Computer Physics Communications 25 (1982) 125–139
North-Holland Publishing Company

DFPOT – A PROGRAM FOR THE CALCULATION OF DOUBLE FOLDED POTENTIALS

J. COOK *

Wheatstone Laboratory, King's College, Strand, London, WC2R 2LS, UK

Received 31 July 1981

PROGRAM SUMMARY

Title of program: DFPOT

Catalogue number: ABQP

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computer: IBM 360/195; *installation*: Rutherford laboratory

Operating system: HASP

Programming language used: FORTRAN IV

High speed storage required: 81768 bytes

No. of bits in a word: 64

Overlay structure: none

No. of magnetic tapes required: none

Other peripherals used: card reader, line printer, disc drive (optional), card punch (optional)

No. of cards in combined program and test deck: 964

Card punching code: EBCDIC (029)

Keywords: double folded potentials, transition potentials, convolution, Fourier transforms, elastic and inelastic scattering, density dependent interactions

Nature of physical problem
The program calculates double folded potentials for use in nuclear scattering problems by integrating a nucleon–nucleon interaction over the density distributions of the two colliding nuclei as described in ref. [1]. Potentials for elastic, inelastic and other scattering processes may be generated by appropriate choice of the interaction and the densities. In addition to a wide range of density independent interactions, a restricted class of density dependent interactions may also be employed.

Method of solution
The potential is calculated by making multipole expansions of the densities and performing the integration in momentum space by a Fourier transform technique.

Restrictions on the complexity of the problem
The program has been written to be very general with few restrictions. The main restriction is that only a limited type of density dependent interactions may be used. Other minor restrictions are described fully in the long write-up.

Typical running time
Using the IBM H-compiler the test calculation described in section 6 of the long write-up took 16.6 s to compile, 0.4 s to link-edit and 2.1 s to execute.

Reference

[1] G.R. Satchler and W.G. Love, Phys. Rep. 55 (1979) 183.

* Present address: Department of Physics, Florida State University, Tallahassee, FL 32306, USA.

0010-4655/82/0000–0000/$02.75

LONG WRITE-UP

1. Introduction

One of the most widely used approaches to describe the elastic scattering of two nuclei is based on the optical potential. Customarily phenomenological Saxon–Woods forms are used for both the real and imaginary parts of the optical potential. However, it would be desirable ro relate the nucleus–nucleus nuclear potential to the nucleon–nucleon nuclear interaction in much the same way as the ion–ion Coulomb potential is related to the point charge Coulomb interaction. In the latter case the potential is obtained by integrating the r^{-1} Coulomb interaction over the charge distributions of the two ions. Similarly the nuclear potential may be obtained by integrating a nucleon–nucleon interaction over the matter distributions of the two colliding nuclei. This approach is called the folding model and has been reviewed by Satchler and Love [1].

Initially calculations of folded potentials were of the "single-folding" form. In this approach a phenomenological nucleon–nucleus potential $U_{1N}(r)$ describing the interaction of a nucleon with nucleus 1 was integrated over the density distribution $\rho_2(r)$ of nucleus 2

$$U_F(\boldsymbol{R}) = \int d\boldsymbol{r}_2 \rho_2(\boldsymbol{r}_2)\, U_{1N}(\boldsymbol{R} - \boldsymbol{r}_2). \tag{1}$$

However, for heavy-ion scattering it was found that this approach overestimated the strength of the potential by a factor of about 2 and therefore the full "double-folding" form had to be used. Then the nucleon–nucleon interaction $V(r)$ is integrated over both density distributions

$$U_F(\boldsymbol{R}) = \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2 \rho_1(\boldsymbol{r}_1)\, \rho_2(\boldsymbol{r}_2)\, V(\boldsymbol{R} - r_1 + r_2). \tag{2}$$

The single-folded form may be viewed as a special case with $\rho_1(r) = \delta(r)$ and may be calculated as such.

In addition to its use for elastic scattering the folding model may also be employed to calculate transition potentials for inelastic scattering and other reaction processes if a suitable interaction is integrated over the appropriate transition densities of the two nuclei.

This paper describes the computer code DFPOT which is a general program for the calculation of double folded potentials. The densities and interaction may be generated by successively adding various contributions together and a limited class of density dependent interactions may also be utilised.

2. General description of the problem

2.1. Formalism of the folded potential

The calculation of double folded potentials by Fourier transform techniques is described in ref. [1]. Only the essential features are reproduced here, following closely the notation of ref. [1].

The double folded potential is written as

$$U(\boldsymbol{R}) = \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2 \rho_1(\boldsymbol{r}_1)\, \rho_2(\boldsymbol{r}_2)\, V(\boldsymbol{R} - \boldsymbol{r}_1 + \boldsymbol{r}_2), \tag{3}$$

where $\rho_1(\boldsymbol{r}_1)$ and $\rho_2(\boldsymbol{r}_2)$ are the density distributions and $V(\boldsymbol{r})$ is the effective nucleon–nucleon interaction. Defining Fourier transforms by

$$\tilde{f}(\boldsymbol{q}) = \int \exp(\boldsymbol{q} \cdot \boldsymbol{r})\, f(\boldsymbol{r})\, d\boldsymbol{r}, \tag{4a}$$

with inverse transform

$$f(\boldsymbol{r}) = \frac{1}{(2\pi)^3} \int \exp(-i\boldsymbol{q} \cdot \boldsymbol{r})\, \tilde{f}(\boldsymbol{q})\, d\boldsymbol{q}, \tag{4b}$$

the potential is conveniently calculated from the expression

$$\tilde{U}(\boldsymbol{q}) = \tilde{\rho}_1(\boldsymbol{q})\, \tilde{\rho}_2(-\boldsymbol{q})\, \tilde{V}(\boldsymbol{q}). \tag{5}$$

It is convenient to make multipole expansions of the densities and the folded potential (it is assumed throughout that V is a scalar in coordinate space). Then

$$U(\boldsymbol{R}) = \sum_L C_L U^{LM}(\boldsymbol{R})\, Y^*_{LM}(\hat{\boldsymbol{R}}), \tag{6}$$

where L is the multipolarity of the folded potential and C_L describes a product of Clebsch–Gordon coefficients (see ref. [1]). The program DFPOT calculates the quantity $U^{LM}(R)$, which is given by

$$U^{LM}(R) = \frac{1}{2\pi^2}\int_0^\infty \tilde{U}^{LM}(q)\, j_L(qR)\, q^2\, \mathrm{d}q, \qquad (7)$$

where

$$\tilde{U}^{LM}(q) = \mathrm{i}^{L_1-L_2-L}\langle L0|L_1L_200\rangle \frac{\hat{L}_1\hat{L}_2}{\hat{L}} \times \frac{F_{L_1}F_{L_2}}{\sqrt{4\pi}\,F_L}\tilde{\rho}_1^{L_1}(q)\,\tilde{\rho}_2^{L_2}(q)\,\tilde{V}^0(q). \qquad (8)$$

In this expression

$$\hat{x} = (2x+1)^{1/2}, \qquad (9a)$$

$$F_L = \begin{cases} \sqrt{4\pi}, & L=0, \\ 1, & L\neq 0, \end{cases} \qquad (9b)$$

$$\tilde{f}^L(q) = 4\pi\int_0^\infty f^L(r)\, j_L(qr)\, r^2\, \mathrm{d}r, \qquad (9c)$$

where $f^L(r)$ is the Lth multipole term for the densities or interaction. L_1 and L_2 are the multipolarities of densities 1 and 2, respectively.

It should be noted that the $U^{LM}(R)$ as defined above may be used directly in DWBA programs such as DWUCK[2] and coupled channels programs such as CHUCK[3].

2.2. Calculation of the Fourier transforms

The integrals that must be evaluated for the Fourier transforms have the form

$$I = \int_0^\infty f(r)\, j_L(kr)\, r^2\, \mathrm{d}r. \qquad (10)$$

Integrals of this kind are notoriously complicated to evaluate numerically due to the oscillatory nature of the spherical Bessel function and the infinite upper limit. Certain elaborate methods have been proposed [4] but for this program simplifications can be made since the functions $f(r)$ fall-off rapidly with increasing r and the infinite upper limit can be replaced by a finite one with little loss of accuracy.

Firstly, the spherical Bessel function is decomposed into sine and cosine parts

$$j_L(x) = u_L(x)\sin(x) + v_L(x)\cos(x).$$

Formulae for $u_L(x)$ and $v_L(x)$ are given in ref. [5]. Then two integrals have to be evaluated

$$S = \int_0^a f(r)\, u_L(kr)\sin(kr)\, r^2\, \mathrm{d}r, \qquad (11a)$$

$$C = \int_0^a f(r)\, v_L(kr)\cos(kr)\, r^2\, \mathrm{d}r. \qquad (11b)$$

Filon's formulae [5] are used in both cases. A further simplification is possible for $L \doteq 0$ since then $v_L(x) = 0$ and only the S integral is required.

2.3. Accuracy

The accuracy of the calculation relies upon two factors

a) Accuracy of the Fourier transforms of the densities and the interaction. To pick up all the major Fourier components a small mesh size ($\Delta r \leq 0.05$ fm) and a large enough integration radius are required. For the interaction we have found $r_{max} = 10$ fm to be sufficient. The maximum radius for the densities depends upon the mass number. For light nuclei $r_{max} \approx 10$ fm is reasonable, whilst for heavy nuclei, such as lead, $r_{max} \approx 15$ fm is more appropriate. An empirical rule to use is $r_{max} = 3.5A^{1/3}$ fm.

b) A sufficient range of momenta to provide accurate inverse transforms. The Fourier transforms for individual functions fall off slowly with q but the product of the three transforms for the densities and the interaction falls off quickly with q and in all cases the author has encountered sufficient accuracy was obtained with $q_{max} = 3.0$ fm^{-1}. This is consistent with the findings of Goldfarb [6]. The choice of momentum interval size is not very crucial.

Exhaustive comparisons have been made with the folding code DOLFIN [7]. The programs take roughly equal times to calculate the potentials and for the test case in section 6 produce values which agree within 2×10^{-6} for $R<6$ fm. For larger radii the agreement becomes poorer and is only $\approx 1\%$ at 9 fm. However, it is not possible to check

whether DOLFIN or DFPOT is producing the more correct results.

For $L_1 + L_2 = L$ certain consistency checks are possible employing the r^2 and r^4 weighted volume integrals of the functions ρ_1, ρ_2, V and U [8]. Defining

$$J_k(f^L) = 4\pi \int_0^\infty f^L(r)\, r^{k+2}\, \mathrm{d}r, \tag{12}$$

$$R_k(f^L) = J_{k+2}(f^L)/J_k(f^L), \tag{13}$$

these checks are

$$J_L(U^L) = \langle L0 | L_1 L_2 00 \rangle \times \frac{(2L+1)!!}{(2L_1+1)!!(2L_2+1)!!} \frac{\hat{L}_1 \hat{L}_2}{\hat{L}} \times \frac{F_{L_1} F_{L_2}}{\sqrt{4\pi}\, F_L} J_{L_1}(\rho_1^{L_1})\, J_{L_2}(\rho_2^{L_2})\, J_0(V^0) \tag{14}$$

and

$$R_L(U^L) = (2L+3)\left\{ \frac{R_{L_1}(\rho_1^{L_1})}{(2L_1+3)} + \frac{R_{L_2}(\rho_2^{L_2})}{(2L_2+3)} + \frac{R_0(V^0)}{3} \right\}. \tag{15}$$

2.4. Charge and matter distributions

The densities appearing in eq. (3) are *matter* densities (sometimes called "point densities"). However, densities derived from electron scattering are *charge* densities and must be corrected for the nucleon charge distribution before they are used. This is conveniently done in momentum space:

$$\tilde{\rho}_{\mathrm{ch}}(q) = \tilde{\rho}_{\mathrm{p}}(q)\, \tilde{\rho}_{\mathrm{p,ch}}(q) + \tilde{\rho}_{\mathrm{n}}(q)\, \tilde{\rho}_{\mathrm{n,ch}}(q), \tag{16}$$

where ρ_{ch} is the charge distribution of the nucleus and $\rho_{\mathrm{p,ch}}$ and $\rho_{\mathrm{n,ch}}$ of the proton and neutron, respectively. ρ_{p} and ρ_{n} are the point distributions of protons and neutrons within the nucleus. If it is assumed that $\rho_{\mathrm{n}} = (N/Z)\,\rho_{\mathrm{p}}$ then the nuclear point density is found from

$$\tilde{\rho}(q) = \left(1 + \frac{N}{Z}\right) \tilde{\rho}_{\mathrm{ch}}(q)/\tilde{\rho}_{\mathrm{N,ch}}(q) \tag{17}$$

where $\rho_{\mathrm{N,ch}} = \rho_{\mathrm{p,ch}} + (N/Z)\,\rho_{\mathrm{n,ch}}$ is approximated by

$$\rho_{\mathrm{N,ch}}(r) = \frac{\alpha^3}{8\pi}\, \mathrm{e}^{-\alpha r}. \tag{18}$$

The parameter α is chosen to reproduce the mean-square charge radius of the nucleon through [1]

$$\langle r^2 \rangle_{\mathrm{N}} = \frac{12}{\alpha^2} = 0.76\text{–}0.11(N/Z)\ \mathrm{fm}^2. \tag{19}$$

2.5. Density-dependent interactions

Folded potentials employing density-dependent interactions of the form

$$V(r,\rho) = V(r)\, \mathrm{e}^{-\beta\rho(r)}, \tag{20}$$

may be conveniently calculated by modifying the densities

$$\rho^L(r) \to \rho^L(r)\, \mathrm{e}^{-\beta\rho_{\mathrm{gs}}(r)}, \tag{21}$$

where ρ^L is the transition density and ρ_{gs} the ground state density (note that for elastic scattering $\rho^L = \rho_{\mathrm{gs}}$). The density appearing in the exponent may be either ρ_1 or ρ_2 (i.e. density dependence for only one nucleus) or $\rho_1 + \rho_2$ (i.e. density dependence for both nuclei).

In the program DFPOT potentials using a sum of density independent and density dependent interactions

$$V(r,\rho) = V_1(r) + V_2(r)\, \mathrm{e}^{-\beta\rho(r)} \tag{22}$$

or a sum of several density dependent interactions

$$V(r,\rho) = V_1(r)\, \mathrm{e}^{-\beta_1\rho(r)} + V_2(r)\, \mathrm{e}^{-\beta_2\rho(r)} \tag{23}$$

may be calculated by calculating a folded potential with each part of the interaction separately, storing on disc and adding the two parts together later. This facility is quite general and could be used in other cases, e.g. for adding isoscalar and isovector potentials together.

3. Program description

The section below summarises the function and operation of each subroutine. The various COM-

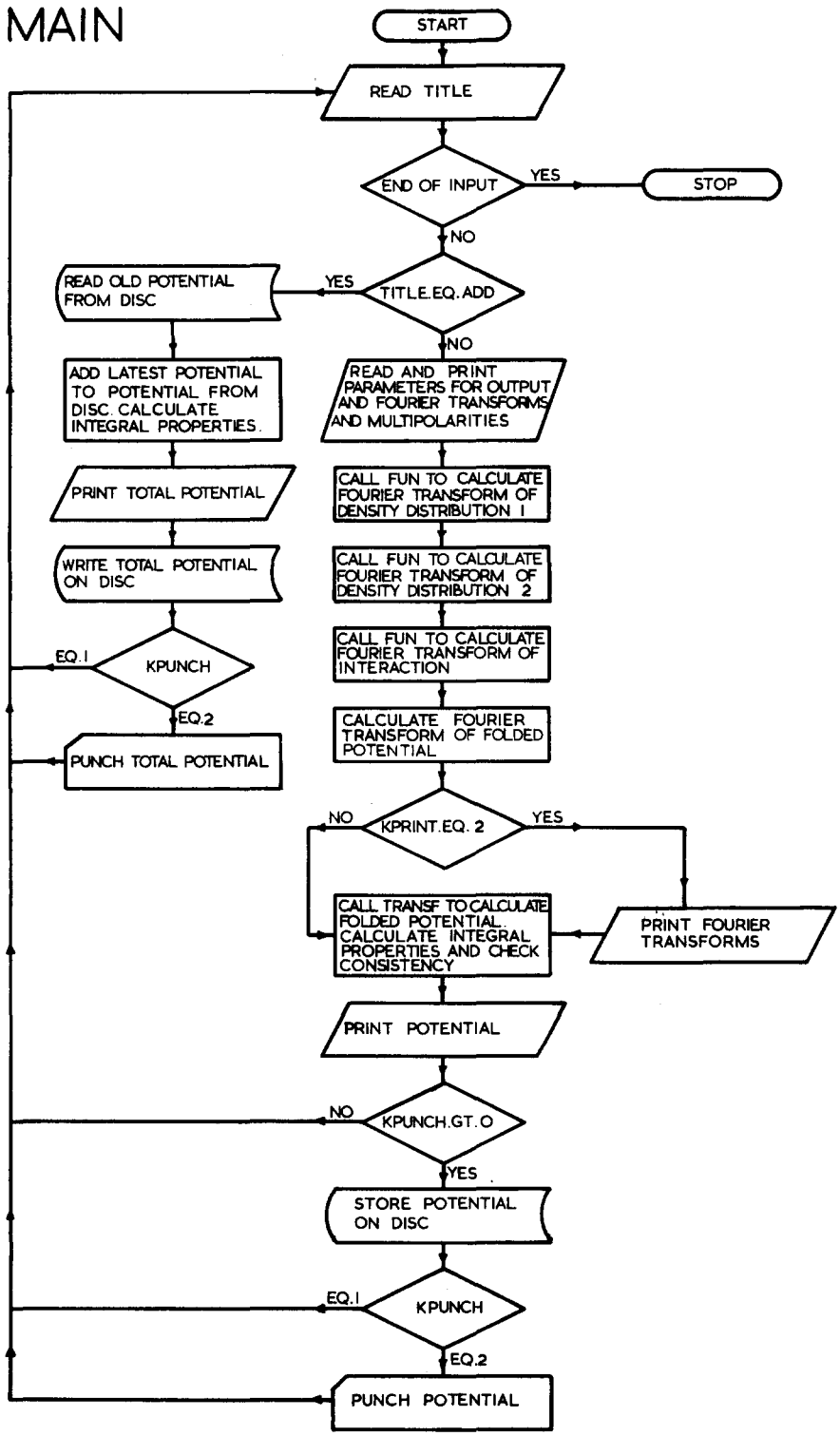

Fig. 1. Flow diagram for subroutine MAIN.

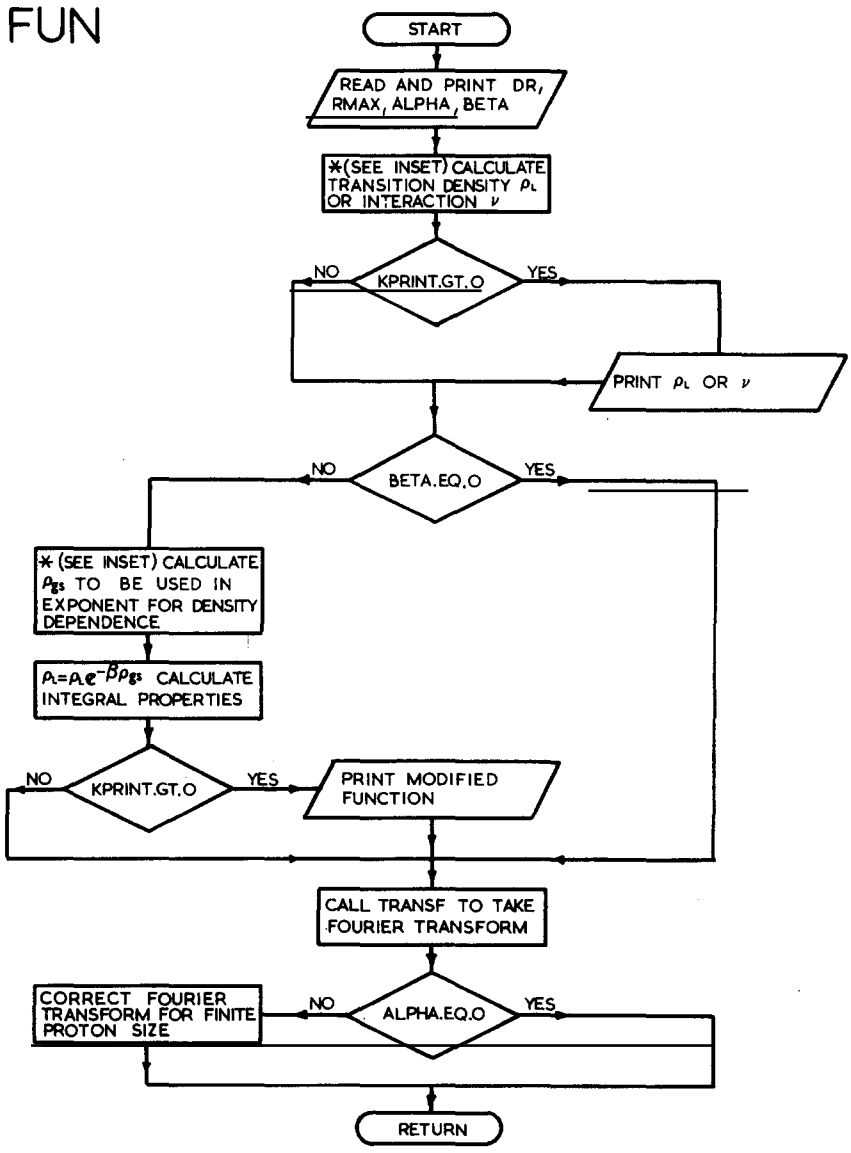

Fig. 2. Flow diagram for subroutine FUN.

MON blocks are described in the comment cards for each subroutine.

MAIN controls the operation of the whole program. Its flow diagram is shown in fig. 1. It calls subroutine FUN three times to successively calculate the Fourier transforms of the two density distributions and of the effective interaction. These three transforms are then multiplied together to form the Fourier transform of the folded potential and subroutine TRANSF is called to obtain the folded potential in configuration space. The accuracy of the calculation of the folded potential is checked through the consistency of its integral properties, with those of the densities and interaction. MAIN also controls the output of the potential: lineprinter, disc and punched card output.

Successive potentials stored on disc may be added together to generate a potential involving complicated combinations of densities and interactions (e.g. for density dependent interactions, or for a sum of isoscalar and isovector potentials).

Subroutine FUN calculates the density distributions and interaction to be used in the folding procedure. Its flow diagram is given in fig. 2. Successive contributions of different functional forms may be added to build up complicated densities and interactions. Each contribution may be normalised to, for example, the mass or multipole moment. If a density dependent interaction is involved then two densities must be calculated: a transition density ρ^L describing the transition and a ground state density ρ_{gs} to give the amount of density dependence. The integral properties of the contributions and the total function are calculated to facilitate checking the consistency of the whole calculation. Subroutine TRANSF is then called to calculate the Fourier transform of the function, and if charge distributions have been calculated the transform is corrected for the proton charge distribution.

Subroutines GAUSS, YUKAWA, FERMI, SAXON, CARDIN, USER, DELTA and TASSIE are all used to provide functions for building up density distributions and interactions in subroutine FUN. The various functions are suggested by the subroutine names and full details are given in the section describing the input instructions.

TRANSF calculates the Fourier transforms and inverse transforms. For economic computing the subroutine is divided into two parts, firstly for $L = 0$ and secondly for $L > 0$. In the first case only the Filon sine integral needs to be calculated, whilst for $L > 0$ the spherical Bessel function must be decomposed into sine and cosine parts and both Filon sine and Filon cosine integrals must be calculated.

The spherical Bessel function is decomposed for $L > 0$ into its sine and cosine parts by subroutines SBES and CBES. The decomposition is effected as

$$j_L(x) = \mathrm{SBES(L, X)}\,\sin(x) + \mathrm{CBES(L, X)}\,\cos(x).$$

INTEGR calculates the r^2 and r^4 weighted volume integrals of various functions using a Simpson integration technique.

The Clebsch–Gordon coefficient $\langle L0|L_1L_200\rangle$ is calculated in subroutine CLEB. FACT2 calculates double factorials.

Subroutine PRINT is used to print the densities, interaction and folded potential in a standard format.

4. Input card requirements

Card 1 Title card
TITLE Format (80A1)

This card contains a title for the user's convenience. If an end-of-file is encountered the program stops execution. If the word ADD is punched in the first three columns then the program adds the last calculated potential $U_{\mathrm{LAST}}(r)$ to one previously stored on disc $U_{\mathrm{DISC}}(r)$. In this case both potentials should have the same values of DROUT and RMAX. A further card is required in this instance

C1, C2 Format (2F10.0)

so that the total potential is given by

$$U_{\mathrm{total}}(r) = \mathrm{C1}\; U_{\mathrm{DISC}}(r) + \mathrm{C2}\; U_{\mathrm{LAST}}(r).$$

Card 2 Parameters for output and Fourier transforms
DROUT, RMAX, DQ, QMAX, KPRINT, KPUNCH, PUNFMT Format (4F10.0, 2I5, 5A4)

DROUT	radial intervals at which the folded potential is to be calculated,
RMAX	maxium radius for calculation of the folded potential. RMAX/DROUT $\leq$ 1000 otherwise RMAX is reset to satisfy this,
DQ	momentum interval for calculation of Fourier transforms. Default value 0.02 fm^{-1},
QMAX	maximum momentum for calculation of Fourier transforms. Default value 3.0 fm^{-1}. QMAX/DQ $\leq$ 1000 otherwise QMAX is reset to satisfy this,

KPRINT = 0 suppresses printing of densities, interaction and Fourier transforms,
* = 1 suppresses printing of Fourier transforms,
= 2 full printout,
KPUNCH = 0 potential printed only,
= 1 potential printed and stored on disc (Fortran stream 8),
= 2 potential printed, stored on disc and punched in format PUNFMT,
PUNFMT format for punching potential, e.g. (6E12.5).

Card 3 Multipolarities
L1, L2, LU Format (3I10)

Multipolarities for density distribution 1, density distribution 2 and the folded potential respectively. Limitation is $L1 + L2 + LU \leq 60$.

Card 4 Parameters for density distribution or interaction
DR, RMAX, ALPHA, BETA Format (4F10.0)

DR radial intervals at which function is to be calculated,
RMAX maximum radius for calculation of function. RMAX/DR $\leq$ 1000 otherwise RMAX is reset to satisfy this,
ALPHA parameter used for unfolding of nucleon charge distribution,
BETA parameter used for density dependent interactions.

Card 5 Option card (see fig. 3)
IOPT, A, SIGN Format (I10, 2F10.0)

IOPT Selects the type of function required,
|IOPT| = 1 Gaussian function,
= 2 Yukawa function,
= 3 3 parameter Fermi function,
= 4 Saxon–Woods functions,
= 5 function read from cards,
= 6 user defined function,
= 7 delta function,
= 8 Tassie transition density,
= 9 density dependence for elastic scattering,

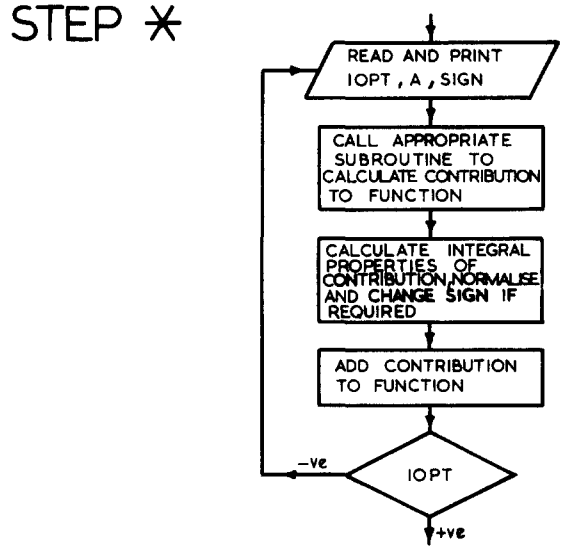

Fig. 3. Flow diagram for subroutine STEP*.

A For $L = 0$ the function is normalized so that $A = 4\pi\int_0^\infty f(r) r^2 dr$, e.g. the mass, and for $L > 0$ so that $A = \int_0^\infty f(r) r^{L+2} dr$, e.g. the multipole moment. If A = 0.0 the function is not renormalised,
SIGN < 0.0 the sign of the function is changed,
$\geq$ 0.0 the sign of the function is not changed.
The use of this parameter is primarily intended for when A = 0.0.

Next follow the input cards for the function as described in the following sections. Successive functions may be added together to generate a complicated total function. If IOPT is negative then the function corresponding to |IOPT| is computed and further functions may be calculated until IOPT becomes positive.

The calculation of the transition density for nucleus 1 is now complete. If density dependence has been specified (BETA $\neq$ 0.0) then card 5 (with the appropriate input cards for the selected function) must be repeated to generate the ground state density distribution to be used in the exponent for modifying the transition density. Cards 4 and 5 must then be repeated to calculate the

density distribution of nucleus 2 and the interaction. After completion of the calculation of the folded potential, execution returns to card 1 to begin a new calculation.

The following sections describe the various types of functions, and their input cards, which may be added together to build up the density distributions and the effective interaction.

IOPT = 1 Gaussian function
Card 1 C, ALPHA, PWR Format (3F10.0)

$$f(r) = Cr^{PWR}\exp\left[-(r/\alpha)^2\right].$$

N.B. C has a default value of 1.0.

IOPT = 2 Yukawa function
Card 1 V, BETA Format (2F10.0)

$$f(r) = Ve^{-\beta r}/\beta r.$$

N.B. V has a default value of 1.0.

IOPT = 3 3 parameter Fermi function
Card 1 C, RR, AR, W Format (4F10.0)

$$f(r) = C\{1 + Wr^2\}\Big/\left[1 + \exp\left(\frac{r - RR}{AR}\right)\right].$$

N.B. C has a default value of 1.0.

IOPT = 4 Saxon–Woods functions
Card 1 C, RR, AR, PWR, IDER Format (4F10.0, I10)

If IDER = 0 then a Saxon–Woods function is calculated

$$f(r) = C\Big/\left[1 + \exp\left(\frac{r - RR}{AR}\right)\right]^{PWR}.$$

If IDER ≠ 0 then a derivative Saxon–Woods function is calculated

$$f'(r) = \frac{df(r)}{dr} = \left[-PWR \times C\exp\left(\frac{r - RR}{AR}\right)\right]\Big/ \left\{AR\left[1 + \exp\left(\frac{r - RR}{AR}\right)\right]^{PWR+1}\right\}.$$

N.B. C has a default value of 1.0, PWR has a default value of 1.0.

IOPT = 5 Card input
Card 1 INFMT, DRIN, NVAL, ISTART Format (5A4, F10.0, 2I10)
Cards 2–N Values to be read in Format (INFMT)

INFMT is the format in which the cards are to be read in, e.g. (6E12.5),
DRIN is the radial interval between the values,
NVAL number of values to be read in,
ISTART = 0 first value at $r = 0$,
= 1 first value at r = DRIN.

If DR ≠ DRIN the function is interpolated at the correct radii using a 4 point Lagrangian method.

IOPT = 6 User defined function
The user may define his own function in subroutine USER using the guidelines in the comment cards and the other subroutines as examples.

IOPT = 7 Delta function
Card 1 V Format (F10.0)

$$f(r) = V\delta(r).$$

N.B.
1) V has a default value of 1.0,
2) this option may be used for one of the densities when only a single folding is required,
3) this option may not be used for generating the function to be used in the exponent for density dependence,
4) the Fourier transform is undefined for $L \neq 0$. In this case the Fourier transform for $L = 0$ is assumed.

IOPT = 8 Tassie transition density
Card 1 ITYPE Format (I10)

The subroutine TASSIE takes the total function calculated by previous values of IOPT and then computes the Tassie type transition density according to ITYPE
ITYPE = 0 (for $L \neq 0$)

$$f(r) = r^{L-1}\,dg(r)/dr,$$

ITYPE = 1

$$f(r) = dg(r)/dr,$$

where $g(r)$ is the total function already calculated.

$f(r)$ may then be normalised to, for example, the B(EL) value through use of the parameter A on the option card.

IOPT = 9 Density dependence for elastic scattering
No input cards required.

For elastic scattering the transition density and the ground state density are identical, i.e. $\rho^L = \rho_{gs}$. For density dependent interactions the same quantity is used for both parts of the modified density

$$\rho_{gs}(r) \to \rho_{gs}(r) \exp\{-\beta\rho_{gs}(r)\}.$$

N.B. This option can only be used for calculating the exponent function and cannot be used for the normal calculation of the function.

5. Description of the output

As a check the program prints out all of the data read in. Units are MeV for energies, fm for lengths and fm^{-1} for momenta. The Clebsch–Gordon coefficient $\langle L0|L_1L_200\rangle$ is printed for the user's convenience.

The output for each of the densities and the effective interaction is identical and is only described here once. The densities and interaction are constructed from a sum of functions. For each function selected the name of the function is printed and also the values of the parameters used. The factor required for normalisation of the function (including the change of sign if SIGN < 0) to A is printed. The r^2 and r^4 weighted volume integrals of each individual function are printed and also their sum for the end of each calculation. If KPRINT > 0 the total density or interaction is then printed.

If a density dependent interaction is being used (BETA ≠ 0) the output above is repeated for the function appearing in the exponent. It KPRINT > 0 the total modified density is printed. A message is printed if the density has been corrected for the nucleon charge distribution (ALPHA ≠ 0).

If KPRINT = 2 the Fourier transforms of the two densities, the interaction and the folded potential are then printed. The integral properties of the folded potential are then printed and their consistency checked. Finally, the folded potential itself is printed. If several potentials are to be added together (TITLE = ADD) the total potential is then printed.

Output other than on a lineprinter can be obtained by use of the KPUNCH parameter. For KPUNCH = 0 only lineprinter output is produced. For KPUNCH > 0 the potentials are written onto disc (Fortran stream 8). On exit from the program only the last calculated potential remains on the disc. The storage is unformatted. For KPUNCH = 2 each potential calculated is punched on cards (Fortran stream 7) in the format specified on card 2. Suitable JCL cards must be included to define the disc data set and the card punch.

6. Test calculation

The test calculation consists of the folding of a Gaussian density to simulate an α-particle with the sum of two Saxon–Woods densities for the proton and neutron distributions for ^{40}Ca. The former is normalised to 4, whilst the latter already has the correct normalisation. The M3Y interaction [1] is used and the $L = 0$ potential for elastic scattering is generated.

Acknowledgement

The author acknowledges the inspiration for many features of this program to the computer program DOLFIN.

References

[1] G.R. Satchler and W.G. Love, Phys. Rep. 55 (1979) 183.
[2] P.D. Kunz, University of Colorado, unpublished.
[3] P.D. Kunz, University of Colorado, unpublished.
[4] M. Blakemore, G.A. Evans and J. Hyslop, J. Comput. Phys. 22 (1976) 352.
B. Sommer and J.G. Zabolitzky, Comput. Phys. Commun. 16 (1979) 383.
D.R. Lehman, W.C. Parke and L.C. Maximon, J. Math. Phys. 22 (1981) 1399.
[5] M. Abramowitz and I.A. Stegun, Handbook of mathematical functions (New York, Dover, 1968).
[6] L.J.B. Goldfarb, Nucl. Phys. A301 (1978) 497.
[7] L.D. Rickertsen, unpublished.
[8] G.R. Satchler, J. Math. Phys. 13 (1972) 1118.

TEST RUN OUTPUT

```
*********************************************

      DDD   FFF  PPP    OO    TTTTT
      D  D  F    P  P  O  O     T
      D  D  FFF  PPP   O  O     T
      D  D  F    P     O  O     T
      DDD   F    P      OO      T

   DOUBLE FOLDING POTENTIAL PROGRAMME

   JULIAN COOK, KING'S COLLEGE, LONDON

*********************************************

TEST CALCULATION
****************

FOR OUTPUT          DR =      0.100          RMAX =     10.000
FOR TRANSFORMS      DQ =      0.025          QMAX =      3.000


MULTIPOLARITIES     L1 =  0     L2 =  0     LU =  0
CLEBSCH-GORDAN COEFFICIENT IS      1.000


DENSITY DISTRIBUTION 1
======================
DR =      0.050     RMAX =     10.000     ALPHA =      0.0      BETA =      0.0

IOPT =  1           A =      4.000     SIGN =      0.0
---------
GAUSSIAN FUNCTION
C =     1.000     ALPHA =     1.199     PWR =     0.0
FACT =  4.263D-01     VOL(L) =     4.000     VOL(L+2)/VOL(L) =     2.124

FUNCTION
--------
```

R	F(R)	R	F(R)	R	F(R)	R	F(R)
0.05	4.255274588D-01	2.55	4.320011899D-03	5.05	6.434262743D-09	7.55	1.405947140D-18
0.10	4.232797226D-01	2.60	3.601753150D-03	5.10	4.496316510D-09	7.60	8.234860640D-19
0.15	4.195598488D-01	2.65	2.992330300D-03	5.15	3.130989350D-09	7.65	4.806291390D-19
0.20	4.144068820D-01	2.70	2.477260620D-03	5.20	2.172565560D-09	7.70	2.735313510D-19
0.25	4.078745240D-01	2.75	2.043621440D-03	5.25	1.502210410D-09	7.75	1.520009390D-19
0.30	4.000302050D-01	2.80	1.679947780D-03	5.30	1.035035450D-09	7.80	8.355588740D-20
0.35	3.909539190D-01	2.85	1.376124410D-03	5.35	7.106344760D-10	7.85	5.363529480D-20
0.40	3.807368750D-01	2.90	1.123275270D-03	5.40	4.861876250D-10	7.90	3.087294450D-20
0.45	3.694709740D-01	2.95	9.136529850D-04	5.45	3.314576940D-10	7.95	1.766413270D-20
0.50	3.572921110D-01	3.00	7.405304840D-04	5.50	2.251743420D-10	8.00	1.004503170D-20
0.55	3.442865220D-01	3.05	5.980963980D-04	5.55	1.524320450D-10	8.05	5.699513490D-21
0.60	3.305888820D-01	3.10	4.813555850D-04	5.60	1.028253530D-10	8.10	3.222484990D-21
2.20	1.397482040D-02	4.70	7.162359790D-08	7.20	5.385455970D-17	9.70	5.240804690D-30
2.25	1.194288250D-02	4.75	5.130364090D-08	7.25	3.233252580D-17	9.75	2.989479550D-30
2.30	1.017041480D-02	4.80	3.661902890D-08	7.30	1.934353330D-17	9.80	1.699037440D-30
2.35	8.630476150D-03	4.85	2.604544060D-08	7.35	1.153149930D-17	9.85	9.490243960D-31
2.40	7.297891960D-03	4.90	1.845966620D-08	7.40	6.850254490D-18	9.90	5.729460540D-31
2.45	6.149314210D-03	4.95	1.303713700D-08	7.45	4.055031580D-18	9.95	1.850387380D-31
2.50	5.163242490D-03	5.00	9.175023690D-09	7.50	2.391929170D-18	10.00	9.145415550D-32

```
TOTAL VOL(L)                    4.000
TOTAL VOL(L+2)/VOL(L)           2.124


DENSITY DISTRIBUTION 2
**********************
DR =      0.050      RMAX =      10.000      ALPHA =       0.0       BETA =       0.0

IOPT =  4           A =       0.0       SIGN =       0.0
---------
SAXON-WOODS FUNCTION
C =      0.085      RP =       3.572      AR =       0.550      PWR =       1.000
FACT =  1.0000D+00      VOL(L) =       20.001      VOL(L+2)/VOL(L) =       11.832

IOPT =  4           A =       0.0       SIGN =       0.0
---------
SAXON-WOODS FUNCTION
C =      0.084      RP =       3.588      AR =       0.550      PWR =       1.000
FACT =  1.0000D+00      VOL(L) =       19.998      VOL(L+2)/VOL(L) =       11.961

FUNCTION
--------

        R           F(R)            R           F(R)            R           F(R)            R           F(R)

      0.05    1.685249790D-01     2.55    1.463081800D-01     5.05    1.090487283D-02     7.55    1.236647930D-04
      0.10    1.684988520D-01     2.60    1.444761420D-01     5.10    1.001347220D-02     7.60    1.129256020D-04
      0.15    1.684702480D-01     2.65    1.425216850D-01     5.15    9.190695570D-03     7.65    1.031184440D-04
      0.20    1.684369320D-01     2.70    1.404410130D-01     5.20    8.451953370D-03     7.70    9.416252470D-05
      0.25    1.684046500D-01     2.75    1.382309370D-01     5.25    7.732777370D-03     7.75    8.598403760D-05
      0.30    1.683671210D-01     2.80    1.358889920D-01     5.30    7.089030600D-03     7.80    7.851556270D-05
      0.35    1.683260400D-01     2.85    1.334135610D-01     5.35    6.496713150D-03     7.85    7.169551510D-05
      0.40    1.682810730D-01     2.90    1.308040050D-01     5.40    5.952064330D-03     7.90    6.546764310D-05
      0.45    1.682318530D-01     2.95    1.280607780D-01     5.45    5.451541870D-03     7.95    5.978056700D-05
      0.50    1.681779820D-01     3.00    1.251855390D-01     5.50    4.991819360D-03     8.00    5.458735890D-05
      0.55    1.681190240D-01     3.05    1.221812520D-01     5.55    4.569779430D-03     8.05    4.984515750D-05
      0.60    1.680545020D-01     3.10    1.190522650D-01     5.60    4.182510390D-03     8.10    4.551481720D-05
      0.65    1.679838960D-01     3.15    1.158043630D-01     5.65    3.827295750D-03     8.15    4.156058620D-05
      0.70    1.679066390D-01     3.20    1.124447940D-01     5.70    3.501607150D-03     8.20    3.794981320D-05

      2.25    1.549905010D-01     4.75    1.797279460D-02     7.25    2.132569480D-04     9.75    2.266630180D-06
      2.30    1.537931200D-01     4.80    1.656425870D-02     7.30    1.947464570D-04     9.80    2.069664060D-06
      2.35    1.525028360D-01     4.85    1.525494380D-02     7.35    1.778409630D-04     9.85    1.889813750D-06
      2.40    1.511143740D-01     4.90    1.403957710D-02     7.40    1.624015820D-04     9.90    1.725591960D-06
      2.45    1.496224970D-01     4.95    1.291289470D-02     7.45    1.483014020D-04     9.95    1.575640660D-06
      2.50    1.480220780D-01     5.00    1.186969310D-02     7.50    1.354244580D-04    10.00    1.438719780D-06


TOTAL VOL(L)                    39.998
TOTAL VOL(L+2)/VOL(L)           11.866
```

EFFECTIVE INTERACTION
=====================
DR = 0.050 RMAX = 10.000 ALPHA = 0.0 BETA = 0.0

IOPT = 2 A = 0.0 SIGN = 0.0

YUKAWA FUNCTION
V = -7999.000 BETA = 4.000
FACT = 1.000D+00 VOL(L) = -1570.558 VOL(L+2)/VOL(L) = 0.375

IOPT = 2 A = 0.0 SIGN = 0.0

YUKAWA FUNCTION
V = 2134.000 BETA = 2.500
FACT = 1.000D+00 VOL(L) = 1716.258 VOL(L+2)/VOL(L) = 0.960

IOPT = 7 A = 0.0 SIGN = 0.0

DELTA FUNCTION
V = 262.000
FACT = 1.000D+00 VOL(L) = 262.000 VOL(L+2)/VOL(L) = 0.0

FUNCTION

R	F(R)	R	F(R)	R	F(R)	R	F(R)
0.05	-1.76791493D+04	2.55	5.41128829D-01	5.05	5.55229861D-04	7.55	7.17772526D-07
0.10	-6.75688164D+03	2.60	4.70183976D-01	5.10	4.85227016D-04	7.60	6.29266000D-07
0.15	-3.40543961D+03	2.65	4.08571315D-01	5.15	4.24088157D-04	7.65	5.51696765D-07
0.20	-1.90405512D+03	2.70	3.55062569D-01	5.20	3.70685634D-04	7.70	4.83710039D-07
0.25	-1.11507103D+03	2.75	3.08590414D-01	5.25	3.24035879D-04	7.75	4.24119286D-07
0.30	-6.63670120D+02	2.80	2.68227669D-01	5.30	2.83281161D-04	7.80	3.71885263D-07
0.35	-3.92282453D+02	2.85	2.33169097D-01	5.35	2.47671446D-04	7.85	3.26097683D-07
0.40	-2.24301677D+02	2.90	2.02715508D-01	5.40	2.16558982D-04	7.90	2.85959174D-07
0.45	-1.18740235D+02	2.95	1.76259888D-01	5.45	1.89369047D-04	7.95	2.50771231D-07
0.50	-5.21524761D+01	3.00	1.53275310D-01	5.50	1.65606240D-04	8.00	2.19921926D-07
0.55	-1.04631561D+01	3.05	1.33304409D-01	5.55	1.44836753D-04	8.05	1.92875151D-07
0.60	1.50844627D+01	3.10	1.15950221D-01	5.60	1.26681943D-04	8.10	1.69161197D-07
0.65	3.00849506D+01	3.15	1.00868219D-01	5.65	1.10811311D-04	8.15	1.48368511D-07
0.70	3.81835934D+01	3.20	8.77593888D-02	5.70	9.69362511D-05	8.20	1.30136477D-07
2.20	1.44865438D+00	4.70	1.42992401D-03	7.20	1.80551242D-06	9.70	2.58726550D-09
2.25	1.25856602D+00	4.75	1.24880405D-03	7.25	1.58237595D-06	9.75	2.27154498D-09
2.30	1.09337745D+00	4.80	1.09073468D-03	7.30	1.38688163D-06	9.80	1.99440385D-09
2.35	9.49855010D-01	4.85	9.52767178D-04	7.35	1.21559635D-06	9.85	1.75112105D-09
2.40	8.25175966D-01	4.90	8.32332085D-04	7.40	1.06551458D-06	9.90	1.53755416D-09
2.45	7.16878809D-01	4.95	7.27190198D-04	7.45	9.34004875D-07	9.95	1.35006834D-09
2.50	6.22818856D-01	5.00	6.35389871D-04	7.50	8.18763313D-07	10.00	1.18547404D-09

TOTAL VOL(L) 407.699
TOTAL VOL(L+2)/VOL(L) 2.597

FOURIER TRANSFORMS

Q	RHOFT1(Q)	RHOFT2(Q)	VFT(Q)	JFT(Q)
0.02	3.99912D+00	3.99492D+01	4.07589D+02	6.51169D+04
0.05	3.99646D+00	3.98012D+01	4.07258D+02	6.47802D+04
0.07	3.99204D+00	3.95558D+01	4.06708D+02	6.42226D+04
0.10	3.98586D+00	3.92144D+01	4.05939D+02	6.34495D+04
0.12	3.97793D+00	3.87793D+01	4.04952D+02	6.24684D+04
0.15	3.96826D+00	3.82533D+01	4.03748D+02	6.12887D+04
0.17	3.95687D+00	3.76398D+01	4.02331D+02	5.99214D+04
0.20	3.94376D+00	3.69427D+01	4.00702D+02	5.83794D+04
0.22	3.92895D+00	3.61663D+01	3.98863D+02	5.66767D+04
0.25	3.91247D+00	3.53157D+01	3.96818D+02	5.48289D+04
0.27	3.89433D+00	3.43959D+01	3.94570D+02	5.28522D+04
0.30	3.87456D+00	3.34126D+01	3.92121D+02	5.07637D+04
0.32	3.85319D+00	3.23717D+01	3.89477D+02	4.85811D+04
0.35	3.83024D+00	3.12792D+01	3.86641D+02	4.63222D+04
0.37	3.80574D+00	3.01415D+01	3.83617D+02	4.40050D+04
2.80	2.49256D-01	4.12051D-02	-3.07425D+01	-3.15746D-01
2.82	2.37152D-01	3.29008D-02	-3.20838D+01	-2.50333D-01
2.85	2.25535D-01	2.50855D-02	-3.33608D+01	-1.88744D-01
2.87	2.14392D-01	1.77885D-02	-3.45747D+01	-1.31858D-01
2.90	2.03709D-01	1.10315D-02	-3.57267D+01	-8.02852D-02
2.92	1.93473D-01	4.82816D-03	-3.68178D+01	-3.43921D-02
2.95	1.83670D-01	-8.14133D-04	-3.78492D+01	5.55965D-03
2.97	1.74286D-01	-5.89442D-03	-3.88220D+01	3.98825D-02
3.00	1.65309D-01	-1.04173D-02	-3.97374D+01	6.84307D-02

FOLDED POTENTIAL

VOL(L)	6.5208D+04
VOL(L+2)/VOL(L)	16.557

CONSISTENCY CHECKS

	POTENTIAL	CHECK	PCT DIFF
VOL(L)	6.5208D+04	6.5229D+04	-0.033
VOL(L+2)/VOL(L)	16.557	16.587	-0.182

NOTE ONLY VALID FOR L1 + L2 = LU

TEST CALCULATION

R	V(R)	R	V(R)	R	V(R)	R	V(R)
0.10	2.44920444D+02	2.60	1.66861628D+02	5.10	3.30673729D+01	7.60	1.27782596D+00
0.20	2.44593744D+02	2.70	1.60988554D+02	5.20	2.99273094D+01	7.70	1.09266239D+00
0.30	2.44047967D+02	2.80	1.55002135D+02	5.30	2.70086297D+01	7.80	9.33003870D-01
0.40	2.43281257D+02	2.90	1.48923051D+02	5.40	2.43057936D+01	7.90	7.95603777D-01
0.50	2.42291120D+02	3.00	1.42772816D+02	5.50	2.18121114D+01	8.00	6.77580326D-01
0.60	2.41074538D+02	3.10	1.36573589D+02	5.60	1.95198497D+01	8.10	5.76383908D-01
0.70	2.39628095D+02	3.20	1.30347933D+02	5.70	1.74204423D+01	8.20	4.89765594D-01
0.80	2.37948133D+02	3.30	1.24118620D+02	5.80	1.55046276D+01	8.30	4.15747293D-01
0.90	2.36030921D+02	3.40	1.17908385D+02	5.90	1.37626139D+01	8.40	3.52593854D-01
1.00	2.33872842D+02	3.50	1.11739712D+02	6.00	1.21842356D+01	8.50	2.98787297D-01
1.10	2.31470586D+02	3.60	1.05634600D+02	6.10	1.07591022D+01	8.60	2.53003220D-01
1.20	2.28821345D+02	3.70	9.96143539D+01	6.20	9.47673639D+00	8.70	2.14089351D-01
1.30	2.25923011D+02	3.80	9.36993741D+01	6.30	8.32670546D+00	8.80	1.81046141D-01
1.40	2.22774365D+02	3.90	8.79089640D+01	6.40	7.29872944D+00	8.90	1.53009255D-01
1.50	2.19375257D+02	4.00	8.22611532D+01	6.50	6.38278777D+00	9.00	1.29233783D-01
1.60	2.15726768D+02	4.10	7.67725383D+01	6.60	5.56920200D+00	9.10	1.09080013D-01
1.70	2.11831358D+02	4.20	7.14581460D+01	6.70	4.84870694D+00	9.20	9.20005756D-02
1.80	2.07692988D+02	4.30	6.63313190D+01	6.80	4.21250632D+00	9.30	7.75288261D-02
1.90	2.03317217D+02	4.40	6.14036260D+01	6.90	3.65731410D+00	9.40	6.52683354D-02
2.00	1.98711274D+02	4.50	5.66847981D+01	7.00	3.16038220D+00	9.50	5.48833795D-02
2.10	1.93884100D+02	4.60	5.21826910D+01	7.10	2.72951572D+00	9.60	4.60903578D-02
2.20	1.88846361D+02	4.70	4.79032738D+01	7.20	2.35307708D+00	9.70	3.86500823D-02
2.30	1.83610430D+02	4.80	4.38506436D+01	7.30	2.02498045D+00	9.80	3.23608959D-02
2.40	1.78190340D+02	4.90	4.00270658D+01	7.40	1.73967795D+00	9.90	2.70525931D-02
2.50	1.72601706D+02	5.00	3.64330374D+01	7.50	1.49213925D+00	10.00	2.25811144D-02