Statistical Electron Density Distributions and Thomas-Fermi-Dirac Screening Functions for Neutral Atoms*

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(Received March 3, 1961)

Statistical electron density distributions and Thomas-Fermi-Dirac (TFD) screening functions have been obtained for the 104 elements corresponding to integral atomic numbers $Z=2$ to $Z=105$, for 117 values of radial distance from the atomic center in each case. These results 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 argon and copper are given here. The complete set of tables for all 104 elements has been deposited with the American Documentation Institute Auxiliary Publications Project.

I. INTRODUCTION

THE usefulness of the statistical model of the atom derives chiefly from its far simpler conceptual and mathematical structure as compared to that of the more exact quantum-mechanical treatment. Thus, the statistical model originally proposed by Thomas[1] and Fermi,[2] and later modified to account for electron exchange by Dirac,[3] has been successfully applied to the approximate solution of a large variety of problems, ranging from the behavior of matter in stars and in the earth[4,5] to the study of radiation damage in solids[6] and of specific properties characteristic of molecular and atomic species.[5,7–12] After suitable modification, the model has proved useful even in the study of the atomic nucleus.[13,14]

The unmodified Thomas-Fermi (TF) model is based on one fundamental equation universal for all atoms, and has been solved by several investigators.[5] Whenever it is desired to use the exchange-corrected Thomas-Fermi-Dirac (TFD) model, however, the basic TFD equation must be solved anew for each atomic species. Solutions of the latter kind with Brillouin's boundary conditions[15] have been given for all 92 elements by Umeda,[16] and with various boundary conditions for about one-quarter of the naturally occurring elements by Metropolis and Reitz.[8] The most complete solutions published to date, however, are those given by Thomas,[17] using Jensen's boundary conditions,[18] essentially for elements of atomic number $Z=2$ to $Z=105$ and the corresponding positive ions with degree of ionization one to four.

These solutions, along with extensive tabulations of related quantities of interest, are given for nonintegral values of Z. To obtain the corresponding values for actually occurring elements, i.e., for integral Z, it is, therefore, necessary to interpolate. More specifically, to obtain results as accurate as the original tables, four- or five-point Lagrangian interpolation is required.[17] Clearly, such a procedure, even if it were to be carried out for only one quantity of physical interest, say the electron density distribution ρ as a function of radial distance r from the atomic center, would involve a most formidable number of operations (about 10^5) for a human computer and is, therefore, a problem best suited for machine calculation. Furthermore, Thomas' tables give the values of $r^{\frac{3}{2}}\rho$ rather than the physically more interesting quantity ρ, thus necessitating for each Z and each r an additional dividing-out of the awkward factor $r^{\frac{3}{2}}$. Lastly, the very useful solution in terms of the TFD screening function ψ is not given in Thomas' work at all.

In conjunction with recent work on interatomic repulsive potentials,[19] a knowledge of the quantities $\rho(Z,r)$ and $\psi(Z,r)$ was desired and their calculation performed on a high-speed electronic computer. It is the purpose of the present paper to make these solutions for neutral atoms generally accessible for utilization in the many domains, indicated above, in which the TFD statistical model is applicable.

II. BASIC THEORETICAL RELATIONS

The basic TFD equation is[20]

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

* Work supported by the U. S. Atomic Energy Commission.
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[20] For proof of the results presented in this section, see reference 4 or 5.

TABLE I. TFD densities ρ for argon ($Z=18$). Outer boundary=4.2818. First row gives radial distance; second gives density (atomic units). 0.21271 E–02 means 0.21271×10^{-2}; etc.

0.42818 E 01 0.21271 E–02	0.42741 E 01 0.21272 E–02	0.42664 E 01 0.21277 E–02	0.42588 E 01 0.21285 E–02	0.42511 E 01 0.21296 E–02	0.42435 E 01 0.21313 E–02
0.42358 E 01 0.21325 E–02	0.42282 E 01 0.21348 E–02	0.42206 E 01 0.21371 E–02	0.42130 E 01 0.21392 E–02	0.42055 E 01 0.21429 E–02	0.41979 E 01 0.21463 E–02
0.41904 E 01 0.21498 E–02	0.41828 E 01 0.21531 E–02	0.41753 E 01 0.21579 E–02	0.41678 E 01 0.21626 E–02	0.41603 E 01 0.21671 E–02	0.41454 E 01 0.21776 E–02
0.41305 E 01 0.21889 E–02	0.41157 E 01 0.22020 E–02	0.41009 E 01 0.22162 E–02	0.40861 E 01 0.22314 E–02	0.40715 E 01 0.22483 E–02	0.40568 E 01 0.22655 E–02
0.40423 E 01 0.22837 E–02	0.40133 E 01 0.23241 E–02	0.39845 E 01 0.23690 E–02	0.39560 E 01 0.24167 E–02	0.39276 E 01 0.24694 E–02	0.38994 E 01 0.25264 E–02
0.38715 E 01 0.25864 E–02	0.38437 E 01 0.26505 E–02	0.38162 E 01 0.27190 E–02	0.37616 E 01 0.28655 E–02	0.37079 E 01 0.30267 E–02	0.36549 E 01 0.32039 E–02
0.36027 E 01 0.33955 E–02	0.35512 E 01 0.36028 E–02	0.35005 E 01 0.38249 E–02	0.34505 E 01 0.40647 E–02	0.34012 E 01 0.43221 E–02	0.33047 E 01 0.48894 E–02
0.32109 E 01 0.55376 E–02	0.31198 E 01 0.62718 E–02	0.30313 E 01 0.71048 E–02	0.29453 E 01 0.80451 E–02	0.28617 E 01 0.91045 E–02	0.27805 E 01 0.10300 E–01
0.27016 E 01 0.11645 E–01	0.25505 E 01 0.14848 E–01	0.24078 E 01 0.18876 E–01	0.22731 E 01 0.23918 E–01	0.21460 E 01 0.30207 E–01	0.20259 E 01 0.38022 E–01
0.19126 E 01 0.47700 E–01	0.18056 E 01 0.59640 E–01	0.17046 E 01 0.74347 E–01	0.15192 E 01 0.11430 E–00	0.13540 E 01 0.17353 E–00	0.12068 E 01 0.26014 E–00
0.10755 E 01 0.38519 E–00	0.95858 E 00 0.56350 E 00	0.85433 E 00 0.81472 E 00	0.76142 E 00 0.11645 E 01	0.67862 E 00 0.16461 E 01	0.53905 E 00 0.31858 E 01
0.42818 E–00 0.59252 E 01	0.34012 E–00 0.10624 E 02	0.27016 E–00 0.18428 E 02	0.21460 E–00 0.31028 E 02	0.17046 E–00 0.50880 E 02	0.13540 E–00 0.81520 E 02
0.10755 E–00 0.12800 E 03	0.85433 E–01 0.19751 E 03	0.67862 E–01 0.30026 E 03	0.53905 E–01 0.45068 E 03	0.42818 E–01 0.66925 E 03	0.34012 E–01 0.98489 E 03
0.27016 E–01 0.14385 E 04	0.21460 E–01 0.20880 E 04	0.17046 E–01 0.30151 E 04	0.13540 E–01 0.43353 E 04	0.10755 E–01 0.62119 E 04	0.85433 E–02 0.88754 E 04
0.67862 E–02 0.12652 E 05	0.53905 E–02 0.18001 E 05	0.42818 E–02 0.25573 E 05	0.34012 E–02 0.36285 E 05	0.27016 E–02 0.51435 E 05	0.21460 E–02 0.72854 E 05
0.17046 E–02 0.10313 E 06	0.13540 E–02 0.14591 E 06	0.10755 E–02 0.20636 E 06	0.85435 E–03 0.29176 E 06	0.67862 E–03 0.41241 E 06	0.53904 E–03 0.58287 E 06
0.42818 E–03 0.82361 E 06	0.34010 E–03 0.11637 E 07	0.27018 E–03 0.16438 E 07	0.21460 E–03 0.23224 E 07	0.17046 E–03 0.32808 E 07	0.13539 E–03 0.46349 E 07
0.10756 E–03 0.65457 E 07	0.85422 E–04 0.92482 E 07	0.67867 E–04 0.13059 E 08	0.53908 E–04 0.18446 E 08	0.42818 E–04 0.26057 E 08	0.33997 E–04 0.36827 E 08
0.27018 E–04 0.51979 E 08	0.21452 E–04 0.73468 E 08	0.17042 E–04 0.10375 E 09	0.13530 E–04 0.14665 E 09	0.10747 E–04 0.20715 E 09	0.85636 E–05 0.29123 E 09
0.68081 E–05 0.41083 E 09	0.53851 E–05 0.58235 E 09	0.42818 E–05 0.82363 E 09			

where

$$V_0=[(Z-N)e/r_0]+\tfrac{15}{16}\tau_0^2, \tag{2}$$

$$\tau_0=(4\kappa_a{}^2/15\kappa_k e)^{\frac{1}{2}}=0.2251(e/a_0)^{\frac{1}{2}}, \tag{3}$$

$$\kappa_a=\tfrac{3}{4}(3/\pi)^{\frac{1}{3}}e^2=0.7386e^2, \tag{4a}$$

$$\kappa_k=\tfrac{3}{10}(3\pi^2)^{\frac{2}{3}}e^2a_0=2.871e^2a_0, \tag{4b}$$

$$\sigma_0=(3e/5\kappa_k)^{\frac{3}{2}}=(3\pi^2)^{-1}(2/ea_0)^{\frac{3}{2}}=0.09553/(ea_0)^{\frac{3}{2}}, \tag{5}$$

and a_0, e, N, r_0, and V, respectively, denote the first Bohr radius in hydrogen, the magnitude of the electronic charge, the number of electrons per atom, the radius of the TFD atom (assumed to be spherically symmetric), and the electric potential.

In view of (1) together with Poisson's equation,

$$\nabla^2V=+4\pi e\rho, \tag{6}$$

where ρ represents the number density of electrons, and by recalling that V_0 and τ_0 are constants, we also have

$$\rho=\sigma_0[(V-V_0+\tau_0{}^2)^{\frac{1}{2}}+\tau_0]^3. \tag{7}$$

The boundary conditions for Eq. (1) are

$$\lim_{r\to0}[r(V-V_0+\tau_0{}^2)]=Ze, \tag{8}$$

$$(V-V_0+\tau_0{}^2)_{r=r_0}=\tfrac{1}{16}\tau_0{}^2, \tag{9}$$

TABLE II. TFD densities ρ for copper ($Z=29$). Outer boundary $=4.45390$. First row gives radial distance; second gives density (atomic units).

0.44539 E 01 0.21264 E-02	0.44459 E 01 0.21268 E-02	0.44379 E 01 0.21272 E-02	0.44299 E 01 0.21288 E-02	0.44220 E 01 0.21294 E-02	0.44140 E 01 0.21317 E-02
0.44061 E 01 0.21330 E-02	0.43982 E 01 0.21357 E-02	0.43903 E 01 0.21382 E-02	0.43824 E 01 0.21405 E-02	0.43745 E 01 0.21443 E-02	0.43666 E 01 0.21477 E-02
0.43588 E 01 0.21513 E-02	0.43510 E 01 0.21562 E-02	0.43431 E 01 0.21609 E-02	0.43353 E 01 0.21655 E-02	0.43275 E 01 0.21702 E-02	0.43120 E 01 0.21820 E-02
0.42965 E 01 0.21946 E-02	0.42811 E 01 0.22087 E-02	0.42657 E 01 0.22239 E-02	0.42504 E 01 0.22402 E-02	0.42351 E 01 0.22581 E-02	0.42199 E 01 0.22771 E-02
0.42048 E 01 0.22962 E-02	0.41746 E 01 0.23404 E-02	0.41447 E 01 0.23882 E-02	0.41150 E 01 0.24408 E-02	0.40855 E 01 0.24971 E-02	0.40562 E 01 0.25578 E-02
0.40271 E 01 0.26236 E-02	0.39982 E 01 0.26923 E-02	0.39695 E 01 0.27651 E-02	0.39128 E 01 0.29234 E-02	0.38569 E 01 0.30977 E-02	0.38018 E 01 0.32887 E-02
0.37475 E 01 0.34961 E-02	0.36939 E 01 0.37208 E-02	0.36412 E 01 0.39633 E-02	0.35891 E 01 0.42238 E-02	0.35379 E 01 0.45038 E-02	0.34375 E 01 0.51253 E-02
0.33400 E 01 0.58365 E-02	0.32452 E 01 0.66489 E-02	0.31531 E 01 0.75733 E-02	0.30637 E 01 0.86222 E-02	0.29767 E 01 0.98124 E-02	0.28923 E 01 0.11160 E-01
0.28102 E 01 0.12685 E-01	0.26530 E 01 0.16352 E-01	0.25046 E 01 0.21010 E-01	0.23645 E 01 0.26909 E-01	0.22322 E 01 0.34347 E-01	0.21074 E 01 0.43697 E-01
0.19895 E 01 0.55404 E-01	0.18782 E 01 0.70014 E-01	0.17731 E 01 0.88186 E-01	0.15803 E 01 0.13851 E-00	0.14084 E 01 0.21476 E-00	0.12553 E 01 0.32877 E-00
0.11188 E 01 0.49701 E-00	0.99710 E 00 0.74213 E 00	0.88867 E 00 0.10948 E 01	0.79203 E 00 0.15960 E 01	0.70590 E 00 0.23001 E 01	0.56071 E 00 0.46191 E 01
0.44539 E-00 0.88936 E 01	0.35379 E-00 0.16464 E 02	0.28102 E-00 0.29402 E 02	0.22322 E-00 0.50818 E 02	0.17731 E-00 0.85303 E 02	0.14084 E-00 0.13952 E 03
0.11188 E-00 0.22307 E 03	0.88867 E-01 0.34964 E 03	0.70590 E-01 0.53874 E 03	0.56071 E-01 0.81804 E 03	0.44539 E-01 0.12268 E 04	0.35379 E-01 0.18205 E 04
0.28102 E-01 0.26777 E 04	0.22322 E-01 0.39096 E 04	0.17731 E-01 0.56734 E 04	0.14084 E-01 0.81912 E 04	0.11188 E-01 0.11777 E 05	0.88867 E-02 0.16874 E 05
0.70589 E-02 0.24111 E 05	0.56071 E-02 0.34371 E 05	0.44539 E-02 0.48908 E 05	0.35379 E-02 0.69487 E 05	0.28102 E-02 0.98606 E 05	0.22323 E-02 0.13979 E 06
0.17731 E-02 0.19803 E 06	0.14085 E-02 0.28035 E 06	0.11188 E-02 0.39670 E 06	0.88869 E-03 0.56110 E 06	0.70590 E-03 0.79342 E 06	0.56070 E-03 0.11217 E 07
0.44539 E-03 0.15853 E 07	0.35377 E-03 0.22404 E 07	0.28104 E-03 0.31653 E 07	0.22323 E-03 0.44724 E 07	0.17731 E-03 0.63189 E 07	0.14083 E-03 0.89277 E 07
0.11188 E-03 0.12609 E 08	0.88855 E-04 0.17816 E 08	0.70594 E-04 0.25160 E 08	0.56075 E-04 0.35539 E 08	0.44539 E-04 0.50205 E 08	0.35364 E-04 0.70959 E 08
0.28104 E-04 0.10016 E 09	0.22314 E-04 0.14157 E 09	0.17727 E-04 0.19993 E 09	0.14074 E-04 0.28260 E 09	0.11179 E-04 0.39919 E 09	0.89078 E-05 0.56121 E 09
0.70817 E-05 0.79171 E 09	0.56119 E-05 0.11223 E 10	0.44539 E-05 0.15872 E 10			

and

$$[-\partial(V-V_0+\tau_0^2)/\partial r]_{r=r0}=(Z-N)e/r_0^2. \quad (10)$$

To simplify the fundamental equations (1) and (7), it is customary to introduce the dimensionless variables

$$x=r/\mu, \quad \psi(x)=(r/Ze)(V-V_0+\tau_0^2), \quad (11,12)$$

where

$$\mu=(4\pi\sigma_0)^{-\frac{2}{3}}e^{-1}Z^{-\frac{1}{3}}=\tfrac{1}{4}(9\pi^2/2)^{\frac{1}{3}}a_0Z^{-\frac{1}{3}}=0.8853a_0Z^{-\frac{1}{3}} \quad (13)$$

and the constant

$$\beta_0=\tau_0(\mu/Ze)^{\frac{1}{2}}=0.2118Z^{-\frac{2}{3}}. \quad (14)$$

The basic TFD equation (1) then becomes

$$d^2\psi/dx^2=x[(\psi/x)^{\frac{1}{2}}+\beta_0]^3, \quad (15)$$

with the correspondingly transformed boundary conditions (8), (9), and (10) now reading

$$\psi(0)=1, \quad \psi(x_0)=\tfrac{1}{16}\beta_0^2x_0, \quad (16,17)$$

$$-\psi'(x_0)=[(Z-N/Z)-\psi(x_0)]/x_0. \quad (18)$$

In terms of the screening function ψ, the electric potential and charge density, respectively, assume the form

$$V=(Ze/r)\psi+V_0-\tau_0^2, \quad (19)$$

and

$$\rho=(Z/4\pi\mu^3)[(\psi/x)^{\frac{1}{2}}+\beta_0]^3=(Z/4\pi\mu^3)(\psi''/x). \quad (20)$$

The physical reason for designating ψ a *screening*

TABLE III. TFD screening functions ψ for argon ($Z=18$). Outer boundary $=4.28180$. First row gives radial distance; second row gives ψ (atomic units).

4.2818	4.2741	4.2664	4.2588	4.2511	4.2435
0.00075220	0.00075090	0.00075021	0.00074974	0.00074974	0.00075039
4.2358	4.2282	4.2206	4.2130	4.2055	4.1979
0.00075036	0.00075171	0.00075305	0.00075416	0.00075707	0.00075975
4.1904	4.1828	4.1753	4.1678	4.1603	4.1454
0.00076243	0.00076491	0.00076917	0.00077327	0.00077704	0.00078654
4.1305	4.1157	4.1009	4.0861	4.0715	4.0568
0.00079696	0.00080934	0.00082307	0.00083791	0.00085486	0.00087206
4.0423	4.0133	3.9845	3.9560	3.9276	3.8994
0.00089055	0.00093216	0.00097934	0.0010301	0.0010869	0.0011493
3.8715	3.8437	3.8162	3.7616	3.7079	3.6549
0.0012156	0.0012871	0.0013644	0.0015316	0.0017182	0.0019258
3.6027	3.5512	3.5005	3.4505	3.4012	3.3047
0.0021520	0.0023981	0.0026624	0.0029480	0.0032540	0.0039232
3.2109	3.1198	3.0313	2.9453	2.8617	2.7805
0.0046765	0.0055108	0.0064321	0.0074392	0.0085331	0.0097204
2.7016	2.5505	2.4078	2.2731	2.1460	2.0259
0.011000	0.013842	0.017081	0.020731	0.024808	0.029329
1.9126	1.8056	1.7046	1.5192	1.3540	1.2068
0.034308	0.039758	0.045694	0.059058	0.074476	0.091980
1.0755	0.95858	0.85433	0.76142	0.67862	0.53905
0.11158	0.13323	0.15686	0.18236	0.20957	0.26838
0.42818	0.34012	0.27016	0.21460	0.17046	0.13540
0.33153	0.39701	0.46278	0.52701	0.58812	0.64499
0.10755	0.085433	0.067862	0.053905	0.042818	0.034012
0.69683	0.74327	0.78423	0.81987	0.85051	0.87659
0.027016	0.021460	0.017046	0.013540	0.010755	0.0085433
0.89859	0.91700	0.93231	0.94497	0.95538	0.96390
0.0067862	0.0053905	0.0042818	0.0034012	0.0027016	0.0021460
0.97086	0.97651	0.98110	0.98481	0.98780	0.99021
0.0017046	0.0013540	0.0010755	0.00085434	0.00067862	0.00053903
0.99215	0.99371	0.99496	0.99596	0.99676	0.99740
0.00042818	0.00034010	0.00027018	0.00021460	0.00017045	0.00013538
0.99791	0.99832	0.99865	0.99891	0.99911	0.99928
0.00010756	0.00008542	0.00006786	0.00005390	0.00004281	0.00003400
0.99941	0.99952	0.99960	0.99966	0.99972	0.99976
0.00002702	0.00002145	0.00001704	0.00001353	0.00001074	0.00000856
0.99980	0.99982	0.99984	0.99986	0.99987	0.99988
0.00000680	0.00000539	0.00000428			
0.99989	0.99990	0.99991			

function can be appreciated by examining Eq. (19). In the immediate vicinity of the nucleus, $\psi(x)\approx\psi(0)=1$, and thus V, the electric potential there, is essentially that due to the "bare" nuclear charge, entirely *unscreened* by the atomic electron cloud. As points successively more distant from the nucleus are considered, however, the positive nuclear charge becomes progressively more and more *screened* by the surrounding electron cloud. Analytically, this progressive screening is brought about by the monotonic decline in ψ, down to a minimal value $\psi(x_0)$ at the atomic boundary, and such that the potential there assumes the appropriate value $(Z-N)e/r_0$.

A distinctive feature of the TFD model, in contradistinction to the simple TF model, is that the former possesses a constant nonvanishing value of the electron density at the atomic boundary, i.e., at $r=r_0$, given by

$$\rho_0=0.002127/a_0^3, \tag{21}$$

which is the same for all free TFD atoms or ions. For all values of $r>r_0$, the density $\rho\equiv 0$.

III. DISCUSSION OF THE RESULTS

A. Electron Density Distributions

Using as input Thomas' data[17] for the "multiplied" electron densities $r^{\frac{3}{2}}\rho$ corresponding to nonintegral Z at 117 relative radial distances r/r_0 ranging from 10^{-6} to

TABLE IV. TFD screening functions ψ for copper ($Z=29$). Outer boundary=4.45390. First row gives radial distance; second row gives ψ (atomic units).

4.4539	4.4459	4.44379	4.4299	4.4220	4.4140
0.00048510	0.00048454	0.00048397	0.00048431	0.00048389	0.00048476
4.4061	4.3982	4.3903	4.3824	4.3745	4.3666
0.00048485	0.00048599	0.00048701	0.00048787	0.00048986	0.00049157
4.3588	4.3510	4.3431	4.3353	4.3275	4.3120
0.00049340	0.00049619	0.00049885	0.00050139	0.00050408	0.00051115
4.2965	4.2811	4.2657	4.2504	4.2351	4.2199
0.00051879	0.00052765	0.00053729	0.00054771	0.00055942	0.00057193
4.2048	4.1746	4.1447	4.1150	4.0855	4.0562
0.00058460	0.00061449	0.00064737	0.00068404	0.00072381	0.00076724
4.0271	3.9982	3.9695	3.9128	3.8569	3.8018
0.00081500	0.00086522	0.00091898	0.0010375	0.0011698	0.0013164
3.7475	3.6939	3.6412	3.5891	3.5379	3.4375
0.0014769	0.0016517	0.0018408	0.0020439	0.0022616	0.0027408
3.3400	3.2452	3.1532	3.0637	2.9767	2.8923
0.0032798	0.0038814	0.0045462	0.0052753	0.0060720	0.0069379
2.8102	2.6530	2.5046	2.3645	2.2322	2.1074
0.0078747	0.0099703	0.012374	0.015105	0.018178	0.021614
1.9895	1.8782	1.7731	1.5803	1.4084	1.2553
0.025429	0.029639	0.034261	0.044800	0.057161	0.071437
1.1188	0.99710	0.88867	0.79203	0.70590	0.56071
0.087686	0.10595	0.12621	0.14843	0.17254	0.22587
0.44539	0.35379	0.28102	0.22322	0.17731	0.14084
0.28490	0.34785	0.41275	0.47764	0.54074	0.60060
0.11188	0.088867	0.070590	0.056071	0.044539	0.035379
0.65612	0.70663	0.75177	0.79152	0.82605	0.85571
0.028102	0.022322	0.017731	0.014084	0.011188	0.0088867
0.88092	0.90217	0.91994	0.93471	0.94691	0.95694
0.0070589	0.0056071	0.0044539	0.0035379	0.0028102	0.0022323
0.96515	0.97185	0.97729	0.98171	0.98527	0.98816
0.0017731	0.00140845	0.0011188	0.00088868	0.00070590	0.00056070
0.99047	0.99234	0.99384	0.99504	0.99600	0.99677
0.00044539	0.00035377	0.00028104	0.00022323	0.00017731	0.00014083
0.99739	0.99788	0.99827	0.99858	0.99884	0.99904
0.00011188	0.00008885	0.00007059	0.00005607	0.00004453	0.00003536
0.99919	0.99932	0.99942	0.99950	0.99957	0.99961
0.00002810	0.00002231	0.00001772	0.00001407	0.00001118	0.00000890
0.99966	0.99969	0.99971	0.99973	0.99975	0.99976
0.00000708	0.00000561	0.00000445			
0.99977	0.99978	0.99979			

1, a high-speed electronic computer was programmed, first, to perform the five-point Lagrangian interpolation (over Z) required to yield the corresponding multiplied density distributions $r^{\frac{3}{2}}\rho$, as accurate as those in the input, for integral values of Z, ranging from $Z=2$ to $Z=105$. In order to obtain from these the electron densities ρ proper (rather than the quantities $r^{\frac{3}{2}}\rho$), the computer was further instructed to divide out the "multiplier" $r^{\frac{3}{2}}$. Lastly, to allow the final results to be put into still more readily useful form, the 117 actual radial distances r (rather than the mere ratios r/r_0) for each of the 104 different species of atoms were computed.

The results thus obtained for the statistical electron density distributions as functions of integral atomic number Z and radial distance r, along with the corresponding values of r_0 (all in atomic units), are given in Table I for a representative noble gas, argon ($Z=18$), and in Table II for a typical metal, copper ($Z=29$).[21] For reasons pertaining to the internal operation of the

[21] Space limitations do not allow inclusion of the corresponding results for the remaining 102 elements here. The complete set of tables of density distributions as well as of screening functions for all 104 elements has been deposited as Document No. 6689 with ADI Auxiliary Publications Project, Photoduplication Service, Library of Congress, Washington 25, D. C. A copy may be secured by citing the document number and by remitting $52.50 for photoprints or $11.00 for 35 mm microfilm. Advance payment is required. Make checks or money orders payable to: Chief, Photoduplication Service, Library of Congress.

high-speed computer, the values for both r and ρ 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[4,5] of $0.002127/a_0^3$ of Eq. (21) above. This showed complete agreement to three significant figures in practically all cases, with the largest error in the third significant figure not exceeding unity, or an error of less than $\sim 0.5\%$ in the density $\rho(r_0)$. A similar estimate of the magnitude of the error was obtained by means of the other method which consisted in actually interpolating "by hand" (at randomly selected points) and comparing the results so obtained with those provided by the machine.

B. TFD Screening Functions

Solving Eq. (20) for ψ and expressing the results in atomic units, gives

$$\psi(x)=4.78498(r/Z)(\rho^{\frac{1}{3}}-0.10290)^2, \tag{22}$$

with

$$x=1.12956rZ^{\frac{1}{3}}. \tag{23}$$

Using these relations and the values of the electron densities ρ just found, the high-speed computer was 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 $\rho(Z,r)$ and also for the 104 elements corresponding to $Z=2$ to $Z=104$. The results for argon and copper are recorded, likewise in atomic units, in Tables III and IV, respectively.[21]

The accuracy of these results was tested, firstly, by checking how closely they satisfied the boundary conditions (16) and (17) above; and secondly, by "hand calculating" randomly chosen values of ψ and comparing these values with those calculated by the machine. It is evident by inspection of these tables that the condition (16) is satisfied accurately to at least four significant figures, thus making the error in ψ less than 0.1% for all Z. This may be fortuitously small, with the other checks giving a value nearer $\sim 1\%$, as might indeed have been expected on the basis of the corresponding error estimate for the electron densities given above.

ACKNOWLEDGMENTS

The author is indebted to Dr. G. J. Dienes and Dr. G. H. Vineyard of Brookhaven National Laboratory for assistance in arranging for computer time; to Professor L. H. Thomas of the Physics Department, Columbia University, for his solutions on punched cards; and to M. Milgram for substantial assistance in programming.

Especial tribute is due to the late Dr. John B. Gibson of Brookhaven National Laboratory for helpful discussions and advice.