oscillator strength and summed over all q shells, gives easily and quickly the anomalous dispersion for any atom.

Sample calculations for the K region of copper and for the L region of tungsten have been made, using in each case only one term in the oscillator distribution for each q shell. Comparison with experiment shows less satisfactory agreement than with the previous less exact calculations. This disagreement is believed to be due to (a) the difficulties inherent in the experimental measurements, and (b) neglect of parts of the calculations in previous comparisons.

Studies of Atomic Self-Consistent Fields. II. Interpolation Problems*

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(Received November 27, 1953)

By studying the self-consistent-field (SCF) functions tabulated in the literature, it is shown that a quantity, which for a hydrogenlike function would equal the atomic number Z, for SCF functions will represent a form of "effective nuclear charge" Z_{eff}, which for a series of consecutive atoms or ions appears to be an almost linear function of the atomic number, convenient for interpolation purposes. The positions and magnitudes of maxima and minima, nodes, derivatives in origin, eigenvalues, etc., are investigated by considering the corresponding effective nuclear charges. It is important that the nodes may be interpolated separately, since the logarithm of an SCF function, divided by a polynomial having the same zero points as the function itself, may be used for interpolating SCF functions as a whole. This logarithm may also be used for defining a continuously varying effective charge $Z_{eff}(r)$, which is convenient for interpolation purposes or for estimating fields with exchange from those without exchange.

THE numerical work involved in each cycle of the integration of the Hartree-Fock equations for atomic self-consistent fields (SCF) with exchange by using the technique developed by Hartree[1] is quite large, and, in order to secure a rapid convergence of the process, it is therefore important to have as good "initial" functions as possible. For this purpose it is now possible to utilize the properties of already tabulated fields; Hartree has shown that rather good estimates of the initial functions could be obtained simply by interpolating their departures from properly scaled hydrogenlike wave functions. A function $F(r)$ is here said to be obtained from another $f(r)$ by change of a scale factor λ, if

$$F(r) = \lambda^{\frac{3}{2}} f(\lambda r), \qquad (1)$$

which transformation leaves the normalization integral invariant.

Brown, Bartlett, and Dunn[2,3] have shown that the SCF wave functions can be approximately transformed into each other by using scale factors λ, which are obtained from the reciprocals of the positions of the maxima and minima of the tabulated functions and which appear to be almost linear functions of the atomic

number Z. Hartree and Hartree[4] have used a similar idea for scaling the departure of the SCF functions with exchange from those without exchange. In a slightly modified form, the scaling method has recently been used also by Scherr[5] in Chicago.

Using a somewhat different approach, Arnot and McLauchlan[6] and Manning and Millman[7] have shown that, instead of the wave functions themselves, the effective nuclear charges associated with the SCF potentials may be used for interpolation purposes. On a large-scale basis, these total charges have recently been tabulated by Freeman[8] for all fields available.

In the first paper of this series,[9] it was shown that SCF wave functions could be interpolated (and to some extent extrapolated) with a surprisingly high accuracy by means of analytic expressions of Slater type. The purpose of the present paper is to investigate whether it is possible to carry out similar interpolations directly in the numerical tables of the functions involved, without the help of the analytic forms. We will first show the existence of some simple regularities for quantities like the positions and the magnitudes of maxima and minima, derivatives in origin, nodes,

[1] For a survey, see D. R. Hartree, Repts. Progr. in Phys. 11, 113 (1946).
[2] Brown, Bartlett, and Dunn, Phys. Rev. 44, 296 (1933).
[3] See also Hartree, reference 1, p. 126, Fig. 1, for another example.
[4] D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) A166, 450 (1938).
[5] C. W. Scherr, J. Chem. Phys. 21, 1237, 1241 (1953).
[6] F. L. Arnot and J. C. McLauchlan, Proc. Roy. Soc. (London) A146, 662 (1934).
[7] M. F. Manning and J. Millman, Phys. Rev. 49, 848 (1936).
[8] A. J. Freeman, Phys. Rev. 91, 1410 (1953).
[9] P. O. Löwdin, Phys. Rev. 90, 120 (1953), in the following referred to as Part I.

TABLE I. Properties of the hydrogenlike radial wave functions $f_{nl}(Z|r)=Z^{\frac{1}{2}}NQ_{nl}(\rho)\exp(-\rho/2)$, expressed in the variable $\rho=2Zr/n$. The values of ρ_m correspond to the maxima and minima; the positions r_m and the magnitudes f_m of these extreme values are given by the relations $r_m=c_m/Z$ and $f_m=d_mZ^{\frac{3}{2}}$. The values of ρ_0 correspond to the nodes.

nl	N^{-1}	$Q(\rho)$	ρ_m	c_m	d_m	ρ_0
$1s$	1	ρ	2	1	0.73576	$\cdots$
$2s_1$	$2\sqrt{2}$	$2\rho-\rho^2$	$3-\sqrt{5}$	0.76393	0.22786	2
$2s_2$			$3+\sqrt{5}$	5.23607	-0.43700	
$2p$	$2\sqrt{6}$	ρ^2	4	4	0.44200	$\cdots$
$3s_1$	$6\sqrt{3}$	$6\rho-6\rho^2+\rho^3$	0.49336	0.74004	0.12179	1.26795
$3s_2$			2.79063	4.18595	-0.19667	4.73205
$3s_3$			8.71602	13.07403	0.31864	
$3p_1$	$6\sqrt{6}$	$4\rho^2-\rho^3$	2	3	0.20025	4
$3p_2$			8	12	-0.31903	
$3d$	$6\sqrt{30}$	ρ^3	6	9	0.32723	$\cdots$

eigenvalues, etc., and we will then describe the general interpolation rule for the numerical wave functions themselves.

I. INTERPOLATION PROPERTIES OF THE MAXIMA AND MINIMA, THE DERIVATIVES IN ORIGIN, THE NODES, AND THE ENERGY EIGENVALUES OF THE SCF FUNCTIONS

If (n,l,m) is a fixed triple of atomic quantum numbers, there is a close connection between the normalized radial wave function $f_{nl}(\text{SCF}|r)$ for a self-consistent field (SCF) with or without exchange and the corresponding hydrogen function $f_{nl}(\text{H}|r)$. With increasing atomic number Z, the attraction from the nucleus on an electron in the orbital (n,l,m) will dominate entirely over the repulsion from the other electrons, and the function $f_{nl}(\text{SCF}|r)$ will therefore tend to be more and more hydrogenlike. In the limit, we obtain

$$\lim_{Z\to\infty} Z^{-\frac{1}{2}}f_{nl}(\text{SCF}|r/Z)=f_{nl}(\text{H}|r). \quad (2)$$

A more rigorous proof[10] of this relation can be derived by considering the Hartree-Fock equations in greater detail. For large Z, we will therefore have

$$f_{nl}(\text{SCF}|r)=Z^{\frac{1}{2}}\{f_{nl}(\text{H}|Zr)+(Z^{-1})\}, \quad (3)$$

where the remainder (Z^{-1}) can be expressed asymptotically as a power series in Z^{-1}. In a similar way, each characteristic SCF quantity can be expressed in the corresponding hydrogenlike quantity and a power series in Z^{-1}. The explicit form of this asymptotic expansion may be useful in interpolation problems, where only one or two SCF data are available, but otherwise it seems to be simpler to use the numerical informations in a more direct way, as described below.

As basic interpolation rule, we will here use the principle that *a quantity, which for a hydrogenlike function equals the atomic number Z, for a series of SCF functions for consecutive atoms or ions will be an almost linearly varying function of the atomic number Z.* The function

[10] D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) **A166**, 450 (1938).

obtained in this way will be called the *effective nuclear charge* with respect to the SCF quantity under consideration and will be denoted by $Z(\text{SCF}|\ )$ plus a suffix indicating the quantity, which is investigated. Numerically, this function is very convenient for interpolation purposes, and, physically, it will give us an idea of the effect of the screening of the electrons around the nucleus in the various atoms under consideration.

(a) The Extreme Values

In order to investigate, for instance, the properties of the maxima and minima of the SCF functions, we will start with considering the scaled hydrogenlike functions $f_{nl}(Z|r)$ having the explicit form

$$f_{nl}(Z|r)=Z^{\frac{1}{2}}f_{nl}(\text{H}|Zr)=Z^{\frac{1}{2}}NQ_{nl}(\rho)\exp(-\rho/2), \quad (4)$$

where $\rho=2Zr/n$; N is a normalization constant, and Q_{nl} is a polynomial in ρ of degree n, which is explicitly given for the lowest quantum numbers[11] in Table I. The numerical values ρ_m, corresponding to the extreme values of $f_{nl}(Z|r)$, are obtained by solving the alegbraic equation $Q(\rho)=2dQ(\rho)/d\rho$. The positions r_m and the magnitudes f_m of the extreme values are then given by

$$r_m=c_m/Z, \quad f_m=d_mZ^{\frac{3}{2}}, \quad (5)$$

where the coefficients c_m and d_m are listed in Table I, too.

In investigating the numerically given SCF functions we should now, according to the analogy rule stated above, study the quantities

$$Z(\text{SCF}|r_m)=c_m/r_m, \quad Z(\text{SCF}|f_m)=(f_m/d_m)^2, \quad (6)$$

where the coefficients c_m and d_m are taken from Table I, whereas r_m and f_m have to be determined from the SCF functions under consideration. In order to compute r_m with some accuracy from the numerical tables, one can utilize the behavior of "quotient series" of the same type as described in Part I. We will start from the assumption that, in the neighborhood of an extreme value belonging to the slope number L in order from origin, the SCF function is of the form

$$f_{nl}(\text{SCF}|r)=\text{const } r^p e^{-ar}, \quad p=l+L, \quad (7)$$

TABLE II. Calculation of r_m for the first maximum of $f_{3s}(r)$ for Cl^- with exchange according to Eq. (12); $k=$ number of iterations.

	Given properties of the function f_{3s}.			Solution of Eq. (12).		
r	$f_{3s}(r)$	f_{3s}/r	$q(r)$	k	r_m	q_m
0.03	0.393	13.10		0		1.243
			1.2214			
0.04	0.429	10.73		1	0.04596	1.2435
			1.2413			
0.05	0.432	8.640		2	0.04589	1.2434
			1.2644			
0.06	0.410	6.833		3	0.04590	

[11] Extensive tables of hydrogenlike radial wave functions $R_{nl}=f_{nl}\cdot r$ are given in L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1935), p. 135.

TABLE III. Positions r_m and magnitudes f_m of maxima and minima for SCF functions with exchange for some Ne-like ions.

Z	Element	1s r_m	f_m	2s₁ r_m	f_m	2s₂ r_m	f_m	2p r_m	f_m
10	Ne	0.10295	2.268	0.08088	0.4752	0.6848	1.087	0.6342	0.965
11	Na⁺	0.09343	2.382	0.07333	0.5190	0.6119	1.169	0.5478	1.070
12	Mg⁺²	0.08550	2.492	0.06672	0.5607	0.5483	1.246	0.4833	1.157
13	Al⁺³	0.07875	2.598	0.06140	0.6019	0.4972	1.320	0.4310	1.243
14	Si⁺⁴	0.07309	2.700	0.05675	0.6400	0.4555	1.390	0.3893	1.321

TABLE IV. Positions r_m and magnitudes f_m of maxima and minima for SCF functions with exchange for some A-like ions.

Z	Element	1s r_m	f_m	2s₁ r_m	f_m	2s₂ r_m	f_m	2p r_m	f_m
17	Cl⁻	0.05992	2.982	0.04672	0.7427	0.3636	−1.575	0.3033	1.5188
18	A	0.05651	3.069	0.04390	0.7722	0.3412	−1.632	0.2825	1.5805
19	K⁺	0.05351	3.157	0.04142	0.8035	0.3196	−1.687	0.2637	1.6407
20	Ca⁺²	0.05083	3.240	0.03944	0.8341	0.3014	−1.743	0.2477	1.6979

Z	Element	3s₁ r_m	f_m	3s₂ r_m	f_m	3s₃ r_m	f_m	3p₁ r_m	f_m	3p₂ r_m	f_m
17	Cl⁻	0.04590	0.2168	0.3026	0.4036	1.3021	0.8635	0.2430	0.3175	1.4825	0.7340
18	A	0.04314	0.2397	0.2825	0.4430	1.1767	0.9242	0.2247	0.3712	1.3010	0.8208
19	K⁺	0.04078	0.2621	0.2652	0.4812	1.0851	0.9813	0.2099	0.4180	1.1641	0.8933
20	Ca⁺²	0.03877	0.2841	0.2500	0.5176	1.0010	1.036	0.1961	0.4622	1.0527	0.9578

where $a=a(r)$ is a function of r, which, in the actual computations, is found to be rather slowly varying. The extreme value is then situated in a point $r=r_m$ satisfying the relation

$$r=p/(a+ra').$$ (8)

In order to determine the denominator without the explicit evaluation of the function $a(r)$, we will introduce the auxiliary functions

$$g(r)=f_{nl}(\text{SCF}|r)/r^p,$$ (9)

$$q_h(r)=g(r-h/2)/g(r+h/2).$$ (10)

The functions $q_h(r)$ are called the "quotient functions" associated with the interval h, and a table for them is easily formed by taking the successive quotients between consecutive values of $g(r)$ in equidistant points having the interval h. Using a Taylor-series expansion of the exponent $ra(r)$ in (7) and Eqs. (9) and (10), we obtain

$$\log_e q_h(r)=h(a+ra')+h^3(3a''+ra''')/24+\cdots.$$ (11)

For the SCF functions under consideration, we have found that the function $q_h(r)$ is so slowly varying that one may use linear interpolations, and, consequently, the higher terms in the expansion (11) may be neglected in comparison to the first term. By using (11), the relation (8) may then be written in the form

$$r=ph/\log_e q_h(r).$$ (12)

From this equation, the position $r=r_m$ may be determined in a few steps by iteration by using only the quotient table. A typical example of the procedure is given in Table II.

The magnitude $f=f_m$ of the extreme value of the SCF function is then given by $f_m=r_m{}^p g(r_m)$, where

$$\log_e g(r_m)=\log_e g(r_1)+\frac{r_1-r_m}{h}\log_e q_h\left(\frac{r_1+r_m}{2}\right).$$ (13)

Two isoelectronic series have been investigated in this way, namely some Ne-like ions (Ne, Na⁺, Mg⁺², Al⁺³, and Si⁺⁴) and some A-like ions (Cl⁻, A, K⁺, and Ca⁺²), for which self-consistent-field functions with exchange are already available in the literature,[12] calculated by D. R. and W. Hartree, and others. Tables III and IV contain the results of our computations of r_m and f_m; we note the existence of such regularities as make these tables directly suitable for interpolation purposes. The corresponding effective nuclear charges $Z(\text{SCF}|\ )$ with respect to r_m and f_m, calculated from Eqs. (6), are then given in Tables V and VI. These quantities may be written in the form

$$Z(\text{SCF}|r_m)=Z-s_1,\quad Z(\text{SCF}|f_m)=Z-s_2,$$ (14)

where the quantities s_1 and s_2 may be interpreted as the "shielding constants" with respect to the positions and the magnitudes of the extreme values, respectively. From the tables, we note that, at least for the inner electrons, the quantities s_1 and s_2 are approximately constant for fixed quantum numbers (nl) in each series, but also that they differ appreciably from each other: $s_1 \neq s_2$. The last fact indicates a result of importance for understanding the special character of the SCF functions in comparison to the hydrogenlike functions.

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[12] The proper references to the original articles used in the calculations in this paper may be found in the extensive bibliography given by Hartree in our reference 1. However, the data for Ne and Al⁺³ are taken from our own SCF calculations (to be published).

TABLE V. Effective nuclear charges $Z(\text{SCF} \mid)$ for the positions r_m and the magnitudes f_m of some Ne-like ions with exchange.

Z	Element	1s		2s₁		2s₂		2p	
		$Z(r_m)$	$Z(f_m)$	$Z(r_m)$	$Z(f_m)$	$Z(r_m)$	$Z(f_m)$	$Z(r_m)$	$Z(f_m)$
10	Ne	9.713	9.502	9.445	4.349	7.646	6.184	6.307	4.771
11	Na⁺	10.704	10.481	10.417	5.188	8.557	7.161	7.302	5.860
12	Mg⁺²	11.696	11.472	11.450	6.055	9.549	8.134	8.277	6.852
13	Al⁺³	12.699	12.464	12.441	6.979	10.531	9.124	9.281	7.908
14	Si⁺⁴	13.683	13.471	13.461	7.889	11.497	10.122	10.276	8.932
Average difference:		0.993	0.992	1.004	0.885	0.963	0.985	0.992	1.040

TABLE VI. Effective nuclear charges $Z(\text{SCF} \mid)$ for the positions r_m and the magnitudes f_m of some A-like ions with exchange.

Z	Element	1s		2s₁		2s₂		2p	
		$Z(r_m)$	$Z(f_m)$	$Z(r_m)$	$Z(f_m)$	$Z(r_m)$	$Z(f_m)$	$Z(r_m)$	$Z(f_m)$
17	Cl⁻	16.688	16.426	16.351	10.624	14.402	12.990	13.188	11.807
18	A	17.695	17.399	17.401	11.485	15.344	13.947	14.160	12.786
19	K⁺	18.687	18.411	18.442	12.435	16.381	14.903	15.168	13.779
20	Ca⁺²	19.673	19.392	19.368	13.400	17.371	15.909	16.146	14.756
Average difference:		0.995	0.989	1.006	0.925	0.990	0.973	0.986	0.983

Z	Element	3s₁		3s₂		3s₃		3p₁		3p₂	
		$Z(r_m)$	$Z(f_m)$	$Z(r_m)$	$Z(f_m)$	$Z(r_m)$	$Z(f_m)$	$Z(r_m)$	$Z(f_m)$	$Z(r_m)$	$Z(f_m)$
17	Cl⁻	16.122	3.169	13.832	4.211	10.040	7.344	12.480	2.514	8.094	5.293
18	A	17.147	3.873	14.818	5.074	11.023	8.412	13.352	3.436	9.224	6.619
19	K⁺	18.147	4.631	15.783	5.987	12.049	9.484	14.294	4.357	10.309	7.840
20	Ca⁺²	19.089	5.441	16.748	6.943	13.061	10.571	15.296	5.312	11.400	9.073
Average difference:		0.989	0.757	0.972	0.911	1.007	1.076	0.939	0.933	1.102	1.260

In the first attempts to treat atomic wave functions, it was natural to consider them as hydrogenlike functions having an effective nuclear charge of the form $(Z-s)$, where the single shielding constants s were determined, e.g., by the rules given by Slater.[13] The results concerning the SCF functions, contained in Tables V and VI, show now that, in order to describe such a function around one of its extreme values, it is necessary to use *two* independent screening constants, s_1 and s_2, and a relation of the form

$$f_{nl}(\text{SCF} \mid r) \approx (Z-s_2)^{\frac{3}{2}} N Q_{nl}(\rho) \exp(-\rho/2),$$
$$\rho = 2(Z-s_1)r/n, \tag{15}$$

which actually corresponds to Eq. (3) with part of the remainder taken into account. This formula gives the values of the SCF function under consideration only within a small range, and, in order to describe the same function around another extreme value or in another region, different values of s_1 and s_2 are necessary. We note that, if the values of s_1 and s_2 would be kept constant from $r=0$ to $r=\infty$, the resulting function (15) would no longer be properly normalized.

As a typical example of the limited validity of formula (15), we have in Table VII listed the values of the right-hand side of this expression for the region around the maximum of f_{2p} for Na⁺ with exchange in comparison to the actual values. If two effective nuclear charges Z_1 and Z_2, taken from Table V, are used, the SCF function will be correctly represented in the maximum $r=r_m$ and with the accuracy desired within

[13] J. C. Slater, Phys. Rev. **36**, 57 (1930).

a small interval $(r_m-0.05; r_m+0.05)$ around this point, whereas the errors, e.g., in the interval $(0; r_m-0.05)$, will be appreciable and amount to as much as -0.070. However, if only *one* effective nuclear charge Z_{eff} is used, for instance the compromise value $Z=(Z_1Z_2)^{\frac{1}{2}}$, the position and the magnitude of the maximum show errors of about 0.05 and 0.070, respectively, whereas the errors in the interval $(0; r_m)$ amount to as much as -0.110. The example shows that, even if two effective nuclear charges are used, it is desirable to have these quantities *continuously varying* in order to describe a SCF function with complete accuracy over a larger region. This idea will be further developed in Sec. II.

We have also investigated the interpolation properties of the extreme values of the SCF functions for a series of *neutral* atoms, namely C, N, and O. These atoms can

TABLE VII. Approximate representation of the $2p$ function of Na⁺ with exchange around its maximum according to Eq. (15) and Table V.

r	SCF Hartree-Hartree	Eq. (15) $Z_1=7.302$ $Z_2=5.860$	Eq. (15) Compromise $Z=(Z_1Z_2)^{\frac{1}{2}}$
0	0.000	0.000	0.000
0.1	0.231	0.183	0.161
0.2	0.578	0.508	0.465
0.3	0.842	0.793	0.753
0.4	0.997	0.978	0.966
0.5	1.061	1.061	1.088
0.6	1.061	1.061	1.130
0.7	1.021	1.002	1.109
0.8	0.956	0.908	1.044
0.9	0.880	0.798	0.953
1.0	0.799	0.684	0.848

TABLE VIII. Positions r_m, magnitudes f_m, and the corresponding effective nuclear charges $Z(\text{SCF}\mid)$ for the maxima of the $2p$ functions of some neutral atoms, namely carbon (^1D, $\beta=0.04$), nitrogen (^2P, $\beta=0$), and oxygen (^1S, $\beta=0$).

Z	Element	State	r_m	f_m	$Z(\text{SCF}\mid r_m)$	$Z(\text{SCF}\mid f_m)$
6	C	^1D	1.221	0.7134	3.276	2.605
7	N	^2P	0.994	0.7813	4.024	3.124
8	O	^1S	0.837	0.8430	4.779	3.637
				Average difference:	0.7515	0.516

occur in several different states, characterized by Slater's[14] parameter β, and we have here treated the actual or interpolated functions belonging to $\beta=0$. The results for the $2p$ functions are given in Table VIII; again it is found that the *linearity rule* for the quantities $Z(\text{SCF}\mid)$ holds with a surprisingly high accuracy. The average differences in each series are now appreciably smaller than 1.000, as one could expect from physical reasons for a sequence of neutral atoms, since one outer electron with some shielding effects is added to the system when the nuclear charge is increased by one.

(b) The Region Around $r = 0$

In order to investigate the SCF functions in greater detail in the neighborhood of the point $r=0$, we will again start from the hydrogenlike functions given in Table I. The quantity $f_{nl}(Z\mid r)/r^{l+1}$ is nonvanishing for $r=0$, and, according to (4), we have

$$\lim_{r\to 0}\frac{f_{nl}(Z\mid r)}{r^{l+1}}=NZ^{\frac{3}{2}}\left\{\frac{Q_{nl}(2Zr/n)}{r^{l+1}}\right\}_{r=0}. \quad (16)$$

From this relation we can then solve the atomic number Z and obtain

$$Z=\left[\alpha_{nl}f_{nl}(Z\mid r)/r^{l+1}\right]_{r=0}^{2/(2l+3)}, \quad (17)$$

where α_{nl} is a constant which for the lowest quantum numbers has the following values:

$$(nl)=\begin{matrix}1s & 2s & 2p & 3s & 3p & 3d\\ \alpha_{nl}=0.5 & \sqrt{2} & 2\sqrt{6} & 1.5\sqrt{3} & 3.375\sqrt{6} & 20.25\sqrt{30}.\end{matrix} \quad (18)$$

According to the analogy rule, stated above, the corresponding quantities for the SCF functions will then represent the effective nuclear charges $Z(\text{SCF}\mid)$ with respect to the first nonvanishing derivative in origin, and, for the sake of simplicity, we will denote these quantities by the symbol K_{nl}, introduced in Part I:

$$K_{nl}=\left[\alpha_{nl}f_{nl}(\text{SCF}\mid r)/r^{l+1}\right]_{r=0}^{2/(2l+3)}. \quad (19)$$

In publishing the results of their calculations of self-consistent fields, Hartree and Hartree have usually given the value of $f_{nl}(\text{SCF}\mid r)/r^{l+1}$ for $r=0$, and the evaluation of K_{nl} is then straightforward. In other cases, one has to study the function $f_{nl}(r)/r^{l+1}$ in the

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[14] J. C. Slater, Phys. Rev. **34**, 1293 (1929).

neighborhood of $r=0$ and to extrapolate its value for $r=0$ by means of "quotient analysis" or logarithmic extrapolation.

The results of our calculations of K_{nl} for the CNO series, the Ne-like ions, and the A-like ions are condensed in Table IX, where the upper values refer to fields with exchange and the lower to fields without exchange. From this table, we conclude that the effective nuclear charge K_{nl} with striking accuracy is a *linear function* of the atomic number Z, and that therefore interpolations and extrapolations to neighboring atoms are possible as soon as two SCF data are available; the existence of additional data will, of course, increase the accuracy. A table of K_{1s} for the He-like ions was also given in Part I.

According to (19), one can determine the first nonvanishing derivative in origin for a SCF function from the corresponding effective nuclear charge K_{nl} by the relation

$$c_{l+1}=\frac{f^{(l+1)}(\text{SCF}\mid 0)}{(l+1)!}=K_{nl}^{(2l+3)/2}/\alpha_{nl}. \quad (20)$$

TABLE IX. Effective nuclear charges K_{nl} for SCF functions belonging to the CNO series, the Ne series, and the A series. The upper values refer to fields *with* exchange, the lower to fields *without* exchange.

Z	Element	State	K_{1s}	K_{2s}	K_{2p}
		CNO series (SCF with exchange)			
6	C	^1D	5.760	4.115	3.85
7	N	^2P	6.757	4.971	4.66
8	O	^1S	7.751	5.787	5.50
	Average difference:		0.996	0.836	0.825

Z	Element	K_{1s}	K_{2s}	K_{2p}
		Ne series		
9	F⁻	$\cdots$ / 8.746	$\cdots$ / 6.516	$\cdots$ / 5.913
10	Ne	9.736 / $\cdots$	7.403 / $\cdots$	7.139 / $\cdots$
11	Na⁺	10.725 / $\cdots$	8.382 / $\cdots$	8.168 / $\cdots$
13	Al⁺³	12.718 / 12.737	10.364 / 10.160	10.198 / 10.022
14	Si⁺⁴	13.735 / 13.743	11.368 / 11.176	11.206 / 11.014
	Average difference:	1.000 / 0.999	0.991 / 0.932	1.017 / 1.202

Z	Element	K_{1s}	K_{2s}	K_{2p}	K_{3s}	K_{3p}
		A series				
17	Cl⁻	16.701 / 16.722	14.301 / 14.024	14.163 / 13.968	9.527 / 9.981	9.976 / 9.817
18	A	17.690 / $\cdots$	15.284 / $\cdots$	15.150 / $\cdots$	10.561 / $\cdots$	11.217 / $\cdots$
19	K⁺	18.698 / 18.712	16.271 / 15.979	16.145 / 15.946	11.645 / 11.898	12.385 / 12.273
20	Ca⁺²	19.691 / 19.706	17.266 / 16.955	17.141 / 16.925	12.717 / 12.888	13.523 / 13.420
	Average difference:	0.997 / 0.995	0.988 / 0.977	0.993 / 0.986	1.063 / 0.969	1.182 / 1.201

This is of particular importance in the calculations of self-consistent fields *with exchange* by solving the Hartree-Fock equations, since, in this case, it is desirable to have as good estimates as possible of the initial conditions in origin in order to obtain the solutions directly in correctly normalized form. The interpolation rule based on (19) may therefore be of value for SCF calculations in the future.

We may conclude that, in a close neighborhood of $r=0$, it is possible to describe a SCF function as a hydrogenlike function with $Z_{\text{eff}}=K_{nl}$. However, the range of validity of such a representation is rather short, as is shown by the example for f_{2p} of Na^+ with exchange in Table X, where the function (4) is compared to the actual SCF function, given by Hartree and Hartree.

Table IX gives also a comparison between the values of K_{nl} for fields with and without exchange, and we note that, except for $(3s)$, the inclusion of exchange corresponds to a slight increase of the effective nuclear charge, which confirms an earlier observation by Hartree. However, a much stronger tool for investigating the influence of the inclusion of exchange will be described in a following section.

In order to give a detailed description of the SCF functions in a longer range around $r=0$, one should investigate also the next derivative of order $(l+2)$, writing the function in the form

$$f_{nl}(\text{SCF}\,|\,r)=c_{l+1}r^{l+1}(1-ar+\cdots).\qquad(21)$$

By substituting this expression into the Hartree-Fock equations, one finds that $a=Z/(l+1)$, where Z is the atomic number of the nucleus. This is a general result which is valid both for the hydrogenlike functions and the SCF functions. However, in their papers concerning self-consistent fields, Hartree and Hartree have usually given tables also of the quantities f_{nl}/r^{r+1} for the range around $r=0$, and by making a "quotient analysis" of this material, we have found that, in the nearest neighborhood of origin, the SCF functions are better expressed under the form

$$f_{nl}(\text{SCF}\,|\,r)=c_{l+1}r^{l+1}e^{-ar}.\qquad(22)$$

TABLE X. Comparison between the SCF function f_{2p} for Na^+ with exchange, given by Hartree and Hartree, and the corresponding hydrogenlike function (4) with $Z_{\text{eff}}=K_{2p}$ in the neighborhood of $r=0$. The numerical value of $K_{2p}=8.168$ is taken from Table IX.

r	SCF	Eq. (4)	r	SCF	Eq. (4)
0.00	0.000	0.000	0.2	0.578	0.688
0.01	0.004	0.004	0.3	0.842	1.029
0.02	0.014	0.014	0.4	0.997	1.216
0.03	0.030	0.031	0.5	1.061	1.263
0.04	0.050	0.053	0.6	1.061	1.209
			0.7	1.021	1.094
0.06	0.102	0.110	0.8	0.956	0.949
0.08	0.163	0.180	0.9	0.880	0.799
0.10	0.231	0.259	1.0	0.799	0.654
0.12	0.302	0.343			

TABLE XI. Example of "quotient analysis" of the numerically given functions $f_{nl}(\text{SCF}\,|\,r)/r^{l+1}$ for $K^+(3s)$ and $(3p)$ with exchange.

r	f_{3s}/r	q_h	f_{3p}/r^2	q_h
0.000	15.295		65.30	
		1.1008		1.0485
0.005	13.895		62.28	
		1.1032		1.0483
0.010	12.595		59.41	
		1.1058		1.0482
0.015	11.39		56.68	
		1.1091		1.0479
0.020	10.27		54.09	

TABLE XII. Quotients $q_h(0)$ for $h=0.005$ and corresponding effective nuclear charges Z_0, defined by (24), for SCF functions of some A-like ions with exchange.

	Z	Element	$1s$	$2s$	$2p$	$3s$	$3p$
$q_h(0)$	17	Cl^-	1.0885	1.0887	1.0427	1.0929[a]	1.0429
	18	A	1.0941	1.0941	1.0462	1.0937	1.0461
	19	K^+	1.0997	1.0993	1.0488	1.0996	1.0486
	20	Ca^{+2}	1.1053	1.1049	1.0514	1.1045	1.0509
Z_0	17	Cl^-	16.960	16.997	16.726	17.767[a]	16.802
	18	A	17.986	17.986	18.066	17.913	18.028
	19	K^+	19.008	18.935	19.058	18.989	18.982
	20	Ca^{+2}	20.023	19.951	20.050	19.879	19.858

[a] The SCF data for $Cl^-(3s)$ contain apparently some slight error.

Here $a=a(r)$ is constant or extremely slowly varying over the interval $(0; 0.02)$ under consideration, as is shown by the example in Table XI. A comparison between (21) and (22) shows then that, for $r=0$, we should simply have

$$a(0)=h^{-1}\log_e q_h(0)=Z/(l+1),\qquad(23)$$

where Z is the atomic number of the nucleus, and q_h is the quotient function defined by (10).

Let us now consider the actual numerical material, given by Hartree and Hartree, from this point of view. The result of our quotient analysis for the A-like ions with exchange is condensed in Table XII, where we also have listed a quantity,

$$Z_0=(l+1)h^{-1}\log_e q_h(0),\qquad(24)$$

obtained from the Hartree-Hartree quotient. Except for the case of $Cl^-(3s)$, where the SCF data apparently contain some accidental error, the quantities Z_0 are all very close to the real atomic number Z, in agreement with (23). In the following, we may, therefore, simply get an approximate idea of the behavior of $f_{nl}(\text{SCF}\,|\,r)r^{l+1}$ by starting from the value of c_{l+1}, found from (20), and by using a quotient q_h, given by the three-term formula

$$q_h=1+hZ/(l+1)+\tfrac{1}{2}\{hZ/(l+1)\}^2,\qquad(25)$$

for, e.g., $h=0.005$. We note that the values in the example in Table XIII are in excellent agreement with the SCF data given in Table XII.

TABLE XIII. The quotient $q_h(0)$ for $h=0.005$ for the A-like ions according to the three-term formula (25). Compare the SCF data in Table XII.

Z	$l=0$	$l=1$
17	1.0886	1.0434
18	1.0941	1.0460
19	1.0995	1.0486
20	1.1050	1.0513

TABLE XIV. Example of the procedure of evaluating the position r_0 of the node for the 2s function of Na^+ with exchange; $r_0^{(k)}$ gives the successive approximations for r_0 in Aitken's iteration scheme.

f_{2s}	r	$r_0^{(k)}$ $k=1$	$k=2$	$k=3$
+0.215	0.16			
+0.102	0.18	0.198 053		
−0.015	0.20	0.197 391	0.197 476	
−0.301	0.25	0.197 500	0.197 913	0.197 45

(c) The Nodes

Another characteristic property of the SCF functions is the position r_0 of their eventual nodes. For the hydrogenlike functions, the nodes are given by the zero points ρ_0 of the polynomials $Q(\rho)$ in Table I; and by solving the atomic number Z, we obtain, therefore, $Z=n\rho_0/2r_0$. According to the analogy rule, the corresponding effective nuclear charges for the SCF functions are then defined by

$$Z(SCF\,|\,r_0)=n\rho_0/2r_0. \qquad (26)$$

The zero points r_0 of the numerically given SCF functions may be determined by solving the equation $f_{nl}(SCF\,|\,r)=0$ by inverse interpolation, and, for this purpose, we have used the Aitken iteration scheme.[15] An example of the procedure is given in Table XIV.

The final results of our calculations of the nodes of of the 2s functions, associated with fields with and without exchange, are condensed in Table XV. We note that the linearity rule for $Z(SCF\,|\,r_0)$ holds with the same striking accuracy as before, and that therefore this auxiliary quantity is very convenient for interpolation purposes. The nodes of the 3s and 3p functions have been evaluated only for the fields with exchange, and the results are given in Table XVI.

Let us finally consider the possibility of expressing a SCF function in the form (15) in the neighborhood of a node. The quantity ρ is defined by $\rho=2Z_{eff}r/n$, but it is not a priori evident that the value of Z_{eff} in the polynomial $Q(\rho)$ is identical with the value of Z_{eff} in $\exp(-\rho/2)$, particularly not in the region around a zero point $r=r_0$, where the former is sharply defined. In order to describe an SCF function in such a region, it may therefore be necessary to use three independent shielding factors in formula (15). In considering a single

continuously varying scale factor, we will meet this problem again, since the nodes will be a little bit "out of scale" and lead to sudden discontinuities.

In general, the nodes cause such complications in the interpolation problem as to make it highly desirable to transform them away. As we shall see in the next section, such a transformation can be carried out even for the numerically given SCF functions, if the nodes are evaluated with sufficient accuracy. The possibility of a separate interpolation of the nodes, based on (26), will in this way prove to be of essential importance for the solution of the interpolation problem for the function as a whole.

(d) The Energy Eigenvalues

The "tails" of the SCF functions for large r may be interpolated simply by considering the outmost Slater exponential in the analytic expressions, described in Part I. This single exponential term is quickly found by a "quotient analysis" without evaluating the whole expression, and we note that the exponents satisfy the

TABLE XV. The positions r_0 and the effective nuclear charges $Z(SCF\,|\,r_0)$ of 2s functions belonging to self-consistent fields with and without exchange.

Z	Element	State β value	r_0 With exchange	r_0 Without exchange	$Z(SCF\,|\,r_0)$ With exchange	$Z(SCF\,|\,r_0)$ Without exchange
3	Li		0.829 96		2.4098	
4	Be		0.589 57	0.679 76	3.3923	2.9422
5	B			0.504 45		3.9647
6	C	^1D 0.04	0.375 41		5.3275	
	C^{+2}		0.370 75	0.400 45	5.3945	4.9944
7	N^-	^1S 0	0.318 15		6.2863	
	N	^2P 0	0.317 98		6.2897	
8	O^-	^2P −0.8	0.276 36		7.2369	
	O	^1S 0	0.276 11	0.289 94	7.2435	6.8980
	O^+	^2P 0	0.275 54	0.289 48	7.2585	6.9089
	O^{+2}	intp. 0	0.274 25	0.288 57	7.2926	6.9307
	O^{+3}	^2P 0	0.272 53	0.287 10	7.3386	6.9662
9	F^-			0.254 02		7.8734
10	Ne		0.218 36		9.159	
11	Na^-		0.197 45		10.129	
	Na^+		0.197 45		10.129	
12	Mg^{+2}		0.180 14	0.185 03	11.102	10.809
13	Al^{+3}		0.165 42	0.169 57	12.090	11.795
14	Si^{+2}			0.156 54		12.776
	Si^{+3}			0.156 51		12.779
	Si^{+4}		0.153 04	0.156 54	13.068	12.776
17	Cl^-		0.124 80	0.127 06	16.027	15.741
18	A		0.117 65		17.000	
19	K^+		0.111 07	0.112 91	18.007	17.713
20	Ca			0.106 91		18.707
	Ca^{+2}		0.105 30		18.993	
29	Cu^+		0.071 612	0.072 302	27.928	27.662

The positions r_0 and the effective nuclear charges $Z(SCF\,|\,r_0)$ for 2s functions of some heavier elements for self-consistent fields without exchange.

Z	Element	r_0	$Z(SCF\,|\,r_0)$
30	Zn	0.069 719	28.687
31	Ca	0.067 510	29.625
32	Ge.	0.065 210	30.670
33	As	0.063 236	31.628
37	Rb	0.056 155	35.616
55	Cs	0.037 342	53.559
80	Hg	0.025 454	78.573

[15] See, for instance, W. E. Milne, *Numerical Calculus* (Princeton University Press, Princeton, 1949), p. 69.

TABLE XVI. The positions r_0 and the effective nuclear charges $Z(\text{SCF}\,|r_0)$ for $3s$ and $3p$ functions belonging to self-consistent fields *with* exchange.

| | | | | 3s | | | 3p | |
Z	Element	r_0'	r_0''	$Z(\text{SCF}\,|r_0')$	$Z(\text{SCF}\,|r_0'')$	r_0	$Z(\text{SCF}\,|r_0)$
17	Cl⁻	0.121 60	0.554 99	15.641	12.790	0.531 53	11.288
18	A	0.114 37	0.515 72	16.630	13.763	0.488 69	12.278
19	K⁺	0.108 00	0.481 89	17.610	14.730	0.431 99	13.275
20	Ca⁺²	0.102 33	0.451 62	18.586	15.717	0.420 42	14.271
29	Cu⁺	0.069 238	0.292 38	27.469	24.277	0.262 63	22.846

linearity rule, whereas the coefficients satisfy Eq. (I, 7). Typical examples may be found in Part I.

Another quantity characteristics for the asymptotic behavior is the eigenvalue parameter ϵ_{nl}. For hydrogen-like functions we would have $\epsilon_{nl} = Z^2/n$, and, for SCF functions, the corresponding effective nuclear charge is then defined by

$$Z(\text{SCF}\,|\,\epsilon_{nl}) = n\sqrt{\epsilon_{nl}}. \qquad (27)$$

Table XVII gives a survey of this quantity for some Ne-like and A-like ions, and we note that, for the outer electrons, the electronic shielding is so strong that the linearity rule for $Z(\text{SCF}\,|\,\epsilon_{nl})$ holds only with a rather moderate accuracy as long as this quantity is comparatively large, whereas there are considerable deviations from this rule when $Z(\text{SCF}\,|\,\epsilon)$ tends to zero on the side of the negative ions. However, if only two SCF data are available, the interpolation based on (27) gives at least a first estimate of the eigenvalue parameter, and, in actual computations, we have found that this value might be just as good as, e.g., the approximate eigenvalue obtained from the average value of the energy operator with respect to an interpolated SCF function.

If three of more SCF data are available, it is usually simpler to carry out the interpolations directly in the quantity ϵ_{nl} itself, which is then considered as being a polynomial of at least the second degree in the atomic number Z.

In our investigation of the SCF functions, we have found that the hydrogenlike behavior decreases when the point under consideration moves outwards from origin, which depends on the simple fact that the electronic screening gets an increasing importance in comparison to the nuclear attraction. The idea of the "effective nuclear charge" must consequently lose some of its validity when it is applied to the asymptotic behavior, and it is therefore probable that a more detailed description of quantities like, e.g., the eigenvalues can be given first after a closer investigation of the basic Hartree-Fock equations.

II. INTERPOLATION OF SELF-CONSISTENT-FIELD WAVE FUNCTIONS

In the previous section we have investigated the interpolation of certain point properties of the SCF functions, and will now study the problem of the interpolation of the SCF functions as a whole. Our different

attempts to treat this question have shown us that the eventual nodes in the SCF functions cause considerable complications in this connection, and we will therefore take advantage of the fact that these nodes may be interpolated separately by using (26).

Let us start by dividing the function $f_{nl}(\text{SCF}\,|r)$ by a polynomial $r^{l+1}(r_0'-r)(r_0''-r)\cdots$, where r_0', r_0'', $\cdots$ are the $(n-l-1)$ zero points of the function itself; the quotient is nodeless and monotonously decreasing with increasing r. Let us also form a table of the quantity

$$\phi_{nl}(\text{SCF}\,|r)$$
$$= \log_e\{f_{nl}(\text{SCF}\,|r)/r^{l+1}(r_0'-r)(r_0''-r)\cdots\}. \qquad (28)$$

We observe that, except for the normalization constant, the quantity $\phi_{nl}(Z\,|r)$ for a hydrogenlike function is linear in rZ/n, and, according to the analogy rule, we may then consider $\phi_{nl}(\text{SCF}\,|r)$ as being the same linear function of $rZ_{\text{eff}}(r)/n$:

$$\phi_{nl}(\text{SCF}\,|r) = \phi_{nl}(\text{SCF}\,|0) - rZ_{\text{eff}}(r)/n. \qquad (29)$$

We postulate that the effective charge $Z_{\text{eff}}(r)$ should be an almost linear function of the atomic number, convenient for interpolation purposes.

TABLE XVII. The effective nuclear charge $Z(\text{SCF}\,|\epsilon_{nl})$ corresponding to the eigenvalue parameters ϵ_{nl} for some Ne-like and some A-like ions.

| | | Ne series, with exchange. | | |
Z	Element	1s	2s	2p
10	Ne	8.093	3.925	2.598
11	Na⁺	9.026	4.960	3.796
12	Mg⁺²	9.973	5.981	4.895
13	Al⁺³	10.94	7.019	5.985
14	Si⁺⁴	11.90	8.042	7.046
Average difference:		0.952	1.029	1.112

A-series, upper values with exchange, lower values without exchange.

Z	Element	1s	2s	2p	3s	3p
17	Cl⁻	14.46	9.049	7.846	3.617	1.635
		14.46	8.567	7.582	3.116	1.013
18	A	15.40	9.930	8.752	4.795	3.260
		⋯	⋯	⋯	⋯	⋯
19	K⁺	16.36	10.85	9.693	5.947	4.590
		16.35	10.33	9.374	5.268	4.096
20	Ca⁺²	17.32	11.79	10.65	7.072	5.814
		17.31	11.27	10.32	6.390	5.330
Average difference:		0.953	0.914	0.935	1.152	1.393
		0.950	0.901	0.913	1.091	1.439

The problem of interpolating an SCF function as a whole may now simply be solved by performing linear interpolations in the functions $\phi_{nl}(\text{SCF}|r)$ given by (28) for each r value under consideration, with an eventual renormalization of the first preliminary result as to the entire wave function. In order to test this rule, we have applied it to the series of A-like ions, where we have interpolated the SCF functions with exchange for K^+ from the tabulated functions for Cl^- and Ca^{+2} and compared them with the correct ones. The results in Table XVIII show that the errors for the $1s$, $2s$, and $2p$ functions are hardly of the order ±0.002, whereas the errors for the $3s$ and $3p$ functions are slightly larger.

Let us now study in greater detail the continuously varying effective charge which, according to (29), is defined by the formula

$$Z_{\text{eff}}(r)/n = \{\phi_{nl}(\text{SCF}|0) - \phi_{nl}(\text{SCF}|r)\}/r. \quad (30)$$

By using (20) and (22), we obtain

$$\phi_{nl}(\text{SCF}|0) = \frac{2l+3}{2} \log_e K_{nl} - \log_e \alpha_{nl} r_0' r_0'' \cdots, \quad (31)$$

where all quantities in the right-hand member may be interpolated according to rules given in the previous section. We note, however, that the value of $\phi_{nl}(\text{SCF}|0)$ is in all events rather unimportant since it corresponds only to a normalization constant in the wave function, which can always be determined afterwards. If there is an uncertainty of $\Delta\phi_0$ in the value of $\phi_{nl}(\text{SCF}|0)$, there will be a corresponding uncertainty of $\Delta\phi_0/r$ in the quantity $Z_{\text{eff}}(r)/n$, which is particularly large in the vicinity of $r=0$. Using (22), (23), and (28), we obtain for the point $r=0$ in particular

$$Z_{\text{eff}}(0)/n = \frac{Z}{l+1} - \frac{1}{r_0'} - \frac{1}{r_0''} - \cdots. \quad (32)$$

TABLE XVIII. The error in the SCF functions for K^+ with exchange obtained from the given functions for Cl^- and Ca^{+2} by linear interpolation in the auxiliary function (28). Unit $= 10^{-3}$.

r interval	$1s$	$2s$	$2p$	$3s$	$3p$
0.00					
	±0.5	0	0	$+2$	$+0.5$
0.02					
	-1	±1	$+0.5$	$+3$	$+3$
0.08					
	-1	-2	$+1.5$	-6	$+6$
0.30					
	$+1$	$+1$	-2	±4	±5
0.60					
		$+1$	-1	$+5$	-7
1.20					
		-0.5	-1	-6	$+8$
4.00					
				-1	$+1$

In addition to $Z_{\text{eff}}(r)$, we have also studied the quantity

$$\omega_{nl}(r) = Z_{\text{eff}}(r)/Z_{\text{eff}}(0). \quad (33)$$

This function is monotonously decreasing with increasing r from the value $\omega(0)=1$, and it describes, therefore, in a simple way some of the essential properties of the SCF functions, particularly their deviations from the hydrogenlike form. Practically we have found that this function is very slowly varying with the atomic number and that the accuracy of the interpolations may be improved by performing them in $\omega(r)$ instead of in $Z_{\text{eff}}(r)$ or in (28). In this way, the error in, for instance, the $3p$ function of K^+ with exchange derived from Cl^- and Ca^{+2} may be reduced by about 50 percent in comparison to the values given in Table XVIII.

As an example, we have given the ω functions for the series of Ne-like ions with exchange in Table XIX. The ω functions for some A-like ions (Cl^-, A, K^+, Ca^{+2}) and Cu^+ with and without exchange have also been calculated and are available on special request.[16] The tables are all affected by small normalization constant uncertainties $\Delta\phi_0/r$ of the type described above, and it is, therefore, remarkable that they still fit rather smoothly together in spite of the fact that the tables are given in their original form without being adjusted to each other.

In the results for the A-like ions and Cu^+, one can observe another characteristic feature of the ω functions, namely, that for an isoelectronic series the difference between the two ω functions for fields with and without exchange seems to be approximately the same function of r for all elements of the series. This property may be used for estimating wave functions with exchange from those without exchange in case only one field with exchange is known in the series.

A comparison of the ω functions for the $1s$, $2s$, and $2p$ functions with exchange for the Ne-like and the A-like ions, respectively, shows further the effect of adding a complete outer electronic shell.

Finally, with respect to the tables published here, we would like to emphasize that, in order to utilize the full accuracy of the given material and to avoid rounding-off errors, we have in general kept at least one figure more in the tables than is actually valid. This is particularly true for the "tails" of the wave functions.

Up till now, several fields with exchange have been determined for atoms and ions up to $Z=39(Cu^+)$, whereas quite a few additional fields without exchange have been calculated up to $Z=80$ (Hg). However,

[16] Tables of the ω functions for some A-like ions (Cl^-, A, K^+, Ca^{+2}) and Cu^+, supplementary to this article, have been deposited as Document number 4222 with the 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 $1.25 for photoprints, or $1.25 for 35-mm microfilm. Advance payment is required. Make checks or money orders payable to: Chief, Photoduplication Service, Library of Congress.

TABLE XIX. The characteristic functions $\omega_{nl}(r)$ for the SCF functions of some Ne-like ions with exchange. These quantities, defined by $\omega(r)=Z_{eff}(r)/Z_{eff}(0)$, describe the relative decrease in the specific effective nuclear charge under consideration here. In addition, the first nonvanishing derivative in origin, the position r_0 of the node of the 2s function, and the values of $Z_{eff}(0)$ are tabulated for the calculation of the wave functions themselves.

1s functions with exchange.

r	Ne	Na+	Mg+2	Al+3	Si+4
0.0	1.0000	1.0000	1.0000	1.0000	1.0000
0.1	0.9858	0.9851	0.9851	0.9858	0.9863
0.2	0.9735	0.9730	0.9732	0.9734	0.9735
0.3	0.9637	0.9631	0.9632	0.9629	0.9630
0.4	0.9550	0.9542	0.9537	0.9528	0.9520
0.5	0.9468	0.9452	0.9442	0.9427	0.9413
0.6	0.9381	0.9351	0.9335	0.9301	0.9287
0.7	0.9284	0.9239	0.9287	0.9148	0.9218
f_0'	60.76	70.25	80.26	90.77	101.8
Z_0	10	11	12	13	14

2s functions with exchange.

r	Ne	Na+	Mg+2	Al+3	Si+4
0.0	1.0000	1.0000	1.0000	1.0000	1.0000
0.1	0.9553	0.9531	0.9533	0.9533	0.9533
0.2	0.9161	0.9128	0.9102	0.9134	0.9122
0.3	0.8831	0.8830	0.8810	0.8824	0.8817
0.4	0.8571	0.8559	0.8547	0.8558	0.8556
0.5	0.8333	0.8323	0.8313	0.8325	0.8328
0.6	0.8123	0.8109	0.8103	0.8121	0.8129
0.7	0.7928	0.7918	0.7915	0.7937	0.7953
0.8	0.7749	0.7742	0.7745	0.7774	0.7798
0.9	0.7585	0.7581	0.7589	0.7627	0.7659
1.0	0.7431	0.7434	0.7448	0.7495	0.7537
1.1	0.7288	0.7297	0.7319	0.7375	0.7427
1.2	0.7157	0.7173	0.7203	0.7269	0.7326
1.4	0.6917	0.6948	0.6998	0.7081	0.7159
1.6	0.6708	0.6756	0.6822	0.6921	0.7016
1.8	0.6522	0.6588	0.6670	0.6794	0.6890
2.0	0.6358	0.6445	0.6530	0.6677	0.6781
2.2	0.6214	0.6311	0.6400	0.6577	0.6685
2.4	0.6083	0.6191	0.6278	0.6490	0.6599
2.6	0.5959	0.6090	0.6163	0.6414	0.6520
2.8	0.5857	0.5992	0.6051	0.6348	0.6446
3.0	0.5754	0.5900	0.5943	0.6275	0.6377
3.2	0.5659	0.5829	0.5839	0.6237	0.6312
3.4	0.5583	0.5730	0.5737	0.6184	0.6245
3.6	0.5510	0.5656	0.5637	0.6110	0.6191
3.8	0.5443	0.5588	0.5538	0.6093	0.6133
4.0	0.5352	0.5552	0.5442	0.6076	0.6078
r_0	0.21836	0.19745	0.18014	0.16542	0.15304
f_0'	14.24	17.16	20.24	23.60	27.10
$Z_0/2$	5.4204	5.9354	6.4488	6.9548	7.4658

2p functions with exchange.

r	Ne	Na+	Mg+2	Al+3	Si+4
0.0	1.0000	1.0000	1.0000	1.0000	1.0000
0.1	0.9489	0.9485	0.9447	0.9445	0.9444
0.2	0.9025	0.9007	0.8989	0.9008	0.8996
0.3	0.8637	0.8639	0.8630	0.8648	0.8654
0.4	0.8323	0.8327	0.8330	0.8352	0.8364
0.5	0.8046	0.8058	0.8067	0.8094	0.8117
0.6	0.7804	0.7820	0.7832	0.7870	0.7902
0.7	0.7582	0.7603	0.7626	0.7672	0.7713
0.8	0.7381	0.7409	0.7437	0.7494	0.7549
0.9	0.7192	0.7230	0.7268	0.7337	0.7401
1.0	0.7021	0.7065	0.7114	0.7193	0.7270
1.1	0.6858	0.6915	0.6975	0.7066	0.7153
1.2	0.6709	0.6777	0.6847	0.6950	0.7047
1.4	0.6439	0.6527	0.6624	0.6749	0.6866
1.6	0.6203	0.6314	0.6436	0.6581	0.6715
1.8	0.5992	0.6129	0.6271	0.6443	0.6588
2.0	0.5808	0.5970	0.6136	0.6319	0.6469
2.2	0.5643	0.5828	0.6014	0.6214	0.6351
2.4	0.5492	0.5700	0.5904	0.6122	0.6276
2.6	0.5362	0.5588	0.5806	0.6041	0.6184
2.8	0.5240	0.5490	0.5721	0.5967	0.6083
3.0	0.5129	0.5391	0.5648	0.5904	0.6016
3.2	0.5030	0.5307		0.5851	0.5918
3.4	0.4935	0.5218		0.5784	
3.6	0.4852	0.5143		0.5737	
3.8	0.4776	0.5072		0.5675	
4.0	0.4697	0.5014			
$f_0''/2$	27.79	38.92	52.00	67.81	85.80
$Z_0/2$	5.0	5.5	6.0	6.5	7.0

there are also a rather large number of atoms and ions left out in the first treatment of the periodic system where the interpolation methods described here may prove to be useful. Further applications of the theory will be given in a later paper of this series.