DEUTERON OPTICAL MODEL PROGRAM DDTP

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1. Introduction

The program DDTP calculates the elastic scattering of deuterons by nuclei. The scattering is described by an optical model potential which includes central, L·S, T_L, T_T, and T_p components.[1] The coupling between partial waves with different orbital angular momenta (caused by the T_T and T_p potentials) is treated exactly, using a coupled-channels approach. All components of the potential may be complex, and many different options for the radial dependence of each component are available.

Some of the features of this routine were derived from DD, a routine by B.A. Robson.[2] The predictor-corrector routine DEPC, which uses Hamming's method[3] is based on a routine of the same name in the program library of the Madison Academic Computing Center.[4]

2. Input Requirements

2.1. Command Cards: Each command card contains an 8-character command and up to five option numbers, in format (2A4,2X,5I5). Only the first 4 characters of each command are necessary. The meanings of the options depend on the command. Each command card may be followed by other cards, depending on the command. Valid commands are:

DATA	Read reaction information and experimental data.
POTENTIAL	Read potential parameters and calculate the potentials.
CALCULATE	Perform a one-shot calculation and print the results.
TITLE	Read a new run number and title.
PLOT	Make a printer plot of the results.
POTPRINT	Print the potentials.
DELPRINT	Print the S-matrix.
WFPRINT	Print the wave functions.
AMPPRINT	Print the scattering amplitudes.
OBSOUT	Write the calculated observables on a specified device.
DELOUT	Write the S-matrix on a specified device.
AMPOUT	Write the scattering amplitudes on a specified device.
EXIT	(or a blank card) Quit.

DATA

Table I is a summary of the input formats and the machine-readable output formats. The commands are identified by asterisks. The formats for machine-readable output are included after the OBSOUT, DELOUT, and AMPOUT commands. Each of the commands, and the associated input and output, will be described in more detail in the following subsections.

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COMMAND STATEMENTS } FORMAT (2A4, 2X, 5I5)

2.2 DATA COMMAND: Read reaction information and experimental data. This should be the first command.

Option 1 is the logical unit number from which the experimental data are to be read. If zero (or omitted), the data are read from cards.

Card 1 (I5,18A4)

NRUN = run number.
TITLE = 72 characters.

Card 1a → Proj Z Proj M (F10.6)

Card 2 (3F10.6,3I5)

ZT = Charge of target (Z).
AMT = Mass of target (in AMU).
ELAB = Lab energy of the incoming deuteron (in MeV).
NCOOR = Coordinate system (both options follow the Madison Convention[5]):
0 = Analyzing powers, z along $\underline{k}_{in}$.
1 = Outgoing polarizations, z along $\underline{k}_{out}$.
NCROS = Type of cross section data to be entered:
0 = Cross section in millibarns per steradian.
1 = Cross section is ratio to Rutherford.
NDAT = Number of angles for which data will be entered.

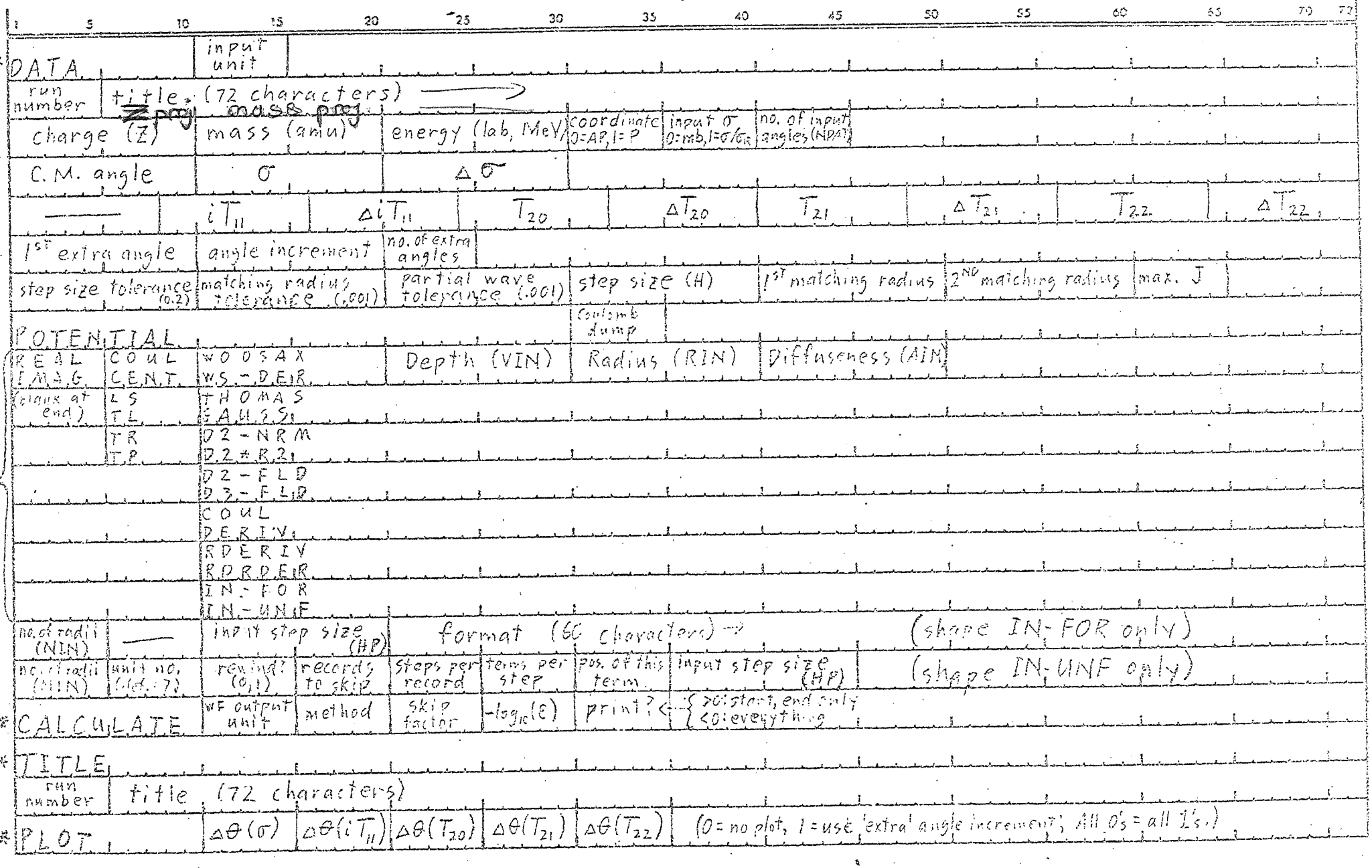
(Limits: NDAT $\leq$ 50, NDAT+NANGL $\leq$ 180)

Cards 3 and 4 (NDAT sets) (3F10.6/8X,8F8.4)
(If option 1 is nonzero, these are read from the indicated unit number instead of cards.)

ANGLE = center-of-mass scattering angle (in degrees).
SIG = C.M. cross section (or ratio to Rutherford).
DSIG = uncertainty in SIG.
T11 = Vector analyzing power iT_{11} (or polarization it_{11}).
DT11 = Uncertainty in T11.
T20 = Tensor analyzing power T_{20} (or polarization t_{20}).
DT20 = Uncertainty in T20.
T21 = Tensor analyzing power T_{21} (or polarization t_{21}).
DT21 = Uncertainty in T21.
T22 = Tensor analyzing power T_{22} (or polarization t_{22}).
DT22 = Uncertainty in T22.

(If any uncertainty is $\leq$ 0, that datum is not plotted, and it is ignored in chi-squared calculations.)

SUMMARY OF INPUT AND OUTPUT FORMATS.



A.014

TABLE I (2)

SUMMARY OF INPUT AND OUTPUT FORMATS.

	1	5	10	15	20	25	30	35	40	45	50	55	60	65	70	72
*	POTPRINT	skip factor														
*	DELPRINT	form (0-4)														
*	WFPRINT	skip factor	max. J													
*	AMPPRINT															
*	OBSOUT	unit	format													
OUTPUT	no. of angles	5	run no.	title (70 characters)												
	θ		σ (or σ/σ_R)		iT_{11}		T_{20}		T_{21}		T_{22}					
*	DELOUT	unit	format	form (0-4)												
OUTPUT	max. J	form (0-4)	run no.	title (70 characters)												
	(form 0,1,2,3)	$Re\,M^J_{--}$	$Im\,M^J_{--}$	$Re\,M^J_{00}$	$Im\,M^J_{00}$	$Re\,M^J_{++}$	$Im\,M^J_{++}$	$Re\,M^J_{+-}$	$Im\,M^J_{+-}$							
	(form 4)	$Re\,M^{(0)}_{LL}$	$Im\,M^{(0)}_{LL}$	$Re\,M^{(1)}_{LL}$	$Im\,M^{(1)}_{LL}$	$Re\,M^{(2)}_{LL}$	$Im\,M^{(2)}_{LL}$	$Re\,M^{(2)}_{L+2,L}$	$Im\,M^{(2)}_{L+2,L}$							
*	AMPOUT	unit	format													
Format 1,2 OUTPUT	no. of angles	6	run no.	title (70 characters)												
	θ		Re A		Im A		Re B		Im B							
	Re C		Im C		Re D		Im D		Re E		Im E					
Format 3,4 OUTPUT	no. of angles	3.333333														
	θ															
	$Re\,F_{11}$		$Im\,F_{11}$		$Re\,F_{10}$		$Im\,F_{10}$		$Re\,F_{1-1}$		$Im\,F_{1-1}$					
	$Re\,F_{01}$		$Im\,F_{01}$		$Re\,F_{00}$		$Im\,F_{00}$		$Re\,F_{0-1}$		$Im\,F_{0-1}$					
	$Re\,F_{-11}$		$Im\,F_{-11}$		$Re\,F_{-10}$		$Im\,F_{-10}$		$Re\,F_{-1-1}$		$Im\,F_{-1-1}$					
*	EXIT (or blank)															

DATA

Card 5 (2F10.4,I5)

TI = First 'extra' angle (in degrees).
DT = Increment between 'extra' angles (degrees).
NANGL = Number of extra angles.

Card 6 (6F10.6,I5)

TOL(1)= Step-size tolerance. The step size H is chosen as TOL(1) times the smallest "critical dimension". These "critical dimensions" include the diffusenesses of the potential terms, 1/internal wave number, and 0.5/external wave number. Default value = 0.2.

TOL(2)= Matching-radius tolerance. The matching radius RMTCH1 is chosen as the radius where all nuclear potentials are less than TOL(2) times the Coulomb potential. Default value = 0.001.

TOL(3)= Partial-wave tolerance. The maximum J-value is chosen as that for which the nuclear amplitudes $(S^J_{LL'}-1)/2i$ remain less than TOL(3) for 2 consecutive partial waves. Default value = 0.001.

* H = Step size (fermis). Overrides TOL(1) if nonzero.

RMTCH1= First matching radius. Overrides TOL(2) if nonzero.

RMTCH2= Second matching radius. If zero, RMTCH2 is chosen as RMTCH1 + 16*H.

LMAX = Maximum partial wave. Overrides TOL(3) if nonzero.

Note 1: The default values of the tolerances have been found to be adequate (errors of order 10^{-4} or less) for several test cases. It is the user's responsibility to determine whether or not they are appropriate for his problem.

Note 2: The importance of the step size H or its tolerance TOL(1) depends on the integration method (see CALCULATE command). For the Cowell method (normally used when T_p potentials are absent), the local truncation error is proportional to H^5, and the integration time is proportional to H^{-1}; hence, the choice of H must be a careful compromise between accuracy and cost. On the other hand, the Hamming predictor-corrector algorithm (normally used when a T_p potential is present) uses a variable step size, with automatic control of the truncation error. Therefore, in this case, it is generally advantageous to set H as small as possible (within array-size limits) to minimize the need for interpolation between the stored values of the potentials.

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POTENTIAL

2.3. POTENTIAL Command: Read the potential parameters, choose the step size and matching radii, calculate and store the potentials, and calculate the Coulomb wave functions and Coulomb phase shifts. This command must precede any CALCULATE commands.

If option 5 is positive, the Coulomb wave functions and Coulomb phase shifts are printed.

Potential parameters are read one "term" per card. A "term" is defined as the real or imaginary part of a given type of potential, such as central or T_r. If more than one term is indicated for a given potential type (such as REAL TR), the resulting potentials are added. In this way, potentials with complicated shapes can be built up from simpler shapes. Currently, the number of potential terms must be ≤ 12, and the total number of stored potential points (= no. of terms × RMTCH2/H) must be ≤ 3600.

Important: The last term must be followed by a blank card, to signal the end of the list.

Potential Cards (one per term).
(Format A4, 1X, A4, 1X, A4, A2, 4X, 3F10.4)

MRI = Real/imaginary mnemonic (4 characters):

blanks = flag after the last term
'REAL' = real part
'IMAG' = imaginary part

MTYPE = Type mnemonic (4 characters):

'COUL' = Coulomb (see note 1 below)
'CENT' = Central
'LS ' = L•S vector
'TL ' = T_L tensor
'TR ' = T_r tensor
'TP ' = T_p tensor (see note 2 below)
'TPD ' = T_p derivative (see note 3 below)

MSHAPE = Shape mnemonic (6 characters. Last 2 ignored).

Blank = standard for type (in parentheses below)
'WOOSAX' = Woods-Saxon (REAL CENT, REAL TP)
'WS-DER' = Woods-Saxon derivative (IMAG CENT, IMAG TP)
'THOMAS' = Thomas (REAL LS)
'GAUSS' = Gaussian (IMAG LS)
'DS-NRM' = Normalized Woods-Saxon second derivative (REAL TL)
'D2*R2 ' = R^2 times Woods-Saxon second derivative (IMAG TL)
'D2-FLD' = Folded Real T_r (REAL TR)

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'D3-FLD' = Folded Im T_γ. (IMAG TR)
'COUL ' = Coulomb (REAL COUL)
'DERIV ' = Derivative (wrt r) of the previous term
'RDERIV' = Modified derivative of the previous term
'RDRDER' = Modified second derivative of the previous term
'IN-FOR' = Formatted input
'IN-UNF' = Unformatted input

VIN = Depth parameter (MeV)

RIN = Radius parameter (fm). RIN will be multiplied by the cube root of the mass.

AIN = Diffuseness parameter (fm). See note 4 below.

Potential Shapes: In the formulas below, $x = (r-R)/AIN$, where $R = RIN \times AMT^{1/3}$, and AMT is the target mass (DATA card 2). The value $\sqrt{2}$ fm is used for λ_π, the Compton wavelength of the pion. In general, the shapes are defined in such a way that if VIN>0, the outermost extremum is negative (attractive). (The obvious exceptions are COUL, DERIV, RDERIV, RDRDER, IN-FOR, and IN-UNF.)

WOOSAX: Woods-Saxon

$$V(r) = -VIN \cdot (1+e^x)^{-1}$$

WS-DER: Woods-Saxon Derivative (normalized to unity)

$$V(r) = 4 \cdot VIN \cdot \frac{d}{dx} (1+e^x)^{-1}$$

$$= \frac{-4 \cdot VIN \cdot e^x}{(1+e^x)^2}$$

THOMAS: Thomas

$$V(r) = \frac{VIN \cdot \lambda_\pi^2}{r} \frac{d}{dr} (1+e^x)^{-1}$$

$$= \frac{-2 \cdot VIN}{AIN \cdot r} \frac{e^x}{(1+e^x)^2}$$

GAUSS: Gaussian

$$V(r) = -VIN \cdot \exp(-x^2)$$

D2-NRM: Woods-Saxon second derivative, normalized to unity at the outermost maximum, as in Raynal's code MAGALI.[5]

$$V(r) = -VIN \cdot 6\sqrt{3} \frac{d^2}{dx^2} (1+e^x)^{-1}$$

$$= -VIN \cdot 6\sqrt{3} \frac{e^x(e^x-1)}{(1+e^x)^3}$$

POTENTIAL

D2*R2: Woods-Saxon second derivative, times r^2, as in Irshad and Robson.[6]

$$V(r) = -VIN \cdot r^2 \frac{d^2}{dr^2} (1+e^x)^{-1}$$

$$= \frac{-VIN \cdot r^2}{(AIN)^2} \frac{e^x(e^x-1)}{(1+e^x)^3}$$

D2-FLD: This potential, which is similar to a Woods-Saxon second derivative, was designed to approximate the real part of the T_r potential predicted by the folding model. It was proposed by Keaton and Armstrong.[7]

$$V(r) = -VIN \cdot \lambda_\pi^2 r \frac{d}{dr} [\frac{1}{r} \frac{d}{dr} (1+e^x)^{-1}]$$

$$= \frac{-2 \cdot VIN}{(AIN)^2} \frac{e^x}{(1+e^x)^2} (\frac{AIN}{r} - \frac{1-e^x}{1+e^x})$$

D3-FLD: This one, which resembles a Woods-Saxon third derivative, was proposed by Keaton and Armstrong[7] to approximate the imaginary T_r folding-model potential.

$$V(r) = -VIN \cdot \lambda_\pi^2 r \frac{d}{dr} [\frac{1}{r} \frac{d}{dr} (\frac{4e^x}{1+e^x)^2})]$$

$$= \frac{-8 \cdot VIN}{r \cdot AIN} \frac{e^x}{(1+e^x)^4} [\frac{r}{AIN} (1-4e^x+e^{2x}) - (1-e^{2x})]$$

COUL: This is the shape of the Coulomb field due to a uniformly charged sphere of radius R. When the COUL shape is used for terms which are not COUL type, the depth VIN is the multiplier of the 1/r tail. For the COUL type term, the value $2\eta E_{CM}/K_{CM}$ is substituted for VIN.

$$V(r) = \begin{cases} \frac{VIN}{2 \cdot R} [3 - (\frac{r}{R})^2] & \text{for } r < R \\ \frac{VIN}{r} & \text{for } r \geq R \end{cases}$$

$2 \frac{z e^2}{r}$

POTENTIAL

DERIV: A five-point numerical derivative formula[8] is used to calculate the first derivative (with respect to the radius r in fermis) of the previous term. This is then renormalized by the ratio of VIN for this term to VIN for the previous term:

$$V(r) = \frac{VIN}{VINP} \frac{d}{dr} [VP(r)]$$

where (VINP and VP(r) refer to the previous term).

RDERIV: Numerical derivative, as in DERIV, but altered:

$$V(r) = \frac{VIN}{VINP} r \frac{d}{dr} [\frac{1}{r} \cdot VP(r)].$$

(See note 5 below).

RDRDER: An altered numerical second derivative of the previous term:

$$V(r) = \frac{VIN}{VINP} r \frac{d}{dr} [\frac{1}{r} \frac{d}{dr} VP(r)].$$

starting at HP *

IN-FOR: The potential is read from cards, interpolated between points if necessary, and multiplied by VIN. (See note 5 below).

Specification card (format I5,5X,F10.6,A60) (see note 11):

NIN = the number of radii to be read in.
HP = the step size (in fm) between successive values of the input potential. If HP=0, HP=H is assumed.

INFORM=the format of the input cards (up to 60 characters). Subsequent cards should contain the potential values, in the format indicated on card 1. All of the cards are read with a single READ statement; therefore, any number of radii may be placed on each card.

NB POTS START AT HP not r=0

IN-UNF: The potential is read from a specified logical unit (which may be tape or mass storage), using Fortran unformatted READ statements. It is then interpolated between points if necessary, and multiplied by VIN. (See note 5 below). One card is required, to give the unit number of the input device and other information regarding the size and contents of the input records.

POTENTIAL

Specification card (format 7I5,F10.6):

NIN	=	the number of radii to be read.
IUN	=	the logical unit number of the input device (default = 7).
IRW	=	rewind flag (rewind before reading if nonzero).
NRSK	=	the number of records to skip before reading. (If negative, number of records to backspace.)
NSPR	=	the number of steps per record (default=1).
NTPS	=	the number of terms per step (default=1).
IPOS	=	the position of the desired term (default=1).
HP	=	step size (in fermis) (default=H).

If NTPS > 1, all words of each record will be ignored, except those in the positions IPOS, IPOS+NTPS, ..., IPOS+(NSPR-1)*NTPS. Each record must contain NSPR*NTPS words.

Notes about the POTENTIAL command:

Note 1. MTYPE = 'COUL': Only one Coulomb term should be present, and it must be REAL. For the combinations 'REAL COUL COUL' or 'REAL COUL VIN is replaced by the Coulomb strength determined by the charge. If the Coulomb term is omitted, it is supplied automatically, with RIN = 1.3 fm. The limit of 12 terms includes the Coulomb term, explicit or implied. If an input central potential ('IN-FOR' or 'IN-UNF') contains a Coulomb part, use type 'COUL' (not type 'CENT') to prevent the automatic generation of another Coulomb term.

Note 2. MTYPE = 'TP': Chapter 3 should be read and understood before using a T_p potential. Briefly, these are the conventions: If a T_p is present, the order of the terms is important. Ordinarily, you should place any T_p potentials after all real central terms, including the Coulomb term (use an explicit REAL COUL COUL term). If this rule is followed, the specified shape and depth will correspond to the energy difference (in MeV) between the $\underline{s}\cdot\underline{p} = \pm 1$ substates and the $\underline{s}\cdot\underline{p} = 0$ substate, as in refs.[1,2].)

The T_p potential used by DDTP is actually the alternative form $S_2 \cdot R_2(p, Up)$ proposed by Satchler.[1]) In all of the calculations I have done, the difference between this form and the usual form $\frac{1}{2}[U(r)T_p + T_pU(r)]$ is insignificant. Chapter 3 has more details.

Note 3. MTYPE = 'TPD': Potential type 'TPD' is not legal for input. A calculation using a T_p potential requires a knowledge of the first derivative of the potential. Therefore, each time a term with MTYPE = 'TP' is specified, two terms are actually generated: The second is type 'TPD' and shape 'DERIV'. The limit of 12 terms includes these internally generated TPD terms.

POTENTIAL
CALCULATE

Note 4. AIN: Even if the diffuseness parameter is not used in calculating the potential (as for shapes IN-FOR or IN-UNF), an approximate value of AIN should be supplied to aid in the choice of step size, unless the step size is specified explicitly. If AIN is not positive, that term is ignored in choosing the step size. See command DATA, variable TOL(1).

Note 5. IN-FOR and IN-UNF: The additional cards needed by IN-FOR and IN-UNF should be placed after the blank card at the end of the list of potential terms. For example, if term 3 has shape IN-FOR, term 4 has a shape IN-UNF, and there are 6 terms in all, then the card describing term 6 should be followed by a blank card, then the specification card for term 3, then the potential deck for term 3, then the specification card for term 4.

NB

INPUT POTENTIALS FROM HP OUTWARD

The spacing (HP) between the input potential values for shapes IN-FOR and IN-UNF does not have to be the same as the spacing (H) used for integration. If HP ≠ H, six-point Lagrangian interpolation[9]) is used to supply the missing values. All of the input potential values are read into the upper part of the potential array before the interpolation is done; these values are then replaced by the interpolated values. It is generally a good idea to place your IN-FOR or IN-UNF terms before any other terms, especially if HP < H; that way, the part of the potential array reserved for the later terms can be used as an input buffer if necessary.

****

2.4. CALCULATE Command: Perform a one-shot calculation and print the results. This command must be preceded by DATA and POTENTIAL.

Option 1 is the logical unit for storage of the "raw" unnormalized wave functions. This must be specified if the WFPRINT command is to be used later. The device may be tape or mass storage. The format of this output is described below. Zero suppresses output.

Option 2 (if nonzero) overrides the normal choice of integration method. 1 = Cowell method, without off-diagonal coupling (normally used in the absence of T_r or T_p potentials); 2 = Cowell method, including off-diagonal coupling (normally used when T_r, but not T_p, terms are present); 3 = Hamming predictor-corrector method (normally required if T_p is present). Method 1 is used in SNOOPY, and method 2 is used in DD. If Method 1 or 2 is used with a T_p potential, the T_p potential is ignored.

CALCULATE
TITLE

Option 3 (if positive) is the "skip factor" for printing and/or storage of the wave functions. Wave functions are printed or stored at intervals of (option 3)*H. Zero means every step (if at all). Note: If Method 3 (Hamming predictor-corrector) is used, and Option 3 = 0, the wave function will be output at nonuniform intervals (see ref. 4).

Option 4 (if positive) is $-\log_{10}(EPS)$, where EPS is the error control parameter in subroutine DEPC (see ref. 4). Default = 5. (Method 3 only).

Option 5 (if positive) causes the wave functions at the starting and matching radii to be printed for diagnostic purposes. If option 5 is negative (and method 3 is used), the unnormalized wave functions are printed (see Option 3).

If Option 1 is positive, the unnormalized wave functions are written using FORTRAN unformatted WRITE statements. The first record for each partial wave contains:

KJ = J + 1 (or -1 after the last partial wave)

KL = L - J + 2 if only one L is present, or = 0 otherwise

JST= starting radius/H

NWF= the number of wave functions in each record
(may be 1, 3, 4, or 5)

Each data record (one per radius) contains:

R = radius (in fm)

CX(I) (I = 1 to NWF) = wave functions (order described below)

The last record for each partial wave is a data record in which R is replaced by -R. The last partial wave is followed by a header record with KJ = -1, followed by two file marks. The output device is then rewound.

If NWF=3, the order of CX(I) is L=J, L=J-1, 1=J+1. If NWF=5, the order is L=J, L=J-1 #1, L=J+1 #1, L=J-1 #2, L=J+1 #2. NWF=4 is like 5, but L=J is omitted.

****

2.5. TITLE Command: Read a new run number and title. The next card should contain the run number and title, in format (I5,A72); these will replace the values on DATA card 1.

****

PLOT
POTPRINT
DELPRINT

2.6. PLOT Command: Make a printer plot of the results.

Options 1-5: Each option specifies the format for plotting one observable. Option 1 is for the cross section, 2 is iT_{11}, 3 is T_{20}, 4 is T_{21}, and 5 is T_{22}. If the option is zero, the corresponding plot is omitted. If the option is 1, one line on the plot will correspond to the difference between the last two angles at which observables were calculated (to the nearest degree). If "extra angles" were specified, this will result in plotting one extra angle per line. If the value of any option is greater than 1, it specifies the number of degrees per line in the plot. Exception: If all 5 options are zero, they are all set to 1.

The experimental data, the calculations at the experimental angles, and the calculations at the extra angles are plotted on the same plot, using 3 different symbols. The Y scales are set automatically, depending on the range of the data and calculations to be plotted.

****

2.7. POTPRINT Command: Print the potentials.

Option 1 is the "skip factor". Potentials are printed at intervals of (option 1)*H.

Note: If "local momentum renormalization" is used, the radial dependence of the T_p potential is not given directly by the formulas given in sec. 2.3. Refer to sec. 3.2 for details.

****

2.8. DELPRINT Command: Print the S matrix, in any one of a number of forms.

Option 1 specifies the form in which the S matrix is to be printed. Possible values are:

0 = $M^J_{L'L}$ (internal form)

DELPRINT

$$1 = \Delta^J_{LL'} = 2iM^J_{L'L} + e^{i(\omega_{L'}+\omega_L)}\,\delta_{L'L} \quad \text{[as in Robson's DD}^2\text{)]}$$

$$2 = \alpha^J_{L'L} = e^{-i(\omega_{L'}+\omega_L)}\,M^J_{L'L} \quad \text{[as in SNOOPY]}$$

$$3 = S^J_{L'L} = 2ie^{-i(\omega_{L'}+\omega_L)}\,M^J_{L'L} + \delta_{L'L} \quad \text{[Nuclear S matrix]}$$

$$4 = M^{(K)}_{L'L} = -\sum_J (2J+1)[3(2L'+1)]^{-\frac{1}{2}}(-1)^{J-L'}W(LL'11;KJ)M^J_{L'L}$$

[Johnson "spin transfer" form[12])]

where L and L' are the incoming and outgoing orbital angular momenta respectively, J is the total angular momentum, ω_L is the relative Coulomb phase shift ($\omega_0 = 0$), and K is the "spin transfer" (K = 0, 1, or 2).

Two other columns are printed (for forms 0-3) as a check on the accuracy of the calculation. If the potentials are all real, the S matrix must be unitary ($SS^\dagger = 1$); i.e.

$$\sum_{L''=J-1}^{J+1} S^J_{L'L''}\,(S^J_{LL''})^* = \delta_{L'L}.$$

The column labelled "ABS ROW SUM" contains the diagonal elements of $SS^\dagger$, and the column labelled "CROSS SUM" contains the off-diagonal elements. If you are in doubt about the accuracy of a calculation, run it once without any imaginary potentials. For such a calculation the diagonal elements of $SS^\dagger$ should all be 1.0, and the off-diagonal elements should be zero. If necessary, readjust the tolerances to improve unitarity. If absorptive potentials are present the diagonal elements of $SS^\dagger$ should be ≤ 1.0.

The DELPRINT output provides another accuracy check whenever a T_r or T_p potential is present: The S matrix should always be symmetric, i.e.

$$S^J_{L'L} = S^J_{LL'}$$

even when absorptive potentials are present. Similar relationships apply

DELPRINT
WFPRINT
AMPRINT

to forms 0, 1, 2, and 3. For form 4, this relationship takes the form

$$(2L'+1)^{\frac{1}{2}} \; M^{(K)}_{L'L} = (2L+1)^{\frac{1}{2}} \; M^{(K)}_{LL'}.$$

The Johnson "spin transfer" form (form 4) is useful for separating the effects of the various potentials. Johnson[12] showed that in first order perturbation theory, $M^{(K)}_{L'L}$ depends only on potentials of order K; i.e., K = 0 = central, 1 = $\underline{L}\cdot\underline{S}$, and 2 = tensor.

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2.9. WFPRINT Command: The wave functions are read from their storage device, renormalized, and printed. This command must be preceded by a CALCULATE command in which the storage device is specified as Option 1.

Option 1 is the "skip factor" S. If s > 1, then s - 1 records are skipped for each record printed. The radial interval between the records written is controlled by CALCULATE Option 3; therefore, the printing interval is the product of these two "skip factors", times the basic interval H.

Option 2 is the maximum J for which the wave functions are to be printed.

The renormalized wave functions are linear combinations of the two independent solutions of the coupled system of differential equations. The coefficients of these two solutions, which are printed at the beginning of each partial wave, are calculated when the wave functions are matched to the external Coulomb waves (see the Theory Chapter).

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2.10. AMPPRINT Command: Print the scattering amplitudes (A through E). They are defined in the Theory Section, and in ref. 2.

****

OBSOUT
DELOUT
AMPOUT

2.11. OBSOUT Command: Write the calculated observables on a specified output device.

Option 1 is the unit number of the output device (default = 1 = card punch).

Option 2 specifies the format (default = 1). If Option 2 = 1, the first card contains the number of angles, the number '5', the run number, and the title, in format (I3,I2,I5,A70). (The number '5' is to distinguish this from DELOUT and AMPOUT output). Each subsequent card contains the angle, and the calculated σ (or σ/σ_R), iT_{11}, T_{20}, T_{21}, and T_{22}, in format (F13.4,E13.6,4F13.6). Only the "extra" angles are written.

If Option 2 = 2, the same format is used, but the calculations at all angles (including the angles of the input data) are written.

****

2.12. DELOUT Command: Write the S matrix on a specified device, in machine-readable form.

Option 1 is the logical unit number of the output device (default = 1 = card punch).

Option 2 specifies the output format (default = 1). At this writing, only one format is available. The first card contains the maximum J, the form (option 3), the run number and the title (format I3,I2,I5,A70). Subsequent cards contain the S-matrix values (format 8F10.7). For forms 0-3, each card corresponds to one value of J, starting with J = 0, in the order (L',L) = (J-1,J-1),(J,J),(J+1,J+1),(J+1,J-1). For form 4, each card has one L value, starting with L = 0, in the order (K,L') = (0,L),(1,L),(2,L),(2,L+2).

Option 3 is the S-matrix form (same as DELPRINT option 1).

****

2.13. AMPOUT Command: Write the scattering amplitudes on a specified device.

AMPOUT
EXIT
T_p

Option 1 is the unit number of the output device (default = 1 = card punch).

Option 2 specifies the format (default = 1). If Option 2 = 1, the first card contains the number of angles, the number '6', the run number, and the title, in format (I3,I2,I5,A70). (The number '6' is to distinguish this from OBSOUT and AMPOUT output.) The scattering amplitudes occupy 2 cards per angle, in the order θ,A,B,C,D,E, in format (F13.4,4E13.6/6E13.6). Only the "extra" angles are written.

If Option 2 = 2, the same format is used, but the amplitudes at all angles (including the angles of the input data) are written.

If Option 2 = 3, the scattering amplitudes are transformed into center-of-mass helicity coordinates and written in a format which is readable by Ed Stephenson's routine HAUSER. The first card contains the number of angles and the normalization factor 3.333333, in format (I3,F10.6). The scattering amplitudes occupy 4 cards per angle, in the order $\theta,(F_{m'm},m=1,0,-1),m'=1,0,-1)$, where m is the incoming spin projection along the incoming momentum direction and m' is the outgoing spin projection along the center-of-mass outgoing momentum direction. The format is (F7.2,3(/ 6E13.6E2)). Only the "extra" angles are written.

If Option 2 = 4, the format is the same as 3, but all of the angles are written.

****

2.14. EXIT Command: Quit. A blank card accomplishes the same thing.

****

3. The T_p Potential - Conventions

The presence of the momentum operator in the T_p tensor spin-orbit potential introduces several complications into any calculation which includes a T_p potential. Most of these complications - such as

the choice of an appropriate algorithm for the numerical solution of the differential equations - are handled automatically by the program; ordinarily, the user need not even be aware of them. However, two of the problems introduced by the T_p potential required the adoption of somewhat arbitrary conventions, of which the user must be aware. These conventions involve the method of attaching a radial dependence to the T_p operator, and the use of a "local momentum" renormalization for the T_p potential. In each case, the convention which is ordinarily used in DDTP is the one which I have found to be most convenient and efficient, but methods are provided for the use of alternative conventions if the user prefers them.

3.1. Commutation: $\frac{1}{2}(UT_p + T_pU)$ vs. T_{pUp}: The T_p operator does not commute with a function of the radius; i.e. $U(r)T_p \neq T_pU(r)$. Satchler[1]) has shown that an "acceptable" T_p potential (i.e., one which produces a symmetric s matrix) can be constructed in either of two ways: The symmetric combination $\frac{1}{2}(U(r)T_p + T_pU(r))$ can be used, or a slightly different operator can be formed by sandwiching the radial function between the two momentum operators. I will refer to this second form as T_{pUp}. The relationship between the two forms is

$$\frac{1}{2}\,(U(r)T_p + T_pU(r)) = T_{pUp} - \frac{1}{2}\,r\,\frac{d}{dr}\,[\frac{1}{r}\,\frac{d}{dr}\,\Downarrow U(r)]\;T_r \qquad (3\text{-}1)$$

where the derivatives on the right operate only on U(r). The difference between the two forms is a T_r potential which looks like the second derivative of U(r). In all of the calculations I have done so far, the effects of this extra T_r potential are negligible in comparison to the effects of the T_p potential. For reasons of efficiency and convenience, DDTP uses the T_{pUp} form, because second derivatives of U(r) are not required. To use the form $\frac{1}{2}\,(U(r)T_p + T_pU(r))$, simply insert a card defining the extra T_r potential immediately after the one defining the T_p potential. This T_r term should have shape = RDERIV and depth = $-\frac{1}{2}$ times the depth of the T_p term. (The correct shape is RDERIV, and not RDRDER, because the first derivative of the T_p term is automatically inserted after the T_p). The theoretical predictions of the T_p potential[10,11]) are not sufficiently detailed to include the effects of the curvature of the nuclear density; therefore, they do not indicate a preference for either form.

****

3.2. Local Momentum Normalization: The T_p operator, as defined

T_p

by Satchler[1]), has the form

$$T_p = (\underset{\sim}{s}\cdot\underset{\sim}{p})^2 - \frac{2}{3}p^2. \tag{3-2}$$

It has dimensions of momentum squared, and its expectation values depend on both the direction and the magnitude of the momentum. Ioanides and Johnson[10]) and Austern[11]) expressed their predicted T_p potentials in terms of the energy difference between a deuteron with $\underset{\sim}{s}\cdot\underset{\sim}{p} = \pm 1$ and one with $\underset{\sim}{s}\cdot\hat{\underset{\sim}{p}} = 0$ (where $\hat{\underset{\sim}{p}} = \underset{\sim}{p}/|\underset{\sim}{p}|$); i.e. their predictions depend only on the direction of $\underset{\sim}{p}$, and not on its magnitude. Unfortunately, we cannot in general simply divide the T_p operator by p^2, because the momentum operator in coordinate space is a differential operator; hence, its inverse is an integral operator, which is nonlocal. However, we can remove the dependence on p^2 in an approximate way by defining a "local momentum" $p_L(r)$ whose magnitude is given by

$$p_L^{\,2}(r) = p_A^{\,2}[1 - \mathrm{Re}\, V_C(r)/E_{CM}] \tag{3-3}$$

where p_A is the asymptotic momentum, E_{CM} is the center-of-mass energy of the incident deuteron, and Re $V_C(r)$ is the real part of the central potential. In the nuclear interior, $V_C(r)$ is large and negative, so $p_L^{\,2}(r)$ there can be much larger than $p_A^{\,2}$. My experience has shown that $p_L^{\,2}(r)$ is a good approximation to the operator p^2, at least at energies well above the Coulomb barrier[13]).

In DDTP, the radial dependence of the T_p potential is given by:

$$U(r) = V_{TP}(r)p_L^{\,-2}(r) = V_{TP}(r)p_A^{\,-2}[1 - \mathrm{Re}\, V_C(r)/E_{CM}]^{-1} \tag{3-4}$$

where $U(r)$ is combined with the T_p operator as described in sect. 3.1. The function $V_{TP}(r)$ is calculated directly from the input parameters, as described in sect. 2.3. The depth of $V_{TP}(r)$ is expressed in MeV, like the other potentials. To the extent that the local momentum approximation is correct, $V_{TP}(r)$ represents the energy difference between the substates with $\underset{\sim}{s}\cdot\hat{\underset{\sim}{p}} = \pm 1$ and the substate with $\underset{\sim}{s}\cdot\hat{\underset{\sim}{p}} = 0$. Thus, for example, $V_{TP}(r)$ can be compared directly to fig. 1 of Ioanides and Johnson[10]). That figure indicates an attractive T_p potential [$V_{TP}(r) < 0$] which is approximately 1 MeV in depth.

T_p

It should be emphasized that the convention used in eq. (3-4) does not represent an approximation to the T_p potential, as defined by Satchler[1]). Instead, it is an approximate way of interpreting the predictions of refs.[10,11]), which do not depend explicitly on p^2, in terms of a local T_p potential, whose expectation values do depend on p^2.

The function $V_c(r)$ used by DDTP in the renormalization in eq. (3-4) is the sum of all of the real central terms (including Coulomb) which appear before the T_p term. Thus, if the local momentum renormalization is to be used, the Coulomb term must be included explicitly, before the first T_p term, along with the other REAL CENT terms. If you prefer not to use the local momentum renormalization, simply place the cards defining your T_p terms before the first REAL CENT or REAL COUL term, and multiply the potential depth by $p_A^{\ 2}$. The local momentum renormalization should definitely not be used for incident energies below the Coulomb barrier, because eq. (3-4) has a singularity where Re $V_c(r) = E_{CM}$.

The T_p potential which is stored by the POTENTIAL command and printed by the POTPRINT command is actually $V_{TP}(r)[1 - \text{Re } V_c(r)/E_{CM}]^{-1}$, which does not include the factor p_A^{-2}. This fact is necessary for understanding your POTPRINT output.

4. Deuteron Optical Model Formalism

Most of the basic formalism for the deuteron optical model may be found in Robson[19], sec. 4.2. Relevant parts of that treatment are repeated here, with some changes in notation and a few corrections, to help the DDTP user to interpret and understand the various input and output options in the program.

4.1. Potentials and Schroedinger Equation: The elastic scattering of deuterons by a nucleus is assumed to be described by a local potential of the form

$$V(r) = V_C(r) + V_{LS}(r)\underset{\sim}{L}\cdot\underset{\sim}{s} + V_{TL}(r)T_L + V_{TR}(r)T_r + \frac{1}{2}\left[U_{TP}(r)T_p + T_pU_{TP}(r)\right]. \tag{4-1}$$

The tensor spin-orbit operators are defined by[4])

$$T_L = (\underset{\sim}{L}\cdot\underset{\sim}{s})^2 + \frac{1}{2}(\underset{\sim}{L}\cdot\underset{\sim}{s}) - \frac{2}{3}\underset{\sim}{L}^2$$

$$T_r = (\underset{\sim}{s}\cdot\hat{\underset{\sim}{r}})^2 - \frac{2}{3} \tag{4-2}$$

$$T_p = (\underset{\sim}{s}\cdot\underset{\sim}{p})^2 - \frac{2}{3}\underset{\sim}{p}^2$$

where L, s, r, and p are the orbital angular momentum, deuteron spin, position, and momentum operators respectively, and $\hat{r} = r/|r|$. The five functions V_C, V_{LS}, V_{TL}, V_{TR}, and U_{TP} are complex functions of radius. In general, $V_C(r)$ contains both nuclear and Coulomb components. The function $U_{TP}(r)$ is discussed further in sec. 3.

The general solution of the Schroedinger equation for this interaction when the incoming spin projection is σ may be written as a partial wave expansion:

$$\psi_\sigma = \sum_{JLL'M\lambda} A_{JLM\lambda\sigma}\, r^{-1} u_{JL'L}(r)\, \mathcal{Y}^M_{JL'S}(\theta,\phi) \tag{4-3}$$

where the dependence on spin and angle is contained in the functions

$$\mathcal{Y}^{M}_{JL'S} = \sum_{\lambda'\sigma'} \langle JM|L'S\ \lambda'\sigma'\rangle \cdot Y^{\lambda'}_{L'}(\theta,\phi)\ \chi^{\sigma'}_{S} \qquad (4\text{-}4)$$

In the expressions above, J, L', and S(=1) are the total angular momentum, orbital angular momentum, and deuteron spin, and M, λ', and σ' are their respective projections on the z axis. The incoming orbital angular momentum L and the coefficients $A_{JLM\lambda\sigma}$ are determined by the boundary conditions, which will be discussed below.

If the expansion (4-3) is substituted into the Schroedinger equation, and if the result is multiplied on the left by $\mathcal{Y}^{M}_{JL''}(\theta,\phi)$ and integrated over angle and spin variables, a set of coupled equations for the radial functions $u_{JL'L}(r)$ is obtained:

$$\left[\frac{d^2}{d\rho^2} - \frac{L'(L'+1)}{\rho^2} + 1\right] u_{JL'L}(r) = E_{cm}^{-1} \sum_{L''} r \langle JL'|V|JL''\rangle\ r^{-1}\ u_{JL''L}(r) \qquad (4\text{-}5$$

where $\rho = kr$, and $k = (2\mu E_{CM}/\hbar^2)^{\frac{1}{2}}$ is the asymptotic wave number. The potential matrix elements $\langle JL'|V|JL''\rangle$ will be discussed in detail in a later subsection. For each value of J (except J=0), there are three equations of the form (4-5), corresponding to L' = J, J±1. Because of parity conservation, only two of these equations (for L' = J±1) are coupled together by the T_r and T_t potentials.

4.2. The Transition Matrix: In general, a system of three second-order equations like (4-5) has six independent solutions. Three of these are eliminated by the requirement that ψ_σ must be regular at the origin; i.e. $u_{JL'L}(0) = 0$. The other three solutions are determined by the condition that in the limit of large r, the function $u_{JL'L}(r)$ must contain Coulomb-distorted plane waves with unit amplitude if L' = L, and only outgoing waves if L' ≠ L. Specifically, a "matching radius" r_m is chosen such that all of the terms in the potential (eq. 4-1) are negligibly small for $r > r_m$ except the Coulomb term. At $r = r_m$, the wave function $u_{JL'L}(r)$ is required to satisfy the "matching equation"

$$u_{JL'L}(r_m) = e^{-i\omega_{L'}} M^{J}_{L'L} [G_{L'}(kr_m) + i F_{L'}(kr_m)] + \delta_{L'L} e^{i\omega_L} F_L(kr_m) \qquad (4\text{-}6)$$

where $F_L(\rho)$ and $G_L(\rho)$ are the regular and irregular Coulomb wave functions[15]

respectively, and ω_L is the relative Coulomb phase shift given by

$$\omega_L = \sigma_L - \sigma_o = \sum_{j=1}^{L} \arctan(\eta/j) \qquad (4\text{-}7)$$

where $\eta = Ze^2/\hbar v$ and $\sigma_o = \arg \Gamma(1 + i\eta)$ are the usual Coulomb parameters.

Both the wave function and its first derivative must be continuous at $r = r_m$; therefore, another matching equation of the form (4-6) must be satisfied by the first derivatives of u, F, and G. These matching equations provide enough information to uniquely specify the boundary condition for $u_{JL'L}(r)$ and to determine the "transition matrix" elements $M^J_{L'L}$. The matrix element $M^J_{L'L}$ is proportional to the coefficient of the outgoing wave with orbital angular momentum L', given a unit-amplitude Coulomb-distorted incident plane wave. This transition matrix is printed by the DELPRINT command with option I=0 (see sect. 2.8).

4.3. The Scattering Amplitudes: Consider first the case of pure Coulomb scattering. In this case, $M^J_{L'L} = 0$, and the expansion (4-3) reduces to

$$\psi_\sigma^c = \sum_{JLM\lambda\lambda'\sigma'} A_{JLM\lambda\sigma}\, e^{i\omega_L}\, r^{-1} F_L(kr) \langle JM|\, L\, S\, \lambda'\sigma'\rangle\, Y_L^{\lambda'}(\theta,\phi)\, \chi_s^{\sigma'}. \qquad (4\text{-}8)$$

We already know what a Coulomb wave looks like[16]):

$$\psi_\sigma^c = 4\pi\, k^{-1} \sum_{L\lambda} i^L e^{i\omega_L}\, r^{-1} F_L(kr)\, Y_L^{\lambda^*}(\theta_k,\phi_k)\, Y_L^{\lambda}(\theta,\phi)\, \chi_s^{\sigma} \qquad (4\text{-}9)$$

where θ_k and ϕ_k describe the direction of the incident beam. Comparing (4-8) and (4-9), we see that the coefficient $A_{JLM\lambda\sigma}$ must have the value

$$A_{JLM\lambda\sigma} = 4\pi\, k^{-1}\, i^L\, \langle JM|LS\lambda\sigma\rangle\, Y_L^{\lambda^*}(\theta_k,\phi_k). \qquad (4\text{-}10)$$

Asymptotically, the Coulomb wave (4-9) has the form

$$\psi_\sigma^c \sim \{[1 - \frac{\eta^2}{i(kr - \underset{\sim}{k}\cdot\underset{\sim}{r})}]e^{i[\underset{\sim}{k}\cdot\underset{\sim}{r} + \eta \log(kr - \underset{\sim}{k}\cdot\underset{\sim}{r}) - \sigma_o]}$$

$$+ r^{-1} f_c(\theta) e^{i[kr - \eta \log 2kr + \sigma_o]}\} \chi_s^\sigma \qquad (4\text{-}11)$$

where

$$f_c(\theta) = -\frac{\eta}{2k}\ \mathrm{cosec}^2\left(\frac{\theta}{2}\right) e^{-2i\eta \log \sin(\theta/2)} \qquad (4\text{-}12)$$

is the Coulomb scattering amplitude. The form (4-11) was chosen because it displays a clear separation between a Coulomb-distorted incident plane wave (first line) and a spherical, outgoing scattered wave.

The general elastic-scattering wave function must be the same as the Coulomb wave function, plus some additional outgoing scattered waves:

$$\psi_\sigma \sim \psi_\sigma^{\,c} + r^{-1} \sum_{\sigma'} [f_{\sigma'\sigma}(\theta,\phi) - \delta_{\sigma'\sigma} f_c(\theta)] e^{i[kr - \eta \log 2kr + \sigma_0]} \chi_s^{\sigma'} \qquad (4\text{-}13)$$

where $f_{\sigma'\sigma}(\theta,\phi)$ is the amplitude for scattering an incident wave with spin projection σ into an outgoing wave with spin projection σ' and direction (θ,ϕ). An expression for $f_{\sigma'\sigma}(\theta,\phi)$ in a partial-wave representation may be obtained by inserting the coefficients (4-10) and the asymptotic radial wave functions (4-6) into the expansion (4-3), and subtracting the Coulomb part (4-9). Making use of the asymptotic behavior of F and G[15]:

$$[G_L(\rho) + i F_L(\rho)] \sim e^{i[\rho - \eta \log 2\rho - \frac{L\pi}{2} + \sigma_L]} \qquad (4\text{-}14)$$

we obtain the result

$$f_{\sigma'\sigma}(\theta,\phi) = \delta_{\sigma'\sigma} f_c(0) \qquad (4\text{-}15)$$

$$+ 4\pi k^{-1} \sum_{JLL'M\lambda\lambda'} i^{L-L'} \langle JM|LS\lambda\sigma\rangle \langle JM|L'S\lambda'\sigma'\rangle Y_L^{\lambda *}(\theta_k,\phi_k) Y_{L'}^{\lambda'}(\theta,\phi) M^J_{L'L}$$

Now we will choose a coordinate system: The z axis is along the incoming beam direction $\underline{k}_{in}$, and the y axis is along $\underline{k}_{in} \times \underline{k}_{out}$, where $\underline{k}_{out}$ is the direction of the detected particle. This coordinate system is in agreement with the Madison Convention[14]. Then $\theta_k = \phi_k = 0$, $M = \sigma$, and we need to evaluate the scattering amplitudes only at $\phi = 0$:

$$f_{\sigma'\sigma}(\theta,0) = \delta_{\sigma'\sigma} f_c(\theta) + k^{-1} \sum_{JLL'} [4\pi(2L+1)]^{\frac{1}{2}}$$

$$\times i^{L-L'} \langle J\sigma | L\ 1\ 0\ \sigma \rangle \quad \langle J\sigma | L'\ 1\ \sigma-\sigma'\sigma' \rangle \quad Y_{L'}^{\sigma-\sigma'}(\theta,0)\ M_{L'L}^{J} \tag{4-16}$$

If we require parity conservation and reciprocity (a weak form of time reversal symmetry), the scattering amplitudes satisfy

$$f_{-\sigma'-\sigma}(\theta) = (-1)^{\sigma-\sigma'} f_{\sigma'\sigma}(\theta) \tag{4-17}$$

so that the matrix f may be written in the form

$$f_{\sigma'\sigma} = \begin{pmatrix} A & B & C \\ D & E & -D \\ C & -B & A \end{pmatrix} \tag{4-18}$$

where the order of σ or σ' is 1, 0, -1. Only four of these amplitudes are independent; it can be shown that they satisfy the relation

$$C = (A-E) - \sqrt{2}\,(B+D) \cot\theta. \tag{4-19}$$

Explicit formulas for the scattering amplitudes are given in the Appendix. The amplitudes A-E are printed by the AMPRINT command, and written in machine-readable form by the AMPOUT command with option 2 = 1 or 2.

If option 2 = 3 or 4 for the AMPOUT command, the amplitudes are transformed into center-of-mass helicity coordinates before they are written. This is accomplished by rotating the coordinate system for the final-state spins by $\theta_{C.M.}$ about the y axis:

$$F_{\sigma'\sigma}(\theta) = \sum_{\sigma''} d^{1}_{\sigma''\sigma'}(0)\ f_{\sigma''\sigma}(\theta) \tag{4-20}$$

where $F_{\sigma'\sigma}(\theta)$ denote the helicity scattering amplitudes, and the quantities $d^{1}_{\sigma''\sigma}(\theta)$ are y-axis rotation matrices for spin-1 particles, as defined in ref. [18]).

4.4 The Observables: The cross section and the analyzing powers are given by[18]:

$$\sigma(\theta) = \frac{1}{3}\,\mathrm{Tr}(ff^{\dagger})$$

$$T_{kq}(\theta) = \frac{\mathrm{Tr}(f\tau_{kq}f^{\dagger})}{\mathrm{Tr}(ff^{\dagger})} \qquad (4\text{-}21)$$

where the matrix f is given by (4-16). The tensor operators τ_{kq} are defined in ref.[14]). Their representation in the usual spin space is given in terms of Clebsch-Gordon coefficients by[19])

$$\langle m'|\tau_{kq}|m\rangle = (2k+1)^{1/2}\,\langle s\ m'|s\ k\ m\ q\rangle \qquad (4\text{-}22)$$

where s = 1 for deuterons. Explicit formulas for the cross section and analyzing powers (4-21) in terms of the amplitudes A-E (4-18) are given in the Appendix.

According to the Madison convention[14]), the polarization of the outgoing particles should be referred to a coordinate system in which $\hat{z}$ is along $\underline{k}_{out}$. If $\underline{k}_{out}$ is in the center-of-mass system, then the polarizations of the scattered particles are given by

$$t'_{kq} = (-1)^{K+q}T_{kq} \qquad (4\text{-}23)$$

where the prime indicates the "outgoing" coordinate system.

Hooton and Johnson[20]) showed that a coordinate system in which the z axis is along $\underline{k}_{in} + \underline{k}_{out}$ may be especially useful for isolating the effects of the tensor potentials. The tensor analyzing powers T_{2q} (or polarizations $\bar{t}_{2q}$) referred to this coordinate system are printed under the heading "Johnson Coordinates" whenever "extra angles" are requested (NANGL>0). They are given by:

$$T_{2q} = \sum_{q'=-2}^{2} d^{(2)}_{q'q}(\theta/2)T_{2q'}$$

$$\bar{t}_{2q} = (-1)^{q}\,T_{2q}, \qquad (4\text{-}24)$$

Explicit formulas are given in the Appendix.

4.5. Potential Matrix Elements: The potential matrix elements $\langle JL'|V|JL\rangle$ in eq. (4-5) are defined as:

$$\langle JL'|V|JL\rangle \equiv \int' d\Omega \, \mathcal{Y}^{M}_{JL'S}(\Omega)^{*} \, V(r) \, \mathcal{Y}^{M}_{JLS}(\Omega) \tag{4-25}$$

where $\mathcal{Y}^{M}_{JLS}$ is given in (4-4) and V(r) is given in (4-1). The symbol $\int'$ implies integration over both spin and angle variables. The matrix elements are independent of M because of rotational invariance.

The derivation of the relevant matrix elements (using (4-25) and eqs. (1-5) of ref. 1) is fairly straightforward, but tedious -- so tedious, in fact, that every published list I have seen contains at least one error. I re-derived the T_r and T_p matrix elements, and Lynn Knutson and R.C. Johnson re-derived them independently. The results agree, and are given in Table II.

TABLE II

POTENTIAL MATRIX ELEMENTS

	J=L+1	J=L	J=L-1
$\langle JL\|\underline{L}\cdot\underline{S}\|JL\rangle$	L	-1	$-(L+1)$
$\langle JL\|T_L\|JL\rangle$	$\frac{1}{6}L(2L-1)$	$-\frac{1}{6}(2L-1)(2L+3)$	$\frac{1}{6}(L+1)(2L+3)$
$\langle JL\|T_r\|JL\rangle$	$-\frac{1}{3}\frac{L}{(2L+3)}$	$\frac{1}{3}$	$-\frac{1(L+1)}{3(2L-1)}$
$\langle JL\|T_p\|JL\rangle$	$\frac{1}{3}\frac{L}{(2L+3)}\nabla^2$	$-\frac{1}{3}\nabla^2$	$\frac{1(L+1)}{3(2L-1)}\nabla^2$

$$\nabla^2 = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{L(L+1)}{r^2}$$

$$\langle J\ J-1|T_r|J\ J+1\rangle = \langle J\ J+1|T_r|J\ J-1\rangle = \frac{[J(J+1)]^{1/2}}{(2J+1)}$$

$$\langle J\ J-1|T_p|J\ J+1\rangle = -\frac{[J(J+1)]^{1/2}}{(2J+1)}\left[\frac{d^2}{dr^2} + \frac{(2J+3)}{r}\frac{d}{dr} + \frac{J(J+2)}{r^2}\right]$$

$$\langle J\ J+1|T_p|J\ J-1\rangle = -\frac{[J(J+1)]^{1/2}}{(2J+1)}\left[\frac{d^2}{dr^2} - \frac{(2J-1)}{r}\frac{d}{dr} + \frac{(J-1)(J+1)}{r^2}\right]$$

The matrix elements in table II do not contain any radial dependence, nor do they include the factors r and r^{-1} on the right side of eq. (4-5). These factors do not commute with the T_p operator. When the complete radial dependence is included (using the T_{pUp} formula discussed in Sec. 3), the resulting matrix elements are given by:

$$r\langle JL|T_{pUp}|JL\rangle r^{-1} = -\langle JL|T_r|JL\rangle \left[U\frac{d^2}{dr^2} + U'\frac{d}{dr} + \frac{1}{2r}U' - \frac{L(L+1)}{r^2}U\right]$$

$$r\langle J\ J-1|T_{pUp}|J\ J+1\rangle r^{-1}$$

$$= -\frac{[J(J+1)]^{1/2}}{(2J+1)}\left[U\frac{d^2}{dr^2} + \left(U' + \frac{(2J+1)}{r}U\right)\frac{d}{dr} + \frac{(J+1)}{r}U' + \frac{(J-1)(J+1)}{r^2}U\right] \qquad (4\text{-}26)$$

$$r\langle J\ J+1\ |T_{pUp}|J\ J-1\rangle\ r^{-1}$$

$$= -\frac{[J(J+1)]^{1/2}}{(2J+1)}\left[U\frac{d^2}{dr^2} + \left(U' - \frac{(2J+1)}{r}U\right)\frac{d}{dr} - \frac{J}{r}U' + \frac{J(J+2)}{r^2}U\right]$$

The "reciprocity" condition (i.e. the requirement that the S matrix be symmetric) is equivalent to the requirement that the Wronskian between any two solution vectors $\underline{u}$ and $\underline{\tilde{u}}$ of (4-5) must disappear; i.e.

$$W \equiv \int_0^{r_m} (\underline{u}\cdot\underline{\tilde{u}}' - \underline{\tilde{u}}\cdot\underline{u}')dr = \int_0^{r_m} (\underline{u}\cdot\underline{V}\underline{\tilde{u}} - \underline{\tilde{u}}\ \underline{V}\ \underline{u})\ dr = 0 \qquad (4\text{-}27)$$

where I have changed to a matrix notation for eq. (4-5), and primes denote differentiation with respect to r. When the potential matrix V contains derivative operators, the usual implication that V must be symmetric does not hold. It can be shown by direct substitution that the T_p potential matrix defined by (4-26) satisfies the reciprocity condition (4-27).

5. Numerical Methods

The differential equation (4-5), written in matrix notation, takes the general form

$$[1 - \underset{\sim}{V}_2(r)]\ \underline{Y}''(r) - \underset{\sim}{V}_1(r)\underline{Y}'(r) + [1 - \underset{\sim}{V}_o(r)]\underline{Y}(r) = 0 \qquad (5\text{-}1)$$

where $\underset{\sim}{y}$ is the solution vector and $\underset{\sim}{V}_o$, $\underset{\sim}{V}_1$, and $\underset{\sim}{V}_2$ are the coefficients of 1, d/dr, and d^2/dr^2 respectively, in the potential matrix. The matrices $\underset{\sim}{V}_1$ and $\underset{\sim}{V}_2$ are diagonal if a T_p potential is present; otherwise, they are zero. The matrix $\underset{\sim}{V}_o$ is diagonal if neither a T_r nor a T_p potential is present.

For general 3-by-3 matrices $\underset{\sim}{V}_i(r)$, the most general regular solution of (5-1) is a linear combination of three independent vector functions $\underset{\sim}{y}(r)$, for a total of nine functions $y_{L'I}(r)$ (where $L' = J, J\pm1$ is the orbital angular momentum and I denotes three independent solutions). Because of parity conservation, the system can be decomposed into a single uncoupled equation for $L' = J$, plus a 2-by-2 system for $L' = J\pm1$, so only five functions are really necessary. However, for notational convenience, the system will be treated as a full 3-by-3 system in the discussion below.

The method used by DDTP to solve (5-1) depends on whether or not a T_p potential is present. In the absence of a T_p potential, the first-derivative term disappears, enabling us to use a relatively fast, efficient algorithm known as the Cowell method[21]). If a T_p potential is present, a somewhat slower predictor-corrector algorithm due to Hamming[3]) is used.

5.1. Starting Values: At small radii, the regular solutions of (5-1) are given approximately by

$$y_{L'I}(r) \approx \alpha_{L'I}\, r\, j_{L'}(\tilde{k}r) \qquad (5\text{-}2)$$

where $\alpha_{L'I}$ is an arbitrary normalization, $j_{L'}$ is a spherical Bessel function and $\tilde{k}$ is a complex local wave number given by

$$\tilde{k} = k_A \left(1 - V_c(r)/E_{CM}\right)^{1/2} \qquad (5\text{-}3)$$

where $k_A = p_A/\hbar$ is the asymptotic wave number. The first term in a series approximation[22]) for j_L is sufficiently accurate except for $L' = 0$, where two terms are used.

For low partial waves, integration starts at $r = 2h$. For higher partial waves, the starting radius is chosen where $j_{L'}(kr) \approx 10^{-8}$.

The normalizations $\alpha_{LL'}$ are arbitrary, except for the requirement that the three solutions must be linearly independent. A unit matrix satisfies that criterion; i.e. $\alpha_{L'I} = 1$ for $(L',I) = (J,1)$, $(J-1,2)$, and $(J+1,3)$ and $\alpha_{L'I} = 0$ otherwise.

5.2. The Cowell Method: In the absence of a T_p potential, (5-1) reduces to the form

$$\underline{y}''(r) = \underset{\sim}{V}(r)\underline{y}(r). \tag{5-4}$$

The Cowell method[21] and its variants are based on the following relationship between a function and its second derivative at three equidistant points:

$$\begin{aligned}[1 - h^2 \underset{\sim}{V}(r+h)/12]\underline{y}(r+h) &= [2 + 5h^2 \underset{\sim}{V}(r)/6]\underline{y}(r) \\ &- [1 - h^2\underset{\sim}{V}(r-h)/12]\ \underline{y}(r-h) - h^6\, y^{(6)}(\xi)/240\end{aligned} \tag{5-5}$$

where the last term is the truncation error. Once $\underline{y}(r-h)$ and $\underline{y}(r)$ are known, $\underline{y}(r+h)$ can be calculated by a matrix inversion.

Instead of solving (5-5) directly, DDTP uses a "subtracted" algorithm which reduces the roundoff error and increases the speed of the calculation. Define the quantities

$$\begin{aligned}\underline{y}_n &\equiv \underline{y}\ (nh) \\ \underset{\sim}{V}_n &\equiv \underset{\sim}{V}\ (nh) \\ \underline{A}_n &\equiv [1 - h^2\ V_n/12]\underline{y}_n \\ \underline{D}_n &\equiv \underline{A}_n - \underline{A}_{n-1}\end{aligned} \tag{5-6}$$

where h is the step size. Then (5-3) can be solved in the following steps:

$$\begin{aligned}\underline{D}_{n+1} &= \underline{D}_n + h^2 \underset{\sim}{V}_n \underline{y}_n \\ \underline{A}_{n+1} &= \underline{A}_n + \underline{D}_{n+1} \\ \underline{y}_{n+1} &= [1 - h^2\ \underset{\sim}{V}_{n+1}/12]^{-1}\ \underline{A}_{n+1}.\end{aligned} \tag{5-7}$$

Roundoff errors are minimized by strictly avoiding situations in which two numbers of approximately equal size are subtracted.

5.3. The Hamming Predictor-Corrector Method: When a T_p potential is present, the second-order system (5-1) is treated as a first-order system with twice as many elements:

$$\underset{\sim}{z}(r) \equiv \begin{pmatrix} \underset{\sim}{y}(r) \\ \underset{\sim}{y}'(r) \end{pmatrix}$$

$$\underset{\sim}{V}(r) \equiv \begin{pmatrix} 0 & 1 \\ [1-\underset{\sim}{V}_2]^{-1} & [\underset{\sim}{V}_0-1] \quad [1-\underset{\sim}{V}_2]^{-1} \quad \underset{\sim}{V}_1 \end{pmatrix} \tag{5-8}$$

$$\underset{\sim}{z}'(r) = \underset{\sim}{V}(r)\underset{\sim}{z}(r).$$

The Hamming predictor-corrector method[3]) was chosen to solve (5-8) because it is stable, accurate, and relatively efficient, because it includes a mechanism to control roundoff error, and because a subroutine (called DEPC) using this method was available in the program library of the Madison Academic Computing Center[4]). The classical fourth-order Runge-Kutta method[2,3]) is used to calculate z and z' at the first four points. For subsequent points, the following steps are used:

Predictor: $$\tilde{\underset{\sim}{p}}_{n+1} = \underset{\sim}{z}_{n-3} + (4h/3)\ (2\underset{\sim}{z}'_n - \underset{\sim}{z}'_{n-1} + 2\underset{\sim}{z}_{n-2}) \tag{5-9a}$$

Modified predictor: $$\underset{\sim}{p}_{n+1} = \tilde{\underset{\sim}{p}}_{n+1} + \frac{112}{121}\ (\tilde{\underset{\sim}{z}}_n - \tilde{\underset{\sim}{p}}_n) \tag{5-9b}$$

$$\underset{\sim}{p}'_{n+1} = \underset{\sim}{V}_{n+1}\ \underset{\sim}{p}_{n+1}$$

Corrector: $$\tilde{\underset{\sim}{z}}_{n+1} = \frac{1}{8}\ (9\underset{\sim}{z}_n - \underset{\sim}{z}_{n-2}) + (3h/8)\ (\underset{\sim}{p}'_{n+1} + 2\underset{\sim}{z}'_n - \underset{\sim}{z}'_{n-1}) \tag{5-9c}$$

Modified corrector: $$\underset{\sim}{z}_{n+1} = \tilde{\underset{\sim}{z}}_{n+1} - \frac{9}{121}\ (\tilde{\underset{\sim}{z}}_{n+1} - \tilde{\underset{\sim}{p}}_{n+1}). \tag{5-9d}$$

The truncation errors in (5-9a) and (5-9c) are

$$\Delta_p = (14/45)h^5\ y^{(5)}(\xi) \tag{5-10a}$$

and

$$\Delta_c = -(9/121)h^5\ y^{(5)}(\xi) \tag{5-10b}$$

respectively. However, the "modifying" steps (5-9b,d) make this effectively

a fifth-order method.

After each integration step, the estimated magnitude of the local truncation error

$$\underline{e}_{n+1} = \frac{9}{121} |\underline{z}_{n+1} - \underline{\tilde{p}}_{n+1}| \tag{5-11}$$

is calculated. Whenever the expression $e_{n+1}/\max(z_{n+1},1)$ exceeds a specified tolerance, the step size is reduced by a factor of two. Conversely, whenever e_{n+1} is sufficiently small, the step size is doubled. In DDTP, the tolerance is given by 10^{-I}, where I = option 4 on the CALCULATE card. The default value of I=5 has been found to be sufficient for several test cases.

In the future, if speed is critical (e.g. if a search is added), it would probably pay to replace this predictor-corrector method by a one-step method based on an approximate matrix inversion.

5.4. The Matching: At the matching radii, the wave functions must satisfy eq. (4-6), which takes the form

$$\sum_I N_{LI} y_{L'I}(r_m) = u_{JL'L}(r_m) = e^{-i\omega_{L'}} M^J_{L'L} [G_{L'}(kr_m) + iF_{L'}(kr_m)] + \delta_{L'L} e^{i\omega_L} v_L(kr_m). \tag{5-12}$$

Equations of the form (5-12) must be satisfied at each of two matching radii r_m (or, equivalently, the functions and their first derivatives must satisfy (5-12) at a single radius). This system can then be solved for the normalizations N_{LI} and the transition matrix elements $M^J_{L'L}$.

The normalizations N_{LI} and the normalized wave functions $u_{JL'L}(r)$ are printed by the WFPRINT command, and the transition matrix elements $M^J_{L'L}$ are printed by DELPRINT, with option 1 = 0 or 1. The Coulomb wave functions F_L, and G_L, and the Coulomb matrix elements $e^{i\omega_L}$ are printed if Option 5 on the POTENTIAL card is positive. Refer to the CALCULATE command for instructions for printing the unnormalized wave functions $y_{L'I}$.

APPENDIX: FORMULAS

A.1. Scattering Amplitudes: The scattering amplitudes (equation 4-16) are given by:

$$A(\theta) \equiv f_{11}(\theta) = f_c(\theta) + \frac{1}{2k}\sum_L \{-[(L-1)L]^{\frac{1}{2}} M_{L\ L-2}^{L-1} - [(L+2)(L+1)]^{\frac{1}{2}} M_{L\ L+2}^{L+1}$$

$$+ (L+2)M_{L\ L}^{L+1} + (2L+1)M_{L\ L}^{L} + (L-1)M_{L\ L}^{L-1}\}P_L^0(\theta)$$

$$B(\theta) \equiv f_{10}(\theta) = \frac{1}{\sqrt{2}k}\sum_L \{[\frac{L'-1}{L'}]^{\frac{1}{2}} M_{L\ L-2}^{L-1} - [\frac{L+2}{L+1}]^{\frac{1}{2}} M_{L\ L+2}^{L+1}$$

$$- M_{L\ L}^{L+1} + M_{L\ L}^{L-1}\}P_L^1(\theta)$$

$$C(\theta) \equiv f_{1-1}(\theta) = \frac{1}{2k}\sum_L \{-[\frac{1}{(L-1)L}]^{\frac{1}{2}} M_{L\ L-2}^{L-1} - [\frac{1}{(L+2)(L+1)}]^{\frac{1}{2}} M_{L\ L+2}^{L+1}$$

$$+\frac{1}{(L+1)} M_{L\ L}^{L+1} - [\frac{2L+1}{L(L+1)}] M_{L\ L}^{L} + \frac{1}{L} M_{L\ L}^{L-1}\}P_L^2(\theta)$$

$$D(\theta) \equiv f_{01}(\theta) = \frac{1}{\sqrt{2}k}\sum_L \{[\frac{L-1}{L}]^{\frac{1}{2}} M_{L\ L-2}^{L-1} - [\frac{L+2}{L+1}]^{\frac{1}{2}} M_{L\ L+2}^{L+1}$$

$$+ [\frac{L+2}{L+1}] M_{L\ L}^{L+1} - [\frac{2L+1}{L(L+1)}] M_{L\ L}^{L} - [\frac{L-1}{L}] M_{L\ L}^{L-1}\}P_L^1(\theta)$$

$$E(\theta) \equiv f_{00}(\theta) = f_c(\theta) + \frac{1}{k}\sum_L \{[(L-1)L]^{\frac{1}{2}} M_{L\ L-2}^{L-1} + [(L+2)(L+1)]^{\frac{1}{2}} M_{L\ L+2}^{L+1}$$

$$+ (L+1) M_{L\ L}^{L+1} + L M_{L\ L}^{L-1}\}P_L^0(\theta) \qquad \text{(A-1)}$$

where $P_L^M(\theta)$ is an associated Legendre function[17]. The index of the sums is actually the outgoing orbital angular momentum L', but the primes were omitted to avoid clutter.

A.2. Observables: The cross section and analyzing powers (eq. 4-21) for a coordinate system in which $\hat{z}$ is along $\underline{k}_{in}$ and $\hat{y}$ is along $\underline{k}_{in} \times \underline{k}_{out}$ are given by:

$$
\begin{aligned}
3\sigma &= 2|A|^2 + 2|B|^2 + 2|C|^2 + 2|D|^2 + |E|^2 \\
3\sigma i T_{11} &= \sqrt{6}\ \mathrm{Im}\ [B^*(A-C) + E^*D] \\
3\sigma T_{20} &= \sqrt{2}\ (|A|^2 - 2|B|^2 + |C|^2 + |D|^2 - |E|^2) \qquad \text{(A-2)} \\
3\sigma T_{21} &= -\sqrt{6}\ \mathrm{Re}\ [B^*(A-C) + E^*D] \\
3\sigma T_{22} &= \sqrt{3}\ [2\mathrm{Re}(A^*C) - |D|^2].
\end{aligned}
$$

The analyzing powers in the Johnson coordinate system (eq. 4-24) are given by

$$
\begin{aligned}
i\bar{T}_{11} &= iT_{11} \\
\bar{T}_{20} &= \frac{1}{4}(1 + 3\cos\theta)T_{20} - \sqrt{\frac{3}{2}}\sin\theta T_{21} + \frac{1}{2}\sqrt{\frac{3}{2}}(1-\cos\theta)\,T_{22} \\
\bar{T}_{21} &= \frac{1}{2}\sqrt{\frac{3}{2}}\sin\theta T_{20} + \cos\theta T_{21} - \frac{1}{2}\sin\theta T_{22} \\
\bar{T}_{22} &= \frac{1}{4}\sqrt{\frac{3}{2}}(1-\cos\theta)T_{20} + \frac{1}{2}\sin\theta T_{21} + \frac{1}{4}(\cos\theta + 3)T_{22}
\end{aligned}
$$

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