A Quantum- and Correlation-Corrected
Thomas-Fermi-Dirac Equation
with a FORTRAN Code
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A Quantum- and Correlation-Corrected Thomas-Fermi-Dirac Equation with a FORTRAN Code

by

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ABSTRACT

In a previously published report (IA-2750, A Proposed Modification of the Available Momentum Region in Thomas-Fermi Theory) a "quantum correction" to the statistical model of the atom was derived in detail. In the present work we use these results and a very simple approximation to the correlation energy in deriving a quantum- and correlation-corrected Thomas-Fermi-Dirac (TFD) equation. One expects the radial density distribution and potential calculated from this equation to be improved over those on the TFD model, both near the nucleus and near the outer boundary of the atom or ion. Minimum-energy (that is, zero boundary pressure) solutions for rare-gas atoms possess values of cell radius in good agreement with those calculated from experimental values of the lattice parameter.

A FORTRAN code is included in an Appendix to the report.

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I. INTRODUCTION

Many properties of free atoms and of solids are predicted with considerable accuracy by the statistical atom model of Thomas, Fermi, and Dirac. The accuracy of the method has probably helped inspire the deeper investigation into its foundations; for if one considers only the premises upon which the original model is based, he would hardly expect more than very rough agreement with experiment or with the predictions of a more refined theory. Yet, to give some examples, the radial density distribution function for a given element calculated from either the Thomas-Fermi (TF) or the Thomas-Fermi-Dirac (TFD) equation appears to be, for any but the very lightest elements, in good agreement with that obtained from self-consistent field calculations. The shell structure is not reproduced, but there appears to be a reasonable averaging of the relative maxima and minima. One-electron energy levels computed in the TF or TFD fields are remarkably close to experimental term values, and the atomic number at which electrons of a given angular momentum make their "first appearance" are predicted correctly to the nearest integer.

The correctness of these predictions would have to be regarded as fortuitous, when they result from a theory which presumes that (1) the potential field in an atom varies sufficiently slowly that the fractional change in an electron's de Broglie wave length $\lambda$ is small over a distance comparable to $\lambda$; and (2) there are a great many electrons in a region having a volume of the order of $\lambda^3$. However, Fényes showed that the TF energy and density expressions follow from quasi-classical arguments as well as from a strictly classical viewpoint. Later, March and Flaskett succeeded in deriving the TF energy equation from an integral of the
WKB eigenvalues over a particular region of the quantum-number plane.\(^6\) Thus, the validity of the statistical model seems to depend upon that of the WKB approximation, and Langer showed that the WKB phase integral, at least in one dimension, is applicable under quite broad conditions on the potential even for small quantum numbers.\(^7\)

Since it is known that the statistical theory rests on more than the classical arguments, it appears well worthwhile to attempt those improvements that can be made with little complication of the equations to be solved. The derivation of March and Plaskett provides the basis for a "quantum correction" of the statistical model reported earlier\(^8,9\) and outlined below.

We have stressed the general success of the TF and TFD equations. There are, nevertheless, some areas in which the calculations do not agree well with experiment. A very apparent discrepancy is in the total binding energy of the electron cloud. The electron density predicted at the nucleus is infinite on either the TF or the TFD model; consequently, the calculated binding energy is considerably too large. The previously derived quantum correction modifies the density in the region near the nucleus and produces binding energies in much better agreement with experimental values and with those obtained from self-consistent field calculations.

A further area for attempting improvement is suggested by the rather large errors in the calculated pressure-compression curves. These relationships are influenced mainly by the outermost parts of the electron distribution. In this region of low density the correlation energy, neglected in the original models, becomes important.

In the present work we incorporate the quantum correction and a very simple form for the correlation energy in the derivation of an easily applied quantum- and correlation-corrected TFD equation. One expects the density distribution and potential calculated from this equation to be improved over those on the TFD model, both near the nucleus and near the outer boundary of the atom or ion.
The numerical procedures used in obtaining solutions of the equation are discussed, and a few calculational results are summarized. It is found that the inclusion of the correlation energy should not greatly change the pressure-compression curves for most elements. However, minimum-energy (that is, zero boundary pressure) solutions for rare-gas atoms possess values of cell radius in good agreement with those calculated from experimental values of the lattice parameter. These results suggest the interpretation of minimum-energy solutions as representing isolated atoms, rather than atoms in crystals, since the rare gases are known to be bound in crystals by the very weak van der Waals forces.

Numerical work was performed on an IBM 7030 computer. A FORTRAN code, version "F4", is listed in the Appendix, but we should caution that certain changes, mainly in the Input-Output statements, might have to be made before using the code with other computer systems. Also, it is necessary to carry more than eight-figure precision throughout the calculations in order to obtain accurately the solutions possessing minimum energy. We have attempted to carry our calculations to about thirteen figures, and while the 7030 word size is equivalent to about 16 decimal digits, it would be necessary to perform the calculations in double-precision arithmetic on a smaller machine. Eight-figure precision is certainly sufficient, however, to obtain general solutions corresponding to arbitrary degrees of compression.

II. A QUANTUM- AND CORRELATION-CORRECTED TFD EQUATION

A. The TF and TFD Equations

A variational technique can be used to derive the TF equation, and an extension of this method provides an often-used and simple means of adding corrections to the statistical model. Thus, we can write the Fermi kinetic energy density of a gas of free electrons at a temperature of zero degrees absolute in the form
where

\[ c_f = \frac{3}{10}(3\pi^2)^{2/3}. \]

The electrostatic potential energy density is the sum of the electron-nuclear and the electron-electron terms. We can write this as

\[ U_p = U_p^n + U_p^e = -(v_n^e + v^e/2)\rho, \]

where \( v_n \) is the potential due to the nucleus of charge \( Z \); \( v^e \) is the potential due to the electrons; and the factor of 1/2 is included in the electron-electron term to avoid counting each pair of electrons twice. With \( x \) denoting distance from the nucleus, the total energy of the spherical distribution is given by

\[ E = \int [c_f^5 \rho^{5/3} - (v_n^e + v^e/2)\rho] 4\pi x^2 dx. \]

The expression for density on the TF model,

\[ \rho = \sigma_0 (E' - v)^{3/2}, \]

with

\[ \sigma_0 = \left(\frac{3}{5c_f^3}\right)^{3/2}, \]

is obtained by minimizing Eq. (1) subject to the auxiliary condition that the total number of particles, \( N \), remains constant. The potential

\[ \text{Throughout this work we shall use atomic units (a.u.), in which } e = \hbar = m = 1. \ \text{The unit of length is } a_0, \ \text{the first Bohr radius for hydrogen; and the unit of energy is } e^2/a_0. \]
energy, \( V \), is a function of position in the electron distribution; \( E' \) is the Fermi energy, or chemical potential, and is constant throughout a given distribution. The TF equation follows from Eq. (2) and Poisson's equation.

The tendency for electrons of like spin to stay apart because of the exclusion principle is accounted for by the inclusion in Eq. (1) of the exchange energy, the volume density of which is given by

\[
U_{\text{ex}} = -c_{\text{ex}} \rho^{1/3},
\]

where

\[
c_{\text{ex}} = (\frac{5}{4})(\frac{3}{\pi})^{1/3}.
\]

Minimization of the total energy now leads to the equation

\[
\frac{5}{3} c_{\text{f}} \rho^{2/3} - \frac{4}{3} c_{\text{ex}} \rho^{1/3} - (E' - V) = 0,
\]

which is quadratic in \( \rho^{1/3} \). From this equation we get

\[
\rho = \sigma_0 \left[ \tau_0 + (E' - V + \tau_0^2)^{1/2} \right]^{3/2}, \tag{3}
\]

where

\[
\tau_0 = \left( \frac{4 c_{\text{ex}}^2}{15 c_{\text{f}}} \right)^{1/2}.
\]

Now Poisson's equation with the density given by Eq. (3) leads to the TF equation.

In the following two sections we propose additional energy terms to be included in Eq. (1); the incorporation of these terms leads to a simple quantum- and correlation-corrected TF equation.
B. The Quantum Correction

The quantum-correction energy density follows from a slight change in the derivation due to March and Plaskett; the development will be only briefly outlined here.

March and Plaskett have demonstrated that the TF approximation to the sum of one-electron eigenvalues in a spherically symmetric potential is given by the integral

\[ I = 2 \int \int (2\ell + 1)E(n_\ell, l)dn_\ell dl, \]  

(4)

where the number of states over which the sum is carried is written as

\[ N = 2 \int \int (2\ell + 1)dn_\ell dl. \]  

(5)

Here \( E(n_\ell, l) \) is the expression for the WKB eigenvalues considered as functions of continuous variables; \( n_\ell \) is the radial quantum number; \( l \) is the orbital quantum number; and the region of integration is bounded by \( n_\ell = -1/2, \ l = -1/2, \) and \( E(n_\ell, l) = E' \). We have included a factor of two in these equations to account for the spin degeneracy of the electronic states. The Fermi energy \( E' \) is chosen so that Eq. (5) gives the total number of states being considered, the \( N \) electrons occupying the \( N \) lowest states. With considerable manipulation, Eq. (4) becomes the TF energy equation

\[ I = \int \left( \frac{3}{2} \frac{p^2}{2} + V \right) \frac{p^3}{2} 4\pi x^2 dx, \]  

(6)

and Eq. (5) reveals the TF density through the expression

\[ N = \int \frac{p^3}{2} \frac{4\pi x^2}{2} dx, \]  

(7)

both integrals being taken between the roots of \( E' = V(x) \). We have written these results in atomic units, so that \( p \), the Fermi momentum,
is defined by

\[ p = 2^{1/2}(E' - \nu)^{1/2}. \]  \hspace{1cm} (8)

It is pertinent to examine the error in the TF sum of eigenvalues, as given by Eq. (6), for the case of the pure Coulomb field. The WKB eigenvalues in a Coulomb field are given by

\[ E_{n_r, \ell} = -\frac{Z^2}{2(n_r + \ell + 1)^2}, \]

and let us consider the levels filled from \( n = 1 \) to \( n = \nu \), where \( n \) is the total quantum number defined by

\[ n = n_r + \ell + 1. \]

Then, for any value of \( \nu \) we can evaluate the error in the TF approximation to the sum of eigenvalues, comparing always with the correct value, \(-Z^2\nu\). Scott's correction to the total binding energy\(^{10}\) is obtained by letting \( \nu \) become very large.

Although the sum of one-electron eigenvalues is not the total energy of the statistical atom because of the electron-electron interaction being counted twice, we might expect to improve the calculated binding energy greatly by correcting this sum in some manner, since the chief cause of the discrepancy is certainly the large error in the electron-nuclear potential energy. This correction can be performed by imposing a new lower limit on \( \ell \) in the integrations above. When we introduce a new lower limit \( \ell_{\text{min}} \) and a related quantity which we call the "modification factor,"

\[ a = \ell_{\text{min}} + 1/2, \]

we obtain, after more manipulation, slightly different expressions corre-
sponding to Eqs. (6) and (7). From these revised expressions we can identify a quantum-corrected TF density expression,

\[ \rho = \sigma_0 (E' - V - a^2/2x^2)^{3/2}, \]  

(9)

and a corrected kinetic energy density,

\[ U_k = c_t \rho^{5/3} + (a^2/2x^2) \rho. \]  

(10)

The revised lower limit on the volume integrals, say \( x_1 \), is the lower root* of

\[ E' - V - a^2/2x^2 = 0; \]  

(11)

for \( x < x_1 \), \( \rho \) must vanish, and we have thus termed \( x_1 \) the "inner density cutoff distance." We can call the second term on the right-hand side of Eq. (10) the "quantum-correction energy density" and write it in the more consistent form

\[ U_q = (c_q/x^2) \rho, \]  

(12)

by defining

\[ c_q = a^2/2. \]

The modification factor, \( a \), is determined by the initial slope of the potential function, as described in Part III of this report.

For interpreting these results it is helpful to consider just what we have done in changing the lower limit of the orbital quantum number.

---

*In application to the atomic problem, there is only one root of Eq. (11) between zero and the outer boundary of the atom or ion. This root is identified as \( x_1 \), and \( x_2 \) is then determined by the usual TF boundary condition.
Since the lower limit \( l = -1/2 \) must correspond to an orbital angular momentum of zero, we have, clearly, eliminated states with angular momentum of magnitude between zero and a cutoff value \( L_c = a\hbar \). Corresponding to \( L_c \) at every radial distance is now a linear cutoff momentum

\[
 p_c = a\hbar/x,
\]

and we can rewrite Eq. (9) in terms of the Fermi momentum and cutoff momentum:

\[
 p = \left(\sigma_0/2^{3/2}\right)(p^2 - p_c^2)^{3/2}.
\]

At radial distances less than \( x_1 \), momenta are prohibited over the entire range from zero to \( P \), so the electron density vanishes.

This interpretation must be modified somewhat when exchange and correlation effects are included; for then the Fermi momentum is no longer simply given by Eq. (8), except very near the nucleus. We can define \( x_1 \) as in the absence of interactions, i.e., as the lower of the roots of Eq. (11), but it is not correct to demand that the density vanish at the upper root. Instead, we require only that the density be real.

C. The Correlation Correction

The original TF equation describes a system of independent* particles, while the introduction of exchange energy, which leads to the TED equation, represents a correction for the correlated motion of electrons of like spin. The remainder of the energy of the electron gas is termed the correlation energy; by its inclusion we are recognizing that electrons, regardless of spin orientation, tend to avoid one another.

* The particles are "independent" in the sense that there is no correlation among their positions. They do interact with each other, however, in establishing the potential field in which each particle moves.
In extensions of the statistical model there have been suggested at least two different expressions\textsuperscript{11,12} for the correlation energy that approach, in the appropriate limits, Wigner's low-density formula and the expression due to Gell-Mann and Brueckner at high densities. In addition to these, Gombás\textsuperscript{13} and Tomishima\textsuperscript{14} have utilized expansions of the correlation energy per particle in powers of $\rho^{1/3}$ about the particle density encountered at the outer boundary of the atom or ion. In this expansion, the term of first-order can be considered as a correction to the exchange energy, and it follows that the TFD solutions for a given Z then correspond to correlation-corrected solutions for a modified value of Z. Aside from the rather poor approximation of the correlation energy, a drawback to this procedure is that the TFD solutions must be at hand. If solutions representing specified degrees of compression are desired, the method would appear to be impractical.

It is, however, interesting and fortunate that over the density range of interest it is apparently possible to approximate the correlation energy per particle quite closely by an expression of the form

$$u_c = -c_c \rho^{1/6}.$$  

This is shown in Fig. 1, where we have set $c_c = 0.0842$, and compared this approximation with the values due to Carr and Maradudin.\textsuperscript{15} The latter are obtained as a higher-order correction to Gell-Mann and Brueckner's formula at the high densities (say $\rho \geq 0.25$ a.u.), and are again reasonable interpolated values at the lower electron densities.

There is no need to be concerned with the correlation energy outside the limited range of density shown in Fig. 1. The lowest density that can be obtained in solutions of the "corrected" TFD equation to be derived is about 0.002 a.u., and at densities above 1.0 a.u. the correlation energy becomes small compared with the exchange energy. Near the lower limit of density, the magnitude of the correlation energy computed from Eq. (13) is about one-third as large as the exchange energy,
Figure 1. Correlation energy per electron.
but at \( \rho = 2.0 \) a.u. it is only 10\% as large. For, say, \( \rho = 10^5 \) the ratio is 1\% and the exchange energy itself is only 0.01\% of the Fermi kinetic energy.

We shall, then, approximate the correlation energy density with

\[
U_c = -c_c \rho^{7/6}
\]

and, in atomic units,

\[
c_c = 0.0842.
\]

D. Derivation of the Equation

From the results of the preceding paragraphs, we can now express the total energy per unit volume of the charge distribution in the form

\[
U = c_x \rho^{5/3} - c_{ex} \rho^{4/3} - c_c \rho^{7/6} - (\sqrt{n + \nu} + \nu/2) \rho + (\nu_x / x^2) \rho,
\]

where all quantities appearing in the equation have been previously defined. By minimizing the integral of \( U \) over the volume occupied by the charge, while requiring that the total number of electrons be fixed, we obtain the following equation:

\[
\rho^{2/3} - \tau_1 \rho^{1/3} - \nu_0 \rho^{1/6} - R/4 = 0,
\]

where

\[
\tau_1 = (4/5)(c_{ex} / c_x),
\]

\[
\nu_0 = (7/6) c_c \sigma_0^{2/3}
\]

\[
R = 4\sigma_0^{2/3}(E' - \nu - \nu_x / x^2).
\]
The electron density is found as a function of \( R \) by solving Eq. (14), a quartic in \( \rho^{1/6} \). To accomplish this we write a "resolvent cubic equation" in terms of another variable, say \( y \):

\[
y^3 + \tau_1 y^2 + Ry + (\tau_1 R - \omega_0^2) = 0. \tag{15}
\]

Let us use the same symbol, \( y \), to denote any real root of this cubic equation. We can then express the four roots of the quartic, and hence four expressions for the electron density, in terms of \( y \). One of these expressions possesses the proper behavior in reducing to previously obtained results in the neglect of correlation and exchange effects, namely,

\[
\rho = (1/8)[\tau_1 + \psi + (y^2 + R)^{1/2}]^3, \tag{16}
\]

where

\[
\psi = (\tau_1 + y)^{1/2}[\tau_1 - y + 2(y^2 + R)^{1/2}]^{1/2}. \tag{17}
\]

We note that \( \psi \) vanishes when correlation is neglected, since \( y = -\tau_1 \) is then a root of Eq. (15).

In the familiar manner we now define a modified TFV potential function \( \phi \) by the relation

\[
Z\phi = (E' - V + \tau_0^2) x, \tag{18}
\]

and from Poisson's equation and Eq. (16) we obtain

\[
\begin{align*}
\phi'' &= (\pi x / 2Z)[\tau_1 + \psi + (y^2 + R)^{1/2}]^3, \quad x \geq x_1, \\
&= 0, \quad x < x_1.
\end{align*} \tag{19}
\]
In terms of $\phi$,

$$R = 4\sigma_0^{2/3}(2\phi/x-a^2/2x^2-\tau^2). \quad (20)$$

Eqs. (20), (15), (17), and (19) constitute the differential relationship to be satisfied at each step in the integration. We could, of course, write immediately the solutions of Eq. (15) in analytic form, but it proves convenient in the numerical treatment to obtain a root by the Newton-Raphson method, since a good first guess in the iteration is available from the previous integration step.

The boundary conditions on Eq. (19) are: (1) As the nucleus is approached the potential must become that of the nucleus alone, or

$$\phi(0) = 1,$$

and (2) at the outer boundary, $x_2$, of the distribution of $N$ electrons,

$$N = \int_{x_1}^{x_2} \rho 4\pi x^2 dx$$

$$= \int_{x_1}^{x_2} \phi'' x dx.$$

Integration by parts yields

$$\int_{x_1}^{x_2} (\phi' x - \phi) = N/Z,$$

and since

$$\phi(x_1) = 1 + x_1 \phi'(x_1),$$

$$\phi(x_2) = \phi.$$
we have the usual condition:

\[ \phi(x_2) = x_2\phi''(x_2) + (Z-N)/x_2. \]

(21)

In addition to potential and density distributions, total binding energies of atoms are of special interest to us here. For the proper evaluation of energies, the arbitrary constant that is present originally in both the electrostatic potential energy and the Fermi energy must be specified. The state of infinite separation of the constituent particles is normally taken to have zero energy; we therefore follow the usual convention and fix the potential at the edge of the neutral atom at zero for all values of \(x_2\). For an ion the potential energy of an electron at the boundary is taken as

\[ V = -(Z-N)/x_2. \]

The defining relation, Eq. (18), now gives at the boundary

\[ Z\phi(x_2) = \left[ E' + (Z-N)/x_2 + x_2^2 \right] x_2, \]

or, solving for the Fermi energy,

\[ E' = Z\phi(x_2)/x_2 = (Z-N)/x_2 - x_2^2. \]

The total electron-nuclear potential energy is given by

\[ E_n^p = \int_{x_1}^{x_2} (Z/x)\rho 4\pi x^2 dx, \]

while for the electron-electron potential energy we have

\[ E_e^p = \frac{1}{2} \int_{x_1}^{x_2} v^e \rho 4\pi x^2 dx. \]
From Eq. (18) and the relation \( V = -(\nu_n^2 + \nu_e^2) \), this becomes

\[
E_p^e = \frac{1}{2} \left[ -E_p^{n+2} N + E_e N - \int_{x_1}^{x_2} (2\phi/x) \rho 4\pi x^2 \, dx \right].
\]

Other energy integrals are, with an obvious notation,

\[
\begin{align*}
E_x &= c_x \int \rho^{5/3} 4\pi x^2 \, dx, \\
E_q &= c_q \int (\rho/x^2) 4\pi x^2 \, dx, \\
E_{ex} &= -c_{ex} \int \rho^{4/3} 4\pi x^2 \, dx, \\
E_c &= -c_c \int \rho^{7/6} 4\pi x^2 \, dx.
\end{align*}
\]

### III. NUMERICAL PROCEDURES

For a given atomic number \( Z \), a family of solutions of the corrected TPD equation, corresponding to different degrees of compression of the element, is obtained by varying the slope of the potential function at the origin. Several parameters of the integration are determined directly by this initial slope, which we denote by \( \phi'_0 \). From the discussion of Eq. (11) we conclude that the electron density, and hence \( \phi'' \), vanishes for \( x \) less than

\[
x_\perp = (1/s) \left[ 1-(1-a_s^2/z)^{1/2} \right],
\]

where

\[
s = -2\phi'_0 + 1/\pi^2 Z.
\]
In starting the stepwise numerical integration, three values of \( \phi \) and \( \phi'' \) are used, including those at the origin. If we therefore choose an initial interval \( h_{in} \) such that

\[
2h_{in} < x_1,
\]

then \( \phi \) is linear in this region, and it is trivial to generate the starting values. For practical reasons \( h_{in} \) is chosen as the largest interval which satisfies both Eq. (22) and the condition

\[
h_{in} = 0.02/2^b,
\]

where \( b \) is an integer. This is done so that upon doubling the space interval a number of times (not necessarily \( b \) times) \( \phi \) is evaluated at convenient values of \( x \).

In the earlier work, justification was presented for determining the modification factor, \( a \), through an "equivalent Coulomb problem." In following this procedure we consider a number of electrons interacting with the charged nucleus but not at all with each other, even to the extent of providing a partial screening of the nuclear charge. Under these conditions we would define \( \phi \) through the equation

\[
Z\phi = (E'-V)x.
\]

Here, in contrast to the situation in the actual atomic problem, the potential energy distribution is known. We have

\[
V = -Z/x.
\]

It can be established by direct substitution that for the Coulomb problem, \( \phi \) is linear throughout the distribution, or
\[ \phi = 1 + x\phi' . \]

In order for Eq. (24) to be satisfied with no additive constant, we must let the Fermi energy of the Coulomb problem be given by

\[ E' = 2\phi' . \]  

(25)

Correction of the region of integration in the quantum-number plane is based on the above value of the Fermi energy, where for \( \phi' \) we use the initial slope of the actual atomic problem, i.e., \( \phi'_0 \). The outer boundary of the region defines a quantity \( \alpha \) through the relation

\[ \alpha = (n + l + 1) \text{outer boundary} . \]

The Fermi energy given by Eq. (25) is the maximum eigenvalue in the Coulomb field. From the form of these eigenvalues we obtain

\[ \alpha = (-2/2\phi'_0) . \]

In correcting the integration region for the Coulomb field we derive the expression for the modification factor,

\[ a = \alpha - (\alpha \nu)^{1/2} , \]

where \( \nu \) is the (generally non-integral) number of filled shells obtained as the solution of the equation

\[ \nu^2 + 3\nu/2 + 2\alpha^{3/2} \nu^{1/2} - (3\nu^2 - 1/2) = 0 . \]

Thus the initial slope of \( \phi \) determines the inner density cutoff distance \( x_1 \), the initial interval of integration \( h_{in} \), and the modification factor \( a \).
The quantum- and correlation-corrected TF equation is of the form

$$\phi'' = f(x, \phi),$$  \hspace{1cm} (26)

a form which can be integrated simply and rapidly by a finite-difference method described by Hartree. In this method the approximation is made that

$$\Delta^2 \phi_0 = h^2(\phi''_0 + \phi''/12),$$  \hspace{1cm} (27)

the subscripted quantities here being associated with the point $x = x_0$ to which the integration has progressed. In the usual notation, $\Delta^2$ is the second difference operator, such that

$$\Delta^2 \phi_0 = (\phi_1 - \phi_0) - (\phi_0 - \phi_{-1})$$

$$= \phi_1 - 2\phi_0 + \phi_{-1},$$

and $h$ is the existent integration interval.

To proceed in the integration an estimate is made of $\Delta^2 \phi''_0$, and from Eq. (27) we find $\Delta^2 \phi_0$. From the backward first difference and $\Delta^2 \phi_0$ we can predict $\phi$ at the next step. Eq. (26) then furnishes the predicted value of $\phi''$, from which the predicted $\Delta^2 \phi''_0$ follows. This predicted value is compared with the original estimate to determine whether the integration is to be allowed to proceed to the next step, or whether it must be repeated with a revised estimate of $\Delta^2 \phi''_0$. The criterion for this decision is discussed below.

Some modification of the integration procedure seems advisable in the vicinity of $x_{\perp}$, where an abrupt change in $\phi''$ occurs. A table of differences in $\phi''$ of second-order and above reveals that the assumption that leads to Eq. (27), namely, that the terms involving differences higher than second-order can be neglected, is not too well justified
for \( x \) close to \( x_{1} \). We can attempt to do a little better by adding one more term and writing

\[
\Delta^{2} \phi_{0} = h^{2} (\phi''_{0} + \Delta \phi''_{0}/12 - \Delta^{4} \phi''_{0}/240).
\]  

(28)

The extra term is retained for only a few integration steps for which the changes in \( \phi'' \) are relatively large; in practice it is dropped upon reaching the point at which \( h \) has achieved its maximum value. We note that, for that portion of the integration in which Eq. (28) is utilized, it is necessary at each step to estimate \( \Delta^{4} \phi''_{0} \); but we can get an estimate of \( \phi'' \) at the forward steps of sufficient accuracy to compute this difference by merely extending \( \phi \) linearly from the origin, thereby obtaining the arguments for Eq. (26).

The integration interval, starting at \( h_{in} \), is doubled on alternate steps until a certain maximum value is obtained, and then is kept constant out to the outer boundary of the charge distribution. This maximum value is selected by requiring that the precision in each integration be independent of \( Z \), the precision being that of a chosen test run. A convenient check on the precision is furnished by the relative discrepancy between the total number of particles \( N \) which enters the boundary condition, Eq. (21), and the volume integral of the calculated electron density. It is thus apparent that there are two conditions on the integration. With \( h \) given, the criterion on proceeding to the next step in integrating the differential equation is that

\[
\left| \frac{\Delta^{2} \phi_{0}^{(e)}}{\Delta^{2} \phi_{0}^{(p)}} \right| \leq 10^{-n},
\]

where \( n \) is the number of significant digits carried in the calculation of \( \phi \). This condition arises from requiring that an error in \( \Delta^{2} \phi''_{0} \) ultimately cause an error in \( \phi_{1} \) of no more than 1/2 in the least significant digit. However, the precision of the integration, as measured by the
calculated number of particles, also depends upon $h$. We might expect this error to be dependent to a large degree upon the magnitudes of $\Delta^2 \phi$ encountered in the integration, and results seem to bear this out. We require, then, as a rough measure of the error,

$$h^2_{\text{max}} \phi'' \approx \text{constant},$$

and seek to estimate $\phi''_{\text{max}}$ as a function of $Z$ and $\phi'_0$.

In the neglect of exchange and correlation effects we have

$$\phi'' = \left(\frac{4\pi}{3}\right)(2\pi x - a^2/x^2)^{3/2}.$$

With $Z$ and $a$ given, the condition for a maximum of $\phi''(x)$ is easily derived as

$$2a^2/x - Z(\phi - 3\phi' x) = 0;$$

and since the maximum occurs at a small value of $x$, it is adequate for this discussion to put $\phi = 1$ and to neglect $3\phi' x$ in comparison with it. We then obtain the result that the maximum is at a position

$$x \approx 2a^2/Z,$$

from which there follows

$$\phi''_{\text{max}} \approx (\pi^{1/2}/\pi)^2 a Z.$$

We then have the requirement

$$h^2_{\text{max}} \approx \text{constant} \cdot (\pi^{1/2}) a/Z.$$
It is found, moreover, that \( a \) varies but slightly with \( Z \) and \( \phi'_0 \). We can treat it as a constant here. It is also found in our calculations that an interval \( h_{\text{max}} = 0.00125 \) produces a respectably small error in number of particles of about four parts in \( 10^6 \) for \( Z = 54 \), with a modification factor of about 0.261. If \( h_{\text{max}} \) is chosen as the largest value obtained by doubling \( h_{\text{in}} \) subject to the condition

\[
h_{\text{max}} < 0.018/Z^{1/2},
\]

a fairly uniform error of a few parts in \( 10^6 \) results for all integrations, although for very small \( Z \) the error tends to be somewhat larger, say one part in \( 10^5 \).

The outer boundary of the electron distribution, \( x_2 \), is determined by Eq. (21). We define a quantity

\[
g = (x_0 - h/2)(\phi_0 - \phi_{-1})/h - (\phi_0 + \phi_{-1})/2 + (Z-N)/Z,
\]

which first becomes positive somewhere in the vicinity of \( x_2 \). At the integration step at which this occurs, a parabola is passed through the points \( \phi_{-2}, \phi_{-1}, \) and \( \phi_0 \). We then have for this limited region the approximation

\[
\phi = Gx^2 + \Delta x + C,
\]

and the coefficients \( G, \Delta, \) and \( C \) are evaluated under the condition that

\[
\phi'' = \Delta^2 \phi/h^2.
\]

Thus,

\[
G = \phi''/2,
\]
The boundary condition becomes

\[ \Theta = (\phi_0 - \phi_{-1})/h + h\alpha = 2x_0, \]

\[ C = \phi_0 - ax_0^2 - ax_0. \]

The boundary condition becomes

\[ Gx_2^2 + ax_2 + C = 2Gx_2^2 + ax_2 + (Z-N)/Z, \]

and hence

\[ x_2 = \left[ (ZC-Z+N)/2G \right]^{1/2}. \]

Integrals yielding the total energies of the various forms and the total number of electrons are evaluated by the Simpson "1/3" rule, with boundary corrections at \( x_1 \) and \( x_2 \) computed by the trapezoidal rule.

IV. RESULTS

It was pointed out in the Introduction that the quantum-corrected TFD equation yields atomic binding energies in good agreement with experimental values and with the results of Hartree-type calculations. It is of interest to know whether the agreement is retained when correlation energy is included. We also wish to ascertain the effect that inclusion of correlation has on the radii of the minimum-energy solutions. The pressure-compression curves on the TFD model suffer from this radius being too large for almost all elements, and correlation effects are known within the statistical theory to contract the electron cloud.

Table I presents summaries of minimum-energy solutions for a number of neutral atoms. We should mention here that the correlation energy for the low-Z elements is roughly twice that given by Clementi. 17

Table II compares the calculated total energies with Hartree-Fock-Slater non-relativistic values, and, for low-Z elements, with experimental
TABLE I
MINIMUM-ENERGY SOLUTIONS

A. THE INITIAL SLOPES, MODIFICATION FACTORS, AND INNER AND OUTER RADII

<table>
<thead>
<tr>
<th>z</th>
<th>( \frac{\psi'}{\psi_0} )</th>
<th>a</th>
<th>( x_1 )</th>
<th>( x_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.662286185</td>
<td>.2893262</td>
<td>.021720161</td>
<td>3.1500</td>
</tr>
<tr>
<td>3</td>
<td>1.944982019</td>
<td>.28290387</td>
<td>.013707739</td>
<td>3.3149</td>
</tr>
<tr>
<td>4</td>
<td>2.179159682</td>
<td>.27921366</td>
<td>.015083695</td>
<td>3.4274</td>
</tr>
<tr>
<td>5</td>
<td>2.37818675</td>
<td>.27665497</td>
<td>.0077987352</td>
<td>3.5175</td>
</tr>
<tr>
<td>6</td>
<td>2.348968232</td>
<td>.27480082</td>
<td>.0063976318</td>
<td>3.5925</td>
</tr>
<tr>
<td>7</td>
<td>2.705926337</td>
<td>.27334467</td>
<td>.0054165521</td>
<td>3.6525</td>
</tr>
<tr>
<td>8</td>
<td>2.852616885</td>
<td>.27218124</td>
<td>.0046931340</td>
<td>3.7075</td>
</tr>
<tr>
<td>10</td>
<td>3.108618420</td>
<td>.27036059</td>
<td>.0036973067</td>
<td>3.7925</td>
</tr>
<tr>
<td>20</td>
<td>4.063980433</td>
<td>.26564491</td>
<td>.0017783697</td>
<td>4.0387</td>
</tr>
<tr>
<td>30</td>
<td>4.745875374</td>
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<tr>
<td>40</td>
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<td>4.2637</td>
</tr>
<tr>
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<td>5.75275881</td>
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<td>.00068564904</td>
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<td>6.158923349</td>
<td>.26062552</td>
<td>.00056803471</td>
<td>4.3893</td>
</tr>
<tr>
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<td>.00048462240</td>
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<td>.00042243370</td>
<td>4.4729</td>
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<td>7.157896787</td>
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<td>.00037425564</td>
<td>4.4972</td>
</tr>
<tr>
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<td>7.440332217</td>
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</table>
TABLE I -- Continued

B. THE VARIOUS FORMS OF ENERGY (a.u.)

<table>
<thead>
<tr>
<th>Z</th>
<th>$E_P$</th>
<th>$E_Q$</th>
<th>$E_R$</th>
<th>$E^e_P$</th>
<th>$E_x$</th>
<th>$E_c$</th>
<th>$E$</th>
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<tbody>
<tr>
<td>2</td>
<td>2.2270</td>
<td>0.67061</td>
<td>-6.5965</td>
<td>1.5881</td>
<td>-0.73537</td>
<td>-0.11198</td>
<td>-2.9582</td>
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<tr>
<td>3</td>
<td>5.9421</td>
<td>1.5576</td>
<td>-17.415</td>
<td>3.9161</td>
<td>-1.4135</td>
<td>-0.18777</td>
<td>-7.6005</td>
</tr>
<tr>
<td>4</td>
<td>11.962</td>
<td>2.8506</td>
<td>-34.693</td>
<td>7.4654</td>
<td>-2.2572</td>
<td>-0.27172</td>
<td>-14.944</td>
</tr>
<tr>
<td>5</td>
<td>20.611</td>
<td>4.5210</td>
<td>-59.182</td>
<td>12.345</td>
<td>-3.2519</td>
<td>-0.36243</td>
<td>-25.319</td>
</tr>
<tr>
<td>6</td>
<td>32.149</td>
<td>6.5894</td>
<td>-91.534</td>
<td>18.646</td>
<td>-4.3867</td>
<td>-0.45896</td>
<td>-38.995</td>
</tr>
<tr>
<td>7</td>
<td>46.827</td>
<td>9.0707</td>
<td>-132.36</td>
<td>26.453</td>
<td>-5.6544</td>
<td>-0.56071</td>
<td>-56.225</td>
</tr>
<tr>
<td>8</td>
<td>64.846</td>
<td>12.030</td>
<td>-182.22</td>
<td>35.838</td>
<td>-7.0479</td>
<td>-0.66715</td>
<td>-77.217</td>
</tr>
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<td>10</td>
<td>111.73</td>
<td>19.085</td>
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<td>59.605</td>
<td>-10.193</td>
<td>-0.89269</td>
<td>-131.31</td>
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<td>20</td>
<td>602.82</td>
<td>80.184</td>
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<td>292.06</td>
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<td>1609.6</td>
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<td>-4269.1</td>
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<td>-63.280</td>
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<td>-1797.3</td>
</tr>
<tr>
<td>40</td>
<td>3225.3</td>
<td>334.76</td>
<td>-8461.7</td>
<td>1445.6</td>
<td>-102.22</td>
<td>-5.5329</td>
<td>-3563.9</td>
</tr>
<tr>
<td>50</td>
<td>5523.5</td>
<td>529.12</td>
<td>-14378.</td>
<td>2422.7</td>
<td>-148.31</td>
<td>-7.4337</td>
<td>-6058.2</td>
</tr>
<tr>
<td>60</td>
<td>8566.6</td>
<td>771.39</td>
<td>-22167.</td>
<td>3696.1</td>
<td>-201.05</td>
<td>-9.4648</td>
<td>-9343.2</td>
</tr>
<tr>
<td>70</td>
<td>12409.</td>
<td>1057.3</td>
<td>-31953.</td>
<td>5283.9</td>
<td>-260.02</td>
<td>-11.611</td>
<td>-13474.</td>
</tr>
<tr>
<td>80</td>
<td>17100.</td>
<td>1386.9</td>
<td>-43849.</td>
<td>7202.5</td>
<td>-324.94</td>
<td>-13.861</td>
<td>-18498.</td>
</tr>
<tr>
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<td>9466.8</td>
<td>-395.53</td>
<td>-16.206</td>
<td>-24461.</td>
</tr>
<tr>
<td>100</td>
<td>29200.</td>
<td>2186.9</td>
<td>-74392.</td>
<td>12090.</td>
<td>-471.58</td>
<td>-18.639</td>
<td>-31405.</td>
</tr>
</tbody>
</table>
# TABLE II

COMPARISON OF CALCULATED AND EXPERIMENTAL TOTAL BINDING ENERGIES (a.u.)

<table>
<thead>
<tr>
<th>Z</th>
<th>$-E_{\text{calc}}$</th>
<th>$-E_{\text{HFS}}$</th>
<th>$-E_{\text{exp}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2.9582</td>
<td>2.8779</td>
<td>2.9027</td>
</tr>
<tr>
<td>3</td>
<td>7.6005</td>
<td>7.2262</td>
<td>7.4761</td>
</tr>
<tr>
<td>5</td>
<td>25.319</td>
<td>24.079</td>
<td>24.652</td>
</tr>
<tr>
<td>6</td>
<td>38.995</td>
<td>37.079</td>
<td>37.846</td>
</tr>
<tr>
<td>7</td>
<td>56.225</td>
<td>53.587</td>
<td>54.598</td>
</tr>
<tr>
<td>8</td>
<td>77.217</td>
<td>73.938</td>
<td>75.092</td>
</tr>
<tr>
<td>10</td>
<td>131.31</td>
<td>127.48</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>684.37</td>
<td>674.02</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>1797.3</td>
<td>1773.6</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>3563.9</td>
<td>3532.6</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>6058.2</td>
<td>6014.6</td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>9343.2</td>
<td>9273.6</td>
<td></td>
</tr>
<tr>
<td>70</td>
<td>13474.0</td>
<td>13380.0</td>
<td></td>
</tr>
<tr>
<td>80</td>
<td>18498.0</td>
<td>18395.0</td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>24461.0</td>
<td>24343.0</td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>31405.0</td>
<td>31264.0</td>
<td></td>
</tr>
</tbody>
</table>
The Hartree-Fock-Slater results through $Z = 30$ were reported by Snow, et al.\textsuperscript{19} as computed from the code published by Herman and Skillman,\textsuperscript{20} while for larger $Z$ the values were calculated by Cowan\textsuperscript{21} with a modification of the same code. In comparing with experiment, the binding energies on the corrected TFD model are seen to be not much worse than those calculated by the self-consistent field method, and in some cases are better. At high $Z$ the two methods give energies differing by roughly one-half of one percent. It should be mentioned, however, that the agreement is slightly better on the model that includes the quantum correction but no correlation. This is especially true for lower $Z$.

Correlation increases the discrepancies with experimental energies from about 2\% to about 3\% for atomic numbers 6, 7, and 8, but at high $Z$ it causes a change in energy of only about 0.1\%.

The radius of minimum-energy solutions as a function of atomic number is shown in Fig. 2; this radius is the "lattice constant" if the atoms are considered to be bound in a solid. Also shown are the corresponding TFD values computed by Thomas,\textsuperscript{22} and spherical cell radii calculated from the observed normal crystal densities. The inclusion of correlation produces a cell radius which represents a somewhat better average to the experimental points in the variation with $Z$, but quite obviously the equation of state for many metals will not be greatly improved.

Although in equation of state calculations a zero boundary pressure solution is tacitly considered to represent an atom bound in a crystal of normal density, the calculated radii of such solutions actually support their interpretation as representing isolated atoms. One might object that, with reference again to Fig. 2, the calculated cell radius of some elements, notably most of the alkalies and alkaline earths, is less than the observed crystal radius. This result is not surprising for these elements, as can be seen from the sketch on page 35. Here are shown the radial distribution functions, as calculated by the self-consistent field code of Boyd, et al.,\textsuperscript{23} for the ground states of neon, sodium, magnesium, and argon. The long "tail" of the distribution, apparent especially for
Figure 2. Lattice constant of the elements.
sodium, and to a lesser extent for magnesium, is not obtained on the statistical model. The statistical density distributions have an abrupt cutoff, and thus much more closely resemble those of the rare gases.

The radii of the rare-gas atoms neon, argon, krypton, and xenon, computed on the present model agree closely with their crystal radii. This comparison is made in Table III, where the "experimental" values are computed from the experimental lattice constants given in the recent review article by Pollack. The rare gases are bound in crystals only by the very weak van der Waals forces; if we were to ascribe a finite radius to the isolated atom, it should be for the solid rare gases that such a radius would most nearly equal its crystal radius. Since the corrected statistical model predicts close to these values for the rare-gas atomic radii, it would appear that the correct interpretation of minimum-energy, or zero boundary pressure, solutions is as representing isolated atoms.
TABLE III

LATTICE CONSTANTS OF THE SOLID RARE GASES (a.u.)

<table>
<thead>
<tr>
<th>Element</th>
<th>$(x_2)_{\text{calc}}$</th>
<th>$(x_2)_{\text{exp}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neon</td>
<td>3.79</td>
<td>3.30</td>
</tr>
<tr>
<td>Argon</td>
<td>4.00</td>
<td>3.92</td>
</tr>
<tr>
<td>Krypton</td>
<td>4.23</td>
<td>4.17</td>
</tr>
<tr>
<td>Xenon</td>
<td>4.36</td>
<td>4.53</td>
</tr>
</tbody>
</table>
APPENDIX

A FORTRAN CODE TO INTEGRATE THE QUANTUM- AND CORRELATION-CORRECTED TFD EQUATION

The FORTRAN machine code listed here in "F4" language generates a single solution of the quantum- and correlation-corrected TFD equation for a given atomic number, initial slope of the potential function, and degree of ionization. The minimum-energy solutions were stressed in this report, and the code as actually used contains a feature that searches for the solutions possessing the lowest energy by adjusting $\phi_0$ and performing a series of integrations. However, there seems little virtue in complicating the present write-up by including a number of code statements that are unnecessary for the task to which a potential user may put the code.

The input data consists of any number of sets of $Z$, $\phi'$, degree of ionization, and a print flag that indicates whether the entire solution is to be printed, or whether summary information only is desired. Each set is entered by a data card, the layout of which is as follows:

<table>
<thead>
<tr>
<th>Columns</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 4</td>
<td>Atomic number $Z$</td>
</tr>
<tr>
<td>5 - 18</td>
<td>Initial slope $\phi'$</td>
</tr>
<tr>
<td>19 - 23</td>
<td>Degree of ionization</td>
</tr>
<tr>
<td>24</td>
<td>Print flag</td>
</tr>
</tbody>
</table>
All but the print flag are floating point numbers. For example, to obtain and print the complete solution corresponding to the free neutral lithium atom, one would prepare the following card:

```
<table>
<thead>
<tr>
<th>Columns</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 4</td>
<td>003.</td>
</tr>
<tr>
<td>5 - 18</td>
<td>-1.9498201900</td>
</tr>
<tr>
<td>19 - 23</td>
<td>0000.</td>
</tr>
<tr>
<td>24</td>
<td>1</td>
</tr>
</tbody>
</table>
```

If only summary information were desired, column 24 would contain a 0 punch.

As a further example, a solution corresponding to a compressed 0⁻ ion of radius 2.5203 a.u. is obtained with the input card:

```
<table>
<thead>
<tr>
<th>Columns</th>
<th>Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 4</td>
<td>008.</td>
</tr>
<tr>
<td>5 - 18</td>
<td>-2.8480000000</td>
</tr>
<tr>
<td>19 - 23</td>
<td>-002.</td>
</tr>
<tr>
<td>24</td>
<td>1</td>
</tr>
</tbody>
</table>
```

The output contains a listing of Z and \( \phi_0' \), and the computed value of \( a \). There follows, unless suppressed by the presence of a 0 in column 24 of the input card: \( x_1, \rho(x_1) \), and a tabulation of \( \phi \) and \( \rho \) for each \( x \) value. Immediately following the tabulation is the computed outer radius of the distribution, \( x_2 \), and the interpolated values of \( \phi(x_2) \) and \( \rho(x_2) \). Also printed out are the total calculated number of electrons within the distribution, and the various energies. If the printing is suppressed, then \( x_1, \rho(x_1) \), and the table of \( \phi(x) \) and \( \rho(x) \) are not printed.

The code consists of a main program and a number of FUNCTION and SUBROUTINE subprograms. "Comment" cards make the purpose of the programs evident; no further explanation of their purpose is required here. However, an attempt will be made to clarify a few items that might
prove puzzling:

In the SOURCE subprogram, note that after 10 attempts to find $y$ by iteration, $y$ being a solution of Eq. (15) of the text, the initial guess is changed; and 10 more attempts can be made. This can occur only once in each integration, where the density decreases below about 0.0123. At this point there becomes only one real root of the cubic equation, this root being approximately 0.13, whereas the iteration procedure utilizing the solution on the previous step of the integration as a first guess attempts to find a solution near $y = -0.18$.

Another item is an apparently extraneous integral that is calculated and never used. This is calculated through FLINT(8) in the integrand routine, and SUM(8) in the main routine. The integral is

$$\int_{x_1}^{x_2} p x^4 \, dx,$$

from which the diamagnetic susceptibility and other quantities of possible interest can be calculated if desired. It should be mentioned that, indeed, the susceptibility has been calculated on this model for the rare gases. The agreement with experiment is slightly better than on the uncorrected TFD model; but the latter values are already in quite good agreement, and the improvement is small.

In addition to the possible necessity of altering the Input-Output statements of the code, it may also be necessary to change the iteration criteria used in the AFUNCT, INTSEC, and SOURCE subprograms.
SUBTYPE, FORTRAN

C MAIN PROGRAM TO INTEGRATE THOMAS-FERMI-DIRAC EQUATION
C WITH QUANTUM AND CORRELATION CORRECTIONS

00000 DIMENSION X(13), PHI(13), FNT(13), SUM(1), FNTM(1)
00001 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)
00002 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)
00003 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)

00004 C0 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)
00005 C0 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)
00006 C0 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)
00007 C0 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)
00008 C0 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)
00009 C0 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)
00010 C0 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)
00011 C0 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)
00012 C0 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)
00013 C0 COMMON Z, P, FISRQD, C1, C2, C3, TAUI, CSLPE, HMAX, R, Y, PHI1, FLINT(1)

00014 5 READ 10,2,SLOPE,DEGIOM,IPRTFG
00015 10 FORMAT(F4.0,F10.0)
00016 CSLOPE=SLOPE
00017 RHOC+=2/00

00018 15 PRINT 20,SLOPE
00019 X=1IFNTC(SLPE,A)
00020 PHI1=1.4*SLOPE*X1
00021 Y=-19
00022 RHOM1=(RHOCON*X1)+SOURCE(X1,PHI1,A)

00023 PRINT 20
00024 20 FORMAT(1H1)
00025 PRINT 22,2
00026 22 FORMAT(7H I = 15)
00027 PRINT 24,3
00028 24 FORMAT(7H SLPE= F10.1)
00029 PRINT 26,4
00030 26 FORMAT(7H A = F10.1)
00031 IF IFRHGF I=1,30,261
00032 261 PRINT 28,X1
00033 28 FORMAT(7H X1 = F10.1)
00034 PRINT 30,RHUM
00035 30 FORMAT(7H RHM1=F13.7/)

00036 PRINT 35
00037 35 FORMAT(4H X=1JH PHI1,M RHO//)
00038 COMPUTE INITIAL AND FINAL INTEGRATION INTERVALS
00039 36 SPLIT=1.0
00040 40 IF(SPLIT>0.4)145,45,50
00041 45 SPLIT=SPLIT*2.0
00042 50 H=0.02/SPLIT
00043 HMAX=.01/SQRT(Z)

00044 C CALCULATE INITIAL VALUES FOR INTEGRATION
GO044  DD 55 I=1,3
GO045  FLI=1
GO046  XI-J=(FLI-1.0)*H
GO047  55 PHI(I)=1.0+SLOPEX(I)
GO048  IF(IPRFFG156,H,0,56)  MAINMFD  000417
   C  PRINT FIRST THREE POINTS
GO049  56 PRINT 60,X(I),PHI(I),I=1,3
GO050  60 FORMAT(2F12.8)  MAINMFD  000420
GO051  600 PHIM2=1.0
GO052  PHIM=PHI(2)
GO053  PHIO=PHI(3)
GO054  PHDPM2=0.0
GO055  PHDPM1=0.0
GO056  PHIDPO=0.0
CC057  XO=X(1)
CC058  INDXBE=1
CC059  XML=X1
CC060  DO 61 J=1,8
CC061  61 SUM(J)=0.0
CC062  CALL FLINTS(X1,PHIX1,RHOX1)
CC063  DO 62 J=1,8
CC064  62 FNT(J,J)=FLINT(J)
   C  ADVANCE ONE STEP IN X
GO065  65 CALL INTSEC(PHIM2,PHIML,PHIO,PHDPM2,PHDPM1,PHIDPO,H,XO,AL)
GO066  IF(XO-XL70.75,75)  MAINMFD  000544
GO067  70 IF(IPRFFG171,H,71)  MAINMFD  000547
GO068  71 PRINT 60,XO,PHIO
GO069  72 INDXBE=INDXBE
GO070  GU TO 65
GO071  75 RHO=RHOCON+PHIDPO/KO
GO072  IF(IPRFFG170,H,80)  MAINMFD  000574
GO073  76 PRINT 80,XO,PHIO,RHU
GO074  80 FORMAT(2F12.8,F7.7)
GO075  810 CALL FLINTS(XO,PHIO,RHU)
GO076  DO 81 J=1,8
GO077  81 FNT(J,J)=FNT(J,3,J)
GO078  SUM(J)=SUM(J)+V*(FNT(J,2)+FNT(J,3,J)+(XC-XM))
GO079  81 FNT(J,J)=FNT(J,3,J)
GO080  XML=XO
GO081  INDXBE=INDXBE
GO082  IF(INDXBE+.85,85)  MAINMFD  000667
GO083  85 CD 86 J=1.8
GO084  86 FNT(J,J)=FNT(J,3,J)
GO085  IF(JH+.5,MAXH,.94)  MAINMFD  000674
   C  DOUBLE INTEGRATION INTERVAL
GO086  90 H=+.01H
GO087  PHIM=PHIM2
GO088  PHIO=PHIO2+.0
GO089  PHIDPO=PHIDPO2
GO090  91 CALL INTSEC(PHIM2,PHIML,PHIO,PHDPM2,PHDPM1,PHIDPO,H,XO,AL)
GO092  RHO=RHOCON+PHIDPC/KO
GO093  IF(IPRFFG170,H,91)  MAINMFD  000740
GO094  910 PRINT 80,XO,PHIO,RHU
GO095  911 CALL FLINTS(XO,PHIO,RHU)
GO096  CD 92 J=1.8
GO097  92 FNT(3,J,J)=FNT(3,J)
GO098  INDXBE=INDXBE
GO099  IF(INDXBE+.93,93)  MAINMFD  001013
GO100  93 CD 93 J=1.8
GO101  931 FNT(2,J,J)=FNT(3,J)  MAINMFD  001015
   C  PRINT FIRST THREE POINTS
PRINT 137,EPN,EPE,EEX,EC
137 FORMAT(5H EPN= 1PE15.7,7H EPE= 1PE15.7,7H EEX= 1PE15.7,1H EC= 1PE15.7)
MAINMFD
MAINMFD
MAINMFD
MAINMFD
MAINMFD
00156
00157
00158
00159
00160
PRINT 138*E
138 FORMAT(5H E= 1PE18.10/)
GO TO 5
END

SUBPROGRAM *MAIN* - COMPILE TIME 006005 SECS. - NO. BINARY CARDS 000000 - LENGTH 81001267 WORDS I=110003695
SUBTYPE, FORTRAN

C COMPUTE MODIFICATION FACTOR FROM INITIAL SLOPE
C BY NEWTON-RAPHSON METHOD

FUNCTION AFUNCT(SLOPE)

0000 COMMON Z,PI,PISQRO,CI,C2,C3,TAU1,CSLOPE,HMAX,R,Y,PHIX2,FLINT(8)
0001 CRIT=1.0E-14
0002 ALPHA=SQR(T/SQRT(SLOPE))
0003 ROOT1=SQRAT(ALPHA)
0004 F1=3.0*ALPHA*ALPHA-.5
0005 F2=ALPHA*ROOT1
0006 C INITIAL GUESS FOR NU
0007 FLNU=ALPHA-.5
0008 9 ROOT2=SQRAT(FLNU)
0009 F=FLNU*(FLNU*(FLNU+1.5)+2.0+F2+ROOT2-F1)
0010 FPRIME=3.0*FLNU*(FLNU+1.0)+3.0*F2*ROOT2-F1
0011 IF(FPRIME>115,10,15
0012 C ADJUST NU IF DERIVATIVE OF F IS ZERO
0013 10 FLNU=.99999*FLNU
0014 GO TO 5
0015 C CONNECT NU
0016 15 CORR=F/FPRIME
0017 C TEST IF CRITERION IS MET
0018 IF(ERROR*CRIT20).5)
0019 RETURN
0020 END

SUBPROGRAM AFUNCT - COMPILERS 000003 SECS. - NO. BINARY CARDS 000000 - LENGTH (8)00135 WORDS (10)00093
C COMPUTE INNER RADIUS OF ELECTRON DISTRIBUTION
FUNCTION XIFNCT(SLOPE,A)
COMMON Z,PI,PISQRD,C1,C2,C3,TAU1,C5LOPE,HMAX,R,Y,PHIX2,FLINT(B)
S=(1.0-PISQRD/(2.0*SLOPE)/(PI*SLOPE*2))
XIFNCT=(1.0-SQRT(1.0-A*A*S/Z))/S
RETURN
END

SUBPROGRAM XIFNCT - COMPIL 00002 SECS. - NO. BINARY CARDS 00000 - LENGTH 181000067 WORDS */(101000055)*/
SUBTYPE, FORTRAN

C COMPUTE OUTER RADIUS OF ELECTRON DISTRIBUTION
C AND INTERPOLATE FOR PHI AT OUTER BOUNDARY

FUNCTION X2FNC(T, PHI1, PHI2, PHI3, PHI0, X0, H, DEGON)

COMMON Z, PI, PIQR, C1, C2, C3, TAU, CSLOPE, HMAX, R, Y, PHIX, FLINTB

SCRIPA = (PHIO - PHI1) / H
SCRIPB = (PHIO - PHI1) / (H + H)

SCRIPC = PHI0 - XQ * (SCRIPA * X0 + SCRIPB)

X2 = SQRT(SCRIPC - DEGON / 2 / SCRIPA)

PHIX2 = X2 * (SCRIPPA * X2 + SCRIPB) / SCRIPC

RETURN
END

SUBPROGRAM X2FNC - COMPILE TIME 000002 SECS. - NO. BINARY CARDS 000000 - LENGTH (8)1000115 WORDS (101000077)
SUBROUTINE WHICH INTEGRATES SECOND ORDER DIFFERENTIAL EQUATION

BY HARTREE (STERNER) METHOD, WITH A CORRECTION TERM

IN INVOLVING AN ESTIMATE OF FOURTH DIFFERENCE IN PHI

DOUBLE PRIME WHEN THIS QUANTITY IS LARGE

SUBROUTINE INTSEC(XM2,XM1,XPH1,XPH2,XPDP2,PHDPO,PHDP1,PHDPM2)

COMMON Z,P1,PISOR,C1,C2,C3,TAU1,CSLOPE,HMAX,R,Y,PHX2,FLINT(8)

CT=1.0E-13

N=1

XP=X+H

TEST IF TO APPLY CORRECTION

IF(H<5*HMAX/10,5,5)

5 IF(PHDPM2)15,10,15

CALCULATE FOURTH ORDER TERM

10 XP=2*XP+2.0*H

ETYPE1=1.0*CSLOP+XP

ETYPE2=1.0*CSLOP+XP

EPDP1=SOURCE(XP1,ETYPE1),A)

EPDP2=SOURCE(XP2,ETYPE2)

FOURTH=(EPDP2-4.0*EPDP1+6.0*PHDPO-4.0*PHDP1+PHDPM2)/240.0

GO TO 20

15 FOURTH=0.0

ESTIMATE SECOND ORDER DIFFERENCE IN PHI DOUBLE PRIME

20 DPDP=PHDPO-2.0*PHDP1+PHDP2

CALCULATE PREDICTED VALUE FOR COMPARISON

25 DPHI=1.0H+1.0PHDPO+(DPDP/12.0)-FOURTH

PHI1=2.0PHI1+DPHI

PHI2=SOURCE(XP1,PHI1,A)

DPDP=PHDP1+2.0PHDP2+PHDPM1

TEST FOR CONVERGENCE

ERROR=ABS((DPDP-EPDP)/PHI)+H/H/6.0

IFERROR<CRIT(45,45,30)

30 DPDP=EPDP

40 FORMAT(I9M INTEGRATION CRITERION NOT MET)

GO TO 45

PHI2=PHI1

PHI1=PHI2

PHDP=PHDP1

PHDP1=PHDP2

PHDP2=PHDP

45 PRINT 40

GO TO 45

END

SUBPROGRAM INSEC ~ COMPILE TIME 003053 SECS. ~ NO. BINARY CARDS 000000 ~ LENGTH (8)100255 WORDS (+1101000173)
FORTRAN SYSTEM -- VERSION 07/15/64 -- CORRECTION LEVEL 09/15/64

S U B T Y P E F O R T R A N

C COMPUTE SOURCE FUNCTION, WHICH IS EQUATED TO 10
C SECOND DERIVATIVE OF PHI
00000 FUNCTION SOURCE(X,PHI,A)
00001 COMMON Z,P1,PISQRD,C1,C2,C3,TAU1,CSLOPE,PHI1,MAX,R,Y,PHIX2,FLINT(8)
00002 CRI1=1.0E-14
00003 N=0
00004 NFLAG=0
00005 R=1!(2*PHI/X+A*A/(2.0*X*X)-C2)
C EVALUATE Y BY NEWTON-RAPHSON METHOD
00006 FZ=TAUL+R-C3
00007 9 F=Y+E*(Y+TAUL)+R+F2
00008 FPRIME=Y*(3.0*Y+Z+TAUL)+R
00009 IF(FPRIME15,10,15
0010 10 Y=0.99999*Y
0011 GO TO 5
0012 15 CORR=-F/FPRIME
0013 Y=Y+CORR
0014 ERROR=ABS(CORR)/Y
0015 IF(VERIFY=0.15,50,20
0016 20 N=N+1
0017 IF(NFLAG=35,25,35
0018 25 IF(N=1015,30,30
0019 30 NFLAG=-1
0020 Y=C.13
0021 N=0
0022 GO TO 5
0023 35 IF(N=1015,40,40
0024 40 PRINT 45
0025 45 FORMAT(23H CRITERION UN Y NOT MET)
0026 90 ROOT=SQRT(Y+R)
0027 PS=SQRT(Y+TAUL)+SQRT(-Y+TAUL+Z+ROOT)
0028 SOURCE=1.5*PI*X/(2.0+PATH)
0029 RETURN
0030 END

S U B P R O G R A M S O U R C E -- C O N P L E T E T I M E 0 0 0 0 0 3 S E C S . -- N O . B I N A R Y C A R D S 0 0 0 0 0 0 C -- L E N G T H (B)0 0 0 1 7 7 W O R D S (+10)0 0 0 1 2 7 )
SUBTYPE, FORTRAN

C COMPUTE INTEGRANDS FOR ENERGY INTEGRALS AND TOTAL C NUMBER OF PARTICLES CHECK

06000 SUBROUTINE FLINTS1X, PHI, RHOD

06000 COMMON Z*, P*, ISQR, C1, C2, C3, TAU1, CSLOPE, HMAX, R, Y, PHI1, PHI2, FLINT8

06002 RHOD = RHOD ** (1.0 / 3.0)

06003 FLINT(6) = RHOD

06004 FLINT(4) = RHOD * X

06005 FLINT(1) = FLINT(4) * X

06006 FLINT(8) = FLINT(1) * X * X

06007 FLINT(2) = FLINT(1) * R RHOD

06008 FLINT(3) = FLINT(2) * R RHOD

06009 FLINT(5) = PHI1 * FLINT(4)

06010 FLINT(7) = FLINT(1) * SQRT(R RHOD)

06011 RETURN

06012 END

SUBPROGRAM FLINTS - COMPILE TIME 000002 SECS. - NO. BINARY CARDS 000000 - LENGTH 81000105 WORDS (10)000069
LIST OF REFERENCES

21. R. D. Cowan (private communication).
23. R. G. Boyd, A. C. Larson, and J. T. Waber, Los Alamos Scientific Laboratory, work to be published.