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A General Hauser-Feshbach Nuclear-Scattering Computer Program

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Abstract

This report describes a CDC-1604 binary program (for which no FORTRAN is available) that computes the scattering angular distribution and integrated cross section for any two-particle nuclear reaction, subject only to the restrictions that the spin of one particle in each reaction channel be no greater than 1 and that the maximum number of partial waves necessary in any one channel be no greater than 16. The input required by the program is the charge, mass, spins, parity, and optical-model parameters for all the channels through which the compound nucleus can decay. The calculation makes use of the Hauser-Feshbach theory modified to include spin-orbit coupling.

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PROGRAM OPERATION

The input to the program and the definitions of the symbols are given in Table 1. Several control options are specified by making certain input parameters positive or negative. These options, other information pertinent to the operation of the program, and the forms of the optical-model potentials are described below.

Control Options and Other Information

The maximum number of channel types (T) which may be simultaneously included is 10; the total number of channels (T,i) of all types and energies is 600.

In running the program the parameters corresponding to a given type of particle (group 1) are read in, followed by the parameters for each level of that type (group 2). To terminate the reading of level parameters, a number $N \geq 10^3$ is placed after the last $(J_T)_i$. Then additional "type" parameters (group 1) are read in, unless previously Z_I had a negative sign, whereupon the energy (group 3) is read. After group 3 is introduced, the computer proceeds to calculate the cross section, after which, if E was positive, another group 3 is read in. If E was negative, then the calculation starts anew with the reading of additional group 1 parameters, and so on as before. However, if the last M_I was negative, then the program running terminates at this point.

Three additional options are available. If, when reading group 3, T_2 is negative, then the sign and value of E replace the parity and spin of particle type T_2 and level i_2. In this way the spin and parity of a single level can be changed without repeating the whole calculation. The next item read in will be another group 3, which, again, may be either a new

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Table 1. Order of Input Parameters and Definitions

Group Number	Parameters	Format
1	Z_I M_I Z_T M_T J_I $\Delta\ell_{max}$ R_o a R'_o a' $\pm S$ V_{so} V W ΔV ΔW	(8E10.3)
2	Q_1 $\pm(J_T)_1$ Q_2 $\pm(JT)_2$ ... Q_i $\pm(J_T)_i$ ... +1.000E+04	(8E10.3)
3	E T_2 i_2	(1E10.3,2I3)

Parameter Definitions:

I — Denotes the incident (or light) particle in the channel.

T — Denotes the target (or heavy) particle in the channel; also used to denote the channel itself - in this sense the maximum number of T's assimilable by the program is 10.

Z — Charge

M — Mass, in amu.

J — Spin; for J_T the sign preceding the parentheses indicates whether the parity is positive or negative; (note also that J_I <u>cannot be greater than 1</u>).

$\Delta\ell_{max}$ — The maximum angular momentum in the channel is $\Delta\ell_{max}(E_{cm} + Q_i)^{1/2}$. A suggested value for neutrons is $\Delta\ell_{max} = (M_T)^{1/3}$ and for protons $\Delta\ell_{max} = \frac{1}{2}(M_T)^{1/3}$.

R_o — The real potential radius is $R_o M_T^{1/3}$ F.

a — Real potential diffuseness in F.

R'_o — The imaginary potential radius is $R'_o M_T^{1/3}$ F.

a' — Imaginary potential diffuseness, in F.

S — Fraction of surface-peaked imaginary potential.

V_{so} — Spin-orbit potential, in MeV.

V,ΔV — The real potential depth is $V + \Delta V(E_{cm} + Q_i)$ MeV.

W,ΔW — The imaginary potential depth is $W + \Delta W(E_{cm} + Q_i)$ MeV.

i — Denotes the channel relative energy index.

Q — Q-value, in MeV, of channel (T,i) with respect to channel (1,1); the program can handle a maximum of 600 (T,i) channels. Negative $(E_{cm} + Q_i)$ values are automatically bypassed in the calculations.

E — Bombarding energy, in MeV, in the laboratory system.

T_2 — Particle type index number for the observed channel.

i_2 — Excitation level index number for the observed channel.

E or a new $(J_T)_i$, depending on the sign of T_2. The calculation proceeds as before, when a positive T_2 is introduced.

If W is negative, then the penetrabilities for all the levels of the current particle type are printed out in the order first of increasing j, then increasing ℓ. Thus for spin-1/2 particles the order for the penetrabilities $T_{\ell j}$ is $T_{0,1/2}$ $T_{1,1/2}$ $T_{1,3/2}$ $T_{2,3/2}$ $T_{2,5/2}$, etc. A heading identifies the channel to which the penetrabilities belong by printing the corresponding values of T and I.

If S is positive, then a surface-peaked Woods-Saxon derivative imaginary potential is employed; if negative, the surface-peaked potential is of the Gaussian form, and, in addition, in calculating the Woods-Saxon volume component of the potential the diffuseness a' is replaced by 0.69a' in order that the volume and surface potentials have approximately the same taper widths. Control options are summarized as follows:

Parameter Value	Program Action
$+Z_I$	Read another group 1 after termination of group 2 reading.
$-Z_I$	Proceed to group 3 after reading group 2.
$+M_I$	Start over at group 1 after termination of group 3 reading.
$-M_I$	End calculations after termination of group 3 reading.
$Q_i \geq 10^3$	Terminate group 2 reading.
$+(J_T)_i$	Parity of $(J_T)_i$ is positive.
$-(J_T)_i$	Parity of $(J_T)_i$ is negative.
+E	Read another group 3 at end of cross-section calculation.
-E	Return to beginning (group 1) at end of cross-section calculation, unless previous M_I was negative.
$+T_2$	E is interpreted as bombarding energy.
$-T_2$	E and its sign are interpreted as replacing the spin and parity, $\pm(J_T)_i$, of level $T = T_2$, $i = i_2$.
+S	The imaginary potential has the form (1 - S)(Woods-Saxon) + S(Derivative)
-S	The imaginary potential has the form (1 - S)(Woods-Saxon) + S(Gaussian)
-W	Print the penetrabilities for all levels of the type particle to which W corresponds.

Optical Model Potential Form Factors

The form factors are functions of the two constants radius (R) and diffuseness (a) and of the variable radius (r):

Woods-Saxon: $f_{ws}(R,a) = 1/\left\{1 + \exp\left[(r-R)/a\right]\right\}$.

Derivative: $f_D(R,a) = -4a \frac{d}{dr} f_{ws}$.

Gaussian: $f_G(R,a) = \exp\left\{-\left[(r-R)/a\right]^2\right\}$.

Spin-Orbit: $f_{so}(R,a) = -\frac{2}{r} \frac{d}{dr} f_{ws} \vec{\sigma}\cdot\vec{\ell}$.

For spin-1 particles the spin-orbit form factor agrees with that used by Robson[1] but is twice the one employed by Satchler.[2]

The meaning of the parameter S can now be stated more explicitly: if S is positive, then the imaginary potential form factor is

$$f(R',a') = (1 - S)f_{ws}(R',a') + Sf_D(R',a') \quad ;$$

if S is negative, then

$$f(R',a') = (1-|S|)f_{ws}(R',0.69a')+|S|\, f_G(R',a') \quad .$$

The Coulomb potential, when present, is the potential of a uniformly charged sphere having the same radius, $R_o M_T^{1/3}$, as the real potential.

The input parameters are reproduced on the printed output, together with headings which identify the various output quantities. The different reaction channels are indexed by integers according to the identity of the two particles in each channel, designated type (with index name T) and for each type according to the excitation energy (with index name i). Both T and i start with the value 1 and correspond in sequence to the order of the input data. The incident (or initial or bombarding) channel must always correspond to $T = 1$, $i = 1$. The particular channel for which a cross-section calculation is desired is called (T_2, i_2). If $T_2 = 1$, $i_2 = 1$, then the program computes compound-elastic scattering. The end result of a calculation is the integrated cross section and also the center-of-mass differential cross section from $\theta = 0$ to 90° in 10° intervals (this is the same as the cross section from $\theta = 180$ to 90°). From $\theta = 0$ to 80°, the angular distribution is relative to that at 90°. Only the 90° cross section is in absolute units.

To use the program on the Oak Ridge CDC-1604 computer the cards illustrated in Table 2 must be present in the front of the program deck in the order shown. The first card is obtained in the computer room at the front desk. The user should supply his own name and account number on cards 1 and 2. After the number of minutes specified for "maximum execution time" (first card) have elapsed, the run is aborted. Any other number can be substituted here. The program can be run with only the FORTRAN 62 monitor system of the CDC-1604.

Table 2

Cards in Front of Program Deck

1604-A JOB CARD

NAME: W R Smith

RETURN TO: Hold

CHARGE: 10509

EXECUTE: [✓] YES [ ] NO

MAXIMUM EXECUTION TIME: 5 MINUTES

RECOVERY DUMP ON STOP: [ ] YES [✓] NO

OPERATOR ACTION

[ ] NO ACTION TAKEN [ ] PULLED ON TIME

[ ] PROGRAM STOPPED

PROGRAM REG. -

FUNCTION REG. -

EXECUTION REG. -

UCN-4242 (3 2-63)

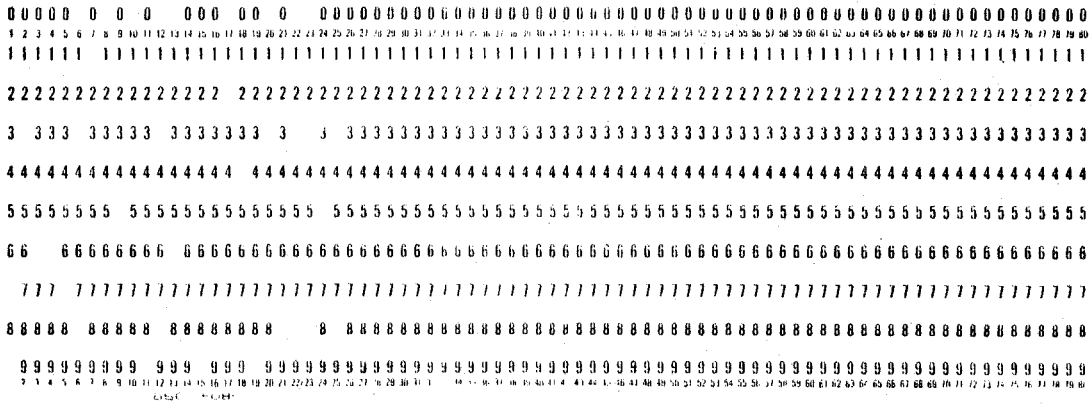
[✓] FORTRAN '62

[ ] FORTRAN '63

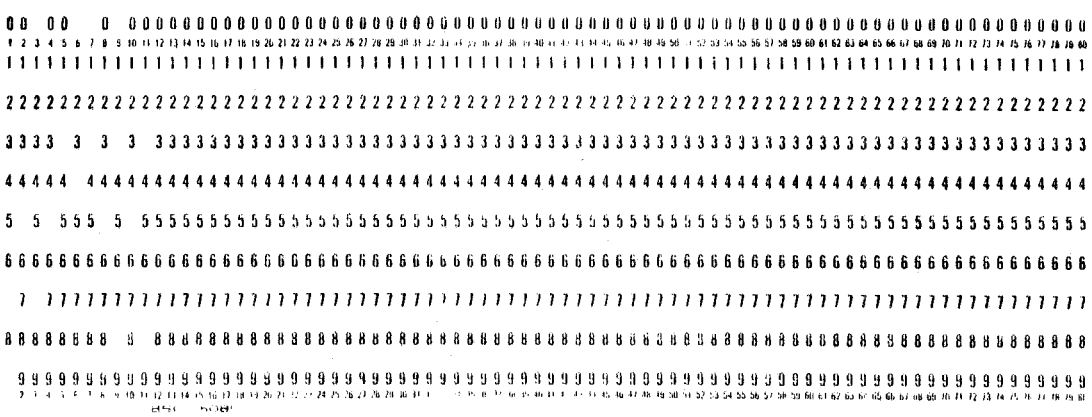
NON-STANDARD TAPES REQUIRED

LOG. NO.	REEL NUMBER	DEN. H	DEN. L	LIST	PLOT	PUNCH	SAVE	SAVED REEL NUMBER	FILE PROTECT BEFORE Y	FILE PROTECT BEFORE N	FILE PROTECT AFTER Y	FILE PROTECT AFTER N

```
*COOP,10509,W R SMITH,,5.
7
9
```



```
*EXECUTE,5.
7
9
```



Calculational Method

The calculational method makes use of the Hauser-Feshbach theory[3] modified[4] to include spin-orbit coupling.

Hauser-Feshbach Cross Sections.

Let $\vec{J}$ be the spin of the compound nucleus and π be its parity. Consider a certain channel with incident particle I and target particle T. Call this channel K. Then $\vec{J}$ is formed by jj vector coupling in the following manner:

$$\vec{\ell}_K + (\vec{J}_I)_K = \vec{j}_K, \quad \vec{j}_K + \vec{J}_T = \vec{J} \quad . \tag{1}$$

The coupling is to be done in such a manner that parity is conserved. For brevity of notation, let $S_K = (J_I)_K$ and $J_K = (J_T)_K$. In the upcoming development the calculation of the integrated and differential cross sections will be revealed in an "unfolding" order; that is, quantities will usually be defined in terms of subsequent equations and recursion relations. Let $K = 1$ be the bombarding channel, $K = 2$ the observed channel, k the wave number, and $T_{\ell_K j_K}$ the penetrability in channel K for partial wave ℓ_K and total spin j_K. The $\beta_\nu^{J_K S_K}(\ell_K j_K J)$ are angular momentum coupling coefficients which are calculated by means of a recursion relation[5] for Racah coefficients and an explicit expression[5] for Clebsch-Gordon coefficients. The P_ν are Legendre polynomials and are calculated by recursion. The Hauser-Feshbach integrated and differential cross sections are calculated as follows:

$$\sigma = \frac{\pi A_o}{k^2(2J_1 + 1)(2S_1 + 1)} \quad ,$$

$$\frac{d\sigma(\theta)}{d\Omega} = \frac{1}{4k^2(2J_1 + 1)(2S_1 + 1)} \cdot \sum_\nu A_\nu P_\nu(\cos\theta) \quad ,$$

where

$$A_\nu = \sum_{J\pi} \frac{(2J+1)}{D_{J\pi}} \left[\sum_{\ell_1 j_1} \beta_\nu^{J_1 S_1}(\ell_1 j_1 J) T_{\ell_1 j_1} \right] \left[\sum_{\ell_2 j_2} \beta_\nu^{J_2 S_2}(\ell_2 j_2 J) T_{\ell_2 j_2} \right]$$

$$\beta_\nu^{J_K S}(\ell j J) = V(\ell j \nu s) V(J j \nu J_K) x_{\ell\nu}$$

$$\beta_o^{J_K S}(\ell j J) = 1, \; V(a d \nu c) = Z_\nu^{1/2} Y_\nu$$

$$Z_{\nu+1} = \frac{Z_\nu}{(2a-\nu)(2d-\nu)(2a+\nu+2)(2d+\nu+2)} ,$$

$Z_o = 1$,

$$Y_{\nu+1} = -(2\nu+1)\left(\frac{x}{\nu+1} + \nu\right) Y_\nu - \left(\frac{\nu}{\nu+1}\right)(4\bar{a}+1-\nu^2)(4\bar{d}+1-\nu^2) Y_{\nu-1},$$

$Y_o = 1$,

$Y_1 = -x$,

$\bar{a} = a(a+1)$,

$x = 2[\bar{c}-\bar{a}-\bar{d}]$,

$$X_{\ell\nu+1} = -\left(\frac{\nu}{\nu+1}\right) \left[\frac{(2\ell+\nu+1)(2\ell-\nu+1)(2\nu+3)}{(2\ell+\nu+2)(2\ell-\nu)(2\nu-1)} \right]^{1/2} X_{\ell,\nu-1} ,$$

$X_{\ell o} = 1;$

and, in addition,

$$P_{\nu+1} = \frac{1}{(\nu+1)} \left[(2\nu+1) \cos\theta \, P_\nu - \nu \, P_{\nu-1} \right] ,$$

$$P_o = 1 ,$$

$$P_1 = \cos\theta .$$

In the above, $D_{J\pi} = \sum_{K,\ell_K,j_K} T_{\ell_K j_K}$ is the sum over all penetrabilities with subscripts which can be coupled to form a compound state with spin J and parity π in the manner of Eq. 1. The above calculational scheme is simple in all respects except one: determining which terms to include in the sums. The way in which this is accomplished is outlined now. The routine to be described applies to the calculation of the β_ν. Similar routines were used four times in the program.

To begin, calculate $\nu_{max}(J,2)$ in a manner similar to that shown below for $\nu_{max}(J,K)$. Set K = 0.

1. Add 1 to K. If K>2, go to the next section of the program. If not, calculate $J = J_{min} = \max\left[|S_1-J_1|,\ |S_2-J_2|\right]$ and,

$$J_{max} = \min\left[(\ell_1+S_1+J_1),(\ell_2+S_2+J_2)\right] \quad .$$

2. Set $\nu_{max}(J,K) = 0$. If $J = J_{max}$, go to step 1. If not, calculate

$$j = j_{min} = |J_K-J|$$

and

$$j_{max} = \min\left[(J_K+J),(\ell_{K\max}+ S_K)\right] \quad .$$

3. If $j > j_{max}$, add 1 to J, set $\nu_{max}(J) = \min\left[\nu_{max}(J,2),\ \nu_{max}(J,K)\right]$, and go to step 2. If not, calculate $\ell_{min}-1 = |j-S_K|-1$ and

$$\ell_{max} = \min\left[(j+S_K),\ \ell_{K\ max}\right] \quad .$$

4. Add 1 to ℓ-1. If $\ell > \ell_{max}$, add 1 to j, and go to step 3. If not, set $\nu_{min} = 0$ and determine $\nu_{max} = \min\left[2J,2j,2\ell,\nu_{max}(J,2)\right]$ and $\nu_{max}(J,K) = \max\left[\nu_{max}(J,K),\nu_{max}\right]$.

5. If $\nu > \nu_{max}$, go to step 4. If not, calculate $\beta_{\nu}^{J_K S}(\ell j J)$, add 2 to ν, and go to step 5.

$D_{J\pi}$ is summed in an analogous manner except that the routine ends with step 4, the calculation of ν_{max} is deleted, and also the parity $\pi_K(-)^{\ell_K}$ is determined in order that the penetrability $T_{\ell_K j_K}$ can be correspondingly added to either an even-parity sum or an odd-parity sum. The sums $\sum_{\ell_1 j_1}$ and $\sum_{\ell_2 j_2}$ are performed in this manner also, that is, separate sums are made for even and odd parity.

Optical-Model Penetrabilities.

The solution $\chi_{\ell j}$ of the scattering radial Schroedinger equation has for boundary conditions that it vanish at the origin and that it be proportional asymptotically to the function

$$F_\ell - \beta_{\ell j}(F_\ell - iG_\ell) \quad ,$$

where F_ℓ and G_ℓ are, respectively, the regular and irregular Coulomb wave functions and $\beta_{\ell j}$ is a boundary matching constant. The latter is obtained by requiring the solution with zero value at the origin to be proprotional to the asymptotic solution at two points exterior to the nuclear potential. In terms of $\beta_{\ell j}$, the penetrability $T_{\ell j}$ is

$$T_{\ell j} = 4\left\{\mathrm{Re}\ \beta_{\ell j} - \left[(\mathrm{Re}\ \beta_{\ell j})^2 + (\mathrm{Im}\ \beta_{\ell j})^2\right]\right\}.$$

Let $\chi_{\ell j}$ be the solution which vanishes at the origin and r_1 and r_2 be two radii outside the nuclear potential. Then $\beta_{\ell j}$ is determined, as described above, by solving the equation

$$\frac{\chi_{\ell j}(r_1)}{\chi_{\ell j}(r_2)} = \frac{F_\ell(r_1) - \beta_{\ell j}[F_\ell(r_1) - i\, G_\ell(r_1)]}{F_\ell(r_2) - \beta_{\ell j}[F_\ell(r_2) - iG_\ell(r_2)]}$$

$\chi_{\ell j}$ is generated stepwise from the origin by means of the approximate recursion relation

$$\chi_{\ell j}(r+\delta) = \frac{[12 - 10\, q(r)]\, \chi_{\ell j}(r) - q(r-\delta)\, \chi_{\ell j}(r-\delta)}{q(r+\delta)}$$

where

$$q(r) = 1 + \frac{\delta^2}{12}\left\{\frac{2m}{\hbar^2}\,[E + V_{\ell j}(r)] - \frac{\ell(\ell+1)}{r^2}\right\},$$

E = the center of mass energy,

m = the reduced mass,

$V_{\ell j}$ = the sum of the Coulomb, spherical nuclear, and spin-orbit potentials.

In the above, $V_{\ell j}$ and hence, q, $\chi_{\ell j}$, and $\beta_{\ell j}$ are complex quantities and the equations must be treated accordingly. In order to avoid an infinite $q(0)$, the following algorithm is employed to start the solution at the origin:

$$\chi_{\ell j}(-\delta) = 0,\ q(-\delta) = 0,\ \chi_{\ell j}(0) = 10^{-20}(1+i),$$

and

$$q(0) = 0.$$

This is equivalent in the present method to having $\chi_{\ell j}(0) = 0$ and

$$\chi_{\ell j}(\delta) = \frac{12\cdot 10^{-20}\,(1+i)}{q(\delta)} .$$

$\chi_{\ell j}$ is generated outward to the radius $R_b+\delta$, where R_b is the larger of $R_o M_T^{1/3} + 9a$ and $R'_o M_T^{1/3} + 9a'$. In the present calculation, $\delta = 0.15$ f. The boundary matching is carried out at the radii $r_1 = R_b$ and $r_2 = R_b + \delta$.

To obtain Coulomb functions at r_1 and r_2 in a universally valid manner is not straightforward. An asymptotic power series can always be used, given a sufficiently large radius, but in order to prevent having to generate the interior solution to unnecessarily large radii, with a consequent loss of computer time, it is desirable to have a scheme valid at any radius. Let recursion in ℓ be called "vertical" and recursion in r be "horizontal." As reasonable methods for obtaining F_ℓ and G_ℓ, we have inward and outward recursion in r, upward and downward recursion in ℓ, an asymptotic power series in 1/kr, and a power series in kr valid either near the origin or for large ℓ but which is often not an accurate method for obtaining G_ℓ. Both F_ℓ and G_ℓ obey the same horizontal and vertical recursion relations, so that any error which enters represents an admixture of, for instance, G_ℓ in the recursion of F_ℓ. However, if in this case G_ℓ rapidly decreases as the recursion progresses, the error incurred in generating F_ℓ is continually damped out. Below a certain radius and above a certain ℓ, F_ℓ decreases rapidly. The opposite is true for G_ℓ. Thus one wants to recur F_ℓ outward and downward and G_ℓ inward and upward.

In a scheme not used in the present calculation, we generated F_{14} and F_{15} by the kr power series and G_0 by the 1/kr power series. If either of these series or both of them were not sufficiently convergent at r_1 and r_2, they were generated at the limits of the valid ranges of the respective series and F_ℓ was then recurred outward, and G_0 inward, to r_1 and r_2. Then F_ℓ was recurred downward. G_ℓ was recurred upward in terms of the F_ℓ by means

of a relation which employs $G_{\ell-1}$, $F_{\ell-1}$, and F_ℓ to obtain G_ℓ. The vertical recursion relations and the power series are summarized in an article by Froberg.[6] Thirty-one terms were used in the kr series and 16 in the asymptotic series. The radius was picked such that the maximum powered term was less than 10^{-6} of the zeroth-powered term.

The method used in the Hauser-Feshbach program differs from the above method when the kr power series for F_{14} does not converge sufficiently at r_2. In that case, G_1 and F_0 are calculated in the same manner as described above for G_0. Then F_1 is found in terms of F_0, G_0, and F_1. Finally, the F_ℓ and G_ℓ are separately recurred upward. This is done on the assumption that if the kr power series is not convergent for F_{14} at r_2, then the F_ℓ do not begin to decrease rapidly when below F_{14}, and hence upward recursion in F_ℓ is safe below $\ell = 15$. This method has shown good agreement with the other method in a number of trial comparisons.

The Coulomb phase shift σ_0, needed for the asymptotic series calculation of G_ℓ and F_ℓ, was generated in the manner shown below:

$$\sigma_{30}(\eta) = \frac{61}{2}\beta + \eta \ln \alpha - \eta + \sum_{i=1}^{5} \frac{(-)^i \sin(2i-1)\beta}{t_i} ,$$

$$\sigma_{\ell-1} = \sigma_\ell - \arctan\left(\frac{\eta}{\ell}\right) ,$$

where

$$\beta = \arctan\left(\frac{\eta}{31}\right) ,$$

$$\alpha = (961 + \eta^2)^{1/2} ,$$

$$t_1 = 12\alpha ,$$

$$t_2 = 30\alpha^2 t_1 ,$$

$$t_3 = \frac{7}{2}\,\alpha^2 t_2 \quad ,$$

$$t_4 = \frac{4}{3}\,\alpha^2 t_3 \quad ,$$

$$t_5 = \frac{99}{140}\,\alpha^2 t_4 \quad .$$

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