A RELATIVISTIC STATISTICAL ATOM MODEL

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PREFACE

In this thesis, the relativistic statistical models of the atom are investigated. The development of the model is put on a sound basis, and numerical solutions of the resulting equations have been obtained. The agreement between theory and experiment has been improved over the non-relativistic calculations, but the agreement for diamagnetic susceptibilities is still only fair. This calculation, however, is regarded as only a preliminary application of a model which promises to be more useful in other areas.

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CHAPTER I

INTRODUCTION

The statistical models of the atom are finding new usefulness today in the studies of many diverse systems. Atomic collision experiments, high energy plasmas, low energy electron diffraction, and molecular theory have all utilized statistical models of the atom to describe certain phenomena. Also, the easily calculated statistical densities are finding usefulness as starting points for more involved self-consistent calculations.

In this thesis we will discuss the relativistic Thomas-Fermi (RTF) model of the atom. The RTF model is derived from the central field Dirac equation and is seen to lead to four similar densities, depending on the precision carried through the derivation. While the model as presented here is applied only to isolated, neutral atoms, immediate extensions of this model are possible to include thermally excited atoms, diatomic molecules, high pressure matter, and ionized states. Thus, while we treat the RTF model as an atomic theory, it is much more generally applicable than that. (In fact, the RTF is more appropriate to other cases than neutral atoms, but we are restricting ourselves in this study to this one application.)

Chapters II and III review the early development and modifications of the Thomas-Fermi model, and Chapter IV presents the basis of the RTF model as first presented by M. Rudkjobing[1] and J. J. Gilvarry[2]. The systematic development of the RTF equations is then presented in Chapter V, and the method of solution and numerical results are given in Chapter VI for one of these four equations.

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CHAPTER II

THE THOMAS-FERMI MODEL OF ATOMS

Development of the Theory

The development of the statistical model of the atom is presented in three main references: Paul Gombas' book, Die Statistische Theorie des Atoms und ihre Anwendungen[1], his review article "Statistische Behandlung des Atoms," in Handbuch der Physik[2] and the review article by N. H. March, "The Thomas-Fermi Approximation in Quantum Mechanics."[3]

The Thomas-Fermi model was developed independently by L. H. Thomas[4] and Enrico Fermi,[5,6] and is based on four explicit assumptions regarding the atomic system:

(1) Relativity corrections can be ignored.

(2) The atomic potential V depends only on the distance r from the nucleus in such a way that:

$$\operatorname*{limit}_{r \to \infty} V(r) = 0,$$

$$\operatorname*{limit}_{r \to o} V(r) = \frac{Ze}{r} .$$

(3) The electrons are distributed uniformly in the six-dimensional phase space at the rate of 2 per h^3 of volume.

(4) The potential V(r) is itself determined by the nuclear charge and this distribution of electrons.

We are thus assuming that the electrons constitute a degenerate electron gas under the influence of a central potential. As given by Thomas[4] himself, the development is as follows: Suppose that around a point $\vec{r}$, the momentum space is occupied up to a certain maximum momentum $p_o(\vec{r})$. Now, the volume in momentum space occupied by these electrons is a sphere with radius p_o: $V_p = \frac{4}{3}\pi p_o^3$. Because of the spin degeneracy, there are 2 electrons per h^3 of phase space volume, so we can find the volume density of electrons at a point $\vec{r}$ by multiplying the phase space density by the momentum space volume:

$$\rho(\vec{r}) = \frac{8\pi\, p_o^3(\vec{r})}{3h^3} . \tag{1}$$

At this point $\vec{r}$, the energy of the electron with the maximum momentum p_o is given by

$$E_o = \frac{p_o^2(r)}{2m} - e\cdot V(r) . \tag{2}$$

If we write E_o as $-eV_o$ and substitute for p_o, the electron density can be written as

$$\rho(\vec{r}) = \frac{8\pi}{3h^3} (2me)^{3/2} \left(V(\vec{r}) - V_o\right)^{3/2} , \tag{3}$$

Now, we apply assumption (4) by requiring that the density and potential be related by Poisson's equation:

$$\nabla^2 V(\vec{r}) = 4\pi e\, \rho(\vec{r}) . \tag{4}$$

The fundamental equation in the Thomas-Fermi model is then

$$\nabla^2 \left(V(\vec{r}) - V_o\right) = \frac{32\pi^2 e}{3h^3} (2me)^{3/2} \left(V(\vec{r}) - V_o\right)^{3/2} . \tag{5}$$

If we now assume that the electron density (and hence, the potential) is spherically symmetric and make the following substitutions:

$$V(r) - V_0 = \frac{Ze}{r} \cdot \Phi(r) \tag{6a}$$

$$r = b \cdot x \tag{6b}$$

$$b = \left(\frac{3}{32\pi^2}\right)^{2/3} \frac{\hbar^3}{2me^2 Z^{1/3}} \tag{6c}$$

the Thomas-Fermi equation takes on the simple form

$$\frac{d^2\Phi}{dx^2} = \frac{\Phi^{3/2}}{x^{1/2}} \tag{7}$$

The boundary conditions for an isolated, neutral atom now become:

$$\underset{x\to\infty}{\text{limit}}\ \Phi(x) = 0 \tag{8a}$$

$$\underset{x\to 0}{\text{limit}}\ \Phi(x) = 1. \tag{8b}$$

Before discussing the solutions of this equation, it is important to note that the same equation can be derived from a variational point of view[7,8]. This approach is useful because it permits a direct incorporation of exchange and correlation corrections and will be discussed in Appendix A.

The Thomas-Fermi equation as written above is a dimensionless equation, independent of Z. This means that it need only be solved once and the actual atomic potential for any Z can be easily found from the universal solution. Unfortunately, this desirable feature is lost as soon as the equation is modified to take into account corrections due to exchange, correlation, or relativity, but with modern computers this is less a disadvantage than it once was.

Solutions of the Thomas-Fermi Equation

Being a second-order differential equation, the Thomas-Fermi equation possesses a doubly infinite number of solutions if no boundary conditions are imposed. Applying the boundary condition at the origin (Eq. 8a) allows an infinite family of curves with $\Phi(0) = 1$, all concave upwards.[9]

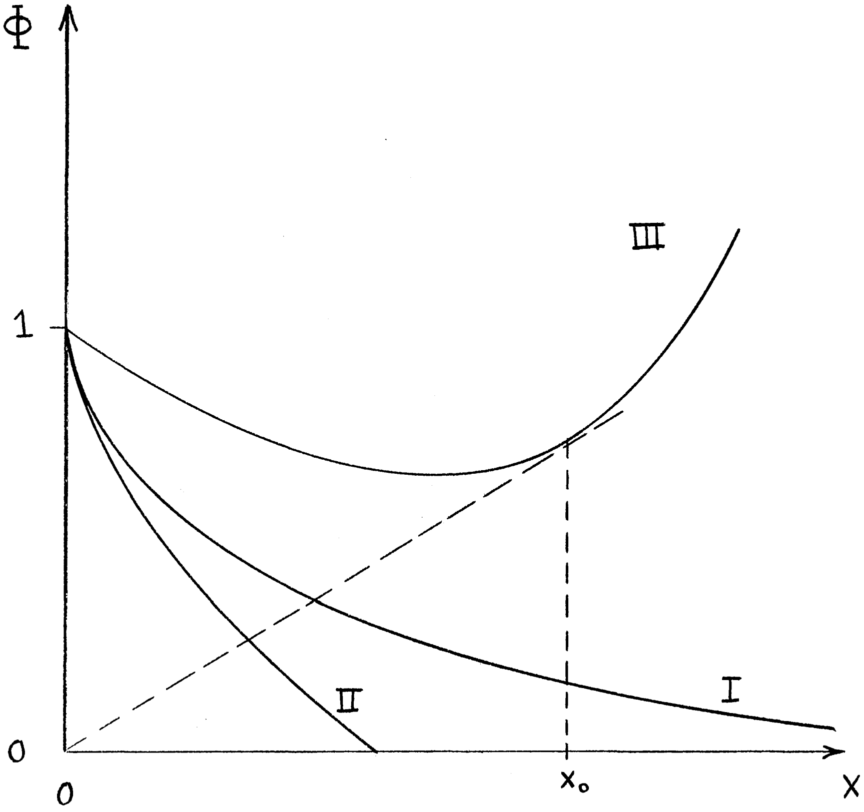

Figure 1. Solutions of the Thomas-Fermi Equation Satisfying the Boundary Condition $\Phi(0) = 1$

These solutions can be identified by their initial slope. Curve I represents the solution describing an isolated, neutral atom, and approaches the x-axis as $144\ x^{-3}$ for large X. Curve II is representative of those with a steeper initial slope than I, and these describe positive ions. Curve III, which diverges for large X, is used (out to a certain finite X_o) in the statistical model of crystals and molecules with high symmetry. The emphasis in this thesis is on the neutral atoms, so we will concern ourselves primarily with the asymptotic solution.

The Thomas-Fermi equation has an analytic solution

$$\Phi(X) = 144 \cdot X^{-3} \tag{9}$$

which satisfies the boundary condition at infinity, but it does not satisfy the requirement that $\phi(0) = 1$. There does not exist an analytic solution satisfying both boundary conditions, so the solution must be obtained by numerical integration. Integration of this equation has been performed by several authors, beginning with Thomas[4] and Fermi[5]. Subsequent numerical integrations were published by E. Baker[10], C. Miranda[11], Slater and Crutter[12] and more recently in a series of articles in the Journal of the Physical Society of Japan by Umeda, Kobayashi, and others[13-16]. It is interesting to note that, for more than twenty years, the most reliable solution of the Thomas-Fermi equation was that produced by a mechanical integrating machine, the "differential analyzer" of Bush and Caldwell[17].

Several investigations have been made regarding the asymptotic behavior of the numerical solution and various refinements have been made in the analytic approximation to the exact numerical solution. The analytic properties of the Thomas-Fermi equation were developed by Arnold

Sommerfeld[18] and an important result is the fact that, if $\phi(x)$ is a solution, then so also is $\chi(y)$, where:

$$\Phi = a \cdot \chi \tag{10}$$

$$x = b \cdot y \tag{11}$$

provided that $ab^3 = 1$. This means that a single numerical integration can be carried out and the resulting solution can be scaled to fit the requisite boundary conditions.

N. H. March[19] used this fact to set up two "master solutions" of the Thomas-Fermi equation. Using the Coulson-March[20] asymptotic expansion

$$\Phi(x) = \frac{144}{x^3}\left(1 - \frac{F_1}{x^c} + \frac{F_2}{x^{2c}} - \frac{F_3}{x^{3c}} + \cdots\right) \tag{12}$$

two solutions were produced: one with positive F_1, and one with negative F_1. These two solutions can be transformed by the scale factors to any particular solution desired.

A procedure similar to this was used by Kobayashi, et al.[15] in their numerical integration. The procedure used was to integrate from $x = \infty$ toward the point $x = 1$ using the transformed variable $y = 1/x$ and starting with Eq. (12). At $x = 1$, the then determined values of $\phi(1)$ and $\phi'(1)$ were used to begin an integration from $x = 1$ to $x = o$, using the variable $z = x^{\frac{1}{2}}$ to remove the divergence in the second derivative at the origin. The solution generated by this method automatically satisfies the boundary condition at infinity, but probably does not intersect the ϕ-axis at $\phi = 1$. To produce the proper behavior at the origin, the invariance properties developed by Sommerfeld can be employed, scaling the entire solution to $\phi(0) = 1$.

The exact numerical solution of the Thomas-Fermi equation for a neutral, isolated atom is plotted in Figure 2 and the numerical values are given in Table I.

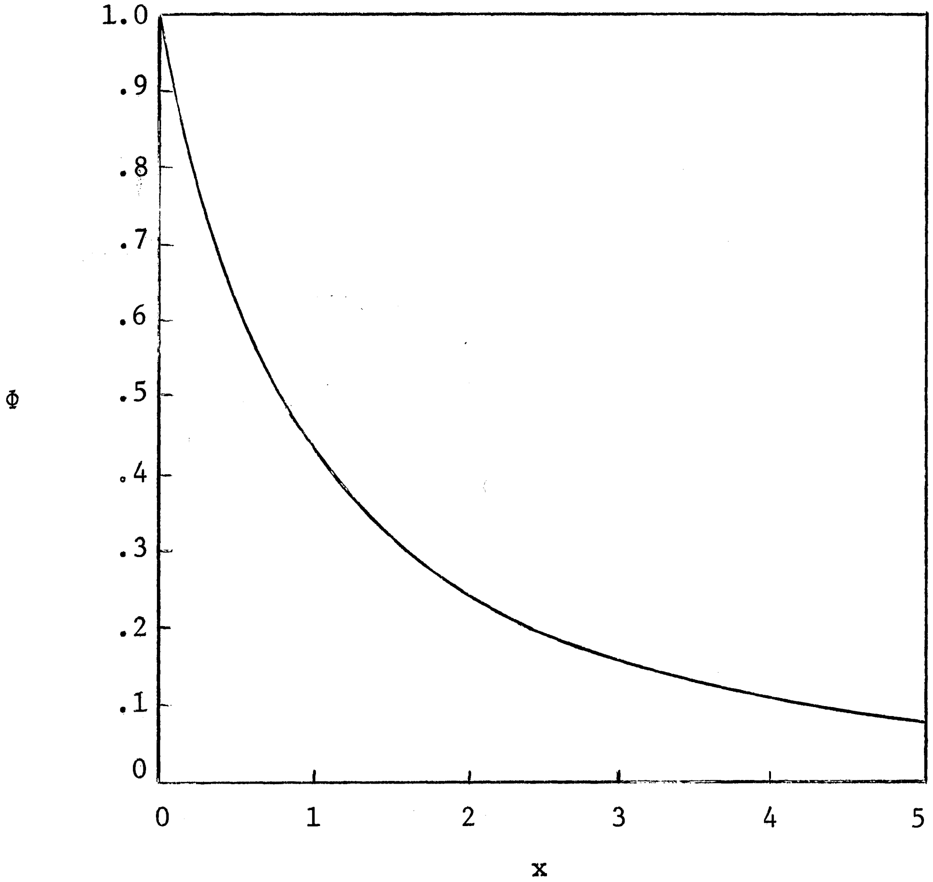

Figure 2. Solution[15] of the Thomas-Fermi Equation

Approximations to the Solution

It is often helpful to have a polynomial approximation for this function, and two expansions have been developed. A small argument expansion was developed by Baker[10] and later extended out to eleven terms

TABLE I

EXACT VALUES OF THE ORDINARY THOMAS-FERMI FUNCTION AND ITS DERIVATIVE[15]

x	$\phi(x)$	$-\phi'(x)$	x	$\phi(x)$	$-\phi'(x)$
0.0	1.00000	1.588071	1.0	0.42401	0.27399
0.1	0.88170	0.99535	1.5	0.31478	0.17374
0.2	0.79306	0.79423	2.0	0.24301	0.11824
0.3	0.72064	0.66180	3.0	0.15663	0.062457
0.4	0.65954	0.56464	5.0	0.078808	0.023560
0.5	0.60699	0.48941	10.0	0.024314	0.0046029

by Feynman, Metropolis and Teller[22]. In their calculations of the Thomas-Fermi-Dirac potential, Metropolis and Reitz[21] amended an error in Ref. 22, and finally, Kobayashi[16] developed the expansion to 17 terms. The expansion is, for x << 1:

$$\Phi(x) = \sum_{n=0}^{17} a_n x^{n/2} \tag{13}$$

The coefficients a_n are given below in Table II.

The large argument expansion, as developed by Coulson and March[20], consists of a polynomial factor multiplying the asymptotic behavior of the Thomas-Fermi function, viz., $\phi(x) \sim 144\, x^{-3}$. The form of this expansion, as originally given by Coulson and March, is:

$$\Phi(x) = \frac{144}{x^3}\left\{1 - \frac{F_1}{x^c} + \frac{F_2}{x^{2c}} - \frac{F_3}{x^{3c}} + \cdots\right\} \tag{14}$$

The succeeding F_n coefficients can all be expressed as a multiple of the first, and in this case, we can write the large argument expansion of the Thomas-Fermi function as:

$$\Phi(x) = 144\, x^{-3}\left(1 + c_1 y + c_2 y^2 + \cdots + c_{17} y^{17}\right) \tag{15}$$

where: $$y = -F \cdot x^{-\lambda}$$

The numerical values of these parameters were determined by Kobayashi, et al.[15] to a precision of 15 significant figures. For completeness, we list these coefficients in Table III. The values used for F and λ are 13.27097391 and 0.772001872658766, respectively.

It should be noted that Eq. 15 is valid only for $x \gtrsim 15$, and that Eq. 13 is valid only for $x \lesssim 0.6$. The derivatives obtained by simple differentiation of Eq. 13 and Eq. 15 are even more restricted.

TABLE II

COEFFICIENTS IN THE SMALL ARGUMENT EXPANSION OF THE THOMAS-FERMI FUNCTION[15,21]

$$\phi(x) \approx \sum_{n=o}^{17} a_n X^n$$

n	a_n	n	a_n
0	1	9	$\frac{2}{27} - \frac{1}{252} a_2^3$
1	0	10	$\frac{1}{175} a_2^2$
2	$\phi'(0)$	11	$\frac{31}{1485} a_2 + \frac{1}{1056} a_2^4$
3	$\frac{4}{3}$	12	$\frac{4}{405} + \frac{4}{1575} a_2^3$
4	0	13	$\frac{557}{100100} a_2^2 - \frac{3}{9152} a_2^5$
5	$\frac{2}{5} a_2$	14	$\frac{4}{693} a_2 - \frac{29}{24255} a_2^4$
6	$\frac{1}{3}$	15	$\frac{101}{52650} - \frac{623}{351000} a_2^3 + \frac{7}{49920} a_2^6$
7	$\frac{3}{70} a_2^2$	16	$-\frac{46}{45045} a_2^2 + \frac{68}{105105} a_2^5$
8	$\frac{2}{15} a_2$	17	$-\frac{113}{1178100} a_2 + \frac{153173}{116424000} a_2^4 - \frac{3}{43520} a_2^7$

TABLE III

COEFFICIENTS IN THE LARGE ARGUMENT EXPANSION OF THE THOMAS-FERMI FUNCTION[15,20]

$$\phi(x) \approx 144\, x^{-3} \sum_{n=o}^{17} C_n\, y^n$$

n	C_n	n	C_n
0	1.0	9	.00085 41653 77807
1	1.0	10	.00027 83738 39349
2	.62569 74977 82349	11	.00008 88230 01411
3	.31338 61150 73309	12	.00002 78360 15974
4	.13739 12767 19371	13	.00000 85895 00194
5	.05508 34346 64149	14	.00000 26150 62632
6	.02070 72584 99192	15	.00000 07867 99377
7	.00741 45294 78496	16	.00000 02342 63579
8	.00255 55311 67949	17	.00000 00691 03239

A more useful approximation for the Thomas-Fermi function was developed by R. Latter[23], who determined, on a best-fit basis, the coefficients in a function of the form

$$\Phi(x) = \left[1 + \sum_{n=1}^{6} a_n x^{n/2}\right]^{-1} \tag{16}$$

At present, the rational expression which provides the closest agreement with the exact numerical solution was developed by J. C. Mason[24] in 1964. Mason chose the functional form to be

$$\Phi(x) = \left(\frac{1 + \sum_{n=1}^{p} a_n x^{n/2}}{1 + \sum_{n=1}^{q} b_n x^{n/2}} \right)^2 \tag{17}$$

The requirement that $\lim_{x\to\infty} \phi(x) = 144\ x^{-3}$ led to the fact that $q = p+3$. The value of the coefficients which give the best agreement with the solutions of Kobayashi[15] are listed in Table IV.

TABLE IV

COEFFICIENTS IN THE THOMAS-FERMI APPROXIMATION OF MASON[24]

n	a_n	b_n
1	1.81061	1.81061
2	0.60112	1.39515
3	(0)	0.77112
4	(0)	0.21465
5	(0)	0.04793

With this approximation, the deviation from the exact result in either the function or its derivative is on the order of 10^{-5}.

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CHAPTER III

MODIFICATIONS OF THE THOMAS-FERMI MODEL

When any simple theory is presented which meets with moderate success in predicting observed behavior of a system, it is natural to see if its predictions can be extended or improved by including more and more corrections and by eliminating as many of the restrictive assumptions as possible. The Thomas-Fermi theory of atoms is no exception, and since its inception, it has been expanded to include exchange, correlations, periodicity, quantum corrections, and relativity. It has been applied to such diverse systems as nuclei, atoms, ions, molecules, atoms in a crystal, and stars. In this chapter, we review some of the modifications which have been proposed for the Thomas-Fermi model of free, neutral atoms with a particular emphasis on the relativistic corrections.

One of the simplest corrections that was proposed was that of Fermi and Amaldi[1]. In the original Thomas-Fermi (TF) theory, the electrons are assumed to constitute a continuous charge distribution and the potential is determined by this charge distribution. Consequently, the electrostatic Coulomb interaction includes the electrostatic self-interaction of the electrons. To eliminate this, Fermi and Amaldi proposed that the mean potential of one electron, V_e/Z, be subtracted from the total atomic potential. Thus, in effect, the Thomas-Fermi potential is multiplied by the correction factor $(Z-1)/Z$. This self-interaction has been studied more recently by R. Latter[2] and C. A. Coulson and C. S.

Sharma[3].

It is well known that the exchange energy in a large atom can contribute a significant portion of the total energy[4]. The TF model as described here does not take this exchange energy into account, and Dirac, using the expression for the exchange energy derived by Fock[2], applied this to the TF theory. The electron density then takes on the form

$$n = \frac{(2me)^{3/2}}{3\pi^2\hbar^3}\left[a + (V - V_0 + a^2)^{1/2}\right]^3 \tag{1}$$

where $a = \frac{1}{\hbar}\sqrt{\frac{me^3}{2\pi^2}}$. The similarity to the TF density is evident if we write the TF density in the form

$$n = \frac{(2me)^{3/2}}{3\pi^2\hbar^3}\left[(V - V_0)^{1/2}\right]^3 \tag{2}$$

It is interesting to note that Eq. (1) can be derived very simply if we use the variational derivation of the TF equation[5]. Bloch[6] showed very early that the exchange energy per unit volume for a system of electrons has the form

$$e_{ex} = -C_e\left(\frac{N}{V}\right)^{4/3} \tag{3}$$

where $C_e = \frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}$. If this energy term is added to the total energy expression (cf. Appendix A), the TFD equation results (Eq. (1)). J. M. C. Scott[7] has shown that, if this energy is evaluated using the TF density, the correction term due to exchange is, in eV,

$$E_{ex} = -6.02 \cdot Z^{5/3} \tag{4}$$

The TFD model has itself been the subject of several improvements. Fermi-Amaldi[1] corrections have been made, and Jensen[8] added a term to the energy of the TF model which varied with the radius and density in such a manner that it was identical to the exchange interaction in the center of the atom and reduced to the Fermi-Amaldi correction at the edge of the atom.

Correlation effects are generally much smaller than exchange effects in atoms (in fact, P. O. Fröman[9] feels that correlation effects are negligible in comparison with the basic approximate nature of the Thomas-Fermi theory), but Gombas[10-12] has evaluated the correction to the potential energy due to correlation to be

$$e_{corr} = - \frac{\alpha_1 \rho^{1/3}}{\rho^{1/3} + \alpha^2} \cdot \rho \tag{5}$$

where $\alpha_1 = 0.05647 \frac{e^2}{a_o}$ and $\alpha_2 = 0.1216/a_o$. (a_o is the first Bohr radius of the hydrogen atom.) The total energy due to this correction is indeed very small, as can be seen by the following argument. The greatest contribution will occur when ρ is very large, so let us allow ρ to dominate α_1 and α_2 in Eq. (5). Then

$$E_{corr} \sim -\alpha_1 \int \rho \, dv \tag{6}$$

$$\sim -\alpha_1 \cdot Z \tag{7}$$

$$\sim -1.5 \; Z \quad (\text{eV}) \tag{8}$$

A second class of corrections are those which modify the kinetic energy term in the energy. The first and basic correction to the kinetic energy was developed by C. F. v. Weizsäcker[13]. This correction is derived as follows: First, one ignores the Pauli exclusion principle and allows the n electrons in a given volume element dv to coexist in the same state ψ. Then the electron density becomes $\rho = n|\psi|^2$. It can be shown that the kinetic energy density from the Schroedinger equation is given by

$$e_k = \frac{1}{2} e^2 a_0 n \left(\vec{\nabla}\psi\right)^2 \tag{9}$$

Thus, the correction to the energy due to Weizsäcker is:

$$E_k = \frac{1}{8} e^2 a_0 \frac{(\vec{\nabla}\rho)^2}{\rho} . \tag{10}$$

This simple approach overestimates the energy and several attempts have been made to correct this problem[14-22]

Recently, the TF theory has been the subject of investigation from several different points of view. The aim of many efforts has been to somehow include the angular-momentum dependence of the quantum mechanical density. As Gombas[23] points out, most of the attempts to derive the electron shells from the TF theory have been unsuccessful, but a more fruitful approach to the problem has been the incorporation of shells into the model. Most of the success in the former approaches have been in the area of nuclear shell structure[24,25], while the attempts to derive atomic shell structure[26-31] have met with only moderate success. L. C. R. Alfred[32] has approached the problem from both points of view, while P. Gombas[33-41] has limited himself to the inclusion of the shells into the statistical models.

Several papers have also appeared recently which demonstrate that the Thomas-Fermi theory is a particular approximation in a rigorous N-body formalism[42-47]. This approach has led to the efforts of subsequent authors to include quantum corrections[48-51], and the majority of the recent work in TF theory has been in these two areas. By combining some of the known properties of the electron density derived from wave mechanics, these authors have been able to circumvent some of the difficulties encountered in the asymptotic behavior of the statistical electron density.

Some independent approaches have appeared recently, like the modified statistical atom model proposed by W. H. E. Schwartz[52], in which account is taken of the Heisenberg uncertainty principle to derive a modification of the exchange potential. P. Gombas has also proposed a new approach to the exchange potential[53] and to the periodicity problem[54].

Another interesting approach to the asymptotic problems of the TF density is that of P. Csavinszky[55], who replaced the differential form of the TF equation (Poisson's equation) by its equivalent variational integral equation. Choosing

$$F = \frac{1}{2}\left(\frac{d\Phi}{dx}\right)^2 + \frac{2}{5}\left(\frac{\Phi^{5/2}}{x^{1/2}}\right), \tag{11}$$

the variation of

$$L = \int_0^\infty F\,dx \tag{12}$$

is equivalent to the ordinary TF equation. This variational equation is then solved subject to the boundary conditions

$$\Phi(0)=1, \qquad \Phi(\infty)=0, \qquad \Phi'(\infty)=0. \tag{13}$$

The functions chosen by Csavinszky were of the form

$$\Phi=\left[a\cdot e^{-\alpha x}+b\cdot e^{-\beta x}\right]^{2} \tag{14}$$

and the total energy of an atom calculated on this basis was found to be much closer than the unmodified TF results.

However, the primary concern of this thesis is a relativistic formulation of the statistical model, so in this last section, we review the early attempts at a relativistic Thomas-Fermi model. The earliest attempt was that of Vallarta and Rosen[56]. By taking into account the variation of the electron's mass with velocity, the relativistic Hamiltonian

$$p^2c^2-(W+eV)^2+m_0^2c^4=0 \tag{15}$$

leads to the relativistic TF equation of Vallarta and Rosen:

$$\frac{1}{x^2}\frac{d}{dx}\left(x^2\frac{d\Phi}{dx}\right)=\Phi^{3/2}(1+\lambda\Phi)^{3/2}, \tag{16}$$

where

$$\lambda=\frac{eb}{2m_0c^2}=1.841\times10^{-5}\cdot Z^{4/3}. \tag{17}$$

This equation, unfortunately, leads to an electron density which diverges as r^{-3} at the origin and is thus unnormalizable. H. Jensen[57] circumvented this problem by recognizing the finite size of the nucleus and utilizing a cut-off radius of r ~ 3Z x 10^{-13} cm. Much later, J. S. Plaskett[15] combined an expression for the electron density in an atom with the Klein-Gordon equation with zero vector potential, obtaining the approximate result

$$\rho = \frac{4\pi}{3} \frac{1}{h^3c^3} \left[(E - e\Phi)^2 - m^2c^4 - \frac{\hbar^2c^2}{4r^2} \right]^{3/2} \tag{18}$$

However, the derivation of this density requires the restrictive assumption that $2Z < 1/\alpha$, or $Z \lesssim 64$, so the expression is not applicable to the very region in which one would expect a statistical model to be most useful. Y. Tomishima[58] attempted to overcome the divergence of Vallarta and Rosen's density by including a modified Weizsäcker correction to reduce the singularity at the origin. The equation thus derived is

$$\begin{aligned} 4\lambda\kappa_i \cdot \nabla^2\psi - \frac{\psi}{\alpha}\left\{ \left[1 + (3\pi^2)^{2/3}\alpha^2\psi^{4/3} \right]^{1/2} - 1 \right\} \\ + \frac{4}{3}\kappa_a \psi^{5/3} + (V - V_0)\psi = 0. \end{aligned} \tag{19}$$

Here, $\kappa_i = \frac{1}{8} a_o$, $\kappa_a = \frac{3}{4}(\frac{3}{\pi})^{1/3}$, and $\psi = \rho^{\frac{1}{2}}$. The asymptotic behavior of ψ for large r is

$$\psi \propto \frac{1}{r} \cdot \exp\left[-r\sqrt{\frac{V_0}{4\lambda\kappa_i}} \right] \tag{20}$$

and as $r \to o$, ψ remains essentially constant. The λ that appears in Eq. (15) is an adjustable parameter and is chosen to provide the best value for the total energy of the atom.

To date, however, the most satisfactory approach to the inclusion of relativistic effects is that of Rudkjobing[59] and Gilvarry[60]. Since the work of these two authors is fundamental to our proposed relativistic

Thomas-Fermi (RTF) model, we will present their development of the RTF equation in detail in the next chapter.

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CHAPTER IV

DEVELOPMENT OF THE RUDKJOBING-GILVARRY MODEL

In 1952, the Danish astrophysicist M. Rudkjobing developed an equation giving the density of states at a zero-temperature for a system of relativistic particles in a central field[1]. He went on to apply this density to the case of a white dwarf star, considering the variation in mass density to be a consequence of the (central) gravitational field. The derivation did not require that the potential be gravitational. In 1954, J. J. Gilvarry used this density as the basis of a relativistic Thomas-Fermi model of the atom.[2] Since our work is essentially based on this approach, we will discuss the derivation of Gilvarry's model in this chapter.

Rudkjobing's Theory

Beginning with the Dirac equation for particles in a central field, Sommerfeld[3] has shown that the spin-angle part of the solution is independent of a central potential, and the radial functions R_1 and R_2 are solutions of the following two simultaneous differential equations:

$$\left(\frac{d}{dr} + \frac{1-k}{r}\right) R_1 = \frac{1}{\hbar c}\left(E - V + E_0\right) R_2 \tag{1a}$$

$$\left(\frac{d}{dr} + \frac{1+k}{r}\right) R_2 = \frac{1}{\hbar c}\left(-E + V + E_0\right) R_1 \tag{1b}$$

In these equations, E_o is the rest energy of the electron, and k is the eigenvalue of $(\vec{\sigma} \cdot \vec{\ell} + \hbar)$ operating on the spin-angle function χ^{μ}_{κ}. Thus, k can take on all integer values except zero.*

Introducing the variables $P_1 = rR_1$ and $P_2 = rR_2$, we get

$$\left(\frac{d}{dr} - \frac{k}{r}\right) P_1 = \frac{1}{\hbar c}\left(E - V + E_0\right) P_2 \tag{2a}$$

$$\left(\frac{d}{dr} + \frac{k}{r}\right) P_2 = \frac{1}{\hbar c}\left(-E + V + E_0\right) P_1 \tag{2b}$$

Now, if we differentiate Eq. (2a) and substitute for $\frac{dP_2}{dr}$ the expression in Eq. (2b), we obtain

$$\frac{d^2P_1}{dr^2} - \frac{k}{r}\cdot\frac{dP_1}{dr} + \frac{k}{r^2} P_1 =$$

$$\frac{1}{\hbar c}\left(E - V + E_0\right)\left[\frac{1}{\hbar c}\left(-E + V + E_0\right) P_1 - \frac{k}{r} P_2\right] - \frac{1}{\hbar c}\cdot\frac{dV}{dr}\cdot P_2 \tag{3}$$

Substitution of the expression for P_2 in Eq. (2a) into Eq. (3) eliminates P_2 from the bracket, leaving

$$\frac{d^2 P_1}{dr^2} + \left[\frac{(E-V)^2 - E_0^2}{\hbar^2 c^2} - \frac{k^2 - k}{r^2}\right] P_1 = -\frac{1}{\hbar c}\cdot\frac{dV}{dr}\cdot P_2 \quad . \tag{4a}$$

Similarly, we can find the corresponding expression for $\frac{d^2P_2}{dr^2}$:

$$\frac{d^2 P_2}{dr^2} + \left[\frac{(E-V)^2 - E_0^2}{\hbar^2 c^2} - \frac{k^2 + k}{r^2}\right] P_2 = \frac{1}{\hbar c}\cdot\frac{dV}{dr}\cdot P_1 \quad , \tag{4b}$$

---

*k corresponds to $-\kappa$ in Rose's[4] notation.

If the potential has a vanishing gradient, then (4a) and (4b) separate into two wave equations. In order to treat the general case, when $\frac{dV}{dr} \neq 0$, we introduce a new radial function Q(r) which is a linear combination of P_1 and P_2:

$$Q = a_1 \cdot P_1 + a_2 \cdot P_2 \tag{5}$$

Here, a_1 and a_2 are as yet unspecified constants. Multiplying Eq. (4a) by a_1 and Eq. (4b) by a_2 and adding, we get

$$\frac{d^2Q}{dr^2} + \left[\frac{(E-V)^2 - E_0^2}{\hbar^2 c^2} - \frac{k^2}{r^2} \right] Q + \tag{6}$$

$$+ \frac{k}{r^2} a_1 P_1 + \frac{1}{\hbar c} \frac{dV}{dr} a_1 P_2 - \frac{k}{r^2} a_2 P_2 - \frac{1}{\hbar c} \frac{dV}{dr} a_2 P_1 = 0 .$$

We now define a function g such that

$$\frac{d^2Q}{dr^2} + \left[\frac{(E-V)^2 - E_0^2}{\hbar^2 c^2} - \frac{k^2 + g}{r^2} \right] Q = 0 . \tag{7}$$

It then follows that

$$\frac{k}{r^2} a_1 - \frac{1}{\hbar c} \frac{dV}{dr} a_2 = - \frac{g}{r^2} a_1 \tag{8a}$$

$$\frac{1}{\hbar c} \frac{dV}{dr} a_1 - \frac{k}{r^2} a_2 = - \frac{g}{r^2} a_2 \; . \tag{8b}$$

If we now make the reasonable assumption that $r^2 \frac{dV}{dr}$ is essentially constant over a small interval, we find that

$$g = \pm\sqrt{k^2 - k_0^2} \tag{9}$$

where k_o is defined to be

$$k_0 = \frac{r^2}{\hbar c}\,\frac{dV}{dr}\,^{*} \tag{10}$$

Whether the + sign or the - sign in Eq. (9) is chosen makes no difference, and we can write a single equation for the radial function Q:

$$\frac{d^2Q}{dr^2} + \left[\frac{(E-V)^2 - E_0^2 - \left(r\frac{dV}{dr}\right)^2}{\hbar^2 c^2} - \frac{g(g+1)}{r^2} \right] Q = 0. \tag{11}$$

This equation determines the radial function Q(r) if the energy and the form of the potential are known, and the solutions Q(r) are parametrized by the number g.

For each energy E, there is a $2|k|$-fold degeneracy due to the angular parts of the functions. For each value of g, the number of states with energy less than some maximum energy Em in a volume element in the form of a shell of unit thickness is equal to $2|k|$ times the number of half oscillations of the Q function for Em, since each radial eigenfunction has one more node than the one immediately below it in energy.

The minimum radial wavelength λ_{min} is dependent on Em and g and is found from Eq. (11).

$$\left(\frac{2\pi}{\lambda_{min}}\right)^2 = \frac{(E_m - V)^2 - E_0^2 - \left(r\frac{dV}{dr}\right)^2}{\hbar^2 c^2} - \frac{g(g+1)}{r^2} \tag{12}$$

---

[*] For a coulombic potential $V = -\frac{Ze^2}{r}$, and $k_o = \frac{Ze^2}{\hbar c} = \alpha Z$, where α is the fine structure constant.

If we make the assumption that $g^2 >> g$, the total number of states with a certain magnitude of g lying in the spherical shell is

$$n = \frac{4|k|}{\pi r}\left[r^2 \frac{(E_m - V)^2 - E_0^2 - (r\frac{dV}{dr})^2}{\hbar^2 c^2} - g^2 \right]^{1/2} \tag{13}$$

To find the total number of states, we integrate over k, using the fact that

$$2|k| \cdot d|k| = d(g^2) \quad , \tag{14}$$

resulting in:

$$N = \frac{2}{\pi r}\int_{g=0}^{g_{max}} \left[r^2 \frac{(E_m - V)^2 - E_0^2 - (r\frac{dV}{dr})^2}{\hbar^2 c^2} - g^2 \right]^{1/2} d(g^2) \tag{15}$$

Thus, the volume density of states (or, at T = 0, the volume density of matter) is

$$\rho = \frac{1}{3\pi^2 r^3}\left[r^2 \frac{(E_m - V)^2 - E_0^2 - (r\frac{dV}{dr})^2}{\hbar^2 c^2} \right]^{3/2} \tag{16}$$

From this point on, Rudkjobing applies this equation to the specific case of the gravitational potential of a white dwarf star. Here we are primarily concerned with statistical models of the atom, so we next summarize Gilvarry's use of this density as a relativistic Thomas-Fermi atom model.

Gilvarry's Theory

Noting that previous attempts to derive a relativistic generalization of the Thomas-Fermi atom were unsatisfactory for one reason or another, J. J. Gilvarry[2] used the equation derived by Rudkjobing (Eq. 16) as the basis of a statistical atom model. In Gilvarry's notation, the number of states n(r,E) per unit volume and per unit energy range of an electron of total energy E at a point r in a spherically symmetric atom where the electrostatic potential is V(r) is found by differentiating Eq. (16) with respect to energy:

$$n(r,E) = \frac{8\pi}{\hbar^3 c^3}\left[(E+eV)^2 - m^2c^4 - \left(re\frac{dV}{dr}\right)^2\right]^{1/2}(E+eV) \qquad (17)$$

Applying the Fermi-Dirac distribution function, one can obtain an expression for the number density of electrons $\rho(r)$ at the point r at a non-zero temperature T:

$$\rho(r) = \int_0^\infty n(r,E)\,\frac{dE}{1+e^{\frac{E-E_m}{kT}}} \qquad (18)$$

Substitution of this expression, evaluated at T = 0, into Poisson's equation results in the relativistic Thomas-Fermi (RTF) equation:

$$\frac{1}{r}\frac{d^2}{dr^2}(rV) = \sigma_2\left\{(\eta+eV) + \frac{(\eta+eV)^2 - \left(re\frac{dV}{dr}\right)^2}{2mc^2}\right\}^{3/2} \qquad (19)$$

where $\sigma_2 = \frac{32\pi^2}{3}(2m)^{3/2}\frac{e}{h^3}$ and $\eta = E_m - mc^2$.

Furthermore, if one assumes that relativistic effects affect the exchange correction only slightly and operate mainly to modify the uncorrected potential V_o, one can obtain a relativistic Thomas-Fermi-Dirac[5] equation:

$$\frac{1}{r}\frac{d^2}{dr^2}(rV_0) = \sigma_2\left\{\gamma + \left[\gamma^2 + (\eta + eV_0) + \frac{(\eta + eV_0)^2 - \left(re\frac{dV}{dr}\right)^2}{2mc^2}\right]^{1/2}\right\}^{3/2} \tag{20}$$

where $\gamma = \dfrac{(2m)^{\frac{1}{2}}e^2}{h}$.

Whereas these equations have been cited by several authors[6-10], the solutions have never been published, although B. Rosznyai[11] has presented the results of his relativistic self-consistent calculations which were begun with Eq. (19).

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CHAPTER V

THE RELATIVISTIC THOMAS-FERMI EQUATION

In this chapter, the arguments of Rudkjobing and Gilvarry will be re-derived and put on a more sound basis. Also, it will be seen that Rudkjobing's density is only one of four possible expressions derivable from the same basic idea, the four expressions resulting from different treatments of a summation which is encountered.

The Central-Field Dirac Equation

We begin by considering the motion of a relativistic fermion moving under the influence of a scalar potential V and has potential energy, U. Such a particle can be described by the Dirac equation:[1]

$$(c\,\vec{\alpha}\cdot\vec{p} + \beta m_0 c^2)\Psi = (W - U)\Psi \tag{1}$$

where W = total energy of the particle. In this form, $\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$ and σ_x, σ_y, σ_z are the Pauli spin matrices for a spin ½ particle. Also,

$$\beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} .$$

Making use of the relation,

$$\vec{\alpha}\cdot\vec{p} = -i\hbar(\vec{\alpha}\cdot\hat{r})\frac{\partial}{\partial r} - \frac{1}{r}(\vec{\alpha}\cdot\hat{r})(\vec{\sigma}\cdot\vec{l}\,) \tag{2}$$

and the γ_5 Dirac matrix

$$\gamma_5 = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \tag{3}$$

we can write the Dirac equation in the form

$$\left[i\hbar c\, \gamma_5 \sigma_r \left(\frac{\partial}{\partial r} + \frac{1}{r} - \frac{\beta}{r} \underset{\sim}{K} \right) + \beta m_0 c^2 + U \right] \Psi = W \Psi \tag{4}$$

where

$$\underset{\sim}{K} = \frac{\beta}{\hbar} \left(\vec{\sigma} \cdot \vec{\ell} + \hbar \right) \quad . \tag{5}$$

We now assume V is a central potential and write the (four component) wave functions in the form

$$\Psi = \begin{pmatrix} f_1(r) \cdot \chi_{\kappa}^{\mu} \\ i\, f_2(r) \cdot \chi_{-\kappa}^{\mu} \end{pmatrix} \tag{6}$$

The χ_{κ}^{μ} are the spin-angle functions which are eigenfunctions of $\vec{\sigma} \cdot \vec{\ell} + \hbar$:

$$\left(\vec{\sigma} \cdot \vec{\ell} + \hbar \right) \chi_{\pm\kappa}^{\mu} = \mp \kappa \hbar\, \chi_{\kappa}^{\mu} \tag{7a}$$

$$\sigma_r\, \chi_{\pm\kappa}^{\mu} = - \chi_{\mp\kappa}^{\mu} \tag{7b}$$

Then the Dirac equation takes on the form

$$\begin{pmatrix} -\hbar c \left(\frac{\partial f_2}{\partial r} + \frac{f_2}{r} \right) \chi_{\kappa}^{\mu} + \hbar c f_2 \frac{\kappa}{r} \chi_{\kappa}^{\mu} + (m_0 c^2 + U) f_1 \chi_{\kappa}^{\mu} \\ i\hbar c \left(\frac{\partial f_1}{\partial r} + \frac{f_1}{r} \right) \chi_{-\kappa}^{\mu} + i\hbar c \frac{\kappa}{r} f_1 \chi_{-\kappa}^{\mu} + i(-m_0 c^2 + U) f_2 \chi_{-\kappa}^{\mu} \end{pmatrix} = W \begin{pmatrix} f_1 \chi_{\kappa}^{\mu} \\ i f_2 \chi_{-\kappa}^{\mu} \end{pmatrix} \tag{8}$$

which allows separation of the spin-angle dependent parts, leaving the radial eigenfunctions to be determined by the two simultaneous differential equations:

$$(W-U-m_0c^2)f_1 = -\hbar c\left(\frac{\partial}{\partial r} + \frac{1-\kappa}{r}\right) f_2 \tag{9a}$$

$$(W-U+m_0c^2)f_2 = \hbar c\left(\frac{\partial}{\partial r} + \frac{1+\kappa}{r}\right) f_1 \tag{9b}$$

If we use $k = -\kappa$, these two equations are identical with Rudkjobing's Eq. (1) with $f_2 = R_2$ and $f_1 = R_1$.

Development of the Density of States

Following the same reasoning presented in Chapter IV, we define an arbitrary linear combination of f_1 and f_2:

$$Q = (a_1 f_1 + a_2 f_2) r \tag{10}$$

which results in the following expression:

$$\begin{aligned} &\frac{d^2Q}{dr^2} + \left[\frac{(W-U)^2 - E_0^2}{\hbar^2c^2} - \frac{k^2}{r^2}\right] Q + \\ &+ \frac{k}{r} a_1 f_1 + \frac{r}{\hbar c}\frac{dU}{dr}\cdot a_1 f_2 - \frac{k}{r}\cdot a_2 f_2 - \frac{r}{\hbar c}\cdot\frac{dU}{dr}\cdot a_2 f_1 = 0. \end{aligned} \tag{11}$$

We now define a new variable g such that

$$a_1 \frac{k}{r} - a_2 \frac{r}{\hbar c}\frac{dU}{dr} = -a_1 \frac{g}{r} \tag{21a}$$

$$a_1 \frac{r}{\hbar c}\frac{dU}{dr} - a_2 \frac{k}{r} = -a_2 \frac{g}{r} \ . \tag{12b}$$

This requires that, unless $a_1 = a_2 = 0$,

$$g^2 = k^2 - \left(\frac{r^2}{\hbar c} \cdot \frac{dU}{dr}\right)^2 \tag{13}$$

We define the second term to be k_o^2:

$$k_0 = \frac{r^2}{\hbar c} \cdot \frac{dU}{dr} \tag{14}$$

(As noted previously, for a coulombic potential, $k_o = \alpha Z$.) Then

$$g = \pm\sqrt{k^2 - k_0^2} \tag{15}$$

and we can write, for either sign of g:

$$\frac{d^2Q}{dr^2} + (-g^2 - g + \epsilon)\frac{Q}{r^2} = 0 \tag{16}$$

where we have defined ε by:

$$\epsilon = \frac{r^2}{\hbar^2 c^2}\left[(W-U)^2 - E_0^{\,2} - \left(r\frac{dU}{dr}\right)^2\right] \tag{17}$$

or, equivalently,

$$\epsilon = \frac{r^2}{\hbar^2 c^2}\left[(W-U)^2 - E_0^2\right] - k_0^2 \tag{18}$$

Now, the radial momentum operator has the representation[2]

$$\underset{\sim}{p_r} = \frac{\hbar}{i}\left(\frac{\partial}{\partial r} + \frac{1}{r}\right) \tag{19}$$

Since the radial behavior of a particle described by our function Q is proportional to Q/r, we find that

$$\underset{\sim}{p_r}\left(\frac{Q}{r}\right) = \frac{\hbar}{i} \cdot \frac{1}{r} \cdot \frac{dQ}{dr} \tag{20}$$

For this reason,

$$\frac{d^2Q}{dr^2} = -\frac{p_r^2}{\hbar^2}Q \tag{21}$$

Comparison of Eq. (21) with Eq. (16) shows that

$$p_r^2 = \frac{\hbar^2}{r^2}\left(-g^2-g+\epsilon\right) \tag{22}$$

Using the deBroglie relationship ($\lambda_r = \frac{h}{P_r}$), see the radial wavelength becomes

$$\lambda_r = 2\pi r\left(-g^2-g+\epsilon\right)^{-1/2}. \tag{23}$$

We wish to establish a connection between the number of states for given values of r, g, and E and the properties of this Q function. It is well known[3] that, for the non-relativistic Kepler problem, the number of nodes in any particular radial eigenfunction is one greater than the number of nodes in the radial eigenfunction for the state lying immediately below it in energy. For the Dirac problem, it is a little more complicated, since f_1 and f_2 do not vanish simultaneously[4] (except possibly at the origin and at infinity). However, it is known that[5] between each pair of nodes in f_1 (or f_2) there is a node in f_2 (or f_1) and that the number of nodes in f_1 follows the same rules as the non-relativistic radial eigenfunctions. It then follows that, regardless of the magnitudes or the signs of a_1 and a_2, a node of Q will fall between adjacent nodes of f_1 and f_2, such that the number of nodes in Q will be the same as the number of nodes in f_1. That is, a particular Q function will have one more node than the Q for the next lowest energy level. If we define an energy Wm such that all states with W ≥ Wm are unoccupied, we can count the number of states by counting the number of nodes in the Q function for Wm.

We are specifically interested in the number of states available to a particle with a particular value of g between a distance r and r + dr from the nucleus. The number of these Q functions per unit radial distance is equal to the number of nodes in Q(Wm) between r and r + dr. As Figure 3 shows, this number (dn_q) is equal to dr divided by one-half the radial wavelength of Qm.

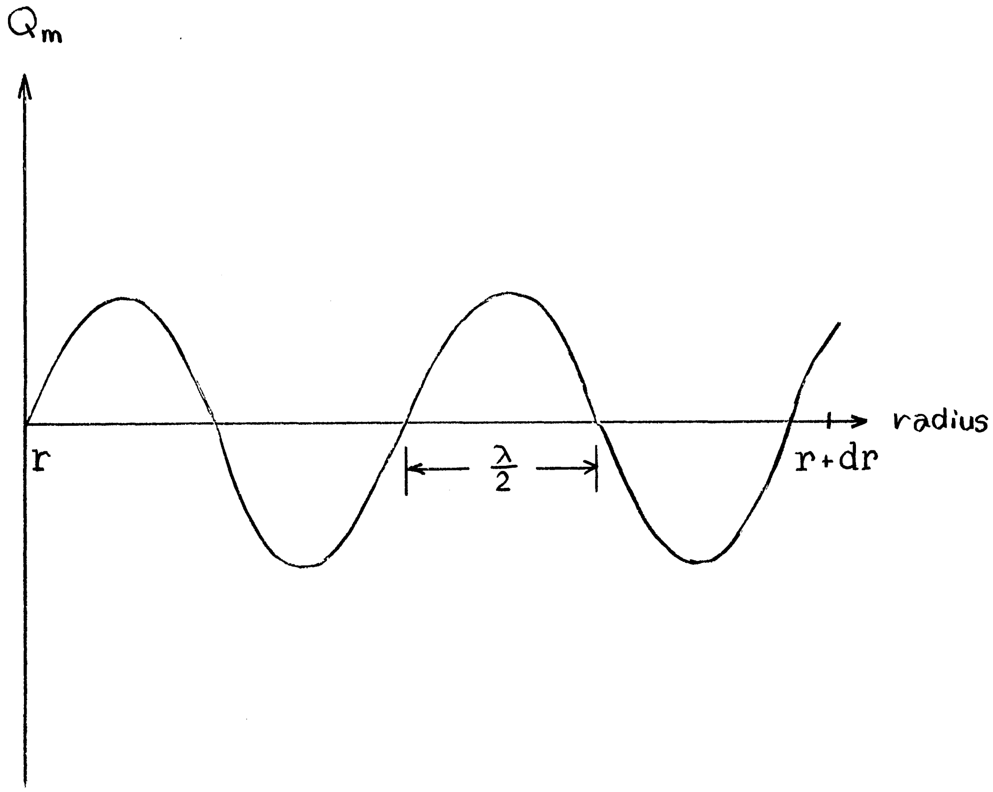

Figure 3. Nodes in the Radial Function Q

Thus,

$$\frac{dn_g}{dr} = \frac{2}{\lambda_r} \,. \tag{24}$$

Substituting the value of λ_r from Eq. (23), the number of Q functions with energy W < Wm between r and r + dr is

$$\frac{dn_g}{dr} = \frac{1}{\pi r}\left(-g^2 - g + \epsilon_m\right)^{1/2} \,, \tag{24}$$

where $\varepsilon_m = \varepsilon(Wm)$. With each Q are associated $2|k|$ spin-angle functions, so the volume density of states with value of g at a distance r from the nucleus available to a particle of energy W is

$$\frac{dn_g}{dv} = \frac{|k|}{2\pi^2 r^3}\left(-g^2 - g + \epsilon\right)^{1/2} \tag{25}$$

Summation Over g

The remaining step is to sum over the different k values to obtain the final expression for the total density of states. Depending on the approximations used, any of four expressions can be derived.

Discrete Densities

We can make use of Eq. (15) to write

$$\frac{dn_g}{dv} = \frac{1}{2\pi^2 r^3}\sqrt{(-g^2 - g + \epsilon)(g^2 + k_0^2)} \tag{26}$$

At a fixed value of r, g can take on the following discrete values:

$$g = \pm\sqrt{1 - k_0^2} \,, \quad \pm\sqrt{4 - k_0^2} \,, \quad \pm\sqrt{9 - k_0^2} \,, \ldots$$

The upper and lower limits of the summation over g are determined by the requirement that the density remain real; i.e., that $-g^2 - g + \epsilon \geq 0$. This gives us the following limits:

$$g_{max} = \frac{-1+\sqrt{4\epsilon+1}}{2} \tag{27}$$

$$g_{min} = \frac{-1-\sqrt{4\epsilon+1}}{2} \tag{28}$$

Thus, the density of states available to a particle of energy W at a distance r from the nucleus becomes

$$\rho_1(r) = \frac{1}{2\pi^2 r^3} \sum_{g \leq g_{min}}^{g_{max}} \sqrt{(-g^2-g+\epsilon)(g^2+k_0^2)} \tag{29}$$

It is interesting to note that this expression can as well be expressed as a Stieltjes integral. The concept of the Stieltjes integral is useful in discussing summations within the formalism of the integral. The connection between the two is evident from the definition[6] of the Stieltjes integral:

$$\int_a^b f(x)\, d\gamma(x) = \sum_{i=1}^{n} f(x_i') \left[\gamma(x_i) - \gamma(x_{i-1}) \right] \tag{30}$$

Here, x_i' lies between x_i and x_{i-1}. Our density (Eq. 29) can be written as a Stieltjes integral if we define $\gamma(g)$ in the following manner:

$$\gamma(g) = -n \quad \text{if} \quad -\sqrt{(-n-1)^2 - k_0^2} \leq g < -\sqrt{n^2 - k_0^2} \tag{31a}$$

$$\gamma(g) = n \quad \text{if} \quad \sqrt{n^2 - k_0^2} \leq g < \sqrt{(n+1)^2 - k_0^2} \tag{31b}$$

This integrating function is shown in Figure 4.

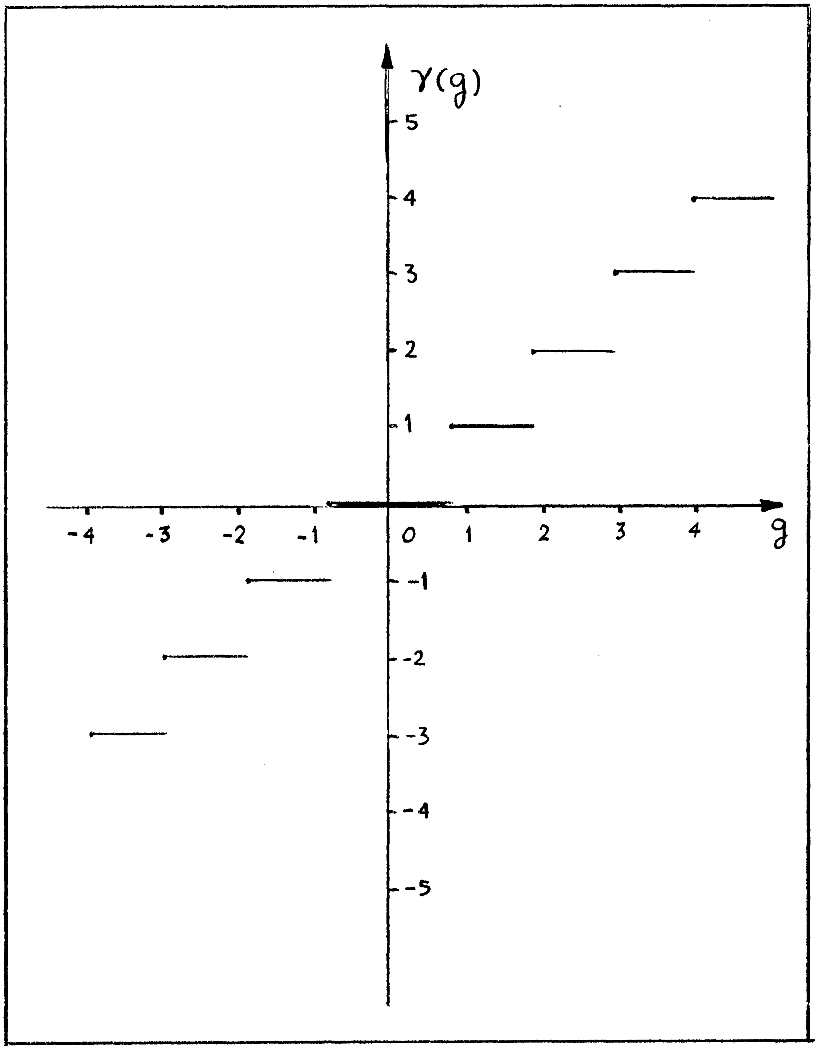

Figure 4. Integrating Function for Stieltjes Density

Then

$$\rho_1 = \frac{1}{2\pi^2 r^3} \int_{g_{min}}^{g_{max}} \sqrt{(-g^2-g+\epsilon)(g^2+k_0^2)}\; d\gamma(g) \tag{32}$$

where $\gamma(g)$ is given by Eq. (31a) and Eq. (31b). A second possibility arises in the case where $g^2 \gg g$ or k_o^2. In this case, $\gamma(g)$ takes on the simple form

$$\gamma(g) = n+1 \qquad \text{if} \qquad n<0 \tag{33a}$$

$$\gamma(g) = n \qquad \text{if} \qquad n \geq 0 \tag{33b}$$

and $\qquad n \leq g \leq n + 1.$

The resulting density can then be expressed as the following sum:

$$\rho_2 = \frac{1}{2\pi^2 r^3} \sum_{g \leq g_{min}}^{g_{max}} \sqrt{-g^2+\epsilon} \cdot |g| \tag{34}$$

<u>Continuous Densities</u>

A second approach to the problem arises when g_{max} and g_{min} are so large in magnitude that the integrating function $\gamma(g)$ in Eq. (32) can be reasonably approximated by $\gamma(g) = g$. In this case, we are left with a Riemann integral of the square root of a fourth-degree polynomial, integrated from one zero of the integrand to the second zero of the integrand:

$$\rho_3 = \frac{1}{2\pi^2 r^3} \int_{g_{min}}^{g_{max}} \sqrt{(-g^2-g+\epsilon)(g^2+k_0^2)}\; dg. \tag{35}$$

An integral of this type can be reduced to a sum of the three standard elliptic integrals, and this reduction is given in Appendix B.

If we further approximate the integrand, by allowing g^2 to be much larger than g or k_o, the integral becomes much simpler:

$$\rho_4 = \frac{1}{2\pi^2 r^3} \int_{g_{min}}^{g_{max}} \sqrt{-g^2+\epsilon}\ |g|\ dg \tag{36}$$

where the limits are now $g_{max} = \sqrt{\varepsilon}$, $g_{min} = -\sqrt{\varepsilon}$. This integration can be performed analytically, resulting in

$$\rho_4 = \frac{1}{2\pi^2 r^3} \cdot \frac{2}{3}\, \epsilon^{3/2} \tag{37}$$

This result is identical to Eq. (16) in Chapter IV, so it is seen that Rudkjobing's density depends on two assumptions:

(1) that the number of allowed g values is so large that the sum can be replaced by an integral, and

(2) that g_{max} and g_{min} are so large that, for the major portion of the integration, $g^2 \gg g$ or k_o.

The validity of these assumptions will be discussed in the next chapter.

For completeness, we list here the conclusions of this model:

The exact density is

$$\rho_1(r) = \frac{1}{2\pi^2 r^3} \sum_g \sqrt{(-g^2-g+\epsilon)(g^2+k_o^2)} \tag{29}$$

If $g^2 \gg g$ and $g^2 \gg k_o^2$, the approximate discrete density is

$$\rho_2(r) = \frac{1}{2\pi^2 r^3} \sum_g \sqrt{\epsilon-g^2}\cdot|g| \tag{34}$$

If we replace the sum in Eq. (29) by a Riemann integral,

$$\rho_3 = \frac{1}{2\pi^2 r^3} \int_{g_{min}}^{g_{max}} \sqrt{(-g^2 - g + \epsilon)(g^2 + k_o^2)}\, dg \tag{35}$$

Finally, if we hold that $|g|$ and k_o^2 are negligibly small when compared to g^2, the approximate continuous density can be written as

$$\rho_4 = \frac{1}{2\pi^2 r^3} \cdot \frac{2}{3} \cdot \epsilon^{3/2} \; . \tag{37}$$

In all four cases,

$$\epsilon = \frac{r^2}{\hbar^2 c^2}\left[(W_m - U)^2 - E_o^2 \right] - k_o^2 \tag{38}$$

and

$$k_o = \frac{r^2}{\hbar c} \cdot \frac{dU}{dr} \; . \tag{39}$$

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CHAPTER VI

SOLUTION OF THE RTF EQUATION

We have seen that the approach of Rudkjobing leads to four possible relativistic Thomas-Fermi equations, depending on the approximations made in the derivation. Substitution of these expressions into Poisson's equation produces a RTF equation of the form

$$\nabla^2 U = -\frac{2}{\pi r^3} \cdot R(r) \tag{1}$$

where $R(r) = 2\pi^2 r^3 \rho(r)$, and the density $\rho(r)$ is given by Eq. (29), Eq. (34), Eq. (35) or Eq. (37) in Chapter V.

Since we are assuming a central potential, we can write the Laplacian as

$$\nabla^2 U = \frac{d^2 U}{dr^2} + \frac{2}{r}\frac{dU}{dr} \tag{2}$$

To eliminate the first-order term, we define $\psi(r)$ by:

$$\psi = rU \tag{3}$$

Then a direct calculation shows that

$$\nabla^2 U = \frac{1}{r} \cdot \frac{d^2\psi}{dr^2} \tag{4}$$

One of the basic assumptions is that, as r approaches zero, the screening effect of the electron cloud disappears, and the potential approaches that of the bare nucleus with a charge of +Z. (We will use atomic units in which $\hbar = m = e = 1$.) That is,

$$\lim_{r\to 0} U(r) = -\frac{Z}{r} \tag{5}$$

To avoid a divergence in the second derivative, we rewrite the RTF equations in terms of a new variable x:

$$x = \sqrt{r} \tag{6}$$

resulting in:

$$\frac{d^2\psi}{dx^2} - \frac{1}{x}\frac{d\psi}{dx} = -\frac{8}{\pi x^2} \cdot R(x) \tag{7}$$

The limits of these terms are, in light of Eq. (5):

$$\lim_{x\to 0} \psi(x) = -Z \tag{8}$$

$$\lim_{x\to 0} \frac{1}{x}\frac{d\psi}{dx} = 0, \tag{9}$$

$$\lim_{x\to 0} \frac{d^2\psi}{dx^2} = 0. \tag{10}$$

The functions R(x) are

$$R_1(x) = \sum_g \sqrt{(-g^2-g+\epsilon)(g^2+k_0^2)} \tag{11}$$

$$R_2(x) = \sum_g \sqrt{\epsilon-g^2}\,|g| \tag{12}$$

$$R_3(x) = \int \sqrt{(-g^2 - g + \epsilon)(g^2 + k_o^2)}\, dg \tag{13}$$

$$R_4(x) = \frac{2}{3}\, \epsilon^{3/2} \tag{14}$$

In Eq. (11) and Eq. (13), the upper and lower limits are $g_{max} = \frac{1}{2}(\eta - 1)$, $g_{min} = \frac{1}{2}(-\eta - 1)$, respectively, with $\eta = \sqrt{4\varepsilon + 1}$. In Eq. (12), the limits are simply $\pm\sqrt{\varepsilon}$. The functions ε and k_o, written in terms of $\psi(x)$, take on the form:

$$k_o = -\frac{1}{c}\left(\psi - \frac{x}{2}\,\frac{d\psi}{dx}\right) \tag{15}$$

$$\epsilon = \frac{x^4}{c^2}\left[\left(W_m - \frac{\psi}{r}\right)^2 - c^4\right] - k_o^2 \tag{16}$$

The relativistic Thomas-Fermi equation is then defined, in a form suitable for computation, by Eq. (7) - Eq. (16). The number Wm, which physically represents the energy of the most energetic electron, is a parameter which is varied to allow normalization of the density:

(17)

Functional Form of R(x)

As can be seen by inspection of Eq. (11) - (16), the function R(x) depends on x in a very complicated manner. Before attempting to numerically integrate Eq. (7), it is helpful to have some idea of how R(x) may vary with x. Although this dependence is not known until the equation is solved, we can get a qualitative idea of the behavior to be expected by using a known expression for the atomic potential and then evaluating R(x) as a function of this potential. Especially if we use the Thomas-Fermi function, we could expect this to give a fairly good idea.

In Figures 5 - 8, we have shown the electron density ($D = 4\pi r^2 \cdot \rho$) as calculated from R_1, R_2, R_3, and R_4, using Mason's[1] approximation for the TF function. Since we are here only interested in the qualitative behavior of the function R(r); no attempt at normalization was made and we arbitrarily chose $Wm = E_o$. (Even with this choice of Wm, the normalization integrals came out remarkably close; the error was less than 10% in each case, with the exception of the densities based on R_3, which diverge at the origin. This point will be discussed later.)

The densities based on R_1 and R_2 are perhaps the most interesting (and most difficult to work with) because of the discontinuities in the slopes which occur. These occur as the limits of the sums in R_1 and R_2 gradually increase and then decrease with increasing radius. As g_{min} and g_{max} pass each succeeding integer, the allowed number of g values in the sum jumps discontinuously from one integer to the next. A careful numerical examination of these transition points reveals the following behavior: The number of allowed g values (Ng) changes only by one region to the next, although it may change very quickly. For example, in rubidium, Ng goes from 1 to 2 at r = .02826, but almost immediately increases to Ng = 3 at r = .0292. Also, the first derivative of ρ goes abruptly from a negative value to a positive value as Ng changes. Finally, it can happen that Ng remains zero for a finite region around the nucleus, thereby producing a density which vanishes in a small region in the center of the atom.

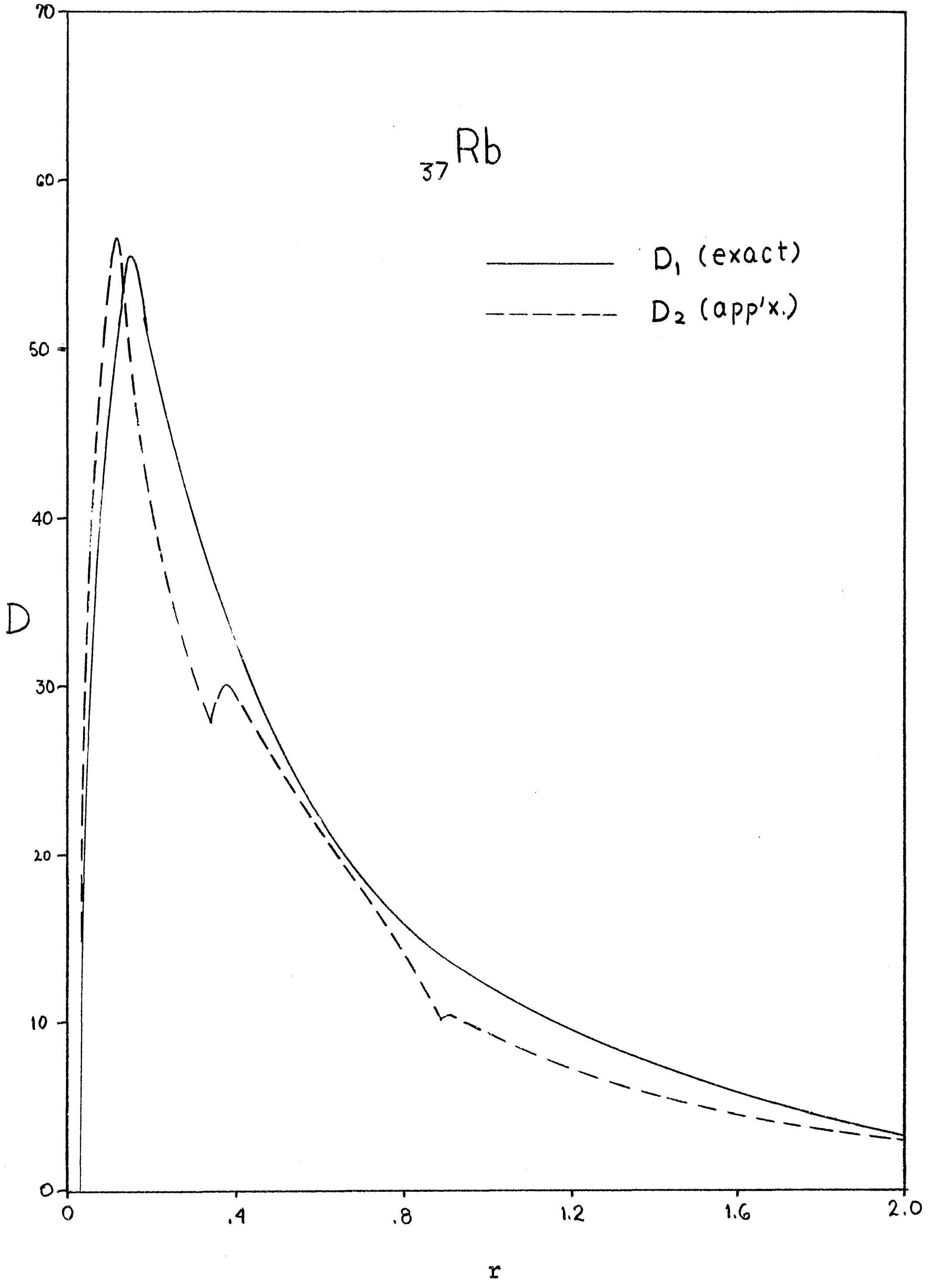

Figure 5. Stieltjes Densities for Rubidium

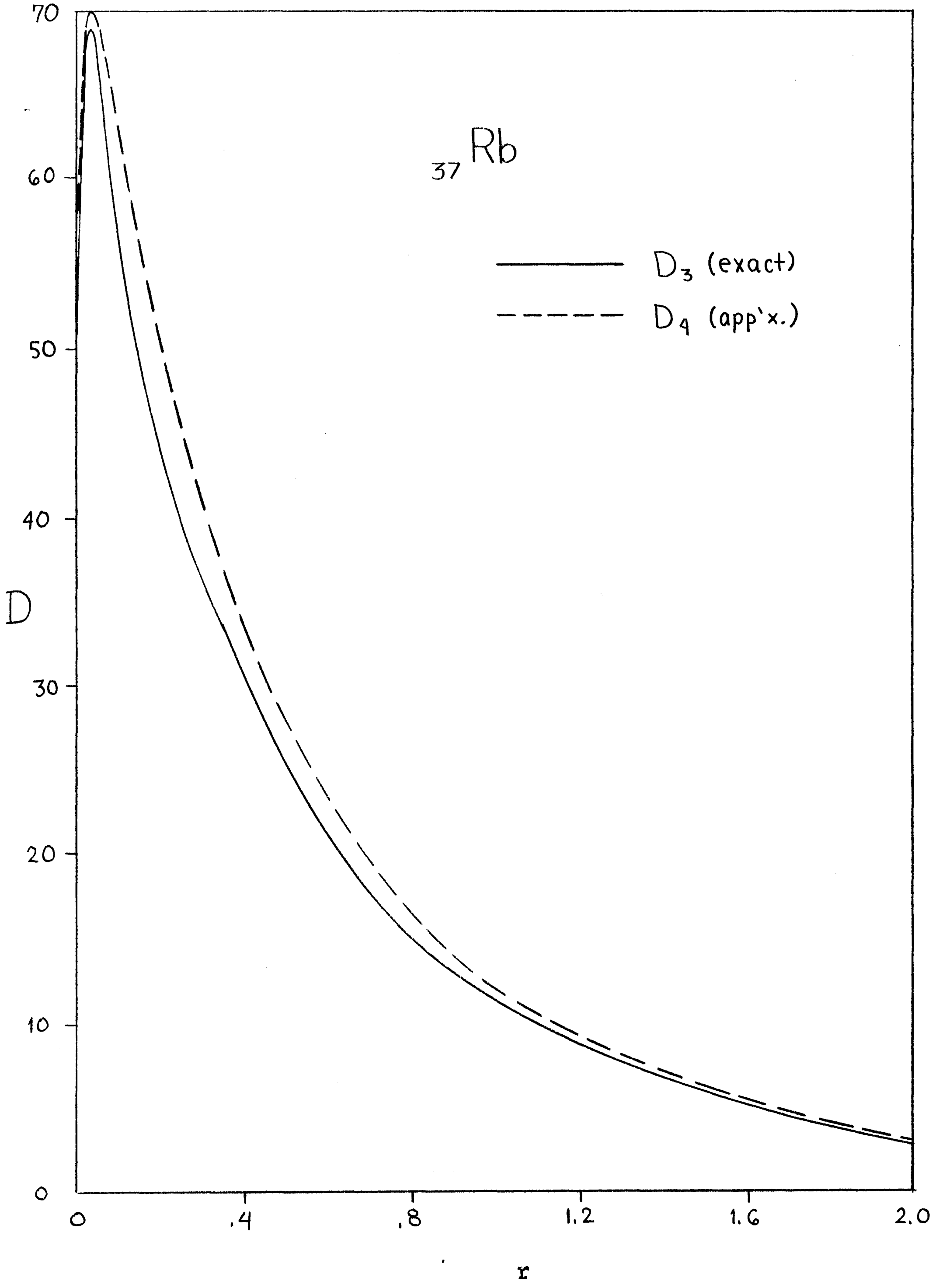

Figure 6. Riemann Densities for Rubidium

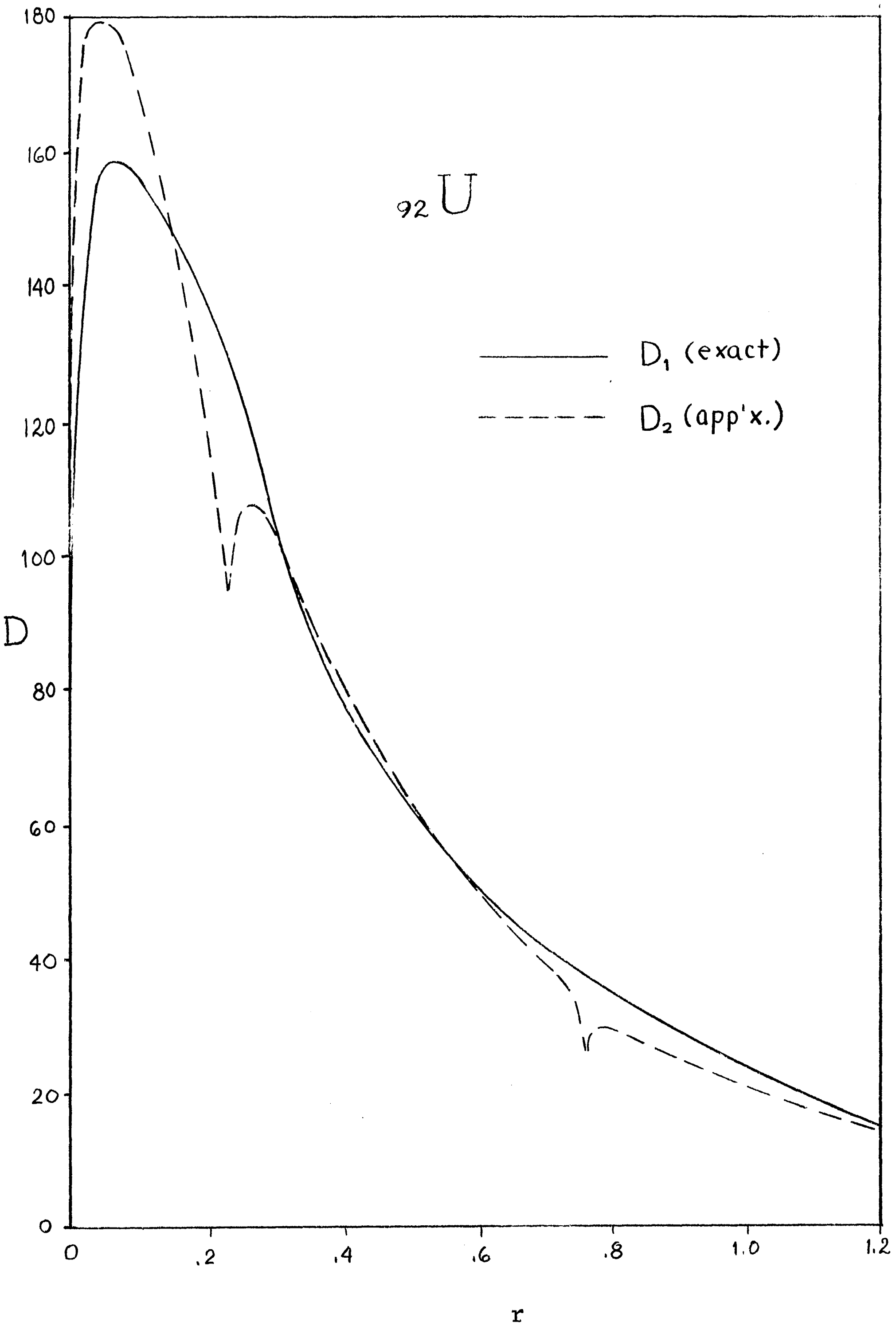

Figure 7. Stieltjes Densities for Uranium

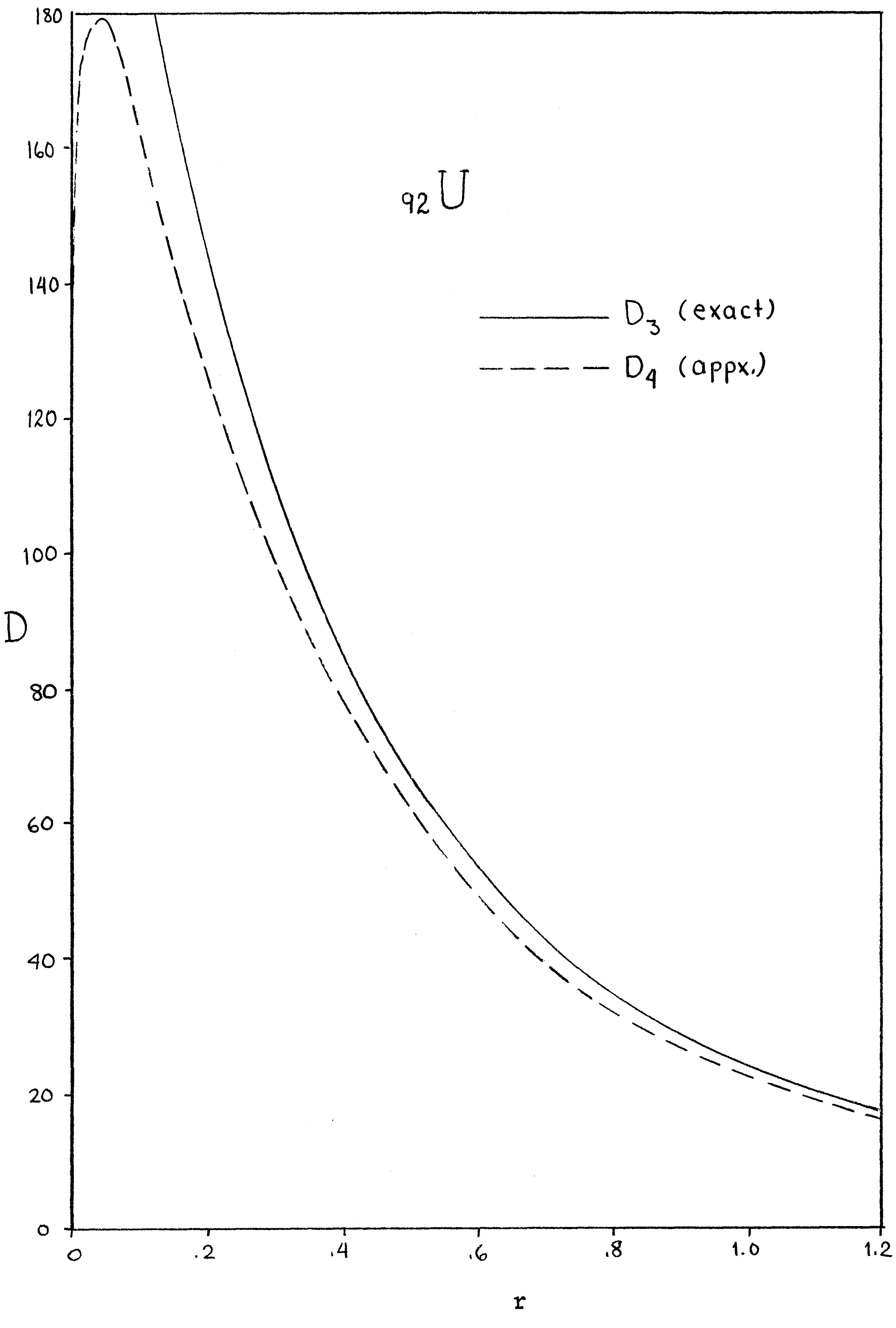

Figure 8. Riemann Densities for Uranium

Normalizability

To examine the normalizability of these densities, we must look at the r → 0 limits of Eq. (11) - Eq. (14). Assuming the potential is coulombic near the nucleus, we find

$$\lim_{r\to 0} k_0 = Z\frac{e^2}{\hbar c} = \alpha Z \tag{18}$$

$$\lim_{r\to 0} \epsilon = 2Z\frac{W_m}{c^2}\cdot r = 0 \tag{19}$$

Thus, the limits for the exact expressions (R_1 and R_3) become, as r approaches zero:

$$\lim_{r\to 0}\left(g_{max}\right) = \lim_{r\to 0}\left\{\tfrac{1}{2}(\eta-1)\right\} = 0 \tag{20}$$

$$\lim_{r\to 0}\left(g_{min}\right) = \lim_{r\to 0}\left\{\tfrac{1}{2}(-\eta-1)\right\} = -1 \tag{21}$$

Thus, at r = 0, R_1 can have two values of g:0 and -1. The resulting expression, however, still vanishes because of ε:

$$\lim_{r\to 0} R_1(x) = 0. \tag{22}$$

The integral expression, however, is non-vanishing at the origin:

$$\lim_{r\to 0} R_3(x) = \int_{-1}^{0}\sqrt{(-g^2-g+0)(g^2+k_0^2)}\,dg \tag{23}$$

$$\lim_{r\to 0} R_3(x) = \int_0^1 \sqrt{(g-g^2)(g^2+k_0^2)}\, dg \neq 0. \tag{24}$$

so the resulting density ($\rho_3 = \frac{1}{2\pi^2 r^3} R_3$) diverges as r^{-3}. Thus, the density based on R_3 is not normalizable if a point nucleus is assumed. A way around this problem was proposed by Jensen[2] in his discussion of Vallarta and Rosen's[3] RTF model. This consists simply of recognizing the finite size of the nucleus so that the potential is no longer divergent. This approach was tried, but the discontinuity of the electron density at the edge of the nucleus hindered the numerical solution of the RTF equation using R_3, and this remains a point to be resolved.

The density based on R_2 vanishes identically at the origin, since $g_{min} = g_{max} = 0$, and no normalization difficulties are encountered.

The density based on R_4 (which is identical to Rudkjobing's density) diverges at the origin:

$$\lim_{r\to 0} \rho_4(r) = \lim_{r\to 0} \left(\frac{1}{2\pi^2 r^3}\right)\left(\frac{2}{3}\epsilon^{3/2}\right) \tag{25}$$

$$= \frac{1}{3\pi^2} \lim_{r\to 0} \left(\frac{\epsilon^{1/2}}{r}\right)^3 \tag{26}$$

$$= \frac{1}{3\pi^2} \lim_{r\to 0} \left[\frac{1}{r}\sqrt{2Z \cdot \frac{W_m}{c^2} \cdot r}\right]^3 \tag{27}$$

$$= \frac{1}{3\pi^2}\left(2Z\frac{W_m}{c^2}\right)^{3/2} \lim_{r\to 0}\left(r^{-3/2}\right) = \infty . \tag{28}$$

However, its divergence is weak enough ($r^{-3/2}$) to allow normalization, so no difficulties are encountered here.

Numerical Integration of the RTF Equation

The remainder of the computational work was directed toward a direct numerical integration of the RTF equation. This equation was attempted with each of the four densities, but the discontinuities have so far prevented any success in the first three (R_1, R_2, and R_3). However, the fourth density has been satisfactorily evaluated, at least on a preliminary basis, for two elements: $_{37}$Rb and $_{92}$U. Normalization has been achieved to within ±.08% and ±0.2%, respectively, and the root-mean-square radius has been evaluated, permitting calculation of the diamagnetic susceptibility.

The equation to be solved is a second-order, non-linear, ordinary differential equation, with one initial condition (Eq. 8) and a second boundary condition which is expressed through the normalization integral:

$$\frac{d^2\psi}{dx^2} - \frac{1}{x}\frac{d\psi}{dx} = -\frac{16}{3\pi} x^{-2} \epsilon^{3/2} ; \tag{29}$$

$$\psi(0) = -Z \tag{30}$$

$$\frac{8}{3\pi}\int_0^\infty \epsilon^{3/2} x^{-1} dx = Z . \tag{31}$$

where ε and k_o are functions of ψ and ψ', defined in Eq. (15) and Eq. (16).

The procedure to solve this equation was the following: First, a value of $\zeta = Wm - E_o$ was guessed, and Eq. (29) was integrated outward from the origin using a modified fourth-order Runge-Kutta program. As the integration of Eq. (29) was performed, the normalization integrand was evaluated at each step and the normalization integral was estimated by a simple trapezoidal integration. Since the most radical changes in ρ occur near the origin, the step size was enlarged as the integration progressed outward. The actual integration was performed using relative and absolute error tolerances in each step of 10^{-4}, 10^{-6}, and 10^{-8}. Although there was virtually no difference between the results obtained with a tolerance of 10^{-6} and those with 10^{-8}, the final values were obtained using the smallest error tolerance. The step sizes originally tried were the following:

$$0 \leq \chi < .0005 \quad ; \Delta\chi = 10^{-4} \tag{32}$$

$$.0005 \leq \chi < .01 \quad ; \Delta\chi = 5 \times 10^{-4} \tag{33}$$

$$.01 \leq \chi < .4 \quad ; \Delta\chi = 10^{-2} \tag{34}$$

$$.4 \leq \chi < \infty \quad ; \Delta\chi = 5 \times 10^{-2} \ . \tag{35}$$

(In the integration routine, these intervals were automatically reduced to meet the error tolerances imposed.)

Once the integration was completed, subsequent guesses at ζ were made, until two values of ζ were found, one of which gave a value of the normalization integral too large, and the other producing a value too small. These two values of ζ were then given to a root-finding subroutine, PEGAS[5], (a modified regula-falsi algorithm) and the normalization was accomplished by finding a root of the equation

$$(\text{norm. integral}) - Z = 0 . \tag{36}$$

The values of ζ which produced normalization are:

$$Z = 37: \quad \zeta = -\ 219.462955075 \tag{37}$$

$$Z = 92: \quad \zeta = -\ 726.06428495 \quad . \tag{38}$$

The electron densities for $_{37}\mathrm{Rb}$ and $_{92}\mathrm{U}$ as calculated from the RTF equation are shown in Figures 9 and 10.

It is a simple matter to evaluate $<r^2>$ as the integration is carried out, and the root-mean-square radii of these two atoms were calculated from the definition

$$r_0^2 = \langle r^2 \rangle = 4\pi \int_0^\infty \rho \; r^4 \, dr \quad . \tag{39}$$

The resulting values were found to be

$$_{37}\mathrm{Rb} : r_o = 1.76 \tag{40}$$

$$_{92}\mathrm{U} : r_o = 1.28 \ . \tag{41}$$

The surprising result that the r.m.s. radius is smaller for the heavy atom than for the light atom is consistent with the predictions of the non-relativistic Thomas-Fermi theory. It was shown that the Thomas-Fermi equation can be put into a dimensionless form that is valid for all values of Z:

$$x^{\frac{1}{2}} \; \Phi'' = \Phi^{3/2} \quad . \tag{42}$$

This defines a function $\psi(x)$, where x is related to the radius by

$$r = (0.885 \; Z^{-1/3}) \; x \ . \tag{43}$$

Thus, if x_o is the r.m.s. radius in dimensionless units, the corresponding length in Bohr radii will be proportional to $Z^{-1/3}$. This result

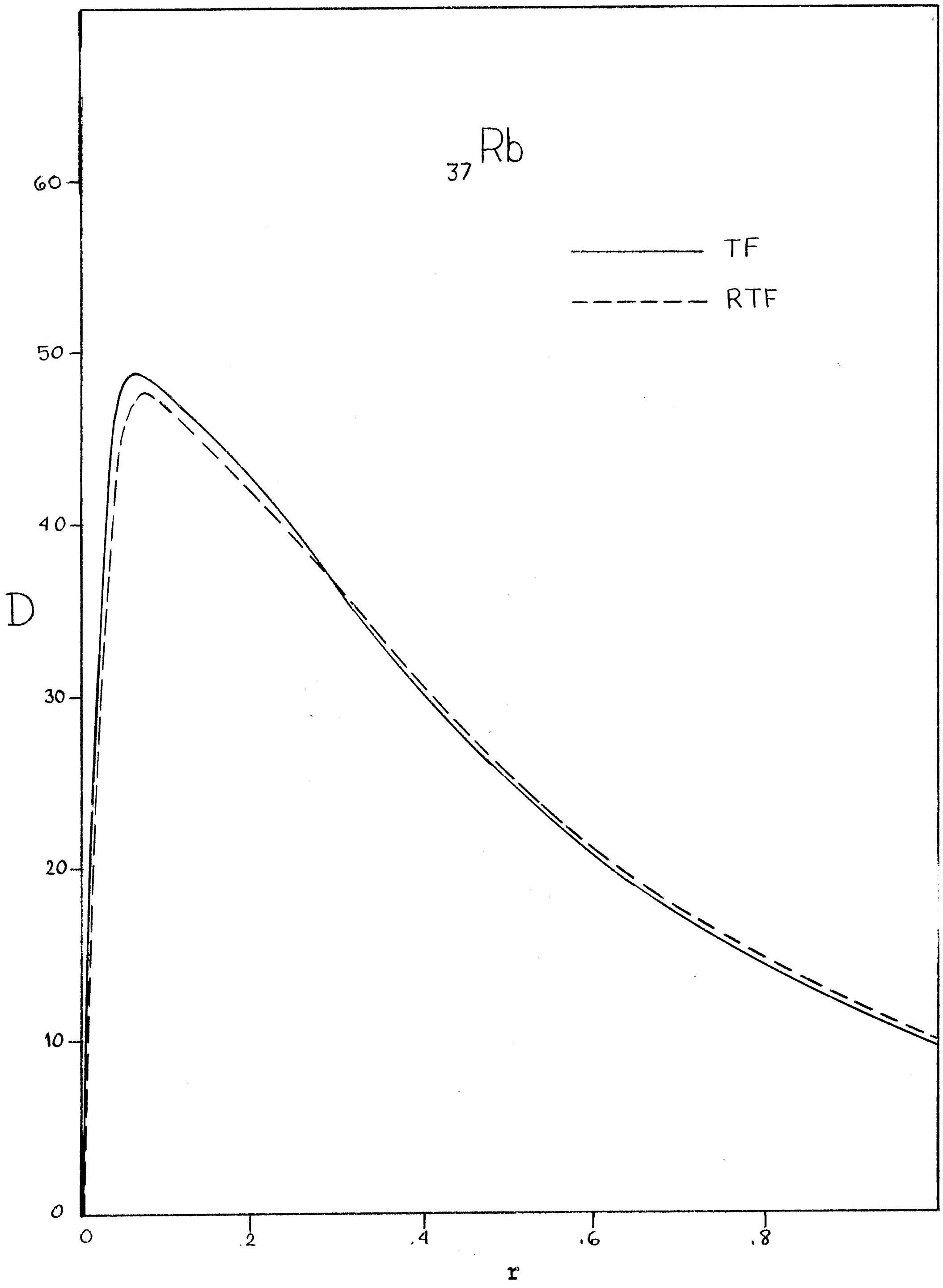

Figure 9. Electron Densities for Rubidium

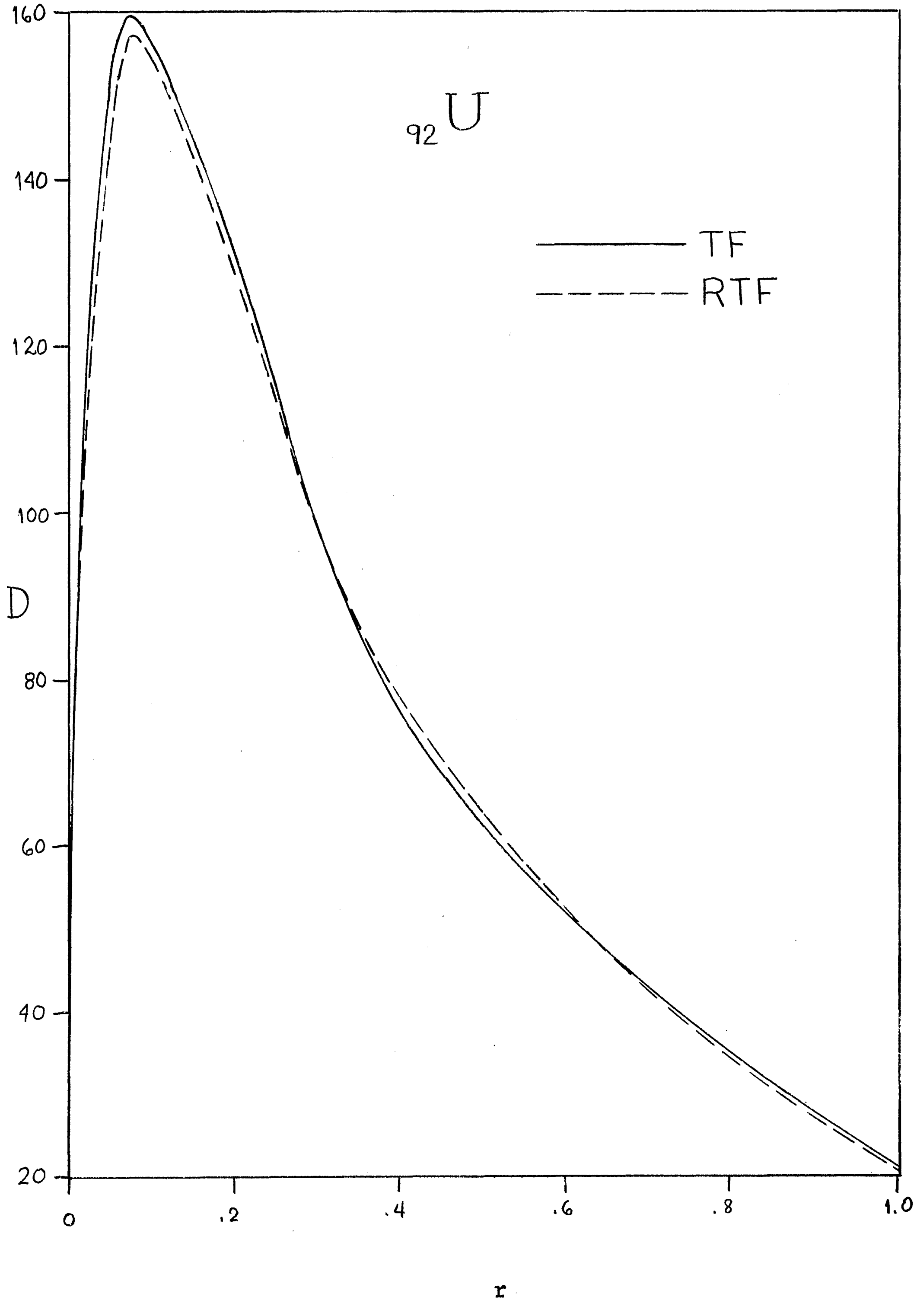

Figure 10. Electron Densities for Uranium

could be physically rationalized, if not proven, by recalling that, in the statistical models, no explicit account is taken of the Pauli exclusion principle, except to allow two electrons per h^3 of phase space volume. It is then conceivable that the increased nuclear attraction of the heavy atom could outweigh the increased electron-electron repulsion, thereby pulling the electron cloud in tighter.

The diamagnetic susceptibility per gram-atom of an element is given by[6]

$$\chi = -N_0 \frac{e^2}{6mc^2} \langle r^2 \rangle \quad , \tag{44}$$

where N_0 is Avogadro's number, and the units of χ (in the CGS system) are cm^3. Using the values of $<r^2>$ from Eq. (40) and Eq. (41), we find

$$_{37}Rb: \quad \chi = 14.9 \times 10^{-6} \text{ cm}^3 \tag{45}$$

$$_{92}U: \quad \chi = 7.8 \times 10^{-6} \text{ cm}^3 \ . \tag{46}$$

The values determined from Mann's data are:

$$_{37}Rb: \quad \chi_{exp} = 29. \times 10^{-6} \text{ cm}^3$$

$$_{92}U: \quad \chi_{exp} = 70. \times 10^{-6} \text{ cm}^3 ,$$

resulting in a relative error of ~50% and ~90%. For comparison, the unmodified TF density gives errors of 264% and 200%, respectively.

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CHAPTER VII

CONCLUSIONS

It was the purpose of this study to investigate the relativistic statistical atom model. It was found that the density obtained by Gilvarry corresponds to one possible approximation in the general expression for the RTF equation. The numerical solution of this equation has never been published, and this was carried out, providing the electron density and root-mean-square radius to compare. It was found that the r.m.s. radius is smaller than that of the non-relativistic TF density, and that the resulting values of diamagnetic susceptibility are closer to the experimentally determined values, although agreement is still poor.

Like all modifications of the TF equation, the RTF model has the drawback that no single universal solution exists, unlike the unmodified TF equation. With modern computers, this is less a drawback than it may have been some time ago, and numerical values for the RTF equation are now available for two elements, and any others are immediately calculable.

This investigation has only been the beginning of this area, and there is much that can be done. The most immediate problem outstanding is the numerical integration of the RTF equation using the other three densities. A means must be developed for handling the discontinuities in the functions and their derivatives. Another project, purely computational, would be to expand the computations to all the elements. Since the most difficult part of the solution procedure is the determination of the maximum energy (Em), a table of the correct values of Em for each element would allow a worker in the field to easily calculate the RTF density and potential for any atom with a single integration over the desired range of r. Also, a perturbation calculation could be attempted in terms of the non-relativistic Thomas-Fermi function, ψ. Finally, a curve-fitting scheme could be employed to obtain an analytical approximation for the solutions of the RTF equation.

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APPENDIX A

VARIATIONAL DERIVATION OF THE THOMAS-FERMI EQUATION

An alternative derivation of the Thomas-Fermi equation involves the variational principle. First, the total energy of the electron system is written down as a function of the electron density. Then this expression for the energy is varied with respect to the density, subject to the restraint that the density be normalized according to

$$\int \rho \, dv = Z \tag{1}$$

One begins by splitting the (non-relativistic) energy into three separate terms: the kinetic energy (T), the potential energy of the electron-nucleus interaction (U_n), and the potential energy of the electron-electron interaction (U_e).

The nucleus-electron interaction is simply

$$U_n = -Ze^2 \int \frac{\rho}{r} \, dv \tag{2}$$

We can also write down the expression for the electron-electron interaction:

$$U_e = \frac{e^2}{2} \iint \frac{\rho(\vec{r}) \, \rho(\vec{r}')}{|\vec{r} - \vec{r}'|} \, dv \, dv' \tag{3}$$

The expression for the kinetic energy can be derived as follows: Since there are two electrons per h^3 of phase space volume, the number of electrons per volume element dv with momenta between p and p + dp is

$$\frac{dn_p}{dv} = \frac{1}{\pi^2 \hbar^3} p^2 dp \tag{4}$$

Then the volume density of electrons with momentum less than p_o is found by integrating Eq. (4):

$$\rho = \int_0^{p_o} dn_p \, dp \tag{5}$$

$$\rho = \frac{p_o^3}{3\pi^2 \hbar^3} \tag{6}$$

Then the kinetic energy per volume element dv is:

$$\frac{dT}{dv} = \int T \, dn_p \tag{7}$$

Substitution of Eq. (4) for dn_p gives:

$$\frac{dT}{dv} = \int_0^{p_o} \frac{p^2}{2m} \cdot \frac{p^2}{\pi^2 \hbar^3} dp \tag{8}$$

$$\frac{dT}{dv} = \frac{p_o^5}{10 m \pi^2 \hbar^3} \tag{9}$$

Finally, solving Eq. (6) for p_o gives an expression for the kinetic energy in terms of the electron density:

$$T = \frac{(3\pi^2)^{5/3}\hbar^2}{10\pi^2 m}\int \rho^{5/3}\,dv \tag{10}$$

Thus, the total energy of the atom can be expressed as

$$E = K_k\int \rho^{5/3}dv - Z\int \frac{\rho}{r}dv + \frac{1}{2}\iint \frac{\rho(\vec{r})\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}dv\,dv' \tag{11}$$

To allow the normalization requirement to be met, we introduce a Lagrange multiplier V_o and require the energy given by Eq. (11) to be stationary with respect to variations in the electron density:

$$\delta\int\left[K_k\rho^{5/3} - \frac{Z}{r}\rho + \frac{1}{2}\int\frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}dv'\cdot\rho + V_o\rho\right]dv = 0 \tag{12}$$

Evaluating these variations, we obtain:

$$\delta\int K_k\rho^{5/3}dv = \frac{5}{3}K_k\int\rho^{2/3}\,\delta\rho\,dv \tag{13}$$

$$\delta\int -\frac{Z}{r}\rho\,dv = -Z\int\frac{1}{r}\,\delta\rho\,dv \tag{14}$$

$$\delta\,\frac{1}{2}\iint\frac{\rho\rho'}{|\vec{r}-\vec{r}'|}dv\,dv' = \int\varphi_e\,\delta\rho\,dv \tag{15}$$

$$\delta\int V_o\rho\,dv = V_o\int\delta\rho\,dv \tag{16}$$

Thus,

$$\int \left(\frac{5}{3} \kappa_k \rho^{2/3} - \frac{Z}{r} + \varphi_e + V_0 \right) \delta\rho \; dv \tag{17}$$

For this expression to vanish for any $\delta\rho$, the factor in parentheses must vanish separately. Denoting the total atomic potential by $V = \frac{Z}{r} - \phi_e$, we obtain:

$$\rho = \left(\frac{3}{5\kappa_k} \right)^{3/2} \left(V - V_0 \right)^{3/2} . \tag{18}$$

Substitution of this expression in Poisson's equation then yields the Thomas-Fermi equation.

APPENDIX B

REDUCTION OF ρ_3 TO ELLIPTIC INTEGRALS

The exact Riemann density (ρ_3) involves an integral of a square root of a fourth-degree polynomial, where the range of integration is from one zero of the polynomial to the other zero. The integral has the specific form

$$I = \int_{g_{min}}^{g_{max}} \sqrt{(-g^2-g+\epsilon)(g^2+k_o^2)}\ dg \qquad \text{(B-1)}$$

where, for purposes of integration, ε and k_o can be treated as positive constants. The limits of integration are the roots of the equation

$$-g^2 - g + \varepsilon = 0, \qquad \text{(B-2)}$$

namely, $g_{max} = \frac{\eta-1}{2}$ and $g_{min} = \frac{-\eta-1}{2}$, where $\eta = \sqrt{4\varepsilon + 1}$. Since this integral must be evaluated repeatedly to a high degree of precision in the numerical solution of the RTF equation, it is highly desirable that a means be obtained of doing this in the minimum amount of time while maintaining sufficient accuracy to permit a numerical integration of the differential equation. This can be accomplished by reduction of the integral to an expression involving the standard Jacobian elliptic integrals. The theory of these elliptic integrals has been extensively developed[1-4], and a means of evaluating these integrals through transformations of the parameters has been adapted for computer work by Bulirsch and others[5-11]. The transformations are discussed in Appendix C.

The standard form of the elliptic integrals of the first, second, and third kind are the following:

$$F(z;k) = \int_0^z \frac{dx}{\sqrt{(1-k^2x^2)(1-x^2)}} \tag{B-3}$$

$$E(z;k) = \int_0^z \sqrt{\frac{1-k^2x^2}{1-x^2}}\, dx \tag{B-4}$$

$$\Pi(z;k,m) = \int_0^z \frac{dx}{(1-mx^2)\sqrt{(1-k^2x^2)(1-x^2)}} \tag{B-5}$$

Under the substitutions $x = \sin\theta$ and $k = \sin\alpha$, these may be written in the equivalent forms:

$$F(\varphi\backslash k) = \int_0^\varphi \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}} \tag{B-6}$$

$$E(\varphi\backslash k) = \int_0^\varphi \sqrt{1-k^2\sin^2\theta}\, d\theta \tag{B-7}$$

$$\Pi(\varphi\backslash k, m) = \int_0^{\varphi} \frac{d\theta}{(1-m\cdot\sin^2\theta)\sqrt{1-k^2\sin^2\theta}} \tag{B-8}$$

The number k is called the "modulus", ψ is the amplitude, and the elliptic integral of the third kind also depends on m, the "characteristic".

The reduction of Eq. (B-1) to the elliptic integrals is carried out in four parts:

(1) Reduction to an expression involving I_o, I_1, and I_2, where

$$I_n = \int \frac{t^n\, dt}{\sqrt{R(t)}} \tag{B-9}$$

and R(t) is a fourth-degree polynomial;

(2) Transformation of variables to eliminate the odd powers of t in R(t);

(3) Factorization and rearrangement to reduce these expressions to the canonical forms;

(4) Transformations to eliminate imaginary arguments.

The integral we must evaluate has the form

$$I = \int_{\frac{-\eta-1}{2}}^{\frac{\eta-1}{2}} \sqrt{(-g^2-g+\epsilon)(g^2+k_o^2)}\; dg \tag{B-10}$$

To make the limits symmetric, make the following changes of variable:

$$t = g + \frac{1}{2}; \qquad \eta = \sqrt{4\varepsilon + 1}; \qquad \kappa = \sqrt{4k_o^{\,2} + 1} .$$

Then,

$$I = \int_{-\frac{\eta}{2}}^{\frac{\eta}{2}} \sqrt{\left(-t^2 + \frac{\eta^2}{4}\right)\left(t^2 - t + \frac{\kappa^2}{4}\right)}\; dt \tag{B-11}$$

or,

$$I = \int_{-\frac{\eta}{2}}^{\frac{\eta}{2}} \sqrt{-t^4 + t^3 + \tfrac{1}{4}(\eta^2 - \kappa^2)t^2 - \tfrac{1}{4}\eta^2 t + \tfrac{1}{16}\eta^2\kappa^2}\; dt \tag{B-12}$$

Hancock[2] has shown that an integral of the form

$$\int_{t_0}^{t_1} R(t)\, dt \tag{B-13}$$

where

$$R(t) = \sqrt{c_4 t^4 + c_3 t^3 + c_2 t^2 + c_1 t + c_0} \tag{B-14}$$

can be reduced to

$$\begin{aligned} I = \frac{1}{24 c_4}\Big[&(4c_4 t + c_3)R + (8c_2 c_4 - 3c_3 c_3)I_2 \\ &+ (12c_1 c_4 - 2c_2 c_3)I_1 + (16 c_0 c_4 - c_1 c_3)I_0 \Big]_{t=t_0}^{t_1} \end{aligned} \tag{B-15}$$

where

$$I_n = \int_{t_0}^{t_1} \frac{t^n\, dt}{R(t)} \tag{B-16}$$

Equation (B-12) then reduces to

$$I = -\frac{1}{24}\Big[(-2\eta^2 + 2\kappa^2 - 3)I_2 + (\tfrac{5}{2}\eta^2 + \tfrac{1}{2}\kappa^2)I_1 + \eta^2(\tfrac{1}{4} - \kappa^2)I_0\Big] \tag{B-17}$$

since $R(t_o) = R(t_1) = 0$. I_0, I_1, and I_2 all involve

$$R(t) = \sqrt{\left(-t^2 + \frac{\eta^2}{4}\right)\left(t^2 - t + \frac{\kappa^2}{4}\right)} \tag{B-18}$$

The first factor vanishes at $t = \pm \frac{\eta}{2}$, while the second is positive definite for all real values of t.

Following the method of Abramowitz and Stegun[12], we define a new variable to produce an expression involving only the even powers of x. For an expression of the form

$$R(t) = \sqrt{(at^2+bt+c)(dt^2+e)} \tag{B-19}$$

we define x by:

$$x = +\sqrt{\frac{dt^2+e}{at^2+bt+c}} \tag{B-20}$$

Then it is evident that

$$R(t) = (at^2 + bt + c)\, x. \tag{B-21}$$

Solving Eq. (20) for t(x), we find two possible values:

$$t_{\pm}(x) = \frac{-bx^2 \pm T}{2(ax^2-d)} \tag{B-22}$$

where $T(x^2)$ is defined to be

$$T = \sqrt{(b^2-4ac)x^4 + 4(cd+ae)x^2 - 4de} \tag{B-23}$$

After a long but straightforward calculation, it can be shown that

$$\frac{dt_{\pm}}{R(t)} = \mp 2\, \frac{dx}{T(x^2)} \tag{B-24}$$

Before substituting this expression for $\frac{dt}{R(t)}$ into (Eq. 17), let us split the integration from $t = -\frac{\eta}{2}$ to $t = +\frac{\eta}{2}$ into two parts: $t \le 0$ and $t \ge 0$:

$$I_n = \int_{-\frac{\eta}{2}}^{\frac{\eta}{2}} \frac{t^n\, dt}{R(t)} \tag{B-25}$$

$$I_n = \int_{-\frac{\eta}{2}}^{0} \frac{t^n\,dt}{R(t)} + \int_{0}^{\frac{\eta}{2}} \frac{t^n\,dt}{R(t)} \tag{B-26}$$

$$= (-1)^n \int_{0}^{\frac{\eta}{2}} \frac{t^n\,dt}{R_-(t)} + \int_{0}^{\frac{\eta}{2}} \frac{t^n\,dt}{R(t)} \tag{B-27}$$

$$= (-1)^n\, I_n^- + I_n^+ \tag{B-28}$$

Here,

$$R_-(t) = R(-t) = \sqrt{(at^2 - bt + c)(dt^2 + e)} \tag{B-29}$$

Thus, $R_-(t)$ can be obtained from $R(t)$ simply by changing the sign of b. It is important to note that $T(x^2)$ depends only on b^2, so $T(x^2)$ derived from $R(t)$ is identical to the $T(x^2)$ derived from $R_-(t)$.

We must now look at our transformation (Eq. B-20) more carefully. For t_+ in Eq. (B-22),

$$x_+(t) = \sqrt{\frac{-t^2 + \frac{\eta^2}{4}}{t^2 - t + \frac{\kappa^2}{4}}} \tag{B-30}$$

The $x(t)$ defined here is not monotonically decreasing as t increases from 0 to $\frac{\eta}{2}$, but reaches a maximum at

$$t_\pm = \frac{1}{4}\left(\xi \pm \sqrt{\xi^2 - 4\eta^2}\right) \tag{B-31}$$

where

$$\xi = \eta^2 + \kappa^2 .$$

t_- is negative and thus lies outside the range $(0, \frac{\eta}{2})$, but t_+ does lie inside this range, so x as a function of t behaves as shown in Figure 11.

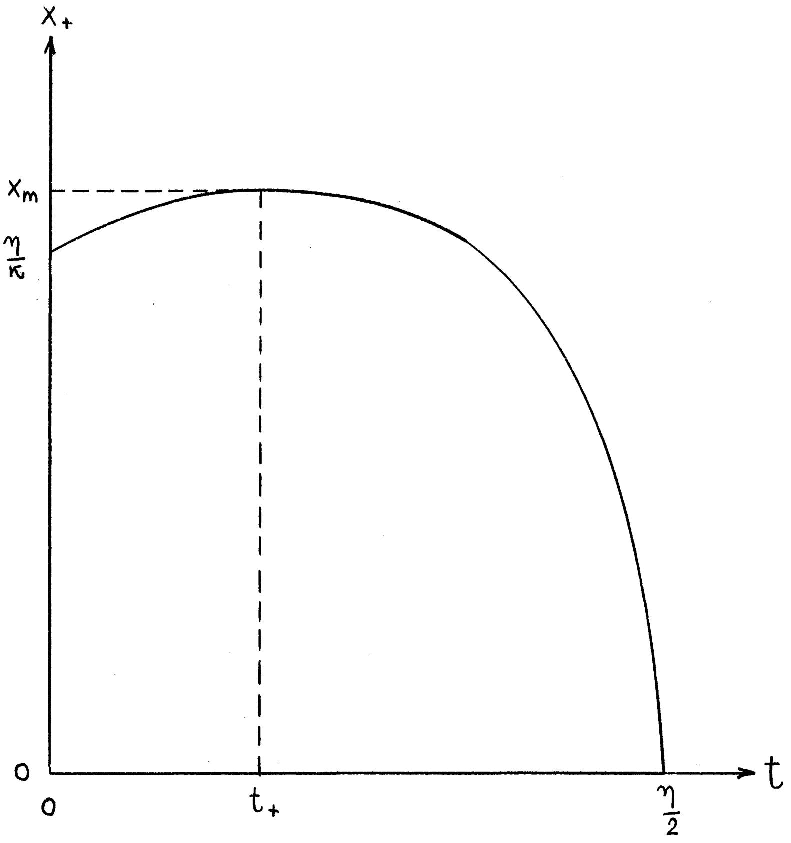

Figure 11. Transformation From t to x in I_n^+

Thus, in the range $0 \leq t \leq t_+$, x(t) is an increasing function of t and $\frac{dx}{dt} \geq 0$. In the range $t_+ \leq t \leq \frac{\eta}{2}$, x(t) is a decreasing function of t, and $\frac{dx}{dt} \leq 0$. By inspection of Eq. B-24, we find that the sign is now uniquely determined: for $0 \leq t \leq t_+$, we must choose t_-, and for $t_+ \leq t \leq \frac{\eta}{2}$, we must choose t_+. Thus, we find that the I_n^+ integral in Eq. (B-28) becomes

$$I_n^+ = \int_0^{t_+} \frac{t_-^{\,n}\, dt_-}{R(t)} + \int_{t_+}^{\frac{\eta}{2}} \frac{t_+^{\,n}\, dt_+}{R(t)} \qquad \text{(B-32)}$$

$$= \int_{X(0)}^{X(t_+)} (t_-)^n \frac{2dx}{T(x^2)} + \int_{X(t_+)}^{X(\frac{\eta}{2})} (t_+)^n \frac{-2\,dx}{T(x^2)} \qquad \text{(B-33)}$$

$$= 2\int_{\frac{\eta}{\kappa}}^{X_m} \left[\frac{x^2-T}{2(x^2+1)}\right]^n \frac{dx}{T} - 2\int_{X_m}^{0} \left[\frac{x^2+T}{2(x^2+1)}\right]^n \frac{dx}{T} \qquad \text{(B-34)}$$

where

$$X_m = \frac{4\eta^2 - \xi\left(\xi + \sqrt{\xi^2 - 4\eta^2}\right)}{(\xi-2)\left(\xi+\sqrt{\xi^2-4\eta^2}\right) - 2(\eta^2-\kappa^2)} \qquad \text{(B-35)}$$

The integral I_n^- in Eq. (B-28) contains $R_-(t)$ so the transformation corresponding to Eq. (B-30) now becomes

$$x_-(t) = \sqrt{\frac{-t^2 + \frac{\eta^2}{4}}{t^2 + t + \frac{\kappa^2}{4}}} \qquad \text{(B-36)}$$

A similar analysis of the extrema of x_- shows that they are located at

$$t_\pm = \frac{1}{4}\left(-\xi \pm \sqrt{\xi^2 - 4\eta^2}\right) \qquad \text{(B-37)}$$

In this case, both t_+ and t_- are negative, so there are no extrema of $x_-(t)$ in the range $0 \le t \le \frac{\eta}{2}$ and x_- as a function of t is monotonically decreasing, as shown in Figure 12.

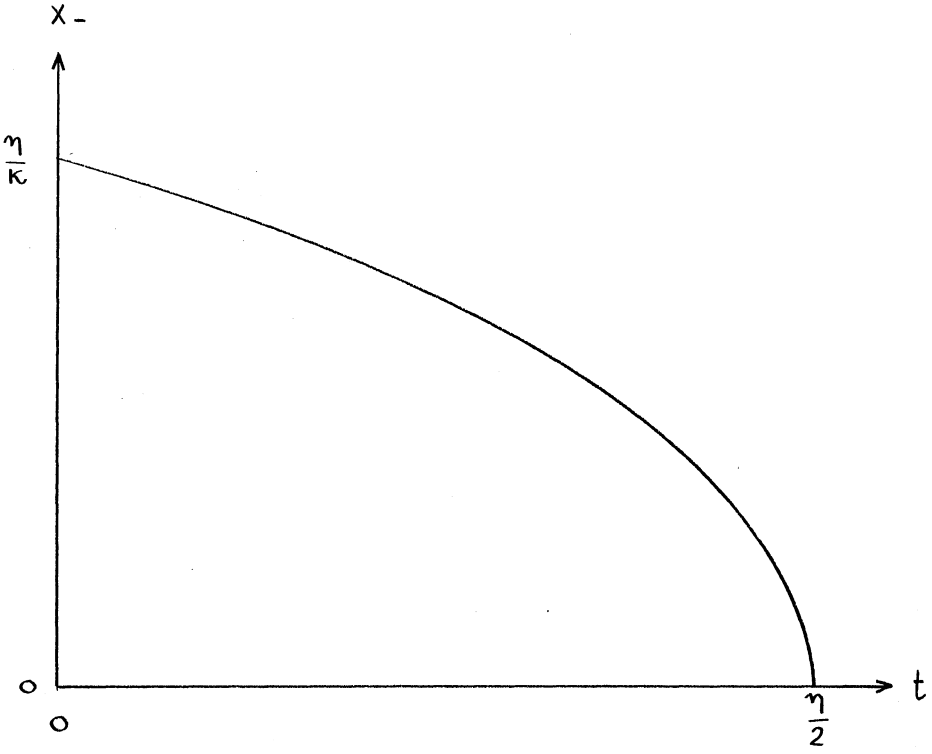

Figure 12. Transformation From t to x in I_n^-

Thus, throughout the whole range of $\int_n$ of I_n^-, $\frac{dx}{dt}$ is negative, so we must choose t_+ in Eq. (B-22):

$$I_n^- = \int_0^{\frac{\eta}{2}} \frac{t_+^{\,n}\, dt_+}{R_-(t)} \tag{B-38}$$

$$= \int_{x(0)}^{x(\frac{\eta}{2})} \left[\frac{x^2+T}{2(x^2+1)}\right]^n \frac{-2dx}{T} \tag{B-39}$$

$$= 2\int_0^{\frac{\eta}{\kappa}} \left[\frac{x^2+T}{2(x^2+1)}\right]^n \frac{dx}{T} \tag{B-40}$$

Combining Eq. (B-40) and Eq. (B-34) gives the result:

$$I_0 = 4\int_0^{x_m} \frac{dx}{T} \tag{B-41}$$

$$I_1 = 2\int_{\frac{\eta}{\kappa}}^{x_m} \frac{x^2}{x^2+1}\,\frac{dx}{T} \tag{B-42}$$

$$I_2 = \int_0^{x_m} \frac{x^4+T^2}{(x^2+1)^2}\,\frac{dx}{T} \tag{B-43}$$

In these expressions, T is defined as follows:

$$T = \sqrt{(1-\kappa^2)x^4 + (\eta^2-\kappa^2)x^2 + \eta^2} \tag{B-44}$$

and x_m is given in Eq. (B-35).

Let us first consider I_1. Adding and subtracting $\int \frac{dx}{T}$, we obtain:

$$I_1 = 2\int_{\frac{\eta}{\kappa}}^{x_m} \frac{dx}{T} - 2\int_{\frac{\eta}{\kappa}}^{x_m} \frac{dx}{(1+x^2)\cdot T} \tag{B-45}$$

The first of these is identical in form to I_0 and integrals of this type will be seen to reduce to the elliptic integral of the first kind F(x;k). The second integral will be seen to reduce to the elliptic integral of the third kind, and we now consider the first integral in Eq. (B-43). Writing out $T(x^2)$, we find we have the integral

$$I = \int \Phi(x^2)\,\frac{dx}{T} \tag{B-46}$$

where:

$$\Phi(x^2) = \frac{(2-\kappa^2)x^4 + (\eta^2-\kappa^2)x^2 + \eta^2}{x^4 + 2x^2 + 1} \tag{B-47}$$

Expanding $\Phi(x^2)$ in partial fractions of $(x^2 + 1)$,

$$\Phi(x^2) = (2-\kappa^2) + \frac{\eta^2+\kappa^2-4}{(x^2+1)} + \frac{2}{(x^2+1)^2} \tag{B-48}$$

Thus, Eq. (B-46) becomes

$$I = (2-\kappa^2)\int_0^{x_m} \frac{dx}{T} + (\eta^2+\kappa^2-4)\int_0^{x_m} \frac{dx}{(1+x^2)\,T} + 2\int_0^{x_m} \frac{dx}{(1+x^2)^2\,T} \tag{B-49}$$

The first two integrals have already been encountered, so we have only the third integral to investigate. Let us for the moment write $T(x^2)$ in the form

$$T = \sqrt{\gamma x^4 + \beta x^2 + \alpha} \tag{B-50}$$

We begin by considering the differential of $Z = \dfrac{xT}{1+x^2}$:

$$\frac{dT}{dx} = \frac{x}{T}\,(2\gamma x^2 + \beta) \tag{B-51}$$

$$\frac{dz}{dx} = \frac{(1-x^2)T + (1+x^2)x\,T'}{(1+x^2)^2} \tag{B-52}$$

$$\frac{dz}{dx} = \frac{\gamma x^6 + 3\gamma x^4 + (2\beta-\alpha)x^2 + \alpha}{(1+x^2)^2\,T} \tag{B-53}$$

If we now write the numerator of Eq. (B-53) in terms of $y = (1 + X^2)$,

$$\frac{dz}{dx} = \frac{\gamma y^3 + (-3\gamma + 2\beta - \alpha) y + 2\gamma - 2\beta + 2\alpha}{y^2 T} \tag{B-54}$$

Upon integrating both sides of Eq. (B-54), we find that

$$\int_0^{X_0} \frac{dx}{(1+X^2)^2 T} = \frac{1}{2(\alpha - \beta + \gamma)} \Big[\frac{XT}{1+X^2} - \gamma \int \frac{dx}{T} + (\alpha - 2\beta + 3\gamma) \int \frac{dx}{(1+X^2)T} - \gamma \int \frac{X^2 dx}{T} \Big]_{X=0}^{X_0} \tag{B-55}$$

In our case, $\alpha = \eta^2$, $\beta = \eta^2 - \kappa^2$, and $\gamma = 1 - \kappa^2$. Also, the first term in Eq. (B-55) vanishes at both limits. Combining Eq. (B-55), Eq. (B-49), Eq. (B-43), and Eq. (B-17), we obtain the following expression:

$$I = \frac{1}{24} \Big\{ [8(\epsilon - k_0^2) + 3] \frac{\eta}{\kappa} \cdot \frac{\eta^2}{\eta^2 + \kappa^2} + 4k_0^2 (16\epsilon + 1) \int \frac{dx}{T} + (12\epsilon + 12k_0^2 + 3) \int \frac{dx}{(1+X^2)T} + 4k_0^2 [8(\epsilon - k_0^2) + 3] \int \frac{X^2 dx}{T} \Big\} \tag{B-56}$$

We now make a further transformation of variables to take $T(X^2)$ into the form $\sqrt{(1-z^2)(1-k^2z^2)}$. With $\alpha = \eta^2$, $\beta = \eta^2 - \kappa^2$, $\gamma = 1 - \kappa^2$, $T(x^2)$ can be written

$$T = \sqrt{\gamma X^4 + \beta X^2 + \alpha} \tag{B-57}$$

If we define

$$\zeta = \frac{\beta}{\sqrt{\alpha}} + \sqrt{\frac{\beta^2}{\alpha} - 4\gamma} \tag{B-58}$$

$$q = \frac{1}{4k_0} \sqrt{\frac{2\xi}{\eta}} \tag{B-59}$$

$$k = \frac{\xi}{4k_0} \tag{B-60}$$

$$z^2 = \frac{x^2}{q^2 \eta^2} \tag{B-61}$$

we find that

$$\frac{dx}{T} = q \frac{dz}{\sqrt{(1-z^2)(1+k^2z^2)}} \tag{B-62}$$

The upper limit of integration, z_o, becomes

$$z_0 = \frac{1}{kq} \tag{B-63}$$

Thus, the integrals appearing in Eq. (B-56) are now the standard elliptic integrals:

$$\begin{aligned} I = & \frac{8(\epsilon - k_0^2)+3}{24} \cdot \frac{\eta}{k} \cdot \frac{\eta^2}{\eta^2+k^2} + \\ & + \left\{ \frac{(16\epsilon+1)k_0^2}{6} q - \frac{16k_0}{q}\left[\frac{8(\epsilon-k_0^2)+3}{24}\right]\right\} F \\ & + \frac{16k_0}{q}\left[\frac{8(\epsilon-k_0^2)+3}{24}\right] E \\ & + \frac{12(\epsilon+k_0^2)+3}{24} q \Pi \end{aligned} \tag{B-64}$$

where F, E, and Π are the standard elliptic integrals:

$$F = F(z_0; ik) = \int_0^{z_0} \frac{dz}{\sqrt{(1-z^2)(1+k^2z^2)}} \tag{B-65}$$

$$E = E(z_0; ik) = \int_0^{z_0} \sqrt{\frac{1+k^2z^2}{1-z^2}}\, dz \qquad \text{(B-66)}$$

$$\Pi = \Pi(z_0; ik, -g^2\eta^2) = \int_0^{z_0} \frac{dz}{(1+g^2\eta^2z^2)\sqrt{(1-z^2)(1+k^2z^2)}} \qquad \text{(B-67)}$$

The last step in our reduction is to use the "imaginary modulus transformation" to remove the ik. As given by Byrd and Friedman[13],

$$F(\varphi, ik) = k_1' \cdot F(\beta, k_1) \qquad \text{(B-68)}$$

$$E(\varphi, ik) = \frac{1}{k_1'}\left[E(\beta, k_1) - k_1^2 \sin\beta \cdot \cos\beta \sqrt{1-k_1^2 \sin^2\beta} \right] \qquad \text{(B-69)}$$

$$\Pi(\varphi, \alpha^2, ik) = \frac{k_1'}{\alpha_1^2}\left[k_1^2 \cdot F(\beta, k_1) + k_1'^2 \cdot \alpha^2 \cdot \Pi(\beta, \alpha_1^2, k_1) \right] \qquad \text{(B-70)}$$

where:

$$k_1 = \frac{k}{\sqrt{1+k^2}} \qquad \text{(B-71)}$$

$$k_1' = \sqrt{1+k_1^2} \qquad \text{(B-72)}$$

$$\alpha_1^2 = \alpha^2 k_1'^2 + k_1^2 \qquad \text{(B-73)}$$

$$\sin\beta = \frac{\sqrt{1+k^2}}{\sqrt{1+k^2 \cdot \sin^2\varphi}} \cdot \sin\varphi \qquad \text{(B-74)}$$

An interesting thing now happens to the upper limit of the integral. Combining Eq. (B-74) with Eq. (B-63) and Eq. (B-59), we find

$$\sin \beta = 1 . \tag{B-75}$$

That is, the integrals become complete elliptic integrals. This simplifies the computation of these integrals, and provides us with our final expression for the integral.

$$I = \frac{1}{24} \left\{ \frac{4C_0}{q} R_1 + \frac{2C_1}{q} (R_1 - R_3) + \frac{C_2}{q} \left[(R_1 - R_3) - 2k_0^2 x_m^2 (R_2 - R_1) \right] \right\} \tag{B-76}$$

where the following identifications are made:

$$R_1 = k_1' \cdot F \ , \tag{B-77}$$

$$R_2 = \frac{1}{k_1'} \cdot E \ , \tag{B-78}$$

$$R_3 = \left[(1 - k_1'^2) F - p^2 k_1'^2 \Pi \right] \frac{k_1'}{1 - p_1} \ ; \tag{B-79}$$

$$C_0 = \eta^2 (\kappa^2 - \tfrac{1}{4}) \tag{B-80}$$

$$C_1 = -(10\epsilon + 2k_0^2 + 3) \tag{B-81}$$

$$C_2 = 8(\epsilon - k_0^2) + 3 \ ; \tag{B-82}$$

$$p_1 = (1 + p^2) \cdot k_1'^2 \tag{B-83}$$

$$p^2 = \left(\zeta + \sqrt{\zeta^2 + \eta^2 k_0^2} \right) / 2k_0^2 \;; \tag{B-84}$$

$$F = \int_0^1 \frac{dx}{\sqrt{(1-x^2)(1-k^2x^2)}} \;, \tag{B-85}$$

$$E = \int_0^1 \sqrt{\frac{1-k^2x^2}{1-x^2}}\, dx \;, \tag{B-86}$$

$$\Pi = \int_0^1 \frac{dx}{(1-mx^2)\sqrt{(1-x^2)(1-k^2x^2)}} \;; \tag{B-87}$$

$$m = 1 - p_1 \;, \tag{B-88}$$

$$k = \sqrt{1 - k_1'^2} \,. \tag{B-89}$$

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APPENDIX C

EVALUATION OF ELLIPTIC INTEGRALS

The evaluation of elliptic integrals is conveniently carried out by a process known as Landen's transformation[1]. The transformation is based on the identities

$$F(\varphi, k_1) = (1 + k_1') F(\theta, k) \qquad \text{(C-1)}$$

$$E(\varphi, k_1) = \left(\frac{1}{1+k_1'}\right)\left[2E(\theta, k) + 2k' \cdot F(\theta, k) + (k'-1)\sin\varphi\right] \qquad \text{(C-2)}$$

$$\Pi(\varphi, \alpha_1^2, k_1) = \left(\frac{1+k_1'}{\alpha_2^2 - \alpha^2}\right)\left[(k^2 - \alpha^2) \cdot \Pi(\theta, \alpha^2, k) + (\alpha_2^2 - k^2) \cdot \Pi(\theta, \alpha_2^2, k)\right] \qquad \text{(C-3)}$$

where:

$$k_1 = \frac{1 - k_1'}{1 + k_1'} \qquad \text{(C-4)}$$

$$\sin\varphi = \frac{(1+k')\sin\theta \cdot \cos\theta}{\sqrt{1 - k^2 \cdot \sin^2\theta}} \qquad \text{(C-5)}$$

$$\alpha^2 = \frac{(1+k')^2}{2}\left[k_1 + \alpha_1^2 - \sqrt{(1-\alpha_1^2)(k_1^2 - \alpha_1^2)}\right] \qquad \text{(C-6)}$$

$$\alpha_2^2 = \frac{(1+k')^2}{2}\left[k_1 + \alpha_1^2 + \sqrt{(1-\alpha_1^2)(k_1^2-\alpha_1^2)}\right] \tag{C-7}$$

Successive substitutions of Eq. (C-4) into (C-1) and (C-2) provide:

$$F(\varphi, k) = k_n\sqrt{\frac{k_1\cdot k_2\cdots k_{n-1}}{k}}\cdot F(\theta_n, k_n) \tag{C-8}$$

$$\begin{aligned} E(\varphi,k) = F(\varphi,k)\Big\{1 + k\Big[1 + \frac{2}{k_1} + \frac{2^2}{k_1k_2} + \cdots + \frac{2^{n-1}}{k_1\cdots k_{n-1}} + {} \\ - \frac{2^n}{k_1\cdots k_{n-1}}\Big]\Big\} - k\Big[\sin\varphi + \frac{2}{\sqrt{k}}\sin\theta_1 + \frac{2^2}{\sqrt{k\cdot k_1}}\sin\theta_2 + {} \\ \cdots + \frac{2^{n-1}}{\sqrt{k\cdots k_{n-1}}}\sin\theta_{n-1} - \frac{2^n}{\sqrt{k\cdots k_n}}\sin\theta_n\Big] \end{aligned} \tag{C-9}$$

The advantage in this lies in the fact that k_n and ψ_n rapidly approach a limit (the convergence is quadratic), and at that point, the elliptic integral can be evaluated analytically by one of the formulas

$$E(\varphi, 1) = \sin\varphi \tag{C-10}$$

$$F(\varphi, 1) = \ln(\tan\varphi + \sec\varphi) \tag{C-11}$$

The evaluation of $\Pi(\psi, \alpha^2, k)$ is somewhat more involved, and an excellent algorithm for this integral was worked out by R. Bulirsch[2]. The FORTRAN coding of these algorithms is listed in Appendix D.

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APPENDIX D

COMPUTER PROGRAMS

The first set of programs lists two subprograms used in the solution of the RTF equation. Function ZINT(ZETA) is used as the function subprogram of the root-finding routine. (The program actually used was PEGAS.) A value of ZETA ($\zeta = Wm - E_o$) is given to the function ZINT, and a value ZINT (= Norm. Int. - Z) is returned to the calling program. When ZINT = 0, normalization is achieved. The second subprogram, subroutine RTF1(NEQ,X,Y,DYDX) is the function subroutine required by the differential equation integration routine, GEM. As indicated, values for Y(1) and Y(2) are passed to the program, and RTF1 returns values for the first and second derivatives.

```
      FUNCTION ZINT(ZETA)
C
C...............................................................................
C
C        SOLUTION OF RUDKJOBING'S EQN. BY GEM. UNDER THE TRF OF VARIABLES
C          U(R) --> PSI(X)/X**2    ;  R --> X**2
C          PSI <-- U(R)*R          ;  X <-- SQRT(R) ,
C        RUDKJOBING'S EQUATION:
C          D2U/DR2 + 2/R * DU/DR = -4*PI * RHO(R)
C          WHERE  RHO(R) IS THE RADIAL ELECTRON DENSITY:
C          RHO(R) = (2/3) * EPS**(3/2) / (2*PI**2 * R**3)   ,
C
C        NOW TAKES ON THE FORM:
C          D2PSI/DX2 - 1/X * DPSI/DX = -16*PI * X**4 * RHO(X)
C          WHERE RHO(X) IS NOW:
C          RHO(X) = (1/3 * PI**2) * (2*(ZETA - PSI/X**2) + 1/C**2 *
C                   (ZETA*(ZETA - 2*PSI / X**2) + PSI'/X *
C                   (PSI / X**2 - 0.25*PSI'/X) )     )**(3/2)
C          AND  PSI' = DPSI/DX,    ZETA = WM-E0
C
C        THE BOUNDARY CONDITIONS OF THIS EQN ARE:
C          PSI(0)=-ZNUM
C          PSI'(0)=0.    ,    PSI'(0)/0 = 0
C          PSI"(0)=0  ,   0**4 * RHO(0) = 0.
C
C...............................................................................
C
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION Y(2),DYDX(2),ERR(2),RERR(2)
      COMMON ZNUM
      COMMON /ZBLK/ RHO,ZZZZ,NG
      EXTERNAL RTF1
      DATA C,C2 / 137.03602D0,1.87787077D4/
C
C        SOME DENSITIES NEED A CUT-OFF RADIUS FOR NORMALIZABILITY;  IF ONE IS
C        NEEDED, A UNIFORMLY CHARGED NUCLEUS WITH RADIUS RNUC CAN BE INTRODUCED.
C        IF X.LE.XNUC  ( XNUC=SQRT(RNUC)  )  THEN U(R)=-ZNUM*R**2/RNUC**3
C        IF THE CUT-OFF RADIUS IS NOT TO BE USED, SET XNUC EQUAL TO A NEGATIVE
C        VALUE.
      XNUC=1.D-1
      XNUC=-1.D0
      RNUC=XNUC*XNUC
C
C
      ZZZZ=ZETA
      SUMRM=0.D0
      SUM=0.D0
C
C        ENTER INITIAL VALUES AND ERROR TOLERANCES
      X=0.D0
      Y(1)=-ZNUM
      Y(2)=0.D0
      XP=X
      FCTP=0.D0
C
      NMAX=200
      NMAX=400
      ER=1.D-04
      ER=1.D-06
```

```
      ER=1.D-08
      DO 10 J=1,2
      ERR(J)=ER
   10 RERR(J)=ER
C
      DO 7 III=1,500
      IF(X.LT.0.5D-3) XF=X+1.D-4
      IF(X.GE.0.5D-3.AND.X.LT.0.99D-2) XF=X+5.D-4
      IF(X.GE.0.99D-2.AND.X.LT.0.4D0) XF=X+1.D-2
      IF(X.GE.0.4D0) XF=X+5.D-2
C
      IF(XF-XNUC) 20,20,21
C         CALCULATE POTENTIAL FROM UNIFORM NUCLEUS
   20 R=XF*XF
      RR=R/RNUC
      Y(1)=-ZNUM*RR**3
      Y(2)=6.D0*Y(1)/XF
      X=XF
      CALL RTF1(2,X,Y,DYDX)
      GO TO 2
C
C         CALCULATE POTENTIAL FROM POISSON'S EQN USING GEM.
   21 CONTINUE
      H=XF
      HMAX=10.D0*XF
      KN=0
      CALL GEM(2,KN,0,X,XF,H,HMAX,Y,ERR,RERR,RTF1,NMAX,NUSED)
      IF(NUSED) 22,23,23
   22 WRITE(6,622) X
  622 FORMAT(1H0,10X,'GEM UNSUCCESSFUL AT X=',D13.6//)
      GO TO 8
   23 CONTINUE
      KN=1
C         Y(1)=PSI   ; Y(2)=PSI'
      R=X*X
      IF(X) 1,1,2
C         R --> 0 LIMIT OF 4*PI*R**2*RHO FOR GILVARRY'S DENSITY
    1 FCT=((ZNUM+ZNUM)*(1.D0+ZETA/C2))**1.5D0 * 8.48826363lD-1
      GO TO 3
    2 FCT=X*R*R*RHO*2.51327412287183D1
    3 DELTA=X-XP
      TERM=(FCT+FCTP)*DELTA*0.5D0
      SUM=SUM+TERM
      SUMRM=SUMRM+R*R*TERM
C
      IF(SUM.GT.500.D0) GO TO 8
C
      XP=X
      FCTP=FCT
C
      IF(X) 4,4,5
    4 U=-1.D75
      DUDR=1.D75
      GO TO 6
    5 U=Y(1)/R
      DUDR=(Y(2)/(X+X)-U)/R
    6 CONTINUE
      IPRINT= 1
      IPRINT=-1
```

```
      IF(IPRINT) 666,66,66
   66 WRITE(6,100) X,Y(1),Y(2),H,NUSED,TERM,R,RHO,U,DUDR,SUM,NG
  100 FORMAT(1H ,'X=',D13.6,2X,'Y(1)=',D13.6,2X,'Y(2)=',D13.6,
     * 5X,'H=',D13.6,2X,'NUSED=',I4,10X,'TERM=',D13.6/
     11H ,20X,'R=',D13.6,2X,'RHO=',D13.6,2X,'U=',D13.6,2X,'DU/DR=',D13.6
     2,5X,'SUM=',D13.6,2X,'NG=',I2/)
  666 CONTINUE
C
      IF(TERM-1.D-6*SUM) 8,7,7
    7 CONTINUE
    8 ZINT=SUM-ZNUM
      RM=DSQRT(SUMRM/ZNUM)
      WRITE(6,600) ZETA,SUM
  600 FORMAT(1H0,5X,'IN ZINT, WITH ZETA=',D22.15,' SUM=',D13.6/)
      WRITE(6,601) RM
  601 FORMAT(1H0,5X,'THE R.M.S. RADIUS IS R0 =',D13.6/)
      RETURN
      END
      SUBROUTINE RTF1(NEQ,X,Y,DYDX)
C
C         THIS SUBROUTINE PROVIDES GEM WITH RUDKJOBING'S RTF EQN
C
C         Y(1)=PSI(X)
C         Y(2)=DYDX(1)=DPSI/DX
C              DYDX(2)=D2PSI/DX2
C
      IMPLICIT REAL*8 (A-H,O-Z)
      DATA C,C2 / 137.03602D0,1.877887077D4/
      DIMENSION Y(2),DYDX(2)
      COMMON /ZBLK/ RHO,ZETA,NG
C
      DYDX(1)=Y(2)
      IF(X) 1,1,2
    1 DYDX(2)=0.D0
      RHO=1.D75
      RETURN
    2 R=X*X
C
      T1=Y(1)/R
      T2=Y(2)/X
      F=(ZETA*(ZETA-T1-T1)+T2*(T1-0.25D0*T2))/C2+2.D0*(ZETA-T1)
      IF(F) 3,3,4
    3 RHO=0.D0
      GO TO 5
    4 RHO=3.377372788D-2*F**1.5D0
C
    5 DYDX(2)=T2-5.026548245D1*R*R*RHO
      RETURN
      END
```

The remaining four subprograms evaluate the four expressions $4\pi r^2\rho_1$, $4\pi r^2\rho_2$, $4\pi r^2\rho_3$, and $4\pi r^2\rho_4$. They require a subroutine POT(R,RU,R2DU) which will, given a value of R, return values of RU = $r \cdot U(r)$ and R2DU = $r^2 \cdot \frac{dU}{dr}$. The third subprogram actually consists of three parts: one part evaluates $4\pi r^2\rho$ and provides communication with the calling program. A second part (RHS) evaluates the coefficients and arguments for the elliptic integral routine (DCEL), which makes up the third part.

```
      FUNCTION FCT(R)
C
C        THIS ROUTINE EVALUATES FCT=4*PI*RHO(R)*R*R, WHERE RHO(R) IS THE
C        EXACT STIELTJES DENSITY
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /FCTBLK/ ZETA
      COMMON ZNUM
      DATA C,C2,FOURPI/137.03602D0,1.877887077D4,1.25663706143592D1/
C
      IF(R) 1,1,2
    1 V=1.D75
      GO TO 3
    2 V=1.D0/(1.97392088021787D1*R**3)
    3 CONTINUE
C
C        THIS SECTION PROVIDES VALUES FOR R*U(R) AND R**2 * DU/DR.
C        IF R IS .GT. RNUC (THE NUCLEAR RADIUS, APPX 1.D-4*A0) THE POTENTIAL
C        IS PROVIDED BY DHFPOT().  IF R IS .LE. RNUC, A UNIFORM NUCLEUS IS USED.
      RNUC=1.D-04
C
      IF(R-RNUC) 4,4,5
    4 X=R/RNUC
      RU=-ZNUM*X**3
      R2DU=RU+RU
      GO TO 6
    5 CALL POT(R,RU,R2DU)
    6 CONTINUE
C
      AK=R2DU/C
      AK2=AK*AK
      EPS=R*ZETA-RU
      EPS=EPS*(R+R+EPS/C2)
C
C        EVALUATE EXACT STIELTJES DENSITY
      IF(EPS+0.25D0) 7,7,8
C
C        IF ETA.LT.0   OR IF G(1).LT.GMIN,  RHO=0.
    7 N=0
      RHO=0.D0
      FCT=0.D0
      GO TO 50
C        SEE IF |EPS| IS SMALL
    8 IF(DABS(EPS)-1.D-15)9,9,11
    9 IF(EPS-0.5D0*AK2) 7,10,10
C        SMALL |EPS|
   10 N=1
      RHO=V*DSQRT(EPS+AK2)
      FCT=FOURPI*R*R*RHO
      GO TO 50
C
C        NORMAL |EPS|
   11 RHO=0.D0
      ETA=DSQRT(4.D0*EPS+1.D0)
      GMAX=(ETA-1.D0)/2.D0
      GMIN=GMAX-ETA
      DO 17 KAPPA=1,50
      SQKAP=KAPPA*KAPPA
      AKAPP=KAPPA
      G=-DSQRT(SQKAP-AK2)
```

```
      GG=G*G
      IF(G-GMIN) 12,13,14
   12 N=KAPPA+KAPPA-2
      GO TO 18
   13 N=KAPPA+KAPPA-1
      RHO=RHO+AKAPP *DSQRT(-GG-G+EPS)
      GO TO 18
   14 RHO=RHO+AKAPP *DSQRT(-GG-G+EPS)
C
      G=-G
      IF(G-GMAX) 17,16,15
   15 N=KAPPA+KAPPA-1
      GO TO 18
   16 N=KAPPA+KAPPA
      RHO=RHO+AKAPP*DSQRT(-GG-G+EPS)
      GO TO 18
   17 RHO=RHO+AKAPP*DSQRT(-GG-G+EPS)
      WRITE(6,170) KAPPA
  170 FORMAT(1H,10X,'IN FCT, SUM IS STILL CONTINUING AFTER KAPPA=',I4)
   18 RHO=V*RHO
      FCT=R*R*FOURPI*RHO
      GO TC 50
C
   50 CONTINUE
      WRITE(6,500) R,RHO,FCT,N,AK,EPS
  500 FORMAT(1H ,'R=',D13.6,2X,'RHO=',D13.6,2X,'FCT=',D13.6,2X,'NG=',I2,
     * 5X,'AK=',D13.6,2X,'EPS=',D13.6)
      RETURN
      END
```

```
      FUNCTION FCT(R)
C
C        THIS ROUTINE EVALUATES FCT=4*PI*RHO(R)*R*R, WHERE RHO(R) IS THE
C        APPROXIMATE STIELTJES DENSITY
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMCN /FCTBLK/ ZETA
      COMMON ZNUM
      CATA C,C2,FOURPI/137.03602D0,1.877887077D4,1.25663706143592D1/
C
      IF(R) 1,1,2
    1 V=1.D75
      GO TC 3
    2 V=1.D0/(1.97392088021787D1*R**3)
    3 CONTINUE
C
C        THIS SECTION PROVIDES VALUES FOR R*U(R) AND R**2 * DU/DR.
C        IF R IS .GT. RNUC (THE NUCLEAR RADIUS, APPX 1.D-4*A0) THE POTENTIAL
C        IS PROVIDED BY DFFPOT().  IF R IS .LE. RNUC, A UNIFORM NUCLEUS IS USED.
      RNUC=1.D-04
C
      IF(R-RNUC) 4,4,5
    4 X=R/RNUC
      RU=-ZNUM*X**3
      R2DU=RU+RU
      GO TO 6
    5 CALL POT(R,RU,R2DU)
    6 CONTINUE
C
      AK=R2DU/C
      AK2=AK*AK
      EPS=R*ZETA-RU
      EPS=EPS*(R+R+EPS/C2)
C
C
C        APPROXIMATE STIELTJES DENSITY
C
      IF(EPS) 20,20,21
   20 N=0
      RHC=0.D0
      FCT=0.D0
      GO TO 50
   21 RHC=0.D0
      DO 24 KAPPA=1,50
      SQKAP=KAPPA*KAPPA
      E=EPS+AK2-SQKAP
      IF(E) 22,23,24
   22 N=KAPPA+KAPPA-2
      GO TC 25
   23 RHO=RHC+DFLOAT(KAPPA)*DSQRT(E)
      N=KAPPA+KAPPA
      GC TC 25
   24 RHO=RHO+DFLOAT(KAPPA)*DSQRT(E)
      WRITE(6,240) KAPPA
  240 FORMAT(1H,10X,'IN FCT, SUM IS STILL CONTINUING AFTER 2*(KAPPA=',I4
     &,')  TERMS.')
   25 RHO=(RHO+RHO)*V
      FCT=FOURPI*R*R*RHO
      GO TO 50
C
```

```
 50 CONTINUE
    WRITE(6,500) R,RHO,FCT,N,AK,EPS
500 FORMAT(1H ,'R=',D13.6,2X,'RHO=',D13.6,2X,'FCT=',D13.6,2X,'NG=',I2,
   * 5X,'AK=',D13.6,2X,'EPS=',D13.6)
    RETURN
    END
```

```
      FUNCTION FCT(R)
C
C        THIS ROUTINE EVALUATES FCT=4*PI*RHO(R)*R*R, WHERE RHO(R) IS THE
C        EXACT RIEMANN DENSITY
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /FCTBLK/ ZETA
      COMMCN ZNUM
      DATA C,C2,FOURPI/137.03602D0,1.87788707704,1.25663706143592D1/
C
      IF(R) 1,1,2
    1 V=1.D75
      GO TO 3
    2 V=1.D0/(1.97392088021787D1*R**3)
    3 CONTINUE
C
C        THIS SECTION PROVIDES VALUES FOR R*U(R) AND R**2 * DU/DR.
C        IF R IS .GT. RNUC (THE NUCLEAR RADIUS, APPX 1.D-4*A0) THE POTENTIAL
C        IS PROVIDED BY DHFPOT().  IF R IS .LE. RNUC, A UNIFORM NUCLEUS IS USED.
      RNUC=1.D-04
C
      IF(R-RNUC) 4,4,5
    4 X=R/RNUC
      RU=-ZNUM*X**3
      R2DU=RU+RU
      GO TO 6
    5 CALL POT(R,RU,R2DU)
    6 CONTINUE
C
      AK=R2DU/C
      AK2=AK*AK
      EPS=R*ZETA-RU
      EPS=EPS*(R+R+EPS/C2)
C
C
C        EXACT RIEMANN DENSITY
C
      IF(R) 40,40,41
   40 RHO=1.D75
      FCT=1.D75
      GO TO 50
   41 CALL RHS(EPS,AK,Z)
      RHO=V*Z
      FCT=FOURPI*R*R*RHO
      GO TO 50
C
   50 CONTINUE
      WRITE(6,500) R,RHO,FCT,N,AK,EPS
  500 FORMAT(1H ,'R=',D13.6,2X,'RHO=',D13.6,2X,'FCT=',D13.6,2X,'NG=',I2,
     * 5X,'AK=',D13.6,2X,'EPS=',D13.6)
      RETURN
      END
      SUBROUTINE RHS(EPS,BK,Z)
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                      C
         THIS SUBROUTINE, WHICH CALLS SUBROUTINE DCEL, EVALUATES THE INTEGRAL  C
C        WHICH OCCURS IN THE RHS OF THE RTF EQN:                       C
C                                                                      C
C        Z=INTEGRAL OF: DSQRT((-T**2+ETA2/4.)*(T**2-T+AKAP2/4.))       C
C                                                                      C
```

```
C        WHERE: ETA2=4.*EPS+1.             AKAP2=4.*AK**2+1.                   C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /DCBLK/ CK12,CK1,XP1,R1,R2,R3,IER
      AK=BK
      IF(AK.LT.0.D0) AK=-AK
      AK2=AK*AK
      ETA2=4.D0*EPS+1.D0
      AKAP2=4.D0*AK2+1.D0
      IF(AKAP2-1.D06*ETA2) 2,1,1
C
C        AK IS MUCH GREATER THAN EPS; THUS, WE USE AN EXPANSION OF THE
C        SECOND FACTOR IN THE INTEGRAND, KEEPING TERMS UP THROUGH ORDER
C        ETA2/AKAP2, BUT IGNORING ETA4/AKAP4, ETC.
    1 AKAP=DSQRT(AKAP2)
      Z=0.196349540849362D0*ETA2*(AKAP+0.125D0*ETA2/AKAP)
      RETURN
C
    2 ZETA=EPS-AK2
      ZZ=ZETA*ZETA
      RAD=DSQRT(ZZ+ETA2*AK2)
      TAK=AK2+AK2
      XPSQ=(ZETA+RAD)/TAK
      XMSQ=(ZETA-RAD)/TAK
      Q=(AK+AK)*DSQRT(-XMSQ)
      CK12=ETA2+(ZETA+ZETA)*XPSQ
      CK12=ETA2/(CK12+CK12)
      CK1=DSQRT(CK12)
      XP1=(1.D0+XPSQ)*CK12
C
C     XK=DSQRT(1.D0-CK12)
C     XM=1.D0-XP1                                                       $,#%+&=
C     WRITE(6,112) AK,XK,CK1,XM,XP1,XPSQ,XMSQ,Q
C 112 FORMAT (1H,5X,'AK=',D22.15,5X,'XK1=',D22.15,2X,'CK1=',D22.15,/
C    1 1H,35X,'XM=',D22.15,2X,'XP1=',D22.15,/ 1H,35X,'XPSQ=',D22.15,2X,
C    2'XMSQ=',D22.15,5X,'Q=',D22.15)
      CALL DCEL
      C0=ETA2*(AKAP2-0.25D0)
      C1=-(10.D0*EPS+AK2+AK2+3.D0)
      C2=8.D0*(EPS-AK2)+3.D0
C     WRITE(6,122) C0,C1,C2,R1,R2,R3
C 122 FORMAT(1H,35X,'C0=',D22.15,2X,'C1=',D22.15,2X,'C2=',D22.15/
C    1 1H,35X,'R1=',D22.15,2X,'R2=',D22.15,2X,'R3=',D22.15)
      R3=((1.D0-CK12)*R1-XPSQ*CK12*R3)*CK1/(1.D0-XP1)
      R2=R2/CK1
      R1=CK1*R1
      V0=4.D0*R1/Q
      V1=(R1-R3)/Q
      V2=V1-(TAK+TAK)*XMSQ*(R2-R1)/Q
      V1=V1+V1
      Z=(C0*V0+C1*V1+C2*V2)/24.D0
      RETURN
      END
      SUBROUTINE DCEL
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                              C
C        THIS SUBROUTINE EVALUATES THE COMPLETE ELLIPTIC INTEGRALS             C
C        USING THE DESCENDING LANDEN'S TRANSFORMATION                          C
```

```
C        REFERENCE:   R. BULIRSCH, NUM MATH 7,78(1965)                         C
C                                                                              C
C        THE INTEGRALS ARE DEFINED AS:                                         C
C             R1=F(PI/2,XK)=INTEGRAL OF DY/DELTA                               C
C             R2=E(PI/2,XK)=INTEGRAL OF DY*DELTA                               C
C             R3=PI(PI/2,XK,XM)=INTEGRAL OF DY/((1.-XM*SIN(Y)**2)*DELTA)       C
C             WHERE:   DELTA=DSQRT(1.-XK**2*SIN(Y)**2)                         C
C             (ALL ARE SUMMED OVER Y FROM Y=0. TO Y=PI/2.                      C
C                                                                              C
C..............................................................................C
C                                                                              C
C        INPUT PARAMETERS:                                                     C
C             CK2=COMPLEMENTARY MODULUS=1.-XK**2                               C
C             CK=DSQRT(CK2)                                                    C
C             XP=1.-XM                                                         C
C                                                                              C
C..............................................................................C
C                                                                              C
C        OUTPUT VALUES:                                                        C
C             R1,R2,R3: VALUES OF ELLIPTIC INTEGRALS (DEFINED ABOVE)           C
C             IER...ERROR CODE:                                                C
C                  IER=0; NORMAL EXECUTION--ALL INTEGRALS ARE FINITE.          C
C                  IER=1; ONE OR MORE INTEGRALS ARE INFINITE--                 C
C                         THE VALUE 1.D75 IS ASSIGNED TO THE INTEGRAL          C
C                                                                              C
C        (ALL COMMUNICATION WITH THE CALLING PROGRAM IS DONE THROUGH           C
C        COMMON /DCBLK/  CK2,CK,XP,R1,R2,R3,IER                                C
C                                                                              C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /DCBLK/ CK2,CK,XP,R1,R2,R3,IER
      DATA PI2/1.570796326794900/
      IER=0
      KOUNT=0
C
C        TEST FOR SPECIAL CASES
C
      IF(CK) 2,1,3
    1 R1=1.D75
      R2=1.D0
      R3=1.D75
      IER=1
      GO TO 17
    2 CK=-CK
    3 IF(CK2-1.D0) 7,4,7
    4 R1=PI2
      R2=PI2
      IF(XP) 7,5,6
    5 R3=1.D75
      IER=1
      GO TO 17
    6 R3=PI2/DSQRT(XP)
      GO TO 17
C
C        INITIALIZATION
C
    7 G=CK
      A=1.D0
      R=2.D0
```

```
      AA=1.DO+CK2
      B=CK2
      C=1.DO
      IF(XP) 9,10,8
    8 P=DSQRT(XP)
      PC=1.DO
      PD=1.DO/P
      GO TO 11
C
    9 PF=1.DO-XP
      P=DSQRT((CK2-XP)/PF)
      PD=(CK2-1.DO)/(P*PF)
      PC=0.DO
      GO TO 11
C
   10 IER=1
C
C          BEGIN LANDEN'S TRF USING MODIFIED A-G MEAN
C
   11 KOUNT=KOUNT+1
      E=A*G
      R=R+R
C
      IF(IER) 12,12,13
   12 PG=E/P
      PF=PC
      PC=PD/P+PC
      PD=PF*PG+PD
      PD=PD+PD
      P=PG+P
C
   13 APREV=A
      A=A+G
C
      B=C*G+B
      B=B+B
      C=AA
      AA=B/A+AA
C
C          TEST FOR CONVERGENCE
C
      IF(G/APREV-0.999999995DO) 14,15,15
C
C          NOT CONVERGED; TRY AGAIN
C
   14 G=DSQRT(E)
      G=G+G
      GO TO 11
C
C          CONVERGENCE ACHIEVED
C
   15 E=0.785398163397448DO/A
      R1=E*R
      R2=E*AA
      IF(IER) 16,16,5
   16 R3=(E+E)*(PC*A+PD)/(A+P)
   17 CONTINUE
C
C          RECORD NUMBER OF ITERATIONS AND IER  (OPTIONAL)
```

```
C
C      WRITE(6,100) KOUNT,IER
C 100  FCRMAT(1H,80X,25HSUBROUTINE DCF  HAS USED ,I4,7H CYCLES/
C    1 1H,80X,12HERROR CODE =,I1)
       RETURN
       END
```

```
      FUNCTION FCT(R)
C
C         THIS ROUTINE EVALUATES FCT=4*PI*RHO(R)*R*R, WHERE RHO(R) IS THE
C         APPROXIMATE RIEMANN DENSITY
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /FCTBLK/ ZETA
      COMMON ZNUM
      DATA C,C2,FOURPI/137.03602D0,1.877887077D4,1.2566370614359201/
C
      IF(R) 1,1,2
    1 V=1.D75
      GO TO 3
    2 V=1.D0/(1.97392088021787D1*R**3)
    3 CONTINUE
C
C         THIS SECTION PROVIDES VALUES FOR R*U(R) AND R**2 * DU/DR.
C         IF R IS .GT. RNUC (THE NUCLEAR RADIUS, APPX 1.D-4*A0) THE POTENTIAL
C         IS PROVIDED BY DHFPOT().  IF R IS .LE. RNUC, A UNIFORM NUCLEUS IS USED.
      RNUC=1.D-04
      RNUC=-1.D0                                                        ########
C
      IF(R-RNUC) 4,4,5
    4 X=R/RNUC
      RU=-ZNUM*X**3
      R2DU=RU+RU
      GO TO 6
    5 CALL POT(R,RU,R2DU)
    6 CONTINUE
C
      AK=R2DU/C
      AK2=AK*AK
      EPS=R*ZETA-RU
      EPS=EPS*(R+R+EPS/C2)
C
C
C         APPROXIMATE RIEMANN DENSITY
C
      IF(R-1.D-20) 30,30,31
   30 RHO=1.D75
      FCT=0.D0
      GO TO 50
   31 IF(EPS) 32,33,33
   32 WRITE(6,310) EPS
  310 FORMAT(1H0,10X,'IN FCT, EPS=',D13.6,'.  RHO IS SET=0.')
      RHO=0.D0
      FCT=0.D0
      GO TO 50
   33 RHO=0.666666666666667D0*V*EPS**1.5D0
      FCT=FOURPI*R*R*RHO
      GO TO 50
C
   50 CONTINUE
      WRITE(6,500) R,RHO,FCT,N,AK,EPS
  500 FORMAT(1H ,'R=',D13.6,2X,'RHO=',D13.6,2X,'FCT=',D13.6,2X,'NG=',I2,
     * 5X,'AK=',D13.6,2X,'EPS=',D13.6)
      RETURN
      END
```

VITA

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