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by

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POLYNOMIAL SOLUTIONS OF THE SCHRÖDINGER EQUATION APPLIED TO PHOTON CROSS SECTIONS IN ATOMS

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ABSTRACT

Solutions of the Schrödinger equation with a realistic potential are carried out in detail. To check our methods, we have calculated a few bound-bound, bound-free, and free-free cross sections and compared our values with existing calculations and experimental data. These comparisons, along with a listing of the computer code in its bound-free form, are included.

I. INTRODUCTION

This report intends to show how the CDC-7600 code DEGA-A (Dense Electron Gas Approximation-Absorption) computes the bound-free, free-free, and bound-bound absorption coefficients, σ_{bf}, σ_{ff}, and σ_{bb}, respectively, as a function of photon energy, $h\upsilon$, from the given potential function V(r) and the electron occupancy of the atom. Assuming V(r) to be exact, the code will do its computation at any desired accuracy, within the machine limits, because the Schrödinger equation is solved using exact power-series expansions, not difference equations.

As the code is now written, any potential function can be used if it adheres to the three following requirements.

1. $\lim_{r \to 0} V(r)r^2 = 0$.

2. After some finite value of r, R_1, the potential must be $V(r) = -|c|/r$.

3. V(r) must be a negative, monotonically, increasing function.

Although it is not necessary to the internal structure of the code, we would also like V(r) to be a function of temperature, density, and the atomic number of the atom.

Throughout this report, $[0,R_1]$ is called Region 1 and $[R_1,\infty]$ Region 2.

The following V(r) is the one most often used in the code.

Experience has shown that a parameterized potential works well and gives energy levels close to those that Herman and Skillman[1] calculated using their Hartree-Fock-Slater method for isolated neutral atoms.

The potential form for an isolated atom is

$$V(r) = Ze/r(1 + \alpha r)^2 \quad . \tag{1}$$

where $\alpha = 0.6057Z^{1/3}$. However, the form actually used in this report, which is also valid for a compressed atom, is

$$V(r) = -(Z^*e)/R_1 \left(\frac{R_1}{r} + \frac{r^2}{2R_1^2} - 3/2 \right) \tag{2}$$

for $r_0 \leqslant r \leqslant R_1$,

where

Z^* is the "effective number" of free electrons,

R_1 is the radius of the sphere representing the spherical atomic volume,

r_0 is the value of the radial distance for which Eq. (2) is equal to the value given in Eq. (3) below, and

e is the electronic charge.

In the inner region, the potential is given by

$$V(r) = -Ze/r(1 + \alpha r)^2 - Z^*e/r\left(\frac{r^2}{2R_1^2} - Bo \right) \tag{3}$$

for $0 \leqslant r \leqslant r_0$.

$$Bo = \left(\frac{Z}{Z^*}\right)\left(\frac{R_1}{r_0}\right)/(1+\alpha r_0)^2 - \frac{R_1}{r_0} + 3/2 \quad . \tag{4}$$

$$Z^* = Z/(1+\alpha r_0)^2 \left[\left(\frac{2\alpha r_0}{1+\alpha r_0}\right) \cdot + 1\right] \quad . \tag{5}$$

After the form of the potential in the two regions is chosen, Eqs. (4) and (5) follow from the potential's continuity and its relation to charge density through Poisson's equation. In the potential outlined above, the value of R_1 is determined by the density of the material being considered. The value of Z^* is chosen by an iterative procedure so that at some finite temperature T, and for an atom occupying a spherical volume of radius R_1, we have

$$Z = N(Z^*) = \int_0^{R_1}\left[\int_0^{\infty} n(r, T, P)\, dP\right] 4\pi r^2\, dr \quad , \tag{6}$$

where n is the Fermi-Dirac distribution function, representing the number of electrons at point r, having momentum between P and P + dP. Using Eq. (5) we have also determined r_0.

We must correct the above potential for self-interaction. This is done in the simplest possible fashion. We replace Z in Eqs. (2) through (5) with (Z − 1) and add the term −1/r to Eqs. (2) and (3). The potential for $r > R_1$ is defined as −1/r. This then represents our potential function used to calculate the one-electron energies and the one-electron orbitals from which we calculate the cross sections and f-values.

This potential can be shown to satisfy the three previously stated conditions.

The hydrogenic potential $V(r) = -1/r$ for $0 \leqslant r \leqslant \infty$ is often used to check parts of the code because analytic solutions for this potential are known.

The code considers the Schrödinger equation in the form

$$\varphi''(r) + \left[\lambda - 2V(r) - \frac{\ell(\ell+1)}{r^2}\right]\varphi(r) = 0,\ 0 \leqslant r \leqslant \infty \quad , \tag{7}$$

where

$r\varphi(r)$ is the radial wave function (however, $\varphi(r)$ will be called the wave function throughout the rest of this report),

λ is the energy eigenvalue, and

ℓ is the angular-momentum quantum number.

Equation (7) has an infinite (in some cases finite, but large) number of discrete bound solutions (negative λ) commonly denoted by 1s, 2s, 2p, 3s, 3p, 3d, etc. Of t! infinite sequence, we calculate only the solutions allowed by the electron occupancy. σ_{bb} can be evaluated only at discrete values of $h\upsilon$, because $h\upsilon = |\lambda_1 - \lambda_2|$ where λ_1 and λ_2 both represent bound solutions. By using a line profile, we then distribute each σ_{bb} over a narrow range of $h\upsilon$. However, every positive λ, given ℓ, is an eigenvalue for a free state. This allows us to choose any finite number of positive λ's. Therefore, we can evaluate σ_{bf} at any energy $h\upsilon$ above the threshold, and σ_{ff} at any desired value of $h\upsilon$. Here $h\upsilon = |\lambda_1 - \lambda_2|$, λ_1 represents either a bound or a free solution, and λ_2 represents a free solution.

II. THE METHOD OF SOLUTION OF THE SCHRÖDINGER EQUATION

A. The Potential Approximation

To solve Eq. (7) on the computer, we choose a finite $R > R_1$ to approximate $r = \infty$, and divide [0,R] into a finite number of intervals. For each of these intervals, r^2 times the potential is approximated by a parabola to some specified degree of accuracy, ξ. This series of fits is started at r = 0 with an interval of arbitrary length. In this first interval, we approximate the potential with

$$V(r) \approx c_1 + \frac{c_2}{r} + \frac{c_3}{r^2} \quad . \tag{8}$$

Let r_1 be the left end point of this interval, r_3 the right end point, and r_2 the midpoint. To evaluate the c's, we solve the set of equations

$$c_1 r_j^2 + c_2 r_j + c_3 = V(r_j) r_j^2 \text{ for } j = 1, 2, 3. \tag{9}$$

These equations have no difficulty at r = 0, and they fit the potential exactly at r_1, r_2, and r_3. Because V(r) is a smooth, monotonic function, we can check our fit by checking the validity of

$$\left|c_1 + \frac{c_2}{r} + \frac{c_3}{r^2} - V(r)\right| < |V(r)|\xi \tag{10}$$

at several points between r_1 and r_3. If this inequality is not satisfied for all points, we decrease the length of the interval until inequality [Eq. (10)] is satisfied for all points checked. This process is continued until Region 1 is complete. Here c_1, c_2, and c_3 should actually be

thought of as $c_{1,i}$, $c_{2,i}$, and $c_{3,i}$, where the subscript i denotes the ith interval.

In Region 2, obviously, $c_2 = -1$ and $c_1 = c_3 = 0$. The lengths of the intervals in this region are governed only by an additional condition discussed later. This condition applies to all intervals.

As the code now exists, for a given set of conditions, all solutions to the Schrödinger equation are found by using the same set of intervals over Region 1; however, each solution has its own set of intervals in Region 2. The code could also be written so that each solution would have its own set of intervals over the entire range of r. It would be impractical to require all solutions to have the same set of intervals in Region 2 because the maximum interval lengths allowed for the various solutions in Region 2 are so different.

B. The Expansion of the Radial Wave Function

In the expansion of the wave function, we will need the condition $c_{3,1} = 0$. This is satisfied if the first requirement on the potential is met.

We assume the wave function to have the form

$$\varphi(r) = \sum_{j=1}^{\infty} a_{ji} r^{j-1} \text{ for } i = 1 \qquad (11)$$

in the first interval. Dropping the subscript i, we substitute the power series and its second derivative for $\varphi(r)$ and $\varphi''(r)$ and the approximation for V(r) in Eq. (8) into the Schrödinger equation to get

$$\begin{aligned}
&\left\{-\left[2c_3 + \ell(\ell+1)\right] a_1\right\}/r^2 \\
&+\left\{-2c_2 a_1 - \left[2c_3 + \ell(\ell+1)\right] a_2\right\}/r \\
&+\sum_{j=3}^{\infty} \left\{(\lambda - 2c_1)a_{j-2} - 2c_2 a_{j-1}\right. \\
&\left.+\left[(j-2)(j-1) - 2c_3 - \ell(\ell+1)\right] a_j\right\} r^{j-3} = 0 \quad . \qquad (12)
\end{aligned}$$

Here we assume that $c_3 = 0$ and $a_j = 0$ for $1 \leq j \leq \ell + 1$. Also $a_{\ell+2}$ is arbitrary because any constant times a solution eigenfunction $\varphi(r)$ is still a solution. As each term in Eq. (12) must be zero for every r in the interval, we now have the recursion relation

$$a_j = \frac{2c_2 a_{j-1} - (\lambda - 2c_1)a_{j-2}}{(j-2)(j-1) - \ell(\ell+1)} \quad \text{for } j > \ell + 2 \quad . \qquad (13)$$

The power-series expansions in all other intervals are also expanded about one of the interval's end points. If expanding about the left end point, we make the substitution $d = r - \rho_i$ and require that $0 \leq d \leq \rho_{i+1} - \rho_i$ where the ρ's are the end points of the intervals. When it is necessary to expand about the right end point, the roles of ρ_i and ρ_{i+1} are switched and $\rho_i - \rho_{i+1} \leq d \leq 0$. Again omitting the subscript i, the Schrödinger equation can now be written as

$$(\rho^2 + 2\rho d + d^2)\varphi''(d) + (B_1 + B_2 d + B_3 d^2)\varphi(d) = 0 \quad ,$$

where

$$\begin{aligned}
B_1 &= b_1\rho^2 + b_2\rho + b_3 \\
B_2 &= 2b_1\rho + b_2 \\
B_3 &= b_1
\end{aligned}$$

and (14)

$$\begin{aligned}
b_1 &= \lambda - 2c_1 \\
b_2 &= -2c_2 \\
b_3 &= -[2c_3 + \ell(\ell+1)] \quad .
\end{aligned}$$

Here we assume the wave function to have the form

$$\varphi(d) = \sum_{j=1}^{\infty} a_{ji} d^{j-1} \quad \text{for } i > 1 \quad . \qquad (15)$$

Substituting the power series and its second derivative for $\varphi(d)$ and $\varphi''(d)$, we get

$$\begin{aligned}
&\left[2\rho^2 a_3 + B_1 a_1\right] + \left[6\rho^2 a_4 + 4\rho a_3 + B_1 a_2 + B_2 a_1\right] d \\
&+\sum_{j=5}^{\infty} \left[(j-2)(j-1)\rho^2 a_j + (j-3)(j-2)2\rho a_{j-1}\right. \\
&+ (j-4)(j-3)a_{j-2} + B_1 a_{j-2} \\
&\left.+ B_2 a_{j-3} + B_3 a_{j-4}\right] d^{j-3} = 0 \qquad (16)
\end{aligned}$$

with the subscript i omitted. Again, because each term of Eq. (16) must be zero for all values of d, we have the recursion relations

$$a_3 = -B_1 a_1/2\rho^2$$

$$a_4 = -[B_2 a_1 + B_1 a_2 + 4\rho a_3]/6\rho^2$$

$$a_j = -\Big\{B_3 a_{j-4} + B_2 a_{j-3} + [B_1 + (j-4)(j-3)]a_{j-2} + 2(j-3)(j-2)\rho a_{j-1}\Big\}/(j-2)(j-1)\rho^2$$

$$\text{for } j > 4 \qquad (17)$$

when a_1 and a_2 are known.

We can easily show that $a_1 = \varphi(d)$ and $a_2 = \varphi'(d)$ at $d = 0$. Therefore, a_1 and a_2 will always be known by the right-boundary condition or can be evaluated with the power-series expansion of the wave function in the previous interval.

In practice, we start with $a_j = 0$ for $1 \leqslant j \leqslant \ell + 1$ and $a_{\ell+2}$ an arbitrary nonzero constant to start the power-series expansion in the first interval. Then we evaluate this power-series and its first derivative at its right end point. This determines a_1 and a_2 for the second interval. This process is repeated until we reach some $\hat{r}$. $0 < \hat{r} < R$, where we evaluate $\varphi_f(\hat{r})$ and $\varphi_f'(\hat{r})$: the determination of $\hat{r}$ is discussed later. At the right boundary, R, $\varphi(R)$. and $\varphi'(R)$ are given by the boundary condition. This enables us to start our successive power-series expansions at R and work our way backward to $\hat{r}$ where we evaluate $\varphi_b(\hat{r})$ and $\varphi_b'(\hat{r})$. We have a solution when $\varphi_f'(\hat{r}) = \varphi_b'(\hat{r})$ for $\varphi_f(\hat{r}) = \varphi_b(\hat{r})$. $\varphi_f(\hat{r})$ is simply the value of the wave function at $\hat{r}$ found by forward expansions, and $\varphi_b(\hat{r})$ is the value of the same wave function at $\hat{r}$ found by backward expansions.

C. Determination of the Expansion Interval Length

In real life, these power series can have only a finite number of terms. The maximum number of terms in the present code is 50. This leads to the other condition regulating the maximum length of a particular interval. Let us define

$$\tilde{V}(r) = \left[\lambda - 2V(r) - \frac{\ell(\ell+1)}{r^2}\right] \qquad (18)$$

Using this definition, we can write the Schrödinger equation as

$$\varphi''(r) \pm h^2\varphi(r) = 0, \text{ where } h^2 = \pm\tilde{V}(r) \qquad (19)$$

choosing the sign so that $h^2 > 0$. If h is assumed to be constant locally, the solution is either

$$\varphi(r) = Ae^{-hr} + Be^{hr} \qquad (20)$$

or

$$\varphi(r) = A \sin hr + B \cos hr, \qquad (21)$$

depending upon the sign. Expanding the decreasing exponential solution in a Taylor series about an end point of the interval, we get

$$\varphi(r) = Ae^{-h\rho_i}\sum_{j=0}^{\infty} (-1)^j \frac{(h\Delta r)^j}{j!} \qquad (22)$$

where $\Delta r = r - \rho_i$ is the maximum allowable interval length. With this series, we can estimate the largest value of $(h\Delta r)$ that allows the series to converge to a specified accuracy in the alloted number of terms. In Region 1. all solutions are considered in estimating the maximum interval length; however. in Region 2 only one solution at a time is considered. The code then plugs the largest encountered value of h into

$$\Delta r = \frac{C}{h} . \qquad (23)$$

This C is an input parameter. and for a 50-term expansion and 8-place accuracy a conservative value for C is 6.

The sinusoidal and increasing exponential solutions have a series similar to Eq. (22), and the interval length is also estimated by Eq. (23).

D. Finding the Join Point $\hat{r}$ for Forward and Backward Integration

Let us consider the question of stability. Here again, Eqs. (20) and (21) can be thought of as local solutions to the Schrödinger equation. If an error is introduced in Eq. (20) during forward integration (increasing r) when the first term is the desired solution. this error will grow exponentially. However, any error introduced will diminish exponentially during backward integration. Likewise, when the second term is the desired solution. backward integration is unstable and forward integration causes any error to diminish exponentially. Equation (21) is considered stable for integration in either direction. Any error introduced into the integration will not grow exponentially: however, once an error is introduced it cannot be diminished as was the case with Eq. (20). Figure 1 shows the regions of stable and unstable integration for the four possible combinations of given conditions.

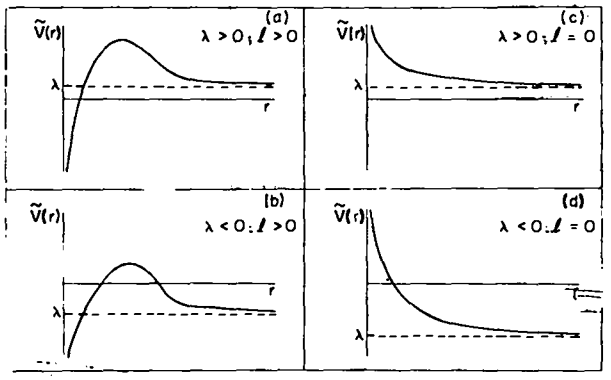

Fig. 1.
Integration is stable in both directions for $\tilde{V}(r) > 0$: integration is stable in only one direction for $\tilde{V}(r) < 0$. λ indicates the asymtotic limit of $\tilde{V}(r)$.

For the cases shown in Figs. 1a and 1b, $\hat{r}$ is chosen such that $\tilde{V}(\hat{r})$ is the maximum value of $\tilde{V}(r)$. For the case shown in Fig. 1c, $\hat{r}$ is the center of the rightmost interval, and for the case shown in Fig. 1d, $\hat{r}$ is chosen such that $\tilde{V}(\hat{r}) = 0$. For positive λ, the value of λ is known and is used to find $\hat{r}$; however, for negative λ one has only a maximum and minimum guess at its value at this stage, so the minimum guess is used in evaluating $\hat{r}$.

E. Boundary Condition at R

1. Bound States–Negative λ. The two right-boundary conditions used in the code are discussed below; however, this method of solving the Schrödinger equation is not limited to these two conditions. For the bound state, the Schrödinger equation becomes

$$\varphi''(r) - |\lambda|\varphi(r) = 0 \text{ as } r \to \infty \quad . \tag{24}$$

Note that this is true only in Region 2. Because $\varphi(R)$ is arbitrary and

$$\varphi(r) = Ae^{-\sqrt{|\lambda|}\, r} \tag{25}$$

is the desired solution to Eq. (24), we derive the boundary condition

$$\varphi'(R) = -\sqrt{|\lambda|}\, \varphi(R) \quad . \tag{26}$$

Although we have no exact relation between R and the accuracy desired, we regulate R by the following method. First, we find the largest root of $\tilde{V}(r)$. R is then taken as some constant (typically 25) times this root. Then, after the Schrödinger equation is solved using this R, we check the validity of

$$|\varphi(r)|_{max} < \gamma|\varphi(R)| \tag{27}$$

(10^{-15} is a typical value for γ). If this condition is not satisfied, we simply keep increasing R until it is. A quick method for getting a value near $|\varphi(r)|_{max}$ is to check $\varphi(r)$ at the end points of the intervals.

2. Free States–Positive λ. The sinusoidal condition given by Carson, Mayers, and Stibbs[2] is used on the right boundary in the free case. This boundary condition also applies only in Region 2.

For large r, the solution may be written

$$\varphi(r) = M(r) \cos [kr + \delta(r)] \tag{28}$$

in which $k = \sqrt{\lambda}$.

$$\lim_{r \to \infty} M(r) = M,$$

and (29)

$$\lim_{r \to \infty} \frac{\delta(r)}{r} = 0 \quad .$$

M fixes the scale of the solution. We shall require the normalization $M = \sqrt{2/\pi k}$.

In Region 2 where $V(r) = -c/r$ for $c > 0$, we assume a solution of the form

$$\varphi(r) = A(r) \cos\left(kr + \frac{c}{k} \ln r\right) + B(r) \sin\left(kr + \frac{c}{k} \ln r\right) \quad . \tag{30}$$

Now substitute Eq. (30) into the Schrödinger equation. Then asymptotic expansions for A(r) and B(r) exist in the form

$$A(r) = \sum a_n/r^n, \; B(r) = \sum b_n/r^n \quad , \tag{31}$$

where

$$a_{n+1} = \left\{ \left[\ell(\ell+1) + \frac{c^2}{k^2} - n(n+1) \right] b_n - \frac{c}{k}(2n+1)a_n \right\} / 2k(n+1)$$

$$b_{n+1} = \left\{ \left[n(n+1) - \frac{c^2}{k^2} - \ell(\ell+1) \right] a_n - \frac{c}{k}(2n+1)b_n \right\} / 2k(n+1) \tag{32}$$

and

$$a_o = M,\ b_o = 0 \quad . \tag{33}$$

The sums in Eq. (31) are only semiconvergent. Therefore A(r) and B(r) must be evaluated at an r large enough that the sums converge to the desired accuracy.

Equation (30) can also be written as

$$\varphi(r) = M(r) \cos \theta(r) \quad , \tag{34}$$

where

$$M(r) = \sqrt{A(r)^2 + B(r)^2} \tag{35}$$

and

$$\theta(r) = kr + \frac{c}{k} + \ln r + \tan^{-1}\left[\frac{A(r)}{B(r)}\right]$$

The asymptotic series expansion for the solution of $\varphi(r)$ given by Eq. (34) is uniquely determined up to some constant phase α_ℓ; therefore, we can write

$$\varphi(r) = M(r) \cos [\theta(r) + \alpha_\ell] \quad , \tag{36}$$

instead of Eq. (34), and we also have

$$\varphi'(r) = M'(r) \cos [\theta(r) + \alpha_\ell] - M(r)\theta'(r) \sin [\theta(r) + \alpha_\ell] \quad . \tag{37}$$

For sufficiently large R, $\varphi(R)$ and $\varphi'(R)$ are the desired right-boundary conditions. The guesses at R may have to be increased several times before Eq. (31) is satisfied.

The phase α_ℓ is determined by an iteration process that is explained later.

III. DETERMINATION OF THE EIGENVALUES AND PHASE FACTORS

A. The Eigenvalue

As stated previously, for the bound state, λ is varied until we find a $[\varphi(\lambda,r),\lambda]$ that solves the Schrödinger equation. We start with a minimum and a maximum guess at λ. This difference in λ is divided into a specified number of logarithmically equal λ-intervals. We define

$$F(\lambda) = \frac{\varphi_b(\lambda,\hat{r})}{\varphi_f(\lambda,\hat{r})}\ \varphi_f'(\lambda,\hat{r}) - \varphi_b'(\lambda,\hat{r}) \tag{38}$$

at the end points of these λ-intervals and look for a sign change in $F(\lambda)$ in each. If we detect a sign change in an interval, we use the Regula Falsa[3] method to find the root of $F(\lambda)$ in that interval. As $F(\lambda)$ also changes sign through poles, we check to reject these intervals.

When we find a $[\varphi(\lambda,r),\lambda]$ solution, we must determine whether it is the desired one for specified quantum numbers n and ℓ, where $\ell \leqslant n-1$. We have the desired solution when

$$I = n - \ell - 1 \quad , \tag{39}$$

where I is the number of roots in $\varphi(r)$. I is found using a Sturm Sequence.[3] If Eq. (39) is not satisfied, we reject this solution and continue our search. The value of λ so obtained is called the eigenvalue.

B. Phase Determination

In the free state, λ is specified and the phase α_ℓ at the right boundary is varied over the range $0 \leqslant \alpha_\ell \leqslant \pi$ until we find a $[\varphi(\alpha_\ell,r),\alpha_\ell]$ that solves the Schrödinger equation. To find this solution, we again use the Regula Falsa method to find the root of $F(\alpha_\ell)$ where

$$F(\alpha_\ell) = \frac{\varphi_b(\alpha_\ell,\hat{r})}{\varphi_f(\alpha_\ell,\hat{r})}\ \varphi_f'(\alpha_\ell,\hat{r}) - \varphi_b'(\alpha_\ell,\hat{r}) \quad . \tag{40}$$

Here, we need not check for poles or unwanted solutions as was necessary for the bound states.

C. Normalization

Even though the wave functions need not be normalized to be solutions to the Schrödinger equation, they must be normalized to produce correct absorption coefficients. We define $\varphi(r)$ as normalized when, for bound states:

$$\int_0^\infty \varphi(r)\varphi(r)\, dr = 1 \quad , \tag{41}$$

and, for free states:

$$\int_0^\infty \varphi_\lambda \varphi_{\lambda'}\, dr = \delta(\lambda - \lambda') \quad . \tag{42}$$

The free states have this normality built into the right-boundary condition. However. for each bound state. we evaluate

$$\int_0^{\infty} \varphi(r)\varphi(r)\, dr = \beta^2 \quad , \tag{43}$$

and the normalized wave function is then $\varphi(r)/\beta$. Equation (43) is evaluated by polynomial multiplication and integration over each interval of r.

IV. EVALUATION OF MATRIX ELEMENTS

Now that we have found all of the necessary solutions to the Schrödinger equation, we compute the matrix elements, H_{mn}, used in evaluating the absorption coefficients. The matrix elements are found by

$$H_{mn} = 2\int_0^{\infty} \varphi_m(r)\, \frac{\partial V(r)}{\partial r}\, \varphi_n(r)\, dr \quad , \tag{44}$$

where m and n refer to eigen solutions of the Schrödinger equation. If one wave function is bound and the other is free. H_{mn} is used in evaluating σ_{bf}. Likewise, if both are bound, the result is σ_{bb}, and if both are free, the result is σ_{ff}.

Equation (44) is evaluated by summing the integrals calculated in each expansion interval. Because $\partial V(r)/\partial r$ decreases as r^{-2} and $\varphi(r)$ decreases exponentially for bound states. this integral converges rapidly to a specified accuracy at some finite value of r, provided at least one $\varphi(r)$ represents a bound state. However, if both wave functions represent free states, the convergence is much slower, because each bound wave function asymptotically approaches a constant amplitude. Here, convergence is achieved only through the r^{-2} decrease in $\partial V(r)/\partial r$.

In the first interval we have

$$\frac{\partial V(r)}{\partial r} = -c_{2,1}\, r^{-2} \quad , \tag{45}$$

multiplied by the polynomial representations of $\varphi_m(r)$ and $\varphi_n(r)$ that can be integrated easily. In the rest of the intervals, we have

$$\frac{\partial V(d)}{\partial d} = -\frac{c_{2,i}(\rho_i + d) + 2c_{3,i}}{(\rho_i + d)^3} \quad , \tag{46}$$

which, by continued long division, can be written as a converging power series in d when $|d/\rho_i| < 1$. Now, multiplying these three polynomials, we get a polynomial that can be integrated easily.

V. EXAMPLES

A. Bound-Free Absorptions

In the code, λ, r. V(r), and H_{mn} are dimensionless parameters. Both λ and V(r). when multiplied by one Rydberg, are energies expressed in Rydbergs, and r, when multiplied by one Bohr radius, is a length expressed in Bohr radii.

The bound-free absorption coefficient is given by

$$\sigma_{bf}(h\upsilon) = 10.756 \times 10^6 \sum \frac{\ell_{max} H_{mn}^2\, \eta}{|\lambda_m - \lambda_n|^3\, g} \quad , \tag{47}$$

where

ℓ_{max} is the maximum of ℓ_m and ℓ_n.

η is the number of electrons in the bound state that can make this transition.

g is the maximum possible degeneracy given by $2(2\ell + 1)$ for the ℓ of the bound state.

Here λ_m, λ_n, and H_{mn} are dimensionless numbers and σ_{bf} is expressed in barns per atom. Also when $h\upsilon = 13.605\ |\lambda_m - \lambda_n|$, $h\upsilon$ is expressed in electron volts. The sum in Eq. (47) is over all possible bound-free transitions at the given $h\upsilon$.

Figures 2 through 7 show examples of bound-free absorptions for cold, normal-density beryllium, carbon, aluminum, iron, copper, and lead as computed by DEGA-A. In these figures, the continuous line was computed by DEGA-A and the X's are experimental data given by Storm and Israel.[4] In Fig. 5, the three experimental points at the m edge for iron were given by Carter and Givens.[5] In Fig. 4, DEGA-A was compared with calculations by Barfield, Koontz, and Huebner[6] for aluminum at low photon energies.

Even though the bound-free cross sections have been computed down to the lowest edge in these examples, we make no claims about the accuracy of the copper and lead cross sections at these low photon energies.

None of the cross sections in this report include electron spin or relativistic effect.

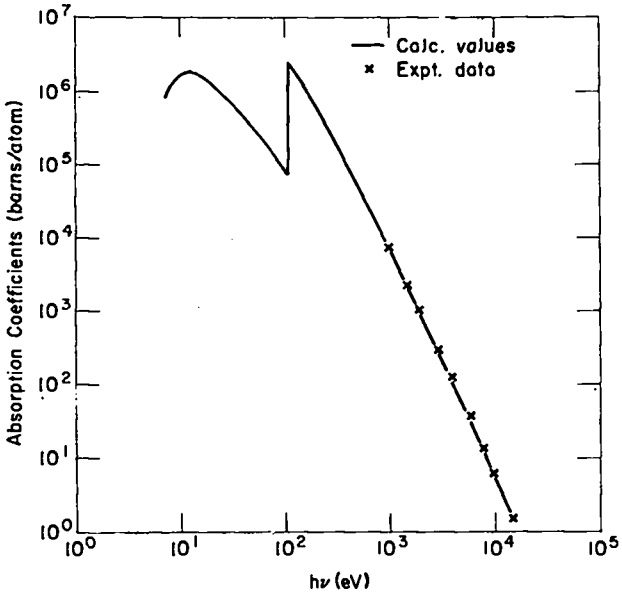

Fig. 2.
Bound-free absorption coefficients for cold, normal density (1.845 g/cm³) Be. (Z = 4, r_0 = 1.406, R_1 = 2.355)

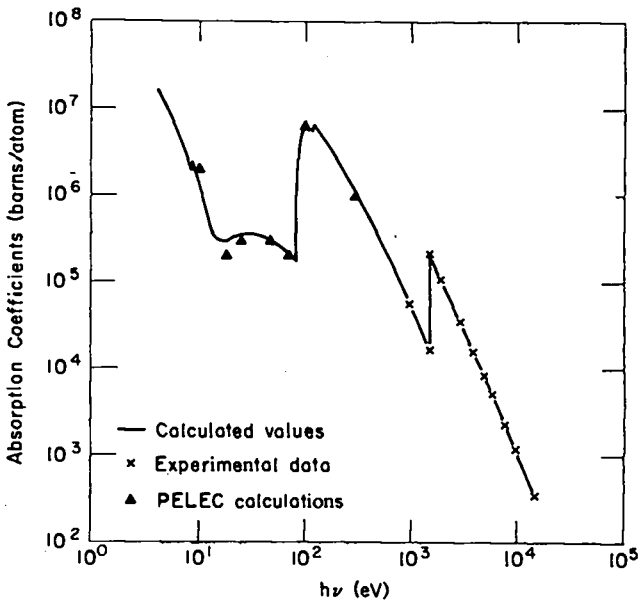

Fig. 4.
Bound-free absorption coefficients for cold, normal density (2.699 g/cm³) Al. (Z = 13, r_0 = 1.699. R_1 = 2.990)

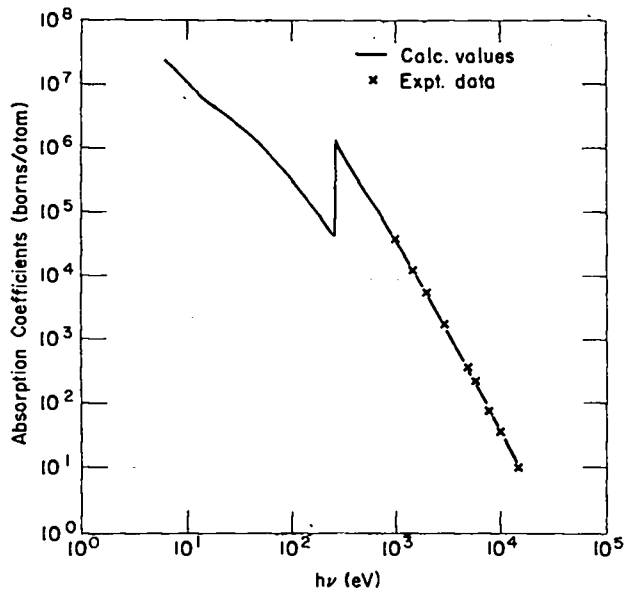

Fig. 3.
Bound-free absorption coefficients for cold, normal density (2.25 g/cm³) C. (Z = 6, r_0 = 1.442, R_1 = 2.426)

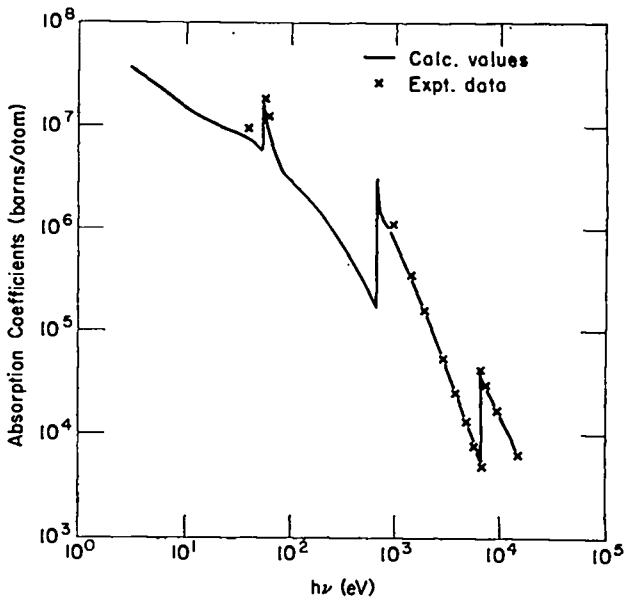

Fig. 5.
Bound-free absorption coefficients for cold. normal density (7.85 g/cm³) Fe. (Z = 26, r_0 = 1.512, R_1 = 2.670)

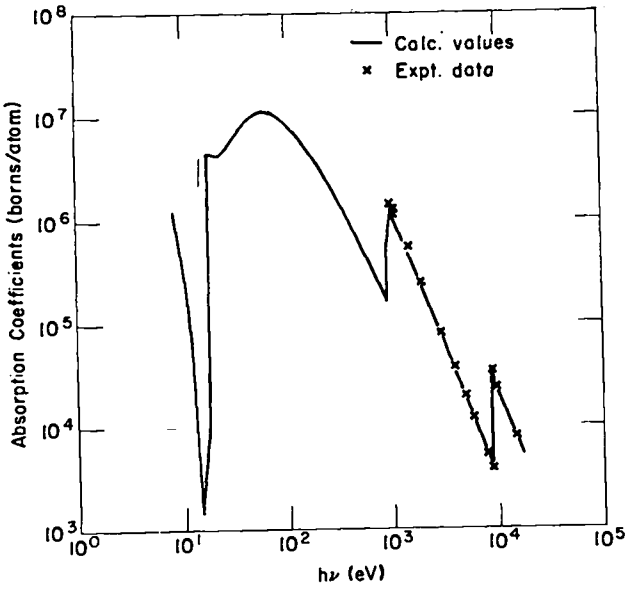

Fig. 6.
Bound-free absorption coefficients for cold, normal density (8.89 g/cm³) Cu. (Z = 29, r_0 = 1.517, R_1 = 2.674)

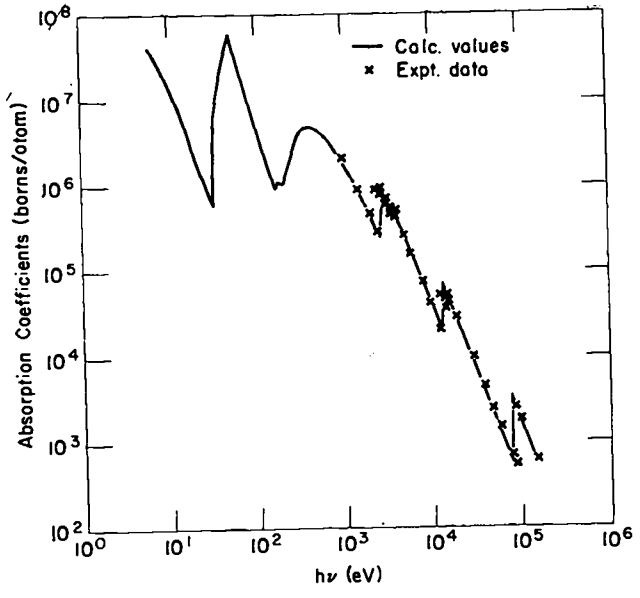

Fig. 7.
Bound-free absorption coefficients for cold, normal density (11.34 g/cm³) Pb. (Z = 82, r_0 = 2.003, R_1 = 3.656)

B. Bound-Bound Absorptions

In checking the bound-bound case, we consider hydrogen, lithium, beryllium, sodium, potassium, and strontium. A formula similar to Eq. (47) can be derived for $\sigma_{bb}(h\upsilon)$.[2] However, because the data found in the literature[7] appeared in a different form, we used the formula

$$\tau = \frac{4H_{mn}^2}{|\lambda_m - \lambda_n|^4 (4\ell_{max}^2 - 1)} \tag{48}$$

to make our numbers directly comparable. See Table I.

Squares of dipole moments for hydrogen were computed by

$$M^2 = \frac{4H_{mn}^2}{|\lambda_m - \lambda_n|^4} \quad . \tag{49}$$

These results checked with the values of the squares of dipole moments* given by Bethe and Salpeter.[8] Note that Eq. (49) is not defined by the method presented in this report when $\lambda_m = \lambda_n$.

To check the code to more digits than given by Bethe and Salpeter (the CDC 7600 is a 14-digit machine). $H_{1s,2p}$ was computed to the maximum possible accuracy using the hydrogenic potential and was compared with its analytic solution. We know that for hydrogen

$$\varphi_{1s} = 2re^{-r}$$

and (50)

$$\varphi_{2p} = \frac{1}{2\sqrt{6}} r^2 e^{-r/2}$$

When these analytic expressions for φ are used in Eq. (44) along with V(r) = −1/r, we obtain

$$H_{1s,2p} = \frac{8}{9\sqrt{6}} = 0.36288736930121$$

and DEGA-A computed

$$H_{1s,2p} = 0.36288736930118 \quad .$$

*Compare with Table 13, page 264, Bethe and Salpeter.[8]

TABLE I

TRANSITION INTEGRAL τ
FOR COLD. NORMAL DENSITY ELEMENTS

Element	Transition	Transition Integral τ Screened-Hydrogenic	Coulomb Approx	Self-Cons Field	DEGA-A
Li I[a]	2p-2s	5.96	5.42	5.5-5.6	4.26
	3p-2s	0.011	0.016	0.011-.020	0.071
	3s-2p	1.72	2.39		1.75
	4s-2p	0.105	0.177		0.148
	5s-2p	0.029	0.056		0.044
	6s-2p	0.013	0.025		0.020
	3d-2p	1.28	1.14		0.748
	4d-2p	0.19	0.18		0.148
Be I[b]	2s2p-2s^2	2.27	2.03	1.86	3.29
Na I[c]	3p-3s	3.41	6.0	6.7	3.63
	4p-3s	0.211	0.047	0.051	0.026
	4s-3p	2.06	6.09	6.2	3.60
K I[d]	4p-4s	4.61	8.05	9.05	7.77
Sr I[e]	5d-5p	0.483	0.42		1.39

[a] Z=3, r_0=1.928, and R_1=3.263.

[b] Z=4, r_0=1.406, and R_1=2.355.

[c] Z=11, r_0=2.264, and R_1=3.986.

[d] Z=19, r_0=2.714, and R_1=4.950.

[e] Z=38, r_0=2.475, and R_1=4.518.

C. Free-Free Absorptions

1. Discussion of Gaunt Factors. A formula similar to Eq. (47)[2] can be derived for σ_{ff} (hυ) in terms of Gaunt factors g_{ff}; however, here we only compute Gaunt factors for hydrogen and sodium and compare some of these results with Karzas and Latter.[9] Gaunt factors can be evaluated with

$$g_{ff}(\lambda_a,h\upsilon) = \frac{\pi\sqrt{3}}{8(Z^{eff})^2} \sum_{\ell=0}^{L'} \left[(\ell+1)H_{\ell+1,\ell}(\lambda_a,h\upsilon)^2 + \ell H_{\ell-1,\ell}(\lambda_a,h\upsilon)^2\right] \quad (51)$$

when the sum converges rapidly enough to be practical. Here λ_a is the initial energy of the electron, hυ is the photon energy, Z^{eff} is the effective number of free electrons in the atom under consideration. and L′ is a finite integer approximation to infinity. The matrix elements are still defined by Eq. (44), but we rewrite the equation as

$$H_{mn}(\lambda_a,h\upsilon) = 2\int_0^{\infty} \varphi_m(\lambda_a,r)\frac{\partial V(r)}{\partial r}\varphi_n(\lambda_a + h\upsilon,r)\,dr \quad (52)$$

to define the association between energy levels and quantum numbers.

The sum in Eq. (51) is not always converging rapidly. Results for other than a coulomb potential can often be obtained in these cases by making use of the formula[10]

$$g_{ff}(\lambda_a,h\upsilon) = g^c_{ff}(\lambda_a,h\upsilon) + \frac{\pi\sqrt{3}}{8}\sum_{\ell=0}^{L}\left\{(\ell+1)\left[H_{\ell+1,\ell}(\lambda_a,h\upsilon)^2 - H^c_{\ell+1,\ell}(\lambda_a,h\upsilon)^2\right] + \ell\left[H_{\ell-1,\ell}(\lambda_a,h\upsilon)^2 - H^c_{\ell-1,\ell}(\lambda_a,h\upsilon)^2\right]\right\}, \quad (53)$$

where g_{ff}^{c} is the coulombic Gaunt factor for the initial energy and photon energy under consideration, H_{mn}^{c} is a coulombic matrix element defined by Eq. (52) using $V(r) = -1/r$, and L is an integer sufficiently large so that the sum has converged to a predetermined accuracy. A graph of $g_{ff}^{c}(\lambda_a, h\nu)$ is given by Karzas and Latter who circumvented the slow convergence problem in Eq. (51) by using hypergeometric functions. Applications of this procedure are limited to the coulomb potential.

The method for obtaining a noncoulombic $\sigma_{ff}(h\nu)$. as described in this report, never requires the evaluation of a $Z^{eff}(\lambda_a, h\nu)$. In terms of coulombic Gaunt factors, $g_{ff}^{c}(\lambda_a, h\nu)$. $Z^{eff}(\lambda_a, h\nu)$ must also be evaluated and then $Z^{eff}(\lambda_a, h\nu)\, g_{ff}^{c}(\lambda_a, h\nu)$ must be used as the desired Gaunt factor. However. Eqs. (51) and (53) give the desired noncoulombic $g_{ff}(\lambda_a, h\nu)$ for $Z^{eff} = 1$ when the matrix elements are computed by DEGA-A using a realistic potential.

2. **Checks on Method.** For the first check on the code, we computed several Gaunt factors with Eq. (51) using the coulomb potential, $V(r) = -1/r$, and compared these results with the Karzas and Latter graph. Here comparisons were made up to, at most, three significant figures. which is the maximum accuracy for reading the graph. Table II shows that for several cases we were able to reproduce the Karzas and Latter values. In the remaining cases, Eq. (51) had not converged for $\ell = 34$. the maximum value of ℓ used in these calculations.

Cold, normal-density sodium ($Z = 11$, $r_0 = 2.264$, $R_1 = 3.986$) was arbitrarily used in the next check (Fig. 8). Here, for low photon energies and low initial energies, the Gaunt factors using the sodium potential and $Z^{eff} = 1$ should approach the coulombic Gaunt factors. Also, for large photon energies and large initial energies. the Gaunt factors using the sodium potential and $Z^{eff} = 11$ should approach the coulombic Gaunt factors. In both cases. the sodium Gaunt factor for $(\lambda_a, h\nu)$ is compared with the coulombic Gaunt factor for $(\lambda_a/(Z^{eff})^2.\ h\nu/(Z^{eff})^2)$.

3. **Discussion of Screening.** The general screening effects are noted for the small electron kinetic energy and the small photon energy shown in Fig. 8. As the photon energy is held fixed and the electron energy is increased, the calculated Gaunt factor increases faster than would be expected from the coulombic case. The qualitative reason for this follows. As the electron energy is increased, the electron wave function samples in greater and greater detail the structure of the atom (the shielding), and as a result the effective charge Z^{eff} increases with increasing energy. The result is that, relative to a coulomb potential. the cross section is raised. However, as the energy of the electron and the photon increase, we eventually arrive at a

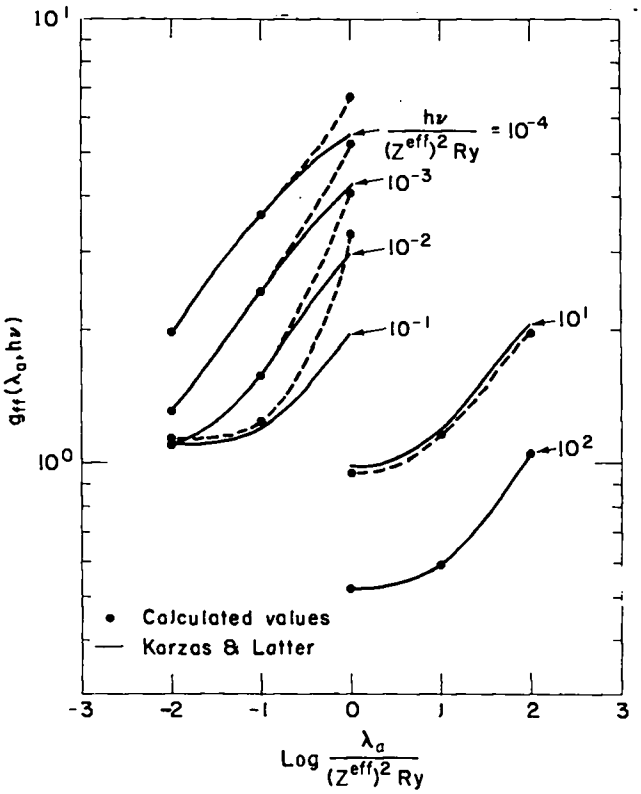

Fig. 8.
A comparison of coulombic and shielded potential (NaI) Gaunt factors.

point where the wave function of the electron oscillates sufficiently rapidly that it is essentially seeing the coulomb field of the nucleus. The effective charge is then the nuclear charge and we have agreement with the coulomb field results. This corresponds to the lower right-hand curves of Fig. 8.

4. **Numerical Results.** The purpose of Table II is to illustrate a trend in the convergence rate for each of Eqs. (51) and (53) as a function of $(\lambda_a, h\nu)$. An integer in parentheses indicates the value of ℓ for which the series was terminated. For example. where $(\lambda_a, h\nu) = (1.0, 0.01)$, Eq. (51) has summed to 3.07 by 34 terms, whereas Eq. (53) has summed to within 2% of the expected (converged) value of 4.10 by three terms. Here convergence means no change in the sum to the accuracy given in Table II. Also. for the coulombic case at this energy pair, Eq. (51) has not converged for $\ell = 34$. For the (1.0, 10) entry, both Eqs. (51) and (53) have converged by $\ell = 3$ for the sodium case. and Eq. (51) has converged by $\ell = 3$ in the coulombic case.

Table II also shows that neither Eq. (51) nor (53) has converged for the entries labeled with footnote b. The use

TABLE II

CALCULATIONS OF COLD, NORMAL DENSITY SODIUM AND COULOMBIC GAUNT FACTORS[a]

λ_a(Ry)	hυ(Ry)	$g^c_{ff}(\lambda_a,h\upsilon)$ from Karzas and Latter	$g^c_{ff}(\lambda_a,h\upsilon)$ Calculated Using Eq. (51)	$g_{ff}(\lambda_a,h\upsilon)$ for Na Calculated Using Eq. (51)	$g_{ff}(\lambda_a,h\upsilon)$ for Na Calculated Using Eq. (53)		
0.01	0.0001	1.97	0.83(34)	0.83(34)	1.97(3)	1.97(34)	
	0.001	1.32	1.20(34)	1.20(34)	1.32(3)	1.32(34)	
	0.01	1.11	1.11(29)	1.09(29)	1.09(3)	1.09(29)	
	0.1	1.08	1.08(14)	1.11(14)	1.11(3)	1.11(14)	
	1.0	1.10	1.10(3)	1.51(3)	1.51(3)	1.51(9)	
0.1	0.0001	3.65	1.34(34)	1.34(34)	3.64(3)	3.65(34)	
	0.001	2.46	1.41(34)	1.40(34)	2.45(3)	2.45(34)	
	0.01	1.58	1.53(34)	1.53(34)	1.58(3)	1.58(34)	
	0.1	1.21	1.21(24)	1.24(24)	1.24(3)	1.24(24)	
	1.0	1.13	1.13(3)	1.99(3)	1.99(3)	1.99(11)	
1.0	0.0001	5.5	1.92(34)	3.01(34)	6.50(3)	6.59(25)	6.59(34)
	0.001	4.2	1.92(34)	3.01(34)	5.20(3)	5.29(25)	5.29(34)
	0.01	3.0	1.97(34)	3.07(34)	4.02(3)	4.10(25)	4.10(34)
	0.1	1.95	1.89(34)	3.23(34)	3.22(3)	3.29(25)	3.29(34)
	1.0	1.31	1.31(15)	5.50(15)	5.44(3)	5.50(15)	5.50(22)
	10.	0.97	0.97(3)	37.4(3)	37.4(3)	37.4(7)	
10.0	0.01	4.55	2.23(34)	27.5(34)	26.7(3)	29.8(25)	29.8(34)
	0.1	3.25	2.19(34)	27.6(34)	25.5(3)	28.6(25)	28.7(34)
	1.0	2.09	2.06(34)	29.6(34)	26.6(3)	29.6(25)	29.6(34)
	10.	1.20	1.20(10)	50.6(10)	49.4(3)	50.6(10)	50.6(16)
	100.	0.59	0.59(3)	106.7(3)	106.7(3)	106.7(7)	
100.0	0.1	4.55	2.28(34)	102.2(34)	82.6(3)	104.3(25)	104.5(34)
	1.	3.30	2.31(34)	102.4(34)	81.7(3)	103.2(25)	103.4(34)
	10.	2.08	2.05(34)	106.1(34)	85.8(3)	106.0(25)	106.1(34)
	100.	1.06	1.06(10)	125.4(10)	121.0(3)	125.4(10)	125.4(15)
	1000.	0.42	0.42(3)	117.7(3)	117.7(3)	117.7(7)	
1000.0	10.0[b]	3.30	2.31(34)	187.3(34)	122.4(3)	185.7(25)	188.3(34)
	100.[b]	2.07	1.89(17)	187.7(34)	129.0(3)	172.8(10)	183.1(17)
	1000.	0.99	0.99(10)	141.3(10)	135.2(3)	141.3(10)	141.3(15)
	10.000.	0.36	0.36(3)	74.1(3)	74.1(3)	74.1(7)	
10,000.0	100.0[b]	3.30	2.31(34)	244.8(34)	132.1(3)	235.4(25)	245.8(34)
	1000.[b]	2.06	2.03(34)	232.2(34)	139.5(3)	228.1(25)	232.2(34)
	10,000.	0.98	0.98(10)	128.1(10)	122.4(3)	128.1(10)	128.1(15)
	100,000.	0.35	0.35(3)	51.8(3)	51.8(3)	51.8(7)	

[a]All values in this table, with the exception of the Karzas and Latter entries, were computed with the DEGA-A code. An integer in parentheses is the value of ℓ for which either Eq. (51) or (53) was terminated to obtain the Gaunt factor. These integers illustrate the speed of convergence of Eqs. (51) and (53).

[b]Neither Eq. (51) nor (53) has converged.

of a geometric sum enables the extrapolation of Eq. (51) to results that should represent a lower bound to the infinite sum. Numerical checks indicate that this extrapolation is good to 10% or better. To derive this extrapolation formula. let us simplify Eq. (51) by setting

$$Y^1_\ell = (\ell + 1)\, H_{\ell+1,\ell}(\lambda_a, h\upsilon)^2$$

and (54)

$$Y^2_\ell = \ell H_{\ell-1,\ell}(\lambda_a, h\upsilon)^2 \quad .$$

From calculations, we note that both $(\log Y^1_\ell, \ell)$ and $(\log Y^2_\ell, \ell)$ approximate straight lines for large values of ℓ. (The $(\log Y_\ell, \ell)$ pair is not to be confused with the $(\lambda_a, h\upsilon)$ pair.) Figure 9 illustrates this point for (1000, 100). The straight line for Y^1_ℓ is written as

$$\log Y^1_\ell = s(\ell - \ell') + q \quad , \tag{55}$$

and two known points, $(\log Y^1_{\ell'}, \ell')$ and $(\log Y^1_{\ell'+1}, \ell' + 1)$, are chosen to evaluate s and q. Equation (55) can also be written as

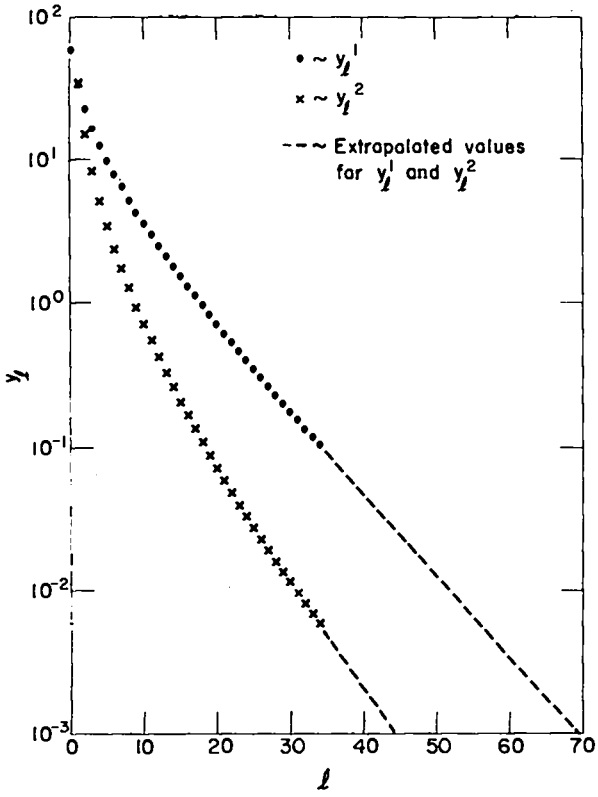

Fig. 9.
A graphic representation of the terms in Eq. (51) and the extrapolation indicated in Eq. (56).

$$Y^1_\ell = e^q (e^s)^{\ell - \ell'} \quad . \tag{56}$$

Now using Eq. (56) to take the infinite sum for all $\ell \geq \ell'$. we have the extrapolation formula

$$\sum_{\ell=\ell'}^{\infty} Y^1_\ell = e^q/(1 - e^s) \quad . \tag{57}$$

The above procedure is repeated using Y^2_ℓ. These two extrapolated values are added to the number obtained by summing Eq. (51) to $\ell = \ell' - 1$. The results obtained by using this extrapolation formula are given in Table III.

TABLE III

EXTRAPOLATED VALUES OF GAUNT FACTORS

λ_a	$h\upsilon$	$g_{ff}(\lambda_a, h\upsilon)$ for Na Calculated Using Eq. (51); ℓ in Parentheses	$g_{ff}(\lambda_a, h\upsilon)$ for Na Calculated Using Extrapolated Form of Eq. (51): ℓ' in Parentheses	
1000.0	10.0	187.3 (34)	189.5 (27)	189.9 (34)
	100.	187.7 (34)	188.3 (27)	188.3 (34)
10.000.0	100.0	244.8 (34)	259.0 (27)	261.7 (34)
	1000.	232.2 (34)	234.2 (27)	234.3 (34)

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APPENDIX
DEGA-A

DEGA-A in its present form is a research and not a production code. The version, whose listing follows, only calculates bound-free absorptions. The code lists these absorption coefficients and makes plots as seen in the previous section. With slight modifications in the coding, bound-bound and free-free absorptions can be calculated.

There are several free parameters that regulate the accuracy of the code. Most of these parameters are set at the beginning of the code; however, a few are found throughout the code. The values in the listing will give at least four-place accuracy. The user should feel free to vary these parameters as he pleases and at his own risk.

Data are read into the bound-free version of DEGA-A with the following FORTRAN statements.

```
  2 FORMAT (8F10.3)
  7 FORMAT (1615)
133 FORMAT (F15.5,215)
    READ 2, Z, RR2, RR
    IF (Z.LT.0.0) end job
    READ 7, ISSMAX
    READ 7. (NSUBSHL (ISS), ISS = 1, ISSMAX)
    READ 7, KWKB
    DO 132 K = 1, KWKB
132 READ 133. XLAMWKB(K), LWKB(K), NWKB(K)
    READ 7, IHNUMAX
    READ 2, (HNUVEC(IHNU), ACOFVEC(IHNU),
             IHNU = 1, IHNUMAX)
```

Z — is the atomic number of the element under consideration.

RR2 — is the same as r_o on page 1.

RR — is the same as R_1 on page 1. Units for RR2 and RR are number of Bohr Radii.

ISSMAX — is the number of subshells under consideration.

NSUBSHL(ISS) — is an array that contains the number of electrons in each subshell. The entries are read into this array in the order 1s, 2s, 2p, 3s, 3p, 3d, etc., up to the last occupied subshell. If any previous subshell is vacant, it must be assigned the value zero.

KWKB — is the number of bound wave functions to be computed. The necessary free wave functions are generated internally by the code.

XLAMWKB(K) — is an array that contains guesses at the eigenvalues of the bound states. Units are number of Rydbergs.

LWKB(K) — is an array that contains the quantum numbers ℓ. $\ell = 0$ for s - states, $\ell = 1$ for p - states, $\ell = 2$ for d - states, etc.

NWKB(K) — is an array that contains the quantum numbers n. n = 1 for the 1s state, n = 2 for the 2s and 2p states, n = 3 for the 3s, 3p, and 3d states, etc.

For each K, XLAMWKB(K), LWKB(K), and NWKB(K) should be consisent with Eq. (39). These guesses at bound eigenvalues can be read in any order. NSUBSHL(ISS) should be defined for each of these guesses at a bound eigenvalue.

IHNUMAX — is the number of $(h\upsilon, \sigma_{bf}(h\upsilon))$ pairs from a separate source that one wants to compare with the results of DEGA-A. This option is illustrated by the X's in Figs. 2 through 7. If IHNUMAX equals zero, no $(h\upsilon, \sigma_{bf}(h\upsilon))$ pairs will be read.

HNUVEC(IHNU) — is the array that contains the $h\upsilon$'s given in electron-volts.

ACOFVEC(IHNU) — is the array that contains the $\sigma_{bf}(h\upsilon)$'s given in barns/atom.

Data decks may be stacked one behind the other. The job terminates normally when it encounters a negative Z.

```
      PROGRAM DEGAA(INP, OUT, FILM)                                          DEGA   00002
      DIMENSION XLAMARY(100), LARY(101), ALFAARY(100), IMAXARY(100)          DEGA   00003
     1     ,NSUBSHL(28), NSHELL(100)                                         DEGA   00004
      COMMON/SCRATCH/SCRATCH(1204)                                           DEGA   00005
      DIMENSION AM1S(401), AM2S(401), JMAXS(401)                             DEGA   00006
      EQUIVALENCE (SCRATCH(1), AM1S(1)), (SCRATCH(402), AM2S(1)),            DEGA   00007
     1     (SCRATCH(803), JMAXS(1))                                          DEGA   00008
      DIMENSION AROOT(2)                                                     DEGA   00009
      DIMENSION PDUM(2)                                                      DEGA   00010
      COMMON/CB3/ Z, ZM1, RR2, RR, A0                                        DEGA   00011
      COMMON/AIMAX/  AF(51,402), JMAXF(402), IMAX,                           DEGA   00012
     1     IMAXF, IMAXFP1, IMAXB, IMAXBP1, C(3,400),                         DEGA   00013
     2     CF(3,402), ATOP(401), ATOPF(402)                                  DEGA   00014
      DIMENSION AB(51,402), JMAXB(402), CB(3,402), ATOPB(402)                DEGA   00015
      EQUIVALENCE(AF(1), AB(1)), (JMAXF(1), JMAXB(1)),                       DEGA   00016
     1     (CF(1), CB(1)), (ATOPF(1), ATOPB(1))                              DEGA   00017
      COMMON/EPS/EPSCONV, FBMAX, EM16, EMATELE, EMDVDD, MAXDIM               DEGA   00018
      DIMENSION AXLAMB(100)                                                  DEGA   00019
      DIMENSION XLAMWKB(100), LWKB(101), NWKB(100)                           DEGA   00020
      COMMON/PI/PI, TWOSPI                                                   DEGA   00021
      COMMON/CB1/ HNUVEC(500), ACOFVEC(500), NOPTS, IHNUMAX, MM(100),        DEGA   00022
     1     NN(100), MNMAX, I4MIN, I4MAX                                      DEGA   00023
      COMMON/METHODS/METHOD, TEMPLAM, CASF, CAPFP, THETA, THETAP             DEGA   00024
      PI = 3.14159265358898   $   TWOSPI = 2.0/PI                           DEGA   00025
      MAXITER = 100                                                          DEGA   00026
      MAXDIM = 100                                                           DEGA   00027
      EPSCONV = 1.0E-5                                                       DEGA   00028
      FBMAX = 1.0E200                                                        DEGA   00029
      EM16 = 1.0E-8                                                          DEGA   00030
      EMATELE = 1.0E-5                                                       DEGA   00031
      EMDVDD = 1.0E-8                                                        DEGA   00032
      RMAXFAC = 25.0                                                         DEGA   00033
      EPHI = 1.0E-15                                                         DEGA   00034
      DRMIN = 1.0E-8                                                         DEGA   00035
      DVMAX = 1.0E-4                                                         DEGA   00036
      ATOPFAC = .5                                                           DEGA   00037
      DHNUI = .1                                                             DEGA   00038
      ZZZFAC = 10.0                                                          DEGA   00039
      NODIVNG = 70                                                           DEGA   00040
      XLAMFC1 = 3.0                                                          DEGA   00041
      XLAMFC2 = .2                                                           DEGA   00042
C      MAKE XLAMFC1 .GT. 1.0 AND XLAMFC2 .LT. 1.0                            DEGA   00043
      CALL ADV(15)                                                           DEGA   00044
    1 FORMAT(E24.14, 2I5)                                                    DEGA   00045
    2 FORMAT(8F10.3)                                                         DEGA   00046
    3 FORMAT(5E25.14)                                                        DEGA   00047
    7 FORMAT(16I5)                                                           DEGA   00048
    9 FORMAT(8F10.3)                                                         DEGA   00049
  997 CONTINUE                                                               DEGA   00050
      MFAC = 1                                                               DEGA   00051
      NOPTS = 500                                                            DEGA   00052
      KPHIMAX = 0                                                            DEGA   00053
      IERROR = 0                                                             DEGA   00054
      RMIN = 0.0                                                             DEGA   00055
      READ 2, Z, RR2, RR                                                     DEGA   00056
      IF(Z .LT. 0.0) GO TO 998                                               DEGA   00057
      RMAX = RR                                                              DEGA   00058
      PRINT 3, Z, RR2, RR                                                    DEGA   00059
      ZM1 = Z - 1.0                                                          DEGA   00060
      A0 = .6057*Z**.333333                                                  DEGA   00061
      READ  7, ISSMAX                                                        DEGA   00062
      PRINT 7, ISSMAX                                                        DEGA   00063
```

```
      READ  7, (NSUBSHL(ISS), ISS=1, ISSMAX)                              DEGA  00064
      PRINT 7, (NSUBSHL(ISS), ISS=1, ISSMAX)                              DEGA  00065
      READ  7, KWKB                                                       DEGA  00066
      PRINT 7, KWKB                                                       DEGA  00067
  133 FORMAT(F15.5, 2I5)                                                  DEGA  00068
      DO 132 K=1, KWKB                                                    DEGA  00069
      READ 133, XLAMWKB(K), LWKB(K), NWKB(K)                              DEGA  00070
      PRINT  1, XLAMWKB(K), LWKB(K), NWKB(K)                              DEGA  00071
      XLAMARY(K) = XLAMWKB(K)                                             DEGA  00072
      LARY(K) = LWKB(K)                                                   DEGA  00073
  132 NSHELL(K) = NWKB(K)                                                 DEGA  00074
      LARY(KWKB + 1) = -1                                                 DEGA  00075
      IF(RR2 .GE. 0.0) SCRATCH(1) = V1(RR2)                               DEGA  00076
      CALL YYY(RMIN,RMAX,DRMIN,DVMAX,ATOPFAC,I2,IERROR,                   DEGA  00077
     1     XLAMWKB, LWKB, KWKB, ZZZFAC)                                   DEGA  00078
      IF(IERROR .NE. 0) GO TO 99                                          DEGA  00079
      I2P1 = I2 + 1                                                       DEGA  00080
      ISKIP = 3*MAXDIM + 4                                                DEGA  00081
      IECS = 1 - ISKIP                                                    DEGA  00082
      DO 118 I=1, I2                                                      DEGA  00083
      IECS = IECS + ISKIP                                                 DEGA  00084
      CALL ECWR(ATOP(I+1), IECS, 1, IE)                                   DEGA  00085
  118 CALL ECWR(C(1,I), IECS+1, 3, IE)                                    DEGA  00086
      PRINT 7, IMAX , I2                                                  DEGA  00087
      IMAXP1 = IMAX + 1                                                   DEGA  00088
      IF(IMAXP1 .GT. 400) GO TO 109                                       DEGA  00089
      DO 108 I=IMAXP1, 400                                                DEGA  00090
      C(1,I)= 0.0                                                         DEGA  00091
      C(2,I) = -1.0                                                       DEGA  00092
  108 C(3,I) = 0.0                                                        DEGA  00093
  109 ATOP(1) = 0.0                                                       DEGA  00094
      DO 10 I=1, IMAX                                                     DEGA  00095
   10 PRINT 3, C(1,I), C(2,I), C(3,I), ATOP(I+1)                          DEGA  00096
      GO TO 49                                                            DEGA  00097
  135 CONTINUE                                                            DEGA  00098
      CALL ZZZ(XLAMARY, LARY, NSHELL, KPHIMAX, HNUVEC, NOPTS,             DEGA  00099
     1     IHNUMAX, DHNUI, ZZZFAC)                                        DEGA  00100
  136 FORMAT(///)                                                         DEGA  00101
      PRINT 136                                                           DEGA  00102
      DO 137 KPHI=1, KPHIMAX                                              DEGA  00103
  137 PRINT 133, XLAMARY(KPHI), LARY(KPHI), NSHELL(KPHI)                  DEGA  00104
      PRINT 136                                                           DEGA  00105
      PRINT 3, (HNUVEC(IHNU), IHNU=1, IHNUMAX)                            DEGA  00106
      PRINT 136                                                           DEGA  00107
      DO 138 IHNU=1, IHNUMAX                                              DEGA  00108
  138 ACOFVEC(IHNU) = 0.0                                                 DEGA  00109
      KWKBMAX = 0                                                         DEGA  00110
      DO 139 KPHI=1, KPHIMAX                                              DEGA  00111
      KWKBMAX = KWKBMAX + 1                                               DEGA  00112
      NWKB(KWKBMAX) = NSHELL(KPHI)                                        DEGA  00113
      LWKB(KWKBMAX) = 1000*(LARY(KPHI) + 1) + LARY(KPHI)                  DEGA  00114
      XLAMWKB(KWKBMAX) = XLAMARY(KPHI)                                    DEGA  00115
      IF(LARY(KPHI) .EQ. 0) GO TO 139                                     DEGA  00116
      KWKBMAX = KWKBMAX + 1                                               DEGA  00117
      NWKB(KWKBMAX) = NSHELL(KPHI)                                        DEGA  00118
      LWKB(KWKBMAX) = 1000*(LARY(KPHI) - 1) + LARY(KPHI)                  DEGA  00119
      XLAMWKB(KWKBMAX) = XLAMARY(KPHI)                                    DEGA  00120
  139 CONTINUE                                                            DEGA  00121
      KWKB = 0                                                            DEGA  00122
      I4MIN = 1                                                           DEGA  00123
  140 KWKB = KWKB + 1                                                     DEGA  00124
      XLAMARY(1) = XLAMWKB(KWKB)                                          DEGA  00125
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      NSHELL(1) = NWKB(KWKB)                                                    DEGA   00126
      LPOS = LWKB(KWKB)/1000                                                    DEGA   00127
      LARY(1) = LWKB(KWKB) - LPOS*1000                                          DEGA   00128
  141 IF(1.0000001*ABS(XLAMARY(1)) .LT. HNUVEC(I4MIN)) GO TO 142                DEGA   00129
      I4MIN = I4MIN + 1                                                         DEGA   00130
      GO TO 141                                                                 DEGA   00131
  142 I4MAX = IHNUMAX                                                           DEGA   00132
      MNMAX = 0                                                                 DEGA   00133
      DO 143 I4=I4MIN , I4MAX                                                   DEGA   00134
      MNMAX = MNMAX + 1                                                         DEGA   00135
      MNMAXP1 = MNMAX + 1                                                       DEGA   00136
      MM(MNMAX) = 1                                                             DEGA   00137
      NN(MNMAX) = MNMAXP1                                                       DEGA   00138
      XLAMARY(MNMAXP1) = HNUVEC(I4) + XLAMARY(1)                                DEGA   00139
      LARY(MNMAXP1) = LPOS                                                      DEGA   00140
  143 NSHELL(MNMAXP1) = 0                                                       DEGA   00141
      LARY(MNMAXP1 + 1) = -2                                                    DEGA   00142
      KPHIMAX = 0                                                               DEGA   00143
   49 CONTINUE                                                                  DEGA   00144
      KPHIMP1 = KPHIMAX + 1                                                     DEGA   00145
      L = LARY(KPHIMP1)                                                         DEGA   00146
      IF(L .EQ. -1) GO TO 135                                                   DEGA   00147
      IF(L .EQ. -2) GO TO 99                                                    DEGA   00148
      METHOD = 2                                                                DEGA   00149
      IF(XLAMARY(KPHIMP1) .LT. 0.0) METHOD = 1                                  DEGA   00150
      XL = L                                                                    DEGA   00151
      XLLP1 = L*(L+1)                                                           DEGA   00152
      XLLM1 = XL*(XL-1.0)                                                       DEGA   00153
      TWOXL = 2.0*XL                                                            DEGA   00154
      LM2 = L-2                                                                 DEGA   00155
      LM1 = L-1                                                                 DEGA   00156
      LP1 = L+1                                                                 DEGA   00157
      XLP1 = LP1                                                                DEGA   00158
      IF (METHOD .EQ. 1) GO TO 107                                              DEGA   00159
      XLAMBDA = XLAMARY(KPHIMP1)                                                DEGA   00160
      SMALLK = SQRT(XLAMBDA)                                                    DEGA   00161
      RMAX = (XLLP1 + 1.0/XLAMBDA - 30.0)*SMALLK                                DEGA   00162
      RTMP = 10.0/XLAMBDA                                                       DEGA   00163
      IF(RTMP .GT. RMAX) RMAX = RTMP                                            DEGA   00164
      IF(ATOP(I2+1) .GT. RMAX) RMAX = 1.05*ATOP(I2+1)                           DEGA   00165
      IF(RMAX .LT. 1.01) RMAX = 1.01                                            DEGA   00166
      GO TO 122                                                                 DEGA   00167
  146 RMAX = 1.2*RMAX                                                           DEGA   00168
      IERROR = 0                                                                DEGA   00169
      GO TO 110                                                                 DEGA   00170
  107 AROOT(1) = 0.0                                                            DEGA   00171
      AROOT(2) = 0.0                                                            DEGA   00172
      IMAX = I2 + 1                                                             DEGA   00173
      ATOP(IMAX+1) = 1000.0                                                     DEGA   00174
      CALL ROOTDIV(XLAMARY(KPHIMP1), XLLP1, AROOT, ICNTR, ICNTD, ICASE,         DEGA   00175
     1     IERROR, 1)                                                           DEGA   00176
      PRINT 3, XLAMARY(KPHIMP1), AROOT(1), AROOT(2)                             DEGA   00177
      IF(IERROR .EQ. 0) GO TO 151                                               DEGA   00178
      PRINT 152, IERROR                                                         DEGA   00179
  152 FORMAT(I5, *  RMAX SET TO 1.1ATOP(I2+1)*)                                 DEGA   00180
      IERROR = 0                                                                DEGA   00181
      RMAX = 1.1*ATOP(I2+1)                                                     DEGA   00182
      GO TO 122                                                                 DEGA   00183
  151 RMAX = AROOT(2)                                                           DEGA   00184
      IF(AROOT(1) .GT. RMAX) RMAX = AROOT(1)                                    DEGA   00185
      RMAX = RMAXFAC*RMAX                                                       DEGA   00186
      IF(RMAX .LT. 1.01*ATOP(I2+1))RMAX = 1.01*ATOP(I2+1)                       DEGA   00187
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      PRINT 153, RMAX                                                    DEGA   00188
  153 FORMAT(*  RMAX = *, E20.10)                                        DEGA   00189
  122 IMAX = I2                                                          DEGA   00190
  110 DR = ATOPFAC*ATOP(IMAX+1)                                          DEGA   00191
      RTMP= ATOP(IMAX + 1)                                               DEGA   00192
      SMALLK = SQRT(ABS(XLAMARY(KPHIMP1) + (2.0 - XLLP1/RTMP)/RTMP))     DEGA   00193
      RTMP = ATOP(IMAX+1) + .5*(ATOP(IMAX+1) - ATOP(IMAX))               DEGA   00194
      SMALLK1 = SQRT(ABS(XLAMARY(KPHIMP1) + (2.0 - XLLP1/RTMP)/RTMP))    DEGA   00195
      IF(SMALLK1 .GT. SMALLK) SMALLK = SMALLK1                           DEGA   00196
      DRMAX = 6.28/SMALLK                                                DEGA   00197
      IF(DR .GT. DRMAX) DR = DRMAX                                       DEGA   00198
      IMAX = IMAX + 1                                                    DEGA   00199
      ATOP(IMAX+1) = ATOP(IMAX) + DR                                     DEGA   00200
      IF(IMAX .EQ. 400) 124, 123                                         DEGA   00201
  124 PRINT 125                                                          DEGA   00202
  125 FORMAT(*      400 INTERVALS WILL NOT SPAN (0,RMAX)*)               DEGA   00203
      GO TO 999                                                          DEGA   00204
  123 IF(ATOP(IMAX+1) .GE. RMAX) 111, 110                                DEGA   00205
  111 ATOP(IMAX+1) = RMAX                                                DEGA   00206
      CAPR = RMAX                                                        DEGA   00207
      ATOPTMP = ATOP(IMAX + 1)                                           DEGA   00208
      ATOP(IMAX+1) = CAPR                                                DEGA   00209
      GO TO (68,69), METHOD                                              DEGA   00210
   68 NODIV = NODIVNG                                                    DEGA   00211
      NODIVP1 = NODIV + 1                                                DEGA   00212
      AXLAMB(1)          = XLAMFC1*XLAMARY(KPHIMP1)                      DEGA   00213
      AXLAMB(NODIVP1) = XLAMFC2*XLAMARY(KPHIMP1)                         DEGA   00214
      DAXLAMB = ABS(ALOG(ABS(AXLAMB(1)))                                 DEGA   00215
     1      - ALOG(ABS(AXLAMB(NODIVP1))))/NODIV                         DEGA   00216
      IF(ABS(AXLAMB(1)) .GT. ABS(AXLAMB(NODIVP1))) DAXLAMB = -DAXLAMB    DEGA   00217
      DO 60 I=2, NODIV                                                   DEGA   00218
   60 AXLAMB(I) = EXP(ALOG(ABS(AXLAMB(I-1))) + DAXLAMB)                  DEGA   00219
      XLAMBDA = AXLAMB(1)                                                DEGA   00220
      GO TO 70                                                           DEGA   00221
   69 TEMPLAM = XLAMBDA                                                  DEGA   00222
      NODIV = 4    $   NODIVP1 = NODIV + 1                               DEGA   00223
      AXLAMB(1) = 0.0    $   DXLAM = PI/4.0                              DEGA   00224
      DO 71 I=1, NODIV                                                   DEGA   00225
   71 AXLAMB(I+1) = AXLAMB(I) + DXLAM                                    DEGA   00226
      CALL CARSON(XLAMBDA, C(2,IMAX), MFAC, CAPR, XLLP1,                 DEGA   00227
     1     CAPF, CAPFP, THETA, THETAP, IERROR)                           DEGA   00228
      IF(IERROR .EQ. 12) GO TO 146                                       DEGA   00229
   70 CONTINUE                                                           DEGA   00230
      AROOT(1) = 0.0    $   AROOT(2) = 0.0                               DEGA   00231
      CALL        ROOTDIV(XLAMBDA, XLLP1, AROOT, ICNTR, ICNTD, ICASE,    DEGA   00232
     1              IERROR, 0)                                          DEGA   00233
      PRINT 3, XLAMBDA, AROOT(1), AROOT(2)                               DEGA   00234
      J25SET = 1                                                         DEGA   00235
   80 J25FST = 1                                                         DEGA   00236
      J25MIN = J25SET                                                    DEGA   00237
      J25MAX = NODIVP1                                                   DEGA   00238
      GO TO 90                                                           DEGA   00239
   81 J25FST = 2                                                         DEGA   00240
      J25MIN = NODIVP1+1                                                 DEGA   00241
      J25MAX = NODIVP1 + 20                                              DEGA   00242
      D25 = (XLAMSTP - XLAMSTT)/19.0                                     DEGA   00243
      AXLAMB(J25MIN) = XLAMSTT                                           DEGA   00244
      AXLAMB(J25MAX) = XLAMSTP                                           DEGA   00245
      I79MIN = J25MIN+1                                                  DEGA   00246
      I79MAX = J25MAX - 1                                                DEGA   00247
      DO 79 I79=I79MIN, I79MAX                                           DEGA   00248
   79 AXLAMB(I79) = AXLAMB(I79 - 1) + D25                                DEGA   00249
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   90 DO 25 J= J25MIN, J25MAX                                                    DEGA    00250
      XLAMSTP = AXLAMB(J)                                                        DEGA    00251
      CALL TAYLORF(XL, XLAMSTP, IERROR, AF, JMAXF, IMAXF, CF, ATOPF)             DEGA    00252
      IBKW = IMAXFP1 + 1                                                         DEGA    00253
      CALL TAYLORB(XL, XLAMSTP, IERROR, AB(1, IBKW),                             DEGA    00254
     1      JMAXB(IBKW), IMAXB, CB(1,IBKW), ATOPB(IBKW))                        DEGA    00255
      CALL BOUNDRY(IFCONV, FBSTP)                                                DEGA    00256
C         TROUBLE MAY ARISE (MISS AN EIGENVALUE) IF FBSTP=0 TWICE                DEGA    00257
C     IN A ROW.                                                                  DEGA    00258
C     **********                                                                 DEGA    00259
C           HERE, LATER, FIND NEW ROOTS AND CHECK STABILITY CONDITIONS.          DEGA    00260
      IF(IFCONV .EQ. 1) 73, 74                                                   DEGA    00261
   73 CAPLAMB = XLAMSTP                                                          DEGA    00262
      GO TO 75                                                                   DEGA    00263
   74 IF(J .EQ. J25MIN) 26, 27                                                   DEGA    00264
   27 IF(FBSTT*FBSTP .LE. 0.0) 28, 26                                            DEGA    00265
   28 XLAMMID = .5*(XLAMSTP + XLAMSTT)                                           DEGA    00266
      CALL TAYLORF(XL, XLAMMID, IERROR, AF, JMAXF, IMAXF, CF, ATOPF)             DEGA    00267
      IBKW = IMAXFP1 + 1                                                         DEGA    00268
      CALL TAYLORB(XL, XLAMMID, IERROR, AB(1,IBKW),                              DEGA    00269
     1      JMAXB(IBKW), IMAXB, CB(1,IBKW), ATOPB(IBKW))                        DEGA    00270
      CALL BOUNDRY(IFCONV, FBMID)                                                DEGA    00271
      IF(FBSTT .GT. FBSTP) 29, 30                                                DEGA    00272
   29 FBTOP = FBSTT   $   FBBOT = FBSTP   $   GO TO 31                          DEGA    00273
   30 FBTOP = FBSTP   $   FBBOT = FBSTT                                         DEGA    00274
   31 IF((FBTOP .GT. FBMID) .AND. (FBMID .GT. FBBOT)) 32, 57                    DEGA    00275
   57 PRINT 58                                                                  DEGA    00276
      PRINT 58                                                                  DEGA    00277
      PRINT 59                                                                  DEGA    00278
      PRINT 58                                                                  DEGA    00279
      PRINT 58                                                                  DEGA    00280
   58 FORMAT(* XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX*)      DEGA    00281
   59 FORMAT(*  FBMID IS NOT BETWEEN FBTOP AND FBBOT.  MAKE SURE A VALUE        DEGA    00282
     1 OF LAMBDA WAS NOT MISSED.*)                                              DEGA    00283
      GO TO 87                                                                  DEGA    00284
   32 XLAMB0 = XLAMSTT   $   XLAMB1 = XLAMSTP                                   DEGA    00285
      FB0 = FBSTT   $   FB1 = FBSTP                                             DEGA    00286
C           REGULA DOES NOT CHECK STABILITY CONDITIONS.                         DEGA    00287
      CALL REGULA(XLAMB0,XLAMB1,FB0,FB1,CAPLAMB,MAXITER,XL,IERROR)              DEGA    00288
C           HERE, LATER, FIND NEW ROOTS AND CHECK STABILITY CONDITIONS.         DEGA    00289
      IF(IERROR .NE. 0) GO TO 87                                                DEGA    00290
      IF(XLAMSTT .LT. XLAMSTP) GO TO 105                                        DEGA    00291
      XLAMB0 = XLAMSTP                                                          DEGA    00292
      XLAMB1 = XLAMSTT                                                          DEGA    00293
      GO TO 104                                                                 DEGA    00294
  105 XLAMB0 = XLAMSTT                                                          DEGA    00295
      XLAMB1 = XLAMSTP                                                          DEGA    00296
  104 IF(XLAMB0 .LE. CAPLAMB .AND. CAPLAMB .LE. XLAMB1) 75, 86                  DEGA    00297
   86 PRINT 58                                                                  DEGA    00298
      PRINT 58                                                                  DEGA    00299
      PRINT 88                                                                  DEGA    00300
   88 FORMAT(*  CAPLAMB IS NOT BETWEEN XLAMSTT AND XLAMSTP.  XLAMSTT, CA        DEGA    00301
     1PLAMB, AND XLAMSTP ARE *)                                                 DEGA    00302
      PRINT 3, XLAMSTT, CAPLAMB, XLAMSTP                                        DEGA    00303
      PRINT 58                                                                  DEGA    00304
      PRINT 58                                                                  DEGA    00305
   87 IF(J25FST .EQ. 1) 82, 84                                                  DEGA    00306
   82 J25SET = J                                                                DEGA    00307
      PRINT 83                                                                  DEGA    00308
   83 FORMAT(*  DIVIDE THIS INTERVAL INTO 19 EQUAL INTERVALS AND TRY AGA        DEGA    00309
     1IN.  *)                                                                   DEGA    00310
      PRINT 58                                                                  DEGA    00311
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      PRINT 58                                                          DEGA   00312
      GO TO 81                                                          DEGA   00313
   84 PRINT 85                                                          DEGA   00314
   85 FORMAT(*  THIS INTERVAL FAILED FOR THE SECOND TIME.  FORGET IT AND DEGA   00315
     1 GO TO THE NEXT INTERVAL. *)                                      DEGA   00316
      PRINT 58                                                          DEGA   00317
      PRINT 58                                                          DEGA   00318
      GO TO 80                                                          DEGA   00319
   75 GO TO(65, 66), METHOD                                             DEGA   00320
   66 ALPHA = CAPLAMB   $  CAPLAMB = XLAMBDA                            DEGA   00321
      PRINT 67, ALPHA, CAPLAMB                                          DEGA   00322
   67 FORMAT(*  ALPHA =*,  E24.14, *     FOR XLAMBDA =*,E24.14)        DEGA   00323
      GO TO 127                                                         DEGA   00324
   65 CONTINUE                                                          DEGA   00325
      IV1 = 0                                                           DEGA   00326
      D = ATOPF(2)                                                      DEGA   00327
      DLP1 = D**LP1                                                     DEGA   00328
      JMAXBOT = JMAXF(1) - 1                                            DEGA   00329
      PDUM(1) = AF(1,2)/DLP1                                            DEGA   00330
      PDUM(2) = (AF(2,2) - XLP1*AF(1,2)/D)/DLP1                         DEGA   00331
      CALL STURMSQ(AF(2,1), JMAXBOT, PDUM, D, IV2, IERROR)              DEGA   00332
      IV1 = IV1 + IV2                                                   DEGA   00333
      IF(IMAXF .EQ. 1) GO TO 98                                         DEGA   00334
      DO 91 IF=2, IMAXF                                                 DEGA   00335
      D = ATOPF(IF+1) - ATOPF(IF)                                       DEGA   00336
      CALL STURMSQ(AF(1,IF), JMAXF(IF), AF(1,IF+1), D, IV2, IERROR)     DEGA   00337
   91 IV1 = IV1 + IV2                                                   DEGA   00338
   98 CONTINUE                                                          DEGA   00339
      DO 95 IB=1, IMAXB                                                 DEGA   00340
      IBKW = IMAXFP1 + IB                                               DEGA   00341
      D = ATOPB(IBKW + 1) - ATOPB(IBKW)                                 DEGA   00342
      CALL STURMSQ(AB(1,IBKW), JMAXB(IBKW), AB(1,IBKW+1),               DEGA   00343
     1     D, IV2, IERROR)                                              DEGA   00344
   95 IV1 = IV1 + IV2                                                   DEGA   00345
      PRINT 128, IV1                                                    DEGA   00346
  128 FORMAT(* THIS WAVE FUNCTION HAS*,I5, * CROSSINGS.*)               DEGA   00347
  127 IBKW = IMAXFP1 + IMAXBP1                                          DEGA   00348
      FAC = AB(1,IBKW)/AF(1,IMAXFP1)                                    DEGA   00349
      DO 33 I=1, IMAXF                                                  DEGA   00350
      JJJ = JMAXF(I)                                                    DEGA   00351
      DO 33 JF=1, JJJ                                                   DEGA   00352
   33 AF(JF,I) = FAC*AF(JF,I)                                           DEGA   00353
      IF(CAPLAMB .LT. 0.0) CALL NORMPHI(CAPLAMB, L)                     DEGA   00354
      PRINT 3, CAPLAMB                                                  DEGA   00355
      KPHIMAX = KPHIMAX + 1                                             DEGA   00356
      GO TO(129,130), METHOD                                            DEGA   00357
  129 IV1L1 = IV1 + L + 1                                               DEGA   00358
      IF(NSHELL(KPHIMAX) .EQ. IV1L1) GO TO 154                          DEGA   00359
      IV1 = NSHELL(KPHIMAX) - L - 1                                     DEGA   00360
      KPHIMAX = KPHIMAX - 1                                             DEGA   00361
      PRINT 134, IV1                                                    DEGA   00362
  134 FORMAT(*  THE PREVIOUS WAVE FUNCTION SHOULD HAVE HAD*, I5,        DEGA   00363
     1   * CROSSINGS.*/*  FORGET THE LAST EIGENVALUE AND TRY SOMEMORE.*) DEGA   00364
      GO TO 26                                                          DEGA   00365
  154 IBKW = IMAXFP1 + 1                                                DEGA   00366
      PHIMIN9 = ABS(AB(1,IBKW))                                         DEGA   00367
      PHIMAX9 = PHIMIN9                                                 DEGA   00368
      IF(IMAXB .EQ. 1) GO TO 155                                        DEGA   00369
      DO 156 IB=2, IMAXB                                                DEGA   00370
      IBKW = IMAXFP1 + IB                                               DEGA   00371
      PHI9 = ABS(AB(1,IBKW))                                            DEGA   00372
      IF(PHI9 .GT. PHIMAX9) PHIMAX9 = PHI9                              DEGA   00373
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156 CONTINUE                                                          DEGA  00374
155 DO 157 IF=1, IMAXF                                                DEGA  00375
    PHI9 = ABS(AF(1,IF))                                              DEGA  00376
    IF(PHI9 .GT. PHIMAX9) PHIMAX9 = PHI9                              DEGA  00377
157 CONTINUE                                                          DEGA  00378
    PRINT 158, PHIMAX9, PHIMIN9                                       DEGA  00379
158 FORMAT(*  PHI MAX AND MIN ARE*, 2E20.10)                          DEGA  00380
    IF(PHIMIN9 .LT. PHIMAX9*EPHI) GO TO 131                           DEGA  00381
    PRINT 159                                                         DEGA  00382
159 FORMAT(*  RMAX IS NOT BIG ENOUGH*)                               DEGA  00383
    KPHIMAX = KPHIMAX - 1                                             DEGA  00384
    GO TO 146                                                         DEGA  00385
130 NSHELL(KHPIMAX) = 0                                               DEGA  00386
131 IMAXARY(KPHIMAX) = IMAX                                           DEGA  00387
    XLAMARY(KPHIMAX) = CAPLAMB                                        DEGA  00388
    LARY(KPHIMAX) = L                                                 DEGA  00389
    IF(CAPLAMB .LT. 0.0) 112, 113                                     DEGA  00390
112 ALFAARY(KPHIMAX) = 0.0                                            DEGA  00391
    GO TO 114                                                         DEGA  00392
113 ALFAARY(KPHIMAX) = ALPHA                                          DEGA  00393
114 CONTINUE                                                          DEGA  00394
    JMAXS(1) = JMAXF(1)                                               DEGA  00395
    DO 115 I=1, IMAXF                                                 DEGA  00396
    AM1S(I) = AF(1,I)                                                 DEGA  00397
115 AM2S(I) = AF(2,I)                                                 DEGA  00398
    IC = IMAXBP1                                                      DEGA  00399
    ID = IMAXF                                                        DEGA  00400
    DO 116 I=1, IMAXB                                                 DEGA  00401
    IC = IC-1                                                         DEGA  00402
    ID = ID+1                                                         DEGA  00403
    IBKW = IMAXFP1 + IC                                               DEGA  00404
    AM1S(ID) = AB(1,IBKW)                                             DEGA  00405
    AM2S(ID) = AB(2,IBKW)                                             DEGA  00406
116 JMAXS(ID) = JMAXB(IBKW)                                           DEGA  00407
    DO 117 I=2, IMAXFP1                                               DEGA  00408
117 JMAXS(I) = 0                                                      DEGA  00409
    IMAXBF = IMAXB + IMAXF                                            DEGA  00410
    IECS = KPHIMAX + 4                                                DEGA  00411
    IECS1 = IECS + MAXDIM                                             DEGA  00412
    IECS2 = IECS1 + MAXDIM                                            DEGA  00413
    CALL ECWR(JMAXS(1), IECS, 1, IE)                                  DEGA  00414
    CALL ECWR(AM1S(1), IECS1, 1, IE)                                  DEGA  00415
    CALL ECWR(AM2S(1), IECS2, 1, IE)                                  DEGA  00416
    DO 121 I=3, I2P1                                                  DEGA  00417
    IECS = IECS + ISKIP                                               DEGA  00418
    IECS1 = IECS + MAXDIM                                             DEGA  00419
    IECS2 = IECS1 + MAXDIM                                            DEGA  00420
    CALL ECWR(JMAXS(I), IECS, 1, IE)                                  DEGA  00421
    CALL ECWR(AM1S(I), IECS1, 1, IE)                                  DEGA  00422
121 CALL ECWR(AM2S(I), IECS2, 1, IE)                                  DEGA  00423
    IF(IMAX .EQ. I2) GO TO 126                                        DEGA  00424
    IECS = 4*(400 - I2)                                               DEGA  00425
    IECS = IECS*(KPHIMAX - 1) + 1                                     DEGA  00426
    IECS = IECS + I2*ISKIP                                            DEGA  00427
    IJUMP = 400 - I2                                                  DEGA  00428
    INUM = IMAX - I2                                                  DEGA  00429
    I2P2 = I2+2                                                       DEGA  00430
    CALL ECWR(ATOP(I2P2), IECS, INUM, IE)                             DEGA  00431
    IECS = IECS + IJUMP                                               DEGA  00432
    CALL ECWR(JMAXS(I2P2), IECS, INUM, IE)                            DEGA  00433
    IECS = IECS + IJUMP                                               DEGA  00434
    CALL ECWR(AM1S(I2P2), IECS, INUM, IE)                             DEGA  00435
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      IECS = IECS + IJUMP                                                DEGA   00436
      CALL ECWR(AM2S(I2P2), IECS, INUM, IE)                              DEGA   00437
  126 GO TO 61                                                           DEGA   00438
   26 XLAMSTT = XLAMSTP    $   FBSTT = FBSTP                             DEGA   00439
   25 CONTINUE                                                           DEGA   00440
      IF(J25FST .EQ. 2) 80, 998                                          DEGA   00441
   61 ATOP(IMAX+1) = ATOPTMP                                             DEGA   00442
      GO TO  49                                                          DEGA   00443
   99 IF(KPHIMAX .EQ. 0) GO TO 999                                       DEGA   00444
      DO 120 KPHI = 1, KPHIMAX                                           DEGA   00445
      PRINT 7, LARY(KPHI)                                                DEGA   00446
  120 PRINT 3, XLAMARY(KPHI) , ALFAARY(KPHI)                             DEGA   00447
      CALL        MATELE(KPHIMAX, XLAMARY, LARY, ALFAARY, IMAXARY, I2,   DEGA   00448
     1     NSUBSHL, ISSMAX, NSHELL)                                      DEGA   00449
  999 CONTINUE                                                           DEGA   00450
      IF(KWKB .LT. KWKBMAX) GO TO 140                                    DEGA   00451
  145 FORMAT(15X, * EV*, 10X, * BARNS/ATOM*)                             DEGA   00452
      PRINT 145                                                          DEGA   00453
      YTOP = ALOG10(ACOFVEC(1))                                          DEGA   00454
      YBOT = YTOP                                                        DEGA   00455
      DO 144 IHNU=1, IHNUMAX                                             DEGA   00456
      HNUVEC(IHNU) = 13.605*HNUVEC(IHNU)                                 DEGA   00457
      PRINT 3, HNUVEC(IHNU), ACOFVEC(IHNU)                               DEGA   00458
      ACOFVEC(IHNU) = ALOG10(ACOFVEC(IHNU))                              DEGA   00459
      IF(ACOFVEC(IHNU) .GT. YTOP) YTOP = ACOFVEC(IHNU)                   DEGA   00460
      IF(ACOFVEC(IHNU) .LT. YBOT) YBOT = ACOFVEC(IHNU)                   DEGA   00461
  144 HNUVEC(IHNU) = ALOG10(HNUVEC(IHNU))                                DEGA   00462
      CALL ADV(2)                                                        DEGA   00463
      CALL DGA(120, 980, 50, 910, HNUVEC(1), HNUVEC(IHNUMAX), YTOP,YBOT) DEGA   00464
      CALL DLGLG                                                         DEGA   00465
      CALL SBLOG                                                         DEGA   00466
      CALL SLLOG                                                         DEGA   00467
      CALL PLOT(IHNUMAX, HNUVEC, 1, ACOFVEC, 1, 42, 1)                   DEGA   00468
      READ 7, IHNUMAX                                                    DEGA   00469
      PRINT 7, IHNUMAX                                                   DEGA   00470
      IF(IHNUMAX .EQ. 0) GO TO 997                                       DEGA   00471
      READ 2, (HNUVEC(IHNU), ACOFVEC(IHNU), IHNU=1, IHNUMAX)             DEGA   00472
      DO 150 IHNU=1, IHNUMAX                                             DEGA   00473
      PRINT 3, HNUVEC(IHNU), ACOFVEC(IHNU)                               DEGA   00474
      HNUVEC(IHNU) = ALOG10(HNUVEC(IHNU))                                DEGA   00475
  150 ACOFVEC(IHNU) = ALOG10(ACOFVEC(IHNU))                              DEGA   00476
      CALL PLOT(IHNUMAX, HNUVEC, 1, ACOFVEC, 1, 55, 0)                   DEGA   00477
      GO TO 997                                                          DEGA   00478
  998 CONTINUE                                                           DEGA   00479
      CALL ADV(15)                                                       DEGA   00480
      CALL EMPTY                                                         DEGA   00481
      END                                                                DEGA   00482
      SUBROUTINE ROOTDIV(XLAMBDA, XLLP1, AROOT, ICNTR, ICNTD, ICASE,     DEGA   00483
     1           IERROR, IFSTOP)                                         DEGA   00484
      DIMENSION AROOT(2)                                                 DEGA   00485
      COMMON/AIMAX/  AF(51,402), JMAXF(402), IMAX,                       DEGA   00486
     1     IMAXF, IMAXFP1, IMAXB, IMAXBP1, C(3,400),                     DEGA   00487
     2     CF(3,402), ATOP(401), ATOPF(402)                              DEGA   00488
      DIMENSION AB(51,402), JMAXB(402), CB(3,402), ATOPB(402)            DEGA   00489
      EQUIVALENCE(AF(1), AB(1)), (JMAXF(1), JMAXB(1)),                   DEGA   00490
     1     (CF(1), CB(1)), (ATOPF(1), ATOPB(1))                          DEGA   00491
      ICNTR = 0    $   ICNTD = 0    $   IERROR = 0                       DEGA   00492
      DO 10 I=1, IMAX                                                    DEGA   00493
      II=I                                                               DEGA   00494
      CALL BINOM (XLAMBDA, XLLP1, II, NOROOTS, ROOT1, ROOT2, NODIV,DIV1) DEGA   00495
      NOROOT1 = NORODTS + 1                                              DEGA   00496
      GO TO(14, 11, 12),NOROOT1                                          DEGA   00497
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11 IF((ATOP(I) .LE. ROOT1) .AND. (ROOT1 .LT. ATOP(I+1)))13,14          DEGA  00498
13 ICNTR = ICNTR + 1                                                   DEGA  00499
   AROOT(ICNTR) = ROOT1                                                DEGA  00500
   IF(ICNTR .EQ. 2)15, 14                                              DEGA  00501
12 IF(ROOT1 .LT. ROOT2) 28, 27                                         DEGA  00502
27 TEMP = ROOT1   $   ROOT1 = ROOT2   $   ROOT2 = TEMP                 DEGA  00503
28 IF((ATOP(I) .LE. ROOT1) .AND.(ROOT1 .LT. ATOP(I+1)))16,17           DEGA  00504
16 ICNTR = ICNTR + 1                                                   DEGA  00505
   AROOT(ICNTR) = ROOT1                                                DEGA  00506
   IF(ICNTR .EQ. 2)15, 17                                              DEGA  00507
17 IF((ATOP(I) .LE. ROOT2) .AND. (ROOT2 .LT. ATOP(I+1)))18,14          DEGA  00508
18 ICNTR = ICNTR + 1                                                   DEGA  00509
   AROOT(ICNTR) = ROOT2                                                DEGA  00510
   IF(ICNTR .EQ. 2)15, 14                                              DEGA  00511
15 IF(ICNTD .EQ. 1)19, 20                                              DEGA  00512
20 IF(NODIV .EQ. 1)21, 19                                              DEGA  00513
21 IF((ATOP(I).LE. DIV1) .AND. (DIV1 .LT. ATOP(I+1)))22, 19            DEGA  00514
22 ICNTD = 1   $   ADIV = DIV1   $   IDIV = I   $   GO TO 19           DEGA  00515
14 IF(ICNTD .EQ. 1)10, 23                                              DEGA  00516
23 IF(NODIV .EQ. 1)24, 10                                              DEGA  00517
24 IF((ATOP(I).LE. DIV1) .AND. (DIV1 .LT. ATOP(I+1)))25, 10            DEGA  00518
25 ICNTD = 1   $   ADIV = DIV1   $   IDIV = I                          DEGA  00519
10 CONTINUE                                                            DEGA  00520
19 IF((ICNTD .EQ. 1) .AND. (ICNTR .EQ.2))29, 44                        DEGA  00521
44 IF((ICNTD .EQ.1).AND. (ICNTR .EQ. 0)) 45, 26                        DEGA  00522
45 ICASE = 5     $   GO TO 31                                          DEGA  00523
29 ICASE = 4                                                           DEGA  00524
   IF((AROOT(1) .LT. ADIV) .AND. (ADIV .LT. AROOT(2)))31, 30           DEGA  00525
30 IERROR = 2                                                          DEGA  00526
   PRINT 2                                                             DEGA  00527
 2 FORMAT(*  IERROR=2, ICASE=4. MAX IS NOT BETWEEN THE TOW ROOTS.*)    DEGA  00528
   RETURN                                                              DEGA  00529
26 IF((ICNTD.EQ. 0) .AND. (ICNTR .EQ. 0))34, 35                        DEGA  00530
34 ICASE = 1   $   IDIV = IMAX                                         DEGA  00531
   ADIV = (ATOP(IMAX) + ATOP(IMAX+1))/2.0                              DEGA  00532
   GO TO 31                                                            DEGA  00533
35 IF((ICNTD .EQ. 0) .AND.(ICNTR .EQ. 1))37, 40                        DEGA  00534
37 ICASE = 2                                                           DEGA  00535
   IF(XLP1 .LT. .25) 47, 46                                            DEGA  00536
47 IMAXP1 = IMAX + 1                                                   DEGA  00537
   DO 48 I=2, IMAXP1                                                   DEGA  00538
   IF(AROOT(1) .LT. ATOP(I)) 49, 48                                    DEGA  00539
49 IDIV = I-1                                                          DEGA  00540
   ADIV = AROOT(1)                                                     DEGA  00541
   GO TO 31                                                            DEGA  00542
48 CONTINUE                                                            DEGA  00543
   IDIV = IMAX                                                         DEGA  00544
   GO TO 38                                                            DEGA  00545
46 IDIV = IMAX                                                         DEGA  00546
   IF(AROOT(1) .LT. ATOP(IMAX))38, 39                                  DEGA  00547
38 ADIV = (ATOP(IMAX) + ATOP(IMAX+1))/2.0                              DEGA  00548
   GO TO 31                                                            DEGA  00549
39 ADIV = (AROOT(1) + ATOP(IMAX+1))/2.0                                DEGA  00550
   GO TO 31                                                            DEGA  00551
40 IF((ICNTD .EQ. 1) .AND.(ICNTR .EQ. 1))41, 42                        DEGA  00552
42 IERROR = 1                                                          DEGA  00553
   PRINT 1, ICNTD, ICNTR                                               DEGA  00554
 1 FORMAT(*  IERROR=1,   ICNTD =*, I2, *,  ICNTR =*, I2)               DEGA  00555
   RETURN                                                              DEGA  00556
41 ICASE = 3                                                           DEGA  00557
   IF(AROOT(1) .LT. ADIV) 31, 43                                       DEGA  00558
43 IERROR = 3                                                          DEGA  00559
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      PRINT 3, AROOT(1), ADIV                                           DEGA    00560
    3 FORMAT(*  IERROR=3, ICASE=3, AROOT(1).GE.ADIV, AROOT(1) =*,E20.10, DEGA    00561
     1       *, ADIV =*, E20.10)                                        DEGA    00562
      RETURN                                                            DEGA    00563
   31 IF(ISTOP .EQ. 1) RETURN                                           DEGA    00564
      IMAXB = IDIV    $   IMAXFP1 = IMAXF + 1                           DEGA    00565
      IMAXB = IMAX + 1 - IDIV    $   IMAXBP1 = IMAXB + 1                DEGA    00566
      DO 32 I=1, IMAXF                                                  DEGA    00567
      ATOPF(I) = ATOP(I)                                                DEGA    00568
      CF(1,I) = C(1,I)    $   CF(2,I) = C(2,I)                          DEGA    00569
   32 CF(3,I) = C(3,I)                                                  DEGA    00570
      ATOPF(IMAXFP1) = ADIV                                             DEGA    00571
      II = IMAX + 1    $   III = IMAX + 2                               DEGA    00572
      DO 33 I=1, IMAXB                                                  DEGA    00573
      III = III-1                                                       DEGA    00574
      IBKW = IMAXFP1 + I                                                DEGA    00575
      ATOPB(IBKW) = ATOP(III)                                           DEGA    00576
      II = II - 1                                                       DEGA    00577
      CB(1,IBKW) = C(1,II)    $   CB(2,IBKW) = C(2,II)                  DEGA    00578
   33 CB(3,IBKW) = C(3,II)                                              DEGA    00579
      IBKW = IMAXFP1 + IMAXBP1                                          DEGA    00580
      ATOPB(IBKW) = ADIV                                                DEGA    00581
      RETURN                                                            DEGA    00582
      END                                                               DEGA    00583
      SUBROUTINE BIVOM(XLAMBDA, XLLP1, I, NOROOTS, ROOT1, ROOT2,        DEGA    00584
     1       NODIV, DIV1)                                               DEGA    00585
      COMMON/AIMAX/  AF(51,402), JMAXF(402), IMAX,                      DEGA    00586
     1      IMAXF, IMAXFP1, IMAXB, IMAXBP1, C(3,400),                  DEGA    00587
     2      CF(3,402), ATOP(401), ATOPF(402)                           DEGA    00588
      DIMENSION AB(51,402), JMAXB(402), CB(3,402), ATOPB(402)           DEGA    00589
      EQUIVALENCE(AF(1), AB(1)), (JMAXF(1), JMAXB(1)),                  DEGA    00590
     1      (CF(1), CB(1)), (ATOPF(1), ATOPB(1))                       DEGA    00591
      B1 = -(2.0*C(3,I) + XLLP1)                                        DEGA    00592
      B2 = -2.0*C(2,I)                                                  DEGA    00593
      B3 = XLAMBDA - 2.0*C(1,I)                                         DEGA    00594
      ARSB1 = ABS(B1)                                                   DEGA    00595
      IF(ARSB1 .LT. ABS(B2)*1.0E-12) 1, 2                               DEGA    00596
    2 IF(ARSB1 .LT. ABS(B3)*1.0E-12) 1, 3                               DEGA    00597
    1 ROOT1 = -B2/B3                                                    DEGA    00598
      NOROOTS = 1                                                       DEGA    00599
      NODIV = 0                                                         DEGA    00600
      GO TO 6                                                           DEGA    00601
    3 RAD = B2*B2 - 4.0*B1*B3                                           DEGA    00602
      TWOB1 = 2.0*B1                                                    DEGA    00603
      NODIV = 1                                                         DEGA    00604
      DIV1 = -TWOB1/B2                                                  DEGA    00605
      IF(RAD .LT. 0.0) 4, 5                                             DEGA    00606
    4 NOROOTS = 0                                                       DEGA    00607
      GO TO 6                                                           DEGA    00608
    5 NOROOTS = 2                                                       DEGA    00609
      RAD = SQRT(RAD)                                                   DEGA    00610
      T1 = ABS(TWOB1)                                                   DEGA    00611
      T2 = ABS(B2 + RAD)                                                DEGA    00612
      IF(T2 .LT. T1*1.0E-20) 7, 8                                       DEGA    00613
    9 FORMAT( I5, 3E20.10, *  XXXXX*)                                   DEGA    00614
    7 I1 = 1                                                            DEGA    00615
      PRINT 9, I1, TWOB1, B2, RAD                                       DEGA    00616
      ROOT1 = 1.0E100                                                   DEGA    00617
      GO TO 10                                                          DEGA    00618
    8 CONTINUE                                                          DEGA    00619
      ROOT1 = -TWOB1/(B2 + RAD)                                         DEGA    00620
   10 T1 = ABS(TWOB1)                                                   DEGA    00621
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      T2 = ABS(-B2 + RAD)                                                DEGA    00622
      IF(T2 .LT. T1*1.0E-20) 11, 12                                      DEGA    00623
   11 I1 = 2                                                             DEGA    00624
      PRINT 9, I1, TWOB1, B2, RAD                                        DEGA    00625
      ROOT2 = 1.0E100                                                    DEGA    00626
      GO TO 6                                                            DEGA    00627
   12 CONTINUE                                                           DEGA    00628
      ROOT2 = TWOB1/(-B2 + RAD)                                          DEGA    00629
    6 RETURN                                                             DEGA    00630
      END                                                                DEGA    00631
      SUBROUTINE REGULA(XLAMB0,XLAMB1,FB0,FB1,CAPLAMB,MAXITER,XL,IERROR) DEGA    00632
      COMMON/AIMAX/  AF(51,402), JMAXF(402), IMAX,                       DEGA    00633
     1      IMAXF, IMAXFP1, IMAXB, IMAXBP1, C(3,400),                   DEGA    00634
     2      CF(3,402), ATOP(401), ATOPF(402)                            DEGA    00635
      DIMENSION AB(51,402), JMAXB(402), CB(3,402), ATOPB(402)            DEGA    00636
      EQUIVALENCE(AF(1), AB(1)), (JMAXF(1), JMAXB(1)),                   DEGA    00637
     1      (CF(1), CB(1)), (ATOPF(1), ATOPB(1))                        DEGA    00638
      COMMON/EPS/ EPSCONV, FBMAX                                         DEGA    00639
    1 FORMAT(2E24.14, 4E20.10)                                           DEGA    00640
      IERROR = 0                                                         DEGA    00641
      DO 14 ITER = 1, MAXITER                                            DEGA    00642
      IF(FB1 .EQ. FB0) 20, 21                                            DEGA    00643
   20 IBKW = IMAXFP1 + IMAXBP1                                           DEGA    00644
      AFAC = AB(1,IBKW)/AF(1,IMAXFP1)*AF(2,IMAXFP1)                      DEGA    00645
      FBOUNDC = FBOJND/ABS(AFAC)                                         DEGA    00646
      CAPLAMB = .5*(XLAMB1 + XLAMB0)                                     DEGA    00647
      PRINT 22                                                           DEGA    00648
      PRINT 22                                                           DEGA    00649
      PRINT 23, FBOUNDC, EPSCONV                                         DEGA    00650
      PRINT 24, CAPLAMB, XLAMB1, XLAMB0                                  DEGA    00651
      PRINT 22                                                           DEGA    00652
      PRINT 22                                                           DEGA    00653
      RETURN                                                             DEGA    00654
   22 FORMAT(* XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX*) DEGA    00655
   23 FORMAT(* FB1=FB0,   FBOUNDC = *,E20.10,*     EPSCONV =*,E20.10)    DEGA    00656
   24 FORMAT(* CAPLAMB =*,E24.14,4H = (,E24.14,2H +,E24.14,4H )/2)       DEGA    00657
   21 ONEGAMA = (XLAMB1 - XLAMB0)/(FB1 - FB0)                            DEGA    00658
      XLAMB2 = XLAMB1 - ONEGAMA*FB1                                      DEGA    00659
      IF(XLAMB2.EQ.XLAMB1.OR.XLAMB2.EQ.XLAMB0) GO TO 15                  DEGA    00660
      CALL TAYLORF(XL, XLAMB2, IERROR, AF, JMAXF, IMAXF, CF, ATOPF)      DEGA    00661
      IF(IERROR .NE. 0) RETURN                                           DEGA    00662
      IBKW = IMAXFP1 + 1                                                 DEGA    00663
      CALL TAYLORB(XL, XLAMB2, IERROR, AB(1,IBKW),                       DEGA    00664
     1      JMAXB(IBKW), IMAXB, CB(1,IBKW), ATOPB(IBKW))                DEGA    00665
      IF(IERROR .NE. 0) RETURN                                           DEGA    00666
      CALL BOUNDRY(IFCONV, FBOUND)                                       DEGA    00667
      IF(IFCONV .EQ. 1) 15, 16                                           DEGA    00668
   15 CAPLAMB = XLAMB2   $   RETURN                                      DEGA    00669
   16 IF(ABS(FBOUND) .GT. FBMAX) 17, 19                                  DEGA    00670
   17 IERROR = 7                                                         DEGA    00671
      PRINT 7                                                            DEGA    00672
    7 FORMAT(*  IERROR = 7, FBOUND .GT. FBMAX*)                          DEGA    00673
      RETURN                                                             DEGA    00674
   19 XLAMB0 = XLAMB1   $   XLAMB1 = XLAMB2                              DEGA    00675
      FB0 = FB1                                                          DEGA    00676
   14 FB1 = FBOUND                                                       DEGA    00677
      IERROR = 8                                                         DEGA    00678
      PRINT 8, MAXITER                                                   DEGA    00679
    8 FORMAT (*  PROBLEM DOES NOT CONVERGE WITHIN*,I5,* ITERATIONS*)     DEGA    00680
      RETURN                                                             DEGA    00681
      END                                                                DEGA    00682
      SUBROUTINE TAYLORF(XL, ALPHLAM, IERROR, A, JMAX, IMAX, C, ATOP)    DEGA    00683
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      DIMENSION A(51,1), JMAX(1), C(3,1), ATOP(1)                       DEGA    00684
      COMMON/METHODS/METHOD, TEMPLAM, CAPF, CAPFP, THETA, THETAP        DEGA    00685
      COMMON/EPS/EPSCONV, FBMAX, EM16                                   DEGA    00686
      GO TO (60, 61), METHOD                                            DEGA    00687
   60 XLAMBDA = ALPHLAM                                                 DEGA    00688
      GO TO 62                                                          DEGA    00689
   61 ALPHA = ALPHLAM                                                   DEGA    00690
      XLAMBDA = TEMPLAM                                                 DEGA    00691
   62 CONTINUE                                                          DEGA    00692
      DO 30 I=1, IMAX                                                   DEGA    00693
   30 JMAX(I) = 0                                                       DEGA    00694
      IERROR = 0                                                        DEGA    00695
      D = ATOP(2)                                                       DEGA    00696
C*********************************************************************  DEGA    00697
C            LEFT BOUNDARY CONDITIONS.  THESE ARE ONLY TRUE FOR         DEGA    00698
C     PHI(0)=0 WHERE PHI(R) IS THE EIGENFUNCTION.                       DEGA    00699
C*********************************************************************  DEGA    00700
      A(1,1) = 0.0                                                      DEGA    00701
      A(2,1) = 1.0                                                      DEGA    00702
C*********************************************************************  DEGA    00703
      CALL TAYLOR1(A(1,1), JMAX(1), D, XLAMBDA,                         DEGA    00704
     1     XL, C(1,1), C(2,1), EM16, IERROR)                            DEGA    00705
      IF(IERROR .EQ. 9) RETURN                                          DEGA    00706
      RP = ATOP(2)                                                      DEGA    00707
      CALL POLY0P(A(1,1), JMAX(1), RR, P)                               DEGA    00708
      A(1,2)= P*RR**XL                                                  DEGA    00709
      CALL POLY1P(A(1,1), JMAX(1), RR, DERIVP)                          DEGA    00710
      A(2,2) = (DERIVP*RR + P*XL)*RR**(XL-1.0)                          DEGA    00711
      IF(IMAX .EQ. 1) GO TO 37                                          DEGA    00712
      IBOT = 2                                                          DEGA    00713
      GO TO 58                                                          DEGA    00714
      ENTRY TAYLORB                                                     DEGA    00715
      DO 54 I=1, IMAX                                                   DEGA    00716
   54 JMAX(I) = 0                                                       DEGA    00717
      GO TO (65, 66), METHOD                                            DEGA    00718
   65 XLAMBDA = ALPHLAM                                                 DEGA    00719
      GO TO 67                                                          DEGA    00720
   66 ALPHA = ALPHLAM                                                   DEGA    00721
      XLAMBDA = TEMPLAM                                                 DEGA    00722
   67 CONTINUE                                                          DEGA    00723
      IERROR = 0                                                        DEGA    00724
      IBOT = 1                                                          DEGA    00725
*********************************************************************   DEGA    00726
            RIGHT BOUNDARY ,R.B. CONDITIONS.  HERE A(1,1) IS AN         DEGA    00727
     ARBITRARY CONSTANT, THE MAGNITUDE OF PHI(R.B.).  A(2,1) IS         DEGA    00728
     THE DERIVATIVE OF PHI(R.B.) NORMILIZED TO A(1,1).                  DEGA    00729
*********************************************************************   DEGA    00730
      GO TO (63, 64) , METHOD                                           DEGA    00731
   63 CONTINUE                                                          DEGA    00732
      A(1,1) = 1.0E-140                                                 DEGA    00733
      A(2,1) = -SQRT(ABS(XLAMBDA))*A(1,1)                               DEGA    00734
      GO TO 58                                                          DEGA    00735
   64 THETA1 = THETA + ALPHA                                            DEGA    00736
      COSTHE1 = COS(THETA1)                                             DEGA    00737
      A(1,1) = CAPF*COSTHE1                                             DEGA    00738
      A(2,1) = CAPFP*COSTHE1 - CAPF*THETAP*SIN(THETA1)                  DEGA    00739
*********************************************************************   DEGA    00740
   58 XLL = XL*(XL+1.0)                                                 DEGA    00741
      DO 25 I=IBOT, IMAX                                                DEGA    00742
      D = ATOP(I+1) - ATOP(I)                                           DEGA    00743
      CALL TAYLORS(A(1,I), JMAX(I), ATOP(I), D, XLAMBDA,                DEGA    00744
     1     XLL, C(1,I), C(2,I), C(3,I), EM16, IERROR)                   DEGA    00745
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      IF(IERROR .EQ. 10) RETURN                                          DEGA    00746
      CALL POLY0P(A(1,I), JMAX(I), D, A(1,I+1))                          DEGA    00747
      CALL POLY1P(A(1,I), JMAX(I), D, A(2,I+1))                          DEGA    00748
   25 CONTINUE                                                           DEGA    00749
   37 RETURN                                                             DEGA    00750
      END                                                                DEGA    00751
      SUBROUTINE BOUNDRY(IFCONV, FBOUND)                                 DEGA    00752
      COMMON/AIMAX/  AF(51,402), JMAXF(402), IMAX,                       DEGA    00753
     1      IMAXF, IMAXFP1, IMAXB, IMAXBP1, C(3,400),                   DEGA    00754
     2      CF(3,402), ATOP(401), ATOPF(402)                            DEGA    00755
      DIMENSION AB(51,402), JMAXB(402), CB(3,402), ATOPB(402)            DEGA    00756
      EQUIVALENCE(AF(1), AB(1)), (JMAXF(1), JMAXB(1)),                   DEGA    00757
     1      (CF(1), CB(1)), (ATOPF(1), ATOPB(1))                        DEGA    00758
      COMMON/EPS/EPSCONV, FBMAX                                          DEGA    00759
C          YOU ARE LIVING DANGERDUSLY IF YOU LET IMAXF=1.  THIS MAY RESU DEGA    00760
C     IN AN UNDETECTED DIVISION BY ZERO OR AN UNDETECTED LOSS OF ACCURAC DEGA    00761
      IF(IMAXF .EQ. 1) 1, 2                                              DEGA    00762
    2 IF(ABS(AF(1,IMAXFP1)) .LT. ABS(AF(1,IMAXF))*1.0E-4) 3, 1           DEGA    00763
    1 IBKW = IMAXFP1 + IMAXB                                             DEGA    00764
      IBKWP1 = IBKW + 1                                                  DEGA    00765
      IF(ABS(AB(1,IBKWP1)) .LT. ABS(AB(1,IBKW))*1.0E-4)3,5               DEGA    00766
    3 PRINT 4                                                            DEGA    00767
    4 FORMAT(*     IN DANGER OF DIVIDING BY ZERO, OR ATLEAST LOOSING ACCU DEGA    00768
     1RACY,  *)                                                          DEGA    00769
    5 IBKW = IMAXFP1 + IMAXBP1                                           DEGA    00770
      FAC = AB(1,IBKW)/AF(1,IMAXFP1)                                     DEGA    00771
      AFAC = FAC*AF(2,IMAXFP1)                                           DEGA    00772
      FBOUND = AFAC - AB(2,IBKW)                                         DEGA    00773
      EPSC = ABS(AFAC)*EPSCONV                                           DEGA    00774
      IF(ABS(FBOUND) .LT. EPSC) 6, 7                                     DEGA    00775
    6 IFCONV = 1    $   GO TO 8                                          DEGA    00776
    7 IFCONV = 0                                                         DEGA    00777
    8 RETURN                                                             DEGA    00778
      END                                                                DEGA    00779
      SUBROUTINE STURMSQ(A1, JMAX1, A2, D, IV2, IERROR)                  DEGA    00780
      DIMENSION A1(2), A2(2), CPI( 51), CPIP1( 51)                       DEGA    00781
      COMMON/SCRATCH/SCRATCH(604)                                        DEGA    00782
      EQUIVALENCE(SCRATCH(1), CPI(1)), (SCRATCH(52), CPIP1(1))           DEGA    00783
      IERROR = 0                                                         DEGA    00784
      JMAXI = JMAX1                                                      DEGA    00785
      IF(D .LT. 0.0) 11, 12                                              DEGA    00786
   11 ISIGN = -1                                                         DEGA    00787
      GO TO 13                                                           DEGA    00788
   12 ISIGN = 1                                                          DEGA    00789
   13 IV2 = 0                                                            DEGA    00790
      J1 = JMAXI+1                                                       DEGA    00791
      DO 14 J=1, JMAXI                                                   DEGA    00792
      J1 = J1 - 1                                                        DEGA    00793
      CPI(J) = A1(J1)                                                    DEGA    00794
   14 CPIP1(J) = (J1-1)*CPI(J)                                           DEGA    00795
      JMAXIP1 = JMAXI-1                                                  DEGA    00796
      P0 = CPI(JMAXI)                                                    DEGA    00797
      PD = A2(1)                                                         DEGA    00798
      P10 = CPIP1(JMAXIP1)                                               DEGA    00799
      P1D = A2(2)                                                        DEGA    00800
      IF(P10 .EQ. 0.0) GO TO 15                                          DEGA    00801
      IF(P0*P10 .LT. 0.0) 15, 16                                         DEGA    00802
   15 IV2 = IV2 + 1                                                      DEGA    00803
   16 IF(P1D .EQ. 0.0) GO TO 17                                          DEGA    00804
      IF(PD*P1D .LT. 0.0) 17, 18                                         DEGA    00805
   17 IV2 = IV2 - 1                                                      DEGA    00806
   18 FAC = CPI(1)/CPIP1(1)                                              DEGA    00807
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      ZERO = ABS(CPI(1))*1.0E-11                                        DEGA   00808
      DO 19 J1=2, JMAXIP1                                               DEGA   00809
   19 CPI(J1) = CPI(J1) - FAC*CPIP1(J1)                                 DEGA   00810
      NOZERO = 1                                                        DEGA   00811
      DO 20 J=2, JMAXI                                                  DEGA   00812
      IF(ABS(CPI(J)) .LT. ZERO) 20, 21                                  DEGA   00813
   20 NOZERO = NOZERO + 1                                               DEGA   00814
      GO TO 99                                                          DEGA   00815
   21 JMAXI = JMAXI - NOZERO                                            DEGA   00816
      DO 22 J=1, JMAXI                                                  DEGA   00817
   22 CPI(J) = CPI(J+NOZERO)                                            DEGA   00818
      IF(JMAXI .LT. JMAXIP1) 23, 18                                     DEGA   00819
   23 JMIN = JMAXI + 1                                                  DEGA   00820
      DO 24 J=JMIN, JMAXIP1                                             DEGA   00821
   24 CPI(J) = 0.0                                                      DEGA   00822
      DO 25 J=1, JMAXIP1                                                DEGA   00823
      TEMP = CPI(J)                                                     DEGA   00824
      CPI(J) = CPIP1(J)                                                 DEGA   00825
   25 CPIP1(J) = -TEMP                                                  DEGA   00826
      JTEMP = JMAXI                                                     DEGA   00827
      JMAXI = JMAXIP1                                                   DEGA   00828
      JMAXIP1 = JTEMP                                                   DEGA   00829
      P0 = P10                                                          DEGA   00830
      PD = P1D                                                          DEGA   00831
      P10 = CPIP1(JMAXIP1)                                              DEGA   00832
      P1D = CPIP1(1)                                                    DEGA   00833
      IF(JMAXIP1 .EQ. 1) 28, 26                                         DEGA   00834
   26 DO 27 J1=2, JMAXIP1                                               DEGA   00835
   27 P1D = P1D*D + CPIP1(J1)                                           DEGA   00836
   28 IF(P10 .EQ. 0.0) GO TO 29                                         DEGA   00837
      IF(P0*P10 .LT. 0.0) 29, 30                                        DEGA   00838
   29 IV2 = IV2 + 1                                                     DEGA   00839
   30 IF(P1D .EQ. 0.0) GO TO 31                                         DEGA   00840
      IF(P0*P1D .LT. 0.0) 31, 35                                        DEGA   00841
   31 IV2 = IV2 - 1                                                     DEGA   00842
   35 IF(JMAXIP1 .EQ. 1) 99, 18                                         DEGA   00843
   99 IV2 = ISIGN*IV2                                                   DEGA   00844
      IF(IV2 .LT. 0) 32, 34                                             DEGA   00845
   32 IERROR = 5                                                        DEGA   00846
      PRINT 33                                                          DEGA   00847
   33 FORMAT( *    IV2 IS LESS THAN 0,  * )                             DEGA   00848
   34 RETURN                                                            DEGA   00849
      END                                                               DEGA   00850
      SUBROUTINE YYY(RMIN, RMAX, DRMIN, DVMAX, ATOPFAC, I2, IERROR,     DEGA   00851
     1     XLAMWKB, LWKB, KWKB, ZZZFAC)                                 DEGA   00852
      DIMENSION XLAMWKB(1), LWKB(1)                                     DEGA   00853
      COMMON/AIMAX/  AF(51,402), JMAXF(402), IMAX,                      DEGA   00854
     1     IMAXF, IMAXFP1, IMAXB, IMAXBP1, C(3,400),                    DEGA   00855
     2     CF(3,402), ATOP(401), ATOPF(402)                             DEGA   00856
      DIMENSION AB(51,402), JMAXB(402), CB(3,402), ATOPB(402)           DEGA   00857
      EQUIVALENCE(AF(1), AB(1)), (JMAXF(1), JMAXB(1)),                  DEGA   00858
     1     (CF(1), CB(1)), (ATOPF(1), ATOPB(1))                         DEGA   00859
      DIMENSION A(3, 4)                                                 DEGA   00860
      DIMENSION XLAMDIM(10), XLDIM(10)                                  DEGA   00861
      COMMON/CB3/ Z, ZM1, RR2, RR, A0                                   DEGA   00862
    2 FORMAT(/////)                                                     DEGA   00863
      IERROR = 0                                                        DEGA   00864
      XLAMMAX = 0.0                                                     DEGA   00865
      LMAX = 0                                                          DEGA   00866
      DO 65 I=1, 10                                                     DEGA   00867
      XLAMDIM(I) = 0.0                                                  DEGA   00868
   65 XLDIM(I) = I*(I-1)                                                DEGA   00869
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      DO 66 I=1, KWKB                                                    DEGA  00870
      IF(XLAMWKB(I) .LT. XLAMMAX) XLAMMAX = XLAMWKB(I)                   DEGA  00871
      IF(LWKB(I) .GT. LMAX) LMAX = LWKB(I)                               DEGA  00872
      J = LWKB(I) + 1                                                    DEGA  00873
      IF(XLAMWKB(I) .LT. XLAMDIM(J)) XLAMDIM(J) = XLAMWKB(I)             DEGA  00874
   66 CONTINUE                                                           DEGA  00875
      LMAXP1 = LMAX + 1                                                  DEGA  00876
      XLDIM(LMAX + 2) = LMAXP1*(LMAX + 2)                                DEGA  00877
      LMAX = LMAX + 3                                                    DEGA  00878
      XLAMDIM(LMAX) = ZZZFAC*ABS(XLAMMAX)                                DEGA  00879
      XLDIM(LMAX) = 0.0                                                  DEGA  00880
   68 FORMAT(2E20.10)                                                    DEGA  00881
      DO 69 L=1, LMAX                                                    DEGA  00882
   69 PRINT 68, XLAMDIM(L), XLDIM(L)                                     DEGA  00883
      IF(RR2 .GT. 0.0) GO TO 62                                          DEGA  00884
      IMAX = 1                                                           DEGA  00885
      DR = ABS(RR2)                                                      DEGA  00886
      ATOP(2) = DR                                                       DEGA  00887
      C(1,1) = 0.0                                                       DEGA  00888
      C(2,1)= -1.0                                                       DEGA  00889
      C(3,1) = 0.0                                                       DEGA  00890
   63 DR = ATOPFAC*ATOP(IMAX+1)                                          DEGA  00891
      IF(DR .GT. DRMAX) DR = DRMAX                                       DEGA  00892
      IMAX = IMAX + 1                                                    DEGA  00893
      ATOP(IMAX+1) = ATOP(IMAX) + DR                                     DEGA  00894
      C(1,IMAX) = 0.0                                                    DEGA  00895
      C(2,IMAX) = -1.0                                                   DEGA  00896
      C(3,IMAX) = 0.0                                                    DEGA  00897
      IF(ATOP(IMAX+1) .GE. RMAX) 64, 63                                  DEGA  00898
   64 ATOP(IMAX+1) = RMAX                                                DEGA  00899
      I2 = IMAX                                                          DEGA  00900
      RETURN                                                             DEGA  00901
   62 IMAX = 0                                                           DEGA  00902
      I2 = 0                                                             DEGA  00903
      IREG1 = 2                                                          DEGA  00904
      IREG2 = 1                                                          DEGA  00905
      OPAF = 1.0 + ATOPFAC                                               DEGA  00906
      RBOT = RMIN                                                        DEGA  00907
      IF(RR2 .GE. RMAX) 50, 51                                           DEGA  00908
   50 RTOP = RMAX                                                        DEGA  00909
      IFINISH = 1                                                        DEGA  00910
      GO TO 37                                                           DEGA  00911
   51 RTOP = RR2                                                         DEGA  00912
      IFINISH = 0                                                        DEGA  00913
   37 DRTB = RTOP - RBOT                                                 DEGA  00914
      R1 = .3*DRTB                                                       DEGA  00915
      R2 = .6*DRTB                                                       DEGA  00916
      CALL DRMAXSB(DRMAX, R1, R2, XLAMDIM, XLDIM, LMAX)                  DEGA  00917
      IF(DRTB .LE. DRMAX) GO TO 21                                       DEGA  00918
      RTOP = RBOT + DRMAX                                                DEGA  00919
      IFINISH = 0                                                        DEGA  00920
   21 IF(IREG2 .EQ. 3) 60, 59                                            DEGA  00921
   60 IF(I2 .EQ. 0) I2 = IMAX                                            DEGA  00922
      IMAX = IMAX + 1                                                    DEGA  00923
      C(1, IMAX ) = 0.0                                                  DEGA  00924
      C(2,IMAX) = -1.0                                                   DEGA  00925
      C(3,IMAX) = 0.0                                                    DEGA  00926
      GO TO 61                                                           DEGA  00927
   59 DR = RTOP - RBOT                                                   DEGA  00928
      DDR = DR/9.0                                                       DEGA  00929
      IF(DR .LT. DRMIN) 22, 23                                           DEGA  00930
   22 PRINT 3                                                            DEGA  00931
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    3 FORMAT(* AN INTERVAL ALONG THE R-AXIS GOT TOO SMALL.*)                    DEGA   00932
      PRINT 4, DR, DRMIN                                                        DEGA   00933
    4 FORMAT(* DR =*,E20.10,*,*,10X,*DRMIN =*,E20.10)                           DEGA   00934
      IERROR = 21                                                               DEGA   00935
    6 FORMAT (*  IERROR =*, I5)                                                 DEGA   00936
      PRINT 6, IERROR                                                           DEGA   00937
      PRINT 2                                                                   DEGA   00938
      GO TO 99                                                                  DEGA   00939
   23 R1 = RBOT    $    R3 = RTOP    $    R2 = (R1 + R3)/2.0                    DEGA   00940
      IF(R1 .LT. 1.0E-200) 33, 34                                               DEGA   00941
   33 A(3,4) = 0.0    $    GO TO 35                                             DEGA   00942
   34 A(3,4) = R1*R1*V(R1)                                                      DEGA   00943
   35 A(2,4) = R2*R2*V(R2)                                                      DEGA   00944
      A(1,4) = R3*R3*V(R3)                                                      DEGA   00945
      A(1,1) = R3*R3    $    A(2,1) = R2*R2    $    A(3,1) = R1*R1             DEGA   00946
      A(1,2) = R3    $    A(2,2) = R2    $    A(3,2) = R1                      DEGA   00947
      A(1,3) = 1.0    $    A(2,3) = 1.0    $    A(3,3) = 1.0                   DEGA   00948
      CALL MATPAC(-1, A, 3, 1, DET, 0.0, IF SING)                               DEGA   00949
      CHAT1 = A(1,4)    $    CHAT2 = A(2,4)    $    CHAT3 = A(3,4)             DEGA   00950
C*********************************************************************        DEGA   00951
C*********************************************************************        DEGA   00952
C       R=0 IS NEVER USED.  WE WILL ONLY BE WORKING WITH VS                     DEGA   00953
C     WHERE V(R) .NE. 0 FOR R .NE. 0.                                           DEGA   00954
C*********************************************************************        DEGA   00955
      R = RBOT                                                                  DEGA   00956
      DO 24 J=1, 8                                                              DEGA   00957
      R = R + DDR                                                               DEGA   00958
      VR = V(R)                                                                 DEGA   00959
      P = CHAT1 + CHAT2/R + CHAT3/(R*R)                                         DEGA   00960
      XJ = J                                                                    DEGA   00961
C   1 FORMAT(4E20.10)                                                           DEGA   00962
C     PRINT 1, XJ, R, VR, P                                                     DEGA   00963
      IF(ABS((VR - P)/VR) .LT. DVMAX) 24, 25                                    DEGA   00964
   24 CONTINUE                                                                  DEGA   00965
C*********************************************************************        DEGA   00966
      IREG2 = IREG1                                                             DEGA   00967
      IMAX = IMAX + 1                                                           DEGA   00968
      C(1,IMAX) = CHAT1    $    C(2,IMAX) = CHAT2    $    C(3,IMAX) = CHAT3    DEGA   00969
   61 ATOP(IMAX + 1) = RTOP                                                     DEGA   00970
      IF (IFINISH .EQ. 1) 99, 31                                                DEGA   00971
   31 IF(IMAX .LT. 400) 28, 32                                                  DEGA   00972
   32 PRINT 7                                                                   DEGA   00973
    7 FORMAT(* THE MAXIMUM NUMBER OF INTERVALS WILL NOT SPAN (RMIN, RMAX       DEGA   00974
     11.*)                                                                      DEGA   00975
      IERROR = 22                                                               DEGA   00976
      PRINT 6, IERROR                                                           DEGA   00977
      PRINT 2                                                                   DEGA   00978
      GO TO 99                                                                  DEGA   00979
   28 RBOT = RTOP                                                               DEGA   00980
      IF(IREG1 .EQ. 3) 58, 57                                                   DEGA   00981
   58 DRTOP = ATOPFAC*RTOP                                                      DEGA   00982
      R1 = RTOP                                                                 DEGA   00983
      R2 = RTOP + .5*(RTOP - ATOP(IMAX))                                        DEGA   00984
      CALL DRMAXSB(DRMAX, R1, R2, XLAMDIM, XLDIM, LMAX)                         DEGA   00985
      IF(DRTOP .GT. DRMAX) DRTOP = DRMAX                                        DEGA   00986
      RTOP = RTOP + DRTOP                                                       DEGA   00987
      GO TO 52                                                                  DEGA   00988
C*********************************************************************        DEGA   00989
C*********************************************************************        DEGA   00990
C          THIS CARD DETERMINES MAXIMUM INTERVAL LENGTH.                        DEGA   00991
C*********************************************************************        DEGA   00992
   57 IF(IMAX .EQ. 1) 40, 41                                                    DEGA   00993
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   40 DR1 = DR                                                                  DEGA    00994
      DR2 = DR                                                                  DEGA    00995
      DR3 = DR                                                                  DEGA    00996
      DR4 = DR                                                                  DEGA    00997
      DRTMP = DR                                                                DEGA    00998
      GO TO 42                                                                  DEGA    00999
   41 DR5 = DR4                                                                 DEGA    01000
      DR4 = DR3                                                                 DEGA    01001
      DR3 = DR2                                                                 DEGA    01002
      DR2= DR1                                                                  DEGA    01003
      DR1 = DR                                                                  DEGA    01004
      DRTMP = (DR1 + DR2 + DR3 + DR4 + DR5)/5.0                                 DEGA    01005
   42 IF(2.0*DRTMP .LT. ATOPFAC*RTOP) 46, 47                                    DEGA    01006
   46 RTOP = RTOP + 2.0*DRTMP                                                   DEGA    01007
      GO TO 48                                                                  DEGA    01008
   47 RTOP = OPAF*RTOP                                                          DEGA    01009
   48 R1 = RBOT                                                                 DEGA    01010
      R2 = RBOT + .5*(RBOT - ATOP(IMAX))                                        DEGA    01011
      CALL DRMAXSB(DRMAX, R1, R2, XLAMDIM, XLDIM, LMAX)                         DEGA    01012
      IF(RTOP - RBOT .GT. DRMAX) RTOP = RBOT + DRMAX                            DEGA    01013
      GO TO (54, 53) , IREG1                                                    DEGA    01014
   54 IF(RTOP .GE. RR2) 55, 52                                                  DEGA    01015
   55 RTOP = RR2                                                                DEGA    01016
      IREG1 = 2                                                                 DEGA    01017
      GO TO 52                                                                  DEGA    01018
   53 IF(RTOP .GE. RR) 56, 52                                                   DEGA    01019
   56 RTOP = RR                                                                 DEGA    01020
      IREG1 = 3                                                                 DEGA    01021
C*********************************************************************         DEGA    01022
   52 IF(RMAX .LE. RTOP) 29, 26                                                 DEGA    01023
   29 RTOP = RMAX    $    IFINISH = 1                                           DEGA    01024
      GO TO 21                                                                  DEGA    01025
   25 IREG1 = IREG2                                                             DEGA    01026
      IF(IMAX .EQ. 0) 43, 44                                                    DEGA    01027
   44 IF( DR .LT. .5*DRTMP) 43, 45                                              DEGA    01028
   43 RTOP = R2                                                                 DEGA    01029
      GO TO 26                                                                  DEGA    01030
   45 RTOP = RBOT + .75*DR                                                      DEGA    01031
   26 IFINISH = 0                                                               DEGA    01032
      GO TO 21                                                                  DEGA    01033
   99 IF(I2 .EQ. 0) I2 = IMAX                                                   DEGA    01034
      RETURN                                                                    DEGA    01035
      END                                                                       DEGA    01036
      SUBROUTINE DRMAXSB(DRMAX, R1, R2, XLAMDIM, XLDIM, LMAX)                   DEGA    01037
      DIMENSION XLAMDIM(1), XLDIM(1)                                            DEGA    01038
      SMALLK = 0.0                                                              DEGA    01039
      R12 = 1.0/R1**2                                                           DEGA    01040
      R22 = 1.0/R2**2                                                           DEGA    01041
      TVR1 = 2.0*V(R1)                                                          DEGA    01042
      TVR2 = 2.0*V(R2)                                                          DEGA    01043
      DO 70 L=1, LMAX                                                           DEGA    01044
      SK = ABS(XLAMDIM(L) - TVR1 - XLDIM(L)*R12)                                DEGA    01045
      IF(SK .GT. SMALLK) SMALLK = SK                                            DEGA    01046
      SK = ABS(XLAMDIM(L) - TVR2 - XLDIM(L)*R22)                                DEGA    01047
      IF(SK .GT. SMALLK) SMALLK = SK                                            DEGA    01048
   70 CONTINUE                                                                  DEGA    01049
      DRMAX = 6.28/SQRT(SMALLK)                                                 DEGA    01050
      RETURN                                                                    DEGA    01051
      END                                                                       DEGA    01052
      FUNCTION V1(R)                                                            DEGA    01053
      COMMON/CB3/ Z, ZM1, RR2, RR, A0                                           DEGA    01054
      FNZZ = 1.0/(1.0 + A0*RR2)                                                 DEGA    01055
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      FNZ =  FNZZ**2*(2.0*A0*RR2*FNZZ + 1.0)*ZM1                        DEGA  01056
      A1 = RR/RR2*(ZM1/FNZ*FNZZ**2 - 1.0) + .5                          DEGA  01057
      VV = ZM1/RR                                                       DEGA  01058
      A0RR = A0*RR                                                      DEGA  01059
      FNZSRRM = -FNZ/RR                                                 DEGA  01060
      ENTRY V                                                           DEGA  01061
      IF(R .GT. RR) GO TO 3                                             DEGA  01062
      X1 = R/RR                                                         DEGA  01063
      IF(R .GT. RR2) GO TO 2                                            DEGA  01064
      V1 = VV/(X1*(1.0 + A0RR*X1)**2)                                   DEGA  01065
      V1 = -V1 + FNZSRRM*(X1**2/2.0 - A1) - 1.0/R                       DEGA  01066
      RETURN                                                            DEGA  01067
    2 V1 = FNZSRRM*(1.0/X1 + X1**2/2.0 - 1.5) - 1.0/R                   DEGA  01068
      RETURN                                                            DEGA  01069
    3 V1 = -1.0/R                                                       DEGA  01070
      RETURN                                                            DEGA  01071
      END                                                               DEGA  01072
      SUBROUTINE MATPAC (IJOB, A, N, M, DET, EP, IF SING)               DEGA  01073
      DIMENSION A(3, 4)                                                 DEGA  01074
      IF SING = 0                                                       DEGA  01075
      DET = 1.                                                          DEGA  01076
      NP1 = N+1                                                         DEGA  01077
      NPM = N+M                                                         DEGA  01078
      NM1 = N-1                                                         DEGA  01079
      IF(IJOB) 2, 1, 2                                                  DEGA  01080
    1 DO 3 I=1, N                                                       DEGA  01081
      NPI = N+I                                                         DEGA  01082
      A(I,NPI) = 1.                                                     DEGA  01083
      IP1 = I+1                                                         DEGA  01084
      IF(N - IP1) 2, 19, 19                                             DEGA  01085
   19 DO 3 J=IP1, N                                                     DEGA  01086
      NPJ = N+J                                                         DEGA  01087
      A(I, NPJ) = 0.                                                    DEGA  01088
    3 A(J, NPI) = 0.                                                    DEGA  01089
    2 DO 4 J=1, NM1                                                     DEGA  01090
      C =  ABS(A(J,J))                                                  DEGA  01091
      JP1 = J+1                                                         DEGA  01092
      DO 5 I=JP1, N                                                     DEGA  01093
      D =  ABS(A(I,J))                                                  DEGA  01094
      IF(C-D) 6,5,5                                                     DEGA  01095
    6 DET = -DET                                                        DEGA  01096
      DO 7 K=J, NPM                                                     DEGA  01097
      B = A(I,K)                                                        DEGA  01098
      A(I,K) = A(J,K)                                                   DEGA  01099
    7 A(J,K) = B                                                        DEGA  01100
      C = D                                                             DEGA  01101
    5 CONTINUE                                                          DEGA  01102
      IF( ABS(A(J,J))-EP) 14, 15, 15                                    DEGA  01103
   14 DET = 0.                                                          DEGA  01104
      IF(IJOB) 16, 16, 17                                               DEGA  01105
   16 IF SING = 1                                                       DEGA  01106
   17 RETURN                                                            DEGA  01107
   15 DO 4 I= JP1, N                                                    DEGA  01108
      CONST = A(I,J)/A(J,J)                                             DEGA  01109
      DO 4 K= JP1, NPM                                                  DEGA  01110
    4 A(I,K) = A(I,K) - CONST*A(J,K)                                    DEGA  01111
      IF( ABS(A(N,N)) - EP) 14, 18, 18                                  DEGA  01112
   18 DO 11 I=1, N                                                      DEGA  01113
   11 DET = DET*A(I,I)                                                  DEGA  01114
      IF(IJOB) 10, 10, 17                                               DEGA  01115
   10 DO 12 I=1, N                                                      DEGA  01116
      K = N-I+1                                                         DEGA  01117
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      KP1 = K+1                                                          DEGA  01118
      DO 12 L=NP1, NPM                                                   DEGA  01119
      S= 0.                                                              DEGA  01120
      IF( N - KP1) 12, 20, 20                                            DEGA  01121
   20 DO 13 J=KP1, N                                                     DEGA  01122
   13 S = S+A(K,J)*A(J,L)                                                DEGA  01123
   12 A(K,L) = (A(K,L)-S)/A(K,K)                                         DEGA  01124
      RETURN                                                             DEGA  01125
      END                                                                DEGA  01126
      SUBROUTINE NORMPHI(CAPLAMB, L)                                     DEGA  01127
      COMMON/AIMAX/  AF(51,402), JMAXF(402), IMAX,                       DEGA  01128
     1      IMAXF, IMAXFP1, IMAXB, IMAXBP1, C(3,400),                   DEGA  01129
     2      CF(3,402), ATOP(401), ATOPF(402)                            DEGA  01130
      DIMENSION AB(51,402), JMAXB(402), CB(3,402), ATOPB(402)            DEGA  01131
      EQUIVALENCE(AF(1), AB(1)), (JMAXF(1), JMAXB(1)),                   DEGA  01132
     1      (CF(1), CB(1)), (ATOPF(1), ATOPB(1))                        DEGA  01133
      DIMENSION CC(101)                                                  DEGA  01134
      COMMON/SCRATCH/SCRATCH(604)                                        DEGA  01135
      EQUIVALENCE (SCRATCH(1), CC(1))                                    DEGA  01136
      SQAB = SQRT(ABS(CAPLAMB))                                          DEGA  01137
      IBKW = IMAXFP1 + 1                                                 DEGA  01138
      EXPSQ = EXP(-SQAB*ATOPB(IBKW))                                     DEGA  01139
      CAPA = AB(1,IBKW)/EXPSQ                                            DEGA  01140
      GUNDA2 = (CAPA*EXPSQ)**2/(2.0*SQAB)                                DEGA  01141
      D = ATOPF(2)                                                       DEGA  01142
      CALL POLYMUL(AF(1,1), JMAXF(1), AF(1,1), JMAXF(1), CC, NC)         DEGA  01143
      L2 = 2*L                                                           DEGA  01144
      LD = L2 + NC                                                       DEGA  01145
      SUM = CC(NC)/LD                                                    DEGA  01146
      N = NC                                                             DEGA  01147
      NCM1 = NC - 1                                                      DEGA  01148
      DO 26 NN=1, NCM1                                                   DEGA  01149
      N = N - 1                                                          DEGA  01150
      LD = LD - 1                                                        DEGA  01151
   26 SUM = SUM*D + CC(N)/LD                                             DEGA  01152
      GUNDA2 = GUNDA2 + SUM*D**(L2 + 1)                                  DEGA  01153
      IF(IMAXF .EQ. 1) GO TO 27                                          DEGA  01154
      DO 20 I=2, IMAXF                                                   DEGA  01155
      D = ATOPF(I+1) - ATOPF(I)                                          DEGA  01156
      CALL POLYMUL(AF(1,I), JMAXF(I), AF(1,I), JMAXF(I), CC, NC)         DEGA  01157
      SUM = CC(NC)/NC                                                    DEGA  01158
      N = NC                                                             DEGA  01159
      NCM1 = NC - 1                                                      DEGA  01160
      DO 21 NN=1, NCM1                                                   DEGA  01161
      N = N - 1                                                          DEGA  01162
   21 SUM = SUM*D + CC(N)/N                                              DEGA  01163
   20 GUNDA2 = GUNDA2 + SUM*D                                            DEGA  01164
   27 DO 22 I=1, IMAXB                                                   DEGA  01165
      IBKW = IMAXFP1 + I                                                 DEGA  01166
      D = ATOPB(IBKW + 1) - ATOPB(IBKW)                                  DEGA  01167
      CALL POLYMUL(AB(1,IBKW), JMAXB(IBKW),                              DEGA  01168
     1      AB(1,IBKW), JMAXB(IBKW), CC, NC)                            DEGA  01169
      SUM = -CC(NC)/NC                                                   DEGA  01170
      N = NC                                                             DEGA  01171
      NCM1 = NC - 1                                                      DEGA  01172
      DO 23 NN=1, NCM1                                                   DEGA  01173
      N = N - 1                                                          DEGA  01174
   23 SUM = SUM*D - CC(N)/N                                              DEGA  01175
   22 GUNDA2 = GUNDA2 + SUM*D                                            DEGA  01176
      GUNDA = SQRT(GUNDA2)                                               DEGA  01177
      DO 24 I=1, IMAXF                                                   DEGA  01178
      JJJ = JMAXF(I)                                                     DEGA  01179
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      DO 24 J=1, JJJ                                                    DEGA   01180
   24 AF(J,I) = AF(J,I)/GUNDA                                           DEGA   01181
      DO 25 I=1, IMAXB                                                  DEGA   01182
      IBKW = IMAXFP1 + I                                                DEGA   01183
      JJJ = JMAXB(IBKW)                                                 DEGA   01184
      DO 25 J=1, JJJ                                                    DEGA   01185
   25 AB(J,IBKW) = AB(J,IBKW)/GUNDA                                     DEGA   01186
      RETURN                                                            DEGA   01187
      END                                                               DEGA   01188
      SUBROUTINE POLYMUL (A, LM, B, LN, C, LL)                          DEGA   01189
      DIMENSION A(1), B(1), C(1)                                        DEGA   01190
      LL = LM + LN - 1                                                  DEGA   01191
      MMIN = 1                                                          DEGA   01192
      DO 1 L=1,LL                                                       DEGA   01193
      IF(L .GT. LM) 3, 2                                                DEGA   01194
    2 MMAX = L                                                          DEGA   01195
    3 IF(L .GT. LN) 5, 4                                                DEGA   01196
    4 NMAXP1 = L + 1                                                    DEGA   01197
      GO TO 6                                                           DEGA   01198
    5 MMIN = MMIN + 1                                                   DEGA   01199
    6 C(L) = 0.0                                                        DEGA   01200
      N = NMAXP1                                                        DEGA   01201
      DO 1 M= MMIN , MMAX                                               DEGA   01202
      N = N - 1                                                         DEGA   01203
    1 C(L) = C(L) + A(M)*B(N)                                           DEGA   01204
      RETURN                                                            DEGA   01205
      END                                                               DEGA   01206
      SUBROUTINE MATELE(KPHIMAX, XLAMARY, LARY, ALFAARY, IMAXARY, I2,   DEGA   01207
     1     NSUBSHL, ISSMAX, NSHELL)                                     DEGA   01208
      DIMENSION JMAX(400), AM1S(400), AM2S(400)                         DEGA   01209
      EQUIVALENCE (SCRATCH(1), ATOPIP1), (SCRATCH(2), C1),              DEGA   01210
     1     (SCRATCH(3), C2), (SCRATCH(4),C3), (SCRATCH(5), JMAX(1)),    DEGA   01211
     2     (SCRATCH(405),AM1S(1)), (SCRATCH(805), AM2S(1))              DEGA   01212
      DIMENSION XLAMARY(1), LARY(1), ALFAARY(1), IMAXARY(1)             DEGA   01213
     1     ,NSUBSHL(1), NSHELL(1)                                       DEGA   01214
      COMMON/AIMAX/ A(51,100), CAPO(100), IFSTOP(100),                  DEGA   01215
     1     XLLP1(100), S1(300), S2(300), OVPOLY(70), SCRATCH(1204)      DEGA   01216
     2     , A1M(400), A2M(400), AMT(51), AMS(51)                       DEGA   01217
     3     , A1N(400), A2N(400), ANT(51), ANS(51)                       DEGA   01218
     4     , ATOPP1M(400), ATOPP1N(400), JMAXM(400), JMAXN(400)         DEGA   01219
      COMMON/CB1/ HNUVEC(500), ACOFVEC(500), NOPTS, IHNUMAX, MM(100),   DEGA   01220
     1     NN(100), MNMAX, I4MIN, I4MAX                                 DEGA   01221
      COMMON/EPS/EPSCONV, FBMAX, EM16, EMATELE, EMOVDD, MAXDIM          DEGA   01222
    1 FORMAT(16I5)                                                      DEGA   01223
    2 FORMAT (25I5)                                                     DEGA   01224
    3 FORMAT(5E25.14)                                                   DEGA   01225
    4 FORMAT(2E25.14, I5)                                               DEGA   01226
    5 FORMAT(/)                                                         DEGA   01227
    6 FORMAT (4E25.14, 2I5)                                             DEGA   01228
      PRINT 1, MNMAX                                                    DEGA   01229
      PRINT 1, (MM(MN), NN(MN), MN=1, MNMAX)                            DEGA   01230
      KPHIM4 = KPHIMAX + 4                                              DEGA   01231
      MAXDIM4 = MAXDIM + 4                                              DEGA   01232
      ISKIP = 3*MAXDIM + 4                                              DEGA   01233
      IECS = 1                                                          DEGA   01234
      IECS1 = IECS + MAXDIM4                                            DEGA   01235
      IECS2 = IECS1+ MAXDIM                                             DEGA   01236
      CALL ECRD (SCRATCH(1), IECS, KPHIM4, IE)                          DEGA   01237
      CALL ECRD(SCRATCH(405), IECS1, KPHIMAX, IE)                       DEGA   01238
      CALL ECRD(SCRATCH(805), IECS2, KPHIMAX, IE)                       DEGA   01239
      DO 31 KPHI=1, KPHIMAX                                             DEGA   01240
      A(1,KPHI) = AM1S(KPHI)                                            DEGA   01241
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31 A(2,KPHI) = AM2S(KPHI)                                                    DEGA    01242
   DO 21 KPHI=1, KPHIMAX                                                     DEGA    01243
   XL = LARY(KPHI)                                                           DEGA    01244
   IERROR = 0                                                                DEGA    01245
   CALL TAYLOR1 (A(1,KPHI), JMAX(KPHI), ATOPIP1,                             DEGA    01246
  1     XLAMARY(KPHI), XL, C1, C2, EM16, IERROR)                            DEGA    01247
   JMAXKP = JMAX(KPHI)                                                       DEGA    01248
21 XLLP1(KPHI) = XL*(XL + 1.0)                                               DEGA    01249
   DO 20 MN=1, MNMAX                                                         DEGA    01250
   M = MM(MN)                                                                DEGA    01251
   N = NN(MN)                                                                DEGA    01252
   LNLM1 = LARY(N) + LARY(M) + 1                                             DEGA    01253
   DEOM = LNLM1 - 1                                                          DEGA    01254
   CALL POLYMUL (A(2,M), JMAX(M)-1, A(2,N), JMAX(N)-1, S2, IS2)              DEGA    01255
   DO 30 J=1, IS2                                                            DEGA    01256
   DEOM = DEOM + 1.0                                                         DEGA    01257
30 S2(J) = S2(J)/DEOM                                                        DEGA    01258
   CALL POLYOP (S2, IS2, ATOPIP1, P)                                         DEGA    01259
20 CAPO(MN) = -C2*P*ATOPIP1**LNLM1                                           DEGA    01260
   DO 36 MN=1, MNMAX                                                         DEGA    01261
36 IFSTOP(MN) = 0                                                            DEGA    01262
   DO 24 I=2, I2                                                             DEGA    01263
   ATOPI = ATOPIP1                                                           DEGA    01264
   IECS = IECS + ISKIP                                                       DEGA    01265
   IECS1 = IECS + MAXDIM4                                                    DEGA    01266
   IECS2 = IECS1 + MAXDIM                                                    DEGA    01267
   CALL ECRD (SCRATCH(1), IECS, KPHIM4, IE)                                  DEGA    01268
   CALL ECRD(SCRATCH(405), IECS1,KPHIMAX, IE)                                DEGA    01269
   CALL ECRD(SCRATCH(805), IECS2, KPHIMAX, IE)                               DEGA    01270
   DO 25 KPHI=1, KPHIMAX                                                     DEGA    01271
   A(1, KPHI) = AM1S(KPHI)                                                   DEGA    01272
25 A(2, KPHI) = AM2S(KPHI)                                                   DEGA    01273
   D = ATOPI - ATOPIP1                                                       DEGA    01274
   DO 27 KPHI=1, KPHIMAX                                                     DEGA    01275
   IERROR = 0                                                                DEGA    01276
27 CALL TAYLORS(A(1,KPHI), JMAX(KPHI), ATOPIP1,                              DEGA    01277
  1     D, XLAMARY(KPHI), XLLP1(KPHI), C1, C2, C3, EM16, IERROR)            DEGA    01278
   CALL DVDD(ATOPIP1, D, C2, C3, DVPOLY, IDVDD, EMDVDD)                      DEGA    01279
   MLAST = 0                                                                 DEGA    01280
   DO 28 MN=1, MNMAX                                                         DEGA    01281
   IF(IFSTOP(MN) .EQ. 5) GO TO 28                                            DEGA    01282
   M= MM(MN)                                                                 DEGA    01283
   N=NN(MN)                                                                  DEGA    01284
   IF(M .EQ. MLAST) GO TO 33                                                 DEGA    01285
   MLAST = M                                                                 DEGA    01286
   CALL POLYMUL(A(1,M), JMAX(M), DVPOLY, IDVDD, S1, IS1)                     DEGA    01287
33 CALL POLYMUL(A(1,N), JMAX(N), S1, IS1, S2, IS2)                           DEGA    01288
   CALL PDLYINT(S2, IS2, D, P)                                               DEGA    01289
   CAPO(MN) = CAPO(MN) - P                                                   DEGA    01290
   IF(ABS(P) .LT. ABS(CAPO(MN))*EMATELE) 34, 35                              DEGA    01291
34 IFSTOP(MN) = IFSTOP(MN) + 1                                               DEGA    01292
   GO TO 28                                                                  DEGA    01293
35 IFSTOP(MN) = 0                                                            DEGA    01294
28 CONTINUE                                                                  DEGA    01295
24 CONTINUE                                                                  DEGA    01296
   ATOPI2 = ATOPIPI                                                          DEGA    01297
   ISKIP = 3*MAXDIM + 4                                                      DEGA    01298
   IJUMP = 400 - I2                                                          DEGA    01299
   MLAST = 0                                                                 DEGA    01300
   NLAST = 0                                                                 DEGA    01301
   DO 40 MN=1, MNMAX                                                         DEGA    01302
   IF(IFSTOP(MN) .EQ. 5) GO TO 40                                            DEGA    01303
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      M = MM(MN)                                                        DEGA   01304
      N = NN(MN)                                                        DEGA   01305
      IF(M .EQ. MLAST) 42, 41                                           DEGA   01306
   41 MLAST = M                                                         DEGA   01307
      IMMAX = IMAXARY(M) - I2                                           DEGA   01308
      IF(IMMAX .EQ. 0) GO TO 60                                         DEGA   01309
      IECS = 4*(400 - I2)                                               DEGA   01310
      IECS = IECS*(M - 1) + 1                                           DEGA   01311
      IECS = IECS + I2*ISKIP                                            DEGA   01312
      CALL ECRD(ATOPP1M(1), IECS, IMMAX, IE)                            DEGA   01313
      IECS = IECS + IJUMP                                               DEGA   01314
      CALL ECRD(JMAXM(1), IECS, IMMAX, IE)                              DEGA   01315
      IECS = IECS + IJUMP                                               DEGA   01316
      CALL ECRD(A1M(1), IECS, IMMAX, IE)                                DEGA   01317
      IECS = IECS + IJUMP                                               DEGA   01318
      CALL ECRD(A2M(1), IECS, IMMAX, IE)                                DEGA   01319
   60 CONTINUE                                                          DEGA   01320
   42 IF(N .EQ. NLAST) 45, 44                                           DEGA   01321
   44 NLAST = N                                                         DEGA   01322
      INMAX = IMAXARY(N) - I2                                           DEGA   01323
      IF(INMAX .EQ. 0) GO TO 61                                         DEGA   01324
      IECS = 4*(400 - I2)                                               DEGA   01325
      IECS = IECS*(N - 1) + 1                                           DEGA   01326
      IECS = IECS + I2*ISKIP                                            DEGA   01327
      CALL ECRD(ATOPP1N(1), IECS, INMAX, IE)                            DEGA   01328
      IECS = IECS + IJUMP                                               DEGA   01329
      CALL ECRD(JMAXN(1), IECS, INMAX, IE)                              DEGA   01330
      IECS = IECS + IJUMP                                               DEGA   01331
      CALL ECRD(A1N(1), IECS, INMAX, IE)                                DEGA   01332
      IECS = IECS + IJUMP                                               DEGA   01333
      CALL ECRD(A2N(1), IECS, INMAX, IE)                                DEGA   01334
   61 CONTINUE                                                          DEGA   01335
   45 IM = 1                                                            DEGA   01336
      IN = 1                                                            DEGA   01337
      ATOPIP1 = ATOPI2                                                  DEGA   01338
      ALASTM = ATOPI2                                                   DEGA   01339
      ALASTN = ATOPI2                                                   DEGA   01340
      IMFIRST = 0                                                       DEGA   01341
      INFIRST = 0                                                       DEGA   01342
      CALL FINDATP(IM, IMMAX, XLLP1(M), ALASTM, ATOPP1M,                DEGA   01343
     1     XLAMARY(M), IERROR)                                          DEGA   01344
      IF(IERROR .EQ. 14) GO TO 100                                      DEGA   01345
      CALL FINDATP(IN, INMAX, XLLP1(N), ALASTN, ATOPP1N,                DEGA   01346
     1     XLAMARY(N), IERROR)                                          DEGA   01347
      IF(IERROR .EQ. 14) GO TO 100                                      DEGA   01348
   47 CONTINUE                                                          DEGA   01349
      ATOPI = ATOPIP1                                                   DEGA   01350
      IF(ABS(ALASTM-ALASTN) .LT. (ALASTM+ALASTN)*.5E-12 ) 48, 49        DEGA   01351
   48 INFIRST = 0                                                       DEGA   01352
      IMFIRST = 0                                                       DEGA   01353
      ATOP1P1 = .5*(ALASTM + ALASTN)                                    DEGA   01354
      CALL FINDA12(IM, IMMAX, XLAMARY(M), ALFAARY(M), XLLP1(M),         DEGA   01355
     1     ATOPIP1, A1M, A2M, JMAXM, AMS, JMSMAX, IERROR)               DEGA   01356
      IF(IERROR .EQ. 12) GO TO 100                                      DEGA   01357
      CALL FINDA12(IN, INMAX, XLAMARY(N), ALFAARY(N), XLLP1(N),         DEGA   01358
     1     ATOPIP1, A1N, A2N, JMAXN, ANS, JNSMAX, IERROR)               DEGA   01359
      IF(IERROR .EQ. 12) GO TO 100                                      DEGA   01360
      IM = IM + 1                                                       DEGA   01361
      IN = IN + 1                                                       DEGA   01362
      CALL FINDATP(IM, IMMAX, XLLP1(M), ALASTM, ATOPP1M,                DEGA   01363
     1     XLAMARY(M), IERROR)                                          DEGA   01364
      IF(IERROR .EQ. 14) GO TO 100                                      DEGA   01365
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      CALL FINDATP(IN, INMAX, XLLP1(N), ALASTN, ATOPP1N,                DEGA   01366
     1     XLAMARY(N), IERROR)                                          DEGA   01367
      IF(IERROR .EQ. 14) 100, 50                                        DEGA   01368
   49 IF(ALASTM .GT. ALASTN) 51, 52                                     DEGA   01369
   51 INFIRST = 0                                                       DEGA   01370
      IMFIRST = IMFIRST + 1                                             DEGA   01371
      ATOPIP1 = ALASTN                                                  DEGA   01372
      DM = ATOPIP1 - ALASTM                                             DEGA   01373
      IF(IMFIRST .EQ. 1) 53, 54                                         DEGA   01374
   53 CALL FINDA12(IM, IMMAX, XLAMARY(M), ALFAARY(M),                   DEGA   01375
     1     XLLP1(M), ALASTM, A1M, A2M, JMAXM, AMT, JMTMAX, IERROR)      DEGA   01376
      IF(IERROR .EQ. 12) GO TO 100                                      DEGA   01377
      IERROR = 0                                                        DEGA   01378
      CALL TAYLORS(AMT, JMTMAX, ALASTM, DM, XLAMARY(M),                 DEGA   01379
     1     XLLP1(M), 0.0, -1.0, 0.0, EM16, IERROR)                      DEGA   01380
      IF(IERROR .EQ. 10) 100, 54                                        DEGA   01381
   54 CALL POLY0P(AMT, JMTMAX, DM, AMS(1))                              DEGA   01382
      CALL POLY1P(AMT, JMTMAX, DM, AMS(2))                              DEGA   01383
      JMSMAX = 0                                                        DEGA   01384
      CALL FINDA12(IN, INMAX, XLAMARY(N), ALFAARY(N), XLLP1(N),         DEGA   01385
     1     ATOPIP1, A1N, A2N, JMAXN, ANS, JNSMAX, IERROR)               DEGA   01386
      IF(IERROR .EQ. 12) GO TO 100                                      DEGA   01387
      IN = IN + 1                                                       DEGA   01388
      CALL FINDATP(IN, INMAX, XLLP1(N), ALASTN, ATOPP1N,                DEGA   01389
     1     XLAMARY(N), IERROR)                                          DEGA   01390
      IF(IERROR .EQ. 14) 100, 50                                        DEGA   01391
   52 IMFIRST = 0                                                       DEGA   01392
      INFIRST = INFIRST + 1                                             DEGA   01393
      ATOP1P1 = ALASTM                                                  DEGA   01394
      DN = ATOPIP1 - ALASTN                                             DEGA   01395
      IF(INFIRST .EQ. 1) 55, 56                                         DEGA   01396
   55 CALL FINDA12(IN, INMAX, XLAMARY(N), ALFAARY(N),                   DEGA   01397
     1     XLLP1(N), ALASTN, A1N, A2N, JMAXN, ANT, JNTMAX, IERROR)      DEGA   01398
      IF(IERROR .EQ. 12) GO TO 100                                      DEGA   01399
      IERROR = 0                                                        DEGA   01400
      CALL TAYLORS(ANT, JNTMAX, ALASTN, DN, XLAMARY(N),                 DEGA   01401
     1     XLLP1(N), 0.0, -1.0, 0.0, EM16, IERROR)                      DEGA   01402
      IF(IERROR .EQ. 10) 100, 56                                        DEGA   01403
   56 CALL POLY0P(ANT, JNTMAX, DN, ANS(1))                              DEGA   01404
      CALL POLY1P(ANT, JNTMAX, DN, ANS(2))                              DEGA   01405
      JNSMAX = 0                                                        DEGA   01406
      CALL FINDA12(IM, IMMAX, XLAMARY(M), ALFAARY(M), XLLP1(M),         DEGA   01407
     1     ATOPIP1, A1M, A2M, JMAXM, AMS, JMSMAX, IERROR)               DEGA   01408
      IF(IERROR .EQ. 12) GO TO 100                                      DEGA   01409
      IM = IM + 1                                                       DEGA   01410
      CALL FINDATP(IM, IMMAX, XLLP1(M), ALASTM,                         DEGA   01411
     1     ATOPP1M, XLAMARY(M), IERROR)                                 DEGA   01412
      IF(IERROR .EQ. 14) 100, 50                                        DEGA   01413
   50 D = ATOPI - ATOPIP1                                               DEGA   01414
      IERROR = 0                                                        DEGA   01415
      CALL TAYLORS(AMS, JMSMAX, ATOPIP1, D, XLAMARY(M),                 DEGA   01416
     1     XLLP1(M), 0.0, -1.0, 0.0, EM16, IERROR)                      DEGA   01417
      IF(IERROR .EQ. 10) GO TO 100                                      DEGA   01418
      CALL TAYLORS(ANS, JNSMAX, ATOPIP1, D, XLAMARY(N),                 DEGA   01419
     1     XLLP1(N), 0.0, -1.0, 0.0, EM16, IERROR)                      DEGA   01420
      IF(IERROR .EQ. 10) GO TO 100                                      DEGA   01421
      CALL DVDD(ATOPIP1, D, -1.0, 0.0, DVPOLY, IDVDD, EMDVDD)           DEGA   01422
      CALL POLYMUL(AMS, JMSMAX, DVPOLY, IDVDD, S1, IS1)                 DEGA   01423
      CALL POLYMUL(ANS, JNSMAX, S1, IS1, S2, IS2)                       DEGA   01424
      CALL POLYINT(S2, IS2, D, P)                                       DEGA   01425
      CAPO(MN) = CAPO(MN) - P                                           DEGA   01426
      IF(ABS(P) .LT. ABS(CAPO(MN))*EMATELE) 58, 57                      DEGA   01427

      PRINT 7, ISSMAX                                                   DEGA   00063
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 58 IFSTOP(MN) = IFSTOP(MN) + 1                                          DEGA   01428
    IF(IFSTOP(MN) .EQ. 5) 40, 47                                         DEGA   01429
 57 IFSTOP(MN) = 0                                                       DEGA   01430
    GO TO 47                                                             DEGA   01431
100 PRINT 101                                                            DEGA   01432
101 FORMAT(*      ERROR IN REGION 3*)                                    DEGA   01433
 40 CONTINUE                                                             DEGA   01434
    DO 29 MN=1, MNMAX                                                    DEGA   01435
    CAPO(MN) = 2.0*CAPO(MN)                                              DEGA   01436
 29 PRINT 3, CAPO(MN)                                                    DEGA   01437
 64 FORMAT(E24.14, * EV*, I5, E24.14, * EV* , I5,                        DEGA   01438
   1     E24.14, * EV*, E24.14, * BARNS/ATOM*)                           DEGA   01439
 65 FORMAT(E24.14, * BARNS/ATOM*)                                        DEGA   01440
 66 FORMAT(/)                                                            DEGA   01441
    DO 62 MN=1, MNMAX                                                    DEGA   01442
    M = MM(MN)                                                           DEGA   01443
    N = NN(MN)                                                           DEGA   01444
    DE = ABS(XLAMARY(M) - XLAMARY(N))                                    DEGA   01445
    HNU = DE*13.605                                                      DEGA   01446
    DE3 = DE**3                                                          DEGA   01447
    LMAX = LARY(M)                                                       DEGA   01448
    IF(LARY(N) .GT. LMAX) LMAX = LARY(N)                                 DEGA   01449
THE GA AND NOE ARE ONLY GOOD HERE FOR THE BOUND-FREE CASE.               DEGA   01450
    MNSS = N                                                             DEGA   01451
    IF(XLAMARY(M) .LT. 0.0) MNSS = M                                     DEGA   01452
    ISS = NSHELL(MNSS)*(NSHELL(MNSS) - 1)/2 + LARY(MNSS) + 1             DEGA   01453
    NOE = NSUBSHL(ISS)                                                   DEGA   01454
    GA = 2*(2*LARY(MNSS) + 1)                                            DEGA   01455
    DSIGMA = 10.756E+6*NOE*LMAX*CAPO(MN)**2/(DE3*GA)                     DEGA   01456
    I4 = I4MIN + MN - 1                                                  DEGA   01457
    ACOFVEC(I4) = ACOFVEC(I4) + DSIGMA                                   DEGA   01458
    EM = XLAMARY(M)*13.605                                               DEGA   01459
    EN = XLAMARY(N)*13.605                                               DEGA   01460
 62 CONTINUE                                                             DEGA   01461
    RETURN                                                               DEGA   01462
    END                                                                  DEGA   01463
    SUBROUTINE ZZZ(XLAMWKB, LWKB, NWKB, KWKB, HNUVEC,                    DEGA   01464
   1     NOPTS, IHNUMAX, DHNUI, ZZZFAC)                                  DEGA   01465
    COMMON/SCRATCH/SCRATCH(1204)                                         DEGA   01466
    DIMENSION XLAMWKB(1), LWKB(1), NWKB(1), HNUVEC(1)                    DEGA   01467
    FAC = ALOG(10.0)                                                     DEGA   01468
    DHNU = DHNUI                                                         DEGA   01469
    DO 6 K=1, KWKB                                                       DEGA   01470
  6 XLAMWKB(K) = ABS(XLAMWKB(K))                                         DEGA   01471
    CALL SORT1(KWKB, 2, XLAMWKB, SCRATCH, LWKB, NWKB)                    DEGA   01472
    XLAMWKB(KWKB+1) = ZZZFAC*XLAMWKB(KWKB)                               DEGA   01473
  3 IHNUMAX = 0                                                          DEGA   01474
    DO 1 I=1, KWKB                                                       DEGA   01475
    EPS = .01                                                            DEGA   01476
    XNUM = ALOG10(ABS(XLAMWKB(I+1))) - ALOG10(ABS(XLAMWKB(I) + EPS))     DEGA   01477
    NOINT = XNUM/DHNU                                                    DEGA   01478
    IF(NOINT .EQ. 0) NOINT = 1                                           DEGA   01479
    NOINT = NOINT + 1                                                    DEGA   01480
    SDHNU = XNUM/NOINT                                                   DEGA   01481
    IHNUMAX = IHNUMAX + 1                                                DEGA   01482
    IF(IHNUMAX .GT. NOPTS) 4, 5                                          DEGA   01483
  4 DHNU = 1.2*DHNU                                                      DEGA   01484
    GO TO 3                                                              DEGA   01485
  5 HNUVEC(IHNUMAX) = XLAMWKB(I) + EPS                                   DEGA   01486
    NOINTM1 = NOINT - 1                                                  DEGA   01487
    DO 2 INT=1, NOINTM1                                                  DEGA   01488
    IHNUMAX = IHNUMAX + 1                                                DEGA   01489
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      IF(IHNUMAX .GT. NOPTS) GO TO 4                                    DEGA  01490
      XNUM = FAC*(ALOG10(ABS(XLAMWKB(I) + EPS)) + INT*SDHNU)            DEGA  01491
    2 HNUVEC(IHNUMAX) =  EXP(XNUM)                                      DEGA  01492
      IHNUMAX = IHNUMAX + 1                                             DEGA  01493
      IF(IHNUMAX .GT. NOPTS) GO TO 4                                    DEGA  01494
    1 HNUVEC(IHNUMAX) = XLAMWKB(I+1)                                    DEGA  01495
      DO 7 K=1, KWKB                                                    DEGA  01496
    7 XLAMWKB(K) = -XLAMWKB(K)                                          DEGA  01497
      RETURN                                                            DEGA  01498
      END                                                               DEGA  01499
      SUBROUTINE CARSON(XLAMBDA, C2, MFAC, CAPR, XLLP1,                 DEGA  01500
     1     CAPF, CAPFP, THETA, THETAP, IERROR)                          DEGA  01501
      COMMON/PI/PI, TWOSPI                                              DEGA  01502
      IERROR = 0                                                        DEGA  01503
      SMALLC = ABS(C2)                                                  DEGA  01504
      SMALLK = SQRT(XLAMBDA)                                            DEGA  01505
      CAPM = SQRT(TWOSPI/SMALLK)                                        DEGA  01506
      CAPM = MFAC*CAPM                                                  DEGA  01507
      AN = CAPM    $   BN = 0.0                                         DEGA  01508
      CSK = SMALLC/SMALLK    $    CSK2 = CSK*CSK                       DEGA  01509
      ACON = XLLP1 + CSK2    $    BCON = -(CSK2 + XLLP1)               DEGA  01510
      DEOM = 1.0    $    TWOK = 2.0*SMALLK                             DEGA  01511
      CAPA = AN    $    CAPB = BN    $    CAPAP = 0.0    $    CAPBP = 0.0  DEGA  01512
      DO 63 NP1 = 1, 15                                                 DEGA  01513
      DEOM = DEOM*CAPR                                                  DEGA  01514
      N = NP1 - 1                                                       DEGA  01515
      XNP1 = NP1                                                        DEGA  01516
      XNNP1 = N*XNP1                                                    DEGA  01517
      TWONP1 = (2.0*N + 1.0)*CSK                                        DEGA  01518
      XDEOM = TWOK*XNP1                                                 DEGA  01519
      ANP1 = ((ACON - XNNP1)*BN - TWONP1*AN)/XDEOM                      DEGA  01520
      BNP1 = ((XNNP1 + BCON)*AN -TWONP1*BN)/XDEOM                       DEGA  01521
      AADD = ANP1/DEOM    $    BADD = BNP1/DEOM                        DEGA  01522
      APADD = XNP1*AADD    $    BPADD = XNP1*BADD                       DEGA  01523
      CAPA = CAPA + AADD    $    CAPB = CAPB + BADD                     DEGA  01524
      CAPAP = CAPAP + APADD    $    CAPBP = CAPBP + BPADD               DEGA  01525
      CAPAB = ABS(CAPA) + ABS(CAPB)                                     DEGA  01526
      CAPABP = ABS(CAPAP) + ABS(CAPBP)                                  DEGA  01527
      IF( ABS(AADD) .LT. CAPAB*1.0E-4 .AND.                             DEGA  01528
     1     ABS(BADD) .LT. CAPAB*1.0E-4 .AND.                            DEGA  01529
     2     ABS(APADD) .LT. CAPABP*1.0E-4 .AND.                          DEGA  01530
     3     ABS(BPADD) .LT. CAPABP*1.0E-4) GO TO 62                      DEGA  01531
      AN = ANP1                                                         DEGA  01532
   63 BN = BNP1                                                         DEGA  01533
      PRINT 64                                                          DEGA  01534
   64 FORMAT(*    CAPA, CAPB, CAPAP, AND CAPBP DO NOT CONVERGE.*)      DEGA  01535
      IERROR = 12                                                       DEGA  01536
      RETURN                                                            DEGA  01537
C*********************************************************************  DEGA  01538
C     RUN THIS CODE FOR CAPR .GT. 1.0                                   DEGA  01539
C*********************************************************************  DEGA  01540
   62 CAPAP = -CAPAP/CAPR                                               DEGA  01541
      CAPBP = -CAPBP/CAPR                                               DEGA  01542
      CAPF2 = CAPA*CAPA + CAPB*CAPB                                     DEGA  01543
      CAPF = SQRT(CAPF2)                                                DEGA  01544
      CAPFP = (CAPA*CAPAP + CAPB*CAPBP)/CAPF                            DEGA  01545
      THETA = SMALLK*CAPR + CSK*ALOG(CAPR) + ATAN2(CAPA, CAPB)          DEGA  01546
      THETAP = SMALLK + CSK/CAPR + (CAPAP*CAPB - CAPBP*CAPA)/CAPF2      DEGA  01547
      RETURN                                                            DEGA  01548
      END                                                               DEGA  01549
      SUBROUTINE TAYLOR1(A, JMAX, D, XLAMBDA, XL, C1, C2, EM16, IERROR) DEGA  01550
      DIMENSION A(1)                                                    DEGA  01551

      PRINT 7, ISSMAX                                                   DEGA  01605
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      IERROR = 0                                                        DEGA    01552
      DEOM = 0.0                                                        DEGA    01553
      DDEOM = 2.0*XL                                                    DEGA    01554
      B1 = 2.0*C1 - XLAMBDA                                             DEGA    01555
      B2 = 2.0*C2                                                       DEGA    01556
      IF(JMAX .GT. 2) GO TO 40                                          DEGA    01557
      IFCONV = 0                                                        DEGA    01558
      FAC = 1.0                                                         DEGA    01559
      AMAX = A(2)                                                       DEGA    01560
      AMAXM16 = AMAX*EM16                                               DEGA    01561
      DO 20 J=3, 50                                                     DEGA    01562
      DDEOM = DDEOM + 2.0                                               DEGA    01563
      DEOM = DEOM + DDEOM                                               DEGA    01564
      JM1 = J-1                                                         DEGA    01565
      A(J) = (B1*A(J-2) + B2*A(JM1))/DEOM                               DEGA    01566
      FAC = FAC*D                                                       DEGA    01567
      ABSA = JM1*ABS(A(J))*FAC                                          DEGA    01568
      IF(ABSA .GT. AMAX) 30, 31                                         DEGA    01569
30    AMAX = ABSA                                                       DEGA    01570
      AMAXM16 = AMAX*EM16                                               DEGA    01571
      GO TO 32                                                          DEGA    01572
31    IF(ABSA .LT. AMAXM16) 33, 32                                      DEGA    01573
32    IFCONV = 0                                                        DEGA    01574
      GO TO 20                                                          DEGA    01575
33    IF(IFCONV .EQ. 1) 35, 34                                          DEGA    01576
35    JMAX = J                                                          DEGA    01577
      RETURN                                                            DEGA    01578
34    IFCONV = 1                                                        DEGA    01579
20    CONTINUE                                                          DEGA    01580
      IERROR = 9                                                        DEGA    01581
      PRINT 9, IERROR                                                   DEGA    01582
 9    FORMAT (I5,* TAYLOR SERIES DOES NOT CONVERGE IN SUBROUTINE TAYLOR1 DEGA    01583
     1, DO-LOOP 20.*)                                                   DEGA    01584
      RETURN                                                            DEGA    01585
40    DO 41 J=3, JMAX                                                   DEGA    01586
      DDEOM = DDEOM + 2.0                                               DEGA    01587
      DEOM = DEOM + DDEOM                                               DEGA    01588
      JM1 = J-1                                                         DEGA    01589
41    A(J) = (B1*A(J-2) + B2*A(JM1))/DEOM                               DEGA    01590
      RETURN                                                            DEGA    01591
      END                                                               DEGA    01592
      SUBROUTINE TAYLOR3(A, JMAX, RR, D, XLAMBDA,                       DEGA    01593
     1     XLLP1, C1, C2, C3, EM16, IERROR)                             DEGA    01594
      DIMENSION A(1)                                                    DEGA    01595
      IERROR = 0                                                        DEGA    01596
      RR2 = RR*RR                                                       DEGA    01597
      TWORR = 2.0*RR                                                    DEGA    01598
      SB1= XLAMBDA - 2.0*C1                                             DEGA    01599
      SB2= -2.0*C2                                                      DEGA    01600
      SB3= -(2.0*C3      + XLLP1)                                       DEGA    01601
      B1 = SB1*RR2 + SB2*RR + SB3                                       DEGA    01602
      B2 = SB1*TWORR + SB2                                              DEGA    01603
      B3 = SB1                                                          DEGA    01604
      A(3)    = -B1*A(1)  /(2.0*RR2)                                    DEGA    01605
      A(4)    = -(B2*A(1)  +B1*A(2)  +2.0*TWORR*A(3)  )/(6.0*RR2)       DEGA    01606
      IF(JMAX .GT. 5) GO TO 60                                          DEGA    01607
      ABSD = ABS(D)                                                     DEGA    01608
      FAC = 1.0                                                         DEGA    01609
      AMAX = ABS(A(2))                                                  DEGA    01610
      AMAXM16 = AMAX*EM16                                               DEGA    01611
      FAC = FAC*ABSD                                                    DEGA    01612
      ABS3 = 2.0*ABS(A(3))*FAC                                          DEGA    01613
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      IF(ABS3          .GT. AMAX) 54, 55                                    DEGA  01614
   54 AMAX = ABS3                                                          DEGA  01615
      AMAXM16 = AMAX*EM16                                                  DEGA  01616
   55 FAC = FAC*ABSD                                                       DEGA  01617
      ABS4 = 3.0*ABS(A(4))*FAC                                             DEGA  01618
      IF(ABS4          .GT. AMAX) 56, 57                                   DEGA  01619
   56 AMAX = ABS4                                                          DEGA  01620
      AMAXM16 = AMAX*EM16                                                  DEGA  01621
   57 DO 26 J=6, 50 , 2                                                    DEGA  01622
      JM1=J-1    $    JM2 = J-2    $    JM3 = J-3                         DEGA  01623
      JM4 = J-4    $    JM5 = J-5                                         DEGA  01624
      DEOM = JM3*JM2*RR2                                                   DEGA  01625
      A(JM1)    = -(B3*A(JM5)   +B2*A(JM4)   +(B1+JM5*JM4)*A(JM3)         DEGA  01626
     1            +JM4*JM3*TWORR*A(JM2)  )/DEOM                           DEGA  01627
      DEOM = JM2*JM1*RR2                                                   DEGA  01628
      A(J)    = -(B3*A(JM4)   +B2*A(JM3)   +(B1+JM4*JM3)*A(JM2)           DEGA  01629
     1            +JM3*JM2*TWORR*A(JM1)  )/DEOM                           DEGA  01630
      FAC = FAC*ABSD                                                       DEGA  01631
      ABSA1 = JM2*ABS(A(JM1))*FAC                                          DEGA  01632
      FAC = FAC*ABSD                                                       DEGA  01633
      ABSA = JM1*ABS(A(J))*FAC                                             DEGA  01634
      IF(ABSA .GT. AMAX) 45, 44                                            DEGA  01635
   45 AMAX = ABSA                                                          DEGA  01636
      AMAXM16 = AMAX*EM16                                                  DEGA  01637
      IF(ABSA1 .GT. AMAX)46, 26                                            DEGA  01638
   46 AMAX = ABSA1    $    AMAXM16 = AMAX*EM16      $   GO TO 26           DEGA  01639
   44 IF(ABSA1 .GT. AMAX) 46, 47                                           DEGA  01640
   47 IF(ABSA .LT. AMAXM16) 48, 26                                         DEGA  01641
   48 IF(ABSA1 .LT. AMAXM16) 49, 26                                        DEGA  01642
   49 JMAX    = J                                                          DEGA  01643
      RETURN                                                               DEGA  01644
   26 CONTINUE                                                             DEGA  01645
      IERROR = 10                                                          DEGA  01646
      PRINT 10, IERROR, I                                                  DEGA  01647
   10 FORMAT (2I5,* TAYLOR SERIES DOES NOT CONVERGE IN SUBROUTINE TAYLOR   DEGA  01648
     1S, DO-LOOP 26 IN LOOP 25.*)                                          DEGA  01649
      JMAX = 50                                                            DEGA  01650
      IERROR = 0                                                           DEGA  01651
    1 FORMAT(4E24.14)                                                      DEGA  01652
      PRINT 1, AMAX, AMAXM16, ABSA, ABSA1                                  DEGA  01653
      RETURN                                                               DEGA  01654
   60 DO 27 J=6, JMAX, 2                                                   DEGA  01655
      JM1=J-1    $    JM2 = J-2    $    JM3 = J-3                         DEGA  01656
      JM4 = J-4    $    JM5 = J-5                                         DEGA  01657
      DEOM = JM3*JM2*RR2                                                   DEGA  01658
      A(JM1)    = -(B3*A(JM5)   +B2*A(JM4)   +(B1+JM5*JM4)*A(JM3)         DEGA  01659
     1            +JM4*JM3*TWORR*A(JM2)  )/DEOM                           DEGA  01660
      DEOM = JM2*JM1*RR2                                                   DEGA  01661
   27 A(J)    = -(B3*A(JM4)   +B2*A(JM3)   +(B1+JM4*JM3)*A(JM2)           DEGA  01662
     1            +JM3*JM2*TWORR*A(JM1)  )/DEOM                           DEGA  01663
      RETURN                                                               DEGA  01664
      END                                                                  DEGA  01665
      SUBROUTINE POLYOP( A, JMAX, D, P)                                    DEGA  01666
      DIMENSION A(1)                                                       DEGA  01667
      M = JMAX                                                             DEGA  01668
      P = A(M)                                                             DEGA  01669
      JUP = M - 1                                                          DEGA  01670
      IF(JUP .LT. 1) RETURN                                                DEGA  01671
      DO 1 J=1, JUP                                                        DEGA  01672
      M = M- 1                                                             DEGA  01673
    1 P = P*D + A(M)                                                       DEGA  01674
      RETURN                                                               DEGA  01675

      PRINT 7, ISSMAX                                                      DEGA  00063
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      ENTRY POLY1P                                                      DEGA    01676
      M = JMAX                                                          DEGA    01677
      P = (M-1)*A(M)                                                    DEGA    01678
      JUP = M-2                                                         DEGA    01679
      IF(JUP .LT. 1) RETURN                                             DEGA    01680
      DO 2 J=1, JUP                                                     DEGA    01681
      M = M-1                                                           DEGA    01682
    2 P = P*D + (M-1)*A(M)                                              DEGA    01683
      RETURN                                                            DEGA    01684
      ENTRY POLYINT                                                     DEGA    01685
      M = JMAX                                                          DEGA    01686
      P = A(M)/M                                                        DEGA    01687
      JUP = M-1                                                         DEGA    01688
      IF(JUP .LT. 1) GO TO 4                                            DEGA    01689
      DO 3 J=1, JUP                                                     DEGA    01690
      M = M-1                                                           DEGA    01691
    3 P = P*D + A(M)/M                                                  DEGA    01692
    4 P = P*D                                                           DEGA    01693
      RETURN                                                            DEGA    01694
      END                                                               DEGA    01695
      SUBROUTINE DVDD( ATOPI, D, C2, C3, DVPOLY, IDVDD, EMDVDD)         DEGA    01696
      COMMON/SCRATCH/SCRATCH(604)                                       DEGA    01697
      DIMENSION DVPOLY(1)                                               DEGA    01698
      OATOPI = -1.0/ATOPI                                               DEGA    01699
      DN = 1.0                                                          DEGA    01700
      IF(C3 .EQ. 0.0) 10, 20                                            DEGA    01701
   10 IDVDD = 1                                                         DEGA    01702
      DVPOLY(1) = -C2/ATOPI**2                                          DEGA    01703
      EPSILON = ABS(DVPOLY(1))*EMDVDD                                   DEGA    01704
      TERMLST = DVPOLY(1)                                               DEGA    01705
   30 IDVDD = IDVDD + 1                                                 DEGA    01706
      TERMLST = TERMLST*OATOPI                                          DEGA    01707
      DN = DN*D                                                         DEGA    01708
      DVPOLY(IDVDD) = IDVDD*TERMLST                                     DEGA    01709
      IF(ABS(DVPOLY(IDVDD)*DN) .LT. EPSILON) 40, 30                     DEGA    01710
   20 ISCH = 1                                                          DEGA    01711
      ICNT1 = 1                                                         DEGA    01712
      ICNT2 = 1                                                         DEGA    01713
      SCRATCH(1) = -1.0/ATOPI**3                                        DEGA    01714
      EPSILON = ABS(SCRATCH(1))*EMDVDD                                  DEGA    01715
      TERMLST = SCRATCH(1)                                              DEGA    01716
   50 ISCH = ISCH + 1                                                   DEGA    01717
      ICNT2 = ICNT 2 + 1                                                DEGA    01718
      ICNT1 = ICNT1 + ICNT2                                             DEGA    01719
      TERMLST = TERMLST*OATOPI                                          DEGA    01720
      DN = DN*D                                                         DEGA    01721
      SCRATCH(ISCH) = ICNT1*TERMLST                                     DEGA    01722
      IF(ABS(SCRATCH(ISCH)*DN) .LT. EPSILON) 60, 50                     DEGA    01723
   60 SCRATCH(499) = C2*ATOPI + 2.0*C3                                  DEGA    01724
      SCRATCH(500) = C2                                                 DEGA    01725
      CALL POLYMUL(SCRATCH(1), ISCH, SCRATCH(499), 2, DVPOLY, IDVDD)    DEGA    01726
   40 RETURN                                                            DEGA    01727
      END                                                               DEGA    01728
      SUBROUTINE FINDA12(I, IMAX, XLAM, ALFA, XLLP1, ATOPIPI,           DEGA    01729
     1     A1, A2, JMAX, AS, JSMAX, IERROR)                             DEGA    01730
      DIMENSION A1(1), A2(1), JMAX(1), AS(2)                            DEGA    01731
      IERROR = 0                                                        DEGA    01732
      IF(I .GT. IMAX) 2, 1                                              DEGA    01733
    1 AS(1) = A1(I)                                                     DEGA    01734
      AS(2) = A2(I)                                                     DEGA    01735
      JSMAX = JMAX(I)                                                   DEGA    01736
      RETURN                                                            DEGA    01737
```

```
2 CALL CARSON(XLAM, -1.0, 1, ATOPIP1, XLLP1,                    DEGA    01738
 1      CAPF, CAPFP, THETA, THETAP, IERROR)                     DEGA    01739
   IF(IERROR .EQ. 12) RETURN                                    DEGA    01740
   THETA1 = THETA + ALFA                                        DEGA    01741
   COSTHE1 = COS(THETA1)                                        DEGA    01742
   AS(1) = CAPF*COSTHE1                                         DEGA    01743
   AS(2) = CAPFP*COSTHE1 - CAPF*THETAP*SIN(THETA1)              DEGA    01744
   JSMAX = 0                                                    DEGA    01745
   RETURN                                                       DEGA    01746
   END                                                          DEGA    01747
   SUBROUTINE FINDATP(IM, IMAX, XLLP1, ALAST, ATOPP1, XLAMB, IERROR) DEGA 01748
   DIMENSION ATOPP1(1)                                          DEGA    01749
   IERROR = 0                                                   DEGA    01750
   IF(IM .GT. IMAX) 2, 1                                        DEGA    01751
1  ALAST = ATOPP1(IM)                                           DEGA    01752
   RETURN                                                       DEGA    01753
2  IF(XLAMB .GT. 0.0) 4, 3                                      DEGA    01754
3  IERROR = 14                                                  DEGA    01755
   RETURN                                                       DEGA    01756
4  DR = .2*ALAST                                                DEGA    01757
   R1 = 1.05*ALAST                                              DEGA    01758
   CALL DRMAXSB(ORMAX, ALAST, R1, XLAMB, XLLP1, 1)              DEGA    01759
   IF(DR .GT. DRMAX) DR = DRMAX                                 DEGA    01760
   ALAST = ALAST + DR                                           DEGA    01761
   RETURN                                                       DEGA    01762
   END                                                          DEGA    01763
```

```
   PRINT 7, ISSMAX                                              DEGA    00003
```

```
 01/09/73 *LASL MCH1  .16 01/09/73 MACH, 1 ECS ON
18.56.54.J15WM2W  01/09/73
18.56.54.$JOB(NAME=J15WM, AC=J15D, USF=DEGAA, TL=
18.56.54.1* SC=156000, PL=200, MX=66,
18.56.54.$1      CL=U, PR=6, CAT=6, UA=8715C131)
18.56.55.ASSIGNMT, DLDPL(PLB,LF223L00,SHB)
18.56.55.65 ASSIGNED
18.56.55.LF223L00
18.56.55.ASSIGNMT, NEWPL(NLB,,SHB)
18.56.56.66 ASSIGNED
18.56.56.LD274L00
18.56.56.UPDATE(F,S)
18.57.07. DECK STRUCTURE CHANGED
18.57.07. DECK STRUCTURE CHANGED
18.57.14. UPDATING FINISHED
18.57.15.REWIND(SOURCE)
18.57.16.UPDATE(N,I=SOURCE)
18.57.38. UPDATING FINISHED
18.57.38.COPYSBF(COMPILE,OUTPUT)
18.57.43.CP  00005.336 SEC.
18.57.43.PP  00057.626 SEC.
18.57.43.SS  00127.002 SEC.
18.57.43.
18.57.43.
18.57.43.
18.57.43.          2W        2W        2W
```

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ALT:358(125)