this may be switched on by setting option (CARD 2, see above)

NORMALIZATION VEFF (FOLDING) = 1

(otherwise 0)

There may be also some reasons [2] to couple the parameters γ and m (eq. 5.4.2) during the fit according to the equation

rev. (5.4.2c) $\gamma = a_1 + a_2 \cdot m$

This can be achieved by setting option (CARD 2, see above)

CONSTRAINTS = 1

with the additional use of parameters

P(16) = a_1
P(17) = a_2

5.4.2.2 Fourier-Bessel series

In the folding models the density distributions ρ_m or ρ_n may also be parametrized in a less model dependent way by use of a Fourier-Bessel-series added to one of the functional forms F-3, G-3

$$(5.4.8) \quad \rho_{m,n}(r) = (F\text{-}3;G\text{-}3) + \sum_{\nu=1}^{N'} \beta_\nu \, j_o\left(\frac{\nu\pi r}{R_{CTF}}\right)$$

This model independent description (including also the FB option for the imaginary potential, (see sect. 5.3.1.2) is coded in the LØAD-module POGYNAFB which is called with the options

```
_INCLUDE_LØAD(POGYNAFB)
     REAL POTENTIAL      =     8
```

The total number of parameters of these model is NP = 49. The meaning of the parameters P(1) to P(12) is the same as for POGYNA except of P(4) (see below). The FB-density cut-off radius and coefficients are stored at the same places as the corresponding real FB-potential values.

P(4)	= V_G	
P(13)	= R_{CTF}	
P(14) to P(28)	= $\beta_\nu, \nu = 1,15$	
P(29)	= R_{cI} (Imaginary Potential),	see sect.5.3.1.2
P(30) to P(37)	= c_i, i = 1,8	see sect.5.3.1.2
P(38)	= m	see sect.5.4.1
P(39)	= R_v	" " 5.4.1
P(40)	= V_Y	" " 5.4.1
P(41)	= a_Y	" " 5.4.1
P(42)	= R_ρ	" " 5.4.7
P(43)	= $c_{m,n}/A^{1/3}$	" " 5.4.6 + 5.4.8
P(44)	= $a_{m,n}$	" " 5.4.6 + 5.4.8
P(45)	= $w_{m,n}$	" " 5.4.6 + 5.4.8
P(46)	= $c_p/A^{1/3}$	" " 5.4.6 + 5.4.8
P(47)	= a_p	" " 5.4.6 + 5.4.8
P(48)	= w_p	" " 5.4.6 + 5.4.8

In the standard POGYNAFB module the functional form to which the FB-series is added is a 3-parameter Fermi form (eqs. 5.4.6 and 5.4.8). When wishing to select a G-3 distribution in eq. 5.4.8 an additional LØAD-module named DEG3FB has to be included in front of POGYNAFB.

Parameters of f(x) may not be varied in this form of the folding model.

The option CONSTRAINT (see above) has another meaning in POGYNAFB than in POGYNA. It may here be used to suppress negative regions in the densities which sometimes occur in FB-analyses [3] in the following way:

if CONSTRAINT = 1 the factor

$$c = \{1 + [A - \int|\rho_m(\vec{r})|d\vec{r}]^2\}$$

is multiplied to the value of χ^2 (eq. 3.2) during the fit, where A is the mass number of the target nucleus. This means that the value of χ^2 is doubled if a negative density of unit 1 occurs [3].

Input examples for two typical folding model cases are given in table 4a and 4b.

Table 4a

Input example for POGYNA

```
//IAK623F0 JOB (0623,145,POC1A),GILS,REGION=800K,TIME=3
// EXEC FHLG,LIB=ZYK
//L.SYSPRINT DD DUMMY
//L.SYSIN DD *
 INCLUDE LOAD(POGYNA)
 INCLUDE LOAD(MCDINA)
 ENTRY MAIN
//G.SYSIN DD *
    1     1     0     1     0     0     0     0     1     2     1     1     0     0
    1     7     2     1     0     0     0     0
    0     0     0
   104 MEV ALPHA-PARTICLES ON 40-CA
4.0026     39.96259  2.          20.         104.
 1500    60    74     2  100   -10
    2    28 (7(F9.4,1X))
+15.        1.34        40.         1.          2.009       1.645       20.00
+1.625      .640        0.          1.          1.          0.          20.6
.20         0.          1.1199      8.          111.        .85         10.
1.070       .49         0.          1.1134      .512188     -.166       .001
    2     6 (7(F9.4,1X))
+10.        .2          .005        .005        .005         .005       .005
    1     5 (2213)
  7   8   9 22 23
    2   420      ((2(0PF10.3,1P2E10.3)))
     3.187 2.335E+05 2.627E+04      3.738 1.243E+05 1.893E+04
     4.289 7.599E+04 8.889E+03      4.859 4.960E+04 5.133E+03
     5.422 3.213E+04 3.677E+03      5.954 1.916E+04 2.392E+03
     6.615 1.144E+04 1.466E+03      7.166 5.789E+03 1.068E+03
     7.717 2.598E+03 5.592E+02      8.268 1.160E+03 2.366E+02
     8.323 8.623E+02 8.646E+01      8.599 6.467E+02 5.190E+01
     8.874 6.054E+02 2.511E+01      9.425 7.671E+02 5.639E+01
     9.976 1.169E+03 1.121E+02     10.251 1.528E+03 9.775E+01
    10.526 1.399E+03 3.521E+01     10.802 1.357E+03 1.499E+01
    11.077 1.386E+03 2.008E+01     11.627 1.248E+03 2.027E+01
    11.903 1.223E+03 4.939E+01     12.178 1.002E+03 5.781E+01
    12.453 9.391E+02 6.027E+01     12.728 7.019E+02 7.580E+01
    13.278 4.182E+02 5.610E+01     13.554 2.802E+02 4.369E+01
    78.935 3.440E-02 1.729E-03     81.503 2.133E-02 1.187E-03
    84.060 1.441E-02 8.365E-04     86.606 1.255E-02 7.579E-04
    89.141 6.961E-03 4.837E-04     91.665 5.092E-03 5.092E-04
    94.177 2.811E-03 3.180E-04     96.679 2.269E-03 2.445E-04
   101.648 9.332E-04 2.808E-04    106.573 4.917E-04 9.329E-05
   108.530 2.655E-04 5.769E-05    116.291 9.449E-05 3.150E-05
    2     2 (7(F9.4,1X))
+5.          1.3227
    2     4 (7(F9.4,1X))
+10.         3.766       .586       -.161
    1     1 (1013)
 20
    2     1 (7(F9.4,1X))
+.05
//
```

Table 4b

Input example for POGYNAFB

```
//IAK62340 JOB (0623,145,POC1A),GILS,REGION=800K,TIME=10
//  EXEC FHLG,LIB=ZYK
//L.SYSPRINT DD DUMMY
//L.SYSIN DD *
 INCLUDE LOAD(POGYNAFB)
 INCLUDE LOAD(MODINA)
 ENTRY MAIN
//G.FT07F001 DD DSN=IAK623.CA40D.DATA,DISP=MOD
//G.FT08F001 DD DSN=IAK623.CA40M.DATA,DISP=MOD
//G.SYSIN DD *
    1    1    0    1    0    0    0    0    0    2    1    1 1100 1001
    1    8    2    1    0    0    0    1
    0    0    0
   104 MEV ALPHA-PARTICLES ON 40-CA
4.0026     39.96259  2.         20.        104.
 1500   60   74    2  100  -10
    2   49 (7(F9.5,1X))
 15.       1.34       40.        20.6       2.009      1.645      20.38
 1.618     .643       0.         1.         1.         6.5        0.



                     .20        8.         111.       .85        10.
1.05722   .493642    0.         1.1134     .512188    -.166      .001
    2   11 (7(F9.4,1X))
+10.       .2         .005       .005       .002       .002       .002
+.002      .002       .002       .002       .002       .002       .002
    1   10 (22I3)
  7  8  9 15 16 17 18 19 20 21 22 23 24 25 26 27 28
    2  420      ((2(0PF10.3,1P2E10.3)))
     3.187 2.335E+05 2.627E+04     3.738 1.243E+05 1.893E+04
     4.289 7.599E+04 8.889E+03     4.859 4.960E+04 5.133E+03
     5.422 3.213E+04 3.677E+03     5.954 1.916E+04 2.392E+03
    75.321 5.763E-02 2.454E-03    76.356 4.660E-02 2.116E-03
    78.935 3.440E-02 1.729E-03    81.503 2.133E-02 1.187E-03
    84.060 1.441E-02 8.365E-04    86.606 1.255E-02 7.579E-04
    89.141 6.961E-03 4.837E-04    91.665 5.092E-03 5.092E-04
    94.177 2.811E-03 3.180E-04    96.679 2.269E-03 2.445E-04
   101.648 9.332E-04 2.808E-04   106.573 4.917E-04 9.328E-05
   108.530 2.655E-04 5.769E-05   116.291 9.449E-05 3.150E-05
    2    2 (7(F9.4,1X))
+5.         1.3227
    2    4 (7(F9.4,1X))
+10.        3.766      .586       -.161
//
```

Program Listings

MODINA

MAIN, page 65

```
                C-----HAUPTPROGRAMM ZUR ANALYSE VON ELASTISCHER STREUUNG
                C-----DIE GENERELLE ARBEITSROUTINE HEISST "SCAMPO"
ISN 0002              REAL*8 TAG,UHR
ISN 0003              COMMON /CZF/TID
ISN 0004              TID=ZEIT(0.)
ISN 0005              CALL DATUM (TAG,UHR)
ISN 0006              WRITE (6,6000) TAG,UHR
ISN 0007           6000 FORMAT (' START OF THE JOB : ',A8,2X,A8,' H.MIN.SEC')
ISN 0008              CALL SCTRLA
ISN 0009              CALL SCAMPO
ISN 0010              CALL DATUM (TAG,UHR)
ISN 0011              WRITE (6,6001) TAG,UHR
ISN 0012           6001 FORMAT (///' END OF THE JOB : ',A8,2X,A8,' H.MIN.SEC')
ISN 0013              WRITE (6,6002)
ISN 0014           6002 FORMAT (///' MODINA, REV.4, NOVEMBER 1983')
ISN 0015              STOP
ISN 0016              END
```


MODINA

OPTION, page 66

```
ISN 0002              SUBROUTINE OPTION
                C-----LESEN DER OPTIONEN ZUR STEUERUNG VON POTFIT
                C     KE(42) : MEHRFACH-OPTIONEN
ISN 0003              COMMON /INPT/KE(42),WI(1000),IN(100)
ISN 0004              READ (5,5001) KE
ISN 0005           5001 FORMAT (14I5)
                C-----AUSDRUCK DER OPTIONEN
ISN 0006              WRITE (6,6001) (KE(I),I=1,10)
ISN 0007           6001 FORMAT (////////' NUMBER OF INDEPENDENT CALCULATIONS ',I2/
                     1 ' CM-DATA                                ',I2/
                     2 ' GRID CALCULATIONS                      ',I2/
                     3 ' PRINT INPUT                            ',I2/
                     4 ' PRINT CPU-TIME                         ',I2/
                     5 ' PRINT CROSS SECTIONS                   ',I2/
```

```
                6 ' PRINT CROSS SECTIONS/RUTHERFORD     ',I2/
                7 ' PRINT SCATTERING AMPLITUDES         ',I2/
                8 ' PRINT POTENTIALS                    ',I2/
                9 ' PRINT POTENTIAL MOMENTS             ',I2)
ISN 0008         WRITE (6,6002) (KE(I),I=11,19)
ISN 0009   6002 FORMAT(
                1 ' PRINT DENSITIES                     ',I2/
                2 ' PRINT DENSITY MOMENTS               ',I2/
                3 ' PUNCH POTENTIALS OR DENSITIES     '  ,I4/
                4 ' PUNCH MOMENTS                     '  ,I4//
                5 ' FOLDED COULOMB POTENTIAL            ',I2/
                6 ' REAL POTENTIAL                      ',I2/
                7 ' TARGET DENSITY (FOLDING)            ',I2/
                8 ' IMAGINARY POTENTIAL                 ',I2/
                9 ' CONSERVE VOLUME-INTEGRAL            ',I2)
ISN 0010         WRITE (6,6005) (KE(I),I=20,22)
ISN 0011   6005 FORMAT (
                1 ' RELATIVISTIC KINEMATICS             ',I2/
                2 ' NORMALIZATION VEFF(FOLDING)         ',I2/
                3 ' CONSTRAINTS                         ',I2)
ISN 0012         WRITE (6,6004)
ISN 0013   6004 FORMAT (/' KE(23-28) : FREE'/)
ISN 0014         WRITE (6,6003) (KE(I),I=29,32)
ISN 0015   6003 FORMAT ( ' PLOTTER TYPE                                 ',I2/
                1 ' PLOT CROSS SECTIONS                 ',I2/
                2 ' PLOT CS/RUTHERFORD                  ',I2/
                3 ' PUNCH THEORETICAL CROSS/SECTIONS    ',I2/
                6 ' KE(33-42) : FREE ' )
ISN 0016   1000 RETURN
ISN 0017         END
```

```
ISN 0002            SUBROUTINE VA02M(M,N,F,X,E,ES,IPP,MC,W,P)
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            REAL*4 F4(300),X4(30),E4(30),W4(21000),WI(1000)
ISN 0005            DIMENSION W(2),X(30),F(300),IW(30),P(2),E(30)
ISN 0006            COMMON /INPT/KO(42),WI,IN(100)
ISN 0007            DO 100 I=1,N
ISN 0008            X4(I)=X(I)
ISN 0009            E4(I)=E(I)
ISN 0010        100 CONTINUE
ISN 0011            KE=0
ISN 0012            IP=IABS(IPP)
ISN 0013            W4(1)=ES
ISN 0014            W4(2)=0.
ISN 0015            W4(3)=0.
ISN 0016            W(3)=0.
ISN 0017            IW(1)=N+1
ISN 0018            IW(2)=MC
ISN 0019            IW(3)=1
ISN 0020            IW(4)=0
ISN 0021            NP=0
ISN 0022          2 W4(4)=0.
ISN 0023            CALL CALFUN(M,N,F,X,P)
ISN 0024            IF (M) 22,22,21
ISN 0025         22 IW(2)=IW(3)
ISN 0026            WRITE (6,600) IW(3)
ISN 0027            M=-M
ISN 0028        600 FORMAT (/' CPU-TIME EXCEEDED AFTER ',I3,' CALLS OF CALFUN'/)
ISN 0029         21 DO 3 I=1,M
ISN 0030            F4(I)=F(I)
ISN 0031          3 W4(4)=W4(4)+F(I)*F(I)
ISN 0032            IF (KO(22).EQ.1) CALL CONSTR(M,N,F,X,P,W4)
ISN 0034            W(4)=W4(4)
ISN 0035            W(3)=W4(3)
ISN 0036            IF (IW(3).NE.NP.AND.IW(3).NE.1.AND.IP.NE.1) GO TO 4
ISN 0038            IF (KO(5).EQ.1) CALL HORA
ISN 0040            WRITE(6,60) IW(3),W(4),IW(4),W(3)
ISN 0041            WRITE(6,61) (X(I),I=1,N)
ISN 0042            NP=NP+IP
ISN 0043            IF(IPP.LE.0) GO TO 4
```

```
ISN 0045            WRITE(6,66)
ISN 0046            WRITE(6,61) (F(I),I=1,M)
ISN 0047          4 CALL FITEX(KE,M,N,F4,X4,E4,W4,IW)
ISN 0048            DO 101 I=1,N
ISN 0049            X(I)=X4(I)
ISN 0050        101 CONTINUE
ISN 0051            IF(KE.EQ.1) GO TO 2
ISN 0053            DO 103 I=1,M
ISN 0054            F(I)=F4(I)
ISN 0055        103 CONTINUE
ISN 0056            IF(MC.EQ.1) GOTO 9
ISN 0058            CALL CALFUN(M,N,F,X,P)
ISN 0059            IF (M.LE.0) M=-M
ISN 0061          6 KW=4+N+N+N*N
ISN 0062            DO 104 I=1,KW
ISN 0063            W(I)=W4(I)
ISN 0064        104 CONTINUE
ISN 0065            WRITE(6,60) IW(3),W(4),IW(4),W(3)
ISN 0066            WRITE(6,61) (X(I),I=1,N)
ISN 0067            IF(IPP.LE.0) GO TO 9
ISN 0069            WRITE(6,66)
ISN 0070            WRITE(6,61) (F(I),I=1,M)
ISN 0071            IF(KE*(KE-3).NE.0.OR.W(5).LE.0.) GO TO 9
ISN 0073            WRITE(6,62)
ISN 0074            WRITE(6,61) (W(4+I),I=1,N)
ISN 0075            WRITE(6,63)
ISN 0076            WRITE(6,61) (W(4+N+I),I=1,N)
ISN 0077            WRITE(6,64)
ISN 0078            L=4+N+N
ISN 0079            DO 7 I=1,N
ISN 0080            K=L+1
ISN 0081            L=L+I
ISN 0082          7 WRITE(6,61) (W(J),J=K,L)
ISN 0083          9 WRITE(6,65) KE
ISN 0084         60 FORMAT('0',I4,' ITERATIONS   TOTAL CHISQUARE =',1PE12.5,'   IW(4)
                   1=',I4,'   W(3) =',1PE13.5/' VARIABLES')
ISN 0085         61 FORMAT(' ',1P10E13.5)
ISN 0086         62 FORMAT('0STANDARD ERRORS')
ISN 0087         63 FORMAT('0ERROR ENHANCEMENTS')
ISN 0088         64 FORMAT('0ERROR CORRELATION MATRIX')
ISN 0089         65 FORMAT('0CONVERGENCE WITH ERROR CODE',I2)
ISN 0090         66 FORMAT(' FUNCTIONS')
ISN 0091            RETURN
ISN 0092            END
```

```
ISN 0002            SUBROUTINE ERMOM(II,IU,IO,IU1,IU2,VARM,RCTF,CHI2,RMS)
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            REAL*8 PI/3.1415926535897930/
ISN 0005            REAL*4 WI(1000)
ISN 0006            DIMENSION VARM(30,30),RMS(10),DRS(9)
ISN 0007            COMMON /INPT/KE(42),WI,IN(100)
ISN 0008            FAK=16.D0*RCTF**6*CHI2*2.D0/(PI*PI)
ISN 0009            DS=0.D0
ISN 0010            DO 20 K=IU,IO
ISN 0011            I1=K-IU1
ISN 0012            I2=I1+IU2
ISN 0013            DO 10 J=IU,IO
ISN 0014            J1=J-IU1
ISN 0015            J2=J1+IU2
ISN 0016            DS=DS+VARM(II+I1,II+J1)*(-1.)**(I2+J2)/(I2*J2)**2
ISN 0017         10 CONTINUE
ISN 0018         20 CONTINUE
ISN 0019            DS=DS*FAK
ISN 0020            DS=DS/RMS(4)**2
                 C-----DS=(DELTA J/ J)**2
ISN 0021            DO 100 L=1,9
ISN 0022            LR=L
ISN 0023            IF (L.GE.4) LR=L+1
ISN 0025            LI=L-3
ISN 0026            DS2=0.D0
ISN 0027            DS3=0.D0
ISN 0028            DRS(L)=0.D0
ISN 0029            F2=FAK*RCTF**(LI*2)
ISN 0030            F3=FAK*RCTF**LI
ISN 0031            DO 50 K=IU,IO
ISN 0032            I1=K-IU1
ISN 0033            I2=I1+IU2
ISN 0034            DO 40 J=IU,IO
ISN 0035            J1=J-IU1
ISN 0036            J2=J1+IU2
```

```
ISN 0037            DS2=DS2+VARM(II+I1,II+J1)*(-1.D0)**(I2+J2)*FUN(L,I2,J2,RCTF)
                   1 /(I2*J2)**2
ISN 0038            DS3=DS3+VARM(II+I1,II+J1)*(-1.D0)**(I2+J2)*FUN(L,I2,0,RCTF)
                   1 /(I2*J2)**2
ISN 0039         40 CONTINUE
ISN 0040         50 CONTINUE
ISN 0041            IF (L.EQ.3) GO TO 60
ISN 0043            RMST=RMS(LR)**LI*RMS(4)
ISN 0044            DS2=DS2*F2/RMST**2
ISN 0045            DS3=DS3*F3/RMST*2.D0/RMS(4)
ISN 0046            GO TO 70
ISN 0047         60 RMST=DLOG(RMS(3))*RMS(4)
ISN 0048            DS2=DS2*F2/RMST**2
ISN 0049            DS3=DS3*F3/RMST*2.D0/RMS(4)
                 C-----DS2=(DELTA <J*RL>/<J*RL>)**2
                 C-----DS3=KORRELATIONEN ZWISCHEN J UND RL
                 C-----DRS(L)=(DELTA <RL>/<RL>)**2
ISN 0050         70 DRS(L)=DS+DS2-DS3
ISN 0051            IF(KE(17).NE.0) DRS(L)=DS2
ISN 0053            IF (L.EQ.3) LI=1
ISN 0055            DRS(L)=DSQRT(DRS(L))*RMS(LR)/IABS(LI)
ISN 0056        100 CONTINUE
ISN 0057            DO 200 I=1,3
ISN 0058            RMS(I)=DRS(I)
ISN 0059        200 CONTINUE
ISN 0060            RMS(4)=DSQRT(DS)*RMS(4)
ISN 0061            DO 300 I=5,10
ISN 0062            RMS(I)=DRS(I-1)
ISN 0063        300 CONTINUE
ISN 0064            RETURN
ISN 0065            END
```

```
ISN 0002            FUNCTION FUN(L,I1,J1,RCTF)
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            REAL*8 PI/3.14159265358979300/
ISN 0005            IZ=1
ISN 0006            N=I1
ISN 0007            XNP=N*PI
ISN 0008            IF (N.EQ.0) GO TO 10
ISN 0010            GO TO (1,2,3,4,5,6,7,8,9),L
ISN 0011          1 F=(-1.D0)**(N+1)*PI*N*SI(XNP)
ISN 0012            GO TO (90,100),IZ
ISN 0013          2 F=(-1.D0)**(N+1)+1.D0
ISN 0014            GO TO (90,100),IZ
ISN 0015          3 F=(-1.D0)**(N+1)*PI*N*SI(XNP)
ISN 0016            F=1.D0-F/(PI*N)**2
ISN 0017            GO TO (90,100),IZ
ISN 0018          4 F=(-1.D0)**(N+1)+1.D0
ISN 0019            F=-F*2.D0/((PI*N)**2)+1.D0
ISN 0020            GO TO (90,100),IZ
ISN 0021          5 F=(PI*N)**2
ISN 0022            F=1.D0-6.D0/F
ISN 0023            GO TO (90,100),IZ
ISN 0024          6 F=(-1.D0)**(N+1)+1.D0
ISN 0025            F=-F*2.D0/((PI*N)**2)+1.D0
ISN 0026            F=-F*12.D0/((PI*N)**2)+1.D0
ISN 0027            GO TO (90,100),IZ
ISN 0028          7 F=(PI*N)**2
ISN 0029            F=1.D0-6.D0/F
ISN 0030            F=-F*20.D0/((PI*N)**2)+1.D0
ISN 0031            GO TO (90,100),IZ
ISN 0032          8 F=(-1.D0)**(N+1)+1.D0
ISN 0033            F=-F*2.D0/((PI*N)**2)+1.D0
ISN 0034            F=-F*12.D0/((PI*N)**2)+1.D0
ISN 0035            F=-F*30.D0/((PI*N)**2)+1.D0
```

```
ISN 0036            GO TO (90,100),IZ
ISN 0037          9 F=(PI*N)**2
ISN 0038            F=1.D0-6.D0/F
ISN 0039            F=-F*20.D0/((PI*N)**2)+1.D0
ISN 0040            F=-F*42.D0/((PI*N)**2)+1.D0
ISN 0041            GO TO (90,100),IZ
ISN 0042         10 F=1.D0
ISN 0043         90 IZ=2
ISN 0044            N=J1
ISN 0045            XNP=N*PI
ISN 0046            FUN=F
ISN 0047            IF (N.EQ.0) RETURN
ISN 0049            GO TO (1,2,3,4,5,6,7,8,9),L
ISN 0050        100 FUN=FUN*F
ISN 0051            RETURN
ISN 0052            END
```

MODINA

CONSTR, DUMMY ROUTINE to be added if other models than POGYNAFB are used

```
ISN 0002            SUBROUTINE CONSTR(M,N,F,X,P,W4)
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            REAL*4 W4(2)
ISN 0005            DIMENSION P(2),F(2),X(2)
ISN 0006            RETURN
ISN 0007            END
```

MODINA

BLOCK OF FIT-ROUTINES, to be added

```
C-----------------------------------------------------------------------
C
C                                                          U R V E R S I O N
C
C  PROGRAMM BESCHREIBUNG NR. 320 VON G. W. SCHWEIMER
C  LINEAR LEAST SQUARES PROBLEM ||B-A*X||=MIN(X)
C  SOLVED BY HOUSEHOLDER TRANSFORMATIONS
C  REDUNDANT VARIABLES ARE DETECTED BY THE METHOD OF G.GOLUB, NUMERISCHE
C  MATHEMATIK, VOL. 7, PAGE 206-216, (1965)
C  INPUT VARIABLES:M: NUMBER OF ROWS OF A AND B
C                  N: NUMBER OF COLUMNS OF A AND ROWS OF X
C                  A: M*N MATRIX (DESTROYED)
C                  B: VECTOR OF M COMPONENTS (DESTROYED)
C  OUTPUT VARIABLES: X: VECTOR OF VARIABLES, THE REDUNDANT VARIABLES ARE
C                     SET TO ZERO. THE ||X||=MIN IS NOT USED BECAUSE THE
C                     COMPONENTS OF X ARE ASSUMED TO BE NOT COMMENSURABLE
C                  IP: PERMUTATION VECTOR OF N COMPONENTS, IT CONTAINS
C                     THE COLUMN LABLES OF MATRIX A ORDERED ACCORDING
C                     THEIR IMPORTANCE IN REDUCING THE EUCLIDEAN NORM
C                  A: THE UPPER PART CONTAINS THE TRANSFORMED INPUT A
C                     A(2,1) CONTAINS THE SQUARE OF THE EUCLIDEAN NORM
C                  B: TRANSFORMED INPUT B
C                  IER: ERROR CODE
C                     IER=0 NO ERROR
C                     IER=-1 ALL COMPONENTS OF X ARE ZERO AND MAY BE
C                     REDUNDANT
C                     IER=-2 NO ACTION BECAUSE M < N OR N < 1
C                     IER>0 THE FIRST IER COMPONENTS OF IP CONTAIN THE
C                     LABELS OF THE NONZERO COMPONENTS OF X, THE REMAIN-
C                     ING COMPONENTS OF X ARE ZERO AND MAY BE REDUNDANT
C  NOTE: ALL ARITHMETIC OPERATIONS ARE PERFORMED IN DOUBLE PRECISION,
C  AN ITERATIVE IMPROVEMENT IS IMPOSSIBLE WITHOUT SAVING A AND B.
C  THE ROUND OFF ERROR OF ||B-A*X||**2 IS APPROXIMATLY GIVEN BY
C  ||B(INITIAL)||**2 - ||B(TRANFORMED)||**2
C***********************************************************************
```

```
ISN 0002            SUBROUTINE LILESQ(M,N,IER,A,B,X,VP)
ISN 0003            DIMENSION A(M,N),B(M),X(N),VP(N)
ISN 0004            DOUBLE PRECISION S,T,U,V,W,DELTA,SIG
ISN 0005            IER=0
ISN 0006            IF(M.LT.N.OR.N.LT.1) GO TO 19
ISN 0008            DO 1 J=1,N
ISN 0009          1 VP(J)=J
                  C  ROTATION LOOP
ISN 0010            DO 10 K=1,N
                  C  PIVOT ELEMENT
ISN 0011            U=0.D0
ISN 0012            DO 4 J=K,N
ISN 0013            C=0.
ISN 0014            DO 2 I=K,M
ISN 0015            IF(ABS(A(I,J)).LE.ABS(C)) GO TO 2
ISN 0017            L2=I
ISN 0018            C=A(I,J)
ISN 0019          2 CONTINUE
ISN 0020            IF(C.EQ.0.) GO TO 4
ISN 0022            S=0.D0
ISN 0023            T=0.D0
ISN 0024            DO 3 I=K,M
ISN 0025            V=DBLE(A(I,J))/DBLE(C)
ISN 0026            S=S+V*V
ISN 0027          3 T=T+V*DBLE(B(I))
ISN 0028            IF(U.GE.T*(T/S)) GO TO 4
ISN 0030            U=T*(T/S)
ISN 0031            SIG=DBLE(C)*DSQRT(S)
ISN 0032            W=T
ISN 0033            L=J
ISN 0034            L1=L2
ISN 0035          4 CONTINUE
ISN 0036            IF(U.EQ.0.D0) GO TO 11
                  C  PERMUTE A(K) AND B(K)
ISN 0038            I=VP(L)
ISN 0039            VP(L)=VP(K)
ISN 0040            VP(K)=I
```

```
ISN 0041            DO 5 I=1,M
ISN 0042            C=A(I,L)
ISN 0043            A(I,L)=A(I,K)
ISN 0044          5 A(I,K)=C
ISN 0045            C=B(K)
ISN 0046            B(K)=B(L1)
ISN 0047            B(L1)=C
ISN 0048            DO 22 J=K,N
ISN 0049            C=A(K,J)
ISN 0050            A(K,J)=A(L1,J)
ISN 0051         22 A(L1,J)=C
                 C  ROTATION OF THE LOWER COLUMN FRAGMENT OF A(K) AND B(K)
ISN 0052            U=SIG+DBLE(A(K,K))
ISN 0053            V=DBLE(A(K,K))/SIG
ISN 0054            DELTA=(DBLE(B(K))+V*W)/U
ISN 0055            A(K,K)=-SIG
ISN 0056            B(K)=-V*W
ISN 0057            L=K+1
ISN 0058            IF(L.GT.M) GO TO 10
ISN 0060            IF(K.GE.N) GO TO 8
ISN 0062            DO 7 J=L,N
ISN 0063            S=V*DBLE(A(K,J))
ISN 0064            DO 6 I=L,M
ISN 0065            T=DBLE(A(I,K))/SIG
ISN 0066          6 S=S+T*DBLE(A(I,J))
ISN 0067            T=(DBLE(A(K,J))+S)/U
ISN 0068            A(K,J)=-S
ISN 0069            DO 7 I=L,M
ISN 0070          7 A(I,J)=DBLE(A(I,J))-T*DBLE(A(I,K))
ISN 0071          8 DO 9 I=L,M
ISN 0072          9 B(I)=DBLE(B(I))-DELTA*DBLE(A(I,K))
ISN 0073         10 CONTINUE
                 C  END OF ROTATION LOOP
ISN 0074            K=N
ISN 0075            GO TO 12
ISN 0076         11 K=K-1
ISN 0077            IER=K
                 C  SQUARE OF THE EUCLIDEAN NORM
ISN 0078         12 S=0.DO
ISN 0079            L=K+1
```

```
ISN 0080            IF(K.EQ.M) GO TO 14
ISN 0082            DO 13 I=L,M
ISN 0083         13 S=S+DBLE(B(I))*DBLE(B(I))
ISN 0084         14 A(2,1)=S
ISN 0085            IF(K.EQ.N) GO TO 16
                 C  COMPONENTS OF X WHICH DO NOT REDUCE THE EUCLIDEAN NORM
ISN 0087            DO 15 I=L,N
ISN 0088            DO 15 J=L,N
ISN 0089            IP=VP(J)
ISN 0090            X(IP)=0.
ISN 0091         15 CONTINUE
ISN 0092            IF(K.EQ.0) GO TO 20
                 C  COMPUTATION OF X
ISN 0094         16 CONTINUE
ISN 0095            IP=VP(K)
ISN 0096            X(IP)=DBLE(B(K))/DBLE(A(K,K))
ISN 0097            IF(K.EQ.1) GO TO 21
ISN 0099            DO 18 J=2,K
ISN 0100            L=K+2-J
ISN 0101            S=B(L-1)
ISN 0102            DO 17 I=L,K
ISN 0103            IP=VP(I)
ISN 0104         17 S=S-DBLE(A(L-1,I))*DBLE(X(IP))
ISN 0105            IP=VP(L-1)
ISN 0106            X(IP)=S/DBLE(A(L-1,L-1))
ISN 0107         18 CONTINUE
ISN 0108            GO TO 21
                 C  ERROR CODE
ISN 0109         19 IER=IER-1
ISN 0110         20 IER=IER-1
ISN 0111         21 RETURN
ISN 0112            END
```

```
C  PROGRAMM BESCHREIBUNG NR. 320 VON G. W. SCHWEIMER
C*********************************************************************
C  INVERSION OF THE PRODUCT MATRIX A(TRANSPOSED)*A
C  THE MATRIX A IS REDUCED TO AN UPPER TRIANGULAR MATRIX R BY
C  HOUSEHOLDER TRANSFORMATIONS. THE REMAINING COMPUTATION IS STRAIGHT
C  FORWARD.
C  INPUT VARIABLES: N: NUMBER OF COLUMNS OF MATRIX A
C                   M: NUMBER OF ROWS OF MATRIX A, M >= N > 0
C                   A: INPUT MATRIX (DESTROYED)
C  OUTPUT VARIABLES: IR: ERROR CODE
C                     IR=-2: M LT N OR N LT 1
C                     IR=-1 RANK OF MATRIX A IS ZERO
C                     IR=0 NO ERROR, RANK OF MATRIX A IS N
C                     IR>0 RANK OF MATRIX A IS IR, THE INVERSE OF A(T)*A
C                     IS COMPUTED CONSIDERING THE IR COLUMNS OF A INDICA-
C                     TED BY THE FIRST IR COMPONENTS OF IP
C                   A: TRIANGULAR MATRIX R, R=A(I,J) I<=J=1,N
C                   D: VECTOR OF LENGTH (N*(N+1))/2, IT CONTAINS THE
C                     UPPER TRIANGULAR PART OF THE INVERSE OF A(T)*A
C                   IP: PERMUTATION VECTOR OF LENGTH N, ITS FIRST IR
C                     COMPONENTS CONTAIN THE LABELS OF THE USEFULL
C                     COLUMNS OF A, THE LAST COMPONENTS CONTAIN THE
C                     LABELS OF THE COLUMNS WHICH ARE LINEAR CONBINATIONS
C                     OF THE FIRST.
C*********************************************************************
ISN 0002        SUBROUTINE INVATA(M,N,IR,A,D,VP)
ISN 0003        DIMENSION A(M,N),D(1),VP(N)
ISN 0004        DOUBLE PRECISION SIG,S,T,U,V
ISN 0005        IR=N
ISN 0006        IF(M.LT.N.OR.N.LT.1) GO TO 19
ISN 0008        DO 1 I=1,IR
ISN 0009      1 VP(I)=I
C  HOUSEHOLDER LOOP
ISN 0010        K=0
ISN 0011      2 K=K+1
C  PIVOT ELEMENT
ISN 0012      3 C=0.
ISN 0013        DO 4 I=K,M
ISN 0014        IF(ABS(A(I,K)).LE.C) GO TO 4
ISN 0016        C=ABS(A(I,K))
ISN 0017        I1=I
```

```
ISN 0018          4 CONTINUE
ISN 0019            IF(C.GT.0.) GO TO 8
ISN 0021            IR=IR-1
ISN 0022            IF(K.GT.IR) GO TO 13
                C  SET UP THE PERMUTATION VECTOR IP AND PERMUTE THE COLUMNS OF MATRIX A
ISN 0024            L=VP(K)
ISN 0025            DO 5 J=K,IR
ISN 0026          5 VP(J)=VP(J+1)
ISN 0027            VP(IR+1)=L
ISN 0028            DO 7 I=1,M
ISN 0029            C=A(I,K)
ISN 0030            DO 6 J=K,IR
ISN 0031          6 A(I,J)=A(I,J+1)
ISN 0032          7 A(I,IR+1)=C
ISN 0033            GO TO 3
                C  ROTATION OF THE LOWER COLUMN FRAGMENTS OF A(K)
ISN 0034          8 DO 9 J=K,IR
ISN 0035            C=A(K,J)
ISN 0036            A(K,J)=A(I1,J)
ISN 0037          9 A(I1,J)=C
ISN 0038            S=A(K,K)
ISN 0039            V=0.D0
ISN 0040            DO 10 I=K,M
ISN 0041            U=DBLE(A(I,K))/S
ISN 0042         10 V=V+U*U
ISN 0043            V=1.D0/DSQRT(V)
ISN 0044            SIG=S/V
ISN 0045            U=S+SIG
ISN 0046            A(K,K)=-SIG
ISN 0047            IF(K.GE.IR) GO TO 13
ISN 0049            L=K+1
ISN 0050            DO 12 J=L,IR
ISN 0051            S=V*DBLE(A(K,J))
ISN 0052            DO 11 I=L,M
ISN 0053         11 S=S+(DBLE(A(I,K))/SIG)*DBLE(A(I,J))
ISN 0054            T=(DBLE(A(K,J))+S)/U
ISN 0055            A(K,J)=-S
ISN 0056            DO 12 I=L,M
```

```
ISN 0057          12 A(I,J)=DBLE(A(I,J))-T*DBLE(A(I,K))
ISN 0058             GO TO 2
                  C  END OF HOUSEHOLDER LOOP
ISN 0059          13 IF(IR.EQ.0) GO TO 20
                  C  INVERSE OF THE TRIANGULAR MATRIX R STORED IN D
ISN 0061             IJ=0
ISN 0062             DO 16 K=1,IR
ISN 0063             D(IJ+K)=1./A(K,K)
ISN 0064             IF(K.EQ.1) GO TO 16
ISN 0066             I=K
ISN 0067             DO 15 L=2,K
ISN 0068             I1=I
ISN 0069             I=I-1
ISN 0070             S=0.DO
ISN 0071             DO 14 J=I1,K
ISN 0072          14 S=S+DBLE(A(I,J))*DBLE(D(IJ+J))
ISN 0073          15 D(IJ+I)=-S/DBLE(A(I,I))
ISN 0074          16 IJ=IJ+K
                  C  INVERSE OF THE PRODUCT MATRIX
ISN 0075             IJ=0
ISN 0076             DO 18 J=1,IR
ISN 0077             DO 18 I=1,J
ISN 0078             IJ=IJ+1
ISN 0079             I1=IJ
ISN 0080             L=J-I
ISN 0081             S=0.DO
ISN 0082             DO 17 K=J,IR
ISN 0083             S=S+DBLE(D(I1))*DBLE(D(I1+L))
ISN 0084          17 I1=I1+K
ISN 0085          18 D(IJ)=S
ISN 0086             GO TO 20
ISN 0087          19 IR=-2
ISN 0088          20 IF(IR.EQ.0) IR=-1
ISN 0090             IF(IR.EQ.N) IR=0
ISN 0092             RETURN
ISN 0093             END
```

```
C  PROGRAMM BESCHREIBUNG NR. 309 VON G. W. SCHWEIMER
C*******************************************************************
C  MINIMISATION OF A FUNCTION F(X) OF ONE VARIABLE X
C  CALLING SEQUENCE
C     KE=0
C     I(2)=MAXIMUM NUMBER OF FUNCTION EVALUATIONS
C     W(1)=START VALUE OF X
C     W(3)=FIRST STEP SIZE
C     W(4)=ABSOLUTE SEARCH ACCURACY
C     W(5)=RELATIVE SEARCH ACCURACY
C   1 W(2)=FUNCTION VALUE F(X) AT X=W(1)
C     OPTIONAL WRITE I(1),X,F
C     CALL FIT1(KE,I,W)
C     IF(KE.EQ.1) GO TO 1
C     XMIN=W(1)
C     FMIN=W(2)
C     NF=I(1)
C  KE = ERROR CODE: KE=0 NO ERRORS, KE=
C    2 MAXIMUM NUMBER OF FUNCTION EVALUATIONS
C    3 ROUNDING ERRORS, PROBABLY BECAUSE BOTH W(4) AND W(5) ARE TOO SMALL
C  THE WORKING FIELDS I AND W HAVE THE LENGTH 3 AND 11 RESPECTIVELY
C  THEY CONTAIN ALL INFORMATION FOR THE CONTINUATION OF THE SEARCH
C  THEREFORE A SEARCH WITHIN ANOTHER SEARCH CAN BE DONE JUST CHANGING
C  THE WORKING FIELDS
C  IF 2 FUNCTION VALUES F1 AND F2 ARE KNOWN FOR X = X1 AND X2 RESPECTIVE
C  LY WITH X1 NE X2 ENTER THE CALLING SEQUENCE AFTER DEFINING :
C  KE = 1; I(1) = 3; W(6) = X1; W(7) = X2; W(9) = F1; W(10) = F2 AND
C  W(1) = USERS CHOICE
C  WORKING FIELD VARIABLES:
C  I(1): CURRENT NUMBER OF FUNCTION EVALUATIONS
C  I(2): MAXIMUM NUMBER OF FUNCTION EVALUATIONS
C  I(3): MINIMUM POINTER, THE MINIMUM FUNCTION VALUE IS AT W(7+I(3))
C  W(1): CURRENT VALUE OF X
C  W(2): USER SUPPLIED FUNCTION VALUE
C  W(3): FIRST STEP SIZE
C  W(4 AND 5): SEARCH ACCURACIES
C  W(6, 7 AND 8): X1, X2 AND X3 WITH X1 < X2 < X3
C  W(9, 10 AND 11): FUNCTION VALUES AT X1, X2 AND X3 RESPECTIVELY
C*******************************************************************
```

```
ISN 0002            SUBROUTINE FIT1(KE,V,W)
ISN 0003            DIMENSION V(3),W(11)
ISN 0004            IF(KE.EQ.1) GO TO 2
ISN 0006            KE=1
ISN 0007            V(1)=1
ISN 0008            V(3)=-1
ISN 0009            W(6)=W(1)
ISN 0010            W(9)=W(2)
ISN 0011          1 W(1)=W(1)+W(3)
ISN 0012            GO TO 12
ISN 0013          2 IF(V(1).GT.2.) GO TO 3
ISN 0015            V(3)=0.
ISN 0016            W(7)=W(1)
ISN 0017            W(10)=W(2)
ISN 0018            IF(W(2).LE.W(9)) GO TO 1
ISN 0020            V(3)=-1.
ISN 0021            W(1)=W(6)-W(3)
ISN 0022            GO TO 12
ISN 0023          3 IF(V(1).GT.3.) GO TO 5
ISN 0025            W(8)=W(1)
ISN 0026            W(11)=W(2)
                C   ORDERING OF THE 3 FIRST VALUES OF X: W(6) < W(7) < W(8)
ISN 0027            DO 4 J=1,3
ISN 0028            K=7-MOD(J,2)
ISN 0029            IF(W(K).LE.W(K+1)) GO TO 4
ISN 0031            W(1)=W(K)
ISN 0032            W(K)=W(K+1)
ISN 0033            W(K+1)=W(1)
ISN 0034            K=K+3
ISN 0035            W(1)=W(K)
ISN 0036            W(K)=W(K+1)
ISN 0037            W(K+1)=W(1)
ISN 0038          4 CONTINUE
ISN 0039            V(3)=0.
ISN 0040            IF(W(9).LT.W(10).AND.W(9).LT.W(11)) V(3)=-1.
ISN 0042            IF(W(11).LT.W(10).AND.W(11).LT.W(9)) V(3)=1.
ISN 0044            GO TO 9
```

```
                C  SORT IN THE NEW VALUES OF X AND F
ISN 0045            5 IF(V(3).EQ.0.) GO TO 6
ISN 0047              J=V(3)
ISN 0048              W(7-J)=W(7)
ISN 0049              W(10-J)=W(10)
ISN 0050              IF((W(7+J)-W(1))*(W(1)-W(7)).GT.0.) GO TO 7
ISN 0052              W(7)=W(7+J)
ISN 0053              W(10)=W(10+J)
ISN 0054              W(7+J)=W(1)
ISN 0055              W(10+J)=W(2)
ISN 0056              IF(W(2).GE.W(10)) V(3)=0.
ISN 0058              GO TO 9
ISN 0059            6 J=-1
ISN 0060              IF(W(1).LT.W(7)) J=1
ISN 0062              IF(W(2).GT.W(10)) GO TO 8
ISN 0064              W(7+J)=W(7)
ISN 0065              W(10+J)=W(10)
ISN 0066            7 W(7)=W(1)
ISN 0067              W(10)=W(2)
ISN 0068              IV=V(3)
ISN 0069              IF(W(2).LE.W(10+IV)) V(3)=0.
ISN 0071              GO TO 9
ISN 0072            8 W(7-J)=W(1)
ISN 0073              W(10-J)=W(2)
ISN 0074            9 IV=V(3)
ISN 0075              J=7+IV
                C  ERROR TESTS
ISN 0076              IF(W(6).EQ.W(7).OR.W(7).EQ.W(9).OR.(W(9).EQ.W(10).AND.W(10).EQ.W(1
                     11))) GO TO 15
ISN 0078              IF(V(1).GE.V(2)) GO TO 16
ISN 0080              IF (V(3).EQ.0.) GOTO 10
                C  STEP SIZE LIMITATION
ISN 0082              W(1)=W(J)+2.*V(3)*(W(8)-W(6))
ISN 0083              GOTO 12
ISN 0084           10 W(1)=AMIN1(W(8)-W(7),W(7)-W(6))/(W(8)-W(6))
ISN 0085              IF(W(1).GT.0.1) GOTO 11
ISN 0087              W(1)=.5*(W(6)+W(8))
ISN 0088              GOTO 12
```

```
C  PREDICTION OF THE POSITION OF THE MINIMUM
ISN 0089      11 W(1)=((W(9)-W(10))/(W(6)-W(7))-(W(10)-W(11))/(W(7)-W(8)))/(W(6)-
                1W(8))
ISN 0090         W(1)=.5*(W(6)+W(8)+(W(11)-W(9))/(W(1)*(W(6)-W(8))))
C  TEST OF CONVERGENCE
ISN 0091         W(2)=ABS(W(1)-W(J))
ISN 0092         IF(W(2).LT.ABS(W(4)).OR.W(2).LT.ABS(W(5)*W(J))) GO TO 13
ISN 0094      12 V(1)=V(1)+1.
ISN 0095         RETURN
ISN 0096      13 KE=0
ISN 0097      14 IV=V(3)
ISN 0098         W(1)=W(7+IV)
ISN 0099         W(2)=W(10+IV)
ISN 0100         RETURN
ISN 0101      15 KE=KE+1
ISN 0102      16 KE=KE+1
ISN 0103         GO TO 14
ISN 0104         END
```



```
C*********************************************************************
C  PROGRAMM BESCHREIBUNG NR. 320 VON G. W. SCHWEIMER
C*********************************************************************
C  CHISQUARE MINIMISING SUBROUTINE
C  SOLVES THE NONLINEAR LEAST SQUARES PROBLEM
C  USING A LEAST SQUARES INTERPOLATION BETWEEN VARIABLES AND FUNCTIONS
C  OR THE EXACT GRADIENT OF THE FUNCTIONS
C  CALLED SUBROUTINES: LILESQ(LINEAR LEAST SQUARES PROBLEM)
C                      INVATA(INVERSION OF A(TRANSPOSED)*A)
C                      FIT1(ONE DIMENSIONAL MINIMUM SEARCH)
C  CALLING SEQUENCE
C     KE=0
C     M=NUMBER OF FUNCTIONS, M GE N
C     N=NUMBER OF VARIABLES, N GE 1
```

```
C      DO 1 I=1,N
C      X(I)=STARTING VALUES OF THE VARIABLES
C    1 E(I)=ABSOLUTE SEARCH ACCURACIES FOR THE VARIABLES, E(I) NE 0
C      W(1)=FIRST STEP SIZE IN UNITS OF E(I), IF LE 1 W(1) = 100 BY FITEX
C           THE MAXIMUM ALLOWED STEP SIZE IS 2*W(1)
C      W(2)=METHOD OF APPROXIMATION, 0 FOR LEAST SQUARES INTERPOLATION
C                                    1 FOR EXACT GRADIENT OF THE FUNCTIONS
C      IW(1)=NUMBER OF POINTS TO BE REMEMBERED, IF LE N IW(1) = N+1
C      IW(2)=MAXIMUM NUMBER OF FUNCTION EVALUATIONS, IF EQ 0 IW(2)=2IW(1)
C            IF IW(2) LT 0 NO ACTION EXCEPT KE = 0
C      JA=4+MAX0(14,(N*(N+5))/2)+(M+N+1)*(IW(1)+1)
C    2 W(4)=0.
C      DO 3 I=1,M
C      F(I)=FUNCTION VALUES AT THE POINT X
C      IF(W(2).EQ.0.) GO TO 3
C      W(JA+I+M*(J-1))= DF(I)/DX(J) FOR J=1,N
C    3 W(4)=W(4)+F(I)*F(I)
C      OPTIONAL WRITE IW(3),IW(4),W(3),W(4),X,F
C      CALL FITEX(KE,M,N,F,X,E,W,IW)
C      IF(KE.EQ.1) GO TO 2
C      W(3)=ERROR RENORMALISATION FACTOR
C      W(4)=MINIMUM QUADRATIC SUM OF THE F(I)
C      X=MINIMUM POINT
C      F=FUNCTIONS AT THE MINIMUM POINT
C      KE=ERROR CODE     KE=0: WITHOUT ERRORS
C                        KE=2: USER INTERRUPT
C                        KE=3: MAXIMUM NUMBER OF FUNCTION EVALUATIONS
C                        KE=4: ROUNDING ERRORS
C                        KE=5: THE FUNCTIONS DO NOT DEPENT ON X(IW(4))
C                        KE=6: USELESS VARIABLES IN THE PREPARATORY CALLS,
C                              THE LABELS OF THE VARIABLES ARE IW(3),IW(4)
C                        KE=7: M LT N OR N LT 0 OR W(2)*(W(2)-1.) NE 0
C      W(4+I)=STANDARD ERRORS OF THE VARIABLES
C      W(4+N+I)=ERROR ENHANCEMENTS
C      W(4+N+N+I+(J*(J-1))/2)=ERROR CORRELATION BETWEEN X(I) AND X(J) I<J
C      IW(3): NUMBER OF FUNCTION EVALUATIONS
C      IW(4): NUMBER OF DEGREES OF FREEDOM
```

```
C  WORKING FIELD:  IW: LENGTH 4+K WITH K = IW(1)
C     W: LENGTH 4+MAX(14,(N*(N+5))/2)+(M+N+1)*(K+1)+M*N
C                    ADRESSES IN IW
C                        4+L: LABELS OF THE QUADRATIC SUMS
C                    ADRESSES IN W
C                        4+I: STANDARD ERROR OF X(I)
C                        4+N+I: ERROR ENHANCEMENT FOR X(I)
C                        FROM 4+N+N+1: MATRIX D AND ERROR CORRELATIONS
C                        FROM JS+1 MATRIX S; JS = 4+MAXO(14,(N*(N+5))/2)
C                        FROM JA+1: MATRIX A WITH JA = JS+(M+N+1)*(K+1)
C  THE WORKING FIELDS CONTAIN ALL INFORMATION FOR THE CONTINUATION OF
C  THE SEARCH. THIS ALLOWS A SEARCH WITHIN ANOTHER SEARCH JUST CHANGING
C  THE WORKING FIELDS
C*********************************************************************
ISN 0002        SUBROUTINE FITEX(KE,M,N,IW,F,X,E,W)
ISN 0003        DIMENSION F(M),X(N),E(N),W(1),IW(1)
ISN 0004        DOUBLE PRECISION S,T,U,V,EPS/1.D-5/
ISN 0005        EQUIVALENCE(A,IR)
ISN 0006        IF(IW(2).LT.0) GO TO 50
ISN 0008        JD=4+N+N
ISN 0009        JS=4+MAXO(14,(N*(N+5))/2)
ISN 0010        LM=M+N+1
ISN 0011        IF(KE.NE.0) GO TO 2
ISN 0013        IF(IW(1).LE.N) IW(1)=N+1
ISN 0015        IF(IW(2).EQ.0) IW(2)=2*IW(1)
ISN 0017        IF(W(1).LE.1.) W(1)=100.
ISN 0019        IW(3)=1
ISN 0020        K=IW(1)
ISN 0021        DO 1 L=1,K
ISN 0022        IW(L+4)=1+K-L
ISN 0023      1 W(JS+LM*L)=7.E75
ISN 0024        KE=1
ISN 0025      2 K=IW(1)
ISN 0026        KV=K
ISN 0027        JA=JS+LM*(K+1)
ISN 0028        JM=JS+LM*IW(5)-LM
ISN 0029        J3=JA-LM
ISN 0030        IF(KE.EQ.2) GO TO 52
ISN 0032        IF(M.LT.N.OR.N.LT.1.OR.W(2)*(W(2)-1.).NE.0.) GO TO 57
ISN 0034        IF(W(4).LE.0.) GO TO 50
```

```
                C  ROW OF MATRIX S TO BE REPLACED BY NEW VALUES
ISN 0036            L=IW(K+4)
ISN 0037            IF(W(JS+LM*L).EQ.7.E75) KV=L-1
ISN 0039            DO 3 I=1,K
ISN 0040            J1=JS+LM*IW(I+4)
ISN 0041            IF(W(4).LT.W(J1)) GO TO 4
ISN 0043          3 CONTINUE
                C  ONE DIMENSIONAL SEARCH IS NECESSARY
ISN 0044            GO TO 37
ISN 0045          4 IF((W(2).EQ.0..AND.I.GT.MAXO(N+1,KV)).OR.(W(2).EQ.1..AND.I.GT.1))
                   1 GO TO 37
                C  VECTOR OF LABELS OF THE QUADRATIC SUMS
ISN 0047            IF(KV.LT.K) KV=KV+1
ISN 0049            I1=K+4
ISN 0050            I2=K-I
ISN 0051            IF(I2.EQ.0) GO TO 6
ISN 0053            DO 5 J=1,I2
ISN 0054            I1=I1-1
ISN 0055          5 IW(I1+1)=IW(I1)
ISN 0056            IW(I1)=L
ISN 0057            JM=JS+LM*IW(5)-LM
                C  NEW ROW
ISN 0058          6 J1=JS+LM*(L-1)
ISN 0059            DO 7 I=1,N
ISN 0060            J1=J1+1
ISN 0061          7 W(J1)=X(I)
ISN 0062            DO 8 I=1,M
ISN 0063            J1=J1+1
ISN 0064          8 W(J1)=F(I)
ISN 0065            W(J1+1)=W(4)
ISN 0066            IF(IW(3).GE.IW(2)) GO TO 53
ISN 0068            IF(N.EQ.1) GO TO 42
ISN 0070            IF(W(2).EQ.1..OR.IW(3).GT.N+1) GO TO 15
```

```
                C  PREPARATORY FUNCTION EVALUATIONS
ISN 0072            MF=IW(3)
ISN 0073            IF(MF.EQ.1) GO TO 12
ISN 0075            X(MF-1)=W(3)
ISN 0076            J2=JS+N
ISN 0077            S=0.D0
ISN 0078            DO 9 I=1,M
ISN 0079            T=F(I)-W(J2+I)
ISN 0080          9 S=S+T*T
ISN 0081            J=2
ISN 0082            IF(S.LT.EPS*EPS*W(JS+LM)) GO TO 55
ISN 0084            W(3)=S
ISN 0085            J1=2+N+MF
ISN 0086            W(J1)=SQRT(W(3))
ISN 0087            IF(MF.LE.2) GO TO 12
ISN 0089            I1=N+1
ISN 0090            DO 11 J=3,MF
ISN 0091            I2=J2+LM*(J-2)
ISN 0092            S=0.D0
ISN 0093            DO 10 I=1,M
ISN 0094         10 S=S+(W(I2+I)-W(J2+I))*(F(I)-W(J2+I))
ISN 0095            IF(DABS(W(J1)*W(I1+J)-DABS(S)).LT.EPS*DABS(S)) GO TO 56
ISN 0097         11 CONTINUE
ISN 0098         12 IF(MF.EQ.N+1) GO TO 15
ISN 0100            W(3)=X(MF)
ISN 0101            X(MF)=X(MF)+W(1)*E(MF)
ISN 0102            GO TO 100
                C  END OF PREPARATORY FUNCTION EVALUATIONS
                C  SUM OF INVERSES OF THE QUADRATIC SUMS
ISN 0103         15 S=0.D0
ISN 0104            DO 16 L=1,KV
ISN 0105            T=W(JS+LM*L)
ISN 0106         16 S=S+1.D0/(T*T)
ISN 0107            W(JA)=1.D0/S
```

```
                C  CENTRE OF THE VARIABLES AND FUNCTIONS
ISN 0108            I1=M+N
ISN 0109            DO 18 I=1,I1
ISN 0110            J1=JS
ISN 0111            S=0.D0
ISN 0112            DO 17 L=1,KV
ISN 0113            T=W(J1+LM)
ISN 0114            S=S+W(J1+I)/(T*T)
ISN 0115         17 J1=J1+LM
ISN 0116         18 W(J3+I)=S*W(JA)
ISN 0117            IF(KE.NE.1) GO TO 60
ISN 0119            IF(W(2).EQ.0.) GO TO 20
ISN 0121            J1=JA-M-1
ISN 0122            DO 19 I=1,M
ISN 0123         19 W(J1+I)=F(I)
ISN 0124            GO TO 23
                C  MATRIX A
ISN 0125         20 J1=JA
ISN 0126            DO 22 I=1,N
ISN 0127            U=W(J3+I)
ISN 0128            DO 22 J=1,M
ISN 0129            J1=J1+1
ISN 0130            J2=JS
ISN 0131            S=0.D0
ISN 0132            T=W(J3+N+J)
ISN 0133            DO 21 L=1,KV
ISN 0134            V=W(J2+LM)
ISN 0135            S=S+(W(J2+N+J)-T)*(W(J2+I)-U)/(V*V)
ISN 0136         21 J2=J2+LM
ISN 0137         22 W(J1)=S*W(JA)
ISN 0138            IF(KE.NE.1) GO TO 62
                C  LINEAR LEAST SQUARES PROBLEM
ISN 0140         23 CALL LILESQ(M,N,IR,W(JA+1),W(JA-M),W(5),W(N+5))
ISN 0141            IF(IR) 54,24,35
```

```
                C  MATRIX D
ISN 0142           24 J1=JD
ISN 0143              DO 26 I=1,N
ISN 0144              T=W(J3+I)
ISN 0145              DO 26 J=1,I
ISN 0146              J1=J1+1
ISN 0147              J2=JS
ISN 0148              S=0.D0
ISN 0149              U=W(J3+J)
ISN 0150              DO 25 L=1,KV
ISN 0151              V=W(J2+LM)
ISN 0152              S=S+(W(J2+I)-T)*(W(J2+J)-U)/(V*V)
ISN 0153           25 J2=J2+LM
ISN 0154           26 W(J1)=S*W(JA)
                C  NEW VARIABLES
ISN 0155              IF(W(2).EQ.0.) GO TO 28
ISN 0157              DO 27 I=1,N
ISN 0158           27 X(I)=W(JM+I)-W(I+4)
ISN 0159              GO TO 31
ISN 0160           28 DO 30 I=1,N
ISN 0161              I2=1
ISN 0162              J1=JD+(I*I-I)/2
ISN 0163              S=0.D0
ISN 0164              DO 29 J=1,N
ISN 0165              J1=J1+I2
ISN 0166              IF(J.GE.I) I2=J
ISN 0168           29 S=S+W(J1)*W(J+4)
ISN 0169           30 X(I)=W(J3+I)-S
                C  TEST OF CONVERGENCE
ISN 0170           31 A=0.
ISN 0171              DO 32 I=1,N
ISN 0172              W(I+4)=X(I)-W(JM+I)
ISN 0173           32 A=AMAX1(A,ABS(W(I+4)/E(I)))
ISN 0174              IF(A.LT.1.) GO TO 50
ISN 0176              IW(4)=0
ISN 0177              W(3)=1.
ISN 0178              IF(A.LT.2.*W(1)) GO TO 33
```

```
                C  STEP SIZE LIMITATION
ISN 0180            IW(4)=1
ISN 0181            W(3)=2.*W(1)/A
ISN 0182         33 DO 34 I=1,N
ISN 0183         34 X(I)=W(JM+I)+W(3)*W(I+4)
ISN 0184            GO TO 100
                C  RANDOM PREDICTION
ISN 0185         35 DO 36 I=1,N
ISN 0186            A=W(J3+I)
ISN 0187         36 X(I)=W(JM+I)+W(1)*E(I)*(MOD(IABS(IR),200)-100)/100.
ISN 0188            IW(4)=3
ISN 0189            GO TO 100
                C  ONE DIMENSIONAL SEARCH
ISN 0190         37 IF(N.EQ.1) GO TO 43
ISN 0192            IF(IW(3).GE.IW(2)) GO TO 53
ISN 0194            IF(IW(4).EQ.2) GO TO 39
ISN 0196            IW(4)=2
ISN 0197            DO 38 I=1,N
ISN 0198         38 W(J3+I)=X(I)-W(JM+I)
ISN 0199            IR=3
ISN 0200            W(5)=A
ISN 0201            IR=20
ISN 0202            W(6)=A
ISN 0203            W(8)=0.5
ISN 0204            W(11)=0.
ISN 0205            W(12)=0.
ISN 0206            W(13)=0.
ISN 0207            W(14)=1.
ISN 0208            W(16)=W(JM+LM)
ISN 0209            W(17)=W(4)
ISN 0210            GO TO 40
ISN 0211         39 W(9)=W(4)
ISN 0212            CALL FIT1(KE,W(5),W(8))
ISN 0213         40 DO 41 I=1,N
ISN 0214         41 X(I)=W(JM+I)+W(8)*W(J3+I)
ISN 0215            IF(KE.EQ.3) KE=2
ISN 0217            IF(KE.EQ.2) GO TO 53
ISN 0219            KE=1
ISN 0220            W(3)=W(8)
ISN 0221            GO TO 100
```

```
C  ONLY ONE VARIABLE X
ISN 0222      42 IF(IW(3).GT.1) GO TO 43
ISN 0224         KE=0
ISN 0225         W(10)=W(1)*E(1)
ISN 0226         W(11)=E(1)
ISN 0227         W(12)=0.
ISN 0228      43 IR=IW(2)
ISN 0229         W(6)=A
ISN 0230         W(8)=X(1)
ISN 0231         W(9)=W(4)
ISN 0232         CALL FIT1(KE,W(5),W(8))
ISN 0233         IW(4)=2
ISN 0234         X(1)=W(8)
ISN 0235         IF(KE.EQ.1) GO TO 100
ISN 0237         IF(KE.GT.0) KE=KE+1
ISN 0239         W(3)=0.
ISN 0240         W(5)=0.
ISN 0241         IF(W(6).NE.0.) GO TO 74
ISN 0243         W(5)=SQRT(ABS((W(13)-W(15))/((W(16)-W(17))/(W(13)-W(14))-(W(17)-
                1W(18))/(W(14)-W(15)))))
ISN 0244         W(6)=1.
ISN 0245         W(7)=1.
ISN 0246         GO TO 71
C  END OF SEARCH
ISN 0247      50 KE=0
ISN 0248         IF(W(4).EQ.0..OR.IW(2).LT.0) GO TO 100
ISN 0250         GO TO 52
C  ERROR CODE DEFINITION
ISN 0251      57 KE=KE+1
ISN 0252      56 KE=KE+1
ISN 0253      55 KE=KE+1
ISN 0254      54 KE=KE+1
ISN 0255      53 KE=KE+1
ISN 0256         KE=KE+1
ISN 0257      52 DO 51 I=1,N
ISN 0258      51 W(I+4)=0.
```

```
ISN 0259          W(3)=0.
ISN 0260          IF(KE*(KE-3).NE.0.OR.(KE.EQ.3.AND.(W(2).EQ.1..OR.(W(3).EQ.0..AND.
                 1IW(3).LE.N)))) GO TO 74
                C  COMPUTATION OF THE ERRORS OF THE VARIABLES
                C  RESTORE MATRIX G
ISN 0262          IF(W(2).EQ.0.) GO TO 15
ISN 0264          J1=JA
ISN 0265          I1=N+1
ISN 0266          DO 45 I=2,I1
ISN 0267          IF(I.GT.M) GO TO 45
ISN 0269          DO 44 J=I,M
ISN 0270       44 W(J1+J)=0.
ISN 0271       45 J1=J1+M
ISN 0272          DO 49 I=1,N
ISN 0273          DO 46 I1=I,N
ISN 0274          A=W(4+N+I1)
ISN 0275          IF(IR.EQ.I) GO TO 47
ISN 0277       46 CONTINUE
ISN 0278       47 IF(I1.EQ.I) GO TO 49
ISN 0280          J1=JA+M*(I-1)
ISN 0281          J2=JA+M*(I1-1)
ISN 0282          W(4+N+I1)=W(4+N+I)
ISN 0283          DO 48 J=1,N
ISN 0284          A=W(J1+J)
ISN 0285          W(J1+J)=W(J2+J)
ISN 0286       48 W(J2+J)=A
ISN 0287       49 CONTINUE
ISN 0288          GO TO 66
                C  INVERSE OF MATRIX D
ISN 0289       60 T=SQRT(W(JA))
ISN 0290          J1=JA
ISN 0291          DO 61 I=1,N
ISN 0292          S=W(J3+I)
ISN 0293          J2=JS+I-LM
ISN 0294          DO 61 L=1,KV
ISN 0295          J1=J1+1
```

```
ISN 0296          61 W(J1)=T*(W(J2+L*LM)-S)/W(JS+L*LM)
ISN 0297             CALL INVATA(KV,N,IR,W(JA+1),W(JD+1),X)
ISN 0298             IF(IR) 74,20,74
                  C  MATRIX G = A*INVERSE OF D
ISN 0299          62 DO 65 L=1,M
ISN 0300             J1=L+JA-M
ISN 0301             DO 64 I=1,N
ISN 0302             I1=JD+(I*I-I)/2
ISN 0303             I2=1
ISN 0304             S=0.D0
ISN 0305             DO 63 J=1,N
ISN 0306             I1=I1+I2
ISN 0307             IF(J.GE.I) I2=J
ISN 0309          63 S=S+W(I1)*DBLE(W(J1+J*M))
ISN 0310          64 X(I)=S
ISN 0311             DO 65 J=1,N
ISN 0312          65 W(J1+J*M)=X(J)
                  C  DIAGONAL ELEMENTS OF G(T)*G
ISN 0313          66 J1=JA
ISN 0314             DO 68 I=1,N
ISN 0315             S=0.D0
ISN 0316             DO 67 L=1,M
ISN 0317             J1=J1+1
ISN 0318          67 S=S+W(J1)*DBLE(W(J1))
ISN 0319          68 W(4+N+I)=DSQRT(S)
                  C  STANDARD ERRORS AND ERROR CORRELATIONS
ISN 0320             CALL INVATA(M,N,IR,W(JA+1),W(JD+1),X)
ISN 0321             IF(IR.NE.0) GO TO 74
ISN 0323             DO 69 I=1,N
ISN 0324             W(I+4)=SQRT(W(JD+(I*I+I)/2))
ISN 0325          69 W(4+N+I)=W(I+4)*W(4+N+I)
ISN 0326             J1=JD
ISN 0327             DO 70 I=1,N
ISN 0328             DO 70 J=1,I
ISN 0329             J1=J1+1
ISN 0330          70 W(J1)=W(J1)/(W(I+4)*W(J+4))
```

```
C  ERROR RENORMALISATION FACTOR
ISN 0331        71 S=0.D0
ISN 0332           DO 72 I=1,M
ISN 0333        72 S=S+W(JM+N+I)
ISN 0334           W(3)=DSQRT(DABS(W(JM+LM)-S*S/M)/MAXO(M-N-1,1))
ISN 0335           DO 73 I=1,N
ISN 0336        73 W(I+4)=W(I+4)*W(3)
C  RESTORE OPTIMUM VALUES TO X AND F
ISN 0337        74 IW(4)=M-N-1
ISN 0338           IF((KE-5)*(KE-6).NE.0) GO TO 75
ISN 0340           IW(3)=J-2
ISN 0341           IW(4)=MF-1
ISN 0342        75 DO 76 I=1,N
ISN 0343        76 X(I)=W(JM+I)
ISN 0344           DO 77 I=1,M
ISN 0345        77 F(I)=W(JM+N+I)
ISN 0346           W(4)=W(JM+LM)
ISN 0347       100 IF(KE.EQ.1) IW(3)=IW(3)+1
ISN 0349           RETURN
ISN 0350           END
```

MODINA

FORHAD, integration subroutine to be added

```
C-------------------------------------------------------------------
C
C  INTEGRATION DURCH FORTGESETZTE HALBIERUNG, ROMBERG-VERFAHREN
C  PROGRAMMBESCHREIBUNG NR. 29 VON G.W. SCHWEIMER
C
C  P(1) UND P(2)   ENDPUNKTE DES INTEGRATIONSINTERVALLS
C  P(3)
C  P(4)            F(X) ODER INTEGRALWERT
C  P(5)            GEWUENSCHTER RELATIVER INTEGRATIONSFEHLER
C  P(6)            STEUERZAHL, STATEMENT 2
C  P(7)            HALBIERUNGSORDNUNG, ZAHL DER INTERVALLE IST 2**P(7)
```

```
C  P(8)              .5**(P(7)-1.)
C  P(9)              INTERVALLNUMMER: 1, 3, 5,...., 2**(P(7)-1.)-1.
C  P(10)             SUMME DER STUETZWERTE IN EINER HALBIERUNG
C  P(11) BIS P(25)  INTEGRALWERTE NACH DER TRAPEZ- (P(11)),SIMPSON- (P(12
C                   COTES- (P(13)), ROMBERG- (P(14) BIS P(25)) FORMEL FUE
C                   2**P(7)+1 STUETZPUNKTE
C
ISN 0002            SUBROUTINE FORHAD(KE,P)
ISN 0003            DIMENSION P(25)
ISN 0004            IF(KE)1,1,2
ISN 0005          1 P(3)=P(1)
ISN 0006            P(6)=-1.
ISN 0007            KE=1
ISN 0008            RETURN
ISN 0009          2 IF(P(6))3,4,7
ISN 0010          3 P(8)=P(4)
ISN 0011            P(6)=0.
ISN 0012            P(3)=P(2)
ISN 0013            KE=1
ISN 0014            RETURN
ISN 0015          4 P(11)=.5*(P(2)-P(1))*(P(4)+P(8))
ISN 0016            P(8)=1.
ISN 0017            P(7)=1.
ISN 0018            P(6)=1.
ISN 0019            KE=1
ISN 0020          5 P(7)=P(7)+1.
ISN 0021            P(8)=.5*P(8)
ISN 0022            P(9)=1.
ISN 0023            P(10)=0.
ISN 0024          6 P(3)=P(1)+P(8)*P(9)*(P(2)-P(1))
ISN 0025            RETURN
ISN 0026          7 P(9)=P(9)+2.
ISN 0027            P(10)=P(10)+P(4)
ISN 0028            KE=1
ISN 0029            IF(P(8)*P(9)-1.)6,8,8
ISN 0030          8 KE=2
```

```
ISN 0031            E=4.
ISN 0032            A=P(11)
ISN 0033            P(11)=.5*A+(P(2)-P(1))*P(8)*P(10)
ISN 0034            N=P(7)
ISN 0035            DO 9 M=2,N
ISN 0036            B=P(M+10)
ISN 0037            P(M+10)=P(M+9)+(P(M+9)-A)/(E-1.)
ISN 0038            A=B
ISN 0039          9 E=4.*E
ISN 0040            P(4)=P(N+10)
ISN 0041            IF(P(4))11,10,11
ISN 0042         10 F=ABS(P(N+9))
ISN 0043            GO TO 12
ISN 0044         11 F=ABS((P(N+9)-P(4))/P(4))
ISN 0045         12 IF(E-ABS(P(5)))15,15,13
ISN 0046         13 IF(N-15)5,14,14
ISN 0047         14 KE=4
ISN 0048            P(5)=E
ISN 0049            GO TO 16
ISN 0050         15 KE=3
ISN 0051         16 RETURN
ISN 0052            END
```

POGYNA

new folding model package, replacing POGA (page 117)

and POAR (page 143)

```
C-----------------------------------------------------------------------
C-----P-O-G-Y-N-A-----------------------------------------------------------
C-----MIKROSKOPISCHES OPTISCHES POTENTIAL
C-----BELIEBIGE WECHSELWIRKUNG IN FXV BERECHNET
C-----MIT DICHTE-ABHAENGIGKEIT
C-----NEUTRONEN- UND PROTONENVERTEILUNG VERSCHIEDEN
C-----NUKLEONENVERTEILUNG IN FUNCTION DENS BERECHNET
C-----COULOMBRADIUS P(2)
C-----MASSENZAHL P(3)
C-----Z*Z P(N+4)
C-----REALTEIL : NORMIERUNG = P(4)
C                CUT-OFF = P(18)
C                GAMMA = P(6)
C-----IMAGINAERTEIL P(7), P(8), P(9)
C     OBERFLAECHE   P(10), P(11), P(12)
C-----COULOMB VC UND VD
C-----COULOMB AUS GEGEBENER LADUNGSVERTEILUNG EXAKT BERECHNET
ISN 0002        SUBROUTINE POTE (P,PR,PI,N)
ISN 0003        IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004        DIMENSION P(2),PR(2),PI(2),F(25),S(25),D(2)
ISN 0005        REAL*8 ROO(2)/0.DO,0.DO/
ISN 0006        DIMENSION V(401),UC(200),ROD(200),RODA(200)
ISN 0007        REAL*4 WI(1000)
ISN 0008        REAL*8 PGN(10)/Z40271AD8921466DF,Z402630336A58B322,
               *               Z402460691E694A69,Z4021B658BB64DBFB,
               *               Z401E41FF31573B48,Z401A1817A317A820,
               *               Z4015519FE196E249,Z40100B467DF7E474,
               *               Z3FA64DAF529DB3FA,Z3F4825A00903A2BA/
ISN 0009        REAL*8 XGN(10)/Z4013973DF98B86AF,Z403A502C6D25177F,
               *               Z405FAB33C5594B0F,Z4082C82E09FBFFB4,
               *               Z40A2D469FD3886D7,Z40BF0F9B9A352A6F,
               *               Z40D6D05EAF7EB739,Z40E988320B9FEC8C,
               *               Z40F6C6DD3DEB84F5,Z40FE3DAD0638E701/
```

```
ISN 0010            REAL*8 PJ/3.14159265358979D0/,FA/.5D0/,FGA/1.D0/
ISN 0011            COMMON /INPT/ KE(42),WI,IN(100)
ISN 0012            DATA NC1/0/
ISN 0013            IF(N) 2,1,2
ISN 0014          1 N=28
ISN 0015            NP=N
ISN 0016            IF ((KE(16).NE.7).OR.(KE(17).EQ.0)) N=1
ISN 0018            ALP=2.D0/3.D0
ISN 0019            RETURN
ISN 0020          2 IF(N-2) 3,4,4
ISN 0021          3 AH13=P(3)**(1.D0/3.D0)
ISN 0022            IF (KE(15).EQ.0) GO TO 66
ISN 0024            CALL COULPO(1,P,R,VC,VD)
ISN 0025            GO TO 9
ISN 0026         66 R=P(2)*AH13
ISN 0027            A=1.43985*P(NP+4)/R
ISN 0028            V2=-.5*A/(R*R)
ISN 0029            V0=A-R*R*V2
ISN 0030            PCR=R
ISN 0031          9 H=P(NP+3)
ISN 0032            R=P(1)
ISN 0033            IF (P(15).LT.0.D0) P(15)=0.D0
ISN 0035            IF (KE(22).GT.0) P(6)=P(16)+P(17)*P(15)
ISN 0037            AK0=P(15)*P(6)
ISN 0038            AM0=(FGA-P(15))*P(6)
ISN 0039            NC2=H*20.
ISN 0040            IF ((NC1.EQ.NC2).AND.(KE(21).EQ.0)) GO TO 21
ISN 0042            HD=FGA/H
ISN 0043            H12=HD*FA
ISN 0044            PI8=8.D0*PJ*H/3.D0
ISN 0045            ISM=P(NP+6)+P(NP+7)
ISN 0046            IF(ISM.GT.200) ISM=200
ISN 0048            ISM2=P(18)/H
ISN 0049            ISM1=P(21)/H
ISN 0050            ISM12=ISM1+ISM2
ISN 0051            IF(ISM12.GT.ISM) ISM12=ISM
                  C-----BERECHNUNG VON FXV
ISN 0053            ISM22=2*ISM12+1
ISN 0054            CALL FXV(H,ISM22,V,P)
ISN 0055            NC1=NC2
```

```
C-----NORMIERUNG DER NEUTRONEN- UND PROTONENVERTEILUNG
ISN 0056        IF (KE(17).EQ.1) GO TO 20
ISN 0058        CALL DPN(ROO,P)
ISN 0059        D(1)=P(3)-P(NP+4)/WI(4)
ISN 0060        D(2)=P(NP+4)/WI(4)
ISN 0061        ROO(2)=ROO(2)*D(2)
ISN 0062        GO TO 21
ISN 0063     20 D(1)=P(3)
ISN 0064     21 S(1)=0.
ISN 0065        S(2)=P(21)
ISN 0066        S(5)=.000001D0
ISN 0067        K=0
ISN 0068        NF=0
ISN 0069     10 CALL FORHAD(K,S)
ISN 0070        GO TO (11,11,12,12),K
ISN 0071     11 S(4)=S(3)*S(3)*DENS(P,S)
ISN 0072        NF=NF+1
ISN 0073        GO TO 10
ISN 0074     12 IF(NF.LE.5) GO TO 11
ISN 0076        ROO(1)=D(1)/(4.D0*PJ*S(4))
C-----INTEGRATION
ISN 0077     43 R1=0.D0
ISN 0078        DO 44 IS12=1,ISM12
ISN 0079        R1=R1+H
ISN 0080        S(3)=R1
ISN 0081        RODN=ROO(1)*DENS(P,S)
ISN 0082        IF (KE(17).EQ.2) RODN=RODN+ROO(2)*DENSP(P,S)
ISN 0084        ROD(IS12)=RODN
ISN 0085        RODA(IS12)=FGA-AMO*RODN**ALP
ISN 0086        UC(IS12)=0.D0
ISN 0087     44 CONTINUE
C-----R-STRICH-PUNKTE
ISN 0088        R1=0.D0
ISN 0089        DO 7 IS1=1,ISM1
ISN 0090        R1=R1+H
ISN 0091        RODN=ROD(IS1)
ISN 0092        SIM=(1+MOD(IS1,2))*R1*R1*RODN
ISN 0093        RODN=FGA-AKO*RODN**ALP
```

```
C-----FO VON R-STRICH, R-ALPHA
ISN 0094        DO 6 IS12=1,ISM12
ISN 0095        A=(IS1*IS1+IS12*IS12)*H*H
ISN 0096        B=2.D0*IS1*IS12*H*H
ISN 0097        FO=0.D0
ISN 0098        RODM=RODN*RODA(IS12)
C-----WINKELINTEGRATION
ISN 0099        DO 5 I=1,10
ISN 0100        C=A-B*XGN(I)
ISN 0101        C=DSQRT(C)
ISN 0102        X=C*HD
ISN 0103        J=X
ISN 0104        X=X-J
ISN 0105        FF=FA*(V(J)+X*(V(J+1)-V(J)))
ISN 0106        C=A+B*XGN(I)
ISN 0107        C=DSQRT(C)
ISN 0108        X=C*HD
ISN 0109        J=X
ISN 0110        X=X-J
ISN 0111        FF=FF+FA*(V(J)+X*(V(J+1)-V(J)))
ISN 0112      5 FO=FO+FF*PGN(I)
ISN 0113      6 UC(IS12)=UC(IS12)+SIM*FO*RODM
ISN 0114      7 CONTINUE
ISN 0115        RETURN
C-----INTERPOLATION
ISN 0116      4 R=P(1)
ISN 0117        IF (KE(15).EQ.0) GO TO 77
ISN 0119        CALL COULPO(2,P,R,VC,VD)
ISN 0120        GO TO 79
ISN 0121     77 IF (R-PCR) 75,18,18
ISN 0122     75 VC=V0+R*R*V2
ISN 0123        VD=R*2.*V2
ISN 0124        GO TO 79
ISN 0125     18 VC=1.43985*P(NP+4)/R
ISN 0126        VD=-VC/R
ISN 0127     79 J=R*HD
ISN 0128        X=R*HD-J
ISN 0129        IF(J.EQ.ISM) GO TO 211
```

```
ISN 0131            IF(J.EQ.0) GO TO 213
ISN 0133            VCC=UC(J)+X*(UC(J+1)-UC(J))
ISN 0134            IF(J.EQ.1) GO TO 212
ISN 0136            VDD=(UC(J+1)-UC(J-1))*H12
ISN 0137            GO TO 150
ISN 0138          211 VCC=UC(J)+X*(UC(J)-UC(J-1))
ISN 0139            VDD=(UC(J)-UC(J-1))*HD
ISN 0140            GO TO 150
ISN 0141          212 VDD=(UC(J+1)-UC(J))*HD
ISN 0142            GO TO 150
ISN 0143          213 VCC=2.*UC(1)-UC(2)
ISN 0144            VDD=(UC(2)-UC(1))*HD
ISN 0145          150 F1=PI8*P(4)
ISN 0146            PR(1)=VC-F1*VCC
ISN 0147            PR(2)=VD-F1*VDD
ISN 0148            KEW=KE(18)
ISN 0149            GO TO (170,180),KEW
ISN 0150          170 SS=R-P(8)*AH13
ISN 0151            A=P(9)
ISN 0152            Y=1.D0/(1.D0+DEXP(SS/A))
ISN 0153            Z=-DEXP(SS/A)/A*Y*Y
ISN 0154            PI(1)=-P(7)*Y
ISN 0155            PI(2)=-P(7)*Z
                C       OBERFLAECHENABSORPTION
ISN 0156            WD=P(10)
ISN 0157            IF(WD) 310,311,310
ISN 0158          310 SS=R-P(11)*AH13
ISN 0159            A=P(12)
ISN 0160            Z=DEXP(SS/A)
ISN 0161            VV=1.D0+Z
ISN 0162            Y=Z/(VV*VV)
ISN 0163            Z=Y*(1.D0-2.D0*Z/VV)/A
```

```
ISN 0164            PI(1)=PI(1)-4.D0*WD*Y
ISN 0165            PI(2)=PI(2)-4.D0*WD*Z
ISN 0166          311 RETURN
                C     IMAGINAERTEIL VOLUMEN
ISN 0167          180 SS=R-P(8)*AH13
ISN 0168            A=P(9)
ISN 0169            Y=1.D0/(1.D0+DEXP(SS/A))
ISN 0170            Z=Y*Y*Y*DEXP(SS/A)*(-2.D0/A)
ISN 0171            Y=Y*Y
ISN 0172            PI(1)=-P(7)*Y
ISN 0173            PI(2)=-P(7)*Z
                C     OBERFLAECHENABSORPTION
ISN 0174            WD=P(10)
ISN 0175            IF(WD) 110,111,110
ISN 0176          110 SS=R-P(11)*AH13
ISN 0177            A=P(12)
ISN 0178            Y1=1.D0/(1.D0+DEXP(SS/A))
ISN 0179            Y2=DEXP(SS/A)
ISN 0180            Y=Y1**3*Y2*(-2.D0/A)
ISN 0181            Z=Y1**4*Y2*Y2*6.D0/(A**2)-Y1**3*Y2*2.D0/(A**2)
ISN 0182            PI(1)=PI(1)+4.D0*WD*Y*A
ISN 0183            PI(2)=PI(2)+4.D0*WD*Z*A
ISN 0184          111 RETURN
ISN 0185            END
```

```
C-----P-O-G-Y-N-A-----------------------------------------------------------
C      GAUSS PLUS YUKAWA INTERACTION NUMERICALLY INTEGRATED
ISN 0002        SUBROUTINE FXV(H,ISM12,DV,P)
ISN 0003        IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004        DIMENSION DV(401),P(2)
ISN 0005        G=P(5)*P(5)
ISN 0006        G=1.D0/G
ISN 0007        AY=1.D0/P(20)
ISN 0008        FY=P(19)
ISN 0009        FG=P(14)
ISN 0010        R=0.D0
ISN 0011        DO 100 I=1,401
ISN 0012        R=R+H
ISN 0013        DV(I)=0.D0
ISN 0014        EXPO=R*R*G
ISN 0015        IF (DABS(EXPO).LT.174.D0) DV(I)=FG*DEXP(-EXPO)
ISN 0017        EXPO=AY*R
ISN 0018        IF (DABS(EXPO).LT.174.D0) DV(I)=DV(I)+FY*DEXP(-EXPO)/EXPO
ISN 0020      100 CONTINUE
ISN 0021        RETURN
ISN 0022        END



ISN 0002        SUBROUTINE DPN(ROO,P)
ISN 0003        IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004        REAL*4 WI(1000)
ISN 0005        DIMENSION ROO(2),F(25),P(2)
ISN 0006        REAL*8 PI/3.14159265358979300/
ISN 0007        DATA NC1/0/
ISN 0008        COMMON /INPT/ KE(42),WI,IN(100)
ISN 0009        NC2=WI(3)+.2
ISN 0010        IF (NC1.EQ.NC2) GO TO 10
ISN 0012        NC1=NC2
```

```
                C-----NORMIERUNG DER PROTONEN-VERTEILUNG
ISN 0013              F(1)=0.
ISN 0014              F(2)=P(21)
ISN 0015              F(5)=.000001D0
ISN 0016              K=0
ISN 0017              NF=0
ISN 0018          100 CALL FORHAD(K,F)
ISN 0019              GO TO (110,110,120,120), K
ISN 0020          110 F(4)=F(3)*F(3)*DENSP(P,F)
ISN 0021              NF=NF+1
ISN 0022              GO TO 100
ISN 0023          120 IF(NF.LE.5) GO TO 110
ISN 0025              RO0(2)=1.D0/(4.D0*PI*F(4))
ISN 0026              RHO2=RO0(2)
ISN 0027              RETURN
ISN 0028           10 RO0(2)=RHO2
ISN 0029              RETURN
ISN 0030              END
```



```
ISN 0002              FUNCTION DENS(P,S)
                C-----3-PARAMETER FERMI-VERTEILUNG DER NEUTRONEN ODER MASSE
ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004              DIMENSION P(2),S(2)
ISN 0005              DENS=0.D0
ISN 0006              C=P(22)*P(3)**(1.D0/3.D0)
ISN 0007              A=P(23)
ISN 0008              W=P(24)
ISN 0009              R=S(3)
ISN 0010              IF (R.GT.P(21)) RETURN
ISN 0012              DENS=(1.D0+R*R*W/(C*C))/(1.D0+DEXP((R-C)/A))
ISN 0013              RETURN
ISN 0014              END
```

```
ISN 0002            FUNCTION DENSP(P,S)
                   C-----3-PARAMETER FERMI-VERTEILUNG DER PROTONEN
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            DIMENSION P(2),S(2)
ISN 0005            DENSP=0.DO
ISN 0006            C=P(25)*P(3)**(1.DO/3.DO)
ISN 0007            A=P(26)
ISN 0008            W=P(27)
ISN 0009            R=S(3)
ISN 0010            IF (R.GT.P(21)) RETURN
ISN 0012            DENSP=(1.DO+R*R*W/(C*C))/(1.DO+DEXP((R-C)/A))
ISN 0013            RETURN
ISN 0014            END


                   C-----P-O-G-Y-N-A-------------------------------------------------------
ISN 0002            SUBROUTINE DENPR(P,W,NP,M,N,VARM,CHI2)
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            REAL*4 WI(1000)
ISN 0005            DIMENSION P(2),W(2),VARM(30,30),S(25),D(2),CP(2,20),ROO(2)
ISN 0006            DIMENSION RMS(10)
ISN 0007            REAL*8 PJ/3.141592653589793DO/
ISN 0008            COMMON /INPT/KE(42),WI,IN(100)
ISN 0009            COMMON /IFIT/IA(30),NC,ID
ISN 0010            RC=P(21)
ISN 0011            AH13=P(3)**(1.DO/3.DO)
ISN 0012            Z2=WI(5)
ISN 0013            H=.1DO
ISN 0014            NS=RC/H+2.
ISN 0015            DRSM=0.DO
ISN 0016            DRSN=0.DO
                   C-----LADUNGSVERTEILUNG
ISN 0017            IF (KE(15).EQ.0) GO TO 10
ISN 0019            NW=7
ISN 0020            DO 1 I=1,4
ISN 0021            NW=NW+WI(NW)+1.1
ISN 0022          1 CONTINUE
ISN 0023            NC=WI(NW)+.1
ISN 0024            DO 2 I=1,NC
ISN 0025            CP(2,I)=WI(NW+I)
```

```
ISN 0026          2 CONTINUE
ISN 0027            NW=NW+WI(NW)+1.1
ISN 0028            S(1)=0.
ISN 0029            S(2)=CP(2,1)
ISN 0030            S(5)=.000001D0
ISN 0031            K=0
ISN 0032            NF=0
ISN 0033          3 CALL FORHAD(K,S)
ISN 0034            GO TO (4,4,5,5), K
ISN 0035          4 S(4)=S(3)*S(3)*DEN2(CP,S)
ISN 0036            NF=NF+1
ISN 0037            GO TO 3
ISN 0038          5 IF (NF.LE.5) GO TO 4
ISN 0040            RHOC=Z2/(4.D0*PJ*S(4))
ISN 0041            WRITE (6,6002) RHOC
ISN 0042       6002 FORMAT (//' DENSITY CHARGE = ',1PD15.5)
               C-----PROTONENVERTEILUNG
ISN 0043         10 IF (KE(17).EQ.1) GO TO 20
ISN 0045            CALL DPN(ROO,P)
ISN 0046            D(1)=P(3)-P(NP+4)/WI(4)
ISN 0047            D(2)=P(NP+4)/WI(4)
ISN 0048            ROO(2)=ROO(2)*D(2)
ISN 0049            GO TO 21
ISN 0050         20 D(1)=P(3)
ISN 0051         21 IF (KE(17).LT.1) GO TO 1000
ISN 0052            S(1)=0.
ISN 0054            S(2)=P(21)
ISN 0055            S(5)=.00000ID0
ISN 0056            K=0
ISN 0057            NF=0
ISN 0058         22 CALL FORHAD(K,S)
ISN 0059            GO TO (23,23,24,24), K
ISN 0060         23 S(4)=S(3)*S(3)*DENS(P,S)
ISN 0061            NF=NF+1
ISN 0062            GO TO 22
ISN 0063         24 IF (NF.LE.5) GO TO 23
ISN 0065            ROO(1)=D(1)/(4.D0*PJ*S(4))
ISN 0066            WRITE (6,6004) ROO
```

```
ISN 0067      6004 FORMAT (//' DENSITIES MATTER/NEUTRONS AND PROTONS',1P2D15.5)
ISN 0068           VK=4.D0*PJ*(P(2)*AH13)**3/3.D0
ISN 0069           DCK=P(NP+4)/(WI(4)*VK)
ISN 0070           PHC=P(2)*AH13
ISN 0071        31 IF (KE(11).EQ.1) WRITE(6,6003)
ISN 0073      6003 FORMAT (///' ',7X,'R',11X,'MATTER',10X,'NEUTRONS',10X,
                  1 'PROTONS',10X,'CHARGE')
ISN 0074        33 R=-H
ISN 0075           DO 100 I=1,NS
ISN 0076           R=R+H
ISN 0077           DM=0.
ISN 0078           DN=0.
ISN 0079           DP=0.
ISN 0080           DC=0.
ISN 0081           IF (R.LT.PHC) DC=DCK
ISN 0083           W(I+NS)=0.D0
ISN 0084           W(I+2*NS)=0.D0
ISN 0085           W(I+3*NS)=0.D0
ISN 0086           S(3)=R
ISN 0087           IF (KE(17).EQ.1) GO TO 32
ISN 0089           DN=DENS(P,S)*R00(1)
ISN 0090           DP=DENSP(P,S)*R00(2)
ISN 0091           DM=DN+DP
ISN 0092           GO TO 35
ISN 0093        32 DM=DENS(P,S)*R00(1)
ISN 0094        35 IF (KE(15).EQ.1) DC=DEN2(CP,S)*RHOC
ISN 0096           W(I)=DM
ISN 0097           W(I+NS)=DN
ISN 0098           W(I+2*NS)=DP
ISN 0099           W(I+3*NS)=DC
ISN 0100        91 IF (KE(11).EQ.1) WRITE (6,6011) R,DM,DN,DP,DC
ISN 0102       100 CONTINUE
ISN 0103      6011 FORMAT (' ',0PF10.3,5X,4(1PD12.4,5X))
ISN 0104           IF ((KE(12).EQ.0).AND.(KE(14).EQ.0)) GO TO 203
ISN 0106           KMM=MOD(KE(14),1000)/100
ISN 0107           KMN=KE(14)/1000
ISN 0108           IF (KE(17).NE.2) KMN=0
ISN 0110           DO 110 I=1,4
```

```
ISN 0111            ND=I-1
ISN 0112            IF (((KE(17).EQ.1).AND.(I.GT.1)).AND.(.NOT.((KE(15).EQ.1).AND.(I.E
                   1 Q.4)))) GO TO 110
ISN 0114            CALL MOMENT(ND,W,H,NS,RMS)
ISN 0115            IF (I.EQ.1) WRITE (6,6300)
ISN 0117         6300 FORMAT (///' MATTER DENSITY')
ISN 0118            IF (I.EQ.2) WRITE (6,6301)
ISN 0120         6301 FORMAT (///' NEUTRON DENSITY')
ISN 0121            IF (I.EQ.3) WRITE (6,6302)
ISN 0123         6302 FORMAT (///' PROTON DENSITY')
ISN 0124            IF (I.EQ.4) WRITE (6,6303)
ISN 0126         6303 FORMAT (///' CHARGE DENSITY')
ISN 0127            WRITE (6,6501) (RMS(J),J=1,3),(RMS(J),J=5,10)
ISN 0128         6501 FORMAT (/' K-TH MOMENT FOR K = -2, -1, ... ,+5, +6'
                   1 /9(F12.5,2X))
ISN 0129            WRITE (6,6502) RMS(4)
ISN 0130         6502 FORMAT (/' VOLUME = ',1PD12.5)
ISN 0131            IF ((KMM.GT.0).AND.(I.EQ.1)) WRITE (8,7001) RMS
ISN 0133            IF ((KMN.GT.0).AND.(I.EQ.2)) WRITE (8,7001) RMS
ISN 0135          110 CONTINUE
ISN 0136          203 IWP=NS
ISN 0137            IWS=1
ISN 0138            KDM=MOD(KE(13),1000)/100
ISN 0139            KDN=KE(13)/1000
ISN 0140            IF (KE(17).NE.2) KDN=0
ISN 0142            IF (KDM.GT.0.OR.KDN.GT.0) WRITE(7,7001) (W(I),I=IWS,IWP)
ISN 0144            IWS=IWP+1
ISN 0145            IWP=IWP+NS
ISN 0146            IF (KDN.GT.0) WRITE (7,7001) (W(I),I=IWS,IWP)
ISN 0148         7001 FORMAT((5X,'*',6(1PD10.3,',')))
ISN 0149         1000 RETURN
ISN 0150            END
```

```
                C-----POTENTIAL PRINT
ISN 0002              SUBROUTINE POTPR(P,W,NP,M,N,VARM,CHI2)
ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004              REAL*4 WI(1000)
ISN 0005              DIMENSION P(2),PR(2),PI(2),W(2),VARM(30,30),RMS(10)
ISN 0006              COMMON /INPT/KE(42),WI,IN(100)
ISN 0007              COMMON /IFIT/IA(30),NC,ID
ISN 0008              NRC=P(NP+3)*(P(NP+6)+P(NP+7)-1.)+1.
ISN 0009              RC=NRC
ISN 0010              H=.1D0
ISN 0011              AH13=P(3)**(1.D0/3.D0)
ISN 0012              NA2=WI(2)+.2
ISN 0013              HA=P(NP+3)
ISN 0014              NSA=P(NP+6)
ISN 0015              MSA=P(NP+7)
ISN 0016              P(NP+3)=H
ISN 0017              NS=RC/H+2
ISN 0018              MS=0
ISN 0019              P(NP+6)=NS
ISN 0020              P(NP+7)=MS
ISN 0021              NN=1
ISN 0022              CALL POTE(P,PR,PI,NN)
ISN 0023              IF (KE(15).EQ.1) GO TO 6
ISN 0025              R=P(2)*AH13
ISN 0026              A=1.43985*P(NP+4)/R
ISN 0027              V2=-.5*A/(R*R)
ISN 0028              V0=A-R*R*V2
ISN 0029            6 IF (KE(9).EQ.1) WRITE(6,6000)
ISN 0031         6000 FORMAT (///' ',10X,'R',15X,'REAL',13X,'REAL+COULOMB',8X,
                     1 'IMAGINARY',11X,'COULOMB')
ISN 0032            9 R=-H
ISN 0033              DO 2 I=1,NS
ISN 0034              R=R+H
ISN 0035              P(1)=R
ISN 0036              W(I)=0.D0
ISN 0037              W(I+NS)=0.D0
ISN 0038              W(I+2*NS)=0.D0
ISN 0039              CALL POTE(P,PR,PI,NP)
```

```
ISN 0040            IF(KE(15).EQ.0) GO TO 3
ISN 0042            CALL COULPO(2,P,R,VC,VD)
ISN 0043            GO TO 1
ISN 0044          3 IF (R-P(2)*AH13) 4,5,5
ISN 0045          4 VC=V0+R*R*V2
ISN 0046            GO TO 1
ISN 0047          5 VC=1.43985*P(NP+4)/R
ISN 0048          1 PR(2)=PR(1)
ISN 0049            PR(1)=PR(1)-VC
ISN 0050            W(I)=PR(1)
ISN 0051            W(I+NS)=PI(1)
ISN 0052            IF (KE(9).EQ.1) WRITE(6,6100) R,PR(1),PR(2),PI(1),VC
ISN 0054          2 CONTINUE
ISN 0055       6100 FORMAT(' ',0PF15.3,5X,4(1PD15.7,5X))
ISN 0056       6300 FORMAT (///' REAL POTENTIAL')
ISN 0057         31 KMR=MOD(KE(14),10)
ISN 0058            IF ((KE(10).EQ.0).AND.(KMR.EQ.0)) GO TO 30
ISN 0060            NV=0
ISN 0061            WRITE (6,6300)
ISN 0062            CALL MOMENT(NV,W,H,NS,RMS)
ISN 0063            WRITE (6,6001) (RMS(I),I=1,3),(RMS(I),I=5,10)
ISN 0064       6001 FORMAT (//' K-TH MOMENT FOR K = -2, -1, ...,+5, +6'/9(F12.5,2X))
ISN 0065            VOL=RMS(4)/(P(3)*NA2)
ISN 0066            WRITE (6,6002) RMS(4),VOL
ISN 0067       6002 FORMAT (/' VOLUME = ',1PD12.5,'   PER NUCLEON PAIR = ',1PD12.5)
ISN 0068            IF (KMR.GT.0) WRITE (8,7001) RMS
ISN 0070       6400 FORMAT (///' IMAGINARY POTENTIAL')
ISN 0071         32 KMI=MOD(KE(14),100)/10
ISN 0072            IF ((KE(10).LT.2).AND.(KMI.EQ.0)) GO TO 30
ISN 0074            NV=1
ISN 0075            WRITE (6,6400)
ISN 0076            CALL MOMENT(NV,W,H,NS,RMS)
ISN 0077            VOL=RMS(4)/(P(3)*NA2)
ISN 0078            WRITE (6,6001) (RMS(I),I=1,3),(RMS(I),I=5,10)
ISN 0079            WRITE (6,6002) RMS(4),VOL
ISN 0080            IF (KMI.GT.0) WRITE (8,7001) RMS
ISN 0082         30 P(NP+3)=HA
ISN 0083            P(NP+6)=NSA
ISN 0084            P(NP+7)=MSA
```

```
ISN 0085            IWP=NS
ISN 0086            IWS=1
ISN 0087            KPR=MOD(KE(13),10)
ISN 0088            IF (KPR.GT.0) WRITE (7,7001) (W(I),I=IWS,IWP)
ISN 0090            IWP=IWP+NS
ISN 0091            IF (KPI.GT.0) WRITE (7,7001) (W(I),I=IWS,IWP)
ISN 0093       7001 FORMAT ((5X,'*',6(1PD10.3,',')))
ISN 0094            RETURN
ISN 0095            END
```

POGYNAFB

new folding model package with FB-option, replacing
POGAFB (page 128) and POARFB (page 156)

```
C-----------------------------------------------------------------------
C-----P-O-G-Y-N-A-F-B-------------------------------------------------
C-----MIKROSKOPISCHES OPTISCHES POTENTIAL
C-----BELIEBIGE WECHSELWIRKUNG IN FXV BERECHNET
C-----MIT DICHTE-ABHAENGIGKEIT
C-----FOURIER-BESSEL-DICHTEN
C-----NEUTRONEN- UND PROTONENVERTEILUNG VERSCHIEDEN
C-----NUKLEONENVERTEILUNG IN FUNCTION DENS BERECHNET
C-----COULOMBRADIUS P(2)
C-----MASSENZAHL P(3)
C-----Z*Z P(N+4)
C-----REALTEIL : NORMIERUNG = P(4)
C                CUT-OFF = P(39)
C                GAMMA = P(6)
C-----IMAGINAERTEIL P(7), P(8), P(9)
C     OBERFLAECHE   P(10), P(11), P(12)
C-----COULOMB VC UND VD
C-----COULOMB AUS GEGEBENER LADUNGSVERTEILUNG EXAKT BERECHNET
ISN 0002        SUBROUTINE POTE (P,PR,PI,N)
ISN 0003        IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004        DIMENSION P(2),PR(2),PI(2),F(25),S(25),D(2)
ISN 0005        REAL*8 ROO(2)/0.DO,0.DO/
ISN 0006        DIMENSION V(401),UC(200),RODA(200),ROD(200)
ISN 0007        REAL*4 WI(1000)
ISN 0008        REAL*8 PGN(10)/Z40271AD8921466DF,Z402630336A588322,
               *               Z402460691E694A69,Z4021B658BB64DBFB,
               *               Z401E41FF31573B48,Z401A1817A317A820,
               *               Z4015519FE196E249,Z40100B467DF7E474,
               *               Z3FA64DAF529D83FA,Z3F4825A009D3A28A/
ISN 0009        REAL*8 XGN(10)/Z4013973DF98B86AF,Z403A502C6D25177F,
               *               Z405FAB33C5594B0F,Z4082C82E09FBFFB4,
               *               Z40A2D469FD3886D7,Z40BF0F9B9A352A6F,
               *               Z40D6D05EAF7EB739,Z40E988320B9FEC8C,
               *               Z40F6C6DD3DEBB4F5,Z40FE3DAD0638E701/
```

```
ISN 0010          REAL*8 PJ/3.14159265358979300/,FA/.500/,FGA/1.00/
ISN 0011          COMMON /INPT/ KE(42),WI,IN(100)
ISN 0012          COMMON /IFIT/ IA(30),NC,ID
ISN 0013          COMMON /CON/ VNEG
ISN 0014          DATA NC1/0/,NC3/0/
ISN 0015          IF(N) 2,1,2
ISN 0016        1 N=49
ISN 0017          NP=N
ISN 0018          IF ((KE(16).NE.8).OR.(KE(17).EQ.0)) N=1
ISN 0020          RETURN
ISN 0021        2 IF(N-2) 3,4,4
ISN 0022        3 AH13=P(3)**(1.D0/3.D0)
ISN 0023          NC4=P(3)
ISN 0024          NF=IN(8)
ISN 0025          IO=IA(NF)
ISN 0026          IF (IO.EQ.NP) IO=IA(NF-1)
ISN 0028          IF (KE(18).LT.3) GO TO 113
ISN 0030          IOW=IO
ISN 0031          RCTFW=P(29)
ISN 0032          DO 111 I=1,NF
ISN 0033          IF (IA(I).GT.28) GO TO 112
ISN 0035        111 CONTINUE
ISN 0036        112 IO=IA(I-1)
ISN 0037          IUW=30
ISN 0038          IF (IO.LT.14) IO=28
ISN 0040        113 IF (KE(15).EQ.0) GO TO 66
ISN 0042          CALL COULPO(1,P,R,VC,VD)
ISN 0043          GO TO 9
ISN 0044         66 R=P(2)*AH13
ISN 0045          A=1.43985*P(NP+4)/R
ISN 0046          V2=-.5*A/(R*R)
ISN 0047          V0=A-R*R*V2
ISN 0048          PCR=R
ISN 0049          9 R=P(1)
ISN 0050          AK0=P(38)*P(6)
ISN 0051          AM0=(FGA-P(38))*P(6)
ISN 0052          H=P(NP+3)
ISN 0053          NC2=H*20.
```

```
ISN 0054            IF (NC1.EQ.NC2) GO TO 21
ISN 0056            HD=FGA/H
ISN 0057            H12=HD*FA
ISN 0058            PI8=8.D0*PJ*H/3.D0
ISN 0059            ALP=2.D0/3.D0
ISN 0060            ISM=P(NP+6)+P(NP+7)
ISN 0061            IF(ISM.GT.200) ISM=200
ISN 0063            ISM2=P(39)/H
ISN 0064            ISM1=P(42)/H
ISN 0065            ISM12=ISM1+ISM2
ISN 0066            IF(ISM12.GT.ISM) ISM12=ISM
ISN 0068            ISM22=2*ISM12+1
                C-----BERECHNUNG VON FXV
ISN 0069            CALL FXV(H,ISM22,V,P)
                C-----NORMIERUNG DER NEUTRONEN- UND PROTONENVERTEILUNG
ISN 0070            IF (KE(17).EQ.1) GO TO 20
ISN 0072            CALL DPN(ROO,P)
ISN 0073            D(1)=P(3)-P(NP+4)/WI(4)
ISN 0074            D(2)=P(NP+4)/WI(4)
ISN 0075            ROO(2)=ROO(2)*D(2)
ISN 0076            GO TO 21
ISN 0077         20 D(1)=P(3)
ISN 0078         21 IF (NC3.EQ.NC4) GO TO 43
ISN 0080            S(1)=0.
ISN 0081            S(2)=P(42)
ISN 0082            S(5)=.000001D0
ISN 0083            K=0
ISN 0084            NF=0
ISN 0085         10 CALL FORHAD(K,S)
ISN 0086            GO TO (11,11,12,12),K
ISN 0087         11 S(4)=S(3)*S(3)*DENS(P,S)
ISN 0088            NF=NF+1
ISN 0089            GO TO 10
ISN 0090         12 IF(NF.LE.5) GO TO 11
ISN 0092            ROO(1)=D(1)/(4.D0*PJ*S(4))
ISN 0093            NC3=NC4
```

```
ISN 0094          43 R1=0.D0
ISN 0095             DO 44 IS12=1,ISM12
ISN 0096             R1=R1+H
ISN 0097             S(3)=R1
ISN 0098             RODN=ROO(1)*DENS(P,S)+DEFB(P,S)
ISN 0099             IF (KE(17).EQ.2) RODN=RODN+DENSP(P,S)*ROO(2)
ISN 0101             ROD(IS12)=RODN
ISN 0102             RODA(IS12)=FGA-AMO*RODN**ALP
ISN 0103             UC(IS12)=0.D0
ISN 0104          44 CONTINUE
                  C-----FALTUNG
                  C-----R-STRICH-PUNKTE
ISN 0105             VNEG=0.D0
ISN 0106             R1=0.D0
ISN 0107             DO 7 IS1=1,ISM1
ISN 0108             R1=R1+H
ISN 0109             RODN=ROD(IS1)
ISN 0110             SIM=(1+MOD(IS1,2))*R1*R1
ISN 0111             VNEG=VNEG+SIM*DABS(RODN)
ISN 0112             SIM=SIM*RODN
ISN 0113             RODN=FGA-AKO*RODN**ALP
                  C-----FO VON R-STRICH, R-ALPHA
ISN 0114             DO 6 IS12=1,ISM12
ISN 0115             A=(IS1*IS1+IS12*IS12)*H*H
ISN 0116             B=2.D0*IS1*IS12*H*H
ISN 0117             RODM=RODN*RODA(IS12)
ISN 0118             FO=0.D0
                  C-----WINKELINTEGRATION
ISN 0119             DO 5 I=1,10
ISN 0120             C=A-B*XGN(I)
ISN 0121             C=DSQRT(C)
ISN 0122             X=C*HD
ISN 0123             J=X
ISN 0124             X=X-J
ISN 0125             FF=FA*(V(J)+X*(V(J+1)-V(J)))
ISN 0126             C=A+B*XGN(I)
```

```
ISN 0127            C=DSQRT(C)
ISN 0128            X=C*HD
ISN 0129            J=X
ISN 0130            X=X-J
ISN 0131            FF=FF+FA*(V(J)+X*(V(J+1)-V(J)))
ISN 0132          5 FO=FO+FF*PGN(I)
ISN 0133          6 UC(IS12)=UC(IS12)+SIM*FO*RODM
ISN 0134          7 CONTINUE
ISN 0135            VNEG=VNEG*PI8
ISN 0136            VNEG=FGA*(P(3)-VNEG)**2
ISN 0137            RETURN
                C-----INTERPOLATION
ISN 0138          4 R=P(1)
ISN 0139            IF (KE(15).EQ.0) GO TO 77
ISN 0141            CALL COULPO(2,P,R,VC,VD)
ISN 0142            GO TO 79
ISN 0143         77 IF (R-PCR) 75,18,18
ISN 0144         75 VC=V0+R*R*V2
ISN 0145            VD=R*2.*V2
ISN 0146            GO TO 79
ISN 0147         18 VC=1.43985*P(NP+4)/R
ISN 0148            VD=-VC/R
ISN 0149         79 J=R*HD
ISN 0150            X=R*HD-J
ISN 0151            IF(J.EQ.ISM) GO TO 211
ISN 0153            IF(J.EQ.0) GO TO 213
ISN 0155            VCC=UC(J)+X*(UC(J+1)-UC(J))
ISN 0156            IF(J.EQ.1) GO TO 212
ISN 0158            VDD=(UC(J+1)-UC(J-1))*H12
ISN 0159            GO TO 150
ISN 0160        211 VCC=UC(J)+X*(UC(J)-UC(J-1))
ISN 0161            VDD=(UC(J)-UC(J-1))*HD
ISN 0162            GO TO 150
ISN 0163        212 VDD=(UC(J+1)-UC(J))*HD
ISN 0164            GO TO 150
ISN 0165        213 VCC=2.*UC(1)-UC(2)
ISN 0166            VDD=(UC(2)-UC(1))*HD
```

```
ISN 0167        150 F1=PI8*P(4)
ISN 0168            PR(1)=VC-F1*VCC
ISN 0169            PR(2)=VD-F1*VDD
ISN 0170            KEW=KE(18)
ISN 0171            GO TO (170,220,170,220),KEW
ISN 0172        170 SS=R-P(8)*AH13
ISN 0173            A=P(9)
ISN 0174            Y=1.D0/(1.D0+DEXP(SS/A))
ISN 0175            Z=-DEXP(SS/A)/A*Y*Y
ISN 0176            PI(1)=-P(7)*Y
ISN 0177            PI(2)=-P(7)*Z
                C       OBERFLAECHENABSORPTION
ISN 0178            WD=P(10)
ISN 0179            IF(WD) 30,31,30
ISN 0180         30 SS=R-P(11)*AH13
ISN 0181            A=P(12)
ISN 0182            Z=DEXP(SS/A)
ISN 0183            VV=1.D0+Z
ISN 0184            Y=Z/(VV*VV)
ISN 0185            Z=Y*(1.D0-2.D0*Z/VV)/A
ISN 0186            PI(1)=PI(1)-4.D0*WD*Y
ISN 0187            PI(2)=PI(2)-4.D0*WD*Z
ISN 0188         31 IF (KE(18).GT.2) GO TO 500
ISN 0190            RETURN
                C       IMAGINAERTEIL VOLUMEN
ISN 0191        220 SS=R-P(8)*AH13
ISN 0192            A=P(9)
ISN 0193            Y=1.D0/(1.D0+DEXP(SS/A))
ISN 0194            Z=Y*Y*Y*DEXP(SS/A)*(-2.D0/A)
ISN 0195            Y=Y*Y
ISN 0196            PI(1)=-P(7)*Y
ISN 0197            PI(2)=-P(7)*Z
                C       OBERFLAECHENABSORPTION
ISN 0198            WD=P(10)
ISN 0199            IF(WD) 230,231,230
```

```
ISN 0200        230 SS=R-P(11)*AH13
ISN 0201            A=P(12)
ISN 0202            Y1=1.D0/(1.D0+DEXP(SS/A))
ISN 0203            Y2=DEXP(SS/A)
ISN 0204            Y=Y1**3*Y2*(-2.D0/A)
ISN 0205            Z=Y1**4*Y2*Y2*6.D0/(A**2)-Y1**3*Y2*2.D0/(A**2)
ISN 0206            PI(1)=PI(1)+4.D0*WD*Y*A
ISN 0207            PI(2)=PI(2)+4.D0*WD*Z*A
ISN 0208        231 IF (KE(18).GT.2)GO TO 500
ISN 0210            RETURN
ISN 0211        500 SYFB=0.D0
ISN 0212            SZFB=0.D0
ISN 0213            IF (R.GE.RCTFW) GO TO 391
ISN 0215            IF ((KE(19).NE.2).AND.(KE(19).NE.3)) GO TO 321
ISN 0217            P(30)=0.D0
ISN 0218            DO 322 I=31,37
ISN 0219            II=I-29
ISN 0220            P(30)=P(30)+P(I)*(-1.D0)**II/II**2
ISN 0221        322 CONTINUE
ISN 0222        321 DO 390 I=30,37
ISN 0223            IX=I-29
ISN 0224            IF (R) 380,380,381
ISN 0225        380 SYFB=SYFB+P(I)
ISN 0226            GO TO 390
ISN 0227        381 YFB=PJ*R*IX/RCTFW
ISN 0228            SYFB=SYFB+P(I)*DSIN(YFB)/YFB
ISN 0229            SZFB=SZFB+P(I)*(DCOS(YFB)*PJ*IX*YFB/RCTFW-
                   1 DSIN(YFB)*PJ*IX/RCTFW)/YFB**2
ISN 0230        390 CONTINUE
ISN 0231        391 PI(1)=PI(1)-SYFB
ISN 0232            PI(2)=PI(2)-SZFB
ISN 0233            RETURN
ISN 0234            END
```

```
C-----P-O-G-Y-N-A-F-B-------------------------------------------------------
C      GAUSS PLUS YUKAWA INTERACTION NUMERICALLY INTEGRATED
ISN 0002        SUBROUTINE FXV(H,ISM12,DV,P)
ISN 0003        IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004        DIMENSION DV(401),P(2)
ISN 0005        G=P(5)*P(5)
ISN 0006        G=1.DO/G
ISN 0007        AY=1.DO/P(41)
ISN 0008        FY=P(40)/P(4)
ISN 0009        R=0.DO
ISN 0010        DO 100 I=1,ISM12
ISN 0011        R=R+H
ISN 0012        DV(I)=0.DO
ISN 0013        EXPO=R*R*G
ISN 0014        IF (DABS(EXPO).LT.174.DO) DV(I)=DEXP(-EXPO)
ISN 0016        EXPO=AY*R
ISN 0017        IF (DABS(EXPO).LT.174.DO) DV(I)=DV(I)+FY*DEXP(-EXPO)/EXPO
ISN 0019      100 CONTINUE
ISN 0020        RETURN
ISN 0021        END
```

```
ISN 0002        SUBROUTINE DPN(ROO,P)
ISN 0003        IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004        REAL*4 WI(1000)
ISN 0005        DIMENSION ROO(2),F(25),P(2)
ISN 0006        REAL*8 PI/3.14159265358979DO/
ISN 0007        DATA NC1/0/
ISN 0008        COMMON /INPT/ KE(42),WI,IN(100)
ISN 0009        NC2=WI(3)+.2
ISN 0010        IF (NC1.EQ.NC2) GO TO 10
ISN 0012        NC1=NC2
```

```
                C-----NORMIERUNG DER PROTONEN-VERTEILUNG
ISN 0013              F(1)=0.
ISN 0014              F(2)=P(42)
ISN 0015              F(5)=.000001D0
ISN 0016              K=0
ISN 0017              NF=0
ISN 0018          100 CALL FORHAD(K,F)
ISN 0019              GO TO (110,110,120,120), K
ISN 0020          110 F(4)=F(3)*F(3)*DENSP(P,F)
ISN 0021              NF=NF+1
ISN 0022              GO TO 100
ISN 0023          120 IF(NF.LE.5) GO TO 110
ISN 0025              ROO(2)=1.D0/(4.D0*PI*F(4))
ISN 0026              RHO2=ROO(2)
ISN 0027              RETURN
ISN 0028           10 ROO(2)=RHO2
ISN 0029              RETURN
ISN 0030              END
```

```
ISN 0002              FUNCTION DENS(P,S)
                C-----3-PARAMETER FERMI-VERTEILUNG DER NEUTRONEN ODER MASSE
ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004              DIMENSION P(2),S(2)
ISN 0005              DENS=0.D0
ISN 0006              C=P(43)*P(3)**(1.D0/3.D0)
ISN 0007              A=P(44)
ISN 0008              W=P(45)
ISN 0009              R=S(3)
ISN 0010              IF (R.GT.P(42)) RETURN
ISN 0012              DENS=(1.D0+R*R*W/(C*C))/(1.D0+DEXP((R-C)/A))
ISN 0013              RETURN
ISN 0014              END
```

```
C-----FOURIER-BESSEL DENS
ISN 0002        FUNCTION DEFB(P,S)
ISN 0003        IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004        REAL*4 WI(1000)
ISN 0005        REAL*8 PI/3.14159265358979D0/
ISN 0006        DIMENSION P(2),S(2)
ISN 0007        COMMON /INPT/KE(42),WI,IN(100)
ISN 0008        DEFB=0.D0
ISN 0009        R=S(3)
ISN 0010        IF (R.GT.P(13)) RETURN
ISN 0012        RCTF=P(13)
ISN 0013        P(14)=0.D0
ISN 0014        DO 50 I=15,28
ISN 0015        II=I-13
ISN 0016        P(14)=P(14)+P(I)*(-1.D0)**II/II**2
ISN 0017     50 CONTINUE
ISN 0018        SYFB=0.D0
ISN 0019        DO 100 I=14,28
ISN 0020        IX=I-13
ISN 0021        IF (R) 10,10,20
ISN 0022     10 SYFB=SYFB+P(I)
ISN 0023        GO TO 100
ISN 0024     20 YFB=PI*R*IX/RCTF
ISN 0025        SYFB=SYFB+P(I)*DSIN(YFB)/YFB
ISN 0026    100 CONTINUE
ISN 0027        DEFB=SYFB
ISN 0028        RETURN
ISN 0029        END
```

```
                C-----P-D-G-Y-N-A-F-B-------------------------------------------------------------
ISN 0002            SUBROUTINE DENPR(P,W,NP,M,N,VARM,CHI2)
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            REAL*4 WI(1000)
ISN 0005            DIMENSION P(2),W(2),VARM(30,30),S(30),D(2),CP(2,20),ROO(2)
ISN 0006            DIMENSION RMS(10)
ISN 0007            REAL*8 PI/3.14159265358979300/
ISN 0008            COMMON /INPT/KE(42),WI,IN(100)
ISN 0009            COMMON /IFIT/IA(30),NC,ID
ISN 0010            RC=P(42)
ISN 0011            AH13=P(3)**(1.D0/3.D0)
ISN 0012            Z2=WI(5)
ISN 0013            H=.1D0
ISN 0014            NS=RC/H+2.
ISN 0015            DRSM=0.D0
ISN 0016            DRSN=0.D0
                C-----LADUNGSVERTEILUNG
ISN 0017            IF (KE(15).EQ.0) GO TO 10
ISN 0019            NW=7
ISN 0020            DO 1 I=1,4
ISN 0021            NW=NW+WI(NW)+1.1
ISN 0022          1 CONTINUE
ISN 0023            NC=WI(NW)+.1
ISN 0024            DO 2 I=1,NC
ISN 0025            CP(2,I)=WI(NW+I)
ISN 0026          2 CONTINUE
ISN 0027            NW=NW+WI(NW)+1.1
ISN 0028            S(1)=0.
ISN 0029            S(2)=CP(2,1)
ISN 0030            S(5)=1.D-6
ISN 0031            K=0
ISN 0032            NF=0
ISN 0033          3 CALL FORHAD(K,S)
ISN 0034            GO TO (4,4,5,5), K
ISN 0035          4 S(4)=S(3)*S(3)*DEN2(CP,S)
ISN 0036            NF=NF+1
ISN 0037            GO TO 3
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ISN 0038          5 IF (NF.LE.5) GO TO 4
ISN 0040            RHOC=Z2/(4.D0*PJ*S(4))
ISN 0041            WRITE (6,6002) RHOC
ISN 0042       6002 FORMAT (//' DENSITY CHARGE = ',1PD15.5)
              C-----PROTONENVERTEILUNG
ISN 0043         10 IF (KE(17).EQ.1) GO TO 20
ISN 0045            CALL DPN(ROO,P)
ISN 0046            D(1)=P(3)-P(NP+4)/WI(4)
ISN 0047            D(2)=P(NP+4)/WI(4)
ISN 0048            ROO(2)=ROO(2)*D(2)
ISN 0049            GO TO 21
ISN 0050         20 D(1)=P(3)
ISN 0051         21 IF (KE(17).LT.1) GO TO 1000
ISN 0053            S(1)=0.
ISN 0054            S(2)=P(42)
ISN 0055            S(5)=1.D-6
ISN 0056            K=0
ISN 0057            NF=0
ISN 0058         22 CALL FORHAD(K,S)
ISN 0059            GO TO (23,23,24,24), K
ISN 0060         23 S(4)=S(3)*S(3)*DENS(P,S)
ISN 0061            NF=NF+1
ISN 0062            GO TO 22
ISN 0063         24 IF (NF.LE.5) GO TO 23
ISN 0065            ROO(1)=D(1)/(4.D0*PJ*S(4))
ISN 0066            WRITE (6,6004) ROO
ISN 0067       6004 FORMAT (//' DENSITIES MATTER/NEUTRONS AND PROTONS',1P2D15.5)
ISN 0068            VK=4.D0*PJ*(P(2)*AH13)**3/3.D0
ISN 0069            DCK=P(NP+4)/(WI(4)*VK)
ISN 0070            PHC=P(2)*AH13
ISN 0071            RCTF=P(13)
ISN 0072            RCT2=RCTF-.01
ISN 0073            NF=IN(8)
ISN 0074            IO=IA(NF)
ISN 0075            IF (IO.EQ.NP) IO=IA(NF-1)
ISN 0077            DO 25 I=1,NF
ISN 0078            IF (IA(I).GT.13) GO TO 26
```

```
ISN 0080          25 CONTINUE
ISN 0081          26 IU=IA(I)
ISN 0082             II=I-1
ISN 0083             IU1=IU-1
ISN 0084             IU2=IU-14
ISN 0085             IF (KE(18).LT.3) GO TO 30
ISN 0087             DO 8 I=1,NF
ISN 0088             IF (IA(I).GT.28) GO TO 9
ISN 0090           8 CONTINUE
ISN 0091           9 IO=IA(I-1)
ISN 0092          30 IF (KE(11).EQ.1) WRITE (6,6001)
ISN 0094        6001 FORMAT (///' ',7X,'R',11X,'MATTER',10X,'NEUTRONS',11X,'ERROR',
                    1 9X,'ERROR PERC',8X,'PROTONS',10X,'CHARGE')
ISN 0095          33 R=-H
ISN 0096             DO 100 I=1,NS
ISN 0097             R=R+H
ISN 0098             DM=0.
ISN 0099             DN=0.
ISN 0100             DP=0.
ISN 0101             DC=0.
ISN 0102             ERR=0.
ISN 0103             W(I+NS)=0.D0
ISN 0104             W(I+2*NS)=0.D0
ISN 0105             W(I+3*NS)=0.D0
ISN 0106             W(I+4*NS)=0.D0
ISN 0107             S(3)=R
ISN 0108             IF (R.LT.PHC) DC=DCK
ISN 0110             KE17=KE(17)
ISN 0111             GO TO (34,35), KE17
ISN 0112          34 DM=DENS(P,S)*ROO(1)+DEFB(P,S)
ISN 0113             GO TO 36
ISN 0114          35 DN=DENS(P,S)*ROO(1)+DEFB(P,S)
ISN 0115             DP=DENSP(P,S)*ROO(2)
ISN 0116             DM=DN+DP
ISN 0117          36 IF (KE(15).EQ.1) DC=DEN2(CP,S)*RHOC
ISN 0119             W(I)=DM
ISN 0120             W(I+2*NS)=DN
ISN 0121             W(I+3*NS)=DP
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```
ISN 0122            W(I+4*NS)=DC
ISN 0123            IF (R.GE.RCT2) GO TO 90
ISN 0125            DO 50 K=IU,IO
ISN 0126            I1=K-IU1
ISN 0127            I2=I1+IU2
ISN 0128            Y=I2*PJ*R/RCTF
ISN 0129          59 DO 60 J=IU,IO
ISN 0130            J1=J-IU1
ISN 0131            J2=J1+IU2
ISN 0132            Z=J2*PJ*R/RCTF
ISN 0133            IF (R) 70,70,80
ISN 0134          70 ERR=ERR+VARM(II+I1,II+J1)
ISN 0135            GO TO 60
ISN 0136          80 ERR=ERR+(DSIN(Y)*DSIN(Z)/(Y*Z))*VARM(II+I1,II+J1)
ISN 0137          60 CONTINUE
ISN 0138          50 CONTINUE
ISN 0139            W(I+NS)=DSQRT(ERR*CHI2*2.D0)
ISN 0140            IF (KE(17).EQ.1) GO TO 85
ISN 0142            ERR=W(I+NS)/DN*100.
ISN 0143            GO TO 90
ISN 0144          85 ERR=W(I+NS)/DM*100.
ISN 0145          90 IF (KE(11).EQ.1) WRITE (6,6010) R,DM,DN,W(I+NS),ERR,DP,DC
ISN 0147         100 CONTINUE
ISN 0148        6010 FORMAT (' ',0PF10.3,5X,6(1PD12.4,5X))
ISN 0149             IF ((KE(12).EQ.0).AND.(KE(14).EQ.0)) GO TO 203
ISN 0151             KMM=MOD(KE(14),1000)/100
ISN 0152             KMN=KE(14)/1000
ISN 0153             IF (KE(17).NE.2) KMN=0
ISN 0155             DO 110 I=1,4
ISN 0156             ND=I
ISN 0157             IF (I.EQ.1) ND=I-1
ISN 0159             IF (((KE(17).EQ.1).AND.(I.GT.1)).AND.(.NOT.((KE(15).EQ.1).AND.(I.E
                    1 Q.4)))) GO TO 110
ISN 0161             CALL MOMENT(ND,W,H,NS,RMS)
ISN 0162             IF (I.EQ.1) WRITE (6,6300)
ISN 0164        6300 FORMAT (///' MATTER DENSITY')
ISN 0165             IF (I.EQ.2) WRITE (6,6301)
ISN 0167        6301 FORMAT (///' NEUTRON DENSITY')
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```
ISN 0168            IF (I.EQ.3) WRITE (6,6302)
ISN 0170         6302 FORMAT (///' PROTON DENSITY')
ISN 0171            IF (I.EQ.4) WRITE (6,6303)
ISN 0173         6303 FORMAT (///' CHARGE DENSITY')
ISN 0174            WRITE (6,6501) (RMS(J),J=1,3),(RMS(J),J=5,10)
ISN 0175         6501 FORMAT (/' K-TH MOMENT FOR K = -2, -1, ... ,+5, +6'
                    1 /9(F12.5,2X))
ISN 0176            WRITE (6,6502) RMS(4)
ISN 0177         6502 FORMAT (/' VOLUME = ',1PD12.5)
ISN 0178            IF ((KMM.GT.0).AND.(I.EQ.1)) WRITE (8,7001) RMS
ISN 0180            IF ((KMN.GT.0).AND.(I.EQ.2)) WRITE (8,7001) RMS
ISN 0182            IF ((I.GT.2).OR.((I.EQ.1).AND.(KE(17).EQ.2))) GO TO 109
ISN 0184            CALL ERMOM (II,IU,IQ,IU1,IU2,VARM,RCTF,CHI2,RMS)
ISN 0185            WRITE (6,6503) (RMS(J),J=1,3),(RMS(J),J=5,10)
ISN 0186            WRITE (6,6504) RMS(4)
ISN 0187         6503 FORMAT (/' ERRORS OF K-TH MOMENT FOR K = -2, -1, ... ,+5, +6'
                    1 /9(1PD12.5,2X))
ISN 0188         6504 FORMAT (/' ERROR VOLUME = ',1PD12.5)
ISN 0189          109 IF ((KMM.GT.0).AND.(I.EQ.1)) WRITE (8,7001) RMS
ISN 0191            IF ((KMN.GT.0).AND.(I.EQ.2)) WRITE (8,7001) RMS
ISN 0193          110 CONTINUE
ISN 0194          203 IWP=NS*2
ISN 0195            IWS=1
ISN 0196            KDM=MOD(KE(13),1000)/100
ISN 0197            KDN=KE(13)/1000
ISN 0198            IF (KE(17).NE.2) KDN=0
ISN 0200            IF (KDM.GT.0.OR.KDN.GT.0) WRITE(7,7001) (W(I),I=IWS,IWP)
ISN 0202            IWS=IWP+1
ISN 0203            IWP=IWP+NS
ISN 0204            IF (KDN.GT.0) WRITE (7,7001) (W(I),I=IWS,IWP)
ISN 0206         7001 FORMAT((5X,'*',6(1PD10.3,',')))
ISN 0207         1000 RETURN
ISN 0208            END
```

```
                C-----POTENTIAL PRINT
ISN 0002              SUBROUTINE POTPR(P,W,NP,M,N,VARM,CHI2)
ISN 0003              IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004              REAL*4 WI(1000)
ISN 0005              DIMENSION P(2),PR(2),PI(2),W(2),VARM(30,30),RMS(10)
ISN 0006              REAL*8 PJ/3.14159265358979300/
ISN 0007              COMMON /INPT/KE(42),WI,IN(100)
ISN 0008              COMMON /IFIT/IA(30),NC,ID
ISN 0009              NRC=P(NP+3)*(P(NP+6)+P(NP+7)-1.)+1.
ISN 0010              RC=NRC
ISN 0011              H=.100
ISN 0012              AH13=P(3)**(1.00/3.00)
ISN 0013              NA2=WI(2)+.2
ISN 0014              HA=P(NP+3)
ISN 0015              NSA=P(NP+6)
ISN 0016              MSA=P(NP+7)
ISN 0017              P(NP+3)=H
ISN 0018              NS=RC/H+2
ISN 0019              MS=0
ISN 0020              P(NP+6)=NS
ISN 0021              P(NP+7)=MS
ISN 0022              NN=1
ISN 0023              CALL POTE(P,PR,PI,NN)
ISN 0024              IF (KE(15).EQ.1) GO TO 6
ISN 0026              R=P(2)*AH13
ISN 0027              A=1.43985*P(NP+4)/R
ISN 0028              V2=-.5*A/(R*R)
ISN 0029              V0=A-R*R*V2
ISN 0030            6 NF=IN(8)
ISN 0031              IO=IA(NF)
ISN 0032              IF (IO.EQ.NP) IO=IA(NF-1)
ISN 0034              IF (KE(18).LT.3) GO TO 13
ISN 0036              IOW=IO
ISN 0037              RCTFW=P(29)
ISN 0038              RCTFW2=RCTFW-.01
ISN 0039              DO 11 I=1,NF
ISN 0040              IF (IA(I).GT.29) GO TO 12
ISN 0042           11 CONTINUE
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ISN 0043          12 IUW=IA(I)
ISN 0044             IU1W=IUW-1
ISN 0045             IU2W=IUW-30
ISN 0046             IIW=I-1
ISN 0047          13 IF (KE(9).EQ.1) WRITE (6,6010)
ISN 0049        6010 FORMAT(///' ',7X,'R',8X,'REAL',7X,
                    1 'REAL+COULOMB',3X,'IMAGINARY',5X,'ERROR IMAG',4X,'ERROR PERC',
                    2 4X,'COULOMB')
ISN 0050             R=-H
ISN 0051             DO 2 I=1,NS
ISN 0052             R=R+H
ISN 0053             P(1)=R
ISN 0054             W(I)=0.D0
ISN 0055             W(I+NS)=0.D0
ISN 0056             W(I+2*NS)=0.D0
ISN 0057             W(I+3*NS)=0.D0
ISN 0058             DV=0.D0
ISN 0059             DVW=0.D0
ISN 0060             CALL POTE(P,PR,PI,NP)
ISN 0061             IF(KE(15).EQ.0) GO TO 3
ISN 0063             CALL COULPO(2,P,R,VC,VD)
ISN 0064             GO TO 1
ISN 0065          3  IF (R-P(2)*AH13) 4,5,5
ISN 0066          4  VC=V0+R*R*V2
ISN 0067             GO TO 1
ISN 0068          5  VC=1.43985*P(NP+4)/R
ISN 0069          1  PR(2)=PR(1)
ISN 0070             PR(1)=PR(1)-VC
ISN 0071             W(I)=PR(1)
ISN 0072             W(I+NS)=PI(1)
ISN 0073             IF (KE(18).LT.3) GO TO 81
ISN 0075             IF (R.GE.RCTFW2) GO TO 81
ISN 0077             DO 150 K=IUW,IOW
ISN 0078             I1=K-IU1W
ISN 0079             I2=I1+IU2W
ISN 0080             Y=I2*PJ*R/RCTFW
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ISN 0081            DO 160 J=IUW,IOW
ISN 0082            J1=J-IU1W
ISN 0083            J2=J1+IU2W
ISN 0084            Z=J2*PJ*R/RCTFW
ISN 0085            IF (R) 170,170,180
ISN 0086          170 DV=DV+VARM(IIW+I1,IIW+J1)
ISN 0087            GO TO 160
ISN 0088          180 DV=DV+(DSIN(Y)*DSIN(Z)/(Y*Z))*VARM(IIW+I1,IIW+J1)
ISN 0089          160 CONTINUE
ISN 0090          150 CONTINUE
ISN 0091            W(I+2*NS)=DSQRT(DV*CHI2*2.D0)
ISN 0092            DVW=-W(I+2*NS)/PI(1)*100.
ISN 0093           81 IF (KE(9).EQ.1) WRITE (6,6110)R,PR(1),PR(2),PI(1)
                   1 ,W(I+2*NS),DVW,VC
ISN 0095            2 CONTINUE
ISN 0096         6110 FORMAT (' ',0PF10.3,2X,6(1PD12.4,2X))
ISN 0097         6300 FORMAT (///' REAL POTENTIAL')
ISN 0098           31 KMR=MOD(KE(14),10)
ISN 0099            IF ((KE(10).EQ.0).AND.(KMR.EQ.0)) GO TO 30
ISN 0101            NV=0
ISN 0102            WRITE (6,6300)
ISN 0103            CALL MOMENT(NV,W,H,NS,RMS)
ISN 0104            WRITE (6,6001) (RMS(I),I=1,3),(RMS(I),I=5,10)
ISN 0105         6001 FORMAT (//' K-TH MOMENT FOR K = -2, -1, ...,+5, +6'/9(F12.5,2X))
ISN 0106            VOL=RMS(4)/(P(3)*NA2)
ISN 0107            WRITE (6,6002) RMS(4),VOL
ISN 0108         6002 FORMAT (/' VOLUME = ',1PD12.5,'   PER NUCLEON PAIR = ',1PD12.5)
ISN 0109            IF (KMR.GT.0) WRITE (8,7001) RMS
ISN 0111            IF ((KE(17).NE.0).OR.(KE(16).LT.3)) GO TO 32
ISN 0113            CALL ERMOM(II,IU,IO,IU1,IU2,VARM,RCTF,CHI2,RMS)
ISN 0114            VOL=RMS(4)/(P(3)*NA2)
ISN 0115            WRITE (6,6501) (RMS(I),I=1,3),(RMS(I),I=5,10)
ISN 0116         6501 FORMAT (//' ERRORS OF K-TH MOMENT FOR K = -2, -1, ... ,+5, +6'
                   1 /9(1PD12.5,2X))
ISN 0117            WRITE (6,6502) RMS(4),VOL
ISN 0118         6502 FORMAT (/' ERROR VOLUME = ' ,1PD12.5,'   PER NUCLEON PAIR = ',
                   1 1PD12.5)
ISN 0119            IF (KMR.GT.0) WRITE (8,7001) RMS
ISN 0121         6400 FORMAT (///' IMAGINARY POTENTIAL')
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ISN 0122          32 KMI=MOD(KE(14),100)/10
ISN 0123             IF ((KE(10).LT.2).AND.(KMI.EQ.0)) GO TO 30
ISN 0125             NV=1
ISN 0126             WRITE (6,6400)
ISN 0127             CALL MOMENT(NV,W,H,NS,RMS)
ISN 0128             VOL=RMS(4)/(P(3)*NA2)
ISN 0129             WRITE (6,6001) (RMS(I),I=1,3),(RMS(I),I=5,10)
ISN 0130             WRITE (6,6002) RMS(4),VOL
ISN 0131             IF(KE(18).LT.3) GO TO 30
ISN 0133             CALL ERMOM(IIW,IUW,IOW,IU1W,IU2W,VARM,RCTFW,CHI2,RMS)
ISN 0134             VOL=RMS(4)/(P(3)*NA2)
ISN 0135             WRITE (6,6501) (RMS(I),I=1,3),(RMS(I),I=5,10)
ISN 0136             WRITE (6,6502) RMS(4),VOL
ISN 0137          30 P(NP+3)=HA
ISN 0138             P(NP+6)=NSA
ISN 0139             P(NP+7)=MSA
ISN 0140             IWP=NS
ISN 0141             IF ((KE(16).GT.2).AND.(KE(16).LT.5)) IWP=IWP+NS
ISN 0143             IWS=1
ISN 0144             KPR=MOD(KE(13),10)
ISN 0145             KPI=MOD(KE(13),100)/10
ISN 0146             IF (KPR.GT.0) WRITE (6,7001) (W(I),I=IWS,IWP)
ISN 0148             IWS=IWP+1
ISN 0149             IWP=IWP+NS
ISN 0150             IF (KE(18).GT.2) IWP=IWP+NS
ISN 0152             IF (KPI.GT.0) WRITE (6,7001) (W(I),I=IWS,IWP)
ISN 0154       7001 FORMAT ((5X,'*',6(1PD10.3,',')))
ISN 0155       1000 RETURN
ISN 0156             END
```

```
ISN 0002            SUBROUTINE CONSTR(M,N,F,X,P,W4)
ISN 0003            IMPLICIT REAL*8 (A-H,O-Z)
ISN 0004            DIMENSION F(2),X(2),P(2)
ISN 0005            REAL*4 W4(2)
ISN 0006            COMMON /CON/ VNEG
ISN 0007            W4(4)=W4(4)*VNEG
ISN 0008            RETURN
ISN 0009            END
```

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