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Screening of Many-Electron Atoms*

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The problem of the screening of many-electron atoms (ions) is considered. Using the scaled Thomas-Fermi (STF) method of Stewart and Rotenberg for approximating the core potential of an atom (ion) with nuclear charge Z and net core charge Z^* , a screened scaled Thomas-Fermi potential (SSTF) is presented: $V(r) = -(Ze^2/r) U_{\text{SSTF}}$, where

$$\begin{aligned} U_{\text{SSTF}} &= U(r) - Ar, & 0 \leq r \leq a \\ &= BU(r) e^{(a-r)/D}, & r \geq a. \end{aligned}$$

Here D is the screening radius; A and B are constants; and $U(r)$ is given by

$$\begin{aligned} U(r) = U_{\text{STF}}(r) &= \varphi(r/\alpha\mu) + qr/r_c, & r \leq r_c \\ &= q, & r \geq r_c \end{aligned}$$

where $\varphi(r/\alpha\mu)$ is the well-known Thomas-Fermi function, r_c is the STF core radius with $\mu = \frac{1}{4}(9\pi^2/2Z)^{1/3} = 0.88534Z^{-1/3}$, α is the adjustable scaling factor, and $q = Z^*/Z$. The constants B and A are given by $B = D[aU'(a) - U(a)]/\{D[aU'(a) - U(a)] - aU(a)\}$ and $A = (1 - B)U(a)/a$, where $U'(a) = \partial U/\partial r$ at $r = a$. Eigenvalues of the Schrödinger equation with the SSTF potential are given for the $3d$, $4s$, $4p$, $4d$, $4f$, and $5s$ orbitals of Fe I and Fe VIII. Comparisons between the ions and corresponding hydrogenic orbitals show that the variations of the SSTF eigenvalues and the limiting screening radii are generally very different, with different level crossings and different relative energies. It is concluded that in order to obtain a correlation between a limiting screening radius and the observed disappearance of lines from a many-electron atom (ion), SSTF solutions are needed for the ion of interest. It is also concluded that until an accurate external screening function is obtained and applied to the screening of Hartree-Fock isolated-atom (-ion) solutions, SSTF solutions will be useful for the very important astrophysical problems of calculating equations of state and opacities for high- Z matter at stellar densities and temperatures.

I. INTRODUCTION

In this paper we consider the screening of bound orbitals of many-electron atoms (ions) by neighboring particles. Previous studies¹⁻¹² have analyzed the screening of bound orbitals of one-electron hydrogenic ions with a point nuclear charge Z ; in considering ions with two or more bound electrons, the core is assumed to be a point with an effective charge $Z^* = Z - N_b + 1$, where N_b is the number of bound electrons. (In this paper $N_b \leq Z$.) The reasons for using hydrogenic assumptions are obvious. In view of the considerable effort needed to accurately understand isolated many-electron atoms (ions) with the self-consistent-field methods of Hartree^{13(a)}

and Slater,^{13(b)} it is hardly feasible to consider accurate solutions with the additional interactions of neighboring atoms, ions, and free electrons in matter at finite densities and nonzero temperatures—systems that are further complicated by the dynamic time-dependent quality of even an equilibrium plasma.

Nevertheless, the hydrogenic screened Coulomb solutions of the time-independent Schrödinger equation have been of value in gaining a crude approximation to the many-electron-atom screening problem. As the next step in this problem, this paper will formulate a better approximation to the screening of many-electron atoms by considering the external screening of an atomic orbital. The electron

that occupies the orbital interacts with the atomic nucleus of charge Z and also interacts with the remaining $N_b - 1$ bound electrons, the latter interaction being approximated by the use of the scaled Thomas-Fermi (STF) ion potential of Stewart and Rotenberg.¹⁴ In the Stewart-Rotenberg theory, an approximate potential for an isolated many-electron atom (ion) is obtained by replacing the core with a Thomas-Fermi (TF) ion whose net charge is Z^* and whose nucleus has the actual nuclear charge. The present approximation modifies this potential by a standard Yukawa or Debye-Hückel-type screening factor as used previously by Rouse^{6,8,9} for hydrogenic ions.

Results for six orbitals of Fe I and Fe VIII show that the variations of the eigenvalues with changes in the screening radius are quite different for the two ions considered, and their limiting screening radii also can differ drastically from the limiting screening radii of hydrogenic ions with point nuclei. The limiting screening radius is the extrapolated screening radius that would yield a zero eigenvalue.

In Sec. II we formulate the problem of time-independent screening of many-electron atoms (ions), and in Sec. III we describe the screened (SSTF) potential that is used to approximate the internal and external screening of an orbital bound to a many-electron atom or ion. In Sec. IV we describe the results for the $3d$, $4s$, $4p$, $4d$, $4f$, and $5s$ orbitals of Fe I and Fe VIII, with the summary and conclusions given in Sec. V.

II. FORMULATION OF MANY-ELECTRON-ATOM SCREENING PROBLEM

We consider an equilibrium plasma composed of monatomic atoms, ions, and free electrons. We focus on an ion of nuclear charge Z with N_b bound electrons and assume that the time-averaged positions of the remaining particles can be described by a radially symmetric distribution function relative to the center of mass of the ion of interest; hence the center of mass of the system is that of the ion. We further assume that the time-averaged radial distribution of external particles includes the effects of elastic collisions, but excludes the particle interactions experienced by the ion of interest in an ionizing, recombination, excitation, or deexcitation event.

For the present discussion, let us start with Hartree's self-consistent-field method for isolated ions where it is assumed that each bound electron moves in a central field that can be calculated from the nuclear potential and the wave functions of all the other bound electrons. As is well known, the Schrödinger equation is then solved for each bound electron in its own central field, and the one-electron wave functions, or orbitals, are made consistent with the fields from which they are calculated.

Hence the k th electron is described by a normalized wave function $u_k(\vec{r}_k)$ that is a solution of

$$\left(-\frac{\hbar^2}{2m} \nabla_k^2 - \frac{Ze^2}{r_k} + \sum_{j \neq k} \int |u_j(\vec{r}_j)|^2 \frac{e^2}{r_{jk}} d\tau_j\right) u_k(\vec{r}_k) = \epsilon_k u_k(\vec{r}_k), \quad (1)$$

where $r_{jk} = |\vec{r}_j - \vec{r}_k|$, and the other symbols have their standard meanings. Exchange, spin orbit, and other terms for the isolated atom (ion) can be added to Eq. (1) but will not be done explicitly here in order to focus attention on the dominant interactions.

We now add the dominant electrostatic interactions with the remaining atoms, ions, and free electrons of the system to Eq. (1), which then becomes

$$\left(-\frac{\hbar^2}{2m} \nabla_k^2 - \frac{Ze^2}{r_k} + \sum_{j \neq k} \int |u_j(\vec{r}_j)|^2 \frac{e^2}{r_{jk}} d\tau_j + \sum_s \int |u_s^e(\vec{r}_s)|^2 \frac{e^2}{r_{sk}} d\tau_s - \sum_p \frac{Z_p e^2}{r_{pk}}\right) u_k(\vec{r}_k) = \epsilon_k u_k(\vec{r}_k), \quad (2)$$

where the u_s^e are the wave functions for the external electrons that are either free or bound to one of the external nuclei of charge Z_p , and r_{sk} and r_{pk} are the distances from the bound electron (k) to the external electrons (s) and to the nuclei (p), respectively.

Clearly, for large average $\langle r_{sk} \rangle$ and $\langle r_{pk} \rangle$, Eq. (2) reduces to Eq. (1) for an isolated ion. Further, for an isolated ion (a neutral atom is an "ion" with zero net charge), the u_k would be expected to satisfy all the standard normalization criteria. However, with the introduction of interacting external particles as in Eq. (2) it is not clear just how the occupied atomic orbitals should be normalized, in general, particularly when the outer orbitals of nearest-neighbor ions could overlap significantly, resulting, in the case of monatomic ions, in a time-averaged radially symmetric overlap charge, as, for example, found in a close-packed bcc lattice crystal. For now we only demand self-consistency for the bound electrons and that the entire wave function Ψ that describes all N bound and free electrons be normalized to N , i. e.,

$$\int \Psi^\dagger \Psi d\tau = N, \quad (3)$$

where the integration is over the occupied volume of configuration space.

The problem of interest is that of obtaining an approximate solution to Eq. (2). Two approximations are used here: (a) The STF method of Stewart and Rotenberg¹⁴ is used to approximate the screening effect of the core of bound electrons; and (b) a Yukawa or Debye-Hückel-type screening factor is used to approximate the effect of the ex-

ternal particles, where we use here the two-parameter form of the complete screened Coulomb potential (CSCP) used by Rouse.^{6,8,9}

In Sec. III the STF potential will be outlined and then modified with a CSCP-type external screening factor.

III. SCREENED SCALED THOMAS-FERMI POTENTIAL

In order to cast Eq. (2) in a form that parallels the Stewart-Rotenberg theory, rewrite Eq. (2) in two steps as

$$\left(-\frac{\hbar^2}{2m} \nabla_k^2 - \frac{Ze^2}{r_k} U_k^{(i)} + \sum_s \int |u_s^e(\vec{r}_s)|^2 \frac{e^2}{r_{sk}} d\tau_s - \sum_p \frac{Z_p^e e^2}{r_{pk}}\right) u_k(\vec{r}_k) = \epsilon_k u_k(\vec{r}_k) \quad (4)$$

and then

$$\left(-\frac{\hbar^2}{2m} \nabla_k^2 - \frac{Ze^2}{r_k} U_k^{(i)} U_k^{(e)}\right) u_k(\vec{r}_k) = \epsilon_k u_k(\vec{r}_k), \quad (5)$$

where $U_k^{(i)}$ is the internal screening function for the remaining bound electrons and $U_k^{(e)}$ is the external screening function for the external particles. The former is defined by

$$U_k^{(i)} = 1 + \frac{r_k}{Ze^2} \left(\sum_{j \neq k} \int |u_j(\vec{r}_j)|^2 \frac{e^2}{r_{jk}} d\tau_j + \text{exchange, spin-orbit, etc., terms} \right), \quad (6)$$

and from Ref. 8, the latter is defined by

$$U_k^{(e)} \sim 1 - r/(D+a), \quad 0 \leq r \leq a \\ \sim [D/(D+a)] e^{(a-r)/D}, \quad r \geq a$$

where D is the unspecified screening radius for the external particles, and where classically a may be interpreted as the mean minimum radius of the ion atmosphere, i. e., the mean minimum magnitude of \vec{r}_s or \vec{r}_p , the positions of the external electrons and nuclei, respectively, relative to the center of mass of the ion of interest. Although a net screening function could possibly be defined by a sum of internal and external screening functions, the product defined in Eq. (5) was chosen partly because it yields in a simple form the limit for a hydrogenic ion at all r and the limit for each orbital of a many-electron atom (ion) at large r . It is also the form to be expected in first order from the following intuitive physical arguments: We start with an isolated nucleus, charge Z , and one bound electron, call it "A." Their interaction is described exactly by the Coulomb potential. Now add more bound electrons, which reduces the mean interaction between A and Z by a factor $U_k^{(i)}$ defined by Eq. (6). Next consider the nucleus and only one bound electron A . Now add the free external particles to the system. This again reduces the mean interaction

between A and the nucleus, but now by a factor $U_k^{(e)}$, which is similar to Eq. (6), but which is usually written as equivalent to an exponential term.

In the first case above, electron A , in zero order, can be said to interact with a nucleus of effective charge Z' , where $Z' = Z \langle U_k^{(i)} \rangle$. Now using nucleus Z' in the second case, the external particles can be said to reduce the interaction between electron A and nucleus of charge Z' by the factor $U_k^{(e)}$; hence $Z' U_k^{(e)} = Z \langle U_k^{(i)} \rangle U_k^{(e)}$. But since $Z \langle U_k^{(i)} \rangle$ would represent a point nucleus and take us back to the hydrogenic screening problem, $Z U_k^{(i)}(\vec{r}) U_k^{(e)}(\vec{r})$ is used as a more realistic first-order term for the screening of a many-electron atom with finite extension in space. A more accurate many-body screening function must await further study.

After presenting the STF approximation for Eq. (6), a single screening function $U_k^{(ie)} = U_k^{(i)} U_k^{(e)}$ will be defined. Of course, for hydrogenic ions, $U_k^{(i)} = 1.0$.

A. Outline of Scaled Thomas-Fermi Potential for Isolated Ions

The discussion of the STF method is given by Stewart and Rotenberg in Ref. 14, with applications to the calculation of electric-dipole transition probabilities (oscillator strengths) where very good results were obtained. Of interest here is the resulting core potential itself. From Ref. 14, the STF potential for a positive ion is given by

$$V_{\text{STF}}(r) = -(2Z/r) [\varphi(x) + q x/x_c], \quad x \leq x_c \\ = -(2Z/r) q, \quad x \geq x_c \quad (7)$$

where the energy is in Ry; r is the radial distance in Bohr radii, x is the distance in STF units, with

$$x = r/\alpha\mu, \quad (8)$$

and $\mu = \frac{1}{4}(9\pi^2/2Z)^{1/3} = 0.88534Z^{-1/3}$; α is the scaling factor for the charge distribution, x_c is the ion core radius in STF units, and q is the fractional degree of ionization of the core given by $q = (Z - N_b + 1)/Z$. The $\varphi(x)$ in Eq. (7) is the TF function^{13(b),15,16} that satisfies the differential equation

$$\varphi''(x) = \varphi(x)^{3/2}/x^{1/2}, \quad (9)$$

with the boundary conditions

$$\varphi(0) = 1 \quad (10)$$

and

$$\varphi(x_c) = 0, \quad \varphi'(x_c) = -q/x_c. \quad (11)$$

We can now rewrite Eq. (5) for the radial wave function $P_{ni}(r)$ with $U_k^{(e)} = 1$, which results in

$$\frac{d^2 P_{ni}}{dr^2} + \left(\frac{2Z}{r} U^{(i)} + E_{n1} - \frac{l(l+1)}{r^2} \right) P_{ni} = 0, \quad (12)$$

where r is in units of Bohr radii; E is in Ry; and for bound orbitals, with $E < 0$, $P(r)$ is the standard radial wave function [$P(r) = rR(r)$] that satisfies the

boundary conditions

$$P_{nl}(0) = 0, \quad P_{nl}(\infty) = 0, \quad \int_0^\infty P_{nl}^2 dr = 1, \quad (13)$$

where l is the angular momentum quantum number and n the principal quantum number.

As described by Stewart and Rotenberg, α is chosen for a given orbital P_{nl} , such that the eigenvalue E_{nl} equals the known energy of the state. This is done here for the ionization energy of the isolated ion, and this same value is used for all assumed screening radii as well as for the other orbitals of the ion.

From Eq. (7), the STF screening function for an isolated ion, $U^{(i)} = U_{\text{STF}}$, is given by

$$U_{\text{STF}} = \varphi(x) + q x/x_c, \quad x \leq x_c \\ = q, \quad x \geq x_c \quad (14)$$

where $\varphi(x)$ satisfies Eqs. (9)–(11).

B. Approximate Many-Electron-Atom Screening Function

For the definition of a SSTF potential, we will look for screening factors that reduce to those for hydrogenic ions given by Rouse for the cases $a=0$ and $a \geq r_c$, where r_c is the core radius. For $0 \leq a \leq r_c$, we can look for solutions of the form, with $U = U_{\text{STF}}$,

$$V(r) = V_i(r) = -\frac{Ze^2}{r} U(r) + Ze^2 A, \quad 0 \leq r \leq a \\ = V_0(r) = -\frac{Ze^2}{r} BU(r) e^{(a-r)/D}, \quad r \geq a \quad (15)$$

where A and B are constants to be determined. To determine A and B , at $r = a$ we have the boundary conditions

$$V_i(a) = V_0(a) \\ \text{and} \\ -\frac{\partial V_i}{\partial r} \Big|_{r=a} = -\frac{\partial V_0}{\partial r} \Big|_{r=a}, \quad (16)$$

which yield

$$B = \frac{D[aU'(a) - U(a)]}{D[aU'(a) - U(a)] - aU(a)} \quad (17)$$

and

$$A = U(a)/a - BU(a)/a = (1 - B)U(a)/a. \quad (18)$$

Since $U'(a) \leq 0$ and $U(a) \geq 0$, then $0 \leq B \leq 1$ for all a . For $a \geq r_c$,

$$U(a) = U(r_c) = q = Z^*/Z, \quad (19)$$

$$U'(a) = U'(r_c) = 0,$$

which results in

$$A|_{a \geq r_c} = \frac{1}{D+a} \frac{Z^*}{Z}, \quad B|_{a \geq r_c} = \frac{D}{D+a}, \quad (20)$$

as expected.

In the limit $a \rightarrow 0$, $B(a=0) = 1$ and $A(a=0) = U'(0)D$.

For this report, since $A(a=0)$ is not needed for the present eigenvalue problem, $U'(0)$ is allowed to take on the values for the isolated ion.

Now Eq. (15) with A and B given by Eqs. (17) and (18) defines the SSTF potential V_{SSTF} , which (with U_{SSTF} and r in Bohr radii and energy in Ry) is given by

$$V_{\text{SSTF}} = -(Ze^2/r) U_{\text{SSTF}}, \quad (21)$$

where

$$U_{\text{SSTF}} = U(r) - Ar, \quad 0 \leq r \leq a \\ = BU(r) e^{(a-r)/D}, \quad r \geq a \quad (21')$$

and

$$U(r) \sim U_{\text{STF}}(x) = \varphi(x) + qx/x_c, \quad x \leq x_c \\ = q, \quad x \geq x_c$$

with $x_c = r_c/\alpha\mu$, the STF core radius in STF units.

In Sec. IV we present the results of numerical solutions of Eq. (12), with $U^{(i)} = U_{\text{SSTF}}$ given by Eqs. (17), (18), and (21).

IV. RESULTS

The Schrödinger equation with the present screened scaled Thomas-Fermi potential (SSTFP) was solved numerically by Numerov's method as described in the Appendix of Ref. 14 using the Gulf General Atomic Univac 1108 computer. The astrophysically important element iron was chosen. The $3d$, $4s$, $4p$, $4d$, $4f$, and $5s$ orbitals of Fe I and Fe VIII were considered to demonstrate similarities and differences between solutions with the present SSTFP and those with the hydrogenic CSCP. However, for comparison with hydrogenic solutions obtained by others, only the solutions with $a=0$ will be discussed in this report.

Tables I and II present the eigenvalues obtained with various assumed screening radii. Table III presents the limiting screening radii^{7,8} as defined for numerical solutions by linear extrapolations of eigenvalues obtained with screening radii near the limiting values. For comparison, Table III also presents hydrogenic screened Coulomb limiting screening radii from Refs. 8 and 10, with modifications for the ion's core charge. Figures 1 and 2 present graphs of the SSTF eigenvalues given in Tables I and II for the six orbitals of Fe I and Fe VIII, respectively.

In Tables I and II the screening radius $D = 10^{10}$ yields the isolated ion eigenvalues for the orbitals. We note that the $4l$ orbital degeneracies at infinite screening are removed as in the real ion. At the level of the present investigation, this can be seen by noting that the core potentials derived by Prokofjew,^{17,18} by Herman and Skillman as reported by Slater^{13(b)} and by Stewart and Rotenberg¹⁴ can be approximated with a core screening function ($U^{(i)}$) given by

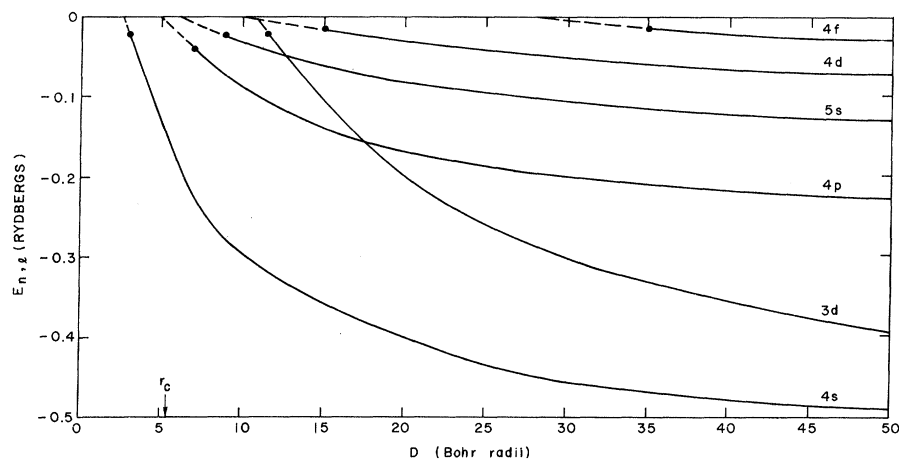


FIG. 1. $E_{n,l}$ vs D for the $3d$, $4s$, $4p$, $4d$, $4f$, and $5s$ orbitals of Fe I. The linearly extrapolated limiting screening radii (dashed lines) are given in Table III. The STF core radius $r_c = 5.6098a_0$. $E_{n,l}$ is the energy in Ry, and D is the screening radius in Bohr radii.

$$U^{(i)} \approx Z^*/Z + [(Z - Z^*)/Z]e^{-\beta r}, \quad (22)$$

where β would represent the reciprocal of an effective core screening radius. (Hence in this approximation, $U^{(i,e)} \sim \{Z^*/Z + [(Z - Z^*)/Z]e^{-\beta r}\}e^{-r/D}$.) Consequently, for any finite nonzero positive β , the

electron experiences a screened Coulomb-type potential near the origin, wherein l degeneracy is removed.

The remaining values of Tables I and II are graphed in Figs. 1 and 2. In Fig. 1, we note the very obvious crossing of the Fe I $4p$ and $5s$ levels

TABLE I. Fe I SSTFP eigenvalues $E_{n,l}$ from solutions with $\alpha = 1.02$ and with $\alpha = 0$ for $3d$, $4s$, $4p$, $4d$, $4f$, and $5s$ orbitals. STF core radius $r_c = 5.6098a_0$. $E_{n,l}$ in Ry and negative. Screening radii D in a. u. Ground-state configuration of Fe I is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6 4s^2 3d_4$.

D ($\alpha = 0$)	$3d$	$4s$	$4p$	$4d$	$4f$	$5s$
10^{10}	0.5404	0.5483	0.27335	0.1090	0.06253	0.1687
50.0	0.3939	0.4904	0.2280	0.07188	0.02900	0.1301
45.0					0.02600	
40.0					0.02245	
35.0					$\lesssim 0.01820$	
30.0	0.3029					
25.0	0.2597	0.4363	0.1869	0.04187		0.09750
20.0	0.1989			0.02925		
18.0	0.1678					
17.0	0.1469					
16.0	0.1270					
15.0	0.1055		0.1388	$\lesssim 0.0147$		0.06277
14.0	0.08238					
13.0	0.05808					0.05179
12.0	0.03390					0.04556
11.5	$\lesssim 0.02278$					
11.0			0.1014			0.03878
10.0		0.2965	0.08885			0.03147
9.0			0.74625			$\lesssim 0.02375$
8.0			0.05844			
7.5			0.04960			
7			$\lesssim 0.0402$			
5		0.1327				
4		0.7804				
3.75		0.06347				
3.5		0.04890				
3.25		0.03625				
3		0.02269				
2.75		$\lesssim 0.0110$				

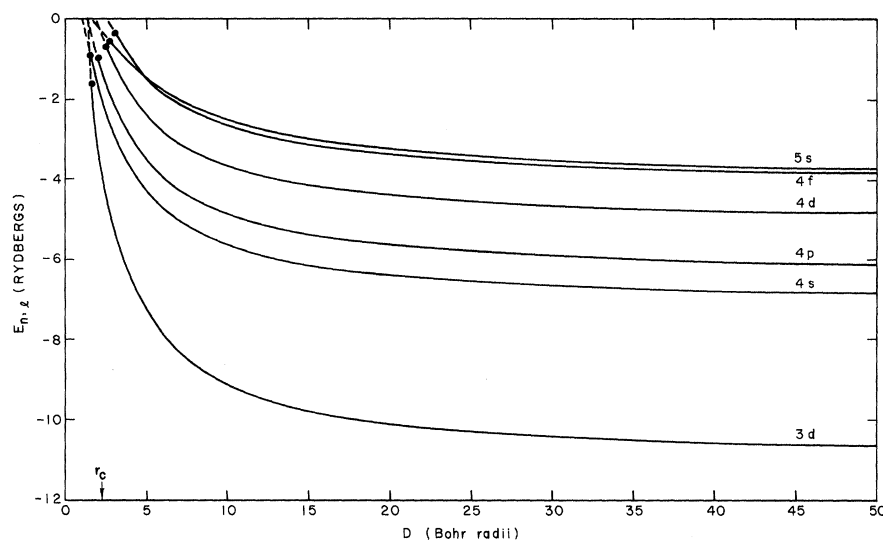


FIG. 2. $E_{n,l}$ vs D for the $3d$, $4s$, $4p$, $4d$, $4f$, and $5s$ orbitals for Fe VIII. The linearly extrapolated limiting screening radii (dashed lines) are given in Table III. The STF core radius $r_c = 1.8221a_0$. $E_{n,l}$ is the energy in Ry, and D is the screening radius in Bohr radii.

by the $3d$ level at screening radii that are over twice the STF core radius. In the hydrogenic solutions, a crossing first occurs between the $4f$ and $5s$ states,^{3,10} which do not cross at all with the Fe I SSTF core. Note further that the $5s$ SSTF level falls between the $4p$ and $4d$ levels. A check of Moore's tables¹⁸ for Fe I show this is to be expected, in general, for terms with the same total spins and angular momenta and the same core configurations.

The $3d$ level may also cross the $4d$ level near their limiting screening radii, but additional calculations are needed to give the correct answer.

Another interesting aspect of the Fe I $3d$ level is the rapid divergence of the $3d$ - $4s$ eigenvalues. At infinite screening, their values are about equal—in agreement with Hartree-Fock solutions.^{13(b)} But under screening the energy of the $3d$ level increases much faster than that of the $4s$ level.

Finally, the disappearance of the Fe I levels does

not follow the hydrogenic sequence. With decreasing screening radius, the corresponding hydrogenic levels considered here disappear in the order $4f$, $5s$, $4d$, $4p$, $4s$, $3d$; whereas the present Fe I SSTF levels disappear in the order $4f$, $3d$, $4d$ (or $4d$, $3d$), $5s$, $4p$, $4s$. In addition, whereas the Fe I $3d$ limiting screening radius appears to differ by less than 1 a.u. from the hydrogenic value, the remaining limiting radii are very different, as shown in Table III.

Next we discuss the Fe VIII curves in Fig. 2. This ion with one electron outside a complete argon core was expected to yield solutions similar to hydrogenic screened-Coulomb solutions. From Fig. 2 we note this to be more or less true except that (a) l degeneracy is removed at $D = \infty$, (b) the energy of the $5s$ level is only slightly greater than that of the $4f$ level; and (c) the levels disappear in a different sequence. However, as with the hydrogenic solutions, the $4f$ level does cross the $5s$ level, but at

TABLE II. Fe VIII SSTFP eigenvalues $E_{n,l}$ from solutions with $\alpha = 1.235$ and with $a = 0$ for $3d$, $4s$, $4p$, $4d$, $4f$, and $5s$ orbitals. STF core radius $r_c = 1.8221a_0$. $E_{n,l}$ in Ry and negative. Screening radii D in a.u. Ground-state configuration of Fe VIII is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^2 D_{3/2}$.

D ($a = 0$)	$3d$	$4s$	$4p$	$4d$	$4f$	$5s$
10^{10}	11.066	7.1452	6.3974	5.1737	4.1051	3.9858
50	10.670	6.8181	6.0697	4.8469	3.7900	3.6707
25	10.281	6.50125	5.7527	4.5319	3.4870	3.3729
15	9.7716	6.0939	5.3487	4.12995	3.1026	3.0022
10	9.1497	5.6089	4.8660	3.6555	2.6532	2.5801
5	7.3848	4.3086	3.5823	2.4135	1.4955	1.5494
3	5.2771	2.9045	2.2173	1.1429	$\lesssim 0.3751$	$\lesssim 0.6399$
2.5			1.6679	$\lesssim 0.6638$		
2.0	3.0414	1.60035	$\lesssim 0.9961$			
1.8	2.3967	1.2646				
1.6	$\lesssim 1.665$	0.9080				

a relatively large screening radius, and they disappear at much different limiting screening radii, as shown in Table III.

It is noteworthy that comparing the Fe VIII isolated-ion STF eigenvalues for the $4p$, $4f$, and $5s$ orbitals with the corresponding states listed by Moore¹⁹ shows very good agreement. For the first three excited states listed by Moore for Fe VIII, relative to a ground-state energy of -11.1 Ry, the corresponding energies are -6.44 , -4.13 , and -3.96 Ry, respectively. Now with an α that gives a ground-state energy of -11.07 Ry, the corresponding STF energies are -6.40 , -4.10 , and -3.99 Ry, respectively.

Finally, in Table III we note that the hydrogenic limiting screening radii for Fe VIII, except for the $3d$ and $4f$ levels, are very different from the SSTF levels. However, additional calculations near the limiting screening radii would be desirable in order to define more accurate SSTF limits.

V. SUMMARY AND CONCLUSIONS

The SSTFP is used here as a first-order approximation for the combined effects of bound core electrons of a many-electron atom (ion) and neighboring free particles (atoms, ions, electrons) on the eigenvalues of an occupied orbital of the many-electron atom. Previous studies considered the screening of one-electron hydrogenic ions with the results used to define a finite electronic partition function⁹ and were applied to the problem of an equation of state of monatomic matter, particularly at high densities where pressure ionization becomes important.²⁰ Noteworthy was the excellent correlation of the hydrogenic results with the disappearance of hydrogen lines observed in the solar photosphere and chromosphere,^{9,21} but not with a Debye-Hückel screening radius, but with a screening radius given by the radius of the mean atomic volume, r_0 , where $\frac{4}{3}\pi r_0^3 N_i = 1$, and N_i is the number of nuclei per unit

volume. This density-dependent screening radius is discussed qualitatively by Rouse^{20,22} in terms of the overlap of nearest-neighbor atomic orbitals.

Clearly, it would be of interest to see if similar correlations can be found for electronic energy levels of many-electron atoms and ions. The present calculations demonstrate that in order to have any chance of obtaining such a correlation for nonhydrogenic atoms, the hydrogenic solutions *cannot* be used, but SSTF solutions are needed for the particular ion of interest. It would also be of interest to obtain more SSTF solutions for other ions in order to search for possible patterns, for generalization of the present results would be premature. Eventually, screened Hartree-Fock self-consistent-field solutions will be desirable to explain more details—particularly to study the effects of screening on two or more orbitals simultaneously. However, before the screening of Hartree-Fock many-electron-atom solutions is considered, it would be desirable to obtain a more realistic effective one-electron screening function: A screening function with the exponential factor having r_0 as the screening radius is as distinct from the Debye potential as the Debye potential is distinct from the Yukawa potential.

In closing, since the partition-function problem for nonisolated hydrogen atoms is difficult enough, the present approximate results for many-electron atoms and ions indicate that a general accurate analytic solution is even more remote.

Note added in manuscript. From Eq. (4), the exact form of the net screening function $U_k^{(i,e)}$ can be written as

$$U_k^{(i,e)} = U_k^{(i)} \left[1 - \frac{r_k}{Z e^2 U_k^{(i)}} \left(\sum_s \int |u_s^e(r_s)|^2 \frac{e^2}{r_{sk}} d\tau_s - \sum_p \frac{Z_p^e e^2}{r_{pk}} \right) \right], \quad (23)$$

which shows how the external screening function

TABLE III. Linearly extrapolated limiting SSTFP screening radii D_L^{SSTF} from the eigenvalues given in Tables I and II for Fe I and Fe VIII, respectively, in a.u. The ZD_L^H are the hydrogenic screened Coulomb potential limiting screening radii obtained by Rouse (Ref. 8) and by Schlüter and Tsai (Ref. 10) in a.u. The ZD_L^H/Z^* are the limiting screening radii that would be obtained in the hydrogenic approximation with a net point core charge Z^* .

Orbital	Fe I		Fe VIII		
	Hydrogenic ZD_L^H	D_L^{SSTF}	ZD_L^H/Z^*	D_L^{SSTF}	ZD_L^H/Z^*
$3d$	10.94 ^a	10.5 ^b	10.94	1.3 ^b	1.37
$4s$	12.7 ^c	2.5 ^b	12.7	1.0	1.59
$4p$	15.0 ^c	4.8 ^b	15.0	1.3 ^b	1.875
$4d$	17.0 ^c	10.0 ^b	17.0	1.7 ^b	2.125
$4f$	20.1 ^c	27.5 ^b	20.1	2.4 ^b	2.51
$5s$	19.7 ^c	6.0 ^b	19.7	1.5 ^b	2.48

^aFrom Ref. 8.

^bLinear extrapolations use the lower limit of eigenvalue for SSTF solutions with the minimum screening radii

assumed in Tables I and II.

^cFrom Ref. 10.

$U_k^{(e)}$ given in Eq. (5) depends on the internal screening function $U_k^{(i)}$. Consequently, for $r \geq r_c$, $U_k^{(i)} = q$ and $ZU_k^{(i)} = Z^*$; hence $U_k^{(i,e)} = U_k^{(i)}U_k^{(e)}$ is exact. For $r < r_c$, in first order we can neglect the variation of $U_k^{(i)}$ in $U_k^{(e)}$ by replacing $ZU_k^{(i)}$ with Z' , an effective nuclear charge, leaving $U_k^{(i,e)} \approx U_k^{(i)}U_k^{(e)}$. Also note that in the core as r_k decreases to zero, $U_k^{(i)}$ increases to 1.0 and the probabilities of finding free particles of the plasma decrease to zero. Hence, near the nucleus $U_k^{(i,e)} \approx U_k^{(i)}$ and the variation in $U_k^{(i)}$ is important for $U_k^{(e)}$ only in the outer part of the core.

This note supports the intuitive arguments for the net product screening function discussed in Sec. III. More importantly, this note suggests that in a given plasma of a mixture of elements all ions with the same net core charge Z^* are influenced by approximately the same *external* screening function. Hence, an accurate external screening function determined for an hydrogenic ion of the system should be applicable in first order to a many-electron ion with the same Z^* . Studies of solar and laboratory spectra may provide a test for this possibility.

Finally, in a generalization of Eq. (23), given a

potential V in the form of a finite sum,

$$V = -Ze^2/r + V_1 + V_2 + \dots + V_n; \quad (24)$$

then

$$V \equiv -(Ze^2/r)U^1U^2 \dots U^n, \quad (25)$$

where

$$U^1 = 1 - (r/Ze^2)V_1,$$

$$U^1U^2 = U^1[1 - (r/Ze^2U^1)V_2],$$

$$U^1U^2U^3 = U^1U^2[1 - (r/Ze^2U^1U^2)V_3],$$

and

$$\prod_{i=1}^n U^i = \left(\prod_{i=1}^{n-1} U^i \right) \left[1 - \left(r/Ze^2 \prod_{i=1}^{n-1} U^i \right) V_n \right].$$

This general form will be given further consideration.

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