

PERFECT V-A : Fortran Programs to Compute Various Properties of the Triton Wave Function Using the RSC5 Potential(Annual Report)

著者	Sasakawa T., Ishikawa S., Sawada T.
journal or publication title	The science reports of the Tohoku University. Ser. 8, Physics and astronomy
volume	3
number	3
page range	268-336
year	1982-12-15
URL	http://hdl.handle.net/10097/25504

PERFECT V-A

Fortran Programs to Compute Various Properties of the
Triton Wave Function Using the RSC5 Potential

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(Received November 17, 1982)

We present the detailed description of the auxiliary codes to PERFECT V that compute the one-body charge form factors, the percentage probabilities, the asymptotic normalization constants, the E1 sum rule, and the two-body correlation function of the triton wave function obtained by PERFECT V using the RSC5 potential.

Keywords: Triton bound state. Reid soft core potential. Interacting S, D-states and spectator s-, d-state. One-body charge form factor. The percentage probabilities. The asymptotic normalization constants. The E1 sum rule. The two-body correlation function.

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§1. Introduction

Based on the formulations presented in reference 1, we have described in our previous report in detail the program named PERFECT V to carry out the iterative calculation of the triton bound state²⁾. In the present paper, we present the detailed description of various auxiliary codes to compute other physical quantities of interest of the triton wave function. They are named NFORM, ASYM5, SUM5 and CORR5, that carry out the computations of the one-body charge form factors and the percentage probabilities(NFORM), the asymptotic normalization constants(ASYM5), the enhancement factor κ of the El sum rule (SUM5), and the two-body correlation function(CORR5), all utilizing the triton wave functions output from PERFECT V, or the extension of them to large x . Necessary formulas to compute these quantities are given in reference 1.

Although in the following sections, we present these codes separately to be used independent of each other, the user will find a strong similarity in parts of the codes that deal with the extension of the wave functions to larger x . In fact, these are the most tedious parts of the computation, but they are essentially the same as the computation done in subroutine RHS of PERFECT V. It would be a simple matter for the user to rearrange these codes in such a way that he prepares a single file in advance on which the wave functions are stored up to the desired large distance x , so that he can compute all the above mentioned quantities all at once.

§2. Computation of One-Body Charge Form Factors and Percentage Probabilities

2-a. One-Body Charge Form Factors

The one-body charge form factors of ${}^3\text{H}$ and ${}^3\text{He}$ are computed by using the formulas given in section 4 of I. We have the main program of PERFECT V²⁾ output on File LFCHI the wave functions - $\Theta_\alpha(q,x)$ and $\phi_\alpha(q,x)$ of Eqs.(II-2.12) and (II-2.16) that correspond to $(\phi(12,3)+\phi(23,1)+\phi(31,2))$ of Eq.(I-2-40a) and $-\phi(12,3)$ of Eq.(I-2-38a), respectively. As explained at the beginning of section I-4, we must utilize the (12,3) component $\bar{\phi}_\alpha(q,x)$ to compute the one-body charge form factors rather than the total wave function $\Theta_\alpha(q,x)$.

Necessary formulas for computation of the relevant quantities $\langle F_i^{uv} \rangle$ ($i=1$ to 4) have already been derived in section 4 of I. Since all these quantities are expressed as integrals involving rapidly oscillating functions, the evaluation of them requires careful treatments, or the resulting charge form factors deteriorate rapidly at large momentum transfers. We describe below how to compute these quantities.

First of all, we need to calculate $\rho_\alpha(x, y)$ of Eq.(I-4-29)

$$\rho_\alpha(x, y) = \int_0^{P_{\text{MALL}}} dp \frac{\phi_\alpha(q, x)}{x^L} \frac{u_\ell(p, y)}{y^\ell} \quad (2.1)$$

to sufficiently far distances $x \leq x_G$ and $y \leq y_G$. To take care accurately the possible oscillatory behavior of $u_\ell(p, y)$, we carry out the p -integration by means of the p -spline as described in section II-5. Thus, we introduce $Y_\ell^{(t)}(y, p_k)$ of Eq.(II-5.9):

$$Y_\ell^{(t)}(y, p_k) = \int_{p_k}^{p_{k+1}} dp' \frac{u_\ell(p', y)}{y^\ell} S^{(t)}(p' - p_k) \quad (2.2)$$

where $S^{(t)}(z)$ ($t=1$ to 4) are the spline functions (see Eq.(II-5.3)). After extending $\phi_\alpha(q, x)$ to $x_{\text{max}} < x \leq x_G$ by using the known asymptotic form (see Eq.(II-3.10)), we compute the p -spline coefficients $a_\alpha^{(t)}(x; p_k)$ by (see Eq.(II-5.7))

$$\frac{\phi_\alpha(q, x)}{x^L} \simeq \sum_{t=1}^4 a_\alpha^{(t)}(x; p_k) S^{(t)}(p - p_k) \quad (p_k \leq p \leq p_{k+1}) \quad (2.3)$$

Then $\rho_\alpha(x, y)$ of Eq.(2.1) can be approximated by

$$\rho_\alpha(x, y) \simeq \sum_{p_k} \sum_{t=1}^4 a_\alpha^{(t)}(x, p_k) Y_\ell^{(t)}(y, p_k) \quad (x \leq x_G, y \leq y_G) \quad (2.4)$$

Perhaps we should mention that, unlike $\rho_\alpha^{\beta(m)}(x, y)$ of Eq.(II-5.8), we need not to separate the p -interval in Eq.(2.1) at $p=p_M$ since $\phi_\alpha(q, x)$ is continuous there as a function of p .

The quantity $\langle F_1^{uv} \rangle$ of Eq.(I-4-40) is given by

$$\langle F_1^{uv} \rangle = \delta_{u,v} \sum_\alpha^u F_{\alpha\alpha}^{(1)}(Q) \quad (2.5)$$

with

$$F_{\alpha\alpha}^{(1)}(Q) = \int_0^{y_M} dy j_0\left(\frac{2}{3} Qy\right) f_\alpha(y) \quad (2.5a)$$

where

$$f_\alpha(y) = \int_0^{x_M} dx x^{2L+2} y^{2\ell+2} [\rho_\alpha(x, y)]^2 \quad (2.5b)$$

where x_M and y_M are appropriately chosen upper limits (see Eq.(2.24) below), and Q is the momentum transfer. The value of Q extends as far as 10 fm^{-1} , and therefore the function $j_0(\frac{2}{3} Qy)$ will oscillate many times as y runs from 0 to the upper limit y_M . To evaluate accurately the y -integral with such an oscillating integrand, we utilize the method of quadrature by a spline interpolation. The y -spline coefficients $b_\alpha^{(t)}(y_i)$ ($t=1$ to 4) of $f_\alpha(y)$ are defined by

$$f_\alpha(y) \approx \sum_{t=1}^4 b_\alpha^{(t)}(y_i) s^{(t)}(y-y_i) \quad (2.6)$$

Introducing

$$I^{(t)}(Q; y_i) = \int_{y_i}^{y_{i+1}} dy j_0(\frac{2}{3} Qy) s^{(t)}(y-y_i) \quad , \quad (2.7)$$

we find for the y -integral in Eq.(2.5a)

$$F_{\alpha\alpha}^{(1)}(Q) \approx \sum_{y_i=y_0}^{y_{M-1}} \sum_{t=0}^4 b_\alpha^{(t)}(y_i) I^{(t)}(Q; y_i) \quad (2.8)$$

For $\langle F_2^{uv} \rangle$ of Eq.(I-4-44), we write

$$\langle F_2^{uv} \rangle = \sum_{\alpha}^u \sum_{\alpha'}^v F_{\alpha\alpha'}^{(2)}(Q) \quad (2.9)$$

with

$$F_{\alpha\alpha'}^{(2)}(Q) = \sum_{\lambda} N_{\alpha\alpha', \lambda} G_{\alpha\alpha', \lambda}(Q) \quad (2.9a)$$

where

$$G_{\alpha\alpha', \lambda}(Q) = \int_0^{x_M} dx j_\lambda(\frac{Q}{2} x) g_{\alpha\alpha', \lambda}(Q; x) \quad (2.9b)$$

and

$$N_{\alpha\alpha', \lambda} = (-)^{\ell+L'} \hat{L}\hat{\ell} \langle L_0 \lambda 0 | L' 0 \rangle \langle \ell 0 \lambda 0 | \ell' 0 \rangle \hat{\lambda}^2 \times \sum_{L_0 S_0} N_{\alpha}^{(L_0 S_0)} N_{\alpha'}^{(L_0 S_0)} (-)^{L_0} \left\{ \begin{matrix} L & \lambda & L' \\ \ell & L_0 & \ell' \end{matrix} \right\} \quad (2.10)$$

$$g_{\alpha\alpha', \lambda}(Q; x) = \int_0^{y_M} dy j_\lambda(\frac{Q}{3} y) f_{\alpha\alpha'}(x, y) \quad (2.11)$$

with

$$f_{\alpha\alpha'}(x, y) = x^{L+2} y^{\ell+2} \rho_{\alpha}(x, y) x^{L'} y^{\ell'} \rho_{\alpha'}(x, y) \quad (2.12)$$

In Eq.(2.10), the factor $N_{\alpha}^{(L_0 S_0)}$ is given by Eq.(I-3-4). The y -integration in Eq.(2.11) involving $j_{\lambda}(\frac{Q}{3} y)$ should be done by the spline method. Thus, the y -spline coefficients $c_{\alpha\alpha'}^{(t)}(x; y_i)$ of $f_{\alpha\alpha'}(x, y)$ is determined by using subroutine SPCOEF: for $y_i \leq y \leq y_{i+1}$

$$f_{\alpha\alpha'}(x, y) \simeq \sum_{t=1}^4 c_{\alpha\alpha'}^{(t)}(x; y_i) s^{(t)}(y - y_i) \quad (2.13)$$

Introducing

$$J_{\lambda}^{(t)}(Q; y_i) = \int_{y_i}^{y_{i+1}} dy j_{\lambda}(\frac{Q}{3} y) s^{(t)}(y - y_i) \quad (\lambda=0, 2, 4) \quad (2.14)$$

we find

$$g_{\alpha\alpha', \lambda}(Q; x) \simeq \sum_{y_i=y_0=0}^{y_{M-1}} \sum_{t=1}^4 c_{\alpha\alpha'}^{(t)}(x; y_i) J_{\lambda}^{(t)}(Q; y_i) \quad (2.15)$$

Here we need only $\lambda=0, 2, 4$ due to the factor $N_{\alpha\alpha', \lambda}$ of Eq.(2.10) and the fact that there are even parity states only in RSC5. To carry out the x -integration in Eq.(2.9) involving $j_{\lambda}(\frac{Q}{2} x)$, we further utilize the method of spline interpolation. Denoting the spline coefficients of $g_{\alpha\alpha', \lambda}(Q; x)$ by $d_{\alpha\alpha', \lambda}^{(t)}(Q; x_j)$, we have

$$g_{\alpha\alpha', \lambda}(Q; x) \simeq \sum_{t=1}^4 d_{\alpha\alpha', \lambda}^{(t)}(Q; x_j) s^{(t)}(x - x_j) \quad (x_j \leq x \leq x_{j+1}) \quad (2.16)$$

Further we introduce

$$K_{\lambda}^{(t)}(Q; x_j) = \int_{x_j}^{x_{j+1}} j_{\lambda}(\frac{Q}{2} x) s^{(t)}(x - x_j) dx \quad (\lambda=0, 2, 4) \quad (2.17)$$

Then we find for the x -integral in Eq.(2.9b)

$$G_{\alpha\alpha', \lambda}(Q) \simeq \sum_{x_j=x_0=0}^{x_{M-1}} \sum_{t=1}^4 d_{\alpha\alpha', \lambda}^{(t)}(Q; x_j) K_{\lambda}^{(t)}(Q; x_j) \quad (2.18)$$

The quantity $\langle F_3^{uv} \rangle$ of Eq.(I-4-49) is given by

$$\langle F_3^{uv} \rangle = \sum_{\alpha}^u \sum_{\alpha'}^v F_{\alpha\alpha'}^{(3)}(Q) \quad (2.19)$$

with

$$F_{\alpha\alpha'}^{(3)}(Q) = \sum_{L_0 S_0} \bar{N}_{\alpha\alpha'}^{(L_0 S_0)} Y_{\alpha\alpha'}^{L_0}(Q) \quad (2.19a)$$

where

$$Y_{\alpha\alpha'}^{L_0}(Q) = \int_0^{Y_M} dy j_0\left(\frac{2}{3} Qy\right) h_{\alpha\alpha'}^L(y), \quad (2.19b)$$

$$\begin{aligned} \bar{N}_{\alpha\alpha'}^{(L_0 S_0)} &= N_{\alpha}^{(L_0 S_0)} N_{\alpha'}^{(L_0 S_0)} \langle (S_0 \frac{1}{2}) S_0 M_{S_0} (12, 3) | (S' \frac{1}{2}) S_0 M_{S_0} (31, 2) \rangle \\ &= N_{\alpha}^{(L_0 S_0)} N_{\alpha'}^{(L_0 S_0)} (-)^S \hat{S} \hat{S}' \left\{ \begin{matrix} \frac{1}{2} & \frac{1}{2} & S' \\ \frac{1}{2} & S_0 & S \end{matrix} \right\} \end{aligned} \quad (2.20)$$

and

$$h_{\alpha\alpha'}^L(y) = \int_0^{x_M} dx x^{L+2} y^{\ell+2} \rho_{\alpha}(x, y) U_{\alpha\alpha'}^{L_0}(Q=0; x, y) \quad (2.21)$$

where $U_{\alpha\alpha'}^{L_0}(Q=0; x, y)$ is given by Eq. (I-4-51) with $Q=0$. From Eq. (I-3-27)

$$U_{\alpha\alpha'}^{L_0}(Q; x, y) = \sum_{a=0}^{L'} \sum_{c=0}^{\ell'} \sum_{\gamma} x^{a+c} y^{b+d} K_{\gamma}^{\alpha'}(x, y) R_{(L\ell, L'\ell')}^{acy} L_0 \quad (2.22)$$

(b=L'-a) (d=l'-c)

with

$$K_{\gamma}^{\alpha'}(x, y) = \frac{1}{2} \int_{-1}^1 d(\cos \theta_{xy}) P_{\gamma}(\cos \theta_{xy}) \rho_{\alpha}(x'', y'') \quad (2.23)$$

and with the coefficients $R_{(L\ell, L'\ell')}^{acy} L_0$ of Eq. (I-3-38). (see section 10 of II on Code RAM.) By a double spline interpolation we can compute $\rho_{\alpha}(x'', y'')$ as in the main program (see Eqs. (II-5.10) ~ (II-5.12)). Unlike during iterations of the main program, here we have to compute $U_{\alpha\alpha'}^{L_0}(Q; x, y)$ just once. Therefore there is no merit of splitting the y -integration interval in Eq. (19b) into two parts as we do in Eq. (II-3.13). Furthermore, here we must integrate over x as well as y . Thus, we prepare $\rho_{\alpha}(x, y)$ at the beginning to sufficiently large distances $x \leq x_G$ and $y \leq y_G$, and compute $K_{\gamma}^{\alpha'}(x, y)$ of Eq. (2.23) up to large distances $x \leq x_M$ and $y \leq y_M$. The relations between (x_G, y_G) and (x_M, y_M) are (see Eq. (II-3.11))

$$x_G = \frac{1}{2} x_M + y_M, \quad y_G = \frac{3}{4} x_M + \frac{1}{2} y_M \quad (2.24)$$

The rest of the computation of $U_{\alpha\alpha'}^{L_0}(Q=0; x, y)$ proceeds just as in subroutine RHS (see section 6-b of II). After obtaining $U_{\alpha\alpha'}^{L_0}(Q=0; x, y)$, we perform the

x-integration in Eq.(2.21). Since $\rho_\alpha(x,y)$ and $U_{\alpha\alpha'}^{L_0}(Q=0;x,y)$ are slowly varying functions of x , we may use a conventional method of quadrature over x to find $h_{\alpha\alpha'}^{L_0}(y)$. This function, in turn, is approximated by a y -spline interpolation,

$$h_{\alpha\alpha'}^{L_0}(y) \approx \sum_{t=1}^4 u_{\alpha\alpha',L_0}^{(t)}(y_i) s^{(t)}(y-y_i) \quad (y_i \leq y \leq y_{i+1}) \quad (2.25)$$

and the y -integration in Eq.(2.19b) is carried out by means of the y -spline method:

$$Y_{\alpha\alpha'}^L(Q) = \sum_{y_i=Y_0}^{Y_{M-1}} \sum_{t=1}^4 u_{\alpha\alpha',L_0}^{(t)}(y_i) I^{(t)}(Q;y_i) \quad (2.26)$$

where $I^{(t)}(Q;y_i)$ is given by Eq.(2.7).

Finally, we need to compute $\langle F_4^{uv} \rangle$ of Eq.(I-4-49). This can be written as

$$\langle F_4^{uv} \rangle = \sum_{\alpha}^u \sum_{\alpha'}^v F_{\alpha\alpha'}^{(4)}(Q) \quad (2.27)$$

with

$$F_{\alpha\alpha'}^{(4)}(Q) = \sum_{L_0 S_0} \bar{N}_{\alpha\alpha'}^{(L_0 S_0)} \int_0^{Y_N} dy h_{\alpha\alpha'}^{L_0}(Q;y) \quad (2.27a)$$

where

$$h_{\alpha\alpha'}^{L_0}(Q;y) = \int_0^{x_M} dx x^{L+2} y^{\ell+2} \rho_\alpha(x,y) U_{\alpha\alpha'}^{L_0}(Q;x,y), \quad (2.28)$$

$$U_{\alpha\alpha'}^{L_0}(Q;x,y) = \sum_{a=0}^{L'} \sum_{c=0}^{\ell'} \sum_{\gamma} x^{a+c} y^{b+d} K_Y^{\alpha'}(Q;x,y) R_{(L\ell, L'\ell')}^{\alpha\gamma} L_0 \quad (b=L'-a) \quad (d=\ell'-c) \quad (2.29)$$

and

$$K_Y^{\alpha'}(Q;x,y) = \frac{1}{2} \int_{-1}^1 d(\cos \theta_{xy}) P_Y(\cos \theta_{xy}) j_0(QR) \rho_{\alpha'}(x'',y'') \quad (2.30)$$

with

$$R = \sqrt{\frac{x^2}{4} + \frac{y^2}{9} - \frac{xy}{3} \cos \theta_{xy}} \quad (2.31)$$

Unlike $U_{\alpha\alpha'}^{L_0}(Q=0;x,y)$, $U_{\alpha\alpha'}^{L_0}(Q;x,y)$ of Eq.(2.29) depends on Q through $j_0(QR)$ in $K_Y^{\alpha'}(Q;x,y)$ of Eq.(2.30). However, due to the $\cos \theta_{xy}$ -integration in $K_Y^{\alpha'}(Q;x,y)$, it is expected that the oscillatory behavior of $j_0(QR)$ is smeared out after the $\cos \theta$ -integration (which requires a small $\cos \theta$ -mesh size depending on the

value of Q) so that the resulting $U_{\alpha\alpha}^{L0}(Q;x,y)$ is a relatively slowly varying function of x and y even for large values of Q . We should be able to tell whether this expectation is born out or not by simply varying the x -mesh size in Eq.(2.28) and watch the change in the resulting values of $\langle F_4^{uv} \rangle$.

Having obtained $\langle F_i^{uv} \rangle$, $i=1$ to 4, the one-body charge form factors of ${}^3\text{H}$ and ${}^3\text{He}$ can be calculated by using Eqs.(I-4-19,20,21,25 and 26). In terms of $F_{\alpha\alpha}^{(i)}(Q)$, $i=1$ to 4, of Eqs.(2.5a), (2.9a), (2.19a) and (2.27a) we have for the quantities appearing in Eqs.(I-4-25 and 26)

$$\langle F_i^{SS} \rangle = \sum_{k=2}^5 \sum_{k'=2}^5 F_{kk'}^{(i)}(Q) \quad (2.32a)$$

$$\langle F_i^{AA} \rangle = F_{11}^{(i)}(Q) \quad (2.32b)$$

$$\langle F_i^{SA} \rangle = \sum_{k=2}^5 F_{k1}^{(i)}(Q) \quad (2.32c)$$

and

$$\langle F_i^{AS} \rangle = \sum_{k=2}^5 F_{1k}^{(i)}(Q) \quad (2.32d)$$

One way of checking the accuracy of the resulting $\langle F_i^{uv} \rangle$ is to see if the symmetry properties of Eq.(I-4-27) are satisfied.

2-b. Percentage Probabilities

All the formulas necessary to compute the percentage probabilities of the Derrick-Blatt classification of the ${}^3\text{H}$ wave function have been derived in section 5 and Appendix of I for the case of RSC5.

We need the following integrals defined by Eqs.(I-5-19) and (I-5-21) (see also Eq.(I-A-3)).

$$I_{kk'} = \delta_{LL'} \delta_{\ell\ell'} N_k N_{k'} \int_0^\infty dx x^2 \int_0^\infty dy y^2 x^L y^\ell \rho_\alpha(x,y) \rho_\alpha(x,y) \quad (2.33a)$$

and

$$K_{kk'} = N_k N_{k'} \int_0^\infty dx x^2 \int_0^\infty dy y^2 x^L y^\ell \rho_\alpha(x,y) U_{\alpha\alpha}^{L0}(Q=0;x,y) \quad (2.33b)$$

Here, $U_{\alpha\alpha}^{L0}(Q=0;x,y)$ is the same as in Eq.(2.21), $\rho_\alpha(x,y)$ is given by Eq.(2.1), and $N_k = N_\alpha^{L0S0}$ of Eq.(I-3-4). The correspondence between the index k and

$\{\alpha, (L_0 S_0)\}$ is given by Table A-1 of I. Comparing Eq.(2.33a) with Eqs.(2.9b), (2.11) and (2.12) we see that

$$\begin{aligned} I_{kk'} &= \delta_{LL'} \delta_{\ell\ell'} N_k N_{k'} G_{\alpha\alpha', \lambda=0}^{(Q=0)} \delta_{L_0 L_0'} \delta_{S_0 S_0'} \\ &= \delta_{LL'} \delta_{\ell\ell'} N_k N_{k'} \frac{F_{\alpha\alpha'}^{(2)}(Q=0)}{N_{\alpha\alpha', \lambda=0}} \delta_{L_0 L_0'} \delta_{S_0 S_0'} \end{aligned} \quad (2.34)$$

Similarly, comparing Eq.(2.33b) with Eqs.(2.19b) and (2.21), we find

$$K_{kk'} = N_k N_{k'} Y_{\alpha\alpha'}^{L_0}(Q=0) \delta_{L_0 L_0'} \delta_{S_0 S_0'} \quad (2.35)$$

Therefore $I_{kk'}$ and $K_{kk'}$ have essentially been obtained already. In terms of these quantities, we can compute the percentage probabilities as per Eqs.(I-A-11,13,14,17 and 18).

2-c. General Description of Code NFORM

The calculations of one-body charge form factors and the percentage probabilities of ^3H and ^3He (without the Coulomb interaction) with RSC5 are carried out in the code named NFORM. It consists of the following parts.

MAIN routine

Subroutines and functions FORM1, FORM2, NRHS3, NRHS4, FORM, PARAM, KOEF2, XTABLE, PTABLE, YTAB, BESSEL, SPLINE, SPCOEF, CLEBSH, F6J, NINEJ, FYFORM, and PL

The code requires the following data files.

File LFRAM, File LFCHI.

Of eighteen subroutines and functions listed above, PTABLE, SPLINE, SPCOEF, CLEBSH, F6J, NINEJ, and PL are identical to those used in the main program, and hence no listings of them are given. The user will find Subroutine FYFORM to run parallel to part of Code FYFI5, Subroutines NRHS3 and NRHS4 similar to Subroutine RHS in the main program. For detailed description of these subroutines, we refer the user to reference II.

Since there are ample comment cards provided in various key places within the code, we shall not give detailed description of each subroutine. Together with the description given in the flow chart below, they should be sufficient

to guide the user to read through each subroutine.

2-d. MAIN routine

The function of this routine is best explained by the flow chart below.

Start

#1 Initialization (Input $|E|$, the x-and y- mesh numbers. See Eq.(2.24):

$$x_{JMX} = x_{\max}, \quad x_{JMXG} = x_M, \quad x_{JMXGG} = x_G, \quad y_{JMYM} = y_M \text{ and } y_{JMYMM} = y_G$$

#2 Call PARAM (Assign values to key-indices)

Call FYFORM(PTABLE, YTAB, BESSEL)

(Set up the same p-table as used in the main program, construct the y-table for $0 \leq y \leq y_G$, and compute $y_\ell^{(t)}(y, p_k)$ of Eq.(2.2))

Read File LFRAM (Read in $R_{(L\ell, L'\ell')}^{acy} L_0$, a, b, c, d, γ of Eq.(2.22))

Call KOEF2(CLEBSH, F6J, NINEJ)

(Compute $N_\alpha^{(L_0 S_0)}$ of Eq.(I-3-4), $N_{\alpha\alpha', \lambda}$ of Eq.(2.10), and $\bar{N}_{\alpha\alpha'}^{(L_0 S_0)}$ of Eq.(2.20))

#3 Read File LFCHI (Read in $-\theta_\alpha(q, x)$ and $\phi_\alpha(q, x)$ of Eqs.(II-2.12) and (II-2.16))

#4 Call XTABLE (Set up the same x-table as used in the main program, and extend it to $x_{\max} \leq x \leq x_G$)

#5 (Compute various spline matrices by calling subroutine SPLINE)

#6 $\left\{ \begin{array}{l} \text{Construct } \rho_\alpha(x, y) \text{ of Eq.(2.1) for all } \alpha \text{ as follows:} \\ \text{First, extend } \phi_\alpha(q, x) \text{ out to } x_{\max} \leq x \leq x_G. \\ \text{Next, construct } \phi_\alpha(q, x)/x^L \text{ and compute the p-spline coefficients} \\ a_\alpha^{(t)}(x; p_k) \text{ of Eq.(2.3) by calling subroutine } \underline{\text{SPCOEF}}. \\ \text{Compute } \rho_\alpha(x, y) \text{ as per Eq.(2.4), extrapolate it to } x=0 \text{ assuming} \\ \text{the form } a+bx^2. \text{ The results are stored as 'RHO(JX, JY, } \alpha \text{)', 'JX'=1} \\ \text{and 'JY'=1 corresponding to } x=0 \text{ and } y=0. \end{array} \right.$

- (Do-loop over the momentum transfer Q)

#7 $\left\{ \text{Construct } I^{(t)}(Q, y_i) \text{ and } J_\lambda^{(t)}(Q, y_i) \text{ of Eqs.(2.7) and (2.14).} \right.$

```

- (Do-loop over the (grand) y-mesh points,  $y_i$ )
  (i) Set up fine y-mesh in the interval  $y_{i-1} \leq y \leq y_i$  (with  $y_0=0$ .)
      These are taken equidistant with the number of intervals 'NY'
      chosen so that there are approximately 30 points in one period
      of  $\sin(Qy)$ . If 'NY' is less than 10, it is set to 10.
  (ii) Process the Simpson quadratures in the interval  $y_{i-1} \leq y \leq y_i$  for
       $I^{(t)}(Q; y_i)$  and  $J_{\lambda}^{(t)}(Q; y_i)$ .
- (End of the do-loop over  $y_i$ )

  (iii) Multiply the (fine) y- mesh size 'DY' to the results obtained
      above to finish the Simpson quadratures. This completes the
      computation of  $I^{(t)}(Q; y_i)$  and  $J_{\lambda}^{(t)}(Q; y_i)$  which are stored as
      'FI1( $y_i, Q, t$ )' and 'FI2( $y_i, Q, t, \lambda$ )', respectively.

#8 Construct  $K_{\lambda}^{(t)}(Q; x_j)$  of Eq.(2.17).
- (Do-loop over the (grand) x-mesh points,  $x_j$ )
  (i) Set up fine x-mesh in the interval  $x_{j-1} \leq x \leq x_j$  (with  $x_0=0$ ). The
      fine x-mesh number 'NX' is chosen with the same principle as
      for 'NY' in #7 above.
  (ii) Process the Simpson quadrature in the interval  $x_{j-1} \leq x \leq x_j$  for
       $K_{\lambda}^{(t)}(Q; x_j)$ .
- (End of the do-loop over  $x_j$ )

  (iii) Multiply the (fine) x-mesh size 'DX' to the results above to
      finish the Simpson quadrature. This completes the computation
      of  $K_{\lambda}^{(t)}(Q, x_j)$  of Eq.(2.17). The results are stored as 'FK( $x_j,$ 
       $Q, t, \lambda$ )'.

- (End of the do-loop over Q)

#9 Call FORM1(SPCOEF) (Compute  $F_{\alpha\alpha}^{(1)}$ , as per Eqs.(2.5) to (2.8), and
      store the results as 'FF1(Q,  $\alpha$ )'.)
      Call FORM2(SPCOEF) (Compute  $F_{\alpha\alpha}^{(2)}$ , as per Eqs.(2.9) to (2.18), and
      store the results as 'FF2(Q,  $\alpha, \alpha$ )'.)

- (Do-loop over the initial state index  $\alpha$ )

#10 (Compute the double -spline coefficients of  $\rho_{\alpha}(x, y)$ )

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| #11 ( Compute the y-integrals in Eqs.(2.19b) and (2,27a).
|      Call NRHS3(PL,SPCOEF) (Compute  $Y_{\alpha\alpha}^{L0}(Q)$  of Eq.(2.19b).)
|      Call NRHS4(PL,SPCOEF) (Compute the y-integral in Eq.(2.27a).)
| )
```

'-(End of the do-loop over α')

```
#12 Call FORM (Compute  $F_{\alpha\alpha}^{(3)}$  of Eq.(2.19) and  $F_{\alpha\alpha}^{(4)}$  of Eq.(2.27))
```

```
#13 ( Compute  $\langle F_i^{uv} \rangle$  using Eq.(2.32) and construct  $F_a(Q)$  and  $F_b(Q)$  by
|      Eqs.(I-4-25 and 26).
| )
```

```
#14 ( Compute nucleon charge form factors using the formulas given by
|      Janssens et al.(Phys.Rev. 142('66) 992).
|      Calculate the  ${}^3\text{H}$  and  ${}^3\text{He}$  charge form factors by Eqs.(I-4-19,20 and
|      21).
| )
```

```
#15 ( Obtaine  $I_{kk}$ , and  $K_{kk}$ , by Eqs.(2.34) and (2.35), and compute
|      percentage probabilities as per Eqs.(I-A-11,13,14,17 and 18).
| )
```

Output the overall normalization constant 'FNORM'.

Stop

```

20.224  ** CODE NFORM ***                                LABEL
(09-30-82)  OPTIONS: INTER,OPT=1,NROUND,NDLR,ALC,MASTER,INLINE=0,LSTIN,LNO,NREST

10  C**** *** CODE NFORM ***
20  C**** TRITON CHARGE FORM FACTOR (WITH RSC5)
30  C**** REFERENCES (SRT=SCIENCE REPORT OF TOHOKU UNIV.)
40  C      I: FORMULATIONS (T.SAWADA+T.SASAKAWA)
50  C      SRT SER.8,VOL.3,NO.1(1982)1
60  C      II: PERFECT V (T.SASAKAWA+S.ISHIKAWA+T.SAWADA)
70  C      SRT(1982)
80  C      III: THIS REPORT
90  COMMON/AAAAA/XR(60),TR1(60),DT,AH2,JMX,JMXG,JMXGG
100 COMMON/BBBBB/YY(47),TY1(47),JMYM,JMYMM,AY2,FY(48,12,4,2)
110 COMMON/DDDDD/RHO(61,48,5),FI1(48,40,4),FI2(48,40,4,3),FK(60,40,4,
120 & 3)
130 COMMON/ZZZZZ/ZFIT(43),EZ(41,3),HZ(42),VZ(42),WZ(42),ZA(42),ZB(42)
140 & ,ZC(42),ZD(42)
150 COMMON/UUUUU/UFIT(47),EU(45,3),HU(46),VU(46),WU(46),UA(46),UB(46)
160 & ,UC(46),UD(46)
170 COMMON/XXXXX/XFIT(61),EX(59,3),HX(60),VX(60),WX(60),XA(60),XB(60)
180 & ,XC(60),XD(60)
190 COMMON/YYYYY/YFIT(48),EY(46,3),HY(47),VY(47),WY(47),YA(47),YB(47)
200 & ,YC(47),YD(47)
210 COMMON/CCCCC/DSP(4,4,60,48)
220 COMMON/FFFFF/FF1(40,5),FF2(40,5,5),FF3(40,5,5),FF4(40,5,5)
230 COMMON/RAMRAM/COEF(8,8),RAM(111),LA(111),LB(111),LC(111),LD(111),
240 & LG(111)
250 COMMON/MMMMM/MAL1(5),KST(14),KED(14),IGX(5),IG(5,5),IPX(5),
260 & LLF(19),LF(19),MSF(19),NR(19)
270 DIMENSION QQ(40),AQ(12),AK2(12),EXK(60,12,2)
280 DIMENSION PFIT(13),EP(11,3),HP(12),VP(12),WP(12),PA(2),PB(12),
290 & PC(12),PD(12)
300 DIMENSION PSI(60,12),FIT(61),SSUM(4,3),S(4),SUMX(4,3),AY(61,48,4)
310 & ,FCHHE3(40),FII(8,8),FKK(8,8),PROB(6)
320 & ,TSI(30,5,12),GSI(30,5,12),
330 & FCHH3(40),RSUM3(40,19),RSUM4(40,19),KEY(20),ZSUM(4),CF2(5,5,3),
340 & CF3(8,8),FAC(8)
350 DATA IQX/40/,
360 & QQ/ 0.0, 1.0, 1.5, 2.0, 2.5, 3.0, 3.25, 3.5, 3.7,
370 & 3.8, 3.9, 4.0, 4.1, 4.2, 4.3, 4.4, 4.5, 4.6,
380 & 4.75, 5.0, 5.25, 5.5, 5.75, 6.0, 6.25, 6.5,
390 & 6.75, 7.0, 7.25, 7.5, 7.75, 8.0, 8.25, 8.5,
400 & 8.75, 9.0, 9.25, 9.5, 9.75, 10.0/
410 DATA KEY/11,21,51,12,22,52,33,43,83,34,44,84,15,25,55,66,77, 38,
420 & 48,88/
430 C**** FOR 'KEY(20)', SEE TABLE 3 OF II. THESE ARE THE LOCATIONS OF
440 C**** TWENTY NON-ZERO MATRIX ELEMENTS OF THE 8*8 MATRIX IN
450 C**** TABLE II-3.
460 KOB=5
470 WRITE(6,1060) KOB
480 1060 FORMAT('1*** CODE NFORM *** TRITON CHARGE FORM FACTOR WITH RSC',I1)
490 C-01
500 BEI=6.80
510 JMX=30
520 JMXG=46
530 JMXGG=59
540 JMYM=42
550 SQ3=SQRT(3.)
560 C-02
570 CALL PARAM
580 CALL FYFORM(AQ,MALL)
590 LFRAM=21
600 REWIND LFRAM
610 READ(LFRAM) COEF,RAM,LA,LB,LC,LD,LG

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```

620          CALL KOEF2(CF2,CF3,FAC)
630          WRITE(6,1005) BEI,JMX,JMXG,JMXGG,JMYM,JMYMM
640          1005 FORMAT('OBEI=',1PE13.5,' JMX,JMXG,JMXGG,JMYM,JMYMM=',5I5)
650          C-03
660          LFCHI=27
670          REWIND LFCHI
680          READ(LFCHI) TSI, GSI
690          C DO 500 MS=1, KOB
700          C WRITE(6,4010) MS
710          C4010 FORMAT(///'1*** GSI(MS=',I3,')')
720          C DO 500 IM=1, MALL
730          C 500 WRITE(6,4020) IM, (GSI(J,MS,IM), J=1, JMX)
740          C4020 FORMAT(' IM=',I3/(2X,1P10E12.4))
750          HM=1./41.47
760          DO 5 I=1, MALL
770          1 5 AK2(I)=SQRT(HM*BEI+0.75*AQ(I)**2)
780          C-04
790          CALL XTABLE(30, JMXGG, XR, TR1, DT, 12., 6., 9., 0.3)
800          WRITE(6,1000) (XR(J), J=1, JMXGG)
810          1000 FORMAT(///'0XR=',1P10E12.5/(4X,1P10E12.5))
820          AH2=2.*DT
830          WRITE(6,1010) (YY(J), J=1, JMYMM)
840          1010 FORMAT('0YY=',1P10E12.5/(4X,1P10E12.5))
850          WRITE(6,1040) IQX, (QQ(I), I=1, IQX)
860          1040 FORMAT('0IQX=',I3/' QQ=',1P10E12.5/(4X,1P10E12.5))
870          C-05
880          C***** VARIOUS SPLINE MATRICES
890          PFIT(1)=0.
900          DO 10 I=1, MALL
910          1 10 PFIT(I+1)=AQ(I)
920          CALL SPLINE(PFIT, MALL-1, EP, HP, VP, WP, MALL-1, PA, PB, PC, PD)
930          XFIT(1)=0.
940          DO 20 I=1, JMXGG
950          1 20 XFIT(I+1)=XR(I)
960          CALL SPLINE(XFIT, JMXGG-1, EX, HX, VX, WX, 59, XA, XB, XC, XD)
970          YFIT(1)=0.
980          DO 30 I=1, JMYMM
990          1 30 YFIT(I+1)=YY(I)
1000          CALL SPLINE(YFIT, JMYMM-1, EY, HY, VY, WY, 46, YA, YB, YC, YD)
1010          ZFIT(1)=0.
1020          DO 35 I=1, JMYM
1030          1 35 ZFIT(I+1)=YY(I)
1040          CALL SPLINE(ZFIT, JMYM-1, EZ, HZ, VZ, WZ, 41, ZA, ZB, ZC, ZD)
1050          UFIT(1)=0.
1060          DO 25 I=1, JMXG
1070          1 25 UFIT(I+1)=XR(I)
1080          CALL SPLINE(UFIT, JMXG-1, EU, HU, VU, WU, 45, UA, UB, UC, UD)
1090          C-06
1100          C***** CONSTRUCT THE RHO-FUNCTION OF EQ.(III-2.1).
1110          X1Q=XR(1)**2
1120          X2Q=XR(2)**2
1130          XQ12=X2Q-X1Q
1140          C***** FIRST, EXTEND THE GSI-FUNCTIONS UP TO XR(JMXGG).
1150          J1=JMX
1160          DO 50 I=1, MALL
1170          1 DO 40 JX=J1, JMXGG
1180          2 AKX=AK2(I)*XR(JX)
1190          2 EXK(JX, I, 1)=EXP(-AKX)
1200          2 40 EXK(JX, I, 2)=EXK(JX, I, 1)*(3./AKX**2+3./AKX+1.)
1210          1 50 CONTINUE
1220          DO 160 MA=1, KOB
1230          1 LL=1
1240          1 IF(MA.EQ.3.OR.MA.EQ.5) LL=2
1250          1 DO 120 I=1, MALL

```

```

1260 2      ASYM=GSI(JMX,MA,I)/EXK(JMX,I,LL)*XR(JMX)
1270 2      DO 80 J=1,J1
1280 3      80 PSI(J,I)=GSI(J,MA,I)*XR(J)
1290 2      DO 90 J=J1,JMXGG
1300 3      90 PSI(J,I)=ASYM*EXK(J,I,LL)
1310 2      120 CONTINUE
1320 1 C      WRITE(6,2020) MA
1330 1 C2020 FORMAT('1*** PSI(MA=',I3,')')
1340 1 C      DO 125 I=1,MALL
1350 1 C 125 WRITE(6,2030) I,(PSI(J,I),J=1,JMXGG)
1360 1 C2030 FORMAT('OIM=',I3/(' ',1P10E12.4))
1370 1 C**** P-SPLINE OF 'PSI' DIVIDED BY X**(L+1)
1380 1      LLP=2*(LL/2)+1
1390 1      LP=1
1400 1      IF(MA.GE.4) LP=2
1410 1      DO 150 JX=1,JMXGG
1420 2      FIT(1)=0.
1430 2      DO 130 I=1,MALL
1440 3      130 FIT(I+1)=PSI(JX,I)/XR(JX)**LLP
1450 2      CALL SPCOEF(PFIT,FIT,MALL-1,EP,HP,VP,WP,PA,PB,PC,PD,MALL-1)
1460 2      DO 150 JY=1,JMYMM+1
1470 3      SUMA=0.
1480 3      DO 140 I=1,MALL
1490 4      140 SUMA=SUMA+PA(I)*FY(JY,I,1,LP)+PB(I)*FY(JY,I,2,LP)+PC(I)
1500 3      &      *FY(JY,I,3,LP)+PD(I)*FY(JY,I,4,LP)
1510 3      150 RHO(JX+1,JY,MA)=SUMA
1520 1 C**** EXTRAPOLATE THE 'RHO'-FUNCTION OF EQ.(III-2.1) TO X=0
1530 1 C**** ASSUMING THE FORM A+B*X**2
1540 1      DO 154 JY=1,JMYMM+1
1550 2      154 RHO(1,JY,MA)=(RHO(2,JY,MA)*X2Q-RHO(3,JY,MA)*X1Q)/XQ12
1560 1 C      WRITE(6,2040) MA
1570 1 C2040 FORMAT('1*** RHO(MA=',I3,')')
1580 1 C      DO 155 JY=1,JMYMM+1
1590 1 C 155 WRITE(6,2050) JY,(RHO(JX,JY,MA),JX=1,JMXGG+1)
1600 1 C2050 FORMAT('OJY=',I3/(' ',1P10E12.4))
1610 1      160 CONTINUE
1620 1 C**** CONSTRUCT THE FUNCTIONS OF Q; 'FI1','FI2', AND 'FK'.
1630 1      DO 270 IQ=1,IQX
1640 1 C-07
1650 1      Y0=0.
1660 1      DO 210 JY=1,JMYM
1670 2      Y1=YY(JY)
1680 2      NY=(Y1-Y0)*QQ(IQ)*5.
1690 2      NY=2*(NY/2)
1700 2      IF(NY.LT.10) NY=10
1710 2      DY=(Y1-Y0)/NY
1720 2      Y=Y0-DY
1730 2      CCC=1./3.
1740 2      DO 170 N=1,4
1750 3      ZSUM(N)=0.
1760 3      DO 170 K=1,3
1770 4      170 SSUM(N,K)=0.
1780 2      DO 190 I=1,NY+1
1790 3      DDD=CCC
1800 3      IF(I.EQ.1.OR.I.EQ.NY+1) DDD=DDD/2.
1810 3      Y=Y+DY
1820 3      YQ2=QQ(IQ)*Y/3.
1830 3      YQ1=2.*YQ2
1840 3      U=Y-YFIT(JY)
1850 3      FX=EXP(U)
1860 3      EXV=1./FX
1870 3      S(1)=(FX-EXV)/2.
1880 3      S(2)=S(1)+EXV

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```

1890      3      S(3)=U
1900      3      S(4)=1.
1910      3      IF(YQ1.LT.1.E-10) GO TO 171
1920      3      FJ0=SIN(YQ1)/YQ1
1930      3      GO TO 181
1940      3      171 FJ0=1.
1950      3      181 DO 182 N=1,4
1960      4      182 ZSUM(N)=ZSUM(N)+DDD*FJ0*S(N)
1970      3      IF(YQ2.LT.1.E-10) GO TO 175
1980      3      FJ0=SIN(YQ2)/YQ2
1990      3      FJ1=FJ0/YQ2-COS(YQ2)/YQ2
2000      3      FJ2=3.*FJ1/YQ2-FJ0
2010      3      FJ3=5.*FJ2/YQ2-FJ1
2020      3      FJ4=7.*FJ3/YQ2-FJ2
2030      3      GO TO 185
2040      3      175 FJ0=1.
2050      3      FJ2=0.
2060      3      FJ4=0.
2070      3      185 DO 180 N=1,4
2080      4      TEMP=DDD*S(N)
2090      4      SSUM(N,1)=SSUM(N,1)+TEMP*FJ0
2100      4      SSUM(N,2)=SSUM(N,2)+TEMP*FJ2
2110      4      180 SSUM(N,3)=SSUM(N,3)+TEMP*FJ4
2120      3      190 CCC=1.-CCC
2130      2      DO 200 N=1,4
2140      3      FI1(JY,IQ,N)=2.*DY*ZSUM(N)
2150      3      DO 200 K=1,3
2160      4      200 FI2(JY,IQ,N,K)=2.*DY*SSUM(N,K)
2170      2      210 Y0=Y1
2180      1      C-08
2190      1      X0=0.
2200      1      DO 260 JX=1,JMXG
2210      2      X1=XR(JX)
2220      2      NX=(X1-X0)*QQ(IQ)*5.
2230      2      NX=2*(NX/2)
2240      2      IF(NX.LT.10) NX=10
2250      2      DX=(X1-X0)/NX
2260      2      X=X0-DX
2270      2      CCC=1./3.
2280      2      DO 220 K=1,3
2290      3      DO 220 N=1,4
2300      4      220 SUMX(N,K)=0.
2310      2      DO 240 I=1,NX+1
2320      3      DDD=CCC
2330      3      IF(I.EQ.1.OR.I.EQ.NX+1) DDD=DDD/2.
2340      3      X=X+DX
2350      3      XQ1=QQ(IQ)*X/2.
2360      3      U=X-XFIT(JX)
2370      3      FX=EXP(U)
2380      3      EXV=1./FX
2390      3      S(1)=(FX-EXV)/2.
2400      3      S(2)=S(1)+EXV
2410      3      S(3)=U
2420      3      S(4)=1.
2430      3      IF(XQ1.LT.1.E-10) GO TO 225
2440      3      FJ0=SIN(XQ1)/XQ1
2450      3      FJ1=FJ0/XQ1-COS(XQ1)/XQ1
2460      3      FJ2=3.*FJ1/XQ1-FJ0
2470      3      FJ3=5.*FJ2/XQ1-FJ1
2480      3      FJ4=7.*FJ3/XQ1-FJ2
2490      3      GO TO 230
2500      3      225 FJ0=1.
2510      3      FJ2=0.
2520      3      FJ4=0.

```

```

2530   3   230 DO 235 N=1,4
2540   4       TEMP=DDD*S(N)
2550   4       SUMX(N,1)=SUMX(N,1)+TEMP*FJ0
2560   4       SUMX(N,2)=SUMX(N,2)+TEMP*FJ2
2570   4   235 SUMX(N,3)=SUMX(N,3)+TEMP*FJ4
2580   3   240 CCC=1.-CCC
2590   2       DO 250 N=1,4
2600   3       DO 250 K=1,3
2610   4   250 FK(JX,IQ,N,K)=2.*DX*SUMX(N,K)
2620   2   260 XO=X1
2630   1   270 CONTINUE
2640   C**** NOW, WE ARE READY TO COMPUTE 'FF1' AND 'FF2'.
2650   C-09
2660       CALL FORM1(IQX,QQ,KOB)
2670       CALL FORM2(IQX,QQ,CF2,KOB)
2680       DO 285 IQ=1,IQX
2690   1       DO 285 M=1,19
2700   2       RSUM3(IQ,M)=0.
2710   2   285 RSUM4(IQ,M)=0.
2720   C**** DO-LOOP OVER THE INITIAL STATE ALPHA'.
2730       DO 330 NA=1,KOB
2740   1 C**** COMPUTE THE DOUBLE-SPLINE COEFFICIENTS OF 'RHO'.
2750   1 C-10
2760   1       DO 300 JX=1,JMXGG+1
2770   2       DO 280 JY=1,JMYMM+1
2780   3   280 FIT(JY)=RHO(JX,JY,NA)
2790   2       CALL SPCOEF(YFIT,FIT,JMYMM-1,EY,HY,VY,WY,YA,YB,YC,YD,46)
2800   2       DO 290 JY=1,JMYMM
2810   3       AY(JX,JY,1)=YA(JY)
2820   3       AY(JX,JY,2)=YB(JY)
2830   3       AY(JX,JY,3)=YC(JY)
2840   3   290 AY(JX,JY,4)=YD(JY)
2850   2   300 CONTINUE
2860   1       DO 320 L=1,4
2870   2       DO 320 JY=1,JMYMM
2880   3       DO 310 JX=1,JMXGG+1
2890   4   310 FIT(JX)=AY(JX,JY,L)
2900   3       CALL SPCOEF(XFIT,FIT,JMXGG-1,EX,HX,VX,WX,XA,XB,XC,XD,59)
2910   3       DO 320 JX=1,JMXGG
2920   4       DSP(1,L,JX,JY)=XA(JX)
2930   4       DSP(2,L,JX,JY)=XB(JX)
2940   4       DSP(3,L,JX,JY)=XC(JX)
2950   4   320 DSP(4,L,JX,JY)=XD(JX)
2960   1 C**** COMPUTE THE Y-INTEGRALS IN EQS.(III-2.19B) AND (III-2.27A)
2970   1 C-11
2980   1       NAR=NA
2990   1       CALL NRHS3(IQX,QQ,RSUM3,NAR)
3000   1       CALL NRHS4(IQX,QQ,RSUM4,NAR)
3010   1   330 CONTINUE
3020   C**** COMPUTE 'FF3' AND 'FF4' OF EQS.(III-2.19) AND (III-2.27).
3030   C-12
3040       CALL FORM(CF3,RSUM3,IQX,FF3,KEY)
3050       CALL FORM(CF3,RSUM4,IQX,FF4,KEY)
3060       WRITE(6,1110)
3070   1110 FORMAT('0*** FF3 ***')
3080       DO 332 IQ=1,IQX
3090   1   332 WRITE(6,1115) QQ(IQ),((FF3(IQ,N,M),M=1,5),N=1,5)
3100   1115 FORMAT(' ',1P6E15.5/(' ',15X,1P5E15.5))
3110       WRITE(6,1120)
3120   1120 FORMAT('0*** FF4 ***')
3130       DO 334 IQ=1,IQX
3140   1   334 WRITE(6,1115) QQ(IQ),((FF4(IQ,N,M),M=1,5),N=1,5)
3150   C**** DO-LOOP OVER THE MOMENTUM TRANSFER

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3160          WRITE(6,2000)
3170      2000  FORMAT('1',7X,'QQ',9X,'FCHP',8X,'FCHN',9X,'FA',10X,'FB',7X,
3180          & 'FCHHE3',7X,'FCHH3',9X,'SS',10X,'AA',10X,'AS',10X,'SA')
3190          DO 370 IQ=1,IQX
3200      1 C*** COMPUTE THE AVERAGE OVER F-SUB-UV USING EQS.(I11-2.32A,B,C,D)
3210      1 C-13
3220      1      F1SS=FF1(IQ,2)+FF1(IQ,3)+FF1(IQ,4)+FF1(IQ,5)
3230      1      F1AA=FF1(IQ,1)
3240      1      F2SS=0.
3250      1      F3SS=0.
3260      1      F4SS=0.
3270      1      DO 340 NA=2,KOB
3280      2      DO 340 NB=2,KOB
3290      3      F2SS=F2SS+FF2(IQ,NA,NB)
3300      3      F3SS=F3SS+FF3(IQ,NA,NB)
3310      3      340 F4SS=F4SS+FF4(IQ,NA,NB)
3320      1      F2AA=FF2(IQ,1,1)
3330      1      F3AA=FF3(IQ,1,1)
3340      1      F4AA=FF4(IQ,1,1)
3350      1      F3AS=0.
3360      1      F3SA=0.
3370      1      F4AS=0.
3380      1      F4SA=0.
3390      1      DO 350 NA=2,KOB
3400      2      F3AS=F3AS+FF3(IQ,1,NA)
3410      2      F3SA=F3SA+FF3(IQ,NA,1)
3420      2      F4AS=F4AS+FF4(IQ,1,NA)
3430      2      350 F4SA=F4SA+FF4(IQ,NA,1)
3440      1 C**** COMPUTE 'FA' AND 'FB' AS PER EQS.(I-4.25,26).
3450      1      FA=F1SS+0.5*F2SS+1.5*F2AA-2.*F3SS+2.*SQ3*F3SA +0.5*F4SS+
3460      1      &      SQ3*F4SA-1.5*F4AA
3470      1      FB=F1AA+1.5*F2SS+0.5*F2AA-2.*F3AA-2.*SQ3*F3AS -1.5*F4SS+
3480      1      &      SQ3*F4SA+0.5*F4AA
3490      1 C-14
3500      1 C**** NUCLEON CHARGE FORM FACTOR (JANSSENS ET AL, PHYS.REV.142('66) 992)
3510      1      QS=QQ(IQ)**2
3520      1      GES=0.5*(2.5/(1.+QS/15.7)-1.6/(1.+QS/26.7)+0.1)
3530      1      GEV=0.5*(1.16/(1.+QS/8.19)-0.16)
3540      1      FCHP=GES+GEV
3550      1      FCHN=GES-GEV
3560      1 C**** HE-3 CHARGE FORM FACTOR (TIMES 2)
3570      1      FL=0.5*(3.*FA+FB)
3580      1      FQ=2.*FB
3590      1      FCHHE3(IQ)=2.*FCHP*FL+FCHN*FQ
3600      1      FCHH3(IQ) =2.*FCHN*FL+FCHP*FQ
3610      1      IF(IQ.EQ.1) GO TO 335
3620      1      FCHHE3(IQ)=FCHHE3(IQ)/FCHHE3(1)
3630      1      FCHH3(IQ)=FCHH3(IQ)/FCHH3(1)
3640      1      335 WRITE(6,2010) QQ(IQ),FCHP,FCHN,FA,FB,FCHHE3(IQ),FCHH3(IQ),
3650      1      &      F1SS,F1AA
3660      1      2010 FORMAT(' ',1P9E12.4)
3670      1      WRITE(6,2011) F2SS,F2AA,F3SS,F3AA,F3AS,F3SA,F4SS,F4AA,F4AS,
3680      1      &      F4SA
3690      1      2011 FORMAT(' ',84X,1P2E12.4,2('/ ',84X,1P4E12.4))
3700      1      370 CONTINUE
3710      C**** PERCENTAGE PROBABILITIES
3720      C-15
3730      C**** FIRST, COMPUTE I-SUB-KK' AND K-SUB-KK' OF EQS.(I11-2.34) AND
3740      C**** (I11-2.35) (SEE ALSO TABLE 3 OF II FOR K-SUB-KK').
3750      DO 375 K=1,8
3760      1      DO 375 KP=1,8
3770      2      FII(K,KP)=0.
3780      2      375 FKK(K,KP)=0.
3790      DO 355 K=1,4

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3800 1 355 FII(K,K)=FAC(K)**2*FF2(1,K,K)/CF2(K,K,1)
3810 TEMP=FF2(1,5,5)/CF2(5,5,1)
3820 DO 365 K=5,8
3830 1 365 FII(K,K)=FAC(K)**2*TEMP
3840 FII(1,2)=FAC(1)*FAC(2)*FF2(1,1,2)/CF2(1,2,1)
3850 FII(2,1)=FAC(2)*FAC(1)*FF2(1,2,1)/CF2(2,1,1)
3860 DO 385 MM=1,20
3870 1 M=MM
3880 1 IF(MM.GE.17) M=MM-1
3890 1 KA=KEY(MM)/10
3900 1 KB=KEY(MM)-10*KA
3910 1 385 FKK(KA,KB)=FAC(KA)*FAC(KB)*RSUM3(1,M)
3920 WRITE(6,3000) ((FII(KA,KB),KB=1,8),KA=1,8)
3930 3000 FORMAT('OFII'/(5X,1P8E13.5))
3940 WRITE(6,3010) ((FKK(KA,KB),KB=1,8),KA=1,8)
3950 3010 FORMAT('OFKK'/(5X,1P8E13.5))
3960 C**** NOW, COMPUTE PERCENTAGE PROBABILITIES AS PER EQS. (I-A-11,13,14,17,
3970 C**** AND 18)
3980 PROB(1)=1.5*(FII(1,1)+FII(2,2)+FII(5,5)-2.*FII(1,2)) +3.*(FKK(1,1)
3990 & +FKK(2,2)+FKK(5,5)+FKK(2,5)+FKK(5,2) -FKK(1,2)-FKK(1,5)-FKK(2,1)
4000 & -FKK(5,1))
4010 PROB(2)=1.5*FII(6,6)+3.*FKK(6,6)
4020 PROB(3)=0.75*(FII(1,1)+FII(2,2)+FII(5,5)+2.*FII(1,2) -FKK(1,1)-
4030 & FKK(2,2)-FKK(5,5)-FKK(2,5)-FKK(5,2) -FKK(1,2)-FKK(1,5)-FKK(2,1)-
4040 & FKK(5,1))
4050 PROB(4)=0.75*(FII(6,6)-FKK(6,6))
4060 PROB(5)=1.5*(FII(7,7)-FKK(7,7))
4070 PROB(6)=1.5*(FII(3,3)+FII(4,4)+FII(8,8)-FKK(3,3)-FKK(4,4) -FKK(8,
4080 & 8)-FKK(3,4)-FKK(3,8)-FKK(4,3)-FKK(4,8)-FKK(8,3) -FKK(8,4))
4090 DO 390 K=3,6
4100 1 390 PROB(K)=2.*PROB(K)
4110 FNORM=0.
4120 DO 400 K=1,6
4130 1 400 FNORM=FNORM+PROB(K)
4140 DO 410 K=1,6
4150 1 410 PROB(K)=PROB(K)/FNORM
4160 WRITE(6,3020) FNORM,(PROB(K),K=1,6)
4170 3020 FORMAT('OFNORM=',1PE13.5/' PROB=',1P6E13.5)
4180 STOP
4190 END
4200 SUBROUTINE FYFORM(AQ,MALL)
4210 C**** THIS COMPUTE (I) THE P-TABLE, (II) THE Y-TABLE, AND
4220 C**** (III) THE Y-FUNCTION OF EQ.(III-2.2).(SEE 'CODE FYF15'
4230 C**** FOR DETAILS)
4240 COMMON/BBBBB/YY(47),TY1(47),JMYM,JMYMM,AY2,FY(48,12,4,2)
4250 DIMENSION AQ(*),AQ1(12),U(48,2),S(4),SUM(48,4,2)
4260 C-01
4270 WRITE(6,1000)
4280 1000 FORMAT('O*** FYFORM ***')
4290 MALL=12
4300 IMX=6
4310 PIMX=0.750428
4320 CALL PTABLE(AQ,AQ1,DK,PIMX,IMX,MALL)
4330 JMY=47
4340 JMYMM=JMY
4350 CALL YTAB(YY,TY1,JMY,2.,30.,18.,0.3,DTY)
4360 AY2=2.*DTY
4370 C**** DO-LOOP OVER THE GRAND P-MESH.
4380 P0=0.
4390 DO 150 JM=1,MALL
4400 1 JMR=JM
4410 1 P1=AQ(JM)
4420 1 C-02
4430 1 C**** DECIDE THE FINER P'-MESH FOR THE P' INTEGRATION.

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4440 1      NP=INT((P1-P0)*YY(JMY)/0.3)
4450 1      NP=2*(NP/2)
4460 1      IF(NP.LT.4) NP=4
4470 1      NP1=NP+1
4480 1      DP=(P1-P0)/NP
4490 1  C-03
4500 1  C**** INITIALIZE THE P' INTEGRATION.
4510 1      IF(JM.EQ.1) GO TO 30
4520 1      DO 20 LL=1,2
4530 2      DO 20 JY=1,JMY+1
4540 3      SUM(JY,1,LL)=0.
4550 3      SUM(JY,2,LL)=U(JY,LL)/6.
4560 3      SUM(JY,3,LL)=0.
4570 3      SUM(JY,4,LL)=SUM(JY,2,LL)
4580 3      20 CONTINUE
4590 1      GO TO 50
4600 1      30 DO 40 JY=1,JMY+1
4610 2      DO 40 LL=1,2
4620 3      DO 40 N=1,4
4630 4      SUM(JY,N,LL)=0.
4640 4      40 CONTINUE
4650 1      50 P=P0
4660 1  C-04
4670 1      CCC=2./3.
4680 1  C**** DO LOOP OVER THE FINER P-MESH(I.E.,P')
4690 1      DO 70 JP=2,NP1
4700 2      DDD=CCC
4710 2      IF(JP.EQ.NP1) DDD=DDD/2.
4720 2      P=P+DP
4730 2  C**** CALCULATE THE SPECTATOR FUNCTION 'U' AT P' AND AT EVERY 'Y'.
4740 2  C**** U(Y)=F(P,Y)/Y**L, WHERE F(P,Y) IS THE NORMALIZED SPHERICAL
4750 2  C**** BESSEL FUNCTION.
4760 2      CALL BESSEL(P,U,YY,JMY)
4770 2  C**** FIND THE SPLINE FUNCTION 'S' AND CARRY OUT THE SIMPSON QUADRATOR
4780 2  C**** FOR THE P' INTEGRATION.
4790 2      EX=EXP(P-P0)
4800 2      S(1)=(EX-1./EX)/2.
4810 2      S(2)=S(1)+1./EX
4820 2      S(3)=P-P0
4830 2      S(4)=1.
4840 2      DO 60 LL=1,2
4850 3      DO 60 JY=1,JMY+1
4860 4      DO 60 N=1,4
4870 5      SUM(JY,N,LL)=SUM(JY,N,LL)+DDD*U(JY,LL)*S(N)
4880 5      60 CONTINUE
4890 2      CCC=1.-CCC
4900 2      70 CONTINUE
4910 1  C-05
4920 1      DO 80 LL=1,2
4930 2      DO 80 JY=1,JMY+1
4940 3      DO 80 N=1,4
4950 4      FY(JY,JM,N,LL)=2.*DP*SUM(JY,N,LL)
4960 4      80 CONTINUE
4970 1      P0=P1
4980 1      150 CONTINUE
4990 1  C      DO 400 LL=1,2
5000 1  C      DO 400 JM=3,MALL,3
5010 1  C      WRITE(6,4001) JM,JMYMM
5020 1  C4001  FORMAT('0*** JM=' I3,' *** JMYMM=' I3)
5030 1  C      DO 410 M=1,4
5040 1  C 410  WRITE(6,4002) M,(FY(JY,JM,M,LL),JY=1,JMY+1)
5050 1  C4002  FORMAT('0FY(M=' I2,')'/' (' ',1P10E12.4))
5060 1  C 400  CONTINUE
5070 1      RETURN
5080 1      END

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5090      SUBROUTINE YTAB(YY,YR1,JMY,YEM,YM,YTM,TYC,DTY)
5100      C**** Y-TABLE. SEE EQS.(II-8.2) AND (II-8.3).
5110      DIMENSION YY(*),YR1(*)
5120      SYO=(YTM-TYC*YM)*YM/(YEM*YM-YTM)
5130      TYO=YEM*SYO/TYC
5140      DTY=YTM/JMY
5150      CTO=TYC*TYO
5160      CSO2=2.*TYC*SYO
5170      CSO4=2.*CSO2
5180      DTDYO=TYC*TYO/SYO
5190      T=0.
5200      DO 40 I=1,JMY
5210      1      T=T+DTY
5220      1      A=CTO-T
5230      1      T1=SQRT(A*A+CSO4*T)
5240      1      YY(I)=(-A+T1)/(2.*TYC)
5250      1      DTDY=TYC*(YY(I)**2+2.*SYO*YY(I)+TYO*SYO)/(YY(I)+SYO)**2
5260      1 C      DTDY2=TYC*2.*SYO*(SYO-TYO)/(YY(I)+SYO)**3
5270      1      YR1(I)=1./DTDY
5280      1 C      YR2(I)=YR1(I)**2
5290      1 C      YR5(I)=-DTDY2*YR2(I)
5300      1      40 CONTINUE
5310      WRITE(6,1000) JMY,YEM,YM,YTM,TYC,DTY,SYO,TYO
5320      1000  FORMAT('OJMY=',I5,' YEM,YM,YTM,TYC=',1P4E13.5/'ODTY,SYO,TYO=',
5330      &      1P3E13.5)
5340      C      WRITE(6,1010) (YY(I),I=1,JMY)
5350      C1010  FORMAT('OYY=',1P10E13.5/(4X,1P10E13.5))
5360      RETURN
5370      END

5380      SUBROUTINE BESSEL(P,U,YR,JMYM)
5390      C**** COMPUTE THE NORMALIZED BESSEL FUNCTION FJL(P,Y) DIVIDED BY Y**L
5400      DIMENSION U(48,2),YR(*)
5410      DATA PI2/7.9788456E-01/
5420      DO 20 J=1,JMYM
5430      1      I=J+1
5440      1      Z=P*YR(J)
5450      1      IF(Z.GT.1.E-5) GO TO 10
5460      1      U(I,1)=1.-Z**2/6.
5470      1      U(I,2)=(1.-Z**2/14.)/15.
5480      1      GO TO 20
5490      1      10 SN=SIN(Z)
5500      1      CO=COS(Z)
5510      1      U(I,1)=SN/Z
5520      1      U(I,2)=((3./Z**2-1.)*SN/Z-(3./Z**2)*CO)/Z**2
5530      1      20 CONTINUE
5540      1      U(1,1)=1.
5550      1      U(1,2)=1./15.
5560      1      FAC=P*PI2
5570      1      FAQ=FAC*P**2
5580      1      DO 30 J=1,JMYM
5590      1      I=J+1
5600      1      U(I,1)=FAC*U(I,1)
5610      1      30 U(I,2)=FAQ*U(I,2)
5620      1      U(1,1)=FAC*U(1,1)
5630      1      U(1,2)=FAQ*U(1,2)
5640      1      RETURN
5650      1      END

5660      SUBROUTINE KOEF2(CF2,CF3,FAC)
5670      C**** 'FAC(I)'(I=1 TO 8) = THE N COEFFICIENTS OF EQ.(II-3.3).
5680      C****      (SEE TABLE 1 OF II FOR THE INDEX I).
5690      C**** 'CF2(N,M,L)'(L=1 TO 3) = THE N COEFFICIENTS OF EQ.(III-2.10) FOR
5700      C****      STATES(N,M). L=1,2,3 FOR LAMBDA=0,2,4.
5710      C**** 'CF3(I,I)'(I,I=1 TO 8) = THE N-BAR COEFFICIENTS OF EQ.(III-2.20).
5720      C****      (SEE TABLE 3 OF II FOR THE INDICES I

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5730          C****                                AND I'.)
5740          DIMENSION CF2(5,5,3),CF3(8,8),FAC(8),FACLOG(100),LL(5),L(5),JJ(5)
5750          & ,J(5),IS(5),LLL(8),KSS(8),NLS(5),M(9),LAMBDA(3),SUMLS(3),ILS(5)
5760          DATA LL/0,0,2,0,2/, L/0,0,0,2,2/, JJ/0,1,1,1,1/, J/1,1,1,3,3/,
5770          & IS/0,1,1,1,1/, LLL/0,0,2,2,0,1,1,2/, KSS/1,1,3,3,1,1,3,3/,
5780          & NLS/1,2,3,4,8/, ILS/1,2,3,4,5/, LAMBDA/0,2,4/
5790          DO 10 NA=1,5
5800          1    DO 10 NB=1,5
5810          2    DO 10 NL=1,3
5820          3    10 CF2(NA,NB,NL)=0.
5830          C**** FIRST, COMPUTE THE N FACTOR OF EQ.(II-3.3)
5840          FACLOG(1)=0.
5850          FACLOG(2)=0.
5860          F1=1.
5870          DO 15 I=3,100
5880          1    F1=F1+1.
5890          1    15 FACLOG(I)=FACLOG(I-1)+ALOG(F1)
5900          DO 20 NA=1,5
5910          1    JJA=2*JJ(NA)
5920          1    JA=J(NA)
5930          1    M(1)=2*LL(NA)
5940          1    M(2)=2*L(NA)
5950          1    M(3)=2*IS(NA)
5960          1    M(4)=1
5970          1    M(7)=JJA
5980          1    M(8)=JA
5990          1    M(9)=1
6000          1    NLSA=NLS(NA)
6010          1    ILSA=ILS(NA)
6020          1    DO 20 K=ILSA,NLSA
6030          2    LLLA=2*LLL(K)
6040          2    KSSA=KSS(K)
6050          2    FAC(K)=SQRT((JJA+1.)*(JA+1.)*(LLLA+1.)*(KSSA+1.))
6060          2    M(5)=LLLA
6070          2    M(6)=KSSA
6080          2    CALL NINEJ(FACLOG, M,UNINE)
6090          2    20 FAC(K)=UNINE*FAC(K)
6100          WRITE(6,1000) (FAC(K),K=1,8)
6110          1000 FORMAT('0*** KOEF2 ***'/' FAC=',1P8E13.5)
6120          C**** NEXT, COMPUTE THE N FACTOR OF EQ.(III-2.10)
6130          DO 70 NA=1,5
6140          1    LLA=2*LL(NA)
6150          1    LA=2*L(NA)
6160          1    NLSA=NLS(NA)
6170          1    ILSA=ILS(NA)
6180          1    DO 70 NB=1,5
6190          2    LLB=2*LL(NB)
6200          2    LB=2*L(NB)
6210          2    NLSB=NLS(NB)
6220          2    ILSB=ILS(NB)
6230          2    DO 30 NL=1,3
6240          3    30 SUMLS(NL)=0.
6250          2    DO 50 KA=ILSA,NLSA
6260          3    DO 50 KB=ILSB,NLSB
6270          4    IF(LLL(KA).NE.LLL(KB)) GO TO 50
6280          4    IF(KSS(KA).NE.KSS(KB)) GO TO 50
6290          4    DO 40 NL=1,3
6300          5    LAM=2*LAMBDA(NL)
6310          5    CALL F6J(FACLOG,LLA,LAM,2*LLL(KA),LB,LLB,LA,RAC)
6320          5    40 SUMLS(NL)=SUMLS(NL)+FAC(KA)*FAC(KB)*(-1.)**LLL(KA)*RAC
6330          4    50 CONTINUE
6340          2    FAK=(-1.)**((LA+LLB)/2)*SQRT((LA+1.)*(LLA+1.))
6350          2    DO 60 NL=1,3
6360          3    LAM=2*LAMBDA(NL)

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6370      3      CALL CLEBSH(LA,LAM,LB,0,0,0,FACLOG,CLEBA)
6380      3      CALL CLEBSH(LLA,LAM,LLB,0,0,0,FACLOG,CLEBB)
6390      3      60 CF2(NA,NB,NL)=FAK*CLEBA*CLEBB*SUMLS(NL)*(LAM+1.)
6400      2      70 CONTINUE
6410          DO 80 NL=1,3
6420      1      WRITE(6,1010) NL
6430      1 1010 FORMAT('OCF2(NL=',I2,')')
6440      1      80 WRITE(6,1020) ((CF2(NA,NB,NL),NB=1,5),NA=1,5)
6450      1020 FORMAT((5X,1P5E15.5))
6460      C**** FINALLY, COMPUTE THE N-BAR OF EQ.(III-2.20)
6470          DO 85 KA=1,8
6480      1      DO 85 KB=1,8
6490      2      85 CF3(KA,KB)=0.
6500          DO 100 NA=1,5
6510      1      ISA=2*IS(NA)
6520      1      NLSA=NLS(NA)
6530      1      ILSA=ILS(NA)
6540      1      DO 100 NB=1,5
6550      2      ISB=2*IS(NB)
6560      2      NLSB=NLS(NB)
6570      2      ILSB=ILS(NB)
6580      2      DO 90 KA=ILSA,NLSA
6590      3      DO 90 KB=ILSB,NLSB
6600      4      IF(LLL(KA).NE.LLL(KB)) GO TO 90
6610      4      IF(KSS(KA).NE.KSS(KB)) GO TO 90
6620      4      CALL F6J(FACLOG,1,1,KSS(KA),1,ISB,ISA,RAC)
6630      4      CF3(KA,KB)=(-1.)*IS(NA)*SQRT((ISA+1.)*(ISB+1.))
6640      4      &          *RAC *FAC(KA)*FAC(KB)
6650      4      90 CONTINUE
6660      2 100 CONTINUE
6670          WRITE(6,1030) ((CF3(KA,KB),KB=1,8),KA=1,8)
6680      1030 FORMAT('OCF3'/(5X,1P8E15.5))
6690          RETURN
6700          END
6710          SUBROUTINE PARAM
6720      C**** ASSIGN VALUES TO KEY-INDICES
6730          COMMON/MMMMM/MAL1(5),KST(14),KED(14),IGX(5),IG(5,5),IPX(5),LLF(19)
6740          & , LF(19),MSF(19),NR(19)
6750          DIMENSION JAL1(5),JST(14),JED(14),JGX(5),JG(5,5),JPX(5),JLF(19),
6760          & JF(19),JSF(19),JR(19)
6770          EQUIVALENCE (MAL1(1),JAL1(1)),(KST(1),JST(1)),(KED(1),JED(1)),
6780          & (IGX(1),JGX(1)),(IG(1,1),JG(1,1)),(IPX(1),JPX(1)),(LLF(1),
6790          & JLF(1)),(LF(1),JF(1)),(MSF(1),JSF(1)),(NR(1),JR(1))
6800      C**** FOR 'IGX,IG,IPX,MAL1,KST AND KED', SEE THE COMMENT CARDS
6810      C**** AT THE BEGINNING OF SUBROUTINE RHS OF THE MAIN PROGRAM.
6820      C**** FOR THE QUANTITIES BELOW, SEE TABLE 2 OF II.
6830      C**** NR(19) = N(M) :THE KEY-INDEX N
6840      C**** LF(19) = THE FINAL L (SPECTATOR)
6850      C**** LLF(19) = THE FINAL L (INTERACTING PAIR)
6860      C**** MSF(19) = THE FINAL STATE INDEX (ALPHA)
6870          DATA JGX/2,2,4,4,5/,IG/0,2,3*0,0,2,3*0,0,1,2,3,0,0,1,2,3,0,0,1,2,
6880          & 3,4/,JPX/3,3,3,3,7/,JAL1/1,4,7,10,13/,JST/1,2,3,6,9,13,16,
6890          & 19,23,33,52,69,81,93/,JED/1,2,5,8,12,15,18,22,32,51,68,80,92,
6900          & 111/,JR/1,1,2,1,1,2,3,4,5,6,7,8,9,9,10,11,12,13,14/,JF/0,0,2,
6910          & 0,0,2,0,2,2,0,2,2,0,2,2,0,2,2/ JLF/0,0,2,0,2,2,0,2,2,0,2,0,2,0,2,0,
6920          & 0,2,2,2,0,2/,JSF/1,2,5,1,2,5,3,4,5,3,4,5,1,2,5,5,3,4,5/
6930          RETURN
6940          END
6950          SUBROUTINE FORM1(IQX,QQ,KOB)
6960      C**** COMPUTE 'FF1(Q,N)'(N=1 TO 5) OF EQ.(III-2.5A)
6970          COMMON/AAAAA/XR(60),TR1(60),DT,AH2,JMX,JMXG,JMXGG
6980          COMMON/BBBBB/YY(47),TY1(47),JMYM,JMYMM,AY2,FY(48,12,4,2)
6990          COMMON/DDDDD/RHO(61,48,5),FI1(48,40,4),FI2(48,40,4,3),FK(60,40,4,
7000          & 3)

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7010      COMMON/ZZZZZ/ZFIT(43),EZ(41,3),HZ(42),VZ(42),WZ(42),ZA(42),ZB(42)
7020      & ,ZC(42),ZD(42)
7030      COMMON/FFFFFF/FF1(40,5),FF2(40,5,5),FF3(40,5,5),FF4(40,5,5)
7040      DIMENSION FIT(61),QQ(*),LL(5),L(5)
7050      DATA LL/0,0,2,0,2/, L/0,0,0,2,2/
7060      C**** DO-LOOP OVER THE STATE
7070      DO 50 NA=1,KOB
7080      1 C**** INTEGRATION OVER X OF EQ.(III-2.5B)
7090      1      KX=2*LL(NA)+2
7100      1      KY=2*L(NA)+2
7110      1      DO 20 JY=1,JMYM
7120      2      SUM=0.
7130      2      CCC=2./3.
7140      2      DO 10 JX=1,JMXG
7150      3      SUM=SUM+TR1(JX)*RHO(JX+1,JY+1,NA)**2*CCC*XR(JX)**KX
7160      3      10 CCC=1.-CCC
7170      2      20 FIT(JY+1)=SUM*AH2*YY(JY)**KY
7180      1      FIT(1)=0.
7190      1 C**** Y-SPLINE COEFFICIENTS OF FIT.
7200      1      CALL SPCOEF(ZFIT,FIT,JMYM-1,EZ,HZ,VZ,WZ,ZA,ZB,ZC,ZD,41)
7210      1 C**** CARRY OUT THE Y-INTEGRATION BY MEANS OF SPLINE. (SEE EQ.
7220      1 C**** (III-2.8))
7230      1      DO 40 IQ=1,IQX
7240      2      SUM=0.
7250      2      DO 30 JY=1,JMYM
7260      3      SUM=SUM+ZA(JY)*FI1(JY,IQ,1)+ZB(JY)*FI1(JY,IQ,2)+ZC(JY)
7270      3      &      *FI1(JY,IQ,3 )+ZD(JY)*FI1(JY,IQ,4)
7280      3      30 CONTINUE
7290      2      FF1(IQ,NA)=SUM
7300      2      40 CONTINUE
7310      1      50 CONTINUE
7320      WRITE(6,1000)
7330      1000 FORMAT('O*** FF1 ***')
7340      DO 60 IQ=1,IQX
7350      1      60 WRITE(6,1010) QQ(IQ),(FF1(IQ,NA),NA=1,KOB)
7360      1010 FORMAT(' ',1P6E15.5)
7370      RETURN
7380      END
7390      SUBROUTINE FORM2(IQX,QQ,CF2,KOB)
7400      C**** COMPUTE 'FF2(Q,N,M)' (N,M=1 TO 5) OF EQ.(III-2.9A).
7410      COMMON/AAAAA/XR(60),TR1(60),DT,AH2,JMX,JMXG,JMXGG
7420      COMMON/BBBBB/YY(47),TY1(47),JMYM,JMYMM,AY2,FY(48,12,4,2)
7430      COMMON/DDDDD/RHO(61,48,5),FI1(48,40,4),FI2(48,40,4,3),FK(60,40,4,
7440      &      3)
7450      COMMON/ZZZZZ/ZFIT(43),EZ(41,3),HZ(42),VZ(42),WZ(42),ZA(42),ZB(42)
7460      & ,ZC(42),ZD(42)
7470      COMMON/UUUUU/UFIT(47),EU(45,3),HU(46),VU(46),WU(46),UA(46),UB(46)
7480      & ,UC(46),UD(46)
7490      COMMON/FFFFFF/FF1(40,5),FF2(40,5,5),FF3(40,5,5),FF4(40,5,5)
7500      COMMON/RAMRAM/COEF(8,8),RAM(111),LA(111),LB(111),LC(111),LD(111),
7510      &      LG(111)
7520      DIMENSION QQ(*),CF2(5,5,3),FIT(61),AZ(48,4),SUML(3),G(40,60,3),
7530      &      LL(5),L(5),IS(5)
7540      DATA LL/0,0,2,0,2/, L/0,0,0,2,2/, IS/0,1,1,1,1/
7550      C**** DO-LOOP OVER THE STATE INDICES
7560      DO 100 NA=1,KOB
7570      1      DO 90 NB=1,KOB
7580      2      DO 5 IQ=1,IQX
7590      3      5-FF2(IQ,NA,NB)=0.
7600      2 C**** Y-SPLINE OF THE F-FUNCTION OF EQ.(III-2.12)
7610      2      IP=LL(NA)+2+LL(NB)
7620      2      JP=L(NA)+2+L(NB)
7630      2      DO 30 JX=1,JMXG

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7640 3      XIP=XR(JX)**IP
7650 3      DO 10 JY=1,JMYM
7660 4      10 FIT(JY+1)=RHO(JX+1,JY+1,NA)*RHO(JX+1,JY+1,NB)*XIP
7670 3      &          *YY(JY)**JP
7680 3      FIT(1)=0.
7690 3      CALL SPCOEF(ZFIT,FIT,JMYM-1,EZ,HZ,VZ,WZ,ZA,ZB,ZC,ZD,41)
7700 3      DO 20 JY=1,JMYM
7710 4      AZ(JY,1)=ZA(JY)
7720 4      AZ(JY,2)=ZB(JY)
7730 4      AZ(JY,3)=ZC(JY)
7740 4      20 AZ(JY,4)=ZD(JY)
7750 3 C**** FIND THE G-FUNCTION BY EQ.(III-2.15)
7760 3      DO 25 IQ=1,IQX
7770 4      DO 25 NL=1,3
7780 5      G(IQ,JX,NL)=0.
7790 5      DO 25 JY=1,JMYM
7800 6      DO 25 K=1,4
7810 7      25 G(IQ,JX,NL)=G(IQ,JX,NL)+AZ(JY,K)*FI2(JY,IQ,K,NL)
7820 3      30 CONTINUE
7830 2 C**** X-SPLINE OF THE G-FUNCTION (SEE EQ.(III-2.16))
7840 2      DO 80 IQ=1,IQX
7850 3      DO 60 NL=1,3
7860 4      FIT(1)=0.
7870 4      DO 40 JX=1,JMXG
7880 5      40 FIT(JX+1)=G(IQ,JX,NL)
7890 4      CALL SPCOEF(UFIT,FIT,JMXG-1,EU,HU,VU,WU,UA,UB,UC,UD,45)
7900 4 C**** X-SPLINE INTEGRATION BY EQ.(III-2.18)
7910 4      SUMX=0.
7920 4      DO 50 JX=1,JMXG
7930 5      50 SUMX=SUMX+UA(JX)*FK(JX,IQ,1,NL)+UB(JX)*FK(JX,IQ,2,NL)
7940 4      &          +UC(JX)*FK(JX,IQ,3,NL)+UD(JX)*FK(JX,IQ,4,NL)
7950 4      SUML(NL)=SUMX
7960 4      60 CONTINUE
7970 3 C**** SUMMATION OVER LAMBDA IN EQ.(III-2.9A)
7980 3      SUM=0.
7990 3      IF(IS(NA).NE.IS(NB)) GO TO 80
8000 3      T=MAX(ABS(CF2(NA,NB,1)),ABS(CF2(NA,NB,2)),ABS(CF2(NA,NB,3)))
8010 3      IF(T.LT.1.E-10) GO TO 80
8020 3      DO 70 NL=1,3
8030 4      70 SUM=SUM+SUML(NL)*CF2(NA,NB,NL)
8040 3      80 FF2(IQ,NA,NB)=SUM
8050 2      90 CONTINUE
8060 1      100 CONTINUE
8070      WRITE(6,1000)
8080      1000 FORMAT('0*** FF2 ***')
8090      DO 110 IQ=1,IQX
8100 1      110 WRITE(6,1010) QQ(IQ),((FF2(IQ,NA,NB),NB=1,KOB),NA=1,KOB)
8110      1010 FORMAT(' ',1P6E15.5/(' ',15X,1P5E15.5))
8120      RETURN
8130      END
8140      SUBROUTINE NRHS3(IQX,QQ,RSUM,MS)
8150 C**** COMPUTE THE Y-FUNCTION OF EQ.(III-2.19B) (SEE SUBROUTINE
8160 C**** 'RHS' FOR DETAILS.)
8170      COMMON/AAAAA/XR(60),TR1(60),DT,AH2,JMX,JMXG,JMXGG
8180      COMMON/BBBBB/YY(47),TY1(47),JMYM,JMYMM,AY2,FY(48,12,4,2)
8190      COMMON/DDDDD/RHO(61,48,5),FI1(48,40,4),FI2(48,40,4,3),FK(60,40,4,
8200      & 3)
8210      COMMON/ZZZZZ/ZFIT(43),EZ(41,3),HZ(42),VZ(42),WZ(42),ZA(42),ZB(42)
8220      & ,ZC(42),ZD(42)
8230      COMMON/XXXXX/XFIT(61),EX(59,3),HX(60),VX(60),WX(60),XA(60),XB(60)
8240      & ,XC(60),XD(60)
8250      COMMON/YYYYY/YFIT(48),EY(46,3),HY(47),VY(47),WY(47),YA(47),YB(47)
8260      & ,YC(47),YD(47)

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8270      COMMON/CCCCC/DSP(4,4,60,48)
8280      COMMON/RAMRAM/COEF(8,8),RAM(111),LA(111),LB(111),LC(111),LD(111),
8290      & LG(111)
8300      COMMON/MMMMM/MAL1(5),KST(14),KED(14),IGX(5),IG(5,5),IPX(5),
8310      & LLF(19),LF(19),MSF(19),NR(19)
8320      DIMENSION SY(4),SX(4),FIT(43),AS(43,7,4),RSUM(40,19),GUM(5),
8330      & SKY(7,43),QQ(*),YR(47)
8340      EQUIVALENCE (YR(1),YY(1))
8350      KY=42
8360      C**** DO-LOOP OVER Y
8370      DO 258 IY=1,JMYM
8380      1      Y=YR(IY)
8390      1      C**** PREPARE QUANTITIES IN EQS.(II-3.11),(II-3.19)
8400      1      YQ=Y*Y
8410      1      DO 60 K=1,7
8420      2      60 SKY(K,IY)=0.
8430      1      XXX=2./3.
8440      1      C**** DO-LOOP OVER X
8450      1      DO 255 IX=1,JMXG
8460      2      X=XR(IX)
8470      2      XH=0.5*X
8480      2      XQ=0.25*X*X
8490      2      XT=1.5*XH
8500      2      XU=XT*XT
8510      2      RXQ=XQ+YQ
8520      2      RYQ=XU+0.25*YQ
8530      2      RXY=X*Y
8540      2      XPMIN=ABS(XH-Y)
8550      2      XPMAX=XH+Y
8560      2      C**** DECIDE THE COS-THETA MESH SIZE FOR EQ.(III-2.23) (IS THIS
8570      2      C**** ENOUGH ?)
8580      2      MCO=INT((XPMAX-XPMIN)/0.2)+1
8590      2      MCO=2*MCO
8600      2      IF(MCO.LT.20) MCO=20
8610      2      C**** COMPUTE THE K-FUNCTION OF EQ.(III-2.23) BY THE SIMPSON
8620      2      C**** QUADRATURE.
8630      2      DO 80 N=1,5
8640      3      80 GUM(N)=0.
8650      2      DCO=2./MCO
8660      2      CO=-1.-DCO
8670      2      CCC=1./3.
8680      2      DO 220 NCO=1,MCO+1
8690      3      DDD=CCC
8700      3      IF(NCO.EQ.1.OR.NCO.EQ.MCO+1) DDD=DDD/2.
8710      3      CO=CO+DCO
8720      3      C**** FOR RXYCO,XP,YP, SEE EQ.(II-3.19).
8730      3      RXYCO=RXY*CO
8740      3      XP=SQRT(ABS(RXQ-RXYCO))
8750      3      YP=SQRT(ABS(RYQ+0.75*RXYCO))
8760      3      C**** PREPARE FOR THE Y-SPLINE OF THE RHO-FUNCTION OF EQ.(III-2.1)
8770      3      SY(4)=1.
8780      3      DO 150 JY=1,JYMM
8790      4      MY=JY
8800      4      150 IF(YP.LT.YR(JY)) GO TO 160
8810      3      160 U=YP-YFIT(MY)
8820      3      FX=EXP(U)
8830      3      EXV=1./FX
8840      3      SY(1)=(FX-EXV)/2.
8850      3      SY(2)=SY(1)+EXV
8860      3      SY(3)=U
8870      3      C**** PREPARE FOR THE X-SPLINE OF THE RHO-FUNCTION OF EQ.(III-2.1)
8880      3      SX(4)=1.
8890      3      DO 170 I=1,JMXGG

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8900 4 II=I
8910 4 170 IF(XP.LT.XR(I)) GO TO 180
8920 3 180 U=XP-XFIT(II)
8930 3 FX=EXP(U)
8940 3 EXV=1./FX
8950 3 SX(1)=(FX-EXV)/2.
8960 3 SX(2)=SX(1)+EXV
8970 3 SX(3)=U
8980 3 KGX=IGX(MS)
8990 3 C**** DOUBLE SPLINE OF THE RHO-FUNCTION OF EQ.(III-2.1)
9000 3 FPI=0.
9010 3 DO 190 M=1,4
9020 4 DO 190 N=1,4
9030 5 190 FPI=FPI+DSP(N,M,II,MY)*SX(N)*SY(M)
9040 3 C**** SIMPSON QUADRATURE OF EQ.(III-2.23)
9050 4 DO 200 NG=1,KGX
9060 4 L=IG(NG,MS)+1
9070 4 200 GUM(L)=GUM(L)+DDD*FPI*PL(CO,L-1)
9080 3 220 CCC=1.-CCC
9090 2 C**** COMPLETE THE SIMPSON QUADRATURE OF EQ.(III-2.23) FOR ALL
9100 2 C**** POSSIBLE GAMMA.
9110 2 DO 230 NG=1,KGX
9120 3 LL=IG(NG,MS)+1
9130 3 230 GUM(LL)=DCO*GUM(LL)
9140 2 C**** 'GUM' IS THE K-FUNCTION OF EQ.(III-2.23).
9150 2 C**** COMPUTE THE U-FUNCTION OF EQ.(III-2.22).
9160 2 MPX=IPX(MS)
9170 2 M1=MAL1(MS)
9180 2 DO 250 MP=1,MPX
9190 3 M=MP+M1-1
9200 3 N=NR(M)
9210 3 MA=MSF(M)
9220 3 K1=KST(N)
9230 3 K2=KED(N)
9240 3 C**** SUM OVER A,C,AND GAMMA (I.E., SUM OVER K) IN EQ.(III-2.22).
9250 3 USUM=0.
9260 3 DO 240 K=K1,K2
9270 4 KA=LA(K)+LC(K)
9280 4 KB=LB(K)+LD(K)
9290 4 KG=LG(K)+1
9300 4 240 USUM=USUM+X**KA*Y**KB*GUM(KG)*RAM(K)
9310 3 C**** 'USUM' IS THE U-FUNCTION OF EQ.(III-2.22).
9320 3 C**** NOW, CARRY OUT THE X-INTEGRATION IN EQ.(III-2.21).
9330 3 SKY(MP,IY)=SKY(MP,IY)+X**(LLF(M)+2)*Y**(LF(M)+2)
9340 3 & *RHO(IX+1,IY+1,MA)*USUM*XXX*TR1(IX)*AH2
9350 3 250 CONTINUE
9360 2 255 XXX=1.-XXX
9370 1 258 CONTINUE
9380 C**** 'SKY(MP,Y)' IS THE H-FUNCTION OF EQ.(III-2.21).
9390 C**** OBTAIN THE Y-SPLINE COEFFICIENTS OF 'SKY'(SEE EQ.(III-2.25))
9400 FIT(1)=0.
9410 DO 280 MP=1,MPX
9420 1 DO 260 JY=1,JMYM
9430 2 260 FIT(JY+1)=SKY(MP,JY)
9440 1 CALL SPCOEF(ZFIT,FIT,JMYM-1,EZ,HZ,VZ,WZ,ZA,ZB,ZC,ZD,KY-1)
9450 1 DO 270 JY=1,JMYM
9460 2 AS(JY,MP,1)=ZA(JY)
9470 2 AS(JY,MP,2)=ZB(JY)
9480 2 AS(JY,MP,3)=ZC(JY)
9490 2 270 AS(JY,MP,4)=ZD(JY)
9500 1 280 CONTINUE
9510 C**** CARRY OUT THE Y-INTEGRATION IN EQ.(III-2.19B) BY MEANS OF
9520 C**** SPLINE INTERPOLATION (SEE EQ.(III-2.26)).

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9530      DO 320 IQ=1,IQX
9540      1      DO 310 MP=1,MPX
9550      2      M=MP+M1-1
9560      2      RTEMP=0.
9570      2      DO 300 JY=1,JMYM
9580      3      DO 300 L=1,4
9590      4      300 RTEMP=RTEMP+AS(JY,MP,L)*FI1(JY,IQ,L)
9600      2      310 RSUM(IQ,M)=RTEMP
9610      1 C**** 'RSUM' IS THE Y-FUNCTION OF EQS.(III-2.19B) OR (III-2.26).
9620      1      320 CONTINUE
9630      RETURN
9640      END
9650      SUBROUTINE NRHS4(IQX,QQ,RSUM,MS)
9660      C**** COMPUTE THE INTEGRAL OVER Y OF THE H-FUNCTION IN EQ.(III-2.27A).
9670      C**** (SEE SUBROUTINE 'RHS' FOR DETAILS.)
9680      COMMON/AAAAA/XR(60),TR1(60),DT,AH2,JMX,JMXG,JMXGG
9690      COMMON/BBBBB/YY(47),TY1(47),JMYM,JMYMM,AY2,FY(48,12,4,2)
9700      COMMON/DDDDD/RHO(61,48,5),FI1(48,40,4),FI2(48,40,4,3),FK(60,40,4,
9710      & 3)
9720      COMMON/ZZZZZ/ZFIT(43),EZ(41,3),HZ(42),VZ(42),WZ(42),ZA(42),ZB(42)
9730      & ,ZC(42),ZD(42)
9740      COMMON/XXXXX/XFIT(61),EX(59,3),HX(60),VX(60),WX(60),XA(60),XB(60)
9750      & ,XC(60),XD(60)
9760      COMMON/YYYYY/YFIT(48),EY(46,3),HY(47),VY(47),WY(47),YA(47),YB(47)
9770      & ,YC(47),YD(47)
9780      COMMON/CCCCC/DSP(4,4,60,48)
9790      COMMON/RAMRAM/COEF(8,8),RAM(111),LA(111),LB(111),LC(111),LD(111),
9800      & LG(111)
9810      COMMON/MMMMM/MAL1(5),KST(14),KED(14),IGX(5),IG(5,5),IPX(5),
9820      & LLF(19),LF(19),MSF(19),NR(19)
9830      DIMENSION SY(4),SX(4),RSUM(40,19),GUM(5,40),SKY(7,43),QQ(*),
9840      & SUMX(40),YR(47)
9850      EQUIVALENCE (YR(1),YY(1))
9860      KY=42
9870      YYY=2./3.
9880      C**** DO-LOOP OVER Y
9890      DO 258 IY=1,JMYM
9900      1      Y=YR(IY)
9910      1      YQ=Y*Y
9920      1      DO 60 K=1,7
9930      2      DO 60 IQ=1,40
9940      3      60 SKY(K,IQ)=0.
9950      1      XXX=2./3.
9960      1 C**** DO-LOOP OVER X
9970      1      DO 255 IX=1,JMXG
9980      2      X=XR(IX)
9990      2      XH=0.5*X
10000     2      XQ=XH*XH
10010     2      XT=1.5*XH
10020     2      XU=XT*XT
10030     2      RXQ=XQ+YQ
10040     2      RYQ=XU+0.25*YQ
10050     2      RXY=X*Y
10060     2      XPMIN=ABS(XH-Y)
10070     2      XPMAX=XH+Y
10080     2 C**** FOR 'RMAX' AND 'RMIN' BELOW, SEE EQ.(III-2.31).
10090     2      RMAX=XH+Y/3.
10100     2      RMIN=ABS(XH-Y/3.)
10110     2      RDIF=RMAX-RMIN
10120     2 C**** COMPUTE THE K-FUNCTION OF EQ.(III-2.30) BY THE SIMPSON
10130     2 C**** QUADRATURE.
10140     2      RQ=XQ+YQ/9.
10150     2      DO 80 IQ=1,IQX

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10160 3      DO 80 N=1,5
10170 4      80 GUM(N,IQ)=0.
10180 2      DO 230 IQ=1,IQX
10190 3      MCO=INT(QQ(IQ)*RDIF)
10200 3      MCO=2*MCO
10210 3      IF(MCO.LT.20) MCO=20
10220 3      DCO=2./MCO
10230 3      CO=-1.-DCO
10240 3      CCC=1./3.
10250 3      DO 220 NCO=1,MCO+1
10260 4      DDD=CCC
10270 4      IF(NCO.EQ.1.OR.NCO.EQ.MCO+1) DDD=DDD/2.
10280 4      CO=CO+DCO
10290 4      RXYCO=RXY*CO
10300 4      RR=SQRT(ABS(RQ-RXYCO/3.))*QQ(IQ)
10310 4      IF(RR.LT.1.E-5) GO TO 90
10320 4      TSIN=SIN(RR)/RR
10330 4      GO TO 100
10340 4      90 TSIN=1.-RR**2/6.
10350 4      100 XP=SQRT(ABS(RXQ-RXYCO))
10360 4      YP=SQRT(ABS(RYQ+0.75*RXYCO))
10370 4 C**** PREPARE FOR THE Y-SPLINE OF THE RHO-FUNCTION OF EQ.(III-2.1).
10380 4      SY(4)=1.
10390 4      DO 150 JY=1,JMYMM
10400 5      MY=JY
10410 5      150 IF(YP.LT.YR(JY)) GO TO 160
10420 4      160 U=YP-YFIT(MY)
10430 4      FX=EXP(U)
10440 4      EXV=1./FX
10450 4      SY(1)=(FX-EXV)/2.
10460 4      SY(2)=SY(1)+EXV
10470 4      SY(3)=U
10480 4 C**** PREPARE FOR THE X-SPLINE OF THE RHO-FUNCTION OF EQ.(III-2.1)
10490 4      SX(4)=1.
10500 4      DO 170 I=1,JMXGG
10510 5      II=I
10520 5      170 IF(XP.LT.XR(I)) GO TO 180
10530 4      180 U=XP-XFIT(II)
10540 4      FX=EXP(U)
10550 4      EXV=1./FX
10560 4      SX(1)=(FX-EXV)/2.
10570 4      SX(2)=SX(1)+EXV
10580 4      SX(3)=U
10590 4      KGX=IGX(MS)
10600 4 C**** DOUBLE SPLINE OF THE RHO-FUNCTION OF EQ.(III-2.1)
10610 4      FPI=0.
10620 4      DO 190 M=1,4
10630 5      DO 190 N=1,4
10640 6      190 FPI=FPI+DSP(N,M,II,MY)*SX(N)*SY(M)
10650 4 C**** SIMPSON QUADRATURE OF EQ.(III-2.30)
10660 4      DO 200 NG=1,KGX
10670 5      L=IG(NG,MS)+1
10680 5      200 GUM(L,IQ)=GUM(L,IQ)+DDD*FPI*PL(CO,L-1)*TSIN
10690 4      CCC=1.-CCC
10700 3 C**** COMPLETE THE SIMPSON QUADRATURE OF EQ.(III-2.23) FOR ALL
10710 3 C**** POSSIBLE GAMMA.
10720 3      DO 230 NG=1,KGX
10730 4      LL=IG(NG,MS)+1
10740 4      230 GUM(LL,IQ)=DCO*GUM(LL,IQ)
10750 2 C**** 'GUM' IS THE K-FUNCTION OF EQ.(III-2.30).
10760 2 C**** COMPUTE THE U-FUNCTION OF EQ.(III-2.29).
10770 2      MPX=IPX(MS)
10780 2      M1=MAL1(MS)

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10790 2      DO 250 MP=1,MPX
10800 3      M=MP+M1-1
10810 3      N=NR(M)
10820 3      MA=MSF(M)
10830 3      K1=KST(N)
10840 3      K2=KED(N)
10850 3      DO 242 IQ=1,IQX
10860 4 242 SUMX(IQ)=0.
10870 3      DO 240 K=K1,K2
10880 4      KA=LA(K)+LC(K)
10890 4      KB=LB(K)+LD(K)
10900 4      KG=LG(K)+1
10910 4      T=X**KA*Y**KB
10920 4      DO 240 IQ=1,IQX
10930 5 240 SUMX(IQ)=SUMX(IQ)+T*GUM(KG,IQ)*RAM(K)
10940 3 C**** 'SUMX' IS THE U-FUNCTION OF EQ.(III-2.29).
10950 3 C**** NOW, CARRY OUT THE X-INTEGRATION IN EQ.(III-2.28).
10960 3      T=X**(LLF(M)+2)*Y**(LF(M)+2)*RHO(IX+1,IY+1,MA)
10970 3      &      *XXX*TR1(IX)*AH2
10980 3      DO 250 IQ=1,IQX
10990 4 250 SKY(MP,IQ)=SKY(MP,IQ)+T*SUMX(IQ)
11000 2 255 XXX=1.-XXX
11010 1 C**** 'SKY' IS THE H-FUNCTION OF EQ.(III-2.28).
11020 1 C**** FINALLY, PERFORM THE Y-INTEGRATION IN EQ.(III-2.27A).
11030 1      DO 310 MP=1,MPX
11040 2      M=MP+M1-1
11050 2      DO 300 IQ=1,IQX
11060 3 300 RSUM(IQ,M)=RSUM(IQ,M)+SKY(MP,IQ)*YYY*TY1(IY)*AY2
11070 2 310 CONTINUE
11080 1 258 YYY=1.-YYY
11090 C**** 'RSUM' IS THE Y-INTEGRAL OF H IN EQ.(III-2.27A).
11100      RETURN
11110      END
11120      SUBROUTINE FORM(CF3,RSUM,IQX,FF,KEY)
11130 C**** THIS SUBROUTINE PERFORMS THE LAST STEPS TO OBTAIN 'FF3'
11140 C**** AND 'FF4' OF EQS.(III-2.19) AND (III-2.27A). THE STEPS
11150 C**** TAKEN HERE ARE THE MULTIPLICATION OF N-BAR AND SUMMATION
11160 C**** OVER GRAND-L AND GRAND-S.
11170      DIMENSION CF3(8,8),RSUM(40,19),FF(40,5,5),KEY(20),LOCK(20)
11180      DATA LOCK/11,21,51,12,22,52,33,43,53,34,44,54,15,25,55,55,55,35,
11190      & 45,55/
11200 C**** 'LOCK(20)' CORRESPOND TO 'KEY(20)', GIVING LOCATIONS
11210 C**** OF TWENTY NON-ZERO MATRIX ELEMENTS OF TABLE II-3, BUT
11220 C**** AS A 5*5 MATRIX.
11230      DO 10 IQ=1,IQX
11240 1      DO 10 NA=1,5
11250 2      DO 10 NB=1,5
11260 3 10 FF(IQ,NA,NB)=0.
11270      DO 100 IQ=1,IQX
11280 1      DO 20 MM=1,20
11290 2      M=MM
11300 2      IF(MM.GE.17) M=MM-1
11310 2      NA=LOCK(MM)/10
11320 2      NB=LOCK(MM)-10*NA
11330 2      KA=KEY(MM)/10
11340 2      KB=KEY(MM)-10*KA
11350 2 20 FF(IQ,NA,NB)=FF(IQ,NA,NB)+CF3(KA,KB)*RSUM(IQ,M)
11360 1 100 CONTINUE
11370      RETURN
11380      END

```

```
14400      SUBROUTINE XTABLE(JMX,JMXG,XR,TR1,DT,EM,XM,TM,TXC)
14410      C**** T(X)=C*(X+T0)*X/(X+S0)
14420      DIMENSION XR(*),TR1(*)
14430      JMXS=JMXG
14440      SX0=(TM-TXC*XM)*XM/(EM*XM-TM)
14450      TX0=EM*SX0/TXC
14460      DT=TM/JMX
14470      DTQ=DT**2
14480      CTO=TXC*TX0
14490      CS02=2.*TXC*SX0
14500      CS04=2.*CS02
14510      TXC2=2.*TXC
14520      T=0.
14530      DO 10 I=1,JMXS
14540      1      T=T+DT
14550      1      A=CTO-T
14560      1      XR(I)=(-A+SQRT(A*A+CS04*T))/TXC2
14570      1      DTDX=TXC*(XR(I)**2+2.*SX0*XR(I)+TX0*SX0)/(XR(I)+SX0)**2
14580      1      TR1(I)=1./DTDX
14590      1      10 CONTINUE
14600      RETURN
14610      END
```


§3. Asymptotic Normalization Constants

3-a. General description of Code ASYM5

The asymptotic normalization constants C_ℓ^j can be calculated by using Eqs. (I-6-20) and (I-6-23);

$$C_\ell^j = I_{00}^{\ell j} + I_{20}^{\ell j} + I_{02}^{\ell j} + I_{22}^{\ell j} \quad (3.1)$$

with

$$I_{L''L}^{\ell j} = \sum_{\alpha'} \frac{2}{\sqrt{|\beta|}} \int_0^\infty y^2 dy j_\ell(i|\beta|y) z_{\alpha\alpha'}^{L''} (y), \quad (3.2)$$

$$z_{\alpha\alpha'}^{L''} (y) = \int_0^\infty x^2 dx w_{L''}(x) ({}^3L''_1 | \frac{4M}{3\hbar^2} V | {}^3L_1) h_{\alpha\alpha'}(x, y), \quad (3.3)$$

and

$$h_{\alpha\alpha'}(x, y) = \delta_{L_0 L_0'} \delta_{S_0 S_0'} \sum_{L_0 S_0} C_{\alpha\alpha'}^{(L_0 S_0)} U_{\alpha\alpha'}^{L_0}(Q=0; x, y). \quad (3.4)$$

In Eq. (3.1),

$$|\beta| = \sqrt{\frac{4M}{3\hbar^2} (|E_t| - |E_d|)} \quad (3.5)$$

In Eq. (3.3), $w_{L''}(x)$ is the deuteron spatial wave function for the 3S_1 -component ($L''=0$) or the 3D_1 -component ($L''=2$), and $({}^3L''_1 | V | {}^3L_1)$ is an element of the 2×2 matrix of the two nucleon potential in the ${}^3S_1 + {}^3D_1$ state. The summation over α' in Eq. (3.2) extends over all states α' that can couple to the state α with the same (L_0, S_0) . The coefficients $C_{\alpha\alpha'}^{(L_0 S_0)}$ are those of Eq. (II-3.2) and are equal to twice $N_{\alpha\alpha'}^{(L_0 S_0)}$ of Eq. (I-3-6). The function $U_{\alpha\alpha'}^{L_0}(Q=0; x, y)$ is defined by Eq. (I-3-27). We have dealt with this function many times before. Specifically, the U-function we have here is precisely the one given by Eq. (2.22) in the previous section. Here, we must properly normalize the wave functions obtained by the main program by using the normalization factor computed at the end of Code NFORM. The computation of $U_{\alpha\alpha'}^{L_0}(Q=0; x, y)$ can be done as in subroutine RHS of the main program (see section 6-b of II). However, since we need to consider the 3S_1 and the 3D_1 states only for the final states, referring to Tables 1 and 2 of II, the combinations $\{\alpha, L_0, \alpha'\}$ with $\alpha=1$, i.e., with the key-index $m=1, 4$ and 13 must be excluded. Further changes from subroutine RHS are required since we need to consider a greatly extended region of x and y as explained below.

The functions $j_\ell(i|\beta|y)$ for $\ell=0$ and $\ell=2$ are explicitly given by

$$j_0(iz) = \frac{e^z - e^{-z}}{2z} \quad (3.6)$$

and

$$j_2(iz) = \left(-\frac{3}{z^2} + \frac{3}{z} - 1\right) \frac{e^z}{2z} + \left(\frac{3}{z^2} + \frac{3}{z} + 1\right) \frac{e^{-z}}{2z} \quad (3.7)$$

with $z = |\beta|y$. The exponential increase of these functions in the integrand of Eq. (3.2) as $y \rightarrow \infty$ must be damped by the counter decrease of $Z^{L''}(y)$, and the integrand as a whole will eventually tend to zero as $y \rightarrow \infty$. However, its decrease will be extremely slow and we have to extend the upper limit y_M of the y -integration to a very far distance. This necessitates the computation of $\rho_\alpha(x'', y'')$ in Eq. (2.23) up to

$$x'' \leq x_G = \frac{1}{2} x_{\max} + y_M, \quad (3.8a)$$

$$y'' \leq y_G = \frac{3}{4} x_{\max} + \frac{1}{2} y_M. \quad (3.8b)$$

(See Eq. (II-3.11)). Yet we may still need to correct for the cutoff at y_M . We take into account the contribution from beyond $y = y_M$ by assuming that the integrand of Eq. (3.2) decreases exponentially.

The code to perform the above calculations is named ASYM5. It consists of the following parts.

MAIN routien

Subroutines and functions

FYASYM, PTABLE, YTAB, BESSEL, ARHS, SPLINE, SPCOEF, PARAM and PL.

It requires the following preparatory code and data files:

Code DEUTRN

File LFCHI, File LFDEUT and File LFRAM

The preparatory code DEUTRN computes the deuteron wave function and the binding energy. For details, see section 3-e. Subroutines PTABLE, YTAB, BESSEL, SPLINE, SPCOEF and PARAM and function PL are identical to those used in Code NFORM (see the previous section). Therefore no listings of them will be given. In the following sections we describe MAIN routine, subroutines FYASYM and ARHS, and Code DEUTRN.

3-b. MAIN routine

The following flow chart should suffice to explain the structure of this routine.

Start

- #1 Initialization (Assign values to key-indices by calling subroutine PARAM.
Assign file numbers and x- and y-mesh numbers:
 $x_{JMX} = x_{\max}$ (same as in the main program), $x_{JMXG} = x_G$,
 $y_{JMYM} = y_M$, and $y_{JMYG} = y_G$ of Eq.(3.8).
Also input the binding energy $|E_t|$ and the normalization constant 'FNORM' taken from the output of Code NFORM.)
- #2 Read File LFCHI (read in $-\theta_\alpha(q,x)$ and $\phi_\alpha(q,x)$ that are obtained at the end of the main program)

(Normalize $\phi_\alpha(q,x)$ using the normalization constant 'FNORM')
- #3 Read File LFRAM (read in $C_{\alpha\alpha'}^{(L_0 S_0)}$, $R_{(L\ell, L'\ell')}^{acy} L_0$, a, b, c, d, and γ of Eqs.(II-3.2) and (III-2.22).)
- #4 Call FYASYM (PTABLE, YTAB, BESSEL)
(i) Set up the same p-table as used in the main program.
(ii) Set up the y-table $y(t)$ and dy/dt as per Eq.(II-8.2) for $0 \leq y \leq y_M$,
and (iii) construct $Y_\ell^{(t)}(y, p_k)$ of Eq.(III-2.2) up to y_M .)
- #5 Read File LFDEUT
(i) Read in the same x-table $x(t)$ and dx/dt as used in the main program, but extended to x_G ,
(ii) read in the RSC potential for the $^3S_1 + ^3D_1$ state,
and (iii) read in the wave function and the binding energy of the deuteron.)
- #6 $\left[\begin{array}{l} \text{Compute } |\beta| \text{ and } \sqrt{|\beta|} \text{ of Eq.(I-6-4).} \\ \text{Compute the (negative energy) regular function } j_\ell(i|\beta|y) \text{ that enters} \\ \text{into Eq.(3.2) as given by Eqs.(3.6) and (3.7).} \end{array} \right]$
- #7 (Prepare various spline matrices.)
- #8 (Construct $\rho_\alpha(x,y)$ of Eq.(III-2.1).)

```

| - - (Do-loop over the summation index  $\alpha'$  (1 to 5))
|
| #9   [ Compute the double-spline coefficients of  $\rho_\alpha(x,y)$  of Eq.(II-2.1)
|       [ for  $0 \leq x \leq x_G$  and  $0 \leq y \leq y_G$  .
|
| #10  Call ARHS (SPLINE,SPCOEF,PL)
|       (Compute the  $y$ -integrals in Eq.(3.2) and output them as
|       'YRHS(L", $\alpha$ ')
|       (Compute  $I_{L''L}^j$  of Eq.(III-3.2) by taking the summation over  $\alpha'$  of
|       'YRHS(L", $\alpha$ ') and obtain  $C_\ell^j$  as per Eq.(III-3.1).)
|
| - - (End of the do-loop over  $\alpha'$ ).

```

Stop

3-c. Subroutine FYASYM

This subroutine sets up the p -table (as used in the main program) and the y -table $y(t)$ and dy/dt using the formula Eq.(II-8.2) for $0 \leq y \leq y_M$. Also, this code constructs $Y_\ell^{(t)}(y, p_k)$ of Eq.(III-2.2) up to y_M .

The coding of this subroutine is almost identical to subroutine FYFORM in Code NFORM of the previous section, except for minor changes in dimensionalities of variables relating to y -mesh. For details, see Code FYFI5 in the main program.

3-d. Subroutine ARHS (YRHS,NB,BETA)

This subroutine computes the y -integrals (divided by $\sqrt{|\beta|}$) in Eq.(III-3.2) for $\alpha' = \text{'NB'}$ for all α and L'' , and outputs them as 'YRHS(L", α ')'. The computation of $U_{\alpha\alpha}^{L0}(Q=0;x,y)$ proceeds as in subroutine RHS of the main program. The following flow chart will be useful to understand the code. We should remember that this subroutine is called within the do-loop over α' in MAIN routine.

Enter

```

| - - - (Do-loop over  $y$ )
|
| | - - (Do-loop over  $x$ )
| |
| |
| |
|

```

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- #1 { Prepare quantities to compute x'' and y'' (see Eqs.(3.11) and (3.19) of II.)
Decide the $\cos \theta$ -mesh size and initiate the $\cos \theta$ -integration in Eq.(2.32). }
- #2 { Compute $K_Y^{\alpha'}$ (x,y) of Eq.(2.32) as follows:
- {Do-loop over $\cos \theta$
Compute x'' and y'' as per Eq.(II-3.19)
Construct ρ_{α} (x'',y'') by the double-spline over x and y .
Process the Simpson quadrature over $\cos \theta$ to find $K_Y^{\alpha'}$ (x,y) of Eq.(2.23).
- {End of the do-loop over $\cos \theta$
Multiply the $\cos \theta$ -mesh size to complete the Simpson quadrature.
The resulting $K_Y^{\alpha'}$ (x,y) is stored as 'GUM(γ)'.
- #3 { Compute $U_{\alpha\alpha}^{L_0}$ ($Q=0;x,y$) of Eq.(2.22). Here we do not need the case with $\alpha=1$. Thus, we skip the computation for $m=1,4$ and 13, where m is the key-index in Table 2 of II. For various other indices, see subroutine RHS of the main program. }
- #4 { Multiply $C_{\alpha\alpha}^{(L_0 S_0)}$ to $U_{\alpha\alpha}^{L_0}$ ($Q=0;x,y$) and sum over (L_0, S_0) to find $h_{\alpha\alpha}$ (x,y) of Eq.(3.4). (For the indices 'LOCK' and "KEY', see the comment cards at the beginning). The results are stored as 'HRHS (α)'.
- #5 { Process the Simpson quadrature over x in Eq.(3.3). The results are stored as 'ZRHS(L", α)'.
- - (End of the do-loop voer x)
- #6 { Construct the integrand of the y -integral in Eq.(3.2).
The results are 'URHS(L", α)'.
- #7 { Process the Simpson quadrature over y in Eq.(3.2). The results are divided by $\sqrt{|\beta|}$ and stored as 'YRHS(L", α)'.
- - - (End of the do-loop over y)
- #8 { Add the contribution from beyond y_M to the y -integral of Eq.(3.2) by }

assuming the integrand goes to zero exponentially.
 (This bit of contribution is called 'SRHS(L", α)'.)

Return

3-e. Code DEUTRN

This code computes the deuteron binding energy and the normalized wave functions for the RSC potential. The method used here is to search for the energy at which the eigenvalue λ of the Sturm-Liouville function for the ${}^3S_1 + {}^3D_1$ state becomes 1.

The computation of the Sturm-Liouville function is identical to Code STURM of PERFECT V. Since we need to calculate the ${}^3S_1 + {}^3D_1$ state only, the part relating to the 1S_0 state may be deleted. For details see Code STURM of PERFECT V. Unlike in PERFECT V, however, here we must normalize the wave function in an ordinary manner.

The search for the binding energy is performed by Newton-Raphson's method, which proceeds as follows. Writing $q = \sqrt{M|E_d|/\hbar^2}$ and defining

$$f(q) = \lambda(q) - 1 \quad (3.9)$$

we start from a trial value q_1 , and compute successive values of q_i ($i=1,2,3,\dots$) by

$$q_i = q_{i-1} - f(q_{i-1})/f'(q_{i-1}) \quad (3.10)$$

until the sequence $\{q_1, q_2, \dots\}$ converges to a value q_0 . This value q_0 satisfies $\lambda(q_0)=1$ and yields the binding energy $|E_d| = \frac{\hbar^2}{M} q_0^2$. To utilize this method, we need to calculate $d\lambda(q)/dq$. Instead of computing this quantity numerically, we use the following analytic expression:

$$\frac{d\lambda(q)}{dq} = 2q\lambda(q)^2 \int_0^\infty (u_\lambda(q,x))^2 dx / \int_0^\infty u_\lambda(q,x) \frac{M}{\hbar^2} V(x) u_\lambda(q,x) dx \quad (3.11)$$

where $u_\lambda(q,x)$ is the Sturm-Liouville function satisfying

$$\left[\frac{d^2}{dx^2} - \frac{L(L+1)}{x^2} - \frac{1}{\lambda} \frac{M}{\hbar^2} V(x) - q^2 \right] u_\lambda(q,x) = 0 \quad (3.12)$$

Equation (3.11) can be derived by a simple manipulation of Eq.(3.12). It is fairly general and is applicable even for a velocity dependent potential.

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The code consists of the following parts:

MAIN routine

Subroutines and functions

STURMD, POTD, RES1, REXS, COW, BULL and YTABLE

All these subroutines and functions are the same as in Code STURM in Perfect V, except for subroutine YTABLE which utilizes Eq.(II-6.2) to compute the same x-table as used in the main program. (See code STURM for subroutine YTABLE.)

The code requires a data file named LFDEUT.

Perhaps no explanation of MAIN routine is necessary since it is simple and contains enough comment cards in it.

```

19.812  ** CODE ASYM5 ***                                LABEL
(09-30-82)  OPTIONS: INTER,OPT=1,NROUND,NDLR,ALC,MASTER,INLINE=0,LSTIN,LNO,NREST

10      C**** *** CODE ASYM5 ***
20      C**** TRITON(NEUTRON-DEUTERN) ASYMPTOTIC NORMALIZATION CONSTANTS
30      C**** REFERENCES (SRT=SCIENCE REPORT OF TOHOKU UNIV.)
40      C      I: FORMULATIONS (T.SAWADA+T.SASAKAWA)
50      C      SRT SER.8,VOL.3,NO.1(1982)1
60      C      II: PERFECT V (SASAKAWA+ISHIKAWA+SAWADA)
70      C      SRT (1982)
80      C      III: THIS REPORT
90      COMMON/AAAAA/XR(80),TR1(80),AH2,RSC(80,3),UU(80),WW(80),JMX,JMXG
100     COMMON/BBBBB/YY(60),TY1(60),JMYM,JMYG,AY2,FY(61,12,4,2),SSH(60,2),
110     & DSP(4,4,71,46)
120     COMMON/RAMRAM/COEF(8,8),RAM(111),LA(111),LB(111),LC(111),LD(111),
130     & LG(111)
140     COMMON/MMMMM/MAL1(5),KST(14),KED(14),IGX(5),IG(5,5),IPX(5),
150     & LLF(19),LF(19),MSF(19),NR(19)
160     DIMENSION PFIT(13),EP(11,3),HP(12),VP(12),WP(12),PA(12),PB(12),
170     & PC(12),PD(12)
180     COMMON/XXXXX/XFIT(71),EX(69,3),HX(70),VX(70),WX(70),XA(70),XB(70),
190     & XC(70),XD(70)
200     COMMON/YYYYY/YFIT(46),EY(44,3),HY(45),VY(45),WY(45),YA(45),YB(45),
210     & YC(45),YD(45)
220     DIMENSION TSI(30,5,12),GSI(30,5,12),AQ(12),C(2,5),AK2(12),
230     & EXK(70,12,2),PSI(70,12),FIT(71),RHO(71,46,5),
240     & AY(71,45,4),YRHS(2,5)
250     C-01
260     C**** ASSIGN VALUES TO KEY-INDICES.
270     CALL PARAM
280     C**** ASSIGN FILE NUMBERS, X- AND Y- MESH NUMBERS.
290     LFDEUT=28
300     LFCHI=27
310     LFRAM=21
320     JMX=30
330     JMXG=70
340     JMYM=60
350     JMYG=45
360     C**** INPUT THE TRITON BINDING ENERGY, AND THE NORMALIZATION CONSTANT.
370     BEI=6.60
380     FNORM=2.6
390     HM=1./41.47
400     MALL=12
410     C-02
420     C**** INPUT THE TRITON WAVE FUNCTIONS.
430     REWIND LFCHI
440     READ(LFCHI) TSI,GSI
450     WRITE(6,1000) BEI,FNORM
460     1000 FORMAT('1*** TRITON ASYMPTOTIC NORMALIZATION (ASYM5) ***'/
470     & '0BEI=',1PE13.5,' FNORM=',1PE13.5)
480     C**** NORMALIZE THE WAVE FUNCTION
490     CONST=SQRT(FNORM)
500     DO 20 MS=1,5
510     1 * WRITE(6,1010) MS
520     1 *1010 FORMAT('0*** NORMALIZED GSI(MS=',I2,') ***')
530     1 DO 20 IM=1,MALL
540     2 DO 10 J=1,JMX
550     3 10 GSI(J,IM,MS)=GSI(J,IM,MS)/CONST
560     2 * WRITE(6,1020) IM,(GSI(J,IM,MS),J=1,JMX)
570     2 *1020 FORMAT(' IM=',I3/(' ',1P10E12.4))
580     2 20 CONTINUE
590     C-03

```


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```

600      C**** READ IN THE C-COEFFICIENTS OF EQ.(II-3.2) AND THE R-COEFFICIENTS,
610      C**** A,B,C,D AND G OF EQ.(III-2.22).
620      REWIND LFRAM
630      READ(LFRAM) COEF, RAM, LA, LB, LC, LD, LG
640      C-04
650      C**** SET UP THE P- AND Y-TABLE, AND CONSTRUCT THE Y-FUNCTION OF EQ.
660      C**** (III-2.2).
670      CALL FYASYM(AQ, MALL)
680      DO 30 I=1, MALL
690      1 30 AK2(I)=SQRT(HM*BEI+0.75*AQ(I)**2)
700      C-05
710      C**** INPUT THE X-TABLE, THE RSC(3S1+3D1) POTENTIAL, AND THE
720      C**** DEUTERON BINDING ENERGY AND WAVE FUNCTION.
730      REWIND LFDEUT
740      READ(LFDEUT) ALPHA, BED, CUTOFF, UU, WW, RSC, DT, XR, TR1
750      WRITE(6, 1030) ALPHA, BED, CUTOFF
760      1030 FORMAT('ODEUTERON WAVE FUNCTION'/' ALPHA=', 1PE13.5, ' BED=',
770      & 1PE13.5, ' CUTOFF=', 1PE13.5)
780      AH2=2.*DT
790      WRITE(6, 1040) (XR(J), J=1, JMX)
800      1040 FORMAT('OXR'/'(' ', 1P10E12.4))
810      WRITE(6, 1050) (UU(J), J=1, JMX)
820      1050 FORMAT('OUU'/'(' ', 1P10E12.4))
830      WRITE(6, 1060) (WW(J), J=1, JMX)
840      1060 FORMAT('OWW'/'(' ', 1P10E12.4))
850      WRITE(6, 1070) (RSC(J, 1), J=1, JMX)
860      1070 FORMAT('OV11'/'(' ', 1P10E12.4))
870      WRITE(6, 1080) (RSC(J, 2), J=1, JMX)
880      1080 FORMAT('OV12'/'(' ', 1P10E12.4))
890      WRITE(6, 1090) (RSC(J, 3), J=1, JMX)
900      1090 FORMAT('OV22'/'(' ', 1P10E12.4))
910      DO 40 IR=1, 3
920      1 DO 40 J=1, 80
930      2 40 RSC(J, IR)=RSC(J, IR)/0.75
940      C-06
950      C**** FOR BETA, SEE EQ.(I-6-4)
960      BETA=SQRT(HM*(BEI-BED)/0.75)
970      C**** (NEGATIVE ENERGY) SOLUTIONS (SEE EQS.(III-3.6) AND (III-3.7))
980      DO 50 JY=1, JMYM
990      1 Z=BETA*YY(JY)
1000     1 EXZ=EXP(Z)
1010     1 T1=EXZ/(2.*Z)
1020     1 T2=1./(EXZ*2.*Z)
1030     1 SSH(JY, 1)=YY(JY)*(T1-T2)
1040     1 50 SSH(JY, 2)=YY(JY)*((-3./Z**2+3./Z-1.)*T1
1050     & (3./Z**2+3./Z+1.)*T2)
1060     * DO 60 K=1, 2
1070     * 60 WRITE(6, 1100) K, (SSH(J, K), J=1, JMYM)
1080     *1100 FORMAT('OSSH(J, K=', I2, ')'/'(' ', 1P10E12.4))
1090     DO 70 K=1, 2
1100     1 DO 70 NA=1, 5
1110     2 70 C(K, NA)=0.
1120     C-07
1130     C**** VARIOUS SPLINE MATRICES
1140     PFIT(1)=0.
1150     DO 80 I=1, MALL
1160     1 80 PFIT(I+1)=AQ(I)
1170     CALL SPLINE(PFIT, MALL-1, EP, HP, VP, WP, MALL-1, PA, PB, PC, PD)
1180     XFIT(1)=0.
1190     DO 90 I=1, JMXG
1200     1 90 XFIT(I+1)=XR(I)
1210     CALL SPLINE(XFIT, JMXG-1, EX, HX, VX, WX, 69, XA, XB, XC, XD)
1220     YFIT(1)=0.
1230     DO 100 I=1, JMYG

```

```

1240 1 100 YFIT(I+1)=YY(I)
1250 CALL SPLINE(YFIT,JMYG-1,EY,HY,VY,WY,44,YA,YB,YC,YD)
1260 C-08
1270 C**** CONSTRUCT THE RHO-FUNCTION OF EQ.(III-2.1).
1280 X1Q=XR(1)**2
1290 X2Q=XR(2)**2
1300 XQ12=X2Q-X1Q
1310 C**** FIRST, EXTEND THE GSI-FUNCTIONS UP TO XR(JMXG).
1320 J1=JMX
1330 DO 120 I=1,MALL
1340 1 DO 110 JX=J1,JMXG
1350 2 AKX=AK2(I)*XR(JX)
1360 2 EXK(JX,I,1)=EXP(-AKX)
1370 2 110 EXK(JX,I,2)=EXK(JX,I,1)*(3./AKX**2+3./AKX+1.)
1380 1 120 CONTINUE
1390 DO 220 MA=1,5
1400 1 LL=1
1410 1 IF(MA.EQ.3.OR.MA.EQ.5) LL=2
1420 1 DO 150 I=1,MALL
1430 2 ASYM=GSI(JMX,MA,I)/EXK(JMX,I,LL)*XR(JMX)
1440 2 DO 130 J=1,J1
1450 3 130 PSI(J,I)=GSI(J,MA,I)*XR(J)
1460 2 DO 140 J=J1,JMXG
1470 3 140 PSI(J,I)=ASYM*EXK(J,I,LL)
1480 2 150 CONTINUE
1490 1 * WRITE(6,1110) MA
1500 1 *1110 FORMAT('1*** PSI(MA=',I3,')')
1510 1 * DO 160 I=1,MALL
1520 1 * 160 WRITE(6,1120) I,(PSI(J,I),J=1,JMXG)
1530 1 *1120 FORMAT('0IM=',I3/(' ',1P10E12.4))
1540 1 C *** P-SPLINE OF 'PSI' DIVIDED BY X**(L+1)
1550 1 LLP=2*(LL/2)+1
1560 1 LP=1
1570 1 IF(MA.GE.4) LP=2
1580 1 DO 190 JX=1,JMXG
1590 2 FIT(1)=0.
1600 2 DO 170 I=1,MALL
1610 3 170 FIT(I+1)=PSI(JX,I)/XR(JX)**LLP
1620 2 CALL SPCOEF(PFIT,FIT,MALL-1,EP,HP,VP,WP,PA,PB,PC,PD,MALL-1)
1630 2 DO 190 JY=1,JMYG+1
1640 3 SUMA=0.
1650 3 DO 180 I=1,MALL
1660 4 180 SUMA=SUMA+PA(I)*FY(JY,I,1,LP)+PB(I)*FY(JY,I,2,LP)+
1670 3 & PC(I)*FY(JY,I,3,LP)+PD(I)*FY(JY,I,4,LP)
1680 3 190 RHO(JX+1,JY,MA)=SUMA
1690 1 C**** EXTRAPOLATE THE 'RHO'-FUNCTION OF EQ.(III-2.1) TO X=0 ASSUMING
1700 1 C**** THE FORM A+B*X**2
1710 1 DO 200 JY=1,JMYG+1
1720 2 200 RHO(1,JY,MA)=(RHO(2,JY,MA)*X2Q-RHO(3,JY,MA)*X1Q)/XQ12
1730 1 * WRITE(6,1130) MA
1740 1 *1130 FORMAT('1*** RHO(MA=',I3,')')
1750 1 * DO 210 JY=1,JMYG+1
1760 1 * 210 WRITE(6,1140) JY,(RHO(JX,JY,MA),JX=1,JMXG+1)
1770 1 *1140 FORMAT('0JY=',I3/(' ',1P10E12.5))
1780 1 220 CONTINUE
1790 C**** DO-LOOP OVER THE SUMMATION INDEX ALPHA'.
1800 DO 290 NB=1,5
1810 1 C-09
1820 1 C**** COMPUTE THE DOUBLE-SPLINE COEFFICIENTS OF 'RHO'.
1830 1 DO 250 JX=1,JMXG+1
1840 2 DO 230 JY=1,JMYG+1
1850 3 230 FIT(JY)=RHO(JX,JY,NB)
1860 2 CALL SPCOEF(YFIT,FIT,JMYG-1,EY,HY,VY,WY,YA,YB,YC,YD,44)

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1870 2      DO 240 JY=1,JMYG
1880 3      AY(JX,JY,1)=YA(JY)
1890 3      AY(JX,JY,2)=YB(JY)
1900 3      AY(JX,JY,3)=YC(JY)
1910 3      240 AY(JX,JY,4)=YD(JY)
1920 2      250 CONTINUE
1930 1      DO 270 L=1,4
1940 2      DO 270 JY=1,JMYG
1950 3      DO 260 JX=1,JMXG+1
1960 4      260 FIT(JX)=AY(JX,JY,L)
1970 3      CALL SPCOEF(XFIT,FIT,JMXG-1,EX,HX,VX,WX,XA,XB,XC,XD,69)
1980 3      DO 270 JX=1,JMXG
1990 4      DSP(1,L,JX,JY)=XA(JX)
2000 4      DSP(2,L,JX,JY)=XB(JX)
2010 4      DSP(3,L,JX,JY)=XC(JX)
2020 4      270 DSP(4,L,JX,JY)=XD(JX)
2030 1      C-10
2040 1      C**** COMPUTE THE Y-INTEGRALS IN EQ.(III-3.2). THE RESULTS ARE 'YRHS'.
2050 1      NBR=NB
2060 1      CALL ARHS(YRHS,NBR,BETA)
2070 1      C**** SUM OVER ALPHA-PRIME(=NB).
2080 1      DO 280 K=1,2
2090 2      DO 280 NA=2,5
2100 3      280 C(K,NA)=C(K,NA)+YRHS(K,NA)
2110 1      290 CONTINUE
2120 C**** 'C' IS THE I-FUNCTION OF EQ.(III-3.2).
2130 WRITE(6,1150) ((K,NA,C(K,NA),NA=2,5),K=1,2)
2140 1150 FORMAT('OTHE ASYMPTOTIC NORMALIZATION CONSTANTS C(K,NA)'/
2150 & 2(5X,4(3X,'C(',I1,',',I1,')=' ,1PE13.5)/))
2160 STOP
2170 END
2180 SUBROUTINE ARHS(YRHS,NB,BETA)
2190 C**** COMPUTE THE Y-INTEGRALS IN EQ.(III-3.2) FOR ALPHA'= NB
2200 C**** AND FOR ALL ALPHA AND L'.
2210 COMMON/AAAAA/XR(80),TR1(80),AH2,RSC(80,3),UU(80),WW(80),
2220 & JMX,JMXG
2230 COMMON/BBBBB/YY(60),TY1(60),JMYM,JMYG,AY2,FY(61,12,4,2),
2240 & SSH(60,2),DSP(4,4,71,46)
2250 COMMON/RAMRAM/COEF(8,8),RAM(111),LA(111),LB(111),LC(111),LD(111),
2260 & LG(111)
2270 COMMON/MMMMM/MAL1(5),KST(14),KED(14),IGX(5),IG(5,5),IPX(5),
2280 & LLF(19),LF(19),MSF(19),NR(19)
2290 COMMON/XXXXX/XFIT(71),EX(69,3),HX(70),VX(70),WX(70),XA(70),XB(70),
2300 & XC(70),XD(70)
2310 COMMON/YYYYY/YFIT(46),EY(44,3),HY(45),VY(45),WY(45),YA(45),YB(45),
2320 & YC(45),YD(45)
2330 DIMENSION SY(4),SX(4),YR(61),GUM(5),HRHS(5),SRHS(2,5),URHS(2,5),
2340 & YRHS(2,5),ZRHS(2,5),LOCK(19),KEY(19),PRURHS(2,5)
2350 EQUIVALENCE (YR(1),YY(1))
2360 DATA LOCK/11,21,51,12,22,52,33,43,53,34,44,54,15,25,55,55,35,45,
2370 & 55/,
2380 & KEY/11,21,51,12,22,52,33,43,83,34,44,84,15,25,55,66,38,48,
2390 & 88/
2400 C**** 'LOCK(M)' GIVES THE INDICES (ALPHA,ALPHA') OF TABLE 2 OF II,
2410 C**** 'KEY(M)' THE INDICES (I,I') IN TABLE 3 OF II, BOTH CORRESPONDING
2420 C**** TO THE KEY-INDIX M.
2430 C**** FOR KEY(M=16), WE USE 66. THE POSSIBILITY OF KEY(M=16) BEING
2440 C**** 77 IS TAKEN CASE AT C-04.
2450 BETAQ=SQRT(BETA)
2460 MS=NB
2470 WRITE(6,1000) NB,((K,NA,NA=2,5),K=1,2)
2480 1000 FORMAT('OTHE INTEGRAND OF THE Y-INTEGRATION IN THE I-FUNCTION ',
2490 & 'FOR NB=',I2/7X,'Y',6X,2(3X,4(4X,'K=',I1,',NA=',I1,' ')))
2500 DO 10 K=1,2

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2510 1 DO 10 NA=1,5
2520 2 10 YRHS(K,NA)=0.
2530 YYY=2./3.
2540 C**** DO-LOOP OVER Y
2550 DO 220 IY=1,JMYM
2560 1 IF(IY.EQ.JMYM) YYY=YYY/2.
2570 1 Y=YR(IY)
2580 1 YQ=Y*Y
2590 1 DO 20 K=1,2
2600 2 DO 20 NA=1,5
2610 3 20 ZRHS(K,NA)=0.
2620 1 XXX=2./3.
2630 1 C**** DO-LOOP OVER X
2640 1 DO 170 IX=1,JMX
2650 2 X=XR(IX)
2660 2 C**** PREPARE QUANTITIES IN EQS.(II-3.11),(II-3.19).
2670 2 C-01
2680 2 XH=0.5*X
2690 2 XQ=XH*XH
2700 2 XT=1.5*XH
2710 2 XU=XT*XT
2720 2 RXQ=XQ+YQ
2730 2 RYQ=XU+0.25*YQ
2740 2 RXY=X*Y
2750 2 XPMIN=ABS(XH-Y)
2760 2 XPMAX=XH+Y
2770 2 C**** DECIDE THE COS-THETA MESH SIZE FOR EQ.(III-2.23) (IS THIS
2780 2 C**** ENOUGH ?)
2790 2 MCO=INT((XPMAX-XPMIN)/0.2)+1
2800 2 MCO=2*MCO
2810 2 IF(MCO.LT.20) MCO=20
2820 2 C**** COMPUTE THE K-FUNCTION OF EQ.(III-2.23) BY THE SIMPSON
2830 2 C**** QUADRATURE.
2840 2 DO 30 N=1,5
2850 3 30 GUM(N)=0.
2860 2 DCO=2./MCO
2870 2 CO=-1.-DCO
2880 2 CCC=1./3.
2890 2 C-02
2900 2 DO 100 NCO=1,MCO+1
2910 3 DDD=CCC
2920 3 IF(NCO.EQ.1.OR.NCO.EQ.MCO+1) DDD=DDD/2.
2930 3 CO=CO+DCO
2940 3 C**** FOR RXYCO,XP,YP, SEE EQ.(II-3.19).
2950 3 RXYCO=RXY*CO
2960 3 XP=SQRT(ABS(RXQ-RXYCO))
2970 3 YP=SQRT(ABS(RYQ+0.75*RXYCO))
2980 3 C**** PREPARE FOR THE Y-SPLINE OF THE RHO-FUNCTION OF EQ.(III-2.1)
2990 3 SY(4)=1.
3000 3 DO 40 JY=1,JMYG
3010 4 MY=JY
3020 4 40 IF(YP.LT.YR(JY)) GO TO 50
3030 3 50 U=YP-YFIT(MY)
3040 3 FX=EXP(U)
3050 3 EXV=1./FX
3060 3 SY(1)=(FX-EXV)/2.
3070 3 SY(2)=SY(1)+EXV
3080 3 SY(3)=U
3090 3 C**** PREPARE FOR THE X-SPLINE OF THE RHO-FUNCTION OF EQ.(III-2.1)
3100 3 SX(4)=1.
3110 3 DO 60 I=1,JMXG
3120 4 II=I
3130 4 60 IF(XP.LT.XR(I)) GO TO 70
3140 3 70 U=XP-XFIT(II)

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3150      3      FX=EXP(U)
3160      3      EXV=1./FX
3170      3      SX(1)=(FX-EXV)/2.
3180      3      SX(2)=SX(1)+EXV
3190      3      SX(3)=U
3200      3      KGX=IGX(MS)
3210      3 C**** DOUBLE SPLINE OF THE RHO-FUNCTION OF EQ.(III-2.1)
3220      3      FPI=0.
3230      3      DO 80 M=1,4
3240      4      DO 80 N=1,4
3250      5      80 FPI=FPI+DSP(N,M,II,MY)*SX(N)*SY(M)
3260      3 C**** SIMPSON QUADRATURE OF EQ.(III-2.23)
3270      3      DO 90 NG=1,KGX
3280      4      L=IG(NG,MS)+1
3290      4      90 GUM(L)=GUM(L)+DDD*FPI*PL(CO,L-1)
3300      3      100 CCC=1.-CCC
3310      2 C**** COMPLETE THE SIMPSON QUADRATURE OF EQ.(III-2.23) FOR ALL
3320      2 C**** POSSIBLE GAMMA.
3330      2      DO 110 NG=1,KGX
3340      3      LL=IG(NG,MS)+1
3350      3      110 GUM(LL)=DCO*GUM(LL)
3360      2 C**** 'GUM' IS THE K-FUNCTION OF EQ.(III-2.23).
3370      2 C-03
3380      2      DO 120 NA=1,5
3390      3      120 HRHS(NA)=0.
3400      2 C**** COMPUTE THE U-FUNCTION OF EQ.(III-2.22).
3410      2      MPX=IPX(MS)
3420      2      M1=MAL1(MS)
3430      2      DO 140 MP=1,MPX
3440      3      M=MP+M1-1
3450      3      IF(M.EQ.1.OR.M.EQ.4.OR.M.EQ.13) GO TO 140
3460      3      N=NR(M)
3470      3      MA=MSF(M)
3480      3      K1=KST(N)
3490      3      K2=KED(N)
3500      3 C**** SUM OVER A,C, AND GAMMA (I.E., SUM OVER K) IN EQ.(III-2.22)
3510      3      USUM=0.
3520      3      DO 130 K=K1,K2
3530      4      KA=LA(K)+LC(K)
3540      4      KB=LB(K)+LD(K)
3550      4      KG=LG(K)+1
3560      4      130 USUM=USUM+X**KA*Y**KB*GUM(KG)*RAM(K)
3570      3 C**** 'USUM' IS THE U-FUNCTION OF EQ.(III-2.22).
3580      3 C-04
3590      3 C**** COMPUTE THE H-FUNCTION OF EQ.(III-3.4) BY MULTIPLYING
3600      3 C**** 'USUM' BY THE C-COEFFICIENTS AND SUM OVER THE GRAND-L AND
3610      3 C**** GRAND-S.
3620      3      NA=LOCK(M)/10
3630      3      KA=KEY(M)/10
3640      3      KB=KEY(M)-10*KA
3650      3      HRHS(NA)=HRHS(NA)+COEF(KA,KB)*USUM
3660      3      IF(M.EQ.16) HRHS(NA)=HRHS(NA)+COEF(KA+1,KB+1)*USUM
3670      3 C**** 'HRHS(NA)' IS THE H-FUNCTION OF EQ.(III-3.4).
3680      3      140 CONTINUE
3690      2 C-05
3700      2 C**** PROCESS THE X-INTEGRATION OF EQ.(III-3.3).
3710      2      XTEMP=X*TR1(IX)*XXX
3720      2      DO 150 NA=2,4,2
3730      3      ZRHS(1,NA)=ZRHS(1,NA)+XTEMP*UU(IX)*RSC(IX,1)*HRHS(NA)
3740      3      150 ZRHS(2,NA)=ZRHS(2,NA)+XTEMP*WW(IX)*RSC(IX,2)*HRHS(NA)
3750      2      DO 160 NA=3,5,2
3760      3      ZRHS(1,NA)=ZRHS(1,NA)+XTEMP*UU(IX)*RSC(IX,2)*HRHS(NA)
3770      3      160 ZRHS(2,NA)=ZRHS(2,NA)+XTEMP*WW(IX)*RSC(IX,3)*HRHS(NA)
3780      2      170 XXX=1.-XXX

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3790 1 DO 180 K=1,2
3800 2 DO 180 NA=2,5
3810 3 180 ZRHS(K,NA)=AH2*ZRHS(K,NA)
3820 1 C**** 'ZRHS' IS THE Z-FUNCTION OF EQ.(III-3.3).
3830 1 C-06
3840 1 C**** CONSTRUCT THE INTEGRAND OF THE Y-INTEGRATION IN EQ.(III-3.2).
3850 1 DO 200 K=1,2
3860 2 DO 190 NA=2,3
3870 3 190 URHS(K,NA)=Y*SSH(IY,1)*ZRHS(K,NA)
3880 2 DO 200 NA=4,5
3890 3 200 URHS(K,NA)=Y*SSH(IY,2)*ZRHS(K,NA)
3900 1 * WRITE(6,1010) Y,((URHS(K,NA),NA=2,5),K=1,2)
3910 1 *1010 FORMAT(' ',1P4E13.5,2(3X,1P4E13.5))
3920 1 C-07
3930 1 C**** PROCESS THE SIMPSON QUADRATURE OF EQ.(III-3.2).
3940 1 DO 210 K=1,2
3950 2 DO 210 NA=2,5
3960 3 YRHS(K,NA)=YRHS(K,NA)+YYY*TY1(IY)*URHS(K,NA)
3970 3 210 IF(IY.EQ.JMYM-5) PRURHS(K,NA)=URHS(K,NA)
3980 1 YYY=1.-YYY
3990 1 220 CONTINUE
4000 DO 230 K=1,2
4010 1 DO 230 NA=2,5
4020 2 230 YRHS(K,NA)=AY2*YRHS(K,NA)/BETAQ
4030 C**** 'YRHS' IS THE CONTRIBUTION TO EQ.(III-3.2) FROM Y=0 TO Y(JMYM).
4040 C-08
4050 C**** NOW, ADD THE CONTRIBUTION FROM Y BEYOND Y(JMYM) BY ASSUMING
4060 C**** THE INTEGRAND 'URHS' TO GO TO ZERO EXPONENTIALLY.
4070 DYM=YY(JMYM)-YY(JMYM-5)
4080 DO 240 K=1,2
4090 1 DO 240 NA=2,5
4100 2 SRHS(K,NA)=0.
4110 2 IF(ABS(URHS(K,NA)).LT.1.E-15) GO TO 240
4120 2 AL=ALOG(PRURHS(K,NA)/URHS(K,NA))/DYM
4130 2 SRHS(K,NA)=URHS(K,NA)/AL/BETAQ
4140 2 240 YRHS(K,NA)=2.*(YRHS(K,NA)+SRHS(K,NA))
4150 WRITE(6,1020) MS,((K,NA,NA=2,5),K=1,2)
4160 1020 FORMAT("OALPHA" =",I2,2(3X,4(4X,"K=",I1,"NA=",I1," "))
4170 WRITE(6,1030) ((YRHS(K,NA),NA=2,5),K=1,2)
4180 1030 FORMAT(5X,'YRHS=',2(3X,1P4E13.5))
4190 WRITE(6,1040) ((SRHS(K,NA),NA=2,5),K=1,2)
4200 1040 FORMAT(' CONTRIBUTION FROM BEYOND Y(JMYM)'/10X,2(3X,1P4E13.5))
4210 RETURN
4220 END
4230 SUBROUTINE FYASYM(AQ,MALL)
4240 C**** THIS COMPUTE (I) THE P-TABLE, (II) THE Y-TABLE, AND
4250 C**** (III) THE Y-FUNCTION OF EQ.(III-2.2).(SEE 'CODE FYFI5'
4260 C**** FOR DETAILS)
4270 COMMON/BBBBB/YY(60),TY1(60),JMYM,JMYG,AY2,FY(61,12,4,2)
4280 & ,SSH(60,2),DSP(4,4,71,46)
4290 DIMENSION AQ(*),AQ1(12),U(61,2),S(4),SUM(61,4,2)
4300 C-01
4310 * WRITE(6,1000)
4320 *1000 FORMAT('O*** FYASYM ***')
4330 MALL=12
4340 IMX=6
4350 PIMX=0.750428
4360 CALL PTABLE(AQ,AQ1,DK,PIMX,IMX,MALL)
4370 JMY=JMYM
4380 CALL YTAB(YY,TY1,JMY,2.,30.,18.,0.3,DTY)
4390 AY2=2.*DTY
4400 C**** DO-LOOP OVER THE GRAND P-MESH.
4410 PO=0.

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4420          DO 80 JM=1,MALL
4430      1      JMR=JM
4440      1      P1=AQ(JM)
4450      1      C-02
4460      1      C**** DECIDE THE FINER P'-MESH FOR THE P' INTEGRATION.
4470      1      NP=INT((P1-P0)*YY(JMY)/0.3)
4480      1      NP=2*(NP/2)
4490      1      IF(NP.LT.4) NP=4
4500      1      NP1=NP+1
4510      1      DP=(P1-P0)/NP
4520      1      C-03
4530      1      C**** INITIALIZE THE P' INTEGRATION.
4540      1      IF(JM.EQ.1) GO TO 20
4550      1      DO 10 LL=1,2
4560      2      DO 10 JY=1,JMY+1
4570      3      SUM(JY,1,LL)=0.
4580      3      SUM(JY,2,LL)=U(JY,LL)/6.
4590      3      SUM(JY,3,LL)=0.
4600      3      SUM(JY,4,LL)=SUM(JY,2,LL)
4610      3      10 CONTINUE
4620      1      GO TO 40
4630      1      20 DO 30 JY=1,JMY+1
4640      2      DO 30 LL=1,2
4650      3      DO 30 N=1,4
4660      4      SUM(JY,N,LL)=0.
4670      4      30 CONTINUE
4680      1      40 P=P0
4690      1      C-04
4700      1      CCC=2./3.
4710      1      C**** DO LOOP OVER THE FINER P-MESH(I.E.,P')
4720      1      DO 60 JP=2,NP1
4730      2      DDD=CCC
4740      2      IF(JP.EQ.NP1) DDD=DDD/2.
4750      2      P=P+DP
4760      2      C**** CALCULATE THE SPECTATOR FUNCTION 'U' AT P' AND AT EVERY 'Y'.
4770      2      C**** U(Y)=F(P,Y)/Y**L, WHERE F(P,Y) IS THE NORMALIZED SPHERICAL
4780      2      C**** BESSEL FUNCTION.
4790      2      CALL BESSEL(P,U,YY,JMY)
4800      2      C**** FIND THE SPLINE FUNCTION 'S' AND CARRY OUT THE SIMPSON QUADRATOR
4810      2      C**** FOR THE P' INTEGRATION.
4820      2      UP=P-P0
4830      2      EX=EXP(UP)
4840      2      S(1)=(EX-1./EX)/2.
4850      2      S(2)=S(1)+1./EX
4860      2      S(3)=UP
4870      2      S(4)=1.
4880      2      DO 50 LL=1,2
4890      3      DO 50 JY=1,JMY+1
4900      4      DO 50 N=1,4
4910      5      SUM(JY,N,LL)=SUM(JY,N,LL)+DDD*U(JY,LL)*S(N)
4920      5      50 CONTINUE
4930      2      CCC=1.-CCC
4940      2      60 CONTINUE
4950      1      C-05
4960      1      DO 70 LL=1,2
4970      2      DO 70 JY=1,JMY+1
4980      3      DO 70 N=1,4
4990      4      FY(JY,JM,N,LL)=2.*DP*SUM(JY,N,LL)
5000      4      70 CONTINUE
5010      1      P0=P1
5020      1      80 CONTINUE
5030      *      DO 110 LL=1,2
5040      *      DO 110 JM=3,MALL,3

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```

5050      *      WRITE(6,1010) JM,JMYM
5060      *1010  FORMAT('O*** JM=' I3,' *** JMYM=',I3)
5070      *      DO 100 M=1,4
5080      * 100  WRITE(6,1020) M,(FY(JY,JM,M,LL),JY=1,JMY+1)
5090      *1020  FORMAT('OFY(M=',I2,',)'/'(' ',1P10E12.4))
5100      * 110  CONTINUE
5110      RETURN
5120      END

6100      SUBROUTINE XTABLE(JMX,JMXGG,XR,TR1,DT,EM,XM,TM,TXC)
6110      C****  T(X)=C*(X+T0)*X/(X+S0)
6120      DIMENSION XR(*),TR1(*)
6130      SX0=(TM-TXC*XM)*XM/(EM*XM-TM)
6140      TX0=EM*SX0/TXC
6150      DT=TM/JMX
6160      DTQ=DT**2
6170      CT0=TXC*TX0
6180      CS02=2.*TXC*SX0
6190      CS04=2.*CS02
6200      TXC2=2.*TXC
6210      T=0.
6220      DO 10 I=1,JMXGG
6230      1      T=T+DT
6240      1      A=CT0-T
6250      1      XR(I)=(-A+SQRT(A*A+CS04*T))/TXC2
6260      1      DTDX=TXC*(XR(I)**2+2.*SX0*XR(I)+TX0*SX0)/(XR(I)+SX0)**2
6270      1      TR1(I)=1./DTDX
6280      1      10 CONTINUE
6290      WRITE(6,1000) TXC,TX0,SX0
6300      1000  FORMAT('OXTABLE WITH T(X)=C*(X+T0)*X/(X+S0)'/5X,'C=',1PE13.5,
6310      & ' T0=',1PE13.5,' S0=',1PE13.5)
6320      RETURN
6330      END

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20.084 ** CODE DEUTRN *** LABEL
 (09-30-82) OPTIONS: INTER,OPT=1,NROUND,NDLR,ALC,MASTER,INLINE=0,LSTIN,LNO,NREST

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10      C**** *** CODE DEUTRN ***
20      C**** *** COMPUTE THE DEUTERON WAVE FUNCTION USING THE STURM-FUNCTION
30      C**** CODE. SEARCH FOR THE RIGHT VALUE OF Q AT WHICH ALAM=1, BY MEANS
40      C**** OF NEWTON-RAPHSON. NORMALIZE THE WAVE FUNCTION IN ORDINARY SENSE.
50      COMMON/ZZZZZ/TR(80),XR(80),TR1(80),TR2(80),TR3(80),TR4(80),TR5(80)
60      & ,DT,TMATCH,A,A2,B,CUTOFF,JMX
70      COMMON/TTTTT/V11(80),V22(80),V12(80),FL2(80)
80      DIMENSION UY(80),WY(80)
90      LFDEUT=28
100     JMX=30
110     JMXS=80
120     HM=1./41.47
130     CUT=50.
140     CALL YTABLE(JMX,JMXS)
150     DO 10 J=1,JMX
160     1   FL2(J)=6./XR(J)**2
170     1   CALL POTD(XR(J),V11(J),V22(J),V12(J),HM,CUT)
180     1   10 CONTINUE
190     C**** INITIAL GUESS FOR 'Q'.
200     Q0=0.230
210     Q=Q0
220     C**** INITIAL GUESS FOR 'ALAM' AT 'Q' = 'Q0'.
230     AM=1.00
240     DLAMO=0.05
250     WRITE(6,1000)
260     1000 FORMAT('0',8X,'Q',18X,'ALAM',16X,'DIFF',7X,'NODE',2X,'I',7X,
270     & 'ANO')
280     ITIME=0
290     20 CALL STURMD(Q,AM,DLAMO,1,UY,WY,ANO)
300     C**** NORMALIZATION FACTOR IN ORDINARY SENSE. THE REGION BEYOND XR(JMX)
310     C**** IS INTEGRATED ANALYTICALLY.
320     SUM=0.
330     CCC=2./3.
340     DO 30 J=1,JMX
350     1   SUM=SUM+(UY(J)**2+WY(J)**2)*CCC*TR1(J)
360     1   30 CCC=1.-CCC
370     SUM=SUM*2.*DT
380     QX=Q*XR(JMX)
390     H0=EXP(-QX)
400     H2=H0*(3./QX**2+3./QX+1.)
410     ASYU=UY(JMX)/H0
420     ASYW=WY(JMX)/H2
430     HQ=H0**2/(2.*Q)
440     HQ2=HQ*(6./QX**3+12./QX**2+6./QX+1.)
450     SUM=SUM+ASYU**2*HQ+ASYW**2*HQ2
460     IF(DABS(AM-1.0).LT.1.E-5) GO TO 40
470     ITIME=ITIME+1
480     IF(ITIME.LT.50) GO TO 25
490     WRITE(6,1030)
500     1030 FORMAT('ONEWTON-RAPHSON DOES NOT CONVERGE. ')
510     STOP
520     25 CONTINUE
530     C**** NOW, WE CAN CALCULATE THE DERIVATIVE OF 'ALAM'. (EQ.(III-
540     C**** 3.11))
550     DAM=2.*Q*AM**2*SUM*ANO
560     C**** NEWTON-RAPHSON (SEE EQ.(III-3.10))
570     Q=Q-(AM-1.)/DAM
580     GO TO 20
590     C**** NORMALIZE THE WAVE FUNCTION IN ORDINARY SENSE.

```

```

600      40 FNORM=SQRT(SUM)
610      DO 50 J=1,JMX
620      1  UY(J)=UY(J)/FNORM
630      1  50 WY(J)=WY(J)/FNORM
640      BED=Q**2/HM
650      WRITE(6,1005) Q,BED,AM,FNORM
660      1005 FORMAT('OQ=',1PE13.5,' BED=',1PE13.5,' AM=',1PE13.5,
670      & ' NORM=',1PE13.5)
680      WRITE(6,1010) (UY(J),J=1,JMX)
690      1010 FORMAT('OUY'/' ' ,1P10E12.4)
700      WRITE(6,1020) (WY(J),J=1,JMX)
710      1020 FORMAT('OWY'/' ' ,1P10E12.4)
720      REWIND LFDEUT
730      WRITE(LFDEUT) Q,BED,CUT,UY,WY,V11,V12,V22,DT,XR,TR1
740      ENDFILE LFDEUT
750      STOP
760      END
770      SUBROUTINE POTD(R,A11,A22,A12,HM,CUT)
780      C***** COMPUTE THE 3S1 +3D1 RSC POTENTIAL
790      X=0.7*R
800      EX1=REX1(1.,CUT,X)
810      EX2=REX1(2.,CUT,X)
820      EX4=REX1(4.,CUT,X)
830      EX6=REX1(6.,CUT,X)
840      EXT=REXS(CUT,X)
850      EXS=(REXS(CUT/4.,4.*X)-REX1(1.,CUT/4.,4.*X))*64.
860      VT=-10.463*(EXT-EXS)
870      VC=-10.463*EX1+105.468*EX2-3187.8*EX4+9924.3*EX6
880      VT=VT+351.77*EX4-1673.5*EX6
890      VLS=708.91*EX4-2713.1*EX6
900      A11=HM*VC
910      A22=HM*(VC-2.*VT-3.*VLS)
920      A12=HM*SQRT(8.)*VT
930      RETURN
940      END
950      FUNCTION REX1(A,C,X)
960      P=C*X
970      IF(P.LT.50.) GO TO 10
980      REX1=EXP(-A*X)/X
990      RETURN
1000     10 REX1=(EXP(-A*X)-EXP(-P))/X
1010     RETURN
1020     END
1030     FUNCTION REXS(C,X)
1040     P=C*X
1050     IF(P.LT.50.) GO TO 10
1060     REXS=(1.+3./X+3./X**2)*EXP(-X)/X
1070     RETURN
1080     10 T=(3.*C**2-1.)/2.+3.*C/X+3./X**2
1090     REXS=((1.+3./X+3./X**2)*EXP(-X)-T*EXP(-P))/X
1100     RETURN
1110     END
1120     SUBROUTINE COW(J,AKQ,DTQ,ALAM)
1130     C***** COMPUTE
1140     C***** H**2*A, AND 1./(1-H**2*A/12)
1150     C***** IN THE NUMEROV INTEGRATION.
1160     COMMON/ZZZZZ/TR(80),XR(80),TR1(80),TR2(80),TR3(80),TR4(80),TR5(80)
1170     & ,DT,TMATCH,ALPHA,ALPHA2,BETA,CUT,KMX
1180     COMMON/TTTTT/V11(80),V22(80),V12(80),FL2(80)
1190     COMMON/CCCCC/A11,A12,A22,B11,B12,B22,C11,C12,C22,UZ1(2),UZ2(2),
1200     & WZ1(2),WZ2(2),UZ3(2),WZ3(2)
1210     A11=(TR2(J)*(V11(J)/ALAM+AKQ)+TR4(J))*DTQ
1220     A12=TR2(J)*(V12(J)/ALAM)*DTQ

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```

1230      A22=(TR2(J))*(V22(J)/ALAM+AKQ+FL2(J))+TR4(J))*DTQ
1240      B11=1.-A11/12.
1250      B12=-A12/12.
1260      B22=1.-A22/12.
1270      DENOM=B11*B22-B12**2
1280      C11=B22/DENOM
1290      C12=-B12/DENOM
1300      C22=B11/DENOM
1310      RETURN
1320      END
1330      SUBROUTINE BULL(J,AKQ,DXQ,ALAM,UZ,WZ)
1340 C**** PROCESS THE NUMEROV ALGORITHM.
1350      COMMON/TTTTT/V11(80),V22(80),V12(80),FL2(80)
1360      COMMON/CCCCC/A11,A12,A22,B11,B12,B22,C11,C12,C22,UZ1(2),UZ2(2),
1370 & WZ1(2),WZ2(2),UZ3(2),WZ3(2)
1380      DIMENSION UZ(*),WZ(*)
1390      D11=2.+A11*C11+A12*C12
1400      D12=A11*C12+A12*C22
1410      D22=2.+A12*C12+A22*C22
1420      DO 11 I=1,2
1430 1      UZ3(I)=D11*UZ2(I)+D12*WZ2(I)-UZ1(I)
1440 1      WZ3(I)=D12*UZ2(I)+D22*WZ2(I)-WZ1(I)
1450 1      UZ1(I)=UZ2(I)
1460 1      WZ1(I)=WZ2(I)
1470 1      UZ2(I)=UZ3(I)
1480 1      11 WZ2(I)=WZ3(I)
1490      CALL COW(J,AKQ,DXQ,ALAM)
1500      DO 12 I=1,2
1510 1      UZ(I )=C11*UZ3(I)+C12*WZ3(I)
1520 1      12 WZ(I )=C12*UZ3(I)+C22*WZ3(I)
1530      RETURN
1540      END
1550      SUBROUTINE STURMD(AK,ALAM,DLAMO,ND,UY,WY,ANO)
1560 C**** STURM FUNCTION (NEGATIVE ENERGY) FOR RSC(3S1 + 3D1)
1570      COMMON/ZZZZZ/TR(80),XR(80),TR1(80),TR2(80),TR3(80),TR4(80),TR5(80)
1580 & ,DT,TMATCH,ALPHA,ALPHA2,BETA,CUT,KMX
1590      COMMON/TTTTT/V11(80),V22(80),V12(80),FL2(80)
1600      COMMON/CCCCC/A11,A12,A22,B11,B12,B22,C11,C12,C22,UZ1(2),UZ2(2),
1610 & WZ1(2),WZ2(2),UZ3(2),WZ3(2)
1620      DIMENSION UY(*),WY(*),UZ(2, 80),WZ(2, 80),UX(2, 80),WX(2, 80),
1630 & AA(4,4),UT(2),WT(2),RR(80)
1640      EQUIVALENCE (RR(1),XR(1)),(JMX,KMX),(DX,DT)
1650      XK=AK*RR(JMX)
1660      H0=EXP(-XK)
1670      H0=H0/TR3(JMX)
1680      H2=-(.3./XK**2+.3./XK+1.)*H0
1690      H2=-H2
1700      XK=AK*RR(JMX-1)
1710      H0M=EXP(-XK)
1720      H0M=H0M/TR3(JMX-1)
1730      H2M=-(.3./XK**2+.3./XK+1.)*H0M
1740      H2M=-H2M
1750      MESH=JMX
1760      DXQ=DX**2
1770      MESH1=MESH-1
1780      MESH2=MESH-2
1790      MATCHO=TMATCH/DT
1800      MATCH=MATCHO
1810      IN=1
1820      NODEO=ND-1
1830      INODE=20
1840      AKQ=AK**2
1850      DLAM=DLAMO

```

```

1860         JMATCH=MATCH+1
1870         MATCH1=MATCH+3
1880         MATCH2=MATCH-3
1890         M=1
1900         100 NODE=0
1910         C**** FIRST, SOLVE FROM INSIDE OUTWARD TO MATCH.
1920         J=1
1930         UZ(1,1)=1.E-3
1940         WZ(1,1)=0.
1950         UZ(2,1)=0.
1960         WZ(2,1)=1.E-3
1970         DO 5 I=1,2
1980         1     UZ1(I)=0.
1990         1     5 WZ1(I)=0.
2000         CALL COW(J,AKQ,DXQ,ALAM)
2010         DO 10 I=1,2
2020         1     UZ2(I)=B11*UZ(I,1)+B12*WZ(I,1)
2030         1     10 WZ2(I)=B12*UZ(I,1)+B22*WZ(I,1)
2040         DO 50 J=2,MATCH1
2050         1     K=J
2060         1     CALL BULL(K,AKQ,DXQ,ALAM,UT,WT)
2070         1     DO 50 I=1,2
2080         2     UZ(I,J)=UT(I)
2090         2     WZ(I,J)=WT(I)
2100         2     50 CONTINUE
2110         C**** CHECK THE NUMBER OF NODES INSIDE MATCH.
2120         DO 60 J=2,MATCH1,2
2130         1     IF(ABS(UY(J)).LT.1.E-10.OR.ABS(UY(J+2)).LT.1.E-10) GO TO 60
2140         1     IF(UY(J)/UY(J+2).LT.0.) NODE=NODE+1
2150         1     60 CONTINUE
2160         IF(NODE.LE.NODE0) GO TO 70
2170         95 ALAM=ALAM*(1.+DLAM/5.)
2180         IN=IN+1
2190         IF(IN.GT.INODE ) GO TO 220
2200         GO TO 100
2210         70 CONTINUE
2220         C**** NOW, SOLVE FROM OUTSIDE INWARD TO MATCH.
2230         J=MESH
2240         UX(1,J)=H0
2250         WX(1,J)=0.
2260         UX(2,J)=0.
2270         WX(2,J)=H2
2280         UX(1,J-1)=H0M
2290         WX(1,J-1)=0.
2300         UX(2,J-1)=0.
2310         WX(2,J-1)=H2M
2320         CALL COW(J,AKQ,DXQ,ALAM)
2330         DO 71 I=1,2
2340         1     UZ1(I)=B11*UX(I,J)+B12*WX(I,J)
2350         1     71 WZ1(I)=B12*UX(I,J)+B22*WX(I,J)
2360         J=J-1
2370         CALL COW(J,AKQ,DXQ,ALAM)
2380         DO 72 I=1,2
2390         1     UZ2(I)=B11*UX(I,J)+B12*WX(I,J)
2400         1     72 WZ2(I)=B12*UX(I,J)+B22*WX(I,J)
2410         DO 40 JV=MATCH2,MESH2
2420         1     J=MESH2-JV+MATCH2
2430         1     CALL BULL(J,AKQ,DXQ,ALAM,UT,WT)
2440         1     DO 40 I=1,2
2450         2     UX(I,J)=UT(I)
2460         2     WX(I,J)=WT(I)
2470         2     40 CONTINUE
2480         C**** JOIN SMOOTHLY THE INNER SOLUTION AND THE OUTER SOLUTION AT MATCH

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```

2490      DO 111 J=1,2
2500      1      K=J
2510      1      AA(1,K)=UZ(J,MATCH)
2520      1      AA(2,K)=WZ(J,MATCH)
2530      1      AA(3,K)=(45.*(UZ(J,MATCH+1)-UZ(J,MATCH-1))-9.*(UZ(J,MATCH+2)
2540      1      &      -UZ(J,MATCH-2))+UZ(J,MATCH+3)-UZ(J,MATCH-3))/(60.*DX)
2550      1      AA(4,K)=(45.*(WZ(J,MATCH+1)-WZ(J,MATCH-1))-9.*(WZ(J,MATCH+2)
2560      1      &      -WZ(J,MATCH-2))+WZ(J,MATCH+3)-WZ(J,MATCH-3))/(60.*DX)
2570      1      111 CONTINUE
2580      DO 112 I=1,2
2590      1      K=5-I
2600      1      AA(1,K)=UX(I,MATCH)
2610      1      AA(2,K)=WX(I,MATCH)
2620      1      AA(3,K)=(45.*(UX(I,MATCH+1)-UX(I,MATCH-1))-9.*(UX(I,MATCH+2)
2630      1      &      -UX(I,MATCH-2))+UX(I,MATCH+3)-UX(I,MATCH-3))/(60.*DX)
2640      1      AA(4,K)=(45.*(WX(I,MATCH+1)-WX(I,MATCH-1))-9.*(WX(I,MATCH+2)
2650      1      &      -WX(I,MATCH-2))+WX(I,MATCH+3)-WX(I,MATCH-3))/(60.*DX)
2660      1      112 CONTINUE
2670      DO 113 I=1,4
2680      1      113 AA(I,4)=-AA(I,4)
2690      DET=AA(1,1)*(AA(2,2)*AA(3,3)-AA(2,3)*AA(3,2))+AA(2,1)*(AA(3,2)
2700      & * AA(1,3)-AA(1,2)*AA(3,3))+AA(3,1)*(AA(1,2)*AA(2,3)-AA(2,2)
2710      & * AA(1,3))
2720      AB=(AA(1,4)*(AA(2,2)*AA(3,3)-AA(2,3)*AA(3,2))+AA(2,4)*(AA(3,2)
2730      & * AA(1,3)-AA(1,2)*AA(3,3))+AA(3,4)*(AA(1,2)*AA(2,3)-AA(2,2)
2740      & * AA(1,3)))/DET
2750      BB=(AA(1,1)*(AA(2,4)*AA(3,3)-AA(3,4)*AA(2,3))+AA(2,1)*(AA(3,4)
2760      & * AA(1,3)-AA(1,4)*AA(3,3))+AA(3,1)*(AA(1,4)*AA(2,3)-AA(2,4)
2770      & * AA(1,3)))/DET
2780      TB=(AA(1,1)*(AA(2,2)*AA(3,4)-AA(3,2)*AA(2,4))+AA(2,1)*(AA(3,2)
2790      & * AA(1,4)-AA(1,2)*AA(3,4))+AA(3,1)*(AA(1,2)*AA(2,4)-AA(2,2)
2800      & * AA(1,4)))/DET
2810      C**** CHECK IF THE LAST EQUATION ALSO HOLDS.
2820      DIFF=AA(4,1)*AB+AA(4,2)*BB+AA(4,3)*TB-AA(4,4)
2830      C**** JOIN THE INNER AND THE OUTER SOLUTIONS.
2840      DO 211 J=1,MATCH
2850      1      UY(J)=UZ(1,J)*AB+UZ(2,J)*BB
2860      1      211 WY(J)=WZ(1,J)*AB+WZ(2,J)*BB
2870      DO 212 J=JMATCH,MESH
2880      1      UY(J)=-UX(1,J)-UX(2,J)*TB
2890      1      212 WY(J)=-WX(1,J)-WX(2,J)*TB
2900      C**** CHECK THE NUMBER OF NODES ALTOGETHER.
2910      DO 120 J=2,MESH1,2
2920      1      IF(ABS(UY(J)).LT.1.E-10.OR.ABS(UY(J+2)).LT.1.E-10) GO TO 120
2930      1      IF(UY(J)/UY(J+2).LT.0.) NODE=NODE+1
2940      1      120 CONTINUE
2950      IF(NODE-NODE0) 90,110,95
2960      90 ALAM=ALAM*(1.-DLAM0)
2970      IN=IN+1
2980      IF(IN.GT.INODE) GO TO 220
2990      GO TO 100
3000      110 CONTINUE
3010      IF(ABS(DIFF).LT.1.E-5) GO TO 210
3020      IF(ABS(DIFF).LT.10.) GO TO 121
3030      WRITE(6,1011) DIFF
3040      1011 FORMAT('0DIFF=',1PE13.5)
3050      STOP
3060      121 M=M+1
3070      IF(M.GT.99) GO TO 230
3080      IF(M.GE.3) GO TO 130
3090      DIFF1=DIFF
3100      ALAM1=ALAM
3110      ALAM=ALAM*(1.-DLAM/3.)
3120      GO TO 100

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3130      130 DIFF2=DIFF
3140          ALAM2=ALAM
3150          IF(DIFF2/DIFF1.LT.0.) GO TO 150
3160          IF(ABS(DIFF2).GT.ABS(DIFF1)) GO TO 140
3170          ALAM=ALAM2*(1.-DLAM/3.)
3180          ALAM1=ALAM2
3190          DIFF1=DIFF2
3200          GO TO 100
3210      140 IF(M.GE.4) GO TO 150
3220          DLAM=-DLAM
3230          GO TO 160
3240      150 DLAM=DLAM/3.
3250      160 ALAM=ALAM1*(1.-DLAM/3.)
3260          GO TO 100
3270      210 DO 205 J=1,MESH
3280      1   UY(J)=TR3(J)*UY(J)
3290      1   205 WY(J)=TR3(J)*WY(J)
3300      C**** CALCULATE THE NORMALIZATION FACTOR 'ANO' BY EQ.(57).
3310          SUM=0.
3320          CCC=2./3.
3330          DO 213 J=1,MESH
3340      1   SUM=SUM+(UY(J)*(V11(J)*UY(J)+V12(J)*WY(J))+WY(J)*(V12(J)*UY(J)+
3350      1   & V22(J)*WY(J))*CCC*TR1(J)
3360      1   CCC=1.-CCC
3370      1   213 CONTINUE
3380          SUM=SUM*DX*2.
3390          ANO=1./SUM
3400          WRITE(6,1006) AK,ALAM,DIFF,NODE,M, ANO
3410      1006 FORMAT(' ',1PE15.4,1PD25.13,1PE15.4,2I5,1PE15.5)
3420          GO TO 200
3430      220 WRITE(6,1003)
3440      1003 FORMAT(' NODE EXCEEDS NODE0')
3450          GO TO 200
3460      230 WRITE(6,1004)
3470          GO TO 210
3480      200 RETURN
3490      1004 FORMAT('OCONVERGENCE TOO SLOW')
3500      END
3510      SUBROUTINE YTABLE(JMX,JMXS)
3520      C****      T(X) = C*(X+T0)*X/(X+S0)
3530          COMMON/ZZZZ/TR(80),XR(80),TR1(80),TR2(80),TR3(80),TR4(80),TR5(80)
3540          & ,DT,DMATCH,A,A2,B,CUT,M
3550          DATA EM,XM,TM,TXC/ 12.0, 6.0, 9.0, 0.3/
3560          SX0=(TM-TXC*XM)*XM/(EM*XM-TM)
3570          TX0=EM*SX0/TXC
3580          DT=TM/JMX
3590          DTQ=DT**2
3600          CTO=TXC*TX0
3610          CS02=2.*TXC*SX0
3620          CS04=2.*CS02
3630          TXC2=2.*TXC
3640          T=0.
3650          DO 10 I=1,JMXS
3660      1   T=T+DT
3670      1   A=CTO-T
3680      1   TR(I)=T
3690      1   XR(I)=(-A+SQRT(A*A+CS04*T))/TXC2
3700      1   DTDX=TXC*(XR(I)**2+2.*SX0*XR(I)+TX0*SX0)/(XR(I)+SX0)**2
3710      1   DTDX2=TXC*2.*SX0*(SX0-TX0)/(XR(I)+SX0)**3
3720      1   DTDX3=-3./(XR(I)+SX0)*DTDX2
3730      1   TR1(I)=1./DTDX
3740      1   TR2(I)=TR1(I)**2
3750      1   TR3(I)=SQRT(TR1(I))

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```
3760 1      FPP=-DTDX2/(DTDX**3)
3770 1      FPPP=- (DTDX3*DTDX-3.*DTDX2**2)/(DTDX**5)
3780 1      TR4(I)=0.75*(FPP/TR1(I))**2-FPPP/(2.*TR1(I))
3790 1      TR5(I)=TR1(I)*TR3(I)
3800 1      10 CONTINUE
3810      WRITE(6,1000) TXC,TX0,SX0
3820      1000 FORMAT('OXTABLE WITH T(X)=C*(X+T0)*X/(X+S0)'/ 'OC=',1PE13.5,
3830      & ' T0=',1PE13.5, ' S0=',1PE13.5/9X, 'TR',13X, 'XR',13X, 'TR1',12X,
3840      & ' TR2',12X, 'TR3',12X, 'TR4',12X, 'TR5')
3850      C      DO 20 J=1,JMXS
3860      C      20 WRITE(6,1001) TR(J),XR(J),TR1(J),TR2(J),TR3(J),TR4(J),TR5(J)
3870      C      1001 FORMAT(' ',1P7E15.5)
3880      DO 30 I=1,JMXS
3890 1      30 IF(XR(I).GE.1.) GO TO 40
3900      40 TMATCH=TR(I)
3910      RETURN
3920      END
```

§4. El Sum Rule

4-a. General description of Code SUM5

The enhancement factor κ of the integrated photo-nuclear absorption cross section with the RSC potential can be calculated by Eqs. (I-7-5), (I-7-11), (I-7-18) to (I-7-22). We rearrange these formulas so that the contribution to κ from each component is apparent.

$$\kappa = \sum_{\alpha=1}^5 \sum_{\alpha' \geq \alpha}^5 \kappa_{\alpha\alpha'} \quad (4.1)$$

with

$$\kappa_{\alpha\alpha'} = 3 \frac{M}{\hbar^2} \int_0^\infty dp \int_0^\infty dx x^2 \theta_\alpha(q, x) \theta_{\alpha'}(q, x) x^2 G_{\alpha\alpha'}(x) \quad (4.2)$$

where there are only seven non-zero elements $G_{\alpha\alpha'}(x)$ with $\alpha' \geq \alpha$, and they are

$$G_{11}(x) = \frac{1}{6} \{-V({}^1S_0) + V({}^1P_1)\} \quad (4.3a)$$

$$G_{22}(x) = G_{44}(x) = \frac{1}{2} \{-V({}^3S_1) + \sum_{J=0}^2 C^2({}^3S_1, {}^3P_J) V({}^3P_J)\} \quad (4.3b)$$

$$G_{33}(x) = G_{55}(x) = \frac{1}{2} \{-V({}^3D_1) + \sum_{J=0}^2 C^2({}^3D_1, {}^3P_J) V({}^3P_J) + C^2({}^3D_1, {}^3F_2) V({}^3F_2) + 2 C({}^3D_1, {}^3P_2) C({}^3D_1, {}^3F_2) V({}^3P_2 - {}^3F_2)\} \quad (4.3c)$$

$$G_{23}(x) = G_{45}(x) = -V({}^3S_1 - {}^3D_1) + \sum_{J=0}^2 C({}^3S_1, {}^3P_J) C({}^3D_1, {}^3P_J) V({}^3P_J) + C({}^3S_1, {}^3P_2) C({}^3D_1, {}^3F_2) V({}^3P_2 - {}^3F_2) \quad (4.3d)$$

where for simplicity we have written $V({}^{2S+1}\lambda_\xi)$ for $\langle {}^{2S+1}\lambda_\xi | V | {}^{2S+1}\lambda_\xi \rangle$ and $V({}^{2S+1}\lambda_\xi - {}^{2S+1}\lambda'_\xi)$ for $\langle {}^{2S+1}\lambda_\xi | V | {}^{2S+1}\lambda'_\xi \rangle$. The coefficients $C({}^{2S+1}L_J, {}^{2S+1}\lambda_\xi)$ are given by Eq. (I-7-22):

$$C({}^{2S+1}L_J, {}^{2S+1}\lambda_\xi) = \hat{L} \hat{\lambda} \hat{\xi} \begin{pmatrix} 1 & L & \lambda \\ 0 & 0 & 0 \end{pmatrix} \begin{Bmatrix} \xi & J & 1 \\ L & \lambda & S \end{Bmatrix} \quad (4.4)$$

There appear ten potential terms in Eq. (4.3) which we number according to Table 1. There are altogether seventeen terms in Eq. (4.3). We denote these seventeen terms by $T_i(x)$ where the numbering i is given by Table 2, so that

regularization given here is slightly simpler than that given in PERFECT since here we use one cut-off mass κ whereas in Eqs.(63)-(65) of PERFECT we use stronger cut-off with two regularization masses κ and Λ in the limit of $\Lambda \rightarrow \kappa$. Functions REX1(n, κ, x) and REXS(κ, a, x) compute $Y_n(\kappa; x)$ of Eq.(4.11) and $Z(\kappa, a; x)$ of Eq.(4.12), respectively.

Table 1 The numbering of the potential terms

	$1S_0$	$3S_1-3S_1$	$3D_1-3D_1$	$3S_1-3D_1$	$1P_1$	$3P_0$	$3P_1$	$3P_2-3P_2$	$3F_2-3F_2$	$3P_2-3F_2$
n	1	2	3	4	5	6	7	8	9	10

Table 2 Classification of terms in Eq.(4.3)

The index n corresponds to the numbering of potential by Table 1. For $i \geq 6$, each term is assigned a set of quantum numbers (L,L',S,J, λ, λ', ξ) according to the form $C(2S+1L_J, 2S+1\lambda_\xi)C(2S+1L'_J, 2S+1\lambda'_\xi) \times V(2S+1\lambda_\xi-2S+1\lambda'_\xi)$.

i	$T_i(x)$	L	L'	S	J	n	λ	λ'	ξ
1	$V(1S_0)$					1			
2	$V(3S_1)$					2			
3	$V(3D_1)$					3			
4	$V(3S_1-3D_1)$					4			
5	$V(1P_1)$					5			
6	$c^2(3S_1, 3P_0)V(3P_0)$	0	0	1	1	6	1	1	0
7	$c^2(3S_1, 3P_1)V(3P_1)$	0	0	1	1	7	1	1	1
8	$c^2(3S_1, 3P_2)V(3P_2)$	0	0	1	1	8	1	1	2
9	$c^2(3D_1, 3P_0)V(3P_0)$	2	2	1	1	6	1	1	0
10	$c^2(3D_1, 3P_1)V(3P_1)$	2	2	1	1	7	1	1	1
11	$c^2(3D_1, 3P_2)V(3P_2)$	2	2	1	1	8	1	1	2
12	$c^2(3D_1, 3F_2)V(3F_2)$	2	2	1	1	9	3	3	2
13	$c(3D_1, 3P_2)c(3D_1, 3F_2)V(3P_2-3F_2)$	2	2	1	1	10	1	3	2
14	$c(3S_1, 3P_0)c(3D_1, 3P_0)V(3P_0)$	0	2	1	1	6	1	1	0
15	$c(3S_1, 3P_1)c(3D_1, 3P_1)V(3P_1)$	0	2	1	1	7	1	1	1
16	$c(3S_1, 3P_2)c(3D_1, 3P_2)V(3P_2)$	0	2	1	1	8	1	1	2
17	$c(3S_1, 3P_2)c(3D_1, 3F_2)V(3P_2-3F_2)$	0	2	1	1	10	1	3	2

Eq.(4.3) is expressed as

$$G_{11}(x) = \frac{1}{6} (-T_1 + T_5) \tag{4.5a}$$

$$G_{22}(x) = G_{44}(x) = \frac{1}{2} (-T_2 + \sum_{i=6}^8 T_i) \tag{4.5b}$$

$$G_{33}(x) = G_{55}(x) = \frac{1}{2} (-T_3 + \sum_{i=9}^{12} T_i + 2T_{13}) \tag{4.5c}$$

$$G_{23}(x) = G_{45}(x) = -T_4 + \sum_{i=14}^{17} T_i \tag{4.5d}$$

The code to carry out the above computation is named SUM5. It consists of the following parts:

MAIN routine

Subroutines and functions

PGEN, PEX1, PEXS, XTABLE, PTABLE, CLEBSH, and F6J.

The code requires a data file named LFCHI which is an output of the main program.

Subroutines PTABLE, CLEBSH and F6J are identical to , and XTABLE is a simplified version of , the ones in the main program. MAIN routine also is simple and self-explanatory with its comment cards. Thus no further explanations are necessary. In the next section, we explain subroutine PGEN and functions REX1 and REXS.

4-b. Subroutine PGEN and functions REX1 and REXS.

These compute ten components of the RSC potential in Table 1. They are given in the notation of reference 3 by the following forms. (In these formulas $h=10.463$ MeV, and x is in units of $\mu^{-1}=(1/0.7)$ fm).

$$V(^1S) = -he^{-x}/x - 1650.6 e^{-4x}/x + 6484.2 e^{-7x}/x \quad (4.6a)$$

$$V(^1D) = -he^{-x}/x - 12.322 e^{-2x}/x - 1112.6 e^{-4x}/x + 6484.2 e^{-7x}/x \quad (4.6b)$$

$$V(^3P_0) = -h[(1+4/x+4/x^2)e^{-x} - (16/x+4/x^2)e^{-4x}]/x + 27.133 e^{-2x}/x - 790.74 e^{-4x}/x + 20662 e^{-7x}/x \quad (4.6c)$$

$$V(^3P_1) = h[(1+2/x+2/x^2)e^{-x} - (8/x+2/x^2)e^{-4x}]/x - 135.25 e^{-2x}/x + 472.81 e^{-3x}/x \quad (4.6d)$$

$$V(^3P_2-^3F_2) = V_C + V_{TS_{12}} + V_{LS} \vec{L} \cdot \vec{S} \quad (4.7)$$

$$V_C = \frac{h}{3} e^{-x}/x - 933.48 e^{-4x}/x + 4152.1 e^{-6x}/x \quad (4.7a)$$

$$V_T = h[(1/3 + 1/x + 1/x^2)e^{-x} - (4/x + 1/x^2)e^{-4x}]/x - 34.925 e^{-3x}/x \quad (4.7b)$$

$$V_{LS} = -2074.1 e^{-6x}/x \quad (4.7c)$$

and for $I=0$ potentials

$$V(^1P_1) = 3 h e^{-x}/x - 634.39 e^{-2x}/x + 2163.4 e^{-3x}/x \quad (4.8a)$$

$$V(^3D_2) = -3 h [(1+2/x + 2/x^2)e^{-x} - (8/x + 2/x^2)e^{-4x}]/x - 220.12 e^{-2x}/x + 871 e^{-3x}/x \quad (4.8b)$$

$$V({}^3S_1 - {}^3D_1) = V_C + V_T S_{12} + V_{LS} \vec{L} \cdot \vec{S} \quad (4.9)$$

$$V_C = -h e^{-x}/x + 105.468 e^{-2x}/x - 3187.8 e^{-4x}/x + 9924.3 e^{-6x}/x \quad (4.9a)$$

$$V_T = -h[(1 + 3/x + 3/x^2) e^{-x} - (12/x + 3/x^2) e^{-4x}]/x + 351.77 e^{-4x}/x + 1673.5 e^{-6x}/x \quad (4.9b)$$

$$V_{LS} = 708.91 e^{-4x}/x - 2713.1 e^{-6x}/x \quad (4.9c)$$

The matrix elements of $\vec{L} \cdot \vec{S}$ are

$$\begin{aligned} (\vec{L} \cdot \vec{S}) &= J - 1 && \text{for } L=J-1 \\ &= -1 && \text{for } L=J \\ &= -J - 2 && \text{for } L=J+1 \end{aligned} \quad (4.10)$$

The matrix elements of S_{12} are given by Table 3.

Since these potentials are all singular at the origin, we regularize them in a manner consistent with the regularization adopted in the main program (see subroutine POTD in Code STURM):

(i) Terms of the form e^{-nx}/x are replaced by

$$Y_n(\kappa; x) = (e^{-nx} - e^{-\kappa x})/x, \quad (4.11)$$

(ii) terms of the form $(1+a/x + a/x^2) e^{-x}/x$ are regularized to

$$Z(\kappa, a; x) = (1 + a/x + a/x^2) e^{-x}/x - \left[\frac{2-a+\kappa^2 a}{2} + \frac{\kappa a}{x} + \frac{a}{x^2} \right] \frac{e^{-\kappa x}}{x} \quad (4.12)$$

and (iii) terms of the form $(\frac{12}{x} + \frac{3}{x^2}) \frac{e^{-4x}}{x}$ are converted to

$$W(\kappa, x) = 64 [Z(\frac{\kappa}{4}, 3; 4x) - Y_1(\frac{\kappa}{4}; 4x)] \quad (4.13)$$

In the above expressions, all x are given in units of μ^{-1} ($\mu=0.7 \text{ fm}^{-1}$). The

$L' \backslash L$	$J-1$	J	$J+1$
$J-1$	$-2(J-1)/(2J+1)$	0	$6\sqrt{J(J+1)}/(2J+1)$
J	0	2	0
$J+1$	$6\sqrt{J(J+1)}/(2J+1)$	0	$-2(J+2)/(2J+1)$

Table 3. Matrix elements of $\langle (LS)J | S_{12} | (L'S)J \rangle$

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```

10.451  ** CODE SUM5 ***                                LABEL
(09-30-82)  OPTIONS: INTER,OPT=1,NROUND,NDLR,ALC,MASTER,INLINE=0,LSTIN,LNO,NREST

10      C**** *** CODE SUM5 ***
20      C**** COMPUTATION OF THE ENHANCEMENT FACTOR KAPPA OF EQ.(III-4.1)
30      C**** FOR THE RSC5 POTENTIAL.
40          DIMENSION XR(30),TR1(30),POT(30,10),AQ(12),AQ1(12),TSI(30,5,12),
50          & FAC(12),SUMP(7),SUMX(7),VK(7),COEF(17),TPX(17),G(5)
60          DIMENSION NSTATE(7),NLA(17),NLB(17),NSS(17),NJJ(17),
70          & NL1(17),NL2(17),NPT(17),NJ2(17),GSI(30,5,12),FACLOG(100)
80      C**** THE FOLLOWING INDICES REFER TO TABLES 1 AND 2 EXCEPT FOR 'NSTATE'.
90      C**** 'NLA'=L, 'NLB'=L', 'NSS'=S, 'NJJ'=J, 'NL1'=LAMBDA, 'NL2'=LAMBDA',
100     C**** 'NJ2'=XI, AND 'NPT'=N.
110     C**** 'NSTATE' IS THE KEY TO STATE INDICES OF SEVEN G-FUNCTIONS OF
120     C**** EQ.(III-4.3).
130         DATA NSTATE/11,22,44,33,55,23,45/,
140         &          NLA/0,0,2,0,0,0,0,0,2,2,2,2,2,0,0,0,0/,
150         &          NLB/0,0,2,2,0,0,0,0,2,2,2,2,2,2,2,2,2/,
160         &          NSS/0,1,1,0,1,1,1,1,1,1,1,1,1,1,1,1,1/,
170         &          NJJ/0,1,1,1,0,1,1,1,1,1,1,1,1,1,1,1,1/,
180         &          NL1/0,0,2,0,1,1,1,1,1,1,1,1,3,1,1,1,1,1/,
190         &          NL2/0,0,2,2,1,1,1,1,1,1,1,1,3,3,1,1,1,3/,
200         &          NPT/1,2,3,4,5,6,7,8,6,7,8,9,10,6,7,8,10/,
210         &          NJ2/0,1,1,1,1,0,1,2,0,1,2,2,2,0,1,2,2/
220         DATA FNORM/2.6/
230     C**** 'FNORM' IS THE NORMALIZATION FACTOR COMPUTED BY CODE NFORM.
240         WRITE(6,1010)
250     1010 FORMAT('O*** CODE SUM5 ***')
260     C-01
270         LFCHI=27
280         REWIND LFCHI
290         READ(LFCHI) TSI,GSI
300         JMX=30
310         CALL XTABLE(30,JMX,XR,TR1,DT,12.,6.,9.,0.3)
320         AH2=2.*DT
330         WRITE(6,2000) (XR(J),J=1,JMX)
340     2000 FORMAT('O XR=',1P10E12.5/(5X,1P10E12.5))
350         IMX=6
360         MALL=12
370         PIMX=0.750428
380         CALL PTABLE(AQ,AQ1,DK,PIMX,IMX,MALL)
390         AKH2=2.*PIMX/IMX
400         CCC=2./3.
410         DO 10 I=1,IMX
420     1         FAC(I)=CCC*AKH2*AQ1(I)
430     1         IF(I.EQ.IMX) FAC(I)=FAC(I)/2.
440     1     10    CCC=1.-CCC
450         AKH2=2.*DK
460         FAC(IMX)=FAC(IMX)+AKH2*AQ1(IMX)/6.
470         IMX1=IMX+1
480         CCC=2./3.
490         DO 20 I=IMX1,MALL
500     1         FAC(I)=CCC*AKH2*AQ1(I)
510     1         IF(I.EQ.MALL) FAC(I)=FAC(I)/2.
520     1     20    CCC=1.-CCC
530         DO 40 MS=1,5
540         WRITE(6,1040) MS
550     1040 FORMAT('O*** TSI(MS=',I3,',) ***')
560         DO 30 IM=1,MALL
570     30 WRITE(6,1060) IM,(TSI(J,MS,IM),J=1,JMX)
580     1060 FORMAT(' IM=',I3/(' ',1P10E12.5))
590         40 CONTINUE

```

```

600      WRITE(6,1050) FNORM
610      1050 FORMAT('OFNORM=',1PE13.5)
620      C-02
630      C**** COMPUTE TEN POTENTIAL COMPONENTS OF TABLE III-1.
640      CALL PGEN(XR,JMX,POT)
650      WRITE(6,1030)
660      1030 FORMAT('O*** POT ***')
670      DO 50 JX=1,JMX
680      50 WRITE(6,1045) JX,(POT(JX,K),K=1,10)
690      1045 FORMAT(I4,1P10E12.4)
700      HM=1./41.47
710      DO 60 K=1,10
720      1 DO 60 JX=1,JMX
730      2 60 POT(JX,K)=HM*POT(JX,K)
740      C-03
750      C**** 'COEF' ARE THE COEFFICIENTS C*C IN TABLE III-2.
760      DO 70 I=1,5
770      1 70 COEF(I)=1.
780      FACLOG(1)=0.
790      FACLOG(2)=0.
800      F1=1.
810      DO 80 I=3,100
820      1 F1=F1+1.
830      1 FACLOG(I)=FACLOG(I-1)+ALOG(F1)
840      1 80 CONTINUE
850      DO 90 K=6,17
860      1 LA=2*NLA(K)
870      1 LB=2*NLB(K)
880      1 L1A=2*NL1(K)
890      1 L1B=2*NL2(K)
900      1 JJ=2*NJJ(K)
910      1 JS=2*NSS(K)
920      1 J2=2*NJ2(K)
930      1 FACTOR=(J2+1.)*SQRT((L1A+1.)*(L1B+1.))
940      1 CALL CLEBSH(L1A,2,LA,0,0,0,FACLOG,CLEBA)
950      1 CALL CLEBSH(L1B,2,LB,0,0,0,FACLOG,CLEBB)
960      1 CALL F6J(FACLOG,L1A,J2,LA,JJ,JS,2,RACA)
970      1 CALL F6J(FACLOG,L1B,J2,LB,JJ,JS,2,RACB)
980      1 90 COEF(K)=FACTOR*CLEBA*CLEBB*RACA*RACB
990      WRITE(6,1065) (COEF(K),K=6,17)
1000     1065 FORMAT('OCOEF=',1P10E12.4/(6X,1P10E12.4))
1010     C-04
1020     C**** CARRY OUT THE P- AND X-INTEGRATIONS OF EQ.(III-4.2).
1030     DO 100 K=1,7
1040     1 100 SUMP(K)=0.
1050     DO 160 IM=1,MALL
1060     1 DO 110 K=1,7
1070     2 110 SUMX(K)=0.
1080     1 CCC=2./3.
1090     1 DO 140 JX=1,JMX
1100     2 XQ=XR(JX)**4*TR1(JX)*AH2*CCC
1110     2 C**** COMPUTE THE SEVENTEEN T-FUNCTIONS IN TABLE III-2 AND EQ.(III-4.5).
1120     2 DO 120 I=1,17
1130     3 KPT=NPT(I)
1140     3 120 TPX(I)=COEF(I)*POT(JX,KPT)
1150     2 C**** CONSTRUCT THE G-FUNCTIONS OF EQ.(III-4.5).
1160     2 G(1)=(-TPX(1)+TPX(5))/6.
1170     2 G(2)=(-TPX(2)+TPX(6)+TPX(7)+TPX(8))/2.
1180     2 G(3)=G(2)
1190     2 G(4)=(-TPX(3)+TPX(9)+TPX(10)+TPX(11)+TPX(12)+2.*TPX(13))/2.
1200     2 G(5)=G(4)
1210     2 G(6)=-TPX(4)+TPX(14)+TPX(15)+TPX(16)+TPX(17)
1220     2 G(7)=G(6)
1230     2 C**** NOW, CARRY OUT THE SIMPSON QUADRATURE OVER X OF EQ.(III-4.2).

```

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```

1240 2      DO 130 K=1,7
1250 3      NA=NSTATE(K)/10
1260 3      NB=NSTATE(K)-10*NA
1270 3      130 SUMX(K)=SUMX(K)+TSI(JX,NA,IM)*G(K)*TSI(JX,NB,IM)*XQ
1280 2      140 CCC=1.-CCC
1290 1      DO 150 K=1,7
1300 2      150 SUMP(K)=SUMP(K)+SUMX(K)*FAC(IM)
1310 1      160 CONTINUE
1320 C**** 'SUMP' IS THE RESULTS OF THE P- AND X-INTEGRATION OF EQ.(III-4.2).
1330 C**** NOW, MULTIPLY 3 AND DIVID BY THE NORMALIZATION FACTOR TO
1340 C**** FIND THE SEVEN KAPPAS OF EQ.(III-4.2).
1350 DO 170 K=1,7
1360 1      170 VK(K)=3.*SUMP(K)/FNORM
1370 C**** SUM OVER ALL KAPPAS AS IN EQ.(III-4.1).
1380 FKAPPA=0.
1390 DO 180 K=1,7
1400 1      180 FKAPPA=FKAPPA+VK(K)
1410 WRITE(6,1020) FKAPPA,(NSTATE(K),VK(K),K=1,7)
1420 1020 FORMAT('OKAPPA=',1PE13.5/' CONTRIBUTION TO KAPPA FROM COMPONENT'/
1430 & (5X,' K(',I2,',')=',1PE13.5))
1440 STOP
1450 END
1470 SUBROUTINE PGEN(XR,JMX,POT)
1480 DIMENSION XR(*),POT(30,10)
1490 CUT=50
1500 H=10.463
1510 DO 10 JX=1,JMX
1520 1      X=0.7*XR(JX)
1530 1      EX1=REX1(1.,CUT,X)
1540 1      EX2=REX1(2.,CUT,X)
1550 1      EX3=REX1(3.,CUT,X)
1560 1      EX4=REX1(4.,CUT,X)
1570 1      EX6=REX1(6.,CUT,X)
1580 1      EX7=REX1(7.,CUT,X)
1590 1      TX2=REXS(CUT,2.,X)
1600 1      TX3=REXS(CUT,3.,X)
1610 1      TX4=REXS(CUT,4.,X)
1620 1      WX=64.*(REXS(CUT/4.,3.,4.*X)-REX1(1.,CUT/4.,4.*X))
1630 1      POT(JX,1)=-H*EX1-1650.6*EX4+6484.2*EX7
1640 1      VC=-H*EX1+105.468*EX2-3187.8*EX4+9924.3*EX6
1650 1      VT=-H*(TX3-WX)+351.77*EX4-1673.5*EX6
1660 1      VLS=708.91*EX4-2713.1*EX6
1670 1      POT(JX,2)=VC
1680 1      POT(JX,3)=VC-2.*VT-3.*VLS
1690 1      POT(JX,4)=2.828427125*VT
1700 1      POT(JX,5)=3.*H*EX1-634.39*EX2+2163.4*EX3
1710 1      POT(JX,6)=-H*(TX4-WX/0.75)+27.133*EX2-790.74*EX4+20662.*EX7
1720 1      POT(JX,7)=H*(TX2-WX/1.5)-135.25*EX2+472.81*EX3
1730 1      VC=H*EX1/3.-933.48*EX4+4152.1*EX6
1740 1      VT=H*(TX3-WX)/3.-34.925*EX3
1750 1      VLS=-2074.1*EX6
1760 1      POT(JX,8)=VC-VT/2.5+VLS
1770 1      POT(JX,9)=VC-1.6*VT-4.*VLS
1780 1      POT(JX,10)=2.939387692*VT
1790 1      10 CONTINUE
1800 RETURN
1810 END
1820 FUNCTION REX1(A,C,X)
1830 P=C*X
1840 IF(P.LT.50.) GO TO 10
1850 REX1=EXP(-A*X)/X
1860 RETURN
1870 10 REX1=(EXP(-A*X)-EXP(-P))/X

```

```

1880         RETURN
1890         END
1900         FUNCTION REXS(C,F,X)
1910         P=C*X
1920         IF(P.LT.50.) GO TO 10
1930         REXS=(1.+F/X+F/X**2)*EXP(-X)/X
1940         RETURN
1950     10 T=(2.-F+F*C**2)/2.+F*C/X+F/X**2
1960         REXS=((1.+F/X+F/X**2)*EXP(-X)-T*EXP(-P))/X
1970         RETURN
1980         END
1990         SUBROUTINE XTABLE(JMX,JMXG,XR,TR1,DT,EM,XM,TM,TXC)
2000     C**** T(X)=C*(X+T0)*X/(X+S0)
2010         DIMENSION XR(*),TR1(*)
2020         JMXS=JMXG
2030         SX0=(TM-TXC*XM)*XM/(EM*XM-TM)
2040         TX0=EM*SX0/TXC
2050         DT=TM/JMX
2060         DTQ=DT**2
2070         CTO=TXC*TX0
2080         CS02=2.*TXC*SX0
2090         CS04=2.*CS02
2100         TXC2=2.*TXC
2110         T=0.
2120         DO 10 I=1,JMXS
2130     1         T=T+DT
2140     1         A=CTO-T
2150     1         XR(I)=(-A+SQRT(A*A+CS04*T))/TXC2
2160     1         DTDX=TXC*(XR(I)**2+2.*SX0*XR(I)+TX0*SX0)/(XR(I)+SX0)**2
2170     1         TR1(I)=1./DTDX
2180     1     10 CONTINUE
2190         RETURN
2200         END

```


§5. Two-body Correlation Function

For the computation of the two-body correlation function

$$\rho(x) = \int d\hat{x} \int d^3y |\Psi|^2 \quad (5.1)$$

we express the total wave function

$$\Psi = \phi(12,3) + \phi(23,1) + \phi(31,2) \quad (5.2)$$

in terms of a single partition, for example,

$$\Psi = - \sum_{\alpha} |F_{\alpha}(12,3)\rangle \theta_{\alpha}(x) \quad (5.3)$$

(See Eq. (I-2-40)). Then due to the ortho-normality of $|F_{\alpha}(12,3)\rangle$, the function $\rho(x)$ is simply given by

$$\rho(x) = \sum_{\alpha} \int_0^{\infty} dp [\theta_{\alpha}(q,x)]^2 \quad (5.4)$$

where

$$\theta_{\alpha}(q,x) = \phi_{\alpha}(q,x) + \chi_{\alpha}(q,x) \quad (5.5)$$

The wave function $\chi_{\alpha}(q,x)$ is the radial part of the component $\phi(23,1)+\phi(31,2)$, and $\phi_{\alpha}(q,x)$ is that of the component $\phi(12,3)$. (See Eqs. (I-2-39a) and (I-2-38a)). In the main program, we compute and output $-\theta_{\alpha}(q,x)$ and $\phi_{\alpha}(q,x)$ for $0 \leq x \leq x_{\max}$ where x_{\max} is the force range. To compute $\rho(x)$ for $x \leq x_{\max}$, therefore, is straightforward. We should not forget to normalize the wave function. The normalization factor is output from Code NFORM (see section 2-d).

However, as mentioned in section 8 of I, $\chi_{\alpha}(q,x)$ is considerably long ranged compared to $\phi_{\alpha}(q,x)$. When it is necessary to compute $\rho(x)$ for $x > x_{\max}$, say for $x \leq x_M$ where x_M is much larger than x_{\max} , we have to extend the computation of $\chi_{\alpha}(q,x)$ to $x_{\max} < x \leq x_M$ as explained in section 3 of II.

5-a. General description of Code CORR5

The code to carry out the computation of $\rho(x)$ of Eq. (5.1) is named CORR5. It consists of the parts

MAIN routine, and

Subroutines XTABLE and PTABLE

It requires the data file LFCHI.

In presenting the listing of the code, we assume that we already have the data file LFCHI on which $-\theta_\alpha(q,x)$ are stored, so that we can start from there.

If we are satisfied with calculating $\rho(x)$ for $x \leq x_{\max}$, then we can use the data file LFCHI output from the main program. If we wish to calculate $\rho(x)$ for $x \leq x_M$ ($x_M > x_{\max}$), then, before entering the computation of $\rho(x)$ using Code CORR5, we must extend $\chi_\alpha(q,x)$ to $x_{\max} < x \leq x_M$ and re-store $-\theta_\alpha(q,x)$ on File LFCHI for $x \leq x_M$. The dimensionality of quantities relating to x and y must be modified accordingly. This preparatory part of the calculation to extend $\chi_\alpha(q,x)$ to $x_{\max} < x \leq x_M$ is very tedious. Since it has to be done only once, perhaps the simplest way is to follow the procedure explained in section 3 of II in exactly the same way, except now we use x_M in place of x_{\max} . We shall not present the listing of this preparatory code but merely indicate how to construct it. Thus, first we note that $Y(x)$ corresponding to Eq.(II-3.12) is to be chosen as

$$Y(x) \leq \frac{1}{2} x + x_M \leq \frac{3}{2} x_M \quad (\text{for } x \leq x_M) \quad (5.6)$$

By Code OVER5 with appropriately modified dimensionalities, we prepare $Q_{\alpha\alpha}^{L0}(p,p';x)$ of Eq.(II-3.17) for $0 \leq x \leq x_M$. This allows us to find ${}^2H_{\alpha\alpha}^{L0}(x)$ of Eq.(II-3.16). From Eq.(II-3.11), we have the upper limits of x'' and y'' given by

$$x'' \leq \frac{1}{2} x + y \leq 2 x_M, \quad y'' \leq \frac{3}{4} x + \frac{1}{2} y \leq \frac{3}{2} x_M \quad (5.7)$$

Therefore, by Code FYFI5 with appropriately modified dimensionalities, we prepare $Y_\ell^{(t)}(y,p_k)$ and $I_\ell^{(s)}(p,y_i)$ of Eqs.(II-5.9) and (II-5.6) for $0 \leq y \leq \frac{3}{2} x_M$. Next, we read off from File LFCHI the functions $\phi_\alpha(q,x)$ for $x \leq x_{\max}$ (which are obtained in the main program). Then we extend $\phi_\alpha(q,x)$ to the region $x_{\max} < x \leq 2 x_M$ using the asymptotic form Eq.(II-3.10).

Now, we are ready to construct $\rho_\alpha(x'',y'')$ in Eq.(II-3.8) for $0 \leq x'' \leq 2x_M$ and $0 \leq y'' \leq \frac{3}{2} x_M$ with the help of the p-spline using $Y_\ell^{(t)}(y,p_k)$ as in Eqs.(II-5.7) and (II-5.8). The computation of $K_Y^{\alpha'}$ of Eq.(II-3.8) and $U_{\alpha\alpha}^{L0}(Q=0;x,y)$ of Eq.(II-3.7) and the subsequent calculation of ${}^1H_{\alpha\alpha}^{L0}(x)$ of Eq.(II-3.14) by means of the y-spline using $I_\ell^{(s)}(p,y_i)$ proceed as in subroutine RHS of the main program. Thus we obtain ${}^1H_{\alpha\alpha}^{L0}(x) = {}^1H_{\alpha\alpha}^{L0} + {}^2H_{\alpha\alpha}^{L0}$, which yields the desired $\chi_\alpha(q,x)$ as per Eq.(II-3.1). All these calculations are entirely parallel to the steps No.25 to No.28 in the main program (see section 6-a of II), and require no further explanations. After calculating $\chi_\alpha(q,x)$ we can construct

$$\theta_\alpha(q,x) = \phi_\alpha(q,x) + \chi_\alpha(q,x) \quad (5.8)$$

for $0 \leq x \leq x_M$ which is to be stored on File LFCHI to be used in MAIN routine.

Fortran Programs - Various Properties of the Triton

19.399 ** CODE CORR5 **** LABEL
 (09-30-82) OPTIONS: INTER,OPT=1,NROUND,NDLR,ALC,MASTER,INLINE=0,LSTIN,LNO,MREST

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10      C**** *** CODE CORR5 ****
20      C**** COMPUTATION OF THE TWO-BODY CORRELATION FUNCTION OF THE TRITON
30      C**** WITH RSC5.
40      DIMENSION XR(30),TR1(30),TSI(30,5,12),GSI(30,5,12),
50      & CORR(30,5),CORSUM(30),AQ(12),AQ1(12),FAC(12)
60      C**** INPUT THE NORMALIZATION CONSTANT OBTAINED IN CODE FNORM.
70      DATA FNORM/2.6/
80      WRITE(6,1000)
90      1000 FORMAT('1*** TRITON TWO-BODY CORRELATION FUNCTION ***')
100     C-01
110     C**** SET UP THE X-TABLE. THIS MUST BE THE SAME AS IN THE MAIN
120     C**** PROGRAM, OR THE EXTENSION OF IT.
130     JMXG=30
140     CALL XTABLE(XR,TR1,JMXG,DT)
150     C**** SET UP THE SAME P-TABLE AS USED IN THE MAIN PROGRAM, AND
160     C**** CONSTRUCT THE SIMPSON-WEIGHTS 'FAC' FOR THE P-INTEGRATION.
170     PIMX=0.750428
180     IMX=6
190     MALL=12
200     CALL PTABLE(AQ,AQ1,DP,PIMX,IMX,MALL)
210     C=2./3.
220     DK=2.*PIMX/IMX
230     DO 10 I=1,IMX
240     1   FAC(I)=CCC*DK
250     1   IF(I.EQ.IMX) FAC(I)=FAC(I)/2.
260     1   10 CCC=1.-CCC
270     DK=0.4
280     FAC(IMX)=FAC(IMX)+DK/6.
290     IMX1=IMX+1
300     CCC=2./3.
310     DO 20 I=IMX1,MALL
320     1   FAC(I)=CCC*DK
330     1   IF(I.EQ.MALL) FAC(I)=FAC(I)/2.
340     1   20 CCC=1.-CCC
350     C-02
360     C**** INPUT THE TOTAL WAVE FUNCTION 'TSI'.
370     LFCHI=27
380     REWIND LFCHI
390     READ(LFCHI) TSI,GSI
400     DO 80 JS=1,5
410     1 C   WRITE(6,1010) JS
420     1 C1010 FORMAT('0TSI(JS=',I2,',)')
430     1 C   DO 30 IM=1,MALL
440     1 C 30 WRITE(6,1020) IM,(TSI(JX,JS,IM),JX=1,JMXG)
450     1 C1020 FORMAT('0IM=',I2,',(5X,1P10E12.4))
460     1 C-03
470     1 C**** CORRELATION FUNCTION OF EACH STATE.
480     1   DO 50 JX=1,JMXG
490     2   SUM=0.
500     2   DO 40 I=1,MALL
510     3   40 SUM=SUM+FAC(I)*(TSI(JX,JS,I)*XR(JX))**2
520     2   50 CORR(JX,JS)=SUM
530     1   WRITE(6,1030) JS,(CORR(JX,JS),JX=1,JMXG)
540     1 1030 FORMAT('0CORR(JS=',I2,',)')/(5X,1P10E12.4))
550     1 C**** NORMALIZE STATE-BY-STATE.
560     1   CCC=2./3.
570     1   CNORM=0.
580     1   DO 60 JX=1,JMXG
590     2   CNORM=CNORM+CCC*TR1(JX)*CORR(JX,JS)

```

```

600 2 60 CCC=1.-CCC
610 1 CNORM=2.*DT*CNORM
620 1 DO 70 JX=1,JMXG
630 2 70 CORSUM(JX)=CORR(JX,JS)/CNORM
640 1 WRITE(6,1040) CNORM,(CORSUM(JX),JX=1,JMXG)
650 1 1040 FORMAT('OAFTER NORMALIZATION WITH CNORM=',1PE13.5/
660 1 & (5X,1P10E12.4))
670 1 80 CONTINUE
680 C-04
690 C**** TOTAL CORRELATION FUNCTION
700 DO 100 JX=1,JMXG
710 1 SUM=0.
720 1 DO 90 JS=1,5
730 2 90 SUM=SUM+CORR(JX,JS)
740 1 100 CORSUM(JX)=SUM
750 C**** COMPUTE THE (TOTAL) NORMALIZATION CONSTANT 'CNORM'(TO BE
760 C**** COMPARED WITH THE TRUE VALUE 'FNORM')
770 CCC=2./3.
780 SUM=0.
790 DO 110 JX=1,JMXG
800 1 SUM=SUM+CCC*TR1(JX)*CORSUM(JX)
810 1 110 CCC=1.-CCC
820 CNORM=2.*DT*SUM
830 C**** NORMALIZE THE TOTAL CORRELATION FUNCTION WITH THE
840 C**** TRUE NORMALIZATION CONSTANT 'FNORM'.
850 DO 120 JX=1,JMXG
860 1 120 CORSUM(JX)=CORSUM(JX)/FNORM
870 WRITE(6,1050) FNORM,CNORM,(CORSUM(JX),JX=1,JMXG)
880 1050 FORMAT('OTHE TRUE NORMALIZATION CONSTANT=',1PE13.5/
890 & ' THE NORMALIZATION CONSTANT FOR X.LE.XR(JMXG)=' ,1PE13.5/
900 & 'OTHE TWO-BODY CORRELATION FUNCTION'/(5X,1P10E12.4))
910 DO 130 JX=1,JMXG
920 1 130 CORSUM(JX)=CORSUM(JX)/XR(JX)**2
930 WRITE(6,1060) (CORSUM(JX),JX=1,JMXG)
940 1060 FORMAT('OAFTER DIVISION BY X**2'/(5X,1P10E12.4))
950 STOP
960 END
970 SUBROUTINE XTABLE(XR,TR,JMXG,DT)
980 C**** T(X)=C*(X+T0)*X/(X+S0)
990 DIMENSION XR(*),TR(*)
1000 DATA EM,XM,TM,ZTXC/ 12.0, 6.0, 9.0, 0.3/
1010 JMX=30
1020 JMXS=JMXG
1030 TXC=ZTXC
1040 SX0=(TM-TXC*XM)*XM/(EM*XM-TM)
1050 TX0=EM*SX0/TXC
1060 DT=TM/JMX
1070 CTO=TXC*TX0
1080 CS02=2.*TXC*SX0
1090 CS04=2.*CS02
1100 TXC2=2.*TXC
1110 T=0.
1120 DO 10 I=1,JMXS
1130 1 T=T+DT
1140 1 A=CTO-T
1150 1 XR(I)=(-A+SQRT(A*A+CS04*T))/TXC2
1160 1 DTDX=TXC*(XR(I)**2+2.*SX0*XR(I)+TX0*SX0)/(XR(I)+SX0)**2
1170 1 TR(I)=1./DTDX
1180 1 10 CONTINUE
1190 WRITE(6,1000) TXC,TX0,SX0
1200 1000 FORMAT('OXTABLE WITH T(X)=C*(X+T0)*X/(X+S0)'/5X,'C=',1PE13.5,
1210 & ' T0=',1PE13.5,' S0=',1PE13.5)
1220 WRITE(6,1002) (XR(I),I=1,JMXS)
1230 1002 FORMAT(' XR=',1P10E12.5/(4X,1P10E12.5))

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```
1240         WRITE(6,1001) (TR(I),I=1,JMXS)
1250     1001 FORMAT(' TR=',1P10E12.5/(4X,1P10E12.5))
1260         RETURN
1270         END
1280         SUBROUTINE PTABLE(AQ,AQ1,DP,PIMX,IMX,M)
1290     C**** CONSTRUCTS THE P-TABLE.
1300         DIMENSION AQ(*),AQ1(*)
1310         DP=PIMX/IMX
1320         DO 10 I=1,IMX
1330     1      10 AQ(I)=I*DP
1340             IMX1=IMX+1
1350             DP2=0.2
1360             DO 20 I=IMX1,M
1370     1      20 AQ(I)=AQ(I-1)+DP2
1380             DO 30 I=1,M
1390     1      30 AQ1(I)=1.
1400             WRITE(6,1000) (AQ(I),I=1,M)
1410     1000 FORMAT('0 AQ=',1P10E12.5/(5X,1P10E12.5))
1420         RETURN
1430         END
```

References

- 1) T. Sawada and T. Sasakawa; Sci.Rep. Tohoku Univ. Series 8, III(1982) 1.
(Referred to as I)
- 2) T. Sasakawa, S. Ishikawa and T. Sawada; Sci.Rep. Tohoku Univ. Preceding article. (This is the program named PERFECT V. We refer this as II).
- 3) V. Reid; Ann. Phys. (N.Y.) 50(1968) 411.
- 4) T. Sasakawa, H. Okuno and T. Sawada, Phys. Rev. 23C(1981) 905.