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CHAINJ, AN UNCLASSIFIED VERSION OF AN
AVERAGE ATOM OPACITY CODE

AUGUST 1974

By:

J.M. GREEN
W.J. KARZAS
R. LATTER

Sponsored By:
UNIVERSITY OF CALIFORNIA
Subcontract 2392205
Lawrence Livermore Laboratory
P.O. Box 808
Livermore, California 94550

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R & D ASSOCIATES
Post Office Box 3580
Santa Monica,
California, 90403

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California, 90403

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1. INTRODUCTION

CHAINJ is the unclassified version of an "average atom opacity" code whose development began with the early unpublished work of R. Latter and W. Karzas at the RAND Corporation. Further developments and calculations first at RAND and later at RDA eventually became the responsibility of J. Green.

By conscious choice, CHAINJ, as it is described in this document, is incapable of computing the contribution made to the absorption cross section by "bound-bound" or line absorption processes. Consequently, the opacity numbers that the present level produces will be useful only for elements of low atomic number (say $z \lesssim 10$). Since the general physical ideas that underlie the calculation of the "continuous opacity" have by now been discussed many places [1-4] in the unclassified literature, this presentation will presuppose a general knowledge of these more common physical ideas and will also presuppose an understanding of the meaning and application of the opacity numbers themselves.

This document is intended to serve as a taxonomic description of the architecture of CHAINJ. The structure of the code will be exhibited, the function of every subroutine will be described, and, wherever applicable, the details of the calculational methods will be presented. In addition, Appendix A provides a complete guide to the input format necessary to run the code.

The rather special techniques which must be invoked to perform the vital line-absorption calculations will be discussed in a separate classified document.

2. GENERAL CONSIDERATIONS

We are interested in computing K_R , the Rosseland mean opacity of a material of temperature T and density ρ , which is assumed to be in local thermodynamic equilibrium with itself and with the surrounding radiation field. The mean is a specially defined average which depends on B_ν , the black body radiation distribution function

$$B_\nu = 2h\nu^3/c^2 (e^{h\nu/kT} - 1) \quad (1)$$

The Rosseland mean is defined to be

$$K_R = \frac{\int_0^\infty \frac{dB_\nu}{dT} d\nu}{\int_0^\infty \frac{1}{\kappa(\nu)(1 - e^{-h\nu/kT})} \frac{dB_\nu}{dT} d\nu} \text{ cm}^2/\text{gm} \quad (2)$$

where $\kappa(\nu)$, measured in units of cm^2/gm , is the frequency dependent absorption coefficient of the material in question.

It is customary to define a dimensionless frequency,

$$u = h\nu/kT \quad (3)$$

and a dimensionless absorption coefficient

$$D = \kappa(\nu) \rho u^3 / \bar{A} \quad (4)$$

Here, ρ , the material density, is in units of cm^3/gm , and $\bar{A}$ is a convenient inverse length which is conventionally chosen to be

$$\bar{A} = \frac{2^4}{3\sqrt{3}} \frac{h^2}{mc} \frac{1}{kT} \frac{1}{\nu} \text{ cm}^{-1} \quad (5)$$

N is the number of atoms contained in a volume v. If we take M to be the atomic weight, and if we measure $(kT)_R$ in Rydbergs, then the numerical value of $\bar{A}$ becomes

$$\bar{A} = 4.762 \times 10^6 \frac{\rho}{M (kT)_R} \text{ cm}^{-1} . \quad (6)$$

It then follows from Eqs. (1), (2), (3) and (4) that

$$\begin{aligned} K_R &= \bar{A} / \rho \int_0^\infty \frac{W(u)}{D(u)} du \\ &= \left(\frac{4.762 \times 10^6}{M(kT)_R} \right) / \int_0^\infty \frac{W(u)}{D(u)} du \quad \text{cm}^2/\text{gm} , \end{aligned} \quad (7)$$

where the weighting function $W(u)$ is given by

$$W(u) = \frac{15}{4\pi} \frac{u^7 e^{2u}}{(e^u - 1)^3} . \quad (8)$$

We will compute D as if each atom was replaced by an "average atom" whose state is given by the set of numbers $\{\bar{N}_k\}$, where $\bar{N}_k$ is the average number of electrons present in the k^{th} single-electron state. Consequently if d_k is the reduced absorption coefficient of one electron in the k^{th} state then

$$D = \sum \bar{N}_k d_k(u) . \quad (9)$$

The occupation numbers $\bar{N}_k$ will be found by doing the statistical mechanics of the independent electron model. Central to this calculation is a knowledge of E_k , the Eigen value of the k^{th} state in the "average atom." Furthermore, d_k , in general, will depend not only upon E_k , but upon the entire set of numbers $\{\bar{N}_k\}$. The Eigen values, E_k , are found by solving the Schrödinger equation and/or the Dirac equations in a potential that is representative of the "average atom." The potential that is usually chosen is the potential of the "hot" Thomas-Fermi atom that was worked out by R. Latter [5].

The general scheme of the calculation now becomes clear:

- A. For a given T , ρ , and atomic number z , the hot Thomas-Fermi atom is solved to find a self-consistent electrostatic potential, ϕ .
- B. Using the potential found in A, the Schrödinger equation is solved to find $E(k)$, the Schrödinger Eigen values and χ_k , the normalized wave function. The χ_k are used to find $E_g(k)$, the Coulomb self energy of each level.
- C. With $E(k)$ as a first guess, the Dirac equation is solved to find $ED(k)$, the Dirac equation Eigen values.
- D. Using $ED(k)$ found in C, $\bar{N}_k$, the occupation numbers, are computed.
- E. Using $\bar{N}_k$ found in D, the $ED(k)$ found in C and E_g found in B, d_k is computed for each state.

Finally, the sum in Eq. (9) and the integral in Eq. (7) is computed.

Each of the preceding steps is performed independently by a separate section of CHAINJ. The computation may be started at any point and may be stopped at any point, provided only that each section of the code somehow receives the data it needs to proceed.

The actual flow of the calculation is directed by a set of seven flags. By name, these flags are: IDPR08, ISKPTF, ISKP34, ISCH, IC0705, IME and LINEC.

In Figure 1 we present a flow diagram which exhibits precisely how these control flags choose the logical path followed by the computation. In Table 1 we tabulate the parameters and function of the flags. The input format for these controls is described in Appendix A.

Figure 1. Control Flag Flow Diagram

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Flow Diagram

Table 1. The Control Flags

NAME	FUNCTION	VARIABLE VALUES	CONSEQUENCE
IDPROB	LIST PROBLEM NUMBER OR END CALCULATION	$N \neq 99,999$ $N = 99,999$	USES THE VALUE OF N TO IDENTIFY THE PROBLEM NUMBER. CALLS EXIT.
ISKPTF	CONTROL COMPUTE OF THOMAS-FERMI POTENTIAL.	$= 0$ $= 1$	GOES THROUGH THOMAS-FERMI COMPUTE. SKIPS THOMAS-FERMI COMPUTE.
ISKP3:	CONTROLS EIGENVALUE COMPUTE.	$= 1$ $= 0$	NO EIGENVALUES ARE COMPUTED. EIGENVALUES ARE COMPUTED.
ISCH	CONTROLS THE NATURE OF EIGENVALUE COMPUTATION.	$= 1$ $= 0$ $= -1$	ONLY SCHRODINGER EIGENVALUES ARE DONE. ONLY DIRAC EIGENVALUES ARE DONE. BOTH DIRAC AND SCHRODINGER EIGENVALUES ARE COMPUTED.
IGOT05	CONTROLS OCCUPATION NUMBER COMPUTE.	$= 1$ $= 0$	OCCUPATION NUMBERS ARE COMPUTED. OCCUPATION NUMBERS ARE NOT COMPUTED.
IME	A DUMMY FLAG TO CONTROL MATRIX ELEMENT CALCULA- TION	$= 0$	SKIP MATRIX ELEMENTS CALCULATION
LINEC	(1) CONTROL WRITING OF ϕ ON DISC. (2) CONTROL CALCULATION OF OPACITY.	$<100,000$ $\geq 100,000$	DO NOT WRITE ϕ ON DISC 72. WRITE ϕ ON DISC 72.
	(LINEC)(LINEC-100,000)=0 (LINEC)(LINEC-100,000) $\neq 0$		DO NOT DO OPACITY COMPUTE. PERFORM OPACITY COMPUTE.

3. THE OVERLAY STRUCTURE

CHAINJ is built of a series of "subsystems" called overlays. These overlays fall into three separate levels or hierarchies. An overlay at some one level may call into the system any one of several overlays contained in the connecting level beneath it. However, when a new overlay is called, any other overlay of the same level (as the newly called overlay) that might be present is overwritten by the overlay that is newly called. Thus, though the system, in general, may have as many as three overlays simultaneously present (each belonging to a different level), no two overlays from the same level may be present at the same time.

The essentials of the overlay structure are exhibited in Figure 2. Each overlay in Figure 2 is described by its number (i,j) and by its function.

The first level consists only of overlay $(0,0)$. Overlay $(0,0)$ is the executive routine which calls all the other overlays.

The second level consists of overlays $(1,0)$, $(2,0)$ and $(3,0)$. Only one of these may be present at one time.

Overlay $(1,0)$ primarily consists of a large set of block data containing the "Thomas-Fermi-interpolation tables." These interpolation tables connect the temperature kT , the volume v , and the atomic number z , with the fundamental variables of the Thomas-Fermi potential, a , and $\phi(1)$. (The physical meaning of these last two variables and the need for the interpolation tables will be discussed later.) Overlay $(1,0)$ reads its data onto a disc for later use by overlay $(2,0)$. If several problems are run in succession, overlay $(1,0)$ is called only once.

Figure 2. Overlay Structure of CHAINJ

Overlay (2,0) calculates, $\phi(y)$, the normalized Thomas-Fermi potential and disposes of it as directed by the control flags. Normally $\phi(y)$ is stored in common for subsequent use.

Overlay (3,0) is an executive structure which controls the flow through overlays (3,1), (3,2), (3,4) and (3,5).

The third level consists of overlays (3,1), (3,2), (3,3), (3,4) and (3,5). If overlay (3,0) is present, then one, but no more than one, of overlays (3,1), (3,2), (3,3), (3,4) or (3,5) may also be present.

Overlay (3,1) computes the Schrödinger equation energy levels and wave functions.

Overlay (3,2) computes the Dirac equation energy levels, and wave functions.

Overlay (3,3) computes the occupation numbers for levels defined by the Dirac equation quantum numbers. If energy levels are not computed in (3,1) and/or (3,2), then the appropriate energy levels must be read in. (See Appendix A for inputs.)

Overlay (3,4) is a dummy overlay reserved for the calculation of matrix elements. This overlay is never called.

Overlay (3,5) computes the continuous opacity, using the results of (3,1), (3,2), and (3,3) which have been stored in common. If any of the overlays (3,1), (3,2), or (3,3) have not been run, then the data that would have been provided by them must be read in when overlay (3,5) is executed. (See Appendix A for the required inputs.)

Each of these overlays contains at least one main program, and each may contain several subprograms. In the subsequent section each of the overlays are examined separately. First we will describe the physics and the mathematical operation performed by each overlay. Then we list subroutines used in each overlay and describe the function of each.

3.1 OVERLAY (0,0). THE EXECUTIVE OVERLAY

Overlay (0,0) performs no theoretical calculations itself. It directs the flow of the computation. There are two subprograms in this overlay, CHAINJ and GCOM.

CHAINJ is the main program of overlay (0,0). It contains all the logic which controls the computations. It also defines the areas of common which are used to transfer data between all of the other overlays of the system.

GCOM contains no executable statements, but provides additional storage area in common for data that will be used in overlay (3,5).

3.2 OVERLAY (1,0). THE THERMODYNAMIC DATA OVERLAY

3.2.1 The Theory for Overlay (1,1)

The temperature dependent Thomas-Fermi theory of R. Latter [5] enables one to calculate Φ , the self-consistent un-normalized Thomas-Fermi potential function associated with an atom of temperature T , radius r_0 , and nuclear charge z .

The function ϕ is defined [5] to be

$$\phi(r/r_0) = \frac{\alpha + eV(r)}{kT} \quad r/r_0, \quad (10)$$

$$\lim_{r \rightarrow 0} reV(r) = e^2 z.$$

Here $V(r)$ is the Coulomb potential of the atom. Naturally the atomic volume, v , is

$$v = \frac{4}{3} \pi r_0^3 = M M_0 / \rho \quad (11)$$

where M is the atomic weight, and M_0 is the mass of unit atomic weight.

Clearly

$$\phi(0) = \frac{ze^2}{kTr_0}. \quad (12)$$

Furthermore,

$$\phi(r/r_0 = 1) = \frac{\alpha}{kT}, \quad (13)$$

since the electrostatic potential $V(r)$, and its derivative, both vanish at the edge of the ion sphere. It is easy to show [5] that α must be identified with the electron free energy, or the so called "degeneracy parameter."

If z is fixed, any two of the three parameters $\phi(1)$, kT , or r_0 will serve to completely identify the thermodynamic state of the atom. $\phi(r/r_0)$ will then, in principle, be determined everywhere.

As a practical matter the equation for $\phi(r/r_0)$ contains explicitly $\phi(1)$, and a second quantity, a , which is defined as

$$a = \left(\frac{4\pi r_0 (2m)^{3/4} (kT)^{1/4}}{h^{3/2}} \right)^2 \quad (14)$$

Thus, although we would prefer to describe the state of our matter by specifying T and ρ (or r_0), the natural parameters of the theory are a and $\phi(1)$.

Furthermore, once $\phi(r/r_0)$ is determined, the other thermodynamic properties of pressure, energy and entropy may be found [5].

Many previous calculations have been performed, and for each of the thermodynamic states investigated values were found for the quantities: $-\phi(1)$, a , $kT/z^{4/3}$ (ev), $zv \times 10^{20}$ cm³/atom, $P/z^{10/3}$ dynes/cm², $(\Delta E_T)/z^{7/3}$ ev/atom, and S/zk . P is the electron pressure at the atom's edge. If E_∞ is the energy of the zero temperature atom at ∞ volume, then

$$\Delta E_T = E_T - E_\infty = E_T + 20.913 z^{7/3} \text{ ev} \quad (15)$$

where E_T is the total energy per atom in ev, and finally S is the entropy per atom. The equation for the computation of ϕ and the connection between ϕ and the thermodynamic quantities T , r_0 , P , S , ΔE_T , a , and $\phi(1)$ will be made explicit in the next section.

For the purposes of this overlay it is sufficient to remark:

- 1) That if z is fixed, any two thermodynamic quantities determine the state; and

- 2) Tables of data exist [5] from previously solved problems which provide values for the seven quantities $-\phi(1)$, a , $kT/z^{4/3}$ (ev), $zv \times 10^{20}$ cm³/atom, $P/z^{10/3}$ dynes/cm², $(\Delta E_T/z)^{7/3}$ ev/atom, and s/zk .

3.2.2 The Structure of Overlay (1,0)

Overlay (1,0) contains the decks STORET and ABCD. STORET is the main routine which writes the tables of deck ABCD onto a disc for use by overlay (2,0).

ABCD is a block data deck which contains 68 tables of thermodynamic quantities. The first table has data for the zero temperature atom and is of no interest here. The remaining 67 tables consist of groups of eight numbers, the first seven of which are the seven previously listed quantities corresponding to some fixed thermodynamic state. The eighth number in each group has no physical meaning. In each of the 67 tables a is constant over the entire table. The tables are ordered according to increasing values of a .

Given any two thermodynamic quantities, any other of the set of seven may be subsequently found by double interpolation in these tables. The data corresponding to these tables have been published by R. Latter [5].

3.3 OVERLAY (2,0). THE ϕ COMPUTATION

3.3.1 The Theory of the ϕ Computation

The theory underlying the calculation of ϕ is derived in Reference 5. For convenience we recall here the essential results of that development. The function ϕ was defined in Eq. (10). If one lets

$$\xi = r/r_0 \quad (16)$$

be the dimensionless radial distance, then the boundary conditions on V ,

$$V(r) = \frac{dV(r)}{dr} = 0, \quad (17)$$

place the following conditions on ϕ

$$\phi(1) = \left. \frac{d\phi}{d\xi} \right|_{\xi=1} = \frac{\alpha}{kT}. \quad (18)$$

According to R. Latter's treatment [5] $\phi(\xi)$ must satisfy the Poisson equation

$$\phi''(\xi) = a\xi F\left(\frac{\phi(\xi)}{\xi}\right) \quad (19)$$

where a is given by Eq. (14) and $F(y)$ is the Fermi-Dirac function

$$F(\eta) = I_{1/2}(\eta) = \int_0^\infty \frac{y^{1/2} dy}{e^{y-\eta} + 1}. \quad (20)$$

The conditions of Eq. (18) and Eq. (19) are simultaneously satisfied by the integral equation,

$$\phi(\xi) = \xi\phi(1) + a \int_\xi^1 dt(t - \xi)tF\left(\frac{\phi(t)}{t}\right). \quad (21)$$

Equation (21) makes it clear that a and $\phi(1)$ rather than T and v (or r_0) are the natural parameters of the Thomas-Fermi theory.

An initial choice of a and $\phi(1)$ will, through Eq. (21), determine $\phi(\xi)$ everywhere. In particular, that choice of a and $\phi(1)$ will determine a value of $\phi(0)$. We recognize that T and r_0 can be found through the use of Eqs. (12) and (14), only after $\phi(0)$ has become available. In principle, then, T and r_0 cannot be known until Eq. (21) has been solved.

Normally only T and r_0 are known beforehand; $\phi(1)$ is unknown and $\phi(x)$ must be found. If this is the case, overlay (2,0) will enter the Thomas-Fermi tables and do a double interpolation on T and v to find a_I and $\phi(1)$. a_I and $\phi(1)$ are the interpolated values of a and $\phi(1)$ which correspond to the input values of T and v (or r_0). Of course a may also be computed directly from T and v by using Eqs. (14) and (11). The value of a computed directly is called a_c to distinguish it from a_I . Because of interpolation errors a_c will differ slightly from a_I . The calculation is usually instructed to stop if

$$\left(\frac{a_c - a_I}{a_I} \right) \geq 0.02 \quad .$$

The system then uses a_I and $\phi(1)$ to determine $\phi(x)$ from Eq. (21). New values of T and r_0 emerge once $\phi(0)$ has been produced by solving Eq. (21). The "new" or "output" values of T and r_0 , of course, represent the precise description of the state of the material.

Fortunately, because of the excellence of the Thomas-Fermi interpolation tables, the input values and output values of T and r_0 usually agree within a fraction of a percent.

We now examine the calculation itself. Since $\phi(\xi)$ changes most rapidly near the origin, the scale is expanded by setting

$$\begin{aligned} \xi = y^2 = r/r_0 \quad \text{and} \\ t = z^2 \end{aligned} \quad (22)$$

Consequently Eq. (21) becomes

$$\phi(y) = y^2 \phi(1) + 2a \int_y^1 z^3 (z^2 - y^2) F\left(\frac{\phi(z^2)}{z^2}\right) dz \quad . \quad (23)$$

Equation (23) may be generalized to account for a discontinuity in the electrostatic field at some arbitrary value of $y = y_0$. This is typically equivalent to inserting a shell of charge at y_0 . Δ is related to the strength of the charge shell. The generalized equation for ϕ becomes

$$\phi(y^2) = \phi(1)y^2 + \left\{ \begin{array}{ll} 0 & , y_0 < y \leq 1 \\ \Delta[y^2 - y_0^2] & , 0 \leq y \leq y_0 \end{array} \right\} + 2a \int_y^1 (z^2 - y^2) P\left(\frac{\phi(z^2)}{z^2}\right) dz. \quad (24)$$

Δ and y_0 are inputs (see Appendix A). (As a practical matter, the charge shell model is almost never used, and Δ and y_0 are almost always set to zero in the input deck.)

Let us now assume that we choose some value y_b , $y_b \leq 1/4$, which divides the range of y into two intervals $(0, y_b)$ and $(y_b, 1)$. If δ_2 is the grid size chosen for the $(y_b, 1)$ range, $\delta_1 = (y_b) \delta_2$ is taken as the grid size in the $(0, y_b)$ interval. y_b is so chosen that there are an even number of intervals in both ranges. Clearly $\delta_1 < \delta_2$. Let y_n be the value of y at the n^{th} grid point and $y_N \equiv 1$ be the last grid point. If $G(y)$ is any function of x , then we adopt the convention that $G_n \equiv G(y_n)$.

With these conventions, a straightforward application of Simpson Rule leads to the equations

$$\phi_n = y_n^2 \phi(1) + \left\{ \begin{array}{ll} 0 & , y_0 \leq y_n \leq 1 \\ (y_n^2 - y_0^2) \Delta & , 0 \leq y_n \leq y_0 \end{array} \right\} + 2a R_{n+1}, \quad (25)$$

where

$$f_n = y_n^3 P(\phi_n/y_n^2) \quad , \quad (26)$$

$$P_n = \frac{\delta}{3} (f_n + 4f_{n+1} + f_{n+2}) + P_{n+2} \equiv \frac{(-1)}{2a} \frac{d}{d(y^2)} \left\{ \phi - y^2 \phi(1) \right\} \Big|_{y_n} \quad (27)$$

and

$$R_n = R_{n+1} + 4y_n P_{n+1} \delta + \frac{4}{3} \delta \left[(2y_n - \delta) f_n + y_n f_{n+1} \right] \quad . \quad (28)$$

Equations (25-28) are an iterative set which will produce values of ϕ_n , f_n , P_n , and R_n if the values at $n+1$ and $n+2$ are known. Consequently, Eqs. (25-28) will integrate Eq. (24) from $y = 1$ to $y = y_b$. When y_b is reached, values for all relevant quantities in Eqs. (25-28) are found at the point $y = y_b + \delta_1$ by the equivalent of a four point interpolation. Then the integration proceeds as before, now using the smaller grid size δ_1 .

In order to start the integration, values at N and $N-1$ are needed. From the boundary conditions we immediately have

$$\left. \begin{aligned} P_N = R_{N+1} &= 0 \\ \phi_N &= \phi(1) \end{aligned} \right\} \quad \text{and} \quad (29)$$

Latter [5] has worked out an expansion for $\phi(x)$ in the neighborhood of $y = 1$. We use the first four terms of this expansion

$$\phi(y^2) = y^2 \phi(1) + a \sum_{k=0}^3 A_k \left[\frac{(1-y^2)^{k+2}}{(k+1)(k+2)} - \frac{(1-y^2)^{k+3}}{(k+2)(k+3)} \right] \quad , \quad (30)$$

to obtain the following connections:

$$\begin{aligned}
 R_N &= \frac{1}{2} \sum_{k=0}^3 A_k \left[\frac{\{(2-\delta_2)\delta_2\}^{k+2}}{(k+1)(k+2)} - \frac{\{(2-\delta_2)\delta_2\}^{k+3}}{(k+2)(k+3)} \right] \\
 P_{N-1} &= \frac{1}{2} \sum_{k=0}^3 A_k \left[\frac{\{(2-\delta_2)\delta_2\}^{k+1}}{k+1} - \frac{\{(2-\delta_2)\delta_2\}^{k+2}}{k+2} \right] .
 \end{aligned} \tag{31}$$

The coefficients are

$$\begin{aligned}
 A_0 &= F(\phi(1)) \\
 A_1 &= 0 \\
 A_2 &= \frac{1}{2} a F'(\phi(1)) F(\phi(1)) \\
 A_3 &= (2/3)A_2
 \end{aligned} \tag{32}$$

Summing up, if a grid size δ_2 is picked and a break point y_b is chosen, Eqs. (25-32) allow the integration of Eq. (24). This provides a complete description of $\phi(y)$, and in particular, it provides a value of $\phi(0)$. Nevertheless, the question remains: "Has the choice of δ_2 been taken small enough to guarantee an accurate calculation."

To test the accuracy of the computation, the integration is repeated using a new δ_2 half the size of the previous one. Indeed $(i+1)$ such computations will be done. If $\delta_2(i)$ is the value of δ_2 used in the $(i+1)^{th}$ integration, we choose $\delta_2(i)$ so that

$$\delta_2(i) = \frac{1}{(64)} \frac{1}{2^i} . \tag{33}$$

Furthermore, if $\phi^{(i)}(0)$ is the value of $\phi(0)$ for the $(i+1)^{\text{th}}$ integration, we can define a relative error ϵ_i by the equation

$$\epsilon_i = \frac{\phi^{(i)}(0) - \phi^{(i-1)}(0)}{\phi^{(i)}(0)} \quad (34)$$

Successively more accurate integrations are performed until

$$|\epsilon_i| \leq 10^{-7}. \quad (35)$$

If Eq. (35) is satisfied, the last set of $\phi(x)$ is accepted. Furthermore, if $10^{-7} \leq |\epsilon_i| \leq 10^{-5}$, and if also $|\epsilon_i/\epsilon_{i-1}| > 0.1$, that solution is accepted. If no solution is obtained after five iterations, the calculation is stopped. Experience has shown that convergence difficulties of this type are rare.

3.3.2 The Results of the ϕ Computation

The $\phi(y)$ calculation contains, in principle, not only the potential function but (up to the accuracy of the theory) the thermodynamics of the atom. The connection between $\phi(y)$ and the thermodynamic quantities are discussed in Reference 5.

At the end of the computation the following data are printed out.

<u>Mathematical Symbol</u>	<u>Physical Quantity</u>
1. z	Atomic number.
2. a	Interpolated from 2nd column of Thomas-Fermi tables.
3. $\phi(1) = \alpha/kT$	Interpolated from 1st column of Thomas-Fermi tables.
4. $\phi(0)$	See equation (12).
5. $(r_o/a_o) = \left(\frac{\pi^2 a^2 \phi(0)}{32z} \right)^{1/3}$	Radius of ion sphere in Bohr radii.

Mathematical Symbol

Physical Quantity

$$6. \quad v/a_0^3 = \frac{4}{3} \pi (r_0/a_0)^3$$

Volume in Bohr radii.

$$7. \quad (kT)_{\text{Ry}} = 2z / [\phi(0) (r_0/a_0)]$$

Temperature in Rydbergs.

$$8. \quad \rho = \frac{M}{(v/a_0^3)} \cdot \frac{1}{6.023 \times 10^{23} a_0^3}$$

Density gm/cm³.

$$9. \quad \eta = \rho/\rho_0$$

Compression.

$$10. \quad \left(\frac{kT}{z^{4/3}} \right)_{\text{ev}} = \frac{(kT)_{\text{Ry}}}{z^{4/3}} \quad 13.602$$

Selected temperature in (ev), column 3 of Thomas-Fermi tables.

$$11. \quad zv(\text{cm}^3) = \pi \left(\frac{v}{a_0^3} \right) a_0^3$$

Scaled volume/atom. Fourth column of Thomas-Fermi table has (zv) $\times 10^{20}$.

$$12. \quad P_0$$

$$\frac{(-1)}{2a} \frac{d}{d(y^2)} \left\{ \phi(y) - y^2 \phi(1) \right\} \Big|_{y=0}$$

$$13. \quad R_1$$

Value of R at $y = \delta_1$.

$$14. \quad A = \left[(kT)_{\text{Ry}}^{3/2} \right] \frac{v}{a_0^3} / 2\pi^2$$

$$15. \quad r_0 \phi_1 \triangleq \frac{-2aP_0}{\phi(0)}$$

$$-\frac{d}{d(y^2)} \left\{ \frac{\phi - y^2 \phi(1)}{\phi(0)} \right\} \triangleq \frac{d}{dy^2} \phi \Big|_{y=0}$$

the derivative of the normalized potential function at the origin.

$$16. \quad -E_0 = \left\{ 12z \int_0^1 x^3 [\phi(x) - x^2 \phi(1)] dx \right\} / \left(\frac{r_0}{a_0} \right) \phi(0)$$

Continuum lowering, or volume average of the electrostatic potential.

$$17. \quad \frac{Fv}{kT} = \frac{2}{9} z \frac{a}{\phi(0)} I_{3/2}(\phi(1))$$

Pv/kT ratio.

$$18. \quad (Pv)_{\text{Ry}} = \left(\frac{Pv}{kT} \right) (kT)_{\text{Ry}}$$

Pressure energy in Rydbergs/atom.

Mathematical Symbol

Physical Quantity

$$19. \frac{P}{(z^{10/3})} = \left(\frac{Pv}{kT} \right) \left(\frac{kT}{z^{4/3}} \right)_{ev} \frac{1}{(zv)} \frac{1.602 \times 10^{-12}}{z} \text{ ergs/cm}^3$$

Scaled pressure in dynes/cm². Sixth column of Thomas-Fermi table.

$$20. L = \int_0^1 x^3 [\phi(x) - \kappa^2 \phi(1)] e^{\left(\frac{\phi(x)}{x^2} \right)} dx$$

Dimensionless electrostatic energy of the electrons.

$$21. \frac{E_{POT}}{kT} = \frac{-az}{\phi(0)} [L + \phi(0)P(0)]$$

Total electrostatic potential energy in units of kT.

$$22. \frac{E_{TOT}}{kT} = \frac{3}{2} \frac{Pv}{kT} + \frac{1}{2} \frac{E_{POT}}{kT}$$

The total energy of the atom in units of kT.

$$23. \frac{E_{TOT}}{z^{7/3}} - \frac{E_{TOT}^{\infty}}{z^{7/3}} = \frac{1}{z^{7/3}} (kT)_{Ry} \left(\frac{E_{TOT}}{kT} \right) - \frac{E_{TOT}^{\infty}}{z^{7/3}},$$

Scaled energy of atom in Rydbergs.

where

The same quantity in (ev) appears in

Column 6 of the Thomas-Fermi tables.

$$\frac{E_{TOT}^{\infty}}{z^{7/3}} = -20.413/13.602 \text{ Ry}$$

$$24. \frac{S}{k} = -z\phi(1) + \frac{5}{2} \frac{Pv}{kT} + \frac{7}{6} \frac{E_{POT}}{kT} + 2azP_0$$

The scaled entropy times $z \cdot \frac{S}{2k}$ is the seventh quantity in the Thomas-Fermi tables.

$$25. TS = \frac{S}{k} (kT)_{Ry}$$

"TS" in Rydbergs/atom.

$$26. E_{TOT} = \left(\frac{E_{TOT}}{kT} \right) (kT)_{Ry}$$

Total energy; in Rydbergs/atom.

$$27. \psi = E_{TOT} - TS$$

Free energy in Rydbergs/atom.

3.3.3 The Structure of Overlay (2,0)

Overlay (2,0) contains the following subroutines, which are now described by name and function:

1. EXEC -- Controls the logic for this segment of the code. It calls the other subroutines and tests for convergence. It prints ϕ at the conclusion of the calculation.
2. START -- Reads data for the Thomas-Fermi compute, calls for interpolation in the Thomas-Fermi tables, and checks the interpolated value of a . Prints calculated parameters.
3. SETD -- Sets values for $\phi(1)$, Δ , and a , which are used in the integration routine.
4. DITS -- Interpolates in Thomas-Fermi tables for first variable and using intermediate table does the interpolation for second variable. Allows for interpolation to be done in logs if desired.
5. FI32 -- Finds value of function $I_{3/2}$ for a given argument.
6. FI12 -- Finds value of function $I_{1/2}$ for a given argument.
7. FIP12 -- Finds value of function $I'_{1/2}$ for a given argument.
8. GRID2 -- Determines N_1 , the initial number of points in X grid, establishes the breakpoint y_b , while generating the grid, and fixes the grid sizes δ_1 and δ_2 .

The procedure for finding y_b , the breakpoint for the integration, is determined as follows:

- a. Let $N_1 = 64 \times 2^i$, where $i = 0, 1, 2, 3, 4$, depending on the iteration index.
- b. Set interval size, $\delta_2 = \frac{1}{N_1}$.

- c. Compute $y_b^* = \frac{2.2}{\{\phi(0)a^2\}^{1/5}}$. y_b^* is an estimate of the value of y where $\phi(y)$ changes sign.
- d. If $y_b^* \geq \frac{1}{4}$, set $y_b = 0.25$, and $\delta_1 = y_b/N_1$.
- e. If $y_b^* < \frac{1}{4}$, an integer, J , is determined such that

$$(J-1) \delta_2 < y_b^* \leq J\delta_2.$$

If J is even, $y_b = J\delta_2$.

If J is odd, $y_b = (J-1)\delta_2$.

Again, $\delta_1 = y_b/N_1$.

9. INTG -- Integrates over the ϕ potential grid and finds values for ϕ, R, P , and $y^3 I_{1/2}(\phi(1)/y^2)$ at each grid point.
10. THERMØ -- Computes and prints thermodynamic results.
11. ØUTPUT -- Computes and prints 16 Thomas-Fermi parameters, which are then carried over to be used in subsequent overlays.
12. FIXI -- Function subprogram used to determine which of the previous $I_{1/2}, I'_{1/2}, I_{3/2}$ functions to execute.
13. SIMPS -- Simpson's Rule integration. Input to routine is x versus $F(x)$ and number of points in function.
14. PCHØUT -- Revises ϕ table (if it is too large) and retains every n th point and its ϕ value and punches all grid information along with the ϕ potential.
15. F32TAB -- Block data control section defines $I_{3/2}$ for argument values of $3.9 < \eta < 19.91$. This table is used for interpolation by subroutine FI32.
16. G4II -- Interpolates in any monotonically ascending or descending table using 4 point interpolation.

3.4 OVERLAY (3,0)

This overlay is an executive routine which controls the flow to overlays (3,1), (3,2), (3,3) and (3,4). It performs no calculations itself.

3.5 OVERLAY (3,1): THE SCHRÖDINGER CALCULATION

Overlay (3,1), the Schrödinger equation calculation, consists of three separate operations: a) the calculation of all of the bound levels with quantum numbers (n,l) which exist in the potential previously defined; b) the calculation of the normalized wave function, χ , for each of these states; and c) the calculation of various integrals of χ with the aim of finding $E_g(n,l)$, the self-screening energy, which is connected with the F_0 integral of each level.

3.5.1 The Theoretical Ideas

3.5.1.1 The Eigen Value Calculation

If one fixes on n and l , the two quantum numbers of a state, one determines N , the number of times the Eigen function changes sign.

$$N = n - l - 1. \quad (36)$$

The Eigen value is that value of the energy E_{nl} which produces the required number of sign changes and satisfies the boundary conditions,

$$\psi(0) = \psi(\mu) = 0, \quad (37)$$

the edge of the atom being taken at $r = \mu$.

The strategy is to guess some initial value of E , integrate outward to $r = \mu$ and then by counting the number of changes of sign and examining the behavior of $\psi(\mu)$, make a new estimate for E_{nl} . If the successive guesses for E_{nl} converge, a bound state exists, and the next level is examined. In order to proceed with this program we must go through the following steps:

1. Once n and l are chosen, a first guess for E_{nl} must be found before the convergence procedure on the Eigen values can commence. The initial guess, E_{nl}^0 , may either be taken as an input, or E_{nl}^0 may be estimated by an algorithm described below.
2. The value for μ , the distance to the "edge" of the atom, must be fixed.
3. The electrostatic screening function ϕ must be found from the unnormalized Thomas-Fermi potential ϕ .
4. Integrate the Schrödinger equation to $r = \mu$.
5. Examine the value of $\psi(\mu)$ and the number of sign changes to make a new guess for E_{nl} . The new guess is used and the procedure begins again at Step 2. If the E 's converge, an Eigen value is found. If there is no convergence, we go to Step 6.
6. This procedure examines the possibility that the level is unbound and properly terminates the computation.

We now examine and describe the six procedures in detail.

1. Estimating E^0

In order to guess $E_{n,l=0}^0$ from E_{n-1} , $l = n-2$ we will need to know $2\xi_n$ which is defined to be the maximum number of free electrons that are available, if all states below that of quantum number n are filled.

Since each principal quantum state, k , can hold, at most, $2k^2$ electrons

$$2\xi_n = z - \frac{(n-1)n(2n-1)}{3}, \quad n > 1. \quad (38)$$

If we assume that the $(n,0)$ state will at most see n more "effective" screening electrons than the $n-1, l = n-2$ state (provided that $n < \xi_n$), then we can justify the following algorithm for estimating E_{nl}^g .

The first guess for the 1st level ($n=1, l=0$) is $E_{n=1, l=0}^g = z^2$. A first guess for each succeeding $n,0$ level is obtained by using the converged Eigen value for the last level of the $n-1$ shell as follows: First,

$$\xi_n = \frac{z - \frac{(n-1)(n)(2n-1)}{3}}{2} \quad (39)$$

is computed for each $n > 1$. (Where ξ_n becomes < 0 , it is < 0 for all remaining n 's.) If $n < \xi_n$,

$$E_{n,l=0}^g = \left(\frac{n-1}{n}\right)^2 E_{n-1, l=n-2} - 2\left(\frac{-1}{n}\right) \sqrt{E_{n-1, l=n-2}} + 1. \quad (40)$$

If $0 \leq \xi_n \leq 0$,

$$E_{n,l=0} \text{ guess} = \left(\frac{n-1}{n}\right)^2 E_{n-1, l=n-2} - \frac{2\xi_n}{n} \left(\frac{n-1}{n}\right) \sqrt{E_{n-1, l=n-2}} + \left(\frac{\xi_n}{n}\right)^2. \quad (41)$$

If $\xi_n \leq 0$,

$$E_{n,l=0} \text{ guess} = \left(\frac{n-1}{n}\right)^2 E_{n-1, l=n-2}. \quad (42)$$

Within each n shell the guess for the next l level is merely the converged E for the level just preceding it. That is:

$$E_{n,l+1}^g = E_{nl} \quad (43)$$

If $E_{n-1,l=n-2}$ is negative (has been set equal to -50 kT as described in the E_0 cut-off routine), the last $E_{n-1,l}$ which was not negative is used to compute the $E_{n,l=0}$ guess.

2. Finding the Value of μ

The edge of the atom, for a bound state, may be defined to be that value of r at which $\psi_{nl}(r)$ may be expected to become "negligible." This definition is not only convenient in that it shortens the range of integration, but it is necessary in that if the integration is carried too far, values of ψ will cease to be significant. We know that in the case of the hydrogenic potential, the dimensionless lengths (μ/a_0) scale like

$$\left(\frac{\mu}{a_0}\right) \frac{z}{n}$$

For any n and l , in the hydrogenic case, one can find a value of

$\left(\frac{\mu}{a_0}\right) \frac{z}{n}$ such that when $r = \mu$, $\psi_{nl}(\mu) \sim 10^{-9}$. Since $\psi \approx P\left(\frac{rz}{a_0 n}\right) e^{-rz/a_0 n}$, where P is a polynomial of order $n-l-1$, the quantities

$\left(\frac{z\mu}{a_0 n}\right) \approx 21$. In generalizing, we now regard the hydrogenic values to be values of $\left(\frac{\mu}{a_0}\right) \frac{z_e}{n}$, where z_e is the "effective" charge defined by

$$E_{nl} = \frac{(z_e)^2}{n^2} \quad (44)$$

Consequently, the code estimates μ by the equation

$$\frac{\mu}{a_0} = \left(\frac{\mu}{a_0}\right) \frac{z_e}{n} / \sqrt{E_{nl}^g} \quad (45)$$

However, if μ/a_0 as calculated by Eq. (24) is greater than r_0 we set $\mu = r_0$ unless provision is made to analytically extend the potential beyond $r = r_0$.

Values of $\left(\frac{\mu}{a_0} \frac{z_e}{n^2}\right)$ are contained in the code. However, provision also exists for reading in an altered table of values of $\left(\frac{z_e \mu}{a_0} \frac{1}{n^2}\right)$.

3. Finding the Screening Function

If $V(x)$ is the potential seen by an electron, $\phi(x)$, the screening function is defined by the equation

$$V(x) = 2z \frac{a_0}{\mu} \frac{\phi(x)}{x^2} \text{ Rydbergs} \quad (46)$$

with the implied conditions

$$\begin{aligned} \phi(0) &= 1, \\ x^2 &= r/\mu. \end{aligned} \quad (47)$$

The $\phi(x)$ function used in the wave equations is computed from ϕ . ϕ is either input or obtained from the Thomas-Fermi compute. ϕ is expressed as a table of numbers, ϕ_n , at specified points, y_n . The y scale is related to r in the Shroedinger equation by

$$y^2 = r/r_0. \quad (48)$$

The code obtains the value of ϕ_n at the appropriate integration points for the wave function by quadratic interpolation (where the scale for the wave function is $x^2 = r/\mu$) and converts ϕ_n to ϕ_n in one of the following ways:

$$a) \quad \phi(x) = \frac{\phi(y) - \phi(1) \frac{\mu}{r_0} x^2}{\phi(0)} \quad (49)$$

$$b) \quad \left\{ \begin{array}{l} \phi(x) = \frac{\phi(y) - \phi(1) \frac{\mu}{r_0} x^2}{\phi(0)}, \quad \frac{\phi(y) - \phi(1) \frac{\mu}{r_0} x^2}{\phi(0)} \geq \frac{1}{2} \\ \phi(x) = \frac{1}{2}, \quad \frac{\phi(y) - \phi(1) \frac{\mu}{r_0} x^2}{\phi(0)} < \frac{1}{2} \end{array} \right. \quad (50)$$

$$c) \quad \phi(x) = \phi(y) \quad (51)$$

$$d) \quad \left\{ \begin{array}{l} \phi(x) = \phi(y), \quad \phi(y) \geq \frac{1}{2} \\ \phi(x) = \frac{1}{2}, \quad \phi(y) < \frac{1}{2} \end{array} \right. \quad (52)$$

If $r_0 < \mu$ and the $\frac{1}{2}$ cut-off is not operable, so that for $y = 1$, $x < 1$, additional $\phi(x)$ values are generated by

$$\phi(x) = A x^2$$

where A is specified. If A is not specified, μ is reset to r_0 .

Case (a) is the usual case, that of the neutral ion sphere at non-zero temperature. Case (b) is an ion sphere at non-zero temperature with a $1/r$ behavior at ∞ . This case should be used with care, since the occupation number calculation corrects for the self-screening implied by a neutral ion sphere. Case (c) allows for the input of a "normalized" potential. Case (d) is Case (c) with a $1/r$ behavior at ∞ .

4. Integration of the Schrödinger Equation

If we set

$$w = r/\mu, \quad (53)$$

$$\lambda = (E_{nl})_{Ry} \left(\frac{\mu}{a_0} \right)^2,$$

then the Schrodinger equation becomes

$$\theta''(w) = \left[\lambda - \frac{2z}{w} \left(\frac{\mu}{a_0} \right) \phi(\sqrt{w}) + \frac{l(l+1)}{w^2} \right] \theta(w). \quad (54)$$

If we now change to a quadratic scale, setting

$$\psi(x) = \theta(w) \quad (55)$$

$$x^2 = w$$

we can show that Eq. (54) is equivalent to the integral equation

$$\psi(x) = x^2 \delta_{0l} + 2 \int_0^x \psi(y) y (x^2 - y^2) F(y) dy \quad (56)$$

where

$$F(y) = \lambda - \frac{2z}{y^2} \frac{\mu}{a_0} \phi(y) + \frac{l(l+1)}{y^4}. \quad (57)$$

It is convenient to define

$$P(x) = 2 \int_0^x y F(y) \psi(y) dy. \quad (58)$$

If one uses the integration formula

$$\int_{x_{n-1}}^{x_n} f(x) dx = \frac{\Delta x}{24} \left[9 f_n + 19 f_{n-1} - 5 f_{n-2} + f_{n-3} \right]. \quad (59)$$

It then follows that

$$\begin{aligned} \psi_n = & \psi_{n-1} + (2x_n - \Delta x) R_{n-1} \\ & + \frac{(\Delta x)^2}{6} \left[(2x_n - \Delta x) f_{n-1} - (3x_n - 4\Delta x) f_{n-2} + (x_n - 2\Delta x) f_{n-3} \right] \end{aligned} \quad (60)$$

where

$$R_n = \Delta x (\delta_{0k} + P_n) + \frac{(\Delta x)^2}{24} [15f_n - 4f_{n-1} + f_{n-2}] \quad (61)$$

and

$$f_n = 2x_n F_n \psi_n = 2x_n \psi_n \left[\lambda - \frac{2z}{x_n^2} \frac{\mu}{a_0} \phi(x_n) + \frac{2(l+1)}{x_n^4} \right]. \quad (62)$$

From Eqs. (58), (59), (61), and (62) we have the simple iteration scheme for R_n

$$R_n = R_{n-1} + (\Delta x)^2 f_n. \quad (63)$$

Equations (60), (62), and (63) along with the definition of Eq. (57) are sufficient to propagate the solution to the point n if values at $n-1$, $n-2$, and $n-3$ are known.

In order to get the starting values at points Δx , $2\Delta x$, and $3\Delta x$, it is necessary to have the following starting series, which is found by inserting a series expansion into the integral equation. These series are

$$\psi_k(x) = x^{2k+2} \left[1 - \frac{2\mu}{a_0} \frac{\phi(0)}{k+1} x^2 + \dots \right] \quad (64)$$

$$P_k(x) = x^{2k} \left[(k+1)(1-\delta_{0k}) - \frac{k+2}{k+1} \frac{2\mu}{a_0} \phi(0)x^2 + \dots \right]. \quad (65)$$

The first three values of R_n must be found by Eq. (61) and Eq. (65) rather than by Eq. (63).

The starting series is carried out to $x_3 = 3\Delta x_1$. At this point $T(x) = z \frac{\psi}{a_0} \frac{x^2}{l+1}$ is computed.

- (1) If $T(x_3) > 0.3$, Δx_1 is halved and the computation restarted (new $\psi(x)$'s and $f(x)$'s).
- (2) If $T(x_3) \leq 0.3$, $f(x_2)$, $f(x_1)$, $f(x_0)$ are tested:
 - a. If $f(x_2)$, $f(x_1)$ and $f(x_0)$ are $> 10^{-30}$, the starting series compute is dropped here and integration started.
 - b. If $f(x_2)$, $f(x_1)$, $f(x_0)$ are $< 10^{-30}$, computation of $T(x)$ is continued, the starting series is continued and the test for three successive f 's $> 10^{-30}$ continued.
- (3) If $x_n > x_3$ is the first x for which $T > 0.3$ and if $f(x_{n-3})$, $f(x_{n-2})$, $f(x_{n-1})$ are not $> 10^{-30}$

$$c = \frac{1}{(x_n - 2\Delta x)} \left(\frac{10^{-15} x_n}{l+1} \right)^{1/(l+1)}$$

is computed.

- (4) Starting from $x = 0$ with the same Δx_1 , new ψ 's, f 's, etc., are computed using the following starting series:

$$\psi(x) = (cx)^{2l+2} \left[1 - \frac{z\psi}{a_0} \frac{\phi(0)}{l+1} x^2 + \dots \right] \quad (66)$$

$$P(x) = c^2 (cx)^{2l} \left[(l+1)(1-\delta_{0l}) - \frac{l+2}{l+1} \frac{z}{a_0} \phi(0) x^2 + \dots \right] \quad (67)$$

- (5) The starting series in Step (4) is continued until three successive f 's are $> 10^{-30}$.

The first choice of Δx_1 is obtained from a table of constant values held in the code. There is also a break point, x_n , beyond which the interval size increases to Δx_2 . These grid values, in general, are specific to each level, and have been chosen by experience. There is an option to input a different choice of grid values.

A special treatment of R_n and P_n is required at the break point. At the break point, x_b , one sets

$$R(x_b) + (\Delta x_1)^2 f(x_b) = \Delta x_1 (\delta_{0l} + P(x_b)) + \left[15f(x_b) - 4f(x_b - \Delta x_1) + f(x_b - 2\Delta x_1) \right] \frac{(\Delta x_1)^2}{24}, \quad (68)$$

and then solves for $P(x_b)$. $R(x_b)$ may then be recomputed:

$$R(x_b) = \Delta x_2 (\delta_{0l} + P(x_b)) + \frac{\Delta x_2^2}{24} [15f(x_b) - 4f(x_b - \Delta x_2) + f(x_b - 2\Delta x_2)]. \quad (69)$$

Beyond the break point the integration continues until a value of $\psi(x=1)$ is found.

5. Eigen Value Convergence, $\psi(1) = 0$

a. The wave function, $\psi(x)$, for each n , l level has N changes of sign in the interval $(0,1)$, where

$$N = n - l - 1. \quad (70)$$

b. For a given level, the code determines N and obtains a guess for λ_0 either from an input E or from the E guess routine (where $\lambda = E(\mu/\alpha_0)^2$). Starting from this guess, two values of λ , λ_1 and λ_2 which give a $\psi(x)$ with N and $N+1$ changes of sign must be obtained.

c. To obtain λ_1 and λ_2 from λ_0 , first $\psi(x, \lambda_0)$ is computed using the equations under 4. The number of changes of sign in $\psi(x, \lambda_0)$ and the value of $\psi(1, \lambda_0)$ are kept. If $\psi(1, \lambda_0)$ has $\begin{pmatrix} \leq N \\ \geq N+1 \end{pmatrix}$ changes of sign, the sequence of values $\psi(1, \lambda_0^{(1)})$ where

$$\lambda_0^{(1)} = \lambda_0^{(i-1)} \left(1 \pm \frac{1}{L} \right) \quad (71)$$

and

$$L = 10$$

are computed.

d. This is continued through $i = 5$. If, $\psi(1, \lambda_0^{(1)})$ giving exactly $\begin{pmatrix} N \\ N+1 \end{pmatrix}$, and $\psi(1, \lambda_0^{(i-1)})$ giving exactly $\begin{pmatrix} N+1 \\ N \end{pmatrix}$ changes of sign, has not been found, L is changed to 2. The step-off is continued until a $\psi(1, \lambda_0^k)$ is obtained which has exactly $\begin{pmatrix} N \\ N+1 \end{pmatrix}$ changes of sign and $\psi(1, \lambda_0^{k-1})$ has exactly $\begin{pmatrix} N+1 \\ N \end{pmatrix}$ changes of sign. Then λ_0^{k-1} and λ_0^k are λ_1 and λ_2 .

e. A flag ($f \neq 0$) is set to indicate we have passed the L step-off routine.

f. Having λ_1 and λ_2 and $\psi(1, \lambda_2)$, the next guess at λ is the average of λ_1 and λ_2 , namely,

$$\lambda_3 = \frac{\lambda_1 + \lambda_2}{2} \quad (72)$$

g. Thereafter a quadratic interpolation is done on the 3 λ 's which yield $\psi(1, \lambda)$'s closest to 0 and for which 2 of the $\psi(x, \lambda)$ functions will have $\begin{pmatrix} N \\ N+1 \end{pmatrix}$ changes of sign and one will have $\begin{pmatrix} N+1 \\ N \end{pmatrix}$ changes of sign.

h. The interpolation scheme used is as follows:

- (1) The 3λ 's defined in "g" are ordered so they are either increasing or decreasing. Call them $\lambda_0, \lambda_1, \lambda_2$ and the $\psi(1)$'s associated with these ψ_0, ψ_1 , and ψ_2 .
- (2) w_0, w_1 and w_2 are computed where

$$\begin{aligned} w_0 &= \lambda_0 - \lambda_1 \\ w_1 &= \lambda_1 - \lambda_1 = 0 \\ w_2 &= \lambda_2 - \lambda_1 \end{aligned} \tag{73}$$

- (3) The coefficients for the second degree polynomial

which passes through $\begin{Bmatrix} w_0, w_1, w_2 \\ \psi_0, \psi_1, \psi_2 \end{Bmatrix}$ are then obtained:

$$\begin{aligned} a &= \frac{\psi_0}{w_0(w_0 - w_2)} + \frac{\psi_1}{w_2 w_0} + \frac{\psi_2}{w_2(w_2 - w_0)} \\ b &= \frac{-\psi_0 w_2}{w_0(w_0 - w_2)} - \frac{\psi_1(w_0 + w_2)}{w_0 w_2} - \frac{\psi_2 w_0}{w_2(w_2 - w_0)} \\ c &= \psi_1 \end{aligned} \tag{74}$$

- (4) Having obtained a, b , and c , the $2w$'s which yield $\psi(1) = 0$ are

$$w_{a,b} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \tag{75}$$

and

$$\begin{aligned} \lambda_a &= \lambda_1 + w_a \\ \lambda_b &= \lambda_1 + w_b \end{aligned} \tag{76}$$

(5) λ_a and λ_b are tested:

- (a) If only one lies between λ_0 and λ_2 , that λ is used to replace λ_0 , λ_1 or λ_2 .
- (b) If both lie between λ_0 and λ_2 , and one lies between λ_+ and λ_- , where λ_+ is the λ associated with the positive ψ of smallest absolute value and λ_- is the λ associated with the negative ψ of smallest absolute value, that λ is used to replace λ_0 , λ_1 or λ_2 for the next interpolation.
- (c) If it should happen that neither λ_a or λ_b lies between λ_0 and λ_2 , both λ_a and λ_b are discarded and

$$\frac{\lambda_+ + \lambda_-}{2} \text{ is used to replace } \lambda_0, \lambda_1 \text{ or } \lambda_2.$$

i. Interpolation is continued until two successive λ 's satisfying

$$\left| \frac{\lambda_f - \lambda_{f-1}}{\lambda_y} \right| \leq t, \quad (77)$$

where $t = 0.2 \times 10^{-6}$ are obtained. The integration is then terminated and the test under (k) is made to assure the μ/a_0 scale was accurate for the converged λ_f .

j. If λ_f has not been found after a total of 20 iterations, the E_0 cut-off routine is called. (See Section 6.)

k. E_f is computed from λ_f and

$$\xi = \left| \frac{\sqrt{E_{\text{guess}}} - \sqrt{E_f}}{\sqrt{E_f}} \right| \quad (78)$$

is determined.

- (a) If $\xi \leq 0.05$, E_f is the converged Eigen value. It is printed and stored according to the index, I, and integration for the next level is begun.
- (b) If $\xi > 0.05$, μ/a_o is recomputed, where

$$\mu/a_o^{(2)} = \frac{(z_e \mu/a_o)}{n \sqrt{E_f}} \quad (79)$$

and the integration and λ convergence for this level is done again using the same interval size and replacing μ/a_o guess and E_{guess} by $\mu/a_o^{(2)}$ and E_f .

- (c) The $E_f^{(2)}$ obtained using $\mu/a_o^{(2)}$ is then the answer (providing the ξ test on $\sqrt{E_f}$ and $\sqrt{E_f^{(2)}}$ is met) and is stored according to I.
- (d) If the ξ test is not satisfied after a converged λ has been found for μ/a_o guess and $\mu/a_o^{(2)}$, Δx_1 and Δx_2 are halved, and the entire Eigen value convergence scheme is repeated using $\mu/a_o^{(2)}$ and $E_f^{(2)}$ as a guess.
- (e) If the ξ test is not met on the second μ/a_o determined on this finer grid, a message is printed and the integration terminated.

6. E_o Cut-Off is Used to Determine if any Particular Level is Bound

a. Converged Eigen values are stored away according to increasing n and l (on the index, I) for later use.

b. Each $E_{n,l}$ computed is tested against $|E_o|$ (from Thomas-Fermi) before it is stored away. Only those $> |E_o|$ are kept.

- (1) If $E_{n=1, l=0} < |E_o|$, it is not stored and no more Eigen values are computed.

- (2) If $E_{n+1, l \neq 0} < |E_0|$, no more E's for that n are computed; the rest are set = -50 kT, but computation is continued for the $n = i+1, l=0$ level.
- (3) Testing against $|E_0|$ is continued until $E_{n=i+1, l \neq 0} < |E_0|$.
- (4) Steps 2 and 3 are repeated with i increased by 1 each time until the first time $E_{n=q, l=0} < |E_0|$ ($q \leq 15$). No more Eigen values are computed.

c. If an Eigen value has not been found for any level before 20 iterations are completed, tests against $|E_0|$ are also made.

- (1) If two successive λ 's have not yielded N and N+1 changes of sign ($f=0$, see 5-e) for the (n, l) level, an E_{nl} is computed from the λ used for the last iteration.
 - (a) If $E_{nl} < |E_0|$, E_{nl} and all E's for that n are set = -50 kT and the code skips to the $n+1, l=0$ level.
 - (b) If $E_{nl} > |E_0|$ a message is printed, the E's obtained to this point are printed and punched along with their index numbers and the computation is stopped.
 - (c) The form of the punched E's is such that they can be read back into the Schrödinger overlay or into subsequent overlays as converged E's.
- (2) If two successive λ 's have yielded N and N+1 changes of sign ($f \neq 0$), E's associated with both these λ 's are computed, call them E_k and E_{k-1} .
 - (a) If both E_k and E_{k-1} are $< |E_0|$ the code follows (1) (a) above.
 - (b) If one or both E_k and E_{k-1} are $> |E_0|$, $\Delta E = (E_k - E_{k-1})/kT$ is computed.

- (i) If $\Delta E \leq 10^{-3}$, the larger of E_k and E_{k-1} is used for $E_{n\lambda}$, a message "weakly convergent" is printed, and the code proceeds to the next level.
- (ii) If $|\Delta E| > 10^{-3}$, either E_k or E_{k-1} is used as an initial guess and the entire iteration scheme is redone for this level. If convergence is not obtained the second time, a message is printed and all previously computed Eigen values are printed and punched in a format which can be used in subsequent computations. The computation is then stopped.

3.5.1.2 Normalizing the Wave Function

The wave function ψ_n computed in the previous section suffers from the fact that no matter how closely $E_{n\lambda}$ is fixed, $\psi(1) \neq 0$. This is a consequence of the fact that in the course of the outward integration $\psi(x)$ will have picked up some integration error which is propagated forward as part of the irregular solution; this solution grows exponentially with x .

In order to have a useful, and normalized representation of ψ we must fit the boundary condition exactly at both ends of the interval $(0,1)$. To do this we must integrate Eq. (54) backwards as well as forward. The procedure is as follows:

1. Using the converged value of λ , integrate Eq. (54) starting at $x = 1$, $\psi(1) = 0$ and proceed inward to a grid point x_{n0} which is near x_0 . The turning point, x_0 , is defined by the equation

$$F(x_0) = 0. \quad (80)$$

2. Integrate outward from the origin to x_{no} .
3. Match the two solutions at x_{no} .

The details of these three procedures are as follows.

1. The Inward Integration

The integral equation for the inward integration which is analogous to Eq. (56) is

$$\begin{aligned}\psi(x) &= (\alpha - x^2) + 2 \int_x^1 dy F(y) \psi(y) (y^2 - x^2) dy \\ P(x) &= 2 \int_x^1 y F(y) \psi(y) dy.\end{aligned}\tag{81}$$

The solution of this equation satisfies the differential equation (Eq. 54). Furthermore, it satisfies the boundary conditions of $x = 1$.

$$\left. \begin{aligned} \text{(a) if } \frac{d\psi}{dx} \Big|_{x=1} &= 2\psi(1), \text{ set } \alpha=0 \\ \text{(b) if } \psi(1) &= 0, \text{ set } \alpha=1 \end{aligned} \right\} \tag{82}$$

The difference equations for the inward integration which are analogous to Eqs. (60) through (63) are

$$\psi_n = \psi_{n+1} + (2x_n + \Delta x) \bar{R}_{n+1} \tag{83}$$

$$+ \frac{(\Delta x)^2}{6} \left[(2x_n + \Delta x) f_{n+1} - (3x_n + 4\Delta x) f_{n+2} + (x_n + 2\Delta x) f_{n+3} \right],$$

$$\bar{R}_n = \bar{R}_{n+1} + (\Delta x)^2 f_n, \tag{84}$$

$$\bar{R}_n = \Delta x (1 + P_n) + \frac{(\Delta x)^2}{24} \left[15f_n - 4f_{n+1} + f_{n+2} \right]. \tag{85}$$

Of course f_n is given by Eq. (62).

The corresponding starting series are

$$\psi_l = (a-1) + (1-x^2) + \frac{1}{2} \left[l(l+1) + \lambda - \frac{2a_0\phi(1)}{a_0} \right] (a-1)(1-x^2)^2 + \dots \quad (86)$$

and

$$P_l = \left[l(l+1) + \lambda - \frac{2a_0\phi(1)}{a_0} \right] (a-1)(1-x^2) + \frac{1}{2} \left[\lambda - \frac{2a_0\phi(1)}{a_0} - \frac{2a_1}{a_0} (\phi(1) + \phi'(1)) (a-1) + l(l+1)(1+2(a-1)) \right] (1-x^2)^2 + \dots \quad (87)$$

P_l , ψ_l , and $\bar{R}$ are computed at $x=1$, $x=1-\Delta$, $x=1-2\Delta$ by using the starting series; the integration then proceeds to the grid point nearest x_0 , which is x_{n0} , and which is also a grid point for the outward integrations.

2. The Outward Integration

This proceeds just as in the previous section.

3. The Matching and Normalization Proceeds as Follows

a. On inward integration the $\psi(x)$'s are scaled by 10^{-30} to prevent overflow. Also, the outward starting series is carried until three successive f 's are $>10^{-30}$.

b. K is computed using Simpson's Rule as follows:

$$K = 2u/a_0 \left[\int_{x_{n0}}^{x_0} dx \, x \, \psi^2(x) + \left(\frac{t_0}{t_1} \right)^2 \int_{x_{n0}}^1 dx \, x \, \psi^2(x) \right] \quad (88)$$

where $\psi(x)$ is the un-normalized wave function ordered on increasing x and $t_0 = \psi(x_{n0})$ from the outward integration; $t_1 = \psi(x_{n0})$ from the inward integration.

c. The normalized wave-function, $\chi(x)$, is then computed

$$\begin{aligned}\chi(x) &= \frac{\psi(x)}{\sqrt{K}} & x \leq x_{no} \\ \chi(x) &= \frac{\psi(x)}{\sqrt{K}} \left(\frac{t_0}{t_1} \right) & x > x_{no}\end{aligned}\quad (89)$$

d. χ is continuous over the interval, satisfies the differential equation, and furthermore

$$2\mu/a_0 \int_0^1 x \chi^2 dx = 1 \quad (90)$$

3.5.1.3 Finding the Integrals of the χ Function

Having the normalized wave functions, χ , at hand we compute the following integrals and related quantities.

$$\frac{1}{4} F_{10} = \int_0^1 dx \frac{\chi^2}{x} \int_0^x dy y \chi^2 = N_1 \quad (91)$$

$$\frac{L_n}{2\mu/a_0} - \frac{1}{4} F_{20} = \int_0^1 dx x \chi^2 \int_0^x dy \frac{\chi^2}{y} = N_2 \quad (92)$$

$$\frac{1}{4z} \frac{E_p}{e^2/2a_0} = \int_0^1 dx \frac{\chi^2}{x} \phi(x) = L_p \quad (93)$$

$$\frac{1}{4z} \frac{E_N}{e^2/2a_0} = \int_0^1 dx \frac{\chi^2}{x} = L_N \quad (94)$$

$$\frac{E_N}{e^2/2a_0} = 4z L_N \quad (95)$$

$$\frac{E_p}{e^2/2a_0} = 4z \quad (96)$$

$$\frac{E_s}{e^2/2a_0} = 4\mu/a_0 \left(N_1 - N_2 + \frac{L_N}{2\mu/a_0} \right) \quad (97)$$

E_p is the electrostatic energy of an electron in the potential of the atom. E_n is the electrostatic energy of the nuclear charge in potential of the electron. E_s is the interaction energy of the electron with the potential produced by its own charge distribution. E_s is proportional to the so-called F_0 integral. E_s is used in the opacity calculation to correct for the fact that we are using a neutral ion sphere rather than a potential which is asymptotic to $1/r$.

3.5.2 The Structure of Overlay (3,1)

Overlay (3,1) consists of the decks, SMAIN, EGUES3, GLII, PHIF, ILLIST, ECØFF3, SIN, SIMSON, SCHACS, SNØRE, SCH, and SCHI. The functions of these decks are as follows.

1. SMAIN

Executive routine to compute any, or all, of 108 Schrodinger energy levels. Directs the flow of the calculation.

2. EGUES3

Generates E_g for each level to be examined. See Eqs. (39-43).

3. GLII

A generalized interpolation routine which uses 3 point interpolation (2 before - 1 after) in any monotonically ascending or descending table.

4. PHIF

A routine to operate on the Thomas-Fermi potential ϕ in four distinct ways (at option) and produce a ϕ function to be used in Schrödinger and Dirac equations. See Eqs. (49-52).

5. ILIST

A function for testing $(A-B)/A < 2 \times 10^{-6}$. The function returns "1" if $(A-B)/A$ is $< 2 \times 10^{-6}$, returns a "2" if not. This is used in finding the converged Eigen values. See Eq. (77) of theoretical discussion (Section 3.5.1).

6. EC0FF3

Called if energy guess failed to make calculation converge. Used to determine if a level is truly bound. See paragraph 6 of theoretical discussion (Section 3.5.1).

7. SIN

Finds integrals--given a converged E and corresponding wave function.

8. SIMSON

Simpson's Rule integration routines.

9. SCHACS

Given an E guess, finds $\psi(E_g)$, $\psi(E_g + \Delta)$, $\psi(E_g - \Delta)$ and interpolates to find a value of E such that $\psi(E) = 0$, at $x = 1$.

10. SNORE

Joins and normalizes the inward and outward integrated wave functions. See Section 3.5.1.2.

11. SCH

Performs outward integration.

12. SCHI

Performs inward integration.

3.6 OVERLAY (3,2): THE DIRAC CALCULATION

Just as overlay (3,1) is used to solve the Schroedinger equation, overlay (3,2) is used to find the Eigen values of the Dirac equation. However, in overlay (3,2) no normalized wave functions or interaction energies are computed.

Consequently it is usually necessary to go through overlay (3,1) just to find E_0 , the self-screening energies. Of course if overlay (3,2) is executed, then the Dirac equation Eigen values rather than the less nearly correct Schrödinger Eigen values will be used in the subsequent opacity calculations. However, the Schrödinger Eigen values are used in this overlay to provide a first guess for the Dirac equation Eigen value convergence routine.

3.6.1 The Theoretical Ideas

The computation of the Dirac equation energy levels proceed as follows.

a. This overlay uses either an input potential ($\phi(y)$) or a potential obtained from the Thomas-Fermi overlay to determine the atomic potential. The options for the normalization of the potential conversions which are allowed are the same as those listed in overlay (3,1).

b. The quantum numbers for the Dirac equation are n, l and k . As in the Schrödinger equation, n and l are the principal quantum number and the orbital quantum number respectively. Furthermore, if j is the total angular momentum, then k is fixed as follows:

$$j = l + \frac{1}{2} \Rightarrow k = -l - 1$$

$$j = l - \frac{1}{2} \Rightarrow k = l.$$

The levels are dictionary ordered:

1. First on increasing n , $n = 1, 2, 3 \dots 15$.
2. Second for each fixed n , on increasing l , where $l = 0, 1, 2 \dots n-1$.
3. Third for each fixed (n, l) on increasing j , where $j = l \pm \frac{1}{2}$. Of course if $l = 0$, only $j = \frac{1}{2}$ is allowed.

c. The maximum number of Dirac Eigen values which can be computed is 200. The largest level as set up now is $n = 15$, $l = 2$, $k = 2$.

d. A first guess, E_g , for λ , where $\lambda = E_g$, is obtained

1. From input cards, or
2. From the Schrödinger overlay.

If E_g comes from (2), the converged Schrödinger energy for the corresponding Dirac level or $|E_g| \times 1.1$ is used, whichever is the larger.

e. The Runge-Kutta method is used to integrate outward the coupled Dirac equations, which are expressed as

$$\frac{d\psi_b(x)}{dx} = -\frac{2k}{x} \psi_b(x) + \frac{2u}{a_0} x \left(\beta + \alpha \frac{a_0}{u} \frac{\phi(x)}{x^2} \right) \psi_a(x) \quad (98)$$

$$\frac{d\psi_a(x)}{dx} = \frac{2k}{x} \psi_a(x) - \frac{2u}{a_0} x \left(\gamma + \alpha \frac{a_0}{u} \frac{\phi(x)}{x^2} \right) \psi_b(x) \quad (99)$$

where,

$$\alpha = \frac{e^2}{\hbar c} = \frac{1}{137.024} \quad (100)$$

$$\beta = \frac{\alpha}{2} \left(-\lambda + \frac{2mc^2}{e^2/2a_0} \right) \frac{\alpha}{2} (-\lambda + 0.7510349138 \times 10^5) \quad (101)$$

$$\gamma = -\frac{\alpha}{2} \lambda \quad (102)$$

$$\lambda = \frac{E_{nlk}}{e^2/2a_0} \quad (E_{nlk} \text{ is the Binding energy}) \quad (103)$$

$$x^2 = r/\mu \quad (104)$$

$$\frac{\hbar^2}{me} \frac{eV}{e^2} = \frac{za_0}{\mu} \frac{\phi(x)}{x^2} \quad (105)$$

The starting series are

$$\psi_b = x^{2S} (1 + B_1 \mu/a_0 x^2 + \dots) \quad (106)$$

$$\phi_a = x^{2S} (A_0 + A_1 \mu/a_0 x^2 + \dots),$$

for $|k| \leq 6$ and,

$$\psi_a = 10^{-30} (1 + B_1 \mu/a_0 x^2 + \dots) \quad (107)$$

$$\phi_a = 10^{-30} (A_0 + A_1 \mu/a_0 x^2 + \dots)$$

for all $|k| \geq 7$. Here,

$$S = (k^2 - z^2 \alpha^2 \phi^2(o))^{1/2}, \quad (108)$$

$$A_0 = \frac{S+k}{Z\alpha\phi(0)}, \quad (109)$$

$$A_1 = \frac{-(\gamma+Z\alpha a_0\phi_1)(S+1+k) + (S+k)(\beta+Z\alpha a_0\phi_1)}{(S+1)^2 - k^2 + Z^2\alpha^2\phi(0)}, \quad (110)$$

$$B = \frac{-(\gamma+Z\alpha a_0\phi_1) + (S+1-k)A_1}{Z\alpha\phi(0)}, \quad (111)$$

where $\phi_1 = \left. \frac{d\phi}{dx} \right|_{x=0}$.

f. The range of the integration is the interval (0, 1) on x, and the code allows a fixed interval size (presently 0.01) for the integration.

g. A given level denoted (nℓk) has N changes of sign, where N is determined by

$$N = n - \ell - 1.$$

h. μ/a_0 is determined for any level from the $\frac{Z_e \mu/a_0}{n}$ table by a search on nℓk (or the I associated with each level). Then, as in the Schrödinger link

$$\mu/a_0 = \frac{Z_e \mu/a_0}{n} \times \frac{1}{\sqrt{E}}. \quad (112)$$

i. When a Thomas-Fermi potential $\phi(y)$ is used and

$$\phi(x) = \frac{\phi(y) - \phi(1) \mu/a_0 x^2}{\phi(0)} \quad (113)$$

the derivative ϕ_1 is given by

$$a_0 \phi_1 = - \frac{2aP_0}{\phi(0)} \frac{a_0}{r_0}. \quad (114)$$

j. The Eigen value convergence scheme is the same as that described in the Schrödinger link. The changes of sign and the condition $\psi(1) = 0$ are both examined for $\psi_b(x)$, which is the "large" component of the pair of coupled Dirac wave functions.

k. Converged Eigen values are stored and printed in the order described under "b" to be called for later use by the occupation number routine or punched if the E_0 cut-off routine so prescribes.

1. The E_0 cut-off routine is the same as that described in the Schrodinger overlay.

3.6.2 The Structure of the Overlay

Overlay (3,2) contains the decks DMAIN, DGLII, DPHIF, ECOPYF4, SCHACD, ACDAUX, RKAM, and EGUES4. These decks perform the following functions.

1. DMAIN

This is the controlling routine for the Dirac Wave Equation integration. Up to 200 energy levels are examined using E_g , (guesses) which are read in, or it uses guesses from the Schroedinger converged values (if that portion was done).

2. DGLII

Same interpolation routine as used in overlay (3,1).

3. DPHIF

The same ϕ function routine as is in overlay (3,1). The little IL ST function is included in this deck.

4. ECØFF4

This routine is called if the energy failed to converge. Determines where failure occurred and adjusts E to a suitable value where possible. Analogous to ECØFF3 of overlay (3,1).

5. SCHACD

This routine uses $E_g \pm \Delta$ and finds values for $\text{PSI}(E_g)$, $\text{PSI}(E_g + \Delta)$, $\text{PSI}(E_g - \Delta)$ and interpolates to find a value of E such that $\text{PSI}(E) = 0$. Analogous to SCHACS of overlay (3,1).

6. ACDAUX

This is the integration deck. It consists of two parts:

a) AC is the controlling routine. First it computes the necessary starting values and constants for the subsequent integration of the Dirac equation. It then calls RKAM at every grid point to propagate the solution forward from point to point.

b) DAUX is a routine used both by RKAM and by AC. Given values of ϕ , ψ_a , and ψ_b at some grid point it then computes $\frac{d\psi_a}{dx}$ and $\frac{d\psi_b}{dx}$ at that grid point by evaluating the right hand side of the differential equations.

7. RKAM

RKAM is the Runge-Kutta-Adams-Moulton integration package. It returns values of ψ_a and ψ_b at the $(n+1)^{\text{th}}$ point if ψ_a , ψ_b , ψ'_a , ψ'_b are known at four previous grid points.

8. EGUES4

This is a dummy routine.

3.7 OVERLAY (3,3): THE OCCUPATION NUMBER OVERLAY

For each bound state with quantum numbers (n, ℓ, j) overlay (3,3) computes $\bar{N}_{n, \ell, j}$ which is the average number of bound electrons present in that state. This overlay also finds $\bar{N}_f$, the number of free electrons present in the neutral ion sphere. Furthermore, as a consequence of this calculation, α , the degeneracy parameter, which corresponds to the set $\{\bar{N}_{n, \ell, j}\}$, is also found.

The calculation requires $E_{n, \ell, j}$ the Dirac energy levels. In the event that these are lacking (because overlay (3,2) was bypassed), overlay (3,3) will store the Schrodinger levels $E_{n\ell}$ in the appropriate Dirac levels $E_{n, \ell, j=\ell-1/2}$ and $E_{n, \ell, j=\ell+1/2}$ to allow the calculation to proceed.

3.7.1 The Theoretical Ideas

It has been shown elsewhere [1] that if α is the degeneracy parameter, then the bound occupations are

$$\bar{N}_{n, \ell, j} = \frac{\Omega_j}{1 + e^{-\frac{\alpha}{kT} - \frac{E_{n, \ell, j}}{kT}}} \quad (115)$$

where

$$\Omega_j = 2j + 1 \quad . \quad (116)$$

Similarly, $\bar{N}_f$, the number of free electrons is

$$\bar{N}_f = A \, I_{1/2} \left(\frac{\alpha - E_0}{kT} \right), \quad (117)$$

where

$$A = \frac{2}{3\pi} \left(\frac{r_0}{a_0} \right)^3 (kT)_R^{3/2}. \quad (118)$$

The degeneracy parameter α is determined by the condition that

$$z = \bar{N}, \quad (119)$$

where

$$\bar{N} = \bar{N}_f + \sum_{n,l,j} N_{n,l,j}. \quad (120)$$

In practice a first guess for α , $\alpha = \alpha_0$ is taken as $\Phi(1)$. Using α_0 , $\bar{N}_f$ and $\bar{N}_{n,l,j}$ are computed and $\bar{N}$ is found. By comparing $\bar{N}$ with z a new α is guessed and the iteration is continued until Eq. (119) is satisfied to a desired precision.

The details of the calculation are as follows:

1. Compute

$$Z_N(\alpha_N) = \sum_{n,l,j} \bar{N}_{n,l,j}(\alpha_N) + \bar{N}_f(\alpha_N) - z,$$

starting with α_0 .

2. If $Z_N \leq 0$ repeat with $\alpha_{N+1} = \alpha_N(1 - a)$;

$$Z_N > 0 \quad \text{repeat with } \alpha_{N+1} = \alpha_N(1 + a)$$

$$a = 0.1.$$

3. Continue until

$$Z_N(\alpha_N) > 0 \geq Z_{N-1}(\alpha_{N-1})$$

or

$$Z_N(\alpha_N) \leq 0 < Z_{N-1}(\alpha_{N-1}).$$

4. Linearly interpolate on Z_N, Z_{N-1} for α . Then quadratically interpolate with Z_{N+1}, Z_N, Z_{N-1} .

5. Continue quadratic interpolation until

$$|Z_N| < 0.00001, \text{ if } Z \leq 10.$$

(The tolerance on Z_N is 1.5×10^{-3} for Z 's > 10 .)

This prescription, in principle, determines $\bar{N}_f, \{\bar{N}_{n,l,j}\}$, and α . There remains a small problem connected to the fact that the code only allows one to consider the first 200 Dirac levels. In most cases this is more than adequate to describe all the bound levels.

If it is conceivable, however, that $ED_{n=15} = ED(200) > |E_0|$, there may exist higher lying bound levels $E_{n>15}$ with the property

$$ED(200) > ED_{n>15} > |E_0|. \quad (121)$$

These bound levels must be provided for, even though the electron occupation of these levels is often negligible. The number of states, $\Omega_>$ that lie above the 200th level but have energy below $|E_0|$ is approximately

$$\Omega_> = \frac{2}{3} (15)^3 \left(\left[\frac{ED(200)}{|E_0|} \right]^{3/2} - 1 \right). \quad (122)$$

The actual number of high lying bound electrons is approximately

$$\bar{N}_j \approx e^{a/kT + |E_0|/kT} \Omega_j, \quad \frac{a}{kT} \ll 0. \quad (123)$$

If j_{200} is the spin of the 200th Dirac level, then the code will set

$$\bar{N}_{200} \approx (2j_{200} + 1) e^{a/kT + E_{200}/kT}. \quad (124)$$

We choose to make provision for the levels $\bar{N}_j$ by placing them all in the 200th level.

Consequently, if Eq. (85) holds, then to get $\bar{N}_j = \bar{N}_{200}$ we set

$$j_{200} = \frac{(15)^3}{3} \left(\left[\frac{E(200)}{E_0} \right]^{3/2} - 1 \right) e^{|E_0|/kT - E(200)/kT} - \frac{1}{2}. \quad (125)$$

All other j 's, of course, are found by setting

$$j = l \pm \frac{1}{2}. \quad (126)$$

The occupation numbers found by this procedure are used in overlay (3,5) to compute the opacity.

3.7.2 The Structure of the Overlay

This overlay consists of the four decks ØCCNØS, STØREJ, ØCCINT, FI512, which have the following functions.

1. ØCCNØS is the executive routine for this overlay.
2. STØREJ arranges the energies in order from ED(1) to ED(200).

If only Schrodinger energies are available, it places the energy

E_{nl} in the cells for the Dirac energies $E_{n,l,j=l+1/2}$ and

$E_{n,l,j=l-1/2}$. Finally, it computes the total spin
 $j=l\pm 1/2=EJ(I)$ to correspond with each energy $ED(I)$.

3. $\phi CCINT$ is the convergence routine which determines α ,
 $\bar{N}_f$ and $\bar{N}_{n,l,j}$ for all levels.
4. FI512 finds the $I_{1/2}$ function. It is the same as FI12 in
overlay (2,0).

3.8 OVERLAY (3,4)

Overlay (3,4) is a "dummy" overlay which has been included in the system to provide room for the planned inclusion of a matrix-element calculation. At present this overlay is empty.

3.9 OVERLAY (3,5): THE OPACITY COMPUTATION

Overlay (3,5) computes the continuous part of the reduced absorption coefficient defined in Eq. (4). $D(u)$ is computed over a frequency grid $0.2 \leq u \leq 30$. The opacity K_R is then found by using Eq. (7).

The reduced continuous absorption coefficient is formed of three parts, D_s , D_{ff} , and D_{bf} ,

$$D = D_s + D_{ff} + D_{bf} \quad (127)$$

D_s arises from scattering, D_{ff} arises from free-free absorption and D_{bf} arises from bound-free absorption. For reasons of classification the bound-bound or line absorption is not included in this treatment.

3.9.1 The Underlying Equations of Overlay (3,5)

3.9.1.1 The Calculation of D_s

D_s is the reduced cross section arising from Compton scattering. This process becomes important only in those regions where both D_{bf} and D_{ff} are small compared to D_s . This occurs at energies which are large compared to the binding energies of the electrons which make important contributions to K_R . Consequently, in that region, where D_s is of importance, the binding energy is small compared to the photon energy and the scattering cross section may be computed as if every scattering electron is unbound. If we use the usual scattering cross section for free electrons along with the definitions of Eq. (4) and Eq. (9), from Reference 6, page 221,

$$D_s = \frac{1}{(137)^3} \frac{\sqrt{3}}{8} z kT \frac{u^3}{1-e^{-u}} f(\xi), \quad (128)$$

where

$$f(\xi) = \frac{3}{4} \left\{ \frac{1+\xi}{\xi^2} \left[\frac{2(1+\xi)}{1+2\xi} - \frac{\ln(1+2\xi)}{\xi} \right] + \frac{\ln(1+2\xi)}{2\xi} - \frac{(1+3\xi)}{(1+2\xi)^2} \right\} \quad (129)$$

and

$$\xi = \frac{1}{2} \frac{ukT}{(137)^2} \quad (130)$$

The factor $(1-e^{-u})$ is inserted to compensate for the fact that $K(u)$ is multiplied by $(1-e^{-u})$ in Eq. (2) to account for induced emission in the bound-free and free-free processes. Since there is no "induced inverse scattering," the $(1-e^{-u})$ factor must be removed from D_s .

For small values of the argument, ξ , the code replaces $f(\xi)$ by a series expansion.

3.9.1.2 The Calculation of D_{ff}

The free-free scattering process is computed with a unit Gaunt factor. If there is no exclusion out of the upper states this is given by [1]

$$D_{ff} = \frac{1}{(kT)_R} N_f^2 \ln \left(1 + e^{(\alpha - E_0)/kT} \right). \quad (131)$$

N_f , of course, is the number of free electrons per atom. Equation (131) is used as long as $[(\alpha - E_0)/kT] - u > -2.0$. For larger values of α , exclusion of the upper state must be accounted for. Using the results of Reference 7 with a unit Gaunt factor, we have

$$D_{ff} = \frac{N_f^2}{(kT)_R} \frac{1}{(1-e^{-u})} \ln \left[\frac{1 + \exp\left(\frac{\alpha - E_0}{kT}\right)}{1 + \exp\left(\frac{\alpha - E_0}{kT} - u\right)} \right] \quad (132)$$

$$\frac{\alpha - E_0}{kT} - u > -2.0.$$

The use of the unit Gaunt factor is based on the hope that wherever other processes do not dominate, the averaging procedure of Eq. (2) will wash out the frequency dependence of the free-free Gaunt factor. This is a poor assumption at low temperatures. Exact free-free Gaunt factors in the hydrogenic approximation are provided by Karzas and Latter [8]. Fermi-Dirac averages of hydrogenic Gaunt factors accounting for exclusion are available in Reference 7. In those cases where the Gaunt factor is neither unity nor hydrogenic, codes exist for the exact computation [9,10] of the non-hydrogenic free-free Gaunt factor in an arbitrary static potential.

3.9.1.3 The Calculation of D_{bf}

Lacking a detailed matrix element calculation, the Kramer's approximation to D_{bf}^i is

$$D_{bf}^i = \frac{1}{n_i} \left| \frac{E_i}{kT} \right|^2 \bar{N}_i g_i; \text{ if } u > (u_i^o + p_i u_i^s - u_o) = u_i^I; \\ = 0, \text{ otherwise.} \quad (133)$$

$$\text{Where } u_i^o = \frac{ED(i)}{kT} = \frac{E_i^i}{n_i \lambda_i}, \quad (134)$$

$$u_i^s = E_s(i)/kT, \quad (135)$$

$$u_o = -E_o/kT, \text{ and} \quad (136)$$

$$p_i = \bar{N}_i / \Omega_i.$$

D_{bf}^i is the absorption provided by $\bar{N}_i$ electrons bound in the i^{th} state of principal quantum number n_i .

In the hydrogenic approximation

$$E_i = \left(\frac{Z_i^*}{n_i} \right)^2, \quad (137)$$

g_i is the hydrogenic gaunt factor, and

$$Z_i^* = Z - \sum_{s < i} \bar{N}_s \sigma_{is} + \frac{\bar{N}_i \sigma_{ii}}{\Omega_i} \quad (138)$$

This code sets $g_i = 1$, but also makes a provision for inputting values of $g_i \neq 1$. When $g_i = 1$, Eq. (138) is apparently not the best approximation. Carson and Hollingsworth [11] get better results using inner-screening only. This is the option that is presently being used:

$$Z_i^* = Z - \sum_{s < i} \bar{N}_s \sigma_{is} - \frac{\bar{N}_i \sigma_{ii}}{2} \left(\frac{\Omega_i - 1}{\Omega_i} \right). \quad (139)$$

Of course, kT_{e1}^i , in Eq. (133), is the mean ionization energy out of state i ; p_i is the probability that state i is occupied; $-E_0 = u_0 kT$ is the continuum lowering; $E_{n,l,j}^i = u_1^0 kT$ is the binding energy of state i in the self-consistent potential; and $E_i^s = kT_{e1}^s$ is the self-screening energy.

D_{bf}^i in Eq. (132) does not account for exclusion. If D_{bf}^i is the bound free absorption with exclusion accounted for, then

$$D_{bf}^i = \frac{D_{bf}^i}{1 + \exp(\alpha/kT + u_0 + u_i^i - u)} \quad (140)$$

Of course, the total bound free absorption is given by summing over all i

$$D_{bf} = \sum_i D_{bf}^i \quad (141)$$

Once D_s , D_{ff} , and D_{jf} are available, $D(u)$ is found according to Eq. (127) over a suitable U grid, and finally K_R is computed according to Eq. (7).

3.9.2 The Structure of Overlay (3,5)

This overlay consists of decks MAIN7, TABLE, FABLE, SIGTAB, ESTAB, COMPI, XPANDE, TAUSUB, FINDS, ACALC, CUD, GETAB, UVAR, SIGMA and UINT, which have the following functions.

1. MAIN7 is the executive routine which directs the flow of computation for this overlay. It has provisions for directly reading in results which would be absent if certain previous overlays were not executed. It also has options for reading in and altering various data tables.
2. TABLE is a deck of block data which lists all possible (α, β) pairs which may be reached by an allowed dipole transition from an initial state α to a final state β . The α and β numbers each run from 1 to 200 allowing a description of the first 200 Dirac energy states. The count on the states is a dictionary ordering: first on the principal quantum number, n ; second on the orbital angular momentum, l , and third on the spin, j . For instance, $\alpha=1$ refers to the $1S_{1/2}$ state with $n=1, l=0, j=1/2$; similarly, $\beta=4$ refers to the $2P_{3/2}$ state with $n=2, l=1, j=3/2$. Each (α, β) pair appears in the table as a six (or more) digit entry whose first digits are the value of α , and whose last five digits are the value of β . Consequently, the fact that a $1S_{1/2} \rightarrow 2P_{3/2}$ transition

is possible, is catalogued by the presence of the number 100004 in the table. Here 1 refers to the value of α and 00004 refers to the value of β .

3. FABLE is a deck of block data containing 2415 values of $f_{\alpha\beta}$, each of which corresponds to a (α, β) pair appearing in TABLE.
4. SIGTAB is a deck of block data containing a 40×40 condensed matrix of $\sigma_{\alpha\beta}$ values and a vector, ITALY, of length 40. Each element of the "condensed" $\sigma_{\alpha\beta}$ table will be repeated ITALY times to expand this table to a 200×200 σ table.
5. ESTAB is a subroutine which
 - (a) Sets $G_\alpha = 1$
 - (b) Finds n_α , the principal quantum number, for each state
 - (c) Establishes the starting value, the breakpoint, and the final grid point over which the absorption spectrum will be calculated. It also sets the number of grid points which will be used on the u scale.
6. COMPU is a subroutine which computes j_α , the value of j for each state α .
7. XPANDE is a subroutine which takes the self-screening energies, E_s , found in the Schroedinger calculation and associates them with their corresponding Dirac energy levels.
8. TAUSLJ is a subroutine which computes and stores on tape $V_{\alpha\beta}/kT = \tau_{\alpha\beta}$. $V_{\alpha\beta}$ is the Coulomb interaction energy between electrons in state α and state β .

9. FINDS is an empty routine which is not used in this calculation.
10. ACALC is the routine in which D_{bf}^i is computed.
11. CUD is an empty routine.
12. GETAB is a routine which returns α, β and $f_{\alpha\beta}$ for each of the possible $\alpha\beta$ pairs.
13. UVAR computes at each grid point, u , all of the u dependent variables, such as $W(u)$, $D_s(u)$, $D_{bf}(u)$, and $D(u)$.
14. SIGMA is the subroutine which gets the appropriate $\sigma_{\alpha\beta}$ value from the compressed data of SIGTAB.
15. UINT is a routine which uses all the u dependent variables, and performs the integration over the u grid according to Equation (7). UINT then prints out the final answers.

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APPENDIX A. INPUT CARDS

We append here a description of the data cards required for running a CHAINJ problem. We describe the data cards in the order in which they appear. We tabulate the format, the variable name that is input, and a description of the nature of the variable. Some data cards must be used for all runs; others must appear or must be omitted depending upon the options chosen for any particular run. We describe the conditions under which each card is to be used or omitted.

The cards occur in sets. Each set contains the collection of cards required by a particular overlay. Although some overlays do not require data cards, we nevertheless list every overlay. If an overlay has no input cards, that fact is mentioned. The cards themselves may be described first by the overlay number, (i,k) , to which they belong, and then by their order of appearance in a set belonging to a particular overlay. This card, $(i,k),j$, is the j^{th} card providing data for overlay (i,k) .

I. Overlay (0,0). Inputs always present.

Card 1. Always present.

- (5I12,
2I6)
1. IDPRØB = Problem ID. A value of 99999 will terminate run.
 2. ISKPTF = 0 if Thomas-Fermi potential to be calculated; =1 if T-F calculation to be omitted.
 3. ISKP34 = 0 if either Schrödinger or Dirac equations to be done; =1 if both omitted.
 4. ISCH = 0, Dirac only; =1, Schrödinger only;
= -1, both Schrödinger and Dirac.
If ISKP34 = 1, then set ISCH = +1 if Schrödinger energies are input.
or set = 0 if Dirac energies are input.
 5. ICGTØ5 = 1 if occupation numbers are to be done;
= 0 to skip occupation number compute.
 6. IME = 0 to skip matrix element compute.
(IME = 1 option not yet available.)
 7. LINEC = $\Delta + 100,000$ if ϕ potential is to be saved on disc 72.
= Δ if ϕ potential is not saved.
If $\Delta = 0$ opacity compute will be omitted.
If $0 < \Delta < 100,000$, opacity compute will be done. Non-zero Δ is usually set = 5.

Card 2. Present only if ISKPTF = 1, and ISKP34 = 0.

- (I12)
1. NY = Number of ϕ 's to be read in. ϕ is the un-normalized Thomas-Fermi potential.

Card 3. Present if, and only if, Card 2 is present.

- (6E13.6)
1. Z = Z, charge on nucleus.
 2. RØA = r_o/a_o , radius of ion sphere in Bhor radii.
 3. AØPI = $a_o \phi_1 = a_o \left. \frac{\partial \phi}{\partial r} \right|_{r=0}$ where ϕ is the normalized potential.

4. EZER ϕ = E_0 , continuum lowering.
5. FKT = kT in Rydbergs, matter temperature.
6. DY1 = $(\delta y)_1$, Grid size for region $0 \leq y \leq y_B$.
 $y^2 = r/r_0$.

Card 4. Present if, and only if, Card 2 is present.

1. DY2 = $(\delta y)_2$, Grid size for $y_B \leq y \leq 1$.
- (2E13.6) 2. YBP = y_B , value of y at breakpoint.

Card 5. Present if, and only if, Card 2 is present.

1. PHIC(1)
 - (6E13.6) 2. PHIC(2)
 3. PHIC(3)
 4. PHIC(4)
 5. PHIC(5)
 6. PHIC(6)
- Values of ϕ at each point of the y grid. ϕ is the un-normalized Thomas-Fermi potential.
- PHIC(1) $\equiv \phi(0)$
 PHIC(1) $\equiv \phi(y_1)$.

Additional cards, in the format of Card 5, listing 6 ϕ 's per card until all ϕ 's are listed.

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$$PHIC(NY) = \phi(y=1).$$

II. Overlay (1,0). Has no input, and is called in connection with the execution of overlay (2,0).

III. Overlay (2,0). Uses the following input cards if, and only if, ISKPTF = 0 on Card (0,0), 1.

Card 1. Always present if ISKPTF = 0.

1. Z = Atomic number
- (5E12.8, 6I3,I2) 2. RKT = Temperature (in Rydbergs)*
3. RH ϕ = Density*

* RKT and RH ϕ must be input; however, if IRPHI = 1, and a and $\phi(1)$ are input, then the RKT and RH ϕ inputs are dummies and any positive value may be used.

4. RH00 = Normal density.
5. EM = Atomic weight.
6. KASE = 1 for zero temperature case; = 3 for non-zero temperature.
7. ITERM = 1 will EXIT if $|(AI-AC)/AC| > 0.02$;
= 0 no exit.
8. ICK0P = 1 for checkout print; = 0, no checkout print.
9. IRPHI = 1 if a and $\phi(1)$ are to be read in;
otherwise 0.
10. JC0L1 = Column in which to interpolate first. Use 3 or 4. 3 is temperature; 4 is volume. } limited to (2 and 3 and 4)
11. JC0L2 = Column in which to interpolate second. Use 4 or 3.
12. IQ = 1 if job to be terminated after interpolation; otherwise, 0.

Card 2. Present if, and only if IRPHI = 1.

1. $\phi(1)$ = Value of ϕ at $y = 1$. $\phi(1) = \alpha/kT$.
- (2E12.8) 2. AI = $r_0^2 h^3 / (4\pi e (2m)^{3/4} (kT)^{1/4})^2$, the Thomas-Fermi parameter.

Card 3. Present if, and only if, card 1 is present.

- (2E12.8) 1. Δ = Strength of charge shell. Generally = 0.
2. x_0 = Position of charge shell. Set = 0,
if $\Delta = 0$.

IV. Overlay (3,0). Has no input. It controls flow only.

V. Overlay (3,1). Has data if, and only if, ISKP34 = 0, and ISCH $\neq$ 0 on Card (0,0), 1.

Card 1. Present if Overlay (3,1) has data.

	1. ID	= Convergence option. If ID = 0, $\psi(\mu) = 0$.
If ID $\neq$ 0, $\psi(\mu) = \mu \partial \psi / \partial r _{\mu}$.
(2I12,
2E12.8,
5I1)	2. IØPT	= (1-6) Option on ϕ function routine.
To get $\phi = [\psi(y) - y^2 \phi(1)] / \phi(0)$, set = 1.
	3. ELIL	= Constant used in ϕ function if IØPT = 5 or 6.
	4. A	= The constant to extend ϕ table when $\mu/r_o > 1$. This is the value of the potential beyond the edge of the atom.
Set = 0 for neutral ion sphere.
	5. IRESTR	= X, where X is the X^{th} time that calculation has been restarted.
	6. IEG	= 1 to read in energy guess for each level. IEG = 0, if E_g is computed internally.
	7. IMU	= 0 if μ to be set = minimum of $(\mu, r_o/a_o)$.
	8. NØLC	= Number of levels in which XB,D1,D2,
$z_e \mu/a_o$ to be changed from default values.
	9. INØ	$\neq$ 0 print wave function output.
= 0 do not print wave function output.

Card 2. Present if, and only if, Card 1 is present.

	1. N1	= Principal quantum number.	} Calculation starts at level N1, L1.
(4I12)	2. L1	= Orbital angular momentum.	
	3. N2	Calculation continues through	
	4. L2	level N2, L2.	
- (N2, L2) implies a value ISTOP, internally computed, which is largest count on energies. The lowest possible level is (N1=1, L1=0); the highest possible level is (N2=15, L2=2).

Card 3. Present if, and only if, IRESTR > 0.

1. NØES = The number of converged E's to be read in.
- (112,E12.8) 2. ERSRT = E_g with which to begin calculation.
An energy guess for the first level to be computed. This is the level, NØES + 1.

Cards 4. Present if, and only if, IRESTR > 0.

1. I These are the successfully converged
- [4(I4, 2. EF(I) E's with their indexes. These cards
- E14.7)] 3. I continue until NØES energies have been
4. EF(I) listed. NØES was read in on Card 3.
5. I
6. EF(I)
7. I
8. EF(I)

Cards 5. Present if, and only if, IRESTR > 0.

1. I
- (4(I4, 2. ES(I) These ES are the self-screening
- E14.7)] 3. I energies. These are read
4. ES(I) until we have NØES of them
5. I also.
6. ES(I)
7. I
8. ES(I)

Cards 6. These energy guess cards are present if, and only if, IEG = 1.

	1. EG(I)	I is the index for level N1, L1.
(6E12.8)	2. EG(I+1)	An EG is read for each level to
	3. EG(I+2)	be computed, if IEG = 1.
	4. EG(I+3)	If IEG = 0, a subroutine is called
	5. EG(I+4)	to calculate the EG's, and these
	6. EG(I+5)	cards are not read in. If EG's
	1. EG(I+6)	are read in, use as many cards as
(6E12.8)	2. .	necessary until EG(ISTOP) is read
	.	in. ISTOP is the index of the
	.	highest level.
	.	
	.	
- $$EG(ISTOP) = \left\lfloor \frac{N2 \cdot (N2-1)}{2} + L2 + 1 \right\rfloor$$

Cards 7. These parameter cards are present if, and only if, NOLC > 0.
There are NOLC of these cards.

(2I4,	1. IN	Principal quantum number, and
4E12.8)	2. IL	orbital angular momentum of level
		to which new values of following
		variables refer.
	3. ZEMAC	$(z_e \mu)/a_0$. Integration of ψ ends at
		$r = \mu$.
	4. XBC	= Breakpoint for ψ integration.
		$0 < XBC \leq 1$.
	5. D1C	= ΔX_1 . Grid size for $x \leq XBC$.
	6. D2C	= ΔX_2 . Grid size for $x \geq XBC$.
- NOTE: If XBC = 1, set D1C = D2C.

VI. Overlay (3,2). Has data if, and only if, ISKP34 = 0 and ISCH $\neq$ 1.

Card 1. Used if, and only if, ISKP34 = 0, ISCH = 0. Otherwise
data for Card 1 comes from Overlay (3,1).

	1. ID	= The same function as on Card (3,1),1.
(2I12,	2. IOPT	= The same function as on Card (3,1),1.
2E12.8	3. ELIL	= The same function as on Card (3,1),1.
3I1)	4. A	= The same function as on Card (3,1),1.

- 5. IØUT = 0 to suppress additional print.
 = 1 to obtain additional print of
 Dirac wave function.
 > 1 Print for one iteration, only.
- 6. IEG = 1 to read energy guess for each level.
 = 0 Compute $\mathcal{E}_g$ internally.
- 7. IMU = 0 if μ to be set = minimum of $(\mu, r_0/a_0)$.

Card 2. Used if, and only if, ISKP34 = 0, ISCH $\neq$ 1.

- 1. NØLC = The number of levels where $z_e \mu/a_0$
 to be altered.
- (2I12) 2. IØUT = 0 no print.
 = 1 additional print of wave function.
 > 1 Print for one iteration, only.

Card 3. Used if, and only if, Card 2 is used.

- 1. N1 Calculation starts at energy level (N1,L1,K1).
 N1 = n = principal quantum number
- 2. L1 Li = l = orbital quantum number
 K1 = l if j = l - 1/2
- 3. K1 K1 = -(l+1) if j = l + 1/2
 The lowest level possible is (1,0,-1).
- 4. N2 Calculation ends at energy level
- 5. L2 (N2,L2,K2).
- 6. K2 The highest level possible is (15,2,2).

Cards 4. Energy guess cards are used if, and only if, Card 1 is present and IEG = 1.

- 1. EG(I) I is index for level N1, L1, K1.
- (6E12.8) 2. EG(I+1) EG(k) is energy guess for kth level.
- .
- .

3. EG(I+2) Use as many energy cards as
 . necessary, until EG(ISTOP) is
 . read in. ISTOP is the index of
 the last energy level. There are
 6. EG(I+5) 6 EG's/card.
 (6E12.8) 1. EG(I+6)
 2. .
 .
 EG(ISTOP) $ISTOP = (N2-1)^2 + 2*L2$, if $K2 = L2$;
 and $ISTOP = (N2-1)^2 + 2*L2+1$, if $K2 =$
 $-(L2+1)$.

Cards 5. Parameter change cards are present if, and only if,
 $N\phi LC > 0$. $N\phi LC$ cards are present.

1. IN Indicates n, l and k of level
 (3I4, 2. IL at which following value to be
 E12.8) 3. IK changed.
 4. ZEMAC $(Z \mu / a_0)$

VII. Overlay (3,3). Only requires data if either ($IC\phi T\phi 5 = 1$ and
 $ISK\phi 34 = 1$), or if ($ISK\phi TF = 1$, $IC\phi T\phi 5 = 1$, and $ISK\phi 34 = 0$).

Card 1. Used if, and only if, $IC\phi T\phi 5 = 1$ and $ISK\phi 34 = 1$.

1. FKT = kT (Rydbergs). Temperature of matter.
 (6E12.8) 2. ALPHAZ = α_0 . Guess at approximate value of
 degeneracy parameter.
 3. CAPA $A = \left[\left((kT)_R \right)^{3/2} \left(\frac{V}{a_0^3} \right) \right] / 2\pi^2$
 4. EZERO = E_0 , continuum lowering.
 5. Z = Z , atomic number.
 6. EMI = m , atomic weight.

Card 2. Used if, and only if, Card 1 is used.

	1. FETA	= $\eta = \rho/\rho_0$.
(2E12.8,
I12)	2. R0A	= r_0/a_0 , where r_0 = radius of ion sphere.
	3. ILAST	= Number of energies with which to calculate occupation numbers.

Cards 3. Used if, and only if, Card 1 is used.

	1. E(1)	ISCH = 0 will call for ED(I), which are
(4(4X,
IPE14.7))	2. E(2)	Dirac equation energies. Dirac energies
	3. E(3)	are ordered first on principal quantum
	4. E(4)	number, second on spin j, third on
		orbital angular momentum $l = j \pm 1/2$.
	1. E(5)	ISCH = 1 will call for EF(I), which
	2. .	are Schroedinger equation energies.
	3. .	Schroedinger energies are ordered first
	.	on principal quantum number n, and
etc. .		second on orbital angular momentum, l.
	.	There are 4 E's per card. Use as many
	E(ILAST)	cards as necessary until E(ILAST) is
		reached.

Card 4. Used if, and only if, IG0T05 = 1, ISKP34 = 0, and ISKPTE = 1.
This card is not used if Cards 1-3 are used.

(4E12.8)	1. ALPHAZ	α_0 , same meaning as in Card 1.
	2. CAPA	A, same meaning as in Card 1.
	3. EMI	m, same meaning as in Card 1.
	4. FETA	n, same meaning as in Card 2.

VIII. Overlay (3,5). Requires data if, and only if,
(LINEC) * (100,000-LINEC) $\neq$ 0.

Card 1. Used if, and only if, (LINEC) * (100,000-LINEC) $\neq$ 0 and Card
(3,1),1 is missing.

(I12)	1. IEND	= Level number of last E_g from
Schroedinger energy array. |
|-------|---------|---|

Cards 2. Used if, and only if, Card 1 is used.

4(I4, 1. I,ES(I) = Level number, and E_s for that level.
 E14.7) .
 .
 .
 IEND,ES(IEND) ES(I) is the Schroedinger energy
 of "self screening" for energy of
 Index I. There are 4 I,ES pairs
 per card.

Card 3. Used if, and only if, LINEC(100,000 - LINEC) $\neq$ 0, and
 ICOT05 = 0.

(6X,I6, 1. N0ES = Number of Dirac energies.
 4E14.7) 2. FET = kT, temperature in Rydbergs
 3. Z = Atomic number.
 4. ALPHA = α , the degeneracy parameter, from
 occupation number calculation.
 5. ENF = N_F , numbers of frees from occupation
 number calculation.

Card 4. Used if, and only if, Card 3 is used.

1. EZER0 = E_0 , continuum lowering.
 (4E14) 2. EMI = M, atomic weight.
 3. R0A = r_0/a_0 , radius of ion sphere/Bohr radius.
 4. FETA = $\eta = \rho/\rho_0$, the compression.

Cards 5. Used if, and only if, Card 3 is used.

1. ENNJ(I) = Occupation number } for level of
 (2E30.7, 2. ED(I) = Dirac energy } index I
 12X) I=1,N0ES (1 pair/card), there are N0ES cards.

Card 6. Used if, and only if, LINEC(100,000 - LINEC) $\neq$ 0.

(6I12) 1. ICHFAB = Number of $F_{\alpha\beta}$'s you wish to change.
 Set = 0 for no change in $F_{\alpha\beta}$ table.

2. ICHSIG = Dimension of new sigma matrix (≤ 40).
Set = 0, to use default values for σ matrix.
3. ICHTAL = Length of new "ITALY" table (≤ 40).
Set = 0, to use old table.
4. ICHCEE = Number of $g_{\alpha\beta}$ you wish to change.
Set = 0 for no change.
5. ICHCEN = 1 if a grid constants will be changed. Set = 0 for no change.
6. IALL = 0 if all other flags on this card = 0. Set = 1 if at least one other flag on this card $\neq 0$.

Cards 7. Used if, and only if, ICHFAB $\neq 0$.

(6X,I6,
E14.7)	1. INDEX	= Index, and value of $F_{\alpha\beta}$ for $\alpha\beta$ pair
	2. ALPHAI(INDEX)	identified by INDEX. This group
		has ICHFAB cards.
	ICHFAB Pairs	

Cards 8*. Used if, and only if, ICHSIG $\neq 0$.

(6X,I6,
E14.7)	{	1. SIG(1,1)	= New σ table stored by columns.
		.	
		.	
J=1		.	
		6. SIG(6,1)	= Six numbers per card.
	{	SIG(ICHSIG,1)	
		SIG(1,2)	
		.	
J=2		SIG(ICHSIG,2)	
		SIG(ICHSIG,ICHSIG)	

* The $\sigma_{\alpha\beta}$ table is a condensation of the actual $\sigma_{\alpha'\beta'}$ used in computation. The set of numbers α' are expanded from α by using ITALY(α). Thus for every α there are ITALY(α), (α')'s.

Cards 9. Used if, and only if, ICHGEE $\neq$ 0.

(5(I3, E12.8))	1. ITH	= Index of Dirac energy level for new g_{bf} .
	2. GEE(ITH)	= New g_{bf} for ITH level.
	:	There are 5 ITH,GEE pairs per card.
	:	There are ICHGEE pairs.
	:	
	GEE(ICHGEE)	

Cards 10^{*}. Used if, and only if, ICHTAL $\neq$ 0.

(20I4)	1. ITALY(I)	New ITALY(I) table for reconstructing σ table.
	:	
	I=1,ICHTAL	20/card
		ICHTAL $\leq$ 40.

Card 11. Used if, and only if, ICHCON $\neq$ 0.

(3E12.8, 2I6)	1. C_1	= Grid point to begin u integration. (Default value = 0.2).
	2. C_2	= Grid point where breakpoint lies. (Default value = 10.7).
	3. C_3	= Grid point to end integration. (Default value 28.7).
	4. NØP1	= Number of intervals from $C_1 - C_2$. (Default value = 790).
	5. NØP2	= Number of intervals from $C_2 - C_3$. (Default value = 400).

*The $\sigma_{\alpha\beta}$ table is a condensation of the actual $\sigma_{\alpha'\beta}$, used in computation. The set of numbers α' are expanded from α by using ITALY(α). Thus for every α there are ITALY(α), (α')'s.

Card 12. Used if, and only if, $LINEC \cdot (100,000 - LINEC) \neq 0$.

- (6112)
1. IDEF
 - = 1 E in DBF compute.
 - = 2 Z^* in DBF compute.
 - = 3 Z^* + smeared edge in DBF compute.
 2. IGAM
 - = 0 Do not compute $\Gamma_{\lambda\beta}$ with correlation.
 - = 1 (Unwritten dummy routine) to compute $\Gamma_{\alpha\beta}$ with correlation.
 3. ICKOUT
 - = 0 No checkout print.
 - = 1 Print $E_g, I, u_{\alpha\alpha} u_{\alpha\alpha}, G_{\alpha}, P_{\alpha}, D_{bf}, Z^*$.
 - = 2 All: Option 1 + $\Gamma_{\alpha\beta}$ table.
 4. IPRINT
 - = 0 No integration print.
 - = 1 Integration print.
 5. IZ
 - = 0 Z^* in TAU compute.
 - = 1 Z in TAU compute.
 6. IFILE
 - = 0 No writing D's on tape.
 - = 1 Write D's on new tape.
 - = 1 Write D's on old tape, containing other sets of D's.

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