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Argonne National Laboratory

**A THEORETICAL STUDY OF
SIMPLE MANY-ELECTRON SYSTEMS**

by

Lester M. Sachs

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ARGONNE NATIONAL LABORATORY
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A THEORETICAL STUDY OF
SIMPLE MANY-ELECTRON SYSTEMS

by

Lester M. Sachs

Solid State Science

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PREFACE

The work of this report was performed during the tenure of a Resident Student Associateship at the Argonne National Laboratory under the sponsorship of the Illinois Institute of Technology. The major portion of the report is a verbatim adoption of the author's thesis as submitted to the Physics Department of the Illinois Institute of Technology. The author would like to express his appreciation to his advisers, Dr. T. L. Gilbert of the Argonne National Laboratory and Prof. P. G. Lykos of the Illinois Institute of Technology, for their interest and advice during the course of the work. He would also like to thank Dr. O. C. Simpson for the arrangement of the Student Associateship and the hospitality of the Solid State Science Division.

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ABSTRACT

A study has been made of the one-electron approximation for a number of simple many-electron systems. A review is given of the mathematical structure underlying the Hartree-Fock (HF), Unrestricted Hartree-Fock (UHF), and Projected Unrestricted Hartree-Fock (PUHF) approximations which may be utilized to obtain approximate solutions of the many-electron Schrödinger equation. The salient features of each method and their applicability to simple systems are outlined.

Solutions using the above approximations were obtained by the "self-consistent field" (SCF) method utilizing a finite set of Slater-type functions as an expansion set. This becomes a matrix procedure and involves the calculations of the matrix elements of the operators and the solution of the matrix (operator) equations. To this end, a number of computer programs were written for the IBM-704 digital computer and utilized to obtain the desired solutions.

Hartree-Fock solutions have been obtained for the atomic configurations $1s^2$, $1s^22s$, and $1s^22s^2$ for the range of atomic number $2 \leq Z \leq 10$. The UHF solution of lithium has also been obtained and the PUHF solution projected from it. A tabulation of the orbitals and two measures of their quality is given for all SCF solutions. Utilizing the HF, UHF, and PUHF solutions, the hyperfine splitting of the lithium ground state is calculated by first-order perturbation and found to be given best by the UHF method, approaching the experimental value. The diamagnetic susceptibilities of He, Li^+ , Li^- , and Be have been calculated.

Hartree-Fock solutions have also been obtained for the ground states of F, F^- , Ne, Na^+ , and Na, and for Na^+ and F^- in the presence of superposed charged spheres. A tabulation of the orbitals and their goodness is given for this series. The diamagnetic susceptibilities of the ten-electron systems has been calculated. The doublet separation of the fluorine ground states has been computed, and the hyperfine splitting of sodium and fluorine have been obtained.

A number of recommendations are offered regarding the SCF computational procedure.

CHAPTER I INTRODUCTION

In this study we shall report on calculations of approximate wave functions for a number of simple atomic systems. The importance of atomic structure calculations stems from the information they provide for calculating atomic properties which are needed for interpreting a wide variety of molecular and solid state phenomena: optical absorption and paramagnetic resonance of color centers, neutron and X-ray scattering, exciton phenomena, etc.

The principal interactions in an atomic system are due to the coulomb forces between the charged particles. The remaining interactions, which are magnetic in character, are smaller by a factor of the order of v/c and may be treated by perturbation theory. In the nonrelativistic situation, the approximate Hamiltonian for an atomic system containing a fixed nucleus of charge Z surrounded by N electrons can be written

$$\mathcal{H} = \sum_{i=1}^N \left(p_i^2 - \frac{Z}{r_i} \right) + \sum_{i>j=1}^N \frac{1}{r_{ij}} \quad . \quad (1.1)$$

Here we have adopted the atomic units of Hartree, wherein the length unit is the Bohr radius, the mass unit is the electronic mass, and the energy unit is $2R_{\infty}hc = 27.21$ ev. The subscripts $i = 1, 2, \dots, N$ label the different electrons; r_i is the distance of electron i from the nucleus and r_{ij} is the mutual distance of electrons i and j .

Approximate eigenfunctions of $\mathcal{H}$ may be obtained by assuming an N -electron wave function of the form

$$\Psi(x_1, x_2, \dots, x_N) = \psi_1(x_1)\psi_2(x_2)\dots\psi_N(x_N) \quad , \quad (1.2)$$

where ψ_i is the wave function for electron i . This approximation was first introduced by Hartree.^{(1)*} The ψ_i were assumed to be products of a space function and a spin function:

$$\psi_i(x_i) \equiv \psi_i(\vec{r}_i, s_i) = \phi_i(\vec{r}_i)\eta(s_i) \quad , \quad (1.3)$$

where the spin function η was either α (with a Z -component of spin of $\frac{1}{2}$) or β (with a Z -component of spin of $-\frac{1}{2}$). The function ϕ has become known as an orbital, a word used as a synonym for the solution to a one-electron space-dependent Schrödinger equation. The ψ_i of (1.3) represent a special form of the general spin-orbital function of space and spin.

Each of the ψ_i of (1.2) was determined by considering electron i alone in the electrostatic field of the nucleus and the other $(N-1)$ electrons.

*For all numbered footnotes, see Bibliography.

This electrostatic field was assumed to be spherically symmetric. In systems with nonspherical charge distributions, the symmetry was achieved by averaging over all directions. Since the orbitals resulting from this set of N equations are determined by the electrostatic field produced by the set of orbitals, this method became known as the Hartree Self-consistent Field (SCF) method.

Slater⁽²⁾ and Fock⁽³⁾ suggested the connection between the Hartree theory and the Variational Principle. If one assumes a wave function of the form (1.2) and calculates the total energy by means of (1.1), then a set of N equations is obtained for the ϕ 's by requiring that the energy remain stationary for an arbitrary variation of each ϕ subject to an orthonormalization constraint. These N equations are the same as the N equations considered by Hartree.

Slater⁽²⁾ and Fock⁽³⁾ also suggested that in order to take account of the Exclusion Principle the proper N -electron wave function should be a linear combination of functions of the type (1.2) with the indices permuted, so as to make it antisymmetric with respect to the interchange of the coordinates of any two electrons. The variation of the ψ 's proceeds in the same manner as previously. This approximation is termed the Hartree-Fock approximation.

In Chapter II we consider the HF approximation in greater detail. We also consider variants of this approximation - the Unrestricted Hartree-Fock (UHF) and the Projected Unrestricted Hartree-Fock (PUHF) approximations. In Chapter III we review the techniques for obtaining approximate self-consistent solutions of the HF equations. We consider in greater detail the method of iterating the matrix representation of the operator equations first introduced by Roothaan,⁽⁴⁾ and we discuss the actual computational procedure and other details of this work. Chapter IV deals with the first series of HF calculations: those on the ground states of the $1s^2$, $1s^2 2s$, and $1s^2 2s^2$ configurations. In Chapter V we present and discuss the UHF and PUHF solutions for lithium and compare them with the HF solution. In Chapter VI we discuss the HF solutions for F, F^- , Ne, Na^+ , and Na, and consider a few applications. Chapter VII summarizes the work and offers a number of recommendations for future studies.

CHAPTER II

THE HARTREE-FOCK APPROXIMATION

The Hartree-Fock formalism as given by Fock⁽³⁾ was restricted to closed-shell configurations* or configurations which differ from a closed shell** by a single spin-orbital. The formalism was later extended to open shells† other than the special ones referred to above by Shortley⁽⁵⁾ and the Hartrees,⁽⁶⁾ and has recently been modified by Roothaan⁽⁷⁾ in such a manner as to fit conveniently into his matrix SCF scheme.

To recapitulate, we recall that both Slater⁽²⁾ and Fock⁽³⁾ suggested that when utilizing the Variational Principle we assume as an N-electron wave function a linear combination of the type (1.2) with permuted indices so as to be antisymmetric to exchange of any pair of electrons. We rewrite (1.2) as

$$\Psi_{k_1, k_2 \dots k_N}(x_1, x_2, \dots x_N) = \psi_{k_1}(x_1) \psi_{k_2}(x_2) \dots \psi_{k_N}(x_N) \quad , \quad (2.1)$$

where the k's are indices contained in the set $\{1, 2, \dots N\}$. We assume, for convenience, that our orbitals form an orthonormal set; the Exclusion Principle demands they be linearly independent. We may express our (normalized) N-electron wave function symbolically as

$$D_K(x_1, x_2, \dots x_N) = A \Psi_{k_1, k_2, \dots k_N}(x_1, x_2, \dots x_N) \quad , \quad (2.2)$$

where the operator A , termed the antisymmetrizing operator, is defined as

$$A \equiv \frac{1}{\sqrt{N!}} \sum_P (-1)^P P \quad . \quad (2.3)$$

The operator P permutes the indices of the set $\{k_1, k_2, \dots k_N\}$, the summation is over all $N!$ permutations of the set, and the subscript K is an abbreviation for the collection of integers $(k_1, k_2, \dots k_N)$. Equation (2.2) is a statement that $D_K(x_1, x_2, \dots x_N)$ is a determinant of the form

*For an atomic system a configuration is a listing of the $n\ell$ values of the orbitals which the electrons occupy.

**A closed shell is a set of $2(2\ell+1)$ spin-orbitals having the same $n\ell$ values.

†An open shell is a set of occupied spin-orbitals of the same $n\ell$ value which has less than the $2(2\ell+1)$ allowable numbers.

$$D_K(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(x_1) & \psi_2(x_1) & \dots & \psi_N(x_1) \\ \psi_1(x_2) & \psi_2(x_2) & \dots & \psi_N(x_2) \\ \dots & \dots & \dots & \dots \\ \psi_1(x_N) & \psi_2(x_N) & \dots & \psi_N(x_N) \end{vmatrix} \quad (2.4)$$

When (2.4) is applied to atomic systems, it has been customary to place a restriction on the orbitals of a closed shell and require them to be equal in pairs or mutually orthogonal. Each orbital of a closed shell will appear twice, once with either spin.

The matrix elements of the one- and two-electron operators of (1.1) with respect to wave functions of the type (2.4) were first given by Slater in his key paper on complex spectra.⁽⁸⁾ He showed that these elements reduce to simple sums over linear and bilinear functionals in the ϕ 's. These functionals are

$$I_i = \int \bar{\phi}_i \left(-\frac{1}{2} \Delta_i - \frac{Z}{r_i} \right) \phi_i dV \quad , \quad (2.5)$$

$$J_{ij} = \int \frac{|\phi_i(1)|^2 |\phi_j(2)|^2}{r_{12}} dV_1 dV_2 \quad , \quad (2.6)$$

$$K_{ij} = \int \frac{\bar{\phi}_i(1) \phi_i(2) \phi_j(1) \bar{\phi}_j(2)}{r_{12}} dV_1 dV_2 \quad . \quad (2.7)$$

If we make the approximation that the electrostatic field is spherically symmetric, then the orbitals may be written as the product of a radial factor and a (complex) spherical harmonic:

$$\phi_{nlm}(r, \theta, \varphi) = R_{nl}(r) Y_{lm}(\theta, \varphi) = R_{nl}(r) \Theta_{\ell|m|}(\theta) \hat{c}_m(\varphi) \quad . \quad (2.8)$$

In this case the two-electron integrals (2.6) and (2.7) become

$$J_{ij} = \sum_{k=0}^{\infty} a^{k(\ell_i m_i, \ell_j m_j)} F^k(n_i \ell_i, n_j \ell_j) \quad (2.9)$$

and

$$K_{ij} = \delta_{s_i, s_j} \sum_{k=0}^{\infty} b^{k(\ell_i m_i, \ell_j m_j)} G^k(n_i \ell_i, n_j \ell_j) \quad , \quad (2.10)$$

where

$$\begin{aligned} a^k(\ell_i m_i, \ell_j m_j) &= C^k(\ell_i m_i, \ell_i m_i) C^k(\ell_j m_j, \ell_j m_j) \quad , \\ b^k(\ell_i m_i, \ell_j m_j) &= [C^k(\ell_i m_i, \ell_j m_j)]^2 \quad , \end{aligned} \quad (2.11)$$

$$C^k(\ell m, \ell' m') = \sqrt{\frac{2}{2k+1}} \int_0^\pi \Theta_{k m - m'} \Theta_{\ell m} \Theta_{\ell' m'} \sin \theta d\theta \quad ,$$

$$F^k(n_i \ell_i, n_j \ell_j) = \int_0^\infty \int_0^\infty \frac{r_{<}^k}{r_{>}^{k+1}} R_{n_i \ell_i}^2(r_1) R_{n_j \ell_j}^2(r_2) \times r_1^2 r_2^2 dr_1 dr_2 \quad , \quad (2.12)$$

$$\begin{aligned} G^k(n_i \ell_i, n_j \ell_j) &= \int_0^\infty \int_0^\infty \frac{r_{<}^k}{r_{>}^{k+1}} R_{n_i \ell_i}(r_1) R_{n_j \ell_j}(r_1) \\ &\quad \times R_{n_i \ell_i}(r_2) R_{n_j \ell_j}(r_2) r_1^2 r_2^2 dr_1 dr_2 \quad , \end{aligned} \quad (2.13)$$

and δ_{s_i, s_j} is the Kronecker delta for the spins s_i and s_j .

For the case of an electron interacting with a complete shell, we get the simple relations⁽⁹⁾

$$\sum_j J_{ij} = 2(2\ell_j + 1) F^0(n_i \ell_i, n_j \ell_j) \quad (2.14)$$

$$\sum_j K_{ij} = 2(2\ell_j + 1) \frac{1}{2} \sum_{k=0}^\infty C_{\ell_i \ell_j k} G^k(n_i \ell_i, n_j \ell_j) \quad , \quad (2.15)$$

where i is the index on the spin-orbital describing the electron and the summation is over the spin-orbitals of the shell. The C 's are given by

$$C_{uvw} = \int_0^\pi P_u(\cos \theta) P_v(\cos \theta) P_w(\cos \theta) \sin \theta d\theta \quad . \quad (2.16)$$

If we have two complete shells interacting with each other, then the contribution of the two-electron terms is

$$2(2\ell+1)(2\ell'+1) [2F^0(n\ell, n'\ell') - \frac{1}{2} \sum_k C_{\ell\ell'k} G^k(n\ell, n'\ell')] \quad . \quad (2.17)$$

Slater⁽⁸⁾ gave the energy expression for the terms* of a number of complex** configurations as a sum of the I, F, and G integrals. This work was subsequently extended by Racah utilizing group theory.⁽¹¹⁾ Shortley, employing the Slater integrals, later modified Fock's procedure by assuming that a given wave function may be represented by a linear combination of determinants formed from the allowable orbitals of a configuration, or

$$\Psi = \sum_K^N a_K D_K \quad , \quad (2.18)$$

where the D_K form a set of orthonormal determinantal wave functions. If (2.18) is substituted into the Schrödinger equation

$$\mathcal{H}\Psi = E\Psi \quad ,$$

we obtain

$$\sum_K^N a_K (\mathcal{H} D_K - E D_K) = 0 \quad . \quad (2.19)$$

We multiply (2.19) in turn by each $D_K^\dagger$ and integrate, and obtain the system of N equations

$$\sum_K a_K (H_{K'K} - E l_{K'K}) = 0 \quad , \quad (2.20)$$

where $H_{K'K} = (D_{K'} | \mathcal{H} | D_K)$ and l is the unit matrix. The condition that (2.20) be solvable for the a_K yields a secular equation for the energy:

$$\det(H - El) = 0 \quad . \quad (2.21)$$

*A set of $(2S+1)(2L+1)$ states belonging to a definite configuration and to definite L and S is called a term.

**A complex configuration is one which yields more than one term.

The eigenvalues of (2.21) yield the expressions for the energies of the terms corresponding to the given configuration. Each energy expression contains averaged coefficients for the F and G integrals involving the open-shell orbitals. A tabulation of these coefficients for a number of important cases has been given by Hartree, Hartree, and Swirles.^(12,13) The Shortley procedure yields exactly the same energy expressions given by Slater.

The Hartree-Fock Approximation for Open-shell Systems

Roothaan⁽⁷⁾ has adopted the Shortley idea, but utilized a notation which is particularly adapted to the matrix SCF process. We shall derive the HF equations as given by him; however, we obtain them in a slightly different manner. We assume our wave function is given by (2.18) and that the secular equation has been solved for the energy of a particular term corresponding to the configuration. The wave function describing such a term is, in general, a linear combination of determinantal wave functions. The energy expression as written by Roothaan is

$$\begin{aligned}
 E &= (\Psi | \mathcal{H} | \Psi) \\
 &= 2 \sum_k H_k + \sum_{k,\ell} (2J_{k\ell} - K_{k\ell}) \\
 &\quad + f \left[2 \sum_m H_m + f \sum_{m,n} (2aJ_{mn} - bK_{mn}) + 2 \sum_{k,m} (2J_{km} - K_{km}) \right] ,
 \end{aligned} \tag{2.22}$$

where we have adopted the notation

- k, ℓ indices for closed-shell orbitals only,
- m, n indices for open-shell orbitals only, and
- i, j indices for closed and open-shell orbitals.

The energy elements $H_i \equiv I_i$ of (2.5) and the two-electron elements may be written

$$J_{ij} = (\phi_i | J_j | \phi_i) = (\phi_j | J_i | \phi_j)$$

and

$$K_{ij} = (\phi_i | K_j | \phi_i) = (\phi_j | K_i | \phi_j) , \tag{2.23}$$

where

$$J_1(r_1)\phi(r_1) = \int |\phi_1(r_2)|^2 r_{12}^{-1} dV_2 \phi(r_1)$$

and

$$K_1(r_1)\phi(r_1) = \int \bar{\phi}_1(r_2)\phi(r_2) r_{12}^{-1} dV_2 \phi_1(r_1) \quad (2.24)$$

The summations of (2.20) are over the orbitals. The constant f is the fractional occupancy of the open shell(s), and the constants f^2a and f^2b are averaged coefficients for the Slater F and G integrals.

The connection between the energy expression (2.22) and those given by Slater may best be seen by evaluating the open-shell summation, the only one which contains parameters. We have the identity

$$\begin{aligned} \sum_{m,n} (2aJ_{mn} - bK_{mn}) &= f^2(2\ell+1)(2\ell'+1) \left[2aF^0(n\ell, n'\ell') \right. \\ &\quad \left. - \frac{b}{2} \sum_k C_{\ell\ell'k} G^k(n\ell, n'\ell') \right] \end{aligned} \quad (2.25)$$

The relation (2.22) is valid if, and only if, (2.25) may be equated to the open-shell energy elements as derived by the Slater or Shortley method, and the equality may be solved for the constants a and b . The validity does not hold in general, but is true in a number of important atomic and molecular configurations (7). The atomic configurations ns and np^q ($q = 1, 5$) do satisfy (2.22) for all term values. In Appendix A we work out a and b for the particular cases studied in this thesis.

To obtain the HF equations we apply the Variational Principle.

$$\delta E = \delta(\Psi | \mathcal{H} | \Psi) = 0 \quad (2.26)$$

Since we wish to apply constraints to our functions ϕ_1 , we utilize the method of Lagrangian undetermined multipliers. We require that our orbitals form an orthonormal set.

$$(\phi_k | \phi_\ell) = (\phi_\ell | \phi_k) = \delta_{k\ell}$$

$$(\phi_k | \phi_m) = (\phi_m | \phi_k) = 0$$

$$(\phi_m | \phi_n) = (\phi_n | \phi_m) = \delta_{mn} \quad (2.27)$$

To meet this requirement we form the auxiliary function

$$E' = E - 2 \sum_{i,j} \lambda_{ij}(\phi_j | \phi_i) \quad ,$$

where $2\lambda_{ij}$ is the Lagrangian multiplier to be associated with the i^{th} constraint. We now take the variation of E' :

$$\begin{aligned} \delta E' = & 2 \sum_k (\delta \phi_k | H | \phi_k) + 2 \sum_{k,\ell} (\delta \phi_k | 2J_\ell - K_\ell | \phi_k) \\ & + f \left[2 \sum_m (\delta \phi_m | H | \phi_m) + 2f \sum_{m,n} (\delta \phi_m | 2aJ_n - bK_n | \phi_m) \right. \\ & \left. + 2 \sum_{k,m} (\delta \phi_k | 2J_m - K_m | \phi_k) + \sum_{k,m} (\delta \phi_m | 2J_k - K_k | \phi_m) \right] \\ & - 2 \sum_{k,\ell} \lambda_{\ell k} (\delta \phi_k | \phi_\ell) - 2 \sum_{k,m} \lambda_{mk} (\delta \phi_k | \phi_m) \\ & - 2 \sum_{k,m} \lambda_{km} (\delta \phi_m | \phi_k) - 2 \sum_{m,n} \lambda_{nm} (\delta \phi_m | \phi_n) \\ & + 2 \sum_k (\phi_k | H | \delta \phi_k) + 2 \sum_{k,\ell} (\phi_k | 2J_\ell - K_\ell | \delta \phi_k) \\ & + f \left[2 \sum_m (\phi_m | H | \delta \phi_m) + 2f \sum_{m,n} (\phi_m | 2aJ_n - bK_n | \delta \phi_m) \right. \\ & \left. + 2 \sum_{k,m} (\phi_k | 2J_m - K_m | \delta \phi_k) + \sum_{k,m} (\phi_m | 2J_k - K_k | \delta \phi_m) \right] \\ & - 2 \sum_{k,\ell} \lambda_{\ell k} (\phi_k | \delta \phi_\ell) - 2 \sum_{k,m} \lambda_{mk} (\phi_k | \delta \phi_m) \\ & - 2 \sum_{k,m} \lambda_{km} (\phi_m | \delta \phi_k) - 2 \sum_{m,n} \lambda_{nm} (\phi_m | \delta \phi_n) = 0 \quad . \end{aligned} \tag{2.28}$$

The variations of the functions ϕ and $\bar{\phi}$ in the above equation are arbitrary, so that necessary conditions for the validity of the equation are

$$\left[H + \sum_{\ell} (2J_{\ell} - K_{\ell}) + f \sum_{\mathbf{m}} (2J_{\mathbf{m}} - K_{\mathbf{m}}) \right] \phi_{\mathbf{k}} = \sum_{\mathbf{k}} \lambda_{\ell \mathbf{k}} \phi_{\ell} + \sum_{\mathbf{m}} \lambda_{\mathbf{m} \mathbf{k}} \phi_{\mathbf{m}} \quad (2.29)$$

$$\left[H + \sum_{\mathbf{k}} (2J_{\mathbf{k}} - K_{\mathbf{k}}) + f \sum_{\mathbf{m}} (2J_{\mathbf{m}} - K_{\mathbf{m}}) \right] \bar{\phi}_{\mathbf{k}} = \sum_{\ell} \lambda_{\mathbf{k} \ell} \bar{\phi}_{\ell} + \sum_{\mathbf{m}} \lambda_{\mathbf{k} \mathbf{m}} \bar{\phi}_{\mathbf{m}} \quad (2.30)$$

$$f \left[H + \sum_{\mathbf{k}} (2J_{\mathbf{k}} - K_{\mathbf{k}}) + f \sum_{\mathbf{n}} (2aJ_{\mathbf{n}} - bK_{\mathbf{n}}) \right] \phi_{\mathbf{m}} = \sum_{\mathbf{k}} \lambda_{\mathbf{k} \mathbf{m}} \phi_{\mathbf{k}} + \sum_{\mathbf{n}} \lambda_{\mathbf{n} \mathbf{m}} \phi_{\mathbf{n}} \quad (2.31)$$

$$f \left[H + \sum_{\mathbf{k}} (2J_{\mathbf{k}} - K_{\mathbf{k}}) + f \sum_{\mathbf{n}} (2aJ_{\mathbf{n}} - bK_{\mathbf{n}}) \right] \bar{\phi}_{\mathbf{m}} = \sum_{\mathbf{k}} \lambda_{\mathbf{m} \mathbf{k}} \bar{\phi}_{\mathbf{k}} + \sum_{\mathbf{n}} \lambda_{\mathbf{m} \mathbf{n}} \bar{\phi}_{\mathbf{n}} \quad . \quad (2.32)$$

If we take the Hermitian conjugate of (2.30) and (2.32) and compare them with (2.29) and (2.31), we see that

$$\sum_{\ell} (\lambda_{\ell \mathbf{k}} - \bar{\lambda}_{\mathbf{k} \ell}) \phi_{\ell} + \sum_{\mathbf{m}} (\lambda_{\mathbf{m} \mathbf{k}} - \bar{\lambda}_{\mathbf{k} \mathbf{m}}) \phi_{\mathbf{m}} = 0$$

and

$$\sum_{\mathbf{k}} (\lambda_{\mathbf{k} \mathbf{m}} - \bar{\lambda}_{\mathbf{m} \mathbf{k}}) \phi_{\mathbf{k}} + \sum_{\mathbf{n}} (\lambda_{\mathbf{n} \mathbf{m}} - \bar{\lambda}_{\mathbf{m} \mathbf{n}}) \phi_{\mathbf{n}} = 0 \quad .$$

The ϕ_i are linearly independent, so we have immediately the relation

$$\lambda_{ij} = \bar{\lambda}_{ji} \quad .$$

If we now define

$$\sum_{\mathbf{k}} J_{\mathbf{k}} = J_C ; \quad \sum_{\mathbf{k}} K_{\mathbf{k}} = K_C$$

$$f \sum_{\mathbf{m}} J_{\mathbf{m}} = J_0 ; \quad f \sum_{\mathbf{m}} K_{\mathbf{m}} = K_0 \quad , \quad (2.34)$$

equations (2.29) and (2.30) take the form

$$[H + 2J_C - K_C + 2J_0 - K_0] \phi_{\mathbf{k}} = \sum_{\mathbf{i}} \lambda_{\mathbf{i} \mathbf{k}} \phi_{\mathbf{i}} \quad (2.35)$$

$$f[H + 2J_C - K_C + 2aJ_0 - bK_0] \phi_n = \sum_i \lambda_{im} \phi_i \quad . \quad (2.36)$$

For convenience, we shall introduce the following abbreviations:

$$F' = H + 2J_C - K_C + 2J_0 - K_0 = H + 2J_T - K_T$$

$$G = 2(a-1)J_0 - (b-1)K_0 \quad ,$$

which allows us to rewrite (2.35) and (2.36) as

$$F' \phi_k = \sum_i \lambda_{ik} \phi_i \quad (2.37)$$

$$[F' + G] \phi_m = \sum_i \frac{\lambda_{im}}{f} \phi_i \quad . \quad (2.38)$$

Equations (2.37) and (2.38) are the same as the HF equations given by Shortley, although the notation is considerably different. These equations (the Shortley form) have been solved by numerical integration for a number of atomic configurations.^(6,12) However, in order to exact the maximum benefit from the matrix SCF scheme, it would be wise to bring these equations into reducible form so that the operators for the closed and open manifolds may be separately diagonalized. This may be accomplished by absorbing into the left sides of (2.37) and (2.38) the terms which couple these manifolds.

We first note that, by (2.33) and (2.37),

$$\bar{\lambda}_{km} = \lambda_{mk} = (\phi_m | F' | \phi_k) = (\phi_k | F' | \phi_m) \quad . \quad (2.39)$$

Equations (2.38) and (2.39) yield the relation

$$P_C G \phi_m = \frac{1-f}{f} \sum_k \lambda_{km} \phi_k \quad , \quad (2.40)$$

where P_C is the projection operator for the closed-shell manifold.* If we next form the inner product of (2.40) with ϕ_k , take complex conjugates, and

*The projection operators P_C and P_0 are defined by

$$P_C \phi = \sum_k (\phi_k | \phi) \phi_k ; \quad P_0 \phi = \sum_m (\phi_m | \phi) \phi_m$$

make use of (2.33), we obtain the relation

$$\frac{f}{1-f} P_0 G \phi_k = \sum_m \lambda_{mk} \phi_m \quad , \quad (2.41)$$

where P_0 is the projection operator for the open-shell manifold.* When (2.40) and (2.41) are substituted into (2.37) and (2.38), we obtain the reducible equations

$$(F' + \frac{f}{f-1} P_0 G) \phi_k = \sum_{\ell} \lambda_{\ell k} \phi_{\ell} \quad (2.42)$$

$$(F' + G + \frac{1}{f-1} P_C G) \phi_m = \sum_n \frac{\lambda_{nm}}{f} \phi_n \quad . \quad (2.43)$$

Now that the HF equations are in reducible form, it would be convenient to have both the closed-shell and open-shell orbitals satisfy the same operator equation. This may be achieved by the addition of

$$\frac{1}{f-1} [fGP_0 + P_C G + GPC - G] \phi_k$$

to both sides of (2.42) and of

$$\frac{1}{f-1} [-fG + fP_0 G + fGP_0 + GPC] \phi_m$$

to both sides of (2.43). Both sets of orbitals now satisfy the equation

$$\left[F' + \frac{1}{f-1} \left\{ f(P_0 G + GP_0) + (P_C G + GPC) - G \right\} \right] \phi_j = \sum_i \epsilon_{ij} \phi_i \quad , \quad (2.44)$$

where

$$\epsilon_{k\ell} = \lambda_{k\ell} + \frac{1}{f-1} (\phi_k | fGP_0 + P_C G + GPC - G | \phi_{\ell}) \quad ,$$

$$\epsilon_{nm} = \frac{\lambda_{nm}}{f} + \frac{1}{f-1} (\phi_n | -fG + fP_0 G + fGP_0 + GPC | \phi_m) \quad ,$$

and

$$\epsilon_{km} = \epsilon_{mk} = 0 \quad . \quad (2.45)$$

Equation (2.44) is the same as equation (36) of Roothaan.(7)

*See footnote on previous page.

It should be noted that equations (2.36), (2.37), and (2.44) are not in a unique form. It is possible to obtain other forms for these equations through use of the projection operators P_C and P_0 . The present form of (2.44) is Hermitian and is therefore easily treated by matrix methods.

The Unrestricted Hartree-Fock Method for Open-shell Systems

In the HF method we restricted the orbitals of a closed shell so that they were equal in pairs or mutually orthogonal. As a consequence, we needed to solve the one-electron equations only for the set of spin-orbitals of one spin type. It has been realized for some time that for systems with incomplete shells, the effective fields which act on the electrons are spin dependent.⁽⁶⁾ Since an electron undergoes an "exchange" interaction only with electrons of like spin, the one-electron Hamiltonians for alpha and beta spin-orbitals should be different. Because of the difficulty of handling such a computation, no attempt was made to eliminate this restriction in earlier calculations.

Recently, this aspect has been re-examined and discussed in the literature.^(14,15,16) The basic change introduced into the Hartree-Fock framework is the relaxation of the double-occupancy requirement and a reliance on the spin dependence of the spin-orbitals to provide the necessary orthogonality between the members of the α set and of the β set. Spin-orbitals of opposite spin are no longer constrained to be equal or orthogonal in their space dependence. Where this procedure may be meaningfully applied, one is no longer able to express any multiplet as a single D_K , but must use a linear combination of those possible from the configuration. This introduced considerable complexity into any computational work, particularly for large systems. If we arbitrarily restrict ourselves to only one D_K , we may expect to obtain a wave function of lower energy than that obtained by the HF approximation, with little more computational difficulty. This is a result of allowing more freedom to our orbitals when applying the Variational Principle. This procedure is termed the "Unrestricted Hartree-Fock" (UHF) approximation.

The objections to the use of the UHF approximation center on the fact that through the use of only one D_K our symmetry has been lost. The wave function is no longer an eigenfunction of S^2 but is a mixture of spin states. If the mixture of spin states contains a large contribution due to the excited states, then the single-determinant wave function will not be meaningful, but if the wave function is nearly a pure spin eigenstate, then we should expect the orbitals to be very nearly the same as in the HF method. Though the UHF orbitals will be almost the same as the HF orbitals for a given configuration, the slight difference between the orbitals of the α set and the orbitals of the β set will give rise to a slight spin polarization of the core due to the difference of charge densities. This core polarization may be important in obtaining better agreement with

experimental data. Pratt⁽¹⁶⁾ has shown that this core polarization is not due to choosing just a single determinant as a wave function, but will also be present if the neglected determinantal wave functions are included in the problem. The lack of symmetry may not be a serious handicap if the UHF wave function is almost a spin eigenstate.

The energy expression, as before, is expressible as a sum of linear and bilinear functionals over the one-electron spaces. We then have

$$\begin{aligned}
 E &= \sum_i H_i + \frac{1}{2} \sum_{a,a'} (J_{aa'} - K_{aa'}) + \sum_{a,b} J_{ab} + \frac{1}{2} \sum_{b,b'} (J_{bb'} - K_{bb'}) \\
 &= \sum_{a,a',b} (\phi_a | H + \frac{1}{2} J_{a'} + \frac{1}{2} J_b - \frac{1}{2} K_{a'} | \phi_a) \\
 &\quad + \sum_{b,b',a} (\phi_a | H + \frac{1}{2} J_a + \frac{1}{2} J_{a'} - \frac{1}{2} K_{b'} | \phi_b) \quad , \quad (2.46)
 \end{aligned}$$

where the subscripts denote the following:

- a, a' , alpha spin-orbitals,
- b, b' , beta spin-orbitals, and
- i , both sets.

We shall apply the Variational Principle subject to the constraints

$$(\phi_a | \phi_{a'}) = \delta_{aa'} \quad \text{and}$$

$$(\phi_b | \phi_{b'}) = \delta_{bb'} \quad .$$

Our auxiliary expression to be varied is then

$$E' = E - \sum_{a,a'} \lambda_{a'a} (\phi_a | \phi_{a'}) - \sum_{b,b'} \lambda_{b'b} (\phi_b | \phi_{b'}) \quad .$$

We thus obtain the expression

$$\begin{aligned}
\delta E' = & \sum_{a,a',b} (\delta \phi_a | H + \frac{1}{2} J_{a'} + \frac{1}{2} J_b - \frac{1}{2} K_{a'} | \phi_a) \\
& + \sum_{b,b',a} (\delta \phi_b | H + \frac{1}{2} J_a + \frac{1}{2} J_{b'} - \frac{1}{2} K_{b'} | \phi_b) \\
& + \sum_{a,b} (\delta \phi_b | \frac{1}{2} J_a | \phi_b) + \sum_{b,a} (\delta \phi_a | \frac{1}{2} J_b | \phi_a) \\
& + \frac{1}{2} \sum_{a,a'} (\delta \phi_a | J_{a'} - K_{a'} | \phi_a) + \frac{1}{2} \sum_{b,b'} (\delta \phi_b | J_{b'} - K_{b'} | \phi_b) \\
& - \sum_{a,a'} \lambda_{a'a} (\delta \phi_a | \phi_{a'}) - \sum_{b,b'} \lambda_{b'b} (\delta \phi_b | \phi_{b'}) \\
& + \sum_{a,a'b} (\phi_a | H + \frac{1}{2} J_{a'} + \frac{1}{2} J_b - \frac{1}{2} K_{a'} | \delta \phi_a) \\
& + \sum_{b,b'a} (\phi_b | H + \frac{1}{2} J_a + \frac{1}{2} J_{b'} - \frac{1}{2} K_{b'} | \delta \phi_b) \\
& + \sum_{a,b} (\phi_b | \frac{1}{2} J_a | \delta \phi_b) + \sum_{b,a} (\phi_a | \frac{1}{2} J_b | \delta \phi_a) \\
& + \frac{1}{2} \sum_{a,a'} (\phi_a | J_{a'} - K_{a'} | \delta \phi_a) + \frac{1}{2} \sum_{b,b'} (\phi_b | J_{b'} - K_{b'} | \delta \phi_b) \\
& - \sum_{a,a'} \lambda_{a'a} (\phi_a | \delta \phi_{a'}) - \sum_{b,b'} \lambda_{b'b} (\phi_b | \delta \phi_{b'}) = 0 \quad .
\end{aligned}$$

Since our variations are arbitrary, this provides the necessary conditions that

$$(H + J_\alpha + J_\beta - K_\alpha) \phi_a = \sum_{a'} \lambda_{a'a} \phi_{a'} \quad (2.47)$$

$$(H + J_\alpha + J_\beta - K_\beta) \phi_b = \sum_b \lambda_{b'b} \phi_{b'} \quad , \quad (2.48)$$

where

$$\begin{aligned} J_\alpha &= \sum_a J_a & K_\alpha &= \sum_a K_a \\ J_\beta &= \sum_b J_b & K_\beta &= \sum_b K_b \end{aligned} .$$

The operators of equations (2.47) and (2.48) are Hermitian, so that it is possible to find a basis for which the λ matrices are diagonal. The λ_i 's are then the one-electron energies of the orbitals.

The Projected UHF Method for Open-shell Systems

As we noted previously, the prime detractor of the UHF method is that the wave function is no longer an eigenfunction of the operator S^2 , but is a mixture of spin eigenfunctions. This was the resultant of using a single D_K instead of the linear combination necessary to produce a spin eigenstate. We can restore the overall symmetry of the wave function by projecting out the desired eigenstate component from the UHF wave function. This procedure is termed the "Projected UHF" approximation.

It is well-known⁽¹⁷⁾ that a self-adjoint operator A may be written in its spectral form as

$$A = \sum_k \alpha_k P_k ,$$

where α_k and P_k are the eigenvalue and projection operator for the k^{th} subspace. The operator P_k is given by

$$P_k(A) = \prod_{j \neq k} \frac{A - \alpha_j}{\alpha_k - \alpha_j} . \quad (2.49)$$

We may therefore project out the desired spin-eigenstate component from the UHF function by the use of equation (2.49):

$$\begin{aligned} \Psi_{\text{PUHF}} &= P_k(S^2) \Psi_{\text{UHF}} \\ &= \prod_{j \neq k} \frac{S^2 - s_j(s_j+1)}{s_k(s_k+1) - s_j(s_j+1)} \Psi_{\text{UHF}} . \end{aligned} \quad (2.50)$$

The projected UHF function should yield a lower energy value than the UHF function, as the excited states are no longer present.

The Generalized UHF Approximation for Open-shell Systems

We have seen that the essence of the UHF method is the relaxation of the restriction which demands that closed-shell orbitals be equal in pairs or mutually orthogonal. This allows the radial functions of the alpha and beta spin-orbital sets to be different. One may now take a further step and allow the spin function of the spin-orbital to be space dependent. Each orbital is then expressible as

$$\psi_i(\mathbf{x}) = \phi_{i1}(\mathbf{r})\alpha + \phi_{i2}(\mathbf{r})\beta \quad , \quad (2.51)$$

where

$$\phi_{i1}^2(\mathbf{r}) + \phi_{i2}^2(\mathbf{r}) = 1 \quad .$$

The wave function is then given as

$$\Psi_{\text{GUHF}} = \mathcal{A}\{\psi_1(\mathbf{x}_1), \psi_2(\mathbf{x}_2), \dots, \psi_N(\mathbf{x}_N)\} \quad , \quad (2.52)$$

where the $\psi_i(\mathbf{x}_i)$ are of the form (2.51). The average energy $\langle \mathcal{H} \rangle$ is given by

$$E = \sum_i H_i + \frac{1}{2} \sum_{i,j} (J_{ij} - K_{ij}) \quad , \quad (2.53)$$

where the summation is over the spin-orbitals $\{\psi_i\}$. We apply the Variational Principle subject to the constraint

$$(\psi_i | \psi_j) = \delta_{ij} \quad .$$

The auxiliary expression to be varied is

$$E' = E - \sum_{i,j} \lambda_{ji} (\psi_i | \psi_j) \quad . \quad (2.54)$$

The variation of (2.54) yields the necessary condition that

$$\left[H + \sum_j (J_j - K_j) \right] \psi_i = \sum_j \lambda_{ji} \psi_j \quad ,$$

which by a suitable unitary transformation may be written in the form

$$\left[H + \sum_j (J_j - K_j) \right] \psi_i = \epsilon_i \psi_i \quad . \quad (2.55)$$

The set of equations, (2.55), is termed the Generalized Unrestricted Hartree-Fock (GUHF) equations. We shall not report on any investigations of the GUHF approximation in this study.

CHAPTER III METHOD OF COMPUTATION

Exact solution of the HF integro-differential equation is not possible; hence only approximate solutions may be obtained. There are two basically different methods which may be employed in obtaining approximate solutions: one may either obtain a numerical solution, i.e., tables of $\phi(r)$ for each orbital, or one may expand each orbital in terms of a set of analytic functions. The chief advantage of having the orbitals in analytic form lies in the ease with which they may be utilized in further applications.

Hartree utilized numerical integration from the outset of his SCF calculations and continued along this line throughout his work. Many specialized numerical techniques for obtaining HF-SCF solutions have been developed by Hartree and others.⁽¹³⁾ Slater⁽¹⁸⁾ first suggested that the numerical functions may be fitted by analytic functions, and Löwdin and Appel⁽¹⁹⁾ have recently shown how this may be done by a process of successive approximations. The numerical solutions of the HF equation can therefore be transformed to a convenient analytic form.

Any analytic procedure utilized to obtain approximate solutions of the HF equations makes use of the fact that the orbitals may be expanded in terms of a complete set of functions. Since it is impractical to utilize a complete set, the central idea is to find a finite basis of a given size which will reproduce the orbitals as faithfully as possible.

There are two schemes presently being utilized to obtain direct analytic solutions. One method is due to McWeeny and is an iterative one involving the first-order density matrix. The other, due to Roothaan,⁽⁷⁾ is an iterative method employing direct diagonalization of the matrix representation of the HF operator. As we chose this latter method to obtain our solutions, we shall elaborate in the next section in some detail regarding the process. We outline McWeeny's technique briefly in the following paragraph.

In the density matrix formulation of the HF approximation for closed shells, one may set down the energy expression as

$$E = \langle \mathcal{H} \rangle = \text{Tr}(\mathcal{H}_1 \rho_1) + \frac{1}{2} \text{Tr}[\rho_1(1) \rho_1(2) (1 - P_{12}) \mathcal{H}_{12}] \quad , \quad (3.1)$$

where $\mathcal{H}_1$ and $\mathcal{H}_{12}$ are one-particle and two-particle operators, Tr is the trace operation, ρ_1 is the first-order density matrix, and P_{12} is the permutation operator which permutes the indices of electrons one and two. McWeeny assumes a finite matrix representation of (3.1) of the form

$$E = 2 \text{Tr}(hR) + \text{Tr}(gR) \quad , \quad (3.2)$$

where h is the matrix representation of $\mathcal{H}_1$, $2R$ is the matrix representation of ρ_1 , and

$$g_{ij} = \sum_{kl} [(1-P_{12})\mathcal{H}_{12}]_{ij,kl} R_{kl} \quad .$$

In this finite-dimensional representation R is given the form

$$R = T \cdot T^+ \quad ,$$

where T is the matrix of coefficients of the basis set. An orthonormality constraint is imposed in the form $T^+T = 1$. If the basis set is nonorthogonal, T may always be decomposed, and one may orthonormalize by the Schmidt process. An initial estimate is made for T , and by a steepest descent process of iteration on R the energy is minimized. Since the HF process minimizes the energy for a given basis set, the final T matrix yields the coefficients of the analytic expansion. McWeeny has given several versions of his iteration process, and further details may be found in his papers.^(20,21)

The Roothaan SCF Procedure

The procedure for obtaining SCF solutions to the HF equations by matrix techniques was first given by Roothaan.⁽⁷⁾ We consider the occupied orbitals which form a finite subspace of an infinite-dimensional space. Were we able to pick a basis for this subspace, we should be able to obtain the orbitals exactly. Since we cannot do so, we select an arbitrary finite subspace by choosing a set of linearly independent functions to form a basis. The aim is to obtain that finite-dimensional subspace along which the projections of the occupied orbitals are as near as possible to the actual functions.

We choose a finite set of linearly independent functions $\{\chi_p\}$, not necessarily orthogonal, and expand our orbitals in terms of them^{(22),*} as follows:

*The criterion for linear independence of the set is not the strict mathematical one, as the accuracy of the calculation limits the criterion. We require only that for the condition

$$\left| \sum_p a_p \chi_p \right| \leq \delta \quad ,$$

the a_p all be zero to the same order of magnitude as δ . The constant δ measures the accuracy limit of the computation.

$$\phi_i = \sum_p C_{i;p} \chi_p \quad . \quad (3.3)$$

With respect to this finite basis our operators have the matrix representation

$$F_{pq} = (\chi_p | F | \chi_q) \quad . \quad (3.4)$$

Thus, if we consider our general operator eigenvalue equation,

$$F\phi_i = \epsilon_i \phi_i \quad , \quad (3.5)$$

and substitute from (3.3), there results

$$\sum_q F_{c_{i;q}} \chi_q = \epsilon_i \sum_q c_{i;q} \chi_q \quad . \quad (3.6)$$

We next take the inner product with χ_p and obtain

$$\sum_q F_{pq} c_{i;q} = \epsilon_i \sum_q S_{pq} c_{i;q}$$

or

$$[F]c_i = \epsilon_i [S]c_i \quad , \quad (3.7)$$

where $S_{pq} = (\chi_p | \chi_q)$ is the overlap matrix of the basis set.

The operator F which enters into the eigenvalue equation (3.5) is a function of its eigenfunctions $\{\phi_i\}$. To handle this situation, we employ a self-consistent field (SCF) type of solution. An initial estimate is made of the orbitals, that is, the coefficients $c_{i;q}$ are estimated. The operator F is calculated from this initial set, $\{\phi_i\}_1$, and (3.7) is solved to yield a new set $\{\phi_i\}_2$. The set $\{\phi_i\}_2$ is then used to obtain a new value for the operator F , and the process repeats once more. This process of iteration is continued until two successive sets, $\{\phi_i\}_n$ and $\{\phi_i\}_{n+1}$, differ by only a prescribed amount.

Implementation of the Roothaan Procedure

To actually carry out an SCF calculation by the Roothaan procedure, one must evaluate the matrix elements of the HF operator. We rewrite (2.44) in a manner more suitable for computation, assuming it is in diagonal form, as follows:

$$\left\{ H + 2J_T - K_T + f(P_0Q + QP_0) + (P_CQ + QP_C) - Q \right\} \phi_i = \epsilon_i \phi_i \quad , \quad (3.8)$$

where

$$Q = 2\alpha J_0 - \beta K_0 \quad ; \quad \alpha = \frac{1-a}{1-f} \quad ; \quad \beta = \frac{1-b}{1-f} \quad . \quad (3.9)$$

If we take the matrix representation of (3.8) with respect to a basis set $\{\chi_p\}$, we obtain the matrix equation

$$[H + P + R - Q] \vec{c}_i = \epsilon_i [S] \vec{c}_i \quad , \quad (3.10)$$

where we have adopted the notation

$$\begin{aligned} S_{pq} &= (\chi_p | \chi_q) \quad , \\ H_{pq} &= T_{pq} - ZU_{pq} = (\chi_p | -\frac{1}{2}\Delta | \chi_q) - Z(\chi_p | r^{-1} | \chi_q) \quad , \\ P_{pq} &= (\chi_p | 2J_T - K_T | \chi_q) \quad , \\ R_{pq} &= (\chi_p | f(P_0Q + QP_0) + (P_CQ - QP_C) | \chi_q) \quad , \quad \text{and} \\ Q_{pq} &= (\chi_p | Q | \chi_q) \quad . \end{aligned} \quad (3.11)$$

Nesbet⁽²³⁾ has shown that the two-electron matrices J_i , K_i , etc., may be obtained by pure matrix methods from the matrix elements of the two-electron operator r_{12}^{-1} . This operator yields two product-space matrices (supermatrices) with elements

$$\begin{aligned} J_{pq,rs} &= (\chi_p \chi_r | r_{12}^{-1} | \chi_q \chi_s) \quad , \\ K_{pq,rs} &= (\chi_p \chi_r | r_{12}^{-1} | \chi_s \chi_q) \quad . \end{aligned} \quad (3.12)$$

One obtains the two-electron matrices from the product-space matrices by a process of contraction over the basis elements of the product space. The procedure as modified for (3.8) starts with the occupied orbitals. We first form the closed-shell, and total-density matrices

$$D_C = \sum_k \vec{c}_k \vec{c}_k^+$$

$$D_0 = f \sum_m \vec{c}_m \vec{c}_m^\dagger$$

$$D_T = D_C + D_0 \quad . \quad (3.13)$$

Next, we form two auxiliary product-space matrices (supermatrices) from J and K

$$\begin{aligned} \rho &= 2J - K \\ \mathcal{Q} &= 2\alpha J - \beta K \quad . \end{aligned} \quad (3.14)$$

On applying the Nesbet contraction procedure, we obtain

$$\begin{aligned} P &= \rho D_T \\ Q &= \mathcal{Q} D_0 \quad , \end{aligned} \quad (3.15)$$

and finally

$$R = S D_T Q + Q D_T S \quad . \quad (3.16)$$

We continue to work within the central-field approximation, and consequently we may simplify the computation considerably by utilizing symmetry-adapted functions as a basis set. For the work reported in this study, we have chosen Slater-type functions defined as

$$\chi_{p\ell m} = R_{\ell p}(r) Y_{\ell m}(\theta, \varphi) = r^{-1} P_{\ell p}(r) \Theta_{\ell} |m| \Phi_m(\varphi) \quad , \quad (3.17)$$

where $Y_{\ell m}$ is a complex normalized spherical harmonic, and the radial function $R_{\ell p}$ is defined by

$$R_{\ell p}(r) = [(2n_{\ell p})!]^{-1/2} (2\zeta_{\ell p})^{n_{\ell p}+1/2} r^{n_{\ell p}-1} e^{-\zeta_{\ell p} r} \quad . \quad (3.18)$$

An orbital of symmetry type ℓ and subspecies m is expanded only in terms of χ 's of the same symmetry type and subspecies. The energy expression (2.22) was written in terms of summations over complete shells, so that, utilizing (2.14) and (2.15), we see that the basis set (3.17) brings (3.8) into a reducible form and one may diagonalize the submatrix for each symmetry type separately.

The matrix elements of (3.11) now assume the particular form

$$\begin{aligned}
 S_{\ell pq} &= (2\ell + 1)^{-1} \sum_m (\chi_{\ell pm} | \chi_{\ell qm}) \\
 &= \int_0^\infty R_{\ell p}(r) R_{\ell q}(r) r^2 dr \quad , \quad (3.19)
 \end{aligned}$$

$$\begin{aligned}
 U_{\ell pq} &= (2\ell + 1)^{-1} \sum_m (\chi_{\ell pm} | r^{-1} | \chi_{\ell qm}) \\
 &= \int_0^\infty R_{\ell p}(r) R_{\ell q}(r) r dr \quad , \quad (3.20)
 \end{aligned}$$

$$\begin{aligned}
 T_{\ell pq} &= (2\ell + 1)^{-1} \sum_m (\chi_{\ell pm} | -\frac{1}{2}\Delta | \chi_{\ell qm}) \\
 &= \frac{1}{2} \int_0^\infty \left[r^2 R'_{\ell p}(r) R'_{\ell q}(r) + \ell(\ell + 1) R_{\ell p}(r) R_{\ell q}(r) \right] dr \quad , \quad (3.21)
 \end{aligned}$$

$$\begin{aligned}
 \mathcal{J}_{\ell pq, \ell' rs} &= (2\ell + 1)^{-1} (2\ell' + 1)^{-1} \sum_{m, m'} x (\chi_{\ell pm} \chi_{\ell' r m'} | r_1^{-1} | \chi_{\ell qm} \chi_{\ell' s m'}) \\
 &= \int_0^\infty \int_0^{r_2} \left[R_{\ell p}(r_2) R_{\ell q}(r_2) R_{\ell' r}(r_1) R_{\ell' s}(r_1) \right. \\
 &\quad \left. + R_{\ell' r}(r_2) R_{\ell' s}(r_2) R_{\ell p}(r_1) R_{\ell q}(r_1) \right] x r_2 r_1^2 dr_2 dr_1 \quad , \quad (3.22)
 \end{aligned}$$

$$\begin{aligned}
 \mathcal{K}_{\ell pq, \ell' rs} &= (2\ell + 1)^{-1} (2\ell' + 1)^{-1} \sum_{m, m'} x (\chi_{\ell pm} \chi_{\ell' r m'} | r_1^{-1} | \chi_{\ell' s m'} \chi_{\ell qm}) \\
 &= \frac{1}{2} \sum_k C_{\ell \ell' k} \mathcal{K}_{\ell pq, \ell' rs}^k \quad , \quad (3.23)
 \end{aligned}$$

and

$$\begin{aligned}
 K_{\ell p q, \ell' r s}^k = & \int_0^\infty \int_0^{r_2} \left[R_{\ell p}(r_2) R_{\ell' r}(r_2) R_{\ell q}(r_1) R_{\ell' s}(r_1) \right. \\
 & + R_{\ell q}(r_2) R_{\ell' s}(r_2) R_{\ell p}(r_1) R_{\ell' r}(r_1) + R_{\ell p}(r_2) R_{\ell' s}(r_2) R_{\ell q}(r_1) R_{\ell' r}(r_1) \\
 & \left. + R_{\ell q}(r_2) R_{\ell' r}(r_2) R_{\ell p}(r_1) R_{\ell' s}(r_1) \right] \times r_2^{-k+1} r_1^{k+2} dr_2 dr_1 \quad ,
 \end{aligned}
 \tag{3.24}$$

where the $C_{\ell \ell' k}$ are given by (2.16). The preceding integrals may be evaluated in a number of ways. The particular formulae which we utilized are given in Appendix B, and further detail may be found in references 7 and 24.

Minimization Procedure for the $1s^2$, $1s^2 2s$, and $1s^2 2s^2$ Configurations

The computer program used to obtain solutions for the $1s^2$, $1s^2 2s$, and $1s^2 2s^2$ configurations possessed limitations on the type and size of the basis set. Within these limits, one could choose the number of exponents and the (same) number of powers of r to be associated with these exponents, starting with the r^0 term. In the original program, the limitations on the exponents and number of powers were: 1,6; 2,6; 3,4; 4,2; 5,1; 6,1; where the first integer specifies the number of exponents and the second the maximum number of powers of r . A revised version of the program raised the total allowable basis size to eighteen functions.

The criterion of convergence for the SCF procedure was determined in the following manner. We defined a vector

$$\vec{g}_i = (F - \epsilon_i S) \vec{c}_i$$

to be associated with the vector of coefficients of each orbital ϕ_i . The SCF process was terminated when all the occupied orbitals satisfied the criterion

$$\sum_p |g_{i;p}| \leq 10^{-6} \quad .$$

Some initial experimentation was done with basis types and sizes within the scope of the computer program. This preliminary work resulted in the solution for lithium reported in this study. Further experimentation was done with the $1s^2$ configuration, and it was found that a basis set of four functions was sufficient to establish an upper bound for the energy which was accurate to four figures. Hartree's extensive calculations have shown that the orbitals of a filled shell are only very slightly disturbed by the

addition of orbitals external to that shell. With this as a guide, it was decided to first determine the $1s^2$ configurations using a basis set of four functions, in this case of the form $N_{11}e^{-\zeta_1 r}$, $N_{12}re^{-\zeta_1 r}$, $N_{21}e^{-\zeta_2 r}$, and $N_{22}re^{-\zeta_2 r}$, where the N's are the appropriate normalization factors. The optimum zeta values were determined by making a two-dimensional grid of the zetas with the energy as the parameter. An example of this procedure is shown in Table 3.1. We noted in these calculations that the primary expansion term was of the form $e^{-\zeta r}$, that is, hydrogenic in character, the other functions contributing small amounts to complete the fit. This hydrogenic tendency increases with atomic number.

Table 3.1. Variation of ζ_1 , ζ_2 for Be^{+2} ; $n = 2$.*

Table entries are the last three significant figures in the energy, $E_{\min} = -13.611297$ au.

ζ_2	3.0	3.2	3.4	3.6	3.8	4.0
ζ_1						
5.0	232	270	283	286	279	-
5.5	248	287	295	294	283	-
6.0	237	290	297	296	281	226
6.5	204	286	297	295	273	187
7.0	142	276	296	293	259	131
7.5	040	256	292	287	236	055
8.0	892	218	281	276	202	958

*n is the number of powers of r for each ζ in the basis set.

To obtain the "compromise" solution for each member of the $1s^2 2s$ and $1s^2 2s^2$ configurations, two basis functions were added to the best basis set obtained for the $1s^2$ configuration of the same Z value. These two new functions were of the form $N_{31}e^{-\zeta_3 r}$ and $N_{32}re^{-\zeta_3 r}$. A one-dimensional variation was made in this third ζ for each configuration, and a minimum was determined for the energy. The minimization procedure for the third ζ was greatly facilitated by noting that for the same configuration the critical exponents increased by definite steps as the Z value increased. This "scaling" has been noticed before and has been utilized in obtaining initial estimates for the solutions obtained by numerical integration.⁽⁶¹⁾ An example of the variation procedure is shown in Table 3.2. The third exponent furnished the greater part of the $2s$ orbital, the function $N_{32}re^{-\zeta_3 r}$ predominating over the other functions. This term characterizes the tail of the $2s$ orbital as the exponent is much smaller than the two needed to describe the $1s$ orbital.

Table 3.2. Variation of ζ_3 for Be; $n = 2$.*
 $\zeta_1 = 6.50$, $\zeta_2 = 3.40$.

ζ_3	Energy	
0.86	-14.572	901
0.87		936
0.88		960
0.89		974
0.90		976
0.91		966
0.92		942
0.93		904

* n is the number of powers of r for each ζ in the basis set.

The basis sets for each configuration were next raised to twelve functions, keeping the number of exponents fixed but utilizing the higher powers of r for each exponent. This size of basis set is sufficient to yield seven-place accuracy in the energies. It was observed that for Li^- a larger basis was needed; therefore another exponent was added to make a total of sixteen basis functions. A significant fact noted in the results of these large-size sets was that the character of the coefficients was no longer retained. The functions which had almost completely dominated the expansion with small basis sets were now no longer prominent. No definite pattern for this behavior was observed, so that no trend seems to be predictable when making the transition from small- to large-size sets.

In the case of lithium, extensive experimentation was carried out utilizing basis sets consisting of twelve functions, each involving three different exponents and four powers of r . The energy surface was found to be a wide shallow trough, contrary to expectations. The expansion exponents were varied over a wide range, and the energy differences were noted only in the eighth significant figure, within the roundoff error of the computation. A slight minimum does seem to exist; however, its precise position is difficult to ascertain. A listing of the data in this series is given in Table 3.3.

Minimization Procedure for the Other Configurations

For the remaining configurations studied; $1s^22s^22p^5$, $1s^22s^22p^6$, and $1s^22s^22p^63s$, a more flexible computer program was written to obtain the solutions. No limitation was placed on the basis functions other than the maximum permissible number, so that any combination of exponents and powers could be used. The SCF convergence criterion was applied to the eigenvectors themselves, and the usual requirement for convergence was

$$\left| \{C_{i;p}\}_{n+1} \right| - \left| \{C_{i;p}\}_n \right| \leq 1.0 \times 10^{-4} \quad ,$$

i.e., the components of the eigenvectors of two iterations all had to agree to within 1.0×10^{-4} .

Table 3.3. Variation of Three Zetas for Li; $n = 4$.[†]

ξ_1	ξ_2	ξ_3	Energy	
4.50	2.40	0.62	-7.4327	268 au.
		0.64		267
		0.67		270*
		0.70		267
		0.72		268
4.50	2.00	0.67		269
	2.20			268
	2.40			270*
	2.60			268
	2.80			268
3.50	2.40	0.67		261
3.80				265
4.20				265
4.50				270*
5.00				266
5.20				269
5.50				265
5.20	2.60	0.67		266
5.50	2.80			267
4.50	2.60	0.70		269
5.20	2.40			269
4.50	2.80	0.72		268
5.50	2.40			265

[†] n is the number of powers of r for each ξ of the basis set.

* This value is listed thrice for reference.

In view of the success achieved by the basis set types utilized for the configurations involving only one symmetry type, an attempt was made to proceed along the same lines to effect the energy minimization. A parameter set was chosen for each system, with the $1s^2 2s^2$ solutions serving as a guide. Each set utilized several exponents and two powers of r for each exponent. An attempt was made to reach the HF energy

minimum, but was unsuccessful with these choices. The p orbital could not be faithfully determined by this procedure, though the s orbitals are easily obtained to good accuracy. The fluorine atom orbitals could not be obtained with these types of basis sets as the matrix SCF process diverged repeatedly.

The next procedure attempted was a building-up from a small basis set, namely: two 1s, two 2s, and two 2p type functions. The basis size was increased, one function at a time, a very slow and tedious process. This was done by assuming an N value for the Slater-type function and varying the ζ value in steps of 1.0 or 2.0. This was repeated for a series of N values and the best function adopted; then the others were readjusted to lower the energy. This work revealed that as ζ was varied for a given N value, a number of energy maxima and minima appeared, sometimes of considerable difference in magnitude. This behavior restricts the use of any automatic minimization procedure and forces the computer to exercise his own judgement.

Löwdin has shown that Slater-type functions may be fitted to numerically determined orbitals through use of an analytical procedure of successive approximations.⁽²⁵⁾ Karo and Allen⁽²⁶⁾ utilized the set listed in Löwdin's paper for F^- as a starting point for their calculations on F and F^- . The type of basis set they finally adopted was one of seven s and five p Slater-type functions consisting of two 1s, four 2s, one 3s, four 2p and one 3p function. The use of such a set for the ten-electron configuration $1s^2 2s^2 2p^6$ proceeds very smoothly, and an energy minimum can be reached in a short time. A sixth p function, a 3p, may be added to the basis set by slightly lowering the exponent of the first 3p function. The parameter set is now no longer unique, and one may obtain the same energy value by several different combinations of exponents. Attempts at enlarging the basis size were unsuccessful, but indications were that the energy would drop at most one or two in the seventh figure.

The solution for sodium, $1s^2 2s^2 2p^6 3s$, was obtained in a manner similar to that used by Hartree and Hartree.⁽²⁷⁾ The best expansion set for Na^+ was used for the core and two 3s functions were appended. The exponents of these two functions were varied to produce the solution reported. A severe problem of SCF convergence was encountered due to the size of the basis set and the fact that there were four orbitals. To obtain the present solution, the SCF convergence criterion had to be relaxed from the value of 1.0×10^{-4} used in the previous calculations. Our solution for Na was first obtained with a criterion of 3.0×10^{-4} and then the criterion strengthened by 0.5×10^{-4} steps. The solution reported was obtained at 2.0×10^{-4} ; the SCF calculation attempted at 1.5×10^{-4} was abandoned after 167 iterations. No significant difference in energy was noted for the calculations at these different convergence criteria nor for the one abandoned.

The severe trouble with the convergence was accentuated by the time involved in making the calculation. In the case of sodium (described above), we have utilized nine s and six p type basis functions, and each SCF iteration took twenty-eight seconds. Each calculation therefore takes considerable time, and many hours were expended in obtaining the solution of minimum energy. Larger basis sets would consume even more time, since the timing for the Jacobi diagonalization procedure utilized in the SCF process increases roughly as m^3 , where m is the order of the matrix to be diagonalized.

The fluorine configuration differs from the previous ones in that there is an open p shell. Although we have been able to obtain an almost adequate set of basis functions for the s orbitals, this is not the case with the p orbital. The fluorine configuration is completely unreceptive to the procedures which worked easily with the ten-electron systems. In order to get any solution at all, it was necessary to add to the computer SCF program an extrapolation procedure originally due to Nesbet.⁽²³⁾ This will be discussed in more detail in the next section.

The Fock operator for fluorine in (2.44) has a small eigenvalue in the p shell, about -0.037, and consequently is highly unstable. A good choice of starting vectors, although usually not too critical for small basis sizes, becomes extremely crucial when working with larger bases. It was not possible to vary the exponents of the p-type basis set over a wide range. At least fifty per cent of the SCF expansions attempted with the larger basis sets ended in failure due to the instability of the iterative process. Due to this impasse, the author was unable to spread out the exponents of the p-type basis functions in the same manner as had been done in the other calculations. Several weeks were spent trying to bring the exponents to the neighborhood indicated by the previous work, and this proved utterly impossible. Attempts were made to add a seventh s and sixth p basis function, but were unsuccessful. The basis set reported represents the best attained. In addition to this instability complication, the convergence criterion had to be raised to 3.0×10^{-4} . In the cases where this was not done, instability occurred frequently even after one hundred iterations.

The Eigenvector Extrapolation Procedure

As mentioned previously, the Fock operator for fluorine in (2.44) is very unstable and necessitates very good initial estimates of the eigenvectors. A good guess, however, may not be sufficient, since instability can still occur. The first method utilized to alleviate this situation was borrowed from the Hartrees. The energy of each SCF iteration was checked, and at the first sign of any significant change, the SCF eigenvectors were averaged with those from the previous iteration. The method proved fruitless and was soon abandoned.

The Nesbet density matrix extrapolation procedure was tried next and also proved inadequate. The procedure was then adapted by the author to operate on the eigenvectors themselves; the resultant vectors are then orthonormalized. The adapted Nesbet procedure assumes a (complex) exponential behavior for each component of each eigenvector. For the iteration numbered by N we may write

$$C(N) = C(\infty) + Ae^{\omega N} \quad ,$$

where A is the amplitude and ω is real, complex, or pure imaginary. These three possibilities for ω are sufficient to describe exponential, sinusoidal, or sinusoidally modulated exponential behavior. Then, if we define

$$\Delta(N + 1) = C(N + 1) - C(N) \quad ,$$

we obtain

$$C(\infty) = C(N + 2) + \frac{[\Delta(N + 2)]^2}{\Delta(N + 1) - \Delta(N + 2)} \quad .$$

The SCF computation proceeds in cycles of three iterations followed by an extrapolation. This procedure functions well, but is not capable of handling all situations. There have been cases where the SCF convergence has been delayed by the extrapolation procedure, so that the assumption of exponential behavior, though reasonable, is by no means always correct.

CHAPTER IV

HF CALCULATIONS OF $1s^2$, $1s^2 2s$, AND $1s^2 2s^2$ CONFIGURATIONS[†]

Discussion of Results

A number of calculations of the electronic structures of atoms and ions of low atomic number have been done previously.* Of the three configurations which have been considered, $1s^2$, $1s^2 2s$, and $1s^2 2s^2$, the two filled-shell configurations are the easier to solve, so that much attention has been focused on them. The literature shows calculations for many of the simple structures of these types. A tabulation of many of the results of previous calculations for the $1s^2$, $1s^2 2s$, and $1s^2 2s^2$ configurations may be found in a paper by Holöien.⁽²⁹⁾ Many of these are variational treatments which consist of minimizing the energy expression with respect to some parameters. There have not been a large number of HF-SCF computations due to the great labor involved in hand calculations. Holöien questions the accuracy of the HF calculations he lists, and the present work affirms his speculations.

Insofar as the qualitative features of the orbitals are concerned, nothing new is introduced by this work; the essential aspects of the orbital solutions have been known from previous work. The prime objective of this series of calculations has been to obtain the HF solutions to as great an accuracy as possible and thus to fix a lower bound on the HF energy. This is needed as a starting point in any investigation of the correlation energy, which is, by definition, the difference between the lowest eigenvalue of (1.1) and the HF energies. The analytical solutions are also in a handy form for further use in molecular and solid state physics.

The $1s^2$ configuration is the simplest to handle of the many-electron configurations, as there is only one space-orbital in the HF approximation. While much of the early work on this configuration is crude by modern computational standards, there has not been a very pressing need to obtain very accurate HF solutions because of the success of the more sophisticated schemes, such as superposition of configurations and correlated orbitals. Since there has been considerable interest centered on the Lamb shift for two-electron systems, which demands calculations of extreme accuracy, few people have been concerned with the HF approximations for these systems. Yet for some applications, such as solid state and molecular theory work, the HF solutions are much easier to handle than the more sophisticated ones and as such serve a useful purpose.

[†] Some of the material presented in this chapter has been published in Rev. Modern Phys. (Ref. 24).

*See Reference 28 for an extensive bibliography.

The first HF-SCF calculation was carried out on the helium ground state by Hartree⁽³⁰⁾ in 1928 subsequent to his introducing the scheme into the new quantum mechanics. There was, unfortunately, no orbital table published therein. Wilson and Lindsay⁽³¹⁾ later repeated this computation with a higher accuracy, stated as ± 2 in the fourth decimal place. The agreement of their work with the present calculation is excellent and substantiates the claim of accuracy made by them. Our wave functions agree usually to four decimal places and at most differ by one in the fourth place. The eigenvalues also agree to four decimal places.

Shortly after Hartree's original publication, Hargreaves⁽³²⁾ published a calculation for Li^+ , listing the self-consistent field, but not the orbital. Fock and Petrashen⁽³³⁾ in their calculation for Li first solved the Li^+ case and then added the valence electron. The $1s$ orbital tabulated in the latter paper differs slightly from that in Table F.2 (see p. 94), the discrepancy occurring frequently in the third significant figure. The tail-off for large r is also different, and consequently the present orbital should be more appropriate for solid state calculations where this region is significant.

Of the structures of the $1s^2 2s^2$ configuration, the ones of most interest are Be and Li^- . The only previous HF calculation of Be recorded in the literature was performed by the Hartrees.⁽³⁴⁾ Their calculation was the first work on the $1s^2 2s^2$ configuration which included the exchange terms in the Hamiltonian. The Hartrees were investigating the effect of the exchange terms on the wave function after having completed an SCF calculation on the same atom in which the exchange terms were neglected. The Hartrees carried only three decimal places in their work, and the present calculation agrees with their work to that accuracy. The additional accuracy of the present calculation has lowered the energy by 0.003 unit, which indicates a considerably better wave function.

Negative ions such as Li^- are of interest as they give some insight into the qualitative features of electron binding, yet no previous HF-SCF calculations have been published on Li^- . We find that the total energy of Li^- calculated in the HF approximation, is 0.004495 unit greater than the total Hartree-Fock energy of Li. On the other hand, the calculated ionization potential for a $2s$ electron of Li^- is 0.01453 au. This unusual situation is accented by the spatial extent of the $2s$ orbital as indicated in Tables 4.2 (see p. 54) and F.6 (see p. 102). One cannot give credence to the ionic size indicated by this calculation.

The simplest unfilled-shell configuration is the $1s^2 2s$ typified by the lithium atom, and as such, provides a system to test various calculational schemes. The earliest calculation for Li performed within the HF approximation which took account of the exchange terms was done by Fock and Petrashen⁽³³⁾ using Hartree's numerical technique. This work yielded

a high value for the total energy because of the neglect of both the off-diagonal multiplier and the large integration grids utilized. Since this was a hand calculation, it represented the best available for many years.

Recently, Nesbet has done open-shell calculations utilizing a modified version of the matrix formalism for filled-shell configurations.^(23,35) This scheme ignores the off-diagonal multipliers which are of significance in obtaining an accurate wave function. His early HF calculations for lithium⁽³⁶⁾ suffer not only from this handicap, but also from the lack of effort necessary to obtain an optimum set of parameters for the basis functions. Each of these calculations is followed by a calculation utilizing superposition of configurations with the HF function as leading term. The other wave functions of the expansion included the virtual orbitals which resulted from the HF calculation. There appears to have been little emphasis on the HF calculations and a greater reliance on the superposition of configurations calculations to minimize the energy. An earlier set of calculations⁽³⁷⁾ gives better results, but no information is available on the procedure.

The ability to obtain the HF energy to the accuracy herein presented has rested on the inclusion of the off-diagonal multipliers. Examination of Table 4.1 reveals that, true to expectation, as the nuclear charge Z increases, the $2s$ electron is pulled in and hence interacts more with the $1s$ electrons. The magnitude of these terms is such that they should not be neglected, particularly as they are now easy to include in the calculations.

Table 4.1. Lagrangian Multipliers for $1s^2 2s$ Configurations.

Z	$\lambda_{1s,1s}$	$\lambda_{1s,2s}$	$\lambda_{2s,2s}$
3	- 2.4777420	-0.001431797	-0.09816141
4	- 5.1383425	-0.004689991	-0.33307313
5	- 8.8077480	-0.008505143	-0.69492580
6	-13.480082	-0.012532270	-1.1825016
7	-19.153753	-0.016658549	-1.7954274
8	-25.828159	-0.020838220	-2.5335495
9	-33.503009	-0.025049129	-3.3967929
10	-42.179288	-0.029776210	-4.4011256

The Quality of the SCF Calculations

There are a number of checks that we may make to determine the worth of the solutions we have obtained by the finite expansion method. We consider any of the Fock-type equations

$$F\phi_i = \epsilon_i \phi_i \quad .$$

In the central-field approximation within which we have been working, the integro-differential equation determining the orbital radial function R_i may be written as

$$-\frac{1}{2}R_i'' - \frac{1}{r}R_i' + \frac{\ell(\ell+1)}{2r^2}R_i - \frac{Z}{r}R_i + \sum_j K_{ij}R_i = \epsilon_i R_i \quad , \quad (4.1)$$

where the K_{ij} are any of the integral operators which appear in the various equations. Let the radial function be represented as

$$R_i = r^\ell R_1 \quad .$$

Then (4.1) becomes

$$-\frac{1}{2}r^\ell R_1'' - (\ell+1)r^{\ell-1}R_1' - Zr^{\ell-1}R_1 + \sum_j K_{ij}r^\ell R_1 = \epsilon_i r^\ell R_1 \quad .$$

The operators K_{ij} all tend to zero as $r \rightarrow 0$; hence, if we now multiply by $r^{1-\ell}$, divide by R_1 , and let $r \rightarrow 0$, we obtain

$$\tilde{R} \equiv (\ell+1) [R_1'/R_1]_0 = -Z \quad . \quad (4.2)$$

Thus, if R is an exact solution of (4.1), the logarithmic derivative at the origin satisfies (4.2). This quantity was evaluated for each orbital at the end of the SCF computation. For the best expansions, (4.2) was satisfied to within three parts per thousand.

Another assay of our solution - and a strict one - consists of direct substitution into the original integro-differential equation. If we define two functions:

$$f(r) = [F - \epsilon]\phi(r) \quad , \text{ and}$$

$$g(r) = \frac{F\phi(r)}{\epsilon\phi(r)} \quad , \quad (4.3)$$

then, for an exact solution, $f(r) \equiv 0$ and $g(r) \equiv 1$. To illustrate the procedure for the tabulation of these functions, we evaluate $F\phi(r)$ for the closed-shell configurations $1s^2$ and $1s^2 2s^2$.

We consider the expansion of an s orbital:

$$\phi_i = \sum_{M,N} a_{i;MN} r^{N-1} e^{-\zeta M r} \quad (4.4)$$

The operator contribution for the configurations $1s^2$ and $1s^2 2s^2$ is

$$\begin{aligned} F\phi_i &= \left[H + \sum_j (2J_j - K_j) \right] \phi_i \\ &= \left[-\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} - \frac{Z}{r} + \sum_j \left\{ 2K_{jj}(r) - K_{ij}(r) \right\} \right] \phi_i \end{aligned}$$

The functions $K_{ij}(r)\phi_i$ are the results of the operations by the coulomb and exchange operators on the orbital ϕ_i . The evaluation of these functions is discussed in Appendix C.

As $r \rightarrow 0$, the expression above becomes troublesome; although the functions $K_{ij}(r)$ tend to zero, the term $-Z/r$ becomes singular. We consider only the one-electron parts of the operator contribution:

$$\begin{aligned} [F\phi]_{r \rightarrow 0} &= -\frac{1}{2}\phi'' - \frac{1}{r}\phi' - \frac{Z}{r}\phi \\ &= -\frac{1}{2}\phi'' - \frac{\phi'}{\phi} \frac{\phi}{r} - \frac{Z}{r}\phi \end{aligned}$$

Were ϕ an exact solution, by (4.2), $\phi'/\phi = -Z$, and we should obtain

$$[F\phi]_{r \rightarrow 0} = -\frac{1}{2}\phi'' \quad (4.5)$$

In Appendix F we list, as functions of the radial distance, the quantities ϕ , ϕ' , the Hartree P function, P' , f , and g for the Hartree-Fock solutions of the $1s^2$, $1s^2 2s$, and $1s^2 2s^2$ configurations. The value at the origin, discussed above, is not tabulated for f and g . The singular terms which should cancel each other do not do so, becoming infinite at slightly different rates. This results from the limitation on the accuracy of the wave functions, namely of four significant figures. As a consequence, the values computed for the origin from (4.5) are meaningless.

Examination of the tables of Appendix F demonstrates that, with the possible exception of Li^- , the HF equations have been adequately solved. The analytical expansions seem accurate to four significant figures, better than the previous solutions obtained by numerical integration over a coarse grid. A comparison cannot be made with respect to very accurate numerically integrated solutions, as these do not exist at present.

In a small region near the origin, the functions $f(r)$ and $g(r)$ show poor behavior, forcing one to question the accuracy of the orbital solutions in this region. However, in the region near the origin the quantity $F\phi$ involves the difference of two large terms, $\frac{1}{2}\Delta\phi$ and $Z\phi/r$, and their cancellation is limited by the number of significant figures of the orbital solutions. One may then turn to the logarithmic derivatives at the origin as a secondary check, and these show good agreement with the required condition.

Hyperfine Splitting of the Lithium Ground State

The major portion of the hyperfine splitting of atomic energy levels normally originates in the dipole-dipole interaction between the electrons and the nucleus. The Hamiltonian for this process is⁽³⁸⁾

$$\mathcal{H}'' = -\frac{\beta_n \beta_e}{I s} \sum_i \left[-\frac{8\pi}{3} (\vec{I} \cdot \vec{s}_i) \delta(\vec{r}_i) + r_i^{-5} \left\{ r_i^2 \vec{I} \cdot (\vec{\ell}_i - \vec{s}_i) - 3(\vec{I} \cdot \vec{r}_i)(\vec{s}_i \cdot \vec{r}_i) \right\} \right], \quad (4.6)$$

where β_n and β_e are the nuclear and electronic magnetic moments, $\vec{I}$ and $\vec{s}_i$ are the nuclear and electronic spin operators, I and s are the magnitude of the intrinsic nuclear and electronic spin, $\vec{\ell}$ is the electronic orbital angular momentum, and $\vec{r}_i$ is the position vector of the i th electron. The second term of (4.6) gives no contribution to the diagonal matrix element for s electrons, so that for the lithium 2S ground-state configuration, $1s^2 2s$, we are left with the Fermi⁽³⁹⁾ contact term, which we rewrite as

$$\mathcal{H}_{c0} = \frac{8}{3} \left(\frac{\beta_n}{I} \right) \left(\frac{\beta_e}{s} \right) \vec{I} \cdot \vec{s} \sum_{i=1}^3 \mathcal{E}_i \delta(\vec{r}_i), \quad (4.7)$$

where $\mathcal{E}_i = \pm 1$, according as the spin of the i th electron is alpha or beta, respectively. Let us henceforth abbreviate the summation above as $\sum_i$.

For s electrons, $j = s = \frac{1}{2}$ as $\ell = 0$, so that

$$2\vec{I} \cdot \vec{s} = 2(\vec{I} \cdot \vec{j}) = [f(f+1) - I(I+1) - s(s+1)]$$

when evaluated for the 2S state. The total angular momentum f assumes only the values $(I + \frac{1}{2})$ and $(I - \frac{1}{2})$; therefore,

$$2\vec{I} \cdot \vec{s} = \begin{cases} I & \text{for } f = I + \frac{1}{2} \\ -(I + 1) & \text{for } f = I - \frac{1}{2} \end{cases} .$$

The energy difference of splitting is, finally, given by

$$\Delta E = \frac{8\pi}{3} \beta_n \beta_e (2 + I^{-1}) (\Psi | \Sigma | \Psi) \quad (4.8)$$

The HF lithium wave function may be written as

$$\Psi_{\text{HF}} = A \left\{ \phi_{10}\alpha, \phi_{10}\beta, \phi_{20}\sigma \right\} ,$$

so that

$$(\Psi_{\text{HF}} | \Sigma | \Psi_{\text{HF}}) = \phi_{20}^2(0)$$

and

$$\Delta E = \frac{8\pi}{3} \beta_n \beta_e (2 + I^{-1}) \phi_{20}^2(0) .$$

If one uses the value $\beta_n(\text{Li}^7) = 3.256310$ nuclear magnetons⁽⁴⁰⁾ and the fundamental constants as given by Cohen, Dumond, Layton and Rollett,⁽⁴¹⁾ one obtains for Li^7 the numerical constant $(8\pi/3)\beta_n\beta_e(2 + I^{-1}) = 3474.38 \text{ mc-a}_0^3/\text{sec}$. Then

$$\Delta E = 3474.38 \times (0.40826)^2 = 579.10 \text{ mc/sec} .$$

The experimental value of ΔE has been measured as 803.512 mc/sec ;⁽⁴²⁾ hence the HF approximation yields 72.1% of the splitting

Nesbet⁽³⁶⁾ has reported hyperfine splitting values calculated from Hartree-Fock wave functions which are in better agreement with experiment. These values were based on a series of HF calculations made with his SCF scheme. The approximate HF solutions reported by him yielded much higher values of total energy than the present calculation. The best of Nesbet's HF calculations was repeated by means of the Roothaan SCF procedure, and the energy and splitting values were close to those reported by him. The basis set utilized by Nesbet was also embedded in a larger set, and the HF-SCF wave function calculated from this set yielded a lower total energy, whereas the hyperfine splitting value fell below that of the present calculation. Other calculations were carried out using basis sets involving six exponentials and a total of twelve functions.

These calculations confirmed the values reported for the energy and hyperfine splitting given in this section. This indicates that the values reported by Nesbet were the result of poor approximate HF wave functions, so that the better agreement with experiment was fortuitous.

Diamagnetic Susceptibility

If an atom has a closed-shell structure, so that J is zero, the expression for the diamagnetic susceptibility assumes a simple form: (4.9)

$$\chi = -\frac{Ne^2}{6mc^2} \sum_i \langle r_i^2 \rangle, \quad (4.9)$$

where χ is the susceptibility in emu/mole, N is Avogadro's number, e and m are the charge and mass of the electron, c is the velocity of light, and r_i is the radial distance of electron i from the nucleus. The constant factor, when evaluated for atomic units, has the value 7.9234×10^{-7} emu/mole- a_0^2 .

In Table 4.3 we list the values of χ calculated for He, Li^+ , Li^- , and Be by means of the orbitals listed in Appendix F. The experimental value of the susceptibility of helium is reported as -1.9×10^{-6} emu/mole and that of Li^+ is estimated as -0.7×10^{-6} emu/mole. (44,45) Within the accuracy reported, these values are the same as those of Table 4.3. No experimental values for Li^- and Be are available.

Table 4.2. Expectation Values of r_1 and r_1^2 for Several Atoms and Ions.

	1s		2s	
	$\bar{r}$	$\overline{r^2}$	$\bar{r}$	$\overline{r^2}$
He	0.92727	1.18483	-	-
Li^+	0.57237	0.44532	-	-
Li	0.57312	0.44680	3.87368	17.73873
Li^-	0.57294	0.44637	6.84560	46.46306
Be	0.41499	0.23295	2.64942	8.42652

Table 4.3. Calculated Diamagnetic Susceptibilities of He, Li^+ , Li^- , and Be.

	χ
He	-1.87757×10^{-6} emu/mole
Li^+	-0.70569
Li^-	-74.3364
Be	-13.7225

CHAPTER V

UHF CALCULATION OF THE $1s^2 2s$ CONFIGURATION OF LITHIUM*

The UHF wave function differs from the HF wave function due to the relaxation of the double-occupancy rule for the orbitals. The $1s^2 2s$ ground-state configuration of lithium is then more properly written as $1s1s'2s$, with a corresponding wave function

$$D_2 \equiv A\{1s\alpha, 1s'\beta, 2s\alpha\} \quad (5.1)$$

The orthogonality of the spin-orbitals $1s\alpha$ and $1s'\beta$ is provided by their different spin functions.

Pratt⁽¹⁶⁾ has discussed the case of lithium at some length and has predicted that the $1s$ and $1s'$ orbitals would be very much alike, whereas the UHF $2s$ orbital should differ from the HF $2s$ orbital due to the spin dependence of the Fock operators. This difference in the spin densities of the two $1s$ orbitals should produce a nonzero magnetic field, so that there will now be a contribution of the $1s$ orbitals to the magnetic interaction with the nucleus. This should give an improved prediction of the value of the hyperfine splitting. Pratt has also predicted that the wave function D_2 would be nearly an eigenfunction of S^2 .

Results and Discussion

It was found that those basis functions which minimize the energy of the HF wave function of lithium also minimize the energy of the UHF wave function. This strongly suggests that the orbitals for these two approximations are very similar. An examination of the orbital tables of Appendices F and G reveals that, except for a small region near the origin, the HF and UHF wave functions are only slightly different. The similarity between these two wave functions is evident in the magnitude of the energy decrease, 2.4×10^{-5} au, obtained through the relaxation of the double-occupancy requirement on the closed-shell orbitals.

The expectation value of S^2 for the UHF function D_2 is given by

$$\begin{aligned} (D_2 | S^2 | D_2) &= (D_2 | \frac{7}{4} D_2 + D_1 + D_3) \\ &= \frac{7}{4} - (\phi_{10}, \phi_{1'0})^2 - (\phi_{1'0}, \phi_{20})^2 \\ &= \frac{7}{4} - (0.99999075)^2 - (-0.00166552)^2 \\ &= 0.75001573 \quad . \end{aligned}$$

*The major portion of the material in this chapter has been published in the Physical Review, reference 46.

For lithium the UHF approximation thus yields almost a pure doublet. The space orthonormality, as shown above, has been almost retained; the inner product of the $1s$ and $1s'$ orbitals is almost unity.

The Quality of the SCF Calculation

The tests for quality applied to the UHF wave function were the same as those applied to the HF wave functions. The logarithmic derivatives at the origin were computed for each orbital, and the best wave function satisfied (4.2) to within three parts per thousand. A goodness test, i.e., calculation of the functions

$$f(r) = (F - \epsilon)\phi(r) \text{ and } g(r) = F\phi(r)/\epsilon\phi(r) \quad ,$$

is given in Appendix G. The tables therein indicate that the UHF solutions have been obtained to the same degree of accuracy as the HF solutions.

Hyperfine Splitting

The energy expression for the splitting of the doublet states is given by (4.8). We have assumed a single determinant, (5.1), as our wave function, so that the necessary matrix element is

$$\langle D_2 | \sum_i | D_2 \rangle = \phi_{10}^2(0) - \phi_{1'0}^2(0) + \phi_{20}^2(0) \quad ,$$

and the energy expression is

$$\Delta E = \frac{8\pi}{3} \beta_n \beta_e (2 + I^{-1}) [\phi_{10}^2(0) - \phi_{1'0}^2(0) + \phi_{20}^2(0)] \quad .$$

A UHF wave function is not an eigenfunction of S^2 , but a mixture of spin-eigenstates. This mixture is due to the neglect of the other determinantal wave functions which may be constructed from the same configuration. In the case of lithium, these are

$$D_1 = A\{\phi_{10}\beta, \phi_{1'0}\alpha, \phi_{20}\alpha\}$$

and

$$D_3 = A\{\phi_{10}\alpha, \phi_{1'0}\alpha, \phi_{20}\beta\} \quad .$$

The UHF wave function for lithium, D_2 , can be seen to be a mixture of a doublet and a quartet, whereas the experimentally observed ground state is known to be a doublet. We may restore the overall symmetry by use of (2.50) to project out the doublet component.

$$P_2 D_2 = \frac{S^2 - \frac{3}{2} \left(\frac{3}{2} + 1 \right)}{\frac{1}{2} \left(\frac{1}{2} + 1 \right) - \frac{3}{2} \left(\frac{3}{2} + 1 \right)} D_2 = \frac{1}{3} [2D_2 - D_1 - D_3] = \frac{1}{3} \Psi_2 \quad .$$

The corresponding energy expression is then proportional to $\langle \Psi_2 | \sum_i | \Psi_2 \rangle$ and assumes the form

$$\begin{aligned} \Delta E = & \frac{8\pi}{3} \beta_n \beta_e (2 + I^{-1}) [6 + 3(\phi_{10}, \phi_{1'0})^2 + 3(\phi_{1'0}, \phi_{20})^2]^{-1} \\ & \times [4\phi_{10}^2(0) - 2\phi_{1'0}^2(0) + 4\phi_{20}^2(0) + 5\phi_{10}^2(0) (\phi_{1'0}, \phi_{20}) \\ & + 5\phi_{20}^2(0) (\phi_{10}, \phi_{1'0}) - 10\phi_{10}(0)\phi_{20}(0) (\phi_{10}, \phi_{1'0}) (\phi_{1'0}, \phi_{20}) \\ & - 2\phi_{1'0}(0)\phi_{20}(0) (\phi_{1'0}, \phi_{20}) - 2\phi_{10}(0)\phi_{1'0}(0) (\phi_{10}, \phi_{1'0})] \quad . \end{aligned}$$

Table 5.1. Expansion Parameters for the UHF Lithium Atom Ground State Orbitals.

ζ_M	N	C_{1s}	$C_{1s'}$	C_{2s}
4.50	1	0.485226	0.482485	0.076064
	2	0.196046	0.196857	0.022892
	3	0.076357	0.078059	0.004458
	4	0.034200	0.035873	0.002265
2.40	1	0.000000	0.000000	-0.000000
	2	0.395230	0.381699	0.148014
	3	-0.102567	-0.087028	-0.036137
	4	0.006717	-0.000425	0.033464
0.67	1	0.018164	0.028171	-0.015645
	2	-0.017809	-0.027705	-1.071172
	3	0.008973	0.014042	0.062361
	4	-0.001992	-0.003142	-0.031610
- ϵ		2.486676	2.468700	0.196367
- $(\phi'/\phi)_0$		3.0065	3.0064	3.0085
- E			7.432751	

In Table 5.2 we list the values at the origin of the orbitals of the HF and UHF wave functions which were used to calculate the hyperfine splittings. Table 5.3 summarizes the results of these calculations and permits a comparison with previous calculations and the experimental value. The UHF hyperfine splitting is in much better agreement with experiment, yielding 97% of the experimental value compared to 72% for the

HF value. This substantial increase has been predicted by Cohen, Goodings, and Heine⁽⁴⁷⁾ in their perturbation calculation of the exchange polarization effect. They did not publish numerical values for the orbitals, but only noted the overall change at the origin. This prevents any comparison with the present UHF orbitals. The SCF calculation shows that the increase of the splitting value is due to the net magnetic moment set up by the difference in the inner orbital charge densities, as may be seen from Table 5.2.

Table 5.2. Magnitude of Orbitals at the Origin.

Orbital	HF	UHF	$\phi_{\text{UHF}}^2 - \phi_{\text{HF}}^2$
$\phi_{10}\alpha(0)$	2.61282	2.61891	0.03186
$\phi_{20}\alpha(0)$	0.40826	0.40482	-0.00280
$\phi_{1'0}\beta(0)$	2.61282	2.60725	-0.02908

Table 5.3. Comparison of Hyperfine Splittings and Total Energies for Li^7 .

Method	Reference	Total Energy (atomic units)	ΔE (mc/sec)	$\frac{\Delta E}{\Delta E_{\text{exp}}}$
HF	Fock & Petrashen	-7.41	573	0.713
HF	This calculation	-7.432727	579.10	0.721
HF	Nesbet	-7.43259	585.813	0.729
UHF by perturbation	Cohen, Goodings and Heine	-	747	0.930
UHF	This calculation	-7.432751	781.10	0.972
Projected UHF	This calculation	-	709.59	0.883
Configuration interaction	Nesbet	-7.431849	793.493	0.988
Experimental	Kusch & Taub	-7.478	803.512	1.000

The results clearly indicate that the UHF approximation is considerably better than the HF approximation for the calculation of hyperfine splittings. The improvement is sufficient to outweigh the drawback of inequivalent orbitals and the resulting unaesthetic lack of symmetry of the total UHF wave function. It is of particular interest to note that if one attempts to restore the overall symmetry by projecting out the doublet, Ψ_2 , a much poorer value for the hyperfine splitting is obtained.

Table 5.4. Expectation Value of r_i and r_i^2 for the UHF Lithium Wave Function.

Orbital	$\overline{r_i}$	$\overline{r_i^2}$
$1s\alpha$	0.57179	0.45886
$1s\beta$	0.57359	0.46327
$2s\alpha$	3.64557	16.30759

CHAPTER VI

HF CALCULATIONS OF GROUND STATES OF F, F⁻, Ne, Na⁺, AND Na

Discussion of Results

The ten-electron isoelectronic sequence, $1s^2 2s^2 2p^6$, is of considerable interest because of the light it sheds on electronic binding. The series F⁻, Ne, and Na⁺ form a triad of three different chemical types, and their SCF solutions are very useful in the field of chemical physics. The solutions for the ions F⁻ and Na⁺ are particularly valuable in the study of the properties of the alkali halides.

There have been a number of previous calculations of the electronic structure of F⁻, starting with that of Brown⁽⁴⁸⁾ in 1933. Brown's calculation has been considered very crude, as he carried three decimal places and included the exchange terms only in the 2p shell. Hartree⁽⁴⁹⁾ subsequently published a more accurate calculation, but must have later felt the need for yet more accuracy as his student Froese⁽⁵⁰⁾ has recently published a calculation performed numerically on the EDSAC. Allen^(26,51) has also done a number of calculations by the Roothaan method, utilizing Whirlwind.

The results of this calculation on F⁻, presented in Table H.2 (see page 118) and Appendix I, agree fairly closely with those of Froese. There are minor discrepancies attributable to the limited storage capacity with which Froese worked. Allen's unpublished results are higher in total electronic energy than are the results of the present work. It is believed that the total energy may be lowered below that reported in Table H.2 by one or two in the seventh figure, but convergence difficulties with larger basis sets have precluded obtaining the SCF wave functions. This convergence difficulty with large basis sets is characteristic of the other members of the isoelectronic sequence.

There have been two previously published calculations of the neon wave function. The early work by Brown⁽⁴⁸⁾ is of the same caliber as the F⁻ calculation. The later work, reported by Worsley,⁽⁵²⁾ was performed by numerical integration on a small computer, and, due to lack of storage, an insufficient number of grid points was used. Allen⁽⁵¹⁾ has also done unpublished work on neon by means of the Roothaan method, but the present wave function is obtained from an SCF calculation yielding a total electronic energy lower than his by 0.0038 au. In Table H.3 (see page 118) and Appendix I, we list the characteristics of the Ne wave function. The one-electron ϵ parameters of Table H.3, which correspond to ionization potentials, fall between the values given by the calculations of Worsley and Allen, with Worsley's values running higher and Allen's values lower than those in Table H.3.

The last member of the ten-electron triad that has been calculated is Na⁺, which has had the distinction of being the first system investigated with the HF approximation including exchange terms. This work was done

by Fock and Petrashen, who utilized a Green's function technique to solve the differential equations.⁽⁵³⁾ This method was soon displaced by the Hartree numerical integration procedure. The Hartrees⁽²⁷⁾ later performed a calculation for Na^+ and pointed out the shortcomings of the Fock and Petrashen work. The present wave function (see Table H.4, page 118, and Appendix I), is in very good agreement with that reported by the Hartrees, though the eigenvalues of the various shells differ in the fourth figure. This difference is to be expected, as the Hartrees carried only three decimals in their calculation. The Fock and Petrashen calculation differs from the present one in the third figure, and their total electronic energy, reported as -161.8 au, is too negative for an HF calculation.

The calculation for the sodium configuration $1s^2 2s^2 2p^6 3s$ presented here is the first to include all the off-diagonal Lagrangian parameters; the calculations of Fock and Petrashen⁽⁵³⁾ and the Hartrees⁽²⁷⁾ were based on a fixed Na^+ core. The Hartrees did use the $\lambda_{2s,3s}$ term to provide orthogonality for the 3s orbital, but the reported value of 4.5×10^{-3} is much larger than the value of -7.7×10^{-4} recorded in Table 6.3 (page 69). To the three decimal places the Hartrees carried their calculation, their orbitals agree with those of Appendix I. The notable exception is the value of the 3s orbital at the origin, which differs in the third figure.

There are two previously published calculations of the $1s^2 2s^2 2p^5$ configuration of fluorine. The early one due to Brown⁽⁴⁸⁾ is of a quality similar to those for F^- and Ne. The later results are given by Allen^(26,51) and were calculated by Nesbet's modification of the Roothaan procedure.^(23,35) Allen has utilized larger basis sets in his calculations than has the author. He has used seven s- and six p-type functions to obtain the orbitals, yet his best SCF calculation⁽⁵¹⁾ has yielded a total electronic energy 0.00108 au higher than that given in Table H.1. (see page 118). The basis set of Table H.1 was insufficient to pin down the HF solution as may be seen in the "goodness" tests of the orbitals. These tests are discussed in the next section. Preliminary results from unstable SCF calculations indicate that the HF total electronic energy for F is about -99.40910 au.

The large discrepancy between the total electronic energy reported by Allen and that of the present calculation is due to the difference between the HF procedures as formulated by Roothaan⁽⁷⁾ and Nesbet.⁽³⁵⁾ Nesbet starts with GUHF equations, (2.55), which are in diagonal form, and then invokes "symmetry and equivalence restrictions," i.e., he neglects all matrix elements between different symmetry types (symmetry restriction) and generates all partners from a single solution for each symmetry type (equivalence restriction). The symmetry and equivalence restrictions allow the retention of the diagonal form of the operator equations. The one-electron Hamiltonian is formulated either by averaging over all possible one-electron operators or by assuming a definite occupancy for the configuration. The former procedure is applicable to the p^5 configuration and results in the

Hamiltonian of (2.35). The latter procedure must be used in the general case and will yield a one-electron Hamiltonian which is dependent on the assumed occupancy for the configuration. In neither case does the Nesbet formulation correspond to that of Roothaan's.

Superposed Potential Sphere

For the interpretation of many solid-state phenomena it would be very advantageous to have true solid-state SCF wave functions. These are not yet available and may be many years in coming, so that it seems plausible in the interim to obtain atomic wave functions that in some manner reflect the environment of the crystal lattice. Electron density studies of some alkali halide crystals have shown that the charge distribution about lattice sites remains essentially spherical, and about the negative ions it remains spherical for a considerable distance.⁽⁵⁴⁾ Kristoffel⁽⁶²⁾ has carried out a calculation for the Cl^- ion of KCl , in which he assumes, in each of three regions, a different form for the orbitals of the outer shell. These regions were chosen so as to reflect the relative importance of the ion central field and the crystal field. The orbital parameters were determined from continuity and normalization conditions. The resulting orbitals tailed off faster than in the free ion. Kristoffel found that the positive ion showed an opposite effect, but the magnitude of the change was not as great. Hurst⁽⁵⁵⁾ has shown that in the presence of a point-charge crystal field, the optimum effective nuclear charge for the H^- wave function increases, indicating a charge distribution of lesser extent than the free ion. This situation should also prevail for the F^- ion in a crystal environment.

If we consider a single ion in a crystal lattice, we find that in addition to the atomic potential there exists the Madelung potential due to Coulomb interaction between the ions. There is also a repulsive potential of unknown origin. These external potentials, collectively acting as a potential well, modify the charge distribution about the nucleus. A complete calculation of the effect of these potentials is a major task which remains to be done. For immediate use, it is desirable to investigate the effect on the orbitals of various types of superposed potential fields which pass within the scope of the central-field SCF scheme.

We have chosen as our superposed field a hollow sphere of radius a carrying charge q . Such a potential has the value q/a for $0 \leq r \leq a$ and q/r for $r > a$. A positively charged sphere should contract the charge cloud of a negative ion, and a negatively charged sphere should swell the charge cloud of a positive ion. The charge q has been taken with magnitude one, corresponding to the net charge exclusive of the ion. The parameter which remained to be chosen was the sphere radius a .

The proper value for the radius of the charged sphere is a debatable point. On intuitive grounds, one can choose the ionic radius; another choice is the lattice constant. Neither of these values can be fully justified. A third

approach can be made by setting the value of the potential inside the sphere to the value of the cohesive energy per ion. This prescription is as questionable as the first two proposed. Only experimentation can shed any light on the best choice for the radius.

A number of spheres of varying radii were superposed on the F^- and Na^+ solutions reported in this study. No attempt was made to minimize the energy, as the size of the basis sets was sufficient to give good results. This is demonstrated by the goodness tests. The radii of the spheres were chosen less than, equal to, and greater than the ionic radii as given by Pauling.⁽⁵⁶⁾ For F^- , an additional value was chosen equal to the LiF lattice constant. These spheres had the desired effect of changing the sizes of the ions. The Na^+ orbitals were only slightly affected by the spheres, but a good deal of change resulted in the 2s and 2p orbitals of F^- . The solution for F^- with a superposed sphere corresponding to the ionic radius given by Pauling is given in Appendix J.

The Quality of the SCF Solutions

In Chapter IV we discussed some tests which may be applied to SCF solutions obtained as analytic expansions. A solution to the HF equations must satisfy (4.2), and this quantity, the reduced logarithmic derivative at the origin, was computed for each orbital at the end of each SCF computation. For s orbitals, there still remains a correlation between energy minimization and satisfying (4.2), but the situation was different with the p orbitals. When using the type of basis sets of Appendix H, we found no correlation between the reduced logarithmic derivative at the origin of the p orbitals and the energy minimization. The lack of correlation is undoubtedly due to the inability to pinpoint precisely the energy minimum which results from the number of significant figures to which the orbitals are accurate. More discussion of the accuracy is given in the latter part of this section.

A stringent test which can be applied to analytic orbitals is the goodness test, which requires computation of the functions

$$f(r) = (F - \epsilon)\phi \text{ and } g(r) = \frac{F\phi}{\epsilon\phi} \quad .$$

The procedure as outlined in Chapter IV is applicable to atoms containing only s orbitals and must be modified to handle configurations involving more than one symmetry type. Let us consider the diagonal form of our equations:

$$F\phi_i = [F' + f(P_0Q + QP_0) + (PCQ + QPC) - Q]\phi_i = \epsilon_i\phi_i \quad , \quad (6.1)$$

where ϕ_i is of the form

$$\phi_{nlm}(r, \theta, \varphi) = R(r)Y_{lm}(\theta, \varphi) \quad .$$

We wish to evaluate the functional $F\phi$ at each point of space (r, θ, φ) . Since we are working within the central-field approximation, it is not necessary to have an angular dependence and we may multiply (6.1) by $\bar{Y}_{\ell m}(\theta, \varphi)$ and integrate over $d\Omega_1$. This integration coupled with the integration over $d\Omega_2$ reduces the equation to a one-dimensional equation in r .

The one-electron terms present no problem and are easy to evaluate, whereas the two-electron terms may be handled in the manner of Slater.⁽⁸⁾ We recall that the interaction energy of a closed shell with an electron described by ϕ_i is given by

$$\sum_j (2J_{ij} - K_{ij}) = (2\ell' + 1) [2F^0(n\ell, n'\ell') - \frac{1}{2} \sum_k C_{\ell\ell'k} G^k(n\ell, n'\ell')] \quad .$$

Thus the functional we need is obtained from the first integral of this expression:

$$\sum_j (2J_j - K_j) \phi_i = (2\ell' + 1) [2\underline{F}^0(n\ell, n'\ell') - \frac{1}{2} \sum_k C_{\ell\ell'k} \underline{G}^k(n\ell, n'\ell')] \phi_i, \quad (6.2)$$

where the underline signifies the first integral of the F 's and G 's. The general integral entering here is of the form

$$K_{ij}^k(r) = \int_0^\infty \frac{r^{< k}}{r^{> k+1}} R_{n\ell}(r_1) R_{n'\ell'}(r_1) r_1^2 dr_1 \quad (6.3)$$

and is discussed in Appendix C. The evaluation of the two-electron terms then proceeds easily.

The projection operator terms may be obtained by transposition, utilizing (2.40), (2.41), and (2.45). We then obtain the relation

$$\begin{aligned} & [f(P_0Q + QP_0) + (P_CQ + QP_C) - Q]\phi_k \\ &= - \sum_m \lambda_{mk} \phi_m + \sum_\ell (\epsilon_{\ell k} - \lambda_{\ell k}) \phi_\ell \end{aligned} \quad (6.4)$$

for the closed-shell orbitals, whereas the open-shell orbitals satisfy the equation

$$\begin{aligned} & [f(P_0Q + QP_0) + (P_CQ + QP_C) - Q]\phi_m \\ &= (f-1)Q\phi_m + \sum_n \left(\epsilon_{nm} - \frac{\lambda_{nm}}{f} \right) \phi_n - \sum_k \frac{\lambda_{km}}{f} \phi_k \quad . \end{aligned} \quad (6.5)$$

In Appendix I we have tabulated the functions

$$f(r) = F(r) R(r) - \epsilon R(r)$$

and

$$g(r) = \frac{F(r)R(r)}{\epsilon R(r)} \quad (6.6)$$

along with the other orbital characteristics. One can see that the orbitals are accurate to about four figures. The exception to this is for fluorine, which is not yet adequately determined. The p orbital is poor by the standard which has been set for the other calculations. One can see also that the goodness in a region near the origin is poor for many orbitals. Attempts can be made to improve this situation by restricting the basis set so that (4.2) is satisfied. This restriction makes the computational procedure very cumbersome, and no evidence has been shown that the goodness of the orbitals obtained in this manner is superior to orbitals obtained without the restriction. It has not been possible to obtain the same standard of goodness over all space for any orbital. Changing of the basis sets merely shifts the regions where the goodness quality is poor.

Diamagnetic Susceptibility

The diamagnetic susceptibilities of the ten-electron systems may be calculated by means of (4.9). In addition, the values for the susceptibilities have been calculated for the ions with superposed spheres. These results are presented in Table 6.1.

Table 6.1. Diamagnetic Susceptibilities for Ten-electron Systems

System	Superposed Sphere		$\chi^*, \times 10^{-6}$
	Charge	Radius	
F^-	-	-	-12.665
Ne	-	-	- 7.4175
Na^+	-	-	- 5.0816
F^-	1.0	2.40	-11.633
F^-	1.0	2.57	-11.784
F^-	1.0	2.70	-11.888
F^-	1.0	3.789	-12.428
Na^+	-1.0	1.70	- 5.1775
Na^+	-1.0	1.7953	- 5.1539
Na^+	-1.0	1.90	- 5.1344

* units are emu/mole.

The precise experimental values of the susceptibilities for these systems are difficult to obtain. In Landolt-Börnstein⁽⁴⁴⁾ is listed a value for Ne of -7.2×10^{-6} emu/mole, so that the value listed in Table 6.1 is within the experimental error. The susceptibilities for the ionic systems are obtained from measurements on crystals or aqueous solutions. The values for the ionic systems F^- and Na^+ are known only approximately, and Landolt-Börnstein list the values obtained by the various methods. This range of data is discussed by Myers,⁽⁴⁵⁾ who concludes that a more accurate experimental technique is needed and that none of the values is a standard. The values given in Table 6.1 fall within the accepted range as given by Landolt-Börnstein and Myers.

The experimentally determined susceptibility values for LiF and NaF are given as 10.1 and 15.5 (in units of -10^{-6} emu/mole).⁽⁴⁵⁾ Using the free-ion values of Table 6.1, we obtain for χ the values $\chi_{LiF} = 13.74$ and $\chi_{NaF} = 17.75$. These values are too large. Use of the χ for the ions with the superposed spheres of ionic radii yields the values $\chi_{LiF} = 12.5$ and $\chi_{NaF} = 16.84$, where the susceptibility for Li^+ has been assumed constant at 0.7. These values are in better agreement with experiment, though still high, as the potential field has not caused very large changes in the charge distributions. The radii of the spheres might be chosen such that the susceptibility calculated would agree with the experimental value, although this procedure does not lead to a unique choice for each ion.

Hyperfine Splitting of the Sodium Ground States

The sodium ground-state configuration is like the lithium ground state in having a lone s electron in an outer shell. As a consequence, the hyperfine-splitting Hamiltonian is the same as for lithium, depending only on the Fermi contact term (4.7). Using a value for β_n (Na^{23}) of 2.21763 and $I = 3/2$, we obtain for Na^{23} the numerical constant $8\pi/3\beta_n\beta_e(2+I^{-1}) = 2366.14$ mc/sec- a_0^2 . If we utilize the value of $\psi_{3s}^2(0)$ obtained from Table I.15 (page 151), we have

$$\Delta E = 1272.68 \text{ mc/sec} \quad ,$$

which is 71.84% of the experimental value of 1771.61 mc/sec.⁽⁴¹⁾ The value of the splitting obtained using the Hartrees' value⁽²⁷⁾ for $\psi_{3s}^2(0)$ is

$$\Delta E = 1248.49 \text{ mc/sec, or } 70.47\% \text{ of the experimental value.}$$

Fine Splitting of the Fluorine 2P States

The interaction of the orbital angular momentum and the electronic spin of the unpaired electron of fluorine produces a splitting of the ground state. This spin-orbit coupling may be treated by first-order perturbation using the Hamiltonian⁽⁵⁷⁾

$$\mathcal{H}' = \frac{1}{2m^2c^2} \left(\frac{1}{r} \frac{\partial V}{\partial r} \right) \vec{\ell} \cdot \vec{s} \quad , \quad (6.7)$$

where m is the mass of the electron, c is the velocity of light, $\vec{\ell}$ and $\vec{s}$ are electronic orbital and spin angular momenta, and $V(r)$ is the electrostatic potential that the unpaired electron experiences..

The expectation value for (6.7) becomes

$$E' = \langle \Psi | \mathcal{H}' | \Psi \rangle = \frac{1}{2} \zeta_{2p} [j(j+1) - \ell(\ell+1) - s(s+1)] \quad , \quad (6.8)$$

where $\vec{j} = \vec{\ell} + \vec{s}$ and the parameter ζ_{2p} is given by

$$\zeta_{2p} = K \int_0^\infty \frac{1}{r} \frac{Z(r)}{r^2} P_{2p}^2(r) dr \quad . \quad (6.9)$$

In (6.9), the constant $K = \hbar^2/2m^2c^2$ and $Z(r)$ is the charge contained within a sphere of radius r , i.e., an effective nuclear charge for the unpaired 2p electron. Now

$$Z(r) = Z - q(r),$$

where Z is the nuclear charge and $q(r)$ is the number of electrons within a sphere of radius r , excluding the unpaired 2p electron. Then

$$\begin{aligned} \zeta_{2p} &= K \left[Z \int_0^\infty r^{-3} P_{2p}^2 dr - \int_0^\infty r^{-3} q(r) P_{2p}^2 dr \right] \\ &= K \left[Z \langle r^{-3} \rangle - \sum_i \int_0^\infty r^{-3} P_{2p}^2(r) \int_0^r P_i^2(r_i) dr_i dr \right] \quad . \end{aligned} \quad (6.10)$$

The evaluation of ζ_{2p} is reduced to evaluating $\langle r^{-3} \rangle$ and the summation of (6.10). The final values in (6.10) are

$$\zeta_{2p} = 5.84358 \text{ cm}^{-1} a_0^3 \cdot [9(7.5309070) - 13.725266] a_0^{-3}.$$

The values that j can assume in (6.8) are $\frac{3}{2}$ and $\frac{1}{2}$, so that we finally obtain for the doublet separation

$$\Delta E = \frac{3}{2} \zeta_{2p} = 473.79 \text{ cm}^{-1}.$$

The experimental value⁽⁵⁸⁾ given for the difference ${}^2P_{3/2} - {}^2P_{1/2}$ is 404 cm^{-1} ; hence we are considerably high in our calculation.

Hyperfine Splitting of the Fluorine $^2P_{3/2}$ States

The Hamiltonian which describes the hyperfine splitting of the fluorine ground state is given by the second expression in (4.6). When used with our first-order wave function, this term becomes⁽³⁸⁾

$$\mathcal{H}_c = 2\beta_e \frac{\beta_n}{I} \frac{\ell(\ell+1)}{j(j+1)} (\vec{I} \cdot \vec{j}) \frac{1}{r^3} .$$

Then

$$E_c = (\Psi | \mathcal{H}_c | \Psi) = \beta_e \frac{\beta_n}{I} \langle r^{-3} \rangle [f(f+1) - I(I+1) - j(j+1)] \frac{\ell(\ell+1)}{j(j+1)} .$$

The values assumed by f are two and one, as $I = \frac{1}{2}$, so that with $j = \frac{3}{2}$

$$[f(f+1) - I(I+1) - j(j+1)] = \begin{cases} \frac{3}{2} & \text{for } f = 2 \\ -\frac{5}{2} & \text{for } f = 1 \end{cases} .$$

Using the value of $\beta_n(F^{19}) = 2.62850$ and the fundamental constants given by Cohen et al.,⁽⁴¹⁾ we obtain

$$\Delta E = 2016.87 \text{ mc/sec.}$$

The experimental value for the hyperfine splitting of F^{19} does not seem to be available. A systematic search of the literature has failed to reveal any experimental data for the free F atom in the ground state. Therefore a comparison of the calculated value with the experimental value is not possible.

Table 6.2. Expectation Values of r_i and r_i^2 for F, F^- , Ne, Na^+ , and Na.

System	1s		2s		2p		3s	
	$\bar{r}$	$\overline{r^2}$	$\bar{r}$	$\overline{r^2}$	$\bar{r}$	$\overline{r^2}$	$\bar{r}$	$\overline{r^2}$
F	0.17594	0.04175	1.00107	1.21690	1.08256	1.53107	-	-
F^-	0.17576	0.04162	1.03553	1.31873	1.25551	2.21064	-	-
Ne	0.15763	0.03347	0.89220	0.96764	0.96496	1.22655	-	-
Na^+	0.14286	0.02748	0.77911	0.73148	0.79625	0.81592	-	-
Na	0.14286	0.02748	0.77907	0.73149	0.79847	0.82203	4.16691	20.1162

Table 6.3. Lagrangian Multipliers for F and Na.

λ	F	Na
1s, 1s	-26.380306	-40.477501
1s, 2s	- 0.047280	- 0.00073464
1s, 3s	-	- 0.00004631
2s, 2s	- 1.571014	- 2.7960461
2s, 3s	-	- 0.00077444
3s, 3s	-	- 0.09097405
2p, 2p	- 0.590295	- 1.5171746

CHAPTER VII CONCLUSIONS

In the course of this study we have discussed the Hartree-Fock approximation which is used to obtain solutions to the many-electron Schrödinger equation. We have employed this approximation to obtain SCF wave functions for a number of atomic configurations. We have chosen a particular calculation scheme to obtain these SCF solutions to the HF equations. This calculational scheme, due to Roothaan^(4,7) and Nesbet,⁽²³⁾ makes use of a finite expansion of nonorthogonal functions to represent the orbitals and terminates in a matrix SCF iterative procedure to obtain the coefficients in the expansions.

We have obtained HF-SCF solutions of the $1s^2$, $1s^22s$, and $1s^22s^2$ configurations in the atomic number range $2 \leq Z \leq 10$. A goodness test has been applied to these solutions and they have been shown to be more accurate than previous HF calculations. The UHF solution for the lithium atom has been calculated and compared with the HF solution.

The work on the lithium atom has shown that the UHF approximation must be kept in mind if calculations are performed on quantities which are very sensitive to small changes in the wave function. We have seen that an energy decrease of only 1.4×10^{-5} atomic units from the HF value, which was obtained through the use of the UHF method, resulted in improvement of the hyperfine splitting value from 72% to 97% of the experimental value. Further investigation of the UHF approximation is recommended to see if this situation prevails in more complicated physical systems.

We have obtained HF-SCF solutions to the ground states of F, F^- , Ne, Na^+ , and Na. Solutions for F^- and Na^+ have also been obtained with the ions subjected to a superposed potential field. The calculation of Hurst⁽⁵⁵⁾ has indicated that when the ion is in a crystal, the orbitals do not extend as far as they do in the free ion. The superposed potential fields were chosen so as to curtail the extent of the negative ion and increase the extent of the positive ion, and thus reflect the change of charge distribution caused by the crystal field. The SCF wave functions have been utilized to make a number of simple applications to the atomic systems which are described by these wave functions. These applications give a measure of the usefulness of HF approximate wave functions in calculating and interpreting physical phenomena.

In the computational procedure we have found that several basis sets are capable of yielding the minimum-energy wave function. This is probably because the different sets span the same manifold, at least to the order of accuracy of the calculations. In addition, as noted in Chapter III, the variation of the energy with respect to the basis function parameters does not follow a smooth surface over a wide range. Consequently, when

dealing with large basis sets, the feasibility of an automatic minimization procedure, whereby the best parameters are predicted on the basis of previous values, can be seriously questioned.

It has been known for some time that the matrix SCF process will, on occasion, diverge or become unstable and not yield a solution. Such behavior occurs even when an extrapolation procedure is incorporated to minimize its possibility. In the work on the fluorine atom, instability of the SCF process took place for orbitals near the energy minimum and at times even after one hundred iterations. When using the Nesbet scheme,⁽²³⁾ which ignores the off-diagonal multipliers, instability did not occur for fluorine.⁽⁵¹⁾ One is led to attribute the instability to the small magnitude of the 2p eigenvalue when compared with $\lambda_{2p,2p}$, so that the Fock operator of (2.44) is only slightly stable. This is indicated by the fact that when instability occurred, we found that the 2p eigenvalue had become positive while the 2s eigenvalue was still sufficiently negative. However, the author has encountered instability of the SCF process for closed-shell systems, where the Fock operator should be highly stable. In view of the common occurrence of instability and/or divergence of the SCF iterative process, it is evident that if the matrix SCF scheme is to continue as a useful research tool, the SCF mathematical process should be examined from the standpoint of mathematical analysis with the possibility in mind of introducing a constraint to assure convergence, or at least to set bounds on the region of stability of the Fock operator.

If we take cognizance of the instability difficulties encountered with the Fock operator, (2.44), for the fluorine configuration, the difficulty reported with the boron configuration,⁽⁵⁹⁾ and the excessive time consumed in obtaining an SCF solution for sodium, it appears that the matrix SCF procedure for atomic structure calculations may not be useful past the third row of the periodic table. This is primarily due to the large basis sets which must be used to minimize the energy, and as a consequence, the computational time becomes a major obstacle. Cohen⁽⁶⁰⁾ has recently shown that, if exchange is neglected, the electronic structure of large systems, e.g., of uranium, may be calculated to high accuracy by numerical integration in two hours. This high accuracy, stated as six figures for the eigenvalues, was achieved by using a large number of grid points (613 points in the case of uranium). The feasibility of accurate HF-SCF calculations by numerical integration appears to have been amply demonstrated by Cohen's work and the works of the Hartrees, Froese, and Worsely.

It is the author's judgement that future atomic SCF calculations would be more efficiently and economically done by numerical integration utilizing a very fine, highly selected, grid of points. The calculational time in this manner could be brought to a reasonable figure. To satisfy the

demand for analytic orbitals, the numerical orbitals could be fitted by analytic expansions, as demonstrated by Löwdin.⁽¹⁹⁾ The Roothaan SCF method still seems preferable for molecular and solid state calculations where numerical integration seems infeasible and the calculations are still crude.

APPENDIX A EVALUATION OF THE ENERGY MATRIX

In this appendix we illustrate how the constants a and b of equation (2.22) may be evaluated for a particular term of a configuration. We adopt the Slater-Shortley method for the evaluation of the energy expression.

We rewrite the expression for the wave function (2.18),

$$\Psi = \sum_{K'} a_K D_K \quad , \quad (A.1)$$

where the D_K are orthonormal determinants and the summation is over all possible determinants which may be formed from the given configuration. This leads to a secular equation for the energy,

$$\det(H - El) = 0 \quad , \quad (A.2)$$

where $H_{K'K} = (D_{K'} | \mathcal{H} | D_K)$ and l is the unit matrix. In general, (A.2) is reducible so that the majority of the matrix elements are zero. One then employs the invariance of the trace (diagonal-sum rule) to find the energy of each spectroscopic term.

Example I: ns

There are two possible determinants which may be formed:

$$\begin{aligned} D_1 &\equiv \mathcal{A} \left\{ n00 \frac{1}{2} \right\} \\ D_2 &\equiv \mathcal{A} \left\{ n00 \frac{\bar{1}}{2} \right\} \quad , \end{aligned}$$

where the core configuration has been assumed and the four quantum numbers for the open-shell spin-orbitals are listed. The overhead bar signifies a negative number.

These determinants lead to the secular equation

$$\begin{vmatrix} (H_{11} - E) & 0 \\ 0 & (H_{22} - E) \end{vmatrix} = 0 \quad ,$$

since $H_{ij} = 0$ unless $(M_L)_i = (M_L)_j$ and $(M_S)_i = (M_S)_j$.

There is only one term present, a 2S , so that either determinant will yield the energy of the term. We use D_1 and evaluate H_{11} . If we designate the sum of the one-electron energies and the two-electron energies of the core and core-open shell orbitals by E_0 , then

$$E = H_{11} = E_0 \quad .$$

We next utilize (2.20) and make use of the fact that for equivalent electrons*

$$G^k(n\ell, n\ell) = F^k(n\ell, n\ell) \quad .$$

We obtain

$$\frac{1}{4}[2aF^0 - bF^0] = 0$$

or

$$a = \frac{b}{2} \quad .$$

As there are no other requirements on a and b , we may assume a value for either a or b and the other is determined.

Example II: $2p^5$

There are now six possible determinants which may be formed, namely,

$$D_1 \equiv A\left\{211\frac{1}{2}, 210\frac{1}{2}, 21\bar{1}\frac{1}{2}, 211\frac{\bar{1}}{2}, 210\frac{\bar{1}}{2}\right\} \quad ,$$

$$D_2 \equiv A\left\{211\frac{1}{2}, 210\frac{1}{2}, 21\bar{1}\frac{1}{2}, 211\frac{\bar{1}}{2}, 21\bar{1}\frac{\bar{1}}{2}\right\} \quad ,$$

$$D_3 \equiv A\left\{211\frac{1}{2}, 210\frac{1}{2}, 21\bar{1}\frac{1}{2}, 210\frac{\bar{1}}{2}, 21\bar{1}\frac{\bar{1}}{2}\right\} \quad ,$$

$$D_4 \equiv A\left\{211\frac{1}{2}, 210\frac{1}{2}, 211\frac{\bar{1}}{2}, 210\frac{\bar{1}}{2}, 21\bar{1}\frac{\bar{1}}{2}\right\} \quad ,$$

$$D_5 \equiv A\left\{211\frac{1}{2}, 21\bar{1}\frac{1}{2}, 211\frac{\bar{1}}{2}, 210\frac{\bar{1}}{2}, 21\bar{1}\frac{\bar{1}}{2}\right\} \quad ,$$

and

$$D_6 \equiv A\left\{210\frac{1}{2}, 21\bar{1}\frac{1}{2}, 211\frac{\bar{1}}{2}, 210\frac{\bar{1}}{2}, 21\bar{1}\frac{\bar{1}}{2}\right\} \quad .$$

*Equivalent electrons are electrons described by the same $n\ell$ values.

These lead to the following secular equation for the energy:

$$\begin{vmatrix} (H_{11} - E) & & & & & & 0 \\ & (H_{22} - E) & & & & & \\ & & (H_{33} - E) & & & & \\ & & & (H_{44} - E) & & & \\ & & & & (H_{55} - E) & & \\ & 0 & & & & (H_{66} - E) & \\ & & & & & & (H_{66} - E) \end{vmatrix} = 0.$$

We consequently see that

$$H_{11} = H_{22} = H_{33} = H_{44} = H_{55} = H_{66} = E, \quad ,$$

so that any one of the determinants may be used to evaluate E for the resultant 2P state.

We now evaluate the matrix element H_{11} . Let us designate our space-orbitals by

$$1 \equiv 21\bar{1}; \quad 2 \equiv 210; \quad 3 \equiv 211 \quad .$$

The energy is then

$$\begin{aligned} E = H_{11} &= E_0 + J_{33} + J_{22} + 4J_{32} + 2J_{31} + 2J_{21} - 2K_{32} - K_{31} - K_{21} \\ &= E_0 + \left(F^0 + \frac{1}{25} F^2\right) + \left(F^0 + \frac{4}{25} F^2\right) + \left(4F^0 - \frac{8}{25} F^2\right) \\ &\quad + \left(2F^0 + \frac{2}{25} F^2\right) + \left(2F^0 - \frac{4}{25} F^2\right) \\ &\quad - \frac{6}{25} F^2 - \frac{6}{25} F^2 - \frac{3}{25} F^2 \\ &= E_0 + 10 F^0 - \frac{4}{5} F^2 \quad . \end{aligned}$$

As the last step, we equate the last two terms of E to the expansion of (2.22):

$$10 F^0 - \frac{4}{5} F^2 = \left(\frac{5}{6}\right)^2 (3)^2 \left[2aF^0 - \frac{b}{2} \left(\frac{2}{3} F^0 + \frac{4}{15} F^2\right) \right] \quad ,$$

whence

$$a = b = 24/25 \quad .$$

APPENDIX B FORMULAE FOR THE ONE- AND TWO-ELECTRON MATRIX ELEMENTS FOR SLATER FUNCTIONS

There are a number of ways in which the integrals of (3.19) to (3.24) may be evaluated. We have chosen a particular formulation which is simple to code for an electronic digital computer.⁽²⁴⁾ These formulae for the matrix elements are:

$$\begin{aligned}
 S_{lpq} &= \left[V_{2n_{lp}}(\zeta_{lp}) V_{2n_{lq}}(\zeta_{lq}) \right]^{-1/2} V_{n_{lp}+n_{lq}} \left(\frac{\zeta_{lp} + \zeta_{lq}}{2} \right) , \\
 U_{lpq} &= 2 \left[V_{2n_{lp}}(\zeta_{lp}) V_{2n_{lq}}(\zeta_{lq}) \right]^{-1/2} V_{n_{lp}+n_{lq}-1} \left(\frac{\zeta_{lp} + \zeta_{lq}}{2} \right) , \\
 T_{lpq} &= \frac{1}{2} \zeta_{lp} \zeta_{lq} \left[V_{2n_{lp}}(\zeta_{lp}) V_{2n_{lq}}(\zeta_{lq}) \right]^{-1/2} \\
 &\quad \times \left\{ V_{n_{lp}+n_{lq}} \left(\frac{\zeta_{lp} + \zeta_{lq}}{2} \right) \right. \\
 &\quad \left. - \left[W_{l,n_{lp}}(\zeta_{lp}) + W_{l,n_{lq}}(\zeta_{lq}) \right] V_{n_{lp}+n_{lq}-1} \left(\frac{\zeta_{lp} + \zeta_{lq}}{2} \right) \right. \\
 &\quad \left. + W_{l,n_{lp}}(\zeta_{lp}) W_{l,n_{lq}}(\zeta_{lq}) V_{n_{lp}+n_{lq}-2} \left(\frac{\zeta_{lp} + \zeta_{lq}}{2} \right) \right\} , \\
 J_{lpq,l'rs} &= U_{lpq} S_{l'rs} C_{n_{lp}+n_{lq}-1, n_{l'r}+n_{l's}} \left(\frac{\zeta_{lp} + \zeta_{lq}}{\zeta_{l'r} + \zeta_{l's}} \right) \\
 &\quad + U_{l'rs} S_{lpq} C_{n_{l'r}+n_{l's}-1, n_{lp}+n_{lq}} \left(\frac{\zeta_{l'r} + \zeta_{l's}}{\zeta_{lp} + \zeta_{lq}} \right)
 \end{aligned}$$

and

$$\begin{aligned}
 K_{lpq,l'rs}^k &= \left[V_{2n_{lp}}(\zeta_{lp}) V_{2n_{lq}}(\zeta_{lq}) V_{2n_{l'r}}(\zeta_{l'r}) V_{2n_{l's}}(\zeta_{l's}) \right]^{-1/2} \\
 &\quad \times \left[V_{n_{lp}+n_{l'r}-k-1} \left(\frac{\zeta_{lp} + \zeta_{l'r}}{2} \right) V_{n_{lq}+n_{l's}+k} \left(\frac{\zeta_{lq} + \zeta_{l's}}{2} \right) \right. \\
 &\quad \times C_{n_{lp}+n_{l'r}-k-1, n_{lq}+n_{l's}+k} \left(\frac{\zeta_{lp} + \zeta_{l'r}}{\zeta_{lq} + \zeta_{l's}} \right) \\
 &\quad \left. + V_{n_{lq}+n_{l's}-k-1} \left(\frac{\zeta_{lq} + \zeta_{l's}}{2} \right) V_{n_{lp}+n_{l'r}+k} \left(\frac{\zeta_{lp} + \zeta_{l'r}}{2} \right) \right]
 \end{aligned}$$

$$\begin{aligned}
& \times C_{n_{\ell_q}+n_{\ell'_s}-k-1, n_{\ell_p}+n_{\ell'_r}+k} \left(\frac{\zeta_{\ell_q} + \zeta_{\ell'_s}}{\zeta_{\ell_p} + \zeta_{\ell'_r}} \right) \\
& + V_{n_{\ell_p}+n_{\ell'_s}-k-1} \left(\frac{\zeta_{\ell_p} + \zeta_{\ell'_s}}{2} \right) V_{n_{\ell_q}+n_{\ell'_r}+k} \left(\frac{\zeta_{\ell_q} + \zeta_{\ell'_r}}{2} \right) \\
& \times C_{n_{\ell_p}+n_{\ell'_s}-k-1, n_{\ell_q}+n_{\ell'_r}+k} \left(\frac{\zeta_{\ell_p} + \zeta_{\ell'_s}}{\zeta_{\ell_q} + \zeta_{\ell'_r}} \right) \\
& + V_{n_{\ell_q}+n_{\ell'_r}-k-1} \left(\frac{\zeta_{\ell_q} + \zeta_{\ell'_r}}{2} \right) V_{n_{\ell_p}+n_{\ell'_s}+k} \left(\frac{\zeta_{\ell_p} + \zeta_{\ell'_s}}{2} \right) \\
& \times C_{n_{\ell_q}+n_{\ell'_r}-k-1, n_{\ell_p}+n_{\ell'_s}+k} \left(\frac{\zeta_{\ell_q} + \zeta_{\ell'_r}}{\zeta_{\ell_p} + \zeta_{\ell'_s}} \right) \Big] \quad ,
\end{aligned}$$

where

$$V_i(x) = x^{-i-1} i! \quad ,$$

$$W_{ij}(x) = 2x^{-1}(j-i-1) \quad ,$$

and

$$C_{\alpha\beta}(t) = (\alpha!\beta!)^{-1} t^{\alpha+1} \int_0^\infty du \cdot u^\alpha e^{-tu} \int_0^u dv \cdot v^\beta e^{-v} \quad .$$

The functions $C_{\alpha\beta}(t)$ can be computed from the recurrence relation

$$C_{\alpha\beta}(t) = (1+t)^{-1} [tC_{\alpha-1,\beta}(t) + C_{\alpha,\beta-1}(t) + \delta_{\beta 0}] \quad .$$

This recurrence relation holds for $\alpha, \beta \geq 0$, if we interpret terms with a negative index as zero.

APPENDIX C EVALUATION OF THE FUNCTIONS $K_{ij}^k(r)$

We consider the function defined by (6.6):

$$f_{n\ell}(r) = \int \bar{Y}_{\ell m} [F - \epsilon] \phi_{n\ell m}(r, \theta, \varphi) d\Omega \quad .$$

Since the operator F involves the summation over the subspecies for each symmetry type, we may handle this integral in the manner of Condon and Shortley.⁽⁹⁾ This integral then involves terms of the forms

$$J_{n\ell, n\ell}(r) = \int_0^\infty \frac{r_1^k}{r_1^k} [R_{n\ell}(r_1)]^2 r_1^2 dr_1$$

and

$$K_{n\ell, n'\ell'}^k(r) = \int_0^\infty \frac{r_1^k}{r_1^k} R_{n\ell}(r_1) R_{n'\ell'}(r_1) r_1^2 dr_1 \quad ,$$

where $R_{n\ell}(r)$ is the radial part of the basis function $\chi_{n\ell m}(r, \theta, \varphi)$.

It suffices to treat just the general K^k integral as the J 's are then a special form of the K^k . We utilize (3.18) and write

$$K_{n\ell, n'\ell'}^k(r) = N_1 N_2 \left[\int_0^r \frac{r_2^k}{r_2^{k+1}} r_2^{n+n'-2} e^{-(\zeta + \zeta')r_2} r_2^2 dr_2 + \int_r^\infty \frac{r_2^k}{r_2^{k+1}} r_2^{n+n'-2} e^{-(\zeta + \zeta')r_2} r_2^2 dr_2 \right] \quad ,$$

where N_1 and N_2 are the appropriate normalization factors. We then obtain

$$\begin{aligned} K_{n\ell, n'\ell'}^k(r) &= N_1 N_2 \left[r^{-k-1} \int_0^\infty r_2^{n+n'+k} \exp[-(\zeta + \zeta')r_2] dr_2 - r^{-k-1} \int_r^\infty r_2^{n+n'+k} \exp[-(\zeta + \zeta')r_2] dr_2 \right. \\ &\quad \left. + r^k \int_r^\infty r_2^{n+n'-k-1} \exp[-(\zeta + \zeta')r_2] dr_2 \right] \\ &= N_1 N_2 r^{n+n'} \left\{ \frac{(n+n'+k)!}{\alpha^{n+n'+k+1}} + A_{n+n'-k-1}(\alpha) - A_{n+n'+k}(\alpha) \right\} \quad , \end{aligned}$$

where $\alpha = r(\zeta + \zeta')$ and

$$A_n(\alpha) = \int_1^\infty x^n e^{-\alpha x} dx \quad .$$

APPENDIX D PARAMETERS FOR COMPROMISE SCF WAVE FUNCTIONS OF THE $1s^2$, $1s^22s$, AND $1s^22s^2$ CONFIGURATIONS

By compromise wave functions, we mean SCF wave functions of high accuracy given by a compact expansion. These wave functions are not as accurate as those of Appendix E, but should suffice in many calculations where it is impractical to carry as many basis functions as are utilized by the functions of Appendix E. The basis functions in this appendix are all s-type functions and may be written as

$$\chi_i = [4\pi(2N_i)!]^{-1/2} (2\zeta_i)^{N_i+1/2} r^{N_i-1} e^{-\zeta_i r}.$$

The ϵ listed in the following tables are the eigenvalues of the Fock operator (2.44), I is the calculated ionization potential, and E is the total electronic energy.

Table D.1. Parameters for He.

ζ	N	C_{1s}
3.00	1	0.175261
	2	0.010673
1.40	1	0.884315
	2	-0.051269
- ϵ		0.917946
I		0.917946
- $(\phi'/\phi)_0$		2.0018
- E		2.861671

Table D.2. Parameters for Li^+ .

ζ	N	C_{1s}
4.40	1	0.133937
	2	-0.008925
2.40	1	0.914304
	2	-0.029575
- ϵ		2.792361
I		2.792361
- $(\phi'/\phi)_0$		3.0113
- E		7.236412

Table D.3. Parameters for Be^{+2} .

ζ	N	C_{1s}
6.50	1	0.090576
	2	0.006158
3.40	1	0.932883
	2	-0.020880
- ϵ		5.667113
I		5.667113
- $(\phi'/\phi)_0$		4.0160
- E		13.61130

Table D.4. Parameters for B^{+3} .

ζ	N	C_{1s}
8.00	1	0.077235
	2	0.001760
4.40	1	0.942992
	2	-0.015453
- ϵ		9.541976
I		9.541976
- $(\phi'/\phi)_0$		5.0191
- E		21.98623

Table D.5. Parameters for C^{+4} .

ζ	N	C_{1s}
9.50	1	0.066900
	2	-0.000681
5.40	1	0.951308
	2	-0.012417
- ϵ		14.41689
I		14.41689
- $(\phi'/\phi)_0$		6.0208
- E		32.36119

Table D.7. Parameters for O^{+6} .

ζ	N	C_{1s}
12.50	1	0.052270
	2	-0.002955
7.40	1	0.963254
	2	-0.009141
- ϵ		27.16679
I		27.16679
- $(\phi'/\phi)_0$		8.0226
- E		59.11114

Table D.6. Parameters for N^{+5} .

ζ	N	C_{1s}
11.00	1	0.058772
	2	-0.002105
6.40	1	0.957950
	2	-0.010486
- ϵ		20.29183
I		20.29183
- $(\phi'/\phi)_0$		7.0218
- E		44.73616

Table D.8. Parameters for F^{+7} .

ζ	N	C_{1s}
14.00	1	0.047004
	2	-0.003450
8.40	1	0.967475
	2	-0.008121
- ϵ		35.04175
I		35.04175
- $(\phi'/\phi)_0$		9.0230
- E		75.48612

Table D.9. Parameters for Ne^{+8} .

ζ	N	C_{1s}
15.50	1	0.042610
	2	-0.003762
9.40	1	0.971012
	2	-0.007360
- ϵ		43.91672
I		43.91672
- $(\phi'/\phi)_0$		10.0234
- E		93.86111

Table D 10 Parameters for Li

ζ	N	C_{1s}	C_{2s}
4 40	1	0 128169	0 061628
	2	-0 012275	0 017507
2 40	1	0 926908	0 039733
	2	-0 037651	0 101098
0 67	1	0 005692	0 010105
	2	-0 002035	-1 043535
- ϵ		2 463469	0 079319
I		2 470616	0 196319
- $(\phi'/\phi)_0$		3 0137	2 9790
- E		7 432722	

Table D 12 Parameters for B^{+2}

ζ	N	C_{1s}	C_{2s}
8 00	1	0 074290	0 044364
	2	0 000132	0 012092
4 40	1	0 947348	0 092899
	2	-0 019849	0 070947
1 71	1	0 005326	0 331356
	2	-0 000468	-1 307998
- ϵ		8 750132	1 113787
I		8 778937	1 389851
- $(\phi'/\phi)_0$		5 0201	5 0076
- E		23 37599	

Table D 14 Parameters for N^{+4}

ζ	N	C_{1s}	C_{2s}
11 00	1	0 056341	0 045366
	2	-0 003290	0 011398
6 40	1	0 960742	0 071379
	2	-0 013702	0 065051
2 72	1	0 004414	0 485098
	2	-0 000007	-1 419215
- ϵ		19 05186	3 162021
I		19 10280	3 590855
- $(\phi'/\phi)_0$		7 0219	7 0157
- E		48 32685	

Table D 11 Parameters for Be^{+1}

ζ	N	C_{1s}	C_{2s}
6 50	1	0 087271	0 040000
	2	0 004118	0 011646
3 40	1	0 938933	0 102410
	2	-0 026475	0 068967
1 20	1	0 005943	0 219443
	2	-0 001096	-1 218766
- ϵ		5 102721	0 467844
I		5 120512	0 666145
- $(\phi'/\phi)_0$		4 0181	4 0008
- E		14 27739	

Table D 13 Parameters for C^{+3}

ζ	N	C_{1s}	C_{2s}
9 50	1	0 064265	0 040158
	2	-0 002034	0 009662
5 40	1	0 954646	0 088107
	2	-0 016070	0 056023
2 22	1	0 004797	0 440327
	2	-0 000143	-1 384259
- ϵ		13 40026	2 012257
I		13 44014	2 365002
- $(\phi'/\phi)_0$		6 0212	6 0192
- E		34 72606	

Table D 15 Parameters for O^{+5}

ζ	N	C_{1s}	C_{2s}
12 50	1	0 049983	0 048303
	2	-0 004029	0 012299
7 40	1	0 965734	0 058279
	2	-0 012059	0 069157
3 22	1	0 004084	0 525134
	2	0 000069	-1 448572
- ϵ		25 70418	4 562441
I		25 76618	5 067099
- $(\phi'/\phi)_0$		8 0224	8 0140
- E		64 17804	

Table D.16. Parameters for F^{+6} .

ζ	N	C_{1s}	C_{2s}
14.00	1	0.044986	0.049775
	2	-0.004373	0.012704
8.40	1	0.969455	0.047993
	2	-0.010619	0.070546
3.72	1	0.003673	0.560359
	2	0.000158	-1.473268
$-\epsilon$		33.35696	6.213265
I		33.43000	6.793585
$-(\phi'/\phi)_0$		9.0225	9.0131
$-E$		82.27949	

Table D.18. Parameters for Li^- .

ζ	N	C_{1s}	C_{2s}
4.40	1	0.133664	0.111961
	2	-0.009144	0.044848
2.40	1	0.913953	-0.101615
	2	-0.028962	0.222883
0.285	1	0.001612	-1.055194
	2	-0.001113	0.004754
$-\epsilon$		2.320989	0.013524
I		2.320989	0.013524
$-(\phi'/\phi)_0$		3.0111	2.8169
$-E$		7.427997	

Table D.20. Parameters for B^{+1} .

ζ	N	C_{1s}	C_{2s}
8.00	1	0.074950	0.076197
	2	0.000370	0.024671
4.40	1	0.945457	0.100824
	2	-0.017800	0.196901
1.42	1	0.005742	-0.202420
	2	-0.002364	-0.922348
$-\epsilon$		8.185896	0.873807
I		8.185896	0.873807
$-(\phi'/\phi)_0$		5.0191	4.9675
$-E$		24.23756	

Table D.17. Parameters for Ne^{+7} .

ζ	N	C_{1s}	C_{2s}
15.50	1	0.040635	0.038161
	2	-0.004643	0.008671
9.40	1	0.972956	0.052591
	2	-0.009759	0.047183
4.23	1	0.003469	0.632319
	2	0.000175	-1.514805
$-\epsilon$		42.00995	8.114297
I		42.09403	8.770233
$-(\phi'/\phi)_0$		10.0228	10.0242
$-E$		102.6311	

Table D.19. Parameters for Be .

ζ	N	C_{1s}	C_{2s}
6.50	1	0.088737	0.075841
	2	0.004895	0.028953
3.40	1	0.935313	0.064546
	2	-0.022712	0.208057
0.90	1	0.004590	-0.386020
	2	-0.002201	-0.740733
$-\epsilon$		4.732344	0.309131
I		4.732344	0.309131
$-(\phi'/\phi)_0$		4.0166	3.9163
$-E$		14.57298	

Table D.21. Parameters for C^{+2} .

ζ	N	C_{1s}	C_{2s}
9.50	1	0.064343	0.073559
	2	-0.002107	0.021417
5.40	1	0.953819	0.115219
	2	-0.015151	0.181766
1.93	1	0.006343	-0.066932
	2	-0.002390	-1.041633
$-\epsilon$		12.65066	1.694059
I		12.65066	1.694059
$-(\phi'/\phi)_0$		6.0203	5.9891
$-E$		36.40849	

Table D 22 Parameters for N^{+3}

ζ	N	C_{1s}	C_{2s}
11 00	1	0 056014	0 065289
	2	-0 003544	0 017043
6 40	1	0 960581	0 126612
	2	-0 013522	0 157940
2 44	1	0 006634	0 056139
	2	-0 002355	-1 138073
- ϵ		18 12006	2 766718
I		18 12006	2 766718
- $(\phi'/\phi)_0$		7 0210	7.0075
- E		51 08231	

Table D 24 Parameters for F^{+5}

ζ	N	C_{1s}	C_{2s}
14 00	1	0 044029	0 054391
	2	-0 004872	0 012328
8 40	1	0 970326	0 127488
	2	-0 011451	0 127278
3 45	1	0 006660	0 227570
	2	-0 002198	-1 263452
- ϵ		32 06540	5 665442
I		32 06540	5 665442
- $(\phi'/\phi)_0$		9 0217	9 0228
- E		87 93405	

Table D 23 Parameters for O^{+4}

ζ	N	C_{1s}	C_{2s}
12 50	1	0 049361	0 066281
	2	-0 004400	0 016928
7 40	1	0 966047	0 119116
	2	-0 012381	0 153934
2.94	1	0 006713	0 128979
	2	-0 002293	-1.195978
- ϵ		24 59215	4 090744
I		24 59215	4 090744
- $(\phi'/\phi)_0$		8 0215	8 0081
- E		68 25771	

Table D 25 Parameters for Ne^{+6}

ζ	N	C_{1s}	C_{2s}
15 50	1	0 039510	0 053432
	2	-0 005194	0 011932
9 40	1	0 974094	0 120245
	2	-0 010836	0 121903
3 95	1	0 006601	0 281647
	2	-0 002135	-1 302306
- ϵ		40 53979	7 490705
I		40 53979	7 490705
- $(\phi'/\phi)_0$		10 0220	10 0235
- E		110 1110	

APPENDIX E
PARAMETERS FOR THE BEST SCF WAVE FUNCTIONS
OF THE $1s^2$, $1s^22s$, AND $1s^22s^2$ CONFIGURATIONS

In this appendix we have listed the parameters used to obtain the best SCF wave functions of the $1s^2$, $1s^22s$, and $1s^22s^2$ configurations. These wave functions are more accurate than those listed in Appendix D. The parameters listed in this appendix were used to compute the orbital tables of Appendix F. The expansion functions are all s-type functions and may be written as

$$\chi_i = [4\pi(2N_i)!]^{-1/2} (2\zeta_i)^{N_i+1/2} r^{N_i-1} e^{-\zeta_i r}.$$

The ϵ listed in the tables are the eigenvalues of the Fock operator (2.44), I is the calculated ionization potential, and E is the total electronic energy.

Table E.1. Parameters for He.

ζ_M	N	C_{1s}
3.00	1	0.457418
	2	0.244272
	3	0.136571
	4	0.094513
	5	0.008192
	6	0.027670
1.40	1	0.000000
	2	0.129851
	3	0.113403
	4	-0.086860
	5	0.025460
	6	-0.002674
<hr/>		
$-\epsilon$		0.917956
I		0.917956
$-(\phi'/\phi)_0$		2.0019
$-E$		2.861680

Table E.2. Parameters for Li^{+1} .

ζ_M	N	C_{1s}
4.40	1	-0.000000
	2	-0.220023
	3	-0.126397
	4	-0.021018
	5	-0.028489
	6	0.015049
2.40	1	1.246497
	2	0.459177
	3	-0.675516
	4	0.408814
	5	-0.135526
	6	0.020320
<hr/>		
$-\epsilon$		2.792365
I		2.792365
$-(\phi'/\phi)_0$		3.0027
$-E$		7.236415

Table E.3. Parameters for Be^{+2} .

ζ_M	N	C_{1s}
6.50	1	0.443327
	2	0.189357
	3	0.059425
	4	0.025014
	5	-0.004885
	6	0.000707
3.40	1	0.000000
	2	0.533882
	3	-0.168932
	4	0.003107
	5	0.019426
	6	-0.005592
<hr/>		
$-\epsilon$		5.667116
I		5.667116
$-(\phi'/\phi)_0$		4.0028
$-E$		13.61130

Table E.5. Parameters for C^{+4} .

ζ_M	N	C_{1s}
9.50	1	0.474400
	2	0.195068
	3	0.071333
	4	0.038714
	5	0.001165
	6	0.008981
5.40	1	-0.000000
	2	0.441249
	3	-0.195623
	4	0.077636
	5	-0.021630
	6	-0.002943
<hr/>		
$-\epsilon$		14.41689
I		14.41689
$-(\phi'/\phi)_0$		6.0020
$-E$		32.36119

Table E.4. Parameters for B^{+3} .

ζ_M	N	C_{1s}
8.00	1	0.461639
	2	0.258029
	3	0.176207
	4	0.137810
	5	0.037801
	6	0.047757
4.40	1	0.000000
	2	0.187874
	3	-0.453636
	4	0.462170
	5	-0.213482
	6	0.040873
<hr/>		
$-\epsilon$		9.541979
I		9.541979
$-(\phi'/\phi)_0$		4.9967
$-E$		21.98623

Table E.6. Parameters for N^{+5} .

ζ_M	N	C_{1s}
11.00	1	0.483726
	2	0.329658
	3	0.181329
	4	0.097099
	5	0.022800
	6	0.018714
6.40	1	-0.000000
	2	-0.097140
	3	0.102628
	4	0.010245
	5	-0.021758
	6	0.005334
<hr/>		
$-\epsilon$		20.29183
I		20.29183
$-(\phi'/\phi)_0$		7.0012
$-E$		44.73616

Table E.7. Parameters for O^{+6} .

ζ_M	N	C_{1s}
12.50	1	0.490916
	2	0.262449
	3	-0.075741
	4	-0.149444
	5	-0.083258
	6	-0.058394
7.40	1	0.000000
	2	0.158968
	3	1.235800
	4	-1.109943
	5	0.444473
	6	-0.075629
$-\epsilon$		27.16679
I		27.16679
$-(\phi'/\phi)_0$		8.0116
$-E$		59.11115

Table E.8. Parameters for F^{+7} .

ζ_M	N	C_{1s}
14.00	1	0.496507
	2	0.195498
	3	0.035986
	4	-0.000214
	5	-0.013475
	6	-0.003290
8.40	1	0.000000
	2	0.399466
	3	0.039220
	4	-0.116937
	5	0.054289
	6	-0.009731
$-\epsilon$		35.04176
I		35.04176
$-(\phi'/\phi)_0$		9.0040
$-E$		75.48613

Table E.9. Parameters of Ne^{+8} .

ζ_M	N	C_{1s}
15.50	1	-0.000000
	2	0.009861
	3	-0.197848
	4	-0.197144
	5	-0.096674
	6	-0.058088
9.40	1	1.061048
	2	-0.154285
	3	1.306401
	4	-1.083190
	5	0.414569
	6	-0.067828
$-\epsilon$		43.91673
I		43.91673
$-(\phi'/\phi)_0$		10.0131
$-E$		93.86112

Table E.10. Parameters for Li.

ζ_M	N	C_{1s}	C_{2s}
4.50	1	0.483756	0.076821
	2	0.196364	0.022188
	3	0.077166	0.003878
	4	0.034979	0.001886
2.40	1	-0.000000	-0.000008
	2	0.388381	0.153833
	3	-0.094911	-0.040527
	4	0.003019	0.035474
0.67	1	0.024068	-0.017657
	2	-0.023095	1.068963
	3	0.012061	0.061040
	4	-0.002699	-0.031465
$-\epsilon$		2.463447	0.079318
I		2.470595	0.196323
$-(\phi'/\phi)_0$		3.0064	3.0077
$-E$		7.432727	

Table E.12. Parameters for B⁺₂.

ζ_M	N	C_{1s}	C_{2s}
8.00	1	0.448959	0.112567
	2	0.205013	0.027197
	3	0.074763	0.000091
	4	0.030916	-0.000003
4.40	1	-0.000001	0.000000
	2	0.351849	0.300086
	3	-0.081477	-0.080195
	4	-0.013877	0.071064
1.71	1	0.125970	0.024729
	2	-0.089925	-1.105348
	3	0.035185	-0.062447
	4	-0.006166	0.005804
$-\epsilon$		8.750137	1.113790
I		8.778943	1.389852
$-(\phi'/\phi)_0$		5.0046	5.0082
$-E$		23.37599	

Table E.11. Parameters for Be⁺₂.

ζ_M	N	C_{1s}	C_{2s}
6.50	1	0.440586	0.081689
	2	0.195205	0.035570
	3	0.068732	0.010554
	4	0.029457	0.005376
3.40	1	0.000000	0.000000
	2	0.487708	0.130829
	3	-0.161563	-0.011894
	4	0.022777	0.015755
1.20	1	0.027352	0.182542
	2	-0.022703	-1.224015
	3	0.010766	0.031685
	4	-0.002141	-0.016516
$-\epsilon$		5.102764	0.467873
I		5.120553	0.666146
$-(\phi'/\phi)_0$		4.0043	4.0032
$-E$		14.27740	

Table E.13. Parameters for C⁺₂.

ζ_M	N	C_{1s}	C_{2s}
9.50	1	0.533313	0.108615
	2	0.159594	0.030937
	3	0.032675	0.003923
	4	0.008289	0.002561
5.40	1	0.017451	-0.000699
	2	0.880749	0.233813
	3	-0.312327	-0.042908
	4	0.152329	0.046757
2.22	1	-0.593017	0.170852
	2	0.402856	-1.212283
	3	-0.145966	-0.050951
	4	0.024388	0.003938
$-\epsilon$		13.40033	2.012297
I		13.44021	2.365003
$-(\phi'/\phi)_0$		6.0103	6.0064
$-E$		34.72606	

Table E.14. Parameters for N^{+4} .

ζ_M	N	C_{1s}	C_{2s}
11.00	1	0.486051	0.173324
	2	0.187465	-0.043641
	3	0.057554	-0.051667
	4	0.019405	-0.022463
6.40	1	-0.000023	-0.000000
	2	0.463619	0.797662
	3	-0.137653	-0.328748
	4	0.029486	0.206778
2.72	1	-0.023679	-0.297734
	2	0.009050	-0.956271
	3	0.000519	-0.138574
	4	-0.000683	0.016855
$-\epsilon$		19.05186	3.162022
I		19.10281	3.590855
$-(\phi'/\phi)_0$		7.0085	7.0275
$-E$		48.32685	

Table E.16. Parameters for F^{+6} .

ζ_M	N	C_{1s}	C_{2s}
14.00	1	0.505707	0.104220
	2	0.206587	-0.005522
	3	0.066752	-0.016594
	4	0.022424	-0.005293
8.40	1	0.000000	0.000000
	2	0.395827	0.323193
	3	-0.077786	-0.113575
	4	0.013914	0.070940
3.72	1	-0.071307	0.325763
	2	0.049249	-1.361125
	3	-0.017450	-0.023285
	4	0.002925	0.001102
$-\epsilon$		33.35692	6.213238
I		33.42996	6.793586
$-(\phi'/\phi)_0$		9.0073	9.0140
$-E$		82.27949	

Table E.15. Parameters for O^{+5} .

ζ_M	N	C_{1s}	C_{2s}
12.50	1	0.508584	0.150478
	2	0.183572	-0.029041
	3	0.052329	-0.037482
	4	0.016647	-0.014409
7.40	1	0.000000	-0.000000
	2	0.527528	0.611948
	3	-0.154423	-0.235503
	4	0.047600	0.150046
3.22	1	-0.139916	-0.053223
	2	0.083134	-1.126041
	3	-0.025213	-0.089833
	4	0.003474	0.009996
$-\epsilon$		25.70416	4.562424
I		25.76616	5.067099
$-(\phi'/\phi)_0$		8.0091	8.0196
$-E$		64.17804	

Table E.17. Parameters for Ne^{+7} .

ζ_M	N	C_{1s}	C_{2s}
15.50	1	-0.000001	-0.000000
	2	0.074443	-0.120383
	3	0.053242	-0.069735
	4	0.027463	-0.022126
9.40	1	1.051870	0.331420
	2	-0.388203	0.548671
	3	0.236094	-0.240153
	4	-0.077422	0.161106
4.23	1	0.026214	-0.023754
	2	0.021212	-1.168941
	3	-0.019783	-0.089115
	4	0.005227	0.007987
$-\epsilon$		42.00999	8.114323
I		42.09407	8.770233
$-(\phi'/\phi)_0$		10.0036	10.0237
$-E$		102.6311	

Table E.18. Parameters for Li^- .

ζ_M	N	C_{1s}	C_{2s}
6.00	1	0.101716	0.139053
	2	0.024322	0.124683
	3	0.012709	-0.004005
	4	0.009070	-0.013930
4.50	1	0.328526	-0.141198
	2	0.230096	-0.212811
	3	0.036193	0.106808
	4	0.045538	-0.136282
2.40	1	0.000000	-0.000000
	2	0.434302	0.688443
	3	-0.134309	-0.418560
	4	0.021620	0.186442
0.85	1	-0.000477	-1.276428
	2	0.000720	0.406510
	3	-0.000527	-0.252797
	4	0.000161	0.001068
$-\epsilon$		2.322789	0.01453434
I		2.322789	0.01343434
$-(\phi'/\phi)_0$		3.0078	3.0227
$-E$		7.428232	

Table E.20. Parameters for B^{+1} .

ζ_M	N	C_{1s}	C_{2s}
8.00	1	0.460775	0.117108
	2	0.199242	0.054041
	3	0.069294	0.017384
	4	0.028164	0.007737
4.40	1	0.000000	-0.000000
	2	0.443290	0.207201
	3	-0.123551	0.012615
	4	0.017767	0.010206
1.42	1	0.001179	-0.197772
	2	-0.000443	-0.983398
	3	-0.000185	0.075585
	4	0.000137	-0.032056
$-\epsilon$		8.185922	0.873823
I		8.185922	0.873823
$-(\phi'/\phi)_0$		5.0053	5.0025
$-E$		24.23758	

Table E.19. Parameters for Be.

ζ_M	N	C_{1s}	C_{2s}
6.50	1	0.442306	-0.106320
	2	0.196025	-0.036690
	3	0.069198	-0.006877
	4	0.029984	-0.001767
3.40	1	-0.000000	0.000171
	2	0.494810	-0.303518
	3	-0.161936	0.058670
	4	0.026115	-0.061146
0.90	1	0.006644	0.496479
	2	-0.007953	0.694577
	3	0.004735	-0.050554
	4	-0.001211	0.044122
$-\epsilon$		4.732670	0.309270
I		4.732670	0.309270
$-(\phi'/\phi)_0$		4.0041	4.0080
$-E$		14.57302	

Table E.21. Parameters for C^{+2} .

ζ_M	N	C_{1s}	C_{2s}
9.50	1	0.459555	0.105788
	2	0.223948	0.070123
	3	0.085812	0.029392
	4	0.034333	0.013314
5.40	1	-0.000000	-0.000000
	2	0.249534	0.050414
	3	-0.008724	0.085275
	4	-0.039459	-0.041610
1.93	1	0.152639	0.120917
	2	-0.121390	-1.241777
	3	0.051224	0.119930
	4	-0.009813	-0.033566
$-\epsilon$		12.65062	1.694049
I		12.65062	1.694049
$-(\phi'/\phi)_0$		6.0047	5.9994
$-E$		36.40850	

Table E.22. Parameters for N^{+3} .

ζ_M	N	C_{1s}	C_{2s}
11.00	1	0.510710	0.076037
	2	0.160686	0.093292
	3	0.038083	0.047377
	4	0.011162	0.020769
6.40	1	-0.000000	0.000000
	2	0.680141	-0.183050
	3	-0.246970	0.182797
	4	0.097086	-0.105663
2.44	1	-0.266102	0.490948
	2	0.195151	-1.504409
	3	-0.076294	0.174334
	4	0.013598	-0.040179
$-\epsilon$		18.12011	2.766736
I		18.12011	2.766736
$-(\phi'/\phi)_0$		7.0105	6.9950
$-E$		51.08231	

Table E.24. Parameters for F^{+5} .

ζ_M	N	C_{1s}	C_{2s}
14.00	1	0.829455	0.622211
	2	0.448085	0.493860
	3	0.172047	0.221045
	4	0.060943	0.084923
8.40	1	-0.718260	1.034748
	2	0.318192	-0.151229
	3	0.108552	0.502918
	4	-0.073506	-0.181980
3.45	1	0.000000	-0.000000
	2	0.043768	-0.987677
	3	-0.034097	-0.148813
	4	0.009075	0.032957
$-\epsilon$		32.06549	5.665469
I		32.06549	5.665469
$-(\phi'/\phi)_0$		8.9957	8.9243
$-E$		87.93404	

Table E.23. Parameters for O^{+4} .

ζ_M	N	C_{1s}	C_{2s}
12.50	1	0.520564	0.125861
	2	0.174232	-0.031133
	3	0.046073	-0.037022
	4	0.014738	-0.015858
7.40	1	0.000000	-0.000000
	2	0.615552	0.502938
	3	-0.194008	-0.227788
	4	0.077870	0.097188
2.94	1	-0.267431	0.082724
	2	0.190808	-1.235532
	3	-0.073026	0.052984
	4	0.012819	-0.018079
$-\epsilon$		24.59208	4.090721
I		24.59208	4.090721
$-(\phi'/\phi)_0$		8.0095	8.0280
$-E$		68.25771	

Table E.25. Parameters for Ne^{+6} .

ζ_M	N	C_{1s}	C_{2s}
15.50	1	-0.000000	-0.000000
	2	0.036173	-0.111155
	3	0.028963	-0.063038
	4	0.015017	-0.017915
9.40	1	0.968036	0.414288
	2	-0.310659	0.559569
	3	0.124151	-0.212796
	4	-0.067962	0.158253
3.95	1	0.335375	-0.382590
	2	-0.231809	-0.892244
	3	0.087142	-0.129215
	4	-0.015221	0.016802
$-\epsilon$		40.53982	7.490716
I		40.53982	7.490716
$-(\phi'/\phi)_0$		10.0104	10.0181
$-E$		110.1110	

APPENDIX F
ORBITAL TABLES FOR He, Li^+ , Li, Li^- , AND Be

The orbital tables contained in this appendix have been calculated from the (eight-figure) parameter tables of Appendix E. We list the orbital ϕ , its derivative ϕ' , the Hartree function P , its derivative P' , and the two goodness functions $f(r)$ and $g(r)$ of (4.3).

Table F.1. Radial Characteristics of the Hartree-Fock He 1s Orbital.

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
0.	1.34097	-2.68449	0.	4.75363		
0.01	1.31442	-2.62558	0.04660	4.56644	0.18577	0.84604
0.02	1.28846	-2.56802	0.09135	4.38539	0.06522	0.94486
0.03	1.26306	-2.51178	0.13432	4.21031	0.02878	0.97518
0.04	1.23822	-2.45682	0.17557	4.04100	0.01292	0.98863
0.05	1.21392	-2.40314	0.21516	3.87728	0.00500	0.99551
0.06	1.19015	-2.35069	0.25314	3.71900	0.00082	0.99925
0.07	1.16690	-2.29945	0.28956	3.56596	-0.00139	1.00130
0.08	1.14416	-2.24940	0.32447	3.41802	-0.00249	1.00237
0.09	1.12191	-2.20051	0.35794	3.27501	-0.00294	1.00286
0.10	1.10014	-2.15276	0.38999	3.13678	-0.00301	1.00298
0.12	1.05802	-2.06055	0.45007	2.87404	-0.00259	1.00267
0.14	1.01769	-1.97260	0.50507	2.62865	-0.00191	1.00205
0.16	0.97909	-1.88870	0.55532	2.39953	-0.00124	1.00137
0.18	0.94212	-1.80867	0.60115	2.18564	-0.00066	1.00077
0.20	0.90672	-1.73234	0.64284	1.98602	-0.00022	1.00027
0.22	0.87280	-1.65953	0.68068	1.79977	0.00009	0.99989
0.24	0.84031	-1.59008	0.71492	1.62602	0.00030	0.99962
0.26	0.80918	-1.52384	0.74580	1.46397	0.00041	0.99944
0.28	0.77934	-1.46064	0.77355	1.31289	0.00046	0.99935
0.30	0.75073	-1.40035	0.79838	1.17205	0.00046	0.99933
0.35	0.68426	-1.26142	0.84897	0.86056	0.00034	0.99946
0.40	0.62434	-1.13778	0.88529	0.59989	0.00017	0.99971
0.45	0.57025	-1.02763	0.90967	0.38222	0.00002	0.99997
0.50	0.52137	-0.92938	0.92411	0.20094	-0.00008	1.00016
0.55	0.47714	-0.84165	0.93028	0.05045	-0.00012	1.00028
0.60	0.43706	-0.76319	0.92959	-0.07395	-0.00013	1.00031
0.65	0.40068	-0.69293	0.92325	-0.17626	-0.00010	1.00028
0.70	0.36764	-0.62992	0.91228	-0.25984	-0.00007	1.00021
0.75	0.33759	-0.57331	0.89753	-0.32755	-0.00003	1.00011
0.80	0.31022	-0.52240	0.87975	-0.38179	-0.00000	1.00001
0.85	0.28526	-0.47652	0.85954	-0.42461	0.00002	0.99992
0.90	0.26249	-0.43513	0.83745	-0.45774	0.00004	0.99985
0.95	0.24168	-0.39773	0.81391	-0.48267	0.00004	0.99980
1.00	0.22266	-0.36388	0.78930	-0.50064	0.00004	0.99978
1.05	0.20524	-0.33322	0.76394	-0.51273	0.00004	0.99979
1.10	0.18929	-0.30540	0.73811	-0.51986	0.00003	0.99982
1.15	0.17466	-0.28013	0.71202	-0.52282	0.00002	0.99986
1.20	0.16124	-0.25714	0.68588	-0.52227	0.00001	0.99992
1.25	0.14891	-0.23621	0.65985	-0.51880	0.00000	0.99998
1.30	0.13758	-0.21713	0.63404	-0.51289	-0.00000	1.00004
1.35	0.12717	-0.19972	0.60859	-0.50499	-0.00001	1.00009
1.40	0.11759	-0.18382	0.58357	-0.49544	-0.00001	1.00014
1.45	0.10877	-0.16928	0.55907	-0.48457	-0.00002	1.00017
1.50	0.10064	-0.15598	0.53513	-0.47265	-0.00002	1.00020
1.55	0.09315	-0.14380	0.51182	-0.45991	-0.00002	1.00020
1.60	0.08624	-0.13263	0.48915	-0.44655	-0.00002	1.00020
1.65	0.07987	-0.12239	0.46717	-0.43274	-0.00001	1.00018
1.70	0.07399	-0.11299	0.44588	-0.41862	-0.00001	1.00016
1.75	0.06856	-0.10435	0.42531	-0.40433	-0.00001	1.00012
1.80	0.06354	-0.09642	0.40545	-0.38996	-0.00000	1.00008
1.85	0.05891	-0.08911	0.38631	-0.37561	-0.00000	1.00003
1.90	0.05462	-0.08240	0.36789	-0.36134	0.00000	0.99998
1.95	0.05066	-0.07621	0.35018	-0.34724	0.00000	0.99993
2.00	0.04699	-0.07051	0.33316	-0.33334	0.00001	0.99988
2.10	0.04046	-0.06042	0.30119	-0.30634	0.00001	0.99980
2.20	0.03486	-0.05182	0.27185	-0.28059	0.00001	0.99975
2.30	0.03005	-0.04450	0.24502	-0.25627	0.00001	0.99974
2.40	0.02592	-0.03824	0.22055	-0.23345	0.00001	0.99977
2.50	0.02237	-0.03289	0.19828	-0.21218	0.00000	0.99984
2.60	0.01932	-0.02831	0.17806	-0.19245	0.00000	0.99993
2.70	0.01669	-0.02439	0.15974	-0.17423	-0.00000	1.00005
2.80	0.01442	-0.02102	0.14317	-0.15747	-0.00000	1.00016
2.90	0.01247	-0.01812	0.12820	-0.14211	-0.00000	1.00027

Table F.1. (continued).

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
3.00	0.01079	-0.01564	0.11470	-0.12806	-0.00000	1.00036
3.20	0.00808	-0.01166	0.09161	-0.10360	-0.00000	1.00044
3.40	0.00605	-0.00870	0.07297	-0.08345	-0.00000	1.00036
3.60	0.00454	-0.00651	0.05799	-0.06697	-0.00000	1.00013
3.80	0.00341	-0.00487	0.04598	-0.05357	0.00000	0.99977
4.00	0.00257	-0.00365	0.03639	-0.04273	0.00000	0.99939
4.20	0.00193	-0.00274	0.02875	-0.03400	0.00000	0.99906
4.40	0.00145	-0.00206	0.02267	-0.02699	0.00000	0.99888
4.60	0.00110	-0.00155	0.01786	-0.02139	0.00000	0.99893
4.80	0.00083	-0.00117	0.01404	-0.01692	0.00000	0.99926
5.00	0.00062	-0.00088	0.01103	-0.01336	0.00000	0.99986
5.50	0.00031	-0.00043	0.00600	-0.00735	-0.00000	1.00235
6.00	0.00015	-0.00021	0.00324	-0.00401	-0.00000	1.00495
6.50	0.00008	-0.00011	0.00174	-0.00217	-0.00000	1.00525
7.00	0.00004	-0.00005	0.00094	-0.00116	-0.00000	1.00049
7.50	0.00002	-0.00003	0.00050	-0.00062	0.00000	0.98823
8.00	0.00001	-0.00001	0.00027	-0.00033	0.00000	0.96702
8.50	0.00000	-0.00001	0.00015	-0.00018	0.00000	0.93689
9.00	0.00000	-0.00000	0.00008	-0.00010	0.00000	0.89959
9.50	0.00000	-0.00000	0.00005	-0.00005	0.00000	0.85830

Table F.2. Radial Characteristics of the Hartree-Fock Li^+ 1s Orbital.

r	$\phi(r)$	$\phi'(r)$	P(r)	P'(r)	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
0.	2.61477	-7.85125	0.	9.26911		
0.01	2.53751	-7.60096	0.08995	8.72581	0.43800	0.93819
0.02	2.46272	-7.35897	0.17460	8.20838	0.12544	0.98176
0.03	2.39031	-7.12502	0.25420	7.71570	0.03941	0.99409
0.04	2.32020	-6.89886	0.32900	7.24665	0.00695	0.99893
0.05	2.25231	-6.68026	0.39921	6.80017	-0.00607	1.00097
0.06	2.18657	-6.46897	0.46507	6.37526	-0.01073	1.00176
0.07	2.12290	-6.26475	0.52678	5.97094	-0.01152	1.00194
0.08	2.06125	-6.06737	0.58455	5.58627	-0.01053	1.00183
0.09	2.00153	-5.87661	0.63857	5.22037	-0.00881	1.00158
0.10	1.94369	-5.69226	0.68902	4.87236	-0.00689	1.00127
0.12	1.83339	-5.34191	0.77990	4.22682	-0.00338	1.00066
0.14	1.72986	-5.01467	0.85851	3.64349	-0.00083	1.00017
0.16	1.63266	-4.70901	0.92602	3.11675	0.00073	0.99984
0.18	1.54137	-4.42347	0.98352	2.64147	0.00151	0.99965
0.20	1.45560	-4.15667	1.03199	2.21296	0.00175	0.99957
0.22	1.37499	-3.90733	1.07232	1.82695	0.00164	0.99957
0.24	1.29920	-3.67425	1.10533	1.47956	0.00134	0.99963
0.26	1.22792	-3.45632	1.13174	1.16724	0.00096	0.99972
0.28	1.16085	-3.25248	1.15223	0.88678	0.00059	0.99982
0.30	1.09773	-3.06175	1.16740	0.63526	0.00025	0.99992
0.32	1.03830	-2.88324	1.17782	0.41001	-0.00003	1.00001
0.34	0.98232	-2.71609	1.18396	0.20863	-0.00023	1.00008
0.36	0.92958	-2.55952	1.18630	0.02891	-0.00037	1.00014
0.38	0.87988	-2.41281	1.18525	-0.13113	-0.00045	1.00018
0.40	0.83301	-2.27527	1.18118	-0.27330	-0.00047	1.00020
0.42	0.78881	-2.14628	1.17443	-0.39926	-0.00046	1.00021
0.44	0.74711	-2.02526	1.16531	-0.51049	-0.00041	1.00020
0.46	0.70775	-1.91166	1.15410	-0.60836	-0.00035	1.00018
0.48	0.67059	-1.80499	1.14105	-0.69410	-0.00028	1.00015
0.50	0.63551	-1.70478	1.12641	-0.76883	-0.00020	1.00011
0.52	0.60236	-1.61060	1.11037	-0.83359	-0.00012	1.00007
0.54	0.57105	-1.52205	1.09312	-0.88929	-0.00005	1.00003
0.56	0.54145	-1.43877	1.07485	-0.93679	0.00001	0.99999
0.58	0.51346	-1.36039	1.05570	-0.97686	0.00006	0.99996
0.60	0.48700	-1.28662	1.03582	-1.01020	0.00010	0.99992
0.65	0.42693	-1.12040	0.98372	-1.06819	0.00016	0.99986
0.70	0.37458	-0.97702	0.92949	-1.09658	0.00016	0.99984
0.75	0.32890	-0.85309	0.87444	-1.10218	0.00013	0.99986
0.80	0.28899	-0.74575	0.81956	-1.09043	0.00008	0.99990
0.85	0.25409	-0.65260	0.76561	-1.06568	0.00002	0.99997
0.90	0.22353	-0.57164	0.71315	-1.03138	-0.00002	1.00003
0.95	0.19675	-0.50117	0.66259	-0.99029	-0.00005	1.00009
1.00	0.17326	-0.43973	0.61420	-0.94460	-0.00007	1.00014
1.05	0.15265	-0.38611	0.56818	-0.89602	-0.00007	1.00016
1.10	0.13454	-0.33925	0.52462	-0.84593	-0.00006	1.00017
1.15	0.11862	-0.29826	0.48359	-0.79539	-0.00005	1.00015
1.20	0.10463	-0.26237	0.44508	-0.74520	-0.00003	1.00011
1.25	0.09231	-0.23092	0.40905	-0.69600	-0.00001	1.00005
1.30	0.08147	-0.20334	0.37546	-0.64825	0.00000	0.99999
1.35	0.07192	-0.17913	0.34420	-0.60227	0.00002	0.99992
1.40	0.06351	-0.15786	0.31519	-0.55832	0.00002	0.99986
1.45	0.05609	-0.13918	0.28833	-0.51654	0.00003	0.99981
1.50	0.04956	-0.12274	0.26350	-0.47701	0.00003	0.99977
1.55	0.04379	-0.10829	0.24059	-0.43977	0.00003	0.99974
1.60	0.03870	-0.09556	0.21949	-0.40482	0.00003	0.99974
1.65	0.03421	-0.08435	0.20007	-0.37212	0.00002	0.99976
1.70	0.03024	-0.07448	0.18224	-0.34162	0.00002	0.99980
1.75	0.02674	-0.06577	0.16588	-0.31324	0.00001	0.99986
1.80	0.02365	-0.05810	0.15088	-0.28690	0.00000	0.99994
1.85	0.02091	-0.05133	0.13715	-0.26249	-0.00000	1.00003
1.90	0.01850	-0.04536	0.12460	-0.23992	-0.00001	1.00013
1.95	0.01637	-0.04009	0.11313	-0.21910	-0.00001	1.00023
2.00	0.01448	-0.03544	0.10266	-0.19990	-0.00001	1.00033

Table F.2. (continued).

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
2.10	0.01134	-0.02770	0.08442	-0.16602	-0.00002	1.00050
2.20	0.00888	-0.02167	0.06928	-0.13748	-0.00001	1.00060
2.30	0.00696	-0.01695	0.05677	-0.11355	-0.00001	1.00058
2.40	0.00546	-0.01327	0.04644	-0.09357	-0.00001	1.00044
2.50	0.00428	-0.01040	0.03794	-0.07695	-0.00000	1.00016
2.60	0.00336	-0.00814	0.03096	-0.06316	0.00000	0.99977
2.70	0.00264	-0.00638	0.02523	-0.05176	0.00001	0.99929
2.80	0.00207	-0.00501	0.02054	-0.04236	0.00001	0.99877
2.90	0.00162	-0.00393	0.01670	-0.03462	0.00001	0.99828
3.00	0.00128	-0.00308	0.01357	-0.02826	0.00001	0.99789
3.10	0.00100	-0.00242	0.01101	-0.02304	0.00001	0.99766
3.20	0.00079	-0.00190	0.00893	-0.01876	0.00001	0.99768
3.30	0.00062	-0.00149	0.00723	-0.01527	0.00000	0.99800
3.40	0.00049	-0.00117	0.00586	-0.01241	0.00000	0.99869
3.50	0.00038	-0.00092	0.00473	-0.01008	0.00000	0.99979
3.60	0.00030	-0.00072	0.00382	-0.00818	-0.00000	1.00130
3.70	0.00024	-0.00057	0.00309	-0.00663	-0.00000	1.00323
3.80	0.00018	-0.00045	0.00249	-0.00537	-0.00000	1.00553
3.90	0.00015	-0.00035	0.00201	-0.00434	-0.00000	1.00815
4.00	0.00011	-0.00028	0.00161	-0.00351	-0.00000	1.01097
4.20	0.00007	-0.00017	0.00104	-0.00228	-0.00000	1.01660
4.40	0.00004	-0.00010	0.00067	-0.00148	-0.00000	1.02075
4.60	0.00003	-0.00006	0.00044	-0.00095	-0.00000	1.02101
4.80	0.00002	-0.00004	0.00028	-0.00061	-0.00000	1.01422
5.00	0.00001	-0.00002	0.00018	-0.00039	0.00000	0.99676
5.20	0.00001	-0.00001	0.00012	-0.00025	0.00000	0.96512
5.40	0.00000	-0.00001	0.00008	-0.00016	0.00000	0.91689
5.60	0.00000	-0.00001	0.00006	-0.00010	0.00000	0.85204
5.80	0.00000	-0.00000	0.00004	-0.00007	0.00000	0.77381
6.00	0.00000	-0.00000	0.00003	-0.00004	0.00000	0.68853
6.20	0.00000	-0.00000	0.00002	-0.00003	0.00000	0.60410
6.40	0.00000	-0.00000	0.00002	-0.00002	0.00000	0.52771

Table F.3. Radial Characteristics of the Hartree-Fock Li 1s Orbital.

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \eta\phi$	$F\phi/\eta\phi$
0.	2.61282	-7.85544	0.	9.26222		
0.01	2.53554	-7.60302	0.08988	8.71873	1.14767	0.81732
0.02	2.46073	-7.35926	0.17446	8.20132	0.36430	0.94025
0.03	2.38832	-7.12384	0.25399	7.70879	0.13828	0.97663
0.04	2.31823	-6.89649	0.32872	7.24001	0.04641	0.99192
0.05	2.25037	-6.67691	0.39887	6.79390	0.00475	0.99915
0.06	2.18467	-6.46485	0.46467	6.36940	-0.01422	1.00263
0.07	2.12105	-6.26002	0.52632	5.96554	-0.02189	1.00417
0.08	2.05944	-6.06219	0.58404	5.58134	-0.02374	1.00465
0.09	1.99978	-5.87110	0.63801	5.21592	-0.02257	1.00456
0.10	1.94200	-5.68651	0.68842	4.86839	-0.01994	1.00414
0.12	1.83182	-5.33594	0.77923	4.22377	-0.01338	1.00295
0.14	1.72841	-5.00873	0.85779	3.64127	-0.00734	1.00172
0.16	1.63132	-4.70326	0.92526	3.11526	-0.00274	1.00068
0.18	1.54014	-4.41800	0.98274	2.64060	0.00039	0.99990
0.20	1.45448	-4.15154	1.03120	2.21262	0.00227	0.99937
0.22	1.37396	-3.90257	1.07153	1.82704	0.00319	0.99906
0.24	1.29826	-3.66985	1.10453	1.48000	0.00344	0.99893
0.26	1.22707	-3.45227	1.13096	1.16797	0.00325	0.99893
0.28	1.16008	-3.24876	1.15147	0.88774	0.00280	0.99903
0.30	1.09703	-3.05833	1.16666	0.63642	0.00222	0.99918
0.32	1.03767	-2.88010	1.17710	0.41133	0.00161	0.99938
0.34	0.98175	-2.71319	1.18327	0.21009	0.00102	0.99958
0.36	0.92907	-2.55685	1.18564	0.03050	0.00049	0.99979
0.38	0.87941	-2.41033	1.18462	-0.12944	0.00006	0.99997
0.40	0.83259	-2.27296	1.18059	-0.27151	-0.00029	1.00014
0.45	0.72683	-1.96562	1.15945	-0.55902	-0.00079	1.00044
0.50	0.63528	-1.70312	1.12601	-0.76667	-0.00086	1.00054
0.55	0.55589	-1.47835	1.08382	-0.91175	-0.00068	1.00050
0.60	0.48692	-1.28540	1.03565	-1.00790	-0.00041	1.00034
0.65	0.42690	-1.11938	0.98367	-1.06592	-0.00015	1.00014
0.70	0.37460	-0.97618	0.92955	-1.09440	0.00007	0.99993
0.75	0.32896	-0.85241	0.87460	-1.10015	0.00020	0.99975
0.80	0.28909	-0.74522	0.81982	-1.08860	0.00027	0.99963
0.85	0.25420	-0.65220	0.76596	-1.06406	0.00028	0.99956
0.90	0.22366	-0.57135	0.71358	-1.02998	0.00024	0.99956
0.95	0.19690	-0.50096	0.66308	-0.98910	0.00018	0.99962
1.00	0.17342	-0.43960	0.61474	-0.94358	0.00012	0.99972
1.05	0.15281	-0.38603	0.56877	-0.89517	0.00005	0.99986
1.10	0.13470	-0.33921	0.52525	-0.84520	-0.00000	1.00001
1.15	0.11879	-0.29825	0.48425	-0.79475	-0.00005	1.00016
1.20	0.10479	-0.26237	0.44577	-0.74463	-0.00008	1.00030
1.25	0.09248	-0.23093	0.40977	-0.69547	-0.00010	1.00042
1.30	0.08163	-0.20335	0.37620	-0.64774	-0.00010	1.00050
1.35	0.07208	-0.17914	0.34497	-0.60178	-0.00010	1.00055
1.40	0.06367	-0.15788	0.31599	-0.55783	-0.00009	1.00055
1.45	0.05625	-0.13919	0.28915	-0.51605	-0.00007	1.00051
1.50	0.04971	-0.12276	0.26435	-0.47653	-0.00005	1.00044
1.55	0.04394	-0.10830	0.24146	-0.43931	-0.00004	1.00033
1.60	0.03885	-0.09558	0.22038	-0.40438	-0.00002	1.00019
1.65	0.03436	-0.08438	0.20098	-0.37171	-0.00000	1.00002
1.70	0.03039	-0.07451	0.18317	-0.34125	0.00001	0.99985
1.75	0.02689	-0.06581	0.16682	-0.31292	0.00002	0.99966
1.80	0.02380	-0.05814	0.15184	-0.28663	0.00003	0.99948
1.85	0.02106	-0.05138	0.13813	-0.26229	0.00004	0.99931
1.90	0.01865	-0.04542	0.12558	-0.23979	0.00004	0.99916
1.95	0.01651	-0.04015	0.11412	-0.21903	0.00004	0.99904
2.00	0.01462	-0.03551	0.10365	-0.19991	0.00004	0.99896
2.10	0.01147	-0.02778	0.08540	-0.16615	0.00003	0.99891
2.20	0.00901	-0.02175	0.07025	-0.13772	0.00002	0.99905
2.30	0.00708	-0.01704	0.05770	-0.11388	0.00001	0.99939
2.40	0.00556	-0.01336	0.04734	-0.09397	0.00000	0.99992
2.50	0.00438	-0.01048	0.03880	-0.07738	-0.00001	1.00060
2.60	0.00345	-0.00823	0.03177	-0.06360	-0.00001	1.00138

Table F.3. (continued).

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi-\eta\phi$	$F\phi/\eta\phi$
2.70	0.00272	-0.00646	0.02600	-0.05219	-0.00001	1.00219
2.80	0.00214	-0.00507	0.02126	-0.04276	-0.00002	1.00294
2.90	0.00169	-0.00399	0.01739	-0.03499	-0.00001	1.00354
3.00	0.00134	-0.00313	0.01422	-0.02859	-0.00001	1.00389
3.10	0.00106	-0.00246	0.01163	-0.02334	-0.00001	1.00389
3.20	0.00084	-0.00194	0.00952	-0.01903	-0.00001	1.00347
3.30	0.00067	-0.00153	0.00780	-0.01550	-0.00000	1.00255
3.40	0.00053	-0.00120	0.00640	-0.01263	-0.00000	1.00109
3.50	0.00042	-0.00095	0.00526	-0.01028	0.00000	0.99906
3.60	0.00034	-0.00075	0.00433	-0.00836	0.00000	0.99648
3.70	0.00027	-0.00059	0.00357	-0.00681	0.00000	0.99342
3.80	0.00022	-0.00047	0.00296	-0.00554	0.00001	0.98999
3.90	0.00018	-0.00037	0.00246	-0.00451	0.00001	0.98634
4.00	0.00014	-0.00030	0.00205	-0.00368	0.00001	0.98269
4.20	0.00010	-0.00019	0.00145	-0.00246	0.00001	0.97641
4.40	0.00007	-0.00012	0.00104	-0.00165	0.00000	0.97346
4.60	0.00005	-0.00008	0.00077	-0.00112	0.00000	0.97610
4.80	0.00003	-0.00005	0.00058	-0.00077	0.00000	0.98585
5.00	0.00003	-0.00004	0.00045	-0.00054	-0.00000	1.00281
5.20	0.00002	-0.00002	0.00036	-0.00038	-0.00000	1.02544
5.40	0.00002	-0.00002	0.00029	-0.00027	-0.00000	1.05079
5.60	0.00001	-0.00001	0.00025	-0.00020	-0.00000	1.07513
5.80	0.00001	-0.00001	0.00021	-0.00015	-0.00000	1.09484
6.00	0.00001	-0.00001	0.00019	-0.00011	-0.00000	1.10714
6.20	0.00001	-0.00001	0.00017	-0.00009	-0.00000	1.11046
6.40	0.00001	-0.00000	0.00015	-0.00007	-0.00000	1.10461
6.60	0.00001	-0.00000	0.00014	-0.00005	-0.00000	1.09044
6.80	0.00001	-0.00000	0.00013	-0.00005	-0.00000	1.06954
7.00	0.00000	-0.00000	0.00012	-0.00004	-0.00000	1.04384
7.20	0.00000	-0.00000	0.00011	-0.00003	-0.00000	1.01522
7.40	0.00000	-0.00000	0.00011	-0.00003	0.00000	0.98542
7.60	0.00000	-0.00000	0.00010	-0.00003	0.00000	0.95583
7.80	0.00000	-0.00000	0.00010	-0.00003	0.00000	0.92754
8.00	0.00000	-0.00000	0.00009	-0.00003	0.00000	0.90134
8.20	0.00000	-0.00000	0.00009	-0.00003	0.00000	0.87779
8.40	0.00000	-0.00000	0.00008	-0.00003	0.00000	0.85725
8.60	0.00000	-0.00000	0.00008	-0.00003	0.00000	0.83996
8.80	0.00000	-0.00000	0.00007	-0.00003	0.00000	0.82608
9.00	0.00000	-0.00000	0.00007	-0.00002	0.00000	0.81572
9.50	0.00000	-0.00000	0.00005	-0.00002	0.00000	0.80599
10.00	0.00000	-0.00000	0.00004	-0.00002	0.00000	0.82176
10.50	0.00000	-0.00000	0.00003	-0.00002	0.00000	0.86941
11.00	0.00000	-0.00000	0.00002	-0.00002	0.00000	0.96357
11.50	0.00000	-0.00000	0.00002	-0.00001	-0.00000	1.13944
12.00	0.00000	-0.00000	0.00001	-0.00001	-0.00000	1.49770
12.50	0.00000	-0.00000	0.00000	-0.00001	-0.00000	2.46448
13.00	0.00000	-0.00000	0.00000	-0.00001	-0.00000	11.23966
13.50	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-3.49016
14.00	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-1.37781
14.50	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-0.80940
15.00	-0.00000	-0.00000	-0.00001	-0.00000	-0.00000	-0.54816
15.50	-0.00000	0.00000	-0.00001	-0.00000	-0.00000	-0.39945
16.00	-0.00000	0.00000	-0.00001	0.00000	-0.00000	-0.30419
16.50	-0.00000	0.00000	-0.00001	0.00000	-0.00000	-0.23836
17.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.19041
17.50	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.15407
18.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.12570
18.50	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.10299
19.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.08446
19.50	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.06908
20.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.05613
20.50	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.04510
21.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.03561
21.50	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-0.02735

Table F.4. Radial Characteristics of the Hartree-Fock Li 2s Orbital.

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \eta\phi$	$F\phi/\eta\phi$
0.	0.40826	-1.22846	0.	1.44724		
0.01	0.39615	-1.19321	0.01404	1.36202	0.25714	-2.30624
0.02	0.38439	-1.15908	0.02725	1.28045	0.08524	-0.12955
0.03	0.37297	-1.12603	0.03966	1.20238	0.03466	0.52668
0.04	0.36187	-1.09403	0.05131	1.12765	0.01348	0.81027
0.05	0.35108	-1.06304	0.06223	1.05613	0.00344	0.95007
0.06	0.34060	-1.03303	0.07244	0.98768	-0.00146	1.02187
0.07	0.33042	-1.00398	0.08199	0.92217	-0.00375	1.05776
0.08	0.32052	-0.97584	0.09090	0.85947	-0.00462	1.07347
0.09	0.31090	-0.94858	0.09919	0.79947	-0.00473	1.07748
0.10	0.30154	-0.92219	0.10689	0.74204	-0.00442	1.07469
0.12	0.28361	-0.87186	0.12064	0.63449	-0.00331	1.05941
0.14	0.26665	-0.82464	0.13233	0.53599	-0.00211	1.04028
0.16	0.25060	-0.78031	0.14214	0.44579	-0.00110	1.02232
0.18	0.23542	-0.73870	0.15022	0.36319	-0.00034	1.00743
0.20	0.22104	-0.69962	0.15671	0.28755	0.00017	0.99608
0.22	0.20742	-0.66290	0.16176	0.21829	0.00048	0.98815
0.24	0.19451	-0.62840	0.16548	0.15489	0.00064	0.98322
0.26	0.18227	-0.59595	0.16799	0.09685	0.00069	0.98078
0.28	0.17066	-0.56544	0.16939	0.04373	0.00066	0.98032
0.30	0.15964	-0.53672	0.16977	-0.00488	0.00058	0.98138
0.32	0.14918	-0.50969	0.16922	-0.04935	0.00048	0.98353
0.34	0.13924	-0.48422	0.16782	-0.09002	0.00037	0.98642
0.36	0.12980	-0.46023	0.16564	-0.12720	0.00026	0.98977
0.38	0.12082	-0.43760	0.16276	-0.16117	0.00016	0.99332
0.40	0.11229	-0.41626	0.15922	-0.19220	0.00007	0.99688
0.45	0.09271	-0.36798	0.14789	-0.25835	-0.00009	1.00501
0.50	0.07538	-0.32604	0.13361	-0.31067	-0.00016	1.01103
0.55	0.06001	-0.28950	0.11701	-0.35169	-0.00017	1.01446
0.60	0.04636	-0.25753	0.09860	-0.38343	-0.00014	1.01526
0.65	0.03420	-0.22947	0.07879	-0.40753	-0.00009	1.01355
0.70	0.02335	-0.20475	0.05795	-0.42530	-0.00004	1.00912
0.75	0.01367	-0.18290	0.03635	-0.43780	-0.00000	1.00009
0.80	0.00502	-0.16351	0.01424	-0.44590	0.00003	0.96974
0.85	-0.00271	-0.14626	-0.00818	-0.45032	0.00005	1.08979
0.90	-0.00963	-0.13086	-0.03074	-0.45165	0.00006	1.02914
0.95	-0.01583	-0.11707	-0.05330	-0.45036	0.00005	1.01739
1.00	-0.02136	-0.10470	-0.07574	-0.44687	0.00005	1.01123
1.05	-0.02632	-0.09356	-0.09795	-0.44153	0.00004	1.00712
1.10	-0.03074	-0.08351	-0.11986	-0.43462	0.00003	1.00414
1.15	-0.03468	-0.07443	-0.14139	-0.42639	0.00001	1.00196
1.20	-0.03820	-0.06621	-0.16248	-0.41705	0.00000	1.00038
1.25	-0.04132	-0.05875	-0.18308	-0.40679	-0.00001	0.99928
1.30	-0.04408	-0.05197	-0.20315	-0.39577	-0.00001	0.99856
1.35	-0.04652	-0.04580	-0.22265	-0.38412	-0.00002	0.99815
1.40	-0.04867	-0.04018	-0.24155	-0.37197	-0.00002	0.99798
1.45	-0.05055	-0.03506	-0.25984	-0.35941	-0.00002	0.99798
1.50	-0.05219	-0.03038	-0.27749	-0.34655	-0.00002	0.99811
1.55	-0.05360	-0.02611	-0.29449	-0.33345	-0.00002	0.99833
1.60	-0.05480	-0.02220	-0.31083	-0.32020	-0.00002	0.99860
1.65	-0.05582	-0.01863	-0.32651	-0.30686	-0.00001	0.99890
1.70	-0.05667	-0.01536	-0.34152	-0.29347	-0.00001	0.99920
1.75	-0.05736	-0.01237	-0.35586	-0.28010	-0.00001	0.99950
1.80	-0.05791	-0.00963	-0.36953	-0.26677	-0.00000	0.99976
1.85	-0.05833	-0.00713	-0.38254	-0.25354	0.00000	1.00000
1.90	-0.05863	-0.00484	-0.39488	-0.24042	0.00000	1.00020
1.95	-0.05882	-0.00274	-0.40658	-0.22745	0.00000	1.00037
2.00	-0.05891	-0.00082	-0.41763	-0.21466	0.00001	1.00049
2.10	-0.05882	0.00253	-0.43784	-0.18969	0.00001	1.00064
2.20	-0.05842	0.00531	-0.45560	-0.16564	0.00001	1.00066
2.30	-0.05777	0.00762	-0.47101	-0.14262	0.00001	1.00060
2.40	-0.05691	0.00952	-0.48416	-0.12070	0.00001	1.00047
2.50	-0.05588	0.01107	-0.49519	-0.09993	0.00000	1.00032
2.60	-0.05470	0.01232	-0.50419	-0.08034	0.00000	1.00016
2.70	-0.05342	0.01331	-0.51129	-0.06193	0.00000	1.00000
2.80	-0.05205	0.01408	-0.51662	-0.04471	-0.00000	0.99988
2.90	-0.05061	0.01466	-0.52027	-0.02867	-0.00000	0.99978
3.00	-0.04912	0.01508	-0.52239	-0.01377	-0.00000	0.99971
3.10	-0.04760	0.01535	-0.52307	0.00000	-0.00000	0.99968
3.20	-0.04605	0.01551	-0.52242	0.01268	-0.00000	0.99968
3.30	-0.04450	0.01556	-0.52057	0.02431	-0.00000	0.99970

Table F.4. (continued).

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi-\eta\phi$	$F\phi/\eta\phi$
3.40	-0.04294	0.01553	-0.51759	0.03494	-0.00000	0.99974
3.50	-0.04140	0.01542	-0.51361	0.04460	-0.00000	0.99979
3.60	-0.03986	0.01525	-0.50871	0.05333	-0.00000	0.99985
3.70	-0.03835	0.01503	-0.50297	0.06120	-0.00000	0.99992
3.80	-0.03686	0.01476	-0.49649	0.06823	-0.00000	0.99998
3.90	-0.03540	0.01446	-0.48935	0.07449	0.00000	1.00004
4.00	-0.03397	0.01413	-0.48162	0.08001	0.00000	1.00010
4.20	-0.03121	0.01341	-0.46467	0.08903	0.00000	1.00018
4.40	-0.02860	0.01263	-0.44617	0.09564	0.00000	1.00022
4.60	-0.02616	0.01183	-0.42656	0.10017	0.00000	1.00022
4.80	-0.02387	0.01102	-0.40622	0.10291	0.00000	1.00019
5.00	-0.02175	0.01023	-0.38549	0.10415	0.00000	1.00013
5.20	-0.01978	0.00945	-0.36464	0.10412	0.00000	1.00005
5.40	-0.01797	0.00871	-0.34391	0.10304	-0.00000	0.99998
5.60	-0.01630	0.00800	-0.32348	0.10112	-0.00000	0.99990
5.80	-0.01476	0.00734	-0.30351	0.09851	-0.00000	0.99984
6.00	-0.01336	0.00671	-0.28412	0.09537	-0.00000	0.99979
6.20	-0.01208	0.00613	-0.26539	0.09182	-0.00000	0.99977
6.40	-0.01091	0.00558	-0.24741	0.08797	-0.00000	0.99976
6.60	-0.00984	0.00508	-0.23022	0.08392	-0.00000	0.99977
6.80	-0.00887	0.00461	-0.21385	0.07975	-0.00000	0.99980
7.00	-0.00799	0.00419	-0.19832	0.07552	-0.00000	0.99984
7.20	-0.00719	0.00379	-0.18364	0.07129	-0.00000	0.99990
7.40	-0.00647	0.00343	-0.16980	0.06710	-0.00000	0.99997
7.60	-0.00582	0.00310	-0.15679	0.06299	0.00000	1.00004
7.80	-0.00523	0.00280	-0.14460	0.05899	0.00000	1.00011
8.00	-0.00470	0.00253	-0.13319	0.05512	0.00000	1.00019
8.20	-0.00422	0.00228	-0.12254	0.05139	0.00000	1.00026
8.40	-0.00378	0.00206	-0.11262	0.04782	0.00000	1.00032
8.60	-0.00339	0.00185	-0.10340	0.04442	0.00000	1.00038
8.80	-0.00304	0.00167	-0.09484	0.04120	0.00000	1.00043
9.00	-0.00272	0.00150	-0.08691	0.03815	0.00000	1.00046
9.50	-0.00207	0.00115	-0.06960	0.03127	0.00000	1.00048
10.00	-0.00156	0.00087	-0.05547	0.02543	0.00000	1.00040
10.50	-0.00118	0.00066	-0.04401	0.02054	0.00000	1.00021
11.00	-0.00089	0.00050	-0.03478	0.01649	-0.00000	0.99991
11.50	-0.00067	0.00038	-0.02739	0.01317	-0.00000	0.99951
12.00	-0.00051	0.00029	-0.02150	0.01047	-0.00000	0.99902
12.50	-0.00038	0.00022	-0.01683	0.00829	-0.00000	0.99844
13.00	-0.00029	0.00016	-0.01314	0.00654	-0.00000	0.99779
13.50	-0.00021	0.00012	-0.01024	0.00514	-0.00000	0.99707
14.00	-0.00016	0.00009	-0.00795	0.00403	-0.00000	0.99631
14.50	-0.00012	0.00007	-0.00617	0.00315	-0.00000	0.99551
15.00	-0.00009	0.00005	-0.00477	0.00245	-0.00000	0.99468
15.50	-0.00007	0.00004	-0.00369	0.00191	-0.00000	0.99383
16.00	-0.00005	0.00003	-0.00285	0.00148	-0.00000	0.99298
16.50	-0.00004	0.00002	-0.00219	0.00115	-0.00000	0.99213
17.00	-0.00003	0.00002	-0.00169	0.00089	-0.00000	0.99128
17.50	-0.00002	0.00001	-0.00130	0.00068	-0.00000	0.99045
18.00	-0.00002	0.00001	-0.00099	0.00053	-0.00000	0.98965
18.50	-0.00001	0.00001	-0.00076	0.00041	-0.00000	0.98887
19.00	-0.00001	0.00001	-0.00058	0.00031	-0.00000	0.98812
19.50	-0.00001	0.00000	-0.00045	0.00024	-0.00000	0.98741
20.00	-0.00000	0.00000	-0.00034	0.00018	-0.00000	0.98673
20.50	-0.00000	0.00000	-0.00026	0.00014	-0.00000	0.98610
21.00	-0.00000	0.00000	-0.00020	0.00011	-0.00000	0.98551
21.50	-0.00000	0.00000	-0.00015	0.00008	-0.00000	0.98497
22.00	-0.00000	0.00000	-0.00011	0.00006	-0.00000	0.98448
22.50	-0.00000	0.00000	-0.00009	0.00005	-0.00000	0.98403
23.00	-0.00000	0.00000	-0.00007	0.00004	-0.00000	0.98363
23.50	-0.00000	0.00000	-0.00005	0.00003	-0.00000	0.98328
24.00	-0.00000	0.00000	-0.00004	0.00002	-0.00000	0.98299
24.50	-0.00000	0.00000	-0.00003	0.00002	-0.00000	0.98274
25.00	-0.00000	0.00000	-0.00002	0.00001	-0.00000	0.98253
25.50	-0.00000	0.00000	-0.00002	0.00001	-0.00000	0.98238
26.00	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.98227
26.50	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.98221
27.00	-0.00000	0.00000	-0.00001	0.00000	-0.00000	0.98219
27.50	-0.00000	0.00000	-0.00001	0.00000	-0.00000	0.98222

Table F.5. Radial Characteristics of the Hartree-Fock Li^- 1s Orbital.

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
0.	2.61272	-7.84192	0.	9.26185		
0.01	2.53555	-7.59254	0.08988	8.71915	0.23271	0.96049
0.02	2.46084	-7.35130	0.17447	8.20226	0.06459	0.98870
0.03	2.38850	-7.11796	0.25401	7.71004	0.01900	0.99658
0.04	2.31846	-6.89231	0.32875	7.24141	0.00222	0.99959
0.05	2.25063	-6.67411	0.39891	6.79532	-0.00424	1.00081
0.06	2.18495	-6.46315	0.46473	6.37077	-0.00633	1.00125
0.07	2.12134	-6.25921	0.52640	5.96678	-0.00645	1.00131
0.08	2.05974	-6.06205	0.58413	5.58244	-0.00571	1.00119
0.09	2.00008	-5.87148	0.63811	5.21685	-0.00464	1.00100
0.10	1.94229	-5.68728	0.68852	4.86915	-0.00352	1.00078
0.12	1.83209	-5.33718	0.77935	4.22420	-0.00158	1.00037
0.14	1.72865	-5.01014	0.85791	3.64144	-0.00023	1.00006
0.16	1.63154	-4.70464	0.92538	3.11525	0.00055	0.99986
0.18	1.54033	-4.41926	0.98286	2.64047	0.00090	0.99975
0.20	1.45464	-4.15262	1.03131	2.21244	0.00097	0.99971
0.22	1.37411	-3.90346	1.07164	1.82686	0.00087	0.99973
0.24	1.29840	-3.67056	1.10465	1.47986	0.00069	0.99977
0.26	1.22719	-3.45281	1.13107	1.16789	0.00048	0.99983
0.28	1.16019	-3.24916	1.15157	0.88773	0.00028	0.99990
0.30	1.09713	-3.05863	1.16677	0.63647	0.00010	0.99996
0.32	1.03776	-2.88031	1.17721	0.41144	-0.00004	1.00002
0.34	0.98184	-2.71335	1.18339	0.21023	-0.00014	1.00006
0.36	0.92916	-2.55697	1.18576	0.03065	-0.00020	1.00009
0.38	0.87950	-2.41044	1.18474	-0.12928	-0.00024	1.00012
0.40	0.83268	-2.27308	1.18071	-0.27137	-0.00025	1.00013
0.40	0.83268	-2.27308	1.18071	-0.27137	-0.00025	1.00013
0.45	0.72691	-1.96577	1.15958	-0.55898	-0.00020	1.00012
0.50	0.63536	-1.70333	1.12614	-0.76680	-0.00011	1.00007
0.55	0.55595	-1.47861	1.08394	-0.91204	-0.00002	1.00002
0.60	0.48697	-1.28568	1.03575	-1.00833	0.00004	0.99997
0.65	0.42693	-1.11965	0.98374	-1.06644	0.00007	0.99993
0.70	0.37462	-0.97643	0.92960	-1.09496	0.00007	0.99991
0.75	0.32897	-0.85263	0.87462	-1.10071	0.00006	0.99992
0.80	0.28908	-0.74539	0.81981	-1.08911	0.00005	0.99993
0.85	0.25419	-0.65233	0.76593	-1.06450	0.00003	0.99996
0.90	0.22365	-0.57145	0.71352	-1.03035	0.00001	0.99999
0.95	0.19687	-0.50103	0.66300	-0.98940	-0.00001	1.00002
1.00	0.17339	-0.43964	0.61466	-0.94383	-0.00002	1.00004
1.05	0.15278	-0.38606	0.56867	-0.89537	-0.00002	1.00006
1.10	0.13467	-0.33923	0.52515	-0.84538	-0.00002	1.00008
1.15	0.11876	-0.29826	0.48414	-0.79492	-0.00002	1.00009
1.20	0.10476	-0.26239	0.44565	-0.74481	-0.00002	1.00009
1.25	0.09245	-0.23095	0.40964	-0.69567	-0.00002	1.00008
1.30	0.08160	-0.20338	0.37606	-0.64796	-0.00001	1.00007
1.35	0.07205	-0.17917	0.34482	-0.60203	-0.00001	1.00005
1.40	0.06364	-0.15791	0.31582	-0.55811	-0.00000	1.00003
1.45	0.05622	-0.13923	0.28897	-0.51635	-0.00000	1.00000
1.50	0.04968	-0.12279	0.26415	-0.47684	0.00000	0.99997
1.55	0.04391	-0.10834	0.24125	-0.43963	0.00001	0.99994
1.60	0.03881	-0.09561	0.22015	-0.40470	0.00001	0.99992
1.65	0.03432	-0.08440	0.20074	-0.37203	0.00001	0.99989
1.70	0.03035	-0.07453	0.18291	-0.34156	0.00001	0.99987
1.75	0.02685	-0.06583	0.16655	-0.31321	0.00001	0.99985
1.80	0.02375	-0.05816	0.15155	-0.28690	0.00001	0.99984
1.85	0.02102	-0.05139	0.13783	-0.26253	0.00001	0.99983
1.90	0.01860	-0.04542	0.12527	-0.24000	0.00001	0.99983
1.95	0.01646	-0.04015	0.11380	-0.21921	0.00001	0.99983
2.00	0.01457	-0.03550	0.10332	-0.20005	0.00001	0.99985
2.10	0.01143	-0.02777	0.08506	-0.16624	0.00000	0.99990
2.20	0.00896	-0.02174	0.06990	-0.13776	0.00000	0.99999
2.30	0.00703	-0.01703	0.05735	-0.11388	-0.00000	1.00011
2.40	0.00552	-0.01334	0.04699	-0.09394	-0.00000	1.00026
2.50	0.00434	-0.01046	0.03845	-0.07734	-0.00000	1.00041

Table F.5. (continued).

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
2.60	0.00341	-0.00821	0.03143	-0.06356	-0.00000	1.00056
2.70	0.00268	-0.00644	0.02566	-0.05215	-0.00000	1.00069
2.80	0.00211	-0.00506	0.02093	-0.04273	-0.00000	1.00078
2.90	0.00166	-0.00397	0.01706	-0.03496	-0.00000	1.00080
3.00	0.00131	-0.00312	0.01389	-0.02857	-0.00000	1.00072
3.10	0.00103	-0.00245	0.01131	-0.02333	-0.00000	1.00054
3.20	0.00081	-0.00193	0.00920	-0.01903	-0.00000	1.00021
3.30	0.00064	-0.00152	0.00748	-0.01551	0.00000	0.99974
3.40	0.00050	-0.00120	0.00608	-0.01263	0.00000	0.99912
3.50	0.00040	-0.00094	0.00493	-0.01027	0.00000	0.99833
3.60	0.00031	-0.00074	0.00401	-0.00836	0.00000	0.99740
3.70	0.00025	-0.00058	0.00325	-0.00679	0.00000	0.99634
3.80	0.00020	-0.00046	0.00264	-0.00552	0.00000	0.99518
3.90	0.00015	-0.00036	0.00214	-0.00448	0.00000	0.99398
4.00	0.00012	-0.00029	0.00173	-0.00364	0.00000	0.99280
4.20	0.00008	-0.00018	0.00114	-0.00240	0.00000	0.99083
4.40	0.00005	-0.00011	0.00075	-0.00158	0.00000	0.99018
4.60	0.00003	-0.00007	0.00049	-0.00104	0.00000	0.99209
4.80	0.00002	-0.00004	0.00032	-0.00069	0.00000	0.99827
5.00	0.00001	-0.00003	0.00021	-0.00045	-0.00000	1.01101
5.20	0.00001	-0.00002	0.00013	-0.00030	-0.00000	1.03346
5.40	0.00000	-0.00001	0.00008	-0.00019	-0.00000	1.07008
5.60	0.00000	-0.00001	0.00005	-0.00013	-0.00000	1.12756
5.80	0.00000	-0.00000	0.00003	-0.00008	-0.00000	1.21693
6.00	0.00000	-0.00000	0.00002	-0.00005	-0.00000	1.35753
6.20	0.00000	-0.00000	0.00001	-0.00003	-0.00000	1.58779
6.40	0.00000	-0.00000	0.00001	-0.00002	-0.00000	1.99617
6.60	0.00000	-0.00000	0.00000	-0.00001	-0.00000	2.83749
6.80	0.00000	-0.00000	0.00000	-0.00001	-0.00000	5.22654
7.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	28.93484
7.20	-0.00000	-0.00000	-0.00000	-0.00000	-0.00000	-12.76073
7.40	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-22.98555

Table F.6. Radial Characteristics of the Hartree-Fock Li^- 2s Orbital.

r	$\phi(r)$	$\phi'(r)$	P(r)	P'(r)	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
0.	-0.28298	0.85434	-0.	-1.00315		
0.01	-0.27457	0.82895	-0.00973	-0.94393	-0.34290	-84.92896
0.02	-0.26640	0.80454	-0.01889	-0.88733	-0.09911	-24.59708
0.03	-0.25847	0.78104	-0.02749	-0.83320	-0.03141	-7.36187
0.04	-0.25078	0.75840	-0.03556	-0.78144	-0.00557	-0.52698
0.05	-0.24330	0.73658	-0.04312	-0.73193	0.00498	2.40699
0.06	-0.23604	0.71552	-0.05021	-0.68456	0.00884	3.57784
0.07	-0.22899	0.69519	-0.05682	-0.63924	0.00958	3.87960
0.08	-0.22214	0.67555	-0.06300	-0.59587	0.00886	3.74307
0.09	-0.21548	0.65658	-0.06875	-0.55437	0.00749	3.39153
0.10	-0.20900	0.63823	-0.07409	-0.51465	0.00592	2.94982
0.12	-0.19659	0.60331	-0.08363	-0.44026	0.00299	2.04519
0.14	-0.18486	0.57059	-0.09174	-0.37212	0.00079	1.29320
0.16	-0.17375	0.53991	-0.09855	-0.30971	-0.00061	0.75852
0.18	-0.16325	0.51111	-0.10417	-0.25256	-0.00135	0.43305
0.20	-0.15330	0.48406	-0.10869	-0.20024	-0.00160	0.28210
0.22	-0.14387	0.45864	-0.11220	-0.15233	-0.00154	0.26415
0.24	-0.13494	0.43474	-0.11481	-0.10849	-0.00129	0.34007
0.26	-0.12647	0.41226	-0.11657	-0.06837	-0.00096	0.47539
0.28	-0.11844	0.39111	-0.11756	-0.03167	-0.00062	0.64214
0.30	-0.11082	0.37119	-0.11786	0.00190	-0.00029	0.81844
0.32	-0.10359	0.35245	-0.11751	0.03259	-0.00002	0.98789
0.34	-0.09672	0.33479	-0.11657	0.06065	0.00020	1.13880
0.36	-0.09019	0.31815	-0.11510	0.08630	0.00035	1.26403
0.38	-0.08399	0.30246	-0.11313	0.10972	0.00044	1.35923
0.40	-0.07809	0.28767	-0.11072	0.13111	0.00048	1.42289
0.40	-0.07809	0.28767	-0.11072	0.13111	0.00048	1.42294
0.45	-0.06456	0.25424	-0.10298	0.17672	0.00042	1.44937
0.50	-0.05259	0.22525	-0.09321	0.21283	0.00024	1.31982
0.55	-0.04197	0.20003	-0.08183	0.24121	0.00005	1.08979
0.60	-0.03253	0.17799	-0.06919	0.26326	-0.00009	0.81206
0.65	-0.02413	0.15867	-0.05559	0.28009	-0.00017	0.52436
0.70	-0.01663	0.14167	-0.04125	0.29260	-0.00018	0.23775
0.75	-0.00993	0.12664	-0.02639	0.30152	-0.00016	-0.09458
0.80	-0.00393	0.11333	-0.01115	0.30744	-0.00011	-0.87931
0.85	0.00143	0.10148	0.00431	0.31085	-0.00005	3.39740
0.90	0.00624	0.09091	0.01990	0.31215	0.00000	0.97351
0.95	0.01054	0.08146	0.03550	0.31169	0.00004	0.72394
1.00	0.01440	0.07298	0.05104	0.30974	0.00007	0.67995
1.05	0.01785	0.06536	0.06645	0.30656	0.00008	0.70365
1.10	0.02095	0.05849	0.08168	0.30234	0.00007	0.75522
1.15	0.02371	0.05230	0.09667	0.29727	0.00006	0.81649
1.20	0.02619	0.04670	0.11139	0.29148	0.00005	0.87740
1.25	0.02839	0.04163	0.12581	0.28512	0.00003	0.93211
1.30	0.03036	0.03703	0.13990	0.27828	0.00001	0.97761
1.35	0.03210	0.03286	0.15363	0.27106	-0.00001	1.01263
1.40	0.03365	0.02907	0.16700	0.26353	-0.00002	1.03723
1.45	0.03502	0.02561	0.17998	0.25577	-0.00003	1.05229
1.50	0.03622	0.02247	0.19257	0.24784	-0.00003	1.05916
1.55	0.03727	0.01960	0.20476	0.23977	-0.00003	1.05944
1.60	0.03818	0.01698	0.21655	0.23163	-0.00003	1.05477
1.65	0.03897	0.01458	0.22793	0.22344	-0.00003	1.04675
1.70	0.03964	0.01240	0.23889	0.21524	-0.00002	1.03675
1.75	0.04021	0.01040	0.24945	0.20706	-0.00002	1.02597
1.80	0.04068	0.00857	0.25960	0.19892	-0.00001	1.01533
1.85	0.04107	0.00690	0.26934	0.19085	-0.00000	1.00555
1.90	0.04138	0.00537	0.27869	0.18287	0.00000	0.99710
1.95	0.04161	0.00398	0.28763	0.17499	0.00001	0.99027
2.00	0.04178	0.00270	0.29619	0.16723	0.00001	0.98517
2.10	0.04193	0.00047	0.31215	0.15211	0.00001	0.98004
2.20	0.04188	-0.00139	0.32663	0.13760	0.00001	0.98056
2.30	0.04166	-0.00294	0.33969	0.12375	0.00001	0.98487
2.40	0.04130	-0.00421	0.35140	0.11060	0.00001	0.99100
2.50	0.04083	-0.00526	0.36184	0.09816	0.00000	0.99732

Table F.6. (continued).

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
2.60	0.04026	-0.00611	0.37106	0.08644	-0.00000	1.00261
2.70	0.03961	-0.00679	0.37915	0.07543	-0.00000	1.00622
2.80	0.03891	-0.00733	0.38617	0.06512	-0.00000	1.00795
2.90	0.03815	-0.00776	0.39219	0.05548	-0.00000	1.00792
3.00	0.03736	-0.00808	0.39729	0.04649	-0.00000	1.00648
3.10	0.03654	-0.00832	0.40151	0.03813	-0.00000	1.00411
3.20	0.03570	-0.00848	0.40493	0.03037	-0.00000	1.00129
3.30	0.03484	-0.00858	0.40761	0.02318	0.00000	0.99845
3.40	0.03398	-0.00862	0.40959	0.01652	0.00000	0.99596
3.50	0.03312	-0.00863	0.41093	0.01038	0.00000	0.99408
3.60	0.03226	-0.00859	0.41168	0.00472	0.00000	0.99294
3.70	0.03140	-0.00852	0.41189	-0.00049	0.00000	0.99260
3.80	0.03056	-0.00843	0.41160	-0.00527	0.00000	0.99305
3.90	0.02972	-0.00832	0.41085	-0.00965	0.00000	0.99418
4.00	0.02889	-0.00819	0.40968	-0.01365	0.00000	0.99588
4.20	0.02728	-0.00788	0.40623	-0.02061	-0.00000	1.00032
4.40	0.02574	-0.00754	0.40152	-0.02635	-0.00000	1.00511
4.60	0.02427	-0.00718	0.39576	-0.03102	-0.00000	1.00917
4.80	0.02287	-0.00681	0.38917	-0.03478	-0.00000	1.01181
5.00	0.02155	-0.00644	0.38190	-0.03775	-0.00000	1.01269
5.20	0.02030	-0.00608	0.37411	-0.04006	-0.00000	1.01184
5.40	0.01912	-0.00572	0.36592	-0.04180	-0.00000	1.00952
5.60	0.01800	-0.00538	0.35742	-0.04307	-0.00000	1.00610
5.80	0.01696	-0.00506	0.34872	-0.04394	-0.00000	1.00206
6.00	0.01598	-0.00475	0.33987	-0.04448	0.00000	0.99780
6.20	0.01506	-0.00446	0.33094	-0.04473	0.00000	0.99370
6.40	0.01419	-0.00419	0.32199	-0.04474	0.00000	0.99007
6.60	0.01338	-0.00393	0.31306	-0.04456	0.00000	0.98710
6.80	0.01262	-0.00369	0.30418	-0.04421	0.00000	0.98494
7.00	0.01190	-0.00346	0.29538	-0.04373	0.00000	0.98363
7.20	0.01123	-0.00325	0.28670	-0.04314	0.00000	0.98316
7.40	0.01060	-0.00305	0.27814	-0.04245	0.00000	0.98349
7.60	0.01001	-0.00286	0.26972	-0.04169	0.00000	0.98454
7.80	0.00946	-0.00269	0.26146	-0.04086	0.00000	0.98621
8.00	0.00893	-0.00253	0.25338	-0.03999	0.00000	0.98838
8.20	0.00844	-0.00237	0.24547	-0.03909	0.00000	0.99093
8.40	0.00798	-0.00223	0.23775	-0.03815	0.00000	0.99376
8.60	0.00755	-0.00210	0.23021	-0.03720	0.00000	0.99674
8.80	0.00714	-0.00197	0.22287	-0.03623	0.00000	0.99979
9.00	0.00676	-0.00186	0.21572	-0.03526	-0.00000	1.00281
9.50	0.00590	-0.00160	0.19870	-0.03282	-0.00000	1.00979
10.00	0.00516	-0.00137	0.18289	-0.03044	-0.00000	1.01530
10.50	0.00452	-0.00119	0.16824	-0.02815	-0.00000	1.01887
11.00	0.00397	-0.00103	0.15472	-0.02598	-0.00000	1.02036
11.50	0.00349	-0.00089	0.14225	-0.02393	-0.00000	1.01984
12.00	0.00307	-0.00077	0.13076	-0.02202	-0.00000	1.01754
12.50	0.00271	-0.00067	0.12020	-0.02025	-0.00000	1.01378
13.00	0.00240	-0.00059	0.11049	-0.01862	-0.00000	1.00890
13.50	0.00212	-0.00051	0.10156	-0.01711	-0.00000	1.00328
14.00	0.00188	-0.00045	0.09336	-0.01572	0.00000	0.99726
14.50	0.00167	-0.00040	0.08582	-0.01445	0.00000	0.99115
15.00	0.00148	-0.00035	0.07889	-0.01329	0.00000	0.98525
15.50	0.00132	-0.00031	0.07252	-0.01222	0.00000	0.97978
16.00	0.00118	-0.00027	0.06666	-0.01124	0.00000	0.97496
16.50	0.00105	-0.00024	0.06127	-0.01034	0.00000	0.97094
17.00	0.00093	-0.00021	0.05631	-0.00952	0.00000	0.96785
17.50	0.00083	-0.00019	0.05174	-0.00876	0.00000	0.96577
18.00	0.00074	-0.00017	0.04754	-0.00807	0.00000	0.96477
18.50	0.00067	-0.00015	0.04366	-0.00743	0.00000	0.96487
19.00	0.00060	-0.00013	0.04010	-0.00685	0.00000	0.96608
19.50	0.00053	-0.00012	0.03681	-0.00631	0.00000	0.96840
20.00	0.00048	-0.00011	0.03378	-0.00581	0.00000	0.97180
20.50	0.00043	-0.00009	0.03099	-0.00535	0.00000	0.97625
21.00	0.00038	-0.00008	0.02843	-0.00493	0.00000	0.98171

Table F.6. (continued).

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
21.50	0.00034	-0.00008	0.02606	-0.00454	0.00000	0.98811
22.00	0.00031	-0.00007	0.02388	-0.00418	0.00000	0.99540
22.50	0.00027	-0.00006	0.02187	-0.00385	-0.00000	1.00353
23.00	0.00025	-0.00005	0.02003	-0.00354	-0.00000	1.01243
23.50	0.00022	-0.00005	0.01833	-0.00326	-0.00000	1.02204
24.00	0.00020	-0.00004	0.01677	-0.00300	-0.00000	1.03229
24.50	0.00018	-0.00004	0.01533	-0.00276	-0.00000	1.04314
25.00	0.00016	-0.00003	0.01401	-0.00253	-0.00000	1.05452
25.50	0.00014	-0.00003	0.01279	-0.00233	-0.00000	1.06637
26.00	0.00013	-0.00003	0.01168	-0.00214	-0.00000	1.07864
26.50	0.00011	-0.00003	0.01066	-0.00196	-0.00000	1.09128
27.00	0.00010	-0.00002	0.00972	-0.00180	-0.00000	1.10424
27.50	0.00009	-0.00002	0.00886	-0.00165	-0.00000	1.11749
28.00	0.00008	-0.00002	0.00807	-0.00151	-0.00000	1.13096
28.50	0.00007	-0.00002	0.00735	-0.00138	-0.00000	1.14464
29.00	0.00007	-0.00001	0.00668	-0.00126	-0.00000	1.15848
29.50	0.00006	-0.00001	0.00608	-0.00116	-0.00000	1.17245
31.00	0.00004	-0.00001	0.00456	-0.00088	-0.00000	1.21483
32.00	0.00003	-0.00001	0.00375	-0.00073	-0.00000	1.24323
33.00	0.00003	-0.00001	0.00309	-0.00061	-0.00000	1.27157
34.00	0.00002	-0.00000	0.00253	-0.00050	-0.00000	1.29970
35.00	0.00002	-0.00000	0.00207	-0.00042	-0.00000	1.32751
36.00	0.00001	-0.00000	0.00169	-0.00034	-0.00000	1.35494
37.00	0.00001	-0.00000	0.00138	-0.00028	-0.00000	1.38190
38.00	0.00001	-0.00000	0.00112	-0.00023	-0.00000	1.40834
39.00	0.00001	-0.00000	0.00091	-0.00019	-0.00000	1.43424
42.00	0.00000	-0.00000	0.00049	-0.00010	-0.00000	1.50840
44.00	0.00000	-0.00000	0.00032	-0.00007	-0.00000	1.55479
46.00	0.00000	-0.00000	0.00020	-0.00004	-0.00000	1.59875
48.00	0.00000	-0.00000	0.00013	-0.00003	-0.00000	1.64033

Table F.7. Radial Characteristics of the Hartree-Fock Be 1s Orbital.

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
0.	4.13860	-16.57147	0.	14.67096		
0.01	3.97637	-15.88007	0.14096	13.53293	0.94243	0.94992
0.02	3.82090	-15.21876	0.27089	12.46576	0.21656	0.98802
0.03	3.67190	-14.58627	0.39050	11.46533	0.03662	0.99789
0.04	3.52908	-13.98136	0.50041	10.52777	-0.01995	1.00119
0.05	3.39218	-13.40287	0.60125	9.64938	-0.03522	1.00219
0.06	3.26094	-12.84964	0.69358	8.82669	-0.03490	1.00226
0.07	3.13511	-12.32057	0.77796	8.05641	-0.02890	1.00195
0.08	3.01445	-11.81461	0.85488	7.33542	-0.02142	1.00150
0.09	2.89874	-11.33072	0.92482	6.66081	-0.01427	1.00104
0.10	2.78777	-10.86794	0.98824	6.02980	-0.00818	1.00062
0.12	2.57920	-10.00194	1.09716	4.88830	0.00025	0.99998
0.14	2.38720	-9.20953	1.18474	3.89184	0.00435	0.99961
0.16	2.21037	-8.48420	1.25369	3.02344	0.00553	0.99947
0.18	2.04742	-7.82001	1.30643	2.26811	0.00503	0.99948
0.20	1.89720	-7.21153	1.34508	1.61255	0.00375	0.99958
0.22	1.75863	-6.65379	1.37152	1.04501	0.00227	0.99973
0.24	1.63074	-6.14230	1.38740	0.55508	0.00091	0.99988
0.26	1.51265	-5.67296	1.39418	0.13359	-0.00016	1.00002
0.28	1.40356	-5.24202	1.39314	-0.22759	-0.00090	1.00014
0.30	1.30274	-4.84612	1.38543	-0.53563	-0.00133	1.00022
0.32	1.20951	-4.48219	1.37203	-0.79687	-0.00149	1.00026
0.34	1.12326	-4.14742	1.35383	-1.01692	-0.00146	1.00027
0.36	1.04343	-3.83931	1.33159	-1.20073	-0.00129	1.00026
0.38	0.96952	-3.55555	1.30601	-1.35269	-0.00104	1.00023
0.40	0.90106	-3.29405	1.27767	-1.47667	-0.00075	1.00017
0.45	0.75104	-2.72578	1.19807	-1.68582	-0.00006	1.00002
0.50	0.62677	-2.26026	1.11093	-1.78435	0.00038	0.99987
0.55	0.52363	-1.87768	1.02093	-1.80467	0.00052	0.99979
0.60	0.43789	-1.56235	0.93136	-1.77076	0.00046	0.99978
0.65	0.36649	-1.30179	0.84446	-1.70039	0.00029	0.99983
0.70	0.30696	-1.08599	0.76171	-1.60667	0.00009	0.99994
0.75	0.25728	-0.90693	0.68402	-1.49922	-0.00007	1.00005
0.80	0.21577	-0.75810	0.61190	-1.38506	-0.00017	1.00016
0.85	0.18105	-0.63422	0.54554	-1.26920	-0.00021	1.00024
0.90	0.15200	-0.53097	0.48495	-1.15519	-0.00020	1.00028
0.95	0.12767	-0.44483	0.42995	-1.04545	-0.00016	1.00027
1.00	0.10728	-0.37288	0.38030	-0.94154	-0.00011	1.00021
1.10	0.07584	-0.26245	0.29574	-0.75454	0.00001	0.99998
1.20	0.05369	-0.18507	0.22841	-0.59694	0.00008	0.99970
1.30	0.03806	-0.13073	0.17541	-0.46753	0.00009	0.99949
1.40	0.02701	-0.09248	0.13407	-0.36321	0.00007	0.99945
1.50	0.01919	-0.06551	0.10206	-0.28030	0.00003	0.99964
1.60	0.01365	-0.04646	0.07742	-0.21511	-0.00000	1.00005
1.70	0.00972	-0.03298	0.05856	-0.16431	-0.00003	1.00061
1.80	0.00692	-0.02344	0.04418	-0.12499	-0.00004	1.00121
1.90	0.00494	-0.01667	0.03325	-0.09476	-0.00004	1.00171
2.00	0.00352	-0.01186	0.02499	-0.07162	-0.00003	1.00194
2.20	0.00180	-0.00603	0.01405	-0.04061	-0.00001	1.00104
2.40	0.00092	-0.00307	0.00787	-0.02286	0.00001	0.99776
2.60	0.00048	-0.00157	0.00439	-0.01282	0.00002	0.99237
2.80	0.00025	-0.00081	0.00245	-0.00718	0.00002	0.98663
3.00	0.00013	-0.00042	0.00136	-0.00402	0.00001	0.98409
3.20	0.00007	-0.00022	0.00075	-0.00225	0.00000	0.99045
3.40	0.00003	-0.00011	0.00041	-0.00126	-0.00000	1.01402
3.60	0.00002	-0.00006	0.00022	-0.00070	-0.00001	1.06723
3.80	0.00001	-0.00003	0.00011	-0.00039	-0.00001	1.17022
4.00	0.00000	-0.00002	0.00005	-0.00021	-0.00001	1.35985
4.20	0.00000	-0.00001	0.00002	-0.00010	-0.00001	1.70996
4.40	0.00000	-0.00000	0.00001	-0.00005	-0.00000	2.35359
4.60	0.00000	-0.00000	0.00000	-0.00002	-0.00000	3.16994
4.80	0.00000	0.00000	0.00000	0.00000	-0.00000	2.31154
5.00	0.00000	0.00000	0.00000	0.00001	0.00000	0.65510
5.20	0.00000	0.00000	0.00001	0.00001	0.00000	0.06284

Table F.8. Radial Characteristics of the Hartree-Fock Be 2s Orbital.

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$R\phi - \epsilon\phi$	$R\phi/\epsilon\phi$
0.	0.75429	-3.02317	0.	2.67389		
0.01	0.72461	-2.91350	0.02569	2.46539	0.36195	-0.61512
0.02	0.69601	-2.80812	0.04935	2.26818	0.09642	0.55205
0.03	0.66843	-2.70687	0.07109	2.08167	0.02586	0.87489
0.04	0.64185	-2.60958	0.09101	1.90529	0.00071	0.99643
0.05	0.61623	-2.51611	0.10922	1.73851	-0.00840	1.04409
0.06	0.59152	-2.42629	0.12581	1.58083	-0.01087	1.05944
0.07	0.56769	-2.34000	0.14087	1.43176	-0.01047	1.05966
0.08	0.54471	-2.25708	0.15448	1.29085	-0.00890	1.05283
0.09	0.52254	-2.17739	0.16671	1.15767	-0.00696	1.04307
0.10	0.50115	-2.10082	0.17765	1.03181	-0.00505	1.03256
0.12	0.46060	-1.95648	0.19593	0.80051	-0.00190	1.01335
0.14	0.42282	-1.82310	0.20984	0.59407	0.00013	0.99902
0.16	0.38761	-1.69979	0.21984	0.40993	0.00121	0.98994
0.18	0.35477	-1.58572	0.22637	0.24579	0.00161	0.98536
0.20	0.32412	-1.48014	0.22980	0.09959	0.00158	0.98421
0.22	0.29551	-1.38234	0.23046	-0.03051	0.00133	0.98549
0.24	0.26878	-1.29169	0.22867	-0.14615	0.00097	0.98833
0.26	0.24380	-1.20761	0.22470	-0.24878	0.00060	0.99203
0.28	0.22044	-1.12954	0.21880	-0.33973	0.00027	0.99605
0.30	0.19858	-1.05701	0.21118	-0.42015	-0.00000	1.00003
0.32	0.17812	-0.98955	0.20206	-0.49110	-0.00020	1.00367
0.34	0.15897	-0.92677	0.19160	-0.55349	-0.00033	1.00680
0.36	0.14102	-0.86828	0.17997	-0.60817	-0.00041	1.00933
0.38	0.12421	-0.81375	0.16732	-0.65587	-0.00043	1.01121
0.40	0.10845	-0.76286	0.15377	-0.69728	-0.00042	1.01240
0.45	0.07321	-0.64976	0.11679	-0.77698	-0.00028	1.01248
0.50	0.04318	-0.55390	0.07654	-0.82869	-0.00011	1.00815
0.55	0.01758	-0.47225	0.03428	-0.85840	0.00003	0.99400
0.60	-0.00424	-0.40236	-0.00901	-0.87082	0.00012	1.08875
0.65	-0.02282	-0.34231	-0.05257	-0.86963	0.00014	1.02048
0.70	-0.03861	-0.29051	-0.09580	-0.85774	0.00013	1.01107
0.75	-0.05198	-0.24569	-0.13821	-0.83750	0.00010	1.00601
0.80	-0.06327	-0.20681	-0.17944	-0.81081	0.00005	1.00270
0.85	-0.07275	-0.17301	-0.21921	-0.77921	0.00001	1.00051
0.90	-0.08065	-0.14358	-0.25730	-0.74395	-0.00002	0.99915
0.95	-0.08717	-0.11791	-0.29356	-0.70608	-0.00004	0.99841
1.00	-0.09249	-0.09551	-0.32788	-0.66645	-0.00005	0.99812
1.10	-0.10013	-0.05888	-0.39044	-0.58456	-0.00005	0.99841
1.20	-0.10456	-0.03099	-0.44479	-0.50249	-0.00003	0.99917
1.30	-0.10655	-0.00983	-0.49103	-0.42300	-0.00000	0.99993
1.40	-0.10670	0.00612	-0.52953	-0.34785	0.00001	1.00045
1.50	-0.10546	0.01801	-0.56078	-0.27807	0.00002	1.00068
1.60	-0.10320	0.02673	-0.58534	-0.21421	0.00002	1.00067
1.70	-0.10020	0.03298	-0.60382	-0.15645	0.00002	1.00049
1.80	-0.09667	0.03729	-0.61683	-0.10473	0.00001	1.00024
1.90	-0.09279	0.04010	-0.62496	-0.05884	-0.00000	0.99999
2.00	-0.08869	0.04174	-0.62878	-0.01847	-0.00001	0.99979
2.20	-0.08022	0.04252	-0.62559	0.04722	-0.00001	0.99960
2.40	-0.07182	0.04115	-0.61106	0.09553	-0.00001	0.99969
2.60	-0.06383	0.03861	-0.58833	0.12962	-0.00000	0.99992
2.80	-0.05642	0.03550	-0.55997	0.15234	0.00000	1.00015
3.00	-0.04965	0.03217	-0.52799	0.16614	0.00000	1.00029
3.20	-0.04355	0.02886	-0.49397	0.17305	0.00000	1.00031
3.40	-0.03809	0.02570	-0.45911	0.17476	0.00000	1.00023
3.60	-0.03325	0.02276	-0.42433	0.17258	0.00000	1.00008
3.80	-0.02897	0.02007	-0.39027	0.16759	-0.00000	0.99992
4.00	-0.02521	0.01763	-0.35742	0.16063	-0.00000	0.99977
4.20	-0.02190	0.01545	-0.32611	0.15234	-0.00000	0.99967
4.40	-0.01901	0.01350	-0.29654	0.14323	-0.00000	0.99963
4.60	-0.01649	0.01178	-0.26884	0.13369	-0.00000	0.99965
4.80	-0.01429	0.01026	-0.24307	0.12402	-0.00000	0.99973
5.00	-0.01237	0.00893	-0.21923	0.11444	-0.00000	0.99985
5.20	-0.01070	0.00776	-0.19728	0.10511	-0.00000	1.00000

Table F.8. (continued).

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
5.40	-0.00925	0.00674	-0.17716	0.09615	0.00000	1.00016
5.60	-0.00800	0.00584	-0.15879	0.08763	0.00000	1.00031
5.80	-0.00691	0.00506	-0.14208	0.07960	0.00000	1.00045
6.00	-0.00597	0.00438	-0.12692	0.07210	0.00000	1.00056
6.20	-0.00515	0.00379	-0.11320	0.06513	0.00000	1.00064
6.40	-0.00444	0.00328	-0.10083	0.05870	0.00000	1.00067
6.60	-0.00383	0.00284	-0.08969	0.05278	0.00000	1.00067
6.80	-0.00331	0.00245	-0.07968	0.04736	0.00000	1.00062
7.00	-0.00285	0.00212	-0.07071	0.04242	0.00000	1.00052
7.20	-0.00246	0.00183	-0.06268	0.03793	0.00000	1.00039
7.40	-0.00212	0.00158	-0.05551	0.03386	0.00000	1.00021
7.60	-0.00182	0.00136	-0.04911	0.03019	0.00000	1.00001
7.80	-0.00157	0.00117	-0.04341	0.02687	-0.00000	0.99977
8.00	-0.00135	0.00101	-0.03834	0.02389	-0.00000	0.99951
8.50	-0.00093	0.00070	-0.02801	0.01772	-0.00000	0.99878
9.00	-0.00064	0.00048	-0.02037	0.01306	-0.00000	0.99799
9.50	-0.00044	0.00033	-0.01476	0.00957	-0.00000	0.99723
10.00	-0.00030	0.00023	-0.01065	0.00698	-0.00000	0.99655
10.50	-0.00021	0.00016	-0.00766	0.00507	-0.00000	0.99600
11.00	-0.00014	0.00011	-0.00550	0.00367	-0.00000	0.99562
11.50	-0.00010	0.00007	-0.00393	0.00264	-0.00000	0.99543
12.00	-0.00007	0.00005	-0.00281	0.00190	-0.00000	0.99546
13.00	-0.00003	0.00002	-0.00142	0.00097	-0.00000	0.99621
14.00	-0.00001	0.00001	-0.00071	0.00049	-0.00000	0.99786
15.00	-0.00001	0.00001	-0.00035	0.00025	0.00000	1.00037
16.00	-0.00000	0.00000	-0.00017	0.00012	0.00000	1.00365
17.00	-0.00000	0.00000	-0.00009	0.00006	0.00000	1.00757
18.00	-0.00000	0.00000	-0.00004	0.00003	0.00000	1.01202
19.00	-0.00000	0.00000	-0.00002	0.00001	0.00000	1.01688

APPENDIX G
ORBITAL TABLES FOR THE Li UHF WAVE FUNCTION

The orbital tables of this appendix have been calculated from the (eight-figure) parameters of Table 5.1. We list the orbital ϕ , its derivative ϕ' , the Hartree P function, its derivative P' , and the goodness functions $f(r)$ and $g(r)$.

Table G.1. Radial Characteristics of the UHF Lithium $1s\alpha$ Orbital.

r	$\phi(r)$	$\phi'(r)$	P(r)	P'(r)	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
0.	2.61891	-7.87375	0.	9.28381		
0.01	2.54145	-7.62106	0.09009	8.73903	1.15240	0.81765
0.02	2.46646	-7.37702	0.17487	8.22037	0.36677	0.94020
0.03	2.39388	-7.14133	0.25458	7.72662	0.13985	0.97651
0.04	2.32361	-6.91369	0.32948	7.25665	0.04746	0.99179
0.05	2.25558	-6.69383	0.39979	6.80937	0.00544	0.99903
0.06	2.18971	-6.48148	0.46574	6.38374	-0.01377	1.00253
0.07	2.12592	-6.27636	0.52753	5.97877	-0.02163	1.00409
0.08	2.06416	-6.07823	0.58538	5.59351	-0.02361	1.00460
0.09	2.00434	-5.88684	0.63947	5.22704	-0.02254	1.00452
0.10	1.94640	-5.70196	0.68998	4.87851	-0.01998	1.00413
0.12	1.83591	-5.35079	0.78098	4.23197	-0.01350	1.00296
0.14	1.73221	-5.02298	0.85967	3.64769	-0.00749	1.00174
0.16	1.63485	-4.71690	0.92726	3.12003	-0.00288	1.00071
0.18	1.54340	-4.43103	0.98482	2.64385	0.00027	0.99993
0.20	1.45748	-4.16397	1.03333	2.21446	0.00218	0.99940
0.22	1.37673	-3.91440	1.07368	1.82761	0.00313	0.99909
0.24	1.30080	-3.68110	1.10669	1.47941	0.00341	0.99895
0.26	1.22938	-3.46294	1.13309	1.16633	0.00324	0.99894
0.28	1.16219	-3.25886	1.15356	0.88518	0.00281	0.99903
0.30	1.09894	-3.06789	1.16869	0.63302	0.00224	0.99918
0.32	1.03939	-2.88911	1.17905	0.40721	0.00164	0.99937
0.34	0.98330	-2.72169	1.18514	0.20534	0.00106	0.99957
0.36	0.93045	-2.56484	1.18741	0.02520	0.00054	0.99977
0.38	0.88064	-2.41783	1.18628	-0.13519	0.00009	0.99996
0.40	0.83368	-2.28000	1.18212	-0.27765	-0.00026	1.00012
0.45	0.72759	-1.97155	1.16066	-0.56580	-0.00076	1.00042
0.50	0.63577	-1.70807	1.12688	-0.77373	-0.00085	1.00054
0.55	0.55615	-1.48244	1.08433	-0.91879	-0.00069	1.00050
0.60	0.48700	-1.28873	1.03582	-1.01470	-0.00042	1.00035
0.65	0.42683	-1.12204	0.98350	-1.07232	-0.00016	1.00015
0.70	0.37441	-0.97828	0.92908	-1.10028	0.00005	0.99995
0.75	0.32868	-0.85403	0.87385	-1.10545	0.00019	0.99977
0.80	0.28873	-0.74642	0.81882	-1.09328	0.00026	0.99964
0.85	0.25380	-0.65307	0.76474	-1.06811	0.00027	0.99957
0.90	0.22322	-0.57193	0.71217	-1.03341	0.00024	0.99957
0.95	0.19643	-0.50131	0.66151	-0.99193	0.00019	0.99962
1.00	0.17294	-0.43976	0.61305	-0.94586	0.00012	0.99971
1.05	0.15232	-0.38604	0.56697	-0.89692	0.00006	0.99984
1.10	0.13422	-0.33910	0.52338	-0.84648	0.00000	0.99999
1.15	0.11832	-0.29805	0.48233	-0.79561	-0.00004	1.00014
1.20	0.10433	-0.26210	0.44382	-0.74511	-0.00007	1.00027
1.25	0.09203	-0.23061	0.40780	-0.69562	-0.00009	1.00039
1.30	0.08121	-0.20299	0.37423	-0.64760	-0.00010	1.00048
1.35	0.07168	-0.17876	0.34301	-0.60140	-0.00009	1.00053
1.40	0.06328	-0.15748	0.31406	-0.55725	-0.00009	1.00055
1.45	0.05588	-0.13879	0.28725	-0.51530	-0.00007	1.00052
1.50	0.04936	-0.12236	0.26249	-0.47564	-0.00006	1.00045
1.55	0.04362	-0.10791	0.23965	-0.43830	-0.00004	1.00035
1.60	0.03854	-0.09519	0.21862	-0.40329	-0.00002	1.00022
1.65	0.03407	-0.08400	0.19928	-0.37056	-0.00001	1.00006
1.70	0.03012	-0.07415	0.18153	-0.34006	0.00001	0.99989
1.75	0.02664	-0.06547	0.16524	-0.31171	0.00002	0.99972
1.80	0.02356	-0.05782	0.15032	-0.28541	0.00003	0.99954
1.85	0.02084	-0.05107	0.13667	-0.26107	0.00003	0.99937
1.90	0.01844	-0.04513	0.12418	-0.23858	0.00004	0.99922
1.95	0.01632	-0.03988	0.11278	-0.21785	0.00004	0.99909
2.00	0.01444	-0.03525	0.10237	-0.19875	0.00004	0.99899
2.10	0.01131	-0.02756	0.08423	-0.16507	0.00003	0.99891
2.20	0.00887	-0.02156	0.06918	-0.13673	0.00002	0.99902
2.30	0.00696	-0.01688	0.05673	-0.11299	0.00001	0.99931
2.40	0.00546	-0.01322	0.04645	-0.09316	0.00000	0.99979
2.50	0.00429	-0.01036	0.03799	-0.07666	-0.00000	1.00043
2.60	0.00337	-0.00813	0.03103	-0.06297	-0.00001	1.00118

Table G.1. (continued).

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
2.70	0.00264	-0.00637	0.02531	-0.05164	-0.00001	1.00198
2.80	0.00208	-0.00500	0.02063	-0.04228	-0.00001	1.00274
2.90	0.00163	-0.00393	0.01680	-0.03457	-0.00001	1.00340
3.00	0.00129	-0.00308	0.01367	-0.02823	-0.00001	1.00385
3.10	0.00101	-0.00242	0.01112	-0.02302	-0.00001	1.00400
3.20	0.00080	-0.00190	0.00904	-0.01875	-0.00001	1.00376
3.30	0.00063	-0.00149	0.00734	-0.01526	-0.00000	1.00306
3.40	0.00049	-0.00118	0.00596	-0.01241	-0.00000	1.00182
3.50	0.00039	-0.00092	0.00484	-0.01009	0.00000	0.99999
3.60	0.00031	-0.00073	0.00393	-0.00819	0.00000	0.99755
3.70	0.00024	-0.00057	0.00319	-0.00665	0.00000	0.99450
3.80	0.00019	-0.00045	0.00259	-0.00540	0.00000	0.99089
3.90	0.00015	-0.00036	0.00210	-0.00438	0.00000	0.98679
4.00	0.00012	-0.00028	0.00171	-0.00356	0.00001	0.98234
4.20	0.00008	-0.00018	0.00113	-0.00235	0.00001	0.97313
4.40	0.00005	-0.00011	0.00074	-0.00155	0.00000	0.96542
4.60	0.00003	-0.00007	0.00049	-0.00103	0.00000	0.96243
4.80	0.00002	-0.00004	0.00032	-0.00068	0.00000	0.96871
5.00	0.00001	-0.00003	0.00020	-0.00046	0.00000	0.99080
5.20	0.00001	-0.00002	0.00013	-0.00030	-0.00000	1.03867
5.40	0.00000	-0.00001	0.00008	-0.00020	-0.00000	1.12933
5.60	0.00000	-0.00001	0.00005	-0.00013	-0.00000	1.29689
5.80	0.00000	-0.00000	0.00003	-0.00009	-0.00000	1.62537
6.00	0.00000	-0.00000	0.00001	-0.00005	-0.00000	2.40172
6.20	0.00000	-0.00000	0.00000	-0.00003	-0.00000	5.68811
6.40	-0.00000	-0.00000	-0.00000	-0.00002	-0.00000	-9.80193
6.60	-0.00000	-0.00000	-0.00000	-0.00001	-0.00000	-2.44447
6.80	-0.00000	0.00000	-0.00000	0.00000	-0.00000	-1.36876
7.00	-0.00000	0.00000	-0.00000	0.00001	-0.00000	-0.96896
7.20	-0.00000	0.00000	-0.00000	0.00001	-0.00000	-0.83923
7.40	-0.00000	0.00000	-0.00000	0.00001	-0.00000	-6.90736
7.60	0.00000	0.00000	0.00000	0.00001	0.00000	-0.17528

Table G.2. Radial Characteristics of the UHF Lithium $1s'\beta$ Orbital.

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
0.	2.60725	-7.83854	0.	9.24244		
0.01	2.53013	-7.58638	0.08969	8.70014	1.13357	0.81852
0.02	2.45549	-7.34287	0.17409	8.18389	0.35841	0.94088
0.03	2.38324	-7.10771	0.25345	7.69249	0.13511	0.97704
0.04	2.31331	-6.88061	0.32802	7.22482	0.04459	0.99219
0.05	2.24560	-6.66130	0.39802	6.77978	0.00370	0.99933
0.06	2.18006	-6.44949	0.46369	6.35633	-0.01477	1.00274
0.07	2.11659	-6.24493	0.52522	5.95348	-0.02213	1.00424
0.08	2.05514	-6.04737	0.58282	5.57028	-0.02377	1.00468
0.09	1.99562	-5.85654	0.63669	5.20581	-0.02247	1.00456
0.10	1.93798	-5.67223	0.68700	4.85922	-0.01975	1.00413
0.12	1.82808	-5.32221	0.77764	4.21636	-0.01311	1.00291
0.14	1.72494	-4.99555	0.85606	3.63552	-0.00708	1.00166
0.16	1.62811	-4.69063	0.92344	3.11105	-0.00250	1.00062
0.18	1.53718	-4.40593	0.98085	2.63781	0.00057	0.99985
0.20	1.45175	-4.14002	1.02926	2.21112	0.00239	0.99933
0.22	1.37146	-3.89159	1.06957	1.82673	0.00327	0.99903
0.24	1.29598	-3.65942	1.10259	1.48077	0.00347	0.99891
0.26	1.22498	-3.44237	1.12904	1.16971	0.00325	0.99893
0.28	1.15819	-3.23938	1.14959	0.89035	0.00277	0.99903
0.30	1.09532	-3.04947	1.16484	0.63978	0.00217	0.99920
0.32	1.03613	-2.87173	1.17535	0.41537	0.00155	0.99940
0.34	0.98038	-2.70532	1.18162	0.21471	0.00095	0.99961
0.36	0.92785	-2.54944	1.18409	0.03561	0.00043	0.99981
0.38	0.87833	-2.40338	1.18317	-0.12390	-0.00001	1.00000
0.40	0.83165	-2.26646	1.17925	-0.26564	-0.00035	1.00017
0.45	0.72619	-1.96015	1.15842	-0.55257	-0.00082	1.00046
0.50	0.63489	-1.69857	1.12531	-0.76002	-0.00087	1.00055
0.55	0.55570	-1.47463	1.08346	-0.90516	-0.00068	1.00049
0.60	0.48690	-1.28240	1.03561	-1.00158	-0.00039	1.00033
0.65	0.42702	-1.11700	0.98393	-1.06004	-0.00012	1.00012
0.70	0.37482	-0.97434	0.93009	-1.08906	0.00009	0.99990
0.75	0.32926	-0.85103	0.87540	-1.09541	0.00022	0.99972
0.80	0.28944	-0.74421	0.82084	-1.08449	0.00028	0.99960
0.85	0.25460	-0.65152	0.76717	-1.06059	0.00028	0.99955
0.90	0.22409	-0.57093	0.71494	-1.02713	0.00024	0.99956
0.95	0.19734	-0.50076	0.66457	-0.98684	0.00018	0.99963
1.00	0.17386	-0.43956	0.61633	-0.94188	0.00011	0.99974
1.05	0.15325	-0.38613	0.57043	-0.89398	0.00004	0.99988
1.10	0.13514	-0.33942	0.52696	-0.84447	-0.00001	1.00004
1.15	0.11921	-0.29854	0.48599	-0.79443	-0.00006	1.00020
1.20	0.10520	-0.26273	0.44751	-0.74468	-0.00009	1.00034
1.25	0.09287	-0.23133	0.41151	-0.69584	-0.00010	1.00046
1.30	0.08200	-0.20378	0.37791	-0.64838	-0.00011	1.00054
1.35	0.07243	-0.17958	0.34664	-0.60265	-0.00010	1.00057
1.40	0.06400	-0.15833	0.31761	-0.55889	-0.00009	1.00057
1.45	0.05656	-0.13964	0.29072	-0.51726	-0.00007	1.00052
1.50	0.05000	-0.12320	0.26585	-0.47786	-0.00005	1.00043
1.55	0.04421	-0.10873	0.24289	-0.44073	-0.00003	1.00031
1.60	0.03909	-0.09599	0.22174	-0.40587	-0.00001	1.00015
1.65	0.03458	-0.08477	0.20227	-0.37324	0.00000	0.99997
1.70	0.03059	-0.07488	0.18438	-0.34281	0.00002	0.99978
1.75	0.02707	-0.06616	0.16795	-0.31448	0.00003	0.99959
1.80	0.02396	-0.05848	0.15289	-0.28819	0.00004	0.99940
1.85	0.02121	-0.05169	0.13910	-0.26383	0.00004	0.99922
1.90	0.01878	-0.04571	0.12648	-0.24130	0.00004	0.99907
1.95	0.01663	-0.04043	0.11494	-0.22050	0.00004	0.99895
2.00	0.01473	-0.03576	0.10440	-0.20133	0.00004	0.99887
2.10	0.01155	-0.02800	0.08601	-0.16747	0.00003	0.99884
2.20	0.00907	-0.02194	0.07073	-0.13893	0.00002	0.99902
2.30	0.00712	-0.01720	0.05807	-0.11497	0.00001	0.99942
2.40	0.00560	-0.01349	0.04761	-0.09493	-0.00000	1.00003
2.50	0.00440	-0.01059	0.03898	-0.07822	-0.00001	1.00079
2.60	0.00346	-0.00831	0.03187	-0.06433	-0.00001	1.00166

Table G.2. (continued).

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
2.70	0.00272	-0.00653	0.02603	-0.05282	-0.00002	1.00255
2.80	0.00214	-0.00513	0.02124	-0.04330	-0.00002	1.00338
2.90	0.00168	-0.00403	0.01732	-0.03544	-0.00002	1.00403
3.00	0.00133	-0.00317	0.01411	-0.02897	-0.00001	1.00440
3.10	0.00105	-0.00249	0.01148	-0.02365	-0.00001	1.00439
3.20	0.00082	-0.00196	0.00934	-0.01928	-0.00001	1.00387
3.30	0.00065	-0.00154	0.00760	-0.01571	-0.00000	1.00278
3.40	0.00051	-0.00121	0.00618	-0.01279	-0.00000	1.00102
3.50	0.00041	-0.00095	0.00503	-0.01040	0.00000	0.99856
3.60	0.00032	-0.00075	0.00409	-0.00846	0.00000	0.99538
3.70	0.00025	-0.00059	0.00332	-0.00688	0.00001	0.99151
3.80	0.00020	-0.00047	0.00270	-0.00559	0.00001	0.98701
3.90	0.00016	-0.00037	0.00220	-0.00454	0.00001	0.98202
4.00	0.00013	-0.00029	0.00179	-0.00369	0.00001	0.97672
4.20	0.00008	-0.00018	0.00118	-0.00245	0.00001	0.96629
4.40	0.00005	-0.00012	0.00078	-0.00163	0.00001	0.95865
4.60	0.00003	-0.00007	0.00051	-0.00108	0.00000	0.95812
4.80	0.00002	-0.00005	0.00033	-0.00073	0.00000	0.97086
5.00	0.00001	-0.00003	0.00021	-0.00049	-0.00000	1.00603
5.20	0.00001	-0.00002	0.00013	-0.00033	-0.00000	1.07859
5.40	0.00000	-0.00001	0.00008	-0.00022	-0.00000	1.21716
5.60	0.00000	-0.00001	0.00004	-0.00014	-0.00000	1.48870
5.80	0.00000	-0.00000	0.00002	-0.00009	-0.00000	2.10463
6.00	0.00000	-0.00000	0.00001	-0.00005	-0.00000	4.29137
6.20	-0.00000	-0.00000	-0.00000	-0.00003	-0.00000	-19.94293
6.40	-0.00000	-0.00000	-0.00001	-0.00001	-0.00000	-2.72565
6.60	-0.00000	0.00000	-0.00001	-0.00000	-0.00000	-1.41693
6.80	-0.00000	0.00000	-0.00001	0.00001	-0.00000	-0.95648
7.00	-0.00000	0.00000	-0.00000	0.00001	-0.00000	-0.75335
7.20	-0.00000	0.00000	-0.00000	0.00001	-0.00000	-0.80317
7.40	0.00000	0.00000	0.00000	0.00001	0.00000	-0.05426
7.60	0.00000	0.00000	0.00000	0.00001	0.00000	-0.22046

Table G.3. Radial Characteristics of the UHF Lithium 2s α Orbital.

r	$\phi(r)$	$\phi'(r)$	P(r)	P'(r)	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
0.	0.40482	-1.21788	0.	1.43504		
0.01	0.39281	-1.18303	0.01392	1.35055	0.23864	-2.09381
0.02	0.38115	-1.14927	0.02702	1.26967	0.07871	-0.05159
0.03	0.36982	-1.11658	0.03933	1.19225	0.03175	0.56282
0.04	0.35882	-1.08492	0.05088	1.11814	0.01216	0.82745
0.05	0.34812	-1.05425	0.06170	1.04720	0.00292	0.95729
0.06	0.33773	-1.02456	0.07183	0.97930	-0.00156	1.02350
0.07	0.32763	-0.99579	0.08130	0.91431	-0.00361	1.05618
0.08	0.31781	-0.96794	0.09013	0.85211	-0.00437	1.07010
0.09	0.30827	-0.94095	0.09835	0.79257	-0.00443	1.07320
0.10	0.29899	-0.91482	0.10599	0.73559	-0.00411	1.07005
0.12	0.28120	-0.86498	0.11962	0.62886	-0.00304	1.05499
0.14	0.26437	-0.81820	0.13120	0.53110	-0.00190	1.03667
0.16	0.24845	-0.77429	0.14092	0.44156	-0.00096	1.01971
0.18	0.23338	-0.73305	0.14892	0.35956	-0.00027	1.00581
0.20	0.21911	-0.69432	0.15535	0.28446	0.00020	0.99535
0.22	0.20559	-0.65793	0.16034	0.21569	0.00048	0.98816
0.24	0.19278	-0.62373	0.16401	0.15273	0.00061	0.98381
0.26	0.18063	-0.59157	0.16648	0.09508	0.00065	0.98181
0.28	0.16910	-0.56131	0.16785	0.04231	0.00061	0.98164
0.30	0.15816	-0.53284	0.16820	-0.00598	0.00053	0.98286
0.32	0.14778	-0.50603	0.16764	-0.05017	0.00043	0.98507
0.34	0.13791	-0.48078	0.16622	-0.09058	0.00033	0.98793
0.36	0.12854	-0.45698	0.16404	-0.12753	0.00022	0.99116
0.38	0.11962	-0.43454	0.16114	-0.16129	0.00013	0.99454
0.40	0.11115	-0.41337	0.15760	-0.19213	0.00005	0.99789
0.45	0.09170	-0.36547	0.14629	-0.25792	-0.00010	1.00537
0.50	0.07450	-0.32387	0.13204	-0.30996	-0.00016	1.01070
0.55	0.05923	-0.28760	0.11548	-0.35078	-0.00016	1.01349
0.60	0.04566	-0.25588	0.09711	-0.38238	-0.00012	1.01376
0.65	0.03358	-0.22803	0.07737	-0.40639	-0.00008	1.01165
0.70	0.02280	-0.20348	0.05658	-0.42410	-0.00003	1.00690
0.75	0.01318	-0.18178	0.03504	-0.43658	0.00001	0.99744
0.80	0.00458	-0.16253	0.01300	-0.44467	0.00003	0.96369
0.85	-0.00311	-0.14539	-0.00936	-0.44910	0.00005	1.07735
0.90	-0.00999	-0.13009	-0.03186	-0.45045	0.00005	1.02643
0.95	-0.01614	-0.11639	-0.05436	-0.44919	0.00005	1.01546
1.00	-0.02165	-0.10409	-0.07675	-0.44575	0.00004	1.00970
1.05	-0.02657	-0.09302	-0.09891	-0.44044	0.00003	1.00589
1.10	-0.03097	-0.08304	-0.12076	-0.43358	0.00002	1.00320
1.15	-0.03489	-0.07401	-0.14224	-0.42539	0.00001	1.00126
1.20	-0.03838	-0.06583	-0.16329	-0.41611	-0.00000	0.99990
1.25	-0.04149	-0.05841	-0.18384	-0.40590	-0.00001	0.99898
1.30	-0.04424	-0.05167	-0.20386	-0.39492	-0.00001	0.99842
1.35	-0.04666	-0.04553	-0.22332	-0.38332	-0.00002	0.99814
1.40	-0.04880	-0.03994	-0.24219	-0.37121	-0.00002	0.99806
1.45	-0.05067	-0.03484	-0.26043	-0.35870	-0.00002	0.99813
1.50	-0.05229	-0.03019	-0.27805	-0.34588	-0.00002	0.99832
1.55	-0.05369	-0.02593	-0.29502	-0.33282	-0.00002	0.99856
1.60	-0.05489	-0.02204	-0.31133	-0.31961	-0.00001	0.99885
1.65	-0.05590	-0.01849	-0.32698	-0.30630	-0.00001	0.99914
1.70	-0.05674	-0.01523	-0.34196	-0.29295	-0.00001	0.99943
1.75	-0.05743	-0.01225	-0.35627	-0.27961	-0.00000	0.99970
1.80	-0.05797	-0.00953	-0.36992	-0.26631	-0.00000	0.99994
1.85	-0.05839	-0.00703	-0.38291	-0.25311	0.00000	1.00015
1.90	-0.05868	-0.00475	-0.39523	-0.24002	0.00000	1.00032
1.95	-0.05887	-0.00266	-0.40691	-0.22707	0.00001	1.00045
2.00	-0.05895	-0.00075	-0.41794	-0.21430	0.00001	1.00054
2.10	-0.05885	0.00259	-0.43812	-0.18937	0.00001	1.00063
2.20	-0.05845	0.00537	-0.45585	-0.16535	0.00001	1.00061
2.30	-0.05780	0.00767	-0.47123	-0.14236	0.00001	1.00051
2.40	-0.05693	0.00956	-0.48436	-0.12046	0.00000	1.00037
2.50	-0.05590	0.01111	-0.49536	-0.09971	0.00000	1.00021
2.60	-0.05472	0.01235	-0.50434	-0.08013	0.00000	1.00006
2.70	-0.05343	0.01334	-0.51142	-0.06174	-0.00000	0.99992
2.80	-0.05206	0.01411	-0.51673	-0.04453	-0.00000	0.99981
2.90	-0.05062	0.01468	-0.52037	-0.02850	-0.00000	0.99974
3.00	-0.04913	0.01510	-0.52246	-0.01361	-0.00000	0.99969
3.10	-0.04760	0.01537	-0.52313	0.00015	-0.00000	0.99968
3.20	-0.04606	0.01552	-0.52247	0.01282	-0.00000	0.99969

Table G.3. (continued).

r	$\phi(r)$	$\phi'(r)$	$P(r)$	$P'(r)$	$F\phi - \epsilon\phi$	$F\phi/\epsilon\phi$
3.30	-0.04450	0.01558	-0.52060	0.02445	-0.00000	0.99973
3.40	-0.04295	0.01554	-0.51762	0.03506	-0.00000	0.99978
3.50	-0.04140	0.01543	-0.51362	0.04471	-0.00000	0.99984
3.60	-0.03986	0.01526	-0.50870	0.05344	-0.00000	0.99991
3.70	-0.03835	0.01504	-0.50296	0.06129	-0.00000	0.99998
3.80	-0.03686	0.01477	-0.49647	0.06832	0.00000	1.00004
3.90	-0.03539	0.01447	-0.48932	0.07457	0.00000	1.00010
4.00	-0.03396	0.01414	-0.48158	0.08009	0.00000	1.00015
4.20	-0.03121	0.01341	-0.46462	0.08909	0.00000	1.00021
4.40	-0.02860	0.01264	-0.44611	0.09569	0.00000	1.00024
4.60	-0.02615	0.01183	-0.42648	0.10021	0.00000	1.00022
4.80	-0.02387	0.01102	-0.40614	0.10295	0.00000	1.00017
5.00	-0.02174	0.01023	-0.38541	0.10417	0.00000	1.00010
5.20	-0.01978	0.00945	-0.36456	0.10414	0.00000	1.00002
5.40	-0.01796	0.00871	-0.34382	0.10306	-0.00000	0.99993
5.60	-0.01629	0.00800	-0.32339	0.10113	-0.00000	0.99986
5.80	-0.01476	0.00734	-0.30342	0.09851	-0.00000	0.99980
6.00	-0.01335	0.00671	-0.28402	0.09537	-0.00000	0.99975
6.20	-0.01207	0.00612	-0.26530	0.09182	-0.00000	0.99973
6.40	-0.01090	0.00558	-0.24731	0.08797	-0.00000	0.99973
6.60	-0.00984	0.00508	-0.23012	0.08392	-0.00000	0.99975
6.80	-0.00887	0.00461	-0.21375	0.07974	-0.00000	0.99979
7.00	-0.00799	0.00418	-0.19823	0.07551	-0.00000	0.99984
7.20	-0.00719	0.00379	-0.18355	0.07128	-0.00000	0.99990
7.40	-0.00647	0.00343	-0.16971	0.06709	-0.00000	0.99998
7.60	-0.00582	0.00310	-0.15671	0.06298	0.00000	1.00006
7.80	-0.00523	0.00280	-0.14451	0.05897	0.00000	1.00014
8.00	-0.00469	0.00253	-0.13311	0.05510	0.00000	1.00023
8.20	-0.00421	0.00228	-0.12246	0.05137	0.00000	1.00030
8.40	-0.00378	0.00206	-0.11255	0.04781	0.00000	1.00037
8.60	-0.00339	0.00185	-0.10333	0.04441	0.00000	1.00044
8.80	-0.00304	0.00167	-0.09477	0.04118	0.00000	1.00049
9.00	-0.00272	0.00150	-0.08685	0.03813	0.00000	1.00052
9.50	-0.00207	0.00115	-0.06954	0.03125	0.00000	1.00055
10.00	-0.00156	0.00087	-0.05542	0.02542	0.00000	1.00048
10.50	-0.00118	0.00066	-0.04397	0.02053	0.00000	1.00029
11.00	-0.00089	0.00050	-0.03475	0.01648	-0.00000	0.99999
11.50	-0.00067	0.00038	-0.02736	0.01316	-0.00000	0.99958
12.00	-0.00050	0.00029	-0.02148	0.01046	-0.00000	0.99908
12.50	-0.00038	0.00022	-0.01681	0.00828	-0.00000	0.99849
13.00	-0.00028	0.00016	-0.01313	0.00653	-0.00000	0.99783
13.50	-0.00021	0.00012	-0.01022	0.00513	-0.00000	0.99710
14.00	-0.00016	0.00009	-0.00794	0.00402	-0.00000	0.99633
14.50	-0.00012	0.00007	-0.00616	0.00314	-0.00000	0.99552
15.00	-0.00009	0.00005	-0.00477	0.00245	-0.00000	0.99468
15.50	-0.00007	0.00004	-0.00368	0.00191	-0.00000	0.99382
16.00	-0.00005	0.00003	-0.00284	0.00148	-0.00000	0.99295
16.50	-0.00004	0.00002	-0.00219	0.00115	-0.00000	0.99209
17.00	-0.00003	0.00002	-0.00168	0.00089	-0.00000	0.99123
17.50	-0.00002	0.00001	-0.00129	0.00068	-0.00000	0.99039
18.00	-0.00002	0.00001	-0.00099	0.00053	-0.00000	0.98957
18.50	-0.00001	0.00001	-0.00076	0.00041	-0.00000	0.98878
19.00	-0.00001	0.00001	-0.00058	0.00031	-0.00000	0.98803
19.50	-0.00001	0.00000	-0.00045	0.00024	-0.00000	0.98730
20.00	-0.00000	0.00000	-0.00034	0.00018	-0.00000	0.98662
20.50	-0.00000	0.00000	-0.00026	0.00014	-0.00000	0.98598
21.00	-0.00000	0.00000	-0.00020	0.00011	-0.00000	0.98539
21.50	-0.00000	0.00000	-0.00015	0.00008	-0.00000	0.98484
22.00	-0.00000	0.00000	-0.00011	0.00006	-0.00000	0.98434
22.50	-0.00000	0.00000	-0.00009	0.00005	-0.00000	0.98389
23.00	-0.00000	0.00000	-0.00007	0.00004	-0.00000	0.98349
23.50	-0.00000	0.00000	-0.00005	0.00003	-0.00000	0.98314
24.00	-0.00000	0.00000	-0.00004	0.00002	-0.00000	0.98284
24.50	-0.00000	0.00000	-0.00003	0.00002	-0.00000	0.98259
25.00	-0.00000	0.00000	-0.00002	0.00001	0.00000	0.98239
25.50	-0.00000	0.00000	-0.00002	0.00001	-0.00000	0.98223
26.00	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.98213
26.50	-0.00000	0.00000	-0.00001	0.00001	0.00000	0.98207
27.00	-0.00000	0.00000	-0.00001	0.00000	-0.00000	0.98205
27.50	-0.00000	0.00000	-0.00001	0.00000	-0.00000	0.98208

APPENDIX H PARAMETERS FOR THE F, F⁻, Ne, Na⁺, and Na GROUND-STATE SCF WAVE FUNCTIONS

We have listed in this appendix the parameters used to obtain the expansion for the radial portion of the orbitals for the series of HF wave functions reported in Chapter VI. Each orbital is written as in (3.17):

$$\phi_{n\ell m}(r, \theta, \varphi) = R_{n\ell}(r) Y_{\ell m}(\theta, \varphi) \quad ,$$

where the radial functions are given as

$$R_i = \sum_p c_{i;p} \chi_p$$

and

$$\chi_p = [(2N_p)!]^{-1/2} (2\zeta_p)^{N_p+1/2} r^{N_p-1} e^{-\zeta_p r} \quad .$$

Table H.1. Parameters for F.

ζ	N	C_{1s}	C_{2s}	ζ	N	C_{2p}
13.00	1	0.083213	- 0.318543	5.85	2	0.058234
8.30	1	0.917427	0.876397	4.40	2	0.056213
11.00	2	- 0.000438	- 0.277799	3.28	2	0.430374
5.00	2	0.007829	- 0.080002	1.66	2	0.570120
3.10	2	0.001847	- 0.585995	6.20	3	- 0.025913
2.00	2	0.001052	- 0.451711			
- ϵ		24.897355	0.619046			0.036830
- $\tilde{R}$		9.0028	8.9592			10.8257
- E			99.40900			

Table H.2. Parameters for F⁻.

ζ	N	C_{1s}	C_{2s}	ζ	N	C_{2p}
12.20	1	0.089611	- 0.199570	6.05	2	0.064814
8.20	1	0.938018	0.610790	3.06	2	0.551546
10.80	2	- 0.022939	- 0.138830	1.44	2	0.500480
4.10	2	- 0.007729	- 0.193139	0.69	2	0.086499
2.66	2	- 0.005912	- 0.565973	3.75	3	- 0.058375
1.68	2	0.001681	- 0.300736	8.00	3	- 0.006756
4.50	3	0.014018	- 0.053758			
- ϵ		25.82956	1.074662			0.1810072
- $\tilde{R}$		8.9947	9.0409			10.1932
- E			99.45921			

Table H.3. Parameters for Ne.

ζ	N	C_{1s}	C_{2s}	ζ	N	C_{2p}
14.00	1	0.104781	- 0.339010	6.60	2	0.071588
9.20	1	0.891761	0.891909	3.40	2	0.616462
12.00	2	0.006277	- 0.270688	2.20	2	0.261474
4.50	2	0.008780	- 0.289318	1.60	2	0.296791
2.80	2	- 0.001525	- 0.706866	4.00	3	- 0.152330
1.80	2	0.000650	- 0.127561	9.00	3	- 0.010184
5.00	3	- 0.000799	0.004109			
- ϵ		32.77205	1.930050			0.8501921
- $\tilde{R}$		10.0011	9.9808			11.4695
- E			128.5470			

Table H.4. Parameters for Na⁺.

ζ	N	C_{1s}	C_{2s}	ζ	N	C_{2p}
15.00	1	0.118514	0.050484	6.60	2	0.135376
10.30	1	0.854775	0.171023	3.40	2	0.715241
				2.30	2	0.362710
11.00	2	0.031730	0.084504	1.80	2	0.062804
5.40	2	0.008566	- 0.115679			
3.10	2	- 0.001522	- 0.775681	4.00	3	0.202196
2.00	2	0.000665	- 0.050108	9.60	3	- 0.014961
6.00	3	0.000535	- 0.144197			
- ϵ		40.75973	3.073676			1.797188
- $\tilde{R}$		11.0025	11.0537			13.1688
- E			161.6769			

Table H.5. Parameters for Na.

ζ	N	C_{1s}	C_{2s}	C_{3s}	ζ	N	C_{2p}
15.00	1	0.119350	0.047534	0.032102	6.60	2	0.136986
10.30	1	0.853316	0.176254	- 0.017092	3.40	2	0.711595
					2.30	2	0.327634
11.00	2	0.032905	0.080178	0.050078	1.80	2	0.087792
5.40	2	0.007227	- 0.110721	- 0.054853			
3.10	2	- 0.002610	- 0.768442	- 0.244542	4.00	3	- 0.187674
2.00	2	0.001321	- 0.054269	0.098813	9.60	3	- 0.014453
6.00	3	0.002122	- 0.151899	0.048011			
1.00	3	- 0.000378	0.001880	0.376549			
0.75	3	0.000224	- 0.001112	0.630171			
- ϵ		40.47482	2.788847	0.07343543			1.513905
- $\tilde{R}$		11.0029	11.0473	11.3573			13.1429
- E				161.8587			

APPENDIX I
ORBITAL TABLES OF THE F, F⁻, Ne, Na⁺, AND Na GROUND-STATE
SCF WAVE FUNCTIONS

The orbital tables contained in this appendix have been calculated from the (eight-figure) parameter tables of Appendix H. We list the radial function R , its derivative R' , the Hartree function P , its derivative P' , and the two goodness functions $f(r)$ and $g(r)$ of (6.6).

Table I.1. Radial Characteristics of the Hartree-Fock F 1s Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR-εR	FR/εR
0.	51.67586	-465.22771	0.	51.67586		
0.01	47.23372	-423.87021	0.47234	42.99502	-16.52641	1.01405
0.02	43.18573	-386.33269	0.86371	35.45908	-11.53850	1.01073
0.03	39.49557	-352.24675	1.18487	28.92816	-6.08799	1.00619
0.04	36.13040	-321.28121	1.44522	23.27915	-2.39051	1.00266
0.05	33.06054	-293.13809	1.65303	18.40363	-0.18517	1.00022
0.06	30.25912	-267.54915	1.81555	14.20618	0.97215	0.99871
0.07	27.70185	-244.27284	1.93913	10.60275	1.44926	0.99790
0.08	25.36669	-223.09148	2.02933	7.51937	1.51389	0.99760
0.09	23.23369	-203.80883	2.09103	4.89090	1.34978	0.99767
0.10	21.28477	-186.24781	2.12848	2.65999	1.07792	0.99797
0.12	17.87508	-155.66703	2.14501	-0.80497	0.48448	0.99891
0.14	15.02373	-130.24736	2.10332	-3.21090	0.02687	0.99993
0.16	12.63681	-109.08850	2.02189	-4.81735	-0.23734	1.00075
0.18	10.63673	-91.45322	1.91461	-5.82485	-0.33991	1.00128
0.20	8.95925	-76.73662	1.79185	-6.38807	-0.33480	1.00150
0.22	7.55114	-64.44143	1.66125	-6.62597	-0.27122	1.00144
0.24	6.36820	-54.15809	1.52837	-6.62974	-0.18526	1.00117
0.26	5.37367	-45.54864	1.39715	-6.46898	-0.09981	1.00075
0.28	4.53696	-38.33376	1.27035	-6.19649	-0.02727	1.00024
0.30	3.83257	-32.28218	1.14977	-5.85208	0.02735	0.99971
0.35	2.51923	-21.06270	0.88173	-4.85272	0.08843	0.99859
0.40	1.66102	-13.78679	0.66441	-3.85370	0.07860	0.99810
0.45	1.09851	-9.04995	0.49433	-2.97397	0.04376	0.99840
0.50	0.72881	-5.95600	0.36441	-2.24918	0.01071	0.99941
0.55	0.48523	-3.92947	0.26688	-1.67598	-0.01087	1.00090
0.60	0.32434	-2.59886	0.19460	-1.23497	-0.02070	1.00256
0.65	0.21781	-1.72327	0.14157	-0.90232	-0.02205	1.00407
0.70	0.14707	-1.14591	0.10295	-0.65507	-0.01859	1.00508
0.75	0.09997	-0.76445	0.07498	-0.47337	-0.01320	1.00530
0.80	0.06849	-0.51189	0.05479	-0.34102	-0.00770	1.00452
0.85	0.04737	-0.34431	0.04027	-0.24529	-0.00304	1.00257
0.90	0.03313	-0.23282	0.02982	-0.17641	0.00044	0.99946
0.95	0.02347	-0.15845	0.02230	-0.12705	0.00274	0.99531
1.00	0.01688	-0.10866	0.01688	-0.09178	0.00403	0.99040
1.10	0.00918	-0.05259	0.01010	-0.04867	0.00453	0.98016
1.20	0.00537	-0.02673	0.00645	-0.02671	0.00362	0.97297
1.30	0.00339	-0.01445	0.00441	-0.01539	0.00234	0.97224
1.40	0.00228	-0.00836	0.00320	-0.00942	0.00121	0.97870
1.50	0.00162	-0.00519	0.00243	-0.00616	0.00038	0.99060
1.60	0.00120	-0.00343	0.00192	-0.00428	-0.00016	1.00522
1.70	0.00091	-0.00239	0.00155	-0.00314	-0.00046	1.02018
1.80	0.00071	-0.00173	0.00128	-0.00240	-0.00060	1.03390
1.90	0.00056	-0.00129	0.00106	-0.00189	-0.00064	1.04562
2.00	0.00045	-0.00099	0.00089	-0.00153	-0.00061	1.05508
2.10	0.00036	-0.00077	0.00076	-0.00125	-0.00056	1.06236
2.20	0.00029	-0.00060	0.00064	-0.00104	-0.00049	1.06771
2.30	0.00024	-0.00048	0.00055	-0.00087	-0.00042	1.07143
2.40	0.00019	-0.00039	0.00047	-0.00073	-0.00036	1.07382
2.50	0.00016	-0.00031	0.00040	-0.00062	-0.00030	1.07515
2.60	0.00013	-0.00025	0.00034	-0.00053	-0.00025	1.07566
2.70	0.00011	-0.00021	0.00029	-0.00045	-0.00020	1.07554
2.80	0.00009	-0.00017	0.00025	-0.00039	-0.00017	1.07497
2.90	0.00007	-0.00014	0.00021	-0.00033	-0.00014	1.07406
3.00	0.00006	-0.00011	0.00018	-0.00028	-0.00011	1.07292
3.20	0.00004	-0.00008	0.00014	-0.00021	-0.00007	1.07021
3.40	0.00003	-0.00005	0.00010	-0.00015	-0.00005	1.06728
3.60	0.00002	-0.00004	0.00007	-0.00011	-0.00003	1.06437
3.80	0.00001	-0.00003	0.00005	-0.00008	-0.00002	1.06163
4.00	0.00001	-0.00002	0.00004	-0.00006	-0.00001	1.05915
4.20	0.00001	-0.00001	0.00003	-0.00005	-0.00001	1.05699
4.40	0.00000	-0.00001	0.00002	-0.00003	-0.00001	1.05518
4.60	0.00000	-0.00001	0.00002	-0.00002	-0.00000	1.05373
4.80	0.00000	-0.00000	0.00001	-0.00002	-0.00000	1.05267

Table I.1. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.00000	-0.00000	0.00001	-0.00001	-0.00000	1.05200
5.20	0.00000	-0.00000	0.00001	-0.00001	-0.00000	1.05171
5.40	0.00000	-0.00000	0.00000	-0.00001	-0.00000	1.05181
5.60	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.05231
5.80	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.05318
6.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.05444
6.20	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.05607
6.40	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.05808
6.60	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.06047
6.80	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.06322
7.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.06634
7.20	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.06984
7.40	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.07370
7.60	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.07794
7.80	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.08256
8.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.08756
8.20	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.09295
8.40	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.09874
8.60	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.10493
8.80	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.11154
9.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.11858
9.20	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.12605
9.40	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.13398
9.60	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.14238
9.80	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.15126
10.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.16064

Table I.2. Radial Characteristics of the Hartree-Fock F 2s Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR-εR	FR/εR
0.	12.05132	-107.97060	0.	12.05132		
0.01	11.01102	-100.18410	0.11011	10.00918	-31.13855	5.56823
0.02	10.04581	-92.94644	0.20092	8.18688	-8.26665	2.32930
0.03	9.15037	-86.22300	0.27451	6.56368	-1.89293	1.33417
0.04	8.31975	-79.98006	0.33279	5.12054	0.41527	0.91937
0.05	7.54928	-74.18519	0.37746	3.84002	1.20245	0.74270
0.06	6.83465	-68.80735	0.41008	2.70621	1.33489	0.68450
0.07	6.17184	-63.81712	0.43203	1.70464	1.18300	0.69037
0.08	5.55711	-59.18667	0.44457	0.82218	0.92378	0.73147
0.09	4.98700	-54.88988	0.44883	0.04691	0.64521	0.79100
0.10	4.45828	-50.90225	0.44583	-0.63194	0.39020	0.85862
0.12	3.51338	-43.76455	0.42161	-1.73836	0.01169	0.99463
0.14	2.70116	-37.60917	0.37816	-2.56413	-0.18720	1.11195
0.16	2.00341	-32.29466	0.32055	-3.16373	-0.25054	1.20202
0.18	1.40457	-27.70010	0.25282	-3.58144	-0.23113	1.26582
0.20	0.89130	-23.72255	0.17826	-3.85321	-0.17166	1.31112
0.22	0.45215	-20.27453	0.09947	-4.00825	-0.10118	1.36147
0.24	0.07729	-17.28184	0.01855	-4.07036	-0.03672	1.76743
0.26	-0.24174	-14.68152	-0.06285	-4.05894	0.01351	1.09025
0.28	-0.51223	-12.42007	-0.14343	-3.98985	0.04714	1.14865
0.30	-0.74050	-10.45198	-0.22215	-3.87609	0.06526	1.14236
0.35	-1.16058	-6.57420	-0.40620	-3.46154	0.06228	1.08669
0.40	-1.41678	-3.83273	-0.56671	-2.94987	0.02918	1.03327
0.45	-1.55734	-1.90395	-0.70080	-2.41412	-0.00184	0.99809
0.50	-1.61690	-0.56067	-0.80845	-1.89723	-0.01896	0.98106
0.55	-1.62044	0.35927	-0.89124	-1.42284	-0.02262	0.97745
0.60	-1.58605	0.97313	-0.95163	-1.00217	-0.01785	0.98182
0.65	-1.52679	1.36636	-0.99241	-0.63866	-0.00980	0.98963
0.70	-1.45204	1.60151	-1.01643	-0.33098	-0.00204	0.99773
0.75	-1.36850	1.72443	-1.02638	-0.07518	0.00362	1.00428
0.80	-1.28091	1.76864	-1.02472	0.13401	0.00673	1.00849
0.85	-1.19254	1.75863	-1.01366	0.30230	0.00759	1.01027
0.90	-1.10565	1.71216	-0.99508	0.43529	0.00684	1.00999
0.95	-1.02172	1.64206	-0.97063	0.53824	0.00517	1.00818
1.00	-0.94168	1.55754	-0.94168	0.61585	0.00317	1.00544
1.10	-0.79522	1.36945	-0.87474	0.71117	-0.00037	0.99925
1.20	-0.66782	1.17995	-0.80138	0.74812	-0.00228	0.99448
1.30	-0.55878	1.00384	-0.72641	0.74622	-0.00262	0.99242
1.40	-0.46640	0.84699	-0.65297	0.71938	-0.00201	0.99304
1.50	-0.38869	0.71071	-0.58303	0.67737	-0.00106	0.99561
1.60	-0.32361	0.59413	-0.51777	0.62700	-0.00017	0.99917
1.70	-0.26927	0.49542	-0.45775	0.57295	0.00047	1.00283
1.80	-0.22400	0.41242	-0.40319	0.51837	0.00082	1.00591
1.90	-0.18633	0.34297	-0.35403	0.46531	0.00092	1.00798
2.00	-0.15502	0.28504	-0.31004	0.41505	0.00085	1.00884
2.10	-0.12900	0.23683	-0.27090	0.36834	0.00068	1.00846
2.20	-0.10738	0.19677	-0.23624	0.32551	0.00046	1.00696
2.30	-0.08942	0.16351	-0.20567	0.28666	0.00025	1.00453
2.40	-0.07449	0.13592	-0.17878	0.25172	0.00007	1.00142
2.50	-0.06208	0.11303	-0.15520	0.22050	-0.00008	0.99789
2.60	-0.05175	0.09404	-0.13456	0.19275	-0.00019	0.99418
2.70	-0.04316	0.07828	-0.11654	0.16818	-0.00025	0.99054
2.80	-0.03601	0.06519	-0.10083	0.14652	-0.00029	0.98718
2.90	-0.03005	0.05432	-0.08715	0.12747	-0.00029	0.98426
3.00	-0.02509	0.04528	-0.07526	0.11075	-0.00028	0.98193
3.20	-0.01749	0.03151	-0.05597	0.08332	-0.00022	0.97941
3.40	-0.01220	0.02195	-0.04149	0.06244	-0.00015	0.98013
3.60	-0.00852	0.01531	-0.03066	0.04662	-0.00008	0.98420
3.80	-0.00594	0.01069	-0.02259	0.03468	-0.00003	0.99147
4.00	-0.00415	0.00747	-0.01659	0.02572	0.00000	1.00164
4.20	-0.00289	0.00521	-0.01215	0.01901	0.00003	1.01429
4.40	-0.00202	0.00364	-0.00887	0.01401	0.00004	1.02903
4.60	-0.00141	0.00254	-0.00646	0.01029	0.00004	1.04542
4.80	-0.00098	0.00177	-0.00470	0.00753	0.00004	1.06311

Table I.2. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	-0.00068	0.00124	-0.00340	0.00550	0.00003	1.08175
5.20	-0.00047	0.00086	-0.00246	0.00401	0.00003	1.10107
5.40	-0.00033	0.00060	-0.00177	0.00291	0.00002	1.12083
5.60	-0.00023	0.00042	-0.00128	0.00211	0.00002	1.14084
5.80	-0.00016	0.00029	-0.00092	0.00152	0.00002	1.16096
6.00	-0.00011	0.00020	-0.00066	0.00110	0.00001	1.18106
6.20	-0.00008	0.00014	-0.00047	0.00079	0.00001	1.20106
6.40	-0.00005	0.00010	-0.00033	0.00057	0.00001	1.22090
6.60	-0.00004	0.00007	-0.00024	0.00041	0.00001	1.24053
6.80	-0.00002	0.00005	-0.00017	0.00029	0.00000	1.25994
7.00	-0.00002	0.00003	-0.00012	0.00021	0.00000	1.27911
7.20	-0.00001	0.00002	-0.00009	0.00015	0.00000	1.29804
7.40	-0.00001	0.00002	-0.00006	0.00010	0.00000	1.31673
7.60	-0.00001	0.00001	-0.00004	0.00007	0.00000	1.33520
7.80	-0.00000	0.00001	-0.00003	0.00005	0.00000	1.35347
8.00	-0.00000	0.00000	-0.00002	0.00004	0.00000	1.37157
8.20	-0.00000	0.00000	-0.00001	0.00003	0.00000	1.38951
8.40	-0.00000	0.00000	-0.00001	0.00002	0.00000	1.40733
8.60	-0.00000	0.00000	-0.00001	0.00001	0.00000	1.42505
8.80	-0.00000	0.00000	-0.00001	0.00001	0.00000	1.44271
9.00	-0.00000	0.00000	-0.00000	0.00001	0.00000	1.46035
9.20	-0.00000	0.00000	-0.00000	0.00000	0.00000	1.47798
9.40	-0.00000	0.00000	-0.00000	0.00000	0.00000	1.49565
9.60	-0.00000	0.00000	-0.00000	0.00000	0.00000	1.51339
9.80	-0.00000	0.00000	-0.00000	0.00000	0.00000	1.53124
10.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	1.54923

Table I.3. Radial Characteristics of the Hartree-Fock F 2p Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR-εR	FR/εR
0.	0.	20.22193	-0.	0.		
0.01	0.19380	18.55958	0.00194	0.37940	-8.30631	1164.72554
0.02	0.37159	17.01764	0.00743	0.71195	-7.15800	524.03236
0.03	0.53453	15.58741	0.01604	1.00215	-6.05964	308.80834
0.04	0.68369	14.26081	0.02735	1.25412	-5.04239	201.25490
0.05	0.82007	13.03036	0.04100	1.47158	-4.12365	137.53284
0.06	0.94459	11.88913	0.05668	1.65794	-3.31107	96.17624
0.07	1.05812	10.83069	0.07407	1.81627	-2.60499	67.84564
0.08	1.16146	9.84906	0.09292	1.94939	-2.00115	47.78208
0.09	1.25534	8.93874	0.11298	2.05983	-1.49247	33.28094
0.10	1.34046	8.09460	0.13405	2.14992	-1.07021	22.67804
0.12	1.48688	6.58619	0.17843	2.27723	-0.44759	9.17342
0.14	1.60532	5.28986	0.22474	2.34590	-0.05992	2.01342
0.16	1.69970	4.17638	0.27195	2.36792	0.15784	-1.52149
0.18	1.77342	3.22064	0.31922	2.35314	0.25862	-2.95969
0.20	1.82943	2.40100	0.36589	2.30963	0.28319	-3.20301
0.22	1.87025	1.69888	0.41145	2.24400	0.26154	-2.79708
0.24	1.89806	1.09825	0.45553	2.16164	0.21497	-2.07514
0.26	1.91476	0.58532	0.49784	2.06694	0.15790	-1.23910
0.28	1.92198	0.14820	0.53815	1.96347	0.09969	-0.40838
0.30	1.92112	-0.22335	0.57634	1.85412	0.04598	0.35018
0.35	1.89129	-0.92045	0.66195	1.56914	-0.05289	1.75933
0.40	1.83322	-1.36809	0.73329	1.28598	-0.09881	2.46349
0.45	1.75737	-1.64162	0.79082	1.01865	-0.10581	2.63473
0.50	1.67107	-1.79366	0.83554	0.77424	-0.09113	2.48074
0.55	1.57941	-1.86119	0.86868	0.55576	-0.06813	2.17123
0.60	1.48592	-1.87030	0.89155	0.36375	-0.04510	1.82408
0.65	1.39304	-1.83953	0.90548	0.19735	-0.02623	1.51130
0.70	1.30241	-1.78209	0.91169	0.05495	-0.01296	1.27018
0.75	1.21512	-1.70746	0.91134	-0.06547	-0.00510	1.11395
0.80	1.13184	-1.62241	0.90547	-0.16608	-0.00169	1.04051
0.85	1.05297	-1.53180	0.89502	-0.24906	-0.00151	1.03889
0.90	0.97869	-1.43910	0.88083	-0.31650	-0.00338	1.09387
0.95	0.90905	-1.34678	0.86360	-0.37038	-0.00633	1.18904
1.00	0.84398	-1.25652	0.84398	-0.41254	-0.00959	1.30866
1.10	0.72697	-1.08647	0.79966	-0.46815	-0.01521	1.56807
1.20	0.62610	-0.93395	0.75132	-0.49464	-0.01822	1.79005
1.30	0.53955	-0.80028	0.70141	-0.50082	-0.01849	1.93064
1.40	0.46544	-0.68484	0.65161	-0.49334	-0.01674	1.97675
1.50	0.40202	-0.58606	0.60303	-0.47707	-0.01386	1.93602
1.60	0.34773	-0.50201	0.55637	-0.45548	-0.01060	1.82780
1.70	0.30120	-0.43069	0.51203	-0.43097	-0.00750	1.67606
1.80	0.26123	-0.37021	0.47022	-0.40515	-0.00486	1.50465
1.90	0.22685	-0.31891	0.43101	-0.37907	-0.00279	1.33451
2.00	0.19720	-0.27530	0.39439	-0.35340	-0.00132	1.18237
2.10	0.17157	-0.23815	0.36030	-0.32854	-0.00038	1.06039
2.20	0.14939	-0.20641	0.32865	-0.30471	0.00013	0.97642
2.30	0.13014	-0.17920	0.29932	-0.28202	0.00031	0.93472
2.40	0.11342	-0.15581	0.27221	-0.26053	0.00027	0.93655
2.50	0.09887	-0.13564	0.24718	-0.24024	0.00007	0.98101
2.60	0.08620	-0.11821	0.22412	-0.22113	-0.00021	1.06564
2.70	0.07515	-0.10309	0.20291	-0.20319	-0.00052	1.18698
2.80	0.06552	-0.08996	0.18344	-0.18636	-0.00082	1.34100
2.90	0.05710	-0.07853	0.16560	-0.17062	-0.00110	1.52343
3.00	0.04976	-0.06856	0.14928	-0.15593	-0.00134	1.73000
3.20	0.03775	-0.05227	0.12080	-0.12953	-0.00167	2.19950
3.40	0.02860	-0.03983	0.09723	-0.10683	-0.00181	2.72032
3.60	0.02162	-0.03031	0.07785	-0.08750	-0.00181	3.26890
3.80	0.01632	-0.02303	0.06202	-0.07120	-0.00170	3.82727
4.00	0.01230	-0.01747	0.04919	-0.05757	-0.00153	4.38238
4.20	0.00925	-0.01322	0.03884	-0.04627	-0.00134	4.92518
4.40	0.00694	-0.00998	0.03055	-0.03699	-0.00114	5.44972
4.60	0.00520	-0.00753	0.02393	-0.02942	-0.00095	5.95237
4.80	0.00389	-0.00566	0.01868	-0.02328	-0.00078	6.43118

Table I.3. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.00291	-0.00425	0.01454	-0.01835	-0.00063	6.88539
5.20	0.00217	-0.00319	0.01128	-0.01440	-0.00050	7.31508
5.40	0.00162	-0.00238	0.00872	-0.01126	-0.00040	7.72086
5.60	0.00120	-0.00178	0.00673	-0.00877	-0.00031	8.10368
5.80	0.00089	-0.00133	0.00518	-0.00682	-0.00025	8.46470
6.00	0.00066	-0.00099	0.00398	-0.00528	-0.00019	8.80516
6.20	0.00049	-0.00074	0.00305	-0.00408	-0.00015	9.12637
6.40	0.00036	-0.00055	0.00233	-0.00314	-0.00011	9.42959
6.60	0.00027	-0.00041	0.00178	-0.00241	-0.00009	9.71606
6.80	0.00020	-0.00030	0.00135	-0.00185	-0.00007	9.98695
7.00	0.00015	-0.00022	0.00103	-0.00141	-0.00005	10.24336
7.20	0.00011	-0.00017	0.00078	-0.00108	-0.00004	10.48632
7.40	0.00008	-0.00012	0.00059	-0.00082	-0.00003	10.71678
7.60	0.00006	-0.00009	0.00045	-0.00063	-0.00002	10.93563
7.80	0.00004	-0.00007	0.00034	-0.00048	-0.00002	11.14367
8.00	0.00003	-0.00005	0.00026	-0.00036	-0.00001	11.34165
8.20	0.00002	-0.00004	0.00019	-0.00027	-0.00001	11.53026
8.40	0.00002	-0.00003	0.00015	-0.00021	-0.00001	11.71013
8.60	0.00001	-0.00002	0.00011	-0.00016	-0.00001	11.88183
8.80	0.00001	-0.00001	0.00008	-0.00012	-0.00000	12.04591
9.00	0.00001	-0.00001	0.00006	-0.00009	-0.00000	12.20283
9.20	0.00001	-0.00001	0.00005	-0.00007	-0.00000	12.35306
9.40	0.00000	-0.00001	0.00003	-0.00005	-0.00000	12.49700
9.60	0.00000	-0.00000	0.00003	-0.00004	-0.00000	12.63505
9.80	0.00000	-0.00000	0.00002	-0.00003	-0.00000	12.76754
10.00	0.00000	-0.00000	0.00001	-0.00002	-0.00000	12.89481

Table I.4. Radial Characteristics of the Hartree-Fock F^- 1s Orbital.

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
0.	51.68873	-464.92493	0.	51.68873		
0.01	47.24886	-423.71236	0.47249	43.01174	-39.76698	1.03258
0.02	43.20189	-386.28009	0.86404	35.47629	-16.90096	1.01515
0.03	39.51186	-352.26852	1.18536	28.94380	-6.99129	1.00685
0.04	36.14620	-321.35352	1.44585	23.29206	-1.87902	1.00201
0.05	33.07544	-293.24278	1.65377	18.41331	0.71474	0.99916
0.06	30.27288	-267.67261	1.81637	14.21252	1.86914	0.99761
0.07	27.71432	-244.40504	1.94000	10.60597	2.19755	0.99693
0.08	25.37782	-223.22518	2.03023	7.51981	2.07322	0.99684
0.09	23.24350	-203.93899	2.09192	4.88900	1.72609	0.99712
0.10	21.29332	-186.37109	2.12933	2.65621	1.29619	0.99764
0.12	17.88134	-155.77132	2.14576	-0.81122	0.47898	0.99896
0.14	15.02811	-130.33090	2.10394	-3.21821	-0.09293	1.00024
0.16	12.63972	-109.15301	2.02236	-4.82476	-0.39452	1.00121
0.18	10.63851	-91.50190	1.91493	-5.83183	-0.48836	1.00178
0.20	8.96019	-76.77301	1.79204	-6.39442	-0.45142	1.00195
0.22	7.55144	-64.46880	1.66132	-6.63169	-0.34811	1.00178
0.24	6.36802	-54.17917	1.52832	-6.63498	-0.22368	1.00136
0.26	5.37312	-45.56554	1.39701	-6.47392	-0.10582	1.00076
0.28	4.53610	-38.34800	1.27011	-6.20134	-0.00884	1.00008
0.30	3.83144	-32.29479	1.14943	-5.85699	0.06205	0.99937
0.35	2.51752	-21.07336	0.88113	-4.85815	0.13469	0.99793
0.40	1.65881	-13.79596	0.66353	-3.85957	0.11179	0.99739
0.45	1.09590	-9.05694	0.49315	-2.97973	0.05699	0.99799
0.50	0.72592	-5.96026	0.36296	-2.25421	0.00700	0.99963
0.55	0.48219	-3.93091	0.26521	-1.67981	-0.02488	1.00200
0.60	0.32130	-2.59783	0.19278	-1.23740	-0.03848	1.00464
0.65	0.21486	-1.72037	0.13966	-0.90338	-0.03876	1.00698
0.70	0.14431	-1.14181	0.10101	-0.65496	-0.03141	1.00843
0.75	0.09743	-0.75974	0.07307	-0.47238	-0.02099	1.00834
0.80	0.06619	-0.50706	0.05295	-0.33946	-0.01053	1.00616
0.85	0.04531	-0.33969	0.03851	-0.24343	-0.00169	1.00144
0.90	0.03129	-0.22863	0.02816	-0.17448	0.00487	0.99397
0.95	0.02183	-0.15477	0.02074	-0.12521	0.00910	0.98386
1.00	0.01540	-0.10553	0.01540	-0.09013	0.01129	0.97163
1.10	0.00797	-0.05042	0.00876	-0.04750	0.01127	0.94523
1.20	0.00434	-0.02523	0.00521	-0.02593	0.00814	0.92742
1.30	0.00249	-0.01333	0.00323	-0.01484	0.00427	0.93354
1.40	0.00148	-0.00743	0.00207	-0.00893	0.00090	0.97655
1.50	0.00091	-0.00434	0.00136	-0.00560	-0.00151	1.06419
1.60	0.00057	-0.00260	0.00091	-0.00360	-0.00292	1.19844
1.70	0.00036	-0.00158	0.00062	-0.00232	-0.00351	1.37315
1.80	0.00024	-0.00095	0.00043	-0.00147	-0.00351	1.56691
1.90	0.00017	-0.00056	0.00032	-0.00090	-0.00314	1.73424
2.00	0.00012	-0.00032	0.00025	-0.00051	-0.00258	1.81148
2.10	0.00010	-0.00017	0.00021	-0.00026	-0.00193	1.75402
2.20	0.00009	-0.00008	0.00019	-0.00010	-0.00130	1.57697
2.30	0.00008	-0.00004	0.00019	-0.00000	-0.00072	1.34231
2.40	0.00008	-0.00002	0.00019	0.00004	-0.00022	1.10992
2.50	0.00008	-0.00001	0.00019	0.00005	0.00018	0.91083
2.60	0.00008	-0.00001	0.00020	0.00005	0.00049	0.75226
2.70	0.00008	-0.00002	0.00020	0.00003	0.00072	0.63009
2.80	0.00007	-0.00002	0.00020	0.00001	0.00087	0.53706
2.90	0.00007	-0.00003	0.00020	-0.00002	0.00097	0.46623
3.00	0.00007	-0.00004	0.00020	-0.00004	0.00102	0.41203
3.20	0.00006	-0.00004	0.00019	-0.00008	0.00101	0.33778
3.40	0.00005	-0.00004	0.00017	-0.00010	0.00092	0.29240
3.60	0.00004	-0.00004	0.00015	-0.00011	0.00079	0.26417
3.80	0.00003	-0.00004	0.00013	-0.00011	0.00066	0.24672
4.00	0.00003	-0.00003	0.00011	-0.00010	0.00053	0.23646
4.20	0.00002	-0.00003	0.00009	-0.00009	0.00042	0.23133
4.40	0.00002	-0.00002	0.00007	-0.00008	0.00033	0.23013
4.60	0.00001	-0.00002	0.00006	-0.00006	0.00025	0.23216
4.80	0.00001	-0.00001	0.00005	-0.00005	0.00019	0.23704

Table I.4. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.00001	-0.00001	0.00004	-0.00004	0.00014	0.24462
5.20	0.00001	-0.00001	0.00003	-0.00004	0.00011	0.25490
5.40	0.00000	-0.00001	0.00002	-0.00003	0.00008	0.26798
5.60	0.00000	-0.00000	0.00002	-0.00002	0.00006	0.28408
5.80	0.00000	-0.00000	0.00001	-0.00002	0.00004	0.30352
6.00	0.00000	-0.00000	0.00001	-0.00001	0.00003	0.32670
6.50	0.00000	-0.00000	0.00001	-0.00001	0.00001	0.40464
7.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.52074
7.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.69244
8.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.94624
8.50	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.32222
9.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.88109
9.50	0.00000	-0.00000	0.00000	-0.00000	-0.00000	2.71491
10.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	3.96362

Table I.5. Radial Characteristics of the Hartree-Fock F^- 2s Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	11.67570	-105.55842	0.	11.67570		
0.01	10.66012	-97.66796	0.10660	9.68344	21.30934	-0.86010
0.02	9.72026	-90.40382	0.19441	7.91218	3.32377	0.68181
0.03	8.85014	-83.71080	0.26550	6.33882	-0.25827	1.02716
0.04	8.04431	-77.53903	0.32177	4.94274	-0.97554	1.11285
0.05	7.29777	-71.84338	0.36489	3.70560	-0.92455	1.11789
0.06	6.60599	-66.58301	0.39636	2.61101	-0.68604	1.09664
0.07	5.96478	-61.72095	0.41753	1.64432	-0.44206	1.06896
0.08	5.37035	-57.22369	0.42963	0.79246	-0.24529	1.04250
0.09	4.81920	-53.06086	0.43373	0.04372	-0.10368	1.02002
0.10	4.30811	-49.20489	0.43081	-0.61238	-0.01013	1.00219
0.12	3.39463	-42.31574	0.40736	-1.68326	0.07602	0.97916
0.14	2.60912	-36.38214	0.36528	-2.48438	0.08760	0.96876
0.16	1.93394	-31.25987	0.30943	-3.06763	0.07055	0.96605
0.18	1.35412	-26.82898	0.24374	-3.47510	0.04748	0.96737
0.20	0.85685	-22.98937	0.17137	-3.74103	0.02746	0.97018
0.22	0.43117	-19.65713	0.09486	-3.89340	0.01285	0.97227
0.24	0.06765	-16.76165	0.01624	-3.95514	0.00322	0.95565
0.26	-0.24181	-14.24326	-0.06287	-3.94506	-0.00267	0.98972
0.28	-0.50425	-12.05129	-0.14119	-3.87861	-0.00608	0.98878
0.30	-0.72575	-10.14261	-0.21773	-3.76853	-0.00795	0.98981
0.35	-1.13342	-6.38064	-0.39670	-3.36665	-0.00933	0.99234
0.40	-1.38214	-3.72263	-0.55286	-2.87119	-0.00843	0.99432
0.45	-1.51881	-1.85535	-0.68347	-2.35372	-0.00608	0.99627
0.50	-1.57713	-0.55721	-0.78856	-1.85573	-0.00288	0.99830
0.55	-1.58135	0.33050	-0.86974	-1.39958	0.00034	1.00020
0.60	-1.54899	0.92244	-0.92939	-0.99553	0.00284	1.00171
0.65	-1.49264	1.30185	-0.97021	-0.64644	0.00425	1.00265
0.70	-1.42133	1.52936	-0.99493	-0.35078	0.00454	1.00297
0.75	-1.34149	1.64915	-1.00612	-0.10463	0.00395	1.00274
0.80	-1.25767	1.69343	-1.00613	0.09708	0.00281	1.00208
0.85	-1.17301	1.68561	-0.99706	0.25975	0.00147	1.00117
0.90	-1.08969	1.64268	-0.98072	0.38872	0.00018	1.00015
0.95	-1.00912	1.57690	-0.95867	0.48893	-0.00088	0.99919
1.00	-0.93223	1.49710	-0.93223	0.56487	-0.00163	0.99837
1.10	-0.79133	1.31869	-0.87046	0.65923	-0.00220	0.99742
1.20	-0.66854	1.13840	-0.80224	0.69754	-0.00183	0.99746
1.30	-0.56322	0.97067	-0.73219	0.69865	-0.00103	0.99829
1.40	-0.47379	0.82126	-0.66330	0.67597	-0.00021	0.99958
1.50	-0.39831	0.69150	-0.59747	0.63894	0.00042	1.00098
1.60	-0.33486	0.58056	-0.53578	0.59404	0.00079	1.00221
1.70	-0.28163	0.48665	-0.47877	0.54567	0.00094	1.00309
1.80	-0.23703	0.40764	-0.42666	0.49672	0.00090	1.00353
1.90	-0.19968	0.34144	-0.37939	0.44906	0.00075	1.00351
2.00	-0.16838	0.28611	-0.33677	0.40384	0.00055	1.00304
2.10	-0.14215	0.23992	-0.29852	0.36167	0.00034	1.00220
2.20	-0.12015	0.20137	-0.26432	0.32287	0.00013	1.00103
2.30	-0.10167	0.16920	-0.23383	0.28750	-0.00004	0.99964
2.40	-0.08613	0.14234	-0.20671	0.25549	-0.00018	0.99811
2.50	-0.07305	0.11990	-0.18262	0.22670	-0.00027	0.99651
2.60	-0.06203	0.10113	-0.16127	0.20090	-0.00034	0.99494
2.70	-0.05272	0.08540	-0.14235	0.17786	-0.00037	0.99348
2.80	-0.04486	0.07222	-0.12561	0.15735	-0.00038	0.99220
2.90	-0.03821	0.06115	-0.11081	0.13912	-0.00036	0.99117
3.00	-0.03257	0.05184	-0.09772	0.12294	-0.00033	0.99047
3.20	-0.02373	0.03739	-0.07594	0.09591	-0.00025	0.99027
3.40	-0.01734	0.02709	-0.05896	0.07475	-0.00015	0.99205
3.60	-0.01270	0.01970	-0.04574	0.05821	-0.00005	0.99615
3.80	-0.00933	0.01438	-0.03544	0.04530	0.00003	1.00283
4.00	-0.00686	0.01052	-0.02743	0.03523	0.00009	1.01229
4.20	-0.00505	0.00772	-0.02120	0.02737	0.00013	1.02467
4.40	-0.00372	0.00567	-0.01636	0.02124	0.00016	1.04011
4.60	-0.00274	0.00418	-0.01261	0.01647	0.00017	1.05873
4.80	-0.00202	0.00308	-0.00971	0.01275	0.00018	1.08069

Table I.5. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	-0.00149	0.00227	-0.00746	0.00986	0.00017	1.10616
5.20	-0.00110	0.00167	-0.00572	0.00761	0.00016	1.13541
5.40	-0.00081	0.00124	-0.00438	0.00586	0.00015	1.16877
5.60	-0.00060	0.00091	-0.00335	0.00451	0.00013	1.20668
5.80	-0.00044	0.00067	-0.00256	0.00346	0.00012	1.24966
6.00	-0.00032	0.00050	-0.00195	0.00266	0.00010	1.29839
6.50	-0.00015	0.00023	-0.00098	0.00136	0.00007	1.45116
7.00	-0.00007	0.00011	-0.00049	0.00069	0.00005	1.66354
7.50	-0.00003	0.00005	-0.00024	0.00034	0.00003	1.96356
8.00	-0.00001	0.00002	-0.00012	0.00017	0.00002	2.39392
8.50	-0.00001	0.00001	-0.00006	0.00008	0.00001	3.01934
9.00	-0.00000	0.00000	-0.00003	0.00004	0.00001	3.93777
9.50	-0.00000	0.00000	-0.00001	0.00002	0.00001	5.29773
10.00	-0.00000	0.00000	-0.00001	0.00001	0.00000	7.32495
10.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	10.36332
11.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	14.93800
11.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	21.85290
12.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	32.34118
12.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	48.29351
13.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	72.64450
13.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	109.88417
14.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	166.98069
14.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	254.71463
15.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	389.80245
15.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	598.20335
17.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	2192.10168
18.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	5260.30414
19.00	-0.00000	0.00000	-0.00000	0.00000	0.0000012703	80701
20.00	-0.00000	0.00000	-0.00000	0.00000	0.0000030853	46875
21.00	-0.00000	0.00000	-0.00000	0.00000	0.0000075312	13965

Table I.6. Radial Characteristics of the Hartree-Fock F 2p Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	0.	18.64716	-0.	0.		
0.01	0.17854	17.08178	0.00179	0.34936	-4.54128	141.52194
0.02	0.34203	15.63581	0.00684	0.65475	-3.99146	65.47140
0.03	0.49162	14.29978	0.01475	0.92062	-3.42238	39.45916
0.04	0.62837	13.06504	0.02513	1.15097	-2.86463	26.18603
0.05	0.75324	11.92363	0.03766	1.34942	-2.34324	18.18659
0.06	0.86713	10.86827	0.05203	1.51922	-1.87117	12.92164
0.07	0.97087	9.89227	0.06796	1.66332	-1.45485	9.27871
0.08	1.06522	8.98950	0.08522	1.78438	-1.09568	6.68263
0.09	1.15088	8.15431	0.10358	1.88477	-0.79190	4.80141
0.10	1.22851	7.38154	0.12285	1.96666	-0.53984	3.42766
0.12	1.36202	6.00459	0.16344	2.08257	-0.17114	1.69418
0.14	1.47001	4.82501	0.20580	2.14551	0.05235	0.80326
0.16	1.55614	3.81433	0.24898	2.16643	0.17060	0.39432
0.18	1.62355	2.94841	0.29224	2.15426	0.21715	0.26109
0.20	1.67491	2.20674	0.33498	2.11625	0.21806	0.28074
0.22	1.71253	1.57188	0.37676	2.05834	0.19252	0.37892
0.24	1.73839	1.02897	0.41721	1.98535	0.15397	0.51068
0.26	1.75421	0.56530	0.45610	1.90119	0.11136	0.64929
0.28	1.76146	0.17001	0.49321	1.80906	0.07029	0.77955
0.30	1.76141	-0.16620	0.52842	1.71155	0.03394	0.89354
0.35	1.73619	-0.79798	0.60767	1.45690	-0.02875	1.09149
0.40	1.68534	-1.20491	0.67414	1.20338	-0.05371	1.17607
0.45	1.61831	-1.45449	0.72824	0.96379	-0.05318	1.18154
0.50	1.54172	-1.59394	0.77086	0.74475	-0.03972	1.14234
0.55	1.46019	-1.65656	0.80311	0.54909	-0.02234	1.08451
0.60	1.37695	-1.66597	0.82617	0.37737	-0.00625	1.02508
0.65	1.29420	-1.63906	0.84123	0.22881	0.00613	0.97382
0.70	1.21344	-1.58794	0.84941	0.10188	0.01418	0.93542
0.75	1.13566	-1.52128	0.85175	-0.00530	0.01826	0.91118
0.80	1.06147	-1.44531	0.84917	-0.09478	0.01914	0.90036
0.85	0.99121	-1.36448	0.84253	-0.16859	0.01774	0.90111
0.90	0.92505	-1.28193	0.83254	-0.22869	0.01489	0.91107
0.95	0.86301	-1.19987	0.81986	-0.27687	0.01128	0.92778
1.00	0.80503	-1.11983	0.80503	-0.31481	0.00745	0.94888
1.10	0.70068	-0.96946	0.77075	-0.36572	0.00049	0.99617
1.20	0.61060	-0.83504	0.73272	-0.39145	-0.00442	1.04000
1.30	0.53311	-0.71752	0.69304	-0.39967	-0.00700	1.07256
1.40	0.46655	-0.61622	0.65318	-0.39615	-0.00763	1.09037
1.50	0.40938	-0.52964	0.61407	-0.38509	-0.00691	1.09320
1.60	0.36019	-0.45606	0.57631	-0.36950	-0.00541	1.08293
1.70	0.31779	-0.39368	0.54025	-0.35146	-0.00360	1.06261
1.80	0.28114	-0.34084	0.50605	-0.33238	-0.00182	1.03574
1.90	0.24935	-0.29607	0.47377	-0.31318	-0.00026	1.00578
2.00	0.22170	-0.25807	0.44340	-0.29443	0.00097	0.97576
2.10	0.19755	-0.22571	0.41486	-0.27645	0.00185	0.94814
2.20	0.17640	-0.19809	0.38808	-0.25939	0.00240	0.92473
2.30	0.15780	-0.17440	0.36295	-0.24331	0.00266	0.90673
2.40	0.14141	-0.15401	0.33938	-0.22821	0.00269	0.89477
2.50	0.12691	-0.13638	0.31728	-0.21404	0.00255	0.88901
2.60	0.11406	-0.12107	0.29655	-0.20073	0.00229	0.88924
2.70	0.10263	-0.10772	0.27711	-0.18822	0.00195	0.89498
2.80	0.09246	-0.09604	0.25888	-0.17645	0.00158	0.90557
2.90	0.08338	-0.08577	0.24179	-0.16536	0.00120	0.92023
3.00	0.07526	-0.07672	0.22578	-0.15490	0.00084	0.93814
3.20	0.06149	-0.06161	0.19676	-0.13568	0.00022	0.98036
3.40	0.05040	-0.04968	0.17137	-0.11852	-0.00024	1.02600
3.60	0.04145	-0.04019	0.14923	-0.10323	-0.00052	1.06980
3.80	0.03420	-0.03259	0.12997	-0.08966	-0.00067	1.10778
4.00	0.02831	-0.02650	0.11326	-0.07767	-0.00070	1.13718
4.20	0.02352	-0.02159	0.09880	-0.06714	-0.00067	1.15638
4.40	0.01962	-0.01763	0.08631	-0.05795	-0.00058	1.16475
4.60	0.01642	-0.01443	0.07554	-0.04997	-0.00048	1.16241
4.80	0.01380	-0.01185	0.06625	-0.04308	-0.00038	1.15011

Table I.6. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.01165	-0.00976	0.05825	-0.03715	-0.00027	1.12902
5.20	0.00987	-0.00807	0.05134	-0.03208	-0.00018	1.10062
5.40	0.00840	-0.00669	0.04536	-0.02774	-0.00010	1.06652
5.60	0.00718	-0.00558	0.04020	-0.02405	-0.00004	1.02836
5.80	0.00616	-0.00467	0.03571	-0.02090	0.00001	0.98774
6.00	0.00530	-0.00392	0.03180	-0.01822	0.00005	0.94611
6.50	0.00370	-0.00259	0.02405	-0.01312	0.00010	0.84538
7.00	0.00263	-0.00176	0.01841	-0.00966	0.00011	0.75958
7.50	0.00190	-0.00122	0.01422	-0.00726	0.00010	0.69483
8.00	0.00138	-0.00087	0.01104	-0.00554	0.00009	0.65158
8.50	0.00101	-0.00062	0.00860	-0.00429	0.00007	0.62713
9.00	0.00074	-0.00045	0.00670	-0.00334	0.00005	0.61761
9.50	0.00055	-0.00033	0.00522	-0.00261	0.00004	0.61915
10.00	0.00041	-0.00025	0.00406	-0.00205	0.00003	0.62840
10.50	0.00030	-0.00018	0.00315	-0.00161	0.00002	0.64275
11.00	0.00022	-0.00013	0.00244	-0.00126	0.00001	0.66021
11.50	0.00016	-0.00010	0.00188	-0.00098	0.00001	0.67938
12.00	0.00012	-0.00007	0.00145	-0.00076	0.00001	0.69929
12.50	0.00009	-0.00005	0.00111	-0.00059	0.00000	0.71927
13.00	0.00007	-0.00004	0.00085	-0.00046	0.00000	0.73890
13.50	0.00005	-0.00003	0.00065	-0.00035	0.00000	0.75792
14.00	0.00004	-0.00002	0.00049	-0.00027	0.00000	0.77618
14.50	0.00003	-0.00002	0.00038	-0.00021	0.00000	0.79360
15.00	0.00002	-0.00001	0.00028	-0.00016	0.00000	0.81015
15.50	0.00001	-0.00001	0.00022	-0.00012	0.00000	0.82584
17.00	0.00001	-0.00000	0.00009	-0.00005	0.00000	0.86808
18.00	0.00000	-0.00000	0.00005	-0.00003	0.00000	0.89262
19.00	0.00000	-0.00000	0.00003	-0.00002	0.00000	0.91468
20.00	0.00000	-0.00000	0.00002	-0.00001	0.00000	0.93460
21.00	0.00000	-0.00000	0.00001	-0.00001	0.00000	0.95264

Table I.7. Radial Characteristics of the Hartree-Fock Ne 1s Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR-εR	FR/εR
0.	60.74663	-607.53011	0.	60.74663		
0.01	54.97409	-548.03955	0.54974	49.49369	-26.50537	1.01471
0.02	49.76577	-494.57336	0.99532	39.87430	-14.15198	1.00868
0.03	45.06466	-446.49811	1.35194	31.66972	-5.97820	1.00405
0.04	40.81973	-403.24965	1.63279	24.68974	-1.31020	1.00098
0.05	36.98526	-364.32518	1.84926	18.76900	1.04999	0.99913
0.06	33.52031	-329.27643	2.01122	13.76372	1.99945	0.99818
0.07	30.38815	-297.70343	2.12717	9.54891	2.14275	0.99785
0.08	27.55585	-269.24909	2.20447	6.01592	1.86985	0.99793
0.09	24.99384	-243.59447	2.24945	3.07034	1.42159	0.99826
0.10	22.67558	-220.45452	2.26756	0.63013	0.93934	0.99874
0.12	18.67732	-180.72585	2.24128	-3.00978	0.13779	0.99977
0.14	15.39775	-148.32851	2.15568	-5.36825	-0.32306	1.00064
0.16	12.70465	-121.87089	2.03274	-6.79470	-0.48827	1.00117
0.18	10.49082	-100.23419	1.88835	-7.55133	-0.46469	1.00135
0.20	8.66919	-82.51701	1.73384	-7.83422	-0.34851	1.00123
0.22	7.16889	-67.99169	1.57716	-7.78928	-0.20637	1.00088
0.24	5.93219	-56.06962	1.42373	-7.52452	-0.07665	1.00039
0.26	4.91195	-46.27383	1.27711	-7.11925	0.02317	0.99986
0.28	4.06966	-38.21712	1.13950	-6.63114	0.08891	0.99933
0.30	3.37378	-31.58460	1.01213	-6.10160	0.12368	0.99888
0.35	2.11637	-19.66517	0.74073	-4.76644	0.11848	0.99829
0.40	1.33220	-12.28660	0.53288	-3.58244	0.05926	0.99864
0.45	0.84154	-7.70058	0.37869	-2.62372	0.00450	0.99984
0.50	0.53360	-4.84048	0.26680	-1.88664	-0.02697	1.00154
0.55	0.33977	-3.05151	0.18687	-1.33856	-0.03679	1.00330
0.60	0.21741	-1.92958	0.13045	-0.94034	-0.03289	1.00462
0.65	0.13992	-1.22425	0.09095	-0.65584	-0.02287	1.00499
0.70	0.09067	-0.77975	0.06347	-0.45516	-0.01184	1.00399
0.75	0.05924	-0.49891	0.04443	-0.31495	-0.00253	1.00130
0.80	0.03908	-0.32098	0.03126	-0.21771	0.00408	0.99682
0.85	0.02607	-0.20787	0.02216	-0.15062	0.00798	0.99066
0.90	0.01761	-0.13569	0.01585	-0.10451	0.00965	0.98329
0.95	0.01207	-0.08941	0.01147	-0.07287	0.00970	0.97548
1.00	0.00840	-0.05957	0.00840	-0.05117	0.00871	0.96835
1.10	0.00427	-0.02749	0.00470	-0.02597	0.00539	0.96147
1.20	0.00231	-0.01346	0.00278	-0.01384	0.00204	0.97306
1.30	0.00133	-0.00701	0.00173	-0.00779	-0.00041	1.00947
1.40	0.00080	-0.00387	0.00113	-0.00461	-0.00185	1.07022
1.50	0.00051	-0.00223	0.00076	-0.00284	-0.00246	1.14797
1.60	0.00033	-0.00133	0.00053	-0.00180	-0.00251	1.22936
1.70	0.00023	-0.00081	0.00039	-0.00115	-0.00222	1.29649
1.80	0.00016	-0.00050	0.00030	-0.00074	-0.00178	1.33038
1.90	0.00012	-0.00032	0.00024	-0.00048	-0.00129	1.31742
2.00	0.00010	-0.00020	0.00020	-0.00031	-0.00082	1.25580
2.10	0.00008	-0.00014	0.00017	-0.00021	-0.00042	1.15632
2.20	0.00007	-0.00010	0.00015	-0.00014	-0.00008	1.03656
2.30	0.00006	-0.00007	0.00014	-0.00010	0.00018	0.91318
2.40	0.00006	-0.00006	0.00013	-0.00008	0.00037	0.79755
2.50	0.00005	-0.00005	0.00012	-0.00007	0.00050	0.69530
2.60	0.00005	-0.00004	0.00012	-0.00007	0.00058	0.60796
2.70	0.00004	-0.00004	0.00011	-0.00007	0.00063	0.53478
2.80	0.00004	-0.00004	0.00010	-0.00007	0.00064	0.47401
2.90	0.00003	-0.00004	0.00010	-0.00007	0.00063	0.42369
3.00	0.00003	-0.00003	0.00009	-0.00007	0.00061	0.38196
3.20	0.00002	-0.00003	0.00008	-0.00007	0.00054	0.31814
3.40	0.00002	-0.00002	0.00006	-0.00006	0.00045	0.27290
3.60	0.00001	-0.00002	0.00005	-0.00005	0.00036	0.23997
3.80	0.00001	-0.00002	0.00004	-0.00005	0.00029	0.21539
4.00	0.00001	-0.00001	0.00003	-0.00004	0.00022	0.19659
4.20	0.00001	-0.00001	0.00003	-0.00003	0.00017	0.18190
4.40	0.00000	-0.00001	0.00002	-0.00003	0.00013	0.17021
4.60	0.00000	-0.00001	0.00002	-0.00002	0.00010	0.16075
4.80	0.00000	-0.00000	0.00001	-0.00002	0.00007	0.15299

Table I.7. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.00000	-0.00000	0.00001	-0.00001	0.00005	0.14654
5.20	0.00000	-0.00000	0.00001	-0.00001	0.00004	0.14112
5.40	0.00000	-0.00000	0.00001	-0.00001	0.00003	0.13654
5.60	0.00000	-0.00000	0.00000	-0.00001	0.00002	0.13263
5.80	0.00000	-0.00000	0.00000	-0.00000	0.00002	0.12927
6.00	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.12637
6.20	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.12386
6.40	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.12167
6.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11977
6.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11812
7.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11667
7.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11541
7.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11432
7.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11338
7.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11257
8.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11187
8.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11129
8.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11080
8.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11040
8.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11009
9.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.10985
9.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.10968
9.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.10959
9.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.10955
9.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.10957
10.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.10965
10.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.10979
10.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.10997
10.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.11020

Table I.8. Radial Characteristics of the Hartree-Fock Ne 2s Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR-εR	FR/εR
0.	14.26056	-142.33111	0.	14.26056		
0.01	12.89496	-130.94637	0.12895	11.58549	-19.19259	1.77116
0.02	11.63861	-120.46802	0.23277	9.22925	-5.11143	1.22755
0.03	10.48281	-110.82590	0.31448	7.15803	-0.91657	1.04530
0.04	9.41953	-101.95417	0.37678	5.34136	0.61293	0.96629
0.05	8.44136	-93.79125	0.42207	3.75180	1.07706	0.93389
0.06	7.54153	-86.27991	0.45249	2.36474	1.07104	0.92642
0.07	6.71377	-79.36704	0.46996	1.15808	0.86846	0.93298
0.08	5.95236	-73.00360	0.47619	0.11207	0.60590	0.94726
0.09	5.25202	-67.14434	0.47268	-0.79097	0.35119	0.96535
0.10	4.60793	-61.74767	0.46079	-1.56684	0.13582	0.98473
0.12	3.47112	-52.19243	0.41653	-2.79197	-0.14391	1.02148
0.14	2.51070	-44.06898	0.35150	-3.65896	-0.24635	1.05084
0.16	1.70033	-37.15211	0.27205	-4.24401	-0.23396	1.07129
0.18	1.01783	-31.25367	0.18321	-4.60783	-0.16575	1.08438
0.20	0.44445	-26.21666	0.08889	-4.79889	-0.08322	1.09702
0.22	0.03570	-21.90999	-0.00785	-4.85590	-0.01029	0.85063
0.24	-0.43609	-18.22412	-0.10466	-4.80988	0.04242	1.05040
0.26	-0.76819	-15.06728	-0.19973	-4.68568	0.07286	1.04914
0.28	-1.04179	-12.36243	-0.29170	-4.50327	0.08376	1.04166
0.30	-1.26527	-10.04468	-0.37958	-4.27867	0.07988	1.03271
0.35	-1.64930	-5.60406	-0.57726	-3.61072	0.03791	1.01191
0.40	-1.84961	-2.60652	-0.73984	-2.89221	-0.00649	0.99818
0.45	-1.92655	-0.60890	-0.86695	-2.20055	-0.02965	0.99203
0.50	-1.92203	0.69349	-0.96102	-1.57529	-0.03169	0.99146
0.55	-1.86521	1.51294	-1.02587	-1.03309	-0.02142	0.99405
0.60	-1.77628	1.99858	-1.06577	-0.57713	-0.00759	0.99778
0.65	-1.66915	2.25554	-1.08495	-0.20305	0.00418	1.00130
0.70	-1.55329	2.35793	-1.08730	0.09726	0.01154	1.00385
0.75	-1.43505	2.35788	-1.07629	0.33336	0.01435	1.00518
0.80	-1.31859	2.29185	-1.05488	0.51489	0.01360	1.00534
0.85	-1.20654	2.18519	-1.02556	0.65087	0.01063	1.00457
0.90	-1.10046	2.05532	-0.99041	0.74933	0.00668	1.00315
0.95	-1.00119	1.91415	-0.95113	0.81724	0.00268	1.00139
1.00	-0.90910	1.76960	-0.90910	0.86050	-0.00080	0.99955
1.10	-0.74632	1.48934	-0.82096	0.89195	-0.00519	0.99639
1.20	-0.61029	1.23670	-0.73235	0.87375	-0.00628	0.99467
1.30	-0.49783	1.01841	-0.64718	0.82610	-0.00518	0.99461
1.40	-0.40547	0.83421	-0.56766	0.76242	-0.00312	0.99601
1.50	-0.32996	0.68096	-0.49493	0.69148	-0.00098	0.99846
1.60	-0.26838	0.55459	-0.42942	0.61895	0.00077	1.00148
1.70	-0.21828	0.45098	-0.37108	0.54838	0.00195	1.00463
1.80	-0.17756	0.36637	-0.31960	0.48191	0.00258	1.00754
1.90	-0.14448	0.29746	-0.27452	0.42069	0.00276	1.00989
2.00	-0.11764	0.24144	-0.23527	0.36525	0.00260	1.01143
2.10	-0.09584	0.19597	-0.20127	0.31568	0.00222	1.01200
2.20	-0.07816	0.15908	-0.17194	0.27183	0.00173	1.01147
2.30	-0.06379	0.12919	-0.14673	0.23334	0.00120	1.00976
2.40	-0.05213	0.10497	-0.12511	0.19979	0.00069	1.00684
2.50	-0.04265	0.08535	-0.10662	0.17072	0.00022	1.00271
2.60	-0.03494	0.06945	-0.09083	0.14563	-0.00017	0.99742
2.70	-0.02866	0.05657	-0.07738	0.12408	-0.00050	0.99101
2.80	-0.02354	0.04613	-0.06592	0.10561	-0.00075	0.98358
2.90	-0.01937	0.03766	-0.05616	0.08984	-0.00093	0.97523
3.00	-0.01596	0.03078	-0.04787	0.07639	-0.00105	0.96606
3.20	-0.01088	0.02066	-0.03482	0.05522	-0.00114	0.94580
3.40	-0.00747	0.01395	-0.02539	0.03995	-0.00110	0.92383
3.60	-0.00516	0.00948	-0.01856	0.02896	-0.00098	0.90116
3.80	-0.00358	0.00648	-0.01360	0.02105	-0.00084	0.87870
4.00	-0.00250	0.00446	-0.00999	0.01534	-0.00069	0.85720
4.20	-0.00175	0.00309	-0.00736	0.01122	-0.00055	0.83721
4.40	-0.00123	0.00215	-0.00543	0.00823	-0.00043	0.81911
4.60	-0.00087	0.00151	-0.00401	0.00606	-0.00033	0.80311
4.80	-0.00062	0.00106	-0.00297	0.00447	-0.00025	0.78926

Table I.8. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	-0.00044	0.00075	-0.00220	0.00330	-0.00019	0.77754
5.20	-0.00031	0.00053	-0.00163	0.00244	-0.00014	0.76782
5.40	-0.00022	0.00038	-0.00121	0.00181	-0.00010	0.75995
5.60	-0.00016	0.00027	-0.00089	0.00134	-0.00008	0.75373
5.80	-0.00011	0.00019	-0.00066	0.00099	-0.00006	0.74897
6.00	-0.00008	0.00014	-0.00049	0.00074	-0.00004	0.74548
6.20	-0.00006	0.00010	-0.00036	0.00055	-0.00003	0.74307
6.40	-0.00004	0.00007	-0.00027	0.00041	-0.00002	0.74158
6.60	-0.00003	0.00005	-0.00020	0.00030	-0.00001	0.74086
6.80	-0.00002	0.00004	-0.00015	0.00022	-0.00001	0.74078
7.00	-0.00002	0.00003	-0.00011	0.00016	-0.00001	0.74122
7.20	-0.00001	0.00002	-0.00008	0.00012	-0.00001	0.74209
7.40	-0.00001	0.00001	-0.00006	0.00009	-0.00000	0.74331
7.60	-0.00001	0.00001	-0.00004	0.00007	-0.00000	0.74481
7.80	-0.00000	0.00001	-0.00003	0.00005	-0.00000	0.74653
8.00	-0.00000	0.00000	-0.00002	0.00004	-0.00000	0.74842
8.20	-0.00000	0.00000	-0.00002	0.00003	-0.00000	0.75044
8.40	-0.00000	0.00000	-0.00001	0.00002	-0.00000	0.75256
8.60	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.75475
8.80	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.75700
9.00	-0.00000	0.00000	-0.00000	0.00001	-0.00000	0.75928
9.20	-0.00000	0.00000	-0.00000	0.00001	-0.00000	0.76158
9.40	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.76390
9.60	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.76621
9.80	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.76853
10.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.77083
10.20	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.77312
10.40	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.77540
10.60	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.77766

Table I.9. Radial Characteristics of the Hartree-Fock Ne 2p Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	-0.	27.70083	-0.	0.		
0.01	0.26373	25.08497	0.00264	0.51458	-3.40765	16.19761
0.02	0.50245	22.69459	0.01005	0.95634	-3.11992	8.30352
0.03	0.71831	20.50921	0.02155	1.33358	-2.70681	5.43231
0.04	0.91326	18.51036	0.03653	1.65367	-2.24716	3.89417
0.05	1.08908	16.68135	0.05445	1.92315	-1.79252	2.93592
0.06	1.24740	15.00706	0.07484	2.14782	-1.37339	2.29501
0.07	1.38969	13.47386	0.09728	2.33286	-1.00500	1.85061
0.08	1.51731	12.06937	0.12138	2.48285	-0.69323	1.53739
0.09	1.63147	10.78241	0.14683	2.60189	-0.43793	1.31573
0.10	1.73331	9.60282	0.17333	2.69359	-0.23544	1.15977
0.12	1.90404	7.52982	0.22848	2.80762	0.03444	0.97873
0.14	2.03670	5.78648	0.28514	2.84681	0.16703	0.90354
0.16	2.13734	4.31999	0.34197	2.82854	0.20943	0.88475
0.18	2.21105	3.08664	0.39799	2.76665	0.19866	0.89432
0.20	2.26212	2.05008	0.45242	2.67213	0.16108	0.91625
0.22	2.29416	1.18002	0.50472	2.55377	0.11399	0.94156
0.24	2.31026	0.45112	0.55446	2.41853	0.06775	0.96551
0.26	2.31301	-0.15787	0.60138	2.27196	0.02789	0.98582
0.28	2.30462	-0.66484	0.64529	2.11847	-0.00330	1.00169
0.30	2.28699	-1.08488	0.68610	1.96153	-0.02552	1.01312
0.35	2.21244	-1.83394	0.77435	1.57056	-0.04823	1.02564
0.40	2.10883	-2.26739	0.84353	1.20188	-0.04176	1.02329
0.45	1.98922	-2.48833	0.89515	0.86947	-0.02479	1.01466
0.50	1.86236	-2.56706	0.93118	0.57883	-0.00813	1.00514
0.55	1.73407	-2.55200	0.95374	0.33047	0.00385	0.99739
0.60	1.60816	-2.47660	0.96489	0.12220	0.01049	0.99233
0.65	1.48702	-2.36405	0.96657	-0.04961	0.01277	0.98990
0.70	1.37210	-2.23034	0.96047	-0.18914	0.01214	0.98959
0.75	1.26416	-2.08644	0.94812	-0.30067	0.00990	0.99079
0.80	1.16350	-1.93972	0.93080	-0.38827	0.00701	0.99292
0.85	1.07015	-1.79509	0.90963	-0.45568	0.00411	0.99548
0.90	0.98391	-1.65567	0.88552	-0.50619	0.00157	0.99812
0.95	0.90447	-1.52334	0.85924	-0.54270	-0.00045	1.00058
1.00	0.83144	-1.39913	0.83144	-0.56769	-0.00191	1.00271
1.10	0.70294	-1.17650	0.77324	-0.59120	-0.00339	1.00568
1.20	0.59502	-0.98739	0.71402	-0.58985	-0.00348	1.00688
1.30	0.50445	-0.82861	0.65579	-0.57274	-0.00282	1.00658
1.40	0.42842	-0.69608	0.59979	-0.54609	-0.00188	1.00516
1.50	0.36450	-0.58573	0.54675	-0.51409	-0.00094	1.00303
1.60	0.31066	-0.49387	0.49706	-0.47953	-0.00015	1.00056
1.70	0.26522	-0.41733	0.45087	-0.44424	0.00045	0.99803
1.80	0.22677	-0.35343	0.40819	-0.40940	0.00084	0.99567
1.90	0.19418	-0.29997	0.36895	-0.37576	0.00105	0.99364
2.00	0.16649	-0.25512	0.33299	-0.34375	0.00112	0.99207
2.10	0.14292	-0.21740	0.30013	-0.31362	0.00109	0.99103
2.20	0.12282	-0.18559	0.27020	-0.28548	0.00099	0.99054
2.30	0.10564	-0.15869	0.24297	-0.25936	0.00084	0.99063
2.40	0.09094	-0.13590	0.21826	-0.23522	0.00067	0.99128
2.50	0.07835	-0.11654	0.19586	-0.21300	0.00050	0.99248
2.60	0.06754	-0.10005	0.17560	-0.19260	0.00033	0.99418
2.70	0.05825	-0.08600	0.15729	-0.17393	0.00018	0.99636
2.80	0.05027	-0.07398	0.14076	-0.15688	0.00004	0.99897
2.90	0.04340	-0.06370	0.12586	-0.14134	-0.00007	1.00196
3.00	0.03748	-0.05489	0.11245	-0.12719	-0.00017	1.00530
3.20	0.02798	-0.04083	0.08954	-0.10268	-0.00030	1.01281
3.40	0.02091	-0.03043	0.07108	-0.08257	-0.00038	1.02119
3.60	0.01563	-0.02272	0.05626	-0.06615	-0.00040	1.03014
3.80	0.01169	-0.01697	0.04442	-0.05281	-0.00039	1.03944
4.00	0.00874	-0.01269	0.03497	-0.04202	-0.00036	1.04891
4.20	0.00654	-0.00949	0.02747	-0.03333	-0.00032	1.05839
4.40	0.00489	-0.00710	0.02152	-0.02636	-0.00028	1.06780
4.60	0.00366	-0.00532	0.01683	-0.02079	-0.00024	1.07706
4.80	0.00274	-0.00398	0.01313	-0.01636	-0.00020	1.08612

Table I.9. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.00205	-0.00298	0.01023	-0.01284	-0.00017	1.09497
5.20	0.00153	-0.00223	0.00795	-0.01005	-0.00013	1.10358
5.40	0.00114	-0.00167	0.00617	-0.00785	-0.00011	1.11195
5.60	0.00085	-0.00125	0.00478	-0.00612	-0.00009	1.12009
5.80	0.00064	-0.00093	0.00369	-0.00476	-0.00007	1.12800
6.00	0.00048	-0.00070	0.00285	-0.00370	-0.00005	1.13570
6.20	0.00035	-0.00052	0.00220	-0.00287	-0.00004	1.14318
6.40	0.00026	-0.00039	0.00169	-0.00222	-0.00003	1.15047
6.60	0.00020	-0.00029	0.00130	-0.00171	-0.00003	1.15755
6.80	0.00015	-0.00022	0.00100	-0.00132	-0.00002	1.16446
7.00	0.00011	-0.00016	0.00077	-0.00102	-0.00002	1.17118
7.20	0.00008	-0.00012	0.00059	-0.00078	-0.00001	1.17774
7.40	0.00006	-0.00009	0.00045	-0.00060	-0.00001	1.18412
7.60	0.00005	-0.00007	0.00034	-0.00046	-0.00001	1.19034
7.80	0.00003	-0.00005	0.00026	-0.00035	-0.00001	1.19640
8.00	0.00002	-0.00004	0.00020	-0.00027	-0.00000	1.20231
8.20	0.00002	-0.00003	0.00015	-0.00021	-0.00000	1.20806
8.40	0.00001	-0.00002	0.00012	-0.00016	-0.00000	1.21366
8.60	0.00001	-0.00002	0.00009	-0.00012	-0.00000	1.21911
8.80	0.00001	-0.00001	0.00007	-0.00009	-0.00000	1.22442
9.00	0.00001	-0.00001	0.00005	-0.00007	-0.00000	1.22959
9.20	0.00000	-0.00001	0.00004	-0.00005	-0.00000	1.23462
9.40	0.00000	-0.00000	0.00003	-0.00004	-0.00000	1.23951
9.60	0.00000	-0.00000	0.00002	-0.00003	-0.00000	1.24428
9.80	0.00000	-0.00000	0.00002	-0.00002	-0.00000	1.24891
10.00	0.00000	-0.00000	0.00001	-0.00002	-0.00000	1.25341
10.20	0.00000	-0.00000	0.00001	-0.00001	-0.00000	1.25779
10.40	0.00000	-0.00000	0.00001	-0.00001	-0.00000	1.26205
10.60	0.00000	-0.00000	0.00001	-0.00001	-0.00000	1.26619

Table I.10. Radial Characteristics of the Hartree-Fock Na^+ 1s Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	70.28162	-773.27136	0.	70.28162		
0.01	62.97044	-690.57790	0.62970	56.06467	-25.12714	1.00979
0.02	56.43969	-617.00129	1.12879	44.09967	-13.29794	1.00578
0.03	50.60351	-551.50174	1.51811	34.05846	-4.64523	1.00225
0.04	45.38580	-493.16231	1.81543	25.65931	0.00177	1.00000
0.05	40.71910	-441.17385	2.03596	18.66041	2.01714	0.99878
0.06	36.54355	-394.82199	2.19261	12.85423	2.52219	0.99831
0.07	32.80599	-353.47556	2.29642	8.06270	2.25681	0.99831
0.08	29.45922	-316.57656	2.35674	4.13309	1.67274	0.99861
0.09	26.46128	-283.63144	2.38152	0.93445	1.02589	0.99905
0.10	23.77487	-254.20329	2.37749	-1.64546	0.44722	0.99954
0.12	19.20748	-204.39425	2.30490	-5.31983	-0.32649	1.00042
0.14	15.53278	-164.55187	2.17459	-7.50448	-0.61122	1.00097
0.16	12.57269	-132.63154	2.01163	-8.64836	-0.57894	1.00113
0.18	10.18553	-107.02022	1.83340	-9.07811	-0.40113	1.00097
0.20	8.25838	-86.44245	1.65168	-9.03011	-0.19373	1.00058
0.22	6.70106	-69.88759	1.47423	-8.67421	-0.01828	1.00007
0.24	5.44144	-56.55313	1.30595	-8.13131	0.10220	0.99954
0.26	4.42175	-45.80060	1.14966	-7.48640	0.16716	0.99907
0.28	3.59562	-37.12106	1.00677	-6.79827	0.18678	0.99873
0.30	2.92582	-30.10812	0.87774	-6.10662	0.17457	0.99854
0.35	1.75264	-17.88972	0.61342	-4.50876	0.08286	0.99884
0.40	1.05433	-10.67014	0.42173	-3.21372	-0.00527	1.00012
0.45	0.63715	-6.38669	0.28672	-2.23686	-0.04989	1.00192
0.50	0.38704	-3.83638	0.19352	-1.53114	-0.05657	1.00359
0.55	0.23655	-2.31322	0.13010	-1.03572	-0.04263	1.00442
0.60	0.14563	-1.40084	0.08738	-0.69487	-0.02251	1.00379
0.65	0.09045	-0.85269	0.05879	-0.46380	-0.00451	1.00122
0.70	0.05677	-0.52227	0.03974	-0.30882	0.00807	0.99651
0.75	0.03607	-0.32234	0.02705	-0.20569	0.01492	0.98985
0.80	0.02324	-0.20079	0.01859	-0.13739	0.01716	0.98189
0.85	0.01521	-0.12647	0.01293	-0.09229	0.01623	0.97382
0.90	0.01012	-0.08069	0.00911	-0.06250	0.01350	0.96728
0.95	0.00685	-0.05224	0.00651	-0.04278	0.00999	0.96424
1.00	0.00472	-0.03437	0.00472	-0.02965	0.00640	0.96673
1.10	0.00235	-0.01566	0.00259	-0.01487	0.00046	0.99520
1.20	0.00124	-0.00761	0.00149	-0.00789	-0.00311	1.06121
1.30	0.00069	-0.00390	0.00090	-0.00438	-0.00458	1.16245
1.40	0.00040	-0.00207	0.00056	-0.00250	-0.00466	1.28322
1.50	0.00025	-0.00112	0.00037	-0.00144	-0.00397	1.39164
1.60	0.00016	-0.00061	0.00026	-0.00082	-0.00297	1.44320
1.70	0.00012	-0.00034	0.00020	-0.00046	-0.00194	1.40182
1.80	0.00009	-0.00019	0.00017	-0.00025	-0.00101	1.26849
1.90	0.00008	-0.00011	0.00015	-0.00014	-0.00026	1.08235
2.00	0.00007	-0.00007	0.00014	-0.00008	0.00031	0.88987
2.10	0.00006	-0.00006	0.00013	-0.00006	0.00071	0.72000
2.20	0.00006	-0.00005	0.00013	-0.00005	0.00097	0.58218
2.30	0.00005	-0.00005	0.00012	-0.00005	0.00112	0.47484
2.40	0.00005	-0.00004	0.00012	-0.00006	0.00119	0.39256
2.50	0.00004	-0.00004	0.00011	-0.00006	0.00119	0.32958
2.60	0.00004	-0.00004	0.00010	-0.00007	0.00115	0.28109
2.70	0.00004	-0.00004	0.00010	-0.00007	0.00109	0.24340
2.80	0.00003	-0.00004	0.00009	-0.00007	0.00101	0.21375
2.90	0.00003	-0.00004	0.00008	-0.00007	0.00091	0.19016
3.00	0.00002	-0.00003	0.00007	-0.00007	0.00082	0.17116
3.10	0.00002	-0.00003	0.00007	-0.00007	0.00073	0.15568
3.20	0.00002	-0.00003	0.00006	-0.00007	0.00065	0.14293
3.30	0.00002	-0.00002	0.00005	-0.00006	0.00057	0.13232
3.40	0.00001	-0.00002	0.00005	-0.00006	0.00049	0.12342
3.50	0.00001	-0.00002	0.00004	-0.00005	0.00043	0.11587
3.60	0.00001	-0.00002	0.00004	-0.00005	0.00037	0.10943
3.70	0.00001	-0.00001	0.00003	-0.00004	0.00032	0.10388
3.80	0.00001	-0.00001	0.00003	-0.00004	0.00027	0.09908
3.90	0.00001	-0.00001	0.00002	-0.00003	0.00023	0.09490

Table I.10. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	0.00001	-0.00001	0.00002	-0.00003	0.00020	0.09123
4.10	0.00000	-0.00001	0.00002	-0.00003	0.00017	0.08799
4.20	0.00000	-0.00001	0.00002	-0.00002	0.00014	0.08513
4.40	0.00000	-0.00000	0.00001	-0.00002	0.00010	0.08030
4.60	0.00000	-0.00000	0.00001	-0.00001	0.00007	0.07642
4.80	0.00000	-0.00000	0.00001	-0.00001	0.00005	0.07326
5.00	0.00000	-0.00000	0.00000	-0.00001	0.00004	0.07065
5.20	0.00000	-0.00000	0.00000	-0.00001	0.00003	0.06848
5.40	0.00000	-0.00000	0.00000	-0.00000	0.00002	0.06665
5.60	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.06511
5.80	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.06379
6.00	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.06267
6.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06171
6.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06088
6.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06017
6.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.05955
7.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.05902
7.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.05857
7.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.05817
7.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.05784
7.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.05755
8.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.05730
8.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.05709
8.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.05692
8.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.05678
8.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.05666
9.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.05657

Table I.11. Radial Characteristics of the Hartree-Fock Na^+ 2s Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	17.17251	-189.82042	0.	17.17251		
0.01	15.36071	-172.82209	0.15361	13.63249	33.30480	0.29460
0.02	13.71071	-157.43098	0.27421	10.56209	2.28331	0.94582
0.03	12.20731	-143.47509	0.36622	7.90306	-2.39078	1.06372
0.04	10.83693	-130.80340	0.43348	5.60480	-2.48842	1.07471
0.05	9.58741	-119.28305	0.47937	3.62326	-1.70399	1.05782
0.06	8.44782	-108.79692	0.50687	1.92001	-0.92429	1.03560
0.07	7.40837	-99.24157	0.51859	0.46146	-0.34866	1.01531
0.08	6.46020	-90.52541	0.51682	-0.78184	0.01726	0.99913
0.09	5.59533	-82.56718	0.50358	-1.83571	0.21816	0.98731
0.10	4.80657	-75.29467	0.48066	-2.72290	0.30384	0.97943
0.12	3.43182	-62.55625	0.41182	-4.07493	0.28543	0.97294
0.14	2.29064	-51.87314	0.32069	-4.97160	0.17528	0.97511
0.16	1.34555	-42.89426	0.21529	-5.51753	0.06771	0.98363
0.18	0.56541	-35.33532	0.10177	-5.79495	-0.00711	1.00409
0.20	-0.07578	-28.96446	-0.01516	-5.86867	-0.04746	0.79625
0.22	-0.59981	-23.59122	-0.13196	-5.78988	-0.06145	0.96667
0.24	-1.02502	-19.05824	-0.24601	-5.59900	-0.05871	0.98137
0.26	-1.36687	-15.23477	-0.35539	-5.32791	-0.04720	0.98876
0.28	-1.63841	-12.01166	-0.45876	-5.00168	-0.03255	0.99354
0.30	-1.85072	-9.29738	-0.55522	-4.63993	-0.01821	0.99680
0.35	-2.18050	-4.26147	-0.76318	-3.67202	0.00676	1.00101
0.40	-2.30700	-1.04364	-0.92280	-2.72446	0.01472	1.00208
0.45	-2.30497	0.96171	-1.03723	-1.87220	0.01235	1.00174
0.50	-2.22421	2.15980	-1.11211	-1.14431	0.00650	1.00095
0.55	-2.09785	2.82329	-1.15382	-0.54504	0.00114	1.00018
0.60	-1.94770	3.13618	-1.16862	-0.06599	-0.00223	0.99963
0.65	-1.78798	3.22270	-1.16219	0.30677	-0.00355	0.99935
0.70	-1.62779	3.16663	-1.13945	0.58886	-0.00338	0.99933
0.75	-1.47274	3.02430	-1.10456	0.79548	-0.00242	0.99947
0.80	-1.32616	2.83332	-1.06093	0.94049	-0.00124	0.99970
0.85	-1.18980	2.61857	-1.01133	1.03598	-0.00023	0.99994
0.90	-1.06443	2.39628	-0.95798	1.09222	0.00045	1.00014
0.95	-0.95013	2.17676	-0.90262	1.11779	0.00074	1.00026
1.00	-0.84660	1.96635	-0.84660	1.11975	0.00072	1.00028
1.10	-0.66949	1.58559	-0.73644	1.07467	0.00014	1.00007
1.20	-0.52746	1.26509	-0.63295	0.99065	-0.00055	0.99966
1.30	-0.41453	1.00267	-0.53889	0.88895	-0.00089	0.99930
1.40	-0.32522	0.79127	-0.45531	0.78255	-0.00080	0.99920
1.50	-0.25485	0.62262	-0.38227	0.67909	-0.00040	0.99949
1.60	-0.19953	0.48893	-0.31925	0.58275	0.00012	1.00019
1.70	-0.15613	0.38336	-0.26542	0.49558	0.00059	1.00123
1.80	-0.12211	0.30024	-0.21981	0.41832	0.00092	1.00244
1.90	-0.09549	0.23492	-0.18143	0.35086	0.00107	1.00365
2.00	-0.07466	0.18368	-0.14932	0.29269	0.00106	1.00462
2.10	-0.05838	0.14353	-0.12260	0.24302	0.00092	1.00514
2.20	-0.04567	0.11210	-0.10046	0.20096	0.00070	1.00500
2.30	-0.03573	0.08754	-0.08219	0.16560	0.00044	1.00403
2.40	-0.02798	0.06834	-0.06715	0.13604	0.00018	1.00208
2.50	-0.02193	0.05336	-0.05481	0.11147	-0.00007	0.99902
2.60	-0.01720	0.04167	-0.04472	0.09115	-0.00028	0.99477
2.70	-0.01351	0.03256	-0.03647	0.07440	-0.00045	0.98928
2.80	-0.01062	0.02545	-0.02974	0.06064	-0.00057	0.98252
2.90	-0.00836	0.01991	-0.02425	0.04938	-0.00066	0.97451
3.00	-0.00660	0.01559	-0.01979	0.04018	-0.00070	0.96528
3.10	-0.00521	0.01223	-0.01616	0.03268	-0.00072	0.95490
3.20	-0.00413	0.00960	-0.01321	0.02659	-0.00072	0.94345
3.30	-0.00327	0.00755	-0.01081	0.02163	-0.00069	0.93103
3.40	-0.00260	0.00594	-0.00885	0.01761	-0.00066	0.91778
3.50	-0.00207	0.00469	-0.00726	0.01434	-0.00061	0.90382
3.60	-0.00166	0.00371	-0.00596	0.01169	-0.00056	0.88929
3.70	-0.00133	0.00294	-0.00491	0.00954	-0.00051	0.87434
3.80	-0.00106	0.00233	-0.00404	0.00780	-0.00046	0.85912
3.90	-0.00085	0.00186	-0.00333	0.00638	-0.00041	0.84378

Table I.11. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	-0.00069	0.00148	-0.00276	0.00523	-0.00036	0.82845
4.10	-0.00056	0.00118	-0.00228	0.00430	-0.00032	0.81326
4.20	-0.00045	0.00095	-0.00189	0.00353	-0.00028	0.79833
4.40	-0.00030	0.00061	-0.00130	0.00240	-0.00021	0.76967
4.60	-0.00020	0.00040	-0.00091	0.00164	-0.00016	0.74312
4.80	-0.00013	0.00026	-0.00063	0.00113	-0.00011	0.71912
5.00	-0.00009	0.00017	-0.00044	0.00078	-0.00008	0.69788
5.20	-0.00006	0.00012	-0.00031	0.00055	-0.00006	0.67944
5.40	-0.00004	0.00008	-0.00022	0.00038	-0.00004	0.66370
5.60	-0.00003	0.00005	-0.00015	0.00027	-0.00003	0.65046
5.80	-0.00002	0.00004	-0.00011	0.00019	-0.00002	0.63950
6.00	-0.00001	0.00002	-0.00008	0.00013	-0.00001	0.63053
6.20	-0.00001	0.00002	-0.00005	0.00009	-0.00001	0.62329
6.40	-0.00001	0.00001	-0.00004	0.00007	-0.00001	0.61754
6.60	-0.00000	0.00001	-0.00003	0.00005	-0.00000	0.61304
6.80	-0.00000	0.00001	-0.00002	0.00003	-0.00000	0.60958
7.00	-0.00000	0.00000	-0.00001	0.00002	-0.00000	0.60698
7.20	-0.00000	0.00000	-0.00001	0.00002	-0.00000	0.60510
7.40	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.60380
7.60	-0.00000	0.00000	-0.00000	0.00001	-0.00000	0.60298
7.80	-0.00000	0.00000	-0.00000	0.00001	-0.00000	0.60253
8.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.60239
8.20	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.60250
8.40	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.60281
8.60	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.60327
8.80	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.60385
9.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.60452

Table I.12. Radial Characteristics of the Hartree-Fock $\text{Na}^+ 2p$ Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	-0.	38.77291	-0.	0.		
0.01	0.36723	34.74006	0.00367	0.71463	-3.19990	5.84844
0.02	0.69607	31.08679	0.01392	1.31780	-3.02384	3.41721
0.03	0.99011	27.77561	0.02970	1.82338	-2.61381	2.46892
0.04	1.25261	24.77299	0.05010	2.24353	-2.11444	1.93926
0.05	1.48650	22.04891	0.07432	2.58894	-1.61192	1.60337
0.06	1.69442	19.57647	0.10167	2.86901	-1.15468	1.37918
0.07	1.87878	17.33157	0.13151	3.09199	-0.76479	1.22650
0.08	2.04174	15.29258	0.16334	3.26515	-0.44914	1.12240
0.09	2.18526	13.44008	0.19667	3.39486	-0.20539	1.05230
0.10	2.31111	11.75663	0.23111	3.48677	-0.02626	1.00632
0.12	2.51610	8.83569	0.30193	3.57638	0.17644	0.96098
0.14	2.66791	6.42207	0.37351	3.56700	0.23554	0.95088
0.16	2.77578	4.42825	0.44412	3.48430	0.21464	0.95697
0.18	2.84736	2.78286	0.51252	3.34827	0.15828	0.96907
0.20	2.88902	1.42742	0.57780	3.17451	0.09404	0.98189
0.22	2.90607	0.31388	0.63933	2.97512	0.03682	0.99295
0.24	2.90292	-0.59741	0.69670	2.75955	-0.00694	1.00133
0.26	2.88330	-1.33930	0.74966	2.53508	-0.03595	1.00694
0.28	2.85030	-1.93908	0.79808	2.30736	-0.05168	1.01009
0.30	2.80653	-2.41954	0.84196	2.08067	-0.05682	1.01127
0.35	2.66353	-3.21639	0.93223	1.53779	-0.04225	1.00883
0.40	2.49169	-3.60275	0.99668	1.05059	-0.01583	1.00353
0.45	2.30762	-3.72571	1.03843	0.63105	0.00443	0.99893
0.50	2.12187	-3.68272	1.06093	0.28051	0.01420	0.99628
0.55	1.94102	-3.53873	1.06756	-0.00529	0.01552	0.99555
0.60	1.76895	-3.33699	1.06137	-0.23324	0.01207	0.99620
0.65	1.60780	-3.10610	1.04507	-0.41117	0.00697	0.99759
0.70	1.45851	-2.86476	1.02096	-0.54682	0.00217	0.99917
0.75	1.32129	-2.62486	0.99097	-0.64735	-0.00139	1.00059
0.80	1.19588	-2.39372	0.95670	-0.71910	-0.00351	1.00163
0.85	1.08171	-2.17555	0.91945	-0.76752	-0.00436	1.00224
0.90	0.97807	-1.97254	0.88026	-0.79722	-0.00428	1.00244
0.95	0.88419	-1.78546	0.83998	-0.81200	-0.00363	1.00229
1.00	0.79926	-1.61429	0.79926	-0.81503	-0.00270	1.00188
1.10	0.65317	-1.31705	0.71849	-0.79558	-0.00080	1.00068
1.20	0.53406	-1.07349	0.64087	-0.75413	0.00052	0.99946
1.30	0.43697	-0.87506	0.56806	-0.70061	0.00113	0.99857
1.40	0.35781	-0.71378	0.50093	-0.64149	0.00119	0.99814
1.50	0.29321	-0.58274	0.43981	-0.58090	0.00096	0.99817
1.60	0.24044	-0.47620	0.38471	-0.52148	0.00062	0.99856
1.70	0.19731	-0.38950	0.33542	-0.46484	0.00029	0.99919
1.80	0.16201	-0.31885	0.29162	-0.41193	0.00002	0.99994
1.90	0.13310	-0.26123	0.25290	-0.36323	-0.00017	1.00072
2.00	0.10941	-0.21417	0.21883	-0.31893	-0.00028	1.00144
2.10	0.08998	-0.17570	0.18897	-0.27899	-0.00033	1.00205
2.20	0.07404	-0.14423	0.16289	-0.24327	-0.00033	1.00250
2.30	0.06095	-0.11846	0.14018	-0.21151	-0.00030	1.00277
2.40	0.05019	-0.09734	0.12046	-0.18343	-0.00026	1.00283
2.50	0.04135	-0.08003	0.10338	-0.15872	-0.00020	1.00268
2.60	0.03408	-0.06582	0.08862	-0.13706	-0.00014	1.00232
2.70	0.02810	-0.05416	0.07588	-0.11814	-0.00009	1.00175
2.80	0.02318	-0.04459	0.06491	-0.10167	-0.00004	1.00098
2.90	0.01913	-0.03672	0.05547	-0.08736	-0.00000	1.00003
3.00	0.01579	-0.03025	0.04737	-0.07497	0.00003	0.99889
3.10	0.01304	-0.02493	0.04042	-0.06426	0.00006	0.99759
3.20	0.01077	-0.02056	0.03447	-0.05501	0.00007	0.99614
3.30	0.00890	-0.01696	0.02938	-0.04706	0.00009	0.99454
3.40	0.00736	-0.01399	0.02502	-0.04021	0.00009	0.99282
3.50	0.00609	-0.01155	0.02130	-0.03434	0.00010	0.99098
3.60	0.00503	-0.00954	0.01813	-0.02930	0.00010	0.98903
3.70	0.00417	-0.00788	0.01542	-0.02498	0.00010	0.98699
3.80	0.00345	-0.00651	0.01311	-0.02129	0.00009	0.98485
3.90	0.00286	-0.00538	0.01114	-0.01813	0.00009	0.98263

Table I.12. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	0.00237	-0.00445	0.00947	-0.01543	0.00008	0.98033
4.10	0.00196	-0.00368	0.00804	-0.01313	0.00008	0.97795
4.20	0.00163	-0.00305	0.00683	-0.01117	0.00007	0.97551
4.40	0.00112	-0.00209	0.00492	-0.00807	0.00006	0.97043
4.60	0.00077	-0.00143	0.00355	-0.00582	0.00005	0.96513
4.80	0.00053	-0.00099	0.00255	-0.00420	0.00004	0.95962
5.00	0.00037	-0.00068	0.00184	-0.00302	0.00003	0.95394
5.20	0.00025	-0.00047	0.00132	-0.00218	0.00002	0.94813
5.40	0.00018	-0.00032	0.00095	-0.00157	0.00002	0.94221
5.60	0.00012	-0.00022	0.00069	-0.00113	0.00001	0.93622
5.80	0.00009	-0.00015	0.00049	-0.00081	0.00001	0.93021
6.00	0.00006	-0.00011	0.00036	-0.00058	0.00001	0.92422
6.20	0.00004	-0.00007	0.00026	-0.00042	0.00001	0.91828
6.40	0.00003	-0.00005	0.00018	-0.00030	0.00000	0.91244
6.60	0.00002	-0.00004	0.00013	-0.00022	0.00000	0.90674
6.80	0.00001	-0.00003	0.00010	-0.00016	0.00000	0.90120
7.00	0.00001	-0.00002	0.00007	-0.00011	0.00000	0.89587
7.20	0.00001	-0.00001	0.00005	-0.00008	0.00000	0.89076
7.40	0.00000	-0.00001	0.00004	-0.00006	0.00000	0.88589
7.60	0.00000	-0.00001	0.00003	-0.00004	0.00000	0.88129
7.80	0.00000	-0.00000	0.00002	-0.00003	0.00000	0.87696
8.00	0.00000	-0.00000	0.00001	-0.00002	0.00000	0.87291
8.20	0.00000	-0.00000	0.00001	-0.00002	0.00000	0.86915
8.40	0.00000	-0.00000	0.00001	-0.00001	0.00000	0.86567
8.60	0.00000	-0.00000	0.00001	-0.00001	0.00000	0.86248
8.80	0.00000	-0.00000	0.00000	-0.00001	0.00000	0.85956
9.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.85690

Table I.13. Radial Characteristics of the Hartree-Fock Na 1s Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	70.28236	-773.31286	0.	70.28236		
0.01	62.97084	-690.60550	0.62971	56.06478	-23.30273	1.00914
0.02	56.43986	-617.01875	1.12880	44.09949	-12.88956	1.00564
0.03	50.60354	-551.51190	1.51811	34.05819	-4.58594	1.00224
0.04	45.38576	-493.16737	1.81543	25.65907	-0.04765	1.00003
0.05	40.71903	-441.17549	2.03595	18.66026	1.93930	0.99882
0.06	36.54347	-394.82145	2.19261	12.85418	2.44598	0.99835
0.07	32.80592	-353.47377	2.29641	8.06276	2.19376	0.99835
0.08	29.45917	-316.57416	2.35673	4.13324	1.62564	0.99864
0.09	26.46126	-283.62889	2.38151	0.93467	0.99425	0.99907
0.10	23.77488	-254.20089	2.37749	-1.64521	0.42899	0.99955
0.12	19.20753	-204.39262	2.30490	-5.31959	-0.32566	1.00042
0.14	15.53285	-164.55120	2.17460	-7.50432	-0.60041	1.00096
0.16	12.57276	-132.63171	2.01164	-8.64831	-0.56466	1.00111
0.18	10.18560	-107.02099	1.83341	-9.07818	-0.38747	1.00094
0.20	8.25843	-86.44357	1.65169	-9.03029	-0.18287	1.00055
0.22	6.70108	-69.88883	1.47424	-8.67446	-0.01107	1.00004
0.24	5.44144	-56.55432	1.30595	-8.13160	0.10578	0.99952
0.26	4.42173	-45.80162	1.14965	-7.48669	0.16758	0.99906
0.28	3.59558	-37.12184	1.00676	-6.79853	0.18474	0.99873
0.30	2.92576	-30.10863	0.87773	-6.10683	0.17081	0.99856
0.35	1.75258	-17.88962	0.61340	-4.50879	0.07771	0.99890
0.40	1.05428	-10.66965	0.42171	-3.21358	-0.00913	1.00021
0.45	0.63713	-6.38609	0.28671	-2.23661	-0.05152	1.00200
0.50	0.38705	-3.83585	0.19353	-1.53087	-0.05616	1.00359
0.55	0.23658	-2.31286	0.13012	-1.03549	-0.04085	1.00427
0.60	0.14568	-1.40068	0.08741	-0.69473	-0.02011	1.00341
0.65	0.09050	-0.85269	0.05882	-0.46375	-0.00213	1.00058
0.70	0.05681	-0.52239	0.03977	-0.30886	0.01001	0.99565
0.75	0.03610	-0.32253	0.02708	-0.20579	0.01621	0.98891
0.80	0.02326	-0.20101	0.01861	-0.13754	0.01772	0.98118
0.85	0.01522	-0.12668	0.01294	-0.09245	0.01613	0.97382
0.90	0.01012	-0.08087	0.00911	-0.06266	0.01285	0.96864
0.95	0.00685	-0.05238	0.00651	-0.04292	0.00894	0.96773
1.00	0.00471	-0.03447	0.00471	-0.02975	0.00512	0.97318
1.10	0.00234	-0.01566	0.00257	-0.01489	-0.00091	1.00963
1.20	0.00123	-0.00756	0.00148	-0.00784	-0.00419	1.08400
1.30	0.00069	-0.00382	0.00089	-0.00428	-0.00521	1.18727
1.40	0.00041	-0.00199	0.00057	-0.00238	-0.00479	1.29125
1.50	0.00026	-0.00105	0.00039	-0.00132	-0.00368	1.35061
1.60	0.00018	-0.00056	0.00029	-0.00072	-0.00237	1.32339
1.70	0.00014	-0.00031	0.00024	-0.00039	-0.00115	1.20440
1.80	0.00011	-0.00019	0.00021	-0.00022	-0.00015	1.03129
1.90	0.00010	-0.00013	0.00019	-0.00014	0.00060	0.85195
2.00	0.00009	-0.00010	0.00018	-0.00011	0.00109	0.69602
2.10	0.00008	-0.00009	0.00017	-0.00011	0.00137	0.57262
2.20	0.00007	-0.00009	0.00015	-0.00012	0.00148	0.47975
2.30	0.00006	-0.00009	0.00014	-0.00014	0.00146	0.41192
2.40	0.00005	-0.00008	0.00013	-0.00015	0.00136	0.36371
2.50	0.00004	-0.00008	0.00011	-0.00016	0.00121	0.33099
2.60	0.00004	-0.00008	0.00010	-0.00016	0.00103	0.31107
2.70	0.00003	-0.00007	0.00008	-0.00016	0.00083	0.30284
2.80	0.00002	-0.00006	0.00006	-0.00015	0.00064	0.30699
2.90	0.00002	-0.00006	0.00005	-0.00014	0.00046	0.32723
3.00	0.00001	-0.00005	0.00004	-0.00013	0.00030	0.37407
3.10	0.00001	-0.00004	0.00002	-0.00012	0.00015	0.47966
3.20	0.00000	-0.00003	0.00001	-0.00011	0.00003	0.79170
3.30	0.00000	-0.00003	0.00000	-0.00009	-0.00007	5.67521
3.40	-0.00000	-0.00002	-0.00001	-0.00008	-0.00016	-0.82241
3.50	-0.00000	-0.00002	-0.00001	-0.00007	-0.00023	-0.33716
3.60	-0.00001	-0.00001	-0.00002	-0.00005	-0.00028	-0.19433
3.70	-0.00001	-0.00001	-0.00003	-0.00004	-0.00031	-0.12726
3.80	-0.00001	-0.00001	-0.00003	-0.00003	-0.00034	-0.08885
3.90	-0.00001	-0.00000	-0.00003	-0.00002	-0.00035	-0.06423

Table I.13. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	-0.00001	-0.00000	-0.00003	-0.00001	-0.00036	-0.04721
4.10	-0.00001	0.00000	-0.00003	-0.00001	-0.00035	-0.03477
4.20	-0.00001	0.00000	-0.00004	-0.00000	-0.00035	-0.02527
4.40	-0.00001	0.00000	-0.00003	0.00001	-0.00032	-0.01155
4.60	-0.00001	0.00001	-0.00003	0.00002	-0.00028	-0.00170
4.80	-0.00001	0.00001	-0.00003	0.00002	-0.00023	0.00641
5.00	-0.00000	0.00001	-0.00002	0.00002	-0.00018	0.01414
5.20	-0.00000	0.00001	-0.00002	0.00002	-0.00014	0.02287
5.40	-0.00000	0.00000	-0.00001	0.00002	-0.00010	0.03481
5.60	-0.00000	0.00000	-0.00001	0.00002	-0.00006	0.05563
5.80	-0.00000	0.00000	-0.00000	0.00002	-0.00003	0.11039
6.00	-0.00000	0.00000	-0.00000	0.00002	0.00000	1.03351
6.20	0.00000	0.00000	0.00000	0.00002	0.00002	-0.14709
6.40	0.00000	0.00000	0.00001	0.00001	0.00004	-0.06885
6.60	0.00000	0.00000	0.00001	0.00001	0.00006	-0.04466
6.80	0.00000	0.00000	0.00001	0.00001	0.00007	-0.03275
7.00	0.00000	0.00000	0.00001	0.00001	0.00008	-0.02560
7.20	0.00000	0.00000	0.00001	0.00001	0.00008	-0.02081
7.40	0.00000	0.00000	0.00002	0.00000	0.00008	-0.01736
7.60	0.00000	0.00000	0.00002	0.00000	0.00009	-0.01475
7.80	0.00000	-0.00000	0.00002	0.00000	0.00009	-0.01270
8.00	0.00000	-0.00000	0.00002	0.00000	0.00008	-0.01105
8.20	0.00000	-0.00000	0.00002	-0.00000	0.00008	-0.00969
8.40	0.00000	-0.00000	0.00002	-0.00000	0.00008	-0.00854
8.60	0.00000	-0.00000	0.00002	-0.00000	0.00008	-0.00757
8.80	0.00000	-0.00000	0.00002	-0.00000	0.00007	-0.00672
9.00	0.00000	-0.00000	0.00002	-0.00000	0.00007	-0.00599
9.20	0.00000	-0.00000	0.00001	-0.00000	0.00006	-0.00535
9.40	0.00000	-0.00000	0.00001	-0.00000	0.00006	-0.00477
9.60	0.00000	-0.00000	0.00001	-0.00000	0.00006	-0.00426
9.80	0.00000	-0.00000	0.00001	-0.00000	0.00005	-0.00381
10.00	0.00000	-0.00000	0.00001	-0.00000	0.00005	-0.00339
10.20	0.00000	-0.00000	0.00001	-0.00000	0.00004	-0.00302
10.40	0.00000	-0.00000	0.00001	-0.00000	0.00004	-0.00267
10.60	0.00000	-0.00000	0.00001	-0.00000	0.00004	-0.00236
10.80	0.00000	-0.00000	0.00001	-0.00000	0.00003	-0.00207
11.00	0.00000	-0.00000	0.00001	-0.00000	0.00003	-0.00181
11.20	0.00000	-0.00000	0.00001	-0.00000	0.00003	-0.00156
11.40	0.00000	-0.00000	0.00001	-0.00000	0.00003	-0.00134
11.60	0.00000	-0.00000	0.00001	-0.00000	0.00002	-0.00112
11.80	0.00000	-0.00000	0.00001	-0.00000	0.00002	-0.00093
12.00	0.00000	-0.00000	0.00001	-0.00000	0.00002	-0.00075
12.20	0.00000	-0.00000	0.00001	-0.00000	0.00002	-0.00057
12.40	0.00000	-0.00000	0.00000	-0.00000	0.00002	-0.00041
12.60	0.00000	-0.00000	0.00000	-0.00000	0.00001	-0.00026
12.80	0.00000	-0.00000	0.00000	-0.00000	0.00001	-0.00012
13.00	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.00001
13.50	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.00031
14.00	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.00057
14.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00079
15.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00099
15.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00117
16.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00133
16.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00146
17.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00159
17.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00170
18.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00180
18.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00189
19.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00197
19.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.00205

Table I.14. Radial Characteristics of the Hartree-Fock Na 2s Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	17.17566	-189.74480	0.	17.17566		
0.01	15.36441	-172.78659	0.15364	13.63655	27.47346	0.35883
0.02	13.71462	-157.42389	0.27429	10.56614	1.06677	0.97211
0.03	12.21118	-143.48743	0.36634	7.90656	-2.50465	1.07355
0.04	10.84061	-130.82837	0.43362	5.60748	-2.28280	1.07551
0.05	9.59080	-119.31557	0.47954	3.62502	-1.43366	1.05360
0.06	8.45087	-108.83327	0.50705	1.92087	-0.68056	1.02888
0.07	7.41104	-99.27907	0.51877	0.46150	-0.16062	1.00777
0.08	6.46250	-90.56221	0.51700	-0.78248	0.14598	0.99190
0.09	5.59727	-82.60206	0.50375	-1.83691	0.29416	0.98116
0.10	4.80817	-75.32686	0.48082	-2.72451	0.33728	0.97485
0.12	3.43284	-62.58211	0.41194	-4.07701	0.26444	0.97238
0.14	2.29120	-51.89271	0.32077	-4.97377	0.13223	0.97931
0.16	1.34578	-42.90841	0.21532	-5.51956	0.02285	0.99391
0.18	0.56541	-35.34520	0.10177	-5.79673	-0.04331	1.02747
0.20	-0.07595	-28.97119	-0.01519	-5.87018	-0.07108	0.66440
0.22	-0.60009	-23.59576	-0.13202	-5.79116	-0.07251	0.95667
0.24	-1.02538	-19.06135	-0.24609	-5.60010	-0.05925	0.97928
0.26	-1.36728	-15.23700	-0.35549	-5.32890	-0.04008	0.98949
0.28	-1.63886	-12.01336	-0.45888	-5.00260	-0.02064	0.99548
0.30	-1.85120	-9.29877	-0.55536	-4.64083	0.00407	0.99921
0.35	-2.18104	-4.26243	-0.76336	-3.67289	0.01888	1.00310
0.40	-2.30758	-1.04405	-0.92303	-2.72519	0.02011	1.00312
0.45	-2.30554	0.96210	-1.03749	-1.87260	0.01140	1.00177
0.50	-2.22475	2.16106	-1.11237	-1.14422	0.00162	1.00026
0.55	-2.09830	2.82532	-1.15406	-0.54437	-0.00508	0.99913
0.60	-1.94803	3.13872	-1.16882	-0.06480	-0.00788	0.99855
0.65	-1.78818	3.22546	-1.16232	0.30837	-0.00756	0.99848
0.70	-1.62785	3.16933	-1.13950	0.59068	-0.00542	0.99881
0.75	-1.47268	3.02672	-1.10451	0.79736	-0.00261	0.99936
0.80	-1.32598	2.83531	-1.06079	0.94226	0.00002	1.00001
0.85	-1.18954	2.62006	-1.01111	1.03751	0.00200	1.00060
0.90	-1.06410	2.39724	-0.95769	1.09342	0.00318	1.00107
0.95	-0.94977	2.17723	-0.90228	1.11860	0.00359	1.00136
1.00	-0.84622	1.96638	-0.84622	1.12016	0.00338	1.00143
1.10	-0.66914	1.58498	-0.73606	1.07433	0.00192	1.00103
1.20	-0.52720	1.26413	-0.63264	0.98976	0.00017	1.00011
1.30	-0.41437	1.00163	-0.53868	0.88775	-0.00107	0.99907
1.40	-0.32516	0.79031	-0.45523	0.78127	-0.00158	0.99826
1.50	-0.25488	0.62185	-0.38232	0.67789	-0.00149	0.99790
1.60	-0.19963	0.48836	-0.31941	0.58175	-0.00106	0.99810
1.70	-0.15627	0.38301	-0.26566	0.49485	-0.00051	0.99883
1.80	-0.12228	0.30007	-0.22011	0.41785	-0.00001	0.99998
1.90	-0.09566	0.23491	-0.18176	0.35066	0.00036	1.00135
2.00	-0.07483	0.18377	-0.14967	0.29272	0.00058	1.00276
2.10	-0.05854	0.14370	-0.12294	0.24323	0.00065	1.00400
2.20	-0.04580	0.11232	-0.10077	0.20131	0.00062	1.00486
2.30	-0.03585	0.08778	-0.08245	0.16604	0.00052	1.00521
2.40	-0.02807	0.06859	-0.06737	0.13655	0.00039	1.00492
2.50	-0.02199	0.05360	-0.05498	0.11201	0.00024	1.00393
2.60	-0.01724	0.04190	-0.04482	0.09169	0.00011	1.00219
2.70	-0.01353	0.03276	-0.03652	0.07492	-0.00001	0.99974
2.80	-0.01062	0.02563	-0.02974	0.06114	-0.00010	0.99663
2.90	-0.00835	0.02006	-0.02421	0.04983	-0.00016	0.99298
3.00	-0.00657	0.01572	-0.01970	0.04059	-0.00020	0.98892
3.10	-0.00517	0.01233	-0.01604	0.03304	-0.00022	0.98464
3.20	-0.00408	0.00968	-0.01305	0.02688	-0.00022	0.98037
3.30	-0.00322	0.00760	-0.01062	0.02187	-0.00021	0.97635
3.40	-0.00254	0.00598	-0.00864	0.01780	-0.00019	0.97287
3.50	-0.00201	0.00471	-0.00704	0.01449	-0.00017	0.97026
3.60	-0.00159	0.00372	-0.00573	0.01179	-0.00014	0.96885
3.70	-0.00126	0.00294	-0.00466	0.00960	-0.00011	0.96903
3.80	-0.00100	0.00232	-0.00379	0.00782	-0.00008	0.97120
3.90	-0.00079	0.00184	-0.00309	0.00637	-0.00005	0.97582

Table I.14. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	-0.00063	0.00146	-0.00251	0.00519	-0.00003	0.98335
4.10	-0.00050	0.00115	-0.00204	0.00423	-0.00001	0.99434
4.20	-0.00039	0.00092	-0.00166	0.00345	0.00001	1.00935
4.40	-0.00025	0.00058	-0.00109	0.00229	0.00004	1.05400
4.60	-0.00016	0.00036	-0.00072	0.00151	0.00005	1.12294
4.80	-0.00010	0.00023	-0.00047	0.00099	0.00006	1.22212
5.00	-0.00006	0.00014	-0.00031	0.00064	0.00006	1.35586
5.20	-0.00004	0.00009	-0.00021	0.00041	0.00006	1.52156
5.40	-0.00003	0.00005	-0.00014	0.00025	0.00005	1.69954
5.60	-0.00002	0.00003	-0.00010	0.00014	0.00004	1.84327
5.80	-0.00001	0.00002	-0.00008	0.00008	0.00003	1.89009
6.00	-0.00001	0.00001	-0.00007	0.00003	0.00003	1.80603
6.20	-0.00001	0.00000	-0.00007	0.00001	0.00002	1.61996
6.40	-0.00001	0.00000	-0.00007	-0.00001	0.00001	1.39571
6.60	-0.00001	-0.00000	-0.00007	-0.00002	0.00001	1.18360
6.80	-0.00001	-0.00000	-0.00007	-0.00002	0.00000	1.00526
7.00	-0.00001	-0.00000	-0.00008	-0.00002	-0.00000	0.86324
7.20	-0.00001	-0.00000	-0.00008	-0.00001	-0.00001	0.75239
7.40	-0.00001	0.00000	-0.00008	-0.00001	-0.00001	0.66608
7.60	-0.00001	0.00000	-0.00008	-0.00001	-0.00001	0.59844
7.80	-0.00001	0.00000	-0.00008	-0.00000	-0.00001	0.54485
8.00	-0.00001	0.00000	-0.00008	0.00000	-0.00001	0.50185
8.20	-0.00001	0.00000	-0.00008	0.00000	-0.00002	0.46692
8.40	-0.00001	0.00000	-0.00008	0.00001	-0.00002	0.43819
8.60	-0.00001	0.00000	-0.00008	0.00001	-0.00002	0.41428
8.80	-0.00001	0.00000	-0.00008	0.00001	-0.00001	0.39419
9.00	-0.00001	0.00000	-0.00008	0.00001	-0.00001	0.37712
9.20	-0.00001	0.00000	-0.00007	0.00002	-0.00001	0.36250
9.40	-0.00001	0.00000	-0.00007	0.00002	-0.00001	0.34988
9.60	-0.00001	0.00000	-0.00007	0.00002	-0.00001	0.33891
9.80	-0.00001	0.00000	-0.00006	0.00002	-0.00001	0.32931
10.00	-0.00001	0.00000	-0.00006	0.00002	-0.00001	0.32086
10.20	-0.00001	0.00000	-0.00006	0.00002	-0.00001	0.31338
10.40	-0.00000	0.00000	-0.00005	0.00002	-0.00001	0.30673
10.60	-0.00000	0.00000	-0.00005	0.00002	-0.00001	0.30080
10.80	-0.00000	0.00000	-0.00005	0.00002	-0.00001	0.29548
11.00	-0.00000	0.00000	-0.00004	0.00002	-0.00001	0.29070
11.20	-0.00000	0.00000	-0.00004	0.00001	-0.00001	0.28639
11.40	-0.00000	0.00000	-0.00004	0.00001	-0.00001	0.28248
11.60	-0.00000	0.00000	-0.00003	0.00001	-0.00001	0.27895
11.80	-0.00000	0.00000	-0.00003	0.00001	-0.00001	0.27573
12.00	-0.00000	0.00000	-0.00003	0.00001	-0.00000	0.27280
12.20	-0.00000	0.00000	-0.00003	0.00001	-0.00000	0.27013
12.40	-0.00000	0.00000	-0.00002	0.00001	-0.00000	0.26768
12.60	-0.00000	0.00000	-0.00002	0.00001	-0.00000	0.26545
12.80	-0.00000	0.00000	-0.00002	0.00001	-0.00000	0.26339
13.00	-0.00000	0.00000	-0.00002	0.00001	-0.00000	0.26151
13.50	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.25744
14.00	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.25413
14.50	-0.00000	0.00000	-0.00001	0.00000	-0.00000	0.25142
15.00	-0.00000	0.00000	-0.00001	0.00000	-0.00000	0.24920
15.50	-0.00000	0.00000	-0.00001	0.00000	-0.00000	0.24738
16.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.24588
16.50	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.24466
17.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.24366
17.50	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.24285
18.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.24220
18.50	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.24168
19.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.24127
19.50	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.24096

Table I.15. Radial Characteristics of the Hartree-Fock Na 3s Orbital.

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
0.	2.59983	-29.52703	0.	2.59983		
0.01	2.31916	-26.66718	0.02319	2.05249	45.45846	-265.91860
0.02	2.06540	-24.13490	0.04131	1.58270	8.20409	-53.09044
0.03	1.83552	-21.88361	0.05507	1.17902	-0.06450	1.47851
0.04	1.62692	-19.87423	0.06508	0.83195	-2.13705	18.88717
0.05	1.43734	-18.07391	0.07187	0.53365	-2.32373	23.01502
0.06	1.26484	-16.45504	0.07589	0.27754	-1.91236	21.58868
0.07	1.10772	-14.99433	0.07754	0.05811	-1.36283	17.75360
0.08	0.96449	-13.67210	0.07716	-0.12928	-0.84695	12.95781
0.09	0.83387	-12.47169	0.07505	-0.28858	-0.42312	7.90966
0.10	0.71470	-11.37896	0.07147	-0.42320	-0.10261	2.95499
0.12	0.50678	-9.47002	0.06081	-0.62962	0.26759	-6.19034
0.14	0.33386	-7.86803	0.04674	-0.76767	0.38112	-14.54537
0.16	0.19040	-6.51551	0.03046	-0.85209	0.35107	-24.10898
0.18	0.07187	-5.36884	0.01294	-0.89453	0.25686	-47.67167
0.20	-0.02550	-4.39417	-0.00510	-0.90434	0.14710	79.54586
0.22	-0.10487	-3.56470	-0.02307	-0.88910	0.04804	7.23765
0.24	-0.16891	-2.85872	-0.04054	-0.85501	-0.02864	-1.30899
0.26	-0.21992	-2.25834	-0.05718	-0.80709	-0.08003	-3.95558
0.28	-0.25985	-1.74856	-0.07276	-0.74945	-0.10805	-4.66242
0.30	-0.29038	-1.31667	-0.08711	-0.68538	-0.11688	-4.48096
0.35	-0.33460	-0.50996	-0.11711	-0.51309	-0.08646	-2.51857
0.40	-0.34618	0.00726	-0.13847	-0.34328	-0.03006	-0.18245
0.45	-0.33713	0.32815	-0.15171	-0.18946	0.01635	1.66044
0.50	-0.31554	0.51769	-0.15777	-0.05670	0.04109	2.77319
0.55	-0.28680	0.62067	-0.15774	0.05457	0.04592	3.18016
0.60	-0.25441	0.66750	-0.15264	0.14610	0.03760	3.01257
0.65	-0.22064	0.67855	-0.14342	0.22042	0.02317	2.42990
0.70	-0.18692	0.66726	-0.13085	0.28016	0.00794	1.57831
0.75	-0.15414	0.64239	-0.11560	0.32765	-0.00488	0.56889
0.80	-0.12281	0.60964	-0.09825	0.36490	-0.01385	-0.53615
0.85	-0.09324	0.57266	-0.07926	0.39352	-0.01879	-1.74361
0.90	-0.06558	0.53381	-0.05902	0.41486	-0.02019	-3.19353
0.95	-0.03987	0.49459	-0.03787	0.43000	-0.01892	-5.46227
1.00	-0.01611	0.45597	-0.01611	0.43986	-0.01586	-12.41059
1.10	0.02577	0.38272	0.02835	0.44677	-0.00750	4.96078
1.20	0.06068	0.31667	0.07281	0.44068	0.00038	0.91373
1.30	0.08937	0.25861	0.11619	0.42557	0.00576	0.12210
1.40	0.11266	0.20848	0.15773	0.40453	0.00832	-0.00574
1.50	0.13132	0.16576	0.19698	0.37995	0.00859	0.10905
1.60	0.14604	0.12972	0.23366	0.35358	0.00736	0.31369
1.70	0.15746	0.09953	0.26768	0.32666	0.00536	0.53648
1.80	0.16611	0.07438	0.29900	0.29999	0.00315	0.74210
1.90	0.17247	0.05349	0.32770	0.27410	0.00108	0.91455
2.00	0.17693	0.03616	0.35386	0.24924	-0.00063	1.04868
2.10	0.17980	0.02179	0.37759	0.22556	-0.00192	1.14537
2.20	0.18137	0.00986	0.39901	0.20307	-0.00276	1.20859
2.30	0.18184	-0.00005	0.41824	0.18174	-0.00325	1.24369
2.40	0.18141	-0.00830	0.43539	0.16150	-0.00341	1.25626
2.50	0.18023	-0.01518	0.45057	0.14229	-0.00333	1.25162
2.60	0.17842	-0.02092	0.46388	0.12403	-0.00307	1.23447
2.70	0.17608	-0.02571	0.47541	0.10666	-0.00270	1.20879
2.80	0.17330	-0.02970	0.48524	0.09013	-0.00226	1.17782
2.90	0.17016	-0.03302	0.49346	0.07440	-0.00180	1.14415
3.00	0.16672	-0.03576	0.50015	0.05943	-0.00134	1.10974
3.10	0.16302	-0.03801	0.50537	0.04520	-0.00091	1.07604
3.20	0.15913	-0.03982	0.50921	0.03171	-0.00052	1.04409
3.30	0.15507	-0.04125	0.51174	0.01893	-0.00017	1.01460
3.40	0.15089	-0.04236	0.51302	0.00687	0.00013	0.98799
3.50	0.14661	-0.04317	0.51314	-0.00449	0.00038	0.96451
3.60	0.14226	-0.04372	0.51215	-0.01515	0.00058	0.94422
3.70	0.13787	-0.04405	0.51013	-0.02511	0.00074	0.92709
3.80	0.13346	-0.04417	0.50715	-0.03438	0.00085	0.91300
3.90	0.12905	-0.04411	0.50328	-0.04298	0.00093	0.90180

Table I.15. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	0.12464	-0.04389	0.49858	-0.05090	0.00098	0.89328
4.10	0.12027	-0.04352	0.49312	-0.05818	0.00100	0.88723
4.20	0.11594	-0.04304	0.48696	-0.06482	0.00099	0.88341
4.40	0.10746	-0.04175	0.47282	-0.07625	0.00093	0.88162
4.60	0.09926	-0.04014	0.45662	-0.08536	0.00083	0.88622
4.80	0.09142	-0.03828	0.43881	-0.09235	0.00070	0.89572
5.00	0.08396	-0.03627	0.41981	-0.09741	0.00056	0.90885
5.20	0.07692	-0.03417	0.39996	-0.10075	0.00043	0.92459
5.40	0.07030	-0.03201	0.37961	-0.10257	0.00030	0.94211
5.60	0.06411	-0.02986	0.35902	-0.10309	0.00018	0.96075
5.80	0.05835	-0.02773	0.33845	-0.10250	0.00009	0.98001
6.00	0.05301	-0.02566	0.31808	-0.10097	0.00000	0.99951
6.20	0.04808	-0.02367	0.29811	-0.09868	-0.00007	1.01895
6.40	0.04354	-0.02177	0.27866	-0.09576	-0.00012	1.03814
6.60	0.03937	-0.01996	0.25984	-0.09237	-0.00016	1.05692
6.80	0.03555	-0.01826	0.24173	-0.08860	-0.00020	1.07519
7.00	0.03206	-0.01666	0.22441	-0.08458	-0.00022	1.09287
7.20	0.02888	-0.01518	0.20791	-0.08039	-0.00023	1.10995
7.40	0.02598	-0.01380	0.19226	-0.07610	-0.00024	1.12639
7.60	0.02335	-0.01252	0.17747	-0.07178	-0.00024	1.14219
7.80	0.02097	-0.01134	0.16355	-0.06748	-0.00024	1.15737
8.00	0.01881	-0.01026	0.15048	-0.06325	-0.00024	1.17194
8.20	0.01686	-0.00927	0.13824	-0.05912	-0.00023	1.18592
8.40	0.01510	-0.00836	0.12682	-0.05511	-0.00022	1.19935
8.60	0.01351	-0.00753	0.11618	-0.05126	-0.00021	1.21225
8.80	0.01208	-0.00678	0.10630	-0.04757	-0.00020	1.22466
9.00	0.01079	-0.00609	0.09715	-0.04405	-0.00019	1.23660
9.20	0.00964	-0.00547	0.08867	-0.04071	-0.00018	1.24810
9.40	0.00860	-0.00491	0.08085	-0.03756	-0.00016	1.25920
9.60	0.00767	-0.00440	0.07364	-0.03459	-0.00015	1.26992
9.80	0.00684	-0.00394	0.06700	-0.03181	-0.00014	1.28029
10.00	0.00609	-0.00353	0.06090	-0.02921	-0.00013	1.29034
10.20	0.00542	-0.00316	0.05530	0.02678	-0.00012	1.30009
10.40	0.00482	-0.00282	0.05018	-0.02452	-0.00011	1.30956
10.60	0.00429	-0.00252	0.04549	-0.02242	-0.00010	1.31878
10.80	0.00381	-0.00225	0.04120	-0.02048	-0.00009	1.32777
11.00	0.00339	-0.00201	0.03729	0.01868	-0.00008	1.33654
11.20	0.00301	-0.00179	0.03372	-0.01702	-0.00008	1.34511
11.40	0.00267	-0.00159	0.03047	-0.01549	-0.00007	1.35350
11.60	0.00237	-0.00142	0.02751	-0.01409	-0.00006	1.36172
11.80	0.00210	-0.00126	0.02483	-0.01280	-0.00006	1.36978
12.00	0.00187	-0.00112	0.02239	-0.01162	-0.00005	1.37769
12.20	0.00165	-0.00100	0.02017	-0.01053	0.00005	1.38547
12.40	0.00147	-0.00089	0.01817	-0.00954	-0.00004	1.39312
12.60	0.00130	-0.00079	0.01635	-0.00864	-0.00004	1.40066
12.80	0.00115	-0.00070	0.01471	-0.00781	0.00003	1.40809
13.00	0.00102	-0.00062	0.01322	-0.00706	0.00003	1.41542
13.50	0.00075	-0.00046	0.01010	-0.00547	-0.00002	1.43333
14.00	0.00055	-0.00034	0.00770	-0.00421	-0.00002	1.45072
14.50	0.00040	-0.00025	0.00585	-0.00324	-0.00001	1.46765
15.00	0.00030	-0.00018	0.00443	-0.00248	-0.00001	1.48416
15.50	0.00022	-0.00014	0.00334	-0.00189	-0.00001	1.50029
16.00	0.00016	-0.00010	0.00252	-0.00143	-0.00001	1.51606
16.50	0.00011	-0.00007	0.00189	-0.00109	-0.00000	1.53148
17.00	0.00008	-0.00005	0.00142	-0.00082	-0.00000	1.54656
17.50	0.00006	-0.00004	0.00106	-0.00062	-0.00000	1.56131
18.00	0.00004	-0.00003	0.00079	-0.00046	-0.00000	1.57573
18.50	0.00003	-0.00002	0.00059	-0.00035	-0.00000	1.58984
19.00	0.00002	-0.00001	0.00044	-0.00026	-0.00000	1.60361
19.50	0.00002	-0.00001	0.00032	-0.00019	0.00000	1.61707

Table I.16. Radial Characteristics of the Hartree-Fock Na 2p Orbital.

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	-0.	38.69169	-0.	0.		
0.01	0.36650	34.67381	0.00366	0.71324	-3.81062	7.86794
0.02	0.69473	31.03279	0.01389	1.31539	-3.51114	4.33836
0.03	0.98829	27.73161	0.02965	1.82023	-2.99832	3.00400
0.04	1.25039	24.73713	0.05002	2.23987	-2.41343	2.27495
0.05	1.48395	22.01964	0.07420	2.58493	-1.84036	1.81919
0.06	1.69161	19.55255	0.10150	2.86477	-1.32520	1.51746
0.07	1.87576	17.31197	0.13130	3.08759	-0.88821	1.31278
0.08	2.03854	15.27646	0.16308	3.26065	-0.53464	1.17324
0.09	2.18190	13.42678	0.19637	3.39032	-0.26070	1.07892
0.10	2.30763	11.74561	0.23076	3.48219	-0.05789	1.01657
0.12	2.51244	8.82803	0.30149	3.57181	0.17683	0.95351
0.14	2.66413	6.41672	0.37298	3.56247	0.25300	0.93727
0.16	2.77190	4.42459	0.44350	3.47984	0.23934	0.94296
0.18	2.84343	2.78052	0.51182	3.34392	0.18402	0.95725
0.20	2.88505	1.42622	0.57701	3.17030	0.11720	0.97317
0.22	2.90209	0.31372	0.63846	2.97110	0.05555	0.98736
0.24	2.89895	-0.59659	0.69575	2.75577	0.00669	0.99848
0.26	2.87935	-1.33752	0.74863	2.53159	-0.02735	1.00627
0.28	2.84639	-1.93640	0.79699	2.30420	-0.04760	1.01105
0.30	2.80269	-2.41600	0.84081	2.07789	-0.05654	1.01332
0.35	2.65991	-3.21099	0.93097	1.53606	-0.04790	1.01190
0.40	2.48838	-3.59605	0.99535	1.04996	-0.02313	1.00614
0.45	2.30466	-3.71829	1.03710	0.63143	-0.00182	1.00052
0.50	2.11929	-3.67513	1.05964	0.28172	0.01019	0.99682
0.55	1.93881	-3.53139	1.06635	-0.00345	0.01393	0.99525
0.60	1.76710	-3.33017	1.06026	-0.23100	0.01250	0.99533
0.65	1.60627	-3.09998	1.04408	-0.40872	0.00878	0.99639
0.70	1.45727	-2.85938	1.02009	-0.54429	0.00472	0.99786
0.75	1.32031	-2.62020	0.99023	-0.64485	0.00135	0.99932
0.80	1.19510	-2.38972	0.95608	-0.71667	-0.00098	1.00054
0.85	1.08112	-2.17212	0.91895	-0.76518	-0.00229	1.00140
0.90	0.97764	-1.96955	0.87988	-0.79495	-0.00281	1.00190
0.95	0.88390	-1.78283	0.83970	-0.80979	-0.00278	1.00207
1.00	0.79909	-1.61193	0.79909	-0.81284	-0.00242	1.00200
1.10	0.65323	-1.31504	0.71855	-0.79332	-0.00141	1.00142
1.20	0.53430	-1.07166	0.64116	-0.75169	-0.00053	1.00066
1.30	0.43739	-0.87336	0.56861	-0.69797	-0.00001	1.00001
1.40	0.35839	-0.71220	0.50175	-0.63868	0.00023	0.99958
1.50	0.29395	-0.58131	0.44092	-0.57801	0.00029	0.99934
1.60	0.24132	-0.47496	0.38610	-0.51863	0.00028	0.99924
1.70	0.19829	-0.38849	0.33710	-0.46214	0.00024	0.99919
1.80	0.16308	-0.31809	0.29355	-0.40949	0.00021	0.99915
1.90	0.13424	-0.26072	0.25505	-0.36113	0.00019	0.99908
2.00	0.11059	-0.21390	0.22117	-0.31722	0.00017	0.99898
2.10	0.09117	-0.17566	0.19146	-0.27771	0.00016	0.99884
2.20	0.07522	-0.14438	0.16549	-0.24241	0.00015	0.99869
2.30	0.06211	-0.11877	0.14285	-0.21106	0.00014	0.99856
2.40	0.05132	-0.09778	0.12316	-0.18336	0.00012	0.99847
2.50	0.04243	-0.08057	0.10607	-0.15900	0.00010	0.99846
2.60	0.03510	-0.06643	0.09126	-0.13763	0.00008	0.99858
2.70	0.02906	-0.05482	0.07845	-0.11896	0.00005	0.99885
2.80	0.02407	-0.04527	0.06739	-0.10268	0.00003	0.99931
2.90	0.01995	-0.03740	0.05784	-0.08853	-0.00000	1.00001
3.00	0.01654	-0.03093	0.04962	-0.07624	-0.00002	1.00098
3.10	0.01372	-0.02559	0.04254	-0.06560	-0.00005	1.00225
3.20	0.01139	-0.02118	0.03645	-0.05639	-0.00007	1.00387
3.30	0.00946	-0.01755	0.03122	-0.04844	-0.00008	1.00587
3.40	0.00786	-0.01454	0.02673	-0.04158	-0.00010	1.00830
3.50	0.00654	-0.01206	0.02287	-0.03567	-0.00011	1.01118
3.60	0.00544	-0.01001	0.01957	-0.03058	-0.00012	1.01456
3.70	0.00452	-0.00831	0.01673	-0.02621	-0.00013	1.01849
3.80	0.00376	-0.00690	0.01430	-0.02245	-0.00013	1.02301
3.90	0.00313	-0.00573	0.01222	-0.01922	-0.00013	1.02817

Table I.16. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	0.00261	-0.00476	0.01045	-0.01645	-0.00013	1.03404
4.10	0.00218	-0.00396	0.00892	-0.01407	-0.00013	1.04066
4.20	0.00181	-0.00330	0.00762	-0.01203	-0.00013	1.04811
4.40	0.00126	-0.00228	0.00555	-0.00879	-0.00013	1.06581
4.60	0.00088	-0.00159	0.00405	-0.00642	-0.00012	1.08782
4.80	0.00061	-0.00110	0.00295	-0.00468	-0.00011	1.11498
5.00	0.00043	-0.00077	0.00214	-0.00341	-0.00010	1.14834
5.20	0.00030	-0.00054	0.00156	-0.00248	-0.00009	1.18915
5.40	0.00021	-0.00037	0.00113	-0.00181	-0.00008	1.23893
5.60	0.00015	-0.00026	0.00082	-0.00131	-0.00007	1.29953
5.80	0.00010	-0.00018	0.00060	-0.00096	-0.00006	1.3731 ⁵
6.00	0.00007	-0.00013	0.00044	-0.00070	-0.00005	1.46248
6.20	0.00005	-0.00009	0.00032	-0.00051	-0.00004	1.57072
6.40	0.00004	-0.00006	0.00023	-0.00037	-0.00004	1.70176
6.60	0.00003	-0.00004	0.00017	-0.00027	-0.00003	1.86026
6.80	0.00002	-0.00003	0.00012	-0.00019	-0.00003	2.05184
7.00	0.00001	-0.00002	0.00009	-0.00014	-0.00002	2.28327
7.20	0.00001	-0.00002	0.00006	-0.00010	-0.00002	2.56272
7.40	0.00001	-0.00001	0.00005	-0.00007	-0.00002	2.90005
7.60	0.00000	-0.00001	0.00003	-0.00005	-0.00002	3.30715
7.80	0.00000	-0.00001	0.00002	-0.00004	-0.00001	3.79838
8.00	0.00000	-0.00000	0.00002	-0.00003	-0.00001	4.39110
8.20	0.00000	-0.00000	0.00001	-0.00002	-0.00001	5.10629
8.40	0.00000	-0.00000	0.00001	-0.00001	-0.00001	5.96932
8.60	0.00000	-0.00000	0.00001	-0.00001	-0.00001	7.01087
8.80	0.00000	-0.00000	0.00000	-0.00001	-0.00001	8.26807
9.00	0.00000	-0.00000	0.00000	-0.00001	-0.00001	9.78587
9.20	0.00000	-0.00000	0.00000	-0.00000	-0.00000	11.61870
9.40	0.00000	-0.00000	0.00000	-0.00000	-0.00000	13.83248
9.60	0.00000	-0.00000	0.00000	-0.00000	-0.00000	16.50708
9.80	0.00000	-0.00000	0.00000	-0.00000	-0.00000	19.73932
10.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	23.64656

APPENDIX J
PARAMETERS AND ORBITAL TABLES FOR THE SCF WAVE
FUNCTION OF THE GROUND STATES OF F^- AND Na^+ IN THE
PRESENCE OF A SUPERPOSED POTENTIAL SPHERE

The solutions given in this appendix correspond to an F^- ion and to a Na^+ ion in the presence of a superposed hollow sphere carrying a unit charge. The radius of the superposed sphere was taken as the Pauling ionic radius of 2.57 au for F^- and 1.7953 au for Na^+ . The expansion parameters are the same as those of Tables H.2 and H.4. The orbital tables are given exactly as in Appendix I.

Table J.1. Parameters for F^- with Superposed Potential Sphere.

ζ	N	C_{1s}	C_{2s}	ζ	N	C_{2p}
12.20	1	0.089840	- 0.227944	6.05	2	0.050460
8.20	1	0.937570	0.661599	3.06	2	0.634463
				1.44	2	0.550004
10.80	2	- 0.022792	- 0.158977	0.69	2	0.029166
4.10	2	- 0.007465	- 0.209390			
2.66	2	- 0.005762	- 0.590389	3.75	3	- 0.141918
1.68	2	0.001639	- 0.296774	8.00	3	- 0.011830
4.50	3	0.013763	- 0.020377			
- ϵ		26.16936	1.431042			0.5395839
- $\tilde{R}$		8.9947	9.0597			10.2368
- E			103.3235			
Charge on Sphere		1.00		Radius of Sphere		2.57

Table J.2. Parameters for Na^+ with Superposed Potential Sphere.

ζ	N	C_{1s}	C_{2s}	ζ	N	C_{2p}
15.00	1	0.118585	0.041607	6.60	2	0.142694
10.30	1	0.854666	0.186576	3.40	2	0.704154
				2.30	2	0.228789
11.00	2	0.031835	0.071497	1.80	2	0.150446
5.40	2	0.008407	- 0.100483			
3.10	2	- 0.001567	- 0.756084	4.00	3	- 0.143792
2.00	2	0.000685	- 0.060506	9.60	3	- 0.013064
6.00	3	0.000658	- 0.166421			
- ϵ		40.22343	2.528619			1.253062
- $\tilde{R}$		11.0025	11.0350			13.0767
- E			156.1229			
Charge on Sphere		- 1.00		Radius of Sphere		1.7953

Table J.3. Radial Characteristics of the Hartree-Fock F^- 1s Orbital*.

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	51.68727	-464.91376	0.	51.68727		
0.01	47.24750	-423.70165	0.47247	43.01048	-39.62706	1.03205
0.02	43.20064	-386.26986	0.86401	35.47524	-16.85802	1.01491
0.03	39.51070	-352.25875	1.18532	28.94294	-6.97551	1.00675
0.04	36.14514	-321.34421	1.44581	23.29137	-1.87394	1.00198
0.05	33.07447	-293.23393	1.65372	18.41278	0.71537	0.99917
0.06	30.27200	-267.66421	1.81632	14.21215	1.86790	0.99764
0.07	27.71352	-244.39706	1.93995	10.60572	2.19571	0.99697
0.08	25.37710	-223.21764	2.03017	7.51969	2.07145	0.99688
0.09	23.24285	-203.93186	2.09186	4.88899	1.72468	0.99716
0.10	21.29274	-186.36437	2.12927	2.65630	1.29513	0.99768
0.12	17.88088	-155.76537	2.14571	-0.81096	0.47878	0.99898
0.14	15.02777	-130.32568	2.10389	-3.21783	-0.09253	1.00024
0.16	12.63948	-109.14847	2.02232	-4.82428	-0.39375	1.00119
0.18	10.63835	-91.49798	1.91490	-5.83129	-0.48742	1.00175
0.20	8.96010	-76.76966	1.79202	-6.39383	-0.45044	1.00192
0.22	7.55142	-64.46597	1.66131	-6.63109	-0.34718	1.00176
0.24	6.36805	-54.17680	1.52833	-6.63439	-0.22285	1.00134
0.26	5.37319	-45.56359	1.39703	-6.47335	-0.10511	1.00075
0.28	4.53621	-38.34642	1.27014	-6.20079	-0.00828	1.00007
0.30	3.83158	-32.29354	1.14947	-5.85649	0.06248	0.99938
0.35	2.51770	-21.07276	0.88120	-4.85776	0.13484	0.99795
0.40	1.65901	-13.79580	0.66360	-3.85931	0.11178	0.99743
0.45	1.09610	-9.05707	0.49324	-2.97958	0.05691	0.99802
0.50	0.72611	-5.96054	0.36305	-2.25416	0.00693	0.99964
0.55	0.48236	-3.93128	0.26530	-1.67984	-0.02492	1.00197
0.60	0.32145	-2.59822	0.19287	-1.23749	-0.03849	1.00458
0.65	0.21499	-1.72075	0.13975	-0.90350	-0.03874	1.00689
0.70	0.14442	-1.14216	0.10109	-0.65509	-0.03138	1.00830
0.75	0.09752	-0.76006	0.07314	-0.47252	-0.02096	1.00821
0.80	0.06627	-0.50733	0.05302	-0.33960	-0.01050	1.00606
0.85	0.04538	-0.33992	0.03857	-0.24356	-0.00167	1.00141
0.90	0.03135	-0.22882	0.02821	-0.17459	0.00488	0.99405
0.95	0.02188	-0.15493	0.02078	-0.12531	0.00910	0.98410
1.00	0.01544	-0.10566	0.01544	-0.09021	0.01128	0.97209
1.10	0.00800	-0.05051	0.00880	-0.04756	0.01126	0.94620
1.20	0.00437	-0.02529	0.00524	-0.02598	0.00814	0.92880
1.30	0.00251	-0.01337	0.00326	-0.01488	0.00427	0.93489
1.40	0.00150	-0.00747	0.00209	-0.00896	0.00090	0.97690
1.50	0.00092	-0.00436	0.00138	-0.00563	-0.00149	1.06205
1.60	0.00058	-0.00263	0.00093	-0.00362	-0.00290	1.19180
1.70	0.00037	-0.00160	0.00063	-0.00235	-0.00350	1.35982
1.80	0.00025	-0.00097	0.00044	-0.00150	-0.00351	1.54565
1.90	0.00017	-0.00058	0.00032	-0.00092	-0.00314	1.70687
2.00	0.00013	-0.00033	0.00025	-0.00053	-0.00258	1.78418
2.10	0.00010	-0.00018	0.00021	-0.00028	-0.00194	1.73441
2.20	0.00009	-0.00009	0.00019	-0.00011	-0.00130	1.56837
2.30	0.00008	-0.00004	0.00019	-0.00002	-0.00073	1.34255
2.40	0.00008	-0.00002	0.00019	0.00003	-0.00023	1.11461
2.50	0.00008	-0.00001	0.00019	0.00004	0.00017	0.91652
2.60	0.00008	-0.00001	0.00020	0.00004	0.00048	0.75687
2.70	0.00007	-0.00002	0.00020	0.00002	0.00071	0.63243
2.80	0.00007	-0.00002	0.00020	0.00000	0.00087	0.53692
2.90	0.00007	-0.00003	0.00020	-0.00002	0.00097	0.46364
3.00	0.00007	-0.00004	0.00020	-0.00004	0.00102	0.40711
3.20	0.00006	-0.00004	0.00018	-0.00008	0.00101	0.32852
3.40	0.00005	-0.00004	0.00017	-0.00010	0.00093	0.27904
3.60	0.00004	-0.00004	0.00015	-0.00011	0.00080	0.24672
3.80	0.00003	-0.00004	0.00013	-0.00010	0.00067	0.22501
4.00	0.00003	-0.00003	0.00011	-0.00010	0.00054	0.21016
4.20	0.00002	-0.00003	0.00009	-0.00009	0.00043	0.19998
4.40	0.00002	-0.00002	0.00007	-0.00007	0.00034	0.19315
4.60	0.00001	-0.00002	0.00006	-0.00006	0.00026	0.18883
4.80	0.00001	-0.00001	0.00005	-0.00005	0.00020	0.18652

*Parameters taken from Table J.1.

Table J.3. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.00001	-0.00001	0.00004	-0.00004	0.00015	0.18589
5.20	0.00001	-0.00001	0.00003	-0.00003	0.00011	0.18678
5.40	0.00000	-0.00001	0.00002	-0.00003	0.00009	0.18908
5.60	0.00000	-0.00000	0.00002	-0.00002	0.00006	0.19278
5.80	0.00000	-0.00000	0.00001	-0.00002	0.00005	0.19793
6.00	0.00000	-0.00000	0.00001	-0.00001	0.00004	0.20461
6.50	0.00000	-0.00000	0.00001	-0.00001	0.00002	0.22898
7.00	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.26734
7.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.32542
8.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.41217
8.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.54123
9.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.73336
9.50	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.02007
10.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.44930
10.50	0.00000	-0.00000	0.00000	-0.00000	-0.00000	2.09414
11.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	3.06625
11.50	0.00000	-0.00000	0.00000	-0.00000	-0.00000	4.53653
12.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	6.76723
12.50	0.00000	-0.00000	0.00000	-0.00000	-0.00000	10.16146
13.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	15.34011
13.50	0.00000	-0.00000	0.00000	-0.00000	-0.00000	23.26121
14.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	35.40555
14.50	0.00000	-0.00000	0.00000	-0.00000	-0.00000	54.06576
15.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	82.79677
15.50	0.00000	-0.00000	0.00000	-0.00000	-0.00000	127.11910
17.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	466.09274
18.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1118.59082
19.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	2701.54498
20.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	6561.27844
21.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	16015.89954

Table J.4. Radial Characteristics of the Hartree-Fock F^- 2s Orbital*.

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
0.	11.64364	-105.48773	0.	11.64364		
0.01	10.62901	-97.54972	0.10629	9.65352	35.00233	-1.30118
0.02	9.69052	-90.25101	0.19381	7.88550	7.18366	0.48198
0.03	8.82206	-83.53405	0.26466	6.31603	0.88888	0.92959
0.04	8.01807	-77.34694	0.32072	4.92419	-0.85001	1.07408
0.05	7.27351	-71.64284	0.36368	3.69136	-1.20360	1.11563
0.06	6.58375	-66.37949	0.39502	2.60098	-1.10212	1.11698
0.07	5.94458	-61.51870	0.41612	1.63827	-0.87119	1.10241
0.08	5.35215	-57.02597	0.42817	0.79007	-0.63059	1.08233
0.09	4.80293	-52.87009	0.43226	0.04463	-0.42186	1.06138
0.10	4.29372	-49.02282	0.42937	-0.60857	-0.25536	1.04156
0.12	3.38368	-42.15418	0.40604	-1.67482	-0.03725	1.00769
0.14	2.60117	-36.24267	0.36416	-2.47280	0.07017	0.98115
0.16	1.92857	-31.14202	0.30857	-3.05415	0.11210	0.95938
0.18	1.35090	-26.73111	0.24316	-3.46070	0.11838	0.93876
0.20	0.85540	-22.90922	0.17108	-3.72644	0.10661	0.91291
0.22	0.43117	-19.59226	0.09486	-3.87913	0.08668	0.85952
0.24	0.06882	-16.70964	0.01652	-3.94149	0.06408	0.34939
0.26	-0.23972	-14.20188	-0.06233	-3.93220	0.04182	1.12192
0.28	-0.50142	-12.01857	-0.14040	-3.86662	0.02159	1.03009
0.30	-0.72233	-10.11687	-0.21670	-3.75739	0.00427	1.00413
0.35	-1.12904	-6.36682	-0.39517	-3.35743	-0.02445	0.98487
0.40	-1.37726	-3.71572	-0.55090	-2.86355	-0.03386	0.98282
0.45	-1.51370	-1.85286	-0.68117	-2.34749	-0.02966	0.98631
0.50	-1.57198	-0.55805	-0.78599	-1.85100	-0.01854	0.99176
0.55	-1.57632	0.32683	-0.86697	-1.39656	-0.00600	0.99734
0.60	-1.54420	0.91625	-0.92652	-0.99445	0.00447	1.00202
0.65	-1.48822	1.29347	-0.96734	-0.64746	0.01133	1.00532
0.70	-1.41737	1.51922	-0.99216	-0.35391	0.01440	1.00710
0.75	-1.33807	1.63776	-1.00356	-0.10975	0.01435	1.00749
0.80	-1.25484	1.68132	-1.00387	0.09022	0.01213	1.00676
0.85	-1.17080	1.67329	-0.99518	0.25150	0.00873	1.00521
0.90	-1.08809	1.63060	-0.97928	0.37946	0.00495	1.00318
0.95	-1.00811	1.56545	-0.95770	0.47907	0.00137	1.00095
1.00	-0.93177	1.48657	-0.93177	0.55480	-0.00164	0.99877
1.10	-0.79181	1.31052	-0.87099	0.64976	-0.00545	0.99519
1.20	-0.66970	1.13280	-0.80364	0.68966	-0.00648	0.99324
1.30	-0.56483	0.96744	-0.73427	0.69284	-0.00562	0.99305
1.40	-0.47561	0.81998	-0.66586	0.67237	-0.00385	0.99435
1.50	-0.40019	0.69170	-0.60028	0.63736	-0.00188	0.99672
1.60	-0.33666	0.58176	-0.53866	0.59415	-0.00014	0.99972
1.70	-0.28328	0.48844	-0.48158	0.54706	0.00119	1.00295
1.80	-0.23849	0.40972	-0.42928	0.49902	0.00208	1.00610
1.90	-0.20092	0.34359	-0.38174	0.45191	0.00257	1.00894
2.00	-0.16941	0.28817	-0.33882	0.40694	0.00275	1.01135
2.10	-0.14298	0.24180	-0.30026	0.36481	0.00271	1.01322
2.20	-0.12080	0.20303	-0.26575	0.32587	0.00251	1.01454
2.30	-0.10216	0.17062	-0.23498	0.29027	0.00224	1.01532
2.40	-0.08650	0.14353	-0.20759	0.25797	0.00193	1.01559
2.50	-0.07331	0.12086	-0.18327	0.22885	0.00162	1.01540
2.60	-0.06220	0.10190	-0.16172	0.20273	0.00104	1.01169
2.70	-0.05283	0.08600	-0.14264	0.17938	0.00006	1.00086
2.80	-0.04491	0.07268	-0.12576	0.15858	-0.00061	0.99051
2.90	-0.03822	0.06149	-0.11084	0.14009	-0.00106	0.98065
3.00	-0.03256	0.05208	-0.09767	0.12369	-0.00134	0.97129
3.20	-0.02368	0.03750	-0.07578	0.09631	-0.00155	0.95415
3.40	-0.01728	0.02711	-0.05875	0.07491	-0.00150	0.93922
3.60	-0.01264	0.01968	-0.04551	0.05822	-0.00133	0.92661
3.80	-0.00927	0.01434	-0.03522	0.04522	-0.00111	0.91637
4.00	-0.00681	0.01048	-0.02723	0.03511	-0.00089	0.90850
4.20	-0.00501	0.00768	-0.02102	0.02724	-0.00070	0.90295
4.40	-0.00369	0.00564	-0.01622	0.02111	-0.00053	0.89965
4.60	-0.00272	0.00414	-0.01249	0.01635	-0.00039	0.89849
4.80	-0.00200	0.00305	-0.00961	0.01264	-0.00029	0.89938

*Parameters taken from Table J.1.

Table J.4. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	-0.00148	0.00225	-0.00738	0.00977	-0.00021	0.90222
5.20	-0.00109	0.00166	-0.00566	0.00753	-0.00014	0.90695
5.40	-0.00080	0.00122	-0.00433	0.00580	-0.00010	0.91352
5.60	-0.00059	0.00090	-0.00331	0.00446	-0.00007	0.92195
5.80	-0.00044	0.00067	-0.00253	0.00342	-0.00004	0.93225
6.00	-0.00032	0.00049	-0.00192	0.00262	-0.00003	0.94452
6.50	-0.00015	0.00023	-0.00097	0.00134	-0.00000	0.98478
7.00	-0.00007	0.00011	-0.00048	0.00068	0.00000	1.04199
7.50	-0.00003	0.00005	-0.00024	0.00034	0.00001	1.12273
8.00	-0.00001	0.00002	-0.00012	0.00017	0.00000	1.23758
8.50	-0.00001	0.00001	-0.00006	0.00008	0.00000	1.40295
9.00	-0.00000	0.00000	-0.00003	0.00004	0.00000	1.64389
9.50	-0.00000	0.00000	-0.00001	0.00002	0.00000	1.99851
10.00	-0.00000	0.00000	-0.00001	0.00001	0.00000	2.52483
10.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	3.31128
11.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	4.49290
11.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	6.27644
12.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	8.97903
12.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	13.08818
13.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	19.35468
13.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	28.93705
14.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	43.62588
14.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	66.19344
15.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	100.93840
15.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	154.53619
17.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	564.43192
18.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	1353.43825
19.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	3267.55280
20.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	7934.75122
21.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	19367.29443

Table J.5. Radial Characteristics of the Hartree-Fock F^- 2p Orbital*.

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	-0.	18.83933	-0.	0.		
0.01	0.18022	17.22612	0.00180	0.35248	-1.55496	16.99079
0.02	0.34495	15.74168	0.00690	0.65979	-1.51794	9.15526
0.03	0.49544	14.37508	0.01486	0.92669	-1.38955	6.19786
0.04	0.63281	13.11634	0.02531	1.15747	-1.20948	4.54213
0.05	0.75810	11.95642	0.03790	1.35592	-1.01057	3.47050
0.06	0.87224	10.88707	0.05233	1.52547	-0.81257	2.72649
0.07	0.97612	9.90080	0.06833	1.66917	-0.62786	2.19207
0.08	1.07051	8.99076	0.08564	1.78977	-0.46316	1.80182
0.09	1.15616	8.15074	0.10405	1.88973	-0.32150	1.51535
0.10	1.23374	7.37505	0.12337	1.97125	-0.20347	1.30564
0.12	1.36709	5.99642	0.16405	2.08666	-0.03335	1.04521
0.14	1.47494	4.81863	0.20649	2.14954	0.06359	0.92010
0.16	1.56097	3.81142	0.24976	2.17080	0.10735	0.87255
0.18	1.62836	2.94950	0.29310	2.15927	0.11605	0.86792
0.20	1.67978	2.21161	0.33596	2.12210	0.10408	0.88517
0.22	1.71753	1.57989	0.37786	2.06511	0.08185	0.91168
0.24	1.74358	1.03929	0.41846	1.99301	0.05638	0.94007
0.26	1.75963	0.57704	0.45750	1.90966	0.03202	0.96627
0.28	1.76711	0.18233	0.49479	1.81817	0.01113	0.98833
0.30	1.76731	-0.15405	0.53019	1.72109	-0.00526	1.00551
0.35	1.74264	-0.78865	0.60992	1.46661	-0.02668	1.02836
0.40	1.69214	-1.20016	0.67686	1.21208	-0.02757	1.03019
0.45	1.62523	-1.45444	0.73135	0.97074	-0.01866	1.02128
0.50	1.54854	-1.59768	0.77427	0.74971	-0.00775	1.00928
0.55	1.46676	-1.66274	0.80672	0.55226	0.00110	0.99861
0.60	1.38318	-1.67324	0.82991	0.37923	0.00655	0.99123
0.65	1.30006	-1.64626	0.84504	0.22999	0.00876	0.98751
0.70	1.21897	-1.59423	0.85328	0.10301	0.00856	0.98699
0.75	1.14091	-1.52615	0.85568	-0.00371	0.00687	0.98884
0.80	1.06651	-1.44855	0.85321	-0.09233	0.00450	0.99218
0.85	0.99613	-1.36611	0.84671	-0.16506	0.00204	0.99620
0.90	0.92992	-1.28214	0.83693	-0.22401	-0.00013	1.00027
0.95	0.86790	-1.19897	0.82451	-0.27112	-0.00183	1.00391
1.00	0.80999	-1.11817	0.80999	-0.30818	-0.00299	1.00684
1.10	0.70585	-0.96731	0.77643	-0.35820	-0.00382	1.01002
1.20	0.61595	-0.83359	0.73914	-0.38435	-0.00321	1.00966
1.30	0.53854	-0.71754	0.70010	-0.39426	-0.00189	1.00650
1.40	0.47189	-0.61805	0.66064	-0.39338	-0.00042	1.00165
1.50	0.41444	-0.53331	0.62165	-0.38553	0.00085	0.99618
1.60	0.36480	-0.46134	0.58368	-0.37334	0.00176	0.99105
1.70	0.32181	-0.40024	0.54707	-0.35861	0.00226	0.98698
1.80	0.28445	-0.34831	0.51201	-0.34251	0.00237	0.98453
1.90	0.25189	-0.30406	0.47859	-0.32584	0.00217	0.98404
2.00	0.22342	-0.26625	0.44684	-0.30907	0.00172	0.98571
2.10	0.19846	-0.23380	0.41676	-0.29252	0.00111	0.98962
2.20	0.17651	-0.20586	0.38832	-0.27638	0.00040	0.99575
2.30	0.15716	-0.18170	0.36147	-0.26074	-0.00034	1.00400
2.40	0.14007	-0.16072	0.33616	-0.24567	-0.00108	1.01423
2.50	0.12493	-0.14244	0.31232	-0.23117	-0.00177	1.02623
2.60	0.11150	-0.12645	0.28990	-0.21726	-0.00189	1.03147
2.70	0.09957	-0.11241	0.26885	-0.20394	-0.00107	1.01997
2.80	0.08896	-0.10006	0.24910	-0.19119	-0.00055	1.01145
2.90	0.07951	-0.08915	0.23059	-0.17901	-0.00024	1.00548
3.00	0.07109	-0.07949	0.21327	-0.16738	-0.00006	1.00167
3.20	0.05687	-0.06332	0.18200	-0.14575	0.00003	0.99909
3.40	0.04554	-0.05052	0.15483	-0.12623	-0.00003	1.00117
3.60	0.03649	-0.04034	0.13137	-0.10874	-0.00011	1.00581
3.80	0.02927	-0.03222	0.11121	-0.09319	-0.00018	1.01133
4.00	0.02349	-0.02574	0.09397	-0.07947	-0.00021	1.01641
4.20	0.01888	-0.02056	0.07930	-0.06748	-0.00020	1.01999
4.40	0.01520	-0.01643	0.06687	-0.05707	-0.00017	1.02128
4.60	0.01226	-0.01312	0.05638	-0.04811	-0.00013	1.01970
4.80	0.00991	-0.01049	0.04754	-0.04043	-0.00008	1.01484

*Parameters taken from Table J.1.

Table J.5. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.00803	-0.00839	0.04013	-0.03390	-0.00003	1.00646
5.20	0.00652	-0.00671	0.03392	-0.02838	0.00002	0.99446
5.40	0.00532	-0.00538	0.02872	-0.02373	0.00006	0.97887
5.60	0.00435	-0.00432	0.02437	-0.01984	0.00009	0.95982
5.80	0.00358	-0.00348	0.02074	-0.01658	0.00012	0.93759
6.00	0.00295	-0.00280	0.01770	-0.01387	0.00014	0.91253
6.50	0.00186	-0.00166	0.01210	-0.00894	0.00016	0.84047
7.00	0.00121	-0.00101	0.00846	-0.00585	0.00016	0.76156
7.50	0.00081	-0.00063	0.00605	-0.00392	0.00014	0.68392
8.00	0.00055	-0.00041	0.00442	-0.00270	0.00012	0.61382
8.50	0.00039	-0.00027	0.00328	-0.00191	0.00009	0.55485
9.00	0.00027	-0.00018	0.00247	-0.00138	0.00007	0.50797
9.50	0.00020	-0.00013	0.00187	-0.00102	0.00006	0.47236
10.00	0.00014	-0.00009	0.00143	-0.00077	0.00004	0.44632
10.50	0.00010	-0.00007	0.00110	-0.00058	0.00003	0.42787
11.00	0.00008	-0.00005	0.00084	-0.00045	0.00002	0.41520
11.50	0.00006	-0.00003	0.00064	-0.00034	0.00002	0.40676
12.00	0.00004	-0.00003	0.00049	-0.00026	0.00001	0.40138
12.50	0.00003	-0.00002	0.00038	-0.00020	0.00001	0.39814
13.00	0.00002	-0.00001	0.00029	-0.00016	0.00001	0.39638
13.50	0.00002	-0.00001	0.00022	-0.00012	0.00001	0.39565
14.00	0.00001	-0.00001	0.00017	-0.00009	0.00000	0.39559
14.50	0.00001	-0.00001	0.00013	-0.00007	0.00000	0.39598
15.00	0.00001	-0.00000	0.00010	-0.00005	0.00000	0.39666
15.50	0.00000	-0.00000	0.00007	-0.00004	0.00000	0.39752
17.00	0.00000	-0.00000	0.00003	-0.00002	0.00000	0.40051
18.00	0.00000	-0.00000	0.00002	-0.00001	0.00000	0.40252
19.00	0.00000	-0.00000	0.00001	-0.00001	0.00000	0.40443
20.00	0.00000	-0.00000	0.00001	-0.00000	0.00000	0.40620
21.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.40782

Table J.6. Radial Characteristics of the Hartree-Fock Na^+ 1s Orbital*.

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
0.	70.28266	-773.28548	0.	70.28266		
0.01	62.97135	-690.59004	0.62971	56.06545	-24.97693	1.00986
0.02	56.44048	-617.01182	1.12881	44.10025	-13.26807	1.00584
0.03	50.60420	-551.51095	1.51813	34.05887	-4.64473	1.00228
0.04	45.38641	-493.17039	1.81546	25.65959	-0.00713	1.00000
0.05	40.71963	-441.18103	2.03598	18.66058	2.00609	0.99878
0.06	36.54401	-394.82839	2.19264	12.85430	2.51126	0.99829
0.07	32.80639	-353.48131	2.29645	8.06270	2.24739	0.99830
0.08	29.45956	-316.58176	2.35676	4.13302	1.66510	0.99859
0.09	26.46158	-283.63614	2.38154	0.93433	1.01981	0.99904
0.10	23.77512	-254.20756	2.37751	-1.64563	0.44272	0.99954
0.12	19.20765	-204.39779	2.30492	-5.32008	-0.32887	1.00043
0.14	15.53289	-164.55481	2.17460	-7.50479	-0.61232	1.00098
0.16	12.57274	-132.63398	2.01164	-8.64869	-0.57942	1.00115
0.18	10.18554	-107.02220	1.83340	-9.07845	-0.40136	1.00098
0.20	8.25836	-86.44405	1.65167	-9.03045	-0.19392	1.00058
0.22	6.70101	-69.88885	1.47422	-8.67454	-0.01852	1.00007
0.24	5.44137	-56.55410	1.30593	-8.13161	0.10189	0.99953
0.26	4.42166	-45.80131	1.14963	-7.48668	0.16681	0.99906
0.28	3.59552	-37.12155	1.00675	-6.79851	0.18640	0.99871
0.30	2.92570	-30.10842	0.87771	-6.10682	0.17419	0.99852
0.35	1.75252	-17.88969	0.61338	-4.50887	0.08255	0.99883
0.40	1.05422	-10.66992	0.42169	-3.21375	-0.00549	1.00013
0.45	0.63705	-6.38639	0.28667	-2.23682	-0.05001	1.00195
0.50	0.38696	-3.83606	0.19348	-1.53107	-0.05664	1.00364
0.55	0.23648	-2.31293	0.13007	-1.03563	-0.04265	1.00448
0.60	0.14558	-1.40059	0.08735	-0.69478	-0.02249	1.00384
0.65	0.09041	-0.85248	0.05876	-0.46371	-0.00448	1.00123
0.70	0.05673	-0.52211	0.03971	-0.30874	0.00811	0.99645
0.75	0.03604	-0.32221	0.02703	-0.20562	0.01497	0.98968
0.80	0.02322	-0.20069	0.01857	-0.13734	0.01719	0.98159
0.85	0.01519	-0.12639	0.01291	-0.09224	0.01626	0.97340
0.90	0.01011	-0.08063	0.00910	-0.06246	0.01351	0.96676
0.95	0.00684	-0.05220	0.00650	-0.04275	0.00999	0.96370
1.00	0.00471	-0.03434	0.00471	-0.02963	0.00639	0.96627
1.10	0.00235	-0.01563	0.00258	-0.01485	0.00044	0.99537
1.20	0.00124	-0.00759	0.00149	-0.00787	-0.00313	1.006281
1.30	0.00069	-0.00389	0.00090	-0.00437	-0.00461	1.16630
1.40	0.00040	-0.00206	0.00056	-0.00248	-0.00468	1.28960
1.50	0.00025	-0.00111	0.00037	-0.00142	-0.00398	1.39959
1.60	0.00016	-0.00061	0.00026	-0.00081	-0.00298	1.45032
1.70	0.00012	-0.00033	0.00020	-0.00045	-0.00194	1.40559
1.80	0.00009	-0.00019	0.00017	-0.00024	-0.00101	1.26844
1.90	0.00008	-0.00011	0.00015	-0.00013	-0.00026	1.08081
2.00	0.00007	-0.00007	0.00014	-0.00008	0.00031	0.88885
2.10	0.00006	-0.00006	0.00013	-0.00005	0.00072	0.72071
2.20	0.00006	-0.00005	0.00013	-0.00005	0.00098	0.58498
2.30	0.00005	-0.00005	0.00012	-0.00005	0.00113	0.47961
2.40	0.00005	-0.00005	0.00012	-0.00006	0.00119	0.39899
2.50	0.00004	-0.00004	0.00011	-0.00007	0.00120	0.33735
2.60	0.00004	-0.00004	0.00011	-0.00007	0.00116	0.28992
2.70	0.00004	-0.00004	0.00010	-0.00008	0.00109	0.25307
2.80	0.00003	-0.00004	0.00009	-0.00008	0.00101	0.22408
2.90	0.00003	-0.00004	0.00008	-0.00008	0.00092	0.20102
3.00	0.00003	-0.00003	0.00008	-0.00007	0.00082	0.18243
3.10	0.00002	-0.00003	0.00007	-0.00007	0.00073	0.16729
3.20	0.00002	-0.00003	0.00006	-0.00007	0.00065	0.15481
3.30	0.00002	-0.00002	0.00005	-0.00006	0.00057	0.14442
3.40	0.00001	-0.00002	0.00005	-0.00006	0.00049	0.13569
3.50	0.00001	-0.00002	0.00004	-0.00005	0.00043	0.12829
3.60	0.00001	-0.00002	0.00004	-0.00005	0.00037	0.12196
3.70	0.00001	-0.00001	0.00003	-0.00004	0.00032	0.11651
3.80	0.00001	-0.00001	0.00003	-0.00004	0.00027	0.11179
3.90	0.00001	-0.00001	0.00003	-0.00003	0.00023	0.10766

*Parameters taken from Table J.2.

Table J.6. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	0.00001	-0.00001	0.00002	-0.00003	0.00020	0.10403
4.10	0.00000	-0.00001	0.00002	-0.00003	0.00017	0.10083
4.20	0.00000	-0.00001	0.00002	-0.00002	0.00014	0.09799
4.40	0.00000	-0.00000	0.00001	-0.00002	0.00010	0.09319
4.60	0.00000	-0.00000	0.00001	-0.00001	0.00007	0.08931
4.80	0.00000	-0.00000	0.00001	-0.00001	0.00005	0.08613
5.00	0.00000	-0.00000	0.00000	-0.00001	0.00004	0.08350
5.20	0.00000	-0.00000	0.00000	-0.00001	0.00003	0.08129
5.40	0.00000	-0.00000	0.00000	-0.00000	0.00002	0.07942
5.60	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.07784
5.80	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.07648
6.00	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.07532
6.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.07432
6.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.07346
6.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.07272
6.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.07208
7.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.07153
7.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.07105
7.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.07065
7.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.07031
7.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.07003
8.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06979
8.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06960
8.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06945
8.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06934
8.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06926
9.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06921

Table J.7. Radial Characteristics of the Hartree-Fock Na⁺ 2s Orbital*.

r	R(r)	R'(r)	P(r)	P'(r)	FR-εR	FR/εR
0.	17.16932	-189.46310	0.	17.16932		
0.01	15.36041	-172.59594	0.15360	13.63445	16.43557	0.57685
0.02	13.71217	-157.29992	0.27424	10.56617	-1.16188	1.03351
0.03	12.20972	-143.41132	0.36629	7.90738	-2.65433	1.08597
0.04	10.83973	-130.78575	0.43359	5.60830	-1.84536	1.06733
0.05	9.59022	-119.29560	0.47951	3.62544	-0.89068	1.03673
0.06	8.45041	-108.82788	0.50702	1.92074	-0.20116	1.00941
0.07	7.41059	-99.28237	0.51874	0.46083	0.20345	0.98914
0.08	6.46199	-90.56999	0.51696	-0.78361	0.39072	0.97609
0.09	5.59668	-82.61141	0.50370	-1.83835	0.43439	0.96930
0.10	4.80749	-75.33585	0.48075	-2.72610	0.39393	0.96759
0.12	3.43201	-62.58734	0.41184	-4.07847	0.21559	0.97516
0.14	2.29032	-51.89301	0.32064	-4.97471	0.04186	0.99277
0.16	1.34493	-42.90445	0.21519	-5.51978	-0.06944	1.02042
0.18	0.56467	-35.33835	0.10164	-5.79624	-0.11723	1.08210
0.20	-0.07653	-28.96291	-0.01531	-5.86911	-0.11922	0.38392
0.22	-0.60051	-23.58730	-0.13211	-5.78971	-0.09512	0.93736
0.24	-1.02563	-19.05361	-0.24615	-5.59850	-0.06050	0.97667
0.26	-1.36739	-15.23056	-0.35552	-5.32733	-0.02567	0.99258
0.28	-1.63886	-12.00849	-0.45888	-5.00123	0.00364	1.00088
0.30	-1.85112	-9.29550	-0.55533	-4.63977	0.02501	1.00534
0.35	-2.18088	-4.26242	-0.76331	-3.67273	0.04452	1.00807
0.40	-2.30746	-1.04553	-0.92298	-2.72567	0.03254	1.00558
0.45	-2.30550	0.96070	-1.03748	-1.87319	0.01098	1.00188
0.50	-2.22476	2.16066	-1.11238	-1.14442	-0.00708	0.99874
0.55	-2.09829	2.82618	-1.15406	-0.54390	-0.01702	0.99679
0.60	-1.94796	3.14065	-1.16877	-0.06356	-0.01920	0.99610
0.65	-1.78799	3.22805	-1.16219	0.31024	-0.01601	0.99646
0.70	-1.62752	3.17213	-1.13927	0.59296	-0.01013	0.99754
0.75	-1.47222	3.02930	-1.10416	0.79976	-0.00369	0.99901
0.80	-1.32541	2.83737	-1.06032	0.94449	0.00191	1.00057
0.85	-1.18888	2.62142	-1.01054	1.03933	0.00600	1.00199
0.90	-1.06339	2.39783	-0.95705	1.09466	0.00838	1.00312
0.95	-0.94904	2.17705	-0.90159	1.11915	0.00921	1.00384
1.00	-0.84553	1.96550	-0.84553	1.11997	0.00882	1.00412
1.10	-0.66859	1.58305	-0.73545	1.07276	0.00581	1.00344
1.20	-0.52687	1.26167	-0.63224	0.98714	0.00192	1.00144
1.30	-0.41429	0.99907	-0.53858	0.88450	-0.00135	0.99871
1.40	-0.32534	0.78797	-0.45547	0.77782	-0.00346	0.99579
1.50	-0.25527	0.61989	-0.38290	0.67457	-0.00446	0.99309
1.60	-0.20019	0.48686	-0.32030	0.57879	-0.00466	0.99079
1.70	-0.15696	0.38196	-0.26683	0.49237	-0.00439	0.98893
1.80	-0.12305	0.29943	-0.22150	0.41592	-0.00375	0.98796
1.90	-0.09648	0.23460	-0.18332	0.34926	-0.00046	0.99810
2.00	-0.07567	0.18374	-0.15134	0.29181	0.00133	1.00696
2.10	-0.05937	0.14387	-0.12468	0.24276	0.00217	1.01444
2.20	-0.04661	0.11264	-0.10254	0.20121	0.00241	1.02041
2.30	-0.03661	0.08820	-0.08421	0.16623	0.00229	1.02478
2.40	-0.02879	0.06907	-0.06910	0.13697	0.00200	1.02745
2.50	-0.02266	0.05411	-0.05666	0.11260	0.00163	1.02836
2.60	-0.01786	0.04241	-0.04644	0.09240	0.00124	1.02748
2.70	-0.01410	0.03326	-0.03806	0.07571	0.00088	1.02481
2.80	-0.01114	0.02611	-0.03120	0.06197	0.00057	1.02039
2.90	-0.00882	0.02052	-0.02558	0.05069	0.00032	1.01430
3.00	-0.00700	0.01615	-0.02099	0.04144	0.00012	1.00665
3.10	-0.00556	0.01272	-0.01724	0.03388	-0.00003	0.99755
3.20	-0.00443	0.01004	-0.01417	0.02770	-0.00014	0.98715
3.30	-0.00353	0.00794	-0.01166	0.02266	-0.00022	0.97563
3.40	-0.00283	0.00629	-0.00961	0.01855	-0.00026	0.96315
3.50	-0.00227	0.00499	-0.00793	0.01519	-0.00029	0.94991
3.60	-0.00182	0.00397	-0.00655	0.01246	-0.00029	0.93609
3.70	-0.00146	0.00316	-0.00542	0.01023	-0.00029	0.92187
3.80	-0.00118	0.00253	-0.00449	0.00841	-0.00028	0.90744
3.90	-0.00096	0.00202	-0.00372	0.00693	-0.00026	0.89294

*Parameters taken from Table J.2.

Table J.7. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	-0.00077	0.00162	-0.00309	0.00571	-0.00024	0.87855
4.10	-0.00063	0.00130	-0.00257	0.00472	-0.00022	0.86440
4.20	-0.00051	0.00105	-0.00215	0.00390	-0.00019	0.85060
4.40	-0.00034	0.00069	-0.00149	0.00268	-0.00015	0.82446
4.60	-0.00023	0.00045	-0.00105	0.00186	-0.00011	0.80075
4.80	-0.00015	0.00030	-0.00073	0.00129	-0.00009	0.77980
5.00	-0.00010	0.00020	-0.00052	0.00090	-0.00006	0.76172
5.20	-0.00007	0.00014	-0.00037	0.00063	-0.00005	0.74648
5.40	-0.00005	0.00009	-0.00026	0.00045	-0.00003	0.73388
5.60	-0.00003	0.00006	-0.00018	0.00032	-0.00002	0.72370
5.80	-0.00002	0.00004	-0.00013	0.00022	-0.00002	0.71566
6.00	-0.00002	0.00003	-0.00009	0.00016	-0.00001	0.70947
6.20	-0.00001	0.00002	-0.00007	0.00011	-0.00001	0.70486
6.40	-0.00001	0.00001	-0.00005	0.00008	-0.00001	0.70158
6.60	-0.00000	0.00001	-0.00003	0.00006	-0.00000	0.69940
6.80	-0.00000	0.00001	-0.00002	0.00004	-0.00000	0.69813
7.00	-0.00000	0.00000	-0.00002	0.00003	-0.00000	0.69760
7.20	-0.00000	0.00000	-0.00001	0.00002	-0.00000	0.69767
7.40	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.69821
7.60	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.69913
7.80	-0.00000	0.00000	-0.00000	0.00001	-0.00000	0.70034
8.00	-0.00000	0.00000	-0.00000	0.00001	-0.00000	0.70179
8.20	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.70341
8.40	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.70516
8.60	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.70701
8.80	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.70893
9.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.71089

Table J.8. Radial Characteristics of the Hartree-Fock Na^+ 2p Orbital*.

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	-0.	38.64499	-0.	0.		
0.01	0.36615	34.64917	0.00366	0.71264	-5.44181	12.86088
0.02	0.69422	31.02445	0.01388	1.31471	-4.81177	6.53140
0.03	0.98775	27.73493	0.02963	1.81980	-4.02314	4.25046
0.04	1.24993	24.74839	0.05000	2.23986	-3.20873	3.04868
0.05	1.48363	22.03594	0.07418	2.58543	-2.44630	2.31587
0.06	1.69147	19.57160	0.10149	2.86577	-1.77589	1.83787
0.07	1.87581	17.33205	0.13131	3.08906	-1.21283	1.51599
0.08	2.03879	15.29627	0.16310	3.26249	-0.75794	1.29668
0.09	2.18235	13.44537	0.19641	3.39244	-0.40360	1.14759
0.10	2.30826	11.76234	0.23083	3.48449	-0.13794	1.04769
0.12	2.51336	8.83997	0.30160	3.57416	0.18111	0.94249
0.14	2.66523	6.42346	0.37313	3.56451	0.30149	0.90973
0.16	2.77309	4.42649	0.44369	3.48133	0.30570	0.91202
0.18	2.84461	2.77835	0.51203	3.34471	0.25187	0.92934
0.20	2.88616	1.42091	0.57723	3.17034	0.17713	0.95102
0.22	2.90306	0.30620	0.63867	2.97043	0.10291	0.97171
0.24	2.89976	-0.60546	0.69594	2.75445	0.03995	0.98900
0.26	2.87998	-1.34703	0.74879	2.52975	-0.00773	1.00214
0.28	2.84683	-1.94595	0.79711	2.30196	-0.04004	1.01123
0.30	2.80294	-2.42516	0.84088	2.07539	-0.05889	1.01677
0.35	2.65975	-3.21809	0.93091	1.53342	-0.06503	1.01951
0.40	2.48792	-3.60068	0.99517	1.04765	-0.04322	1.01386
0.45	2.30402	-3.72093	1.03681	0.62961	-0.01781	1.00617
0.50	2.11856	-3.67651	1.05928	0.28030	0.00115	0.99957
0.55	1.93803	-3.53224	1.06591	-0.00470	0.01184	0.99513
0.60	1.76627	-3.33102	1.05976	-0.23233	0.01584	0.99284
0.65	1.60540	-3.10111	1.04351	-0.41033	0.01550	0.99229
0.70	1.45633	-2.86089	1.01943	-0.54629	0.01286	0.99295
0.75	1.31928	-2.62204	0.98946	-0.64725	0.00930	0.99437
0.80	1.19398	-2.39172	0.95519	-0.71939	0.00568	0.99620
0.85	1.07990	-2.17409	0.91791	-0.76807	0.00245	0.99819
0.90	0.97633	-1.97129	0.87869	-0.79783	-0.00022	1.00018
0.95	0.88251	-1.78416	0.83838	-0.81244	-0.00226	1.00204
1.00	0.79765	-1.61270	0.79765	-0.81505	-0.00372	1.00372
1.10	0.65177	-1.31447	0.71695	-0.79415	-0.00510	1.00625
1.20	0.53297	-1.06972	0.63957	-0.75069	-0.00493	1.00738
1.30	0.43632	-0.87026	0.56721	-0.69502	-0.00373	1.00682
1.40	0.35767	-0.70830	0.50074	-0.63395	-0.00195	1.00435
1.50	0.29364	-0.57701	0.44045	-0.57188	0.00004	0.99988
1.60	0.24144	-0.47062	0.38631	-0.51155	0.00198	0.99345
1.70	0.19884	-0.38439	0.33803	-0.45462	0.00369	0.98519
1.80	0.16402	-0.31445	0.29524	-0.40198	0.00483	0.97649
1.90	0.13551	-0.25765	0.25748	-0.35403	0.00193	0.98865
2.00	0.11214	-0.21148	0.22427	-0.31082	0.00036	0.99746
2.10	0.09293	-0.17388	0.19516	-0.27221	-0.00042	1.00357
2.20	0.07713	-0.14321	0.16969	-0.23793	-0.00073	1.00753
2.30	0.06411	-0.11815	0.14744	-0.20764	-0.00079	1.00983
2.40	0.05335	-0.09764	0.12804	-0.18099	-0.00073	1.01088
2.50	0.04445	-0.08082	0.11113	-0.15761	-0.00061	1.01101
2.60	0.03708	-0.06701	0.09642	-0.13714	-0.00049	1.01052
2.70	0.03097	-0.05564	0.08362	-0.11925	-0.00037	1.00963
2.80	0.02589	-0.04626	0.07249	-0.10364	-0.00028	1.00851
2.90	0.02166	-0.03851	0.06283	-0.09003	-0.00020	1.00732
3.00	0.01814	-0.03211	0.05443	-0.07818	-0.00014	1.00616
3.10	0.01521	-0.02680	0.04714	-0.06786	-0.00010	1.00511
3.20	0.01275	-0.02239	0.04081	-0.05888	-0.00007	1.00421
3.30	0.01070	-0.01872	0.03533	-0.05108	-0.00005	1.00352
3.40	0.00899	-0.01567	0.03056	-0.04429	-0.00003	1.00304
3.50	0.00755	-0.01313	0.02644	-0.03840	-0.00003	1.00280
3.60	0.00635	-0.01101	0.02286	-0.03328	-0.00002	1.00278
3.70	0.00534	-0.00924	0.01976	-0.02883	-0.00002	1.00298
3.80	0.00449	-0.00775	0.01707	-0.02497	-0.00002	1.00339
3.90	0.00378	-0.00651	0.01475	-0.02162	-0.00002	1.00400

*Parameters taken from Table J2.

Table J.8. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	0.00318	-0.00547	0.01273	-0.01871	-0.00002	1.00479
4.10	0.00268	-0.00460	0.01099	-0.01619	-0.00002	1.00574
4.20	0.00226	-0.00387	0.00949	-0.01400	-0.00002	1.00683
4.40	0.00160	-0.00274	0.00706	-0.01046	-0.00002	1.00938
4.60	0.00114	-0.00194	0.00524	-0.00781	-0.00002	1.01232
4.80	0.00081	-0.00138	0.00389	-0.00582	-0.00002	1.01551
5.00	0.00058	-0.00098	0.00288	-0.00433	-0.00001	1.01889
5.20	0.00041	-0.00070	0.00213	-0.00322	-0.00001	1.02236
5.40	0.00029	-0.00050	0.00158	-0.00239	-0.00001	1.02589
5.60	0.00021	-0.00035	0.00116	-0.00177	-0.00001	1.02944
5.80	0.00015	-0.00025	0.00086	-0.00131	-0.00001	1.03298
6.00	0.00011	-0.00018	0.00063	-0.00097	-0.00000	1.03649
6.20	0.00008	-0.00013	0.00047	-0.00071	-0.00000	1.03997
6.40	0.00005	-0.00009	0.00034	-0.00053	-0.00000	1.04341
6.60	0.00004	-0.00006	0.00025	-0.00039	-0.00000	1.04680
6.80	0.00003	-0.00005	0.00018	-0.00029	-0.00000	1.05016
7.00	0.00002	-0.00003	0.00014	-0.00021	-0.00000	1.05349
7.20	0.00001	-0.00002	0.00010	-0.00015	-0.00000	1.05677
7.40	0.00001	-0.00002	0.00007	-0.00011	-0.00000	1.06003
7.60	0.00001	-0.00001	0.00005	-0.00008	-0.00000	1.06325
7.80	0.00000	-0.00001	0.00004	-0.00006	-0.00000	1.06644
8.00	0.00000	-0.00001	0.00003	-0.00004	-0.00000	1.06960
8.20	0.00000	-0.00000	0.00002	-0.00003	-0.00000	1.07273
8.40	0.00000	-0.00000	0.00002	-0.00002	-0.00000	1.07583
8.60	0.00000	-0.00000	0.00001	-0.00002	-0.00000	1.07891
8.80	0.00000	-0.00000	0.00001	-0.00001	-0.00000	1.08195
9.00	0.00000	-0.00000	0.00001	-0.00001	-0.00000	1.08495

APPENDIX K

COULOMB POTENTIAL AND CHARGE DENSITY TABLES

In this appendix we have tabulated the Coulomb potential and charge densities for the solutions given in Appendices F and H.

The function $Z(r)$, which has at times been called the "effective nuclear charge," is defined as

$$V(r) = Z(r)/r \quad ,$$

where $V(r)$ is the electrostatic potential at a distance r from the origin.

The charge densities are defined as follows:

- (a) for closed-shell systems or open-shell systems involving s orbitals only:

$$\rho(r) = \sum_i \phi_i^2(r) \quad ; \quad D(r) = 4\pi r^2 \rho(r) \quad ;$$

- (b) for the open-shell system $2p^5$:

$$\rho_t(r, \theta) = \rho(r) + \rho'(r) \cos^2 \theta$$

$$D_t(r, \theta) = 4\pi r^2 \rho_t(r, \theta) \quad ,$$

where

$$\rho(r) = \sum_i \phi_i^2(r)$$

$$\rho'(r) = \phi_{210}^2(r) \cos^{-2} \theta \quad .$$

Table K.1. Coulomb Potential and Charge Densities for He.

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	2.00000	3.59642	0.	1.40	0.35436	0.02765	0.68111
0.01	1.99999	3.45542	0.00434	1.45	0.32172	0.02366	0.62511
0.02	1.99989	3.32024	0.01669	1.50	0.29178	0.02026	0.57273
0.03	1.99963	3.19064	0.03609	1.55	0.26438	0.01735	0.52391
0.04	1.99914	3.06636	0.06165	1.60	0.23934	0.01488	0.47854
0.05	1.99838	2.94720	0.09259	1.65	0.21647	0.01276	0.43649
0.06	1.99728	2.83292	0.12816	1.70	0.19563	0.01095	0.39762
0.07	1.99580	2.72332	0.16769	1.75	0.17666	0.00940	0.36178
0.08	1.99391	2.61819	0.21057	1.80	0.15941	0.00808	0.32878
0.09	1.99158	2.51736	0.25624	1.85	0.14374	0.00694	0.29848
0.10	1.98878	2.42063	0.30419	1.90	0.12952	0.00597	0.27069
0.12	1.98170	2.23880	0.40512	1.95	0.11663	0.00513	0.24525
0.14	1.97255	2.07140	0.51019	2.00	0.10496	0.00442	0.22199
0.16	1.96128	1.91722	0.61677	2.10	0.08485	0.00327	0.18143
0.18	1.94788	1.77518	0.72276	2.20	0.06844	0.00243	0.14781
0.20	1.93238	1.64427	0.82650	2.30	0.05509	0.00181	0.12007
0.22	1.91484	1.52357	0.92665	2.40	0.04426	0.00134	0.09728
0.24	1.89535	1.41225	1.02222	2.50	0.03550	0.00100	0.07863
0.26	1.87399	1.30954	1.11243	2.60	0.02842	0.00075	0.06341
0.28	1.85089	1.21473	1.19676	2.70	0.02272	0.00056	0.05103
0.30	1.82616	1.12720	1.27483	2.80	0.01814	0.00042	0.04099
0.35	1.75808	0.93641	1.44150	2.90	0.01446	0.00031	0.03287
0.40	1.68269	0.77959	1.56746	3.00	0.01151	0.00023	0.02631
0.45	1.60198	0.65038	1.65501	3.20	0.00727	0.00013	0.01678
0.50	1.51777	0.54366	1.70797	3.40	0.00457	0.00007	0.01065
0.55	1.43168	0.45533	1.73084	3.60	0.00286	0.00004	0.00672
0.60	1.34511	0.38203	1.72828	3.80	0.00179	0.00002	0.00423
0.65	1.25920	0.32110	1.70479	4.00	0.00111	0.00001	0.00265
0.70	1.17491	0.27032	1.66450	4.20	0.00069	0.00001	0.00165
0.75	1.09297	0.22793	1.61113	4.40	0.00043	0.00000	0.00103
0.80	1.01396	0.19247	1.54791	4.60	0.00026	0.00000	0.00064
0.85	0.93830	0.16275	1.47763	4.80	0.00016	0.00000	0.00039
0.90	0.86628	0.13780	1.40264	5.00	0.00010	0.00000	0.00024
0.95	0.79808	0.11682	1.32489	5.50	0.00003	0.00000	0.00007
1.00	0.73381	0.09915	1.24598	6.00	0.00001	0.00000	0.00002
1.05	0.67348	0.08425	1.16721	6.50	0.00000	0.00000	0.00001
1.10	0.61707	0.07166	1.08960	7.00	0.00000	0.00000	0.00000
1.15	0.56449	0.06101	1.01396	7.50	0.00000	0.00000	0.00000
1.20	0.51563	0.05199	0.94087	8.00	0.00000	0.00000	0.00000
1.25	0.47035	0.04435	0.87079	8.50	0.	0.00000	0.00000
1.30	0.42849	0.03786	0.80402	9.00	0.	0.00000	0.00000
1.35	0.38989	0.03234	0.74076	9.50	0.	0.00000	0.00000

Table K.2. Coulomb Potential and Charge Densities for Li^+ .

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	3.00000	13.67403	0.	1.25	1.09278	0.01704	0.33465
0.01	2.99995	12.87796	0.01618	1.30	1.07740	0.01328	0.28193
0.02	2.99958	12.13000	0.06097	1.35	1.06446	0.01035	0.23695
0.03	2.99865	11.42715	0.12924	1.40	1.05359	0.00807	0.19869
0.04	2.99693	10.76662	0.21648	1.45	1.04449	0.00629	0.16627
0.05	2.99427	10.14577	0.31874	1.50	1.03688	0.00491	0.13887
0.06	2.99052	9.56214	0.43258	1.55	1.03053	0.00383	0.11577
0.07	2.98559	9.01344	0.55500	1.60	1.02525	0.00300	0.09635
0.08	2.97940	8.49749	0.68341	1.65	1.02085	0.00234	0.08006
0.09	2.97191	8.01227	0.81555	1.70	1.01720	0.00183	0.06642
0.10	2.96308	7.55590	0.94950	1.75	1.01417	0.00143	0.05503
0.12	2.94141	6.72266	1.21650	1.80	1.01166	0.00112	0.04553
0.14	2.91449	5.98486	1.47408	1.85	1.00959	0.00087	0.03762
0.16	2.88256	5.33117	1.71503	1.90	1.00788	0.00068	0.03105
0.18	2.84603	4.75164	1.93463	1.95	1.00646	0.00054	0.02560
0.20	2.80534	4.23753	2.13002	2.00	1.00530	0.00042	0.02108
0.22	2.76100	3.78118	2.29976	2.10	1.00356	0.00026	0.01425
0.24	2.71352	3.37582	2.44350	2.20	1.00238	0.00016	0.00960
0.26	2.66343	3.01555	2.56167	2.30	1.00159	0.00010	0.00645
0.28	2.61122	2.69515	2.65527	2.40	1.00106	0.00006	0.00431
0.30	2.55737	2.41002	2.72567	2.50	1.00070	0.00004	0.00288
0.32	2.50234	2.15613	2.77450	2.60	1.00046	0.00002	0.00192
0.34	2.44652	1.92992	2.80354	2.70	1.00031	0.00001	0.00127
0.36	2.39031	1.72825	2.81464	2.80	1.00020	0.00001	0.00084
0.38	2.33405	1.54837	2.80964	2.90	1.00013	0.00001	0.00056
0.40	2.27802	1.38781	2.79037	3.00	1.00009	0.00000	0.00037
0.42	2.22252	1.24444	2.75856	3.10	1.00006	0.00000	0.00024
0.44	2.16775	1.11634	2.71588	3.20	1.00004	0.00000	0.00016
0.46	2.11394	1.00182	2.66388	3.30	1.00002	0.00000	0.00010
0.48	2.06125	0.89939	2.60400	3.40	1.00002	0.00000	0.00007
0.50	2.00983	0.80774	2.53758	3.50	1.00001	0.00000	0.00004
0.52	1.95978	0.72568	2.46583	3.60	1.00001	0.00000	0.00003
0.54	1.91122	0.65219	2.38984	3.70	1.00000	0.00000	0.00002
0.56	1.86421	0.58633	2.31060	3.80	1.00000	0.00000	0.00001
0.58	1.81881	0.52729	2.22901	3.90	1.00000	0.00000	0.00001
0.60	1.77506	0.47434	2.14585	4.00	1.00000	0.00000	0.00001
0.65	1.67303	0.36453	1.93541	4.20	1.00000	0.00000	0.00000
0.70	1.58147	0.28062	1.72791	4.40	1.00000	0.00000	0.00000
0.75	1.50009	0.21635	1.52930	4.60	1.00000	0.00000	0.00000
0.80	1.42833	0.16703	1.34337	4.80	1.00000	0.00000	0.00000
0.85	1.36550	0.12912	1.17233	5.00	1.00000	0.00000	0.00000
0.90	1.31083	0.09993	1.01718	5.20	1.00000	0.00000	0.00000
0.95	1.26352	0.07742	0.87805	5.40	1.00000	0.00000	0.00000
1.00	1.22277	0.06004	0.75449	5.60	1.00000	0.00000	0.00000
1.05	1.18782	0.04660	0.64565	5.80	1.00000	0.00000	0.00000
1.10	1.15797	0.03620	0.55046	6.00	1.00000	0.00000	0.00000
1.15	1.13257	0.02814	0.46772	6.20	1.00000	0.00000	0.00000
1.20	1.11101	0.02189	0.39619	6.40	1.00000	0.00000	0.00000

Table K.3. Coulomb Potential and Charge Densities for Li.

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	3.00000	13.82036	0.	2.70	0.74926	0.00287	0.26277
0.01	2.99994	13.01484	0.01635	2.80	0.72272	0.00272	0.26780
0.02	2.99958	12.25817	0.06162	2.90	0.69575	0.00257	0.27129
0.03	2.99863	11.54729	0.13060	3.00	0.66851	0.00242	0.27329
0.04	2.99690	10.87933	0.21874	3.10	0.64114	0.00227	0.27387
0.05	2.99421	10.25158	0.32206	3.20	0.61378	0.00212	0.27311
0.06	2.99042	9.66155	0.43708	3.30	0.58656	0.00198	0.27111
0.07	2.98544	9.10687	0.56076	3.40	0.55960	0.00184	0.26799
0.08	2.97919	8.58534	0.69047	3.50	0.53300	0.00171	0.26385
0.09	2.97162	8.09491	0.82396	3.60	0.50686	0.00159	0.25882
0.10	2.96270	7.63365	0.95927	3.70	0.48126	0.00147	0.25301
0.12	2.94081	6.79153	1.22897	3.80	0.45628	0.00136	0.24652
0.14	2.91361	6.04588	1.48910	3.90	0.43198	0.00125	0.23948
0.16	2.88136	5.38522	1.73242	4.00	0.40840	0.00115	0.23197
0.18	2.84445	4.79949	1.95411	4.20	0.36359	0.00097	0.21593
0.20	2.80336	4.27986	2.15129	4.40	0.32208	0.00082	0.19907
0.22	2.75858	3.81857	2.32250	4.60	0.28398	0.00068	0.18195
0.24	2.71063	3.40882	2.46738	4.80	0.24929	0.00057	0.16502
0.26	2.66005	3.04461	2.58636	5.00	0.21794	0.00047	0.14860
0.28	2.60734	2.72070	2.68044	5.20	0.18980	0.00039	0.13297
0.30	2.55299	2.43243	2.75102	5.40	0.16469	0.00032	0.11828
0.32	2.49745	2.17575	2.79975	5.60	0.14242	0.00027	0.10464
0.34	2.44114	1.94706	2.82844	5.80	0.12276	0.00022	0.09212
0.36	2.38443	1.74318	2.83895	6.00	0.10549	0.00018	0.08072
0.38	2.32769	1.56133	2.83316	6.20	0.09040	0.00015	0.07043
0.40	2.27120	1.39903	2.81292	6.40	0.07725	0.00012	0.06121
0.45	2.13284	1.06516	2.71051	6.60	0.06584	0.00010	0.05300
0.50	2.00106	0.81286	2.55366	6.80	0.05599	0.00008	0.04573
0.55	1.87804	0.62163	2.36303	7.00	0.04749	0.00006	0.03933
0.60	1.76504	0.47633	2.15487	7.20	0.04020	0.00005	0.03372
0.65	1.66264	0.36566	1.94141	7.40	0.03396	0.00004	0.02883
0.70	1.57084	0.28120	1.73149	7.60	0.02863	0.00003	0.02458
0.75	1.48932	0.21662	1.53119	7.80	0.02409	0.00003	0.02091
0.80	1.41750	0.16717	1.34443	8.00	0.02023	0.00002	0.01774
0.85	1.35462	0.12925	1.17346	8.20	0.01696	0.00002	0.01502
0.90	1.29987	0.10014	1.01933	8.40	0.01420	0.00001	0.01268
0.95	1.25240	0.07779	0.88218	8.60	0.01186	0.00001	0.01069
1.00	1.21138	0.06060	0.76156	8.80	0.00990	0.00001	0.00899
1.05	1.17599	0.04739	0.65658	9.00	0.00825	0.00001	0.00755
1.10	1.14548	0.03723	0.56615	9.50	0.00520	0.00000	0.00484
1.15	1.11915	0.02942	0.48900	10.00	0.00325	0.00000	0.00308
1.20	1.09638	0.02342	0.42383	10.50	0.00202	0.00000	0.00194
1.25	1.07659	0.01881	0.36935	11.00	0.00124	0.00000	0.00121
1.30	1.05928	0.01527	0.32432	11.50	0.00076	0.00000	0.00075
1.35	1.04402	0.01256	0.28758	12.00	0.00047	0.00000	0.00046
1.40	1.03041	0.01048	0.25805	12.50	0.00028	0.00000	0.00028
1.45	1.01811	0.00888	0.23473	13.00	0.00017	0.00000	0.00017
1.50	1.00684	0.00767	0.21676	13.50	0.00010	0.00000	0.00010
1.55	0.99636	0.00673	0.20333	14.00	0.00006	0.00000	0.00006
1.60	0.98645	0.00602	0.19375	14.50	0.00004	0.00000	0.00004
1.65	0.97693	0.00548	0.18740	15.00	0.00002	0.00000	0.00002
1.70	0.96766	0.00506	0.18374	15.50	0.00001	0.00000	0.00001
1.75	0.95852	0.00474	0.18229	16.00	0.00001	0.00000	0.00001
1.80	0.94940	0.00449	0.18266	16.50	0.00000	0.00000	0.00000
1.85	0.94023	0.00429	0.18449	17.00	0.00000	0.00000	0.00000
1.90	0.93093	0.00413	0.18748	17.50	0.00000	0.00000	0.00000
1.95	0.92147	0.00400	0.19135	18.00	0.00000	0.00000	0.00000
2.00	0.91179	0.00390	0.19591	18.50	0.00000	0.00000	0.00000
2.10	0.89169	0.00372	0.20629	19.00	0.00000	0.00000	0.00000
2.20	0.87050	0.00358	0.21744	19.50	0.00000	0.00000	0.00000
2.30	0.84820	0.00344	0.22851	20.00	0.00000	0.00000	0.00000
2.40	0.82482	0.00330	0.23890	20.50	0.00000	0.00000	0.00000
2.50	0.80046	0.00316	0.24822	21.00	0.00000	0.00000	0.00000
2.60	0.77522	0.00302	0.25623	21.50	0.	0.00000	0.00000

Table K.4. Coulomb Potential and Charge Densities for Li^- .

r	Z(r)	$\rho(r)$	D(r)
0.	3.00000	13.81275	0.
0.01	3.94501	13.00883	0.01635
0.02	3.94464	12.25340	0.06159
0.03	3.94370	11.54347	0.13055
0.04	3.94196	10.87621	0.21868
0.05	3.93927	10.24899	0.32198
0.06	3.93549	9.65933	0.43698
0.07	3.93050	9.10490	0.56064
0.08	3.92425	8.58354	0.69033
0.09	3.91668	8.09319	0.82379
0.10	3.90777	7.63196	0.95906
0.12	3.88589	6.78976	1.22865
0.14	3.85869	6.04393	1.48862
0.16	3.82645	5.38303	1.73172
0.18	3.78957	4.79704	1.95312
0.20	3.74849	4.27714	2.14992
0.22	3.70374	3.81558	2.32068
0.24	3.65584	3.40557	2.46503
0.26	3.60532	3.04113	2.58340
0.28	3.55267	2.71699	2.67679
0.30	3.49840	2.42854	2.74661
0.32	3.44295	2.17170	2.79453
0.34	3.38675	1.94287	2.82236
0.36	3.33018	1.73890	2.83198
0.38	3.27358	1.55700	2.82530
0.40	3.21727	1.39469	2.80418
0.40	3.21727	1.39469	2.80418
0.45	3.07939	1.06098	2.69986
0.50	2.94817	0.80911	2.54189
0.55	2.82574	0.61861	2.35152
0.60	2.71328	0.47427	2.14556
0.65	2.61123	0.36479	1.93678
0.70	2.51949	0.28168	1.73443
0.75	2.43757	0.21856	1.54491
0.80	2.36472	0.17063	1.37229
0.85	2.30002	0.13424	1.21883
0.90	2.24250	0.10664	1.08543
0.95	2.19114	0.08570	0.97197
1.00	2.14498	0.06984	0.87760
1.05	2.10309	0.05781	0.80098
1.10	2.06462	0.04870	0.74046
1.15	2.02880	0.04177	0.69424
1.20	1.99499	0.03650	0.66044
1.25	1.96259	0.03245	0.63721
1.30	1.93112	0.02933	0.62279
1.35	1.90019	0.02688	0.61551
1.40	1.86947	0.02492	0.61388
1.45	1.83873	0.02334	0.61656
1.50	1.80777	0.02201	0.62234
1.55	1.77646	0.02087	0.63022
1.60	1.74472	0.01987	0.63933
1.65	1.71252	0.01897	0.64896
1.70	1.67983	0.01813	0.65851
1.75	1.64667	0.01735	0.66754
1.80	1.61309	0.01660	0.67568
1.85	1.57913	0.01587	0.68269
1.90	1.54484	0.01517	0.68839
1.95	1.51031	0.01450	0.69267
2.00	1.47560	0.01384	0.69548
2.10	1.40594	0.01257	0.69673
2.20	1.33644	0.01139	0.69252
2.30	1.26760	0.01028	0.68356
2.40	1.19985	0.00927	0.67073
2.50	1.13355	0.00834	0.65494

Table K.4. (continued).

r	Z(r)	$\rho(r)$	D(r)
2.60	1.06894	0.00750	0.63704
2.70	1.00619	0.00674	0.61780
2.80	0.94540	0.00607	0.59784
2.90	0.88662	0.00547	0.57769
3.00	0.82986	0.00493	0.55773
3.10	0.77506	0.00446	0.53825
3.20	0.72218	0.00404	0.51946
3.30	0.67114	0.00366	0.50148
3.40	0.62186	0.00333	0.48438
3.50	0.57424	0.00304	0.46819
3.60	0.52819	0.00278	0.45289
3.70	0.48363	0.00255	0.43846
3.80	0.44047	0.00234	0.42485
3.90	0.39863	0.00216	0.41200
4.00	0.35805	0.00199	0.39985
4.20	0.28036	0.00170	0.37740
4.40	0.20695	0.00147	0.35703
4.60	0.13744	0.00127	0.33830
4.80	0.07154	0.00111	0.32089
5.00	0.00902	0.00097	0.30451
5.20	-0.05032	0.00085	0.28898
5.40	-0.10662	0.00075	0.27415
5.60	-0.16002	0.00066	0.25994
5.80	-0.21063	0.00058	0.24629
6.00	-0.25857	0.00052	0.23315
6.20	-0.30393	0.00046	0.22051
6.40	-0.34681	0.00040	0.20836
6.60	-0.38730	0.00036	0.19669
6.80	-0.42551	0.00032	0.18551
7.00	-0.46154	0.00028	0.17481
7.20	-0.49547	0.00025	0.16460
7.40	-0.52741	0.00023	0.15486
7.60	-0.55745	0.00020	0.14559
7.80	-0.58568	0.00018	0.13679
8.00	-0.61219	0.00016	0.12844
8.20	-0.63708	0.00014	0.12054
8.40	-0.66044	0.00013	0.11306
8.60	-0.68234	0.00011	0.10601
8.80	-0.70287	0.00010	0.09935
9.00	-0.72210	0.00009	0.09307
9.50	-0.76502	0.00007	0.07897
10.00	-0.80141	0.00005	0.06690
10.50	-0.83222	0.00004	0.05661
11.00	-0.85828	0.00003	0.04787
11.50	-0.88031	0.00002	0.04047
12.00	-0.89893	0.00002	0.03420
12.50	-0.91467	0.00001	0.02890
13.00	-0.92797	0.00001	0.02442
13.50	-0.93920	0.00001	0.02063
14.00	-0.94870	0.00001	0.01743
14.50	-0.95672	0.00001	0.01473
15.00	-0.96350	0.00000	0.01245
15.50	-0.96922	0.00000	0.01052
16.00	-0.97406	0.00000	0.00889
16.50	-0.97815	0.00000	0.00751
17.00	-0.98161	0.00000	0.00634
17.50	-0.98452	0.00000	0.00535
18.00	-0.98699	0.00000	0.00452
18.50	-0.98907	0.00000	0.00381
19.00	-0.99082	0.00000	0.00322
19.50	-0.99230	0.00000	0.00271
20.00	-0.99354	0.00000	0.00228
20.50	-0.99459	0.00000	0.00192
21.00	-0.99547	0.00000	0.00162

Table K.4. (continued).

r	$Z(r)$	$\rho(r)$	$D(r)$
21.50	-0.99621	0.00000	0.00136
22.00	-0.99684	0.00000	0.00114
22.50	-0.99736	0.00000	0.00096
23.00	-0.99780	0.00000	0.00080
23.50	-0.99817	0.00000	0.00067
24.00	-0.99847	0.00000	0.00056
24.50	-0.99873	0.00000	0.00047
25.00	-0.99895	0.00000	0.00039
25.50	-0.99913	0.00000	0.00033
26.00	-0.99928	0.00000	0.00027
26.50	-0.99940	0.00000	0.00023
27.00	-0.99950	0.00000	0.00019
27.50	-0.99959	0.00000	0.00016
28.00	-0.99966	0.00000	0.00013
28.50	-0.99972	0.00000	0.00011
29.00	-0.99977	0.00000	0.00009
29.50	-0.99981	0.00000	0.00007
31.00	-0.99990	0.00000	0.00004
32.00	-0.99993	0.00000	0.00003
33.00	-0.99995	0.00000	0.00002
34.00	-0.99997	0.00000	0.00001
35.00	-0.99998	0.00000	0.00001
36.00	-0.99999	0.00000	0.00001
37.00	-0.99999	0.00000	0.00000
38.00	-0.99999	0.00000	0.00000
39.00	-1.00000	0.00000	0.00000
42.00	-1.00000	0.00000	0.00000
44.00	-1.00000	0.00000	0.00000
46.00	-1.00000	0.00000	0.00000
48.00	-1.00000	0.00000	0.00000

Table K.5. Coulomb Potential and Charge Densities for Be.

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	4.00000	37.30067	0.	2.00	1.35300	0.01576	0.79207
0.01	3.99607	34.21486	0.04300	2.20	1.19495	0.01288	0.78315
0.02	3.99511	31.40248	0.15785	2.40	1.04156	0.01032	0.74691
0.03	3.99273	28.83760	0.32615	2.60	0.89740	0.00815	0.69230
0.04	3.98846	26.49690	0.53275	2.80	0.76534	0.00637	0.62714
0.05	3.98199	24.35938	0.76527	3.00	0.64684	0.00493	0.55755
0.06	3.97311	22.40614	1.01363	3.20	0.54232	0.00379	0.48801
0.07	3.96169	20.62016	1.26969	3.40	0.45143	0.00290	0.42157
0.08	3.94771	18.98606	1.52695	3.60	0.37335	0.00221	0.36010
0.09	3.93117	17.49000	1.78026	3.80	0.30698	0.00168	0.30462
0.10	3.91213	16.11947	2.02563	4.00	0.25108	0.00127	0.25550
0.12	3.86697	13.71090	2.48107	4.20	0.20436	0.00096	0.21269
0.14	3.81328	11.68238	2.87738	4.40	0.16560	0.00072	0.17587
0.16	3.75232	9.97004	3.20735	4.60	0.13365	0.00054	0.14455
0.18	3.68544	8.52148	3.46952	4.80	0.10745	0.00041	0.11817
0.20	3.61398	7.29351	3.66612	5.00	0.08609	0.00031	0.09612
0.22	3.53920	6.25052	3.80164	5.20	0.06875	0.00023	0.07784
0.24	3.46228	5.36301	3.88187	5.40	0.05474	0.00017	0.06277
0.26	3.38426	4.60652	3.91317	5.60	0.04346	0.00013	0.05043
0.28	3.30604	3.96066	3.90206	5.80	0.03442	0.00010	0.04037
0.30	3.22841	3.40846	3.85488	6.00	0.02719	0.00007	0.03221
0.32	3.15204	2.93568	3.77762	6.20	0.02143	0.00005	0.02563
0.34	3.07747	2.53040	3.67585	6.40	0.01685	0.00004	0.02033
0.36	3.00514	2.18260	3.55458	6.60	0.01322	0.00003	0.01609
0.38	2.93539	1.88381	3.41833	6.80	0.01036	0.00002	0.01270
0.40	2.86848	1.62690	3.27107	7.00	0.00810	0.00002	0.01000
0.45	2.71469	1.13037	2.87643	7.20	0.00632	0.00001	0.00786
0.50	2.58093	0.78799	2.47554	7.40	0.00493	0.00001	0.00616
0.55	2.46678	0.55129	2.09564	7.60	0.00383	0.00001	0.00482
0.60	2.37075	0.38745	1.75276	7.80	0.00298	0.00000	0.00377
0.65	2.29075	0.27401	1.45482	8.00	0.00231	0.00000	0.00294
0.70	2.22447	0.19556	1.20416	8.50	0.00122	0.00000	0.00157
0.75	2.16957	0.14141	0.99954	9.00	0.00064	0.00000	0.00083
0.80	2.12381	0.10413	0.83749	9.50	0.00033	0.00000	0.00044
0.85	2.08519	0.07858	0.71341	10.00	0.00017	0.00000	0.00023
0.90	2.05192	0.06113	0.62222	10.50	0.00009	0.00000	0.00012
0.95	2.02250	0.04927	0.55882	11.00	0.00004	0.00000	0.00006
1.00	1.99566	0.04125	0.51839	11.50	0.00002	0.00000	0.00003
1.10	1.94576	0.03219	0.48940	12.00	0.00001	0.00000	0.00002
1.20	1.89626	0.02797	0.50620	13.00	0.00000	0.00000	0.00000
1.30	1.84370	0.02579	0.54762	14.00	0.00000	0.00000	0.00000
1.40	1.78641	0.02432	0.59909	15.00	0.00000	0.00000	0.00000
1.50	1.72387	0.02303	0.65116	16.00	0.	0.00000	0.00000
1.60	1.65635	0.02170	0.69804	17.00	0.	0.00000	0.00000
1.70	1.58454	0.02028	0.73653	18.00	0.	0.00000	0.00000
1.80	1.50938	0.01879	0.76513	19.00	0.	0.00000	0.00000
1.90	1.43186	0.01727	0.78352				

Table K.6. Coulomb Potential and Charge Densities for F.

r	Z(r)	$\rho(r)$	D(r)	$\rho'(r)$	D'(r)
0.	9.00000	448.12127	0.	0.	0.
0.01	8.99836	374.39283	0.47048	0.00897	0.00001
0.02	8.98850	312.95267	1.57307	0.03296	0.00017
0.03	8.96596	261.72810	2.96007	0.06821	0.00077
0.04	8.92913	219.00134	4.40328	0.11159	0.00224
0.05	8.87821	183.34780	5.76004	0.16055	0.00504
0.06	8.81453	153.58513	6.94803	0.21301	0.00964
0.07	8.74001	128.73133	7.92666	0.26729	0.01646
0.08	8.65685	107.97027	8.68348	0.32205	0.02590
0.09	8.56724	90.62317	9.22431	0.37621	0.03829
0.10	8.47329	76.12513	9.56617	0.42896	0.05390
0.12	8.27963	53.87310	9.74865	0.52780	0.09551
0.14	8.08794	38.31493	9.43700	0.61522	0.15153
0.16	7.90619	27.43348	8.82532	0.68969	0.22187
0.18	7.73885	19.82241	8.07070	0.75082	0.30570
0.20	7.58764	14.49949	7.28824	0.79899	0.40162
0.22	7.45237	10.77759	6.55506	0.83504	0.50788
0.24	7.33159	8.17544	5.91757	0.86006	0.62253
0.26	7.22318	6.35564	5.39903	0.87527	0.74353
0.28	7.12471	5.08157	5.00638	0.88188	0.86883
0.30	7.03370	4.18723	4.73564	0.88109	0.99649
0.35	6.82416	2.93234	4.51399	0.85394	1.31455
0.40	6.61837	2.36318	4.75146	0.80231	1.61313
0.45	6.39871	2.05264	5.22334	0.73729	1.87618
0.50	6.15725	1.83394	5.76149	0.66666	2.09436
0.55	5.89281	1.64644	6.25866	0.59553	2.26379
0.60	5.60826	1.47133	6.65616	0.52711	2.38461
0.65	5.30852	1.30511	6.92920	0.46328	2.45967
0.70	4.99923	1.14892	7.07452	0.40496	2.49353
0.75	4.68596	1.00464	7.10138	0.35249	2.49162
0.80	4.37370	0.87354	7.02541	0.30583	2.45964
0.85	4.06668	0.75609	6.86467	0.26469	2.40321
0.90	3.76834	0.65207	6.63728	0.22867	2.32756
0.95	3.48129	0.56080	6.36008	0.19728	2.23742
1.00	3.20744	0.48128	6.04793	0.17005	2.13692
1.10	2.70391	0.35299	5.36731	0.12616	1.91838
1.20	2.26228	0.25815	4.67140	0.09358	1.69344
1.30	1.88153	0.18869	4.00722	0.06950	1.47592
1.40	1.55747	0.13806	3.40032	0.05172	1.27379
1.50	1.28431	0.10121	2.86176	0.03858	1.09094
1.60	1.05573	0.07440	2.39347	0.02887	0.92865
1.70	0.86552	0.05485	1.99215	0.02166	0.78653
1.80	0.70792	0.04057	1.65178	0.01629	0.66332
1.90	0.57778	0.03010	1.36530	0.01229	0.55731
2.00	0.47063	0.02239	1.12552	0.00928	0.46664

Table K.6. (continued).

r	$Z(r)$	$\rho(r)$	$D(r)$	$\rho'(r)$	$D'(r)$
2.10	0.38260	0.01670	0.92569	0.00703	0.38945
2.20	0.31046	0.01249	0.75969	0.00533	0.32403
2.30	0.25143	0.00936	0.62216	0.00404	0.26878
2.40	0.20324	0.00703	0.50850	0.00307	0.22229
2.50	0.16397	0.00528	0.41475	0.00233	0.18329
2.60	0.13203	0.00397	0.33759	0.00177	0.15069
2.70	0.10610	0.00299	0.27420	0.00135	0.12352
2.80	0.08510	0.00226	0.22224	0.00102	0.10095
2.90	0.06811	0.00170	0.17974	0.00078	0.08227
3.00	0.05441	0.00128	0.14504	0.00059	0.06686
3.20	0.03451	0.00073	0.09383	0.00034	0.04378
3.40	0.02172	0.00041	0.06016	0.00020	0.02836
3.60	0.01357	0.00023	0.03824	0.00011	0.01818
3.80	0.00841	0.00013	0.02410	0.00006	0.01154
4.00	0.00518	0.00007	0.01507	0.00004	0.00726
4.20	0.00317	0.00004	0.00935	0.00002	0.00453
4.40	0.00193	0.00002	0.00576	0.00001	0.00280
4.60	0.00116	0.00001	0.00352	0.00001	0.00172
4.80	0.00070	0.00001	0.00214	0.00000	0.00105
5.00	0.00042	0.00000	0.00129	0.00000	0.00063
5.20	0.00025	0.00000	0.00078	0.00000	0.00038
5.40	0.00015	0.00000	0.00046	0.00000	0.00023
5.60	0.00009	0.00000	0.00028	0.00000	0.00014
5.80	0.00005	0.00000	0.00016	0.00000	0.00008
6.00	0.00003	0.00000	0.00010	0.00000	0.00005
6.20	0.00002	0.00000	0.00006	0.00000	0.00003
6.40	0.00001	0.00000	0.00003	0.00000	0.00002
6.60	0.00001	0.00000	0.00002	0.00000	0.00001
6.80	0.00000	0.00000	0.00001	0.00000	0.00001
7.00	0.00000	0.00000	0.00001	0.00000	0.00000
7.20	0.00000	0.00000	0.00000	0.00000	0.00000
7.40	0.00000	0.00000	0.00000	0.00000	0.00000
7.60	0.00000	0.00000	0.00000	0.00000	0.00000
7.80	0.00000	0.00000	0.00000	0.00000	0.00000
8.00	0.00000	0.00000	0.00000	0.00000	0.00000
8.20	0.00000	0.00000	0.00000	0.00000	0.00000
8.40	0.00000	0.00000	0.00000	0.00000	0.00000
8.60	0.00000	0.00000	0.00000	0.00000	0.00000
8.80	0.00000	0.00000	0.00000	0.00000	0.00000
9.00	0.00000	0.00000	0.00000	0.00000	0.00000
9.20	0.00000	0.00000	0.00000	0.00000	0.00000
9.40	0.00000	0.00000	0.00000	0.00000	0.00000
9.60	0.00000	0.00000	0.00000	0.00000	0.00000
9.80	0.00000	0.00000	0.00000	0.00000	0.00000
10.00	0.00000	0.00000	0.00000	0.00000	0.00000

Table K.7. Coulomb Potential and Charge Densities for F^- .

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	9.00000	446.91460	0.	2.30	-0.37273	0.01354	0.89976
0.01	8.99836	373.40748	0.46924	2.40	-0.45639	0.01073	0.77654
0.02	8.98853	312.14067	1.56899	2.50	-0.52862	0.00854	0.67070
0.03	8.96605	261.05181	2.95243	2.60	-0.59102	0.00682	0.57965
0.04	8.92930	218.43113	4.39182	2.70	-0.64497	0.00547	0.50125
0.05	8.87851	182.86020	5.74472	2.80	-0.69163	0.00440	0.43366
0.06	8.81498	153.16149	6.92886	2.90	-0.73201	0.00355	0.37534
0.07	8.74063	128.35684	7.90360	3.00	-0.76696	0.00287	0.32497
0.08	8.65765	107.63309	8.65637	3.20	-0.82345	0.00189	0.24383
0.09	8.56823	90.31386	9.19283	3.40	-0.86585	0.00126	0.18317
0.10	8.47445	75.83620	9.52986	3.60	-0.89773	0.00085	0.13780
0.12	8.28115	53.60832	9.70073	3.80	-0.92173	0.00057	0.10386
0.14	8.08974	38.05943	9.37407	4.00	-0.93984	0.00039	0.07847
0.16	7.90820	27.17847	8.74329	4.20	-0.95355	0.00027	0.05947
0.18	7.74098	19.56320	7.96516	4.40	-0.96395	0.00019	0.04524
0.20	7.58980	14.23403	7.15480	4.60	-0.97188	0.00013	0.03456
0.22	7.45448	10.50557	6.38962	4.80	-0.97795	0.00009	0.02653
0.24	7.33360	7.89763	5.71649	5.00	-0.98262	0.00007	0.02047
0.26	7.22504	6.07346	5.15932	5.20	-0.98623	0.00005	0.01588
0.28	7.12640	4.79673	4.72575	5.40	-0.98904	0.00003	0.01239
0.30	7.03521	3.90158	4.41258	5.60	-0.99124	0.00002	0.00972
0.35	6.82525	2.65242	4.08308	5.80	-0.99297	0.00002	0.00766
0.40	6.61916	2.09815	4.21859	6.00	-0.99434	0.00001	0.00608
0.45	6.39928	1.80873	4.60265	6.50	-0.99666	0.00001	0.00347
0.50	6.15750	1.61462	5.07249	7.00	-0.99800	0.00000	0.00203
0.55	5.89237	1.45303	5.52345	7.50	-0.99880	0.00000	0.00121
0.60	5.60646	1.30357	5.89719	8.00	-0.99927	0.00000	0.00073
0.65	5.30438	1.16167	6.16763	8.50	-0.99956	0.00000	0.00044
0.70	4.99151	1.02787	6.32915	9.00	-0.99973	0.00000	0.00027
0.75	4.67318	0.90372	6.38805	9.50	-0.99984	0.00000	0.00016
0.80	4.35421	0.79040	6.35680	10.00	-0.99990	0.00000	0.00010
0.85	4.03875	0.68843	6.25036	10.50	-0.99994	0.00000	0.00006
0.90	3.73018	0.59771	6.08398	11.00	-0.99997	0.00000	0.00004
0.95	3.43112	0.51776	5.87196	11.50	-0.99998	0.00000	0.00002
1.00	3.14353	0.44778	5.62699	12.00	-0.99999	0.00000	0.00001
1.10	2.60775	0.33409	5.07992	12.50	-0.99999	0.00000	0.00001
1.20	2.12833	0.24915	4.50852	13.00	-1.00000	0.00000	0.00000
1.30	1.70546	0.18619	3.95409	13.50	-1.00000	0.00000	0.00000
1.40	1.33616	0.13966	3.43978	14.00	-1.00000	0.00000	0.00000
1.50	1.01580	0.10527	2.97640	14.50	-1.00000	0.00000	0.00000
1.60	0.73908	0.07979	2.56690	15.00	-1.00000	0.00000	0.00000
1.70	0.50067	0.06084	2.20965	15.50	-1.00000	0.00000	0.00000
1.80	0.29554	0.04668	1.90060	17.00	-1.00000	0.00000	0.00000
1.90	0.11912	0.03603	1.63464	18.00	-1.00000	0.00000	0.00000
2.00	-0.03265	0.02798	1.40644	19.00	-1.00000	0.00000	0.00000
2.10	-0.16326	0.02185	1.21089	20.00	-1.00000	0.00000	0.00000
2.20	-0.27576	0.01715	1.04336	21.00	-1.00000	0.00000	0.00000

Table K.8. Coulomb Potential and Charge Densities for Ne.

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	10.00000	619.67248	0.	2.40	0.13792	0.00438	0.31713
0.01	9.99776	507.48767	0.63773	2.50	0.10954	0.00322	0.25291
0.02	9.98456	415.84743	2.09028	2.60	0.08691	0.00237	0.20151
0.03	9.95493	340.95139	3.85607	2.70	0.06889	0.00175	0.16041
0.04	9.90744	279.71155	5.62393	2.80	0.05456	0.00129	0.12757
0.05	9.84306	229.61671	7.21362	2.90	0.04316	0.00096	0.10135
0.06	9.76408	188.62308	8.53311	3.00	0.03411	0.00071	0.08045
0.07	9.67341	155.06595	9.54822	3.20	0.02124	0.00039	0.05053
0.08	9.57412	127.58846	10.26127	3.40	0.01317	0.00022	0.03160
0.09	9.46912	105.08378	10.69623	3.60	0.00813	0.00012	0.01968
0.10	9.36101	86.64841	10.88856	3.80	0.00500	0.00007	0.01221
0.12	9.14397	59.16859	10.70689	4.00	0.00306	0.00004	0.00754
0.14	8.93603	40.71798	10.02887	4.20	0.00187	0.00002	0.00464
0.16	8.74438	28.33019	9.11379	4.40	0.00114	0.00001	0.00284
0.18	8.57179	20.01525	8.14922	4.60	0.00069	0.00001	0.00173
0.20	8.41792	14.43596	7.25631	4.80	0.00042	0.00000	0.00105
0.22	8.28060	10.69264	6.50339	5.00	0.00025	0.00000	0.00064
0.24	8.15665	8.17944	5.92046	5.20	0.00015	0.00000	0.00038
0.26	8.04261	6.48833	5.51175	5.40	0.00009	0.00000	0.00023
0.28	7.93509	5.34463	5.26555	5.60	0.00005	0.00000	0.00014
0.30	7.83104	4.56366	5.16138	5.80	0.00003	0.00000	0.00008
0.35	7.57023	3.48292	5.36154	6.00	0.00002	0.00000	0.00005
0.40	7.28877	2.95030	5.93194	6.20	0.00001	0.00000	0.00003
0.45	6.97551	2.59275	6.59775	6.40	0.00001	0.00000	0.00002
0.50	6.63024	2.28929	7.19203	6.60	0.00000	0.00000	0.00001
0.55	6.25890	2.00781	7.63234	6.80	0.00000	0.00000	0.00001
0.60	5.87004	1.74449	7.89188	7.00	0.00000	0.00000	0.00000
0.65	5.47264	1.50232	7.97626	7.20	0.00000	0.00000	0.00000
0.70	5.07496	1.28421	7.90755	7.40	0.00000	0.00000	0.00000
0.75	4.68396	1.09135	7.71432	7.60	0.00000	0.00000	0.00000
0.80	4.30512	0.92333	7.42585	7.80	0.00000	0.00000	0.00000
0.85	3.94251	0.77860	7.06906	8.00	0.	0.00000	0.00000
0.90	3.59896	0.65501	6.66718	8.20	0.	0.00000	0.00000
0.95	3.27622	0.55015	6.23936	8.40	0.	0.00000	0.00000
1.00	2.97520	0.46161	5.80081	8.60	0.	0.00000	0.00000
1.10	2.43871	0.32458	4.93537	8.80	0.	0.00000	0.00000
1.20	1.98603	0.22832	4.13166	9.00	0.	0.00000	0.00000
1.30	1.60936	0.16095	3.41806	9.20	0.	0.00000	0.00000
1.40	1.29913	0.11380	2.80297	9.40	0.	0.00000	0.00000
1.50	1.04557	0.08076	2.28354	9.60	0.	0.00000	0.00000
1.60	0.83951	0.05754	1.85119	9.80	0.	0.00000	0.00000
1.70	0.67279	0.04117	1.49509	10.00	0.	0.00000	0.00000
1.80	0.53833	0.02957	1.20402	10.20	0.	0.00000	0.00000
1.90	0.43017	0.02133	0.96745	10.40	0.	0.00000	0.00000
2.00	0.34334	0.01544	0.77598	10.60	0.	0.00000	0.00000
2.10	0.27374	0.01121	0.62151				
2.20	0.21803	0.00817	0.49717				
2.30	0.17349	0.00598	0.39727				

Table K.9. Coulomb Potential and Charge Densities for Na⁺.

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	11.00000	833.08091	0.	2.20	1.05692	0.00295	0.17938
0.01	10.99703	668.71063	0.84033	2.30	1.04150	0.00198	0.13141
0.02	10.97984	537.12818	2.69990	2.40	1.03022	0.00133	0.09608
0.03	10.94199	431.73554	4.88281	2.50	1.02198	0.00089	0.07013
0.04	10.88248	347.27880	6.98245	2.60	1.01596	0.00060	0.05112
0.05	10.80335	279.57042	8.78296	2.70	1.01158	0.00041	0.03720
0.06	10.70814	225.26944	10.19095	2.80	1.00840	0.00027	0.02705
0.07	10.60091	181.70818	11.18872	2.90	1.00608	0.00019	0.01964
0.08	10.48565	146.75450	11.80270	3.00	1.00440	0.00013	0.01425
0.09	10.36597	118.70304	12.08250	3.10	1.00318	0.00009	0.01033
0.10	10.24491	96.18867	12.08742	3.20	1.00230	0.00006	0.00748
0.12	10.00788	63.61375	11.51127	3.30	1.00166	0.00004	0.00541
0.14	9.78733	42.63243	10.50040	3.40	1.00120	0.00003	0.00391
0.16	9.58863	29.12500	9.36949	3.50	1.00087	0.00002	0.00283
0.18	9.41199	20.43345	8.31949	3.60	1.00062	0.00001	0.00204
0.20	9.25457	14.84055	7.45968	3.70	1.00045	0.00001	0.00147
0.22	9.11204	11.23629	6.83405	3.80	1.00032	0.00001	0.00106
0.24	8.97963	8.90327	6.44439	3.90	1.00023	0.00000	0.00077
0.26	8.85284	7.37850	6.26793	4.00	1.00017	0.00000	0.00055
0.28	8.72773	6.36389	6.26973	4.10	1.00012	0.00000	0.00040
0.30	8.60112	5.66837	6.41078	4.20	1.00009	0.00000	0.00029
0.35	8.26410	4.63292	7.13183	4.40	1.00005	0.00000	0.00015
0.40	7.88528	3.98834	8.01903	4.60	1.00002	0.00000	0.00008
0.45	7.46428	3.45273	8.78612	4.80	1.00001	0.00000	0.00004
0.50	7.01091	2.96091	9.30196	5.00	1.00001	0.00000	0.00002
0.55	6.53884	2.50821	9.53453	5.20	1.00000	0.00000	0.00001
0.60	6.06183	2.10121	9.50565	5.40	1.00000	0.00000	0.00001
0.65	5.59187	1.74435	9.26128	5.60	1.00000	0.00000	0.00000
0.70	5.13841	1.43791	8.85399	5.80	1.00000	0.00000	0.00000
0.75	4.70835	1.17898	8.33371	6.00	1.00000	0.00000	0.00000
0.80	4.30620	0.96283	7.74350	6.20	1.00000	0.00000	0.00000
0.85	3.93458	0.78402	7.11825	6.40	1.00000	0.00000	0.00000
0.90	3.59451	0.63709	6.48480	6.60	1.00000	0.00000	0.00000
0.95	3.28590	0.51696	5.86290	6.80	1.00000	0.00000	0.00000
1.00	3.00780	0.41908	5.26637	7.00	1.00000	0.00000	0.00000
1.10	2.53670	0.27504	4.18204	7.20	1.00000	0.00000	0.00000
1.20	2.16576	0.18046	3.26552	7.40	1.00000	0.00000	0.00000
1.30	1.87798	0.11852	2.51696	7.60	1.00000	0.00000	0.00000
1.40	1.65730	0.07796	1.92020	7.80	1.00000	0.00000	0.00000
1.50	1.48963	0.05138	1.45287	8.00	1.00000	0.00000	0.00000
1.60	1.36318	0.03394	1.09186	8.20	1.00000	0.00000	0.00000
1.70	1.26842	0.02247	0.81594	8.40	1.00000	0.00000	0.00000
1.80	1.19777	0.01491	0.60688	8.60	1.00000	0.00000	0.00000
1.90	1.14532	0.00991	0.44957	8.80	1.00000	0.00000	0.00000
2.00	1.10654	0.00660	0.33190	9.00	1.00000	0.00000	0.00000
2.10	1.07794	0.00441	0.24431				

Table K.10. Coulomb Potential and Charge Densities for Na.

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	11.00000	833.65247	0.	4.00	0.48586	0.00124	0.24925
0.01	10.99703	669.16434	0.84090	4.10	0.46121	0.00115	0.24365
0.02	10.97983	537.48686	2.70170	4.20	0.43715	0.00107	0.23749
0.03	10.94195	432.01752	4.88600	4.40	0.39100	0.00092	0.22374
0.04	10.88241	347.49891	6.98688	4.60	0.34775	0.00078	0.20860
0.05	10.80323	279.74061	8.78831	4.80	0.30762	0.00067	0.19261
0.06	10.70796	225.39950	10.19683	5.00	0.27073	0.00056	0.17627
0.07	10.60066	181.80601	11.19474	5.20	0.23711	0.00047	0.15999
0.08	10.48534	146.82661	11.80850	5.40	0.20671	0.00039	0.14411
0.09	10.36561	118.75470	12.08776	5.60	0.17942	0.00033	0.12890
0.10	10.24451	96.22416	12.09188	5.80	0.15509	0.00027	0.11455
0.12	10.00740	63.62681	11.51364	6.00	0.13353	0.00022	0.10118
0.14	9.78683	42.63243	10.50040	6.20	0.11455	0.00018	0.08887
0.16	9.58816	29.11803	9.36724	6.40	0.09791	0.00015	0.07765
0.18	9.41158	20.42338	8.31539	6.60	0.08341	0.00012	0.06752
0.20	9.25426	14.82979	7.45426	6.80	0.07084	0.00010	0.05844
0.22	9.11184	11.22622	6.82792	7.00	0.05997	0.00008	0.05036
0.24	8.97956	8.89464	6.43814	7.20	0.05063	0.00007	0.04323
0.26	8.85288	7.37162	6.26209	7.40	0.04262	0.00005	0.03696
0.28	8.72788	6.35883	6.26474	7.60	0.03579	0.00004	0.03150
0.30	8.60136	5.66502	6.40698	7.80	0.02998	0.00003	0.02675
0.35	8.26444	4.63297	7.13190	8.00	0.02505	0.00003	0.02264
0.40	7.88551	3.99040	8.02318	8.20	0.02088	0.00002	0.01911
0.45	7.46422	3.45567	8.79362	8.40	0.01737	0.00002	0.01608
0.50	7.01041	2.96398	9.31162	8.60	0.01442	0.00001	0.01350
0.55	6.53783	2.51097	9.54502	8.80	0.01194	0.00001	0.01130
0.60	6.06030	2.10344	9.51576	9.00	0.00988	0.00001	0.00944
0.65	5.58987	1.74600	9.27001	9.20	0.00815	0.00001	0.00786
0.70	5.13603	1.43900	8.86068	9.40	0.00671	0.00001	0.00654
0.75	4.70568	1.17959	8.33804	9.60	0.00552	0.00000	0.00542
0.80	4.30338	0.96307	7.74546	9.80	0.00453	0.00000	0.00449
0.85	3.93171	0.78400	7.11812	10.00	0.00372	0.00000	0.00371
0.90	3.59170	0.63692	6.48310	10.20	0.00304	0.00000	0.00306
0.95	3.28319	0.51673	5.86034	10.40	0.00249	0.00000	0.00252
1.00	3.00522	0.41888	5.26381	10.60	0.00203	0.00000	0.00207
1.10	2.53428	0.27505	4.18225	10.80	0.00165	0.00000	0.00170
1.20	2.16301	0.18083	3.27230	11.00	0.00134	0.00000	0.00139
1.30	1.87409	0.11931	2.53376	11.20	0.00109	0.00000	0.00114
1.40	1.65110	0.07917	1.94987	11.40	0.00089	0.00000	0.00093
1.50	1.47972	0.05297	1.49759	11.60	0.00072	0.00000	0.00076
1.60	1.34799	0.03584	1.15310	11.80	0.00058	0.00000	0.00062
1.70	1.24624	0.02463	0.89460	12.00	0.00047	0.00000	0.00050
1.80	1.16684	0.01727	0.70332	12.20	0.00038	0.00000	0.00041
1.90	1.10386	0.01243	0.56378	12.40	0.00031	0.00000	0.00033
2.00	1.05277	0.00922	0.46352	12.60	0.00025	0.00000	0.00027
2.10	1.01017	0.00709	0.39275	12.80	0.00020	0.00000	0.00022
2.20	0.97350	0.00565	0.34384	13.00	0.00016	0.00000	0.00017
2.30	0.94087	0.00468	0.31096	13.50	0.00009	0.00000	0.00010
2.40	0.91092	0.00400	0.28965	14.00	0.00005	0.00000	0.00006
2.50	0.88267	0.00352	0.27656	14.50	0.00003	0.00000	0.00003
2.60	0.85542	0.00317	0.26918	15.00	0.00002	0.00000	0.00002
2.70	0.82870	0.00290	0.26561	15.50	0.00001	0.00000	0.00001
2.80	0.80221	0.00268	0.26448	16.00	0.00001	0.00000	0.00001
2.90	0.77576	0.00251	0.26475	16.50	0.00000	0.00000	0.00000
3.00	0.74924	0.00235	0.26570	17.00	0.00000	0.00000	0.00000
3.10	0.72262	0.00221	0.26678	17.50	0.00000	0.00000	0.00000
3.20	0.69589	0.00208	0.26761	18.00	0.00000	0.00000	0.00000
3.30	0.66911	0.00196	0.26795	18.50	0.00000	0.00000	0.00000
3.40	0.64233	0.00184	0.26763	19.00	0.00000	0.00000	0.00000
3.50	0.61561	0.00173	0.26655	19.50	0.	0.00000	0.00000
3.60	0.58904	0.00163	0.26466				
3.70	0.56271	0.00152	0.26196				
3.80	0.53668	0.00142	0.25846				
3.90	0.51104	0.00133	0.25420				

Table K.11. Coulomb Potential and Charge Densities for F^- of J.1

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	9.00000	446.77145	0.	2.40	-0.53022	0.01056	0.76419
0.01	8.99836	373.28191	0.46908	2.50	-0.60091	0.00831	0.65244
0.02	8.98853	312.03249	1.56845	2.60	1.00000	0.00655	0.55657
0.03	8.96606	260.96010	2.95139	2.70	1.00000	0.00518	0.47436
0.04	8.92933	218.35455	4.39028	2.80	1.00000	0.00410	0.40392
0.05	8.87855	182.79723	5.74274	2.90	1.00000	0.00325	0.34360
0.06	8.81504	153.11055	6.92656	3.00	1.00000	0.00258	0.29200
0.07	8.74072	128.31635	7.90111	3.20	1.00000	0.00163	0.21022
0.08	8.65776	107.60158	8.65383	3.40	1.00000	0.00104	0.15074
0.09	8.56836	90.28997	9.19040	3.60	1.00000	0.00066	0.10769
0.10	8.47462	75.81870	9.52766	3.80	1.00000	0.00042	0.07668
0.12	8.28134	53.60053	9.69932	4.00	1.00000	0.00027	0.05447
0.14	8.08995	38.05813	9.37375	4.20	1.00000	0.00017	0.03862
0.16	7.90841	27.18138	8.74423	4.40	1.00000	0.00011	0.02736
0.18	7.74116	19.56875	7.96742	4.60	1.00000	0.00007	0.01938
0.20	7.58992	14.24120	7.15841	4.80	1.00000	0.00005	0.01375
0.22	7.45451	10.51371	6.39457	5.00	1.00000	0.00003	0.00977
0.24	7.33352	7.90634	5.72279	5.20	1.00000	0.00002	0.00697
0.26	7.22483	6.08249	5.16700	5.40	1.00000	0.00001	0.00499
0.28	7.12601	4.80595	4.73484	5.60	1.00000	0.00001	0.00359
0.30	7.03463	3.91089	4.42312	5.80	1.00000	0.00001	0.00259
0.35	6.82404	2.66170	4.09737	6.00	1.00000	0.00000	0.00189
0.40	6.61715	2.10709	4.23655	6.50	1.00000	0.00000	0.00088
0.45	6.39629	1.81705	4.62383	7.00	1.00000	0.00000	0.00043
0.50	6.15338	1.62216	5.09616	7.50	1.00000	0.00000	0.00022
0.55	5.88702	1.45971	5.54884	8.00	1.00000	0.00000	0.00012
0.60	5.59981	1.30943	5.92374	8.50	1.00000	0.00000	0.00006
0.65	5.29639	1.16684	6.19511	9.00	1.00000	0.00000	0.00004
0.70	4.98212	1.03251	6.35768	9.50	1.00000	0.00000	0.00002
0.75	4.66232	0.90797	6.41806	10.00	1.00000	0.00000	0.00001
0.80	4.34181	0.79440	6.38891	10.50	1.00000	0.00000	0.00001
0.85	4.02468	0.69227	6.28525	11.00	1.00000	0.00000	0.00000
0.90	3.71427	0.60148	6.12228	11.50	1.00000	0.00000	0.00000
0.95	3.41320	0.52148	5.91413	12.00	1.00000	0.00000	0.00000
1.00	3.12340	0.45147	5.67332	12.50	1.00000	0.00000	0.00000
1.10	2.58257	0.33767	5.13445	13.00	1.00000	0.00000	0.00000
1.20	2.09735	0.25253	4.56970	13.50	1.00000	0.00000	0.00000
1.30	1.66814	0.18925	4.01916	14.00	1.00000	0.00000	0.00000
1.40	1.29227	0.14232	3.50545	14.50	1.00000	0.00000	0.00000
1.50	0.96545	0.10750	3.03940	15.00	1.00000	0.00000	0.00000
1.60	0.68269	0.08158	2.62442	15.50	1.00000	0.00000	0.00000
1.70	0.43890	0.06222	2.25955	17.00	1.00000	0.00000	0.00000
1.80	0.22922	0.04768	1.94146	18.00	1.00000	0.00000	0.00000
1.90	0.04919	0.03672	1.66572	19.00	1.00000	0.00000	0.00000
2.00	-0.10518	0.02840	1.42761	20.00	1.00000	0.00000	0.00000
2.10	-0.23743	0.02206	1.22247	21.00	1.00000	0.00000	0.00000
2.20	-0.35063	0.01720	1.04602				
2.30	-0.44746	0.01345	0.89440				

Table K.12. Coulomb Potential and Charge Densities for F^- of L.L.

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	9.00000	446.74571	0.	2.30	-0.46221	0.01337	0.88905
0.01	8.99836	373.25800	0.46905	2.40	-0.54440	0.01047	0.75802
0.02	8.98853	312.01097	1.56834	2.50	1.00000	0.00822	0.64566
0.03	8.96606	260.94123	2.95118	2.60	1.00000	0.00647	0.54937
0.04	8.92933	218.33839	4.38995	2.70	1.00000	0.00510	0.46693
0.05	8.87856	182.78370	5.74232	2.80	1.00000	0.00402	0.39639
0.06	8.81505	153.09946	6.92606	2.90	1.00000	0.00318	0.33609
0.07	8.74074	128.30749	7.90056	3.00	1.00000	0.00252	0.28461
0.08	8.65778	107.59471	8.65328	3.20	1.00000	0.00158	0.20330
0.09	8.56839	90.28484	9.18988	3.40	1.00000	0.00099	0.14447
0.10	8.47465	75.81509	9.52720	3.60	1.00000	0.00063	0.10216
0.12	8.28139	53.59930	9.69910	3.80	1.00000	0.00040	0.07190
0.14	8.09000	38.05856	9.37386	4.00	1.00000	0.00025	0.05041
0.16	7.90845	27.18293	8.74472	4.20	1.00000	0.00016	0.03522
0.18	7.74118	19.57102	7.96835	4.40	1.00000	0.00010	0.02454
0.20	7.58992	14.24392	7.15977	4.60	1.00000	0.00006	0.01708
0.22	7.45448	10.51669	6.39638	4.80	1.00000	0.00004	0.01187
0.24	7.33345	7.90946	5.72505	5.00	1.00000	0.00003	0.00825
0.26	7.22470	6.08566	5.16969	5.20	1.00000	0.00002	0.00575
0.28	7.12583	4.80912	4.73796	5.40	1.00000	0.00001	0.00401
0.30	7.03438	3.91404	4.42667	5.60	1.00000	0.00001	0.00281
0.35	6.82359	2.66469	4.10197	5.80	1.00000	0.00000	0.00197
0.40	6.61644	2.10988	4.24218	6.00	1.00000	0.00000	0.00139
0.45	6.39527	1.81964	4.63042	6.50	1.00000	0.00000	0.00060
0.50	6.15202	1.62454	5.10365	7.00	1.00000	0.00000	0.00027
0.55	5.88526	1.46191	5.55718	7.50	1.00000	0.00000	0.00013
0.60	5.59761	1.31146	5.93291	8.00	1.00000	0.00000	0.00006
0.65	5.29371	1.16873	6.20511	8.50	1.00000	0.00000	0.00003
0.70	4.97892	1.03427	6.36852	9.00	1.00000	0.00000	0.00002
0.75	4.65856	0.90962	6.42975	9.50	1.00000	0.00000	0.00001
0.80	4.33744	0.79595	6.40143	10.00	1.00000	0.00000	0.00001
0.85	4.01966	0.69373	6.29855	10.50	1.00000	0.00000	0.00000
0.90	3.70857	0.60285	6.13627	11.00	1.00000	0.00000	0.00000
0.95	3.40679	0.52276	5.92870	11.50	1.00000	0.00000	0.00000
1.00	3.11625	0.45266	5.68830	12.00	1.00000	0.00000	0.00000
1.10	2.57390	0.33868	5.14970	12.50	1.00000	0.00000	0.00000
1.20	2.08717	0.25335	4.58443	13.00	1.00000	0.00000	0.00000
1.30	1.65655	0.18989	4.03265	13.50	1.00000	0.00000	0.00000
1.40	1.27942	0.14280	3.51715	14.00	1.00000	0.00000	0.00000
1.50	0.95153	0.10783	3.04893	14.50	1.00000	0.00000	0.00000
1.60	0.66793	0.08180	2.63160	15.00	1.00000	0.00000	0.00000
1.70	0.42354	0.06235	2.26437	15.50	1.00000	0.00000	0.00000
1.80	0.21350	0.04775	1.94401	17.00	1.00000	0.00000	0.00000
1.90	0.03332	0.03673	1.66619	18.00	1.00000	0.00000	0.00000
2.00	-0.12100	0.02837	1.42623	19.00	1.00000	0.00000	0.00000
2.10	-0.25303	0.02201	1.21951	20.00	1.00000	0.00000	0.00000
2.20	-0.36587	0.01713	1.04173	21.00	1.00000	0.00000	0.00000

Table K.13. Coulomb Potential and Charge Densities for F^- of L.2.

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	9.00000	446.78849	0.	2.30	-0.43770	0.01349	0.89705
0.01	8.99836	373.29775	0.46910	2.40	-0.52076	0.01060	0.76752
0.02	8.98853	312.04673	1.56852	2.50	-0.59181	0.00836	0.65629
0.03	8.96606	260.97258	2.95153	2.60	-0.65254	0.00660	0.56081
0.04	8.92933	218.36522	4.39049	2.70	-0.70442	0.00523	0.47887
0.05	8.87854	182.80618	5.74303	2.80	1.00000	0.00415	0.40859
0.06	8.81503	153.11789	6.92689	2.90	1.00000	0.00330	0.34835
0.07	8.74071	128.32224	7.90147	3.00	1.00000	0.00262	0.29673
0.08	8.65774	107.60617	8.65420	3.20	1.00000	0.00167	0.21477
0.09	8.56834	90.29343	9.19075	3.40	1.00000	0.00107	0.15494
0.10	8.47459	75.82120	9.52797	3.60	1.00000	0.00068	0.11145
0.12	8.28132	53.60151	9.69950	3.80	1.00000	0.00044	0.07998
0.14	8.08993	38.05806	9.37373	4.00	1.00000	0.00028	0.05730
0.16	7.90839	27.18061	8.74398	4.20	1.00000	0.00019	0.04101
0.18	7.74114	19.56753	7.96693	4.40	1.00000	0.00012	0.02936
0.20	7.58991	14.23971	7.15766	4.60	1.00000	0.00008	0.02104
0.22	7.45452	10.51206	6.39357	4.80	1.00000	0.00005	0.01511
0.24	7.33355	7.90461	5.72154	5.00	1.00000	0.00003	0.01089
0.26	7.22489	6.08073	5.16550	5.20	1.00000	0.00002	0.00787
0.28	7.12611	4.80418	4.73309	5.40	1.00000	0.00002	0.00572
0.30	7.03476	3.90913	4.42112	5.60	1.00000	0.00001	0.00418
0.35	6.82429	2.66000	4.09475	5.80	1.00000	0.00001	0.00307
0.40	6.61754	2.10548	4.23332	6.00	1.00000	0.00001	0.00227
0.45	6.39685	1.81556	4.62004	6.50	1.00000	0.00000	0.00111
0.50	6.15415	1.62079	5.09185	7.00	1.00000	0.00000	0.00056
0.55	5.88802	1.45846	5.54407	7.50	1.00000	0.00000	0.00030
0.60	5.60106	1.30829	5.91856	8.00	1.00000	0.00000	0.00016
0.65	5.29790	1.16579	6.18951	8.50	1.00000	0.00000	0.00009
0.70	4.98393	1.03153	6.35167	9.00	1.00000	0.00000	0.00005
0.75	4.66444	0.90706	6.41161	9.50	1.00000	0.00000	0.00003
0.80	4.34426	0.79354	6.38199	10.00	1.00000	0.00000	0.00002
0.85	4.02749	0.69145	6.27786	10.50	1.00000	0.00000	0.00001
0.90	3.71746	0.60070	6.11442	11.00	1.00000	0.00000	0.00001
0.95	3.41680	0.52075	5.90585	11.50	1.00000	0.00000	0.00000
1.00	3.12742	0.45078	5.66467	12.00	1.00000	0.00000	0.00000
1.10	2.58748	0.33707	5.12531	12.50	1.00000	0.00000	0.00000
1.20	2.10318	0.25202	4.56049	13.00	1.00000	0.00000	0.00000
1.30	1.67488	0.18884	4.01032	13.50	1.00000	0.00000	0.00000
1.40	1.29986	0.14200	3.49738	14.00	1.00000	0.00000	0.00000
1.50	0.97379	0.10725	3.03241	14.50	1.00000	0.00000	0.00000
1.60	0.69167	0.08140	2.61872	15.00	1.00000	0.00000	0.00000
1.70	0.44837	0.06210	2.25524	15.50	1.00000	0.00000	0.00000
1.80	0.23906	0.04761	1.93856	17.00	1.00000	0.00000	0.00000
1.90	0.05925	0.03668	1.66418	18.00	1.00000	0.00000	0.00000
2.00	-0.09503	0.02840	1.42732	19.00	1.00000	0.00000	0.00000
2.10	-0.22731	0.02207	1.22332	20.00	1.00000	0.00000	0.00000
2.20	-0.34064	0.01723	1.04785	21.00	1.00000	0.00000	0.00000

Table K.14. Coulomb Potential and Charge Densities for F^- of L.3.

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	9.00000	446.87724	0.	2.30	-0.39129	0.01356	0.90138
0.01	8.99836	373.37588	0.46920	2.40	-0.47501	0.01072	0.77608
0.02	8.98853	312.11426	1.56886	2.50	-0.54709	0.00851	0.66841
0.03	8.96605	261.02994	2.95218	2.60	-0.60919	0.00678	0.57582
0.04	8.92931	218.41320	4.39146	2.70	-0.66269	0.00542	0.49614
0.05	8.87852	182.84566	5.74427	2.80	-0.70879	0.00434	0.42754
0.06	8.81499	153.14984	6.92834	2.90	-0.74851	0.00349	0.36843
0.07	8.74065	128.34762	7.90303	3.00	-0.78275	0.00281	0.31751
0.08	8.65767	107.62589	8.65579	3.20	-0.83767	0.00183	0.23579
0.09	8.56826	90.30835	9.19227	3.40	-0.87846	0.00121	0.17511
0.10	8.47449	75.83208	9.52934	3.60	-0.90876	0.00080	0.13010
0.12	8.28119	53.60625	9.70036	3.80	1.00000	0.00053	0.09674
0.14	8.08979	38.05868	9.37389	4.00	1.00000	0.00036	0.07205
0.16	7.90826	27.17857	8.74332	4.20	1.00000	0.00024	0.05379
0.18	7.74103	19.56382	7.96542	4.40	1.00000	0.00017	0.04028
0.20	7.58985	14.23496	7.15527	4.60	1.00000	0.00011	0.03028
0.22	7.45451	10.50670	6.39031	4.80	1.00000	0.00008	0.02286
0.24	7.33361	7.89889	5.71740	5.00	1.00000	0.00006	0.01735
0.26	7.22504	6.07480	5.16046	5.20	1.00000	0.00004	0.01324
0.28	7.12637	4.79813	4.72714	5.40	1.00000	0.00003	0.01017
0.30	7.03515	3.90303	4.41422	5.60	1.00000	0.00002	0.00785
0.35	6.82509	2.65392	4.08539	5.80	1.00000	0.00001	0.00610
0.40	6.61887	2.09962	4.22154	6.00	1.00000	0.00001	0.00477
0.45	6.39883	1.81008	4.60610	6.50	1.00000	0.00000	0.00264
0.50	6.15687	1.61581	5.07621	7.00	1.00000	0.00000	0.00150
0.55	5.89155	1.45402	5.52722	7.50	1.00000	0.00000	0.00088
0.60	5.60545	1.30437	5.90085	8.00	1.00000	0.00000	0.00052
0.65	5.30320	1.16233	6.17113	8.50	1.00000	0.00000	0.00031
0.70	4.99016	1.02843	6.33255	9.00	1.00000	0.00000	0.00019
0.75	4.67165	0.90422	6.39153	9.50	1.00000	0.00000	0.00011
0.80	4.35251	0.79088	6.36060	10.00	1.00000	0.00000	0.00007
0.85	4.03684	0.68891	6.25477	10.50	1.00000	0.00000	0.00004
0.90	3.72802	0.59824	6.08929	11.00	1.00000	0.00000	0.00002
0.95	3.42867	0.51833	5.87842	11.50	1.00000	0.00000	0.00001
1.00	3.14073	0.44840	5.63480	12.00	1.00000	0.00000	0.00001
1.10	2.60402	0.33480	5.09070	12.50	1.00000	0.00000	0.00001
1.20	2.12337	0.24990	4.52214	13.00	1.00000	0.00000	0.00000
1.30	1.69902	0.18693	3.96996	13.50	1.00000	0.00000	0.00000
1.40	1.32806	0.14036	3.45702	14.00	1.00000	0.00000	0.00000
1.50	1.00595	0.10589	2.99401	14.50	1.00000	0.00000	0.00000
1.60	0.72749	0.08032	2.58395	15.00	1.00000	0.00000	0.00000
1.70	0.48744	0.06128	2.22537	15.50	1.00000	0.00000	0.00000
1.80	0.28083	0.04702	1.91439	17.00	1.00000	0.00000	0.00000
1.90	0.10314	0.03629	1.64612	18.00	1.00000	0.00000	0.00000
2.00	-0.04965	0.02816	1.41540	19.00	1.00000	0.00000	0.00000
2.10	-0.18103	0.02197	1.21730	20.00	1.00000	0.00000	0.00000
2.20	-0.29404	0.01722	1.04729	21.00	1.00000	0.00000	0.00000

Table K.15. Coulomb Potential and Charge Densities for Na^+ of J.2.

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	11.00000	833.08659	0.	2.10	-1.00000	0.00468	0.25961
0.01	10.99704	668.72684	0.84035	2.20	-1.00000	0.00319	0.19379
0.02	10.97984	537.14749	2.70000	2.30	-1.00000	0.00218	0.14462
0.03	10.94199	431.75380	4.88302	2.40	-1.00000	0.00149	0.10791
0.04	10.88248	347.29401	6.98276	2.50	-1.00000	0.00103	0.08053
0.05	10.80334	279.58178	8.78332	2.60	-1.00000	0.00071	0.06009
0.06	10.70813	225.27698	10.19129	2.70	-1.00000	0.00049	0.04485
0.07	10.60089	181.71227	11.18897	2.80	-1.00000	0.00034	0.03348
0.08	10.48563	146.75569	11.80279	2.90	-1.00000	0.00024	0.02499
0.09	10.36595	118.70189	12.08238	3.00	-1.00000	0.00016	0.01866
0.10	10.24490	96.18569	12.08705	3.10	-1.00000	0.00012	0.01393
0.12	10.00788	63.60843	11.51031	3.20	-1.00000	0.00008	0.01040
0.14	9.78736	42.62590	10.49880	3.30	-1.00000	0.00006	0.00776
0.16	9.58870	29.11784	9.36718	3.40	-1.00000	0.00004	0.00579
0.18	9.41211	20.42587	8.31640	3.50	-1.00000	0.00003	0.00432
0.20	9.25476	14.83261	7.45568	3.60	-1.00000	0.00002	0.00322
0.22	9.11232	11.22797	6.82899	3.70	-1.00000	0.00001	0.00240
0.24	8.98003	8.89457	6.43809	3.80	-1.00000	0.00001	0.00179
0.26	8.85337	7.36945	6.26025	3.90	-1.00000	0.00001	0.00133
0.28	8.72843	6.35457	6.26054	4.00	-1.00000	0.00000	0.00099
0.30	8.60202	5.65887	6.40003	4.10	-1.00000	0.00000	0.00074
0.35	8.26563	4.62350	7.11733	4.20	-1.00000	0.00000	0.00055
0.40	7.88762	3.97968	8.00161	4.40	-1.00000	0.00000	0.00030
0.45	7.46754	3.44519	8.76693	4.60	-1.00000	0.00000	0.00017
0.50	7.01515	2.95457	9.28206	4.80	-1.00000	0.00000	0.00009
0.55	6.54407	2.50296	9.51458	5.00	-1.00000	0.00000	0.00005
0.60	6.06805	2.09685	9.48593	5.20	-1.00000	0.00000	0.00003
0.65	5.59907	1.74067	9.24175	5.40	-1.00000	0.00000	0.00002
0.70	5.14660	1.43474	8.83446	5.60	-1.00000	0.00000	0.00001
0.75	4.71751	1.17619	8.31401	5.80	-1.00000	0.00000	0.00000
0.80	4.31636	0.96035	7.72356	6.00	-1.00000	0.00000	0.00000
0.85	3.94573	0.78180	7.09812	6.20	-1.00000	0.00000	0.00000
0.90	3.60668	0.63511	6.46468	6.40	-1.00000	0.00000	0.00000
0.95	3.29906	0.51521	5.84312	6.60	-1.00000	0.00000	0.00000
1.00	3.02193	0.41757	5.24735	6.80	-1.00000	0.00000	0.00000
1.10	2.55261	0.27397	4.16587	7.00	-1.00000	0.00000	0.00000
1.20	2.18307	0.17981	3.25374	7.20	-1.00000	0.00000	0.00000
1.30	1.89621	0.11821	2.51052	7.40	-1.00000	0.00000	0.00000
1.40	1.67590	0.07793	1.91935	7.60	-1.00000	0.00000	0.00000
1.50	1.50804	0.05154	1.45722	7.80	-1.00000	0.00000	0.00000
1.60	1.38094	0.03421	1.10058	8.00	-1.00000	0.00000	0.00000
1.70	1.28513	0.02280	0.82798	8.20	-1.00000	0.00000	0.00000
1.80	-1.00000	0.01526	0.62111	8.40	-1.00000	0.00000	0.00000
1.90	-1.00000	0.01025	0.46498	8.60	-1.00000	0.00000	0.00000
2.00	-1.00000	0.00692	0.34760	8.80	-1.00000	0.00000	0.00000
				9.00	-1.00000	0.00000	0.00000

Table K.16. Coulomb Potential and Charge Densities for Na^+ of L.4.

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	9.00000	833.08294	0.	2.20	-1.00000	0.00326	0.19830
0.01	8.99704	668.72765	0.84035	2.30	-1.00000	0.00224	0.14861
0.02	8.97984	537.15031	2.70001	2.40	-1.00000	0.00154	0.11138
0.03	8.94199	431.75713	4.88306	2.50	-1.00000	0.00106	0.08350
0.04	8.88248	347.29704	6.98282	2.60	-1.00000	0.00074	0.06262
0.05	8.80334	279.58408	8.78339	2.70	-1.00000	0.00051	0.04697
0.06	8.70813	225.27841	10.19135	2.80	-1.00000	0.00036	0.03524
0.07	8.60089	181.71279	11.18900	2.90	-1.00000	0.00025	0.02644
0.08	8.48563	146.75536	11.80277	3.00	-1.00000	0.00018	0.01984
0.09	8.36595	118.70083	12.08227	3.10	-1.00000	0.00012	0.01489
0.10	8.24490	96.18401	12.08684	3.20	-1.00000	0.00009	0.01117
0.12	8.00788	63.60580	11.50983	3.30	-1.00000	0.00006	0.00838
0.14	7.78738	42.62267	10.49800	3.40	-1.00000	0.00004	0.00629
0.16	7.58874	29.11424	9.36602	3.50	-1.00000	0.00003	0.00471
0.18	7.41218	20.42205	8.31484	3.60	-1.00000	0.00002	0.00353
0.20	7.25486	14.82866	7.45370	3.70	-1.00000	0.00002	0.00265
0.22	7.11246	11.22396	6.82655	3.80	-1.00000	0.00001	0.00198
0.24	6.98022	8.89055	6.43519	3.90	-1.00000	0.00001	0.00148
0.26	6.85363	7.36546	6.25686	4.00	-1.00000	0.00001	0.00111
0.28	6.72876	6.35065	6.25668	4.10	-1.00000	0.00000	0.00083
0.30	6.60244	5.65504	6.39570	4.20	-1.00000	0.00000	0.00062
0.35	6.26629	4.62000	7.11194	4.40	-1.00000	0.00000	0.00034
0.40	5.88857	3.97655	7.99533	4.60	-1.00000	0.00000	0.00019
0.45	5.46882	3.44243	8.75992	4.80	-1.00000	0.00000	0.00011
0.50	5.01680	2.95215	9.27444	5.00	-1.00000	0.00000	0.00006
0.55	4.54612	2.50081	9.50641	5.20	-1.00000	0.00000	0.00003
0.60	4.07052	2.09494	9.47727	5.40	-1.00000	0.00000	0.00002
0.65	3.60198	1.73897	9.23270	5.60	-1.00000	0.00000	0.00001
0.70	3.14997	1.43323	8.82515	5.80	-1.00000	0.00000	0.00001
0.75	2.72135	1.17486	8.30462	6.00	-1.00000	0.00000	0.00000
0.80	2.32066	0.95919	7.71430	6.20	-1.00000	0.00000	0.00000
0.85	1.95049	0.78082	7.08922	6.40	-1.00000	0.00000	0.00000
0.90	1.61187	0.63430	6.45638	6.60	-1.00000	0.00000	0.00000
0.95	1.30465	0.51455	5.83564	6.80	-1.00000	0.00000	0.00000
1.00	1.02787	0.41705	5.24085	7.00	-1.00000	0.00000	0.00000
1.10	0.55909	0.27370	4.16168	7.20	-1.00000	0.00000	0.00000
1.20	0.18985	0.17971	3.25202	7.40	-1.00000	0.00000	0.00000
1.30	-0.09696	0.11824	2.51112	7.60	-1.00000	0.00000	0.00000
1.40	-0.31744	0.07803	1.92189	7.80	-1.00000	0.00000	0.00000
1.50	-0.48563	0.05168	1.46125	8.00	-1.00000	0.00000	0.00000
1.60	-0.61319	0.03437	1.10561	8.20	-1.00000	0.00000	0.00000
1.70	-0.70953	0.02295	0.83358	8.40	-1.00000	0.00000	0.00000
1.80	-1.00000	0.01540	0.62691	8.60	-1.00000	0.00000	0.00000
1.90	-1.00000	0.01038	0.47069	8.80	-1.00000	0.00000	0.00000
2.00	-1.00000	0.00702	0.35302	9.00	-1.00000	0.00000	0.00000
2.10	-1.00000	0.00477	0.26462				

Table K.17. Coulomb Potential and Charge Densities for Na⁺ of L.5.

r	Z(r)	$\rho(r)$	D(r)	r	Z(r)	$\rho(r)$	D(r)
0.	11.00000	833.08762	0.	2.20	-1.00000	0.00312	0.19000
0.01	10.99704	668.72459	0.84034	2.30	-1.00000	0.00212	0.14124
0.02	10.97984	537.14395	2.69998	2.40	-1.00000	0.00145	0.10495
0.03	10.94199	431.75012	4.88298	2.50	-1.00000	0.00099	0.07796
0.04	10.88248	347.29084	6.98270	2.60	-1.00000	0.00068	0.05791
0.05	10.80335	279.57940	8.78325	2.70	-1.00000	0.00047	0.04301
0.06	10.70813	225.27547	10.19122	2.80	-1.00000	0.00032	0.03195
0.07	10.60089	181.71159	11.18893	2.90	-1.00000	0.00022	0.02373
0.08	10.48563	146.75575	11.80280	3.00	-1.00000	0.00016	0.01762
0.09	10.36595	118.70260	12.08245	3.10	-1.00000	0.00011	0.01308
0.10	10.24490	96.18694	12.08721	3.20	-1.00000	0.00008	0.00971
0.12	10.00787	63.61043	11.51067	3.30	-1.00000	0.00005	0.00721
0.14	9.78735	42.62837	10.49940	3.40	-1.00000	0.00004	0.00535
0.16	9.58867	29.12058	9.36807	3.50	-1.00000	0.00003	0.00397
0.18	9.41206	20.42878	8.31758	3.60	-1.00000	0.00002	0.00295
0.20	9.25469	14.83562	7.45720	3.70	-1.00000	0.00001	0.00218
0.22	9.11221	11.23104	6.83085	3.80	-1.00000	0.00001	0.00162
0.24	8.97987	8.89766	6.44033	3.90	-1.00000	0.00001	0.00120
0.26	8.85317	7.37254	6.26287	4.00	-1.00000	0.00000	0.00089
0.28	8.72817	6.35763	6.26356	4.10	-1.00000	0.00000	0.00066
0.30	8.60170	5.66188	6.40344	4.20	-1.00000	0.00000	0.00049
0.35	8.26512	4.62630	7.12163	4.40	-1.00000	0.00000	0.00027
0.40	7.88687	3.98217	8.00663	4.60	-1.00000	0.00000	0.00015
0.45	7.46653	3.44737	8.77249	4.80	-1.00000	0.00000	0.00008
0.50	7.01385	2.95647	9.28802	5.00	-1.00000	0.00000	0.00004
0.55	6.54246	2.50462	9.52086	5.20	-1.00000	0.00000	0.00002
0.60	6.06613	2.09830	9.49249	5.40	-1.00000	0.00000	0.00001
0.65	5.59681	1.74196	9.24856	5.60	-1.00000	0.00000	0.00001
0.70	5.14399	1.43588	8.84147	5.80	-1.00000	0.00000	0.00000
0.75	4.71455	1.17720	8.32112	6.00	-1.00000	0.00000	0.00000
0.80	4.31304	0.96123	7.73063	6.20	-1.00000	0.00000	0.00000
0.85	3.94207	0.78256	7.10501	6.40	-1.00000	0.00000	0.00000
0.90	3.60267	0.63576	6.47123	6.60	-1.00000	0.00000	0.00000
0.95	3.29474	0.51575	5.84918	6.80	-1.00000	0.00000	0.00000
1.00	3.01732	0.41800	5.25277	7.00	-1.00000	0.00000	0.00000
1.10	2.54754	0.27422	4.16968	7.20	-1.00000	0.00000	0.00000
1.20	2.17772	0.17992	3.25571	7.40	-1.00000	0.00000	0.00000
1.30	1.89075	0.11822	2.51068	7.60	-1.00000	0.00000	0.00000
1.40	1.67050	0.07787	1.91790	7.80	-1.00000	0.00000	0.00000
1.50	1.50286	0.05144	1.45447	8.00	-1.00000	0.00000	0.00000
1.60	1.37608	0.03410	1.09689	8.20	-1.00000	0.00000	0.00000
1.70	1.28067	0.02268	0.82370	8.40	-1.00000	0.00000	0.00000
1.80	1.20914	0.01514	0.61655	8.60	-1.00000	0.00000	0.00000
1.90	1.15566	0.01015	0.46038	8.80	-1.00000	0.00000	0.00000
2.00	-1.00000	0.00683	0.34316	9.00	-1.00000	0.00000	0.00000
2.10	-1.00000	0.00461	0.25546				

APPENDIX L
PARAMETERS AND ORBITAL TABLES FOR THE SCF WAVE
FUNCTIONS OF THE GROUND STATES OF F^- AND Na^+ IN
THE PRESENCE OF SUPERPOSED POTENTIAL SPHERES

The solutions given in this appendix correspond to an F^- ion and to a Na^+ ion in the presence of a superposed hollow sphere carrying a unit charge. The radius of the superposed sphere has been taken at several values which are different from those in Appendix J. The expansion parameters are the same as those of Tables H.2 and H.4.

Table L.1. Parameters for F^- with Superposed Potential Sphere

ζ	n	C_{1s}	C_{2s}	ζ	n	C_{2p}
12.20	1	0.089916	- 0.239794	6.05	2	0.050244
8.20	1	0.937421	0.683005	3.06	2	0.635847
				1.44	2	0.557051
10.80	2	- 0.022742	- 0.167362	0.69	2	0.019084
4.10	2	- 0.007380	- 0.215606			
2.66	2	- 0.005722	- 0.604434	3.75	3	- 0.144059
1.68	2	0.001627	- 0.292119	8.00	3	- 0.011877
4.50	3	0.013687	- 0.005869			
- ϵ		26.18396	1.450631			0.5591383
$-\tilde{R}$		8.9947	9.0672			10.2401
$-E$				103.5879		
Charge on Sphere	1.00			Radius of Sphere	2.40	

Table L.2. Parameters for F^- with Superposed Potential Sphere

ζ	n	C_{1s}	C_{2s}	ζ	n	C_{2p}
12.20	1	0.089872	- 0.221050	6.05	2	0.051184
8.20	1	0.937518	0.649161	3.06	2	0.630219
				1.44	2	0.544725
10.80	2	- 0.022764	- 0.154093	0.69	2	0.036150
4.10	2	- 0.007473	- 0.205678			
2.66	2	- 0.005762	- 0.582818	3.75	3	- 0.137323
1.68	2	0.001640	- 0.299086	8.00	3	- 0.011581
4.50	3	0.013758	- 0.028662			
- ϵ		26.15867	1.417240			0.5257729
$\tilde{R}$		8.9947	9.0553			10.2332
-E				103.1422		
Charge on Sphere	1.00			Radius of Sphere	2.70	

Table L.3. Parameters for F^- with Superposed Potential Sphere.

ζ	n	C_{1s}	C_{2s}	ζ	n	C_{2p}
12.20	1	0.089711	- 0.201754	6.05	2	0.059712
8.20	1	0.937830	0.614562	3.06	2	0.580765
				1.44	2	0.514525
10.80	2	- 0.022869	- 0.140392	0.69	2	0.701605
4.10	2	- 0.007649	- 0.194646			
2.66	2	- 0.005860	- 0.565947	3.75	3	- 0.087558
1.68	2	0.001668	- 0.302182	8.00	3	- 0.008525
4.50	3	0.013928	- 0.051227			
- ϵ		26.08340	1.331305			0.4386323
- $\tilde{R}$		8.9947	9.0425			10.2058
- E			102.0955			
Charge on Sphere		1.00		Radius of Sphere		3.789

Table L.4. Parameters for Na^+ with Superposed Potential Sphere

ζ	n	C_{1s}	C_{2s}	ζ	n	C_{2p}
15.00	1	0.118547	0.039100	6.60	2	0.143044
10.30	1	0.854737	0.190950	3.40	2	0.707453
11.00	2	0.031796	0.067772	2.30	2	0.203736
5.40	2	0.008415	- 0.096180	1.80	2	0.168879
3.10	2	- 0.001564	- 0.749297	4.00	3	- 0.139094
2.00	2	0.000686	- 0.064375	9.60	3	- 0.013097
6.00	3	0.000640	- 0.173150			
<hr/>						
$-\epsilon$		40.20039	2.501944			1.226943
$-\tilde{R}$		11.0025	11.0300			13.0616
$-E$			155.8185			
Charge on Sphere	- 1.00			Radius of Sphere		1.70

Table L.5. Parameters for Na^+ with Superposed Potential Sphere

ζ	n	C_{1s}	C_{2s}	ζ	n	C_{2p}
15.00	1	0.118583	0.043908	6.60	2	0.141979
10.30	1	0.854665	0.182553	3.40	2	0.702768
11.00	2	0.031828	0.074895	2.30	2	0.253752
5.40	2	0.008433	- 0.104426	1.80	2	0.132852
3.10	2	- 0.001559	- 0.761746	4.00	3	- 0.150723
2.00	2	0.000681	- 0.057363	9.60	3	- 0.013162
6.00	3	0.000641	- 0.160464			
<hr/>						
$-\epsilon$		40.24794	2.555828			1.279855
$-\tilde{R}$		11.0025	11.0396			13.0923
$-E$			156.4242			
Charge on Sphere	- 1.00			Radius of Sphere		1.90

Table L.6. Radial Characteristics of the Hartree-Fock F^- 1s Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	51.68674	-464.90915	0.	51.68674		
0.01	47.24702	-423.69736	0.47247	43.01005	-39.62169	1.03203
0.02	43.20020	-386.26585	0.86400	35.47488	-16.85553	1.01490
0.03	39.51031	-352.25502	1.18531	28.94265	-6.97345	1.00674
0.04	36.14478	-321.34072	1.44579	23.29115	-1.87223	1.00198
0.05	33.07415	-293.23068	1.65371	18.41261	0.71694	0.99917
0.06	30.27170	-267.66117	1.81630	14.21203	1.86946	0.99764
0.07	27.71325	-244.39423	1.93993	10.60565	2.19740	0.99697
0.08	25.37686	-223.21499	2.03015	7.51966	2.07314	0.99688
0.09	23.24264	-203.92939	2.09184	4.88900	1.72634	0.99716
0.10	21.29255	-186.36206	2.12925	2.65634	1.29678	0.99767
0.12	17.88074	-155.76337	2.14569	-0.81087	0.48024	0.99897
0.14	15.02766	-130.32396	2.10387	-3.21769	-0.09124	1.00023
0.16	12.63940	-109.14698	2.02230	-4.82412	-0.39268	1.00119
0.18	10.63830	-91.49671	1.91489	-5.83111	-0.48655	1.00175
0.20	8.96007	-76.76858	1.79201	-6.39364	-0.44976	1.00192
0.22	7.55141	-64.46506	1.66131	-6.63090	-0.34666	1.00175
0.24	6.36806	-54.17604	1.52833	-6.63419	-0.22246	1.00133
0.26	5.37321	-45.56297	1.39703	-6.47316	-0.10482	1.00075
0.28	4.53624	-38.34592	1.27015	-6.20062	-0.00806	1.00007
0.30	3.83162	-32.29314	1.14949	-5.85632	0.06265	0.99938
0.35	2.51776	-21.07257	0.88122	-4.85764	0.13493	0.99795
0.40	1.65907	-13.79574	0.66363	-3.85922	0.11185	0.99743
0.45	1.09616	-9.05711	0.49327	-2.97954	0.05697	0.99802
0.50	0.72617	-5.96064	0.36308	-2.25415	0.00698	0.99963
0.55	0.48242	-3.93140	0.26533	-1.67985	-0.02488	1.00197
0.60	0.32150	-2.59835	0.19290	-1.23752	-0.03845	1.00457
0.65	0.21504	-1.72088	0.13977	-0.90354	-0.03872	1.00688
0.70	0.14446	-1.14228	0.10112	-0.65514	-0.03137	1.00829
0.75	0.09755	-0.76016	0.07316	-0.47257	-0.02096	1.00821
0.80	0.06630	-0.50742	0.05304	-0.33964	-0.01052	1.00606
0.85	0.04540	-0.34000	0.03859	-0.24360	-0.00169	1.00142
0.90	0.03136	-0.22888	0.02823	-0.17463	0.00486	0.99409
0.95	0.02189	-0.15499	0.02080	-0.12535	0.00908	0.98417
1.00	0.01546	-0.10570	0.01546	-0.09025	0.01126	0.97218
1.10	0.00801	-0.05054	0.00881	-0.04758	0.01124	0.94637
1.20	0.00437	-0.02531	0.00525	-0.02600	0.00813	0.92901
1.30	0.00251	-0.01339	0.00326	-0.01489	0.00427	0.93504
1.40	0.00150	-0.00748	0.00210	-0.00897	0.00091	0.97682
1.50	0.00092	-0.00437	0.00138	-0.00564	-0.00149	1.06146
1.60	0.00058	-0.00263	0.00093	-0.00363	-0.00289	1.19038
1.70	0.00037	-0.00161	0.00063	-0.00236	-0.00349	1.35731
1.80	0.00025	-0.00097	0.00044	-0.00151	-0.00350	1.54209
1.90	0.00017	-0.00058	0.00032	-0.00093	-0.00314	1.70300
2.00	0.00013	-0.00033	0.00025	-0.00054	-0.00258	1.78144
2.10	0.00010	-0.00018	0.00021	-0.00028	-0.00194	1.73407
2.20	0.00009	-0.00009	0.00019	-0.00012	-0.00131	1.57044
2.30	0.00008	-0.00004	0.00019	-0.00002	-0.00073	1.34596
2.40	0.00008	-0.00002	0.00019	0.00003	-0.00024	1.11816
2.50	0.00008	-0.00001	0.00019	0.00004	0.00016	0.91886
2.60	0.00007	-0.00001	0.00019	0.00004	0.00047	0.75795
2.70	0.00007	-0.00002	0.00020	0.00002	0.00070	0.63265
2.80	0.00007	-0.00002	0.00020	0.00000	0.00086	0.53635
2.90	0.00007	-0.00003	0.00020	-0.00002	0.00096	0.46240
3.00	0.00006	-0.00004	0.00019	-0.00004	0.00101	0.40529
3.20	0.00006	-0.00004	0.00018	-0.00008	0.00101	0.32573
3.40	0.00005	-0.00004	0.00017	-0.00010	0.00092	0.27544
3.60	0.00004	-0.00004	0.00015	-0.00010	0.00080	0.24239
3.80	0.00003	-0.00004	0.00012	-0.00010	0.00067	0.21993
4.00	0.00003	-0.00003	0.00010	-0.00010	0.00054	0.20430
4.20	0.00002	-0.00003	0.00009	-0.00009	0.00043	0.19327
4.40	0.00002	-0.00002	0.00007	-0.00007	0.00034	0.18547
4.60	0.00001	-0.00002	0.00006	-0.00006	0.00026	0.18007
4.80	0.00001	-0.00001	0.00004	-0.00005	0.00020	0.17652

* Parameters taken from Table L.1.

Table L.6. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.00001	-0.00001	0.00004	-0.00004	0.00015	0.17449
5.20	0.00001	-0.00001	0.00003	-0.00003	0.00012	0.17375
5.40	0.00000	-0.00001	0.00002	-0.00003	0.00009	0.17418
5.60	0.00000	-0.00000	0.00002	-0.00002	0.00007	0.17572
5.80	0.00000	-0.00000	0.00001	-0.00002	0.00005	0.17837
6.00	0.00000	-0.00000	0.00001	-0.00001	0.00004	0.18215
6.50	0.00000	-0.00000	0.00001	-0.00001	0.00002	0.19710
7.00	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.22174
7.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.25973
8.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.31691
8.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.40223
9.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.52936
9.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.71908
10.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.00301

Table L.7. Radial Characteristics of the Hartree-Fock F^- 2s Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	11.63902	-105.53338	0.	11.63902		
0.01	10.62406	-97.57108	0.10624	9.64835	40.49264	-1.62741
0.02	9.68545	-90.25367	0.19371	7.88037	8.73488	0.37830
0.03	8.81703	-83.52261	0.26451	6.31135	1.35362	0.89417
0.04	8.01322	-77.32515	0.32053	4.92021	-0.79463	1.06836
0.05	7.26891	-71.61378	0.36345	3.68822	-1.31074	1.12431
0.06	6.57946	-66.34560	0.39477	2.59873	-1.26480	1.13252
0.07	5.94065	-61.48194	0.41585	1.63691	-1.03979	1.12066
0.08	5.34859	-56.98788	0.42789	0.78956	-0.78230	1.10083
0.09	4.79976	-52.83186	0.43198	0.04490	-0.54736	1.07861
0.10	4.29092	-48.98535	0.42909	-0.60761	-0.35223	1.05659
0.12	3.38161	-42.12001	0.40579	-1.67280	-0.08228	1.01677
0.14	2.59974	-36.21308	0.36396	-2.47009	0.06280	0.98335
0.16	1.92768	-31.11736	0.30843	-3.05110	0.12790	0.95426
0.18	1.35045	-26.71120	0.24308	-3.45756	0.14571	0.92562
0.20	0.85531	-22.89358	0.17106	-3.72340	0.13718	0.88943
0.22	0.43135	-19.58026	0.09490	-3.87631	0.11519	0.81592
0.24	0.06921	-16.70063	0.01661	-3.93894	0.08753	0.12819
0.26	-0.23917	-14.19524	-0.06218	-3.92993	0.05893	1.16984
0.28	-0.50075	-12.01376	-0.14021	-3.86461	0.03218	1.04430
0.30	-0.72159	-10.11342	-0.21648	-3.75562	0.00889	1.00849
0.35	-1.12818	-6.36533	-0.39486	-3.35605	-0.03029	0.98149
0.40	-1.37635	-3.71502	-0.55054	-2.86235	-0.04352	0.97820
0.45	-1.51277	-1.85256	-0.68075	-2.34642	-0.03842	0.98249
0.50	-1.57104	-0.55813	-0.78552	-1.85010	-0.02411	0.98942
0.55	-1.57539	0.32625	-0.86646	-1.39595	-0.00791	0.99654
0.60	-1.54332	0.91508	-0.92599	-0.99427	0.00563	1.00251
0.65	-1.48741	1.29171	-0.96681	-0.64780	0.01452	1.00673
0.70	-1.41666	1.51692	-0.99166	-0.35482	0.01857	1.00904
0.75	-1.33749	1.63505	-1.00312	-0.11121	0.01860	1.00959
0.80	-1.25440	1.67835	-1.00352	0.08828	0.01585	1.00871
0.85	-1.17051	1.67023	-0.99493	0.24918	0.01155	1.00680
0.90	-1.08795	1.62761	-0.97915	0.37690	0.00672	1.00426
0.95	-1.00812	1.56265	-0.95771	0.47640	0.00211	1.00144
1.00	-0.93191	1.48406	-0.93191	0.55214	-0.00183	0.99865
1.10	-0.79216	1.30877	-0.87138	0.64748	-0.00691	0.99398
1.20	-0.67019	1.13187	-0.80423	0.68804	-0.00845	0.99131
1.30	-0.56537	0.96723	-0.73498	0.69203	-0.00749	0.99087
1.40	-0.47615	0.82034	-0.66661	0.67232	-0.00526	0.99238
1.50	-0.40067	0.69243	-0.60101	0.63798	-0.00269	0.99537
1.60	-0.33706	0.58270	-0.53929	0.59526	-0.00034	0.99930
1.70	-0.28358	0.48946	-0.48209	0.54850	0.00151	1.00366
1.80	-0.23868	0.41072	-0.42963	0.50062	0.00279	1.00806
1.90	-0.20102	0.34450	-0.38193	0.45354	0.00355	1.01218
2.00	-0.16943	0.28896	-0.33885	0.40849	0.00389	1.01583
2.10	-0.14293	0.24245	-0.30014	0.36621	0.00391	1.01888
2.20	-0.12068	0.20353	-0.26551	0.32709	0.00372	1.02125
2.30	-0.10201	0.17099	-0.23462	0.29127	0.00339	1.02294
2.40	-0.08631	0.14378	-0.20714	0.25876	0.00300	1.02397
2.50	-0.07310	0.12101	-0.18276	0.22943	0.00137	1.01290
2.60	-0.06198	0.10196	-0.16116	0.20312	0.00020	1.00219
2.70	-0.05261	0.08600	-0.14204	0.17960	-0.00063	0.99180
2.80	-0.04470	0.07263	-0.12515	0.15866	-0.00118	0.98176
2.90	-0.03801	0.06140	-0.11023	0.14005	-0.00154	0.97206
3.00	-0.03236	0.05197	-0.09707	0.12356	-0.00175	0.96275
3.20	-0.02351	0.03736	-0.07522	0.09605	-0.00186	0.94538
3.40	-0.01713	0.02698	-0.05825	0.07459	-0.00174	0.92986
3.60	-0.01252	0.01956	-0.04507	0.05788	-0.00152	0.91639
3.80	-0.00917	0.01423	-0.03485	0.04490	-0.00126	0.90507
4.00	-0.00673	0.01039	-0.02692	0.03481	-0.00102	0.89594
4.20	-0.00495	0.00760	-0.02077	0.02698	-0.00080	0.88897
4.40	-0.00364	0.00557	-0.01601	0.02089	-0.00061	0.88408
4.60	-0.00268	0.00410	-0.01233	0.01616	-0.00046	0.88118
4.80	-0.00197	0.00301	-0.00948	0.01249	-0.00034	0.88015

* Parameters taken from Table L.1.

Table L.7. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	-0.00145	0.00222	-0.00727	0.00964	-0.00025	0.88088
5.20	-0.00107	0.00164	-0.00558	0.00743	-0.00018	0.88326
5.40	-0.00079	0.00121	-0.00427	0.00572	-0.00013	0.88722
5.60	-0.00058	0.00089	-0.00326	0.00440	-0.00009	0.89269
5.80	-0.00043	0.00066	-0.00249	0.00338	-0.00006	0.89965
6.00	-0.00032	0.00048	-0.00190	0.00259	-0.00004	0.90812
6.50	-0.00015	0.00023	-0.00095	0.00132	-0.00001	0.93629
7.00	-0.00007	0.00010	-0.00048	0.00067	-0.00000	0.97625
7.50	-0.00003	0.00005	-0.00024	0.00033	0.00000	1.03202
8.00	-0.00001	0.00002	-0.00012	0.00017	0.00000	1.11035
8.50	-0.00001	0.00001	-0.00006	0.00008	0.00000	1.22187
9.00	-0.00000	0.00000	-0.00003	0.00004	0.00000	1.38295
9.50	-0.00000	0.00000	-0.00001	0.00002	0.00000	1.61855
10.00	-0.00000	0.00000	-0.00001	0.00001	0.00000	1.96669
10.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	2.48531
11.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	3.26296
11.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	4.43514
12.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	6.20974

Table L.8. Radial Characteristics of the Hartree-Fock F^- 2p Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	0.	18.85864	0.	0.		
0.01	0.18040	17.24371	0.00180	0.35284	-1.54962	16.36285
0.02	0.34530	15.75772	0.00691	0.66046	-1.51458	8.84460
0.03	0.49595	14.38969	0.01488	0.92764	-1.38758	6.00383
0.04	0.63346	13.12967	0.02534	1.15864	-1.20855	4.41215
0.05	0.75887	11.96858	0.03794	1.35730	-1.01041	3.38129
0.06	0.87313	10.89817	0.05239	1.52702	-0.81298	2.66526
0.07	0.97711	9.91093	0.06840	1.67088	-0.62869	2.15072
0.08	1.07160	9.00001	0.08573	1.79160	-0.46427	1.77485
0.09	1.15734	8.15917	0.10416	1.89167	-0.32280	1.49883
0.10	1.23500	7.38275	0.12350	1.97328	-0.20487	1.29669
0.12	1.36849	6.00282	0.16422	2.08883	-0.03480	1.04548
0.14	1.47645	4.82393	0.20670	2.15180	0.06223	0.92462
0.16	1.56259	3.81580	0.25001	2.17312	0.10616	0.87850
0.18	1.63005	2.95309	0.29341	2.16161	0.11506	0.83736
0.20	1.68154	2.21453	0.33631	2.12445	0.10328	0.89015
0.22	1.71934	1.58225	0.37826	2.06744	0.08123	0.91550
0.24	1.74544	1.04115	0.41890	1.99531	0.05591	0.94271
0.26	1.76151	0.57849	0.45799	1.91192	0.03167	0.96785
0.28	1.76903	0.18343	0.49533	1.82039	0.01087	0.98901
0.30	1.76924	-0.15325	0.53077	1.72326	-0.00546	1.00552
0.35	1.74459	-0.78842	0.61061	1.46865	-0.02682	1.02749
0.40	1.69410	-1.20030	0.67764	1.21398	-0.02772	1.02926
0.45	1.62718	-1.45482	0.73223	0.97251	-0.01884	1.02070
0.50	1.55046	-1.59821	0.77523	0.75136	-0.00793	1.00914
0.55	1.46865	-1.66337	0.80776	0.55380	0.00097	0.99882
0.60	1.38503	-1.67393	0.83102	0.38068	0.00650	0.99160
0.65	1.30188	-1.64701	0.84622	0.23133	0.00883	0.98787
0.70	1.22075	-1.59502	0.85452	0.10423	0.00876	0.98717
0.75	1.14265	-1.52700	0.85699	-0.00260	0.00720	0.98873
0.80	1.06821	-1.44946	0.85457	-0.09136	0.00496	0.99170
0.85	0.99778	-1.36709	0.84811	-0.16425	0.00260	0.99534
0.90	0.93152	-1.28321	0.83837	-0.22337	0.00051	0.99903
0.95	0.86945	-1.20012	0.82597	-0.27067	-0.00114	1.00235
1.00	0.81147	-1.11940	0.81147	-0.30793	-0.00229	1.00504
1.10	0.70720	-0.96871	0.77792	-0.35839	-0.00317	1.00802
1.20	0.61715	-0.83514	0.74058	-0.38501	-0.00272	1.00788
1.30	0.53958	-0.71921	0.70145	-0.39539	-0.00162	1.00538
1.40	0.47276	-0.61979	0.66187	-0.39495	-0.00041	1.00154
1.50	0.41513	-0.53508	0.62270	-0.38749	0.00061	0.99739
1.60	0.36532	-0.46310	0.58451	-0.37565	0.00127	0.99380
1.70	0.32215	-0.40196	0.54765	-0.36118	0.00154	0.99143
1.80	0.28462	-0.34995	0.51232	-0.34529	0.00147	0.99075
1.90	0.25190	-0.30561	0.47862	-0.32875	0.00112	0.99206
2.00	0.22329	-0.26767	0.44658	-0.31206	0.00056	0.99551
2.10	0.19819	-0.23510	0.41620	-0.29553	-0.00013	1.00116
2.20	0.17612	-0.20703	0.38746	-0.27935	-0.00088	1.00895
2.30	0.15666	-0.18274	0.36031	-0.26364	-0.00165	1.01878
2.40	0.13946	-0.16163	0.33471	-0.24845	-0.00238	1.03051
2.50	0.12424	-0.14322	0.31061	-0.23381	-0.00098	1.01413
2.60	0.11074	-0.12711	0.28793	-0.21974	-0.00010	1.00154
2.70	0.09875	-0.11296	0.26664	-0.20624	0.00043	0.99228
2.80	0.08809	-0.10050	0.24667	-0.19331	0.00069	0.98590
2.90	0.07861	-0.08949	0.22796	-0.18093	0.00079	0.98200
3.00	0.07015	-0.07975	0.21046	-0.16910	0.00078	0.98020
3.20	0.05590	-0.06343	0.17888	-0.14709	0.00057	0.98161
3.40	0.04455	-0.05051	0.15148	-0.12719	0.00030	0.98776
3.60	0.03552	-0.04025	0.12786	-0.10937	0.00007	0.99671
3.80	0.02832	-0.03206	0.10761	-0.09352	-0.00011	1.00689
4.00	0.02258	-0.02553	0.09033	-0.07955	-0.00022	1.01705
4.20	0.01802	-0.02032	0.07567	-0.06734	-0.00026	1.02621
4.40	0.01438	-0.01617	0.06329	-0.05675	-0.00027	1.03358
4.60	0.01149	-0.01285	0.05287	-0.04764	-0.00025	1.03858
4.80	0.00920	-0.01022	0.04414	-0.03985	-0.00021	1.04072

*Parameters taken from Table L.1.

Table L.8. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.00737	-0.00812	0.03685	-0.03324	-0.00016	1.03967
5.20	0.00592	-0.00646	0.03078	-0.02766	-0.00012	1.03519
5.40	0.00477	-0.00514	0.02573	-0.02297	-0.00007	1.02715
5.60	0.00385	-0.00409	0.02154	-0.01905	-0.00003	1.01549
5.80	0.00312	-0.00326	0.01807	-0.01578	-0.00000	1.00025
6.00	0.00253	-0.00260	0.01519	-0.01307	0.00003	0.98157
6.50	0.00153	-0.00150	0.00998	-0.00818	0.00007	0.92145
7.00	0.00096	-0.00088	0.00670	-0.00517	0.00008	0.84700
7.50	0.00061	-0.00053	0.00461	-0.00333	0.00008	0.76586
8.00	0.00041	-0.00032	0.00325	-0.00219	0.00007	0.68595
8.50	0.00028	-0.00021	0.00235	-0.00149	0.00006	0.61356
9.00	0.00019	-0.00014	0.00172	-0.00103	0.00005	0.55239
9.50	0.00014	-0.00009	0.00128	-0.00074	0.00004	0.50352
10.00	0.00010	-0.00006	0.00097	-0.00054	0.00003	0.46624
10.50	0.00007	-0.00004	0.00073	-0.00040	0.00002	0.43882
11.00	0.00005	-0.00003	0.00056	-0.00030	0.00002	0.41928
11.50	0.00004	-0.00002	0.00043	-0.00023	0.00001	0.40575
12.00	0.00003	-0.00002	0.00033	-0.00018	0.00001	0.39664
12.50	0.00002	-0.00001	0.00025	-0.00013	0.00001	0.39073
13.00	0.00001	-0.00001	0.00019	-0.00010	0.00000	0.38706
13.50	0.00001	-0.00001	0.00014	-0.00008	0.00000	0.38497
14.00	0.00001	-0.00000	0.00011	-0.00006	0.00000	0.38394
14.50	0.00001	-0.00000	0.00008	-0.00005	0.00000	0.38365
15.00	0.00000	-0.00000	0.00006	-0.00004	0.00000	0.38384
15.50	0.00000	-0.00000	0.00005	-0.00003	0.00000	0.38434
17.00	0.00000	-0.00000	0.00002	-0.00001	0.00000	0.38673
18.00	0.00000	-0.00000	0.00001	-0.00001	0.00000	0.38855
19.00	0.00000	-0.00000	0.00001	-0.00000	0.00000	0.39034
20.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.39201
21.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.39357

Table L.9. Radial Characteristics of the Hartree-Fock F^- 1s Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	51.68752	-464.91463	0.	51.68752		
0.01	47.24775	-423.70276	0.47248	43.01072	-39.71544	1.03213
0.02	43.20087	-386.27114	0.86402	35.47545	-16.87950	1.01494
0.03	39.51093	-352.26015	1.18533	28.94312	-6.97832	1.00675
0.04	36.14535	-321.34569	1.44581	23.29152	-1.86984	1.00198
0.05	33.07467	-293.23545	1.65373	18.41290	0.72221	0.99917
0.06	30.27218	-267.66574	1.81633	14.21223	1.87546	0.99763
0.07	27.71368	-244.39859	1.93996	10.60578	2.20325	0.99696
0.08	25.37725	-223.21913	2.03018	7.51972	2.07854	0.99687
0.09	23.24299	-203.93330	2.09187	4.88899	1.73110	0.99715
0.10	21.29286	-186.36576	2.12929	2.65628	1.30090	0.99766
0.12	17.88098	-155.76663	2.14572	-0.81102	0.48316	0.99897
0.14	15.02784	-130.32680	2.10390	-3.21791	-0.08926	1.00023
0.16	12.63952	-109.14944	2.02232	-4.82439	-0.39136	1.00118
0.18	10.63838	-91.49880	1.91491	-5.83141	-0.48568	1.00175
0.20	8.96011	-76.77035	1.79202	-6.39396	-0.44916	1.00192
0.22	7.55142	-64.46654	1.66131	-6.63122	-0.34623	1.00175
0.24	6.36804	-54.17726	1.52833	-6.63450	-0.22211	1.00133
0.26	5.37317	-45.56396	1.39702	-6.47346	-0.10453	1.00074
0.28	4.53618	-38.34671	1.27013	-6.20090	-0.00779	1.00007
0.30	3.83155	-32.29376	1.14946	-5.85658	0.06290	0.99937
0.35	2.51767	-21.07284	0.88118	-4.85783	0.13518	0.99795
0.40	1.65897	-13.79580	0.66359	-3.85935	0.11207	0.99742
0.45	1.09606	-9.05703	0.49323	-2.97960	0.05715	0.99801
0.50	0.72607	-5.96048	0.36304	-2.25417	0.00712	0.99963
0.55	0.48233	-3.93121	0.26528	-1.67983	-0.02479	1.00196
0.60	0.32142	-2.59816	0.19285	-1.23747	-0.03841	1.00457
0.65	0.21497	-1.72069	0.13973	-0.90348	-0.03870	1.00688
0.70	0.14440	-1.14210	0.10108	-0.65507	-0.03136	1.00830
0.75	0.09750	-0.76000	0.07313	-0.47250	-0.02097	1.00822
0.80	0.06625	-0.50728	0.05300	-0.33957	-0.01053	1.00607
0.85	0.04536	-0.33988	0.03856	-0.24353	-0.00170	1.00143
0.90	0.03133	-0.22878	0.02820	-0.17457	0.00485	0.99409
0.95	0.02187	-0.15490	0.02077	-0.12529	0.00907	0.98414
1.00	0.01544	-0.10563	0.01544	-0.09019	0.01125	0.97213
1.10	0.00799	-0.05049	0.00879	-0.04754	0.01124	0.94622
1.20	0.00436	-0.02527	0.00524	-0.02597	0.00813	0.92877
1.30	0.00250	-0.01336	0.00325	-0.01487	0.00427	0.93478
1.40	0.00149	-0.00746	0.00209	-0.00895	0.00091	0.97673
1.50	0.00092	-0.00436	0.00138	-0.00562	-0.00149	1.06187
1.60	0.00058	-0.00262	0.00092	-0.00362	-0.00290	1.19164
1.70	0.00037	-0.00160	0.00063	-0.00234	-0.00349	1.35973
1.80	0.00025	-0.00097	0.00044	-0.00150	-0.00350	1.54560
1.90	0.00017	-0.00057	0.00032	-0.00092	-0.00314	1.70676
2.00	0.00013	-0.00033	0.00025	-0.00053	-0.00257	1.78386
2.10	0.00010	-0.00018	0.00021	-0.00028	-0.00193	1.73392
2.20	0.00009	-0.00009	0.00019	-0.00011	-0.00130	1.56794
2.30	0.00008	-0.00004	0.00019	-0.00002	-0.00073	1.34248
2.40	0.00008	-0.00002	0.00019	0.00003	-0.00024	1.11504
2.50	0.00008	-0.00001	0.00019	0.00004	0.00017	0.91744
2.60	0.00008	-0.00001	0.00020	0.00004	0.00048	0.75838
2.70	0.00007	-0.00002	0.00020	0.00002	0.00070	0.63482
2.80	0.00007	-0.00002	0.00020	0.00000	0.00086	0.53957
2.90	0.00007	-0.00003	0.00020	-0.00002	0.00096	0.46651
3.00	0.00007	-0.00004	0.00020	-0.00004	0.00101	0.41016
3.20	0.00006	-0.00004	0.00018	-0.00008	0.00101	0.33189
3.40	0.00005	-0.00004	0.00017	-0.00010	0.00092	0.28273
3.60	0.00004	-0.00004	0.00015	-0.00011	0.00080	0.25076
3.80	0.00003	-0.00004	0.00013	-0.00010	0.00066	0.22944
4.00	0.00003	-0.00003	0.00011	-0.00010	0.00054	0.21505
4.20	0.00002	-0.00003	0.00009	-0.00009	0.00043	0.20540
4.40	0.00002	-0.00002	0.00007	-0.00007	0.00034	0.19918
4.60	0.00001	-0.00002	0.00006	-0.00006	0.00026	0.19557
4.80	0.00001	-0.00001	0.00005	-0.00005	0.00020	0.19409

* Parameters taken from Table L.2.

Table L.9. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.00001	-0.00001	0.00004	-0.00004	0.00015	0.19443
5.20	0.00001	-0.00001	0.00003	-0.00003	0.00011	0.19643
5.40	0.00000	-0.00001	0.00002	-0.00003	0.00008	0.20002
5.60	0.00000	-0.00000	0.00002	-0.00002	0.00006	0.20523
5.80	0.00000	-0.00000	0.00001	-0.00002	0.00005	0.21211
6.00	0.00000	-0.00000	0.00001	-0.00001	0.00003	0.22080
6.50	0.00000	-0.00000	0.00001	-0.00001	0.00002	0.25177
7.00	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.29973
7.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.37189
8.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.47938
8.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.63912
9.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.87684
9.50	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.23157
10.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.76272

Table L.10. Radial Characteristics of the Hartree-Fock F^- 2s Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	11.64710	-105.46750	0.	11.64710		
0.01	10.63260	-97.54333	0.10633	9.65716	31.78302	-1.10917
0.02	9.69411	-90.25520	0.19388	7.88901	6.27774	0.54307
0.03	8.82556	-83.54614	0.26477	6.31918	0.62061	0.95038
0.04	8.02143	-77.36473	0.32086	4.92684	-0.87836	1.07726
0.05	7.27666	-71.66457	0.36383	3.69344	-1.13715	1.11027
0.06	6.58667	-66.40372	0.39520	2.60245	-1.00370	1.10752
0.07	5.94725	-61.54431	0.41631	1.63915	-0.76980	1.09133
0.08	5.35456	-57.05207	0.42837	0.79040	-0.53956	1.07110
0.09	4.80509	-52.89600	0.43246	0.04445	-0.34665	1.05090
0.10	4.29562	-49.04803	0.42956	-0.60919	-0.19730	1.03241
0.12	3.38510	-42.17699	0.40621	-1.67614	-0.01018	1.00212
0.14	2.60217	-36.26240	0.36430	-2.47457	0.07475	0.97973
0.16	1.92920	-31.15850	0.30867	-3.05616	0.10282	0.96239
0.18	1.35123	-26.74449	0.24322	-3.46278	0.10219	0.94664
0.20	0.85550	-22.91984	0.17110	-3.72847	0.08843	0.92706
0.22	0.43107	-19.60051	0.09484	-3.88104	0.06969	0.88593
0.24	0.06858	-16.71594	0.01646	-3.94324	0.05006	0.48493
0.26	-0.24006	-14.20661	-0.06242	-3.93378	0.03158	1.09281
0.28	-0.50185	-12.02209	-0.14052	-3.86803	0.01522	1.02140
0.30	-0.72283	-10.11946	-0.21685	-3.75866	0.00145	1.00142
0.35	-1.12963	-6.36803	-0.39537	-3.35844	-0.02100	0.98688
0.40	-1.37788	-3.71631	-0.55115	-2.86441	-0.02810	0.98561
0.45	-1.51435	-1.85312	-0.68146	-2.34825	-0.02438	0.98864
0.50	-1.57263	-0.55801	-0.78631	-1.85163	-0.01513	0.99321
0.55	-1.57696	0.32721	-0.86733	-1.39699	-0.00476	0.99787
0.60	-1.54482	0.91699	-0.92689	-0.99462	0.00388	1.00177
0.65	-1.48878	1.29460	-0.96771	-0.64730	0.00950	1.00450
0.70	-1.41787	1.52068	-0.99251	-0.35340	0.01196	1.00595
0.75	-1.33850	1.63948	-1.00387	-0.10889	0.01182	1.00623
0.80	-1.25517	1.68319	-1.00414	0.09138	0.00990	1.00556
0.85	-1.17103	1.67522	-0.99538	0.25291	0.00701	1.00422
0.90	-1.08823	1.63251	-0.97940	0.38103	0.00384	1.00249
0.95	-1.00816	1.56725	-0.95775	0.48073	0.00087	1.00061
1.00	-0.93173	1.48820	-0.93173	0.55647	-0.00161	0.99878
1.10	-0.79163	1.31170	-0.87079	0.65125	-0.00464	0.99586
1.20	-0.66943	1.13350	-0.80331	0.69077	-0.00535	0.99436
1.30	-0.56450	0.96769	-0.73386	0.69350	-0.00452	0.99435
1.40	-0.47528	0.81989	-0.66540	0.67256	-0.00299	0.99556
1.50	-0.39988	0.69136	-0.59982	0.63716	-0.00136	0.99760
1.60	-0.33640	0.58127	-0.53824	0.59364	0.00004	1.00009
1.70	-0.28307	0.48789	-0.48122	0.54635	0.00108	1.00269
1.80	-0.23833	0.40917	-0.42899	0.49818	0.00174	1.00515
1.90	-0.20081	0.34308	-0.38155	0.45104	0.00207	1.00728
2.00	-0.16936	0.28772	-0.33871	0.40609	0.00215	1.00898
2.10	-0.14297	0.24142	-0.30023	0.36402	0.00207	1.01020
2.20	-0.12082	0.20273	-0.26580	0.32518	0.00187	1.01093
2.30	-0.10221	0.17039	-0.23508	0.28968	0.00162	1.01120
2.40	-0.08656	0.14336	-0.20775	0.25750	0.00135	1.01104
2.50	-0.07339	0.12075	-0.18348	0.22849	0.00109	1.01052
2.60	-0.06229	0.10183	-0.16196	0.20246	0.00086	1.00971
2.70	-0.05292	0.08597	-0.14289	0.17921	0.00065	1.00867
2.80	-0.04501	0.07268	-0.12603	0.15848	-0.00012	0.99814
2.90	-0.03832	0.06151	-0.11112	0.14006	-0.00064	0.98819
3.00	-0.03265	0.05212	-0.09795	0.12371	-0.00098	0.97881
3.20	-0.02376	0.03755	-0.07605	0.09641	-0.00129	0.96182
3.40	-0.01735	0.02718	-0.05899	0.07505	-0.00130	0.94726
3.60	-0.01270	0.01974	-0.04572	0.05837	-0.00117	0.93518
3.80	-0.00931	0.01439	-0.03540	0.04538	-0.00098	0.92562
4.00	-0.00684	0.01052	-0.02738	0.03525	-0.00079	0.91855
4.20	-0.00504	0.00771	-0.02115	0.02736	-0.00061	0.91392
4.40	-0.00371	0.00567	-0.01632	0.02122	-0.00046	0.91164
4.60	-0.00273	0.00417	-0.01257	0.01644	-0.00034	0.91163
4.80	-0.00201	0.00307	-0.00967	0.01272	-0.00025	0.91379

* Parameters taken from Table L.2.

Table L.10. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	-0.00149	0.00226	-0.00743	0.00983	-0.00017	0.91805
5.20	-0.00110	0.00167	-0.00570	0.00758	-0.00012	0.92437
5.40	-0.00081	0.00123	-0.00436	0.00584	-0.00008	0.93274
5.60	-0.00060	0.00091	-0.00333	0.00449	-0.00005	0.94320
5.80	-0.00044	0.00067	-0.00254	0.00345	-0.00003	0.95581
6.00	-0.00032	0.00049	-0.00194	0.00264	-0.00001	0.97072
6.50	-0.00015	0.00023	-0.00098	0.00135	0.00000	1.01942
7.00	-0.00007	0.00011	-0.00049	0.00068	0.00001	1.08870
7.50	-0.00003	0.00005	-0.00024	0.00034	0.00001	1.18696
8.00	-0.00001	0.00002	-0.00012	0.00017	0.00001	1.32746
8.50	-0.00001	0.00001	-0.00006	0.00008	0.00001	1.53064
9.00	-0.00000	0.00000	-0.00003	0.00004	0.00000	1.82766
9.50	-0.00000	0.00000	-0.00001	0.00002	0.00000	2.26589
10.00	-0.00000	0.00000	-0.00001	0.00001	0.00000	2.91738
10.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	3.89195
11.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	5.35734
11.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	7.57032
12.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	10.92477

Table L.11. Radial Characteristics of the Hartree-Fock F^- 2p Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	0.	18.82230	0.	0.		
0.01	0.18006	17.21203	0.00180	0.35218	-1.69466	18.90057
0.02	0.34467	15.73002	0.00689	0.65927	-1.63326	10.01273
0.03	0.49505	14.36542	0.01485	0.92601	-1.48404	6.70161
0.04	0.63233	13.10834	0.02529	1.15667	-1.28616	4.86857
0.05	0.75755	11.94976	0.03788	1.35503	-1.07209	3.69168
0.06	0.87163	10.88151	0.05230	1.52452	-0.86122	2.87925
0.07	0.97545	9.89612	0.06828	1.66818	-0.66565	2.29791
0.08	1.06981	8.98680	0.08558	1.78875	-0.49185	1.87444
0.09	1.15542	8.14734	0.10399	1.88868	-0.34262	1.56400
0.10	1.23297	7.37210	0.12330	1.97018	-0.21833	1.33680
0.12	1.36627	5.99409	0.16395	2.08556	-0.03898	1.05426
0.14	1.47407	4.81668	0.20637	2.14840	0.06382	0.91765
0.16	1.56007	3.80971	0.24961	2.16962	0.11102	0.86465
0.18	1.62742	2.94792	0.29294	2.15805	0.12144	0.85807
0.20	1.67881	2.21013	0.33576	2.12084	0.11003	0.87534
0.22	1.71654	1.57851	0.37764	2.06381	0.08762	0.90291
0.24	1.74256	1.03800	0.41821	1.99168	0.06151	0.93286
0.26	1.75858	0.57585	0.45723	1.90830	0.03627	0.96077
0.28	1.76604	0.18126	0.49449	1.81680	0.01442	0.98447
0.30	1.76622	-0.15499	0.52986	1.71972	-0.00291	1.00314
0.35	1.74151	-0.78924	0.60953	1.46528	-0.02630	1.02872
0.40	1.69099	-1.20039	0.67640	1.21084	-0.02836	1.03189
0.45	1.62408	-1.45435	0.73084	0.96962	-0.01990	1.02331
0.50	1.54740	-1.59735	0.77370	0.74873	-0.00895	1.01100
0.55	1.46564	-1.66224	0.80610	0.55141	0.00021	0.99973
0.60	1.38208	-1.67265	0.82925	0.37849	0.00606	0.99166
0.65	1.29900	-1.64564	0.84435	0.22933	0.00865	0.98733
0.70	1.21793	-1.59362	0.85255	0.10240	0.00874	0.98635
0.75	1.13990	-1.52557	0.85493	-0.00427	0.00724	0.98792
0.80	1.06553	-1.44800	0.85243	-0.09287	0.00496	0.99115
0.85	0.99518	-1.36559	0.84590	-0.16557	0.00250	0.99521
0.90	0.92900	-1.28166	0.83610	-0.22449	0.00027	0.99945
0.95	0.86700	-1.19850	0.82365	-0.27157	-0.00153	1.00336
1.00	0.80911	-1.11768	0.80911	-0.30857	-0.00281	1.00661
1.10	0.70502	-0.96677	0.77552	-0.35843	-0.00388	1.01046
1.20	0.61518	-0.83295	0.73822	-0.38436	-0.00344	1.01064
1.30	0.53784	-0.71679	0.69919	-0.39399	-0.00220	1.00777
1.40	0.47127	-0.61719	0.65978	-0.39279	-0.00071	1.00285
1.50	0.41391	-0.53236	0.62086	-0.38463	0.00066	0.99698
1.60	0.36437	-0.46032	0.58300	-0.37214	0.00170	0.99114
1.70	0.32148	-0.39919	0.54652	-0.35715	0.00235	0.98611
1.80	0.28423	-0.34726	0.51161	-0.34083	0.00261	0.98250
1.90	0.25177	-0.30303	0.47837	-0.32399	0.00255	0.98074
2.00	0.22341	-0.26525	0.44682	-0.30710	0.00222	0.98107
2.10	0.19854	-0.23287	0.41694	-0.29049	0.00171	0.98362
2.20	0.17668	-0.20500	0.38870	-0.27432	0.00108	0.98841
2.30	0.15742	-0.18092	0.36206	-0.25870	0.00038	0.99537
2.40	0.14039	-0.16003	0.33695	-0.24367	-0.00032	1.00436
2.50	0.12532	-0.14183	0.31330	-0.22925	-0.00100	1.01518
2.60	0.11195	-0.12592	0.29107	-0.21544	-0.00163	1.02763
2.70	0.10007	-0.11197	0.27020	-0.20224	-0.00218	1.04147
2.80	0.08950	-0.09968	0.25061	-0.18961	-0.00147	1.03130
2.90	0.08009	-0.08885	0.23225	-0.17757	-0.00100	1.02375
3.00	0.07169	-0.07926	0.21508	-0.16608	-0.00069	1.01842
3.20	0.05751	-0.06320	0.18403	-0.14473	-0.00039	1.01292
3.40	0.04619	-0.05049	0.15705	-0.12547	-0.00029	1.01212
3.60	0.03714	-0.04038	0.13371	-0.10822	-0.00027	1.01382
3.80	0.02990	-0.03231	0.11363	-0.09289	-0.00026	1.01625
4.00	0.02411	-0.02587	0.09643	-0.07936	-0.00023	1.01804
4.20	0.01947	-0.02071	0.08177	-0.06753	-0.00019	1.01811
4.40	0.01575	-0.01659	0.06932	-0.05726	-0.00013	1.01569
4.60	0.01278	-0.01330	0.05877	-0.04840	-0.00007	1.01022
4.80	0.01039	-0.01067	0.04987	-0.04081	-0.00001	1.00136

* Parameters taken from Table L.2.

Table L.11. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.00848	-0.00856	0.04238	-0.03434	0.00005	0.98894
5.20	0.00694	-0.00689	0.03607	-0.02887	0.00010	0.97298
5.40	0.00570	-0.00555	0.03077	-0.02425	0.00014	0.95361
5.60	0.00470	-0.00448	0.02632	-0.02037	0.00017	0.93109
5.80	0.00389	-0.00362	0.02258	-0.01713	0.00019	0.90580
6.00	0.00324	-0.00294	0.01943	-0.01442	0.00021	0.87821
6.50	0.00209	-0.00178	0.01356	-0.00946	0.00022	0.80257
7.00	0.00138	-0.00110	0.00967	-0.00632	0.00020	0.72426
7.50	0.00094	-0.00070	0.00705	-0.00433	0.00017	0.65075
8.00	0.00065	-0.00046	0.00523	-0.00305	0.00014	0.58695
8.50	0.00046	-0.00031	0.00393	-0.00220	0.00011	0.53500
9.00	0.00033	-0.00022	0.00298	-0.00162	0.00009	0.49479
9.50	0.00024	-0.00015	0.00228	-0.00122	0.00007	0.46495
10.00	0.00018	-0.00011	0.00175	-0.00092	0.00005	0.44355
10.50	0.00013	-0.00008	0.00135	-0.00071	0.00004	0.42868
11.00	0.00009	-0.00006	0.00103	-0.00054	0.00003	0.41869
11.50	0.00007	-0.00004	0.00079	-0.00042	0.00002	0.41222
12.00	0.00005	-0.00003	0.00061	-0.00032	0.00002	0.40826
12.50	0.00004	-0.00002	0.00047	-0.00025	0.00001	0.40604
13.00	0.00003	-0.00002	0.00036	-0.00019	0.00001	0.40502
13.50	0.00002	-0.00001	0.00027	-0.00015	0.00001	0.40481
14.00	0.00001	-0.00001	0.00021	-0.00011	0.00000	0.40513
14.50	0.00001	-0.00001	0.00016	-0.00009	0.00000	0.40580
15.00	0.00001	-0.00000	0.00012	-0.00007	0.00000	0.40668
15.50	0.00001	-0.00000	0.00009	-0.00005	0.00000	0.40768
17.00	0.00000	-0.00000	0.00004	-0.00002	0.00000	0.41094
18.00	0.00000	-0.00000	0.00002	-0.00001	0.00000	0.41305
19.00	0.00000	-0.00000	0.00001	-0.00001	0.00000	0.41503
20.00	0.00000	-0.00000	0.00001	-0.00000	0.00000	0.41686
21.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.41853

Table L.12. Radial Characteristics of the Hartree-Fock F^- 1s Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	51.68849	-464.92234	0.	51.68849		
0.01	47.24864	-423.71006	0.47249	43.01154	-39.79314	1.03229
0.02	43.20169	-386.27804	0.86403	35.47613	-16.91156	1.01501
0.03	39.51168	-352.26669	1.18535	28.94368	-6.99652	1.00679
0.04	36.14604	-321.35187	1.44584	23.29196	-1.88219	1.00200
0.05	33.07529	-293.24129	1.65376	18.41323	0.71272	0.99917
0.06	30.27275	-267.67126	1.81636	14.21247	1.86760	0.99763
0.07	27.71420	-244.40379	1.93999	10.60593	2.19634	0.99696
0.08	25.37771	-223.22404	2.03022	7.51979	2.07222	0.99687
0.09	23.24341	-203.93793	2.09191	4.88899	1.72516	0.99715
0.10	21.29323	-186.37011	2.12932	2.65622	1.29529	0.99767
0.12	17.88127	-155.77046	2.14575	-0.81119	0.47815	0.99897
0.14	15.02806	-130.33015	2.10393	-3.21816	-0.09370	1.00024
0.16	12.63968	-109.15235	2.02235	-4.82470	-0.39526	1.00120
0.18	10.63848	-91.50132	1.91493	-5.83175	-0.48905	1.00176
0.20	8.96017	-76.77250	1.79203	-6.39433	-0.45205	1.00193
0.22	7.55144	-64.46836	1.66132	-6.63160	-0.34867	1.00177
0.24	6.36802	-54.17879	1.52833	-6.63489	-0.22416	1.00135
0.26	5.37313	-45.56522	1.39701	-6.47383	-0.10622	1.00076
0.28	4.53612	-38.34773	1.27011	-6.20125	-0.00918	1.00008
0.30	3.83146	-32.29457	1.14944	-5.85691	0.06178	0.99938
0.35	2.51755	-21.07324	0.88114	-4.85808	0.13454	0.99795
0.40	1.65885	-13.79592	0.66354	-3.85952	0.11172	0.99742
0.45	1.09593	-9.05696	0.49317	-2.97970	0.05696	0.99801
0.50	0.72595	-5.96030	0.36298	-2.25420	0.00701	0.99963
0.55	0.48222	-3.93097	0.26522	-1.67981	-0.02486	1.00198
0.60	0.32132	-2.59790	0.19279	-1.23742	-0.03847	1.00459
0.65	0.21488	-1.72044	0.13967	-0.90340	-0.03875	1.00691
0.70	0.14433	-1.14187	0.10103	-0.65499	-0.03141	1.00834
0.75	0.09744	-0.75980	0.07308	-0.47241	-0.02100	1.00826
0.80	0.06620	-0.50711	0.05296	-0.33948	-0.01055	1.00611
0.85	0.04532	-0.33973	0.03852	-0.24345	-0.00171	1.00145
0.90	0.03130	-0.22866	0.02817	-0.17450	0.00484	0.99407
0.95	0.02183	-0.15480	0.02074	-0.12522	0.00907	0.98407
1.00	0.01541	-0.10554	0.01541	-0.09014	0.01126	0.97199
1.10	0.00797	-0.05043	0.00877	-0.04750	0.01125	0.94590
1.20	0.00435	-0.02523	0.00522	-0.02593	0.00813	0.92829
1.30	0.00249	-0.01333	0.00324	-0.01484	0.00427	0.93431
1.40	0.00148	-0.00744	0.00208	-0.00893	0.00090	0.97669
1.50	0.00091	-0.00434	0.00137	-0.00560	-0.00150	1.06296
1.60	0.00057	-0.00261	0.00091	-0.00360	-0.00291	1.19485
1.70	0.00037	-0.00158	0.00062	-0.00233	-0.00350	1.36613
1.80	0.00024	-0.00096	0.00044	-0.00148	-0.00350	1.55571
1.90	0.00017	-0.00056	0.00032	-0.00091	-0.00314	1.71937
2.00	0.00012	-0.00032	0.00025	-0.00052	-0.00257	1.79546
2.10	0.00010	-0.00017	0.00021	-0.00026	-0.00193	1.74052
2.20	0.00009	-0.00009	0.00019	-0.00010	-0.00129	1.56837
2.30	0.00008	-0.00004	0.00019	-0.00001	-0.00072	1.33872
2.40	0.00008	-0.00002	0.00019	0.00004	-0.00023	1.10994
2.50	0.00008	-0.00001	0.00019	0.00005	0.00018	0.91302
2.60	0.00008	-0.00001	0.00020	0.00004	0.00049	0.75560
2.70	0.00007	-0.00002	0.00020	0.00003	0.00071	0.63394
2.80	0.00007	-0.00002	0.00020	0.00000	0.00087	0.54106
2.90	0.00007	-0.00003	0.00020	-0.00002	0.00097	0.47019
3.00	0.00007	-0.00004	0.00020	-0.00004	0.00101	0.41583
3.20	0.00006	-0.00004	0.00019	-0.00008	0.00101	0.34108
3.40	0.00005	-0.00004	0.00017	-0.00010	0.00092	0.29504
3.60	0.00004	-0.00004	0.00015	-0.00011	0.00079	0.26605
3.80	0.00003	-0.00004	0.00013	-0.00011	0.00066	0.24768
4.00	0.00003	-0.00003	0.00011	-0.00010	0.00053	0.23589
4.20	0.00002	-0.00003	0.00009	-0.00009	0.00042	0.22914
4.40	0.00002	-0.00002	0.00007	-0.00008	0.00033	0.22617
4.60	0.00001	-0.00002	0.00006	-0.00006	0.00025	0.22627
4.80	0.00001	-0.00001	0.00005	-0.00005	0.00019	0.22901

* Parameters taken from Table L.3.

Table L.12. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.00001	-0.00001	0.00004	-0.00004	0.00015	0.23421
5.20	0.00001	-0.00001	0.00003	-0.00003	0.00011	0.24180
5.40	0.00000	-0.00001	0.00002	-0.00003	0.00008	0.25184
5.60	0.00000	-0.00000	0.00002	-0.00002	0.00006	0.26449
5.80	0.00000	-0.00000	0.00001	-0.00002	0.00004	0.27999
6.00	0.00000	-0.00000	0.00001	-0.00001	0.00003	0.29866
6.50	0.00000	-0.00000	0.00001	-0.00001	0.00001	0.36213
7.00	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.45742
7.50	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.59890
8.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.80842
8.50	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.11910
9.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	1.58109
9.50	0.00000	-0.00000	0.00000	-0.00000	-0.00000	2.27050
10.00	0.00000	-0.00000	0.00000	-0.00000	-0.00000	3.30302

Table L.13. Radial Characteristics of the Hartree-Fock F^- 2s Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	11.66674	-105.49685	0.	11.66674		
0.01	10.65177	-97.60625	0.10652	9.67571	22.52785	-0.58862
0.02	9.71252	-90.34278	0.19425	7.90567	3.67350	0.71590
0.03	8.84301	-83.65108	0.26529	6.33348	-0.15015	1.01275
0.04	8.03776	-77.48112	0.32151	4.93852	-0.95961	1.08968
0.05	7.29180	-71.78764	0.36459	3.70242	-0.94604	1.09745
0.06	6.60056	-66.52970	0.39603	2.60878	-0.72090	1.08204
0.07	5.95988	-61.67025	0.41719	1.64296	-0.47895	1.06036
0.08	5.36594	-57.17571	0.42927	0.79188	-0.27903	1.03906
0.09	4.81525	-53.01563	0.43337	0.04384	-0.13199	1.02059
0.10	4.30460	-49.16243	0.43046	-0.61164	-0.03234	1.00564
0.12	3.39192	-42.27868	0.40703	-1.68152	0.06512	0.98558
0.14	2.60709	-36.35014	0.36499	-2.48193	0.08508	0.97549
0.16	1.93251	-31.23249	0.30920	-3.06469	0.07331	0.97150
0.18	1.35319	-26.80575	0.24357	-3.47184	0.05299	0.97059
0.20	0.85635	-22.96978	0.17127	-3.73761	0.03387	0.97029
0.22	0.43102	-19.64072	0.09483	-3.88994	0.01896	0.96696
0.24	0.06781	-16.74799	0.01627	-3.95171	0.00836	0.90743
0.26	-0.24141	-14.23194	-0.06277	-3.94171	0.00116	1.00361
0.28	-0.50364	-12.04199	-0.14102	-3.87539	-0.00361	0.99461
0.30	-0.72497	-10.13501	-0.21749	-3.76547	-0.00675	0.99301
0.35	-1.13235	-6.37628	-0.39632	-3.36405	-0.01037	0.99312
0.40	-1.38091	-3.72046	-0.55236	-2.86909	-0.01031	0.99439
0.45	-1.51751	-1.85469	-0.68288	-2.35212	-0.00779	0.99615
0.50	-1.57582	-0.55762	-0.78791	-1.85463	-0.00391	0.99814
0.55	-1.58008	0.32932	-0.86905	-1.39896	0.00009	1.00004
0.60	-1.54780	0.92069	-0.92868	-0.99538	0.00324	1.00157
0.65	-1.49154	1.29970	-0.96950	-0.64674	0.00507	1.00255
0.70	-1.42035	1.52694	-0.99424	-0.35149	0.00556	1.00294
0.75	-1.34063	1.64658	-1.00548	-0.10570	0.00497	1.00278
0.80	-1.25694	1.69080	-1.00555	0.09570	0.00371	1.00221
0.85	-1.17242	1.68301	-0.99655	0.25814	0.00215	1.00138
0.90	-1.08922	1.64016	-0.98030	0.38693	0.00063	1.00043
0.95	-1.00878	1.57453	-0.95834	0.48702	-0.00067	0.99950
1.00	-0.93200	1.49490	-0.93200	0.56290	-0.00162	0.99869
1.10	-0.79130	1.31689	-0.87043	0.65728	-0.00247	0.99765
1.20	-0.66867	1.13703	-0.80240	0.69577	-0.00222	0.99751
1.30	-0.56347	0.96970	-0.73251	0.69714	-0.00141	0.99811
1.40	-0.47411	0.82063	-0.66376	0.67477	-0.00051	0.99919
1.50	-0.39869	0.69115	-0.59803	0.63805	0.00024	1.00045
1.60	-0.33526	0.58043	-0.53641	0.59343	0.00073	1.00163
1.70	-0.28203	0.48667	-0.47946	0.54531	0.00096	1.00256
1.80	-0.23743	0.40778	-0.42737	0.49657	0.00100	1.00315
1.90	-0.20005	0.34165	-0.38010	0.44909	0.00089	1.00335
2.00	-0.16873	0.28636	-0.33747	0.40399	0.00071	1.00318
2.10	-0.14248	0.24019	-0.29920	0.36192	0.00050	1.00266
2.20	-0.12044	0.20165	-0.26497	0.32319	0.00030	1.00184
2.30	-0.10193	0.16948	-0.23445	0.28786	0.00011	1.00079
2.40	-0.08637	0.14261	-0.20729	0.25589	-0.00005	0.99958
2.50	-0.07327	0.12015	-0.18316	0.22710	-0.00017	0.99826
2.60	-0.06222	0.10135	-0.16177	0.20130	-0.00026	0.99692
2.70	-0.05289	0.08561	-0.14281	0.17826	-0.00031	0.99561
2.80	-0.04501	0.07241	-0.12603	0.15773	-0.00034	0.99440
2.90	-0.03834	0.06132	-0.11119	0.13948	-0.00034	0.99335
3.00	-0.03269	0.05199	-0.09807	0.12328	0.00033	0.99252
3.20	-0.02382	0.03751	-0.07623	0.09621	-0.00026	0.99170
3.40	-0.01741	0.02718	-0.05919	0.07500	-0.00018	0.99230
3.60	-0.01276	0.01977	-0.04592	0.05842	-0.00009	0.99460
3.80	-0.00936	0.01443	-0.03559	0.04547	-0.00002	0.99822
4.00	-0.00689	0.01056	-0.02754	0.03536	-0.00005	0.99458
4.20	-0.00507	0.00775	-0.02129	0.02748	-0.00004	0.99403
4.40	-0.00374	0.00570	-0.01644	0.02133	-0.00002	0.99651
4.60	-0.00275	0.00419	-0.01267	0.01654	0.00001	1.00199
4.80	-0.00203	0.00309	-0.00975	0.01280	0.00003	1.01045

* Parameters taken from Table L.3.

Table L.13. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	-0.00150	0.00228	-0.00749	0.00990	0.00004	1.02195
5.20	-0.00111	0.00168	-0.00575	0.00764	0.00005	1.03655
5.40	-0.00082	0.00124	-0.00440	0.00589	0.00006	1.05440
5.60	-0.00060	0.00092	-0.00337	0.00453	0.00006	1.07573
5.80	-0.00044	0.00068	-0.00257	0.00348	0.00006	1.10085
6.00	-0.00033	0.00050	-0.00196	0.00267	0.00006	1.13014
6.50	-0.00015	0.00023	-0.00099	0.00136	0.00005	1.22524
7.00	-0.00007	0.00011	-0.00049	0.00069	0.00003	1.36144
7.50	-0.00003	0.00005	-0.00024	0.00034	0.00002	1.55705
8.00	-0.00001	0.00002	-0.00012	0.00017	0.00002	1.84024
8.50	-0.00001	0.00001	-0.00006	0.00008	0.00001	2.25393
9.00	-0.00000	0.00000	-0.00003	0.00004	0.00001	2.86322
9.50	-0.00000	0.00000	-0.00001	0.00002	0.00001	3.76690
10.00	-0.00000	0.00000	-0.00001	0.00001	0.00000	5.11520
10.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	7.13706
11.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	10.18211
11.50	-0.00000	0.00000	-0.00000	0.00000	0.00000	14.78557
12.00	-0.00000	0.00000	-0.00000	0.00000	0.00000	21.76851

Table L.14. Radial Characteristics of the Hartree-Fock F^- 2p Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	0.	18.70288	0.	0.		
0.01	0.17902	17.12184	0.00179	0.35024	-3.50461	45.63183
0.02	0.34285	15.66338	0.00686	0.65611	-3.13301	21.83354
0.03	0.49266	14.31755	0.01478	0.92219	-2.71714	13.57375
0.04	0.62954	13.07521	0.02518	1.15255	-2.29068	9.29546
0.05	0.75448	11.92805	0.03772	1.35088	-1.88136	6.68490
0.06	0.86839	10.86846	0.05210	1.52050	-1.50450	4.94979
0.07	0.97212	9.88947	0.06805	1.66438	-1.16859	3.74058
0.08	1.06643	8.98470	0.08531	1.78521	-0.87690	2.87463
0.09	1.15204	8.14831	0.10368	1.88539	-0.62933	2.24541
0.10	1.22961	7.37496	0.12296	1.96710	-0.42370	1.78559
0.12	1.36298	5.99819	0.16356	2.08276	-0.12369	1.20689
0.14	1.47086	4.81987	0.20592	2.14564	0.05616	0.91295
0.16	1.55690	3.81093	0.24910	2.16665	0.14885	0.78203
0.18	1.62426	2.94683	0.29237	2.15469	0.18254	0.74379
0.20	1.67560	2.20683	0.33512	2.11697	0.17922	0.75616
0.22	1.71324	1.57336	0.37691	2.05938	0.15503	0.79371
0.24	1.73915	1.03149	0.41740	1.98671	0.12116	0.84117
0.26	1.75503	0.56852	0.45631	1.90284	0.08499	0.88960
0.28	1.76234	0.17360	0.49346	1.81095	0.05097	0.93406
0.30	1.76236	-0.16253	0.52871	1.71360	0.02157	0.97210
0.35	1.73731	-0.79504	0.60806	1.45905	-0.02692	1.03533
0.40	1.68658	-1.20339	0.67463	1.20522	-0.04380	1.05920
0.45	1.61959	-1.45447	0.72881	0.96508	-0.04070	1.05729
0.50	1.54296	-1.59512	0.77148	0.74540	-0.02849	1.04209
0.55	1.46136	-1.65848	0.80375	0.54919	-0.01439	1.02245
0.60	1.37801	-1.66816	0.82680	0.37711	-0.00228	1.00376
0.65	1.29515	-1.64113	0.84185	0.22841	0.00636	0.98880
0.70	1.21430	-1.58959	0.85001	0.10158	0.01141	0.97859
0.75	1.13645	-1.52235	0.85234	-0.00531	0.01340	0.97312
0.80	1.06222	-1.44572	0.84978	-0.09436	0.01313	0.97182
0.85	0.99196	-1.36425	0.84316	-0.16765	0.01138	0.97384
0.90	0.92582	-1.28114	0.83324	-0.22720	0.00882	0.97827
0.95	0.86383	-1.19863	0.82064	-0.27486	0.00597	0.98426
1.00	0.80592	-1.11827	0.80592	-0.31235	0.00317	0.99104
1.10	0.70175	-0.96765	0.77193	-0.36266	-0.00143	1.00463
1.20	0.61184	-0.83343	0.73421	-0.38828	-0.00417	1.01554
1.30	0.53449	-0.71642	0.69484	-0.39685	-0.00517	1.02204
1.40	0.46801	-0.61576	0.65522	-0.39406	-0.00487	1.02372
1.50	0.41085	-0.52987	0.61627	-0.38396	-0.00379	1.02103
1.60	0.36161	-0.45690	0.57857	-0.36943	-0.00237	1.01492
1.70	0.31910	-0.39503	0.54247	-0.35246	-0.00092	1.00655
1.80	0.28229	-0.34259	0.50812	-0.33437	0.00035	0.99714
1.90	0.25032	-0.29808	0.47560	-0.31603	0.00135	0.98775
2.00	0.22245	-0.26021	0.44490	-0.29798	0.00202	0.97930
2.10	0.19809	-0.22791	0.41598	-0.28052	0.00239	0.97247
2.20	0.17672	-0.20025	0.38877	-0.26383	0.00250	0.96774
2.30	0.15791	-0.17647	0.36319	-0.24797	0.00240	0.96539
2.40	0.14131	-0.15594	0.33915	-0.23295	0.00214	0.96550
2.50	0.12663	-0.13815	0.31657	-0.21875	0.00178	0.96802
2.60	0.11361	-0.12266	0.29538	-0.20532	0.00136	0.97281
2.70	0.10203	-0.10913	0.27549	-0.19262	0.00091	0.97962
2.80	0.09172	-0.09726	0.25683	-0.18061	0.00048	0.98817
2.90	0.08253	-0.08682	0.23934	-0.16924	0.00007	0.99814
3.00	0.07432	-0.07760	0.22296	-0.15847	-0.00030	1.00920
3.20	0.06040	-0.06219	0.19329	-0.13860	-0.00088	1.03333
3.40	0.04923	-0.05001	0.16738	-0.12080	-0.00126	1.05816
3.60	0.04023	-0.04031	0.14485	-0.10490	-0.00144	1.08167
3.80	0.03298	-0.03257	0.12531	-0.09078	-0.00145	1.10057
4.00	0.02711	-0.02635	0.10843	-0.07831	-0.00104	1.08722
4.20	0.02235	-0.02136	0.09388	-0.06737	-0.00071	1.07205
4.40	0.01850	-0.01735	0.08138	-0.05784	-0.00044	1.05434
4.60	0.01536	-0.01412	0.07066	-0.04958	-0.00023	1.03375
4.80	0.01281	-0.01152	0.06147	-0.04247	-0.00006	1.01025

* Parameters taken from Table L.3.

Table L.14. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
5.00	0.01072	-0.00942	0.05360	-0.03638	0.00008	0.98402
5.20	0.00901	-0.00773	0.04686	-0.03117	0.00018	0.95545
5.40	0.00761	-0.00636	0.04108	-0.02675	0.00025	0.92503
5.60	0.00645	-0.00526	0.03612	-0.02299	0.00030	0.89334
5.80	0.00549	-0.00436	0.03185	-0.01981	0.00033	0.86097
6.00	0.00469	-0.00363	0.02816	-0.01711	0.00035	0.82850
6.50	0.00322	-0.00235	0.02096	-0.01205	0.00035	0.75024
7.00	0.00226	-0.00156	0.01583	-0.00868	0.00032	0.68088
7.50	0.00161	-0.00107	0.01210	-0.00639	0.00027	0.62359
8.00	0.00117	-0.00075	0.00932	-0.00481	0.00022	0.57888
8.50	0.00085	-0.00053	0.00722	-0.00367	0.00017	0.54555
9.00	0.00062	-0.00038	0.00560	-0.00283	0.00013	0.52166
9.50	0.00046	-0.00028	0.00435	-0.00220	0.00010	0.50513
10.00	0.00034	-0.00021	0.00338	-0.00172	0.00007	0.49414
10.50	0.00025	-0.00015	0.00262	-0.00134	0.00006	0.48718
11.00	0.00018	-0.00011	0.00202	-0.00105	0.00004	0.48307
11.50	0.00014	-0.00008	0.00156	-0.00081	0.00003	0.48094
12.00	0.00010	-0.00006	0.00120	-0.00063	0.00002	0.48018
12.50	0.00007	-0.00005	0.00092	-0.00049	0.00002	0.48032
13.00	0.00005	-0.00003	0.00070	-0.00038	0.00001	0.48106
13.50	0.00004	-0.00002	0.00054	-0.00029	0.00001	0.48217
14.00	0.00003	-0.00002	0.00041	-0.00022	0.00001	0.48351
14.50	0.00002	-0.00001	0.00031	-0.00017	0.00000	0.48496
15.00	0.00002	-0.00001	0.00024	-0.00013	0.00000	0.48647
15.50	0.00001	-0.00001	0.00018	-0.00010	0.00000	0.48799
17.00	0.00000	-0.00000	0.00008	-0.00004	0.00000	0.49236
18.00	0.00000	-0.00000	0.00004	-0.00002	0.00000	0.49502
19.00	0.00000	-0.00000	0.00002	-0.00001	0.00000	0.49745
20.00	0.00000	-0.00000	0.00001	-0.00001	0.00000	0.49966
21.00	0.00000	-0.00000	0.00001	-0.00000	0.00000	0.50168

Table L.15. Radial Characteristics of the Hartree-Fock Na^+ 1s Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	70.28300	-773.28617	0.	70.28300		
0.01	62.97168	-690.59152	0.62972	56.065771	12569.18164	-3.96514
0.02	56.44080	-617.01386	1.12882	44.10052	5630.77142	-1.48167
0.03	50.60449	-551.51334	1.51813	34.05909	3368.98251	-0.65607
0.04	45.38668	-493.17299	1.81547	25.65976	2269.33261	-0.24377
0.05	40.71987	-441.18370	2.03599	18.66069	1630.81073	0.00375
0.06	36.54422	-394.83107	2.19265	12.85436	1220.66214	0.16910
0.07	32.80658	-353.48392	2.29646	8.06270	939.58733	0.28756
0.08	29.45973	-316.58426	2.35678	4.13299	738.16598	0.37670
0.09	26.46172	-283.63850	2.38155	0.93425	589.06432	0.44625
0.10	23.77524	-254.20976	2.37752	-1.64574	475.95235	0.50202
0.12	19.20773	-204.39964	2.30493	-5.32023	319.80264	0.58583
0.14	15.53293	-164.55632	2.17461	-7.50495	221.28785	0.64562
0.16	12.57276	-132.63516	2.01164	-8.64887	156.58039	0.69020
0.18	10.18554	-107.02311	1.83340	-9.07862	112.77118	0.72459
0.20	8.25834	-86.44472	1.65167	-9.03061	82.38919	0.75183
0.22	6.70098	-69.88933	1.47421	-8.67468	60.89921	0.77393
0.24	5.44133	-56.55442	1.30592	-8.13173	45.44617	0.79224
0.26	4.42161	-45.80151	1.14962	-7.48678	34.17922	0.80771
0.28	3.59547	-37.12166	1.00673	-6.79859	25.86846	0.82103
0.30	2.92565	-30.10846	0.87770	-6.10688	19.67877	0.83268
0.35	1.75248	-17.88962	0.61337	-4.50889	10.09704	0.85668
0.40	1.05418	-10.66981	0.42167	-3.21375	5.26574	0.87574
0.45	0.63702	-6.38628	0.28666	-2.23681	2.78141	0.89139
0.50	0.38693	-3.83596	0.19346	-1.53105	1.49122	0.90413
0.55	0.23646	-2.31283	0.13005	-1.03560	0.81724	0.91403
0.60	0.14556	-1.40051	0.08733	-0.69475	0.46268	0.92093
0.65	0.09039	-0.85241	0.05875	-0.46368	0.27359	0.92471
0.70	0.05672	-0.52205	0.03970	-0.30871	0.17009	0.92540
0.75	0.03603	-0.32216	0.02702	-0.20559	0.11097	0.92338
0.80	0.02321	-0.20065	0.01857	-0.13731	0.07515	0.91945
0.85	0.01518	-0.12635	0.01291	-0.09222	0.05194	0.91491
0.90	0.01010	-0.08060	0.00909	-0.06244	0.03593	0.91152
0.95	0.00684	-0.05217	0.00650	-0.04273	0.02437	0.91134
1.00	0.00471	-0.03432	0.00471	-0.02961	0.01581	0.91649
1.10	0.00235	-0.01562	0.00258	-0.01483	0.00472	0.95000
1.20	0.00124	-0.00759	0.00149	-0.00786	-0.00105	1.02101
1.30	0.00069	-0.00388	0.00090	-0.00436	-0.00353	1.12735
1.40	0.00040	-0.00206	0.00056	-0.00248	-0.00409	1.25280
1.50	0.00025	-0.00111	0.00037	-0.00142	-0.00364	1.36435
1.60	0.00016	-0.00061	0.00026	-0.00081	-0.00276	1.41640
1.70	0.00012	-0.00033	0.00020	-0.00045	-0.00179	1.37339
1.80	0.00009	-0.00019	0.00017	-0.00024	-0.00091	1.23955
1.90	0.00008	-0.00011	0.00015	-0.00013	-0.00018	1.05496
2.00	0.00007	-0.00007	0.00014	-0.00008	0.00038	0.86596
2.10	0.00006	-0.00006	0.00013	-0.00005	0.00077	0.70032
2.20	0.00006	-0.00005	0.00013	-0.00005	0.00103	0.56657
2.30	0.00005	-0.00005	0.00012	-0.00005	0.00117	0.46273
2.40	0.00005	-0.00005	0.00012	-0.00006	0.00123	0.38330
2.50	0.00005	-0.00004	0.00011	-0.00007	0.00123	0.32264
2.60	0.00004	-0.00004	0.00011	-0.00007	0.00118	0.27602
2.70	0.00004	-0.00004	0.00010	-0.00008	0.00111	0.23986
2.80	0.00003	-0.00004	0.00009	-0.00008	0.00103	0.21149
2.90	0.00003	-0.00004	0.00008	-0.00008	0.00093	0.18896
3.00	0.00003	-0.00003	0.00008	-0.00007	0.00084	0.17088
3.10	0.00002	-0.00003	0.00007	-0.00007	0.00074	0.15619
3.20	0.00002	-0.00003	0.00006	-0.00007	0.00066	0.14413
3.30	0.00002	-0.00002	0.00005	-0.00006	0.00058	0.13413
3.40	0.00001	-0.00002	0.00005	-0.00006	0.00050	0.12577
3.50	0.00001	-0.00002	0.00004	-0.00005	0.00043	0.11871
3.60	0.00001	-0.00002	0.00004	-0.00005	0.00037	0.11270
3.70	0.00001	-0.00001	0.00003	-0.00004	0.00032	0.10756
3.80	0.00001	-0.00001	0.00003	-0.00004	0.00028	0.10312
3.90	0.00001	-0.00001	0.00003	-0.00003	0.00024	0.09926

*Parameters taken from Table L.4.

Table L.15. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	0.00001	-0.00001	0.00002	-0.00003	0.00020	0.09590
4.10	0.00000	-0.00001	0.00002	-0.00003	0.00017	0.09294
4.20	0.00000	-0.00001	0.00002	-0.00002	0.00014	0.09034
4.40	0.00000	-0.00000	0.00001	-0.00002	0.00010	0.08597
4.60	0.00000	-0.00000	0.00001	-0.00001	0.00007	0.08249
4.80	0.00000	-0.00000	0.00001	-0.00001	0.00005	0.07968
5.00	0.00000	-0.00000	0.00000	-0.00001	0.00004	0.07738
5.20	0.00000	-0.00000	0.00000	-0.00001	0.00003	0.07548
5.40	0.00000	-0.00000	0.00000	-0.00000	0.00002	0.07390
5.60	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.07259
5.80	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.07148
6.00	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.07056
6.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06978
6.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06912
6.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06858
6.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06812
7.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06775
7.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06744
7.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06720
7.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06701
7.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06688
8.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06678
8.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06673
8.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06671
8.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06672
8.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06677
9.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06684

Table L.16. Radial Characteristics of the Hartree-Fock $\text{Na}^+ 2s$ Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	17.16724	-189.35525	0.	17.16724		
0.01	15.35921	-172.52452	0.15359	13.63397	3083.91159	-79.25191
0.02	13.71154	-157.25502	0.27423	10.56644	1369.13976	-38.91019
0.03	12.20945	-143.38529	0.36628	7.90789	811.27601	-25.55798
0.04	10.83965	-130.77278	0.43359	5.60874	540.32965	-18.92351
0.05	9.59022	-119.29132	0.47951	3.62566	382.94556	-14.95992
0.06	8.45043	-108.82905	0.50703	1.92068	281.67617	-12.32275
0.07	7.41058	-99.28665	0.51874	0.46051	212.08074	-10.43857
0.08	6.46192	-90.57571	0.51695	-0.78413	162.03505	-9.02235
0.09	5.59655	-82.61743	0.50369	-1.83901	124.85515	-7.91678
0.10	4.80730	-75.34143	0.48073	-2.72684	96.55861	-7.02809
0.12	3.43173	-62.59091	0.41181	-4.07918	57.38744	-5.68384
0.14	2.28999	-51.89422	0.32060	-4.97520	32.71667	-4.71029
0.16	1.34460	-42.90365	0.21514	-5.51998	16.69920	-3.96392
0.18	0.56437	-35.33618	0.10159	-5.79615	6.12317	-3.33647
0.20	-0.07678	-28.96000	-0.01536	-5.86878	-0.90612	-3.71704
0.22	-0.60069	-23.58418	-0.13215	-5.78921	-5.56424	-2.70233
0.24	-1.02576	-19.05068	-0.24618	-5.59792	-8.60783	-2.35407
0.26	-1.36746	-15.22805	-0.35554	-5.32675	-10.53754	-2.07998
0.28	-1.63888	-12.00653	-0.45889	-5.00071	-11.69172	-1.85137
0.30	-1.85111	-9.29412	-0.55533	-4.63934	-12.30302	-1.65646
0.35	-2.18083	-4.26217	-0.76329	-3.67259	-12.40664	-1.27381
0.40	-2.30741	-1.04574	-0.92297	-2.72571	-11.49952	-0.99194
0.45	-2.30547	0.96060	-1.03746	-1.87320	-10.23586	-0.77455
0.50	-2.22472	2.16098	-1.11236	-1.14422	-8.90953	-0.60067
0.55	-2.09823	2.82697	-1.15402	-0.54339	-7.65164	-0.45755
0.60	-1.94784	3.14179	-1.16870	-0.06276	-6.51625	-0.33711
0.65	-1.78781	3.22934	-1.16208	0.31126	-5.51991	-0.23405
0.70	-1.62728	3.17337	-1.13910	0.59408	-4.66085	-0.14479
0.75	-1.47192	3.03033	-1.10394	0.80083	-3.92867	-0.06681
0.80	-1.32506	2.83808	-1.06005	0.94540	-3.30947	0.00174
0.85	-1.18851	2.62175	-1.01023	1.03998	-2.78849	0.06224
0.90	-1.06301	2.39776	-0.95671	1.09497	-2.35153	0.11583
0.95	-0.94868	2.17662	-0.90125	1.11911	-1.98567	0.16342
1.00	-0.84519	1.96476	-0.84519	1.11957	-1.67947	0.20579
1.10	-0.66836	1.58188	-0.73519	1.07171	-1.20818	0.27748
1.20	-0.52676	1.26033	-0.63211	0.98564	-0.87587	0.33541
1.30	-0.41432	0.99777	-0.53861	0.88279	-0.63954	0.38304
1.40	-0.32548	0.78684	-0.45568	0.77609	-0.46987	0.42301
1.50	-0.25552	0.61900	-0.38327	0.67299	-0.34697	0.45725
1.60	-0.20052	0.48623	-0.32082	0.57745	-0.25730	0.48711
1.70	-0.15733	0.38156	-0.26747	0.49132	-0.19150	0.51350
1.80	-0.12346	0.29924	-0.22223	0.41517	-0.13899	0.55005
1.90	-0.09690	0.23458	-0.18411	0.34881	-0.10119	0.58262
2.00	-0.07608	0.18385	-0.15216	0.29162	-0.07393	0.61161
2.10	-0.05976	0.14407	-0.12551	0.24278	-0.05424	0.63725
2.20	-0.04698	0.11290	-0.10335	0.20140	-0.04000	0.65969
2.30	-0.03696	0.08848	-0.08501	0.16656	-0.02968	0.67904
2.40	-0.02911	0.06937	-0.06985	0.13738	-0.02218	0.69541
2.50	-0.02295	0.05441	-0.05737	0.11308	-0.01671	0.70890
2.60	-0.01812	0.04270	-0.04710	0.09291	-0.01271	0.71961
2.70	-0.01432	0.03354	-0.03867	0.07624	-0.00976	0.72766
2.80	-0.01134	0.02637	-0.03176	0.06250	-0.00757	0.73321
2.90	-0.00900	0.02076	-0.02609	0.05120	-0.00593	0.73642
3.00	-0.00715	0.01636	-0.02145	0.04193	-0.00470	0.73747
3.10	-0.00569	0.01291	-0.01765	0.03434	-0.00375	0.73656
3.20	-0.00454	0.01021	-0.01454	0.02813	-0.00302	0.73390
3.30	-0.00363	0.00809	-0.01199	0.02305	-0.00246	0.72970
3.40	-0.00291	0.00642	-0.00989	0.01890	-0.00201	0.72421
3.50	-0.00234	0.00510	-0.00818	0.01552	-0.00165	0.71762
3.60	-0.00188	0.00406	-0.00677	0.01275	-0.00136	0.71018
3.70	-0.00152	0.00325	-0.00561	0.01049	-0.00113	0.70208
3.80	-0.00123	0.00260	-0.00466	0.00865	-0.00094	0.69353
3.90	-0.00099	0.00208	-0.00387	0.00713	-0.00078	0.68471

* Parameters taken from Table L.4.

Table L.16. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	-0.00081	0.00167	-0.00322	0.00589	-0.00065	0.67579
4.10	-0.00065	0.00135	-0.00268	0.00488	-0.00055	0.66691
4.20	-0.00053	0.00109	-0.00224	0.00404	-0.00046	0.65821
4.40	-0.00036	0.00071	-0.00156	0.00279	-0.00032	0.64174
4.60	-0.00024	0.00047	-0.00110	0.00194	-0.00022	0.62703
4.80	-0.00016	0.00032	-0.00077	0.00135	-0.00016	0.61443
5.00	-0.00011	0.00021	-0.00055	0.00095	-0.00011	0.60411
5.20	-0.00007	0.00014	-0.00039	0.00067	-0.00007	0.59603
5.40	-0.00005	0.00010	-0.00027	0.00047	-0.00005	0.59006
5.60	-0.00003	0.00007	-0.00019	0.00033	-0.00004	0.58600
5.80	-0.00002	0.00004	-0.00014	0.00024	-0.00002	0.58361
6.00	-0.00002	0.00003	-0.00010	0.00017	-0.00002	0.58264
6.20	-0.00001	0.00002	-0.00007	0.00012	-0.00001	0.58287
6.40	-0.00001	0.00001	-0.00005	0.00008	-0.00001	0.58409
6.60	-0.00001	0.00001	-0.00003	0.00006	-0.00001	0.58609
6.80	-0.00000	0.00001	-0.00002	0.00004	-0.00000	0.58871
7.00	-0.00000	0.00000	-0.00002	0.00003	-0.00000	0.59182
7.20	-0.00000	0.00000	-0.00001	0.00002	-0.00000	0.59529
7.40	-0.00000	0.00000	-0.00001	0.00002	-0.00000	0.59903
7.60	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.60296
7.80	-0.00000	0.00000	-0.00000	0.00001	-0.00000	0.60702
8.00	-0.00000	0.00000	-0.00000	0.00001	-0.00000	0.61115
8.20	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.61531
8.40	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.61947
8.60	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.62362
8.80	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.62772
9.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.63177

Table L.17. Radial Characteristics of the Hartree-Fock Na^+ 2p Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	0.	38.63185	0.	0.		
0.01	0.36602	34.63628	0.00366	0.71238	67.86897	-150.12893
0.02	0.69396	31.01198	0.01388	1.31420	64.67403	-74.95726
0.03	0.98737	27.72299	0.02962	1.81906	61.87521	-50.07535
0.04	1.24943	24.73709	0.04998	2.23892	59.32267	-37.69754
0.05	1.48303	22.02533	0.07415	2.58429	56.92267	-30.28323
0.06	1.69077	19.56172	0.10145	2.86447	54.62074	-25.32992
0.07	1.87501	17.32292	0.13125	3.08762	52.38808	-21.77216
0.08	2.03790	15.28791	0.16303	3.26094	50.21159	-19.08149
0.09	2.18138	13.43777	0.19632	3.39078	48.08753	-16.96701
0.10	2.30722	11.75548	0.23072	3.48277	46.01734	-15.25580
0.12	2.51219	8.83452	0.30146	3.57234	42.05454	-12.64380
0.14	2.66397	6.41929	0.37296	3.56267	38.35701	-10.73523
0.16	2.77176	4.42345	0.44348	3.47951	34.94882	-9.27668
0.18	2.84323	2.77629	0.51178	3.34296	31.83811	-8.12665
0.20	2.88474	1.41965	0.57695	3.16867	29.01905	-7.19882
0.22	2.90163	0.30561	0.63836	2.96886	26.47609	-6.43683
0.24	2.89832	-0.60551	0.69560	2.75300	24.18804	-5.80189
0.26	2.87854	-1.34666	0.74842	2.52841	22.13117	-5.26625
0.28	2.84540	-1.94527	0.79671	2.30073	20.28151	-4.80941
0.30	2.80152	-2.42425	0.84046	2.07425	18.61615	-4.41590
0.35	2.65839	-3.21690	0.93044	1.53248	15.12603	-3.63748
0.40	2.48663	-3.59947	0.99465	1.04684	12.39148	-3.06151
0.45	2.30279	-3.71980	1.03625	0.62888	10.21893	-2.61682
0.50	2.11737	-3.67551	1.05869	0.27962	8.47278	-2.26140
0.55	1.93689	-3.53131	1.06529	-0.00533	7.05683	-1.96948
0.60	1.76518	-3.33012	1.05911	-0.23289	5.90096	-1.72464
0.65	1.60435	-3.10019	1.04283	-0.41077	4.95251	-1.51595
0.70	1.45533	-2.85988	1.01873	-0.54658	4.17089	-1.33583
0.75	1.31834	-2.62090	0.98875	-0.64734	3.52429	-1.17882
0.80	1.19310	-2.39043	0.95448	-0.71924	2.98748	-1.04082
0.85	1.07908	-2.17263	0.91722	-0.76765	2.54028	-0.91868
0.90	0.97559	-1.96967	0.87803	-0.79711	2.16647	-0.80993
0.95	0.88185	-1.78239	0.83776	-0.81142	1.85300	-0.71259
1.00	0.79709	-1.61081	0.79709	-0.81372	1.58931	-0.62509
1.10	0.65141	-1.31240	0.71655	-0.79223	1.17859	-0.47464
1.20	0.53282	-1.06759	0.63939	-0.74829	0.88305	-0.35076
1.30	0.43638	-0.86820	0.56729	-0.69228	0.66822	-0.24805
1.40	0.35793	-0.70641	0.50110	-0.63104	0.51058	-0.16263
1.50	0.29407	-0.57535	0.44111	-0.56895	0.39384	-0.09154
1.60	0.24203	-0.46924	0.38725	-0.50875	0.30659	-0.03245
1.70	0.19955	-0.38330	0.33924	-0.45206	0.24078	0.01660
1.80	0.16483	-0.31365	0.29669	-0.39974	0.18527	0.08387
1.90	0.13639	-0.25713	0.25913	-0.35216	0.14369	0.14134
2.00	0.11305	-0.21120	0.22610	-0.30935	0.11226	0.19065
2.10	0.09386	-0.17381	0.19711	-0.27114	0.08831	0.23319
2.20	0.07806	-0.14332	0.17173	-0.23724	0.06990	0.27013
2.30	0.06501	-0.11840	0.14953	-0.20732	0.05564	0.30248
2.40	0.05423	-0.09801	0.13014	-0.18099	0.04451	0.33106
2.50	0.04529	-0.08127	0.11322	-0.15788	0.03576	0.35655
2.60	0.03787	-0.06751	0.09847	-0.13764	0.02883	0.37954
2.70	0.03171	-0.05617	0.08561	-0.11994	0.02332	0.40048
2.80	0.02657	-0.04680	0.07441	-0.10448	0.01892	0.41976
2.90	0.02229	-0.03906	0.06465	-0.09098	0.01538	0.43768
3.00	0.01872	-0.03264	0.05616	-0.07920	0.01253	0.45450
3.10	0.01573	-0.02731	0.04876	-0.06893	0.01022	0.47040
3.20	0.01323	-0.02287	0.04233	-0.05997	0.00835	0.48555
3.30	0.01113	-0.01918	0.03673	-0.05217	0.00683	0.50006
3.40	0.00937	-0.01610	0.03186	-0.04536	0.00559	0.51403
3.50	0.00789	-0.01352	0.02763	-0.03944	0.00458	0.52753
3.60	0.00665	-0.01137	0.02395	-0.03427	0.00375	0.54060
3.70	0.00561	-0.00956	0.02075	-0.02977	0.00307	0.55331
3.80	0.00473	-0.00805	0.01797	-0.02586	0.00252	0.56567
3.90	0.00399	-0.00678	0.01556	-0.02245	0.00207	0.57770

* Parameters taken from Table L.4.

Table L.17. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	0.00337	-0.00571	0.01347	-0.01948	0.00170	0.58943
4.10	0.00284	-0.00482	0.01165	-0.01690	0.00139	0.60087
4.20	0.00240	-0.00406	0.01008	-0.01466	0.00114	0.61202
4.40	0.00171	-0.00289	0.00753	-0.01101	0.00077	0.63350
4.60	0.00122	-0.00206	0.00561	-0.00825	0.00052	0.65393
4.80	0.00087	-0.00147	0.00418	-0.00618	0.00035	0.67333
5.00	0.00062	-0.00105	0.00311	-0.00462	0.00024	0.69175
5.20	0.00044	-0.00075	0.00231	-0.00344	0.00016	0.70923
5.40	0.00032	-0.00053	0.00171	-0.00257	0.00011	0.72580
5.60	0.00023	-0.00038	0.00127	-0.00191	0.00007	0.74153
5.80	0.00016	-0.00027	0.00094	-0.00142	0.00005	0.75646
6.00	0.00012	-0.00019	0.00069	-0.00105	0.00003	0.77064
6.20	0.00008	-0.00014	0.00051	-0.00078	0.00002	0.78413
6.40	0.00006	-0.00010	0.00038	-0.00058	0.00001	0.79698
6.60	0.00004	-0.00007	0.00028	-0.00043	0.00001	0.80922
6.80	0.00003	-0.00005	0.00020	-0.00031	0.00001	0.82091
7.00	0.00002	-0.00004	0.00015	-0.00023	0.00000	0.83208
7.20	0.00002	-0.00003	0.00011	-0.00017	0.00000	0.84278
7.40	0.00001	-0.00002	0.00008	-0.00013	0.00000	0.85304
7.60	0.00001	-0.00001	0.00006	-0.00009	0.00000	0.86289
7.80	0.00001	-0.00001	0.00004	-0.00007	0.00000	0.87235
8.00	0.00000	-0.00001	0.00003	-0.00005	0.00000	0.88146
8.20	0.00000	-0.00000	0.00002	-0.00004	0.00000	0.89024
8.40	0.00000	-0.00000	0.00002	-0.00003	0.00000	0.89870
8.60	0.00000	-0.00000	0.00001	-0.00002	0.00000	0.90686
8.80	0.00000	-0.00000	0.00001	-0.00001	0.00000	0.91475
9.00	0.00000	-0.00000	0.00001	-0.00001	0.00000	0.92238

Table L.18. Radial Characteristics of the Hartree-Fock Na^+ 1s Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	70.28236	-773.28251	0.	70.28236		
0.01	62.97108	-690.58722	0.62971	56.06521	-24.94757	1.00984
0.02	56.44024	-617.00919	1.12880	44.10006	-13.25107	1.00583
0.03	50.60398	-551.50847	1.51812	34.05873	-4.63228	1.00227
0.04	45.38622	-493.16809	1.81545	25.65949	0.00301	1.00000
0.05	40.71946	-441.17888	2.03597	18.66052	2.01472	0.99877
0.06	36.54386	-394.82640	2.19263	12.85427	2.51894	0.99829
0.07	32.80626	-353.47947	2.29644	8.06270	2.25441	0.99829
0.08	29.45945	-316.58006	2.35676	4.13305	1.67131	0.99859
0.09	26.46148	-283.63458	2.38153	0.93437	1.02553	0.99904
0.10	23.77504	-254.20613	2.37750	-1.64557	0.44786	0.99953
0.12	19.20760	-204.39660	2.30491	-5.31999	-0.32462	1.00042
0.14	15.53285	-164.55384	2.17460	-7.50468	-0.60886	1.00097
0.16	12.57273	-132.63319	2.01164	-8.64858	-0.57659	1.00114
0.18	10.18554	-107.02158	1.83340	-9.07834	-0.39909	1.00097
0.20	8.25837	-86.44357	1.65167	-9.03035	-0.19211	1.00058
0.22	6.70103	-69.88848	1.47423	-8.67444	-0.01710	1.00006
0.24	5.44139	-56.55383	1.30593	-8.13153	0.10299	0.99953
0.26	4.42169	-45.80112	1.14964	-7.48660	0.16766	0.99906
0.28	3.59555	-37.12143	1.00675	-6.79845	0.18704	0.99871
0.30	2.92574	-30.10836	0.87772	-6.10677	0.17466	0.99852
0.35	1.75256	-17.88972	0.61340	-4.50884	0.08274	0.99883
0.40	1.05425	-10.66999	0.42170	-3.21374	-0.00542	1.00013
0.45	0.63708	-6.38648	0.28669	-2.23683	-0.05000	1.00195
0.50	0.38699	-3.83615	0.19349	-1.53109	-0.05664	1.00364
0.55	0.23650	-2.31301	0.13008	-1.03565	-0.04265	1.00448
0.60	0.14560	-1.40066	0.08736	-0.69480	-0.02249	1.00384
0.65	0.09042	-0.85254	0.05877	-0.46373	-0.00447	1.00123
0.70	0.05674	-0.52216	0.03972	-0.30877	0.00811	0.99645
0.75	0.03605	-0.32225	0.02704	-0.20564	0.01497	0.98968
0.80	0.02322	-0.20072	0.01858	-0.13735	0.01719	0.98160
0.85	0.01520	-0.12642	0.01292	-0.09226	0.01626	0.97341
0.90	0.01011	-0.08065	0.00910	-0.06248	0.01352	0.96679
0.95	0.00685	-0.05221	0.00650	-0.04276	0.01000	0.96372
1.00	0.00472	-0.03435	0.00472	-0.02964	0.00640	0.96628
1.10	0.00235	-0.01564	0.00259	-0.01485	0.00044	0.99530
1.20	0.00124	-0.00760	0.00149	-0.00788	-0.00313	1.06258
1.30	0.00069	-0.00389	0.00090	-0.00437	-0.00460	1.16581
1.40	0.00040	-0.00206	0.00056	-0.00249	-0.00467	1.28885
1.50	0.00025	-0.00112	0.00037	-0.00143	-0.00398	1.39877
1.60	0.00016	-0.00061	0.00026	-0.00081	-0.00298	1.44979
1.70	0.00012	-0.00033	0.00020	-0.00045	-0.00194	1.40556
1.80	0.00009	-0.00019	0.00017	-0.00024	-0.00101	1.26866
1.90	0.00008	-0.00011	0.00015	-0.00013	-0.00025	1.08011
2.00	0.00007	-0.00007	0.00014	-0.00008	0.00032	0.88759
2.10	0.00006	-0.00006	0.00013	-0.00005	0.00072	0.71878
2.20	0.00006	-0.00005	0.00013	-0.00005	0.00098	0.58245
2.30	0.00005	-0.00005	0.00012	-0.00005	0.00113	0.47660
2.40	0.00005	-0.00004	0.00012	-0.00006	0.00120	0.39564
2.50	0.00004	-0.00004	0.00011	-0.00007	0.00120	0.33376
2.60	0.00004	-0.00004	0.00010	-0.00007	0.00116	0.28617
2.70	0.00004	-0.00004	0.00010	-0.00007	0.00109	0.24921
2.80	0.00003	-0.00004	0.00009	-0.00008	0.00101	0.22017
2.90	0.00003	-0.00004	0.00008	-0.00008	0.00092	0.19707
3.00	0.00002	-0.00003	0.00007	-0.00007	0.00082	0.17847
3.10	0.00002	-0.00003	0.00007	-0.00007	0.00073	0.16333
3.20	0.00002	-0.00003	0.00006	-0.00007	0.00065	0.15086
3.30	0.00002	-0.00002	0.00005	-0.00006	0.00057	0.14049
3.40	0.00001	-0.00002	0.00005	-0.00006	0.00049	0.13178
3.50	0.00001	-0.00002	0.00004	-0.00005	0.00043	0.12441
3.60	0.00001	-0.00002	0.00004	-0.00005	0.00037	0.11811
3.70	0.00001	-0.00001	0.00003	-0.00004	0.00032	0.11269
3.80	0.00001	-0.00001	0.00003	-0.00004	0.00027	0.10799
3.90	0.00001	-0.00001	0.00003	-0.00003	0.00023	0.10390

* Parameters taken from Table L.5.

Table L.18. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	0.00001	-0.00001	0.00002	-0.00003	0.00020	0.10030
4.10	0.00000	-0.00001	0.00002	-0.00003	0.00017	0.09713
4.20	0.00000	-0.00001	0.00002	-0.00002	0.00014	0.09432
4.40	0.00000	-0.00000	0.00001	-0.00002	0.00010	0.08958
4.60	0.00000	-0.00000	0.00001	-0.00001	0.00007	0.08576
4.80	0.00000	-0.00000	0.00001	-0.00001	0.00005	0.08264
5.00	0.00000	-0.00000	0.00000	-0.00001	0.00004	0.08006
5.20	0.00000	-0.00000	0.00000	-0.00001	0.00003	0.07790
5.40	0.00000	-0.00000	0.00000	-0.00000	0.00002	0.07608
5.60	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.07454
5.80	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.07323
6.00	0.00000	-0.00000	0.00000	-0.00000	0.00001	0.07211
6.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.07115
6.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.07032
6.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06961
6.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06899
7.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06847
7.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06802
7.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06764
7.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06732
7.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06705
8.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06683
8.20	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06665
8.40	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06651
8.60	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06641
8.80	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06634
9.00	0.00000	-0.00000	0.00000	-0.00000	0.00000	0.06629

Table L.19. Radial Characteristics of the Hartree-Fock Na^+ 2s Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	17.17072	-189.55849	0.	17.17072		
0.01	15.36103	-172.65776	0.15361	13.63446	20.56948	0.47607
0.02	13.71230	-157.33737	0.27425	10.56555	-0.34287	1.00978
0.03	12.20957	-143.43149	0.36629	7.90663	-2.61276	1.08373
0.04	10.83945	-130.79404	0.43358	5.60768	-2.01961	1.07290
0.05	9.58990	-119.29606	0.47949	3.62509	-1.10054	1.04490
0.06	8.45011	-108.82351	0.50701	1.92070	-0.38389	1.01778
0.07	7.41034	-99.27535	0.51872	0.46107	0.06649	0.99649
0.08	6.46182	-90.56185	0.51695	-0.78313	0.30027	0.98182
0.09	5.59659	-82.60320	0.50369	-1.83770	0.38432	0.97313
0.10	4.80748	-75.32826	0.48075	-2.72535	0.37589	0.96941
0.12	3.43213	-62.58199	0.41186	-4.07771	0.23744	0.97293
0.14	2.29052	-51.89019	0.32067	-4.97411	0.07880	0.98654
0.16	1.34517	-42.90379	0.21523	-5.51944	-0.03260	1.00948
0.18	0.56490	-35.33923	0.10168	-5.79616	-0.08813	1.06104
0.20	-0.07633	-28.96469	-0.01527	-5.86926	-0.10055	0.48455
0.22	-0.60034	-23.58945	-0.13208	-5.79002	-0.08661	0.94355
0.24	-1.02551	-19.05574	-0.24612	-5.59888	-0.06041	0.97695
0.26	-1.36730	-15.23240	-0.35550	-5.32773	-0.03169	0.99093
0.28	-1.63881	-12.00991	-0.45887	-5.00158	-0.00620	0.99852
0.30	-1.85109	-9.29647	-0.55533	-4.64003	0.01335	1.00282
0.35	-2.18088	-4.26244	-0.76331	-3.67273	0.03431	1.00616
0.40	-2.30744	-1.04517	-0.92298	-2.72551	0.02750	1.00466
0.45	-2.30547	0.96092	-1.03746	-1.87306	0.01088	1.00185
0.50	-2.22472	2.16046	-1.11236	-1.14449	-0.00405	0.99929
0.55	-2.09828	2.82551	-1.15406	-0.54426	-0.01284	0.99761
0.60	-1.94799	3.13962	-1.16879	-0.06422	-0.01533	0.99692
0.65	-1.78808	3.22683	-1.16225	0.30936	-0.01328	0.99709
0.70	-1.62768	3.17090	-1.13937	0.59196	-0.00882	0.99788
0.75	-1.47243	3.02823	-1.10432	0.79875	-0.00373	0.99901
0.80	-1.32566	2.83657	-1.06053	0.94359	0.00080	1.00024
0.85	-1.18917	2.62094	-1.01079	1.03864	0.00418	1.00137
0.90	-1.06369	2.39769	-0.95732	1.09423	0.00620	1.00228
0.95	-0.94935	2.17723	-0.90188	1.11903	0.00697	1.00287
1.00	-0.84581	1.96597	-0.84581	1.12016	0.00674	1.00312
1.10	-0.66881	1.58393	-0.73569	1.07351	0.00448	1.00262
1.20	-0.52699	1.26273	-0.63238	0.98829	0.00149	1.00111
1.30	-0.41430	1.00014	-0.53860	0.88588	-0.00097	0.99908
1.40	-0.32525	0.78891	-0.45534	0.77923	-0.00249	0.99701
1.50	-0.25509	0.62065	-0.38264	0.67588	-0.00312	0.99521
1.60	-0.19995	0.48742	-0.31992	0.57992	-0.00314	0.99385
1.70	-0.15667	0.38232	-0.26634	0.49326	-0.00284	0.99292
1.80	-0.12274	0.29961	-0.22093	0.41656	-0.00242	0.99228
1.90	-0.09616	0.23465	-0.18270	0.34967	-0.00203	0.99172
2.00	-0.07535	0.18368	-0.15069	0.29201	0.00025	1.00130
2.10	-0.05906	0.14373	-0.12402	0.24278	0.00143	1.00948
2.20	-0.04631	0.11245	-0.10188	0.20108	0.00191	1.01613
2.30	-0.03634	0.08797	-0.08358	0.16600	0.00196	1.02115
2.40	-0.02854	0.06883	-0.06849	0.13665	0.00178	1.02446
2.50	-0.02243	0.05387	-0.05609	0.11223	0.00149	1.02597
2.60	-0.01766	0.04217	-0.04591	0.09200	0.00116	1.02568
2.70	-0.01391	0.03304	-0.03757	0.07529	0.00084	1.02356
2.80	-0.01098	0.02591	-0.03075	0.06155	0.00055	1.01966
2.90	-0.00868	0.02033	-0.02518	0.05028	0.00031	1.01405
3.00	-0.00688	0.01597	-0.02063	0.04105	0.00012	1.00682
3.10	-0.00546	0.01257	-0.01691	0.03351	-0.00003	0.99808
3.20	-0.00434	0.00990	-0.01388	0.02736	-0.00013	0.98799
3.30	-0.00346	0.00782	-0.01140	0.02234	-0.00021	0.97670
3.40	-0.00276	0.00618	-0.00938	0.01826	-0.00025	0.96438
3.50	-0.00221	0.00490	-0.00773	0.01493	-0.00028	0.95123
3.60	-0.00177	0.00389	-0.00637	0.01223	-0.00028	0.93741
3.70	-0.00142	0.00309	-0.00526	0.01002	-0.00028	0.92313
3.80	-0.00115	0.00247	-0.00435	0.00823	-0.00027	0.90855
3.90	-0.00092	0.00197	-0.00361	0.00676	-0.00025	0.89386

Table L.19. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	-0.00075	0.00158	-0.00299	0.00557	-0.00023	0.87920
4.10	-0.00061	0.00127	-0.00249	0.00459	-0.00021	0.86472
4.20	-0.00049	0.00102	-0.00207	0.00379	-0.00019	0.85056
4.40	-0.00033	0.00066	-0.00144	0.00260	-0.00015	0.82359
4.60	-0.00022	0.00044	-0.00100	0.00179	-0.00011	0.79896
4.80	-0.00015	0.00029	-0.00070	0.00124	-0.00008	0.77706
5.00	-0.00010	0.00019	-0.00049	0.00087	-0.00006	0.75806
5.20	-0.00007	0.00013	-0.00035	0.00061	-0.00004	0.74193
5.40	-0.00005	0.00009	-0.00025	0.00043	-0.00003	0.72852
5.60	-0.00003	0.00006	-0.00017	0.00030	-0.00002	0.71762
5.80	-0.00002	0.00004	-0.00012	0.00021	-0.00002	0.70893
6.00	-0.00001	0.00003	-0.00009	0.00015	-0.00001	0.70219
6.20	-0.00001	0.00002	-0.00006	0.00011	-0.00001	0.69710
6.40	-0.00001	0.00001	-0.00004	0.00008	-0.00001	0.69341
6.60	-0.00000	0.00001	-0.00003	0.00005	-0.00000	0.69089
6.80	-0.00000	0.00001	-0.00002	0.00004	-0.00000	0.68932
7.00	-0.00000	0.00000	-0.00002	0.00003	-0.00000	0.68854
7.20	-0.00000	0.00000	-0.00001	0.00002	-0.00000	0.68840
7.40	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.68876
7.60	-0.00000	0.00000	-0.00001	0.00001	-0.00000	0.68953
7.80	-0.00000	0.00000	-0.00000	0.00001	-0.00000	0.69062
8.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.69195
8.20	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.69348
8.40	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.69515
8.60	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.69692
8.80	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.69877
9.00	-0.00000	0.00000	-0.00000	0.00000	-0.00000	0.70068

Table L.20. Radial Characteristics of the Hartree-Fock Na^+ 2p Orbital.*

r	R(r)	R'(r)	P(r)	P'(r)	FR- ϵ R	FR/ ϵ R
0.	0.	38.66131	0.	0.		
0.01	0.36630	34.66304	0.00366	0.71293	-5.37202	12.45895
0.02	0.69450	31.03629	0.01389	1.31522	-4.75850	6.35350
0.03	0.98814	27.74508	0.02964	1.82049	-3.98311	4.14951
0.04	1.25041	24.75715	0.05002	2.24070	-3.17938	2.98669
0.05	1.48420	22.04354	0.07421	2.58637	-2.42541	2.27683
0.06	1.69211	19.57824	0.10153	2.86680	-1.76165	1.81345
0.07	1.87651	17.33786	0.13136	3.09016	-1.20376	1.50122
0.08	2.03955	15.30140	0.16316	3.26366	-0.75279	1.28839
0.09	2.18316	13.44992	0.19648	3.39365	-0.40135	1.14364
0.10	2.30910	11.76639	0.23091	3.48574	-0.13778	1.04662
0.12	2.51427	8.84320	0.30171	3.57546	0.17893	0.94439
0.14	2.66620	6.42603	0.37327	3.56585	0.29864	0.91248
0.16	2.77411	4.42853	0.44386	3.48268	0.30314	0.91462
0.18	2.84567	2.77993	0.51222	3.34605	0.25006	0.93134
0.20	2.88724	1.42208	0.57745	3.17166	0.17624	0.95231
0.22	2.90417	0.30700	0.63892	2.97171	0.10291	0.97231
0.24	2.90088	-0.60499	0.69621	2.75568	0.04071	0.98903
0.26	2.88110	-1.34684	0.74909	2.53092	-0.00640	1.00173
0.28	2.84795	-1.94603	0.79743	2.30307	-0.03833	1.01052
0.30	2.80406	-2.42546	0.84122	2.07642	-0.05699	1.01588
0.35	2.66084	-3.21882	0.93129	1.53425	-0.06330	1.01859
0.40	2.48897	-3.60165	0.99559	1.04831	-0.04219	1.01324
0.45	2.30502	-3.72198	1.03726	0.63013	-0.01760	1.00596
0.50	2.11950	-3.67756	1.05975	0.28072	0.00071	0.99974
0.55	1.93892	-3.53323	1.06641	-0.00435	0.01100	0.99557
0.60	1.76712	-3.33193	1.06027	-0.23204	0.01488	0.99342
0.65	1.60620	-3.10197	1.04403	-0.41008	0.01465	0.99287
0.70	1.45709	-2.86173	1.01996	-0.54612	0.01227	0.99342
0.75	1.32000	-2.62288	0.99000	-0.64716	0.00905	0.99464
0.80	1.19466	-2.39260	0.95573	-0.71942	0.00579	0.99621
0.85	1.08053	-2.17504	0.91845	-0.76826	0.00288	0.99792
0.90	0.97691	-1.97234	0.87922	-0.79820	0.00048	0.99962
0.95	0.88303	-1.78531	0.83888	-0.81302	-0.00140	1.00123
1.00	0.79811	-1.61397	0.79811	-0.81585	-0.00277	1.00271
1.10	0.65210	-1.31593	0.71731	-0.79542	-0.00423	1.00507
1.20	0.53315	-1.07130	0.63978	-0.75241	-0.00439	1.00644
1.30	0.43633	-0.87188	0.56723	-0.69711	-0.00367	1.00656
1.40	0.35753	-0.70987	0.50054	-0.63629	-0.00240	1.00525
1.50	0.29334	-0.57845	0.44001	-0.57433	-0.00089	1.00237
1.60	0.24101	-0.47188	0.38562	-0.51399	0.00065	0.99790
1.70	0.19829	-0.38543	0.33710	-0.45693	0.00205	0.99191
1.80	0.16338	-0.31526	0.29409	-0.40408	0.00323	0.98455
1.90	0.13481	-0.25823	0.25613	-0.35584	0.00414	0.97603
2.00	0.11138	-0.21184	0.22276	-0.31230	0.00183	0.98713
2.10	0.09215	-0.17405	0.19352	-0.27335	0.00052	0.99557
2.20	0.07634	-0.14321	0.16795	-0.23873	-0.00018	1.00185
2.30	0.06332	-0.11802	0.14564	-0.20812	-0.00052	1.00638
2.40	0.05258	-0.09740	0.12620	-0.18117	-0.00064	1.00954
2.50	0.04372	-0.08050	0.10929	-0.15752	-0.00065	1.01163
2.60	0.03638	-0.06662	0.09460	-0.13682	-0.00060	1.01293
2.70	0.03031	-0.05521	0.08184	-0.11874	-0.00053	1.01363
2.80	0.02528	-0.04581	0.07078	-0.10298	-0.00045	1.01392
2.90	0.02110	-0.03805	0.06118	-0.08925	-0.00038	1.01393
3.00	0.01762	-0.03165	0.05286	-0.07732	-0.00031	1.01377
3.10	0.01473	-0.02635	0.04566	-0.06694	-0.00026	1.01354
3.20	0.01232	-0.02196	0.03943	-0.05794	-0.00021	1.01329
3.30	0.01031	-0.01831	0.03404	-0.05012	-0.00017	1.01307
3.40	0.00864	-0.01529	0.02937	-0.04335	-0.00014	1.01292
3.50	0.00724	-0.01277	0.02534	-0.03747	-0.00012	1.01285
3.60	0.00607	-0.01068	0.02185	-0.03238	-0.00010	1.01289
3.70	0.00509	-0.00894	0.01884	-0.02797	-0.00008	1.01303
3.80	0.00427	-0.00748	0.01624	-0.02416	-0.00007	1.01328
3.90	0.00359	-0.00627	0.01399	-0.02086	-0.00006	1.01363

* Parameters taken from Table L.5.

Table L.20. (continued).

r	$R(r)$	$R'(r)$	$P(r)$	$P'(r)$	$FR-\epsilon R$	$FR/\epsilon R$
4.00	0.00301	-0.00525	0.01205	-0.01800	-0.00005	1.01409
4.10	0.00253	-0.00441	0.01038	-0.01553	-0.00005	1.01464
4.20	0.00213	-0.00370	0.00893	-0.01340	-0.00004	1.01527
4.40	0.00150	-0.00260	0.00661	-0.00996	-0.00003	1.01676
4.60	0.00106	-0.00184	0.00489	-0.00739	-0.00003	1.01848
4.80	0.00075	-0.00130	0.00362	-0.00548	-0.00002	1.02036
5.00	0.00053	-0.00092	0.00267	-0.00406	-0.00002	1.02236
5.20	0.00038	-0.00065	0.00197	-0.00300	-0.00001	1.02443
5.40	0.00027	-0.00046	0.00145	-0.00222	-0.00001	1.02655
5.60	0.00019	-0.00033	0.00107	-0.00164	-0.00001	1.02869
5.80	0.00014	-0.00023	0.00078	-0.00121	-0.00001	1.03084
6.00	0.00010	-0.00016	0.00058	-0.00089	-0.00000	1.03300
6.20	0.00007	-0.00012	0.00042	-0.00065	-0.00000	1.03517
6.40	0.00005	-0.00008	0.00031	-0.00048	-0.00000	1.03736
6.60	0.00003	-0.00006	0.00023	-0.00035	-0.00000	1.03955
6.80	0.00002	-0.00004	0.00017	-0.00026	-0.00000	1.04176
7.00	0.00002	-0.00003	0.00012	-0.00019	-0.00000	1.04399
7.20	0.00001	-0.00002	0.00009	-0.00014	-0.00000	1.04624
7.40	0.00001	-0.00002	0.00007	-0.00010	-0.00000	1.04852
7.60	0.00001	-0.00001	0.00005	-0.00007	-0.00000	1.05083
7.80	0.00000	-0.00001	0.00003	-0.00005	-0.00000	1.05316
8.00	0.00000	-0.00001	0.00003	-0.00004	-0.00000	1.05551
8.20	0.00000	-0.00000	0.00002	-0.00003	-0.00000	1.05789
8.40	0.00000	-0.00000	0.00001	-0.00002	-0.00000	1.06029
8.60	0.00000	-0.00000	0.00001	-0.00002	-0.00000	1.06270
8.80	0.00000	-0.00000	0.00001	-0.00001	-0.00000	1.06513
9.00	0.00000	-0.00000	0.00001	-0.00001	-0.00000	1.06758

APPENDIX M
GRAPHICAL PRESENTATION OF THE ORBITALS AND
CHARGE DENSITIES

In this appendix we present plots of the orbitals and charge distributions tabulated in previous appendices.

Figure 1. Radial Probability Distribution of the HeI Ground State Hartree-Fock Orbital

Figure 2. Radial Probability Distribution of the LiI Ground State Hartree-Fock Orbitals

Figure 3. Radial Probability Distribution of the BeII Ground State Hartree-Fock Orbitals

Figure 4. Radial Probability Distribution of the BeI Ground State Hartree-Fock Orbitals

Figure 5. Probability Distribution of the HeI Ground State Hartree-Fock Orbital

Figure 6. Probability Distribution of the LiI Ground State Hartree-Fock Orbitals

Figure 7. Probability Distribution of the BeII Ground State Hartree-Fock Orbitals

Figure 8. Probability Distribution of the BeI
Ground State Hartree-Fock Orbitals

Figure 9. Orbital Densities for Fluorine

Figure 10. Orbital Densities for the Negative Fluorine Ion

Figure 11. Orbital Densities for Neon

Figure 12. Orbital Densities for the Sodium Ion

Figure 13. Orbital Densities for Sodium

Figure 14. Radial Orbital Densities for Fluorine

Figure 15. Radial Orbital Densities for the Negative Fluorine Ion

Figure 16. Radial Orbital Densities for Neon

Figure 17. Radial Orbital Densities for the Sodium Ion

Figure 18. Radial Orbital Densities for Sodium

Figure 19. Radial Charge Density for Fluorine

Figure 20. Radial Charge Density for the Negative Fluorine Ion

Figure 21. Radial Charge Density for Neon

Figure 22. Radial Charge Density for the Sodium Ion

Figure 23. Radial Charge Density for Sodium

Figure 24. Effective Nuclear Charge for Fluorine

Figure 25. Effective Nuclear Charge for the Negative Fluorine Ion

Figure 26. Effective Nuclear Charge for Neon

Figure 27. Effective Nuclear Charge for the Sodium Ion

Figure 28. Effective Nuclear Charge for Sodium

Figure 29. Charge Density for Fluorine

Figure 30. Charge Density for the Negative Fluorine Ion

Figure 31. Charge Density for Neon

Figure 32. Charge Density for the Sodium Ion

Figure 33. Charge Density for Sodium

BIBLIOGRAPHY

1. Hartree, D. R., Proc. Cambridge Phil. Soc., 24, 89 (1928).
2. Slater, J. C., Phys. Rev., 35, 210 (1930).
3. Fock, V., Z. Physik, 61, 126 (1930); 62, 795 (1930); 81, 195 (1933).
4. Roothaan, C. C. J., Rev. Mod. Phys., 23, 69 (1951).
5. Shortley, G. H., Phys. Rev., 50, 1072 (1936).
6. Hartree, D. R., and W. Hartree, Proc. Roy. Soc. (London) A154, 588, (1936).
7. Roothaan, C. C. J., Rev. Mod. Phys., 32, 179 (1960).
8. Slater, J. C., Phys. Rev., 34, 1293 (1929).
9. Condon, E. V., and G. H. Shortley, The Theory of Atomic Spectra, Cambridge Univ. Press, Cambridge (1935), Chapter VI.
10. Eyring, H., J. Walter, and G. E. Kimball, Quantum Chemistry, John Wiley and Sons, Inc. (1944).
11. Racah, G., Phys. Rev., 62, 438 (1942).
12. Hartree, D. R., W. Hartree, and B. Swirles, Phil. Trans. Roy. Soc., 238, 229 (1939).
13. Hartree, D. R., The Calculation of Atomic Structure, John Wiley and Sons, Inc., New York (1957).
14. Berthier, G. B., J. chimie phys., 51, 363 (1954).
15. Pople, J. A., and R. K. Nesbet, J. Chem. Phys., 22, 571 (1954).
16. Pratt, G. W., Jr., Phys. Rev., 102, 1303 (1956).
17. Cooke, R. G., Linear Operators, Macmillan and Company, London (1953), Chapter IV.
18. Slater, J. C., Phys. Rev., 42, 33 (1932).
19. Löwdin, P. O., and K. Appel, Phys. Rev. 103, 1746 (1956).
20. McWeeny, R., Proc. Roy. Soc. (London), A235, 496 (1956); A237, 355 (1956); A241, 239 (1957).
21. McWeeny, R., Rev. Mod. Phys., 32, 335 (1960).
22. Löwdin, P. O., Tech. Note No. 35, Quantum Chem. Group, Uppsala Univ.
23. Nesbet, R. K., Quart. Prog. Rept. No. 18, Solid State and Mol. Theory Group, MIT, p. 4.
24. Roothaan, C. C. J., L. M. Sachs, and A. W. Weiss, Rev. Mod. Phys., 32, 179 (1960).

25. Löwdin, P. O., *Phys. Rev.*, 90, 120 (1953).
26. Karo, A. M., and L. C. Allen, *J. Chem. Phys.*, 31, 968 (1959).
27. Hartree, D. R., and W. Hartree, *Proc. Roy. Soc. (London)*, A193, 299 (1948).
28. Knox, R. S., *Solid State Physics, Vol. 4*, Academic Press, New York (1957), p. 413.
29. Holöien, E., *Proc. Phys. Soc. (London)*, A68, 297 (1955).
30. Hartree, D. R., *Proc. Cambridge Phil. Soc.*, 24, 111 (1928).
31. Wilson, W. S., and R. B. Lindsay, *Phys. Rev.*, 47, 681 (1935).
32. Hargreaves, J., *Proc. Cambridge Phil. Soc.*, 25, 75 (1928).
33. Fock, V., and M. J. Petrashen, *Physik. Z. Sowjetunion*, 8, 547 (1935).
34. Hartree, D. R., and W. Hartree, *Proc. Roy. Soc. (London)*, A150, 9 (1935).
35. Nesbet, R. K., *Proc. Roy. Soc. (London)* A230, 312 (1955); *Rev. Mod. Phys.*, 33, 28 (1961).
36. Nesbet, R. K., *Phys. Rev.*, 118, 681 (1960); *Quart. Prog. Rept. No. 22*, Solid State and Mol. Theory Group, MIT, p. 47.
37. Nesbet, R. K., *Quart. Prog. Rept. No. 21*, Solid State and Mol. Theory Group, MIT, p. 3.
38. Bethe, H. A., and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms*, Academic Press, New York (1957), Section 22.
39. Fermi, E., *Z. Physik*, 60, 320 (1930).
40. Ramsey, N. F., *Nuclear Moments*, Oxford Univ. Press, London (1956), p. 172.
41. Cohen, E. R., J. W. M. DuMont, T. W. Layton, and J. S. Rollet, *Rev. Mod. Phys.*, 27, 363 (1955).
42. Kusch, P., and H. Taub, *Phys. Rev.*, 75, 1477 (1949).
43. Seitz, F., *The Modern Theory of Solids*, McGraw-Hill Book Company, New York (1940), Chapter XVI.
44. Landolt-Bornstein, *Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik*, Springer-Verlag, Berlin (1950), 6th Ed.
45. Myers, W. R., *Rev. Mod. Phys.* 24, 15 (1952).
46. Sachs, L. M., *Phys. Rev.*, 117, 1504 (1960).
47. Cohen, M. H., D. A. Goodings, and V. Heine, *Proc. Phys. Soc. (London)*, 73, 811 (1959).

48. Brown, F. W., Phys. Rev., 44, 214 (1933).
49. Hartree, D. R., Proc. Roy. Soc. (London) A151, 96 (1935).
50. Froese, C., Proc. Cambridge Phil. Soc., 53, 206 (1957).
51. Allen, L. C., J. Chem. Phys. (to be published).
52. Worsley, B. H., Can. J. Phys., 36, 289 (1958).
53. Fock, V., and M. J. Petrashen, Physik. Z. Sowjetunion, 6, 368 (1934).
54. Witte, H., and E. Wolfel, Rev. Mod. Phys., 30, 51 (1958).
55. Hurst, R. P., Phys. Rev., 114, 746 (1959).
56. Pauling, L., Nature of the Chemical Bond, Cornell Univ. Press, Ithaca (1960), 3rd Ed., p. 514.
57. Kemble, E. C., The Fundamental Principles of Quantum Mechanics, Dover Publ., New York (1958), Chapter XIII.
58. Moore, C. E., Atomic Energy Levels, NBS Circular 467.
59. Yoshimine, M., private communication.
60. Cohen, S., Phys. Rev., 118, 489 (1960).
61. Hartree, D. R., Rev. Mod. Phys., 30, 63 (1958).
62. Kristoffel, N. N., Akad. Nauk Estonian SSR (Tartu), 7, 112 (1958).