Self-Consistent Field for Tungsten

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Calculations of the self-consistent field of the tungsten atom have been carried out with the aid of the Massachusetts Institute of Technology differential analyzer. A discussion of the machine set-up and an outline of a method for estimating initial fields are given.

IF the wave-function of a many-electron atom is expressed as a product of one-electron wave-functions, the radial factor of each of these wave-functions is found by solution of the differential equation[1]

$$d^2P/dr^2+(2v-\epsilon-l(l+1)/r^2)P=0. \quad (1)$$

As has been pointed out by Hartree[2] it is convenient to introduce the new independent variable $\rho=\log r$, and the new dependent variables $Q=Pr^{-l-1}$ and $Y=Pr^{-\frac{1}{2}}$. The differential equations which Q and Y satisfy are:

$$d^2Q/d\rho^2+(2l+1)dQ/d\rho+(2rZ_p-\epsilon r^2)Q=0, \quad (2)$$

$$d^2Y/d\rho^2+[2rZ_p-\epsilon r^2-(l+\tfrac{1}{2})^2]Y=0. \quad (3)$$

For $n<4$ and for all of the "s" functions, Eq. (3) was used throughout the range of integration. For the other functions the "Q" equation was used near the origin because in this region Q is nearly constant while Y increases exponentially.

The contribution to Z_p of the electrons of a particular type is found from the relations:

$$\zeta=\int_0^r P^2dr=\int_0^\rho Y^2e^{2\rho}d\rho, \quad (4)$$

$$Z=2(2l+1)\left[1-\int_0^r P^2dr\Big/\int_0^\infty P^2dr\right], \quad (5)$$

$$dZ_p/d\rho=Z_p-Z. \quad (6)$$

The estimation of the initial Z_p's was carried out by a method which, as far as the authors know, has not been described in the literature. Since it proved to be very satisfactory, it will be outlined briefly here. The basis of the method of interpolation is the fact that the Z *vs.* ρ curve for a particular type of electron has the same shape for different elements which are not too far apart in the periodic table. As can be seen from the graph of Fig. 1, one curve can be nearly superposed on the other by a shift parallel to the ρ axis. A reason why this can be expected and a method of utilizing it for interpolations can be seen from the screening constant relation:

$$r_1/r_2=(N_2-\sigma)/(N_1-\sigma) \quad (7)$$

or

$$\rho_1-\rho_2=\log\,(N_2-\sigma)/(N_1-\sigma), \quad (7a)$$

where N_1 and N_2 are the atomic numbers of the two elements considered and σ is the screening constant for the type of electron considered. This relation is ordinarily assumed to be valid only for the two radii for which the charge densities have their maxima, but the figure shows that it will be valid for any pair of radii corresponding to the same value of Z. Using data from two atoms which have been studied previously, $\rho_1-\rho_2$ and hence σ can be determined. Eq. (7a) can then be used to determine the Z against ρ curve for the same type of electron in another atom. For tungsten the interpolations were based upon Hartree's result for caesium[3] and mercury.[4] For the electrons inside of the 4s electron, the original estimates agreed so closely with those computed that it was necessary to determine these functions only once. For the outer electrons the estimates were not as satisfactory. This is because the 4f shell occurs in only one of the atoms which were used for interpolation. Since the charge density of the 4f electrons overlaps both four and five quantum electrons, it is easy to understand why the screening constants should be affected in a manner difficult to estimate.

[1] Except where stated the notation is that used by Hartree. See Proc. Roy. Soc. **A141**, 282 (1933).

[2] Hartree, Phys. Rev. **46**, 738 (1934).

[3] Hartree, Proc. Roy. Soc. **A143**, 506 (1934).

[4] Hartree, Proc. Roy. Soc. **A149**, 210 (1935).

In determining the Z's by the method described, there is some difficulty about making estimates in the region of the nodes. Even after the Z's have been determined, it is necessary to integrate to obtain the Z_p's. For these reasons, it seems possible that it would be more satisfactory to make the estimates in terms of the Z_p's. Hence tables of $2Z_p$ and $2v_0$ for the separate electrons have been included in the results.

Method of Solution

The solutions of Eqs. (2), (3), and (4) have been carried out on the Massachusetts Institute of Technology differential analyzer.[5] A schematic diagram[6, 7] of the setup for the simultaneous solution of Eqs. (3) and (4) is given in Fig. 2. The solution of Eq. (2) requires only the insertion of an extra set of gears and an adder. This equation is not used beyond the point where contributions to ζ become appreciable. It would be possible to integrate a modified form of Eq. (6) but this would require another input table. It is also difficult to estimate the starting conditions, and hence it was found more convenient to carry out this comparatively easy integration by hand. For the inner electrons and for the earlier approximations to the outer ones, it is not necessary to use different input plots of $2rZ_p$ for different functions having the same value of n but different values of l. The constant $(l+\frac{1}{2})^2$ can be taken care of by the initial setting of the first integrator. The method of generating ϵr^2 by an integrator avoids the necessity of making either a large number of plots or using another input table. In practice, the displacement of this integrator is multiplied by a factor greater than unity at small ρ and less than unity at large ρ. Compensating gears must, of course, be introduced.

The method ordinarily used by Hartree is to integrate from the origin outward to some point near the outer maximum of the wave function and to integrate a transformed equation from large r inward to the same point. The value of ϵ for which these solutions join is the eigenvalue. To carry out this process on an analyzer having six integrators would have required either an additional input table or the hand integration of the ζ equation. It seemed preferable to keep to the same equation and hunt for solutions asymptotic to the ρ axis. In practice this method did not prove too difficult, but some improvement in this part of the integration would probably be necessary before the accuracy could be greatly increased. The tabulated values of Y at large ρ have been smoothed to the correct asymptotic form.

One of the difficulties of any step-by-step process of integration is the accumulation of rounding-off errors. In hand computation this can be partly avoided by carrying extra figures

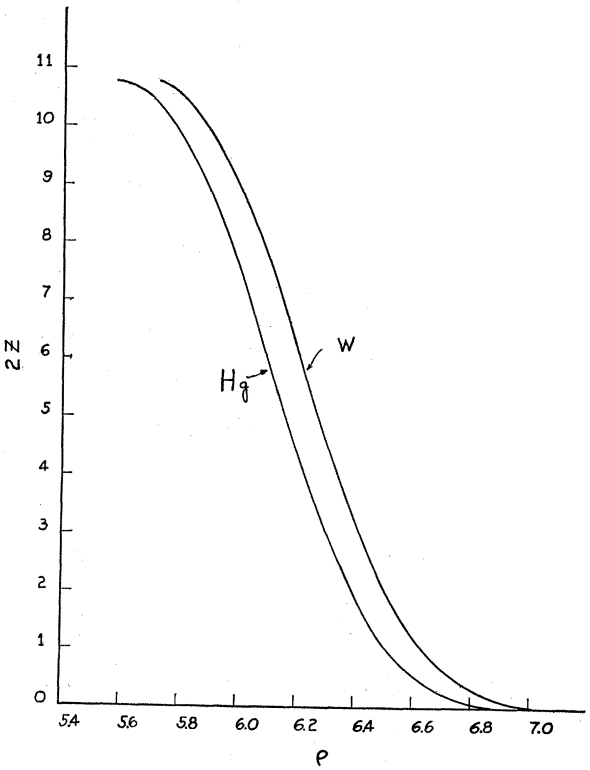

FIG. 1. Plot of $2Z$ as a function of ρ for $4p$ electrons in Hg and W.

[5] The authors wish to express their thanks to Professor S. H. Caldwell of the department of electrical engineering for placing the facilities of the differential analyzer at their disposal, and for making many helpful suggestions about the problem. As Hartree has pointed out, the solution of such a problem without mechanical methods of computation, is very laborious.

[6] For an explanation of the operation of the differential analyzer and the meanings of the symbols used, see: V. Bush, J. Frank. Inst. **212**, 447 (1931).

[7] For other cases where a differential analyzer has been used for the solution of the self-consistent field problem, see: Hartree, Phys. Rev. **46**, 738 (1934); Porter, Proc. Manchester Phil. Soc. **79**, 75 (1935).

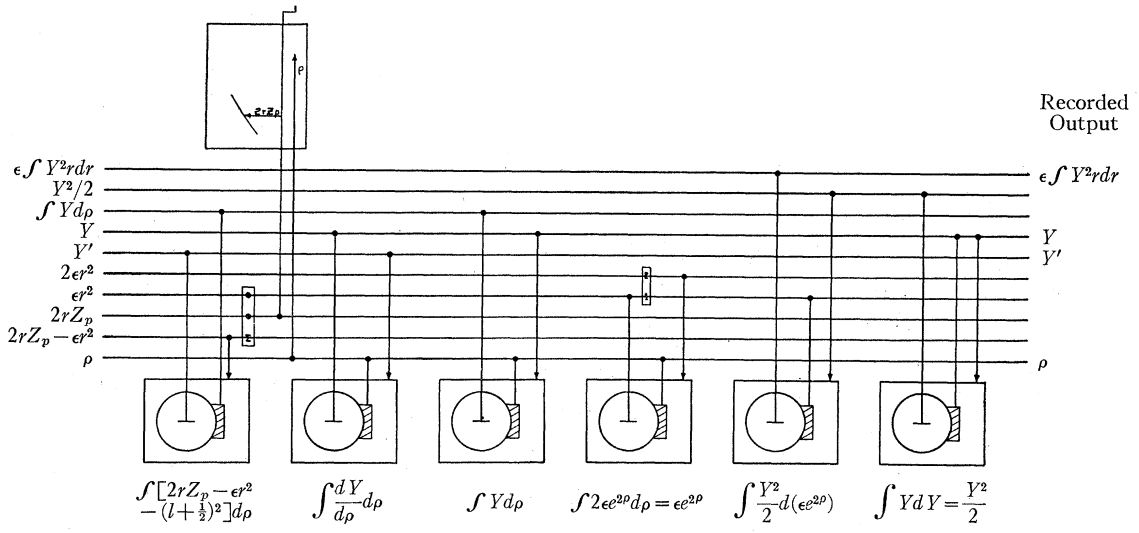

FIG. 2. Schematic diagram for the set-up of the differential analyzer for solution of the equations:

$$d^2Y/d\rho^2+[2rZ_p-\epsilon r^2-(l+\tfrac{1}{2})^2]Y=0 \quad \text{and} \quad \zeta=\int_0^\rho Y^2e^{2\rho}d\rho.$$

for the earlier stages of the computation. With the differential analyzer this method is not possible, and instead a method suggested by Professor Caldwell was used. The essential feature is to run solutions for five different energies which are evenly spaced about a value of the energy estimated from preliminary runs. These solutions are carried forward in stages of about two units in ρ. The solutions are smoothed by a least-squares method at the end of each of these stages and the solutions carried forward with the smoothed values.

As was anticipated, the most troublesome function was the $4f$. This is because $2rZ_p$ is never very much greater than $(l+\frac{1}{2})^2$ and hence small changes in $2rZ_p$ can produce large changes in the coefficient of Y in Eq. (3) in the region where that coefficient is positive. These small changes in $2rZ_p$ can be produced by any of the four or five quantum electrons—most particularly by the $4f$ electrons themselves. The functions are probably not "overstable" in the sense used by Hartree, but any process of using the field found at the end of one approximation as the initial field for the next approximation would probably converge but slowly. A little judicious guessing as to what is likely to happen next speeds up the convergence considerably. The $5d$ functions caused much less trouble than in the case of Hartree's calculations for mercury. This is partly because there are four instead of ten electrons in this shell, and partly because of a fortuitous estimate made at the end of the first approximation. The solution of the problem was of course much easier than it would have been without Hartree's previous work on mercury.

TABLE I. *Values of Y for* $\rho<2.0$.

	$1s$	$2s$	$2p$	$3s$	$3p$	$3d$	$4s$, $5s$, $6s$
0.0	3200	3200	80.0	3200	64.0	5.33	3200
.2	3478	3475	106.5	3477	85.5	8.70	3476
.4	3764	3761	142.0	3765	114.1	14.23	3762
.6	4058	4052	189.2	4058	152.0	23.28	4053
.8	4351	4341	251.5	4348	202.3	38.02	4343
1.0	4634	4617	333.5	4625	268.0	61.91	4620
.2	4896	4868	440.3	4874	353.9	100.50	4868
.4	5121	5074	578.5	5079	464.9	162.3	5071
.6	5293	5215	756	5216	605.8	261.8	5206
.8	5392	5264	980	5267	784.0	420.3	5235
2.0	5395	5188	1258	5174	1006	671.0	5155

TABLE II. *Values of* $Q\times10^{-4}$.

ρ	$4p$, $5p$	$4d$, $5d$	$4f$	ρ	$4p$, $5p$	$4d$, $5d$	$4f$
0.0	329.5	1780	1905	2.4		1393	1586
.4	323.5	1758	1887	2.6		1313	1519
.8	314.7	1727	1862	2.8		1222	1441
1.2	302.0	1681	1824	3.0		1119	1352
1.6	284.0	1615	1770	3.2			1253
2.0	251.9	1522	1694	3.4			1143
2.2		1462	1644	3.6			1024

TABLE III. *Values of Y.*

	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	5d	6s
2.0	5395	5188	1258	5174	1008	67.1	5155	1600			5155	1600		5155
.1	5353	5094	1420	5073	1135	84.3	5052	1803			5052	1803		5052
.2	5280	4957	1398	4928	1276	106.0	4903	2028			4902	2027		4902
.3	5173	4773	1794	4734	1431	133.0	4704	2273			4702	2272		4702
.4	5031	4538	2006	4488	1397	166.5	4452	2537			4448	2535		4448
.5	4852	4251	2236	4185	1776	208	4144	2820			4137	2817		4137
.6	4643	3910	2481	3825	1996	260	3776	3120			3766	3115		3766
.7	4392	3507	2739	3405	2165	323	3349	3433			3335	3427		3335
.8	4112	3054	3009	2928	2369	399	2864	3754			2844	3745		2844
.9	3803	2545	3286	2395	2576	476	2323	4078			2298	4067		2298
3.0	3471	1988	3565	1817	2781	605	1733	4396	640		1702	4380	640	1702
.1	3121	1390	3841	1188	2976	741	1102	4697	780		1065	4677	779	1065
.2	2761	761	4106	+ 534	3155	896	+ 442	4969	948		+ 400	4944	946	+ 400
.3	2398	+ 114	4352	− 135	3307	1083	− 230	5197	1144		− 276	5167	1143	− 276
.4	2042	− 538	4569	− 799	3424	1301	− 895	5364	1374		− 943	5328	1372	− 943
.5	1702	−1173	4748	−1437	3495	1552	−1527	5454	1638		−1578	5412	1636	−1578
.6	1382	−1775	4879	−2023	3507	1840	−2106	5447	1939	96.0	−2151	5398	1936	−2151
.7	1094	−2320	4952	−2529	3451	2163	−2596	5323	2275	127.6	−2635	5266	2272	−2635
.8	841	−2789	4958	−2927	3314	2524	−2971	5068	2648	169.0	−3001	5002	2644	−3001
.9	625	−3162	4890	−3129	3097	2918	−3201	4667	3049	222.4	−3225	4591	3042	−3225
4.0	448	−3425	4738	−3298	2776	3340	−3265	4112	3470	290.2	−3226	4026	3461	−3226
.1	308	−3566	4517	−3233	2369	3782	−3141	3406	3898	377.4	−3129	3288	3887	−3129
.2	202	−3581	4217	−2975	1875	4229	−2825	2561	4322	485	−2798	2430	4302	−2798
.3	125	−3474	3850	−2559	1305	4670	−2324	1597	4716	618	−2280	1461	4685	−2280
.4	73	−3257	3433	−1971	683	5082	−1660	+ 556	5055	780	1598	+ 416	5010	−1598
.5	39	−2949	2979	−1252	+ 23	5447	− 871	− 523	5708	975	− 796	− 615	5247	− 797
.6	20	−2577	2511	− 448	− 639	5738	− 15	−1565	5446	1205	+ 72	−1676	5363	+ 69
.7	10	−2169	2050	+ 389	−1265	5935	+ 843	−2504	5436	1472	932	−2588	5327	927
.8	4	−1753	1616	1196	−1824	6015	1623	−3264	5249	1776	1704	−3310	5110	1698
.9	2	−1357	1226	1915	−2227	5967	2251	−3777	4865	2115	2307	−3771	4690	2300
5.0	1	−1004	892	2485	−2597	5781	2653	−3986	4276	2483	2671	−3917	4060	2663
.1		− 706	619	2880	−2773	5459	2785	−3857	3477	2874	2743	−3713	3224	2735
.2		− 470	409	3069	−2796	5015	2618	−3386	2503	3274	2502	−3158	2212	2493
.3		− 294	256	3056	−2676	4474	2164	−2603	1388	3670	1964	−2298	+1065	1954
.4		− 171	152	2865	−2441	3863	1467	−1574	+ 192	4047	1184	−1188	− 150	1172
.5		− 94	82	2536	−2120	3222	+ 603	− 392	−1017	4371	+ 254	+ 38	−1356	+ 241
.6		− 49	45	2122	−1751	2587	− 331	+ 828	−2159	4630	− 739	1272	−2458	− 724
.7		− 24	21	1677	−1374	1991	−1228	1967	−3158	4822	−1578	2352	−3371	−1587
.8		− 10	9	1252	−1021	1465	−1991	2915	−3945	4906	−2234	3153	−4014	−2231
.9		− 4	4	873	− 715	1026	−2543	3593	−4475	4885	−2585	3579	−4331	−2564
6.0		− 1	1	571	− 471	679	−2844	3958	−4725	4757	−2586	3580	−4297	−2537
.1				345	− 289	422	−2899	4017	−4710	4534	−2241	3160	−3911	−2154
.2				190	− 164	241	−2737	3806	−4461	4231	−1624	2377	−3218	−1475
.3				88	− 80	134	−2417	3394	−4036	3868	− 763	1331	−2281	− 598
.4				41	− 43	69	−2006	2860	−3494	3465	+ 171	+ 140	−1178	+ 360
.5				18	− 20	33	−1569	2282	−2898	3042	1085	−1068	+ 1	1268
.6				7	− 8	15	−1158	1724	−2303	2616	1880	−2167	1194	2021
.7				3	− 3	6	− 801	1232	−1753	2199	2490	−3077	2305	2535
.8				1	− 1	2	− 520	831	−1274	1810	2864	−3724	3282	2756
.9						1	− 317	529	− 884	1454	2998	−4083	4079	2673
7.0							− 180	319	− 584	1140	2914	−4120	4674	2309
.1							− 96	185	− 365	871	2657	−3991	5058	1708
.2							− 48	100	− 214	646	2288	−3633	5242	949
.3							− 22	51	− 118	467	1867	−3151	5245	+ 106
.4							− 9	23	− 58	326	1446	−2609	5093	− 747
.5							− 4	11	− 30	220	1064	−2064	4816	−1546
.6							− 1	3	− 13	141	747	−1562	4441	−2236
.7								1	− 5	87	497	−1127	3999	−2782
.8									− 2	52	318	− 775	3516	−3162
.9										29	191	− 505	3020	−3369
8.0										16	108	− 311	2532	−3411
.1										8	57	− 183	2071	−3306
.2										3	29	− 101	1652	−3079
.3										1	13	− 53	1282	−2763
.4											5	− 25	967	−2391
.5											2	− 11	708	−1996
.6											1	− 5	500	−1604
.7												− 2	337	−1238
.8												− 1	214	− 915
.9													132	− 645
9.0													77	− 440
.1													42	− 266
.2													22	− 158
.3													11	− 89
.4													5	− 46
.5													2	− 22
.6													1	− 10
.7														− 4
.8														− 1

RESULTS

Tables of Y, $2Z$, and $2Z_p$ for each type of electron are given. For the cases where the Q equation was used near the origin, the values of Q rather than Y are given at small ρ. In the tables $\rho = \log 1000r$. The discrepancy between final estimates and final values of $2Z_p$ for any given type of electron does not exceed 0.06. This is about the same as the discrepancy in Z and is about five times the tolerance allowed by

TABLE IV. *Values of $2Z_p$ for the separate electrons and for the complete atom.*

(ρ)	$(1s)$	$(2s)$	$(2p)$	$(3s)$	$(3p)$	$(3d)$	$(4s)$	$(4p)$	$(4d)$	$(4f)$	$(5s)$	$(5p)$	$(5d)$	$(6s)$	Total
0.0	3.71	3.93	11.79	3.97	11.92	19.87	3.99	11.97	19.95	27.94	4.00	11.99	8.00	4.00	147.02
.4	3.56	3.89	11.69	3.96	11.83	19.81	3.98	11.95	19.93	27.91	3.99	11.98	7.99	4.00	146.49
.8	3.35	3.84	11.54	3.94	11.83	19.71	3.98	11.93	19.89	27.87	3.99	11.97	7.99	4.00	145.83
1.2	3.05	3.77	11.31	3.92	11.74	19.57	3.96	11.89	19.83	27.81	3.99	11.96	7.98	4.00	144.78
.6	2.62	3.67	10.97	3.87	11.61	19.36	3.95	11.84	19.75	27.71	3.98	11.94	7.98	3.99	143.24
2.0	2.07	3.52	10.47	3.81	11.42	19.05	3.92	11.76	19.63	27.57	3.97	11.91	7.97	3.99	141.05
.2	1.75	3.42	10.13	2.77	11.29	18.84	3.90	11.71	19.55	27.47	3.96	11.89	7.96	3.99	139.64
.4	1.42	3.31	9.72	3.73	11.14	18.58	3.88	11.64	19.45	27.36	3.95	11.87	7.95	3.99	137.98
.6	1.08	3.18	9.22	3.67	10.95	18.26	3.86	11.56	19.33	27.21	3.94	11.84	7.94	3.98	136.03
.8	0.77	3.03	8.62	3.60	10.72	17.88	3.83	11.47	19.18	27.04	3.93	11.81	7.92	3.98	133.07
3.0	.50	2.85	7.90	3.52	10.44	17.41	3.79	11.35	19.00	26.83	3.92	11.77	7.91	3.98	131.15
.2	.29	2.64	7.05	3.43	10.11	16.83	3.74	11.21	18.78	26.57	3.90	11.72	7.89	3.97	128.11
.4	.15	2.38	6.07	3.31	9.71	16.13	3.69	11.04	18.51	26.26	3.87	11.65	7.86	3.96	124.59
.6	.06	2.06	4.99	3.16	9.25	15.28	3.62	10.84	18.18	25.86	3.85	11.58	7.83	3.96	120.50
.8	.02	1.69	3.84	2.99	8.73	14.24	3.54	10.60	17.77	25.39	3.81	11.49	7.79	3.95	115.83
4.0		1.28	2.71	2.79	8.14	12.98	3.44	10.32	17.29	24.81	3.77	11.37	7.74	3.93	110.57
.1		1.07	2.19	2.67	7.82	12.26	3.38	10.15	17.00	24.48	3.75	11.32	7.72	3.93	107.74
.2		0.86	1.72	2.56	7.46	11.49	3.32	9.99	16.70	24.10	3.72	11.24	7.69	3.92	104.77
.3		.68	1.30	2.43	7.09	10.64	3.26	9.79	16.36	23.70	3.69	11.17	7.66	3.91	101.66
.4		.50	0.94	2.30	6.67	9.74	3.20	9.58	15.99	23.24	3.66	11.08	7.62	3.90	98.42
.5		.36	.65	2.15	6.22	8.79	3.11	9.34	15.60	22.75	3.63	10.99	7.58	3.89	95.05
.6		.24	.43	2.00	5.71	7.79	3.02	9.09	15.17	22.19	3.59	10.88	7.54	3.88	91.54
.7		.16	.27	1.82	5.16	6.77	2.93	8.80	14.72	21.58	3.55	10.77	7.51	3.86	87.89
.8		.09	.16	1.63	4.56	5.75	2.82	8.50	14.23	20.91	3.50	10.64	7.44	3.85	84.07
.9		.05	.08	1.42	3.92	4.75	2.71	8.16	13.71	20.17	3.45	10.51	7.40	3.83	80.16
5.0		.02	.04	1.20	3.26	3.80	2.59	7.80	13.16	19.35	3.39	10.35	7.32	3.82	76.11
.1		.01	.02	0.98	2.61	2.94	2.46	7.42	12.57	18.47	3.33	10.19	7.27	3.80	72.05
.2			.01	.76	1.99	2.18	2.32	7.02	11.94	17.49	3.27	10.01	7.17	3.78	68.37
.3				.56	1.45	1.54	2.17	6.59	11.24	16.44	3.19	9.81	7.11	3.75	63.85
.4				.38	0.99	1.03	2.02	6.13	10.48	15.30	3.12	9.59	7.00	3.73	59.76
.5				.25	.63	0.65	1.85	5.63	9.64	14.09	3.03	9.36	6.91	3.70	55.72
.6				.15	.37	.38	1.66	5.08	8.72	12.81	2.93	9.09	6.79	3.67	51.63
.7				.08	.20	.21	1.46	4.47	7.71	11.49	2.83	8.81	6.68	3.63	47.54
.8				.04	.09	.10	1.24	3.81	6.65	10.14	2.71	8.48	6.53	3.59	43.38
.9				.02	.04	.04	1.01	3.13	5.56	8.79	2.58	8.15	6.39	3.55	39.25
6.0				.01	.01	.02	0.78	2.46	4.48	7.47	2.45	7.77	6.22	3.51	35.17
.1							.57	1.83	3.47	6.22	2.31	7.38	6.06	3.45	31.30
.2							.39	1.29	2.56	5.05	2.16	6.96	5.86	3.40	27.66
.3							.25	0.85	1.80	4.01	1.99	6.50	5.66	3.34	24.39
.4							.14	.52	1.20	3.09	1.81	6.00	5.42	3.27	21.45
.5							.08	.29	0.75	2.31	1.61	5.45	5.18	3.19	18.86
.6							.04	.15	.44	1.67	1.40	4.83	4.89	3.11	16.52
.7							.02	.07	.23	1.16	1.17	4.18	4.59	3.02	14.44
.8							.01	.03	.11	0.78	0.94	3.50	4.25	2.92	12.53
.9								.01	.05	.50	.71	2.82	3.89	2.82	10.80
7.0									.02	.31	.52	2.17	3.50	2.70	9.21
.1										.18	.35	1.59	3.11	2.57	7.81
.2										.10	.22	1.11	2.69	2.44	6.56
.3										.05	.13	0.73	2.30	2.29	5.50
.4										.02	.07	.44	1.92	2.12	4.58
.5										.01	.04	.25	1.56	1.94	3.80
.6											.02	.13	1.23	1.74	3.12
.7											.01	.07	0.94	1.53	2.55
.8												.03	.70	1.31	2.04
.9												.01	.50	1.09	1.60
8.0													.35	0.87	1.22
.1													.23	.68	0.90
.2													.14	.50	.64
.3													.08	.35	.43
.4													.05	.23	.28
.5													.02	.14	.16
.6													.01	.08	.09
.7														.04	.04
.8														.01	.01

TABLE V. *Values of ϵ, $\int_0^\infty P^2dr$, and $2v_0$.*

	ϵ	$\int_0^\infty P^2dr$	$-2v_0$
$1s$	4764	7.187×10^3	294
$2s$	773.5	67.90	74
$2p$	740.5	93.67	206
$3s$	175.4	269.6	26
$3p$	161.8	244.7	78
$3d$	135.5	851.4	129
$4s$	34.46	1.318×10^3	10.9
$4p$	28.30	2.711	32.4
$4d$	17.33	4.251	49.9
$4f$	3.378	4.422	57.2
$5s$	4.865	7.875	4.3
$5p$	3.125	19.10	11.7
$5d$	.4870	88.0	4.7
$6s$	.4293	113.3	1.2
Total			979

Hartree in his calculations for mercury.[8] Much further improvement in the results would require less efficient operation of the differential analyzer and some checking by hand calculations. In this work there has been no direct check of the machine integrations. The only checks are the interval consistency of different runs and the check of estimated and calculated values of Z

[8] Calculations of about the same accuracy have also been made for iron. Since applications to theories of ferromagnetism and atomic spectra require a higher degree of accuracy than the work for which the tungsten results are being used, the results for iron will not be published until their accuracy has been improved.

TABLE VI. *Values of 2Z.*

(p)	(1s)	(2s)	(2p)	(3s)	(3p)	(3d)	(4s)	(4p)	(4d)	(4f)	(5s)	(5p)	(5d)	(6s)
0.0	4.00	4.00	12.00	4.00	12.00	20.00	4.00	12.00	20.00	28.00	4.00	12.00	8.00	4.00
.4	4.00													
.8	3.98	4.00												
1.2	3.95	3.99												
.6	3.85	3.98		4.00										
2.0	3.61	3.96		3.99										
.2	3.40	3.94	12.00	3.99										
.4	3.10	3.91	11.99	3.98	12.00		4.00							
.6	2.71	3.88	11.97	3.98	11.99		3.99							
.8	2.24	3.85	11.92	3.97	11.98		3.99	12.00						
3.0	1.71	3.83	11.83	3.96	11.96		3.99	11.99						
.2	1.18	3.81	11.64	3.96	11.92	20.00	3.99	11.98						
.4	0.72	3.81	11.28	3.96	11.84	19.99	3.99	11.96				12.00		
.6	.37	3.79	10.65	3.96	11.71	19.98	3.99	11.93	20.00			11.99		
.8	.16	3.68	9.61	3.93	11.52	19.94	3.98	11.89	19.99			11.99		
4.0	.05	3.39	8.13	3.86	11.29	19.84	3.97	11.85	19.97		4.00	11.98		
.1	.02	3.15	7.12	3.82	11.18	19.74	3.96	11.83	19.95		3.99	11.98		
.2	.01	2.85	6.23	3.77	11.10	19.59	3.95	11.81	19.91		3.99	11.98		
.3		2.45	5.20	3.72	11.04	19.37	3.94	11.80	19.87		3.99	11.98		
.4		2.08	4.18	3.68	11.01	19.03	3.93	11.80	19.80	28.00	3.99	11.98	8.00	
.5		1.66	3.21	3.66	11.01	18.56	3.92	11.80	19.71	27.99	3.99	11.98	7.99	
.6		1.27	2.35	3.65	11.00	17.90	3.92	11.79	19.58	27.99	3.99	11.98	7.99	
.7		0.90	1.63	3.65	10.95	17.02	3.92	11.77	19.43	27.98	3.99	11.97	7.99	
.8		.60	1.05	3.63	10.79	15.90	3.92	11.72	19.25	27.96	3.99	11.96	7.99	
.9		.37	0.63	3.58	10.46	14.53	3.90	11.63	19.05	27.93	3.98	11.95	7.98	
5.0		.21	.35	3.46	9.87	12.93	3.86	11.50	18.86	27.87	3.98	11.93	7.98	
.1		.11	.18	3.23	9.00	11.11	3.80	11.33	18.68	27.78	3.97	11.91	7.98	
.2		.06	.08	2.88	7.86	9.19	3.74	11.16	18.56	27.63	3.96	11.89	7.97	
.3		.02	.03	2.44	6.52	7.27	3.67	11.01	18.49	27.40	3.95	11.87	7.97	
.4			.01	1.94	5.10	5.46	3.63	10.92	18.47	27.05	3.94	11.86	7.97	
.5				1.43	3.71	3.86	3.61	10.90	18.46	26.55	3.94	11.86	7.97	
.6				0.97	2.49	2.56	3.61	10.89	18.38	25.84	3.94	11.86	7.97	4.00
.7				.60	1.53	1.57	3.59	10.81	18.10	24.89	3.93	11.84	7.96	3.99
.8				.34	0.84	0.88	3.51	10.54	17.50	23.67	3.92	11.79	7.95	3.99
.9				.17	.41	.44	3.32	9.96	16.48	22.16	3.88	11.70	7.93	3.99
6.0				.07	.17	.20	3.00	9.02	15.01	20.38	3.83	11.58	7.91	3.99
.1				.02	.06	.07	2.54	7.74	13.12	18.35	3.77	11.44	7.88	3.99
.2				.01	.02	.02	2.01	6.23	10.93	16.16	3.73	11.35	7.85	3.98
.3							1.47	4.68	8.64	13.87	3.71	11.29	7.83	3.98
.4							0.98	3.25	6.45	11.59	3.71	11.27	7.82	3.98
.5							.60	2.08	4.52	9.39	3.70	11.27	7.82	3.98
.6							.33	1.22	2.96	7.37	3.65	11.18	7.82	3.98
.7							.16	0.65	1.80	5.57	3.50	10.92	7.80	3.96
.8							.07	.31	1.00	4.06	3.22	10.37	7.75	3.95
.9							.02	.14	0.49	2.83	2.83	9.51	7.64	3.92
7.0							.01	.05	.20	1.89	2.34	8.34	7.45	3.90
.1								.02	.08	1.19	1.81	6.94	7.16	3.88
.2									.02	0.72	1.31	5.45	6.76	3.87
.3										.41	0.87	4.02	6.15	3.87
.4										.22	.54	2.77	5.68	3.87
.5										.11	.31	1.77	5.02	3.85
.6										.04	.16	1.04	4.32	3.80
.7										.01	.08	0.56	3.60	3.70
.8											.03	.29	2.91	3.53
.9											.01	.13	2.26	3.28
8.0												.05	1.70	2.96
.1												.01	1.22	2.57
.2													0.84	2.13
.3													.55	1.69
.4													.34	1.27
.5													.19	0.90
.6													.10	.59
.7													.04	.36
.8													.02	.20
.9														.04
9.0														.01

for the inner electrons.

Tables of total $2Z_p$ and the values of ϵ, $\int_0^r P^2 dr$, and $2v_0$ are also given. The maximum discrepancy between final estimates and final values of the total $2Z_p$ does not exceed 0.10. The last figure of ϵ has significance only as indicating the resolving power of the method of computation. The last figure in the other quantities is also uncertain.

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