TECHNICAL REPORT (UTNT-1)

JPWKB

User's Manual

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1. INTRODUCTION

The purpose of this note is to give a brief description of a computer program called JPWKB, which is an extension/modification of a program called JUPITER-1 (JP1) that was written sometime ago[1]. The program JP1 was written and used to perform coupled-channel (CC) calculations[2] to obtain cross sections of inelastic scattering (primarily) of light ions by various nuclei. To use JP1 for the inelastic scattering between heavy ions is not very appropriate, however, because there the inclusion of the Coulomb excitation process is inevitable, and the calculations become very time consuming. The new program JPWKB calculates the effect of the Coulomb excitation much faster than does JP1, because of the use of a technique developed recently by Alder and Pauli[3,4].

The essential method of the JPWKB calculation is to divide the whole radial region into two parts: (i) the interior in which the radius parameter r is less than the separation radius R_S, and both nuclear and Coulomb interactions have to be taken into account, and (ii) the exterior region where $r > R_S$ and only Coulomb interactions need be considered. In the interior region, the CC equations are solved exactly--in our case JP1 is used in its original form. In the exterior region, however, a specific form of WKB approximation of Alder and Pauli[3] is used (hence the name JPWKB), which allows the calculations to be made very fast without losing needed accuracy.

Detailed accounts of CC calculations were given earlier[1,2]. We thus review very briefly, in Sec. 2, the technique of Alder and Pauli and then discuss how to integrate this technique into our original formulation.

The basic structure of JPWKB is discussed in Sec. 3, while explanations of how to prepare input data are given in Sec. 4. The present note was prepared with the assumption that the reader is familiar with our previous publications[1,2].

2. FORMALISM

2.1) S-matrix

We start with the S-matrix, $S^{(1)}$, obtained by solving the CC equation in the interior region. This $S^{(1)}$ is exactly the same as that produced by the original program JP1. The total S-matrix, S, can be given as

$$S = U^T S^{(1)} U , \tag{1}$$

where the transformation matrix U contains all the effects of the Coulomb excitation in the exterior region. In what follows, we describe how to calculate U.

In the external region, it is assumed that the radial part of the partial wave in the channel q is given as[3]

$$u_q(r) = \frac{1}{\sqrt{k_q}} \left(h_q^{(-)} a_q^{(-)} - h_q^{(+)} a_q^{(+)}\right) , \tag{2a}$$

with

$$h_q^{(\pm)} = G_q \pm i F_q , \tag{2b}$$

where k_q is the wave number, while G_q and F_q are the regular and irregular Coulomb wave functions, respectively. Since the spin-orbit interaction is not important for heavy-ion scattering, it is not necessary to take into account explicitly the spin of the projectiles. The channel index q can then be specified essentially by the spin, I_n, of the nuclear state n, and the orbital angular momentum, ℓ; i.e. $q = (I_n, \ell)$.

The CC equation for $a_q^{(\pm)}$ is obtained by inserting Eq. (2a) into the CC equation for $u_q(r)$ (see Eq. (25) of ref. 2) and multiplying either by $h^{(+)}$ or $h^{(-)}$ from left. For the thus obtained CC equations, the following three approximations are now made: (i) $h^{(\pm)}$ are approximated by those obtained by the WKB Approximation; (ii) the second derivative of $a_q^{(\pm)}$ with respect to r is neglected; and (iii) the rapidly oscillating terms like $h^{(-)}h^{(-)}$ and $h^{(+)}h^{(+)}$ are neglected. It is then easy to see that $a_q^{(\pm)}$ satisfies[3]

$$\frac{da_q^{(\pm)}}{dr} = \mp \sum_{q'} V_{qq'}^{(\pm)} a_{q'}^{(\pm)}, \tag{3}$$

where

$$V_{qq'}^{(\pm)} = \frac{1}{2i} \frac{p_q p_{q'}}{\sqrt{k_q k_{q'}}} v_{qq'}^{J} e^{\pm i(\phi_q - \phi_{q'})}, \tag{4}$$

$$p_q = \left[1 - (2\eta_q/k_q r) - \ell(\ell+1)/k_q^2 r^2\right]^{-1/4}, \tag{5a}$$

and

$$\phi_q = k_q r/p_q^2 + \eta_I \log\left[\sqrt{\eta_I^2 + \ell(\ell+1)}/(k_q r - \eta_q + \sqrt{k_q r}/p_q)\right]$$

$$- \sqrt{\ell(\ell+1)} \cos^{-1}\left[\eta_q/\sqrt{\eta_I^2 + \ell(\ell+1)} + \ell(\ell+1)/k_q r\sqrt{\eta_I^2 + \ell(\ell+1)}\right], \tag{5b}$$

with η_q being the Sommerfeld parameter. $v_{qq'}^{J}$ in Eq. (4) is exactly the same as the interaction matrix element given by Eq. (27) of ref. 2, except that no nuclear interaction is involved in Eq. (4). Since $a_q^{(\pm)}$ are slowly varying, Eq. (3) can be integrated in large steps, which is the origin of very fast integration.

We note here that $V_{qq'}^{(\pm)}$ has a property that

$$V_{qq'}^{(\pm)*} = \mp V_{qq'}^{(\mp)}, \tag{6a}$$

which results in

$$a_q^{(-)*} = a_q^{(+)} . \tag{6b}$$

In other words, $a_q^{(+)}$ and $a_q^{(-)}$ are not independent from each other, and thus Eq. (4) needs be solved only for one set (rather than both sets) of the double signs. In JPWKP, the coding is made so that Eq. (4) is solved for $a_q^{(-)}$. The integration is carried out n times (n is the dimension of the CC equations) from $r = R_s$ to $r = R_M$, the matching radius, with n-different starting values given as

$$a_{qk}^{(-)}(r = R_s) = \delta_{qk}, \quad q = 1, 2, \ldots n . \tag{7}$$

To distinguish the n independent solutions, an additional suffix k is attached to $a_q^{(-)}$, defining $a_{qk}^{(-)}$.

The solution $u_{qq_o}(r)$ which corresponds to the boundary condition at $r = R_M$, i.e., the condition that

$$u_{qq_o}(r) \to \frac{1}{\sqrt{k_q}} \left(h_q^{(-)} \delta_{qq_o} - h_q^{(+)} S_{qq_o}\right) , \tag{8}$$

may be put in the form

$$u_{qq_o} = \frac{1}{\sqrt{k_q}} \sum_{qk} \left(h_q^{(-)} a_{qk}^{(-)} \alpha_{kq_o}^{(-)} - h_q^{(+)} a_{qk}^{(+)} \alpha_{kq_o}^{(+)}\right) . \tag{9}$$

The unknown coefficients $\alpha_{kq_o}^{(\pm)}$ are determined by the condition (8), as well as the requirement that $u_{qq_o}(r)$ matches smoothly to the interior solutions at $r = R_s$. The result is given, in the matrix form, as

$$\alpha^{(-)} = a^{(-)}(r \to \infty) \equiv U, \tag{10a}$$

$$\alpha^{(+)} = S^{(1)} \alpha^{(-)} = S^{(1)} U . \tag{10b}$$

From Eq. (9), it is seen that the total S matrix can be written as

$$S = a^{(+)}(\infty)\ \alpha^{(+)} \tag{11}$$

Using the relations (10a) and (10b) and also the fact that $U^{+} = U$, it is easy to see that Eq. (11) is reduced to Eq. (1).

Once an S matrix is obtained, the C matrix can be calculated as

$$C = -\frac{1}{2i}(1 - S)\,. \tag{12}$$

2.2) Cross Section

In terms of the C matrix given by Eq. (12), the cross section can be expressed as

$$\frac{d\sigma}{d\Omega} = \frac{1}{(2I_o + 1)} \sum_{M_n M_{n_o}} \left| X_{M_n M_{n_o}}(\theta) \right|^2 \tag{13a}$$

where

$$X_{M_n M_{n_o}}(\theta) = \sum_{\ell\ell'} \frac{4\pi}{\sqrt{k'_n k_n}}\, \hat{\ell}'\hat{\ell}\; e^{i(\sigma_{\ell'}^{(n)} + \sigma_{\ell}^{(n_o)})}$$

$$\langle \ell I_1 O M_1 | J M_1 \rangle \langle \ell' I_n M_{\ell'}, M_n | J M_1 \rangle\; C^{J}_{\ell' I_n \ell I_1}\, Y_{\ell' M_{\ell'}}(\theta) \tag{13b}$$

2.3) Interpolation and Padé approximation

Use of the WKB approximation saves computer time dramatically. Yet the calculation is still rather time consuming because the CC equations have to be solved for a large number of partial waves. In order to speed up the calculations still more, use is made in JPWKB of two other techniques: interpolation and Padé approximation.

The "interpolation" is used to generate C matrices for higher ℓ-values for which only the Coulomb excitation effects are important. The integration of the CC equations is made for all the ℓ-values up to a certain

ℓ-value, say ℓ_o. Beyond ℓ_o the integration is carried out with a step of $\Delta\ell = 10$ and the C matrices for the ℓ-values in between are generated by the four point interpolation method.

The use of the Padé approximation is made in the following way. Noting first that the scattering amplitudes $X_{MM_o}(\theta)$ of Eq. (13) may be written as

$$X_{MM_o}(\theta) = \sum_{\ell} A_{\ell m} Y_{\ell m}(\theta) \qquad (m = M - M_o) \tag{14}$$

we extract k times from the r.h.s. a factor $1/(1-\cos\theta)$. The resultant $X_{MM_o}(\theta)$ may then be written as

$$X_{MM_o}(\theta) = \frac{1}{(1-\cos\theta)^k} \sum_{\ell} A^{(k)}_{\ell m} Y_{\ell m}(\theta), \tag{15}$$

where $A^{(k)}_{\ell m}$ is calculated from the recursion relation

$$A^{(k)}_{\ell m} = A^{(k-1)}_{\ell m} - \left[\frac{(\ell+m)(\ell-m)}{(2\ell+1)(2\ell-1)}\right]^{\frac{1}{2}} A^{(k-1)}_{\ell-1,m} - \left[\frac{(\ell+m+1)(\ell-m+1)}{(2\ell+3)(2\ell+1)}\right]^{\frac{1}{2}} A^{(k-1)}_{\ell+1,m}. \tag{16}$$

The larger is k, the smaller is the ratio $|A_{\ell+1,m}|/|A_{\ell,m}|$. Therefore if k is sufficiently large, a fairly small value of ℓ_{max} can be chosen for the upper limit of the summation in Eq. (15). In JPWKB, ℓ_{max} is given as an input data and the iteration of Eq. (16) is terminated if

$$\left|\left[\sigma^{(k+1)}(\theta) - \sigma^{(k)}(\theta)\right]/\sigma^{(k)}(\theta)\right| < 10^{-4}$$

where θ is also an input data.

In Sec. 4, an explanation is given of how to prepare the input data of JPWKB. There a sample data set is given for ^{18}O scattering (with an incident ^{18}O ion energy of E_{lab} = 50 Mev) from ^{58}Ni. The integration is carried out up to 300 fm and $\ell_o = 50$, $\ell_{max} = 200$ are used. The time required to

carry out the calculation of this example scattering is 110 sec (CP) with a CDC 6600, which is reasonably fast.

3. OUTLINE OF THE PROGRAM JPWKB

In Fig. 1 we give the flow diagram of JPWKB. As is seen, JPWKB consists of 23 subroutines, 12 of which (subroutine nos. 2-6, 8-13 and 15) are essentially the same as those of the original JP1 and the rest (subroutine nos. 1, 7, 14, and 16-23) are new. We outline below the role played by these newly added subroutines. Most of them were taken from ref. 4.

In JPWKB, use is made of OVERLAY, whose structure is seen clearly in the flow diagram of Fig. 1. The first new subroutine, JPCTRL, controls the OVERLAY structure.

The second new subroutine is JKLOOP (no.7). Note that the CC equations have to be solved for various sets of the total angular momentum J, and parity, π. The original JP1 had a JJ-K double DO-loop in subroutine CCCTRL, JJ and K standing for J and π, respectively. In JPWKB, this JJ-K loop has been moved from CCCTRL to JKLOOP. JKLOOP calls COUPLE for each set of JJ and K, where the CC equation for the interior region is solved.

In the original JP1, the integration started from the origin (r = 0), as is usually necessary for light ion scattering, where the absorption is not so strong and thus the interior of the nucleus may contribute significantly to the reaction. For heavy-ion scattering where the absorption is strong, however, there is no need to start integration at r = 0, and in JPWKB, a starting radius $r = R_i$ (=0) is fixed by the following relation:

$$R_i = \max \left\{ \begin{matrix} a_\ell - \Delta R_i \\ R_c \end{matrix} \right\} \qquad (17)$$

Here a_ℓ is the closest distance of approach for the partial wave ℓ, while R_c (the lower cutoff radius) and ΔR_i are given as input parameters. Since a_ℓ increases with increased ℓ, $R_i = a_\ell - \Delta R_i$ for beyond a certain critical value, while $R_i = R_c$ for lower ℓ values.

The separation distance R_s is determined similarly by the relation

$$R_s = \max \left\{ \begin{matrix} a_\ell + \Delta R_s \\ R_N \end{matrix} \right\}, \tag{18}$$

where R_N, the range of the nuclear potential, and ΔR_s are input data. ΔR_s is also input data.

In JP1, COUPLE calls a subroutine SMATRX in order to evaluate the S and C matrices. In JPWKB, COUPLE calls a new routine WKBCTRL (no. 14) instead, which calculates first the S-matrix, which is $S^{(1)}$ of Eq. (1), in exactly the same way as does SMATRX in JP1. WKBCTRL next prepares initial values of the amplitudes $a_{qk}^{(-)}$ (see Eq. (7)), and then calls WKBINT, where the CC equation for the exterior region, Eq. (3), is integrated by means of the RUNGE-KUTTA-GILL method. In this integration processes, four new subroutines are used, which are CMATRX, AMPDER, RMATRX and CHEKRM, which are essentially taken from ref. 4. CMATRX evaluates the Coulomb interaction matrix element $V_{qq'}^{(-)}$, given by Eqs. (4) and (5), AMPDER carries out the calculation of the right hand side of Eq. (3), obtaining the derivative of $a^{(-)}$ and then RMATRX generates the final S and C matrices, given by Eqs. (11) and (12). CHEKRM is a subroutine which tests the convergence of the integration; i.e., it compares the S matrices evaluated at two successive points. If the fractional change becomes less than 10^{-4}, the integration is terminated.

The last three subroutines JP1AMP, CROSPL and LEGNDR called from JP1CTRL replace the routines XSEC, CROSPL, CMMMFC and BFCTOR of the original

JP1, and are used to calculate the cross sections. JP1AMP calculates X_{MM_o} of Eq. (13) and then the cross section is calculated is JP1CRS. LEGNDR calculates $Y_{\ell m}$ in Eq. (13b).

The original JP1 allowed one to carry out calculations for various types of couplings. What type of the coupling is chosen is controlled by the input data, INTYPE and INTMAX. For instance, if one wants to carry out a simple $0^+ - 2^+$ coupling calculation for even vibrational nuclei, one inputs 2 and 1, respectively, for INTYPE and INTMAX. In JPWKB, in its present form, the choice of INTYPE and INTMAX is more limited than it is in JP1. Only the following three cases are allowed:

1. INTYPE = 2 and INTMAX = 1. $0^+ - I^\pi$ coupling. In the original JP1 the $0^+ - 2^+ - 3^-$ type calculations were also possible under this choice of INTYPE = 2. This type of calculation, however, is not possible in the present JPWKB.
2. INTYPE = 3. $0^+ - 2^+ - I_1 - I_2 - I_3$ type calculations, where I_i is the i-th member of the two-phonon states of the quadrupole vibration. The number of two-phonon states to be considered is arbitrary. INTMAX does not need to be input in this case, since it is automatically set in the program to be 7. (cf. p. 29-31 of ref. 1 for more detail.)
3. INTYPE = 4. $0^+ - 2^+ - 4^+ \ldots$ coupling calculation for the deformed nuclei. So far only up to the Y_4 deformation can be included. INTMAX should be 1 or 2 according to the Y_2 deformation only, or both Y_2 and Y_4 deformations are included.

4. INPUT DATA

The input data of JPWKB are very much the same as those of JP1. Therefore, it is convenient to start with the original card deck of JP1 to explain how one can prepare the input data deck for JPWKB. In page 16, a sample input data set is given of the scattering of E_{lab} = 50 Mev ^{18}O from ^{58}Ni. A simple $0^+ - 2^+$ coupling is assumed in this example.

The original input data of JP1 consists of 19 cards. Since in JPWKB, KTRL(8) = 0 is assumed (no polarization in the incident channel), Cards 11 - 16 are not needed. Therefore, there should be 13 cards.

Card-1 and -2: KTRL(N), N = 1 - 28, are read in. In addition to KTRL(N)'s that are used in JP1, KTRL(2) and KTRL(14) are used in JPWKB. If KTRL(2) = 1, the nuclear radius R_o is calculated according to

$$R_o = r_o(A_T^{\frac{1}{3}} + A_P^{\frac{1}{3}}) \qquad (19)$$

instead of $R_o = r_o A_T^{\frac{1}{3}}$, usually used for the light-ion reaction, where A_T and A_P are the target and projectile masses, respectively, and r_o is the radius parameter. If KTRL(14) = 1, the Coulomb excitation effects in the exterior region is neglected. In this case the calculation is exactly the same as that of the JP1.

Card-3: KEXCOM(N), N = 1 - 14, are read in from this card. In JP1 KEXCOM(1) is not used, but in JPWKB it is used to determine R_c of Eq. (17) as

$$R_c = \text{XMESB} * \text{KEXCOM(1)},$$

where XMESB is the mesh size read in from the Card-9. In the example data of Table I, KEXCOM(1) has 20, which is the value determined from our experience. In the original JP1, KEXCOM(2) is used to fix the matching radius R_m. (This

R_m corresponds in the present JPWKB to R_s, the separation distance between the interior and exterior region.) In JPWKB, this KEXCOM(2) is used to determine the nuclear range, R_N, in Eq. (18). The use of the rest of KEXCOM is the same as that in the original JP1.

Card-4 and -5: KTLOUT(N), N = 1 - 28, are read in and used to control the intermediate outputs. KTLOUT(N) is set equal to 1, such outputs are generated in various subroutines, according to the values of N, as summarized in the Table given below.

N	SUBROUTINE	N	SUBROUTINE	N	SUBROUTINE
3	JKLOOP	10	COUPLE	16	CMATRX
5	FLGLCH, FLGLNG	12	JP1AMP	17	AMPDER
6	CCCTRL	13	JP1CRS	18	RMATRX
7	POTENT	14	WKBCTR		
9	AMATRX	15	WKBINT		

Card-6 through -10: Same as in JP1 (cf., however, notes at the end of Sec. 3.)

Card-11 through -16: These cards are not needed in the card deck of JPWKB, since there KTRL(8) = 0 is always assumed.

Card-17 and -18: Same as in JP1.

Card-19: In the original JP1, VCOUPL(N), N = 1 - 10, are read in from this card. In JPWKB, this is the same, but the usage of VCOUPL(N) is somewhat different from that of JP1 as described below; when INTYPE = 2, only VCOUPL(1)-(4) are used which are respectively the transition ($\beta_{\lambda N}$ and $\beta_{\lambda C}$), and the static ($\bar{\beta}_{\lambda N}$ and $\bar{\beta}_{\lambda C}$) deformation parameters of the nuclear and Coulomb interactions respectively; i.e.

$$\text{VCOUPL(1) and (2)} = \beta_{\lambda N} \text{ and } \beta_{\lambda C},$$
$$\text{VCOUPL(3) and (4)} = \bar{\beta}_{\lambda N} \text{ and } \bar{\beta}_{\lambda C}.$$

The transition deformation parameter is the usual deformation parameter for the vibration nuclei, describing the transition strength, for instance, of the one-phonon excitation, whereas the static deformation is the deformation parameter related to the static moment of the one-phonon state; i.e.

$$\bar{\beta}_{\lambda C} = \sqrt{\frac{5}{12ZeR^2}} \sqrt{\frac{(2\lambda+1)(\lambda+1)(2\lambda+3)}{\lambda(2\lambda+1)}}\, Q_\lambda^{(c)}$$

where $Q_\lambda^{(c)}$ is the static λ-pole electric moment of the one phonon state of the spin λ. $\bar{\beta}_{\lambda N}$ is the corresponding deformation of the matter moment. Note that, when KTRL(2) = 1, β's are modified after being read in according to

$$\beta_{\lambda N} \rightarrow \frac{A_T^{\frac{1}{3}}}{A_T^{\frac{1}{3}} + A_P^{\frac{1}{3}}}\, \beta_{\lambda N},$$
$$\beta_{\lambda C} \rightarrow \left(\frac{A_T^{\frac{1}{3}}}{A_T^{\frac{1}{3}} + A_P^{\frac{1}{3}}}\right)^2 \beta_{\lambda C}.$$

When INTYPE = 3, besides a card for VCOUPL(1)-(10), one more card is added to read in VCOUPL(11)-(19), which correspond the values of β_{20}, β'_{00}, β_{22}, β'_{02}, β_{24}, β'_{04}, β''_{00}, β''_{02} and β''_{04} in this order. The meaning of these parameters are described in ref. 1.

When INTYPE = 4, one card is needed to read in VCOUPL(1)-(N), where N = 2*INTMAX. INTMAX can take either 1 or 2. When it is 1, only $\lambda = 2$ deformation is taken into account and we put β_{2N} and β_{2C} in VCOUPL(1) and VCOUPL(2); whereas when it is 2, both $\lambda = 2$ and $\lambda = 4$ deformations are included. VCOUPL(1)-(4) then have the values of β_{2N}, β_{2C}, β_{4N} and β_{4C}.

Card-20: This and the next one are new in JPWKB. Card-20 reads KPPADE, KTCONV, and LINTPO with FORMAT(14I5). KPPADE is the number of times that the Padé recursion procedure is applied (see Eq. (14)-(16)). KTCONV is used for defining angles that are used in checking the convergence of the Padé procedure. LINTPO is the ℓ_o-value discussed before, from which the CC equation is solved every interval of $\Delta\ell = 10$. In the example of page 16, KPPADE = 3, KTCONV = 25 and LINTPO = 50. These are all our empirical value, and may be used as a guide.

Card-21: RFTPMI, RFTPMX, and RWKBMX are read in with FORMAT(10F7.3). RFTPMI and RFTPMX presents respectively R_i and R_s in Eq. (17) and (18). RWKBMX is the upper limit of WKB integration (R_{max}). All these three values are in fm unit. The values of R_i = 7.0 fm, R_s = 7.0 fm and R_{max} = 300 fm used in the example of Table I may again be used as a guide for these parameters.

Finally, the output data are given in pages 17-20, which are generated by running the program with the input data of page 16. These output data may be used for testing the program after installation. As mentioned in Sec. 2, this run took 110 sec of CP time with a CDC 6600 computer at the University of Texas Computation Center.

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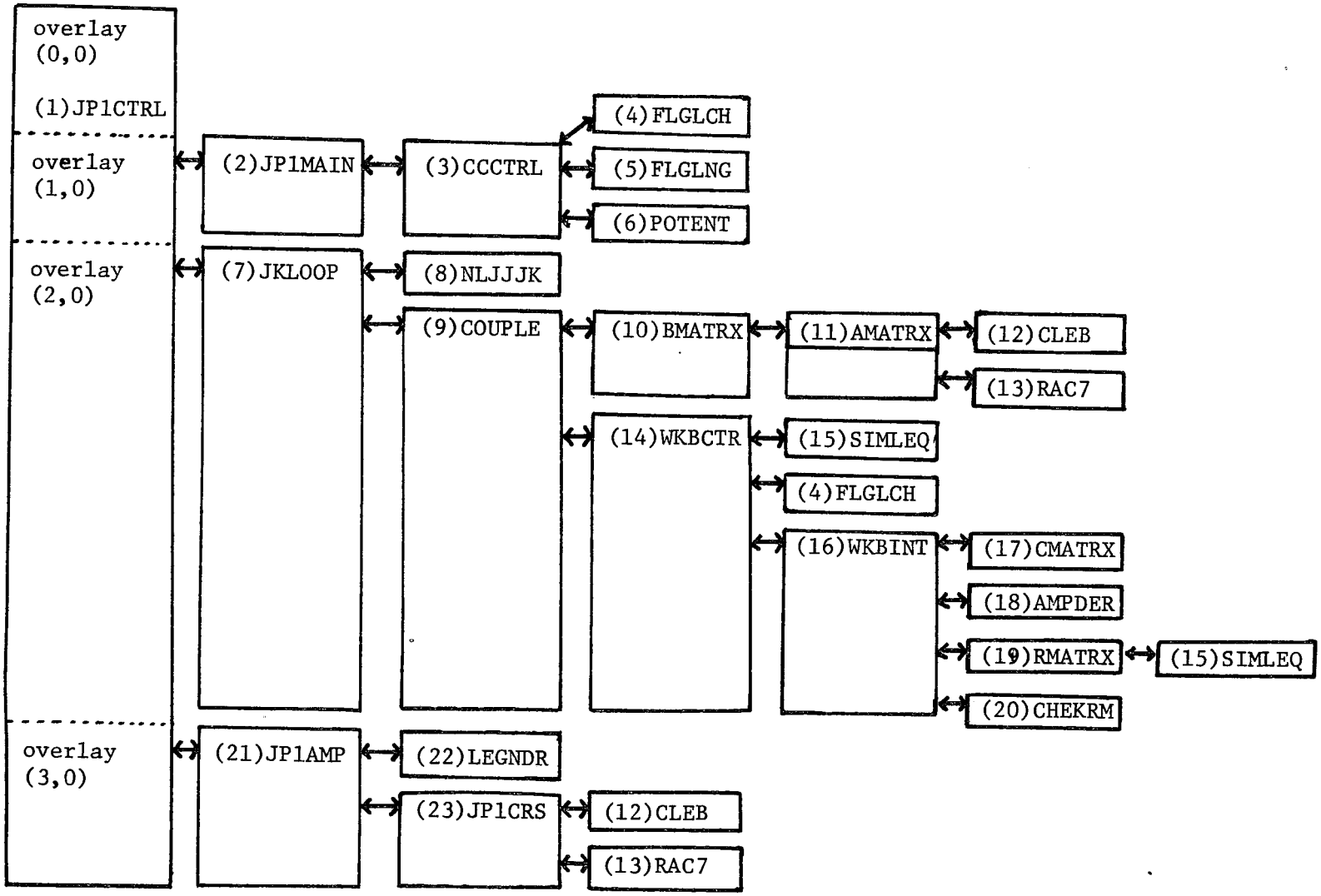

Figure 1. The Flow Diagram of JPWKB

SAMPLE INPUT DATA FOR THE SCATTERING OF ^{18}O ON ^{58}Ni

```
      1                                                    1    1        KTRL    1
                                                                         KTRL    2
 20  200                                                          203    KEXCOM  3
           2                    10                1                     KTLOUT  4
                                                                         KTLOUT  5
                                                                         EXTCOM  6
   2    2    1    0   41    2    0    0    0    1                       IICPLE  7
   0    1     0.0      2    1     1.450                                 IIREAD  8
50.0   18.0   58.0  224.0    .0125   .10                                 ELAB    9
10.0    1.0                                                              ANGLE  10
65.0    9.0    0.0    0.0    1.0    1.0    1.0                          VSX    17
 .760   .544   .760   .760  1.073  1.343  1.073  1.073  1.250           DFN    18
 .150          .150                                                     VCPLE  19
   3   25   50                                                          PADE   20
 7.0    7.0  300.0                                                      WKB    21
```

********** COUPLED CHANNEL CALCULATION **********

(ON PROGRAM JUPITOR-1)

ELAB=50.000, CHARGE=224.0, TMAS= 58.000, PMAS=18.000

```
VSX,WSX,WSF,VSO                    =  65.000   9.000   0.000   0.000
DFN,DFNW,DFNS,DFNSP                =    .760    .540    .760    .760
RZERO,RZEROW,RZEROS,RZROSP,RZEROC=   1.073   1.343   1.073   1.073   1.250
WC                                 =   1.000   1.000   1.000  -0.000  -0.000  -0.000
```

PROJECTILE SPIN=0

IIRMAX=2,INTYPE=2,INTMAX=1,BETA= .150-0.000 .150-0.000-0.000-0.000-0.000-0.000-0.000-0.000

TARGET STATES, 0 (+) AT 0.000 MEV, 2 (+) AT 1.450 MEV,

```
KTRL    =0   1  =0  =0  =0  =0  =0  =0  =0  =0  =0   1   1  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0
KEXCOM  20 200  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0 203   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0
KTLOUT  =0  =0   2  =0  =0  =0  10  =0  =0   1  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0  =0
EXTCOM     =0.00     =0.00     =0.00     =0.00     =0.00     =0.00     =0.00     =0.00     =0.00     =0.00     =0.00
XMES1= .01250    XMES2= .10000    UNIT=AML
```

```
KPPADE,KTCONV,LINTPO     =    3   25   50
RFTPMI,RFTPMX,SKBMX      =   7.00    7.00  300.00
```

```
ECM         3,81579E+01     3,67079E+01
WN          5,00723E+00     4,91117E+00
WNINI       8,23297E+00     8,17490E+00
ETA         2,11618E+01     2,15757E+01
SIGM0       2,27413E-01     1,49484E+00

JJJMAX,KEX14,NXCPLE,NXMAX=  201   203   200   200 XMAX,XBAR=  2,0000000E+01  6,9655062E+00


WOODS-SAXON POTENTIAL

X
 2,5000E-02  2,0002E-01  1,0000E+00  2,0000E+00  3,0000E+00  4,0000E+00  5,0000E+00  6,0000E+00  7,0000E+00  8,0000E+00
 9,0000E+00  1,0000E+01  1,1000E+01  1,2000E+01  1,3000E+01  1,4000E+01  1,5000E+01  1,6000E+01  1,7000E+01  1,8000E+01
 1,9000E+01  2,0000E+01
VCENTR
-6,4993E+01 -6,4991E+01 -6,4975E+01 -6,4906E+01 -6,4650E+01 -6,3713E+01 -6,0448E+01 -5,0753E+01 -3,1763E+01 -1,3263E+01
-4,1825E+00 -1,1775E+00 -3,2011E-01 -8,6184E-02 -2,3142E-02 -6,2098E-03 -1,6660E-03 -4,4693E-04 -1,1989E-04 -3,2163E-05
-8,6282E-06 -2,3146E-06
VCENTI
-9,0000E+00 -9,0000E+00 -9,0000E+00 -9,0000E+00 -8,9998E+00 -8,9985E+00 -8,9903E+00 -8,9396E+00 -8,6332E+00 -7,1031E+00
-3,3600E+00 -7,7919E-01 -1,3370E-01 -2,1541E-02 -3,4340E-03 -5,4652E-04 -8,6954E-05 -1,3834E-05 -2,2012E-06 -3,5218E-07
-5,5712E-08 -8,8637E-09
VCPL1R
-5,7600E-03 -7,2510E-03 -2,0765E-02 -7,7241E-02 -2,8566E-01 -1,0342E+00 -3,4703E+00 -9,1193E+00 -1,3314E+01 -8,6541E+00
-3,2080E+00 -9,4774E-01 -2,6112E-01 -7,0556E-02 -1,8964E-02 -5,0901E-03 -1,3657E-03 -3,6637E-04 -9,8285E-05 -2,6366E-05
-7,0731E-06 -1,8974E-06
VCPL1I
-1,4808E-06 -2,0427E-06 -8,8894E-06 -5,5873E-05 -3,5117E-04 -2,2066E-03 -1,3845E-02 -8,6040E-02 -5,0436E-01 -2,1462E+00
-3,4182E+00 -1,0202E+00 -1,8880E-01 -3,0803E-02 -4,9225E-03 -7,8335E-04 -1,2464E-04 -1,9831E-05 -3,1550E-06 -5,0195E-07
-7,9860E-08 -1,2706E-08
VCPL2R
 2,3604E-03  2,9712E-03  8,5045E-03  3,1568E-02  1,1583E-01  4,0712E-01  1,2232E+00  2,0993E+00 -1,2382E-01 -2,8996E+00
-1,1457E+00 -3,7439E-01 -1,0597E-01 -2,8843E-02 -7,7676E-03 -2,0859E-03 -5,5973E-04 -1,5017E-04 -4,0285E-05 -1,0807E-05
-2,8991E-06 -7,7772E-07
VCPL2I
 1,0613E-06  1,4640E-06  6,3712E-06  4,0045E-05  2,5168E-04  1,5810E-03  9,9014E-03  6,0838E-02  3,3202E-01  8,8972E-01
-5,4801E-01 -6,2460E-01 -1,3130E-01 -2,1972E-02 -3,5239E-03 -5,6137E-04 -8,9331E-05 -1,4213E-05 -2,2612E-06 -3,5976E-07
-5,7237E-08 -9,1063E-09
```

```
N=     1     2
L=     0     2
J=     0     2

C-MATRIX(X=305,4) -8,968E-03  4,942E-01  3,630E-03  3,244E-03

N=     1     2     2     2
L=    25    27    25    23
J=    25    27    25    23

C-MATRIX(X=300,6)  1,172E-01  8,133E-02 -3,370E-03  1,703E-03 -3,358E-03 -2,121E-02  4,970E-02 -7,548E-03

N=     1     2     2     2
L=    50    52    50    48
J=    50    52    50    48

C-MATRIX(X=310,2)  8,993E-04  1,081E-03  2,686E-04 -4,316E-03 -3,046E-03 -1,059E-02  1,552E-02 -2,591E-02

N=     1     2     2     2
L=   100   102   100    98
J=   100   102   100    98

C-MATRIX(X=320,4) -3,923E-04  6,956E-05  1,065E-03 -1,224E-03 -7,133E-04 -1,611E-03 -2,012E-03 -7,626E-03

N=     1     2     2     2
L=   150   152   150   148
J=   150   152   150   148

C-MATRIX(X=306,2) -8,594E-05  7,111E-06  5,185E-04 -6,291E-04  1,022E-05 -4,886E-04 -1,528E-03 -1,915E-03

N=     1     2     2     2
L=   200   202   200   198
J=   200   202   202   198

C-MATRIX(X=308,1) -1,637E-04  9,840E-07  3,159E-04 -3,236E-04  1,655E-04 -2,263E-04 -6,102E-04 -5,192E-04


********** TIME SPENT IN COUPLE= 101,18500**********

 AMAX= 7,557E-23  FOR II,NITE1=   2   2
```

COUPLED CHANNEL CROSS SECTION FOR ELAB= 50.000-MEV

ANGLE	SIG/RUTH	I=0	I=2	I=
10.00	9.998E-01	7.737E+05	1.233E+00	
12.00	9.998E-01	3.740E+05	1.016E+00	
14.00	9.999E-01	2.024E+05	1.611E+00	
16.00	9.999E-01	1.190E+05	2.933E+00	
18.00	9.998E-01	7.455E+04	4.308E+00	
20.00	9.998E-01	4.910E+04	5.069E+00	
22.00	1.000E+00	3.369E+04	5.850E+00	
24.00	1.000E+00	2.390E+04	6.591E+00	
26.00	9.998E-01	1.743E+04	7.210E+00	
28.00	1.000E+00	1.304E+04	7.581E+20	
30.00	9.988E-01	9.940E+03	7.817E+00	
32.00	9.984E-01	7.723E+03	8.241E+00	
34.00	9.994E-01	6.108E+03	8.385E+00	
36.00	9.987E-01	4.891E+03	8.270E+00	
38.00	9.962E-01	3.959E+03	8.267E+00	
40.00	9.962E-01	3.251E+03	8.436E+00	
42.00	1.000E+00	2.707E+03	8.419E+00	
44.00	1.003E+00	2.275E+03	8.126E+00	
46.00	1.002E+00	1.919E+03	7.834E+00	
48.00	9.952E-01	1.624E+03	7.787E+00	
50.00	9.901E-01	1.386E+03	7.987E+00	
52.00	9.929E-01	1.201E+03	8.223E+00	
54.00	1.007E+00	1.059E+03	8.263E+00	
56.00	1.031E+00	9.473E+02	7.992E+00	
58.00	1.057E+00	8.546E+02	7.425E+00	
60.00	1.079E+00	7.708E+02	6.707E+00	
62.00	1.088E+00	6.905E+02	5.968E+00	
64.00	1.080E+00	6.115E+02	5.342E+00	
66.00	1.052E+00	5.341E+02	4.876E+00	
68.00	1.006E+00	4.595E+02	4.584E+00	
70.00	9.444E-01	3.896E+02	4.423E+00	
72.00	8.712E-01	3.259E+02	4.344E+00	
74.00	7.912E-01	2.693E+02	4.303E+00	
76.00	7.084E-01	2.202E+02	4.265E+00	
78.00	6.262E-01	1.783E+02	4.201E+00	
80.00	5.472E-01	1.431E+02	4.099E+00	
82.00	4.735E-01	1.141E+02	3.953E+00	
84.00	4.061E-01	9.046E+01	3.761E+00	
86.00	3.458E-01	7.138E+01	3.535E+00	
88.00	2.928E-01	5.614E+01	3.282E+00	
90.00	2.464E-01	4.421E+01	3.012E+20	

B-matrices with the well defined geometrical factors.* Further, the amount of the output of the B-matrices is much smaller than that of the A-matrices.

CARD-6 reads in EXTCOM(N); N = 1 ~ 10. In the present shape of our program none of them are used. Therefore, this card can be blank. It may be that the modification of JP1MAIN is to be made so as to drop the card SN-100+1 altogether, but we prefer to retain it. The reason is the following.

The name EXTCOM means extra-common. Many of them are unused at present, but they are useful when a small modification of the program is to be made in which communication of a quantity from a routine to another is needed, since EXTCOM lies in the COMMON field (occupying 50 core storages altogether). EXTCOM(N) in the CARD-6 is useful when the quantity to be communicated is to be given as input data.

As was seen in CARD-3, there are quantities which are not used in KEXCOM(N), N = 1 ~ 14. They can be used to read in some new integer quantities. KEXCOM(N), N = 15 ~ 50 can be used to communicate new integer quantities between subroutines.

In the comment cards given in the beginning of JP1MAIN, there is given a list of KEXCOM(N) and EXTCOM(N) that are already used in the present shape of our program.

CARD-7 reads in ten integer quantities. Their meaning and use are as follows:

---

*It should be noted that the A-matrices in the present program are the product of the B- and A-matrices of T, and not the A-matrices of T themselves. It should also be noted that some non-vanishing values must be given to KEXCOM(5), (6) and (7) to get output of A- and B-matrices. (Cf. AMATRX, SN-4210 ~ 4214.)

(i) IICPLE equals the number of coupled states in the target and thus equals N_c of (T-19). (If KTRL(7) = 1, IICPLE = 1 always.)

(ii-iii) INTYPE and INTMAX specify the type of the coupling and the number of coupling terms, respectively, and for their complete understanding the reader has to understand the subroutines COUPLE, BMATRX and AMATRX. A brief explanation of these quantities will, nevertheless, be given in the explanation of the CARD-19 below.

(iv) ISTRTW is twice the value of the projectile spin s.

(v) NANGLR is the number of angles for which the differential cross sections (and polarizations) are to be computed.

(vi) IIXCAL is the number of states for which the differential scattering cross sections are to be computed. For NACC, usually IIXCAL equals IICPLE, but there are cases, for example, in which the energy of the incident particle is so low that the projectile gets a negative energy when the target is in an excited state. In such a case IIXCAL is smaller than IICPLE. For ACC usually IIXCAL $\geq$ IICPLE = 1.

(vii) IIXPLT is the number of states for which the theoretical and experimental differential cross sections are to be machine-plotted. Clearly IIXPLT $\leq$ IIXCAL. Note that IIXPLT must be ≤ 6.

(viii-ix) IIPCAL and IIPPLT serve the same role for polarizations as IIXCAL and IIXPLT serve for differential cross sections. Note that IIPPLT must be ≤ 2.

(x) KANGRD equals either 0 or 1. How to use these two values will be seen below in the explanation of CARD-10.

CARD-7-1 (SN-102) is needed to be in the data deck only when INTYPE = 6. If INTYPE = 6 this card reads in KEXCOM(N), N = 21 ~ 27. Note that when INTYPE = 6 the target is a deformed even nucleus and excitation of vibrational states are also considered. KEXCOM(N), N = 21 ~ 27, respectively, give the number of states considered in the coupling in each of the following seven bands: (i) ground band; (ii) $K = 0^+$ (β-vibrational) band; (iii) $K = 0^-$ band; (iv) $K = 2^+$ (γ-vibrational) band; and (v-vii) $K = 1^-$, 2^-, and 3^- bands. See the explanation of CARD-19 for more detail.

CARD-8 (SN-103) reads in the quantities that specify the nature of the target states. (FORMAT is 3(2I5, F10.3)). This card reads in three quantities for each state. (i) IIREAD(N) = I_N if KTRL(1) = 0; IIREAD(N) = $I_N + \frac{1}{2}$ if KTRL(1) = 1. (ii) KPRITR(N) = 1 or 2, depending on whether the parity of the N-th states is + or -. (iii) QVALUE(N) is the excitation energy (thus the negative of the usual Q-value) of the N-th state above the ground state. Therefore QVALUE(1) is zero always and QVALUE(N) > 0 for N $\geq$ 2. If IICPLE $\geq$ 4 for NACC or IIXCAL $\geq$ 4 for ACC more than two cards of type CARD-8 are needed.

The order with which these states appear in CARD-8 must satisfy certain rules. These rules are shown in the explanation of CARD-19.

CARD-9 (SN-105) reads in seven floating point quantities that follow:

(i) ELAB = E_{lab} of the projectile in MeV.

(ii) PMAS = Mass of the projectile in amu or pmu depending on whether AMUPMU = 0 or 1; see (vii) below. However, the use of an integer value may be made.

(iii) TMAS = Mass of the target. Remarks concerning the unit is the

same as in (ii).

(iv) CHARGE = ZZ′ of (T-7), i.e., the product of the charge numbers of the projectile and the target. Thus if the projectile is a neutron, CHARGE = 0.0.

(v-vi) XMES1 and XMES2 are the mesh sizes used in the differential equation integration. They are equal to h_1 and h of Appendix B, respectively. The use of XMES1 = 0.0125 and XMES2 = 0.1 is usually recommended.

(vii) AMUPMU = 0.0 (= 1.0) if atomic (proton) mass unit is to be used.

CARD-10 reads in ANGLER(N), i.e., the center of mass angles θ_{CM} in degree. If KANGRD, which was read in from CARD-7 were zero, SN-111 of JP1MAIN is executed and thus the cards should contain values of ANGLER(N) for N = 1 ~ NANGLR. Therefore the needed number of the cards, N_{10} say, of the type CARD-10 is given by N_{10} = ((NANGLR-1)/10)+1. On the other hand, if KNAGRD = 1, which is used when all the θ_{CM} are equally spaced, SN-112 is executed and CARD-10 needs to carry only two quantities, the smallest value of θ_{CM} and the increment $\Delta\theta_{CM}$.

CARDs-10-1 (SN-127). These cards read in the experimental differential cross sections SGMEXP(N,I) (in mb/sterad) and the experimental polarization POLEXP(N,I). They are needed in the card deck only when either or both of IIXPLT and IIPPLT are non-zero. The number of cards needed equals N_{10} times (IIXPLT + IIPPLT).

As is seen in PLOTER, the plotting of $\sigma_{th}(\theta)$ and $\sigma_{exp}(\theta)$, and $P_{th}(\theta)$ and $P_{exp}(\theta)$ (the theoretical and experimental cross sections and polarizations) is made on a sheet of paper taking a fixed spacing between the

neighboring angle, irrespective of whether the actual difference of the neighboring θ is a constant or not. Therefore, it is recommended to use θ of an equal spacing when the machine plot is to be made. Thus, when original σ_{exp} and P_{exp} are not given with equally spaced θ, plot σ_{exp} and P_{exp} on a sheet of paper, draw a line through, read off the values at equally spaced angles θ and use them as $\sigma_{exp}(\theta)$ and $P_{exp}(\theta)$, i.e., as SGMEXP(N,I) and POLEXP(N,I).

It should also be noted that the number of angles NANGLR for which the cross sections are to be calculated and then plotted is commonly used for all the states. In many practical cases, however, it happens that the range of the angles for which experimental cross sections are supplied differs from a state to another. In such a case fix NANGLR so that the widest range of angles are covered. For the angles (in other states) where no experimental data exist never make SGMEXP(N,I) equal to zero. (The computer is requested to take a logarithm of zero and may stop.) It is recommended to give to such SGMEXP(N,I) the following values. Suppose there are experimental cross sections for $N = N_{min} \sim N_{max}$. Make SGMEXP(N,I) = SGMEXP(N_{min},I) for $N \leq N_{min}$ and SGMEXP(N,I) = SGMEXP(N_{max},I) for $N \geq N_{max}$. The same remark applies to POLEXP(N,I), too.

CARD-11 (SN-132). This card with FORMAT (I5,4F7.2) is needed in the card deck only when KTRL(8) $\neq$ 0. The first quantity NFAI is the number of different azimuthal angles φ for which the differential cross sections $\sigma(\theta,\varphi)$ are to be computed. Up to two values of φ can be considered at present. FAI(N), N = 1 $\sim$ 2 are such φ values in degree. Note that for KTRL(8) $\neq$ 0 there is an initial polarization and thus the

CARD-17 (SN-400) reads in the strength parameters of the optical potentials. To make easy the explanation of this card and the next card (CARD-18), we shall call the real and imaginary parts of the Saxon potential, surface type imaginary potential and the spin-orbit potential, as No. 1 ~ No. 4 potentials, respectively.

VSX = depth of No. 1 potential = V of (T-1)

WSX = depth of No. 2 potential = W of (T-1)

WSF = depth of No. 3 potential = W_D of (T-1)

VSO = depth of No. 4 potential = V_{so} of (T-1)

CARD-17 also reads in WC(N), N = 1 ~ 6. They are the "fudge" factors for the strength of the No. 2 and/or No. 3 potentials. See Sec. IV-(ii) and IV-(iv) of T. See also ref. 2. WC(N) for N > IICPLE is of no meaning (and not used). (Note that the actual strength of imaginary potentials in channel N equals WSX or WSF times WC(N). Thus if no fudging is to be done, WC(N) = 1.0, not = 0.)

CARD-18 (SN-400+1) reads in the geometrical parameters of the optical potentials. (DFN,RZERO), (DFNW,RZEROW), (DFNS,RZEROS) and (DFNSP,RZROSP) are the diffuseness parameter (a or $\bar{a}$ of (T-1)) and the radius parameter (r_o or $\bar{r}_o$ in (T-3)) for the potentials No. 1 through No. 4. RZEROC is the radius parameter for the Coulomb potential and equals R_c of (T-8) divided by $A^{1/3}$. (Order of reading is that four a's are read first and then five r_o's.)

CARD-19 (SN-400+2) reads in VCOULE(N), N = 1 ~ 10 and an integer quantity KREAD1.

VCOUPL is essentially the value of β_λ introduced in (T-2) and (T-32)