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Analyses with the Nuclear Optical Model, by Michel A. Melkanoff
and David S. Saxon and John S. Nodvik and David G. Cantor

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A FORTRAN Program
for Elastic Scattering Analyses
with the Nuclear Optical Model

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This program is largely based on experience gained on the SWAC, and the authors recall this with gratitude to Numerical Analysis Research, Department of Mathematics, UCLA.

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I. INTRODUCTION

The purpose of the present report is to describe in complete detail a FORTRAN code named Program SCAT 4 written by the UCLA group in order to analyze elastic scattering of various particles against complex nuclei by means of the diffuse surface optical model of the nucleus.

While a number of similar programs have been prepared and used by other groups, there have been many requests for the UCLA program because of its flexibility and the availability of IBM 704 and 709 computers for which the program is written.

The present program still contains some undesirable features and the UCLA group is constantly modifying it to make it more efficient and flexible. However, a “final” program will probably never be reached and it was decided to release Program SCAT 4 without further delay; as they develop, modifications and additions will be described in later reports.

Other laboratories will probably add further modifications and the UCLA group will be grateful for description of such modifications as well as for any suggestions in this regard. Modifications and additions deemed worthwhile will be passed on to other users of the program but while the UCLA group is willing to serve partially as a central clearing house, the entire clerical responsibility cannot be assumed by the UCLA group.

It should also be noted that, while every effort has been made to check out the program, the UCLA group cannot guarantee its complete correctness.

Program SCAT 4 is available on a symbolic deck and will be mailed on request. Air mailing will require prepaid postage by requesting parties.

Potential users of program SCAT 4 may find it useful to follow these suggestions in reading the present report:

- 1) If the potential user is only interested in analyses with standard potentials he may proceed as follows:
 - a) Read the introduction to the mathematical description.
 - b) Consider the fundamental equations: (34), (35), (51), (78) through (85), (132), (137) through (139) in [chapter II](#).
 - c) Read [chapter III](#), section A and the general flow chart.
 - d) Read the description of subroutines INPT4 and OUTPT4 in [chapter III](#), section B.
 - e) Read [chapter IV](#) and [VII](#).
- 2) If the potential user is interested in all the features of the program, then a perusal of the whole report is advisable. The mathematical description of [chapter II](#) is a brief review of the theory and the basic equations are all listed there. Symbolic FORTRAN variables are indicated in capital letters and may be looked up in the glossary making up [chapter V](#).

Note that the program may be used for incident neutral particle by letting $ZZ' = 0$.

II. MATHEMATICAL DESCRIPTION

Program **SCAT 4** calculates in the center-of-mass system the differential elastic scattering cross sections $\sigma(\theta)$, the polarization $P(\theta)$, and the total reaction cross section σ_R for particles of spin 0 or 1/2 having any mass, charge and (non-relativistic) energy scattered by spinless nuclei of any mass and charge for various sets of diffuse surface optical model parameters. The incident and target particles are assumed to interact through a two-body potential consisting of a complex nuclear potential which includes spin-orbit interaction and whose shape can be specified by input parameters. When the incident particle is charged, the two body potential contains, in addition, the coulomb potential between an incident point charge and an extended, constant charge density target.

The calculations include numerical integrations of the radial Schroedinger equations for the effective partial waves. The complex phase shifts are obtained as usual by matching the logarithmic derivatives of the numerically obtained nuclear wave functions to that of the coulomb (or spherical Bessel) functions. The phase shifts are then used to compute polarizations and cross sections which may be compared to the experimental values by means of the χ^2 test.

A. GENERAL FORMULATION

We begin with a brief review of the basic theory relating to the scattering of spin 1/2 particles by a zero spin target¹. We shall first consider the case of an uncharged incident particle and indicate later the modifications necessary if the incident particle is charged.

The interaction is assumed to be of the form

$$V_T = V_1 + V_2 \vec{S} \cdot \vec{L} \quad (1)$$

where V_1 and V_2 are complex quantities depending only on the distance r between the incident particle and the target particle. In terms of the Pauli spin operator $\vec{\sigma}$, the spin operator of the incident particle, \vec{S} , is given by

$$\vec{S} = \frac{1}{2} \hbar \vec{\sigma} \quad (2)$$

and the (relative) orbital angular momentum operator is given by

$$\vec{L} = \vec{r} \times \left(\frac{\hbar}{i} \vec{\nabla} \right). \quad (3)$$

The Schroedinger equation is then

$$\left[-\frac{\hbar^2}{2\mu} \vec{\nabla}^2 + V_1(r) + V_2(r) \vec{S} \cdot \vec{L} \right] \Psi = E\Psi \quad (4)$$

¹See J. Lepore, Phys. Rev. **79**, 137 (1950).

where

$$\mu = \frac{m_i m_b}{m_i + m_b} \quad (5)$$

is the reduced mass, m_i and m_b being respectively the masses of the incident and target particles in atomic mass units.

$$E = \frac{m_b}{m_i + m_b} E_{\text{LAB}} \quad (6)$$

is the energy in the center of mass system, E_{LAB} being the lab energy of the incident particle in MeV.

1. UNCHARGED INCIDENT PARTICLES

The wave function corresponding to a wave incident in the positive z direction and normalized to one incident particle per unit time per unit area is

$$\Psi_{\text{inc}} = \frac{1}{\sqrt{v}} e^{ikz} \chi_{\text{inc}} \quad (7)$$

where v is the relative velocity, the wave number k is given by

$$k = \sqrt{\frac{2\mu E}{\hbar^2}} = 0.2195376 \sqrt{\mu E} \text{ fermi}^{-1} \quad (8)$$

and the incident spin function is

$$\chi_{\text{inc}} = a_{1/2} \alpha + a_{-1/2} \beta \quad (9)$$

where α and β are normalized spin eigenfunctions of S_z and $a_{1/2}$, $a_{-1/2}$ the corresponding amplitudes.

The partial wave expansion corresponding to (7) is given by:

$$\Psi_{\text{inc}} = \frac{1}{\sqrt{v}} \sum_{\ell=0}^{\infty} (2\ell + 1) i^\ell j_\ell(kr) \sqrt{\frac{4\pi}{2\ell + 1}} Y_\ell^0(\theta, \varphi) [a_{1/2} \alpha + a_{-1/2} \beta] \quad (10)$$

where $j_\ell(kr)$ is the regular spherical Bessel function of order ℓ and the normalized spherical harmonics are defined as

$$Y_\ell^m(\theta, \varphi) = (-1)^{\frac{m+|m|}{2}} \sqrt{\frac{2\ell + 1}{4\pi}} \sqrt{\frac{(\ell - |m|)!}{(\ell + |m|)!}} P_\ell^{|m|}(\cos \theta) e^{im\varphi} \quad (11)$$

where $P_\ell^{|m|}(\cos \theta)$ are the associated Legendre polynomials.

The product functions $Y_\ell^0 \alpha$ and $Y_\ell^0 \beta$ which appear in (10) are simultaneous eigenfunctions of the operators \vec{L}^2 , L_z , \vec{S}^2 , and S_z but not of the operator $\vec{L} \cdot \vec{S}$ which appears in the spin-orbit interaction. This may be remedied by introducing functions $\mathcal{Y}_{jls}^{m_j}$ which

are simultaneous eigenfunctions of \vec{L}^2 , \vec{S}^2 , \vec{J}^2 , and J_z and thus of $\vec{L} \cdot \vec{S}$ where \vec{J} is the total angular momentum,

$$\vec{J} = \vec{L} + \vec{S}. \quad (12)$$

Since $s = 1/2$, the possible values of j are $j = \ell + 1/2$ and $j = \ell - 1/2$; the corresponding eigenfunctions are given by

$$\left. \begin{aligned} \mathcal{Y}_{\ell+1/2,\ell,s}^{m_j} &= \sqrt{\frac{\ell+m_j+1/2}{2\ell+1}} Y_\ell^{m_j-1/2} \alpha + \sqrt{\frac{\ell-m_j+1/2}{2\ell+1}} Y_\ell^{m_j+1/2} \beta, \text{ for } j = \ell + 1/2 \\ \mathcal{Y}_{\ell-1/2,\ell,s}^{m_j} &= -\sqrt{\frac{\ell-m_j+1/2}{2\ell+1}} Y_\ell^{m_j-1/2} \alpha + \sqrt{\frac{\ell+m_j+1/2}{2\ell+1}} Y_\ell^{m_j+1/2} \beta, \text{ for } j = \ell - 1/2 \end{aligned} \right\} \quad (13)$$

The incident wave function may now be written as

$$\begin{aligned} \Psi_{\text{inc}} &= \sqrt{\frac{4\pi}{V}} \sum_{\ell=0}^{\infty} \sqrt{\ell+1} i^\ell j_\ell(kr) \left[a_{1/2} \mathcal{Y}_{\ell+1/2,\ell,1/2}^{1/2} + a_{-1/2} \mathcal{Y}_{\ell+1/2,\ell,1/2}^{-1/2} \right] \\ &+ \sqrt{\frac{4\pi}{V}} \sum_{\ell=0}^{\infty} \sqrt{\ell} i^\ell j_\ell(kr) \left[-a_{1/2} \mathcal{Y}_{\ell-1/2,\ell,1/2}^{1/2} + a_{-1/2} \mathcal{Y}_{\ell-1/2,\ell,1/2}^{-1/2} \right] \end{aligned} \quad (14)$$

The total wave function can be written in a form similar to (14):

$$\begin{aligned} \Psi_{\text{total}} &= \Psi_{\text{inc}} + \Psi_{\text{scatt}} \\ &= \sqrt{\frac{4\pi}{V}} \sum_{\ell=0}^{\infty} \sqrt{\ell+1} i^\ell \frac{\Psi_\ell^+(r)}{kr} \left[a_{1/2} \mathcal{Y}_{\ell+1/2,\ell,1/2}^{1/2} + a_{-1/2} \mathcal{Y}_{\ell+1/2,\ell,1/2}^{-1/2} \right] \\ &+ \sqrt{\frac{4\pi}{V}} \sum_{\ell=0}^{\infty} \sqrt{\ell} i^\ell \frac{\Psi_\ell^-(r)}{kr} \left[-a_{1/2} \mathcal{Y}_{\ell-1/2,\ell,1/2}^{1/2} + a_{-1/2} \mathcal{Y}_{\ell-1/2,\ell,1/2}^{-1/2} \right] \end{aligned} \quad (15)$$

where Ψ_ℓ^+ is the radial function associated with $j = \ell + 1/2$ and Ψ_ℓ^- is associated with $j = \ell - 1/2$.

The terms appearing in (15) are not coupled by the spin-orbit interaction, and substitution into the Schroedinger equation (4) yields the following radial equations:

$$\frac{d^2 \Psi_\ell^\pm}{dr^2} + \left\{ k^2 - \frac{2\mu}{\hbar^2} \left[V_1 + \frac{\hbar^2}{2} \begin{pmatrix} \ell \\ \text{or} \\ -\ell-1 \end{pmatrix} V_2 \right] - \frac{\ell(\ell+1)}{r^2} \right\} \Psi_\ell^\pm = 0 \quad (16)$$

where the quantity ℓ appears in the equation for Ψ_ℓ^+ and $-\ell - 1$ appears in the equation for Ψ_ℓ^- .

The radial wave function Ψ_ℓ^\pm must reduce to that of the incident wave, $kr j_\ell(kr)$, when there is no interaction and must be such that only the outgoing wave is modified by the interaction. These conditions are satisfied by the asymptotic expression

$$\Psi_\ell^\pm \cong kr j_\ell(kr) + C_\ell^\pm [-y_\ell(kr) + i j_\ell(kr)] \quad (17)$$

which reduces to

$$\Psi_\ell^\pm \cong kr j_\ell(kr) + C_\ell^\pm e^{i(kr-\ell\pi/2)} \quad (18)$$

or equivalently

$$\Psi_\ell^\pm \cong \sin(kr - \frac{\ell\pi}{2}) + C_\ell^\pm e^{i(kr-\ell\pi/2)} \quad (19)$$

as may be seen by applying the asymptotic expression for the regular and irregular spherical Bessel functions:

$$\left. \begin{aligned} kr j_\ell(kr) &\cong \sin(kr - \ell\pi/2) \\ kr y_\ell(kr) &\cong -\cos(kr - \ell\pi/2). \end{aligned} \right\} \quad (20)$$

On the other hand, in terms of complex phase shifts δ_ℓ^\pm , (19) must be of the form

$$\Psi_\ell^\pm \cong A_\ell^\pm \sin(kr - \ell\pi/2 + \delta_\ell^\pm) \quad (21)$$

Comparison of the coefficients of e^{ikr} and e^{-ikr} in eqs. (21) and (19) yields

$$C_\ell^\pm = \frac{1}{2i}(e^{2i\delta_\ell^\pm} - 1) \quad (22)$$

$$A_\ell^\pm = e^{i\delta_\ell^\pm} \quad (23)$$

Substituting (18) into (15) and subtracting Ψ_{inc} as given by (14), yields for Ψ_{scatt} the asymptotic form:

$$\Psi_{\text{scatt}} \cong \frac{1}{\sqrt{V}} \frac{e^{ikr}}{r} \left\{ A(\theta) [a_{1/2}\alpha + a_{-1/2}\beta] + iB(\theta) [a_{-1/2}e^{-i\varphi}\alpha - a_{1/2}e^{i\varphi}\beta] \right\} \quad (24)$$

where

$$\left. \begin{aligned} A(\theta) &= \frac{1}{k} \sum_{\ell=0}^{\infty} [(\ell+1)C_\ell^+ + \ell C_\ell^-] P_\ell(\cos\theta) \\ B(\theta) &= -\frac{i}{k} \sum_{\ell=0}^{\infty} [C_\ell^+ - C_\ell^-] P_\ell^1(\cos\theta) \end{aligned} \right\} \quad (25)$$

The wave function of the scattered wave can more conveniently be expressed in terms of $\vec{\sigma}$ and \vec{n} , the unit vector normal to the scattering plane defined by

$$\vec{n} \sin\theta = \vec{k}_1 \times \vec{k}_0 \quad (26)$$

where \vec{k}_0 and \vec{k}_1 are unit vectors in the direction of propagation before and after scattering; thus

$$\Psi_{\text{scatt}} \cong \frac{1}{\sqrt{V}} \frac{e^{ikr}}{r} [A(\theta) + B(\theta)\vec{\sigma} \cdot \vec{n}] \chi_{\text{inc}} = \frac{1}{\sqrt{V}} \frac{e^{ikr}}{r} f(\theta) \chi_{\text{inc}} \quad (27)$$

where $f(\theta)$ is the operator

$$f(\theta) = A(\theta) + B(\theta)\vec{\sigma} \cdot \vec{n}. \quad (28)$$

The differential elastic scattering cross section and polarization vector which are given by

$$\sigma(\theta) = \left\langle [f(\theta)\chi_{\text{inc}}]^\dagger [f(\theta)\chi_{\text{inc}}] \right\rangle \quad (29)$$

$$\vec{P}(\theta) = \frac{\left\langle [f(\theta)\chi_{\text{inc}}]^\dagger [f(\theta)\chi_{\text{inc}}] \right\rangle}{\sigma(\theta)} \quad (30)$$

thus become

$$\sigma(\theta) = |A|^2 + |B|^2 + (A^*B + AB^*)\vec{n} \cdot \vec{P}_0 \quad (31)$$

$$\vec{P}(\theta) = \frac{(|A|^2 - |B|^2)\vec{P}_0 + [A^*B + AB^* + 2|B|^2\vec{P}_0 \cdot \vec{n}] \vec{n} + i(A^*B - AB^*)\vec{n} \times \vec{P}_0}{|A|^2 + |B|^2 + (A^*B + AB^*)\vec{P}_0 \cdot \vec{n}} \quad (32)$$

where the incident polarization vector \vec{P}_0 , is given by

$$\vec{P}_0 = \left\langle \chi_{\text{inc}}^\dagger \vec{\sigma} \chi_{\text{inc}} \right\rangle \quad (33)$$

If the incident beam is unpolarized, i.e., $\vec{P}_0 = 0$, the scattered beam is polarized along the direction \vec{n} , perpendicular to the scattering plane and

$$\sigma(\theta) = |A|^2 + |B|^2 \quad (34)$$

$$\vec{P}(\theta) = P(\theta)\vec{n} = \frac{(A^*B + AB^*)}{|A|^2 + |B|^2} \vec{n} \quad (35)$$

Experimentally, the polarization is sometimes obtained from a double scattering experiment in the same plane wherein the polarization in the first scattering is known².

The differential elastic scattering cross section for the second scattering may then be obtained from (31) and (35):

$$\begin{aligned} \sigma_2(\theta) &= (|A|^2 + |B|^2) \left[1 + \frac{A^*B + AB^*}{|A|^2 + |B|^2} \vec{n}_2 \cdot \vec{P}_1 \right] \\ &= (|A|^2 + |B|^2)(1 + \vec{P}_2 \cdot \vec{P}_1). \end{aligned} \quad (36)$$

Referring to FIGURE 1, it is clear that

$$\vec{n}_1 = \vec{n}_2^r = -\vec{n}_2^\ell, \quad (37)$$

so that the differential scattering cross sections along the r and ℓ beams are as follows:

$$\left. \begin{aligned} \sigma_2^r(\theta) &= (|A|^2 + |B|^2)(1 + P_2 P_1) \\ \sigma_2^\ell(\theta) &= (|A|^2 + |B|^2)(1 - P_2 P_1), \end{aligned} \right\} \quad (38)$$

²L. Rosen, Proceedings of the International Conference on the Nuclear Optical Model, Florida State University, Tallahassee, 1959, pp. 72-90.

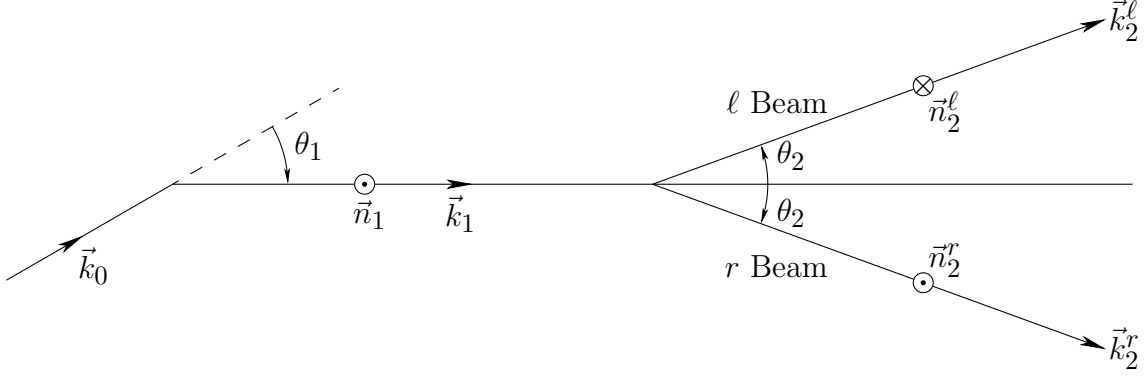


FIG. 1

the ratio of the scattering intensities becomes

$$\frac{\sigma_2^l(\theta)}{\sigma_2^r(\theta)} = \frac{1 - P_2 P_1}{1 + P_2 P_1}, \quad (39)$$

and solving for P_2 :

$$P_2 = \frac{1}{P_1} \frac{\sigma_2^l - \sigma_2^r}{\sigma_2^l + \sigma_2^r} \quad (40)$$

which reduces when $P_1 = 1$ to

$$P_2 = \frac{\sigma_2^l - \sigma_2^r}{\sigma_2^l + \sigma_2^r} \quad (41)$$

2. CHARGED INCIDENT PARTICLES

We next consider the case in which the incident particle has charge Ze and the target particle has charge $Z'e$. The potential $V(r)$ must now include a term $V_c(r)$ which describes the coulomb interaction. For small values of r , V_c will depend on the assumed charge distribution, while for large values of r , we must have

$$V_c = \frac{ZZ'e^2}{r} \quad (r \text{ large}). \quad (42)$$

It is convenient to introduce the parameter η ,

$$\eta = \frac{\mu ZZ'e^2}{\hbar^2 k} = 0.15805086 ZZ' \sqrt{\frac{m_i}{E_{\text{LAB}}}} \quad (43)$$

For the “incident wave” we take $\Psi_c(r)\chi_{\text{inc}}$, where Ψ_c is the solution to the Schroedinger equation

$$-\frac{\hbar}{2\mu} \vec{\nabla}^2 \Psi_c + \frac{ZZ'e^2}{r} \Psi_c = E \Psi_c \quad (44)$$

corresponding to the scattering of two point charges.

It is well known that in that case

$$\Psi_c = \frac{1}{\sqrt{V}} \Gamma(1 + i\eta) e^{-1/2\eta\pi} e^{ikz} F(-i\eta, 1, ik\xi) \quad (45)$$

where $\xi = r - z$ and F is the confluent hypergeometric function.

It is important to note that Ψ_c includes a distorted incoming wave *plus* a scattered wave due to the point charge potential, and as such is not strictly an incident wave.

The asymptotic form of Ψ_c is given by

$$\begin{aligned} \Psi_c \cong & \frac{1}{\sqrt{V}} \left\{ e^{i[kz - \eta \ln k(r-z)]} \left(1 - \frac{\eta^2}{ik(r-z)} \right) \right. \\ & \left. + \frac{1}{r} f_c(\theta) e^{i(kr - \eta \ln 2kr)} \right\} \end{aligned} \quad (46)$$

where

$$f_c(\theta) = -\frac{\eta}{2k \sin^2 \theta/2} e^{-i\eta \ln(\sin^2 \theta/2) + 2i \sigma_0} \quad (47)$$

is the Rutherford scattering amplitude and σ_0 is given by [equation \(49\)](#), below, with $\ell = 0$.

The partial wave expansion of Ψ_c is given by

$$\Psi_c = \frac{1}{\sqrt{V}} \sum_{\ell=0}^{\infty} (2\ell + 1) i^\ell e^{i\sigma_\ell} \frac{F_\ell(\eta, kr)}{kr} \sqrt{\frac{4\pi}{2\ell + 1}} Y_\ell^0(\theta, \varphi) \quad (48)$$

where $F_\ell(\eta, kr)$ is the regular coulomb function and σ_ℓ is the usual coulomb phase shift given by

$$\sigma_\ell = \arg \Gamma(\ell + 1 + i\eta) \quad (49)$$

Comparing [equation \(48\)](#) with [\(10\)](#) we see that in [equation \(14\)](#) it is necessary to replace $j_\ell(kr)$ by $e^{i\sigma_\ell} \frac{F_\ell(\eta, kr)}{kr}$; thus, in this case,

$$\begin{aligned} \Psi_{\text{inc}} = & \sqrt{\frac{4\pi}{V}} \sum_{\ell=0}^{\infty} \sqrt{\ell + 1} i^\ell e^{i\sigma_\ell} \frac{F_\ell(\eta, kr)}{kr} \left[a_{1/2} \mathcal{Y}_{\ell+1/2, \ell, 1/2/2}^1 + a_{-1/2} \mathcal{Y}_{\ell+1/2, \ell, 1/2/2}^{-1/2} \right] \\ & + \sqrt{\frac{4\pi}{V}} \sum_{\ell=0}^{\infty} \sqrt{\ell} i^\ell e^{i\sigma_\ell} \frac{F_\ell(\eta, kr)}{kr} \left[-a_{1/2} \mathcal{Y}_{\ell-1/2, \ell, 1/2/2}^1 + a_{-1/2} \mathcal{Y}_{\ell-1/2, \ell, 1/2/2}^{-1/2} \right] \end{aligned} \quad (50)$$

The total wave function can be written as a sum of the “incident” wave, Ψ_{inc} , plus a “scattered” wave, Ψ_{scatt} , where Ψ_{scatt} now includes only interference terms and deviations

from pure Rutherford scattering:

$$\begin{aligned}
\Psi_{\text{total}} &= \Psi_{\text{inc}} + \Psi_{\text{scatt}} \\
&= \sqrt{\frac{4\pi}{V}} \sum_{\ell=0}^{\infty} \sqrt{\ell+1} i^{\ell} e^{i\sigma_{\ell}} \frac{\Psi_{\ell}^{+}(r)}{kr} \left[a_{1/2} \mathcal{Y}_{\ell+1/2, \ell, 1/2}^1 / 2 + a_{-1/2} \mathcal{Y}_{\ell+1/2, \ell, 1/2}^{-1/2} \right] \\
&\quad + \sqrt{\frac{4\pi}{V}} \sum_{\ell=0}^{\infty} \sqrt{\ell} i^{\ell} e^{i\sigma_{\ell}} \frac{\Psi_{\ell}^{-}(r)}{kr} \left[-a_{1/2} \mathcal{Y}_{\ell-1/2, \ell, 1/2}^1 / 2 + a_{-1/2} \mathcal{Y}_{\ell-1/2, \ell, 1/2}^{-1/2} \right]
\end{aligned} \tag{51}$$

This wave function, Ψ_{total} , is formally almost identical to the expression given by [equation \(15\)](#) and the radial wave functions Ψ_{ℓ}^{\pm} obey an equation which is formally identical to [equation \(16\)](#) except that $V_1(r)$ must now include the coulomb potential $V_c(r)$ which may differ from a point charge potential at close distances.

The radial wave function Ψ_{ℓ}^{\pm} must now reduce to the “incident” wave, $F_{\ell}(\eta, kr)$, when the potential becomes a coulomb point charge potential, and must be such that only the outgoing wave is modified by the non-coulomb interaction. These conditions are satisfied by the asymptotic expression:

$$\Psi_{\ell}^{\pm} \cong F_{\ell}(\eta, kr) + C_{\ell}^{\pm} [G_{\ell}(\eta, kr) + iF_{\ell}(\eta, kr)] \tag{52}$$

which reduces to

$$\Psi_{\ell}^{\pm} \cong F_{\ell}(\eta, kr) + C_{\ell}^{\pm} e^{i(kr - \eta \ell n 2kr - \ell\pi/2 + \sigma_{\ell})} \tag{53}$$

or equivalently

$$\Psi_{\ell}^{\pm} \cong \sin(kr - \eta \ell n 2kr - \ell\pi/2 + \sigma_{\ell}) + C_{\ell}^{\pm} e^{i(kr - \eta \ell n 2kr - \ell\pi/2 + \sigma_{\ell})} \tag{54}$$

as may be seen by introducing the asymptotic expressions for the regular and irregular coulomb functions:

$$\left. \begin{aligned}
F_{\ell}(\eta, kr) &\cong \sin(kr - \eta \ell n 2kr - \ell\pi/2 + \sigma_{\ell}) \\
G_{\ell}(\eta, kr) &\cong \cos(kr - \eta \ell n 2kr - \ell\pi/2 + \sigma_{\ell})
\end{aligned} \right\} \tag{55}$$

In this case, the “nuclear phase shift” δ_{ℓ}^{\pm} is taken to be such that the asymptotic form of Ψ_{ℓ}^{\pm} is given by

$$\Psi_{\ell}^{\pm} \cong A_{\ell}^{\pm} \sin(kr - \eta \ell n 2kr - \ell\pi/2 + \sigma_{\ell} + \delta_{\ell}^{\pm}) \tag{56}$$

Comparison of the coefficients of $e^{i(kr - \eta \ell n 2kr)}$ and $e^{-i(kr - \eta \ell n 2kr)}$ in [equations \(54\)](#) and [\(56\)](#) yields

$$C_{\ell}^{\pm} = \frac{1}{2i} \left[e^{2i\delta_{\ell}^{\pm}} - 1 \right] \tag{57}$$

$$A_{\ell}^{\pm} = e^{i\delta_{\ell}^{\pm}} \tag{58}$$

Substituting (53) into (51) and making use of (46) and (50) we obtain for the asymptotic form of the total wave function

$$\begin{aligned} \Psi_{\text{total}} \cong & \frac{1}{\sqrt{V}} \left\{ e^{i[kz - \eta \ln k(r-z)]} \left[1 - \frac{\eta^2}{ik(r-z)} \right] \right\} \chi_{\text{inc}} \\ & + \frac{1}{\sqrt{V}} \frac{e^{i(kr - \eta \ln 2kr)}}{r} \left\{ A(\theta) \left[a_{1/2}\alpha + a_{-1/2}\beta \right] + iB(\theta) \left[a_{-1/2}e^{-i\varphi}\alpha - a_{1/2}e^{i\varphi}\beta \right] \right\} \end{aligned} \quad (59)$$

where

$$\begin{aligned} A(\theta) &= f_c(\theta) + \frac{1}{k} \sum_{\ell=0}^{\infty} e^{2i\sigma_\ell} [(\ell+1)C_\ell^+ + \ell C_\ell^-] P_\ell(\cos\theta) \\ B(\theta) &= -\frac{i}{k} \sum_{\ell=0}^{\infty} e^{2i\sigma_\ell} [C_\ell^+ - C_\ell^-] P_\ell^1(\cos\theta) \end{aligned} \quad (60)$$

and $f_c(\theta)$ is given by equation (47).

From this point, the formulation follows through as in the case of uncharged particles.

B. OPTICAL MODEL POTENTIAL

1. DIFFUSE SURFACE OPTICAL MODEL WITH VOLUME ABSORPTION AND COULOMB SPIN-ORBIT.

The interaction (1) is assumed to have the form

$$V_T = V_{\text{CN}} + V_{\text{SO}} + V_{\text{Coul}} + V_{\text{Coul SO}} \quad (61)$$

where the terms appearing in equation (61) are respectively the central nuclear, spin-orbit nuclear, coulomb, and coulomb spin-orbit potentials.

We shall first consider the case for which the real and imaginary parts of the central potential have a special common form factor (corresponding to volume absorption), and the spin-orbit potential is of the Thomas type. This particular central potential form factor has been used extensively and will be referred to as the standard form factor. We shall then discuss other form factors available in the program.

(a) CENTRAL NUCLEAR POTENTIAL

$$V_{\text{CN}} = (-V - iW) \frac{1}{(1 + e^{(r-R_N)/a})} \quad (62)$$

where V and W are respectively the depths of the real and imaginary part of the nuclear potential in MeV (V and W are positive for an attractive, absorbing potential), and a common volume absorption form factor is assumed, where

$$R_N = R_{\text{ON}} m_b^{1/3} \times 10^{-13} \text{ cm} \quad (63)$$

R_{ON} being the nuclear radius constant and a is the rounding parameter in 10^{-13} cm.

(b) **NUCLEAR SPIN-ORBIT POTENTIAL**

The nuclear spin-orbit potential is often written in the Thomas form

$$V_{\text{SO}} = \lambda \frac{1}{2M_p^2 c^2} \left\{ \frac{1}{r} \frac{d}{dr} \left[\frac{-V}{1 + e^{(r-R_N)/a}} \right] \right\} \vec{S} \cdot \vec{L} \quad (64)$$

where M_p is the proton rest mass and c the velocity of light. If λ were 1, the spin-orbit term would be that predicted by the Dirac equation. To provide more freedom in the model one writes

$$\lambda = 4 \left(\frac{M_p}{M_\pi} \right)^2 \frac{V_S + iW_S}{V} \quad (65)$$

where M_π is the pion rest mass and V_S and W_S are respectively the strengths of the real and imaginary parts of the nuclear spin-orbit potential in MeV.

It may be noted that a negative value of the real part of λ would be in accordance with the shell model of the nucleus where a (real) negative spin-orbit term is required to give the proper level sequence in contra-distinction to the atomic case.

(c) **COULOMB POTENTIAL**

The coulomb potential is taken here to correspond to a constant charge density within the nucleus extending to a distance R_c given by

$$R_c = R_{\text{oc}} m_b^{1/3} \times 10^{-13} \text{ cm} \quad (66)$$

where R_{oc} is the coulomb radius constant; thus

$$\begin{aligned} V_{\text{Coul}} &= (ZZ'e^2/2R_c)(3 - r^2/R_c^2) && \text{for } r \leq R_c \\ &= ZZ'e^2/r && \text{for } r \geq R_c \end{aligned} \quad (67)$$

(d) **COULOMB SPIN-ORBIT POTENTIAL**

The coulomb spin-orbit term is assumed to have the form³

$$V_{\text{Coul SO}} = (\mu_P - \frac{1}{2}) \frac{1}{M_P^2 c^2} \left[\frac{1}{r} \frac{d}{dr} V_{\text{Coul}} \right] \vec{S} \cdot \vec{L} \quad (68)$$

where μ_P is the proton magnetic moment in nuclear magnetons. It may be noted that the coulomb spin-orbit term is negligible except at very high energies.

Substituting equations (62), (64), (67), and (68) into equation (16) and transforming to the dimensionless variable

$$\rho = kr \quad (69)$$

³W. Heckrotte, Phys. Rev. **101**, 1406 (1956).

we find

$$\left\{ -\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2} - \left(\frac{V+iW}{E}\right) \left(\frac{1}{1+e^{(\rho-\bar{\rho}_N)/ka}}\right) + \left(\frac{\hbar}{M_\pi c}\right)^2 \left(\frac{V_S+iW_S}{E}\right) k^2 \left[-\frac{1}{\rho} \frac{d}{d\rho} \left(\frac{1}{1+e^{(\rho-\bar{\rho}_N)/ka}}\right)\right] \begin{pmatrix} \ell \\ \text{or} \\ -\ell-1 \end{pmatrix} + U_{\text{Coul}} + U_{\text{Coul SO}} - 1 \right\} \Psi_\ell^\pm(\rho) = 0 \quad (70)$$

where

$$U_{\text{Coul}} = \frac{\eta}{\bar{\rho}_c} \left(3 - \frac{\rho^2}{\bar{\rho}_c^2}\right) \quad \text{for } \rho \leq \bar{\rho}_c \quad (71)$$

$$= 2\eta/\rho \quad \text{for } \rho \geq \bar{\rho}_c$$

$$U_{\text{Coul SO}} = -\frac{1}{2} \left(\frac{\hbar}{M_{PC}}\right)^2 (\mu_P - \frac{1}{2})(2\eta) \left(k^2/\bar{\rho}_c^3\right) \begin{pmatrix} \ell \\ \text{or} \\ -\ell-1 \end{pmatrix} \quad \text{for } \rho \leq \bar{\rho}_c \quad (72)$$

$$= -\frac{1}{2} \left(\frac{\hbar}{M_{PC}}\right)^2 (\mu_P - \frac{1}{2})(2\eta) \left(k^2/\rho^3\right) \begin{pmatrix} \ell \\ \text{or} \\ -\ell-1 \end{pmatrix} \quad \text{for } \rho \geq \bar{\rho}_c$$

and where

$$\bar{\rho}_N = kR_N \quad (73)$$

$$\bar{\rho}_c = kR_c. \quad (74)$$

Substituting now

$$\left(\frac{\hbar}{M_\pi c}\right)^2 = 2.00 \times 10^{-26} \text{ cm}^2 \quad (75)$$

$$2\eta k^2 \cdot \frac{1}{2} \left(\frac{\hbar}{M_{PC}}\right)^2 \cong 2\eta \left(\frac{E}{M_{PC}^2}\right) = 2\eta \frac{E}{931} \quad (76)$$

$$\mu_P - \frac{1}{2} = 2.7934 - 0.5 = 2.2934 \quad (77)$$

into [equation \(70\)](#) yields:

$$\frac{d^2}{d\rho^2} \Psi_\ell^\pm(\rho) = \left\{ -1 + \frac{\ell(\ell+1)}{\rho^2} - \left(\frac{V+iW}{E}\right) \left(\frac{1}{1+e^{(\rho-\bar{\rho}_N)/ka}}\right) + \frac{\eta}{\bar{\rho}_c} \left(3 - \frac{\rho^2}{\bar{\rho}_c^2}\right) + \left[2 \left(\frac{V_S+iW_S}{E}\right) \left(\frac{k}{a}\right) \left(\frac{1}{\rho} \frac{e^{(\rho-\bar{\rho}_N)/ka}}{(1+e^{(\rho-\bar{\rho}_N)/ka})^2}\right) - 0.004926 \frac{\eta E}{\bar{\rho}_c^3} \right] \begin{pmatrix} \ell \\ \text{or} \\ -\ell-1 \end{pmatrix} \right\} \Psi_\ell^\pm(\rho), \quad \text{for } \rho \leq \bar{\rho}_c$$

$$= \left\{ -1 + \frac{\ell(\ell+1)}{\rho^2} - \left(\frac{V+iW}{E}\right) \left(\frac{1}{1+e^{(\rho-\bar{\rho}_N)/ka}}\right) + \frac{2\eta}{\rho} \right\} \Psi_\ell^\pm(\rho), \quad (78)$$

$$+ \left[2 \left(\frac{V_S+iW_S}{E}\right) \left(\frac{k}{a}\right) \left(\frac{1}{\rho} \frac{e^{(\rho-\bar{\rho}_N)/ka}}{(1+e^{(\rho-\bar{\rho}_N)/ka})^2}\right) - 0.004926 \frac{\eta E}{\rho^3} \right] \begin{pmatrix} \ell \\ \text{or} \\ -\ell-1 \end{pmatrix} \Psi_\ell^\pm(\rho), \quad \text{for } \rho \geq \bar{\rho}_c$$

2. NUCLEAR FORM FACTORS

Equation (78) may be rewritten in such a way as to display explicitly the various nuclear form factors:

$$\begin{aligned}
 \frac{d^2}{d\rho^2} \Psi_\ell^\pm(\rho) &= \left\{ -1 + \frac{\ell(\ell+1)}{\rho^2} - \frac{V}{E} f_{\text{CR}}(\rho) - i \frac{W}{E} f_{\text{CI}}(\rho) + \frac{\eta}{\bar{\rho}_c} \left(3 - \frac{\rho^2}{\bar{\rho}_c^2} \right) \right. \\
 &+ \left. \left[\frac{V_S}{E} \frac{2k}{a} f_{\text{SR}}(\rho) + i \frac{W_S}{E} \frac{2k}{a} f_{\text{SI}}(\rho) - 0.004926 \frac{\eta E}{\bar{\rho}_c^3} \right] \begin{pmatrix} \ell \\ \text{or} \\ -\ell-1 \end{pmatrix} \right\} \Psi_\ell^\pm(\rho), \text{ for } \rho \leq \bar{\rho}_c \\
 &= \left\{ -1 + \frac{\ell(\ell+1)}{\rho^2} - \frac{V}{E} f_{\text{CR}}(\rho) - i \frac{W}{E} f_{\text{CI}}(\rho) + \frac{2\eta}{\rho} \right. \\
 &+ \left. \left[\frac{V_S}{E} \frac{2k}{a} f_{\text{SR}}(\rho) + i \frac{W_S}{E} \frac{2k}{a} f_{\text{SI}}(\rho) - 0.004926 \frac{\eta E}{\rho^3} \right] \begin{pmatrix} \ell \\ \text{or} \\ -\ell-1 \end{pmatrix} \right\} \Psi_\ell^\pm(\rho), \text{ for } \rho \geq \bar{\rho}_c
 \end{aligned} \tag{79}$$

Three basic nuclear form factors and some special modifications of them are presently available in the program. In addition the coulomb spin-orbit term may be excluded at will. The required form factors may be chosen by assigning the proper values to the symbolic quantities KTRL as described on [pages 33 ff.](#)

(a) BASIC FORM FACTORS

(i) VOLUME ABSORPTION (KTRL(I) = 0, I = 1, 7, 8, 9, 10)

$$f_{\text{CR}}(\rho) = f_{\text{CI}}(\rho) = \frac{1}{(1 + e^{(\rho - \bar{\rho}_N)/ka})} \tag{80}$$

$$f_{\text{SR}}(\rho) = f_{\text{SI}}(\rho) = \frac{1}{\rho} \frac{e^{(\rho - \bar{\rho}_N)/ka}}{(1 + e^{(\rho - \bar{\rho}_N)/ka})^2} \tag{81}$$

(ii) GAUSSIAN ABSORPTION (KTRL(1) = 1)

f_{CR} is given by (80), f_{SR} and f_{SI} are given by (81) and

$$f_{\text{CI}}(\rho) = e^{-[(\rho - \bar{\rho}_G)/kb]^2} \tag{82}$$

where

$$\bar{\rho}_G = kR_{\text{OG}}m_b^{1/3}, \tag{83}$$

R_{OG} being the nuclear Gaussian radius constant, and b determines the Gaussian width.

(iii) SQUARE WELL (KTRL(1) = 2)

$$\begin{aligned}
 f_{\text{CR}}(\rho) = f_{\text{CI}}(\rho) &= 1 & \text{for } \rho \leq \bar{\rho}_N \\
 &= 0 & \text{for } \rho \geq \bar{\rho}_N
 \end{aligned} \tag{84}$$

$$f_{\text{SR}}(\rho) = f_{\text{SI}}(\rho) = 0. \tag{85}$$

(b) **SPECIAL CENTRAL NUCLEAR FORM FACTORS**⁴

(KTRL(1) = 0)

The purpose of these form factors is to allow one to modify the knee or tail of the potential curve and produce central rises or depressions in the real and/or imaginary parts of the central nuclear potential, as specified by proper choice of the KTRL's.

(i) FORM A (KTRL(7) = 1 for real part, KTRL(8) = 1 for imaginary part).

$$\left. \begin{aligned} f_{\text{CR}}(\rho) \text{ and/or } f_{\text{CI}}(\rho) &= [1 + h_A(\rho)] f_{nA_1}(\rho) & 0 < \rho \leq \rho_{m_A} \\ &= f_{nA_1}(\rho) & \rho_{m_A} \leq \rho \leq \bar{\rho}_N \\ &= f_{nA_2}(\rho) & \bar{\rho}_N \leq \rho \leq \rho_{\text{max}} \end{aligned} \right\} \quad (86)$$

(ii) FORM B (KTRL(7) = 2 for real part, KTRL(8) = 2 for imaginary part).

$$\left. \begin{aligned} f_{\text{CR}}(\rho) \text{ and/or } f_{\text{CI}}(\rho) &= [1 + h_B(\rho)] f_{nB_1}(\rho) & 0 < \rho \leq \rho_{m_B} \\ &= f_{nB_1}(\rho) & \rho_{m_B} \leq \rho \leq \bar{\rho}_N \\ &= f_{nB_2}(\rho) & \bar{\rho}_N \leq \rho \leq \rho_{\text{max}} \end{aligned} \right\} \quad (87)$$

The presence of forms *A* and *B* allows distinct form factors in the real and imaginary parts. The presence of A_1 , A_2 and B_1 , B_2 allows distinct shapes in the knee and tail of the form factors. Letting x be either *A* or *B*, and n be either nA_1 , nA_2 , nB_1 , or nB_2 ,

$$h_x(\rho) = h_{0x} \left[2 \left(\frac{\rho}{\rho_{m_x}} \right)^3 - 3 \left(\frac{\rho}{\rho_{m_x}} \right)^2 + 1 \right] = h_{0x} \left(1 - \frac{\rho}{\rho_{m_x}} \right)^2 \left(1 + \frac{\rho}{\rho_{m_x}} \right) \quad (88)$$

$$f_n(\rho) = \frac{1}{1 + g_n(\rho)} \quad (89)$$

where

$$g_n(\rho) = \exp \left\{ \frac{1}{n} \left(\frac{\bar{\rho}_N}{ka} \right) \left[\left(\frac{\rho}{\bar{\rho}_N} \right)^n - 1 \right] \right\} \quad (90)$$

where h_{0A} , h_{0B} , nA_1 , nA_2 , nB_1 , nB_2 , ρ_{m_A} , ρ_{m_B} are selected constants. (The n 's are always taken as ≥ 0 .)

Note 1: If h_{0x} is taken to be zero and nx_1 , nx_2 are taken to be 1, forms *A* and *B* reduce to the volume absorption form.

Note 2: The three curves defined by equations (86) and (87) join smoothly with continuous derivatives as long as ρ_{m_x} is chosen less than $\bar{\rho}_N$.

Note 3: Positive values of h_{0x} will produce central rises in the form factors while negative values will produce a central depression.

⁴J.S. Nodvik, Proceedings of the International Conference on the Nuclear Model, Florida State University, Tallahassee, 1959, pp. 16-23.

Note 4: If $nx_1 > 1$, the knee of the potential will be sharper than for the usual volume absorption case, while $0 \leq nx_1 \leq 1$ will soften the knee of the curve.

Note 5: If $nx_2 > 1$, this will shorten the potential tail while $0 \leq nx_2 \leq 1$ will extend it.

Some typical shapes are presented in FIGURES 2, 3, and 4.

(c) **SPECIAL NUCLEAR SPIN-ORBIT FORM FACTORS (KTRL(1) = 0)**

Two special nuclear spin-orbit form factors are available. They can be applied to the real and/or imaginary parts of the nuclear spin-orbit potential. The first of these form factors corresponds to the Thomas term applied to form A in the central nuclear potential, while the second uses form B itself; this permits one to study the result of deviations from the Thomas form.

(i) DERIVATIVE FORM FACTOR A (KTRL(9) = 1 for real part, KTRL(10) = 1 for imaginary part)

$$\begin{aligned}
 f_{\text{SR}}(\rho) \text{ and/or } f_{\text{SI}}(\rho) &= (ka) \left[-\frac{1}{\rho} \frac{d}{d\rho} (\text{form factor A}) \right] \\
 &= (ka) \left[-\left(\frac{1}{\rho} \frac{dh_A(\rho)}{d\rho} \right) f_{nA_1}(\rho) - (1 + h_A(\rho)) \left(\frac{1}{\rho} \frac{df_{nA_1}(\rho)}{d\rho} \right) \right] \\
 & \hspace{15em} \text{for } 0 \leq \rho \leq \rho_{m_a} \\
 &= (ka) \left[-\frac{1}{\rho} \frac{df_{nA_1}(\rho)}{d\rho} \right] \\
 & \hspace{15em} \text{for } \rho_{m_a} \leq \rho \leq \bar{\rho}_N \\
 &= (ka) \left[-\frac{1}{\rho} \frac{df_{nA_2}(\rho)}{d\rho} \right] \\
 & \hspace{15em} \text{for } \bar{\rho}_N \leq \rho \leq \rho_{\text{max}}
 \end{aligned} \tag{91}$$

where

$$-\frac{1}{\rho} \frac{dh_A(\rho)}{d\rho} = \frac{6h_{0A}}{\rho_{m_A}^2} \left(1 - \frac{\rho}{\rho_{m_A}} \right) \tag{92}$$

$$-\frac{1}{\rho} \frac{df_{n\rho}}{d\rho} = \left(\frac{\bar{\rho}_N}{ka} \right) \frac{1}{\rho^2} \left(\frac{\rho}{\bar{\rho}_N} \right)^n g_n(\rho) [f_n(\rho)]^2 \tag{93}$$

and $f_n(\rho)$ and $g_n(\rho)$ are given by equations (89) and (90).

(ii) FORM FACTOR B (KTRL(9) = 2 for real part, KTRL(10) = 2 for imaginary part)

$$f_{\text{SR}}(\rho) \text{ and/or } f_{\text{SI}}(\rho) = \frac{1}{2} \cdot [\text{form factor B as per equation (87)}] \tag{94}$$

Note: If h_{0A} is taken to be zero while nA_1 and nA_2 are taken to be 1, the derivative form factor in (91) becomes identical to the usual spin-orbit form factor (81).

Some typical shapes are presented in FIGURES 5, 6, and 7.

p - Cu 9.75 MeV

$R_0 = 1.2$, $A = 0.52$, $H_A = 0$, $FN1A = 1$, $\rho_{m_A} = \bar{\rho}_N = 3.24$

(Standard form factor)

- ① $FN2A = 0.01$
- ② $FN2A = 1$
- ③ $FN2A = 3$
- ④ $FN2A = 10$

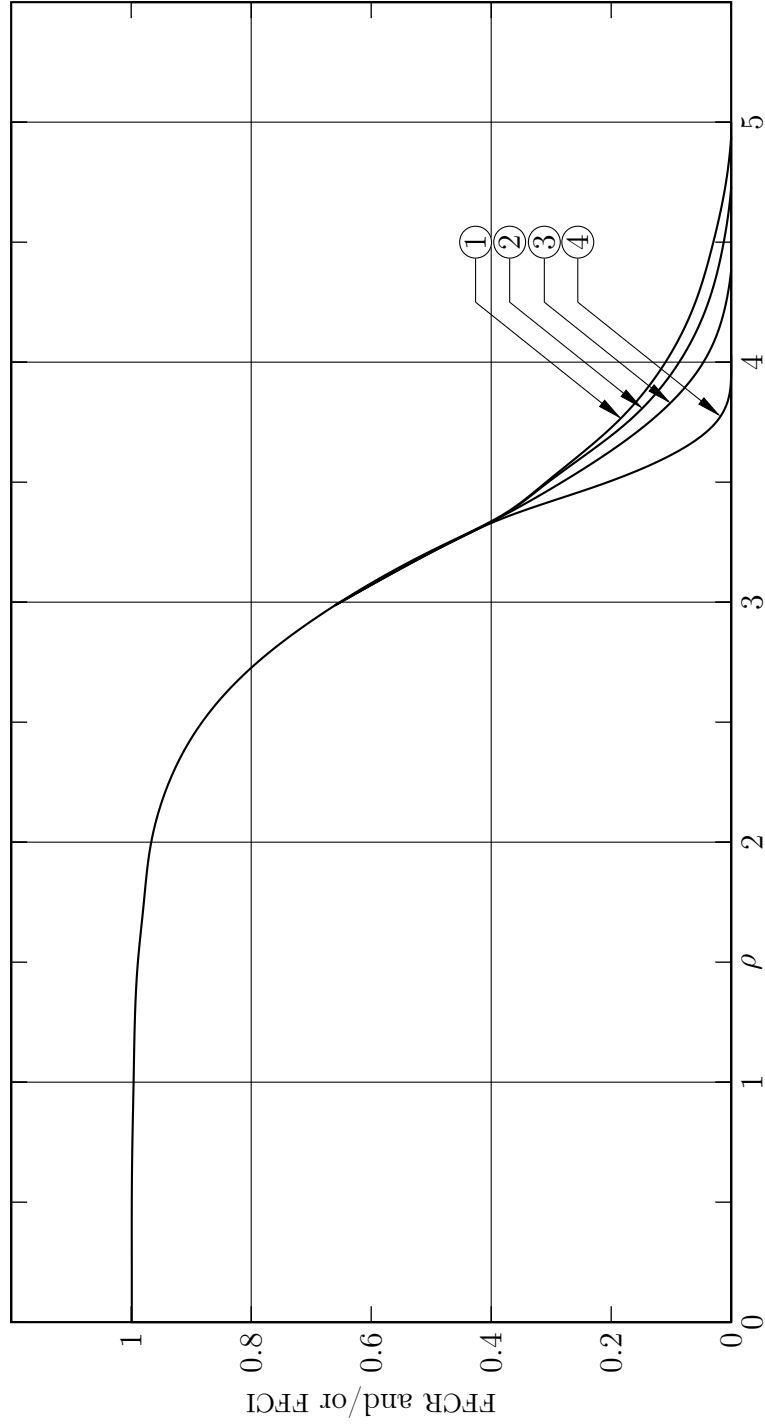


FIG. 2 - Central form factors, tail variation.

p - Ag 135 MeV

R0 = 1.25, A = 0.65, FN1A = 1, FN2A = 1

- ① HA = 0, PMA = 1, $\rho_{m_A} = \bar{\rho}_N = 15.04$ (Standard form factor)
- ② HA = 1 " " " " " "
- ③ HA = -1 " " " " " "
- ④ HA = 2, PMA = 0.7, $\rho_{m_A} = 0.7\bar{\rho}_N = 10.53$

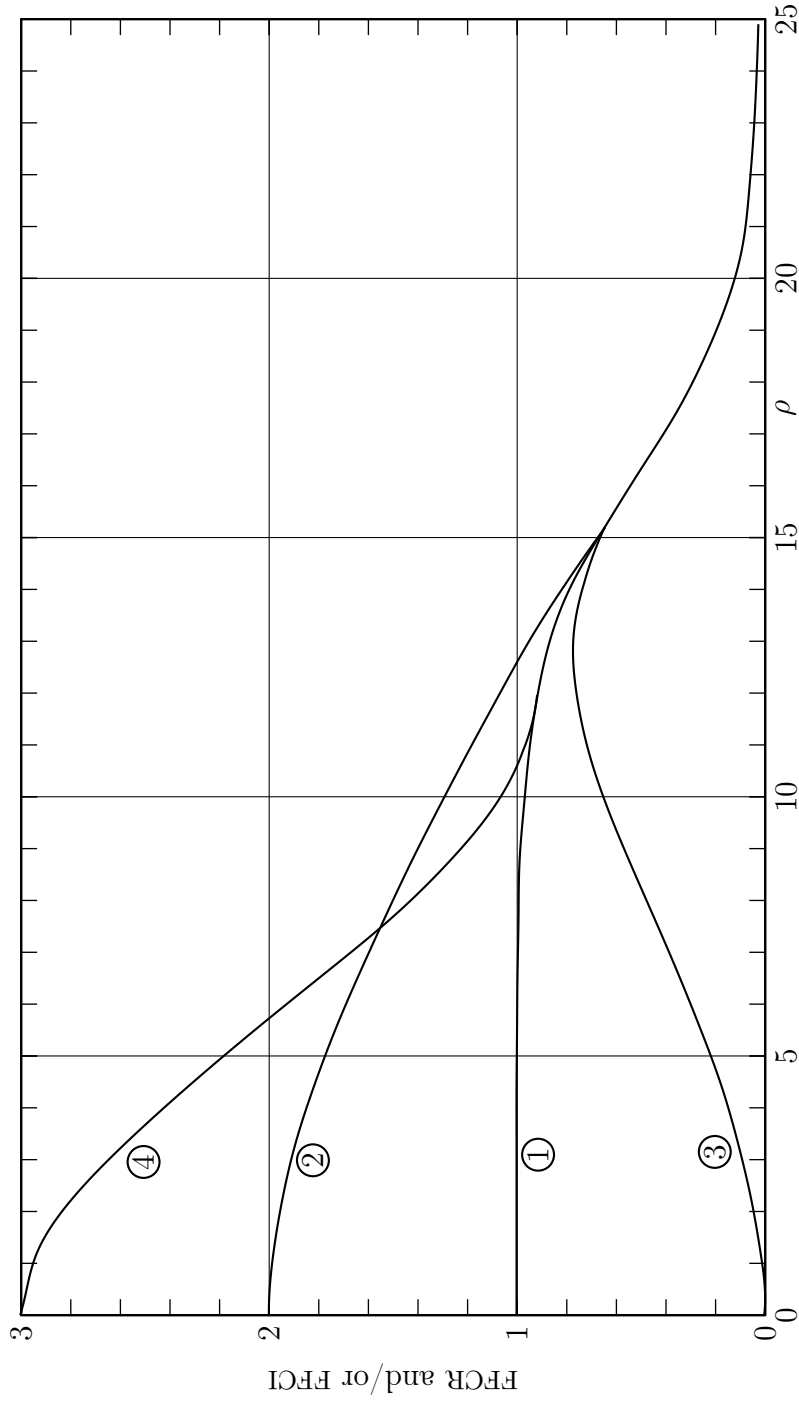


FIG. 3 - Central form factors; central dips and rises.

p - Cu 9.75 MeV

$R_0 = 1.20$, $A = 0.52$, $FN_{2A} = 1$, $PMA = 1$, $\rho_{m_A} = \bar{\rho}_N = 3.24$

- | | | |
|---------------------------|--------------|------------------------|
| ① $FN_{1A} = 0.01$ | $HA = 0$ | (Standard form factor) |
| ② $FN_{1A} = 1$ | $HA = 0$ | |
| ③ $FN_{1A} = 3$ | $HA = 0.046$ | |

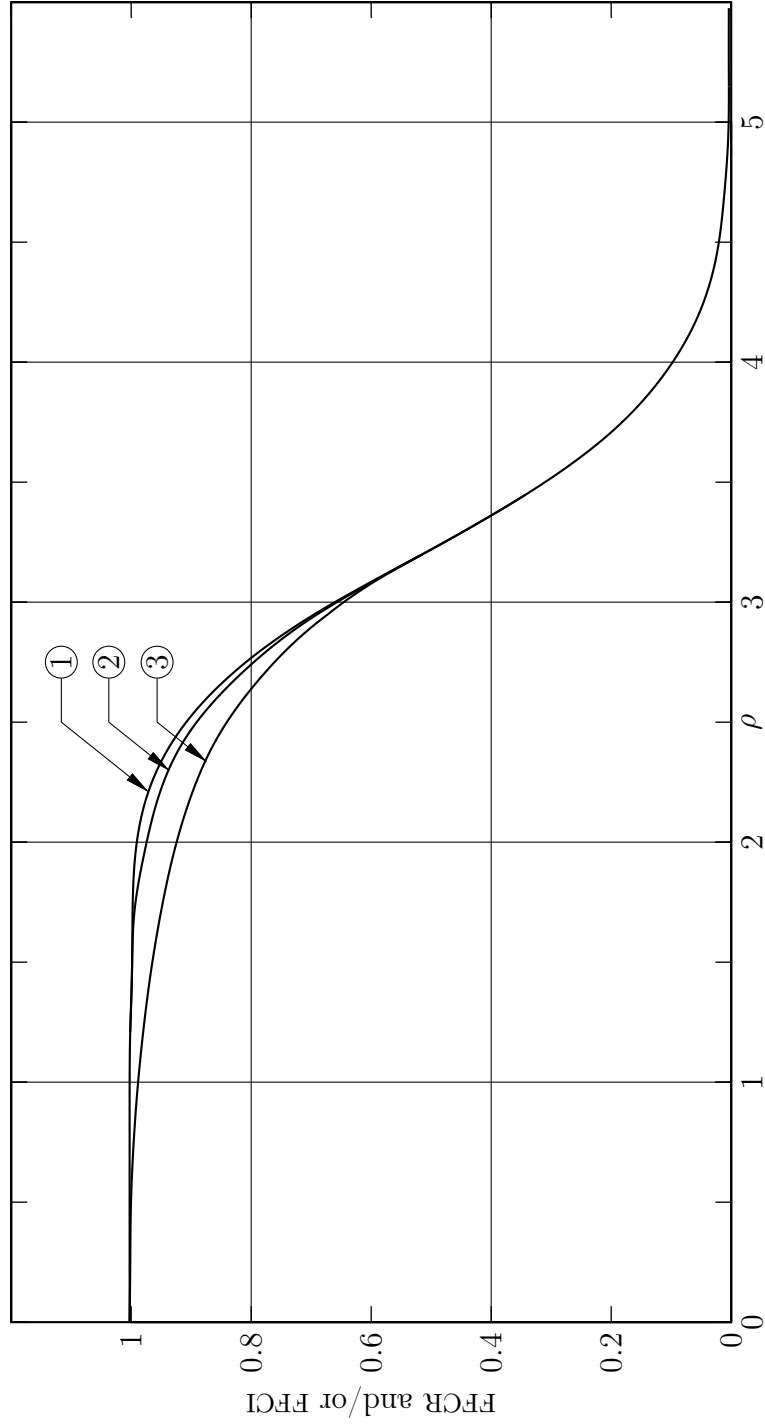


FIG. 4 - Central form factors, knee variation.

3. FINAL FORMULATION FOR MACHINE CALCULATION

The complex radial wave function $\Psi_{\ell}^{\pm}(\rho)$ may be written as

$$\Psi_{\ell}^{\pm}(\rho) = x_{\ell}^{\pm}(\rho) + iy_{\ell}^{\pm}(\rho) \quad (95)$$

and [equation \(79\)](#) for $\vec{\sigma} \cdot \vec{\ell} = \ell$ or $-\ell - 1$ can now be separated into two real coupled differential equations, and dropping the subscripts and superscripts for convenience:

$$\left. \begin{aligned} \frac{d^2 x}{d\rho^2} &= px - qy \\ \frac{d^2 y}{d\rho^2} &= qx + py \end{aligned} \right\} \quad (96)$$

where

$$\left. \begin{aligned} p &= U_{\text{CR}} + U_{\text{SR}} \left(\begin{array}{c} \ell \\ \text{or} \\ -\ell-1 \end{array} \right) + \frac{\ell(\ell+1)}{\rho^2} \\ q &= U_{\text{CI}} + U_{\text{SI}} \left(\begin{array}{c} \ell \\ \text{or} \\ -\ell-1 \end{array} \right) \end{aligned} \right\} \quad (97)$$

Formulas [\(97\)](#) are convenient for programming purposes as the U 's are now independent of ℓ , indeed:

$$\left. \begin{aligned} U_{\text{CR}} &= -1 - \frac{V}{E} f_{\text{CR}} + \frac{\eta}{\bar{\rho}_c} \left(3 - \frac{\rho^2}{\bar{\rho}_c^2} \right) \quad \text{for } \rho \leq \bar{\rho}_c \\ &= -1 - \frac{V}{E} f_{\text{CR}} + \frac{2\eta}{\rho} \quad \text{for } \rho \geq \bar{\rho}_c \end{aligned} \right\} \quad (98)$$

$$U_{\text{CI}} = -\frac{W}{E} f_{\text{CI}} \quad (99)$$

$$\left. \begin{aligned} U_{\text{SR}} &= \frac{V_S}{E} \frac{2k}{a} f_{\text{SR}} - 0.004926 \frac{\eta E}{\bar{\rho}_c^3} \quad \text{for } \rho \leq \bar{\rho}_c \\ &= \frac{V_S}{E} \frac{2k}{a} f_{\text{SR}} - 0.004926 \frac{\eta E}{\rho^3} \quad \text{for } \rho \geq \bar{\rho}_c \end{aligned} \right\} \quad (100)$$

$$U_{\text{SI}} = \frac{W_S}{E} \frac{2k}{a} f_{\text{SI}} \quad (101)$$

4. NUMERICAL INTEGRATION

[Equations \(96\)](#) must be integrated numerically twice for each $\ell = 0$ to ℓ_{max} where $\ell_{\text{max}+1}$ corresponds to a partial wave negligibly disturbed by the scattering.

The method chosen for numerical integration is the 3-point Runge-Kutta method: it lends itself to easy starting, permits one to change the interval quite easily and gives excellent accuracy with relatively large steps.

p - Cu 9.75 MeV

$R_0 = 1.2$, $A = 0.52$, $FN1A = 3$, $PMA = 1$, $\rho_{m_A} = \bar{\rho}_N = 3.24$

① $FN2A = 0.01$

② $FN2A = 1$

③ $FN2A = 3$

④ $FN2A = 10$

(Standard derivative form factor)

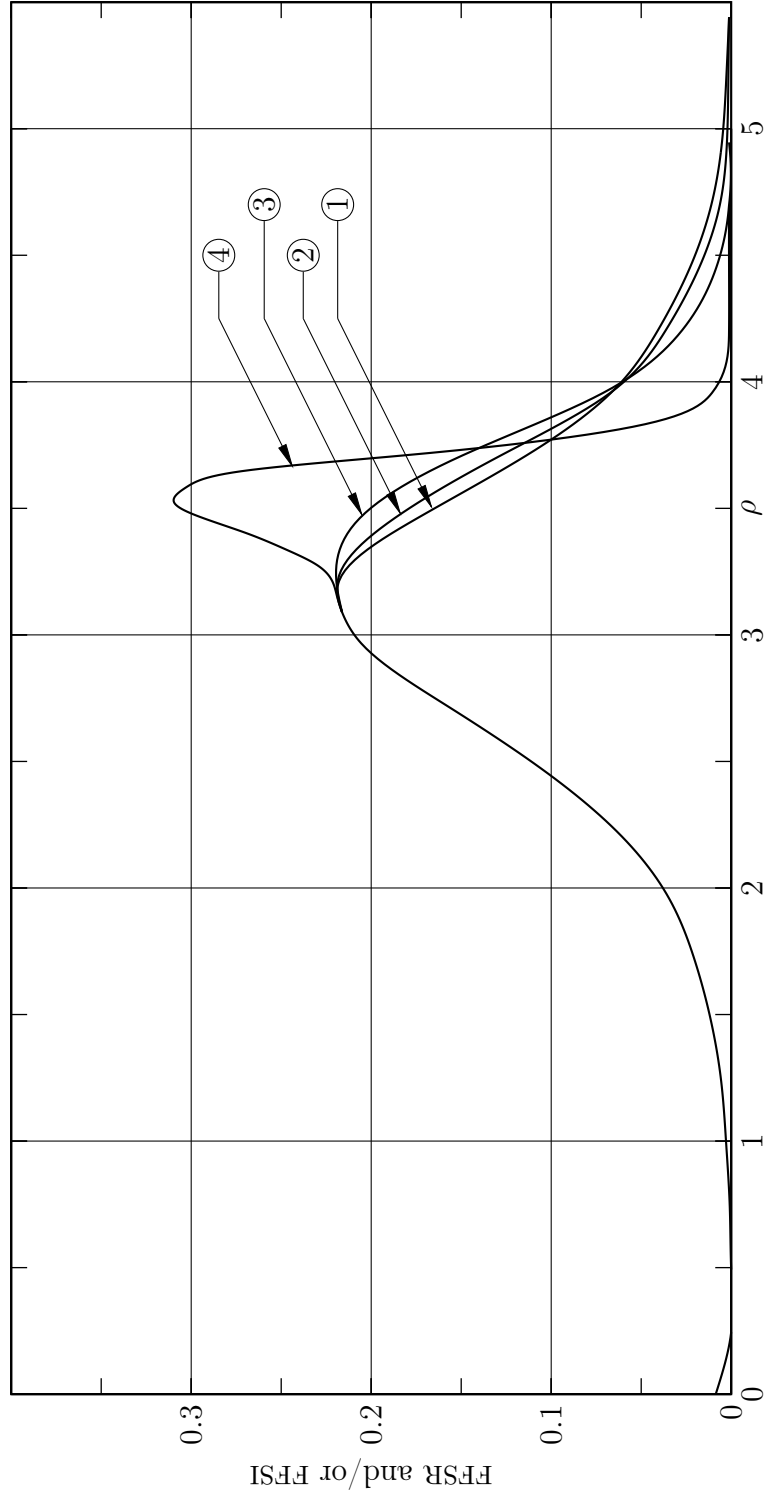


FIG. 5 - Spin-orbit form factor (derivative form). Tail variation.

p - Ag 135 MeV

$R0 = 1.25$, $A = 0.65$, $FN1A = 1$, $FN2A = 1$

- ① $HA = 0$, $PMA = 1$, $\rho_{m_A} = \bar{\rho}_N = 15.04$ (Standard derivative form factor)
- ② $HA = 1$, " " " " " "
- ③ $HA = -1$, " " " " " "
- ④ $HA = 2$, $PMA = 0.7$, $\rho_{m_A} = 0.7 \bar{\rho}_N = 10.53$

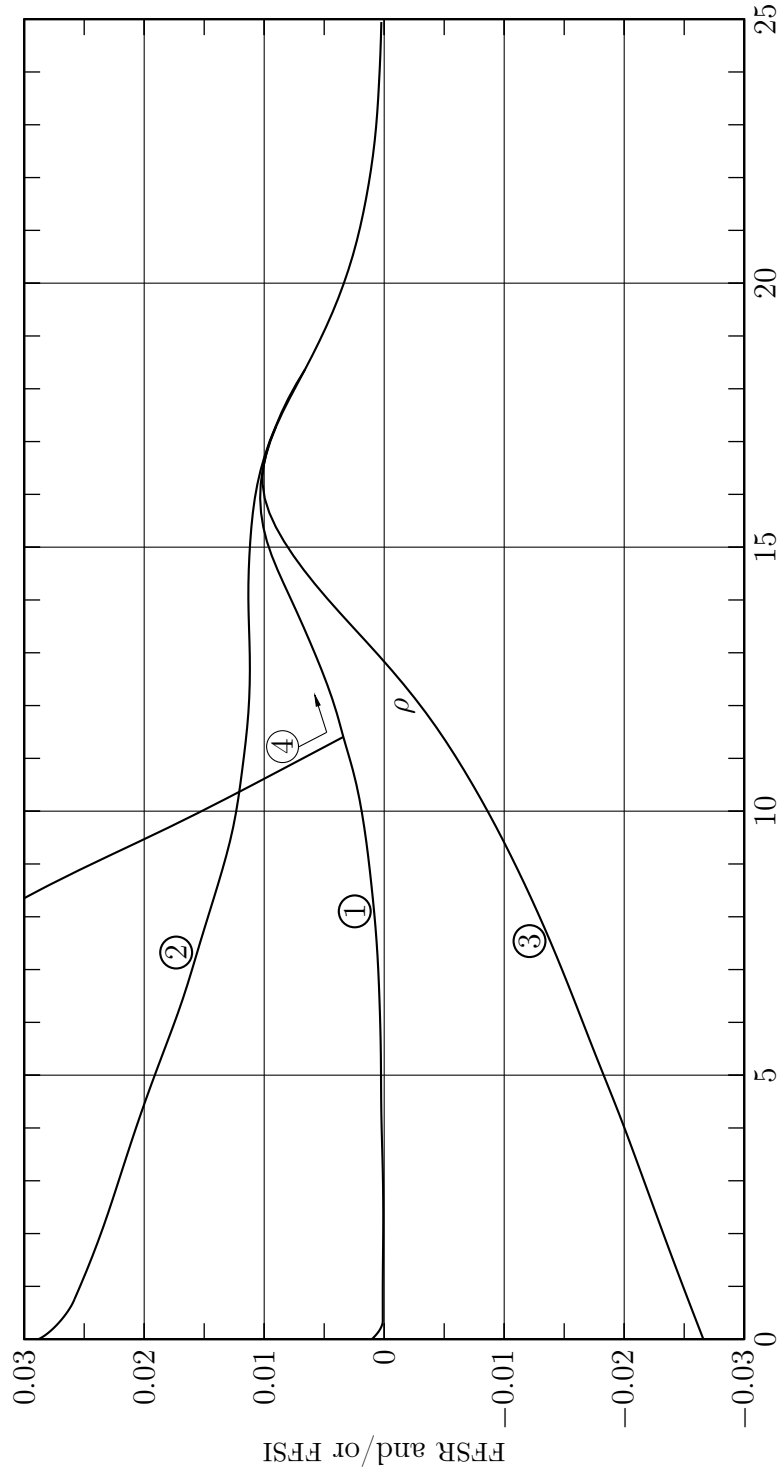


FIG. 6 - Spin-orbit form factors (derivative form). Effect of dips and rises in central form factor.

p - Cu 9.75 MeV

$R0 = 1.20, A = 0.52, FN2A = 1, PMA = 1, \rho_{m_A} = 1, \bar{\rho}_N = 3.24$

- | | | |
|----------------|------------|-----------------------------------|
| ① FN1A = 0.01, | HA = 0 | |
| ② FN1A = 1, | HA = 0 | (Standard derivative form factor) |
| ③ FN1A = 3 | HA = 0.046 | |

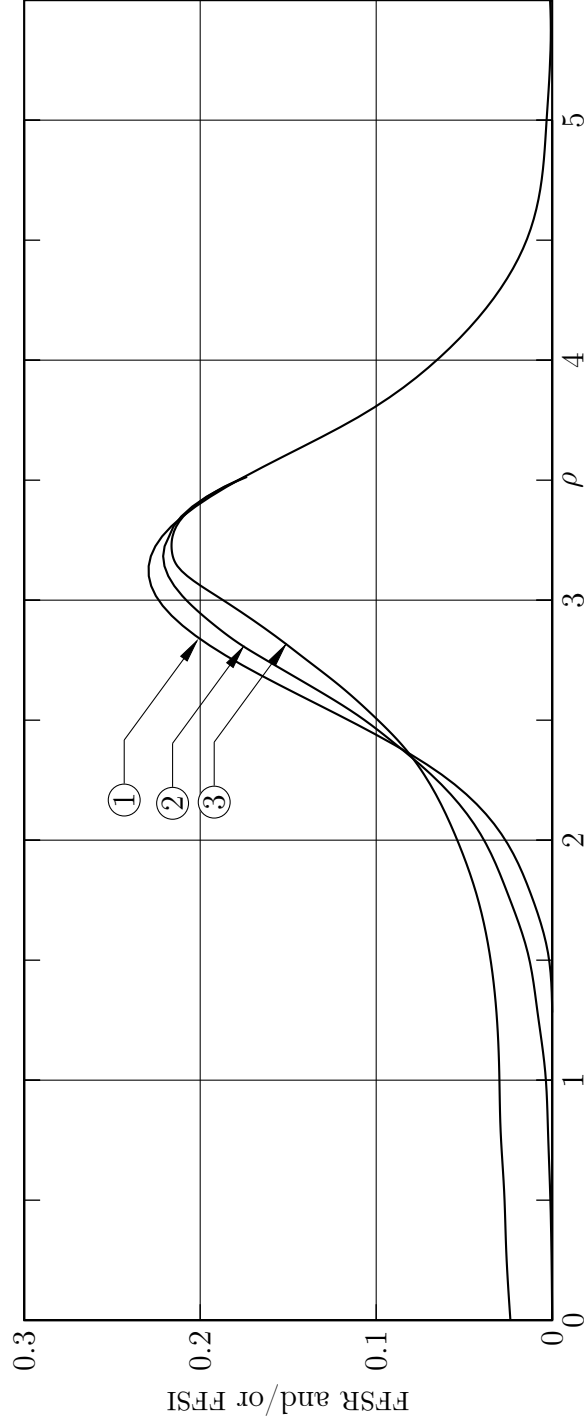


FIG. 7 - Spin-orbit form factor (derivative form). Knee variation.

Given $x_{i1}, y_{i1}, \dot{x}_{i1}, \dot{y}_{i1}$, at ρ_i , where $\dot{x}_{i1} \equiv \left(\frac{dx}{d\rho}\right)_{i,1}$ etc.

$$\ddot{x}_{i1} = f(x_{i1}, y_{i1}, \rho_i); \quad \ddot{y}_{i1} = g(x_{i1}, y_{i1}, \rho_i) \quad (102)$$

$$x_{i2} = x_{i1} + \dot{x}_{i1} \frac{\Delta\rho}{2}; \quad y_{i2} = y_{i1} + \dot{y}_{i1} \frac{\Delta\rho}{2} \quad (103)$$

$$\ddot{x}_{i2} = f(x_{i2}, y_{i2}, \rho_i + \frac{\Delta\rho}{2}); \quad \ddot{y}_{i2} = g(x_{i2}, y_{i2}, \rho_i + \frac{\Delta\rho}{2}) \quad (104)$$

$$x_{i3} = x_{i2} + \ddot{x}_{i1} \frac{(\Delta\rho)^2}{4}; \quad y_{i3} = y_{i2} + \ddot{y}_{i1} \frac{(\Delta\rho)^2}{4} \quad (105)$$

$$\ddot{x}_{i3} = f(x_{i3}, y_{i3}, \rho_i + \frac{\Delta\rho}{2}); \quad \ddot{y}_{i3} = g(x_{i3}, y_{i3}, \rho_i + \frac{\Delta\rho}{2}) \quad (106)$$

$$x_{i4} = x_{i2} + \dot{x}_{i1} \frac{\Delta\rho}{2} + \ddot{x}_{i2} \frac{(\Delta\rho)^2}{2}; \quad y_{i4} = y_{i2} + \dot{y}_{i1} \frac{\Delta\rho}{2} + \ddot{y}_{i2} \frac{(\Delta\rho)^2}{2} \quad (107)$$

$$\ddot{x}_{i4} = f(x_{i4}, y_{i4}, \rho_i + \Delta\rho); \quad \ddot{y}_{i4} = g(x_{i4}, y_{i4}, \rho_i + \Delta\rho) \quad (108)$$

and finally

$$x_{i+1,1} = x_{i1} + \Delta x_i = x_{i1} + \frac{(\Delta\rho)^2}{6}(\ddot{x}_{i1} + \ddot{x}_{i2} + \ddot{x}_{i3}) + \Delta\rho \dot{x}_{i1} \quad (109)$$

$$\dot{x}_{i+1,1} = \dot{x}_{i1} + \Delta\dot{x}_i = \dot{x}_{i1} + \frac{\Delta\rho}{6}(\ddot{x}_{i1} + 2\ddot{x}_{i2} + 2\ddot{x}_{i3} + \ddot{x}_{i4}) \quad (110)$$

$$y_{i+1,1} = y_{i1} + \Delta y_i = y_{i1} + \frac{(\Delta\rho)^2}{6}(\ddot{y}_{i1} + \ddot{y}_{i2} + \ddot{y}_{i3}) + \Delta\rho \dot{y}_{i1} \quad (111)$$

$$\dot{y}_{i+1,1} = \dot{y}_{i1} + \Delta\dot{y}_i = \dot{y}_{i1} + \frac{\Delta\rho}{6}(\ddot{y}_{i1} + 2\ddot{y}_{i2} + 2\ddot{y}_{i3} + \ddot{y}_{i4}) \quad (112)$$

The process is continued until the nuclear potential becomes negligible at which time the wave functions and their first derivatives must be saved for later matching with those of the coulomb function.

Starting values: If ρ_{initial} is very small, the following starting values may be used:

$$\left. \begin{aligned} x_\ell(\rho = \rho_{\text{initial}}) &= (\Delta\rho_1)^{\ell+1}; & \dot{x}_\ell(\rho = \rho_{\text{initial}}) &= (\ell + 1)(\Delta\rho_1)^\ell \\ y_\ell(\rho = \rho_{\text{initial}}) &= 0; & \dot{y}_\ell(\rho = \rho_{\text{initial}}) &= 0 \end{aligned} \right\} \quad (113)$$

5. COULOMB FUNCTIONS

The regular and irregular coulomb functions are given by the following asymptotic formulas which may be used successfully for large values of ρ :

$$\left. \begin{aligned} F_0 &\sim \sin[\text{Re}(\varphi_0)]e^{-\text{Im}(\varphi_0)} \\ F_1 &\sim \sin[\text{Re}(\varphi_1)]e^{-\text{Im}(\varphi_1)} \\ G_0 &\sim \cos[\text{Re}(\varphi_0)]e^{-\text{Im}(\varphi_0)} \\ G_1 &\sim \cos[\text{Re}(\varphi_1)]e^{-\text{Im}(\varphi_1)} \end{aligned} \right\} \quad (114)$$

where

$$\left. \begin{aligned} \varphi_0 &= \rho - \eta \ell n 2\rho + \sigma_0 + \sum_{k=2}^{\infty} \frac{a_k}{\rho^{k-1}} \left(\frac{1}{1-k} \right) \\ \varphi_1 &= \rho - \eta \ell n 2\rho + \sigma_1 - \frac{\pi}{2} + \sum_{k=2}^{\infty} \frac{b_k}{\rho^{k-1}} \left(\frac{1}{1-k} \right) \end{aligned} \right\} \quad (115)$$

and where

$$\left. \begin{aligned} a_1 &= -\eta, & a_2 &= \frac{-\eta^2}{2} + i\eta \\ b_1 &= -\eta, & b_2 &= -\frac{2 + \eta^2}{2} + i\frac{\eta}{2} \\ a_k &= - \left(\frac{1}{2} \sum_{m=1}^{k-1} a_m a_{k-m} \right) - i \frac{k-1}{2} a_{k-1} \end{aligned} \right\} \quad (116)$$

with a similar recurrence formula holding for b_k

$$\left. \begin{aligned} \sigma_0 &= \arg \Gamma(1 + i\eta) \\ \sigma_1 &= \sigma_0 + \tan^{-1} \eta \end{aligned} \right\} \quad (117)$$

Furthermore the quantity σ_0 may be successfully approximated over the whole range of η by the following formula:

$$\begin{aligned} \sigma_0 &= -\eta + \left(\frac{\eta}{2} \right) \ln(\eta^2 + 16) + \frac{7}{2} \tan^{-1} \left(\frac{\eta}{4} \right) - \left[\tan^{-1} \eta + \tan^{-1} \left(\frac{\eta}{2} \right) + \tan^{-1} \left(\frac{\eta}{3} \right) \right] \\ &\quad (118) \\ &\quad - \frac{\eta}{12(\eta^2 + 16)} \left[1 + \frac{1}{30} \frac{\eta^2 - 48}{(\eta^2 + 16)^2} + \frac{1}{105} \frac{\eta^4 - 160\eta^2 + 1280}{(16 + \eta^2)^4} \right]. \end{aligned}$$

The above formulas which can of course be generalized for any value of ℓ are equivalent though not formally identical to the formulas listed by Abramowitz⁵ and by Fröberg⁶.

Rather than use these formulas for obtaining F_ℓ and G_ℓ for any value of $\ell > 1$, it is preferable to make use of recurrence formulas.

The following upward recurrence formula is suitable for finding G_ℓ :

$$G_{\ell+1} = \frac{(2\ell + 1) \left[\eta + \frac{\ell(\ell+1)}{\rho} \right] G_\ell - (\ell + 1) [\ell^2 + \eta^2]^{1/2} G_{\ell-1}}{\ell [(\ell + 1)^2 + \eta^2]^{1/2}}. \quad (119)$$

⁵Tables of Coulomb Wave Functions, Vol. I, National Bureau of Standards, Applied Mathematics Series 17, Washington, 1952, p. XV.

⁶C. E. Fröberg, Rev. Mod. Phys. **27**, 399 (1955).

A similar recurrence relation can only be used for downward recurrence on the F_ℓ 's, otherwise results rapidly lose all significance. This may be done by means of a method due to Stegun and Abramowitz⁷ and which is essentially as follows.

Let it be required to compute F_ℓ from $\ell = 0$ to $\ell = \ell_{\max}$.

(1) Let $\ell^{(1)} = \ell_{\max} + 10$

(The number 10 is arbitrary but has found satisfactory from practical experience)

Let $F_{\ell^{(1)}+1}^{(1)} = 0$ and $F_{\ell^{(1)}}^{(1)} = 0.1$. Successive values of $F_\ell^{(1)}$ can be computed from $\ell = 0$ to $\ell = \ell^{(1)} - 1$ by means of the downward recurrence formula:

$$F_{\ell-1}^{(1)} = \frac{(2\ell+1) \left[\eta + \frac{\ell(\ell+1)}{\rho} \right] F_\ell^{(1)} - \ell [(\ell+1)^2 + \eta^2]^{1/2} F_{\ell+1}^{(1)}}{(\ell+1) [\ell^2 + \eta^2]^{1/2}}. \quad (120)$$

Letting the constant

$$\alpha = (F_0^{(1)} G_1 - F_1^{(1)} G_0)(1 + \eta^2)^{1/2} \quad (121)$$

one may compute successively

$$F_\ell = F_{\ell^{(1)}}^{(1)} \alpha^{-1} \quad (122)$$

for $\ell = \ell_{\max} + 1$ to $\ell = 0$.

(2) To verify the accuracy of the F_ℓ 's obtained above one may compute as above a new set of functions $F_\ell^{(2)}$ starting perhaps from $\ell^{(2)} = \ell^{(1)} + 5$ (again the number 5 is obtained from practical experience) and letting now $F_{\ell^{(2)}+1}^{(2)} = 0$, $F_{\ell^{(2)}}^{(2)} = 0.1$. This yields a new set of F_ℓ 's.

(3) Comparison of the two sets of F_ℓ 's obtained in (1) and (2) above indicates the accuracy of the computation. If this proves insufficient, let $\ell^{(3)} = \ell^{(2)} + 5$ and starting from $F_{\ell^{(3)}+1}^{(3)} = 0$, $F_{\ell^{(3)}}^{(3)} = 0.1$ one may obtain a third set set of F_ℓ 's which is to be compared with the second set.

This procedure may be continued until two successive sets of F_ℓ 's are found to agree. The derivatives of the coulomb functions may be obtained from the formula

$$Y'_\ell = \frac{\left[\frac{(\ell+1)^2}{\rho} + \eta \right] Y_\ell - [(\ell+1)^2 + \eta^2]^{1/2} Y_{\ell+1}}{(\ell+1)} \quad (123)$$

where Y_ℓ stands for either F_ℓ or G_ℓ .

⁷Stegun and Abramowitz, Phys. Rev. **98**, 1851 (1955).

6. PHASE SHIFTS

The phase shifts are obtained in the usual fashion by matching the logarithmic derivatives of the coulomb functions with those of the numerically integrated functions at a value of ρ sufficiently large so that the nuclear potential becomes negligible.

Matching the logarithmic derivative of the nuclear function $\Psi_\ell = x_\ell + iy_\ell$ with that of its asymptotic form

$$F_\ell + (G_\ell + iF_\ell)C_\ell$$

yields

$$\frac{\Psi'_\ell}{\Psi_\ell} = \frac{F'_\ell + (G'_\ell + iF'_\ell)C_\ell}{F_\ell + (G_\ell + iF_\ell)C_\ell} \quad (124)$$

which lead to

$$C_\ell^\pm = \frac{\Psi_\ell^\pm F'_\ell - \Psi_\ell^{\pm'} F_\ell}{\Psi_\ell^{\pm'} G_\ell - \Psi_\ell^\pm G'_\ell + i(\Psi_\ell^{\pm'} F_\ell - \Psi_\ell^\pm F'_\ell)} \quad (125)$$

the quantities C_ℓ being related to the complex phase shifts through [equation \(57\)](#).

7. CROSS SECTION AND POLARIZATION

The differential elastic scattering cross section $\sigma(\theta)$ and the polarization $P(\theta)$ for an unpolarized incident beam are obtained from [equations \(34\)](#) and [\(35\)](#) while the reaction cross section may be obtained as follows.

$$\sigma_R = \frac{N_{\text{abs}}}{N_{\text{inc}}} \quad (126)$$

where N_{abs} is the absorbed flux, and N_{inc} is the incident flux which was assumed to be 1 (see [equation \(7\)](#)). By definition,

$$N_{\text{abs}} = -\frac{\hbar}{2i\mu} \int \left[\Psi_{\text{total}}^\dagger \frac{\partial \Psi_{\text{total}}}{\partial r} - \Psi_{\text{total}} \frac{\partial \Psi_{\text{total}}^\dagger}{\partial r} \right] r_0^2 \sin \theta \, d\theta \, d\varphi \quad (127)$$

where the integral is taken over the surface of a large sphere of radius $r = r_0$. Substituting [equation \(51\)](#) for Ψ_{total} into [equation \(127\)](#) and making use of the orthonormality of the $\mathcal{Y}_{j,\ell,s}^{m_j}$'s and of the relation

$$\left| a_{1/2} \right|^2 + \left| a_{-1/2} \right|^2 = 1, \quad (128)$$

yields after carrying out the surface integration:

$$\begin{aligned} \sigma_R = N_{\text{abs}} = & \frac{4\pi}{V} \sum_{\ell=0}^{\infty} (\ell + 1) \left\{ r^2 \left(-\frac{\hbar}{2i\mu} \right) \left[\frac{\Psi_\ell^{+*}}{kr} \frac{\partial}{\partial r} \left(\frac{\Psi_\ell^+}{kr} \right) - \frac{\Psi_\ell^+}{kr} \frac{\partial}{\partial r} \left(\frac{\Psi_\ell^{+*}}{kr} \right) \right] \right\}_{r=r_0} \\ & - \frac{4\pi}{V} \sum_{\ell=0}^{\infty} \ell \left\{ r^2 \left(-\frac{\hbar}{2i\mu} \right) \left[\frac{\Psi_\ell^{-*}}{kr} \frac{\partial}{\partial r} \left(\frac{\Psi_\ell^-}{kr} \right) - \frac{\Psi_\ell^-}{kr} \frac{\partial}{\partial r} \left(\frac{\Psi_\ell^{-*}}{kr} \right) \right] \right\}_{r=r_0} \end{aligned} \quad (129)$$

Now substituting the asymptotic form (52) for Ψ_ℓ^\pm and making use of the Wronskian relations

$$G_\ell F'_\ell - F_\ell G'_\ell = 1 \quad (130)$$

we are led to the following:

$$\frac{4\pi}{V} \left\{ r^2 \left(-\frac{\hbar}{2i\mu} \right) \left[\frac{\Psi_\ell^{\pm*}}{kr} \frac{\partial}{\partial r} \left(\frac{\Psi_\ell^\pm}{kr} \right) - \frac{\Psi_\ell^\pm}{kr} \frac{\partial}{\partial r} \left(\frac{\Psi_\ell^{\pm*}}{kr} \right) \right] \right\}_{r=r_0} = \frac{4\pi}{k^2} [\text{Im}(C_\ell^\pm) - |C_\ell^\pm|^2]. \quad (131)$$

Finally, substitution of (131) into (129) yields

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} \left\{ (\ell+1) \left[\text{Im}(C_\ell^+) - (\text{Im}(C_\ell^+))^2 - (\text{Re}(C_\ell^+))^2 \right] + \ell \left[\text{Im}(C_\ell^-) - (\text{Im}(C_\ell^-))^2 - (\text{Re}(C_\ell^-))^2 \right] \right\}. \quad (132)$$

Note: The quantities $e^{2i\sigma_\ell}$ appearing in equation (60) may be obtained by the following recurrence formulas:

$$\begin{aligned} \text{Re}(e^{2i\sigma_{\ell+1}}) &= \cos 2\sigma_{\ell+1} = \left[\frac{(\ell+1)^2 - \eta^2}{(\ell+1)^2 + \eta^2} \cos 2\sigma_\ell \right] - \left[\frac{2\eta(\ell+1)}{(\ell+1)^2 + \eta^2} \sin 2\sigma_\ell \right] \\ \text{Im}(e^{2i\sigma_{\ell+1}}) &= \sin 2\sigma_{\ell+1} = \left[\frac{(\ell+1)^2 - \eta^2}{(\ell+1)^2 + \eta^2} \sin 2\sigma_\ell \right] + \left[\frac{2\eta(\ell+1)}{(\ell+1)^2 + \eta^2} \cos 2\sigma_\ell \right] \end{aligned} \quad (133)$$

while the Legendre polynomials obey the usual relations

$$\begin{aligned} P_0(\cos \theta) &= 1, \quad P_1(\cos \theta) = \cos \theta \\ P_{\ell+1}(\cos \theta) &= \frac{1}{\ell+1} [(2\ell+1) \cos \theta P_\ell(\cos \theta) - \ell P_{\ell-1}(\cos \theta)] \end{aligned} \quad (134)$$

$$P_\ell^{(1)}(\cos \theta) = \frac{\ell+1}{\sin \theta} [\cos \theta P_\ell(\cos \theta) - P_{\ell+1}(\cos \theta)]. \quad (135)$$

One may also compute the Rutherford scattering cross section:

$$\sigma_c(\theta) = |f_c(\theta)|^2. \quad (136)$$

8. CHI SQUARE DEVIATION

Experimental and theoretical quantities may be compared by means of the chi square deviation:

$$\chi_T^2 = \chi_\sigma^2 + \chi_P^2 \quad (137)$$

where

$$\chi_\sigma^2 = \sum_{\theta} \chi_\sigma^2(\theta) = \sum_{\theta} \left[\frac{\sigma^{\text{th}}(\theta) - \sigma^{\text{ex}}(\theta)}{\Delta\sigma^{\text{ex}}(\theta)} \right]^2 \quad (138)$$

$$\chi_P^2 = \sum_{\theta} \chi_P^2(\theta) = \sum_{\theta} \left[\frac{P^{\text{th}}(\theta) - P^{\text{ex}}(\theta)}{\Delta P^{\text{ex}}(\theta)} \right]^2 \quad (139)$$

where the $\sigma^{\text{th}}(\theta)$ and $P^{\text{th}}(\theta)$ are the theoretically obtained cross sections and polarizations while $\sigma^{\text{ex}}(\theta)$, $\Delta\sigma^{\text{ex}}(\theta)$, $P^{\text{ex}}(\theta)$, $\Delta P^{\text{ex}}(\theta)$ are respectively the experimentally given cross sections, standard deviations in the cross sections, polarization and standard deviations in the polarization.

It should be noted that the constants were chosen such that the differential and reaction cross section will be obtained in units of 10^{-26} cm². The polarizations are of course dimensionless ratios.

9. NORMALIZATION

The radial wave functions Ψ_ℓ^\pm and their derivatives obtained from numerical integration of the radial Schroedinger equation contain an arbitrary normalization factor, $1/M_\ell^\pm$. This factor however does not affect the cross section and polarization since these are obtained from the phase shifts which in turn are obtained from ratios of logarithmic derivatives (see [equation \(125\)](#)) wherein the M_ℓ 's cancel out. If on the other hand the normalized radial wave functions and their derivatives are required, the normalization terms may be obtained as follows:

The asymptotic form of Ψ_ℓ^\pm must obey [equation \(52\)](#) but improper normalization results in the fact that the calculated wave functions are actually given by

$$x_\ell^\pm(\rho) + iy_\ell^\pm(\rho) = M_\ell^\pm \{F_\ell(\eta, \rho) + C_\ell^\pm [G_\ell(\eta, \rho) + iF_\ell(\eta, \rho)]\} \quad (140)$$

Now, for $\rho \leq \rho_{\text{max}}$ the nuclear potentials are negligible and [equation \(52\)](#) represents the exact solution; in particular, at $\rho = \rho_{\text{max}}$, we must have

$$x_\ell^\pm(\rho_{\text{max}}) + iy_\ell^\pm(\rho_{\text{max}}) = M_\ell^\pm \{F_\ell(\eta, \rho_{\text{max}}) + C_\ell^\pm [G_\ell(\eta, \rho_{\text{max}}) + iF_\ell(\eta, \rho_{\text{max}})]\} \quad (141)$$

whereby

$$M_\ell^\pm = \frac{x_\ell^\pm(\rho_{\text{max}}) + iy_\ell^\pm(\rho_{\text{max}})}{F_\ell(\eta, \rho_{\text{max}}) + C_\ell^\pm [G_\ell(\eta, \rho_{\text{max}}) + iF_\ell(\eta, \rho_{\text{max}})]} \quad (142)$$

and the normalized radial wave functions and their derivatives are given by

$$\left. \begin{aligned} \Psi_\ell^\pm(\rho) &= \frac{1}{M_\ell^\pm} [x_\ell^\pm(\rho) + iy_\ell^\pm(\rho)] \\ \frac{d\Psi_\ell^\pm(\rho)}{d\rho} &= \frac{1}{M_\ell^\pm} [\dot{x}_\ell^\pm(\rho) + i\dot{y}_\ell^\pm(\rho)] \end{aligned} \right\} \quad (143)$$

and the complete normalized wave function is given in [equation \(51\)](#) with Ψ_ℓ^\pm as above in [equation \(143\)](#).

Note: During the numerical integration the program may renormalize the wave functions and their derivatives at any value of ρ for which overflow takes place by dividing the functions and their derivatives by the largest of these. This is accompanied by an explicit printout as explained in the description of subroutine RKINT. Such occasional internal renormalization must of course be taken into account if correctly normalized functions are required.

III. PROGRAM DESCRIPTION

A. GENERAL DESCRIPTION

1. MACHINE SPECIFICATIONS

Program SCAT 4 has been written for an IBM 704 with floating point traps or an IBM 709, with a 32,768 words memory, no drum and a minimum of two tape units.

The program can probably be modified for a 16K memory by reducing the number of θ 's (up to 75 allowed here) and the number of ℓ 's (up to 50 allowed here). A large part of the memory (7500 words) is occupied by the Legendre polynomials and this may also be reduced by computing the polynomials as required. Furthermore, the program contains a large number of printouts which may be abbreviated to save storage space.

2. GENERAL PROGRAM DESCRIPTION

The program was designed to compute cross sections, polarizations and chi square deviations at a number of specified points in the space of the optical model parameters V, W, A, VS, WS, and if needed BG (RO, RC and RG are kept fixed), for a given set of input data.

The time to carry out a run for a single set of parameters depends of course upon the maximum values of ℓ and ρ ; for p-Cu at 10 MeV ($\ell_{\max} = 10$, $\rho = 0.0625$ (.0625) 0.50 (0.25) 10.0) a run takes about 45 seconds including about 15 seconds for maximum output to tape.

The program has been written in the form of subroutines to allow easy checking and modification. Some of these subroutines are not yet available, but some provision have been made to include them in the future. The following subroutines written in FORTRAN are specific (sub)routines of the program:

Main routine	-	MAIN4			
Subroutine	-	CTRL4			
Subroutine	-	INPT4	Subroutine	-	PGEN4
Subroutine	-	POT1CH	Subroutine	-	INTCTR
Subroutine	-	POP1	Subroutine	-	RKINT
Subroutine	-	SIGZRO	Subroutine	-	CSUBL
Subroutine	-	FSUBC	Subroutine	-	AB
Subroutine	-	EXSGML	Subroutine	-	SGSGCP
Subroutine	-	RHOTB	Subroutine	-	SIGMAR
Subroutine	-	COULFN	Subroutine	-	CHISQ
Subroutine	-	RMXINC	Subroutine	-	OUTPT4

The following subroutines are general utility routines used by the program:

Subroutine - SKIP written in FORTRAN

Subroutine - LEAVE written in FORTRAN

Subroutine - SPILL written in FAP

The following subroutines are used in conjunction with the Load-and-Go system in use at WDPC (Western Data Processing Center, UCLA). The effect of using this system is described in [section III-A-3](#) below.

Subroutine - **SAVE**

Subroutine - PDUMP

Subroutine - EXIT

The program assumes the presence of the following Fortran elementary function subroutines:

LOGF	–	(natural logarithm)
SINF	–	(sine)
<i>COSF</i>	–	(cosine)
EXPF	–	(exponential)
SQRTF	–	(square root)
ATANF	–	(arc tangent)

3. USE OF THE WDPC LOAD-AND-GO SYSTEM

Program **SCAT 4** has been written for the Load-and-Go system in use at the WDPC, UCLA. This *only* affects it as follows:

- (i) SPECIAL SUBROUTINES OF THE LOAD-AND-GO SYSTEM.

Subroutine SAVE

The purpose of this subroutine is to allow the operator to interrupt the calculation without loss. The program is normally run with Sense Switch 1 off; turning on Sense Switch 1 will cause the program to call **SAVE** after completing the innermost **DO** loop of subroutine *CTRL4*. **SAVE** then writes on tape the content of the core memory as well as all other information required to continue the computation such as the contents of the AC, MQ, index registers, etc. . . .

A restart routine will then later reload the core memory, reset all registers etc. . . , and return right after the *CALL SAVE* statement. The following statements up to statement number 66 are then required to properly position the input data tape as the latter was probably rewound when the computation was interrupted.

To eliminate the use of subroutine **SAVE**, remove from subroutine *CTRL4* all statements from statement number 118 to statement number 66 inclusive.

Subroutine PDUMP(α, β)

The purpose of this subroutine is to provide a partial core dump of all quantities between the location of the arguments in the call statement. Subroutine PDUMP is called by subroutine LEAVE whenever difficulties such as overflow or division by zero take place.

To eliminate subroutine PDUMP, replace in subroutine LEAVE the statement *CALL PDUMP(A,ZZ)* by whatever statements will cause the required core dump.

Subroutine EXIT

This subroutine terminates the program.

To eliminate subroutine EXIT, replace statement number 151 in subroutine INPT4 by whatever statement will be used to terminate the program.

(ii) END STATEMENTS.

The usual FORTRAN **END** statements do not appear in the program as the load-and-go system provides them automatically.

(iii) INPUT AND OUTPUT STATEMENTS.

In conjunction with the load-and-go system, the program is input from tape, while the input data is brought in from tape 7 and all the output is to tape 6.

All these particular features can of course be easily modified to use the program either directly or in conjunction with any other system.

4. ERROR INDICATIONS:

(i) DIVISION BY ZERO.

Every division which could conceivably have a zero divisor either because of the range of numbers used or because of an error in the input data is followed by an **IF DIVIDE CHECK**. Detection of a zero denominator is then followed by an explicit print out and a *CALL LEAVE* statement which leads to the next set of input data. In order to be sure that no division by zero remains undetected, every subroutine which contains an **IF DIVIDE CHECK** statement also begins with an **IF DIVIDE CHECK** to verify that the trigger is off at the start of the subroutine; if the divide check trigger is found on at the start, there is an explicit printout to that effect followed by a *CALL LEAVE* statement.

(ii) OVERFLOW. UNDERFLOW.

Overflow and underflow are monitored by subroutine SPILL (JSPILL, ISPILL, x , y) which needs only be called once by MAIN4. When SPILL is called, it replaces the quantities JSPILL and ISPILL by zeros. Thereafter, in case of overflow (underflow) the subroutine replaces the overflowed (underflowed) quantity with x (y) and places into JSPILL (ISPILL) the address of the command which caused overflow (underflow) to occur for the first time. Program SCAT 4 uses $x = y = 0$.

Every subroutine in which computations are carried out starts by setting ISPILL and JSPILL equal to zero to insure correct identification of possible subsequent overflow or underflow. The subroutine then ends with a check of ISPILL and JSPILL. If either of these is not zero, there is an explicit printout describing the overflow or underflow. Underflow results therefore in substituting zero for the underflowed quantity, but the computation

proceeds. Overflow on the other hand results in substituting zero for the overflowed quantity and leads to a *CALL LEAVE* statement to stop the computation.

B. DETAILED DESCRIPTIONS OF THE SPECIFIC ROUTINES OF THE PROGRAM

MAIN4

The main routine which is only used at the start of the program carries out the following steps:

- 1) Calls SPILL which controls overflow and underflow (see III-A-4-ii). One such call statement is sufficient to put SPILL in permanent control for all subroutines.
- 2) Sets up EPS1, EPS2, EPS3, which are constants used to control the accuracy of the Coulomb functions computations, and EPS4 which is used in subroutine POT1CH.
- 3) Inputs identification and program numbers.
- 4) Calls *CTRL4*.

CTRL4 (Control 4)

This subroutine controls the whole flow of the program. It was coded as a subroutine to allow it to be called by subroutine LEAVE. It carries out the following steps:

- 1) Advances group identification and resets run identification numbers.
- 2) Call INPT4.
- 3) Calls POT1CH.
- 4) If $KTRL(5) = 1$, calls POP1
if $KTRL(5) = 0$, proceeds.
- 5) Calls SIGZRO, FSUBC, EXSGML.
- 6) Sets up five (or six) nested **DO** loops for varying successively V , W , a , V_s , W_s (and b for a surface absorption potential). The following steps are always done within the innermost **DO** loop:
 - a) If Sense Switch 1 is on, calls **SAVE**
if Sense Switch 1 is off, proceeds.
 - b) Advances run identification number.
 - c) Calls RHOTB, *COULFN*, RMXINC, PGEN4, INTCTR, *CSUBL*, AB, SGSGCP, SIGMAR.
 - d) If $KTRL(2) = 0$, proceeds
if $KTRL(2) = 1$, calls *CHISQ*.
 - e) Calls OUTPT4.
- 7) When all the **DO** loops have been completed, returns to step 1.

INPT4 (Input 4)

- 1) Inputs KTRL(1); if KTRL(1) = 100, calls EXIT
if KTRL(1) \neq 100, proceeds.
- 2) Inputs KTRL(I), I = 2 to 13.
- 3) Inputs FMI, FMB, ELAB, ZZ, RC, V, W, RO, A, VS, WS, RG, BG, DV, DW, DA, DVS, DWS, DBG, HA, PMA, FN1A, FN2A, HB, PMB, FN1B, FN2B, NVMAX, NWMAX, NAMAX, NVSMAX, NWSMAX, NBGMAX.
- 4) Sets up TV = V to TBG = BG (starting values of the parameters).
- 5) Inputs NMAX, forms NMAXP = NMAX–1.
- 6) Inputs RHOIN(I), I = 1 to NMAX and DRHOIN(I), I = 1 to NMAXP.
- 7) Computes FMU as per [equation \(5\)](#)
Computes ECM as per [equation \(6\)](#)
Computes FKAY as per [equation \(8\)](#)
Computes RHOBN as per [equation \(73\)](#)
Computes RMA and RMB (see [Glossary](#), under PMA, PMB)
Computes RHOBK as per [equation \(74\)](#)
Computes ETA as per [equation \(43\)](#).
- 8) Inputs LMAXM, forms IMAX = LMAXM + 1.
- 9) Sets IIN(J) = 1, J = 1 to LMAX (see description of subroutine INTCTR)
- 10) If KTRL(5) = 0, proceeds
if KTRL(5) \neq 0: a) inputs JMAX
b) inputs THETAD(I), I = 1 to JMAX
c) computes THETA(I), I = 1 to JMAX.
- 11) If KTRL(2) = 0 and/or KTRL(3) = 0, proceeds,
if KTRL(2) \neq 0 and KTRL(3) \neq 0, inputs
SGMARX(I), DSGMEX(I), POLEX(I), DPOLEX(I), I = 1 to JMAX.
- 12) Returns to CTRL4.

POT1CH (potential 1 check)

The purpose of this subroutine is to check whether ℓ_{\max} is sufficiently large so that all the partial waves sensibly affected by the potential are included and to check whether ρ_{\max} (the point at which the coulomb functions will be matched to the nuclear wave functions) is sufficiently large to insure that the non-coulomb part of the potential is negligible. If ℓ_{\max} and/or ρ_{\max} are too small, the subroutine increases them, and sets IIN(ℓ_{\max}) = 1. The quantities ρ_{\max} and ℓ_{\max} may be checked or not according to the value assigned to KTRL(13):

- KTRL(13) = 1: check both ℓ_{\max} and ρ_{\max}
- KTRL(13) = 2: check ρ_{\max} only
- KTRL(13) = 3: check ℓ_{\max} only
- KTRL(13) = 4: do not check either.

ρ_{\max} and ℓ_{\max} are checked in various ways depending upon the potential form. The routine operates as follows:

- 1) The routine first calculates the maximum values of V, W, A, VS, WS, and, in the case of a Gaussian absorption, of BG over the specified grid of these parameters.
- 2) If KTRL(1) = 0, standard potential (or variation thereof), the routine checks, if required, that:

- a) ρ_{\max} is sufficiently large so that

$$\frac{(V^2 + W^2)^{1/2}}{E} \frac{1}{(1 + e^{(\rho_{\max} - \bar{\rho}_N)/ka})} \leq \epsilon_4. \quad (144)$$

If this condition is not met, ρ_{\max} is increased by the last value of $\Delta\rho$ and the check is repeated. This is accompanied by the print out:

RHOIN(NMAX) = (value of old ρ_{\max}) + (last value of DRHOIN)
RHOIN(NMAX) IS TOO SMALL IN NUCLEAR POTENTIAL.

- b) The routine also checks, if required, that ℓ_{\max} is sufficiently large so that

$$\frac{\sqrt{V^2 + W^2}}{E} \frac{1}{(1 + e^{(\ell_{\max} - \bar{\rho}_N)/ka})} \leq \epsilon_4. \quad (145)$$

If this condition is not met, ℓ_{\max} is increased by 1 and the check is repeated; this is accompanied by the following printout:

LMAXM = (value of old LMAXM) + 1
LMAXM TOO SMALL BECAUSE OF CENTRAL POTENTIAL.

The routine then checks that ℓ_{\max} is sufficiently large so that

$$2k^2 \frac{\sqrt{V_S^2 + W_S^2}}{E} \frac{1}{(1 + e^{(\ell_{\max} - \bar{\rho}_N)/ka})} \leq \epsilon_4. \quad (146)$$

If this condition is not met, ℓ_{\max} is increased by 1 and the check is repeated; this is accompanied by the following printout:

LMAXM = (value of old LMAXM) + 1
LMAXM TOO SMALL BECAUSE OF SPIN ORBIT POTENTIAL.

- 3) If KTRL(1) = 1, Gaussian absorption,

- a) The check on ρ_{\max} is as follows:

$$\frac{V}{E} \frac{1}{(1 + e^{(\rho_{\max} - \bar{\rho}_N)/ka})} \leq \epsilon_4; \quad (147)$$

and

$$\frac{W}{E} e^{-(\rho_{\max} - \bar{\rho}_G/kb)^2} \leq \epsilon_4. \quad (148)$$

If these conditions are not met ρ_{\max} is increased as before and the checks are repeated; this is accompanied by the same printout as above.

b) The check on ℓ_{\max} is as follows:

$$\frac{V}{E} \frac{1}{(1 + e^{(\ell_{\max} - \bar{\rho}_N)/ka})} \leq \epsilon_4; \quad (149)$$

and

$$\frac{W}{E} e^{-(\ell_{\max} - \bar{\rho}_G/kb)^2} \leq \epsilon_4 \quad (150)$$

and as in [equation \(146\)](#).

If these conditions are not met ℓ_{\max} is increased by 1 and the checks repeated. The prints-out are given on the previous page.

4) If KTRL(1) = 2, Square well

a) The check on ρ_{\max} is as follows

$$\rho_{\max} > \bar{\rho}_N \quad (151)$$

b) The check on ℓ_{\max} is as follows

$$\ell_{\max} > \bar{\rho}_N + 3. \quad (152)$$

Failure to meet these conditions leads to increases in ρ_{\max} and/or ℓ_{\max} accompanied by the same printouts as given above, after which the checks are repeated.

The program uses $\text{EPS4} = 0.001$. This quantity is specified in the MAIN4 routine.

The checks described above are based on a rough estimate of the phase shifts using a WKB expression.

POP1

Computes P(L,J), PP(L,J), L = 1 to LMAXP, J = 1 to JMAX as per [equations \(134\)](#) and [\(135\)](#) and returns to CTRL4.

SIGZRO (Sigma zero)

Computes SIGMA0 and SIGMA1 as per [equations \(117\)](#) and [\(118\)](#) and returns to CTRL4.

FSUBC

Computes FCR(J) and FCI(J), J = 1 to JMAX as per [equation \(47\)](#) and returns to CTRL4.

EXSGML (Exponential sigma ℓ)

Computes EXSGMR(J), EXSGMI(J) for J = 1 to LMAX as per [equation \(133\)](#) and returns to CTRL4.

RHOTB (Rho tabulation)

The purpose of this subroutine is to construct a table of ρ 's and $\Delta\rho$'s corresponding to each step of the numerical integration. This table is formed from the arrays of RHOIN(I) and DRHOIN(I) which are input by subroutine INPT4

INPUT ARRAYS		COMPUTED TABLES	
RHOIN(I)	DRHOIN(I)	RHO(I)	DRHO(I)
RHOIN(1)	DRHOIN(1)	RHO(1)	DRHO(1)
RHOIN(2)	DRHOIN(2)	RHO(2)	DRHO(2)
·	·	·	·
·	·	·	·
·	·	·	·
·	·	·	·
RHOIN(NMAX-1)	DRHOIN(NMAX-1)	RHO(ILAST-1)	DRHO(ILAST-1)
RHOIN(NMAX)		RHO(ILAST)	

$\rho =$ RHOIN(1) (DRHOIN(1)) RHOIN(2) ... (DRHOIN(NMAX-1)) RHOIN(NMAX)

RHO(I+1) = RHO(I) + DRHO(I)

DRHO(1) = DRHO(2) = ... = DRHO(I) = DRHOIN(I)

up to RHO(I) = RHOIN(2), etc. ...

RHO(1) = RHOIN(1); RHO(ILAST) = RHO(NMAX)

ILAST \geq NMAX.

If RHOIN(NMAX) is given in such a way that it cannot be reached by an integral number of DRHO(I)'s, the last interval is shortened (up to 50%) or lengthened (by no more than 50%) so that RHO(ILAST) = RHOIN(NMAX).

COULFN (Coulomb functions)

This is the most complex subroutine of the program. It computes the regular and irregular coulomb functions and their derivatives for L = 1 to LMAXM at $\rho =$ RHOMAX by means of asymptotic formulas. The main steps are as follows:

- 1) The a and b series appearing in [equation \(115\)](#) are calculated according to [equations \(116\)](#) and are cut off when either:
 - (a) The term N_a (or N_b) is such that the next term exceeds in magnitude the previous one, i.e., when

$$[\text{Re}(U_{N_a} + 1)]^2 + [\text{Im}(U_{N_a} + 1)]^2 \geq [\text{Re}(U_{N_a})]^2 + [\text{Im}(U_{N_a})]^2 \quad (153)$$

where

$$U_k = \frac{a_k}{(k-1)\rho_{\max}^{k-1}} \quad (154)$$

and similarly for the b series.

- (b) The contributions of both the real and imaginary terms give undetectable contributions to the real and imaginary parts of φ_0 (and similarly for φ_1). During these computations, the value of ρ_{\max} may be increased by addition of the last value of DRHOIN and the computation starts all over again under the following condition:

- a) The a or b series is identically equal to zero. This is accompanied by the printout:

SERIES IN PHI0 OR PHI1 IS ZERO, CHECK **DATA, IF OK**

INCREASE RHOMAX = (value of old RHOMAX) + (value of last DRHOIN)

- b) Either of the two series diverges too quickly, i.e., the N_a -th (or N_b -th) term still gives a non-negligible contribution to the series obtained so far, viz.

$$\left| \frac{[\operatorname{Re}(U_{N_a})]^2 + [\operatorname{Im}(U_{N_a})]^2}{\left[\operatorname{Re} \left(\sum_{k=2}^{N_a-1} U_k \right) \right]^2 + \left[\operatorname{Im} \left(\sum_{k=2}^{N_a-1} U_k \right) \right]^2} \right| \geq EPS3 \quad (155)$$

(EPS3 is given the value 0.00001 in the MAIN4 routine.)

This is accompanied by the printout:

IF OK A OR B SERIES DIVERGES TOO QUICKLY

INCREASE RHOMAX = (value of old RHOMAX) +(value of last DRHOIN).

- c) Over 48 terms are required in either the a or b series. This is accompanied by the printout:

INCREASE RHOMAX = (value of old RHOMAX) + (value of last DRHOIN)

A OR B SERIES CONVERGES TOO SLOWLY.

- 2) The quantities $\varphi_0, \varphi_1, F_0, F_1, G_0, G_1$ are formed according to [equations \(114\)](#) and [\(115\)](#), and the Wronskian is checked for accuracy requiring that

$$\left| \mathscr{W} - [1 + \eta^2]^{-1/2} \right| = \left| F_0 G_1 - F_1 G_0 - [1 + \eta^2]^{-1/2} \right| \leq EPS1 \quad (156)$$

(EPS1 is given the value 0.00001 in the MAIN4 routine.)

If this condition is violated ρ_{\max} is increased and the computation starts all over again; this is accompanied by the following printout:

INCREASE RHOMAX = (old value of RHOMAX) + (last value of DRHOIN)

BAD INITIAL WRONSKIAN.

- 3) The regular coulomb functions are formed by downward recurrence as per [equations \(120\)](#) and [\(122\)](#) according to the accompanying description.

Agreement between successive sets of F_ℓ 's is verified by checking that

$$\left| (F_\ell^{(n)} / F_\ell^{(n+1)}) - 1 \right| \leq EPS2 \quad (157)$$

(EPS2 is given the value 0.00001 in the MAIN4 routine) for $\ell = 0$ to ℓ_{\max} .

During this computation the value of ρ_{\max} is increased and the computation starts all over if it turns out that $\ell_{(1)} > \ell_{\max} + 40$. This is accompanied by the printout:

INCREASE RHOMAX = (old value of RHOMAX) + (last value of DRHOIN)

L TOO LARGE IN FBAR(L).

- 4) The irregular coulomb functions are formed by upward recurrence as per [equation \(119\)](#) and the Wronskian for every $\ell = 0$ to $\ell_{\max} + 1$ is checked for accuracy requiring that

$$\left| F_{\ell}G_{\ell+1} - F_{\ell+1}G_{\ell} - \frac{\ell + 1}{[(\ell + 1)^2 + \eta^2]^{1/2}} \right| \leq EPS1 \quad (158)$$

(EPS1 is given the value 0.00001 in the MAIN4 routine.)

If this condition is violated the value of ρ_{\max} is increased and the computation starts all over again; this is accompanied by the printout:

INCREASE RHOMAX = (old value of RHOMAX) + (last value of DRHOIN)

BAD WRONSKIAN FOR L = (value of $\ell + 1$ for which [equation \(158\)](#) failed).

- 5) Finally the derivatives of the coulomb functions for $\ell = 0$ to ℓ_{\max} are formed as per [equation \(123\)](#).

RMXINC (Rho max increase)

The purpose of this subroutine is to extend the table of RHO(I) and DRHO(I) by increments of the last value DRHOIN until the final value of RHO(I) equals RHOMAX which may have been increased by the subroutine *COULFN*.

PGEN4 (Potential generator 4)

The purpose of this subroutine is to form tables of the ℓ -independent parts of the potential corresponding to the RHO(I) tables and suitable for using in the numerical integrations.

These include:

UCRB(I), UCIB(I), USRB(I), USIB(I) for I = 1 to ILAST and corresponding to the values at the beginning of an interval of integration; a corresponding table of form factors is also formed:

FFCR(I), FFCI(I), FFSR(I), FFSI(I),

and

UCRM(I), UCIM(I), USRM(I), USIM(I),

and

FFCRM(I), FFCIM(I), FFSRM(I), FFSIM(I) for I = 1 to ILAST – 1 corresponding to the values in the middle of an interval of integration.

The original and tightest part of the subroutine corresponds to a standard form factor; modifications have been added to permit use of a variety of form factors briefly described earlier.

The subroutine operates as follows: The UCR–’s are calculated as per [equation \(98\)](#), the UCI–’s as per [equation \(99\)](#), the USR–’s as per [equation \(100\)](#) and the USI–’s as per [equation \(101\)](#), wherein:

- (i) KTRL(I) = 0: VOLUME ABSORPTION OR SPECIAL NUCLEAR FORM FACTOR:

- If KTRL(7) = 0, f_{CR} is computed as per [equation \(80\)](#); [FFCR]⁸ = f_{CR}
 = 1, f_{CR} is computed as per [equation \(86\)](#); [FFCR] = f_{CR}
 = 2, f_{CR} is computed as per [equation \(87\)](#); [FFCR] = f_{CR}
- If KTRL(8) = 0, f_{CI} is computed as per [equation \(80\)](#); [FFCI] = f_{CI}
 = 1, f_{CI} is computed as per [equation \(86\)](#); [FFCI] = f_{CI}
 = 2, f_{CI} is computed as per [equation \(87\)](#); [FFCI] = f_{CI}
- If KTRL(9) = 0, f_{SR} is computed as per [equation \(81\)](#); [FFSR] = f_{SR}
 = 1, f_{SR} is computed as per [equation \(91\)](#); [FFSR] = f_{SR}/ka
 = 2, f_{SR} is computed as per [equation \(94\)](#); [FFSR] = $f_{\text{SR}}/2$
- If KTRL(10) = 0, f_{SI} is computed as per [equation \(81\)](#); [FFSI] = f_{SI}
 = 1, f_{SI} is computed as per [equation \(91\)](#); [FFSI] = f_{SI}/ka
 = 2, f_{SI} is computed as per [equation \(94\)](#); [FFSI] = $f_{\text{SI}}/2$

(ii) KTRL(1) = 1: GAUSSIAN ABSORPTION

- f_{CR} is computed as per [equation \(80\)](#); [FFCR] = f_{CR}
 f_{CI} is computed as per [equation \(82\)](#); [FFCI] = f_{CI}
 f_{SR} is computed as per [equation \(81\)](#); [FFSR] = f_{SR}
 f_{SI} is computed as per [equation \(81\)](#); [FFSI] = f_{SI}

(iii) KTRL(1) = 2: SQUARE WELL

- f_{CR} is computed as per [equation \(84\)](#); [FFCR] = f_{CR}
 f_{CI} is computed as per [equation \(84\)](#); [FFCI] = f_{CI}
 f_{SR} and f_{SI} are taken to be zero.

Furthermore,

If KTRL(11) = 1, USR- are computed as per [equation \(100\)](#) *including* the coulomb spin-orbit term.

If KTRL(11) = 0, USR- are computed as per [equation \(100\)](#) *excluding* the coulomb spin-orbit term, i.e, the second term on the right hand side. KTRL(7) to KTRL(11) can of course be given any combination of permitted values.

INTCTR (Integration Control)

For each value of L = 1 to LMAX this subroutine carries out the following steps:

- 1) Sets up starting values for the numerical integration as per [equation \(113\)](#). The quantities IIN(L) are not especially useful at the present time, but they have been included in order to permit start of the numerical integration at various values of ρ depending on ℓ and thus permitting considerable time saving by foreshortening the numerical integrations. A study of this method is presently under way.
- 2) Calls RKINT which performs the numerical integration.

⁸FFCR refers to the symbolic variables FFCR(I) and FFCRM(I) appearing in the program (see [glossary of symbols](#)), similarly for FFCI, FFSR, and FFSI.

- 3) Stores the final values of the functions and their derivatives at the completion of each integration.

RKINT (Runge-Kutta integration)

This is the most crucial subroutine in the program as most of the time is spent in numerical integration. Special efforts have therefore been made to produce a rapid program.

The subroutine integrates numerically as per [equations \(102\) to \(112\)](#) the differential [equations \(96\)](#) operating simultaneously on the two sets corresponding to $\vec{\sigma} \cdot \vec{\ell} = \ell$ and $-\ell - 1$.

Special provisions have been made to avoid overflow; this is accomplished by dividing all the functions and their derivatives by the largest of these at every step (RENORM); whenever such renormalization is carried out it is accompanied by the following printout: RENORMALIZATION FACTOR = (value of RENORM) IN RKINT FOR CODED L=(value of $\ell + 1$) and RHO =(value of ρ at which renormalization took place).

CSUBL

This subroutine computes C_ℓ^\pm as per [equation \(125\)](#) for $\ell = 0$ to ℓ_{\max} .

AB

This subroutine computes A(J) and B(J) for J = 1 to JMAX i.e., for the various angles θ required, as per [equation \(60\)](#).

SQSGCP (Sigma, sigma-coulomb, polarization)

This subroutine computes $\sigma(\theta)$, $P(\theta)$, $\sigma_c(\theta)$, as per [equations \(34\)](#), [\(35\)](#); [\(136\)](#) and finally $\sigma(\theta)/\sigma_c(\theta)$ for the various angles required.

SIGMAR

This subroutine computes σ_R as per [equation \(132\)](#).

CHISQ (Chi Square)

This subroutine computes $\chi_\sigma^2(\theta)$, χ_σ^2 , $\chi_P^2(\theta)$, χ_P^2 , χ_T^2 as per [equations \(137\)](#), [\(138\)](#) and [\(139\)](#).

Note: The quantities $\Delta\sigma^{\text{ex}}(\theta)$ and $\Delta P^{\text{ex}}(\theta)$ are always assumed to be non-zero. Thus to avoid including an unknown experimental quantity, the corresponding standard deviation must be taken as very large.

OUTPT4 (Output 4)

Several output formats are available:

- (1) **Minimum output** (KTRL(6) = 1).

- (a) Basic quantities

NUMPRG

KTRL(I) for I = 1 to 13

FMI, FMB, ELAB, ZZ, V, W, A, RO, VS, WS, RC, BG, RG RHOBN, RHOBC, RHOBN, ECM,ETA, FKAY, FKAYA, FKAYB

and, if either KTRL(7), (8), (9), or (10) is not zero,

HA, RMA, FN1A, FN2A, PNA, HB, RMB, FN1B, FN2B, PMB,

then RHOMAX, LMAXM, NMAX, RHOIN(I) for I = 1 to NMAX,

DRHOIN(I) for I = 1 to NMAX-1, SGMRTH
and, if KTRL(2) = 1, CHI2ST, CHI2PT, CHI2T.

(b) Basic Table

THETAD(I), SGMATH(I), SRATIO(I), POLTH(I),
and, if KTRL(2) = 1, SGMAEX(I), POLEX(I), for I = 1 to JMAX.

(2) **Normal output** (KTRL(6) = 0)

(a) Basic quantities

(See above)

(b) Basic Table

(See above)

(c) Form factor table (output only if KTRL(12) = 1)

RHO(I), FFCR(I), FFCI(I), FFSR(I), FFSI(I),
for I = 1 to ILAST.

(d) Fitting table (output only if KTRL(2)=1)

THETAD(I), DSGMEX(I), DPOLEX(I), CHI2S(I),
CHI2P(I), CHI2(I) for I = 1 to JMAX.

(e) L table

L, CR1(L), CI1(L), CR2(L), CI2(L) for L = 1 to LMAXM (corresponding to $\ell = 0$
to ℓ_{\max}).

This output is made for *every* run, and maybe preceded by underflow descriptions which may be ignored, and by other comments referring to an increase in ρ_{\max} , ℓ_{\max} , renormalization, etc.

Every page of output is headed by the run number on the left and the page number on the right. The number of lines per page is held to be less than 50, otherwise the subroutine calls subroutine SKIP which starts a new page.

SKIP

This subroutine increases the page number, resets K, the line counter, and outputs the run and page number. Note that arguments giving the number of lines, page and run numbers are required.

LEAVE

This subroutine is called whenever a run gets into difficulty because overflow, or division by zero occur. The subroutine calls PDUMP to give a partial core dump.

This subroutine was included so as to allow for various possible requirements upon overflow and division by zero without having to change every command where the difficulty might occur.

IV. DESCRIPTION OF INPUT DATA

All data is input from tape 7. The input data tape is prepared from IBM cards which contain one piece of input data per card in either of the two following formats:

Columns.	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	72	
Integers	x	x	x	x	x	←								any Hollerith character	→		
Floating nos.	±	0	.	x	x	x	x	x	x	x	x	x	x	±	x	x	← any Hollerith character →
				} fractional part								} exponent					

Note: Any floating point format which uses 15 columns or less and is acceptable to FORTRAN may be used in place of the above.

(1) The following identification data is input first:

NUMRUN(1) : month
 NUMRUN(2) : day
 NUMRUN(3) : year
 NUMRUN(4) : set number (put in 0 to start with 1)
 NUMRUN(5) : run number (put in 0 to start with 1)
 NUMPRG : program number (we use 4).

Note: The identification which consists of the five quantities NUMRUN(I), I = 1 to 5, is printed at the top left of every output sheet. NUMRUN(4) is advanced every time a new set of data is input, NUMRUN(5) is advanced every time a run is made with a new set of parameters.

(2) Then, for every set of run, i.e., for every set of input data:

(a) **Controls**

KTRL(1) = 0 : Standard potential (possibly with generalized form factors)
 = 1 : Gaussian absorption
 = 2 : Square well⁹
 KTRL(2) = 0 : no χ^2 required
 = 1 : χ^2 required

⁹The quantity A is eventually discarded but it must still be input as 1/2 to avoid overflow in the early part of the program.

- KTRL(3) = 0 : same experimental values as in last set
- = 1 : new experimental values coming¹⁰
- KTRL(4) : not used in present program
- KTRL(5) = 0 : same angles as in last set
- = 1 : new angles coming
- KTRL(6) = 0 : normal output
- = 1 : minimum output
- KTRL(7) = 0 : UCR – Standard form
- = 1 : UCR – form A
- = 2 : UCR – form B
- KTRL(8) = 0 : UCI – Standard form
- = 1 : UCI – form A
- = 2 : UCI – form B
- KTRL(9) = 0 : USR – derivative standard form
- = 1 : USR – derivative form A
- = 2 : USR – form B
- KTRL(10) = 0 : USI – derivative standard form
- = 1 : USI – derivative form A
- = 2 : USI – form B
- KTRL(11) = 0 : do not include coulomb spin-orbit
- = 1 : do include coulomb spin-orbit
- KTRL(12) = 0 : do not print out form factors
- = 1 : do print out form factors
- KTRL(13) = 1 : check ρ_{\max} and ℓ_{\max}
- = 2 : check ρ_{\max} only
- = 3 : check ℓ_{\max} only
- = 4 : do not check ρ_{\max} nor ℓ_{\max} .

(b) **Basic data**

FMI, FMB, ELAB, ZZ, RC, V, W, RO, A, VS, WS, RG, BG, DV, DW, DA, DVS, DWS, DBG, HA, PMA, FN1A, FN2A, HB, PMB, FN1B, FN2B, NVMAX, NWMAX, NAMAX, NVSMAX, NWSMAX, NBGMAX.

(c) **Integration data**

NMAX, RHOIN(I) for I = 1 to NMAX, DRHOIN(I) for I = 1 to NMAX – 1,

(d) LMAXM

(e) **Angles:**

if KTRL(5) = 1 input: JMAX, THETAD(I) for I = 1 to JMAX

(f) **Experimental data:**

¹⁰KTRL(3) = 1 also requires KTRL(2) = 1 for proper operation.

if KTRL(2) = 1 and KTRL(3) = 1 input:

SGMAEX(I) for I = 1 to JMAX

DSGMEX(I) for I = 1 to JMAX

POLEX(I) for I = 1 to JMAX

DPOLEX(I) for I = 1 to JMAX

(3) Final card:

KTRL(1) = 100.

V. GLOSSARY AND DESCRIPTION OF SYMBOLIC VARIABLES APPEARING IN COMMON AND DIMENSION STATEMENTS

FORTRAN Symbol	Math. Symbol	Description
A	a	Rounding parameter appearing in standard potential, see eq. (62)
AR(I), AI(I) I = 1 to 75	$\text{Re}\{a_i\}, \text{Im}\{a_i\}$	1) Real and imaginary parts of the terms of the auxiliary series used to calculate asymptotically the coulomb functions, see eq. (116)
BR(I), BI(I) I = 1 to 75	$\text{Re}\{A(\theta_i)\}, \text{Im}\{A(\theta_i)\}$ $\text{Re}\{b_i\}, \text{Im}\{b_i\}$ $\text{Re}\{B(\theta_i)\}, \text{Im}\{B(\theta_i)\}$	2) See eq. (60) for definition 1) Ibid, see eq. (116) 2) See eq. (60) for definition
BG	b	Width parameter in Gaussian absorption see eq. (82)
CHI2(I) I = 1 to 75	$\chi^2(\theta_i)$	$= \chi_\sigma^2(\theta_i) + \chi_P^2(\theta_i)$
CHI2P(I) I = 1 to 75	$\chi_P^2(\theta_i)$	See eq. (139)
CHI2PT	χ_P^2	See eq. (139)
CHI2S(I) I = 1 to 75	$\chi_\sigma^2(\theta_i)$	See eq. (138)
CHI2ST	χ_σ^2	See eq. (138)
CHI2T	χ^2	$= \chi_\sigma^2 + \chi_P^2$
CR1(L), CI1(L) for L = 1 to 51	$\text{Re}(C_\ell^+), \text{Im}(C_\ell^+)$	See eqs. (57) and (125)
CR2(L), CI2(L)	$\text{Re}(C_\ell^-), \text{Im}(C_\ell^-)$	See eqs. (57) and (125)
DA, DV, DW, DVS, DWS, DBG		Amount by which A, V, W, VS, WS, BG must be incremented for succeeding runs (these increments may be input as positive, zero or negative).
DPOLEX(I) for I = 1 to 75	$\Delta P^{\text{ex}}(\theta_i)$	Standard deviation in the experimental polarization (must <i>never</i> be input as 0)
DRHO(I) for I = 1 to 250	$\Delta \rho_i$	Interval of numerical integration (see description of subroutine RHOTB)
DRHOL		Last interval to be used in the numerical integration

FORTRAN Symbol	Math. Symbol	Description
DRHOIN(I) I = 1 to 250		Interval of numerical integration specified by input for RHOIN(I) < ρ ≤ RHOIN(I+1) (See description of subroutine RHOTB)
DSGMEX(I) I = 1 to 75	$\Delta\sigma^{\text{ex}}(\theta_i)$	Standard deviation in the experimental differential elastic scattering cross section in square fermis/sterad, (must <i>never</i> be input as 0)
ECM	E	Incident energy in center-of-mass system (MeV)
ELAB	E_{LAB}	Incident energy in laboratory system (MeV)
EPS1, EPS2, EPS3	$\epsilon_1, \epsilon_2, \epsilon_3$	Error thresholds appearing in various parts of the calculation of the coulomb functions. See eqs. (155) to (158)
EPS4	ϵ_4	Error threshold used in POT1CH subroutine, see eqs. (144) to (150)
ETA	η	See eq. (43)
ETA2	η^2	
EXSGMR(L), EXSGMI(L) L = 1 to 51	$\text{Re}\{e^{2i\sigma_\ell}\}, \text{Im}\{e^{2i\sigma_\ell}\}$	See eq. (133)
F(L), L = 1 to 52	F_ℓ	See eq. (114) and (122)
FBAR(L), L = 1 to 91	$F_\ell^{(n)}$	See eq. (120)
FCR(I), FCI(I) I = 1 to 75	$\text{Re}\{f_c(\theta_i)\}, \text{Im}\{f_c(\theta_i)\}$	See eq. (47)
FFCR(I), FFCRM(I) I = 1 to 250	$f_{\text{CR}}(\rho_i)$ $f_{\text{CR}}(\rho_i + \frac{\Delta\rho_i}{2})$	Form factors for the real central part of the potential at the beginning and middle of an integration interval (See eqs. (80), (84), (86), (87) and description of subroutine PGEN4)
FFCI(I), FFCIM(I) I = 1 to 250	$f_{\text{CI}}(\rho_i)$ $f_{\text{CR}}(\rho_i + \frac{\Delta\rho_i}{2})$	As above for the imaginary central part of the potential (See eqs. (80), (82), (84), (86), (87) , and description of subroutine PGEN4)
FFSR(I), FFSRM(I) I = 1 to 250	$f_{\text{SR}}(\rho_i)$ $f_{\text{SR}}(\rho_i + \frac{\Delta\rho_i}{2})$	As above for the real spin-orbit part of the potential (See eqs. (81), (85), (91), (94) and description of subroutine PGEN4)

FORTRAN Symbol	Math. Symbol	Description
FFSI(I), FFSIM(I) I = 1 to 250	$f_{SI}(\rho_i) f_{SI}(\rho_i + \frac{\Delta\rho_i}{2})$	As above for the imaginary spin-orbit part of the potential (See eqs. (81), (85), (91), (94), and description of subroutine PGEN4)
FKAY	k	See eq. (8) (inverse fermis)
FKAYA	ka	
FKAYB	kb	
FMB	m_b	Mass number of target nucleus (atomic units)
FMI	m_i	Mass number of incident particle (atomic units)
FMU	μ	Reduced mass of incident particle (atomic units (see eq. (5)))
FN1A, FN2A	nA_1, nA_2	See eq. (86) and following description
FN1B, FN2B	nB_1, nB_2	See eq. (87) and following description
FF(L), L = 1 to 51	F'_ℓ	See eq. (123)
G(L), L = 1 to 52	G_ℓ	See eq. (114) and (119)
GP(L), L = 1 to 51	G'_ℓ	See eq. (123)
HA, HB	h_{0A}, h_{0B}	See eq. (88)
IDATA		Number of sets of data to be processed after making use of subroutine SAVE
IFIRST		Initial value of I, the subscript appearing in RHO(I)
ILAST		Final value of I, the subscript appearing in RHO(I)
IIN(L), L = 1 to 51		Originally designed to allow input of any desired value of IFIRST for various L's in order to speed up the numerical integration. In the present program the IIN(L) are all set equal to 1 by subroutine INPT4
ISPILL, JSPILL		Underflow and overflow indicators used in conjunction with subroutine SPILL
JMAX		Total number of angles input ($JMAX \leq 75$)
JMAXT		Temporary storage for JMAX used after calling subroutine SAVE

FORTRAN Symbol	Math. Symbol	Description
KTRL(I) I = 1 to 13		Controls used throughout the program to specify the potential, input and output type (see description of input data)
KTRLT(I) I = 1 to 13		Temporary storage for KTRL(I) used after calling subroutine SAVE
L	$\ell + 1$	
LMAX	$\ell_{\max} + 1$	
LMAXM	ℓ_{\max}	
NA, NV, NW, NVS, NWS, NBG		DO loop variables used in subroutine <i>CTRL4</i> to specify the number of times the parameters have been incremented
NAMAX, NVMAX, NWMAX, NVSMAX, NWSMAX, NBGMAX		Total number of incrementations of the parameters specified as input data (≥ 1)
NINPUT		DO loop variable used after calling subroutine SAVE in order to count the number of sets of processed input data
NMAX		Total number of input values of RHOIN(I) specified in input
NMAXT		Temporary storage for NMAX used after calling subroutine SAVE
NMAXP		= NMAX – 1
NUMPRG		Program number (see description of input data)
NUMRUN(I) I = 1 to 5		Identification (see description of input data)
POLEX(I) I = 1 to 75	$P^{\text{ex}}(\theta_i)$	Experimental value of the polarization
POLTH(I) I = 1 to 75	$P^{\text{th}}(\theta_i)$	Calculated value of the polarization See eq. (35)
P(L,J) L = 1 to 51 J = 1 to 75	$P_\ell(\theta_j)$	Legendre polynomial, see eq. (134)
PP(L,J) L = 1 to 50 J = 1 to 75	$P_\ell^{(l)}(\theta_j)$	Associated Legendre polynomial, see eq. (135)
PMA, PMB	$\rho_{m_A}/\bar{\rho}_N$ and $\rho_{m_B}/\bar{\rho}_N$	These are the quantities specified by the input as they are more convenient than RMA and RMB.

FORTRAN Symbol	Math. Symbol	Description
RO	R_{ON}	Nuclear radius constant (fermis), see eq. (63)
RC	R_{OC}	Charge radius constant (fermis) see eq. (66)
RG	R_{OG}	Gaussian radius constant (fermis) see eq. (83)
RHOBC	$\bar{\rho}_C$	Value of ρ at which the uniform charge density ends, see eq. (74)
RHOBN	$\bar{\rho}_N$	Value of ρ at which the standard potential falls to half of its initial value, see eq. (73)
RHOBNG	$\bar{\rho}_G$	Value of ρ at which the Gaussian absorption is centered
RHOIN(I) I = 1 to 250		Input values of ρ for which the integration interval must change from DRHOIN(I-1) to DRHOIN(I). See description of subroutine RHOTB)
ROMAX		Final value of ρ in the numerical integration
RHO(I) I = 1 to 250	ρ_i	Value of ρ at the i -th interval of integration, see eq. (14)
RMA, RMB	ρ_{m_A}, ρ_{m_B}	Values of ρ at which special form factors are matched to standard form factors, see eqs. (86) and (87)
SGMAC(I) I = 1 to 75	$\sigma_c(\theta_i)$	See eq. (136) (square fermis/sterad)
SGMAEX(I) I = 1 to 75	$\sigma^{\text{ex}}(\theta_i)$	Experimental values of the differential elastic scattering cross section (square fermis/sterad)
SGMATH(I) I = 1 to 75	$\sigma^{\text{th}}(\theta_1)$	Calculated values of the differential elastic scattering cross section (square fermis/sterad), see eq. (34)
SGMRTH	σ_R	Calculated value of the reaction cross section (square fermis) see eq. (132)
SIGMA0	σ_0	See eqs. (117) and (118)
SIGMA1	σ_1	See eq. (117)
SRATIO(I) I = 1 to 75	$\sigma(\theta_i)/\sigma_c(\theta_i)$	Ratio of calculated to Rutherford cross section
TA, TV, TW, TVS, TWS, TBG,		Storage for initial values input for the parameters

FORTRAN Symbol	Math. Symbol	Description
THETAD(I) I = 1 to 75	θ_i	Scattering angle in center-of-mass system (degrees)
THETA(I) I = 1 to 75	θ_i	As above (radians)
UCRB(I), UCRM(I) I = 1 to 250	$U_{\text{CR}}(\rho_i) U_{\text{CR}}(\rho_i + \frac{\Delta\rho_i}{2})$	L -independent part of the real central potential at the beginning and in the middle of the i -th interval of integration, see eq. (98)
UCIB(I), UCIM(I) I = 1 to 250	$U_{\text{CI}}(\rho_i) U_{\text{CI}}(\rho_i + \frac{\Delta\rho_i}{2})$	As above for the imaginary central potential, see eq. (99)
USRB(I), USRM(I) I = 1 to 250	$U_{\text{SR}}(\rho_i) U_{\text{SR}}(\rho_i + \frac{\Delta\rho_i}{2})$	As above for the real spin-orbit potential, see eq. (100)
USIB(I), USIM(I) I = 1 to 250	$U_{\text{SI}}(\rho_i) U_{\text{SI}}(\rho_i + \frac{\Delta\rho_i}{2})$	As above for the imaginary spin-orbit potential, see eq. (101)
V	V	Depth of real central potential (MeV)
W	W	Depth of imaginary central potential (MeV)
VS	V_S	Real part of spin-orbit potential depth (MeV)
WS	W_S	Imaginary part of spin-orbit potential depth (MeV)
XC1, XCP1	$x_\ell^+(\rho), \dot{x}_\ell^+(\rho)$	Real part of the radial (unnormalized) wave function and its first derivative for the case $L + 1/2$
YC1, YCP1	$y_\ell^+(\rho), \dot{y}_\ell^+(\rho)$	As above for the imaginary part and the case $L + 1/2$
XD1, XDP1	$x_\ell^-(\rho), \dot{x}_\ell^-(\rho)$	As above for the real part and the case $L - 1/2$
YD1, YDP1	$y_\ell^-(\rho), \dot{y}_\ell^-(\rho)$	As above for the imaginary part and the case $L - 1/2$
X1(L), X1P(L) L = 1 to 51	$x_\ell^+(\rho_{\text{max}}), \dot{x}_\ell^+(\rho_{\text{max}})$	Real part of the radial (unnormalized) wave function and its first derivative for the case $L + 1/2$ at the end of a numerical integration
Y1(L), Y1P(L) L = 1 to 51	$y_\ell^+(\rho_{\text{max}}), \dot{y}_\ell^+(\rho_{\text{max}})$	As above for the imaginary part and the case $L + 1/2$
X2(L), X2P(L) L = 1 to 51	$x_\ell^-(\rho_{\text{max}}), \dot{x}_\ell^-(\rho_{\text{max}})$	As above for the real part and the case $L - 1/2$
Y2(L), Y2P(L) L = 1 to 51	$y_\ell^-(\rho_{\text{max}}), \dot{y}_\ell^-(\rho_{\text{max}})$	As above for the imaginary part and the case $L - 1/2$

FORTRAN Symbol	Math. Symbol	Description
<i>ZZ</i>	ZZ'	Product of the atomic numbers of the target nucleus and the incident particle.

VI. SYMBOLIC LISTING OF THE PROGRAM

MAIN ROUTINE — SCAT 4

COMMON A, AR, AI,

1BR, BI, BG,

2CHI2, CHI2P, CHI2PT, CHI2S, CHI2ST, CHI2T, CR1, CI1, CR2, CI2,

3DPOLEX, DSGMEX, DRHO, DRHOIN, DRHOL, DV, DW, DA, DVS, DWS, DBG,

4ECM, ELAB, EPS1, EPS2, EPS3, EPS4, ETA, ETA2, EXSGMR, EXSGMI,

5F, FBAR, FCR, FCI, FFCR, FFCI, FFCRM, FFCIM, FFSR, FFSI, FFSRM, FFSIM,

6FKAY, FMB, FMI, FMU, FN1A, FN2A, FN1B, FN2B, FP, FKAYA, FKAYB,

7G, GP,

8HA, HB,

9IDATA, IFIRST, IIN, ILAST, ISPILL

COMMON JMAX, JMAXT, JSPILL,

1KTRL, KTRLT,

2L, LMAX, LMAXM,

3NMAX, NMAXP, NMAXT, NINPUT, NUMRUN, NUMPRG, NVMAX, NWMAX, NAMAX, NVSMAX,

4NWSMAX, NV, NW, NA, NVS, NWS, NBGMAX, NBG,

5P, PP, POLEX, POLTH, PMA, PMB,

6RC, RO, RHO, RHOBC, RHOEN, RHOIN, RHOMAX, RMA, RMB, RG, RHOBNG,

7SGMAC, SGMAEX, SGMATH, SGMRTH, SIGMA0, SIGMA1, SRATIO,

8THETA, THETAD, TV, TW, TA, TVS, TWS, TBG,

9UCRB, UCIB, UCRM, UCIM, USRB, USIB, USRM, USIM

COMMON V, VS,

1W, WS,

2X1, X2, X1P, X2P, XC1, XCP1, XD1, XDP1,

3Y1, Y2, Y1P, Y2P, YC1, YCP1, YD1, YDP1,

4ZZ

DIMENSION AR(75), AI(75),

1BR(75), BI(75),

2CHI2(75), CHI2P(75), CHI2S(75), CR1(51), CI1(51), CR2(51), CI2(51),

3DPOLEX(75), DSGMEX(75), DRHO(250), DRHOIN(250),

4EXSGMR(51), EXSGMI(51),

5F(52), FBAR(91), FCR(75), FCI(75), FFCR(250), FFCI(250), FFCRM(250),

6FFCIM(250), FFSR(250), FFSI(250), FFSRM(250), FFSIM(250), FP(51),

7G(52), GP(51),

8IIN(51),

9KTRL(13), KTRLT(13)

DIMENSION NUMRUN(5),

1P(51,75), PP(50,75), POLEX(75), POLTH(75),

2RHO(250), RHOIN(250),

3SGMAC(75), SGMAEX(75), SGMATH(75), SRATIO(75),

4THETA(75), THETAD(75),

5UCRB(250), UCIB(250), UCRM(250), UCIM(250), USRB(250), USIB(250),

6USRM(250), USIM(250),

7X1(51), X2(51), X1P(51), X2P(51),

8Y1(51), Y2(51), Y1P(51), Y2P(51)

CALL SPILL(JSPILL, ISPILL, 0., 0.)

EPS1= 0.00001

EPS2= 0.00001

EPS3= 0.00001

EPS4=0.001

```
      READ INPUT TAPE 7,10,(NUMRUN(I)),I=1,5)
      READ INPUT TAPE 7,10,NUMPRG
10    FORMAT(I5)
      CALL CTRL4
      GO
```

```

SUBROUTINE CTRL4
3  NUMRUN(4)=NUMRUN(4)+1
   NUMRUN(5)=0
   CALL INPT4
   CALL POT1CH
35  IF(KTRL(5)) 80,81,80
80  CALL POP1
81  CALL SIGZRO
   CALL FSUBC
   CALL EXSGML
   DO 20 NV=1,NVMAX
     IF (NV-1) 102,101,102
101 V=TV
   GO TO 103
102 V=V+DV
103 DO 20 NW=1,NWMAX
     IF (NW-1) 105,104,105
104 W=TW
   GO TO 109
105 W=W+DW
109 DO 20 NA=1,NAMAX
     IF (NA-1) 111,110,111
110 A=TA
   GO TO 112
111 A=A+DA
112 DO 20 NVS=1,NVSMAX
     IF (NVS-1) 114,113,114
113 VS=TVS
   GO TO 115
114 VS=VS+DVS
115 DO 20 NWS=1,NWSMAX
     IF (NWS-1) 117,116,117
116 WS=TWS
   GO TO 118
117 WS=WS+DWS
118 DO 20 NBG=1,NBGMAX
     IF (NBG-1) 120,119,120
119 BG=TBG
   GO TO 121
120 BG=BG+DBG
121 IF (SENSE SWITCH 1) 26,27
26  REWIND 7
   CALL SAVE(8)
   READ INPUT TAPE 7,50,(LGAR,I=1,6)
   IDATA= NUMRUN(4)
   DO 66 NINPUT=1, IDATA
     READ INPUT TAPE 7,50,(KTRLT(I),I=1,13)
50  FORMAT (I5)
51  FORMAT (E15.9)
   READ INPUT TAPE 7,51,(GAR,I=1,27)
   READ INPUT TAPE 7,50,(LGAR,I=1,6), NMAXT
   NT=2*NMAXT-1
   READ INPUT TAPE 7,51,(GAR,I=1,NT)
   READ INPUT TAPE 7,51, LGAR

```

```
      IF (KTRLT(5)) 71,70,71
71  READ INPUT TAPE 7,50, JMAXT
      READ INPUT TAPE 7,51,(GAR,I=1,JMAXT)
70  IF (KTRLT(2)) 61,66,61
61  IF(KTRLT(3)) 63,66,63
63  NT=4*JMAXT
      READ INPUT TAPE 7,51,(GAR,I=1,NT)
66  CONTINUE
27  NUMRUN(5)= NUMRUN(5)+1
      CALL RHOTB
      CALL COULFN
      CALL RMXINC
      CALL PGEN4
      CALL INTCTR
      CALL CSUBL
      CALL AB
      CALL SGSGCP
      CALL SIGMAR
      IF (KTRL(2)) 33,100,33
33  CALL CHISQ
100 CALL OUTPT4
20  CONTINUE
      GO TO 3
```

```
SUBROUTINE INPT4
  IF DIVIDE CHECK 100,110
100 WRITE OUTPUT TAPE 6,101
101 FORMAT(59H DIVIDE CHECK TRIGGER FOUND ON AT START OF INPT4 SUBROUT
LINE)
  CALL LEAVE
  STOP
110 ISPILL=0
  JSPILL=0
  READ INPUT TAPE 7,10,KTRL(1)
  IF (KTRL(1)-100) 150,151,151
151 CALL EXIT
  STOP
150 READ INPUT TAPE 7,10,(KTRL(I),I=2,13)
10  FORMAT (I5)
  READ INPUT TAPE 7,12,FMI,FMB,ELAB,ZZ,RC,V,W,RO,A,VS,WS,RG,BG,
1DV,DW,DA,DVS,DWS,DBG
  READ INPUT TAPE 7,12,HA,PMA, FN1A, FN2A, HB, PMB, FN1B, FN2B
  READ INPUT TAPE 7,10,NVMAX,NWMAX,NAMAX,NVSMAX,NWSMAX,NBGMAX
12  FORMAT (E15.9)
  TV= V
  TW=W
  TA=A
  TVS=VS
  TWS=WS
  TBG=BG
  READ INPUT TAPE 7,10,NMAX
  NMAXP=NMAX-1
  READ INPUT TAPE 7,12,(RHOIN(I),I=1,NMAX),(DRHOIN(I),I=1,NMAXP)
  CO2=FMI+FMB
  FMU=(FMI*FMB)/CO2
  ECM=ELAB*(FMB/CO2)
  FKAY= .2195376*SQRTF(FMU*ECM)
  T=FKAY*(FMB**.33333333)
  RHOBN= T*RO
  RHOBNG=T*RG
  RMA=PMA*RHOBN
  RMB=PMB*RHOBN
  RHOBC= T*RC
  ETA= .15805086*ZZ*SQRTF(FMI/ELAB)
  IF DIVIDE CHECK 200,47
200 WRITE OUTPUT TAPE 6,201
201 FORMAT(43H INPUT DIVISOR WAS ZERO IN INPT4 SUBROUTINE)
  CALL LEAVE
  STOP
47  READ INPUT TAPE 7,10,LMAXM
  LMAX=LMAXM+1
  DO 147 J=1,LMAX
147  IIN(J)=1
  IF (KTRL(5)) 48,50,48
48  READ INPUT TAPE 7,10,JMAX
  READ INPUT TAPE 7,12,(THETAD(I),I=1,JMAX)
  DO 49 I=1,JMAX
49  THETA(I)= 0.01745329252*THETAD(I)
```

```
50  IF(KTRL(2)) 51,207,51
51  IF(KTRL(3)) 53,207,53
53  READ INPUT TAPE 7,12,(SGMAEX(I),I=1,JMAX),(DSGMEX(I),I=1,JMAX),
    1(POLEX(I),I=1,JMAX),(DPOLEX(I),I=1,JMAX)
207 IF(ISPILL)202,204,202
202 WRITE OUTPUT TAPE 6,203,ISPILL
    203 FORMAT(23H UNDERFLOW OCCURRED AT I5,20H IN INPT4 SUBROUTINE)
204 IF(JSPILL)205,210,205
205 WRITE OUTPUT TAPE 6,206,JSPILL
    206 FORMAT(22H OVERFLOW OCCURRED AT I5,20H IN INPT4 SUBROUTINE)
    CALL LEAVE
    STOP
210 RETURN
```

```
SUBROUTINE POT1CH
  IF DIVIDE CHECK 30,31
30  WRITE OUTPUT TAPE 6,130
130 FORMAT (60H DIVIDE CHECK TRIGGER FOUND ON AT START OF POT1CH SUBRO
1UTINE)
  CALL LEAVE
  STOP
31  ISPILL=0
  JSPILL=0
  IKTRL=KTRL(13)
  NMAX=NMAX
  NMAXP= NMAX-1
  AMAX=NAMAX-1
  TTA=MAXIF(A, ((AMAX*DA)+A))
  VMAX=NVMAX-1
  TTV=MAXIF(V, ((VMAX*DV)+V))
  WMAX=NWMAX-1
  TTW=MAXIF(W, ((WMAX*DW)+W))
  VSWAX=NVSMAX-1
  TTVS=MAXIF(VS, ((VSMAX*DVS)+VS))
  WSMAX=NWSMAX-1
  TTWS=MAXIF(WS, ((WSMAX*DWS)+WS))
  BGMAX=NBGMAX-1
  TTBG=MAXIF(BG, ((BGMAX*DBG)+BG))
  FKAYA=FKAY*TTA
  FKAYB=FKAY*TTBG
  T2=SQRIF(TTV**2+TTW**2)/ECM
  T7=TTV/ECM
  T8=TTW/ECM
  IF DIVIDE CHECK 60,61
60  WRITE OUTPUT TAPE 6,160
160 FORMAT(26H ECM IS ZERO IN POT1CH SUB)
  CALL LEAVE
  STOP
61  GO TO (3,3,111,15),IKTRL
3   IF (KTRL(1)-2) 24,25,24
25  IF (RHOIN(NMAX)-RHOBN) 10,10,8
24  T1=1./(1.+EXPF((RHOIN(NMAX)-RHOBN)/FKAYA))
  IF DIVIDE CHECK 50,28
50  WRITE OUTPUT TAPE 6,150
150 FORMAT(28H FKAYA IS ZERO IN POT1CH SUB)
  CALL LEAVE
  STOP
28  IF (KTRL(1)-1) 40,41,40
40  T3= T2*T1
  GO TO 43
41  T3=T7*T1
43  IF (T3-EPS4) 42,42,10
10  WRITE OUTPUT TAPE 6,100, RHOIN(NMAX),DRHOIN(NMAXP)
100 FORMAT(13H RHOIN(NMAX)=E16.9,2H+ E16.9,46H RHOIN(NMAX) IS TOO SMAL
1L IN NUCLEAR POTENTIAL)
  RHOIN(NMAX)= RHOIN(NMAX)+DRHOIN(NMAXP)
  GO TO 3
42  IF (KTRL(1)-1) 8,6,8
```



```
6   T11= EXPF(-((RHOIN(NMAX)-RHOBNG)/FKAYB)**2)
    IF((T8*T11)-EPS4) 8,8,7
7   WRITE OUTPUT TAPE 6,103,RHOIN(NMAX),DRHOIN(MMAXP)
103 FORMAT(13H RHOIN(NMAX)=E16.9,2H+ E16.9,46H RHOIN(NMAX) IS TOO SMALL
    IN NUCLEAR POTENTIAL)
    RHOIN(NMAX)= RHOIN(NMAX)+DRHOIN(NMAXP)
    GO TO 6
8   GO TO(111,15),IKTRL
111 FLMAX=LMAXM
    IF(KTRL(1)-2) 29,300,29
300 IF(FLMAX-(RHOBN+3.)) 12,12,15
29  T4=1./(1.+EXPF((FLMAX-RHOBN)/FKAYA))
    IF(KTRL(1)-1) 33,32,33
33  T5= T2*T4
    GO TO 310
32  T5=T7*T4
310 IF(T5-EPS4)13,13,12
    12 WRITE OUTPUT TAPE 6,101,LMAXM
101 FORMAT (7H LMAXM=I5,3H +1,45H LMAXM TOO SMALL BECAUSE OF CENTRAL P
    OTENTIAL)
    LMAX= LMAX+1
    LMAXM= LMAXM+1
    IIN(LMAX)=1
    GO TO 111
13  IF(KTRL(1)-1) 17,19,17
19  T4=EXPF(-((FLMAX-RHOBNG)/FKAYB)**2)
    IF((T8*T4)-EPS4) 17,17,20
20  WRITE OUTPUT TAPE 6,200,LMAXM
200 FORMAT (7H LMAXM=I5,3H +1,45H LMAXM TOO SMALL BECAUSE OF CENTRAL P
    OTENTIAL)
    LMAX=LMAX+1
    LMAXM=LMAXM+1
    IIN(LMAX)=1
    GO TO 19
17  T2=SQRTF(TTVS**2+TTWS**2)/ECM
18  FLMAX=LMAXM
    T4=1./(1.+EXPF((FLMAX-RHOBN)/FKAYA))
38  T6=2.*T2*T4*(FKAYW**2)
    IF(T6-EPS4) 15,15,14
14  WRITE OUTPUT TAPE 6,102, LMAXM
102 FORMAT (7H LMAXM=I5,3H +1,48H LMAXM TOO SMALL BECAUSE OF SPIN ORB
    IT POTENTIAL)
    LMAX= LMAX+1
    LMAXM= LMAXM+1
    IIN(LMAX)=1
    GO TO 18
15  IF(ISPILL)202,204,202
202 WRITE OUTPUT TAPE 6,203,ISPILL
203 FORMAT(23H UNDERFLOW OCCURRED AT I5,14H IN POT1CH SUB)
204 IF(JSPILL)205,210,205
205 WRITE OUTPUT TAPE 6,206,JSPILL
206 FORMAT(22H OVERFLOW OCCURRED AT I5,14H IN POT1CH SUB)
    CALL LEAVE
    STOP
```

210 RETURN

```
SUBROUTINE POP1
  IF DIVIDE CHECK 1,2
1  WRITE OUTPUT TAPE 6,101
101 FORMAT (58H DIVIDE CHECK TRIGGER FOUND ON AT START OF POP1 SUBROUT
LINE)
  CALL LEAVE
  STOP
2  ISPILL=0
  JSPILL=0
  LMAXP=LWAX+1
  DO 20 J=1,JMAX
  SI2=1./SINF(THETA(J))
  IF DIVIDE CHECK 3,4
3  WRITE OUTPUT TAPE 6,103, J
103 FORMAT (71H DIVISOR SINF THETA IS ZERO IN FIRST DIVISION OF POP1 S
UBROUTINE FOR J=I3)
  CALL LEAVE
  STOP
4  CO=COSF(THETA(J))
  P(1,J)=1.0
  P(2,J)=CO
  PP(1,J)=0.0
  TWOLP1=3.
  FL=1.
  DO 20 L=1,LMAXP
  TL=FL+1.
  P(L+2,J)=(TWOLP1*CO*P(L+1,J)-FL*P(L,J))/TL
  PP(L+1,J)=TL*SI2*(CO*P(L+1,J)-P(L+2,J))
  TWOLP1=TWOLP1+2.
20  FL=TL
  IF (ISPILL) 30,31,30
30  WRITE OUTPUT TAPE 6,130, ISPILL
130 FORMAT(23H UNDERFLOW OCCURRED AT I6,19H IN POP1 SUBROUTINE)
31  IF (JSPILL) 32,33,32
32  WRITE OUTPUT TAPE 6,132, JSPILL
132 FORMAT (22H OVERFLOW OCCURRED AT I6,19H IN POP1 SUBROUTINE)
  CALL LEAVE
  STOP
33  RETURN
```

```
SUBROUTINE SIGZRO
  IF DIVIDE CHECK 5,6
5  WRITE OUTPUT TAPE 6,105
105 FORMAT (60H DIVIDE CHECK TRIGGER FOUND ON AT START OF SIGZRO SUBRO
1UTINE)
  CALL LEAVE
  STOP
6  ISPILL = 0
  JSPILL = 0
  SIGMA0=-(ETA/(12.*(ETA**2+16.)))*(1.+(ETA**2-48.)/(30.*((ETA**2+16
1.)**2)))+(ETA**4-160.*(ETA**2)+1280.)/(((16.+ETA**2)**4)*105.)
  SIGMA0=SIGMA0-ETA+(ETA/2.)*LOGF(ETA**2+16.)+((7./2.)*ATANF(ETA/4.)
1)-(ATANF(ETA)+ATANF(ETA/2.)+ATANF(ETA/3.))
  SIGMA1=SIGMA0+ATANF(ETA)
15 IF (ISPILL) 30,31,30
  30 WRITE OUTPUT TAPE 6,130,ISPILL
130 FORMAT (23H UNDERFLOW OCCURRED AT I6,21H IN SIGZRO SUBROUTINE)
31 IF (JSPILL) 32,11,32
32 WRITE OUTPUT TAPE 6,132,JSPILL
132 FORMAT (22H OVERFLOW OCCURRED AT I6,21H IN SIGZRO SUBROUTINE)
  CALL LEAVE
  STOP
11 RETURN
```

```
SUBROUTINE FSUBC
  IF DIVIDE CHECK 20,21
20  WRITE OUTPUT TAPE 6,120
120  FORMAT (53H DIVIDE TRIGGER FOUND ON AT START OF FSUBC SUBROUTINE)
     CALL LEAVE
     STOP
21  ISPILL=0
     JSPILL=0
     DO 10 J=1,JMAX
        SN=(SINF(THETA(J)/2.0))**2
        FLN=ETA*(LOGF(SN))-2.0*SIGMA0
        FNO=ETA/(2.0*FKAY*(SN))
        IF DIVIDE CHECK 22,23
22  WRITE OUTPUT TAPE 6,122,J
122  FORMAT (23H DIVISOR IS ZERO FOR J=I3,20H IN FSUBC SUBROUTINE)
     CALL LEAVE
     STOP
23  FCR(J)=(-FNO*COSF(FLN))
10  FCI(J)=(FNO*SINF(FLN))
     IF (ISPILL) 24,25,24
24  WRITE OUTPUT TAPE 6,124, ISPILL
124  FORMAT (23H UNDERFLOW OCCURRED AT I6,20H IN FSUBC SUBROUTINE)
25  IF (JSPILL) 26,27,26
26  WRITE OUTPUT TAPE 6,126, JSPILL
126  FORMAT (22H OVERFLOW OCCURRED AT I6,20H IN FSUBC SUBROUTINE)
     CALL LEAVE
     STOP
27  RETURN
```

```
SUBROUTINE EXSGML
  IF DIVIDE CHECK 10,11
10  WRITE OUTPUT TAPE 6,110
110  FORMAT (60H DIVIDE CHECK TRIGGER FOUND ON AT START OF EXSGML SUBRO
      1UTINE)
      CALL LEAVE
      STOP
11  ISPILL=0
      JSPILL=0
1   FL=0.
      EXSGMR(1)=COSF(2.0*SIGMA0)
      EXSGMI(1)=SINF(2.0*SIGMA0)
      ETA2=ETA**2
      ETA2A=2.0*ETA
      DO 20 L=2,LMAX
      FL=FL+1.0
      TER0=FL**2
      TER1=TER0+ETA2
      TER2=(TER0-ETA2)/TER1
      TER3=(ETA2A*FL)/TER1
      IF DIVIDE CHECK 12,13
12  WRITE OUTPUT TAPE 6,112,L
112  FORMAT (44H DIVISOR IS ZERO IN EXSGML SUBROUTINE FOR L=I3)
      CALL LEAVE
      STOP
13  EXSGMR(L)=(TER2*EXSGMR(L-1))-(TER3*EXSGMI(L-1))
20  EXSGMI(L)=(TER2*EXSGMI(L-1))+(TER3*EXSGMR(L-1))
      IF (ISPILL) 14,15,14
14  WRITE OUTPUT TAPE 6,114, ISPILL
114  FORMAT(23H UNDERFLOW OCCURRED AT I6,21H IN EXSGML SUBROUTINE)
15  IF (JSPILL) 16,17,16
16  WRITE OUTPUT TAPE 6,116,JSPILL
116  FORMAT(22H OVERFLOW OCCURRED AT I6,21H IN EXSGML SUBROUTINE)
      CALL LEAVE
      STOP
17  RETURN
```

```
SUBROUTINE RHOTB
DRHO(1)=DRHOIN(1)
RHO(1)=RHOIN(1)
N=1
I=1
20 RHO(I+1)=RHO(I)+DRHOIN(N)
   IF (RHO(I+1)-RHOIN(NMAX)) 30,50,70
30 IF (ABSF(RHO(I+1)-RHOIN(N+1))-.5*DRHOIN(N)) 35,35,40
   35 N=XMINOF(N+1,NMAX-1)
40 DRHO(I+1)=DRHOIN(N)
   I=I+1
   GO TO 20
50 ILAST=I+1
60 RHO(ILAST)=RHOIN(NMAX)
   DRHO(ILAST-1)=RHO(ILAST)-RHO(ILAST-1)
   RHOMAX=RHOIN(NMAX)
   DRHOL=DRHOIN(NMAX-1)
   IF (ISPILL) 80,81,80
80 WRITE OUTPUT TAPE 6,180,ISPILL
180 FORMAT(23H UNDERFLOW OCCURRED AT I6,21H IN RHOTB SUBROUTINE)
81 IF (JSPILL) 82,83,82
82 WRITE OUTPUT TAPE 6,182,JSPILL
182 FORMAT(22H OVERFLOW OCCURRED AT I6,21H IN RHOTB SUBROUTINE)
   CALL LEAVE
   STOP
83 RETURN
70 IF ((RHO(I+1)-RHOIN(NMAX))-.5*DRHOIN(N)) 50,50,75
75 ILAST=I
   GO TO 60
```

```
SUBROUTINE COULFN
  IF DIVIDE CHECK 50,51
50  WRITE OUTPUT TAPE 6,150
150  FORMAT (60H DIVIDE CHECK TRIGGER FOUND ON AT START OF COULFN SUBRO
      1UTINE)
      CALL LEAVE
      STOP
51  ISPILL=0
      JSPILL=0
      IKTRL=KTRL(13)
      LMAX=LMAXM+1
      ETA2=ETA**2
      SQ=SQRTF(1.+ETA2)
1   IJ = 1
      AR(1)=-ETA
      AI(1)=0.
      AR(2)=-.5*ETA2
      AI(2)=.5*ETA
2   SI=0.
      SR=0.
      PR= RHOMAX
      DO 10 K=2,49
          T= PR*FLOATF(1-K)
          TR=AR(K)/T
          TI=AI(K)/T
          IF DIVIDE CHECK 52,53
52  WRITE OUTPUT TAPE 6,152
152  FORMAT(57H DIVISOR T IS ZERO IN FIRST DIVISION OF COULFN SUBROUTIN
      1E)
      CALL LEAVE
      STOP
53  SQN=TR**2+TI**2
      IF (K-2) 4,4,3
3   IF (SQN-SQO) 4,4,11
4   TR=SR+TR
      TI=SI+TI
      IF (TR-SR) 6,5,6
5   IF (TI-SI) 6,13,6
6   SR=TR
      SI=TI
      AR(K+1)=0.
      AI(K+1)=0.
      KP=K/2
      DO 7 M=1,KP
          KM=K+1-M
          AR(K+1)=AR(K+1)-AR(M)*AR(KM)+AI(W)*AI(KM)
          AI(K+1)=AI(K+1)-AI(KM)*AR(M)-AI(M)*AR(KM)
          IF (K-2*KP) 8,9,8
          AR(K+1)=AR(K+1)-.5*(AR(KP+1)**2-AI(KP+1)**2)
          AI(K+1)=AI(K+1)-AR(KP+1)*AI(KP+1)
9   FK=.5*FLOATF(K)
      AI(K+1)=AI(K+1)-FK*AR(K)
      AR(K+1)=AR(K+1)+FK*AI(K)
      PR= PR*RHOMAX
```



```
10  SQO=SQN
    GO TO 101
11  T=SR**2+SI**2
    IF(T) 105,105,12
12  IF(ABSF(SQO/T)-EPS3) 13,13,106
13  GO TO (14,15),IJ
14  PAR=RHOMAX-ETA*LOGF(2.*RHOMAX)
    PHI0R=PAR+SIGMA0+SR
    PHI0I=SI
    AR(2)=-1.+AR(2)
    IJ=2
    GO TO 2
15  PHI1R=PAR+SIGMA1-1.570796325+SR
    PHI1I=SI
25  T1=EXPF(-PHI0I)
    T2=EXPF(-PHI1I)
    G(1)=T1*COSF(PHI0R)
    G(2)=T2*COSF(PHI1R)
    F1=T1*SINF(PHI0R)
    F2=T2*SINF(PHI1R)
    IF(ABSF(F1*G(2)-F2*G(1)-1./SQ)-EPS1) 31,31,102
31  IDEC=11
32  I=LMAX+IDEC
    FBAR(I)=.1
    FBAR(I+1)=0.
    LIMIT=LMAX+IDEC
    FL=LMAX+11
    T1=SQRTF((FL+1.)**2+ETA2)
    IF(JSPILL) 139,133,139
139 WRITE OUTPUT TAPE 6,1390,JSPILL
1390 FORMAT(23H OVERFLOW2 OCCURRED AT I6,21H IN COULFN SUBROUTINE)
    CALL LEAVE
    STOP
133 DO 33 I=1,LIMIT
    L=LMAX+IDEC-I
    FL=L
    T2=SQRTF(FL**2+ETA2)
    FBAR(L)=((2.*FL+1.)*(ETA+FL*(FL+1.)/RHOMAX)*FBAR(L+1)-FL*T1*FBAR(L
1+2))/((FL+1.)*T2)
    IF DIVIDE CHECK 54,600
54  WRITE OUTPUT TAPE 6,154
154 FORMAT(56H DIVISOR IS ZERO IN SECOND DIVISION OF COULFN SUBROUTINE
1)
    CALL LEAVE
    STOP
600 IF(JSPILL) 601,33,601
601 WRITE OUTPUT TAPE 6,1601,JSPILL
1601 FORMAT(22H OVERFLOW OCCURRED AT I6,21H IN COULFN SUBROUTINE,24H MU
1LTIPLY FBAR(I) BY 0.1)
    K=LMAX+IDEC
    FBAR(K)=FBAR(K)*0.1
    JSPILL=0
    GO TO 133
33  T1=T2
```

```
ALPHA=1./((FBAR(1)*G(2)-FBAR(2)*G(1))*SQ)
IF DIVIDE CHECK 55,43
55 WRITE OUTPUT TAPE 6,155
155 FORMAT (55H DIVISOR IS ZERO IN THIRD DIVISION OF COULFN SUBROUTINE
1)
CALL LEAVE
STOP
43 LMAXP=LMAX+1
DO 34 I=1,LMAXP
34 FBAR(I)=ALPHA*FBAR(I)
IF (IDEC-11) 371,35,371
371 IF (ABS(F1/FBAR(1)-1.)-EPS2) 37,37,35
35 DO 36 I=1,LMAXP
36 F(I)=FBAR(I)
IDEC=IDEC+5
IF (IDEC-40) 32,32,103
37 DO 38 I=1,LMAXP
IF (ABS(F(I)/FBAR(I)-1.)-EPS2) 44,44,35
44 IF DIVIDE CHECK 56,38
56 WRITE OUTPUT TAPE 6,156,L,I
156 FORMAT(74H DIVISOR FBAR(I)-1. IS ZERO IN FOURTH DIVISION OF COULFN
1 SUBROUTINE FOR L=I3,7H AND I=I3)
CALL LEAVE
STOP
38 CONTINUE
DO 381 I=1,MAXP
381 F(I)=FBAR(I)
382 T1=SQ
DO 40 L=1,LMAX
FL=L
T2=SQRTF((FL+1.):**2+ETA2)
G(L+2)=((2.*FL+1.)*(ETA+FL*(FL+1.)/RHOWAX)*G(L+1)-(FL+1.)*T1*G(L))
1/(FL*T2)
TS=FL/T1
IF DIVIDE CHECK 57,45
57 WRITE OUTPUT TAPE 6,157
157 FORMAT(58H DIVISOR T1 IS ZERO IN FIFTH DIVISION OF COULFN SUBROUTI
1NE)
CALL LEAVE
STOP
45 IF (ABS(F(L)*G(L+1)-F(L+1)*G(L)-TS)-EPS1) 40,40,104
40 T1=T2
41 DO 42 L=1,LMAX
FL=L
T=FL**2
T1=T/RHOMAX+ETA
IF DIVIDE CHECK 58,46
58 WRITE OUTPUT TAPE 6,158
158 FORMAT (62H DIVISOR RHOMAX IS ZERO IN SIXTH DIVISION OF COULFN SUB
1ROUTINE)
CALL LEAVE
STOP
46 T2=SQRTF(T+ETA2)
FP(L)=(T1*F(L)-T2*F(L+1))/FL
```

```
42 GP(L)=(T1*G(L)-T2*G(L+1))/FL
   IF DIVIDE CHECK 59,47
59 WRITE OUTPUT TAPE 6,159
159 FORMAT(60H DIVISOR FL IS ZERO IN SEVENTH DIVISION OF COULFN SUBROUTINE)
   CALL LEAVE
   STOP
47 IF(ISPILL) 60,61,60
60 WRITE OUTPUT TAPE 6,160,ISPILL
160 FORMAT(23H UNDERFLOW OCCURRED AT I6,21H IN COULFN SUBROUTINE)
61 IF(JSPILL) 62,63,62
62 WRITE OUTPUT TAPE 6,162,JSPILL
162 FORMAT(22H OVERFLOW OCCURRED AT I6,21H IN COULFN SUBROUTINE)
   CALL LEAVE
   STOP
63 RETURN
101 WRITE OUTPUT TAPE 6,121,RHOMAX,DRHOL
   GO TO (110,110,109,109),IKTRL
109 WRITE OUTPUT TAPE 6,114
   GO TO 13
102 WRITE OUTPUT TAPE 6,122,RHOMAX,DRHOL
   GO TO(110,110,111,111),IKTRL
111 WRITE OUTPUT TAPE 6,114
   GO TO 31
103 WRITE OUTPUT TAPE 6,123,RHOMAX,DRHOL
   GO TO (110,110,112,112),IKTRL
112 WRITE OUTPUT TAPE 6,114
   GO TO 382
104 WRITE OUTPUT TAPE 6,124,RHOMAX,DRHOL ,L
   GO TO (110,110,113,113),IKTRL
113 WRITE OUTPUT TAPE 6,114
   GO TO 40
105 WRITE OUTPUT TAPE 6,125,RHOMAX,DRHOL
   GO TO (110,110,115,115),IKTRL
115 WRITE OUTPUT TAPE 6,114
   GO TO 12
106 WRITE OUTPUT TAPE 6,126,RHOMAX,DRHOL
   GO TO (110,110,116,116),IKTRL
116 WRITE OUTPUT TAPE 6,114
   GO TO 13
110 RHOMAX=RHOMAX+DRHOL
   GO TO 1
121 FORMAT(18H INCREASE RHO MAX=E11.4,2H+ E11.4,35H A OR B SERIES CONVERGES TOO SLOWLY)
122 FORMAT(18H INCREASE RHO MAX=E11.4,2H+ E11.4,22H BAD INITIAL WRONSKIAN)
123 FORMAT(18H INCREASE RHO MAX=E11.4,2H+ E11.4,24H L TOO LARGE IN FBAIR (L))
124 FORMAT(18H INCREASE RHO MAX=E11.4,2H+ E11.4,21H BAD WRONSKIAN FOR IL=I3)
125 FORMAT(67H SERIES IN PHI0 OR PHI1 IS ZERO, CHECK DATA, IF OK INCREASE RHOMAX=E11.4,2H+ E11.4)
126 FORMAT(52H A OR B SERIES DIVERGES TOO QUICKLY INCREASE RHOMAX=E11.4,2H+ E11.4)
```

114 **FORMAT**(42H RHOMAX INCREASE NOT PERMITTED BY KTRL(13))

```
SUBROUTINE RMXINC  
3 IF (RHOMAX-RHO(ILAST)) 1,2,1  
1 ILAST=ILAST+1  
  RHO(ILAST)=RHO(ILAST-1)+DRHOL  
  DRHO(ILAST-1)=DRHOL  
  GO TO 3  
2 RETURN
```

```

SUBROUTINE PGEN4
  IF DIVIDE CHECK 60,61
60  WRITE OUTPUT TAPE 6,160
160  FORMAT (59H DIVIDE CHECK TRIGGER FOUND ON AT START OF PGEN4 SUBROU
      1TINE)
      CALL LEAVE
      STOP
61  ISPILL=0
      JSPILL=0
      IF (KTRL(1)) 3,4,3
3    KTRL(7)=0
      KTRL(8)=0
      KTRL(9)=0
      KTRL(10)=0
4    T1=V/ECM
      T2=W/ECM
      T10=VS/ECM
      T11=WS/ECM
      T12=FKAY*BG
      T3=2.*FKAY/A
      IF DIVIDE CHECK 62,65
62  WRITE OUTPUT TAPE 6,162
162  FORMAT (65H DIVISORS ECM OR A WERE WRONGLY INPUT AS ZERO IN PGEN4
      1SUBROUTINE)
      CALL LEAVE
      STOP
65  T4=T10*T3
      T5=T11*T3
      T6=FKAY*A
      T7=ETA/RHOBC
      IF DIVIDE CHECK 63,64
63  WRITE OUTPUT TAPE 6,163
163  FORMAT(61H DIVISOR RHOBC IS ZERO IN SECOND DIVISION OF PGEN4 SUBRO
      1UTINE)
      CALL LEAVE
      STOP
64  T8=RHOBC**2
      T9=ETA*2.
      I=1
40  EX=EXPF((RHO(I)-RHOBN)/T6)
      IF DIVIDE CHECK 80,66
80  WRITE OUTPUT TAPE 6,165
165  FORMAT (58H QUANTITY T6 IS ZERO IN THIRD DIVISION OF PGEN4 SUBROUT
      1INE)
      CALL LEAVE
      STOP
66  K=1
41  IF (I-1) 42,43,42
42  IF (DRHO(I)-DRHO(I-1)) 43,44,43
43  HDRHO=DRHO(I)*.5
      DEX=EXPF(HDRHO/T6)
44  IF (KTRL(1)-2)53,52,53
52  IF (RHO(I)-RHOBN) 54,55,55
54  S1=1.0
```

```
GO TO 68
55 S1=0.0
GO TO 68
53 S1=1./(1.+EX)
IF DIVIDE CHECK 67,68
67 WRITE OUTPUT TAPE 6,167
167 FORMAT(60H DIVISOR 1.+EX IS ZERO IN FOURTH DIVISION OF PGEN4 SUBRO
UTINE)
CALL LEAVE
STOP
68 S2=EX*(S1**2)
S4=S2/RHO(I)
IF DIVIDE CHECK 69,70
69 WRITE OUTPUT TAPE 6,169,I
169 FORMAT(58H DIVISOR RHO IS ZERO IN FIFTH DIVISION OF PGEN4 SUBROUTI
NE)
CALL LEAVE
STOP
70 IF (RHO(I)-RHOBC) 9,9,10
9 S3=T7*(3.-(RHO(I)**2)/T8)
GO TO 11
10 S3=T9/RHO(I)
11 IF (KTRL(7)) 350,300,350
300 UCRB(I)=-1.-T1*S1+S3
FFCR(I)=S1
301 IF (KTRL(8)) 355,302,355
302 IF (KTRL(1)-1) 309,308,309
308 S1=EXPF(-((RHO(I)-RHOBNB)/T12)**2)
IF DIVIDE CHECK 82,309
82 WRITE OUTPUT TAPE 6,182
182 FORMAT(22H BG IS ZERO IN PGEN SR)
CALL LEAVE
STOP
309 UCIB(I)=-T2*S1
FFCI(I)=S1
303 IF (KTRL(9)) 360,304,360
304 USRB(I)=T4*S4
FFSR(I)=S4
305 IF (KTRL(11)) 501,500,501
500 IF (KTRL(10)) 365,306,365
306 USIB(I)=T5*S4
FFSI(I)=S4
307 IF (I-ILAST) 50,200,200
350 ITT=1
GO TO 340
355 ITT=2
GO TO 340
340 ITQ=1
IF (ITT-1) 380,380,381
380 IF (KTRL(7)-1) 352,351,352
351 TW=HA
TRM=RMA
TN1=FN1A
TN2=FN2A
```

```
GO TO 400
352 TH=HB
    TRM=RMB
    TN1=FN1B
    TN2=FN2B
GO TO 400
381 IF (KTRL(8)-1) 352,351,352
400 IF (RHO(I)-RHOBN) 410,410,411
410 TTN=TN1
GO TO 412
411 TTN=TN2
412 T20=RHO(I)/RHOBN
    IF (TTN*LOGF(T20)-80.) 403,403,409
403 TQ=(T20**TTN-1.)*RHOBN/(TTN*FKAY*A)
    IF DIVIDE CHECK 405,406
405 TG=T20**((RHOBN/(FKAY*A)))
GO TO 407
406 IF (TQ-80.) 408,408,409
408 TG=EXPF(TQ)
GO TO 407
409 TF=0.
GO TO 422
407 TFN=1./(1.+TG)
    IF (RHO(I)-TRM) 420,420,419
419 TF=TFN
GO TO 418
420 T21=RHO(I)/TRM
    THH=TH*(1.+(2.*T21))*((1.-T21)**2)
    TF=TFN*(1.+THH)
418 TFF=TF
421 GO TO (422,423),ITQ
422 GO TO (425,426,427,428),ITT
425 FFCR(I)=TF
    UCRB(I)=-1.-T1*FFCR(I)+S3
GO TO 301
426 FFCI(I)=TF
    UCIB(I)=-T2*FFCI(I)
GO TO 303
427 FFSR(I)=TF
    IF (ITQ-1) 470,470,471
471 USRB(I)=FKAY*A*T4*FFSR(I)
GO TO 305
470 USRB(I)=(T4/2.)*FFSR(I)
GO TO 305
428 FFSI(I)=TF
    IF (ITQ-1) 472,472,473
473 USIB(I)=FKAY*A*T5*FFSI(I)
GO TO 307
360 ITT=3
    IF (KTRL(9)-1) 431,431,430
430 ITQ=1
GO TO 352
365 ITT=4
    IF (KTRL(10)-1) 431,431,430
```

```
472 USIB(I)=(T5/2.)*FFSI(I)
GO TO 307
431 ITQ=2
GO TO 351
423 T23=(RHOBN/(FKAY*A))*(T20**TTN)*TG*((TFN/RHO(I))**2)
T25=T23
IF (RHO(I)-TRM) 460,460,461
460 T24=6.*TH*(1.-T21)/(TRM**2)
T25=(T24*TFN)+((1.+THH)*T23)
461 TF=T25
IF (ITT-3) 427,427,428
501 T30=0.004927*ETA*ECM
IF (RHO(I)-RHOBC) 502,502,503
502 SOCOUL=T30/(RHOBC**3)
GO TO 504
503 SOCOUL=T30/(RHO(I)**3)
504 USRB(I)=USRB(I)+SOCOUL
GO TO 500
50 I=I+1
EX=EX*DEX
RHOM=RHO(I-1)+HDRHO
IF (KTRL(1)-2) 153,152,153
152 IF (RHOM-RHOBN) 34,35,35
34 S1=1.0
GO TO 72
35 S1=0.0
GO TO 72
153 S1=1./(1.+EX)
IF DIVIDE CHECK 71,72
71 WRITE OUTPUT TAPE 6,171
171 FORMAT(54H DIVISOR 15 ZERO IN SIXTH DIVISION OF PGEN4 SUBROUTINE)
CALL LEAVE
STOP
72 S2=EX*(S1**2)
S4=S2/RHOM
IF DIVIDE CHECK 73,74
73 WRITE OUTPUT TAPE 6,173
173 FORMAT (62H QUANTITY RHOM IS ZERO IN SEVENTH DIVISION OF PGEN4 SUB
ROUTINE)
CALL LEAVE
STOP
74 IF (RHOM-RHOBC) 21,21,22
21 S3=T7*(3.-(RHOM**2)/T8)
GO TO 23
22 S3=T9/RHOM
23 IF (KTRL(7)) 1350,1300,1350
1300 UCRM(I-1)=-1.-T1*S1+S3
FFCRM(I-1)=51
1301 IF (KTRL(8)) 1355,1302,1355
1302 IF (KTRL(1)-1) 1309,1308,1309
1308 S1=EXPF(-((RHOM-RHOBN)/T12)**2)
1309 UCIM(I-1)=-T2*S1
FFCIM(I-1)=S1
1303 IF (KTRL(9)) 1360,1304,1360
```



```
1304 USRM(I-1)=T4*S4
      FFSRM(I-1)=S4
1305 IF (KTRL(I1)) 1501,1500,1501
1500 IF (KTRL(I0))1365,1306,1365
1306 USIM(I-1)=T5*S4
      FFSIM(I-1)=S4
1307 IF (K-10) 24,40,40
1350 ITT=1
      GO TO 1340
1355 ITT=2
      GO TO 1340
1340 ITQ=1
      IF (ITT-1)1380,1380,1381
1380 IF (KTRL(7)-1) 1352,1351,1352
1351 TH=HA
      TRM=RMA
      TN1=FN1A
      TN2=FN2A
      GO TO 1400
1352 TH=HB
      TRM=RMB
      TN1=FN1B
      TN2=FN2B
      GO TO 1400
1381 IF (KTRL(8)-1) 1352,1351,1352
1400 IF (RHOM-RHOBN) 1410,1410,1411
1410 TTN=TN1
      GO TO 1412
1411 TTN=TN2
1412 T20=RHOM/RHOBN
      IF (TTN*LOGF(T20)-80.) 1403,1403,1409
1403 TQ=(T20**TTN-1.)*RHOBN/(TTN*FKAY*A)
      IF DIVIDE CHECK 1405,1406
1405 TG=T20**(RHOBN/(FKAY*A))
      GO TO 1407
1406 IF (TQ-80.) 1408,1408,1409
1408 TG=EXPF(TQ)
      GO TO 1407
1409 TF=0.
      GO TO 1422
1407 TFN=1./(1.+TG)
      IF (RHOM-TRM) 1420,1420,1419
1419 TF=TFN
      GO TO 1418
1420 T21=RHOM/TRM
      TRH=TH*(1.+(2.*T21))*((1.-T21)**2)
      TF=TFN*(1.+THH)
1418 TFF=TF
1421 GO TO (1422,1423),ITQ
1422 GO TO (1425,1426,1427,1428),ITT
1425 FFCRM(I-1)=TF
      UCRM(I-1)=-1.-T1*FFCRM(I-1)+S3
      GO TO 1301
1426 FFCIM(I-1)=TF
```

```
      UCIM(I-1)=-T2*FFCIM(I-1)
      GO TO 1303
1427 FFSRM(I-1)=TF
      IF (ITQ-1) 1470,1470,1471
1471 USRM(I-1)=FKAY*A*T4*FFSRM(I-1)
      GO TO 1305
1470 USRM(I-1)=(T4/2.)*FFSRM(I-1)
      GO TO 1305
1428 FFSIM(I-1)=TF
      IF (ITQ-1) 1472,1472,1473
1473 USIM(I-1)=FKAY*A*T5*FFSIM(I-1)
      GO TO 1307
1360 ITT=3
      IF (KTRL(9)-1) 1431,1431,1430
1430 ITQ=1
      GO TO 1352
1365 IIT=4
      IF (KTRL(10)-1) 1431,1431,1430
1472 USIM(I-1)=(T5/2.)*FFSIM(I-1)
      GO TO 1307
1431 ITQ=2
      GO TO 1351
1423 T23=(RHOBN/(FKAY*A))*(T20**TTN)*TG*((TFN/RHOM)**2)
      T25=T23
      IF (RHOM-TRM) 1460,1460,1461
1460 T24=6.*TH*(1.-T21)/(TRM**2)
      T25=(T24*TFN)+((1.+THH)*T23)
1461 TF=T25
      IF (ITT-3) 1427,1427,1428
1501 T30=0.004927*ETA*ECM
      IF (RHOM-RHOBC) 1502,1502,1503
1502 SOCOUL=T30/(RHOBC**3)
      GO TO 1504
1503 SOCOUL=T30/(RHOM**3)
1504 USRM(I-1)=USRM(I-1)+SOCOUL
      GO TO 1500
      24 K=K+1
      EX=EX*DEX
      GO TO 42
200 IF (ISPILL) 75,76,75
      75 WRITE OUTPUT TAPE 6,175,ISPILL
175 FORMAT(23H UNDERFLOW OCCURRED AT I6,20H IN PGEN4 SUBROUTINE)
      76 IF (JSPILL) 77,51,77
      77 WRITE OUTPUT TAPE 6,177, JSPILL
177 FORMAT(22H OVERFLOW OCCURRED AT I6,20H IN PGEN4 SUBROUTINE)
      CALL LEAVE
      STOP
51 RETURN
```

```
SUBROUTINE INTCTR
DO1 L=1,LMAX
IFIRST=IIN(L)
T=RHO(IFIRST)**(L-1)
XC1=T*RHO(IFIRST)
XD1=XC1
FL=L
XCP1=FL*T
XDP1=XCP1
YC1=0.
YD1=0.
YCP1=0.
YDP1=0.
CALL RKINT
X1(L)=XC1
X2(L)=XD1
Y1(L)=YC1
Y2(L)=YD1
X1P(L)=XCP1
X2P(L)=XDP1
Y1P(L)=YCP1
1 Y2P(L)=YDP1
RETURN
```

```
SUBROUTINE RKINT
  IF DIVIDE CHECK 10,11
10  WRITE OUTPUT TAPE 6,110,L,I
110 FORMAT(66H DIVIDE CHECK TRIGGER FOUND ON AT START OF RKINT SUBROUT
LINE FOR L=I3,7H AND I=I3)
  CALL LEAVE
  STOP
11  ISPILL=0
  JSPILL=0
  1  FL=L-1
     F2L=-1.-FL
     F3L=FL*(FL+1.)
     TB=UCRB(IFIRST)+F3L/(RHO(IFIRST)**2)
     IF DIVIDE CHECK 12,13
12  WRITE OUTPUT TAPE 6,112,L,I
112 FORMAT(76H DIVISOR RHO(IFIRST)**2 IS ZERO IN FIRST DIVISION OF RKI
INT SUBROUTINE FOR L=I3,7H AND I=I3)
  CALL LEAVE
  STOP
13  PCB=TB+USRB(IFIRST)*FL
     PDB=TB+USRB(IFIRST)*F2L
     QCB=UCIB(IFIRST)+USIB(IFIRST)*FL
     QDB=UCIB(IFIRST)+USIB(IFIRST)*F2L
     IK=ILAST-1
     DO 6 I=IFIRST,IK
  2  HDRHO=.5*DRHO(I)
     DRHO2=(DRHO(I)**2)*.5
     RHOM=RHO(I)+HDRHO
     TM=UCRM(I)+F3L/(RHOM**2)
     IF DIVIDE CHECK 14,15
14  WRITE OUTPUT TAPE 6,114,L,I
114 FORMAT(70H DIVISOR RHOM**2 IS ZERO IN SECOND DIVISION OF RKINT SUB
ROUTINE FOR L=I3,7H AND I=I3)
  CALL LEAVE
  STOP
15  PCM=TM+USRM(I)*FL
     PDM=TM+USRM(I)*F2L
     QCM=UCIM(I)+USIM(I)*FL
     QDM=UCIM(I)+USIM(I)*F2L
     XCPP1=PCB*XC1-QCB*YC1
     YCPP1=QCB*XC1+PCB*YC1
     XDPP1=PDB*XD1-QDB*YD1
     YDPP1=QDB*XD1+PDB*YD1
     XC2=XC1+XCP1*HDRHO
     YC2=YC1+YCP1*HDRHO
     XD2=XD1+XDP1*HDRHO
     YD2=YD1+YDP1*HDRHO
     XCPP2=PCM*XC2-QCM*YC2
     YCPP2=QCM*XC2+PCM*YC2
     XDPP2=PDM*XD2-QDM*YD2
     YDPP2=QDM*XD2+PDM*YD2
     DRHO4=.5*DRHO2
     SDRHO=.33333333*HDRHO
     XC3=XC2+XCPP1*DRHO4
```

```
YC3=YC2+YCPP1*DRHO4
XD3=XD2+XDPP1*DRHO4
YD3=YD2+YDPP1*DRHO4
XCPP3=PCM*XC3-QCW*YC3
YCPP3=QCM*XC3+PCM*YC3
XDPP3=PDM*XD3-QDM*YD3
YDPP3=QDM*XD3+PDW*YD3
XC4=XC2+XCPP2*DRHO2+XCP1*HDRHO
YC4=YC2+YCPP2*DRHO2+YCP1*HDRHO
XD4=XD2+XDPP2*DRHO2+XDP1*HDRHO
YD4=YD2+YDPP2*DRHO2+YDP1*HDRHO
TB=UCRB(I+1)+F3L/(RHO(I+1)**2)
IF DIVIDE CHECK 16,17
16 WRITE OUTPUT TAPE 6,116,L,I
116 FORMAT(74H DIVISOR RHO(I+1)**2 IS ZERO IN THIRD DIVISION FOR RKINT
1 SUBROUTINE FOR L=I3,7H AND I=I3)
CALL LEAVE
STOP
17 PCB=TB+USRB(I+1)*FL
PDB=TB+USRB(I+1)*F2L
QCB=UCIB(I+1)+USIB(I+1)*FL
QDB=UCI8(I+1)+USIB(I+1)*F2L
XCPP4=PCB*XC4-QCB*YC4
YCPP4=QCB*XC4+PCB*YC4
XDPP4=PDB*XD4-QDB*YD4
YDPP4=QDB*XD4+PDB*YD4
SXC=XCPP2+XCPP3
SYC=YCPP2+YCPP3
SXD=XDPP2+XDPP3
SYD=YDPP2+YDPP3
TXC=SXC+XCPP1
TYC=SYC+YCPP1
TXD=SXD+XDPP1
TYD=SYD+YDPP1
TXC1=XC1+DRHO(I)*(XCP1+SDRHO*TXC)
TYC1=YC1+DRHO(I)*(YCP1+SDRHO*TYC)
TXD1=XD1+DRHO(I)*(XDP1+SDRHO*TXD)
TYD1=YD1+DRHO(I)*(YDP1+SDRHO*TYD)
TXCP1=XCP1+SDRHO*(TXC+SXC+XCPP4)
TYCP1=YCP1+SDRHO*(TYC+SYC+YCPP4)
TXDP1=XDP1+SDRHO*(TXD+SXD+XDPP4)
TYDP1=YDP1+SDRHO*(TYD+SYD+YDPP4)
IF (JSPILL) 20,21,20
20 RENORM=MAX1F(ABSF(XC1),ABSF(YC1),ABSF(XCP1),ABSF(YCP1),ABSF(XD1),
1ABSF(YD1),ABSF(XDP1),ABSF(YDP1))
XC1=XC1/RENORM
YC1=YC1/RENORM
XCP1=XCP1/RENORM
YCP1=YCP1/RENORM
XD1=XD1/RENORM
YD1=YD1/RENORM
XDP1=XDP1/RENORM
YDP1=YDP1/RENORM
WRITE OUTPUT TAPE 6,200,RENORM,L,RHO(I)
```

```
200 FORMAT(24H RENORMALIZATION FACTOR=E16.9,22H IN RKINT FOR CODED L=I
13,9H AND RHO=E16.9)
    JSPILL=0
    GO TO2
21  XC1=TXC1
    YC1=TYC1
    XD1=TXD1
    YD1=TYD1
    XCP1=TXCP1
    YCP1=TYCP1
    XDP1=TXDP1
    YDP1=TYDP1
6   CONTINUE
    IF (ISPILL) 30,31,30
30  WRITE OUTPUT TAPE 6,130, ISPILL,L,I
130 FORMAT(23H UNDERFLOW OCCURRED AT I6,27H IN RKINT SUBROUTINE FOR L=
1I3.7H AND I=I3)
31  IF (JSPILL) 32,4,32
32  WRITE OUTPUT TAPE 6,132, JSPILL,L,I
132 FORMAT(22H OVERFLOW OCCURRED AT I6,27H IN RKINT SUBROUTINE FOR L=I
13,7H AND I=I3)
    CALL LEAVE
    STOP
4   RETURN
```

```
SUBROUTINE CSUBL
  IF DIVIDE CHECK 50,51
50  WRITE OUTPUT TAPE 6,150
150  FORMAT (59H DIVIDE CHECK TRIGGER FOUND ON AT START OF CSUBL SUBROU
      1TINE)
      CALL LEAVE
      STOP
51  ISPILL=0
      JSPILL=0
      DO 40 L=1,LMAX
      XNORM1=MAXIF(ABSF(X1(L))*ABSF(Y1(L)),ABSF(X1P(L)),ABSF(Y1P(L)))
      TX1L=N1(L)/XNORM1
      TY1L=Y1(L)/XNORM1
      TX1PL=N1P(L)/XNORM1
      TY1PL=Y1P(L)/XNORM1
      FNORM=MAXIF(F(L),G(L),FP(L),GP(L))
      TFL=F(L)/FNORM
      TGL=G(L)/FNORM
      TFPL=FP(L)/FNORM
      TGPL=GP(L)/FNORM
      CO1=TFL*TY1PL-TFPL*TY1L
      CO2=TFPL*TX1L-TFL*TX1PL
      CO3=TY1L*TGPL-TY1PL*TGL+TX1L*TFPL-TX1PL*TFL
      CO4=TX1PL*TGL-TX1L*TGPL+TY1L*TFPL-TY1PL*TFL
      CO7=1.0/(CO3**2+CO4**2)
      IF DIVIDE CHECK 52,53
52  WRITE OUTPUT TAPE 6,152
152  FORMAT(54H DIVISOR IS ZERO IN FIRST DIVISION OF CSUBL SUBROUTINE)
      CALL LEAVE
      STOP
53  CR1(L)=(CO1*CO3+CO2*CO4)*CO7
      CI1(L)=(CO2*CO3-CO1*CO4)*CO7
      XNORM2=MAXIF(ABSF(X2(L)),ABSF(Y2(L)),ABSF(X2P(L)),ABSF(Y2P(L)))
      TX2L=N2(L)/XNORM2
      TY2L=Y2(L)/XNORM2
      TX2PL=N2P(L)/XNORM2
      TY2PL=Y2P(L)/XNORM2
      CO1=TFL*TY2PL-TFPL*TY2L
      CO2=TFPL*TX2L-TFL*TX2PL
      CO3=TY2L*TGPL-TY2PL*TGL+TX2L*TFPL-TX2PL*TFL
      CO4=TX2PL*TGL-TX2L*TGPL+TY2L*TFPL-TY2PL*TFL
      CO7=1.0/(CO3**2+CO4**2)
      IF DIVIDE CHECK 54,55
54  WRITE OUTPUT TAPE 6,154
154  FORMAT (55H DIVISOR IS ZERO IN SECOND DIVISION OF CSUBL SUBROUTINE
      1)
      CALL LEAVE
      STOP
55  CR2(L)=(CO1*CO3+CO2*CO4)*CO7
40  CI2(L)=(CO2*CO3-CO1*CO4)*CO7
      IF (ISPILL) 56,57,56
56  WRITE OUTPUT TAPE 6,156,ISPILL,L
156  FORMAT (23H UNDERFLOW OCCURRED AT I6,27H IN CSUBL SUBROUTINE FOR L
      1=I3)
```

```
57  IF (JSPILL) 58,59,58
58  WRITE OUTPUT TAPE 6,158, JSPILL, L
158  FORMAT (22H OVERFLOW OCCURRED AT I6 ,27H IN CSUBL SUBROUTINE FOR L=
      1I3)
      CALL LEAVE
      STOP
59  RETURN
```



```
SUBROUTINE AB
  IF DIVIDE CHECK 1,2
1  WRITE OUTPUT TAPE 6,101
101 FORMAT (56H DIVIDE CHECK TRIGGER FOUND ON AT START OF AB SUBROUTIN
1E)
  CALL LEAVE
  STOP
2  ISPILL=0
  JSPILL=0
  FKAYD=1./FKAY
  IF DIVIDE CHECK 3,4
3  WRITE OUTPUT TAPE 6,103
103 FORMAT(38H DIVISOR FKAY IS ZERO IN AB SUBROUTINE)
  CALL LEAVE
  STOP
4  DO 20 J=1,JMAX
  ASUMR=0.
  ASUMI=0.
  BSUMR=0.
  BSUMI=0.
  DO 10 L=1,LMAX
  FL=L
  ATR1=FL*CR1(L)+(FL-1.)*CR2(L)
  ATI1=FL*CI1(L)+(FL-1.)*CI2(L)
  BTR1=CR1(L)-CR2(L)
  BTI1=CI1(L)-CI2(L)
  ATR2=ATR1*EXSGMR(L)-(ATI1*EXSGMI(L))
  ATI2=ATR1*EXSGMI(L)+(ATI1*EXSGMR(L))
  BTR2=BTR1*EXSGMR(L)-(BTI1*EXSGMI(L))
  BTI2=BTR1*EXSGMI(L)+(BTI1*EXSGMR(L))
  ASUMR=ASUMR+(ATR2*P(L,J))
  ASUMI=ASUMI+(ATI2*P(L,J))
  BSUMR=BSUMR+(BTR2*PP(L,J))
10  BSUMI=BSUMI+(BTI2*PP(L,J))
  AR(J)= FCR(J)+(FKAYD*ASUMR)
  AI(J)=FCI(J)+(FKAYD*ASUMI)
  BR(J)= FKAYD*BSUMI
20  BI(J)= -FKAYD*BSUMR
  IF (ISPILL) 30,31,30
30  WRITE OUTPUT TAPE 6,130, ISPILL
130 FORMAT(23H UNDERFLOW OCCURRED AT I6,17H IN AB SUBROUTINE)
31  IF (JSPILL) 32,33,32
32  WRITE OUTPUT TAPE 6,132,JSPILL
132 FORMAT (22H OVERFLOW OCCURRED AT I6,17H IN AB SUBROUTINE)
  CALL LEAVE
  STOP
33  RETURN
```

```
SUBROUTINE SGSGCP
  IF DIVIDE CHECK 10,11
10  WRITE OUTPUT TAPE 6,110
110  FORMAT (60H DIVIDE CHECK TRIGGER FOUND ON AT START OF SGSGCP SUBRO
      1UTINE)
      CALL LEAVE
      STOP
11  ISPILL=0
      JSPILL=0
      DO 5 J=1,JMAX
      SGMATH(J)=AR(J)**2.+AI(J)**2.+BR(J)**2.+BI(J)**2.
      POLTH(J)= (2.*(AR(J)*BR(J)+AI(J)*BI(J)))/SGMATH(J)
      IF DIVIDE CHECK 12,13
12  WRITE OUTPUT TAPE 6,112,J
112  FORMAT(30H DIVISOR SGMATH IS ZERO FOR J=13,21H IN SGSGCP SUBROUTIN
      1E)
      CALL LEAVE
      STOP
13  SGMAC(J)=FCR(J)**2.+FCI(J)**2.
      IF (ETA) 7,7,8
8    SRATIO(J)=SGMATH(J)/SGMAC(J)
      IF DIVIDE CHECK 14,15
14  WRITE OUTPUT TAPE 6,114,J
114  FORMAT(29H DIVISOR SGMAC IS ZERO FOR J=13,21H IN SGSGCP SUBROUTINE
      1)
      CALL LEAVE
      STOP
15  GO TO 5
7    SRATIO(J)=0.
5    CONTINUE
      IF (ISPILL) 16,17,16
16  WRITE OUTPUT TAPE 6,116,ISPILL
116  FORMAT (23H UNDERFLOW OCCURRED AT 16,21H IN SGSGCP SUBROUTINE)
17  IF (JSPILL) 18,19,18
18  WRITE OUTPUT TAPE 6,118,JSPILL
118  FORMAT(22H OVERFLOW OCCURRED AT 16,21H IN SGSGCP SUBROUTINE)
      CALL LEAVE
      STOP
19  RETURN
```

```
SUBROUTINE SIGMAR
ISPILL=0
JSPILL=0
FL=0.
SGMRTH=0.
CPI=(12.56637060)/(FKAY**2)
DO 20 L=I ,LMAX
SGMRTH=SGMRTH+FL*(C12(L)-(C12(L))**2-(CR2(L))**2)
FL=FL+1.0
20 SGMRTH=SGMRTH+FL*(C11(L)-(C11(L))**2-(CR1(L))**2)
SGMRTH=CPI*SGMRTH
IF(ISPILL) 10,11,10
10 WRITE OUTPUT TAPE 6,110,ISPILL
110 FORMAT(23H UNDERFLOW OCCURRED AT 16,21H IN SIGMAR SUBROUTINE)
11 IF(JSPILL) 12,13,12
12 WRITE OUTPUT TAPE 6,112,JSPILL
112 FORMAT(22H OVERFLOW OCCURRED AT 16,21H IN SIGMAR SUBROUTINE)
CALL LEAVE
STOP
13 RETURN
```

```
SUBROUTINE CHISQ
  IF DIVIDE CHECK 10,11
10  WRITE OUTPUT TAPE 6,110
110 FORMAT(59H DIVIDE CHECK TRIGGER FOUND ON AT START OF CHISQ SUBROUT
LINE)
  CALL LEAVE
  STOP
11  ISPILL=0
  JSPILL=0
  CHI2ST=0
  CHI2PT=0
  DO 20 J=1,JMAX
  CHI2S(J)= ((SGMATH(J)-SGMAEX(J))/DSGMEX(J))**2.
  CHI2P(J)= ((POLTH(J)-POLEX(J))/DPOLEX(J))**2.
  IF DIVIDE CHECK 14,15
14  WRITE OUTPUT TAPE 6,114,J
114 FORMAT(40H DIVISOR DSGMEX OR DPOLEX IS ZERO FOR J=13,20H IN CHISQ
SUBROUTINE)
  CALL LEAVE
  STOP
15  CHI2ST=CHI2ST + CHI2S(J)
  CHI2(J)=CHI2S(J)+CHI2P(J)
20  CHI2PT=CHI2PT+CHI2P(J)
  CHI2T=CHI2ST+CHI2PT
  IF (ISPILL) 16,17,16
16  WRITE OUTPUT TAPE 6,116, ISPILL
116 FORMAT(23H UNDERFLOW OCCURRED AT 16,20H IN CHISQ SUBROUTINE)
17  IF (ISPILL) 18,19,18
18  WRITE OUTPUT TAPE 6,118,JSPILL
118 FORMAT(22H OVERFLOW OCCURRED AT 16,20H IN CHISQ SUBROUTINE)
  CALL LEAVE
  STOP
19  RETURN
```

```
SUBROUTINE OUTPT4
NPGS=0
CALL SKIP(K,NPGS,NUMRUN)
WRITE OUTPUT TAPE 6,245,NUMPRG
245 FORMAT (16H0PROGRAM NUMBER I5)
DO 8 I=1,13
WRITE OUTPUT TAPE 6,250,I,(KTRL(I))
250 FORMAT (6H KTRL(I2,2H)=I2)
8 CONTINUE
WRITE OUTPUT TAPE 6,12
12 FORMAT (11H0BASIC DATA)
FKAYA=FKAY*A
FKAYB=FKAY*BG
WRITE OUTPUT TAPE 6,14,FMI,FMB,ELAB,ZZ,V,W,A,RO,VS,WS,RC,BG,RG,
14 FORMAT(7H0MSUBI=E16.9,10H MSUBB=E16.9,10H ELAB=E16.9,10H
1 ZP=E16.9/7H0 V=E16.9,10H W=E16.9,10H A=E16.9,
210H RO=E16.9/7H0 VS=E16.9,10H WS=E16.9,36H
3 RC=E16.9/59H0
4 BG=E16.9,10H RG=E16.9)
WRITE OUTPUT TAPE 6,16,RHOBN,RHOBC,RHOBN,ECM,ETA,FKAY,FKAYA,FKAYB
16 FORMAT(7H0RHOBN=E16.9,10H RHOBC=E16.9,10H RHOBN=E16.9,10H
1 ECM=E16.9/7H0 ETA=E16.9,10H K=E16.9/10H KA=E16.9,
210H KB=E16.9)
KT=KTRL(7)+KTRL(8)+KTRL(9)+KTRL(10)
IF (KT) 13,1818,13
13 WRITE OUTPUT TAPE 6,150,HA,RMA, FN1A, FN2A, PMA, HB, RMB, FN1B, FN2B, PMB
150 FORMAT(7H0 HA=E16.9,7H RMA=E16.9,7H N1A=E16.9,7H N2A=E16.9
1,7H PMA=E16.9/7H HB=E16.9,7H RMB=E16.9,7H N1B=E16.9,7H
2N2B=E16.9,7H PMB=E16.9)
1818 WRITE OUTPUT TAPE 6,18,RHOMAX,LMAXM
18 FORMAT (17H0INTEGRATION DATA/8H0RHOMAX=E16.9,10H LMAXM=I5)
WRITE OUTPUT TAPE 6,220,NMAX
220 FORMAT (6H0NMAX=I5)
WRITE OUTPUT TAPE 6,24
24 FORMAT (6H0RH0IN)
NOLINE=50
K=20
DO 40 I=1, NMAX,6
IF (K-NOLINE) 30,29,29
29 CALL SKIP(K,NPGS,NUMRUN)
30 M=XMINOF(I+5,NMAX)
K=K+1
WRITE OUTPUT TAPE 6,32,(RH0IN(J),J=I,M)
32 FORMAT(1H E19.9,5E20.9)
40 CONTINUE
WRITE OUTPUT TAPE 6,41
41 FORMAT (7H0DRH0IN)
DO 60 I=1,NMAX,6
IF (K-NOLINE) 45,43,43
43 CALL SKIP(K,NPGS,NUMRUN)
45 M=XMINOF(I+5,NMAX-1)
K=K+1
WRITE OUTPUT TAPE 6,32,(DRH0IN(J),J=I,M)
60 CONTINUE
```

```

WRITE OUTPUT TAPE 6,118,SGMRIH
118 FORMAT(12H0SIGMAR(TH)=E16.9)
15 IF(KTRL(2)-1) 1900,20,1900
20 WRITE OUTPUT TAPE 6,119,CHI2ST,CHI2PT,CHI2T
119 FORMAT (25H0SUM OF CHI SQUARE SIGMA=E16.9/23H0SUM OF CHI SQUARE PO
1L=E16.9/25H0SUM OF CHI SQUARE TOTAL=E16.9)
21 CALL SKIP(K,NPGS,NUMRUN)
WRITE OUTPUT TAPE 6,200
200 FORMAT (113H THETA SIGMATH SIG-SIGC
1 POL TH SIGMA EX POL EX)
DO 90 I=1,JMAX
IF(K-NOLINE)75,70,70
70 CALL SKIP(K,NPGS,NUMRUN)
75 K=K+1
WRITE OUTPUT TAPE 6,32,THETAD(I),SGMATH(I),SRATIO(I),POLTH(I),
1SGMAEX(I),POLEX(I)
90 CONTINUE
GO TO 299
1900 CALL SKIP (K,NPGS,NUMRUN)
WRITE OUTPUT TAPE 6,1905
1905 FORMAT (120H THETA SIGMATH
1 SIG-SIGC POL TH
2)
DO 1920 I=1,JMAX
IF (K-NOLINE) 1910,1908,1908
1908 CALL SKIP (K,NPGS,NUMRUN)
1910 K=K+1
WRITE OUTPUT TAPE 6,1919,THETAD(I),SGMATH(I),SRATIO(I),POLTH(I)
1919 FORMAT (1H E20.9,3E30.9)
1920 CONTINUE
299 IF(KTRL(6)-1) 300,121,300
300 IF(KTRL(12)-1) 25,1700,25
1700 CALL SKIP(K,NPGS,NUMRUN)
WRITE OUTPUT TAPE 6,1701
1701 FORMAT (92H RHO(I) FFCR FFCI
1 FFSR FFSI)
DO 1709 I=1,ILAST
IF (K-NOLINE) 1703,1702,1702
1702 CALL SKIP (K,NPGS,NUMRUN)
1703 WRITE OUTPUT TAPE 6,158,RHO(I),FFCR(I),FFCI(I),FFSR(I),FFSI(I)
158 FORMAT(1H 5E20.9)
1709 CONTINUE
25 IF(KTRL(2)-1) 23,22,23
22 CALL SKIP (K,NPGS,NUMRUN)
WRITE OUTPUT TAPE 6,95
95 FORMAT(120H THETA DSIGMA EX DPOL EX
1 CHI SQUARE SIGMA CHI SQUARE POL CHI SQUARE TOTAL )
DO 120 J=1,JMAX
IF(K-NOLINE) 97,96,96
96 CALL SKIP(K,NPGS,NUMRUN)
97 K=K+1
WRITE OUTPUT TAPE 6,32,THETAD(J),DSGMEX(J),DPOLEX(J)*CHI2S(J),
1CHI2P(J))CHI2(J)
120 CONTINUE

```

```
23  CALL SKIP(K,NPGS,NUMRUN)
1623 WRITE OUTPUT TAPE 6,1150
1150 FORMAT (120H          L          REAL C(L+1/2)          IMA
1G C(L+1/2)          REAL C(L-1/2)          IMAG C(L-1/2)
2)
DO 160 L=1,LMAX
IF (K-NOLINE) 155,153,153
153  CALL SKIP (K,NPGS,NUMRUN)
155  K=K+1
L1=L-1
WRITE OUTPUT TAPE 6,1156,L1,CR1(L),CI1(L),CR2(L),CI2(L)
1156 FORMAT (1H I11 ,E30.9,3E25.9)
160  CONTINUE
121  RETURN
```

```
SUBROUTINE SKIP(K,NPGS,NUMRUN)
NPGS=NPGS+1
WRITE OUTPUT TAPE 6,1510,(NUMRUN(I),I=1,5),NPGS
1510 FORMAT(12H1RUN NUMBER=I2,1H-I2,1H-I4,3H -I3,3H -I3,79H
1
2GE 15/)
K=0
RETURN
```

PA

```
SUBROUTINE LEAVE
CALL PDUMP(A,ZZ)
CALL CTRL4
RETURN
```


*	CARDS	COLUMN	
*	FAP		
	COUNT	43	
*SPILL	SUBROUTINE		
	ENTRY	SPILL	
SPILL	STZ*	1,4	STORE ZERO IN JSPILL
	STZ*	2,4	STORE ZERO IN ISPILL
	STZ	0	STORE ZERO IN LOCATION 00000
	CAL	1,4	
	STA	AA41	SET ADDRESS AA41,
	STA	AA36	AA36 TO JSPILL
	CAL	2,4	SET ADDRESS AA31
	STA	AA31	TO ISPILL
	CLA*	3,4	SET COMMON STORAGE
	STO	AA45	
	CLA*	4,4	SET COMMON STORAGE
	STO	AA46	
	CAL	AA47	PLACE TRANSFER
	SLW	8	INSTRUCTION IN LOCATION 8
	TRA	5,4	EXIT TO MAIN PROGRAM
AA16	LDI	0	ENTRY IN CASE OF OVER-OR UNDERFLOW
	LFT	4	TEST FOR OVERFLOW
	TRA	AA36	TRANSFER IN CASE OF OVERFLOW
	LFT	16	
	TRA	AA24	TRANSFER IN CASE OF UNDERFLOW
	TRA*	0	TRANSFER TO MAIN PROGRAM , NO UFLOW
AA24	LNT	1	TEST FOR UNDERFLOW
	TRA*	0	UNDERFLOW IN AC ONLY
	CAL	0	PLACE LOCATION AT WHICH
	SUB	AA35	UNDERFLOW OCCURRED IN AC
	LLS	18	SHIFT LEFT 18
AA31	STD	AA31	STORE IN ISPILL
	CLA	AA46	SET AC, MQ WITH
	LDQ	AA46	SPECIFIED CONSTANTS
	TRA*	0	EXIT TO MAIN PROGRAM
AA35	HTR	1	CONSTANT
AA36	CLA	AA36	TEST IF JSPILL ZERO
	TNZ	AA42	TRANSFER IN CASE JSPILL NON-ZERO
	CAL	0	PLACE LOCATION AT WHICH OVERFLOW OCCURRED
	SUB	AA35	IN AC
	LLS	18	SHIFT LEFT 18
AA41	STD	AA41	STORE IN JSPILL
AA42	CLA	AA45	SET AC, MQ WITH SPECIFIED CONSTANTS
	LDQ	AA45	
	TRA*	0	EXIT TO MAIN PROGRAM
AA45	HTR	0	COMMON STORAGE
AA46	HTR	0	COMMON STORAGE
AA47	TRA	AA16	INSTRUCTION TO BE INSERTED AT LOC. 8
	END		

VII. TYPICAL INPUT AND OUTPUT

A. INPUT DATA FOR PROTONS AGAINST COPPER AT 9.75 MEV

3		+0.62500000	-01	+0.40750000	+01	+0.00000000	+00	
22		+0.25000000	+00	+0.00000000	+00	-0.16000000	+00	
1960		10		+0.33390000	+01	-0.20000000	+00	
0		32		+0.00000000	+00	+0.00000000	+00	
0			+0.15200000	+02	+0.33560000	+01	-0.17000000	+00
4			+0.20300000	+02	+0.37570000	+01	-0.17000000	+00
0			+0.25400000	+02	+0.38570000	+01	+0.00000000	+00
1			+0.28000000	+02	+0.00000000	+00	-0.10000000	+00
1			+0.30400000	+02	+0.38460000	+01	+0.00000000	+00
0			+0.33000000	+02	+0.00000000	+00	+0.10000000	-01
1			+0.35500000	+02	+0.37570000	+01	+0.00000000	+00
0			+0.39000000	+02	+0.00000000	+00	+0.20000000	+00
0			+0.40600000	+02	+0.39800000	+03	+0.00000000	+00
0			+0.43000000	+02	+0.35500000	+02	+0.00000000	+00
0			+0.45600000	+02	+0.16700000	+02	+0.00000000	+00
0			+0.47000000	+02	+0.10000000	+30	+0.13000000	+00
0			+0.50700000	+02	+0.90800000	+01	+0.00000000	+00
0			+0.51500000	+02	+0.10000000	+30	+0.70000000	-01
1			+0.54000000	+02	+0.53800000	+01	+0.00000000	+00
+0.10000000	+01		+0.55700000	+02	+0.10000000	+30	-0.20000000	-01
+0.64000000	+02		+0.57000000	+02	+0.37300000	+01	+0.10000000	+30
+0.97500000	+01		+0.60000000	+02	+0.10000000	+30	+0.10000000	+30
+0.29000000	+02		+0.60800000	+02	+0.19100000	+01	+0.10000000	+30
+0.12000000	+01		+0.65500000	+02	+0.10000000	+30	+0.30000000	-01
+0.62000000	+02		+0.65800000	+02	+0.91500000	+00	+0.10000000	+30
+0.85000000	+01		+0.69000000	+02	+0.10000000	+30	+0.40000000	-01
+0.12000000	+01		+0.70800000	+02	+0.10000000	+30	+0.10000000	+30
+0.52000000	+00		+0.75500000	+02	+0.49600000	+00	+0.30000000	-01
-0.40000000	+01		+0.75900000	+02	+0.10000000	+30	+0.10000000	+30
+0.00000000	+00		+0.80900000	+02	+0.10000000	+30	+0.30000000	-01
+0.00000000	+00		+0.85900000	+02	+0.25800000	+00	+0.10000000	+30
+0.00000000	+00		+0.86000000	+02	+0.10000000	+30	+0.30000000	-01
+0.00000000	+00		+0.90900000	+02	+0.16300000	+00	+0.10000000	+30
+0.00000000	+00		+0.95500000	+02	+0.10000000	+30	+0.40000000	-01
+0.00000000	+00		+0.95900000	+02	+0.13400000	+00	+0.40000000	-01
+0.00000000	+00		+0.10000000	+03	+0.10000000	+30	+0.10000000	+30
+0.00000000	+00		+0.38650000	+04	+0.13400000	+00	+0.40000000	-01
+0.00000000	+00		+0.97340000	+03	+0.15000000	+00	+0.30000000	-01
+0.00000000	+00		+0.42470000	+03	+0.15400000	+00	+0.10000000	+30
+0.00000000	+00		+0.00000000	+00	+0.10000000	+30	+0.50000000	-01
+0.00000000	+00		+0.22690000	+03	+0.15400000	+00	+0.10000000	+30
+0.00000000	+00		+0.00000000	+00	+0.10000000	+30	+0.40000000	-01
+0.00000000	+00		+0.13460000	+03	+0.15000000	+00	+0.10000000	+30
+0.00000000	+00		+0.00000000	+00	+0.10000000	+30	+0.60000000	-01
+0.00000000	+00		+0.82920000	+02	+0.00000000	+00	+0.10000000	+30
+0.00000000	+00		+0.00000000	+00	+0.00000000	+00	+0.10000000	+30
1			+0.47660000	+02	+0.00000000	+00	+0.10000000	+30
1			+0.00000000	+00	-0.20000000	-01	+0.60000000	-01
1			+0.22870000	+02	+0.00000000	+00	+0.10000000	+30
1			+0.00000000	+00	+0.10000000	-01	+0.50000000	-01
1			+0.00000000	+00	+0.00000000	+00	+0.10000000	+30
1			+0.12410000	+02	-0.30000000	-01	+0.60000000	-01
3			+0.00000000	+00	+0.00000000	+00	100	
+0.62500000	-01		+0.00000000	+00	-0.60000000	-01		
+0.50000000	+00		+0.64560000	+01	+0.00000000	+00		
+0.10000000	+02		+0.00000000	+00	-0.10000000	+00		

B. OUTPUT LISTING

RUN NUMBER= 2-40-1961 - 1 - 1
PAGE 1

PROGRAM NUMBER 4

KTRL(1)=0
KTRL(2)=1
KTRL(3)=1
KTRL(4)=0
KTRL(5)=1
KTRL(6)=0
KTRL(7)=0
KTRL(8)=0
KTRL(9)=0
KTRL(10)=0
KTRL(11)=0
KTRL(12)=0
KTRL(13)=1

BASIC DATA

MSUB1= 0.099999994E 01	MSUBB= 0.639999993E 02	ELAB= 0.974999994E 01	ZZP= 0.289999999E 02
V= 0.619999997E 02	W= 0.849999994E 01	A= 0.519999996E 00	RO= 0.119999997E 01
VS= -0.399999999E 01	WS= 0.		RC= 0.119999997E 01
9		BG= 0.	RG= 0.
RHOBN= 0.393980615E 01	RHOBC= 0.323980615E 01	RHOBNG= 0.	ECM= 0.959999986E 01
ETA= 0.146788672E 01	K= 0.674959674E 00	KA= 0.350979023E-00	KB= 0.

INTEGRATION DATA

RHOMAX= 0.099999994E 02 LMAXM= 10
NMAX= 3
RHOIN
0.625000000E-01 0.500000000E 00 0.099999994E 02
DRHOIN
0.625000000E-01 0.250000000E-00
SIGMAR(TH)= 0.668857820E 02
SUM OF CHI SQUARE SIGMA= 0.587550342E 02
SUM OF CHI SQUARE POL= 0.999665476E 02
SUM OF CHI SQUARE TOTAL= 0.158721581E 03

THETA	SIGMATH	SIG-SIGC	POL TH	SIGMA EX	POL EX
0.151999995E 02	0.366688885E 04	0.948844409E 00	0.624454483E-03	0.386499993E 04	0.
0.202999994E 02	0.107591100E 04	0.877576292E 00	-0.488765538E-02	0.973399989E 03	0.
0.253999993E 02	0.437771246E 03	0.864875652E 00	-0.126092605E-01	0.424699992E 03	0.
0.279999994E 02	0.302826010E 03	0.877252147E 00	-0.152099080E-01	0.	0.199999996E-01
0.303999998E 02	0.223364875E 03	0.892697871E 00	-0.161199562E-01	0.226899996E 03	0.
0.329999998E 02	0.164800696E 03	0.906894624E 00	-0.153716959E-01	0.	-0.999999985E-02
0.354999997E 02	0.12484892E 03	0.912098765E 00	-0.130572930E-01	0.134599991E 03	0.
0.389999993E 02	0.854579188E 02	0.897354133E 00	-0.757811405E-02	0.	0.299999997E-01
0.405999996E 02	0.718648233E 02	0.880526960E 00	-0.435241245E-02	0.829199985E 02	0.
0.430000006E 02	0.552558191E 02	0.843160637E 00	0.115248807E-02	0.	0.599999994E-01
0.455999993E 02	0.412997656E 02	0.787652783E 00	0.776244439E-02	0.476599991E 02	0.
0.469999999E 02	0.351879030E 02	0.752354726E 00	0.114611000E-01	0.	0.999999993E-01
0.506999992E 02	0.227685094E 02	0.647046342E 00	0.208112434E-01	0.	0.
0.514999993E 02	0.206800543E 02	0.623049393E 00	0.225530863E-01	0.	0.159999996E-00
0.539999999E 02	0.152632877E 02	0.548359923E 00	0.265358075E-01	0.	0.199999996E-00
0.556999996E 02	0.124075061E 02	0.499775782E-00	0.272366613E-01	0.124100000E 02	0.
0.569999993E 02	0.106054634E 02	0.464955918E-00	0.261134841E-01	0.	0.169999994E-00
0.599999994E 02	0.749187976E 01	0.396005623E-00	0.156014524E-01	0.	0.169999994E-00
0.607999995E 02	0.686953478E 01	0.380956881E-00	0.104624555E-01	0.645599991E 01	0.
0.654999994E 02	0.452632517E 01	0.327856168E-00	-0.413961068E-01	0.	0.999999993E-01
0.657999992E 02	0.443769753E 01	0.326697305E-00	-0.457080074E-01	0.407499999E 01	0.
0.689999998E 02	0.381219082E 01	0.331831254E-00	-0.927333571E-01	0.	-0.999999985E-02
0.707999989E 02	0.366038024E 01	0.348589554E-00	-0.115995258E-00	0.	0.
0.754999995E 02	0.365827605E 01	0.434639670E-00	-0.151801050E-00	0.333899997E 01	0.
0.758999996E 02	0.367384672E 01	0.444403417E-00	-0.153142102E-00	0.	-0.199999996E-00
0.808999993E 02	0.392783776E 01	0.58852453E 00	-0.153684869E-00	0.335599996E 01	0.
0.858999990E 02	0.411561452E 01	0.750190347E 00	-0.136236615E-00	0.375699997E 01	0.
0.859999999E 02	0.411754631E 01	0.753359631E 00	-0.135786600E-00	0.385699995E 01	0.
0.908999994E 02	0.410156414E 01	0.894658349E 00	-0.110665120E-00	0.	-0.129999995E-00
0.954999998E 02	0.388636135E 01	0.986762404E 00	-0.826589502E-01	0.384599999E 01	0.
0.958999991E 02	0.385919407E 01	0.992326975E 00	-0.800342456E-01	0.	-0.699999988E-01
0.099999994E 03	0.351563454E 01	0.102388248E 01	-0.512336008E-01	0.375699997E 01	0.
				0.	0.199999996E-01

THETA	DSIGMA EX	DPOL EX	CHI SQUARE SIGMA	CHI SQUARE POL	CHI SQUARE TOTAL	PAGE
0.151999995E 02	0.397999994E 03	0.099999994E 30	0.247771524E-00	0.	0.247771524E-00	3
0.202999994E 02	0.354999997E 02	0.099999994E 30	0.833843596E 01	0.	0.833843596E 01	
0.253999993E 02	0.166999996E 02	0.099999994E 30	0.612634748E 00	0.	0.612634748E 00	
0.279999994E 02	0.099999994E 30	0.299999997E-01	0.	0.137748629E 01	0.137748629E 01	
0.303999998E 02	0.907999992E 01	0.099999994E 30	0.151578002E-00	0.	0.151578002E-00	
0.329999998E 02	0.099999994E 30	0.399999991E-01	0.	0.180344537E-01	0.180344537E-01	
0.354999997E 02	0.537999995E 01	0.099999994E 30	0.328498974E 01	0.	0.328498974E 01	
0.389999993E 02	0.099999994E 30	0.299999997E-01	0.	0.156901620E 01	0.156901620E 01	
0.404999996E 02	0.372999996E 01	0.099999994E 30	0.878443092E 01	0.	0.878443092E 01	
0.430000000E 02	0.099999994E 30	0.299999997E-01	0.	0.384781063E 01	0.384781063E 01	
0.455999993E 02	0.191000000E 01	0.099999994E 30	0.110886693E 02	0.	0.110886693E 02	
0.469999999E 02	0.099999994E 30	0.299999997E-01	0.	0.871015161E 01	0.871015161E 01	
0.506999992E 02	0.914999999E 00	0.099999994E 30	0.123029307E-01	0.	0.123029307E-01	
0.514999993E 02	0.099999994E 30	0.399999991E-01	0.	0.118072823E 02	0.118072823E 02	
0.539999999E 02	0.099999994E 30	0.099999994E-01	0.	0.188061401E 02	0.188061401E 02	
0.556999996E 02	0.495999999E-00	0.099999994E 30	0.232838377E-04	0.	0.232838377E-04	
0.569999993E 02	0.099999994E 30	0.399999991E-01	0.	0.129395790E 02	0.129395790E 02	
0.599999994E 02	0.099999994E 30	0.299999997E-01	0.	0.264876761E 02	0.264876761E 02	
0.607999995E 02	0.257999994E-00	0.099999994E 30	0.256912217E 01	0.	0.256912217E 01	
0.654999994E 02	0.099999994E 30	0.499999993E-01	0.	0.799714297E 01	0.799714297E 01	
0.657999992E 02	0.162999995E-00	0.099999994E 30	0.495124198E 01	0.	0.495124198E 01	
0.689999998E 02	0.099999994E 30	0.399999991E-01	0.	0.427800477E 01	0.427800477E 01	
0.707999998E 02	0.133999996E-00	0.099999994E 30	0.575213231E 01	0.	0.575213231E 01	
0.754999995E 02	0.099999994E 30	0.599999994E-01	0.	0.645316236E 00	0.645316236E 00	
0.758999996E 02	0.133999996E-00	0.099999994E 30	0.562634163E 01	0.	0.562634163E 01	
0.808999993E 02	0.149999999E-00	0.099999994E 30	0.129713513E 01	0.	0.129713513E 01	
0.858999990E 02	0.153999999E-00	0.099999994E 30	0.282009937E 01	0.	0.282009937E 01	
0.859999999E 02	0.099999994E 30	0.599999994E-01	0.	0.930132821E-02	0.930132821E-02	
0.908999994E 02	0.153999999E-00	0.099999994E 30	0.275396556E 01	0.	0.275396556E 01	
0.954999998E 02	0.099999994E 30	0.499999993E-01	0.	0.640996160E-01	0.640996160E-01	
0.958999991E 02	0.149999999E-00	0.099999994E 30	0.464161523E-00	0.	0.464161523E-00	
0.099999994E 03	0.099999994E 30	0.599999994E-01	0.	0.140950717E 01	0.140950717E 01	

RUN NUMBER=	L	- 1	- 1	- 1	IMAG C(L+1/2)	REAL C(L+1/2)	IMAG C(L-1/2)	REAL C(L-1/2)	PAGE
2-40-1961	0	-0.149473831E-00	0.621800341E 00	-0.139704145E-00	0.618552327E 00	-0.139704145E-00	0.618552327E 00	4	
	1	-0.890974633E-01	0.280818105E-00	-0.112762213E-00	0.266789824E-00	-0.112762213E-00	0.266789824E-00		
	2	-0.187045686E-00	0.241325634E-00	-0.174136B25E-00	0.274325125E-00	-0.174136B25E-00	0.274325125E-00		
	3	0.670826085E-01	0.135792047E-00	0.546362303E-01	0.848520368E-01	0.546362303E-01	0.848520368E-01		
	4	0.756759964E-02	0.149855547E-01	0.229124613E-02	0.170210496E-01	0.229124613E-02	0.170210496E-01		
	5	0.503797509E-02	0.559476413E-02	0.384988777E-02	0.176129699E-02	0.384988777E-02	0.176129699E-02		
	6	0.628714196E-03	0.123979807E-03	0.362633042E-03	0.807685591E-04	0.362633042E-03	0.807685591E-04		
	7	0.627130263E-04	0.826003924E-05	0.370286375E-04	0.729130283E-05	0.370286375E-04	0.729130283E-05		
	8	0.713366367E-05	0.780125931E-06	0.441690803E-05	0.750615060E-06	0.441690803E-05	0.750615060E-06		
	9	0.130098701E-05	0.808378339E-07	0.101125993E-05	0.797655620E-07	0.101125993E-05	0.797655620E-07		
	10	0.413292557E-06	0.833891876E-08	0.381933421E-06	0.844628319E-08	0.381933421E-06	0.844628319E-08		

VIII. FURTHER SUBROUTINES AND PROGRAMS IN PREPARATION

The following subroutines are presently being prepared at UCLA:

Subroutine TV

This subroutine is designed to output on CRT and on film various required curves such as $\sigma(\theta)$ vs θ , $\sigma(\theta)/\sigma_c(\theta)$ vs θ , $P(\theta)$ vs θ .

Subroutine RHOBEG

This subroutine will make use of the quantities IIN(L) to allow the numerical integrations to start at different values of ρ depending upon ℓ in order to speed up the numerical integration.

Subroutine FLUX

This subroutine will if desired compute the normalized total wave functions, the scattered flux \vec{j} , the divergence and the curl of \vec{j} at specified values of ρ and θ .

All the above subroutines will of course require some modification of the basic program.

The following programs are presently being prepared at UCLA:

Program SCAT 3

This program will be similar to program SCAT 4 except that it will treat incident and target particles of zero spin, thus speeding up the calculation for that case.

Program SCAT 5

This is a modified version of program SCAT 4 offering a simplified input and using only as many ℓ 's as may be significant in the C_ℓ 's calculations.

Program SCAT K

This is a modified version of program SCAT 4 designed to analyze the scattering of K-mesons against complex nuclei, including the use of an approximate Klein-Gordon equation, relativistic kinematic corrections, and averaging of the cross sections over angles, energies, and representative nuclei.

Program SCAT 6

This is a modified version of program SCAT 4 designed to calculate cross sections and polarization of spin 1 particles scattered by 0 spin targets.

Program SEEK 4

This is a program designed to search automatically the parameter space so as to minimize χ^2 .

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