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⁸L. V. Keldysh, *Zh. Eksperim. i Teor. Fiz.* **47**, 1945 (1964) [English transl.: *Soviet Phys. - JETP* **20**, 1307 (1965)].

⁹See, for example, the review article by Yu. P. Raizer, *Usp. Fiz. Nauk* **89**, 29 (1966) [English transl.: *Soviet Phys. - Usp* **8**, 650 (1966)].

¹⁰See, for example, Jon Mathews and R. L. Walker, *Mathematical Methods of Physics* (W. A. Benjamin, Inc. New York, 1964), Chap. 1.

Statistical Electron-Density Distributions and Thomas-Fermi-Dirac Screening Functions for Positive Ions with Degree of Ionization One through Four*

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Statistical electron-density distributions and Thomas-Fermi-Dirac (TFD) screening functions have been obtained for a total of 394 positive ions of elements having integral atomic numbers up to $Z=105$, for 117 values of radial distance from the ionic center in each case. For degrees of ionization 1 through 4, the starting values of Z are 5, 6, 9, and 10, respectively. These solutions were calculated, in part, by using Thomas' solutions of the TFD equation in terms of the statistical electron distributions for nonintegral values of Z and Jensen's boundary conditions. Values for singly ionized cesium and francium; doubly ionized barium and cadmium; triply ionized lanthanum and actinium; and quadruply ionized cerium and thorium are given here. The complete set of tables for all 394 ions has been deposited with ASIS National Auxiliary Publications Service.

I. INTRODUCTION

In a previous paper,¹ statistical electron-density distributions and Thomas-Fermi-Dirac²⁻⁶ (TFD) screening functions were given for neutral ground-state atoms having atomic numbers $Z=2$ to $Z=105$. In a very broad class of problems,⁷⁻¹⁹ however, a detailed knowledge of electron densities and/or screening functions for ions (rather than for neutral atoms) is required. In principle, an exact quantum-mechanical solution of the many-electron problem, in the presence of appropriate nuclei, should furnish the desired data. In practice, however, such exact solutions, except for the very simplest systems, are not presently attainable.²⁰ It is one of the salient features of the TFD approximation that it turns this very obstacle to exact solution, i.e., the many-body aspect of the problem, the good advantage by treating the atomic electrons statistically. Consequently, (other things being equal) the resultant statistical-density distributions can, in fact, be expected to be the more realistic the larger the number of electrons present.

In contrast to the simpler Thomas-Fermi (TF) approximation, the TFD model does take electron

exchange effects into account and also minimizes the spurious electronic self-interaction energy.⁴⁻⁶ In many instances, these distinctive features render the TFD model decidedly more accurate,²¹⁻²² but the improvement is obtained at a price. For, whereas the TF solution can be expressed in universal form, i.e., applicable to all Z , the corresponding TFD problem must be solved anew for each atomic and ionic species. TFD solutions for neutral atoms have been discussed elsewhere.^{1, 5-6, 23-26} Solutions for positive²⁷ ions of about one-quarter of the known elements and carrying various nonintegral net charges²⁸ Z_i , have been computed by Metropolis and Reitz.²⁶ The most complete ionic solutions published to date, however, are those given by Thomas,² using Jensen's boundary conditions²⁹ and covering degrees of ionization $N=1$ to $N=4$.

While the N 's in the latter solutions are integral, the effective atomic numbers Z associated with these "ions" are not. To obtain the corresponding values for the actually occurring ions, i.e., for integral Z , four- or five-point Lagrangian interpolation is required if the accuracy of the original tables is to be preserved.² In view of the overwhelming number (to a human computer) of

operations involved in such interpolations (about 10^5), even when applied solely to the determination of, say, the electron density distribution ρ as a function of radial distance r from the ionic center, this procedure is evidently carried out best by machine calculation. Moreover, as Thomas' tables give the values of $r^{3/2} \rho$ rather than the physically more interesting quantity ρ itself, it is necessary also to divide out the factor $r^{3/2}$ for each Z , N , and r . Lastly, solutions in terms of the frequently useful⁵ TFD screening functions ψ are not given in Thomas' work at all.

In conjunction with recent work on various single-center properties³⁰ of positive ions, as well as on certain binary ion-atom and ion-ion interaction energies indicated elsewhere,³¹ a knowledge of the quantities $\rho(Z, N, r)$ and $\psi(Z, N, r)$ was desired, and their calculation performed on a high-speed electronic computer. It is the purpose of the present paper to make these solutions generally available for use in the many areas, suggested above, in which the TFD model of positive ions is applicable.

II. THEORETICAL BACKGROUND

The fundamental differential equation embodying the TFD model is³²

$$\nabla^2(V - V_0 + \tau_0^2) = 4\pi\sigma_0 e[(V - V_0 + \tau_0^2)^{1/2} + \tau_0]^3, \quad (\text{II. 1})$$

where

$$V_0 = [(Z - N_e)e/r_0] + (\frac{15}{16})\tau_0^2, \quad (\text{II. 2})$$

$$\tau_0 = (4\kappa_a^2/15\kappa_k e)^{1/2} = 0.22508(e/a_0)^{1/2}, \quad (\text{II. 3})$$

$$\kappa_a = (\frac{3}{4})(3/\pi)^{1/3}e^2 = 0.73856e^2, \quad (\text{II. 4})$$

$$\kappa_k = (0.3)(3\pi^2)^{2/3}e^2a_0 = 2.8712e^2a_0, \quad (\text{II. 5})$$

$$\sigma_0 = (3e/5\kappa_k)^{3/2} = 0.095527/(ea_0)^{3/2}, \quad (\text{II. 6})$$

and a_0 , e , N_e , r_0 , and V , respectively, denote the first Bohr radius in hydrogen ($a_0 = 0.52917 \text{ \AA}$), the magnitude of the electronic charge, the number of electrons per ion, the radius of the TFD ion (assumed to be spherically symmetric), and the electric potential.

In view of (II. 1), along with Poisson's equation

$$\nabla^2 V = +4\pi e\rho, \quad (\text{II. 7})$$

where ρ is the number density of electrons, and by observing also that V_0 and τ_0 are constants for a given ion, it follows that

$$\rho = \sigma_0[(V - V_0 + \tau_0^2)^{1/2} + \tau_0]^3. \quad (\text{II. 8})$$

The boundary conditions for Eq. (II. 1) are

$$\lim_{r \rightarrow 0} [r(V - V_0 + \tau_0^2)] = Ze, \quad (\text{II. 9})$$

$$(V - V_0 + \tau_0^2)_{r=r_0} = (\frac{1}{16})\tau_0^2, \quad (\text{II. 10})$$

$$\text{and } (-dV/dr)_{r=r_0} = (Z - N_e)e/r_0^2, \quad (\text{II. 11})$$

reflecting, respectively, the requirements that V reduce to the proper Coulombic form appropriate to the immediate vicinity of the nucleus; and that both V and the electric field $E = -\partial V/\partial r$ be continuous at the ionic boundary $r = r_0$. It may be noted that the second of these three conditions, i. e.,

$$V(r_0) = (Z - N_e)e/r_0 \quad (\text{II. 12})$$

may, with the aid of (II. 2), be written as shown in (II. 10).

For the electron density $\rho_0 \equiv \rho(r_0)$ at the ionic boundary r_0 one finds from (II. 8), and using (II. 2) through (II. 6), that

$$\rho_0 = \frac{1}{8}(\kappa_a/\kappa_k)^3 = 0.0021275/a_0^3, \quad (\text{II. 13})$$

a value evidently independent of Z and of N , and thus the same for all TFD atoms and ions. Furthermore, in view of the constant terms appearing on the right-hand side of Eq. (II. 8), it follows from the normalization condition

$$\int_{\Omega} \rho dv = 4\pi \int_0^{r_0} \rho r^2 dr = N_e, \quad (\text{II. 14})$$

(dv = volume element, Ω = atomic or ionic volume), that r_0 must be finite, and thus $\rho(r) \equiv 0$ when $r > r_0$.

In order to simplify the basic Eqs. (II. 1) and (II. 2), one customarily defines two dimensionless variables, namely, a distance parameter

$$x = r/\mu \quad (\text{II. 15})$$

and the so-called screening function³³

$$\psi(x) = (r/Ze)(V - V_0 + \tau_0^2) \quad (\text{II. 16})$$

with

$$\mu = (4\pi\sigma_0)^{-2/3}e^{-1}Z^{-1/3} = 0.88534Z^{-1/3}a_0, \quad (\text{II. 17})$$

and a constant

$$\beta_0 = \tau_0(\mu/Ze)^{1/2} = 0.21178Z^{-2/3} \quad (\text{II. 18})$$

The fundamental TFD Eq. (II. 1) then becomes

$$d^2\psi/dx^2 = x[(\psi/x)^{1/2} + \beta_0]^3 \quad (\text{II. 19})$$

with the correspondingly transformed boundary conditions (II.9) and (II.10) now reading

$$\psi(0) = 1, \quad (\text{II.20})$$

$$\psi(x_0) = \frac{1}{16} \beta_0^2 x_0, \quad (\text{II.21})$$

where $x_0 = r_0/\mu$. Letting primes denote differentiation with respect to x , it can be shown that the third boundary condition (II.11), or the equivalent Eq. (II.14), can be written

$$Z \int_0^{x_0} x \psi'' dx = N_e \quad (\text{II.22})$$

whence, by partial integration and use of (II.20), one has

$$-\psi'(x_0) = [(N/Z) - \psi(x_0)]/x_0, \quad (\text{II.23})$$

$$\text{where } N = Z - N_e \quad (\text{II.24})$$

again denotes the degree of ionization. In terms of the new variables x and ψ , one finds from (II.8) that the electron density is

$$\begin{aligned} \rho(Z, N, r) &= (Z/4\pi\mu^3) [(\psi/x)^{1/2} + \beta_0]^3 \\ &= (Z/4\pi\mu^3) \psi''/x, \end{aligned} \quad (\text{II.25})$$

and from (II.16) that the electric potential is

$$V(Z, N, r) = (Ze/r)\psi + V_0 - \tau_0^2 \quad (\text{II.26})$$

where, in addition to the explicit appearance of Z and r , V_0 depends on N through Eq. (II.2); x depends on r and Z through Eq. (II.15); the parameters β_0, μ depend upon Z through Eqs. (II.17) and (II.18); and finally, ψ depends on Z, N , and r through Eqs. (II.19)–(II.21) and (II.23)

“Inverting” Eq. (II.25), after clearing constants and simplifying, yields for the screening function

$$\psi(Z, N, r) = (r/Z)A(\rho^{1/3} - B)^2, \quad (\text{II.27})$$

$$\text{where } A = \frac{1}{2}(3\pi^2)^{2/3}, \quad B = (3\pi^5)^{-1/3}. \quad (\text{II.28})$$

Equations (II.25)–(II.27) constitute the main analytic results of this section.

III. DISCUSSION OF THE RESULTS

A. Electron-Density Distributions

Using as input, for each degree of ionization $N=1$ to $N=4$, Thomas' data² for the “multiplied” electron densities $r^{3/2}\rho$ corresponding to nonintegral Z at 117 relative radial distances r/r_0 ranging from 10^{-6} to 1, a high-speed electronic computer was programmed, first, to perform the five-point Lagrangian interpolation (over Z) required to yield the corresponding multiplied den-

sity distributions $r^{3/2}\rho$, as accurate as those in the input, for integral values of Z . In order to extract from these intermediate results the electron densities ρ proper (rather than the quantities $r^{3/2}\rho$), the computer was further instructed to divide out the extraneous factor $r^{3/2}$. Lastly, to further facilitate use of the final results, the 117 actual distances r (rather than the mere ratios r/r_0) were computed for each of the various species of ions (Z, N).

Following Thomas' work,² the density distributions determined here all go up to $Z=105$, inclusive. The starting values of Z , on the other hand, vary with N . Specifically, as N takes on the values 1 through 4, these starting values are $Z=5, 6, 9$, and 10, respectively.

The results thus obtained for the statistical electron-density distributions ρ as functions of integral atomic number Z , radial distance r , and degree of ionization N , along with the corresponding values of r_0 (all in atomic units), are given in Tables I through VIII. In accord with the procedure followed in the previous paper¹ (dealing with neutral TFD atoms), electron densities of only two representative elements for each degree of ionization are given here in full.³⁴ Inasmuch as this selection had to be made from among a total of $101 + 100 + 97 + 96 = 394$ different kinds of ions, a certain degree of arbitrariness in arriving at this selection was patently unavoidable. Two criteria, however, were employed with a view to optimize the usefulness of the eight cases selected. (1) As is well known, the TFD model applies optimally to atoms or ions possessing closed-shell (or rare-gas) electron configurations.⁵ (2) As already mentioned in Sec. I, the larger the number of electrons present, and hence the more difficult the exact quantum-mechanical determination of ρ , the more realistic is the statistical approximation. Accordingly, from among each of the four N groups, only the two heaviest ions with closed-shell electron configurations were selected: Cesium ($Z=55$) and francium ($Z=87$) for $N=1$; barium ($Z=56$) and radium ($Z=88$) for $N=2$; lanthanum ($Z=57$) and actinium ($Z=89$) for $N=3$; and cerium ($Z=58$) and thorium ($Z=90$) for $N=4$. For reasons pertaining to the internal operation of the high-speed computer, the values of r, ρ , and ψ each had to be printed out in “floating - point” form, with the symbols $E+ab$ or $E-ab$ signifying that the decimal fraction immediately preceding is to be multiplied by 10^{ab} or 10^{-ab} , as the case may be.

The accuracy of these results was checked in two ways. The first of these consisted in comparing the value of $\rho(r_0)$ in each case with the standard value^{5,6} $0.0021275/a_0^3$ of Eq. (II.13) above. This procedure showed complete agreement to three significant figures in practically all cases, with the largest error in the third signifi-

TABLE I. TFD densities ρ and screening functions ψ for Cs^+ ($Z=55$, $N=1$) at 117 radial distances r . Outer boundary = $3.6180a_0$, ($a_0=0.52917 \text{ \AA}$). Atomic units are used throughout. $0.35958\text{E-}05$ means 0.35958×10^{-5} , etc.

r	ρ	ψ	r	ρ	ψ	r	ρ	ψ
0.35958E-05	0.57142E 10	0.99986E 00	0.28562E-01	0.65132E 04	0.85719E 00	0.29396E 01	0.12629E-01	0.43213E-02
0.45268E-05	0.40455E 10	0.99987E 00	0.35958E-01	0.43865E 04	0.82785E 00	0.29823E 01	0.11649E-01	0.39768E-02
0.56990E-05	0.28639E 10	0.99984E 00	0.45268E-01	0.29232E 04	0.79369E 00	0.30255E 01	0.10724E-01	0.36423E-02
0.71746E-05	0.20275E 10	0.99983E 00	0.56990E-01	0.19239E 04	0.75439E 00	0.30693E 01	0.98485E-02	0.33177E-02
0.90322E-05	0.14354E 10	0.99982E 00	0.71746E-01	0.12478E 04	0.70975E 00	0.31138E 01	0.90165E-02	0.30009E-02
0.11371E-04	0.10162E 10	0.99980E 00	0.90322E-01	0.79554E 03	0.65982E 00	0.31590E 01	0.82282E-02	0.26934E-02
0.14315E-04	0.71942E 09	0.99978E 00	0.11371E 00	0.49724E 03	0.60493E 00	0.32048E 01	0.74761E-02	0.23933E-02
0.18022E-04	0.50931E 09	0.99976E 00	0.14315E 00	0.30379E 03	0.54576E 00	0.32279E 01	0.71142E-02	0.22465E-02
0.22688E-04	0.36056E 09	0.99972E 00	0.18022E 00	0.18086E 03	0.48338E 00	0.32512E 01	0.67579E-02	0.21005E-02
0.28562E-04	0.25526E 09	0.99969E 00	0.22688E 00	0.10457E 03	0.41922E 00	0.32747E 01	0.64111E-02	0.19572E-02
0.35958E-04	0.18071E 09	0.99964E 00	0.28562E 00	0.58523E 02	0.35501E 00	0.32983E 01	0.60702E-02	0.18150E-02
0.45268E-04	0.12793E 09	0.99957E 00	0.35958E 00	0.31598E 02	0.29267E 00	0.33222E 01	0.57362E-02	0.16748E-02
0.56990E-04	0.90561E 08	0.99949E 00	0.45268E 00	0.16406E 02	0.23413E 00	0.33462E 01	0.54069E-02	0.15356E-02
0.71746E-04	0.64108E 08	0.99939E 00	0.56990E 00	0.81691E 01	0.18110E 00	0.33703E 01	0.50824E-02	0.13978E-02
0.90322E-04	0.45381E 08	0.99927E 00	0.71746E 00	0.56693E 00	0.15707E 00	0.33947E 01	0.47626E-02	0.12616E-02
0.11371E-03	0.32123E 08	0.99911E 00	0.90322E 00	0.38897E 01	0.13485E 00	0.34069E 01	0.46035E-02	0.11938E-02
0.14315E-03	0.22737E 08	0.99891E 00	0.11371E 00	0.26376E 01	0.11454E 00	0.34192E 01	0.44450E-02	0.11263E-02
0.18022E-03	0.16093E 08	0.99866E 00	0.14315E 00	0.17674E 01	0.96157E-01	0.34315E 01	0.42874E-02	0.10593E-02
0.22688E-03	0.11389E 08	0.99835E 00	0.18022E 00	0.11699E 01	0.79716E-01	0.34439E 01	0.41299E-02	0.99237E-03
0.28562E-03	0.80596E 07	0.99796E 00	0.22688E 00	0.76491E 00	0.65176E-01	0.34563E 01	0.39723E-02	0.92568E-03
0.35958E-03	0.57027E 07	0.99747E 00	0.28562E 00	0.49384E 00	0.52474E-01	0.34687E 01	0.38148E-02	0.85933E-03
0.45268E-03	0.40343E 07	0.99686E 00	0.35958E 00	0.31476E 00	0.41517E-01	0.34812E 01	0.36576E-02	0.79351E-03
0.56990E-03	0.28535E 07	0.99610E 00	0.45268E 00	0.25005E 00	0.36657E-01	0.34938E 01	0.34992E-02	0.72769E-03
0.71746E-03	0.20177E 07	0.99515E 00	0.56990E 00	0.19797E 00	0.32188E-01	0.35001E 01	0.34185E-02	0.69440E-03
0.90322E-03	0.14263E 07	0.99396E 00	0.71746E 00	0.15618E 00	0.28094E-01	0.35064E 01	0.33397E-02	0.66205E-03
0.11371E-02	0.10078E 07	0.99247E 00	0.90322E 00	0.12278E 00	0.24357E-01	0.35127E 01	0.32592E-02	0.62921E-03
0.14315E-02	0.71177E 06	0.99062E 00	0.11371E 00	0.96149E-01	0.20959E-01	0.35190E 01	0.31785E-02	0.59653E-03
0.18022E-02	0.50235E 06	0.98832E 00	0.14315E 00	0.74991E-01	0.17882E-01	0.35253E 01	0.30967E-02	0.56366E-03
0.22688E-02	0.35427E 06	0.98547E 00	0.18022E 00	0.58224E-01	0.15105E-01	0.35317E 01	0.30155E-02	0.53133E-03
0.28562E-02	0.24959E 06	0.98193E 00	0.22688E 00	0.44980E-01	0.12610E-01	0.35381E 01	0.29331E-02	0.49881E-03
0.35958E-02	0.17562E 06	0.97756E 00	0.28562E 00	0.39446E-01	0.11462E-01	0.35444E 01	0.28495E-02	0.46622E-03
0.45268E-02	0.12339E 06	0.97217E 00	0.35958E 00	0.34537E-01	0.10377E-01	0.35508E 01	0.27649E-02	0.43361E-03
0.56990E-02	0.86529E 05	0.96553E 00	0.45268E 00	0.30180E-01	0.93513E-02	0.35572E 01	0.26792E-02	0.40109E-03
0.71746E-02	0.60539E 05	0.95740E 00	0.56990E 00	0.26318E-01	0.83841E-02	0.35636E 01	0.25925E-02	0.33623E-03
0.90322E-02	0.42235E 05	0.94746E 00	0.71746E 00	0.22892E-01	0.74722E-02	0.35700E 01	0.25039E-02	0.36872E-03
0.11371E-01	0.29364E 05	0.93538E 00	0.90322E 00	0.19855E-01	0.66132E-02	0.35764E 01	0.24137E-02	0.30388E-03
0.14315E-01	0.20329E 05	0.92076E 00	0.11371E 00	0.17158E-01	0.58036E-02	0.35829E 01	0.23210E-02	0.27146E-03
0.18022E-01	0.14002E 05	0.90317E 00	0.14315E 00	0.14762E-01	0.50406E-02	0.35893E 01	0.22258E-02	0.23918E-03
0.22688E-01	0.95854E 04	0.88214E 00	0.18022E 00	0.128976E 01	0.46754E-02	0.35958E 01	0.21267E-02	0.20675E-03

TABLE II. TFD densities ρ and screening functions ψ for Fr^+ ($Z=87$, $N=1$) at 117 radial distances r . Outer boundary $= 3.7782a_0$, ($a_0 = 0.52917 \text{ \AA}$). Atomic units are used throughout.

r	ρ	ψ	r	ρ	ψ	r	ρ	ψ
0.37782E-05	0.10554E 11	0.99983E 00	0.30011E-01	0.11480E 05	0.83243E 00	0.30888E 01	0.12407E-01	0.28102E-02
0.47565E-05	0.74719E 10	0.99982E 00	0.37782E-01	0.76588E 04	0.79906E 00	0.31335E 01	0.11431E-01	0.25810E-02
0.59880E-05	0.52897E 10	0.99981E 00	0.47565E-01	0.50471E 04	0.76059E 00	0.31790E 01	0.10512E-01	0.23596E-02
0.75385E-05	0.37448E 10	0.99980E 00	0.59880E-01	0.32785E 04	0.71685E 00	0.32250E 01	0.96435E-02	0.21449E-02
0.94904E-05	0.26511E 10	0.99978E 00	0.75385E-01	0.20941E 04	0.66782E 00	0.32718E 01	0.88231E-02	0.19370E-02
0.11948E-04	0.18769E 10	0.99977E 00	0.94904E-01	0.13117E 04	0.61382E 00	0.33192E 01	0.80453E-02	0.17351E-02
0.15041E-04	0.13287E 10	0.99974E 00	0.11948E 00	0.80344E 03	0.55546E 00	0.33673E 01	0.73087E-02	0.15397E-02
0.18936E-04	0.94064E 09	0.99971E 00	0.15041E 00	0.47972E 03	0.49376E 00	0.33916E 01	0.69527E-02	0.14437E-02
0.23839E-04	0.66591E 09	0.99967E 00	0.18936E 00	0.27830E 03	0.43009E 00	0.34161E 01	0.66064E-02	0.13496E-02
0.30011E-04	0.47141E 09	0.99962E 00	0.23839E 00	0.15635E 03	0.36615E 00	0.34408E 01	0.62671E-02	0.12564E-02
0.37782E-04	0.33372E 09	0.99956E 00	0.30011E 00	0.84774E 02	0.30381E 00	0.34657E 01	0.59344E-02	0.11644E-02
0.47565E-04	0.23624E 09	0.99949E 00	0.37782E 00	0.44224E 02	0.24495E 00	0.34907E 01	0.56085E-02	0.10737E-02
0.59880E-04	0.16723E 09	0.99939E 00	0.47565E 00	0.22135E 02	0.19141E 00	0.35159E 01	0.52883E-02	0.98403E-03
0.75385E-04	0.11838E 09	0.99927E 00	0.59880E 00	0.10599E 02	0.14439E 00	0.35413E 01	0.49749E-02	0.89594E-03
0.94904E-04	0.83792E 08	0.99911E 00	0.75385E 00	0.72097E 01	0.12362E 00	0.35669E 01	0.46645E-02	0.80847E-03
0.11948E-03	0.59309E 08	0.99892E 00	0.94904E 00	0.48465E 01	0.10475E 00	0.35797E 01	0.45101E-02	0.76493E-03
0.15041E-03	0.41976E 08	0.99868E 00	0.84583E 00	0.32192E 01	0.87790E-01	0.35926E 01	0.43572E-02	0.72187E-03
0.18936E-03	0.29707E 08	0.99838E 00	0.94904E 00	0.21125E 01	0.72713E-01	0.36056E 01	0.42047E-02	0.67899E-03
0.23839E-03	0.21021E 08	0.99800E 00	0.10648E 01	0.13694E 01	0.59462E-01	0.36186E 01	0.40519E-02	0.63612E-03
0.30011E-03	0.14873E 08	0.99753E 00	0.11948E 01	0.87669E 00	0.47950E-01	0.36316E 01	0.39008E-02	0.59390E-03
0.37782E-03	0.10522E 08	0.99694E 00	0.13406E 01	0.55427E 00	0.38071E-01	0.36447E 01	0.37486E-02	0.55152E-03
0.47565E-03	0.74418E 07	0.99620E 00	0.15041E 01	0.34602E 00	0.29701E-01	0.36578E 01	0.35961E-02	0.50935E-03
0.59880E-03	0.52621E 07	0.99527E 00	0.15933E 01	0.27206E 00	0.26038E-01	0.36710E 01	0.34436E-02	0.46754E-03
0.75385E-03	0.37196E 07	0.99412E 00	0.16877E 01	0.21320E 00	0.22700E-01	0.36776E 01	0.33675E-02	0.44680E-03
0.94904E-03	0.26282E 07	0.99268E 00	0.17877E 01	0.16652E 00	0.19670E-01	0.36842E 01	0.32901E-02	0.42585E-03
0.11948E-02	0.18561E 07	0.99089E 00	0.18936E 01	0.12960E 00	0.16929E-01	0.36909E 01	0.32131E-02	0.40513E-03
0.15041E-02	0.13100E 07	0.98866E 00	0.20058E 01	0.10049E 00	0.14460E-01	0.36975E 01	0.31351E-02	0.38428E-03
0.18936E-02	0.92383E 06	0.98589E 00	0.21246E 01	0.77623E-01	0.12244E-01	0.37042E 01	0.30564E-02	0.36341E-03
0.23839E-02	0.65087E 06	0.98246E 00	0.22505E 01	0.59704E-01	0.10264E-01	0.37108E 01	0.29779E-02	0.34276E-03
0.30011E-02	0.45800E 06	0.97821E 00	0.23839E 01	0.45700E-01	0.85018E-02	0.37175E 01	0.28983E-02	0.32205E-03
0.37782E-02	0.32180E 06	0.97298E 00	0.24535E 01	0.39902E-01	0.76973E-02	0.37242E 01	0.27378E-02	0.30130E-03
0.47565E-02	0.22568E 06	0.96653E 00	0.25251E 01	0.34786E-01	0.69410E-02	0.37309E 01	0.26552E-02	0.28099E-03
0.59880E-02	0.15792E 06	0.95863E 00	0.25989E 01	0.30273E-01	0.62305E-02	0.37376E 01	0.25721E-02	0.26030E-03
0.75385E-02	0.11019E 06	0.94898E 00	0.26748E 01	0.26291E-01	0.55635E-02	0.37444E 01	0.24873E-02	0.23980E-03
0.94904E-02	0.76631E 05	0.93723E 00	0.27529E 01	0.22782E-01	0.49384E-02	0.37511E 01	0.24009E-02	0.21928E-03
0.11948E-01	0.53071E 05	0.92301E 00	0.28333E 01	0.19686E-01	0.43526E-02	0.37579E 01	0.23119E-02	0.19880E-03
0.15041E-01	0.36570E 05	0.90588E 00	0.29160E 01	0.16954E-01	0.38041E-02	0.37646E 01	0.22206E-02	0.17821E-03
0.18936E-01	0.25048E 05	0.88539E 00	0.30011E 01	0.14541E-01	0.32907E-02	0.37714E 01	0.21772E-02	0.15772E-03
0.23839E-01	0.17031E 05	0.86107E 00	0.30446E 01	0.13441E-01	0.30464E-02	0.37782E 01	0.21272E-02	0.13746E-03

TABLE III. TFD densities ρ and screening functions ψ for Ba^{++} ($Z=56$, $N=2$) at 117 radial distances r . Outer boundary = $3.0500a_0$, ($a_0 = 0.52917 \text{ \AA}$). Atomic units are used throughout.

r	ρ	ψ	r	ρ	ψ	r	ρ	ψ
0.30500E-05	0.75143E 10	0.99979E 00	0.24227E-01	0.88170E 04	0.87480E 00	0.24934E 01	0.24459E-01	0.74817E-02
0.38397E-05	0.53197E 10	0.99978E 00	0.30500E-01	0.59755E 04	0.84854E 00	0.25296E 01	0.22389E-01	0.69226E-02
0.48339E-05	0.37661E 10	0.99978E 00	0.38397E-01	0.40119E 04	0.81775E 00	0.25663E 01	0.20426E-01	0.63725E-02
0.60855E-05	0.26662E 10	0.99977E 00	0.48339E-01	0.26638E 04	0.78204E 00	0.26035E 01	0.18562E-01	0.58302E-02
0.76613E-05	0.18876E 10	0.99976E 00	0.60855E-01	0.17456E 04	0.74109E 00	0.26412E 01	0.16790E-01	0.52956E-02
0.96449E-05	0.13363E 10	0.99974E 00	0.76613E-01	0.11264E 04	0.69481E 00	0.26795E 01	0.15105E-01	0.47680E-02
0.12142E-04	0.94605E 09	0.99973E 00	0.96449E-01	0.71394E 03	0.64330E 00	0.27183E 01	0.13494E-01	0.42450E-02
0.15286E-04	0.66976E 09	0.99970E 00	0.12142E 00	0.44323E 03	0.58701E 00	0.27379E 01	0.12718E-01	0.39864E-02
0.19244E-04	0.47415E 09	0.99968E 00	0.15286E 00	0.26871E 03	0.52673E 00	0.27577E 01	0.11959E-01	0.37289E-02
0.24227E-04	0.33567E 09	0.99964E 00	0.19244E 00	0.15858E 03	0.46364E 00	0.27776E 01	0.11214E-01	0.34717E-02
0.30500E-04	0.23764E 09	0.99960E 00	0.24227E 00	0.90792E 02	0.39928E 00	0.27977E 01	0.10485E-01	0.32157E-02
0.38397E-04	0.16823E 09	0.99955E 00	0.30500E 00	0.50264E 02	0.33548E 00	0.28179E 01	0.97693E-02	0.29606E-02
0.48339E-04	0.11709E 09	0.99948E 00	0.38397E 00	0.26819E 02	0.27412E 00	0.28382E 01	0.90688E-02	0.27069E-02
0.60855E-04	0.84307E 08	0.99939E 00	0.48339E 00	0.13749E 02	0.21714E 00	0.28587E 01	0.83775E-02	0.24530E-02
0.76613E-04	0.59681E 08	0.99928E 00	0.54238E 00	0.96881E 01	0.19079E 00	0.28794E 01	0.76969E-02	0.21997E-02
0.96449E-04	0.42246E 08	0.99915E 00	0.60855E 00	0.67516E 01	0.16609E 00	0.28898E 01	0.73599E-02	0.20731E-02
0.12142E-03	0.29904E 08	0.99898E 00	0.68281E 00	0.46520E 01	0.14317E 00	0.29002E 01	0.70251E-02	0.19468E-02
0.15286E-03	0.21166E 08	0.99877E 00	0.76613E 00	0.31680E 01	0.12212E 00	0.29105E 01	0.66909E-02	0.18201E-02
0.19244E-03	0.14980E 08	0.99851E 00	0.84307E 00	0.18170E 01	0.85800E-01	0.29211E 01	0.63588E-02	0.16938E-02
0.24227E-03	0.10602E 08	0.99817E 00	0.96449E 00	0.14170E 01	0.58000E-01	0.29317E 01	0.60295E-02	0.15682E-02
0.30500E-03	0.75020E 07	0.99775E 00	0.10822E 01	0.93006E 00	0.70516E-01	0.29422E 01	0.56972E-02	0.14412E-02
0.38397E-03	0.53078E 07	0.99723E 00	0.12142E 01	0.60252E 00	0.57083E-01	0.29528E 01	0.53666E-02	0.13149E-02
0.48339E-03	0.37548E 07	0.99657E 00	0.12862E 01	0.48246E 00	0.51034E-01	0.29635E 01	0.50352E-02	0.11885E-02
0.60855E-03	0.26555E 07	0.99576E 00	0.13624E 01	0.38495E 00	0.45412E-01	0.29688E 01	0.48688E-02	0.11252E-02
0.76613E-03	0.18776E 07	0.99473E 00	0.14431E 01	0.30599E 00	0.40203E-01	0.29741E 01	0.47026E-02	0.10622E-02
0.96449E-03	0.13271E 07	0.99346E 00	0.15286E 01	0.24225E 00	0.35388E-01	0.29795E 01	0.45349E-02	0.99874E-02
0.12142E-02	0.93758E 06	0.99187E 00	0.16192E 01	0.19095E 00	0.30951E-01	0.29849E 01	0.43665E-02	0.93534E-03
0.15286E-02	0.66203E 06	0.98989E 00	0.17151E 01	0.14978E 00	0.26871E-01	0.29902E 01	0.41966E-02	0.87175E-03
0.19244E-02	0.46714E 06	0.98743E 00	0.18168E 01	0.11684E 00	0.23129E-01	0.29956E 01	0.40258E-02	0.80824E-03
0.24227E-02	0.32934E 06	0.98438E 00	0.19244E 01	0.90528E-01	0.19701E-01	0.30010E 01	0.38554E-02	0.74540E-03
0.30500E-02	0.23194E 06	0.98061E 00	0.19806E 01	0.79446E-01	0.18098E-01	0.30064E 01	0.36803E-02	0.68143E-03
0.38397E-02	0.16314E 06	0.97594E 00	0.20384E 01	0.69557E-01	0.16564E-01	0.30118E 01	0.35049E-02	0.61818E-03
0.48339E-02	0.11455E 06	0.97019E 00	0.20980E 01	0.60736E-01	0.15097E-01	0.30173E 01	0.33251E-02	0.55431E-03
0.60855E-02	0.80276E 05	0.96312E 00	0.21592E 01	0.52861E-01	0.13692E-01	0.30227E 01	0.31428E-02	0.49073E-03
0.76613E-02	0.56118E 05	0.95446E 00	0.22223E 01	0.45837E-01	0.12347E-01	0.30281E 01	0.29567E-02	0.42730E-03
0.96449E-02	0.39111E 05	0.94390E 00	0.22872E 01	0.39565E-01	0.11058E-01	0.30336E 01	0.27647E-02	0.36377E-03
0.12142E-01	0.27158E 05	0.93108E 00	0.23540E 01	0.33961E-01	0.98197E-02	0.30390E 01	0.25642E-02	0.29990E-03
0.15286E-01	0.18774E 05	0.91559E 00	0.24227E 01	0.28951E-01	0.86299E-02	0.30445E 01	0.23529E-02	0.23593E-03
0.19244E-01	0.12908E 05	0.89698E 00	0.24578E 01	0.26644E-01	0.80507E-02	0.30500E 01	0.21265E-02	0.17219E-03

TABLE IV. TFD densities ρ and screening functions ψ for Ra^{++} ($Z=88$, $N=2$) at 117 radial distances r . Outer boundary $= 3.2464a_0$, ($a_0 = 0.52917 \text{ \AA}$). Atomic units are used throughout.

r	ρ	ψ	r	ρ	ψ	r	ρ	ψ
0.32464E-05	0.13481E 11	0.99987E 00	0.25787E-01	0.15148E 05	0.85139E 00	0.26540E 01	0.23449E-01	0.48510E-02
0.40870E-05	0.95437E 10	0.99986E 00	0.32464E-01	0.10175E 05	0.82111E 00	0.26925E 01	0.21448E-01	0.44814E-02
0.51452E-05	0.67564E 10	0.99985E 00	0.40870E-01	0.67600E 04	0.78595E 00	0.27315E 01	0.19556E-01	0.41192E-02
0.64774E-05	0.47832E 10	0.99984E 00	0.51452E-01	0.44330E 04	0.74561E 00	0.27711E 01	0.17763E-01	0.37631E-02
0.81546E-05	0.33863E 10	0.99983E 00	0.64774E-01	0.28631E 04	0.69996E 00	0.28113E 01	0.16064E-01	0.34136E-02
0.10266E-04	0.23973E 10	0.99981E 00	0.81546E-01	0.18166E 04	0.64911E 00	0.28520E 01	0.14450E-01	0.30693E-02
0.12924E-04	0.16971E 10	0.99979E 00	0.10266E 00	0.11292E 04	0.59346E 00	0.28934E 01	0.12915E-01	0.27302E-02
0.16271E-04	0.12015E 10	0.99976E 00	0.12924E 00	0.68561E 03	0.53378E 00	0.29143E 01	0.12173E-01	0.25620E-02
0.20483E-04	0.85057E 09	0.99973E 00	0.16271E 00	0.40532E 03	0.47120E 00	0.29353E 01	0.11450E-01	0.23953E-02
0.25787E-04	0.60214E 09	0.99969E 00	0.20483E 00	0.23254E 03	0.40723E 00	0.29565E 01	0.10742E-01	0.22293E-02
0.32464E-04	0.42627E 09	0.99964E 00	0.25787E 00	0.12904E 03	0.34364E 00	0.29778E 01	0.10049E-01	0.20642E-02
0.40870E-04	0.30176E 09	0.99957E 00	0.32464E 00	0.69029E 02	0.28235E 00	0.29993E 01	0.93700E-02	0.19000E-02
0.51452E-04	0.21362E 09	0.99948E 00	0.40870E 00	0.35491E 02	0.22522E 00	0.30210E 01	0.87026E-02	0.17361E-02
0.64774E-04	0.15121E 09	0.99938E 00	0.51452E 00	0.17489E 02	0.17387E 00	0.30428E 01	0.80486E-02	0.15734E-02
0.81546E-04	0.10704E 09	0.99924E 00	0.57730E 00	0.12073E 02	0.15073E 00	0.30648E 01	0.74040E-02	0.14110E-02
0.10266E-03	0.75764E 08	0.99908E 00	0.64774E 00	0.82388E 01	0.12942E 00	0.30758E 01	0.70844E-02	0.13299E-02
0.12924E-03	0.53625E 08	0.99887E 00	0.72678E 00	0.55566E 01	0.11000E 00	0.30869E 01	0.67664E-02	0.12488E-02
0.16271E-03	0.37952E 08	0.99861E 00	0.81546E 00	0.37030E 01	0.92491E-01	0.30981E 01	0.64520E-02	0.11683E-02
0.20483E-03	0.26858E 08	0.99828E 00	0.91496E 00	0.24380E 01	0.76874E-01	0.31092E 01	0.61364E-02	0.10872E-02
0.25787E-03	0.19005E 08	0.99788E 00	0.10266E 01	0.15853E 01	0.63097E-01	0.31204E 01	0.58225E-02	0.10064E-02
0.32464E-03	0.13446E 08	0.99736E 00	0.11519E 01	0.10180E 01	0.51083E-01	0.31317E 01	0.55084E-02	0.92543E-03
0.40870E-03	0.95113E 07	0.99672E 00	0.12924E 01	0.64528E 00	0.40728E-01	0.31430E 01	0.51958E-02	0.84492E-03
0.51452E-03	0.67265E 07	0.99592E 00	0.13690E 01	0.51117E 00	0.36133E-01	0.31543E 01	0.48806E-02	0.76390E-03
0.64774E-03	0.47558E 07	0.99492E 00	0.14501E 01	0.40352E 00	0.31904E-01	0.31600E 01	0.47240E-02	0.72379E-03
0.81546E-03	0.33613E 07	0.99367E 00	0.15360E 01	0.31739E 00	0.28025E-01	0.31657E 01	0.45652E-02	0.68322E-03
0.10266E-02	0.23746E 07	0.99211E 00	0.16271E 01	0.24869E 00	0.24477E-01	0.31714E 01	0.44068E-02	0.64293E-03
0.12924E-02	0.16766E 07	0.99018E 00	0.17235E 01	0.19405E 00	0.21240E-01	0.31771E 01	0.42477E-02	0.60264E-03
0.16271E-02	0.11830E 07	0.98777E 00	0.18256E 01	0.15073E 00	0.18296E-01	0.31828E 01	0.40874E-02	0.56228E-03
0.20483E-02	0.83402E 06	0.98478E 00	0.19338E 01	0.11646E 00	0.15624E-01	0.31885E 01	0.39265E-02	0.52205E-03
0.25787E-02	0.58735E 06	0.98107E 00	0.20483E 01	0.89425E-01	0.13204E-01	0.31943E 01	0.37628E-02	0.48146E-03
0.32464E-02	0.41310E 06	0.97649E 00	0.21082E 01	0.78148E-01	0.12002E-01	0.32000E 01	0.35981E-02	0.44104E-03
0.40870E-02	0.29007E 06	0.97085E 00	0.21697E 01	0.68136E-01	0.11015E-01	0.32058E 01	0.34308E-02	0.40050E-03
0.51452E-02	0.20328E 06	0.96392E 00	0.22331E 01	0.59259E-01	0.10001E-01	0.32115E 01	0.32608E-02	0.35994E-03
0.64774E-02	0.14211E 06	0.95543E 00	0.22983E 01	0.51387E-01	0.90360E-02	0.32173E 01	0.30884E-02	0.27909E-03
0.81546E-02	0.94507E 05	0.94507E 00	0.23654E 01	0.44403E-01	0.81178E-02	0.32231E 01	0.29116E-02	0.23842E-03
0.10266E-01	0.68784E 05	0.93249E 00	0.24345E 01	0.38205E-01	0.72433E-02	0.32289E 01	0.27287E-02	0.19794E-03
0.12924E-01	0.47556E 05	0.91728E 00	0.25055E 01	0.32703E-01	0.64098E-02	0.32347E 01	0.25397E-02	0.15732E-03
0.16271E-01	0.32703E 05	0.89900E 00	0.25787E 01	0.27809E-01	0.56134E-02	0.32406E 01	0.23404E-02	0.11659E-03
0.20483E-01	0.22344E 05	0.87720E 00	0.26161E 01	0.25567E-01	0.52281E-02	0.32464E 01	0.21263E-02	

TABLE V. TFD densities ρ and screening functions ψ for La^{++} ($Z=57$, $N=3$) at 117 radial distances r . Outer boundary = $2.6893a_0$, ($a_0=0.52917 \text{ \AA}$). Atomic units are used throughout.

r	ρ	ψ	r	ρ	ψ	r	ρ	ψ
0.26893E-05	0.93203E 10	0.99983E 00	0.21362E-01	0.11151E 05	0.88689E 00	0.21986E 01	0.39988E-01	0.10549E-01
0.33856E-05	0.65983E 10	0.99982E 00	0.26893E-01	0.75891E 04	0.86281E 00	0.22304E 01	0.36424E-01	0.97849E-02
0.42623E-05	0.46713E 10	0.99982E 00	0.33856E-01	0.51213E 04	0.83445E 00	0.22628E 01	0.33038E-01	0.90270E-02
0.53659E-05	0.33071E 10	0.99981E 00	0.42623E-01	0.34209E 04	0.80135E 00	0.22956E 01	0.29822E-01	0.82754E-02
0.67552E-05	0.23413E 10	0.99980E 00	0.53659E-01	0.22577E 04	0.76316E 00	0.23288E 01	0.26768E-01	0.75300E-02
0.85043E-05	0.16575E 10	0.99979E 00	0.67552E-01	0.14690E 04	0.71967E 00	0.23626E 01	0.23863E-01	0.67893E-02
0.10706E-04	0.11734E 10	0.99978E 00	0.85043E-01	0.94011E 03	0.67086E 00	0.23968E 01	0.21094E-01	0.60514E-02
0.13478E-04	0.83073E 09	0.99975E 00	0.10706E 00	0.59017E 03	0.61699E 00	0.24142E 01	0.19761E-01	0.56841E-02
0.16968E-04	0.58811E 09	0.99973E 00	0.13478E 00	0.36238E 03	0.55868E 00	0.24316E 01	0.18458E-01	0.53172E-02
0.21362E-04	0.41635E 09	0.99970E 00	0.16968E 00	0.21696E 03	0.49689E 00	0.24491E 01	0.17187E-01	0.49511E-02
0.26893E-04	0.29475E 09	0.99966E 00	0.21362E 00	0.12624E 03	0.43299E 00	0.24668E 01	0.15942E-01	0.45848E-02
0.33856E-04	0.20867E 09	0.99961E 00	0.26893E 00	0.71152E 02	0.36867E 00	0.24846E 01	0.14724E-01	0.42184E-02
0.42623E-04	0.14772E 09	0.99956E 00	0.33856E 00	0.38713E 02	0.30579E 00	0.25026E 01	0.13530E-01	0.38516E-02
0.53659E-04	0.10457E 09	0.99948E 00	0.42623E 00	0.20270E 02	0.24633E 00	0.25207E 01	0.12364E-01	0.34857E-02
0.67552E-04	0.74028E 08	0.99938E 00	0.53659E 00	0.14443E 02	0.21842E 00	0.25389E 01	0.11219E-01	0.31193E-02
0.85043E-04	0.52403E 08	0.99926E 00	0.67552E 00	0.70971E 01	0.19199E 00	0.25480E 01	0.10653E-01	0.29354E-02
0.10706E-03	0.37094E 08	0.99911E 00	0.85043E 00	0.48910E 01	0.16721E 00	0.25572E 01	0.10092E-01	0.27515E-02
0.13478E-03	0.26256E 08	0.99893E 00	0.10706E 01	0.33311E 01	0.14420E 00	0.25664E 01	0.95367E-02	0.25680E-02
0.16968E-03	0.18584E 08	0.99869E 00	0.13478E 01	0.22412E 01	0.12305E 00	0.25757E 01	0.89832E-02	0.23835E-02
0.21362E-03	0.13152E 08	0.99839E 00	0.16968E 01	0.14889E 01	0.10380E 00	0.25849E 01	0.84345E-02	0.21952E-02
0.26893E-03	0.93073E 07	0.99802E 00	0.21362E 01	0.95420E 00	0.86477E-01	0.25943E 01	0.78873E-02	0.20142E-02
0.33856E-03	0.65856E 07	0.99755E 00	0.26893E 01	0.10706E 01	0.71047E-01	0.26036E 01	0.73435E-02	0.18293E-02
0.42623E-03	0.46592E 07	0.99698E 00	0.33856E 01	0.78610E 00	0.64022E-01	0.26130E 01	0.68025E-02	0.16446E-02
0.53659E-03	0.32956E 07	0.99625E 00	0.42623E 01	0.63071E 00	0.57441E-01	0.26177E 01	0.65313E-02	0.15519E-02
0.67552E-03	0.23305E 07	0.99534E 00	0.53659E 01	0.50403E 00	0.51294E-01	0.26224E 01	0.62602E-02	0.14592E-02
0.85043E-03	0.16475E 07	0.99420E 00	0.67552E 01	0.40104E 00	0.45564E-01	0.26271E 01	0.59891E-02	0.13665E-02
0.10706E-02	0.11642E 07	0.99278E 00	0.85043E 01	0.31756E 00	0.40232E-01	0.26319E 01	0.57149E-02	0.12728E-02
0.13478E-02	0.82230E 06	0.99102E 00	0.10706E 01	0.25008E 00	0.35280E-01	0.26366E 01	0.54427E-02	0.11800E-02
0.16968E-02	0.58045E 06	0.98882E 00	0.13478E 01	0.19567E 00	0.30685E-01	0.26414E 01	0.51686E-02	0.10868E-02
0.21362E-02	0.40941E 06	0.98610E 00	0.16968E 01	0.15190E 00	0.26423E-01	0.26461E 01	0.48935E-02	0.99381E-03
0.26893E-02	0.28850E 06	0.98271E 00	0.21362E 01	0.13336E 00	0.24408E-01	0.26509E 01	0.46154E-02	0.90036E-03
0.33856E-02	0.20306E 06	0.97854E 00	0.26893E 01	0.11674E 00	0.22465E-01	0.26556E 01	0.43347E-02	0.80688E-03
0.42623E-02	0.14271E 06	0.97337E 00	0.33856E 01	0.10187E 00	0.20593E-01	0.26604E 01	0.40485E-02	0.71272E-03
0.53659E-02	0.10012E 06	0.96702E 00	0.42623E 01	0.88541E-01	0.18785E-01	0.26652E 01	0.37611E-02	0.61965E-03
0.67552E-02	0.70084E 05	0.95923E 00	0.53659E 01	0.76603E-01	0.17036E-01	0.26700E 01	0.34648E-02	0.52573E-03
0.85043E-02	0.48925E 05	0.94971E 00	0.67552E 01	0.65907E-01	0.15344E-01	0.26748E 01	0.31597E-02	0.43177E-03
0.10706E-01	0.34041E 05	0.93812E 00	0.85043E 01	0.56319E-01	0.13703E-01	0.26796E 01	0.28416E-02	0.33779E-03
0.13478E-01	0.23589E 05	0.92407E 00	0.10706E 01	0.47717E-01	0.12107E-01	0.26845E 01	0.25022E-02	0.24350E-03
0.16968E-01	0.16267E 05	0.90715E 00	0.13478E 01	0.43751E-01	0.11324E-01	0.26893E 01	0.21262E-02	0.14909E-03

TABLE VI. TFD densities ρ and screening functions ψ for Ac^{+++} ($Z=89$, $N=3$) at 117 radial distances r . Outer boundary = $2.8915a_0$, ($a_0=0.52917 \text{ \AA}$). Atomic units are used throughout.

r	ρ	ψ	r	ρ	ψ	r	ρ	ψ
0.28915E-05	0.16309E 11	0.99977E 00	0.22968E-01	0.18736E 05	0.86442E 00	0.23639E 01	0.37646E-01	0.68565E-02
0.36402E-05	0.11546E 11	0.99976E 00	0.28915E-01	0.12644E 05	0.83638E 00	0.23981E 01	0.34270E-01	0.63506E-02
0.45827E-05	0.81739E 10	0.99975E 00	0.36402E-01	0.84473E 04	0.80364E 00	0.24329E 01	0.31074E-01	0.58514E-02
0.57693E-05	0.57867E 10	0.99974E 00	0.45827E-01	0.55762E 04	0.76587E 00	0.24682E 01	0.28044E-01	0.53577E-02
0.72631E-05	0.40967E 10	0.99973E 00	0.57693E-01	0.36293E 04	0.72822E 00	0.25039E 01	0.25171E-01	0.48692E-02
0.91437E-05	0.29002E 10	0.99972E 00	0.72631E-01	0.23235E 04	0.67448E 00	0.25402E 01	0.22446E-01	0.43859E-02
0.11511E-04	0.20532E 10	0.99970E 00	0.91437E-01	0.14593E 04	0.62110E 00	0.25771E 01	0.19854E-01	0.39057E-02
0.14492E-04	0.14535E 10	0.99967E 00	0.11511E 00	0.89657E 03	0.56328E 00	0.25957E 01	0.18606E-01	0.36668E-02
0.18244E-04	0.10290E 10	0.99964E 00	0.14492E 00	0.53717E 03	0.50195E 00	0.26144E 01	0.17388E-01	0.34288E-02
0.22968E-04	0.72848E 09	0.99961E 00	0.18244E 00	0.31284E 03	0.43846E 00	0.26333E 01	0.16199E-01	0.31914E-02
0.28915E-04	0.51571E 09	0.99956E 00	0.22968E 00	0.17651E 03	0.37446E 00	0.26523E 01	0.15037E-01	0.29543E-02
0.36402E-04	0.36508E 09	0.99950E 00	0.28915E 00	0.96157E 02	0.31182E 00	0.26715E 01	0.13900E-01	0.27177E-02
0.45827E-04	0.25844E 09	0.99943E 00	0.36402E 00	0.50419E 02	0.25245E 00	0.26907E 01	0.12790E-01	0.24817E-02
0.57693E-04	0.18295E 09	0.99933E 00	0.45827E 00	0.25372E 02	0.19812E 00	0.27102E 01	0.11698E-01	0.22448E-02
0.72631E-04	0.12950E 09	0.99921E 00	0.57693E 00	0.17707E 02	0.17328E 00	0.27298E 01	0.10630E-01	0.20088E-02
0.91437E-04	0.91667E 08	0.99906E 00	0.72631E 00	0.12219E 02	0.15019E 00	0.27396E 01	0.10102E-01	0.18904E-02
0.11511E-03	0.64883E 08	0.99888E 00	0.91437E 00	0.83346E 01	0.12892E 00	0.27495E 01	0.95798E-02	0.17723E-02
0.14492E-03	0.45921E 08	0.99865E 00	0.11511E 00	0.56184E 01	0.10955E 00	0.27594E 01	0.90600E-02	0.16538E-02
0.18244E-03	0.32499E 08	0.99836E 00	0.14492E 00	0.37420E 01	0.92079E-01	0.27693E 01	0.85456E-02	0.15357E-02
0.22968E-03	0.22998E 08	0.99799E 00	0.18244E 00	0.24617E 01	0.76495E-01	0.27793E 01	0.80327E-02	0.14171E-02
0.28915E-03	0.16272E 08	0.99753E 00	0.22968E 00	0.15991E 01	0.62742E-01	0.27893E 01	0.75227E-02	0.12985E-02
0.36402E-03	0.11511E 08	0.99695E 00	0.28915E 00	0.10251E 01	0.50740E-01	0.27994E 01	0.70153E-02	0.11800E-02
0.45827E-03	0.81420E 07	0.99623E 00	0.36402E 00	0.81654E 00	0.45360E-01	0.28095E 01	0.65067E-02	0.10608E-02
0.57693E-03	0.57574E 07	0.99534E 00	0.45827E 00	0.64806E 00	0.40375E-01	0.28145E 01	0.62546E-02	0.10016E-02
0.72631E-03	0.40699E 07	0.99422E 00	0.57693E 00	0.51236E 00	0.35767E-01	0.28196E 01	0.60014E-02	0.94222E-03
0.91437E-03	0.28759E 07	0.99282E 00	0.72631E 00	0.40340E 00	0.31518E-01	0.28247E 01	0.57455E-02	0.88222E-03
0.11511E-02	0.20311E 07	0.99107E 00	0.91437E 00	0.31617E 00	0.27609E-01	0.28298E 01	0.54910E-02	0.82264E-03
0.14492E-02	0.14337E 07	0.98891E 00	0.11511E 00	0.24653E 00	0.24018E-01	0.28348E 01	0.52356E-02	0.76300E-03
0.18244E-02	0.10112E 07	0.98621E 00	0.14492E 00	0.19108E 00	0.20726E-01	0.28400E 01	0.49793E-02	0.70340E-03
0.22968E-02	0.71248E 06	0.98288E 00	0.18244E 00	0.14702E 00	0.17710E-01	0.28451E 01	0.47224E-02	0.64397E-03
0.28915E-02	0.50144E 06	0.97875E 00	0.22968E 00	0.12853E 00	0.16297E-01	0.28502E 01	0.44602E-02	0.58374E-03
0.36402E-02	0.35240E 06	0.97365E 00	0.28915E 00	0.11208E 00	0.14945E-01	0.28553E 01	0.41978E-02	0.52403E-03
0.45827E-02	0.24721E 06	0.96738E 00	0.36402E 00	0.97421E-01	0.13648E-01	0.28605E 01	0.39304E-02	0.46396E-03
0.57693E-02	0.17303E 06	0.95969E 00	0.45827E 00	0.84381E-01	0.12405E-01	0.28656E 01	0.36578E-02	0.40370E-03
0.72631E-02	0.12079E 06	0.95028E 00	0.57693E 00	0.72769E-01	0.11212E-01	0.28708E 01	0.33805E-02	0.34375E-03
0.91437E-02	0.84037E 05	0.93883E 00	0.72631E 00	0.62428E-01	0.10064E-01	0.28759E 01	0.30941E-02	0.28362E-03
0.11511E-01	0.58233E 05	0.92495E 00	0.91437E 00	0.53211E-01	0.89583E-02	0.28811E 01	0.27951E-02	0.22338E-03
0.14492E-01	0.40155E 05	0.90823E 00	0.11511E 00	0.44991E-01	0.78907E-02	0.28863E 01	0.24772E-02	0.16308E-03
0.18244E-01	0.27266E 05	0.88822E 00	0.14492E 00	0.41216E-01	0.73697E-02	0.28915E 01	0.21265E-02	0.10271E-03

TABLE VII. TFD densities ρ and screening functions ψ for Ce^{++++} ($Z=58$, $N=4$) at 117 radial distances r . Outer boundary = $2.4246a_0$, ($a_0=0.52917 \text{ \AA}$). Atomic units are used throughout.

r	ρ	ψ	r	ρ	ψ	r	ρ	ψ
0.24246E-05	0.11178E 11	0.99997E 00	0.19259E-01	0.13566E 05	0.89605E 00	0.19822E 01	0.59515E-01	0.13521E-01
0.30524E-05	0.79132E 10	0.99997E 00	0.24246E-01	0.92623E 04	0.87366E 00	0.20109E 01	0.54010E-01	0.12557E-01
0.38427E-05	0.56022E 10	0.99996E 00	0.30524E-01	0.62741E 04	0.84717E 00	0.20400E 01	0.48788E-01	0.11599E-01
0.48377E-05	0.39661E 10	0.99996E 00	0.38427E-01	0.42099E 04	0.81613E 00	0.20696E 01	0.43834E-01	0.10647E-01
0.60903E-05	0.28078E 10	0.99994E 00	0.48377E-01	0.27933E 04	0.78014E 00	0.20996E 01	0.39128E-01	0.96976E-02
0.76673E-05	0.19878E 10	0.99993E 00	0.60903E-01	0.18290E 04	0.73892E 00	0.21301E 01	0.34658E-01	0.87510E-02
0.96525E-05	0.14073E 10	0.99992E 00	0.76673E-01	0.11791E 04	0.69235E 00	0.21609E 01	0.30410E-01	0.78061E-02
0.12152E-04	0.99627E 09	0.99991E 00	0.96525E-01	0.74649E 03	0.64058E 00	0.21765E 01	0.27336E-01	0.73326E-02
0.15298E-04	0.70531E 09	0.99988E 00	0.12152E 00	0.46285E 03	0.58406E 00	0.21923E 01	0.26369E-01	0.68603E-02
0.19259E-04	0.49932E 09	0.99985E 00	0.15298E 00	0.28020E 03	0.52361E 00	0.22081E 01	0.24424E-01	0.63876E-02
0.24246E-04	0.35349E 09	0.99982E 00	0.19259E 00	0.16509E 03	0.46042E 00	0.22240E 01	0.22527E-01	0.59146E-02
0.30524E-04	0.25025E 09	0.99978E 00	0.24246E 00	0.94348E 02	0.39606E 00	0.22401E 01	0.20675E-01	0.54404E-02
0.38427E-04	0.17716E 09	0.99973E 00	0.30524E 00	0.52125E 02	0.33233E 00	0.22563E 01	0.18867E-01	0.49659E-02
0.48377E-04	0.12541E 09	0.99965E 00	0.38427E 00	0.27749E 02	0.27118E 00	0.22726E 01	0.17103E-01	0.44905E-02
0.60903E-04	0.88781E 08	0.99956E 00	0.48377E 00	0.15945E 02	0.24216E 00	0.22890E 01	0.15377E-01	0.40135E-02
0.76673E-04	0.62848E 08	0.99946E 00	0.60903E 00	0.14187E 02	0.21445E 00	0.22972E 01	0.14529E-01	0.37746E-02
0.96525E-04	0.44488E 08	0.99932E 00	0.76673E 00	0.99813E 01	0.18824E 00	0.23055E 01	0.13689E-01	0.35352E-02
0.12152E-03	0.31490E 08	0.99915E 00	0.96525E 00	0.69400E 01	0.16370E 00	0.23138E 01	0.12858E-01	0.32953E-02
0.15298E-03	0.22289E 08	0.99894E 00	0.12152E 00	0.47747E 01	0.14093E 00	0.23221E 01	0.12036E-01	0.30551E-02
0.19259E-03	0.15775E 08	0.99867E 00	0.15298E 00	0.32436E 01	0.12002E 00	0.23305E 01	0.11221E-01	0.28147E-02
0.24246E-03	0.11164E 08	0.99833E 00	0.19259E 00	0.21756E 01	0.10100E 00	0.23389E 01	0.10416E-01	0.25743E-02
0.30524E-03	0.78998E 07	0.99791E 00	0.24246E 00	0.14396E 01	0.83877E-01	0.23473E 01	0.96132E-02	0.23323E-02
0.38427E-03	0.55892E 07	0.99737E 00	0.30524E 00	0.11647E 01	0.76014E-01	0.23558E 01	0.88187E-02	0.20906E-02
0.48377E-03	0.39538E 07	0.99672E 00	0.38427E 00	0.93868E 00	0.68608E-01	0.23601E 01	0.84232E-02	0.19697E-02
0.60903E-03	0.27962E 07	0.99589E 00	0.48377E 00	0.75329E 00	0.61641E-01	0.23643E 01	0.80272E-02	0.18481E-02
0.76673E-03	0.19770E 07	0.99486E 00	0.60903E 00	0.60171E 00	0.55102E-01	0.23686E 01	0.76304E-02	0.17260E-02
0.96525E-03	0.13973E 07	0.99356E 00	0.76673E 00	0.47814E 00	0.48973E-01	0.23728E 01	0.72359E-02	0.16044E-02
0.12152E-02	0.98716E 06	0.99195E 00	0.96525E 00	0.37768E 00	0.43236E-01	0.23771E 01	0.68406E-02	0.14824E-02
0.15298E-02	0.69701E 06	0.98995E 00	0.12152E 00	0.29622E 00	0.37867E-01	0.23814E 01	0.64472E-02	0.13610E-02
0.19259E-02	0.49180E 06	0.98746E 00	0.15298E 00	0.23029E 00	0.32837E-01	0.23857E 01	0.60507E-02	0.12388E-02
0.24246E-02	0.34670E 06	0.98438E 00	0.19259E 00	0.20224E 00	0.30443E-01	0.23900E 01	0.56535E-02	0.11167E-02
0.30524E-02	0.24415E 06	0.98056E 00	0.24246E 00	0.17704E 00	0.28121E-01	0.23943E 01	0.52530E-02	0.99424E-03
0.38427E-02	0.17171E 06	0.97583E 00	0.30524E 00	0.15440E 00	0.25869E-01	0.23986E 01	0.48495E-02	0.87183E-03
0.48377E-02	0.12056E 06	0.97002E 00	0.38427E 00	0.13406E 00	0.23681E-01	0.24029E 01	0.44372E-02	0.74825E-03
0.60903E-02	0.84742E 05	0.96287E 00	0.48377E 00	0.11580E 00	0.21553E-01	0.24072E 01	0.40217E-02	0.62586E-03
0.76673E-02	0.59042E 05	0.95412E 00	0.60903E 00	0.99402E-01	0.19479E-01	0.24116E 01	0.35927E-02	0.50277E-03
0.96525E-02	0.41141E 05	0.94345E 00	0.76673E 00	0.84670E-01	0.17453E-01	0.24159E 01	0.31445E-02	0.37914E-03
0.12152E-01	0.28560E 05	0.93049E 00	0.96525E 00	0.71424E-01	0.15469E-01	0.24202E 01	0.26672E-02	0.25579E-03
0.15298E-01	0.19738E 05	0.91484E 00	0.12152E 00	0.65311E-01	0.14491E-01	0.24246E 01	0.21259E-02	0.13204E-03

TABLE VIII. TFD densities ρ and screening functions ψ for Th⁺⁺⁺⁺ ($Z = 90$, $N = 4$) at 117 radial distances r . Outer boundary $= 2.6293a_0$, ($a_0 = 0.52917 \text{ \AA}$). Atomic units are used throughout.

r	ρ	ψ	r	ρ	ψ	r	ρ	ψ
0.26293E-05	0.19122E 11	0.99563E 00	0.20885E-01	0.22334E 05	0.87426E 00	0.21495E 01	0.55173E-01	0.88204E-02
0.33101E-05	0.13538E 11	0.99962E 00	0.26293E-01	0.15126E 05	0.84797E 00	0.21807E 01	0.50056E-01	0.81824E-02
0.41672E-05	0.95839E 10	0.99962E 00	0.33101E-01	0.10148E 05	0.81716E 00	0.22123E 01	0.45207E-01	0.75498E-02
0.52461E-05	0.67849E 10	0.99961E 00	0.41672E-01	0.67326E 04	0.78143E 00	0.22443E 01	0.40609E-01	0.69214E-02
0.66045E-05	0.48034E 10	0.99960E 00	0.52461E-01	0.44077E 04	0.74050E 00	0.22769E 01	0.36257E-01	0.62981E-02
0.83146E-05	0.34005E 10	0.99959E 00	0.66045E-01	0.28412E 04	0.69426E 00	0.23099E 01	0.32130E-01	0.56783E-02
0.10467E-04	0.24074E 10	0.99957E 00	0.83146E-01	0.17987E 04	0.64285E 00	0.23434E 01	0.28210E-01	0.50603E-02
0.13178E-04	0.17043E 10	0.99954E 00	0.10467E 00	0.11152E 04	0.58670E 00	0.23603E 01	0.26327E-01	0.47523E-02
0.16590E-04	0.12065E 10	0.99952E 00	0.13178E 00	0.67511E 03	0.52664E 00	0.23773E 01	0.24495E-01	0.44453E-02
0.20885E-04	0.85415E 09	0.99949E 00	0.16590E 00	0.39778E 03	0.46384E 00	0.23945E 01	0.22705E-01	0.41377E-02
0.26293E-04	0.60468E 09	0.99944E 00	0.20885E 00	0.22736E 03	0.39984E 00	0.24118E 01	0.20956E-01	0.38296E-02
0.33101E-04	0.42806E 09	0.99939E 00	0.26293E 00	0.12564E 03	0.33644E 00	0.24292E 01	0.19255E-01	0.35224E-02
0.41672E-04	0.30303E 09	0.99932E 00	0.33101E 00	0.66909E 02	0.27555E 00	0.24468E 01	0.17591E-01	0.32143E-02
0.52461E-04	0.21451E 09	0.99923E 00	0.41672E 00	0.34234E 02	0.21904E 00	0.24644E 01	0.15966E-01	0.29059E-02
0.66045E-04	0.15185E 09	0.99913E 00	0.52461E 00	0.24100E 02	0.16842E 00	0.24822E 01	0.14380E-01	0.25973E-02
0.83146E-04	0.10749E 09	0.99899E 00	0.66045E 00	0.16778E 02	0.14569E 00	0.24912E 01	0.13599E-01	0.24428E-02
0.10467E-03	0.76081E 08	0.99882E 00	0.83146E 00	0.11549E 02	0.14569E 00	0.25001E 01	0.12827E-01	0.22881E-02
0.13178E-03	0.53849E 08	0.99861E 00	0.10467E 00	0.78574E 01	0.12480E 00	0.25092E 01	0.12063E-01	0.21333E-02
0.16590E-03	0.38110E 08	0.99834E 00	0.13178E 00	0.52821E 01	0.10580E 00	0.25182E 01	0.11306E-01	0.19781E-02
0.20885E-03	0.26970E 08	0.99800E 00	0.16590E 00	0.35073E 01	0.88700E-01	0.25273E 01	0.10555E-01	0.18227E-02
0.26293E-03	0.19083E 08	0.99759E 00	0.20885E 00	0.22994E 01	0.73467E-01	0.25364E 01	0.98103E-02	0.16671E-02
0.33101E-03	0.13501E 08	0.99706E 00	0.26293E 00	0.14875E 01	0.60040E-01	0.25455E 01	0.90701E-02	0.15109E-02
0.41672E-03	0.95502E 07	0.99641E 00	0.33101E 00	0.11901E 01	0.53973E-01	0.25547E 01	0.83362E-02	0.13549E-02
0.52461E-03	0.67539E 07	0.99453E 00	0.41672E 00	0.94851E 00	0.48320E-01	0.25593E 01	0.79709E-02	0.12769E-02
0.66045E-03	0.47749E 07	0.99558E 00	0.52461E 00	0.75294E 00	0.43063E-01	0.25639E 01	0.76051E-02	0.11987E-02
0.83146E-03	0.33746E 07	0.99328E 00	0.66045E 00	0.59509E 00	0.38186E-01	0.25685E 01	0.72395E-02	0.11200E-02
0.10467E-02	0.23839E 07	0.99168E 00	0.83146E 00	0.46805E 00	0.29490E-01	0.25732E 01	0.68745E-02	0.10416E-02
0.13178E-02	0.16831E 07	0.98969E 00	0.10467E 01	0.36607E 00	0.25627E-01	0.25779E 01	0.65095E-02	0.96313E-03
0.16590E-02	0.11874E 07	0.98722E 00	0.13178E 01	0.28442E 00	0.25627E-01	0.25824E 01	0.61439E-02	0.88457E-03
0.20885E-02	0.83704E 06	0.98415E 00	0.16590E 01	0.21919E 00	0.22057E-01	0.25871E 01	0.57754E-02	0.80555E-03
0.26293E-02	0.58940E 06	0.98036E 00	0.20885E 01	0.19170E 00	0.20372E-01	0.25917E 01	0.54057E-02	0.72658E-03
0.33101E-02	0.41446E 06	0.97568E 00	0.26293E 01	0.16715E 00	0.18750E-01	0.25964E 01	0.50340E-02	0.64765E-03
0.41672E-02	0.29097E 06	0.96990E 00	0.33101E 01	0.14525E 00	0.17188E-01	0.26011E 01	0.46588E-02	0.56870E-03
0.52461E-02	0.20385E 06	0.96281E 00	0.41672E 01	0.12570E 00	0.15681E-01	0.26058E 01	0.42788E-02	0.48976E-03
0.66045E-02	0.14246E 06	0.95412E 00	0.52461E 01	0.10825E 00	0.14225E-01	0.26104E 01	0.38900E-02	0.41047E-03
0.83146E-02	0.99257E 05	0.94353E 00	0.66045E 01	0.92663E-01	0.12815E-01	0.26151E 01	0.34899E-02	0.33104E-03
0.10467E-01	0.68897E 05	0.93067E 00	0.83146E 01	0.78744E-01	0.11448E-01	0.26199E 01	0.30731E-02	0.25155E-03
0.13178E-01	0.47606E 05	0.91514E 00	0.10467E 00	0.66311E-01	0.10119E-01	0.26246E 01	0.26270E-02	0.17183E-03
0.16590E-01	0.32715E 05	0.89550E 00	0.13178E 01	0.60586E-01	0.94658E-02	0.26293E 01	0.21267E-02	0.92393E-04

TABLE IX. Magnitudes (in %) of maximum discrepancies $\Delta\rho$ (max) between electron densities interpolated by hand and by machine, respectively.

N	1	2	3	4
$\Delta\rho(\text{max}), \%$	0.367	0.470	0.541	0.781

cant figure not exceeding unity, or an error ϵ of less than $\sim 0.5\%$ in the density $\rho(r_0)$. A similar error estimate was obtained by means of the second method, which consisted in interpolating "by hand" at some 12 judiciously selected points within each N group and comparing the results so obtained with those provided by the machine. The maximum discrepancies $|\Delta\rho(\text{max})|$ thus found are shown in Table IX. [The author has no ready explanation for the observed monotonic increase of $\Delta\rho(\text{max})$ with N .] We do note that the maximum value of $\Delta\rho$ for *all* N is less than 0.8% .

B. TFD Screening Functions

From Eqs. (II. 27) and (II. 28) we have, to five significant figures, that

$$\psi(Z, N, r) = 4.7854(r/Z)(\rho^{1/3} - 0.10289)^2, \quad (\text{III. 1})$$

where r is in atomic units ($a_0 = 0.52917 \text{ \AA}$), and ρ is in units of a_0^{-3} . Using Eq. (III. 1) along with the densities ρ determined as described above, the high-speed computer was also programmed to calculate the values of the TFD screening function ψ at the same 117 radial distances r that were used above in conjunction with the tabulation of $\rho(Z, N, r)$ and for the same 394 different types of ions. The results for the eight elements selected³⁴ are also recorded (to save space) in Tables I through VIII.

Accuracy of the ψ values was tested, firstly, by checking how closely they satisfied the two boundary conditions (II. 20) and (II. 21); and secondly, by "hand calculating" carefully chosen values of ψ at some eight points within each N group, or at a total of ~ 32 points. Inspection of Tables I through VIII shows that condition (II. 20) is satisfied accurately to within at least three significant figures, thus making the error in $\psi(0)$ less than $\sim 0.04\%$ for all (Z, N) here considered. Essentially the same is found to hold with respect to condition (II. 21). The results of checking the ψ values by means of the second method stated above are summarized in Table X. [No simple explanation is apparent for the observed monotonic decrease of $\Delta\psi(\text{max})$ with N ,] It is seen that the maximum value of $\Delta\psi$ does not exceed 0.02% .

C. Some Applications

Combining some of the analytical results of

Sec. II with the appropriate numerical results of Sec. III, some problems of considerable current interest,³⁵⁻³⁸ whose quantum-mechanically exact solutions are entirely impractical, can be solved with relative ease (but, of course, at the expense of reduced exactness). For example, from Eq. (II. 26), and using also Eqs. (II. 2) and (II. 3) we have

$$V(Z, N, r) = \frac{Z}{r} \psi + \frac{Z-N}{r_0} e - \frac{1}{32\pi^2}, \quad r \leq r_0, \quad (\text{III. 2})$$

where the units of V are $e/a_0 (= 27.210 \text{ V})$. In this approximation, the interaction energies $U(R)$ for binary systems comprising a TFD ion or atom (characterized by given Z and N) and a completely stripped ion of nuclear charge Z_s is

$$U(Z, N, R; Z_s) = Z_s V(Z, N, R), \quad R \leq R_0, \quad (\text{III. 3})$$

where R here denotes the distance between centers of the interacting atom-ion or ion-ion pair, and $R_0 = r_0$. Specifically, for a proton, $Z_s = 1$; for an α particle, $Z_s = 2$, etc. Keeping in mind the nature of the model on which Eq. (III. 3) is based, it is at once apparent that, other things equal, (III. 3) will apply optimally (i) in the presence of an electron-rich atom or ion [$N_e = (Z - N)$ large]; (ii) in a situation in which distortion of the ionic (or atomic) electron cloud is negligible; and (iii) when $R < R_0$. This is so because for $R \geq R_0$, $V = (Z - N_e)/R$, and this latter expression clearly underestimates the exact (quantum-mechanical) potential since ions (or atoms), in fact, do NOT possess sharply defined finite "boundaries" at r_0 . Using the screening functions ψ , determined as described in Sec. III B, the potentials V and the corresponding quantities $U(Z, N, R; Z_s)$ with $Z_s = 1$ and 2 , respectively, have also been obtained³⁷ by the writer for the 104 neutral atoms as well as for the nearly 400 ions discussed in Sec. III A above.

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TABLE X. Magnitudes (in %) of maximum discrepancies $\Delta\psi$ (max) between screening functions calculated by hand and by machine, respectively.

N	1	2	3	4
$ \Delta\psi(\text{max}) , \%$	0.0200	0.0153	0.0145	0.0139

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