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Wave Functions for the Ground State of Lithium and Three-Electron Ions

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Improved wave functions and ionization potentials have been obtained for the configuration $1s^2 2s$, by using the variation method with a variation function containing four parameters. The wave function for the whole atom is of the determinant form, built up of K and L single-electron functions. The K function used is hydrogen-like with one parameter, the effective nuclear charge, and the L function is of the form $are^{-\gamma r} - e^{-\zeta r}$. A simple rule is obtained by

means of which it is possible to write down the wave function for any three-electron ion without further calculation. The deviation of the calculated ionization potentials from the observed values is 0.9 percent for Li I and decreases to 0.3 percent for C IV. Comparison is made with the results of other investigators and curves showing the wave functions and electron density functions are given.

INTRODUCTION

THE solution of the Schrödinger equation for the hydrogen atom and for the ground state of the helium atom¹ has been carried out to a high degree of exactness, but the best approximation which has been obtained for the lowest state of lithium is not nearly so accurate. While it is probably not feasible at present to obtain a result for the energy which is superior to the experimental value in accuracy, it was thought worth while to test out on lithium various possible approximate solutions, partly because the better agreement with the experimental energy and the correspondingly improved wave function and electron-density function were considered important in themselves and partly because this study would provide a basis for similar investigations of heavier atoms.

GENERAL METHOD

Slater² has shown how to build up a properly antisymmetric wave function for a many-electron atom by using a determinant whose elements are functions of the coordinates of a single electron only. In particular, if the interaction of the electrons with each other is regarded as a perturbation and neglected in obtaining the zeroth order approximation to the solution of the wave equation, there results for lithium:

$$\psi^0 = \frac{1}{6^{\frac{1}{2}}} \begin{vmatrix} A_1 & A_2 & A_3 \\ \bar{A}_1 & \bar{A}_2 & \bar{A}_3 \\ B_1 & B_2 & B_3 \end{vmatrix} \quad (1)$$

where A_1 is the $1s$ hydrogen-like wave function with positive spin for the first electron; \bar{A}_2 is the same function with negative spin for the second electron, and B_3 is the $2s$ hydrogen-like function with plus spin for the third electron.

The method adopted in this work was to seek a better approximation by the use of new functions for B based on the hydrogen-like functions but generalized by the introduction of parameters whose values were then determined by the application of the variation method.

The solution of the variation problem:

$$\delta E = \delta \left[\int \psi^* H \psi d\tau / \int \psi^* \psi d\tau \right] = 0, \quad (2)$$

where ψ is the function varied and H is the Hamiltonian operator for the system, is equivalent to solving the wave equation

$$H\psi = W\psi \quad (3)$$

with the usual boundary conditions. In particular if this variation problem is not completely solved but instead a trial function ψ used which contains a number of parameters which are varied until E is a minimum, then it can be shown³ that E is an upper limit to the energy, and ψ is assumed to be an approximate solution. The method which was used in this problem is

¹ E. A. Hylleraas, *Zeits. f. Physik* **65**, 209 (1930).

² J. C. Slater, *Phys. Rev.* **34**, 1293 (1929).

³ C. Eckart, *Phys. Rev.* **36**, 878 (1930).

applicable to the lowest state of any multiplicity or total angular momentum.

PREVIOUS WORK ON LITHIUM

Hargreaves⁴ has applied the method of Hartree to lithium, but his results have not appeared in a very usable form. Hartree's method of the "self-consistent field" is not based on the variation principle, but Slater⁵ has shown the relation between these two procedures and in addition has pointed out that several important corrections are needed before the energy values obtained can be compared with the experimental ionization potentials. The curve Hargreaves publishes for the wave function cannot be used for comparison since he gives no scales and has not made the L function orthogonal to the K function, so that its shape is of little significance. However, he does give a table of the self-consistent field, and these values will be compared with other results in Table III.

Eckart,³ using essentially the same method as is described in this paper, employed hydrogen-like functions with two parameters, the effective nuclear charges for the K - and L -shells. Thus if we use a, b, c, \dots , to represent single electron-orbit functions without the spin factor and $A, B, C, \dots; \bar{A}, \bar{B}, \bar{C}, \dots$, for the same functions with plus and minus spin, respectively, Eckart's solutions are

$$\begin{aligned} (K\text{-shell functions}) \quad a &= e^{-\xi r} \\ (L\text{-shell functions}) \quad b &= e^{-\eta r}(\eta r - 1). \end{aligned} \quad (4)$$

There appears to be an error in his energy value for lithium so this has been recalculated and will be found in Table I.

Guillemin and Zener⁶ introduced an additional parameter (α) into b , obtaining thereby a considerable improvement in the energy. Their function is:

$$b = e^{-\eta r}(\alpha r - 1) \quad (5)$$

and values for the energy will also be found in Table I and of the parameters in Table II. In addition these authors varied the exponent of r

TABLE I. *Energies and ionization potentials (atomic units: e^2/a_0).*

	Total energy	Diff.	%	Ionization potential	Diff.	%
Li I						
Experimental	-7.4837	—	—	0.1983	—	—
4-Parameter	-7.4192	0.0645	0.86	.1965	0.0018	0.91
Guillemin-Zener	-7.4183	.0654	.87	.1956	.0027	1.36
Slater	-7.4179	.0658	.88	.1953	.0030	1.51
Hydrogen-like	-7.3922	.0915	1.22	.1696	.0287	14.5
Be II						
Experimental	-14.3422	—	—	.6704	—	—
4-Parameter	-14.2639	.0783	.55	.6663	.0041	.61
Slater	-14.2584	.0838	.58	.6607	.0097	1.45
B III						
Experimental	-23.476	—	—	1.395	—	—
4-Parameter	-23.363	.113	.48	1.390	.005	.36
Slater	-23.350	.126	.54	1.378	.017	1.22
C IV						
Experimental	-34.778	—	—	2.3722	—	—
4-Parameter	-34.713	.065	.19	2.3650	.0072	.30
Guillemin-Zener	-34.698*	.080	.23	2.3496*	.0226	.95
Slater	-34.690	.088	.25	2.3422	.0300	1.26

* This is probably not quite the best value obtainable with this function.

TABLE II. *Parameter values, except for four-parameter function.*

	ξ	η	α	ξ	η	α
Li I			Be II			
Guillemin-Zener ⁶	2.688	0.630	5.56	3.688	1.158	5.88
Slater	2.688	.630	—	3.682	1.09	—
Hydrogen-like ³	2.686	.888	—	3.70	1.42	—
B III			C IV			
Guillemin-Zener ⁶	4.688	1.671	5.56	5.688	2.179	5.88
Slater	4.676	1.52	—	5.672	1.95	—
Hydrogen-like ³	4.72	1.96	—	5.71	2.48	—

in the coefficient, but found in this case that its best value was one, the hydrogen-like value.

Zener⁷ and Slater⁸ noted that α is fairly large and concluded that a good result would be obtained with the very simple function

$$b = re^{-\eta r}. \quad (6)$$

⁴ J. Hargreaves, Proc. Camb. Phil. Soc. **25**, 75 (1929).

⁵ J. C. Slater, Phys. Rev. **35**, 210 (1930).

⁶ V. Guillemin and C. Zener, Zeits. f. Physik **61**, 199 (1930).

⁷ C. Zener, Phys. Rev. **36**, 51 (1930).

⁸ J. C. Slater, Phys. Rev. **36**, 57 (1930).

This function was tried and, as is seen in Table I, found to be remarkably good considering its simplicity. It is better than the hydrogen-like function with screening constant used by Eckart, although, of course, not as good as Guillemin and Zener's function, of which it is a special case.

FUNCTIONS INVESTIGATED

The type of function which has been used in this paper, a natural generalization of Guillemin and Zener's function, is

$$b = \alpha r e^{-\eta r} - e^{-\zeta r}. \quad (7)$$

The same type has been used by Slater⁹ in seeking analytical expressions for Hartree's graphical wave functions. Results which are obtained by using (7) are listed in Table I under the heading "4-parameter" function.

The following form was also tried but found not to give as good results as (7):

$$b = \alpha r e^{-\eta r} + r e^{-\zeta r}. \quad (8)$$

Since the variation principle is applicable to the lowest P state of the atom, the following function was tried for the configuration $1s^2 2p$ of lithium:

$$c = (\gamma e^{-\kappa r} + e^{-\lambda r}) r \cos \vartheta. \quad (9)$$

However, the surprising result was obtained, on varying the parameters, that this function reduced to the simple screening constant type used by Eckart. In other words, the best values of the parameters γ , κ and λ were such that $\gamma = 0$; $\kappa = \lambda$. Therefore, the calculated total energy for this configuration, $-7.35039 \text{ } e^2/a_0$, is not different from Eckart's value, but by combining this with the best calculated value for the ground state, $-7.41915 \text{ } e^2/a_0$, a new result for the resonance potential of lithium is obtained, $0.06876 \text{ } e^2/a_0$, which is to be compared with the experimental value, $0.06794 \text{ } e^2/a_0$. The difference is $0.00082 \text{ } e^2/a_0$ or 1.2 percent.

The calculated energy of removal of the $2p$ electron from $1s^2 2p$ of lithium is 2.2 percent greater than that for a $2p$ hydrogen atom, $e^2/8a_0$, whereas the experimental value is 4.2 percent greater than $e^2/8a_0$. The discrepancy of 2 percent is probably to be attributed to the effect

of polarization of the K -shell by the valence electron, the effect of which is not taken into consideration by any of the variation functions used in this paper, approximate calculations of the polarization energy¹⁰ leading to somewhat larger values than the 2 percent needed. It is of interest that these calculations show, as suggested by Pauling and Goudsmit,¹¹ that there is appreciable interaction of the valence electron with the core of the atom other than polarization even for "nonpenetrating" orbits.

DETAILS OF METHOD

When the units $a_0 = \hbar^2/(4\pi^2\mu e^2)$, $2Rhc = e^2/a_0$ and e are used for length, energy and charge, respectively, Schrödinger's equation for the three-electron problem becomes

$$H\psi = (-\frac{1}{2}\nabla^2 + V)\psi = W\psi \quad (10)$$

where

$$V = 1/r_{12} + 1/r_{23} + 1/r_{13} - Z/r_1 - Z/r_2 - Z/r_3. \quad (11)$$

∇^2 is the Laplacian for the coordinates of the three electrons, and Z is the atomic number of the atom or ion. As pointed out by Hylleraas,¹² application of Green's theorem to the term in (2) involving the Laplacian yields for E :

$$E = (M' - 2L')/2N' \quad (12)$$

where

$$\left. \begin{aligned} M' &= \int |\text{grad } \psi|^2 d\tau \\ L' &= - \int \psi^* V \psi d\tau \\ N' &= \int \psi^* \psi d\tau \end{aligned} \right\}. \quad (13)$$

Further, if the change in scale:

$$r' = \xi r; \quad \eta' = \eta/\xi; \quad \zeta' = \zeta/\xi \quad (14)$$

is made, it is possible to differentiate E with respect to ξ , solve for the minimizing value of ξ and insert this value in E . The result is

$$E = -L^2/2MN \quad (15)$$

where L , M , N differ from L' , M' , N' only in that the substitutions (14) have been made.

The other parameters enter in such a complicated fashion that it is not feasible to obtain the

¹⁰ L. Pauling and S. Goudsmit, *The Structure of Line Spectra*, McGraw-Hill, New York, 1930, p. 47.

¹¹ Reference 10, p. 48.

¹² E. A. Hylleraas, *Zeits. f. Physik* 54, 347 (1929).

⁹ J. C. Slater, *Phys. Rev.* 42, 33 (1932).

minimum by differentiation so resort was had to actually computing E for various values of the parameters and graphically determining the minimum. This is a tedious process at best; the quickest and most certain method was found to involve constructing rough contour maps of the energy surface. An estimate was first made of the probable values of parameters. One of these (usually η') was inserted in the formula for E and a survey of the ζ' , α' plane made by giving ζ' a number of fixed values and plotting E as a function of α' . Each of these curves then gives a section of the energy surface, with E thought of as a function of α' and ζ' only. From these a contour map can be constructed and an estimate made of the best values of α' and ζ' for the value of η' originally chosen. With these values of α' and ζ' , η' is then varied until a minimum is found. A contour map may be constructed for the α' , ζ' plane with this new value of η' and the best values redetermined.

K-SHELL FUNCTIONS

In all the cases discussed here, with the exception of Hargreave's paper, the function used for the K electrons was the same as in Eckart's work, i.e., a hydrogen-like function with one parameter, the effective nuclear charge, as in Eq. (4). It is well known that this is not the best function to represent the K electrons, some term such as one of those used by Hylleraas,¹² for example, to correct more exactly for the repulsion of the electrons giving a better result. However, the introduction of even the simplest of these interaction factors, such as $(1+\gamma r_{12})$, enormously complicates the problem in the case

of lithium and so was not regarded as practicable. Instead, the ionization potential was calculated by subtracting the energy of the Li^+ ion computed by using the same type of $1s$ wave function, the value of the energy so calculated being: $7.22266 e^2/a_0$ for Li^+ ; $13.59766 e^2/a_0$ for Be^{++} ; $21.97266 e^2/a_0$ for B^{+++} ; and $32.34766 e^2/a_0$ for C^{++++} . Although the total energy of the lithium atom is, therefore, in error by about $0.065 e^2/a_0$ or 0.86 percent in all these examples due to the inaccuracy of the K functions, the assumption made that this error is nearly equal in the ion and in the atom is well justified by the close agreement between the experimental and theoretical ionization potentials as given in Table I.

COMPARISON OF L FUNCTIONS

The $2s$ functions which have been enumerated do not, at first glance, appear to be very similar, and it may seem strange that such different functions can all be even moderately good approximations to the true solution. The reason for the discrepancy is the use of single-electron wave functions for comparison instead of the wave function for the atom as a whole. Slater⁹ has pointed out that it is possible to make the $2s$ function orthogonal to the $1s$ function by adding to the $2s$ a certain fraction of the $1s$ function. Since the wave function for the whole atom is a determinant, it possesses the property that the addition of the members of any row multiplied by any factor to the members of any other row does not change the value of the determinant. Thus:

$$\psi = \frac{1}{6^{\frac{1}{2}}} \begin{vmatrix} A_1 & A_2 & A_3 \\ \bar{A}_1 & \bar{A}_2 & \bar{A}_3 \\ B_1 & B_2 & B_3 \end{vmatrix} = \frac{1}{6^{\frac{1}{2}}} \begin{vmatrix} A_1 & A_2 & A_3 \\ \bar{A}_1 & \bar{A}_2 & \bar{A}_3 \\ B_1 + \beta A_1 & B_2 + \beta A_2 & B_3 + \beta A_3 \end{vmatrix} \quad (16)$$

and in particular β may be so chosen that

$$\int A_1(B_1 + \beta A_1) d\tau = 0. \quad (17)$$

With this value of β , the single-electron functions are mutually orthogonal, since A_1 and \bar{A}_1 have opposite spins. In addition, the functions a and

b later tabulated have been normalized to 4π , i.e.,

$$\int A_1^2 d\tau = \int B_1^2 d\tau = 4\pi. \quad (18)$$

The orthogonalization and normalization make a and b unique (as long as functions of different spins are not combined), and it is thus possible to

compare the different approximations which have been obtained.

As shown by Fig. 3, the four approximations already enumerated are remarkably near to each other. The only one showing any great deviation is the hydrogen-like function, which is also the one giving the poorest energy value. The simple, so-called "nodeless" function of Slater⁸ is seen to be miscalculated, since, when it is orthogonalized, it has a node in practically the same place as the more precise functions.

RESULTS

The parameter values obtained for the functions of Guillemin and Zener, Slater, and Eckart are found in Table II. In the case of the four-parameter function, the best parameter values fit into a very convenient rule if we introduce the idea of screening constants. The function for the L electron which has been used, Eq. (7), consists of two terms (before orthogonalization), and it is seen that the first term is the more important at large distances, because of the factor r and the smaller coefficient in the exponent, while the second term is the more important for small values of r . In the simple hydrogen-like function analogous to this, there is only one exponential, whose exponent is $Z_{\text{eff}}/2$, or $(Z-\sigma)/2$ if we define the quantity σ , the screening constant. σ thus represents the shielding effect of the inner electrons which reduces the attraction of the nucleus for the L electron. Likewise in our more complicated function the idea of the screening constant can be introduced, only here two different screening constants for the L electron are needed, since there are two exponentials. The results which are obtained are that these screening constants are essentially independent of the nuclear charge and, therefore, provide a convenient method of summarizing the results of the variation problem. Furthermore, to a sufficiently close approximation, the screening constant for the inner part of the $2s$ function is zero, so that in a sense the four parameters originally used have been reduced to three.

The parameter α can also be related for the ions of different atomic number. It is found that in all four cases investigated α' comes so close to 0.5 that it is very convenient to assume that

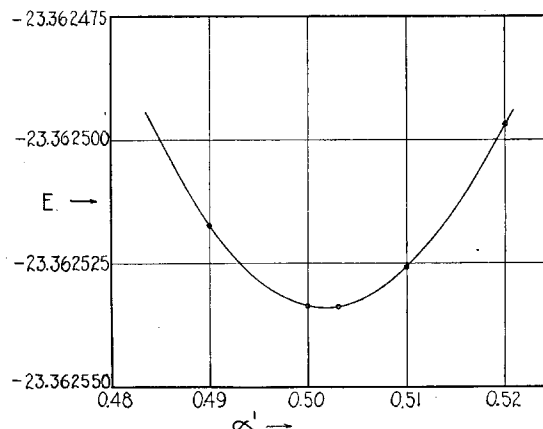


FIG. 1. Curve showing the variation of E with the parameter α' for B III, with the four-parameter function with $\sigma_1=0.31$, $\sigma_2=1.67$, $\zeta=Z/2$.

value for all three-electron ions. Fig. 1 shows the way E varies with α' in the case of B III. Since $\alpha = \alpha'\xi$ and $\xi = Z - \sigma_1$, if σ_1 is the K -shell screening constant, therefore,

$$\alpha = 0.5(Z - \sigma_1) = 0.5(Z - 0.31). \quad (19)$$

Introducing the values indicated above for the parameters η , ζ , α and ξ , we obtain for the best wave function for the state $1s^2 2s^2 S$ of any three-electron atom or ion the expression

$$\psi = (1/6^{\frac{1}{2}}) \sum P \pm P A_1 \bar{A}_2 B_3. \quad (20)$$

$$a = (\xi^3/\pi)^{\frac{1}{2}} e^{-\xi r} \quad (21)$$

$$b = k \{ \alpha r e^{-\eta r} - e^{-\zeta r} + \beta e^{-\xi r} \} \quad (22)$$

where

$$\left. \begin{aligned} \xi &= Z - \sigma_1 & \zeta &= Z/2 \\ \eta &= (Z - \sigma_2)/2 & \alpha &= 0.5(Z - \sigma_1) \end{aligned} \right\} \quad (23)$$

$$\beta = 8\xi^3 \left\{ \frac{1}{(\zeta + \xi)^3} - \frac{3\alpha}{(\eta + \xi)^4} \right\} \quad \text{orthogonality constant}$$

$$K = \left\{ \pi \left[3 \frac{\alpha^2}{\eta^5} + \frac{1}{\zeta^3} + \frac{\beta^2}{\xi^3} - \frac{48\alpha}{(\eta + \zeta)^4} + \frac{48\alpha\beta}{(\eta + \xi)^4} - \frac{16\beta}{(\zeta + \xi)^3} \right] \right\}^{-\frac{1}{2}}$$

and Z = atomic number of ion; and $\sigma_1=0.31$, K -shell screening constant. $\sigma_2=1.67$, L -shell screening constant. The sum in Eq. (20) is over all permutations P of the numbers 1, 2, 3, odd permutations having the negative sign. (This is another

way of writing the determinant of Eq. (1).) The single-electron functions a and b as given above are individually normalized to unity and are mutually orthogonal.

The energies obtained with the various functions are tabulated in Table I, which also contains the calculated ionization potentials. The experimental energy values are listed in the same table, together with deviations and percent deviations of the calculated and observed quantities. It is seen that the poorest values are those obtained with the hydrogen-like function of Eq. (4), even the simpler function put forward by Slater and given in Eq. (6) being considerably better. The error in the ionization potential computed by the use of the four-parameter function is only from thirty to seventy percent of the corresponding error found when Guillemin and Zener's function is used.

Fig. 2 is a plot of the four-parameter single-electron function for the $2s$ electron normalized to 4π and with β adjusted so that the L and K functions are orthogonal. Fig. 3 gives $4\pi r^2 b^2$, the distribution function integrated over all angles. On comparing the size of the two maxima in Li I and in hydrogen ($2s$ state), the effect of the core electrons of lithium in reducing the probability of close approach to the nucleus by the valence electron is clearly seen, in agreement with the old concept of the penetrating orbit, in the inner segment of which the electron was speeded up by the increased effective nuclear charge, diminishing the time spent in traversing this segment. Fig. 4 gives the total electron density function for Li I, integrated over all angles. The very steep rise at the K -shell and the more spread-out maximum of the single L electron are shown.

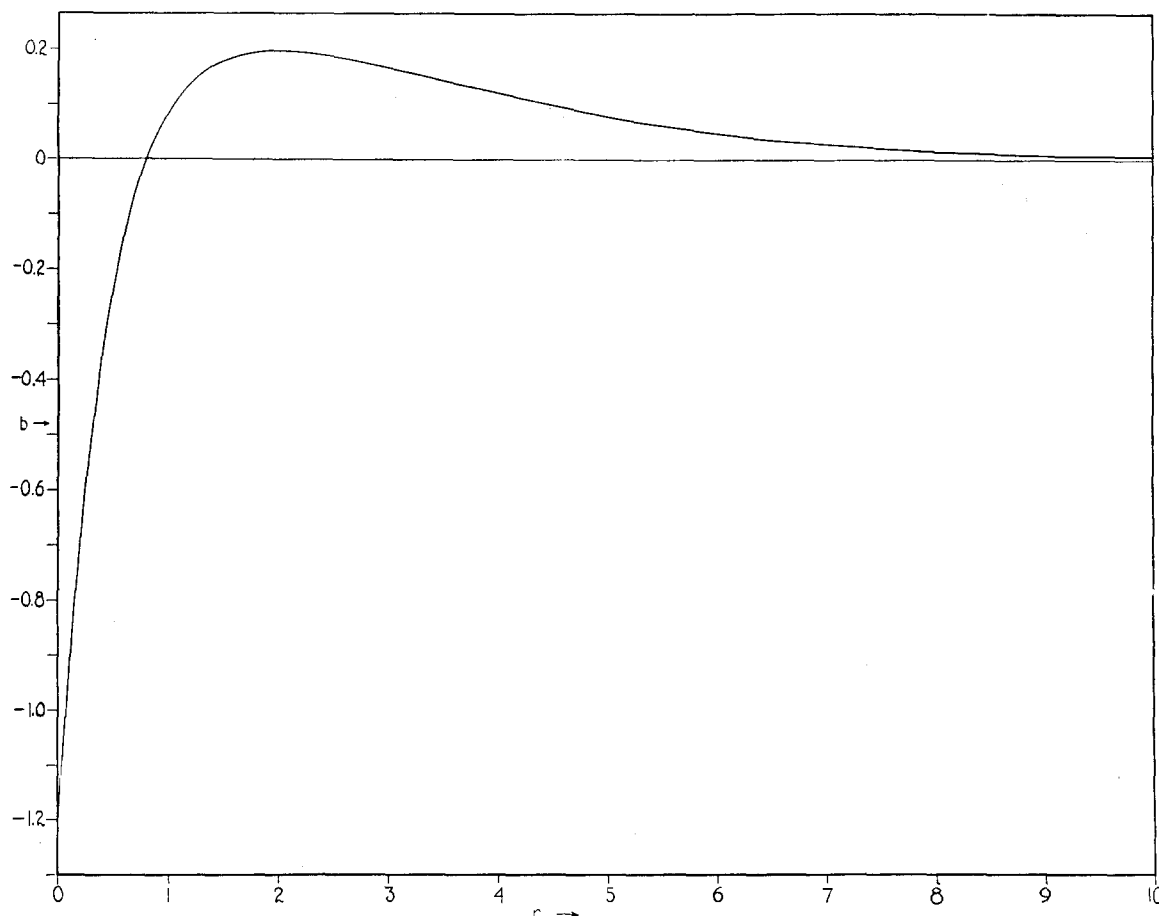


FIG. 2. Plot of four-parameter orthogonalized single-electron wave function b for $2s$ electron, normalized to 4π . r in atomic units. Li I.

THE INTERNAL FIELD

Hargreaves⁴ has given a table of values for the self-consistent field for lithium, obtained graphically. This is expressed in terms of the "effective nuclear charge for field," which is the number Z_f such that the charge $Z_f e$ placed at the position of the nucleus would give the same field (not potential) at the point in question as is actually found. In other words:

$$Z_f = r^2(\partial V/\partial r) \quad (24)$$

in atomic units.

In Table III the values of Z_f found by Hargreaves are listed. In addition there is also

given the field due to the nucleus and the two K

TABLE III. Field due to K electrons. r in atomic units.

r	Z_f —Hargreaves	Z_f —Eq. (24)	Difference
0	3	3	0
0.1	2.963	2.965	−0.002
.2	2.807	2.811	−.004
.3	2.559	2.559	.000
.4	2.280	2.272	+.008
.6	1.773	1.748	+.025
.8	1.425	1.394	.031
1.0	1.219	1.192	.027
1.2	1.108	1.089	.019
1.4	1.050	1.039	.011
1.6	1.022	1.017	.005
1.8	1.009	1.007	.002
2.0	1.003	1.003	.000

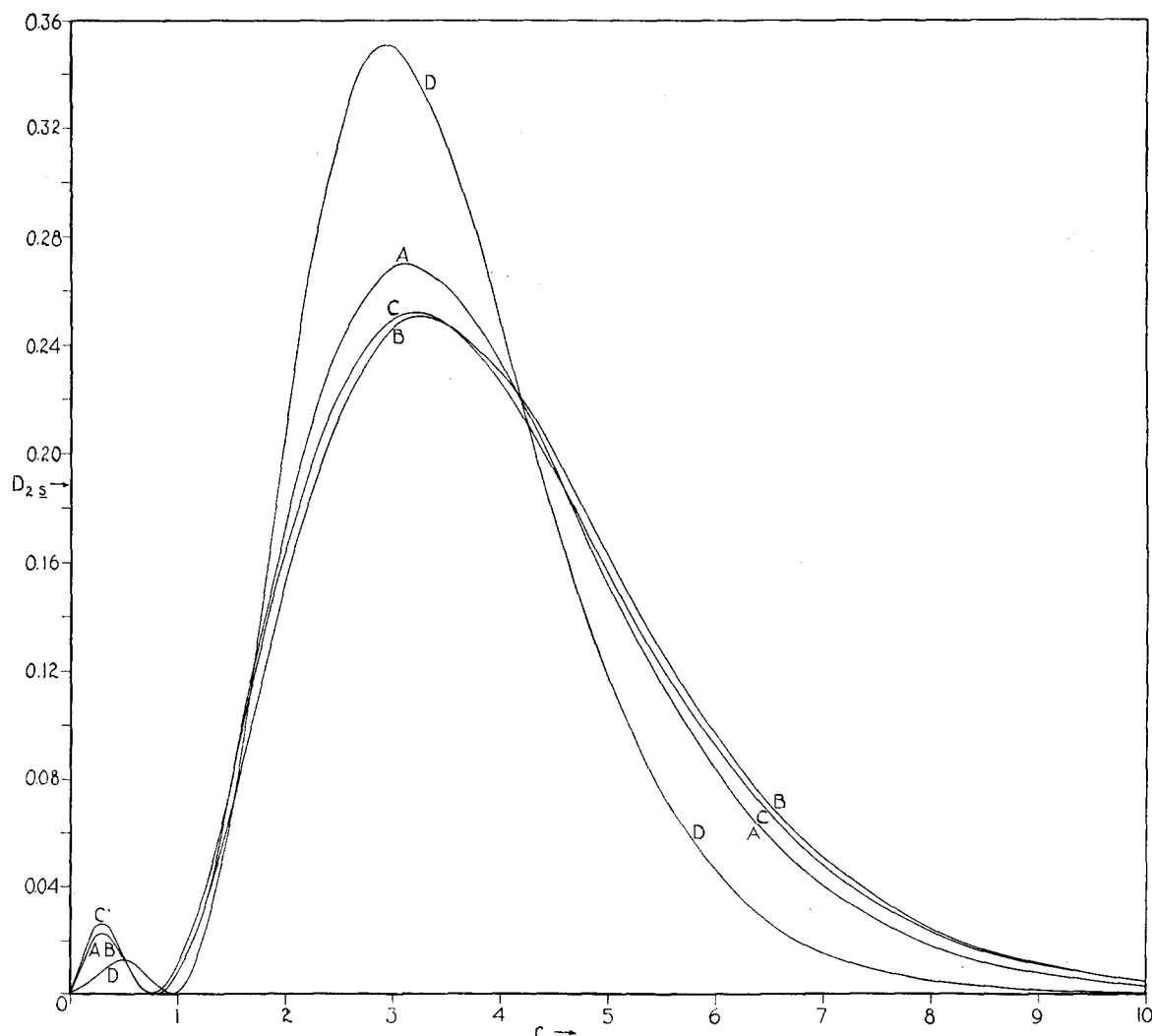


FIG. 3. Plot of electron distribution function for 2s electron, $D_{2s} = 4\pi r^2 b^2$, with different types of functions. Li I. A, 4-parameter; B, Guillemin-Zener; C, Slater; D, hydrogen-like.

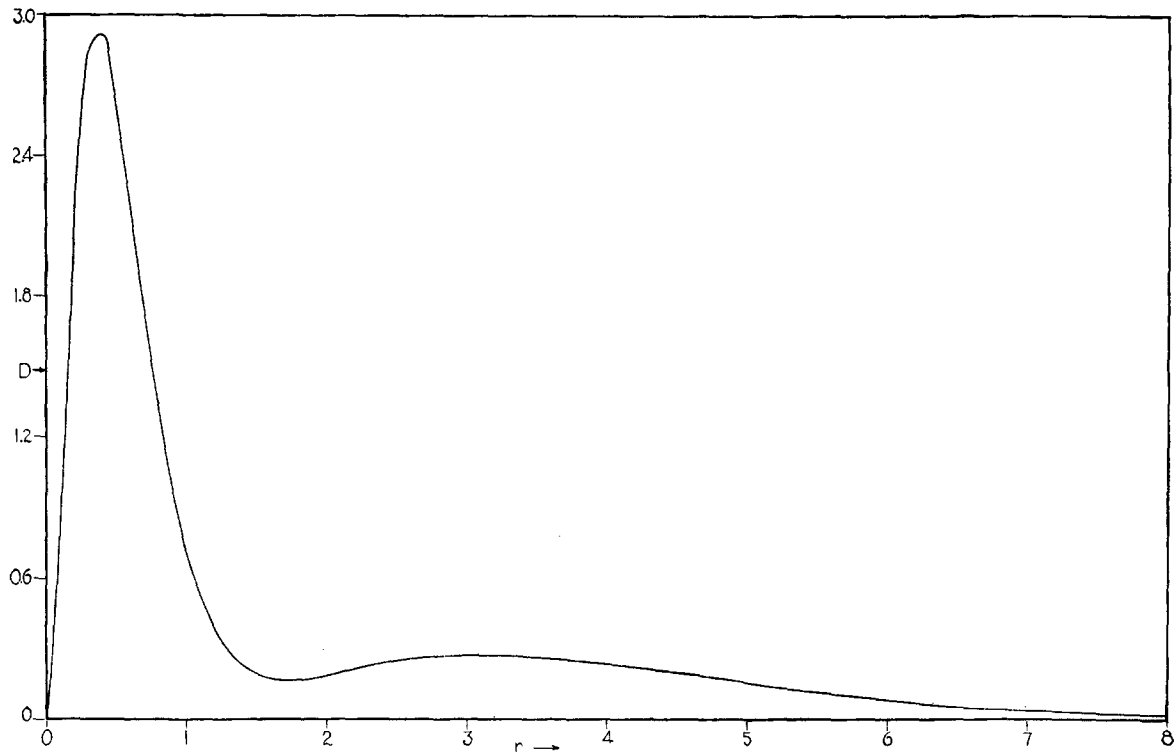


FIG. 4. Total electron distribution function for Li I, $D=4\pi r^2\psi^*$, as a function of r in atomic units.

electrons, found by using the K functions previously described. To calculate this latter quantity at a distance R from the nucleus, use is made of the equation derived from electrostatics for the field due to a distribution of electricity of density $\rho=a^2$

$$V = -\frac{Z}{R} + \frac{8\pi}{R} \int_0^R r^2 a^2 dr + 8\pi \int_R^\infty r a^2 dr. \quad (25)$$

If a is given by Eq. (21), (25) becomes

$$V = -Z/R + (2/R) \{1 - e^{-2\xi R}(1 + \xi R)\}. \quad (26)$$

As is seen from Table III, there is quite good agreement between the field calculated in this manner and that of Hargreaves, the deviation being about 2 percent at most. This comparison refers only to the $1s$ functions used, and not to the $2s$ function, however.

EXPRESSIONS FOR N , L , M

Eq. (15) gives the energy in terms of N , L , M , defined by (13). Algebraic expressions for N , L , M for the configuration $(1s)^2 2s$ and for the $2s$ functions of (7) are given below:

$$\alpha' = \alpha/\xi; \quad \zeta' = \zeta/\xi; \quad \eta' = \eta/\xi. \quad (27)$$

$$2K = \zeta' + \eta'; \quad b = 1 + \eta'; \quad f = 1 + \zeta'; \quad g = 1 + K. \quad (28)$$

$$N = \pi^3 \left\{ \frac{3\alpha'^2}{\eta'^5} - 576 \frac{\alpha'^2}{b^8} + 384 \frac{\alpha'}{b^4 f^3} - 3 \frac{\alpha'}{K^4} + \frac{1}{\zeta'^3} - \frac{64}{f^6} \right\}. \quad (29)$$

$$L = \pi^3 \left\{ 3(2Z - \frac{5}{8}) \frac{\alpha'^2}{\eta'^5} + (1.5Z - 3) \frac{\alpha'^2}{\eta'^4} + 3 \frac{\alpha'^2}{b^4} + 6 \frac{\alpha'^2}{b^5} + (516 - 384 \cdot Z) \frac{\alpha'^2}{b^7} - 576 \cdot Z \frac{\alpha'^2}{b^8} - \frac{384\alpha'^2}{b^4(2+b)^3} \right\}$$

$$\begin{aligned}
& -\frac{1152\alpha'^2}{b^4(2+b)^4} + (4-2Z)\frac{\alpha'}{K^3} - 4\frac{\alpha'}{g^3} - 6\frac{\alpha'}{g^4} + (128\cdot Z - 256)\frac{\alpha'}{f^3b^3} + 192Z\frac{\alpha'}{b^4f^2} + (384Z - 384)\frac{\alpha'}{b^4f^3} \\
& + \frac{128\alpha'}{f^3(2+b)^3} + \frac{384\alpha'}{f^3(2+b)^4} + \frac{1536\alpha'}{b^4f^3(2+f)^2} + \frac{1536\alpha'}{b^4f^2(2+f)^3} + \frac{128\alpha'}{f^3(f+b)^3} + \frac{192\alpha'}{f^2(f+b)^4} - 3(2Z - \frac{5}{8})\frac{\alpha'}{K^4} \\
& + (2Z - \frac{5}{8})\frac{1}{\zeta'^3} + (Z-2)\frac{1}{\zeta'^2} + \frac{2}{f^2} + \frac{2}{f^3} + (20-64Z)\frac{1}{f^5} + (128-64Z)\frac{1}{f^6} - \frac{512}{f^6(2+f)^2} - \frac{512}{f^5(2+f)^3} \Big\}. \quad (30)
\end{aligned}$$

$$\begin{aligned}
M = \pi^3 \Big\{ & \frac{6\alpha'^2}{\eta'^5} + \frac{\alpha'^2}{\eta'^3} + 384\frac{\alpha'^2}{b^7} - 576\frac{\alpha'^2}{b^8} - 1152\frac{\eta'\alpha'^2}{b^8} - 6\frac{\alpha'}{K^4} - 3\frac{\zeta'\eta'\alpha'}{K^4} - 128\frac{\alpha'}{b^3f^3} + 384\frac{\alpha'}{b^4f^3} + 2\frac{\alpha'\zeta'}{K^3} \\
& + 384\frac{\alpha'\zeta'}{b^4f^3} + 384\frac{\alpha'\eta'}{b^4f^3} + \frac{2}{\zeta'^3} + \frac{1}{\zeta'} - 128\frac{\zeta'}{f^6} - 64\frac{1}{f^6} \Big\}. \quad (31)
\end{aligned}$$

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