

# Thomas-Fermi Model of Compressed Atoms

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$S(\pi k)$  and  $C(\pi k)$  by their limiting form for large  $k$ ,  $\frac{1}{2}$ , which yields the asymptotic formula:

$$\lambda_k' = (\pi^2 k^3/2)(1 - 1/2\pi k). \quad (8)$$

The first-order formula for the Fourier coefficients is

$${}^k a_m = G_m {}^k a_k / (G_m - \lambda_k'). \quad (9)$$

The value of  ${}^k a_k$  is to be determined by the normalization requirement that the integral of  $\alpha_k^2(r)$  is to be unity; in fact  ${}^k a_k$  is within a few percent of unity for all cases except  ${}^0 a_0$ , which is  $(1/2)^{\frac{1}{2}}$ . At large values of  $m$ ,  ${}^k a_m$  varies as  $(-1)^{(m-k+2)/2} m^{-3}$ , so that the series and its first and second derivatives are obviously convergent.

The quantities  $\mu_k$  are defined in terms of  $\alpha_k(r)$  and a constant,  $N$ , by the two equivalent formulas:

$$\mu_k = -(4/N^2) \int_{-1}^1 \alpha_k''(r) \alpha_k(r) dr, \quad (10a)$$

$$= (4/N^2) \int_{-1}^1 [\alpha'(r)]^2 dr. \quad (10b)$$

A result valid within one percent is

$$\mu_k = \pi^2 k^2 / N^2. \quad (11)$$

We have also used an expansion in associated Legendre polynomials,  $P_m^2(r)$ , instead of a Fourier series. The resulting matrix seems to be even more nearly diagonal than the Fourier matrix, but it is more laborious to construct since the necessary integrals are not tabulated but must be computed individually. The first and third eigenvalues, using only two terms in the series of polynomials, are found to be  $\lambda_1 = 4.034$  and  $\lambda_3 = 25.18$ , in reasonable agreement with the Fourier results.

Another interesting observation is that a variation procedure may be applied, as with a Sturm-Liouville problem, and the eigenvalues shown to be stationary values of the quantity:

$$\int_{-1}^1 \int_{-1}^1 \frac{\alpha''(r) \alpha''(s) dr ds}{(|r-s|)^{\frac{1}{2}}} / \int_{-1}^1 [\alpha'(r)]^2 dr. \quad (12)$$

The lowest eigenvalues,  $\lambda_0$  and  $\lambda_1$ , are minima of the quantity (12) for the classes of even functions and odd functions respectively. Equation (12) with a fifth degree polynomial as the trial function gives  $\lambda_1 = 4.034$ .

We wish to acknowledge the valuable aid of Miss Virginia G. Thomas and Miss Nancy E. French in carrying out the computations.

## Thomas-Fermi Model of Compressed Atoms

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Solutions of the zero-temperature Thomas-Fermi equation for an atomic system have been obtained by numerical integration with the aid of the IBM 701 Defense Calculator. The complete range of atomic volumes of physical interest has been covered in sufficient detail to permit accurate interpolation to intermediate regions. Tables of the potential distributions are given as well as of the important physical properties.

### I. INTRODUCTION

THE statistical model of Thomas and Fermi has provided an important means for obtaining qualitative as well as semiquantitative estimates of atomic behavior. While the model is a considerable simplification of the more rigorous quantum-mechanical methods, it still suffers from the difficulty of being unamenable to analytic treatment. To obtain information from the Thomas-Fermi model, it has been necessary to resort to numerical methods. Since accurate numerical solutions of the Thomas-Fermi equation involve lengthy integrations, not many solutions have been available in the past. Miranda<sup>1</sup> has reported the solution for the infinite atom; for the case of compressed states of the atom, a few numerical solutions have been reported by Slater and Krutter,<sup>2</sup> by Feynman, Metrop-

olis, and Teller,<sup>3</sup> and by March.<sup>4</sup> These results have been extended to greater detail and with improved accuracy in the present calculations, which consist of sixty-three solutions covering a range of  $ZV$  from  $7.02 \times 10^{-30} \text{ cm}^3$  to  $1.29 \times 10^{-14} \text{ cm}^3$ , where  $Z$  is the atomic number and  $V$  the atomic volume. All physical properties of interest, as well as the potential functions themselves, are presented here. The data may be interpolated directly to provide accurate intermediate values if required.

### II. METHOD OF SOLUTION OF THE THOMAS-FERMI EQUATION

The derivation of the Thomas-Fermi equation for an atomic system starts from the Poisson equation

$$\nabla^2 V(r) = 4\pi e \rho(r) \quad (1)$$

<sup>1</sup> C. Miranda, *Reale Accad. Ital.* **5**, 285 (1934).

<sup>2</sup> J. C. Slater and H. M. Krutter, *Phys. Rev.* **47**, 559 (1935).

<sup>3</sup> Feynman, Metropolis, and Teller, *Phys. Rev.* **75**, 1561 (1949).

<sup>4</sup> N. H. March, *Proc. Cambridge Phil. Soc.* **48**, 665 (1952).

connecting the electrostatic potential distribution  $V(r)$  with the charge density  $-\epsilon\rho(r)$  within the atom. The assumptions of the model lead to an approximate relationship between  $\rho(r)$  and  $V(r)$ . A number of independent derivations of this relationship have been given<sup>5</sup> and lead to the result

$$\rho(r) = \frac{8\pi}{3h^3} [2m(eV(r) + \alpha)]^{\frac{3}{2}}. \quad (2)$$

Combination of Eqs. (1) and (2) yields the basic differential equation of the model,

$$\psi''(w) = aw \left( \frac{\psi(w)}{w} \right)^{\frac{3}{2}}, \quad (3)$$

where

$$\begin{aligned} w &= r/r_0, \\ \psi(w) &= \frac{eV(r) + \alpha}{\alpha}, \\ a &= \left( \frac{r_0}{\mu} \right)^{\frac{3}{2}} \left( \frac{r_0 \alpha}{Ze^2} \right)^{\frac{1}{2}}, \\ \mu &= \left( \frac{9\pi^2}{128Z} \right)^{\frac{1}{3}} a_0, \end{aligned}$$

$r_0$  is the radius of the atom,  $\alpha$  the work function, and  $a_0$  the Bohr radius. The boundary conditions which Eq. (3) must meet are  $\psi(1)=1$ , which results from the choice of the zero of the potential at  $r=r_0$ , and  $\psi'(1)=\psi'(0)$ , which is equivalent to zero electric field at  $r=r_0$ , as follows from the electric neutrality of the atom. The singularity of the electrostatic potential  $V(r)$  at the nucleus,  $r=0$ , leads to the relationship

$$\psi(0) = \frac{Ze^2}{r_0 \alpha}. \quad (4)$$

It is readily seen that the boundary conditions do not distinguish different atomic states. These latter are determined by the value of the single parameter  $a$ . Thus the Thomas-Fermi equation admits of only a one-parameter set of states for atoms at zero temperature. This set of states is seen to be characterized simply by the physical parameter  $Z^{\frac{1}{3}}r_0$ , since for each choice of  $a$  there is a unique value for  $\psi(0)$ ; and  $a$  and  $\psi(0)$  together determine uniquely a value for  $Z^{\frac{1}{3}}r_0$ . It is inconvenient, however, that in solving Eq. (3) it is not possible to decide beforehand on a value of  $Z^{\frac{1}{3}}r_0$  and from that to determine the parameter  $a$  and hence the appropriate solution  $\psi(x)$ . Rather the value of  $Z^{\frac{1}{3}}r_0$  is determined only after finding  $\psi(0)$  which, of course, necessitates integrating Eq. (3). It is this fact which makes it important to have a large number of solutions of Eq. (3), sufficiently extensive so as to enable accurate

interpolation for those values of the parameter  $a$  which correspond to the prescribed atomic state  $Z^{\frac{1}{3}}r_0$ .

Besides the function  $\psi(w)$  which determines the potential and charge distributions within the atom, a number of additional physical properties of the Thomas-Fermi model have important physical applications. These may be expressed in terms of  $a$  and  $\psi(w)$  through the following easily derived relations:

$$Z^{\frac{1}{3}}r_0 = (Z^{\frac{1}{3}}\mu) a^{\frac{1}{2}} \psi^{\frac{1}{2}}(0), \quad (5)$$

$$ZV = -\frac{4\pi}{3} (Z^{\frac{1}{3}}\mu)^3 a^2 \psi(0), \quad (6)$$

$$\frac{\alpha}{Z^{4/3}} = \frac{e^2}{Z^{\frac{1}{3}}\mu} \frac{1}{a^{\frac{1}{2}} \psi^{1/2}(0)}, \quad (7)$$

$$\frac{P}{Z^{10/3}} = \frac{1}{10\pi} \frac{e^2}{(Z^{\frac{1}{3}}\mu)^4} \frac{1}{a^{5/3} \psi^{10/3}(0)}, \quad (8)$$

$$\begin{aligned} -\frac{E_{\text{potential}}}{Z^{7/3}} &= \frac{e^2 a^{\frac{1}{2}}}{Z^{\frac{1}{3}}\mu \psi^{7/3}(0)} \\ &\quad \times \frac{1}{2} \int_0^1 dw \frac{\psi^{\frac{3}{2}}(w)}{w^{\frac{1}{2}}} [\psi(w) - w + \psi(0)], \quad (9) \end{aligned}$$

$$\frac{E_{\text{kinetic}}}{Z^{7/3}} = -\frac{3}{2} \frac{PV}{Z^{7/3}} - \frac{1}{2} \frac{E_{\text{potential}}}{Z^{7/3}}, \quad (10)$$

$$\frac{E_{\text{total}}}{Z^{7/3}} = -\frac{3}{2} \frac{PV}{Z^{7/3}} + \frac{1}{2} \frac{E_{\text{potential}}}{Z^{7/3}}. \quad (11)$$

Equations (10) and (11) constitute a statement of the virial theorem. From these properties one has a complete description of the equation of state of an atomic system.

Returning to the determination of the solutions  $\psi(w)$ , it has been found that the numerical solution of Eq. (3) was simplified by converting it into an integral equation. Thus after a double integration and an integration by parts, Eq. (1) may be written as

$$\phi(x) = x^2 + 2a \int_x^1 dy (y^2 - x^2) \phi^{\frac{3}{2}}(y) \quad (12)$$

where  $\phi(x) = \psi(w)$  and the quadratic change of variable  $w = x^2$ , which has been found convenient in previous numerical work, has been made. The boundary conditions for  $\phi(x)$  are inherent in this form of the equation. In the numerical treatment, the integral of Eq. (12) is approximated by a sum in accordance with Simpson's rule. The integration of the resultant difference equation is initiated by a series expansion for  $\phi(x)$  valid in the neighborhood of  $x=1$ , namely,

$$\phi(x) = x^2 + a \sum_{k=0}^3 A_k \left[ \frac{(1-x^2)^{k+2}}{(k+1)(k+2)} - \frac{(1-x^2)^{k+3}}{(k+2)(k+3)} \right] \quad (13)$$

where  $A_0 = 1$ ,  $A_1 = 0$ ,  $A_2 = \frac{3}{4}a$  and  $A_3 = \frac{1}{2}a$ .

<sup>5</sup> L. H. Thomas, Proc. Cambridge Phil. Soc. **23**, 542 (1926).  
E. Fermi, Rend. Lincei **6**, 602 (1927); Z. Physik **48**, 73 (1928).  
L. Brillouin, Actualités sci. et ind. **160** (Hermann et Cie, 1934).

TABLE I.<sup>a</sup>

a	.0365	.0458	.0578	.0720	.0910	.1130	.1430	.1780	.2230
$2^7x$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$
0	.12234 (-1)	.15373 (-1)	.19436 (-1)	.24264 (-1)	.30757 (-1)	.38323 (-1)	.48724 (-1)	.60985 (-1)	.76952 (-1)
1	.12294	.15432	.19495	.24323	.30815	.38380	.48781	.61040	.77005
2	.12473	.15611	.19673	.24499	.30989	.38552	.48950	.61206	.77166
3	.12773	.15909	.19969	.24793	.31280	.38839	.49232	.61482	.77434
4	.13192	.16327	.20384	.25204	.31687	.39241	.49627	.61868	.77809
5	.13732	.16863	.20917	.25733	.32210	.39758	.50134	.62365	.78291
6	.14390	.17519	.21568	.26380	.32850	.40390	.50755	.62972	.78880
7	.15169	.18294	.22338	.27144	.33606	.41136	.51488	.63689	.79576
8	.16068	.19188	.23227	.28025	.34479	.41998	.52334	.64517	.80380
9	.17086	.20201	.24234	.29025	.35467	.42974	.53294	.65455	.81291
10	.18224	.21334	.25359	.30141	.36572	.44065	.54365	.66504	.82309
11	.19482	.22586	.26603	.31376	.37794	.45271	.55550	.67664	.83434
12	.20860	.23957	.27965	.32727	.39131	.46592	.56848	.68933	.84667
13	.22358	.25447	.29446	.34197	.40585	.48028	.58258	.70314	.86007
14	.23975	.27057	.31046	.35784	.42156	.49579	.59782	.71804	.87454
15	.25713	.28786	.32763	.37488	.43842	.51245	.61418	.73406	.89009
16	.27570	.30634	.34600	.39311	.45645	.53025	.63168	.75117	.90671
17	.29547	.32601	.36554	.41250	.47565	.54921	.65030	.76940	.92440
18	.31643	.34687	.38627	.43308	.49600	.56931	.67005	.78873	.94317
19	.33860	.36893	.40819	.45483	.51753	.59056	.69093	.80916	.96301
20	.36196	.39218	.43129	.47775	.54021	.61297	.71294	.83070	.98393
21	.38653	.41662	.45558	.50185	.56406	.63652	.73608	.85335	.10059 (o)
22	.41229	.44226	.48105	.52713	.58907	.66122	.76035	.87711	.10290
23	.43925	.46909	.50771	.55358	.61525	.68707	.78575	.90197	.10531
24	.46740	.49711	.53555	.58121	.64259	.71407	.81228	.92794	.10784
25	.49676	.52632	.56458	.61001	.67109	.74223	.83994	.95501	.11047
26	.52731	.55672	.59479	.63999	.70076	.77153	.86874	.98319	.11320
27	.55906	.58832	.62619	.67115	.73159	.80198	.89866	.10125 (o)	.11605
28	.59201	.62111	.65877	.70349	.76359	.83358	.92971	.10429	.11900
29	.62616	.65510	.69253	.73700	.79675	.86634	.96190	.10744	.12206
30	.66151	.69027	.72749	.77168	.83108	.90024	.99522	.11070	.12523
31	.69806	.72664	.76363	.80755	.86657	.93530	.10297 (o)	.11407	.12851
32	.73580	.76420	.80095	.84459	.90323	.97150	.10652	.11756	.13190
33	.77463	.80285	.83904	.88277	.94102 (o)	.10070 (o)	.11788	.12868	.13620
34	.81455	.84257	.87861	.92231	.98056 (o)	.10470 (o)	.12572	.13661	.14506
35	.85558	.88332	.91924	.96294	.10260 (o)	.10870 (o)	.12788	.13874	.14729
36	.89773	.92518	.96094	.10045	.10655 (o)	.11265 (o)	.12902	.14087	.14942
37	.94099	.96815	.10036	.10445	.11055 (o)	.11665 (o)	.13302	.14487	.15342
38	.98536	.10118	.10424	.10833	.11443 (o)	.12053 (o)	.13690	.14875	.15730
39	.10307	.10593	.10899	.11308	.11918 (o)	.12528 (o)	.14165	.15350	.16205
40	.10790	.11076	.11382	.11791	.12401 (o)	.13011 (o)	.14648	.15833	.16688
41	.11283	.11569	.11875	.12284	.12894 (o)	.13504 (o)	.15141	.16326	.17181
42	.11786	.12072	.12378	.12787	.13397 (o)	.14007 (o)	.15644	.16829	.17684
43	.12299	.12585	.12891	.13300	.13910 (o)	.14520 (o)	.16157	.17342	.18197
44	.12822	.13108	.13414	.13823	.14433 (o)	.15043 (o)	.16680	.17865	.18720
45	.13355	.13641	.13947	.14356	.14966 (o)	.15576 (o)	.17213	.18398	.19253
46	.13898	.14184	.14490	.14899	.15509 (o)	.16119 (o)	.17756	.18941	.19796
47	.14451	.14737	.15043	.15452	.16062 (o)	.16672 (o)	.18309	.19494	.20349
48	.15014	.15299	.15605	.16014	.16624 (o)	.17234 (o)	.18871	.20056	.20911
49	.15587	.15873	.16179	.16588	.17198 (o)	.17808 (o)	.19445	.20630	.21485
50	.16170	.16456	.16762	.17171	.17781 (o)	.18391 (o)	.20028	.21213	.22068
51	.16763	.17049	.17355	.17764	.18374 (o)	.18984 (o)	.20621	.21806	.22661
52	.17366	.17652	.17958	.18367	.18977 (o)	.19587 (o)	.21224	.22409	.23264
53	.17979	.18265	.18571	.18980	.19590 (o)	.20200 (o)	.21837	.23022	.23877
54	.18592	.18878	.19184	.19593	.20203 (o)	.20813 (o)	.22450	.23635	.24490
55	.19215	.19501	.19807	.20216	.20826 (o)	.21436 (o)	.23073	.24258	.25113
56	.19848	.20134	.20440	.20849	.21459 (o)	.22069 (o)	.23706	.24891	.25746
57	.20491	.20777	.21083	.21492	.22102 (o)	.22712 (o)	.24349	.25534	.26389
58	.21144	.21430	.21736	.22145	.22755 (o)	.23365 (o)	.24992	.26177	.27032
59	.21807	.22093	.22400	.22809	.23419 (o)	.24029 (o)	.25656	.26841	.27696
60	.22480	.22766	.23072	.23481	.24091 (o)	.24701 (o)	.26328	.27513	.28368
61	.23163	.23449	.23755	.24164	.24774 (o)	.25384 (o)	.27011	.28196	.29051
62	.23856	.24142	.24448	.24857	.25467 (o)	.26077 (o)	.27704	.28889	.29744
63	.24559	.24845	.25151	.25560	.26170 (o)	.26780 (o)	.28407	.29592	.30447
64	.25272	.25558	.25864	.26273	.26883 (o)	.27493 (o)	.29120	.30305	.31160
65	.25995	.26281	.26587	.26996	.27606 (o)	.28216 (o)	.29843	.31028	.31883
66	.26728	.27014	.27320	.27729	.28339 (o)	.28949 (o)	.30576	.31761	.32616
67	.27471	.27757	.28063	.28472	.29082 (o)	.29692 (o)	.31319	.32504	.33359
68	.28224	.28510	.28816	.29225	.29835 (o)	.30445 (o)	.32072	.33257	.34112
69	.28987	.29273	.29579	.29988	.30598 (o)	.31208 (o)	.32835	.34020	.34875
70	.29760	.30046	.30352	.30761	.31371 (o)	.31981 (o)	.33608	.34793	.35648
71	.30543	.30829	.31135	.31544	.32154 (o)	.32764 (o)	.34391	.35576	.36431
72	.31336	.31622	.31928	.32337	.32947 (o)	.33557 (o)	.35184	.36369	.37224
73	.32139	.32425	.32731	.33140	.33750 (o)	.34360 (o)	.35987	.37172	.38027
74	.32952	.33238	.33544	.33953	.34563 (o)	.35173 (o)	.36800	.37985	.38840
75	.33775	.34061	.34367	.34776	.35386 (o)	.35996 (o)	.37623	.38808	.39663
76	.34608	.34894	.35200	.35609	.36219 (o)	.36829 (o)	.38456	.39641	.40496
77	.35451	.35737	.36043	.36452	.37062 (o)	.37672 (o)	.39299	.40484	.41339
78	.36304	.36590	.36896	.37305	.37915 (o)	.38525 (o)	.40152	.41337	.42192
79	.37167	.37453	.37759	.38168	.38778 (o)	.39388 (o)	.41015	.42200	.43055
80	.38040	.38326	.38632	.39041	.39651 (o)	.40261 (o)	.41888	.43073	.43928
81	.38923	.39209	.39515	.39924	.40534 (o)	.41144 (o)	.42771	.43956	.44811
82	.39816	.40102	.40408	.40817	.41427 (o)	.42037 (o)	.43664	.44849	.45704
83	.40719	.41005	.41311	.41720	.42330 (o)	.42940 (o)	.44567	.45752	.46607
84	.41632	.41918	.42224	.42633	.43243 (o)	.43853 (o)	.45480	.46665	.47520
85	.42555	.42841	.43147	.43556	.44166 (o)	.44776 (o)	.46403	.47588	.48443
86	.43488	.43774	.44080	.44489	.45099 (o)	.45709 (o)	.47336	.48521	.49376
87	.44431	.44717	.45023	.45432	.46042 (o)	.46652 (o)	.48279	.49464	.50319
88	.45384	.45670	.45976	.46385	.46995 (o)	.47605 (o)	.49232	.50417	.51272
89	.46347	.46633	.46939	.47348	.47958 (o)	.48568 (o)	.50195	.51380	.52235
90	.47320	.47606	.47912	.48321	.48931 (o)	.49541 (o)	.51168	.52353	.53208
91	.48303	.48589	.48895	.49304	.49914 (o)	.50524 (o)	.52151	.53336	.54191
92	.49296	.49582	.49888	.50297	.50907 (o)	.51517 (o)	.53144	.54329	.55184
93	.50300	.50586	.50892	.51301	.51911 (o)	.52521 (o)	.54148	.55333	.56188
94	.51313	.51599	.51905	.52314	.52924 (o)	.53534 (o)	.55161	.56346	.57201
95	.52336	.52622	.52928	.53337	.53947 (o)	.54557 (o)	.56184	.57369	.58224
96	.53369	.53655	.53961	.54370	.54980 (o)	.55590 (o)	.57217	.58402	.59257
97	.54402	.54688	.54994	.55403	.56013 (o)	.56623 (o)	.58250	.59435	.60290
98	.55445	.55731	.56037	.56446	.57056 (o)	.57666 (o)	.59293	.60478	.61333
99	.56498	.56784	.57090	.57500	.58110 (o)	.58720 (o)	.60347	.61532	.62387
100	.57561	.57847	.58153	.58562	.59172 (o)	.59782 (o)	.61409	.62594	.63449
101	.58634	.58920	.59226	.59635	.60245 (o)	.60855 (o)	.62482	.63667	.64522
102	.59717	.60003	.60309	.60718	.61328 (o)	.61938 (o)	.63565	.64750	.65605
103	.60800	.61086	.61392	.61801	.62411 (o)	.63021 (o)	.64648	.65833	.66688
104	.61893	.62179	.62485	.62894	.63504 (o)	.64114 (o)	.65741	.66926	.67781
105	.62996	.63282	.63588	.64000	.64610 (o)	.65220 (o)	.66847	.68032	.68887
106	.64109	.64395	.64701	.65110	.65720 (o)	.66330 (o)	.67957	.69142	.69997
107	.65232	.65518	.65824	.66233	.66843 (o)	.67453 (o)	.69080	.70265	.71120
108	.66365	.66651	.66957	.67366	.67976 (o)	.68586 (o)	.70213	.71398	.72253
109	.67508	.67794	.68100	.68509	.69119 (o)	.69729 (o)	.71356	.72541	.73396
110	.68661	.68947	.69253	.69662	.70272 (o)	.70882 (o)	.72509	.73694	.74549
111	.69824	.70110	.70416	.70825	.71435 (o)	.72045 (o)	.73672	.74857	.75712
112	.71007	.71293	.71600	.72009	.72619 (o)	.73229 (o)	.74856	.76041	.76896
113	.72200	.72486	.72792	.73201	.73811 (o)	.74421 (o)	.76048	.77233	.78088
114	.73403	.73689	.73995	.74404	.75014 (o)</				

TABLE I.—Continued.

a	.2800	.3460	.4300	.5380	.6800	.8500	1.070	1.320	1.470
$2^7x$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$
0	.97514 (-1)	.12181 (0)	.15352 (0)	.19564 (0)	.25349 (0)	.32672 (0)	.42854 (0)	.55498 (0)	.63692 (0)
1	.97565	.12186	.15356	.19568	.25352	.32675	.42854	.55496	.63688
2	.97719	.12200	.15370	.19580	.25362	.32681	.42856	.55490	.63677
3	.97976	.12225	.15392	.19600	.25378	.32692	.42858	.55481	.63659
4	.98336	.12259	.15424	.19628	.25401	.32707	.42862	.55467	.63634
5	.98798	.12303	.15464	.19664	.25430	.32726	.42866	.55451	.63602
6	.99364	.12356	.15514	.19708	.25466	.32751	.42872	.55432	.63565
7	.10003 (0)	.12420	.15573	.19760	.25508	.32779	.42880	.55410	.63521
8	.10080	.12493	.15640	.19820	.25557	.32813	.42889	.55385	.63472
9	.10168	.12576	.15717	.19888	.25612	.32851	.42900	.55358	.63418
10	.10265	.12669	.15803	.19965	.25675	.32894	.42913	.55328	.63358
11	.10374	.12771	.15898	.20049	.25744	.32941	.42928	.55297	.63294
12	.10492	.12883	.16002	.20142	.25820	.32994	.42945	.55264	.63225
13	.10621	.13006	.16116	.20243	.25902	.33052	.42963	.55229	.63152
14	.10760	.13138	.16238	.20352	.25992	.33114	.42985	.55193	.63076
15	.10909	.13249	.16370	.20469	.26088	.33182	.43008	.55155	.62995
16	.11068	.13341	.16510	.20595	.26191	.33255	.43035	.55117	.62911
17	.11238	.13592	.16660	.20729	.26302	.33333	.43063	.55078	.62824
18	.11419	.13764	.16819	.20871	.26419	.33416	.43095	.55038	.62734
19	.11609	.13945	.16988	.21021	.26543	.33505	.43129	.54998	.62642
20	.11810	.14136	.17165	.21180	.26675	.33599	.43167	.54958	.62547
21	.12022	.14337	.17352	.21347	.26813	.33698	.43207	.54918	.62450
22	.12243	.14547	.17548	.21522	.26958	.33803	.43251	.54878	.62352
23	.12475	.14768	.17753	.21706	.27111	.33914	.43298	.54838	.62252
24	.12718	.14999	.17967	.21898	.27271	.34030	.43349	.54799	.62150
25	.12971	.15239	.18191	.22099	.27438	.34152	.43403	.54761	.62048
26	.13234	.15489	.18424	.22308	.27613	.34280	.43461	.54724	.61946
27	.13507	.15750	.18667	.22526	.27795	.34414	.43522	.54689	.61842
28	.13791	.16020	.18918	.22752	.27984	.34553	.43588	.54654	.61739
29	.14086	.16300	.19179	.22986	.28181	.34699	.43658	.54622	.61636
30	.14390	.16590	.19450	.23230	.28385	.34851	.43732	.54591	.61533
31	.14706	.16890	.19729	.23481	.28596	.35009	.43810	.54562	.61431
32	.15031	.17200	.20019	.23742	.28816	.35173	.43892	.54536	.61329
35	.16071	.18190	.20943	.24575	.29519	.35704	.44168	.54472	.61033
39	.17604	.19651	.22308	.25809	.30566	.36503	.44605	.54431	.60667
43	.19305	.21274	.23826	.27185	.31740	.37413	.45129	.54451	.60348
47	.21175	.23059	.25499	.28705	.33046	.38438	.45748	.54546	.60092
51	.23215	.25009	.27329	.30374	.34487	.39584	.46473	.54729	.59916
55	.25427	.27125	.29318	.32193	.36068	.40858	.47311	.55014	.59836
59	.27813	.29410	.31470	.34166	.37794	.42267	.48273	.55414	.59868
63	.30373	.31865	.33787	.36298	.39671	.43818	.49369	.55943	.60029
67	.33111	.34493	.36272	.38593	.41704	.45520	.50611	.56616	.60336
71	.36028	.37298	.38930	.41056	.43901	.47382	.52011	.57449	.60807
75	.39128	.40283	.41765	.43694	.46270	.49413	.53581	.58459	.61461
79	.42414	.43452	.44784	.46513	.48818	.51625	.55336	.59663	.62317
83	.45890	.46811	.47990	.49521	.51557	.54030	.57291	.61079	.63396
87	.49560	.50364	.51393	.52726	.54496	.56642	.59462	.62729	.64722
91	.53430	.54118	.54998	.56137	.57647	.59474	.61870	.64635	.66317
95	.57504	.58080	.58816	.59766	.61025	.62515	.64533	.66822	.68210
99	.61790	.62257	.62855	.63625	.64644	.65873	.67476	.69316	.70430
103	.66294	.66660	.67126	.67728	.68522	.69478	.70722	.72148	.73009
107	.71026	.71297	.71643	.72089	.72677	.73383	.74130	.75351	.75984
111	.75993	.76180	.76418	.76725	.77130	.77615	.78245	.78964	.79397
115	.81207	.81322	.81468	.81657	.81906	.82203	.82590	.83029	.83294
119	.86678	.86736	.86810	.86905	.87030	.87180	.87375	.87596	.87728
123	.92420	.92439	.92463	.92494	.92535	.92583	.92646	.92718	.92761
127	.98447	.98448	.98449	.98450	.98452	.98454	.98456	.98460	.98461
128	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)

other limit to approximately a uniform electron gas.<sup>6</sup> Table I contains these solutions from which the cor-

<sup>6</sup> This limit is determined by Eqs. (5)–(11) with  $\phi(0) = a/3$  and Eq. (9) made to read

$$-E_{\text{potential}} = \frac{Ze^2}{\mu} \frac{a^{1/3}}{\phi^{7/3}(0)} \frac{1}{4} \frac{a}{15} + \phi(0).$$

The definition of  $a$  is as given after Eq. (3).

responding electrostatic potential and charge distributions can be derived with the help of Eqs. (2) and (3). In Table II the physical quantities of Eqs. (5)–(11) are shown for each value of  $a$  for which the corresponding solution is given in Table I. The quantity  $\Delta E$  denotes the difference between  $E$ , the energy under the condi-

a	1.630	1.820	2.010	2.220	2.450	2.690	2.950	3.250	3.520
2 <sup>7</sup> x	φ(x)	φ(x)	φ(x)	φ(x)	φ(x)	φ(x)	φ(x)	φ(x)	φ(x)
0	.72982 (0)	.84813 (0)	.97592 (0)	.11293 (1)	.13134 (1)	.15257 (1)	.17819 (1)	.21160 (1)	.24572 (1)
1	.72976	.84804	.97579	.11291	.13132	.15254	.17815	.21154	.24565
2	.72958	.84778	.97543	.11286	.13125	.15245	.17803	.21138	.24544
3	.72930	.84734	.97482	.11278	.13114	.15230	.17783	.21111	.24509
4	.72890	.84675	.97399	.11266	.13098	.15210	.17755	.21074	.24461
5	.72840	.84599	.97293	.11252	.13079	.15183	.17721	.21027	.24400
6	.72780	.84509	.97167	.11235	.13055	.15152	.17679	.20970	.24327
7	.72711	.84403	.97019	.11214	.13028	.15116	.17631	.20905	.24243
8	.72632	.84284	.96852	.11191	.12997	.15074	.17576	.20831	.24148
9	.72545	.84150	.96665	.11166	.12962	.15028	.17515	.20749	.24042
10	.72448	.84004	.96460	.11137	.12924	.14978	.17448	.20659	.23926
11	.72344	.83845	.96237	.11107	.12883	.14923	.17375	.20561	.23800
12	.72232	.83674	.95996	.11074	.12839	.14864	.17297	.20456	.23666
13	.72113	.83491	.95740	.11039	.12790	.14801	.17214	.20344	.23522
14	.71987	.83298	.95468	.11001	.12740	.14734	.17126	.20226	.23371
15	.71854	.83093	.95181	.10962	.12687	.14663	.17033	.20102	.23212
16	.71715	.82879	.94879	.10921	.12631	.14589	.16936	.19971	.23045
17	.71570	.82655	.94564	.10877	.12572	.14512	.16834	.19836	.22871
18	.71420	.82422	.94236	.10832	.12512	.14432	.16729	.19695	.22692
19	.71264	.82181	.93896	.10786	.12448	.14349	.16619	.19549	.22506
20	.71104	.81932	.93544	.10737	.12383	.14263	.16507	.19398	.22314
21	.70939	.81675	.93181	.10687	.12316	.14174	.16390	.19243	.22117
22	.70770	.81411	.92808	.10636	.12247	.14083	.16271	.19084	.21915
23	.70598	.81141	.92426	.10584	.12176	.13990	.16149	.18922	.21709
24	.70422	.80865	.92034	.10530	.12103	.13894	.16024	.18756	.21499
25	.70243	.80583	.91634	.10475	.12029	.13796	.15896	.18587	.21285
26	.70062	.80296	.91226	.10419	.11954	.13697	.15766	.18415	.21067
27	.69879	.80004	.90811	.10361	.11877	.13596	.15634	.18240	.20847
28	.69693	.79708	.90390	.10303	.11799	.13493	.15500	.18063	.20624
29	.69506	.79409	.89962	.10245	.11719	.13389	.15365	.17884	.20398
30	.69317	.79106	.89529	.10185	.11639	.13284	.15227	.17703	.20170
31	.69128	.78800	.89092	.10125	.11557	.13177	.15089	.17520	.19940
32	.68938	.78492	.88650	.10064	.11475	.13069	.14949	.17336	.19709
35	.68368	.77558	.87305	.98776 (0)	.11225	.12741	.14522	.16677	.19008
39	.67620	.76306	.85487	.96253	.10885	.12296	.13946	.16023	.18066
43	.66905	.75070	.83671	.93720	.10543	.11848	.13368	.15269	.17130
47	.66242	.73875	.81889	.91216	.10203	.11405	.12796	.14527	.16210
51	.65651	.72748	.80171	.88778	.98719 (0)	.10971	.12237	.13803	.15318
55	.65153	.71710	.78546	.86441	.95522	.10551	.11696	.13106	.14460
59	.64766	.70787	.77041	.84238	.92481	.10151	.11180	.12440	.13644
63	.64509	.70000	.75684	.82200	.89632	.97733 (0)	.10693	.11812	.12875
67	.64404	.69374	.74500	.80356	.87008	.94227	.10238	.11225	.12158
71	.64469	.68930	.73516	.78736	.84642	.91024	.98201 (0)	.10684	.11496
75	.64727	.68693	.72757	.77367	.82563	.88155	.94416	.10191	.10893
79	.65198	.68686	.72249	.76278	.80803	.85652	.91059	.97503 (0)	.10350
83	.65905	.68935	.72021	.75499	.79391	.83547	.88162	.93637	.98707 (0)
87	.66874	.69466	.72100	.75058	.78359	.81870	.85755	.90344	.94574
91	.68130	.70309	.72517	.74990	.77740	.80657	.83871	.87654	.91126
95	.69704	.71495	.73305	.75327	.77570	.79942	.82547	.85600	.88393
99	.71626	.73057	.74500	.76109	.77889	.79765	.81820	.84221	.86440
103	.73932	.75034	.76144	.77378	.78740	.80173	.81738	.83560	.85217
107	.76662	.77469	.78281	.79182	.80175	.81216	.82351	.83669	.84864
111	.79859	.80410	.80963	.81576	.82249	.82955	.83722	.84611	.85415
115	.83576	.83912	.84249	.84622	.85031	.85459	.85923	.86461	.86946
119	.87870	.88038	.88207	.88393	.88591	.88811	.89042	.89310	.89551
123	.92807	.92861	.92916	.92976	.93042	.93111	.93185	.93271	.93349
127	.98463	.98466	.98468	.98470	.98473	.98476	.98479	.98483	.98486
128	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)

a	3.850	4.170	4.500	4.870	5.250	5.650	6.100	6.500	6.900
$2^7x$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$
0	.29350 (1)	.34729 (1)	.41189 (1)	.49751 (1)	.60311 (1)	.73820 (1)	.92728 (1)	.11375 (2)	.13988 (2)
1	.29340	.34716	.41172	.49728	.60279	.73776	.92666	.11367	.13977
2	.29311	.34678	.41121	.49660	.60187	.73649	.92485	.11342	.13943
3	.29264	.34616	.41039	.49548	.60036	.73442	.92191	.11302	.13888
4	.29199	.34530	.40926	.49396	.59829	.73159	.91790	.11247	.13814
5	.29118	.34423	.40784	.49204	.59570	.72806	.91289	.11179	.13721
6	.29020	.34294	.40615	.48976	.59262	.72385	.90695	.11098	.13611
7	.28907	.34145	.40419	.48712	.58907	.71901	.90013	.11006	.13486
8	.28779	.33977	.40199	.48416	.58508	.71359	.89250	.10903	.13347
9	.28637	.33791	.39955	.48088	.58068	.70762	.88411	.10790	.13194
10	.28482	.33587	.39688	.47731	.57589	.70113	.87503	.10667	.13029
11	.28314	.33367	.39401	.47347	.57075	.69418	.86531	.10536	.12853
12	.28134	.33132	.39094	.46937	.56527	.68679	.85500	.10398	.12668
13	.27943	.32883	.38769	.46503	.55948	.67899	.84645	.10253	.12474
14	.27741	.32619	.38427	.46048	.55341	.67084	.83823	.10102	.12272
15	.27529	.32344	.38068	.45571	.54708	.66234	.82107	.99452 (1)	.12064
16	.27308	.32056	.37695	.45076	.54051	.65355	.80893	.97838	.11849
17	.27077	.31757	.37308	.44564	.53373	.64444	.79644	.96182	.11630
18	.26839	.31448	.36908	.44035	.52675	.63519	.78365	.94490	.11406
19	.26593	.31130	.36497	.43493	.51959	.62567	.77061	.92768	.11179
20	.26340	.30803	.36075	.42937	.51228	.61597	.75734	.91022	.10950
21	.26080	.30468	.35644	.42370	.50483	.60611	.74389	.89256	.10718
22	.25815	.30125	.35204	.41793	.49726	.59611	.73030	.87474	.10485
23	.25544	.29776	.34756	.41207	.48959	.58600	.71658	.85682	.10251
24	.25267	.29422	.34302	.40613	.48184	.57580	.70278	.83883	.10017
25	.24987	.29062	.33841	.40012	.47401	.56553	.68893	.82082	.97836 (1)
26	.24702	.28697	.33376	.39406	.46613	.55521	.67505	.80281	.95506
27	.24414	.28328	.32906	.38795	.45821	.54486	.66116	.78485	.93187
28	.24122	.27956	.32432	.38181	.45025	.53450	.64729	.76695	.90884
29	.23828	.27581	.31955	.37564	.44228	.52414	.63346	.74916	.88600
30	.23531	.27203	.31476	.36945	.43431	.51380	.61970	.73149	.86338
31	.23232	.26823	.30996	.36326	.42634	.50349	.60602	.71397	.84101
32	.22932	.26442	.30514	.35706	.41839	.49322	.59243	.69662	.81892
35	.22025	.25295	.29069	.33855	.39472	.46282	.55242	.64578	.75454
39	.20814	.23771	.27161	.31426	.36391	.42356	.50125	.58136	.67371
43	.19616	.22273	.25297	.29074	.33433	.38622	.45311	.52136	.59924
47	.18446	.20819	.23501	.26824	.30626	.35111	.40835	.46614	.53141
51	.17316	.19423	.21787	.24693	.27990	.31845	.36714	.41579	.47019
55	.16236	.18095							





TABLE I.—Continued.

a	11.00	11.30	11.70	12.00	12.20	12.50	12.90	13.20	13.50
$2^7x$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$
0	.16677 (3)	.20931 (3)	.28805 (3)	.37114 (3)	.44279 (3)	.58437 (3)	.86925 (3)	.11993 (4)	.16955 (4)
1	.16634	.20873	.28714	.36984	.44113	.58193	.86504	.11927	.16850
2	.16513	.20706	.28454	.36616	.43643	.57506	.85324	.11744	.16558
3	.16321	.20444	.28047	.36041	.42912	.56441	.83505	.11465	.16115
4	.16068	.20098	.27514	.35290	.41960	.55061	.81165	.11107	.15551
5	.15762	.19681	.26874	.34392	.40825	.53424	.78411	.10688	.14896
6	.15410	.19205	.26146	.33375	.39544	.51585	.75340	.10225	.14178
7	.15020	.18679	.25346	.32264	.38148	.49593	.72041	.97303 (3)	.13417
8	.14599	.18113	.24491	.31080	.36667	.47490	.68590	.92171	.12634
9	.14154	.17516	.23594	.29846	.35127	.45317	.65054	.86952	.11845
10	.13690	.16896	.22668	.28578	.33551	.43106	.61488	.81731	.11063
11	.13212	.16261	.21725	.27292	.31959	.40886	.57941	.76578	.10297
12	.12725	.15616	.20774	.26003	.30368	.38681	.54451	.71547	.95570 (3)
13	.12233	.14968	.19824	.24721	.28793	.36512	.51047	.66680	.88472
14	.11740	.14322	.18882	.23456	.27245	.34392	.47754	.62008	.81720
15	.11250	.13681	.17954	.22218	.25734	.32337	.44589	.57555	.75340
16	.10764	.13049	.17045	.21011	.24267	.30354	.41564	.53332	.69346
17	.10286	.12430	.16160	.19841	.22851	.28451	.38689	.49350	.63741
18	.98173 (2)	.11825	.15301	.18712	.21490	.26633	.35967	.45608	.58521
19	.93594	.11237	.14471	.17628	.20187	.24903	.33400	.42107	.53678
20	.89137	.10667	.13671	.16589	.18944	.23263	.30987	.38841	.49198
21	.84814	.10117	.12904	.15597	.17761	.21711	.28726	.35802	.45065
22	.80632	.95865 (2)	.12170	.14652	.16639	.20248	.26612	.32983	.41259
23	.76597	.90772	.11470	.13755	.15577	.18872	.24640	.30371	.37763
24	.72714	.85892	.10802	.12905	.14574	.17579	.22804	.27957	.34556
25	.68984	.81224	.10168	.12101	.13629	.16368	.21098	.25729	.31618
26	.65408	.76769	.95656 (2)	.11341	.12740	.15235	.19515	.23675	.28929
27	.61986	.72522	.89953	.10625	.11904	.14176	.18047	.21784	.26471
28	.58717	.68482	.84558	.99516 (2)	.11120	.13188	.16688	.20044	.24226
29	.55597	.64643	.79462	.93181	.10386	.12267	.15431	.18444	.22176
30	.52626	.60999	.74653	.87230	.96982 (2)	.11409	.14269	.16975	.20305
31	.49797	.57546	.70121	.81647	.90551	.10611	.13196	.15626	.18598
32	.47108	.54275	.65853	.76413	.84541	.98684 (2)	.12205	.14387	.17042
33	.44534	.51494	.62626	.72661	.80803	.79430	.96688 (2)	.11252	.13146
34	.41802	.48519	.59119	.68270	.75233	.81807	.91171	.81538 (2)	.93687 (2)
35	.39133	.45373	.55984	.64991	.72966	.79446	.87215	.95950	.67416
36	.36482	.42252	.52750	.61574	.69645	.76073	.83329	.91387	.49013
37	.33840	.39117	.48180	.56215	.63623	.70995	.78574	.86616	.36012
38	.31241	.36188	.44585	.52799	.60317	.67966	.75420	.83475	.26739
39	.28690	.33443	.41266	.48772	.56290	.63843	.71337	.78837	.20061
40	.26187	.30843	.38463	.45974	.53486	.60999	.68512	.76025	.15202
41	.23734	.28390	.35910	.43421	.50932	.58443	.65956	.73469	.11633
42	.21331	.25987	.33507	.41018	.48529	.56040	.63553	.71066	.89848 (1)
43	.18978	.23634	.31154	.38665	.46176	.53687	.61198	.68711	.70023
44	.16675	.21331	.28851	.36362	.43873	.51384	.58895	.66406	.55052
45	.14422	.19078	.26598	.34109	.41620	.49131	.56642	.64153	.43656
46	.12219	.16875	.24395	.31906	.39417	.46928	.54439	.61950	.34922
47	.10066	.14722	.22242	.29753	.37264	.44775	.52286	.59797	.28190
48	.07963	.12619	.20139	.27650	.35161	.42672	.50183	.57694	.22985
49	.05910	.10566	.18086	.25607	.33118	.40629	.48140	.55651	.18958
50	.03907	.08563	.16083	.23604	.31115	.38626	.46137	.53648	.15202
51	.01954	.06610	.14130	.21651	.29162	.36673	.44184	.51695	.11633
52	.00951	.05607	.13127	.20648	.28159	.35670	.43181	.50692	.89848 (1)
53	.00448	.04104	.11624	.19145	.26666	.34177	.41688	.49199	.70023
54	.00145	.03800	.11320	.18841	.26362	.33873	.41384	.48895	.55052
55	.00042	.03456	.10976	.18497	.26018	.33529	.41040	.48551	.43656
56	.00010	.03070	.10600	.18121	.25642	.33153	.40664	.48175	.34922
57	.00003	.02684	.10230	.17751	.25272	.32783	.40294	.47805	.28190
58	.00000	.02298	.10000	.17500	.25021	.32532	.40043	.47554	.22985
59	.00000	.01912	.10000	.17326	.24847	.32358	.39869	.47380	.18958
60	.00000	.01526	.10000	.17152	.24673	.32184	.39695	.47206	.15202
61	.00000	.01140	.10000	.16978	.24500	.32010	.39521	.47032	.11633
62	.00000	.00754	.10000	.16804	.24326	.31836	.39347	.46858	.89848 (1)
63	.00000	.00368	.10000	.16630	.24152	.31662	.39173	.46684	.70023
64	.00000	.00182	.10000	.16456	.23978	.31488	.38999	.46510	.55052
65	.00000	.00096	.10000	.16282	.23804	.31314	.38825	.46336	.43656
66	.00000	.00050	.10000	.16108	.23630	.31140	.38651	.46162	.34922
67	.00000	.00024	.10000	.15934	.23456	.30966	.38477	.45988	.28190
68	.00000	.00010	.10000	.15760	.23282	.30792	.38303	.45814	.22985
69	.00000	.00005	.10000	.15586	.23108	.30618	.38129	.45640	.18958
70	.00000	.00000	.10000	.15412	.22934	.30444	.37955	.45466	.15202
71	.00000	.00000	.10000	.15238	.22760	.30270	.37781	.45292	.11633
72	.00000	.00000	.10000	.15064	.22586	.30096	.37607	.45118	.89848 (1)
73	.00000	.00000	.10000	.14890	.22412	.29922	.37433	.44944	.70023
74	.00000	.00000	.10000	.14716	.22238	.29748	.37259	.44770	.55052
75	.00000	.00000	.10000	.14542	.22064	.29574	.37085	.44596	.43656
76	.00000	.00000	.10000	.14368	.21890	.29400	.36911	.44422	.34922
77	.00000	.00000	.10000	.14194	.21716	.29226	.36737	.44248	.28190
78	.00000	.00000	.10000	.14020	.21542	.29052	.36563	.44074	.22985
79	.00000	.00000	.10000	.13846	.21368	.28878	.36389	.43900	.18958
80	.00000	.00000	.10000	.13672	.21194	.28704	.36215	.43726	.15202
81	.00000	.00000	.10000	.13498	.21020	.28530	.36041	.43552	.11633
82	.00000	.00000	.10000	.13324	.20846	.28356	.35867	.43378	.89848 (1)
83	.00000	.00000	.10000	.13150	.20672	.28182	.35693	.43204	.70023
84	.00000	.00000	.10000	.12976	.20498	.28008	.35519	.43030	.55052
85	.00000	.00000	.10000	.12802	.20324	.27834	.35345	.42856	.43656
86	.00000	.00000	.10000	.12628	.20150	.27660	.35171	.42682	.34922
87	.00000	.00000	.10000	.12454	.19976	.27486	.34997	.42508	.28190
88	.00000	.00000	.10000	.12280	.19802	.27312	.34823	.42334	.22985
89	.00000	.00000	.10000	.12106	.19628	.27138	.34649	.42160	.18958
90	.00000	.00000	.10000	.11932	.19454	.26964	.34475	.41986	.15202
91	.00000	.00000	.10000	.11758	.19280	.26790	.34301	.41812	.11633
92	.00000	.00000	.10000	.11584	.19106	.26616	.34127	.41638	.89848 (1)
93	.00000	.00000	.10000	.11410	.18932	.26442	.33953	.41464	.70023
94	.00000	.00000	.10000	.11236	.18758	.26268	.33779	.41290	.55052
95	.00000	.00000	.10000	.11062	.18584	.26094	.33605	.41116	.43656
96	.00000	.00000	.10000	.10888	.18410	.25920	.33431	.40942	.34922
97	.00000	.00000	.10000	.10714	.18236	.25746	.33257	.40768	.28190
98	.00000	.00000	.10000	.10540	.18062	.25572	.33083	.40594	.22985
99	.00000	.00000	.10000	.10366	.17888	.25398	.32909	.40420	.18958
100	.00000	.00000	.10000	.10192	.17714	.25224	.32735	.40246	.15202
101	.00000	.00000	.10000	.10018	.17540	.25050	.32561	.40072	.11633
102	.00000	.00000	.10000	.09844	.17366	.24876	.32387	.39898	.89848 (1)
103	.00000	.00000	.10000	.09670	.17192	.24702	.32213	.39724	.70023
104	.00000	.00000	.10000	.09496	.17018	.24528	.32039	.39550	.55052
105	.00000	.00000	.10000	.09322	.16844	.24354	.31865	.39376	.43656
106	.00000	.00000	.10000	.09148	.16670	.24180	.31691	.39202	.34922
107	.00000	.00000	.10000	.08974	.16496	.24006	.31517	.39028	.28190
108	.00000	.00000	.10000	.08800	.16322	.23832	.31343	.38854	.22985
109	.00000	.00000	.10000	.08626	.16148	.23658	.31169	.38680	.18958
110	.00000	.00000	.10000	.08452	.15974	.23484	.30995	.38506	.15202
111	.00000	.00000	.10000	.08278	.15800	.23310	.30821	.38332	.11633
112	.00000	.00000	.10000	.08104	.15626	.23136	.30647	.38158	.89848 (1)
113	.00000	.00000	.10000	.07930	.15452	.22962	.30473	.37984	.70023
114	.00000	.00000	.10000	.07756	.15278	.22788	.30299	.37810	.55052
115	.00000	.00000	.10000	.07582	.15104	.22614	.30125	.37636	.43656
116	.00000	.00000	.10000	.07408	.14930	.22440	.29951	.37462	.34922
117	.00000	.00000</							

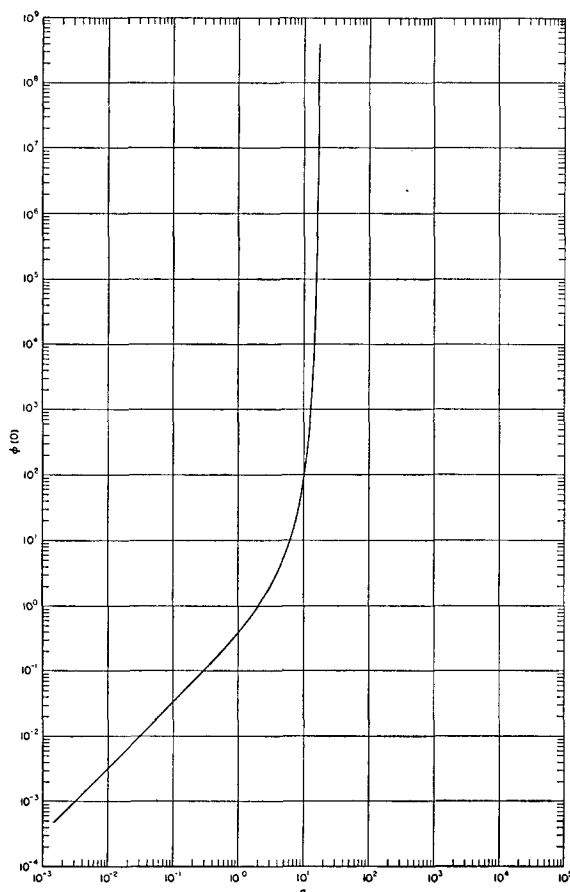
TABLE I.—Continued.

a	13.70	13.90	14.10	14.70	15.00	15.40	15.80	16.29	16.74
2 x	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$	$\phi(x)$
0	.21698 (4)	.28175 (4)	.37195 (4)	.497131 (4)	.17278 (5)	.43256 (5)	.141434 (6)	.12539 (7)	.10698 (9)
1	.21551	.27965	.36889	.496015	.17037	.42433	.13737	.11840	.85732 (8)
2	.21145	.27388	.36052	.493016	.16395	.40301	.12750	.10261	.53419
3	.20529	.26518	.34799	.488629	.15473	.37326	.11436	.84091 (6)	.30142
4	.19751	.25426	.33234	.483296	.14372	.33891	.99987 (5)	.66428	.16533
5	.18853	.24173	.31454	.477390	.13175	.30292	.85758	.51252	.91232 (7)
6	.17873	.22815	.29536	.471216	.11950	.26741	.72511	.38983	.51454
7	.16842	.21397	.27550	.465011	.10744	.23377	.60674	.29425	.29854
8	.15788	.19956	.25550	.458951	.95914 (4)	.20281	.50396	.22145	.17853
9	.14733	.18524	.23577	.453159	.85129	.17493	.44650	.16672	.10998
10	.13693	.17125	.21664	.447718	.75208	.15023	.34315	.12586	.69693 (6)
11	.12683	.15774	.19834	.442674	.66203	.12862	.28227	.95427 (5)	.45336
12	.11712	.14487	.18103	.438048	.58113	.10989	.23209	.72743	.30211
13	.10788	.13269	.16480	.433843	.50905	.93764 (4)	.19094	.55788	.20583
14	.99144 (3)	.12128	.14970	.430047	.44526	.79961	.15728	.43064	.14309
15	.90947	.11064	.13575	.426641	.38909	.68189	.12978	.33466	.10133
16	.83295	.10078	.12292	.423597	.33982	.58177	.10734	.26184	.72986 (5)
17	.76186	.91687 (3)	.11117	.420889	.29675	.49677	.88999 (4)	.20625	.53388
18	.69609	.83330	.10046	.418485	.25918	.42467	.74001	.16354	.39612
19	.63544	.75677	.90719 (3)	.416358	.22646	.36354	.61714	.13052	.29778
20	.57968	.68687	.81887	.414477	.19801	.31171	.51626	.10483	.22657
21	.52854	.62317	.73896	.412817	.17327	.26774	.43324	.84706 (4)	.17432
22	.48174	.56525	.66678	.411354	.15177	.23040	.36473	.68852	.13551
23	.43898	.51266	.60168	.410064	.13309	.19865	.30804	.56283	.10636
24	.39998	.46496	.54302	.408275 (3)	.11685	.17163	.26100	.46260	.84227 (4)
25	.36444	.42176	.49022	.407263	.10272	.14859	.22184	.38221	.67256
26	.33209	.38266	.44271	.406429 (3)	.90429	.12891	.18915	.31738	.54123
27	.30267	.34729	.39999	.405667	.79720	.11208	.16177	.26482	.43872
28	.27593	.31531	.36157	.405811	.70383	.97654 (3)	.13878	.22198	.35806
29	.25164	.28641	.32704	.405760	.62232	.85264	.11940	.18690	.29411
30	.22957	.26028	.29600	.404418	.55109	.74604	.10303	.15802	.24303
31	.20953	.23667	.26809	.403696	.48876	.65413	.89158 (3)	.13416	.20197
32	.19133	.21534	.24299	.403520	.43145	.57473	.77364	.11434	.16875
35	.14616	.16282	.18177	.402637	.30708	.39456	.51349	.72340 (3)	.10135
39	.10296	.11330	.12489	.401692	.19766	.24549	.30765	.44127	.54544 (3)
43	.73322 (2)	.79830 (2)	.87015 (2)	.401351	.13021	.15718	.19093	.24463	.31037
47	.52820	.56967	.61489	.4007729 (2)	.87669 (2)	.10330	.12226	.15129	.18529
51	.38494	.41170	.44058	.400190	.60233	.69526 (2)	.80500 (2)	.96774 (2)	.11516
55	.28377	.30125	.31994	.38421	.42167	.47819	.54343	.63759	.74079 (2)
59	.21152	.22308	.23533	.27671	.30036	.33544	.37515	.43114	.49097
63	.15937	.16709	.17521	.20223	.21739	.23957	.26424	.29835	.33400
67	.12131	.12652	.13197	.14982	.15968	.17393	.18954	.21075	.23251
71	.93261 (1)	.96805 (1)	.10049	.11241	.11891	.12819	.13822	.15165	.16520
75	.72375	.74804	.77314 (1)	.85353 (1)	.89680 (1)	.95795 (1)	.10233	.11097	.11955
79	.56681	.58356	.60078	.65539	.68445	.72516	.76823 (1)	.82445 (1)	.87967 (1)
83	.44789	.45949	.47136	.50866	.52831	.55562	.58426	.62123	.65716
87	.35711	.36515	.37335	.39892	.41227	.43069	.44984	.47434	.49791
91	.28739	.29297	.29863	.31616	.32524	.33769	.35054	.36684	.38239
95	.23364	.23749	.24139	.25337	.25953	.26792	.27653	.28738	.29764
99	.19218	.19481	.19746	.20558	.20972	.21534	.22107	.22825	.23499
103	.16034	.16211	.16388	.16928	.17203	.17573	.17949	.18417	.18854
107	.13622	.13736	.13852	.14201	.14377	.14614	.14854	.15151	.15428
111	.11847	.11917	.11988	.12202	.12310	.12455	.12601	.12780	.12947
115	.10619	.10659	.10699	.10819	.10879	.10960	.11044	.11140	.11232
119	.98869 (0)	.99057 (0)	.99244 (0)	.99809 (0)	.10009	.10047	.10085	.10131	.10174
123	.96297	.96355	.96413	.96589	.96676 (0)	.96793 (0)	.96910 (0)	.97054 (0)	.97186 (0)
127	.98609	.98611	.98614	.98621	.98624	.98629	.98634	.98640	.98645
128	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)	.10000 (1)

TABLE II.<sup>a</sup>

a	$-\frac{d\phi(x)}{dx^2} \Big _{x=0}$	$\frac{a}{Z^{1/3}}$	$Z^{1/3}r_0(\text{cm})$	$ZV(\text{cm}^3)$	$\frac{P}{Z^{10/3}} \left( \frac{\text{dynes}}{\text{cm}^2} \right)$	$-\frac{\Delta E_{\text{tot}}(\text{ergs})}{Z^{7/3}(\text{atom})}$	$\frac{\Delta E_{\text{kin}}(\text{ergs})}{Z^{7/3}(\text{atom})}$	$-\frac{\Delta E_{\text{pot}}(\text{ergs})}{Z^{7/3}(\text{atom})}$
.0365	-.98119 (0)	.15870 (-6)	.11878 (-9)	.70194 (-29)	.89937 (22)	.93844 (-7)	.95548 (-7)	.17038 (-8)
.0458	-.97668	.10060	.14911	.13888 (-28)	.28876	.59271	.60619	.13486
.0578	-.97043	.63012 (-7)	.18830	.27965	.89344 (21)	.36948	.38007	.10594
.0720	-.96295	.40491	.23473	.54172	.29573	.23609	.24451	.84175 (-9)
.0910	-.95279	.25249	.29696	.10969 (-27)	.90806 (20)	.14612	.15269	.65698
.1130	-.94081	.16300	.36917	.21075	.30408	.93524 (-8)	.98732 (-8)	.52084
.1430	-.92409	.10115	.46791	.42911	.92242 (19)	.57359	.61388	.40292
.1780	-.90400	.64805 (-8)	.58350	.83218	.30306	.36251	.39409	.31583
.2230	-.87716	.40897	.73276	.16481 (-26)	.95881 (18)	.22482	.24925	.24431
.2800	-.84146	.25625	.92289	.32926	.29796	.13781	.15651	.18706
.3460	-.79754	.16541	.11445 (-8)	.62803	.99752 (17)	.86737 (-9)	.10120	.14467
.4300	-.73730	.10512	.14291	.12225 (-25)	.32113	.53390	.64384 (-9)	.10993
.5380	-.65194	.65523 (-9)	.17990	.24388	.98512 (16)	.31954	.40121	.81665 (-10)
.6800	-.52453	.39679	.22927	.50482	.28114	.18353	.24224	.58714
.8500	-.34600	.24378	.28953	.10167 (-24)	.83177 (15)	.10589	.14779	.41901
1.0700	-.65523 (-1)	.14564	.35949	.21131	.22945	.58372 (-10)	.87084 (-10)	.28712
1.3200	.33450 (0)	.89695 (-10)	.46327	.41646	.68301 (14)	.32835	.52500	.19664
1.4700	.62362	.69481	.52111	.59275	.36072	.24096	.40048	.15952
1.6300	.97905	.54089	.58419	.83511	.19288	.17710	.30612	.12901
1.8200	.14729 (1)	.41133	.66103	.12099 (-23)	.97270 (13)	.12581	.22726	.10144
2.0100	.20563	.31928	.74010	.16981	.51634	.91236 (-11)	.17180	.80563 (-11)
2.2200	.28218	.24597	.83022	.23970	.26897	.65199	.12822	.63017
2.4500	.38305	.18831	.93240	.33954	.13793	.45967	.94534 (-11)	.18567
2.6900	.51077	.14489	.10432 (-7)	.47549	.71634 (12)	.32450	.69733	.37282
2.9500	.68014	.11078	.11682	.66784	.36616	.22592	.50770	.28177
3.2500	.92434	.82588 (-11)	.13196	.96257	.17571	.15108	.35632	.20524
3.5200	.11989 (2)	.64155	.14628	.13112 (-22)	.93451 (11)	.10635	.26127	.15492
3.8500	.16225	.47687	.16476	.18736	.14516	.70001 (-12)	.18022	.11021
4.1700	.21494	.36127	.18380	.26009	.22238	.47071	.12644	.79374 (-12)
4.5000	.28456	.27353	.20469	.35922	.11092	.31463	.88073 (-12)	.56610
4.8700	.38650	.20173	.22978	.50818	.51810 (10)	.20133	.58853	.38720
5.2500	.52578	.14844	.25759	.71593	.24065	.12769	.38917	.26148
5.6500	.72341	.10796	.28936	.10149 (-21)	.10855	.79148 (-13)	.25137	.17222
6.1000	.10323 (3)	.75686 (-12)	.32858	.14860	.44673 (9)	.46136	.15302	.10688
6.5000	.14446	.55246	.36696	.20698	.20336	.28447	.97827 (-13)	.69380 (-13)
6.9000	.19396	.40296	.40911	.28683	.92398 (8)	.17441	.62066	.14625
7.3500	.27737	.28181	.46173	.41234	.37791	.09967	.36782	.26815
7.8500	.41500	.18836	.52774	.61568	.13803	.05274	.20220	.14946
8.2000	.55287	.14139	.57948	.81508	.67383 (7)	.03341	.13136	.09795
8.6000	.77213	.10124	.64513	.11247 (-20)	.29235	.01956	.07908	.05951
9.0300	.11157 (4)	.70067 (-13)	.72477	.15947	.11649	.01080	.04493	.03412
9.4700	.16450	.47523	.81787	.22916	.44132 (6)	.00575	.02459	.01884
9.8500	.23263	.33604	.90961	.31525	.18557	.00327	.01428	.01102
10.2000	.32355	.24161	.10052 (-6)	.42546	.81337 (5)	.00190	.00848	.00658
10.6000	.47866	.16331	.11301	.60462	.30554	.00100	.00455	.00355
11.0000	.72103	.10842	.12754	.86907	.10972	.00050	.00236	.00185
11.3000	.99384	.78658 (-14)	.14007	.11511 (-19)	.49188 (4)	.00030	.00140	.00111
11.7000	.15570 (5)	.50208	.15945	.16982	.16012	.00014	.00068	.00054
12.0000	.22201	.35211	.17646	.23018	.65947 (3)	.00008	.00038	.00030
12.2000	.28404	.27522	.18923	.28384	.35622	.00005	.00025	.00020
12.5000	.41789	.18707	.21096	.39324	.13567	.00003	.00013	.00011
12.9000	.72465	.10788	.24592	.62299	.34264 (2)	.00001	.00005	.00004
13.2000	.11301 (6)	.69171 (-15)	.27800	.89994	.11280	.00000	.00003	.00002
13.5000	.18204	.42943	.31672	.13308 (-18)	.34256 (1)	.00000	.00001	.00001
13.7000	.25542	.30606	.34725	.17540	.14690	.00000	.00001	.00001
13.9000	.36534	.21397	.38252	.23445	.60034 (0)	.00000	.00000	.00000
14.1000	.53415	.14635	.42364	.31848	.23227	.00000	.00000	.00000
14.7000	.19750 (7)	.39582 (-16)	.59982	.90396	.88358 (-2)	.00000	.00000	.00000
15.0000	.43145	.18119	.73663	.16743 (-17)	.12526	.00000	.00000	.00000
15.4000	.14926 (8)	.52373 (-17)	.10179 (-5)	.44482	.56269 (-4)	.00000	.00000	.00000
15.8000	.73620	.10618	.15366	.15196 (-16)	.10415 (-5)	.00000	.00000	.00000
16.2900	.13799 (10)	.56649 (-19)	.32464	.14331 (-15)	.68469 (-9)	.00000	.00000	.00000
16.7400	.52776 (12)	.14812 (-21)	.14553 (-4)	.12911 (-13)	.23937 (-15)	.00000	.00000	.00000

<sup>a</sup> The numbers in parentheses are the powers of ten associated with the entries.

FIG. 1.  $\phi(0)$  versus  $a$ .

tions indicated in the table, and  $E^\infty$ , the energy of the infinite isolated atom. The subscripts distinguish total, potential and kinetic energies. It has been found numerically that

$$E_{\text{total}}^\infty/Z^{7/3} = -E_{\text{kinetic}}^\infty/Z^{7/3} = \frac{1}{2}E_{\text{potential}}^\infty/Z^{7/3} \\ = -0.33502717 \times 10^{-10} \text{ erg/atom.}$$

Finally, Figs. 1-5 illustrate some of the results of Table II as well as the relationship between the parameter  $a$  and  $\phi(0)$  in Eq. (4).

The calculations leading to the results contained in Tables I and II were accurate to one part in  $10^7$  to  $10^8$ . This precision was needed in order to obtain accurate changes in the energies. The data presented in Tables I and II are therefore accurate to the number of figures presented. It is possible with the present results to resolve the inconsistency pointed out by Umeda<sup>7</sup> in the data of Slater and Krutter and of Feynman, Metropolis, and Teller. Table III compares the results of the present calculations with those of the latter authors and with those of March. The data for the comparison were obtained by quadratic interpolation on Table II,<sup>8</sup> which provides results with five significant figures. It is suggested by Table III that no major inconsistencies exist in the previous calculations. However, the data of

<sup>7</sup> K. Umeda, Phys. Rev. **83**, 65 (1951).

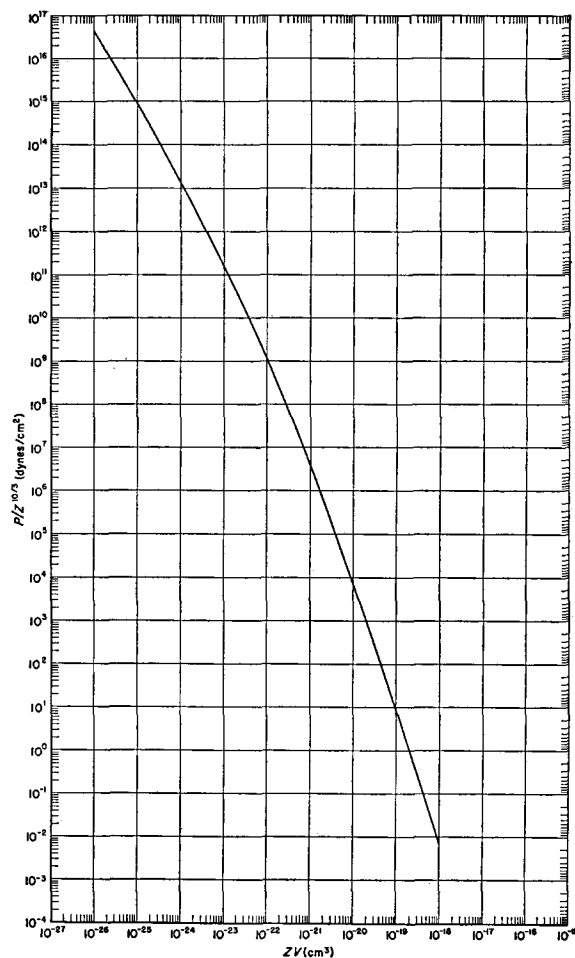


FIG. 2. Pressure versus volume.

Feynman, Metropolis, and Teller possess inaccuracies in the third or fourth significant figures rather than retaining the full accuracy implied by the number of figures which they present. As a final point the infinite atom solution of Miranda may be compared with the solution in Table I with  $a=16.74$ . This latter solution has been estimated to have an initial slope within one part in  $10^9$  of the infinite atom solution. The present calculations gave

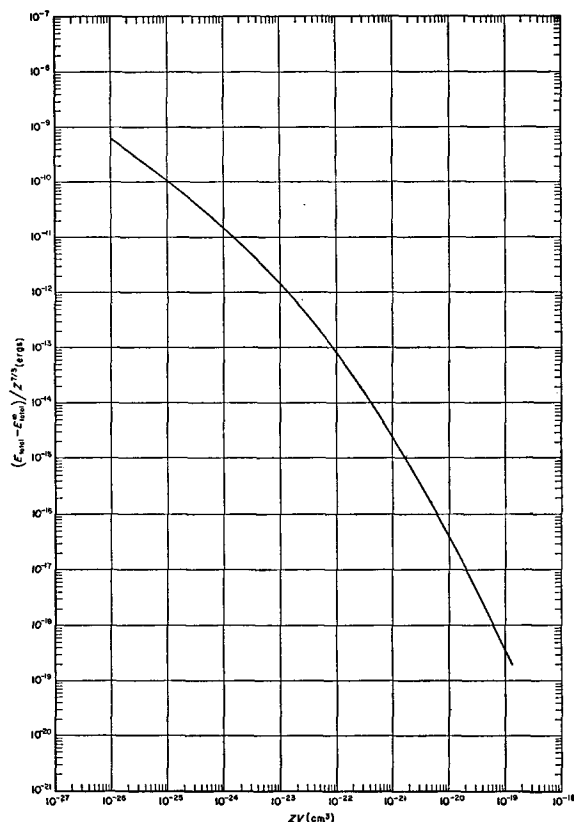
$$-\frac{1}{r_0/\mu} \frac{d\phi(x)}{dx^2} \bigg|_{x=0} = 1.58807102$$

as compared with Miranda's estimate

$$-\frac{1}{r_0/\mu} \frac{d\phi(x)}{dx^2} \bigg|_{x=0} = 1.5880464.$$

<sup>8</sup> The relationship of the present notation to that of references 2, 3, and 4 is

SK	FMT and March	Present
$B$	$-a_2$	$-\frac{1}{r_0/\mu} \frac{d\phi(x)}{dx^2} \bigg _{x=0}$
$X$	$x_0$	$r_0/\mu$
$\phi_x$	$\phi(x_0)$	$1/\phi(0)$

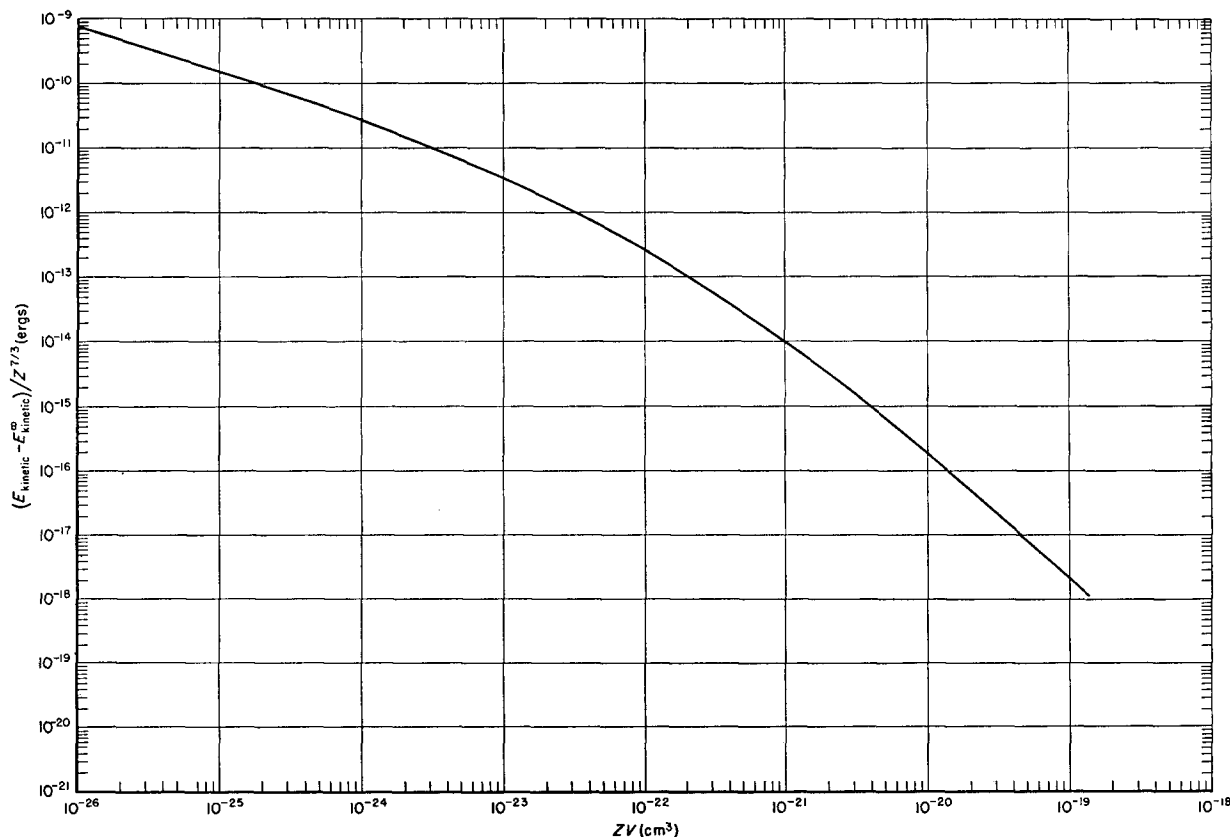
FIG. 3. Total energy *versus* volume.

It may be observed that the solutions of Eq. (12) exist for all atomic radii from zero to infinity,<sup>9</sup> so that the model predicts the fallacious result that no stable crystal states exist. This deficiency in the qualitative behavior of the model, which is reflected in the poor quantitative results for compressibilities in the neighborhood of the normal atomic state, is a consequence of omitting exchange effects. While the inclusion of exchange is known to lead to a finite atomic radius for zero applied pressure, the quantitative predictions are still rather unsatisfactory for compressibilities as well as for normal atomic volumes. Comparison of the present results in Table II with the experimental data of Bridgman shows quite generally that the pressures at a given atomic volume are vastly overestimated by the Thomas-Fermi model. However, on theoretical grounds it is expected that with decreasing volume the predictions of the model improve.

On the other hand, the potential functions may be a more accurate representation of the actual atomic distributions. For the case of isolated atoms the Schrödinger eigenvalues for the atomic energy levels in the Thomas-Fermi potential have been comprehensively investigated by the author.<sup>10</sup> These eigenvalues are found to compare quite favorably with the predictions of the

<sup>9</sup> The zero radius limit corresponds to  $a=0$ , but the limit of infinite radius has not been determined. Some approximations indicate that this limit is very close to, if not exactly,  $a=17$ .

<sup>10</sup> R. Latter, Phys. Rev. **99**, 510 (1955).

FIG. 4. Potential energy *versus* volume.

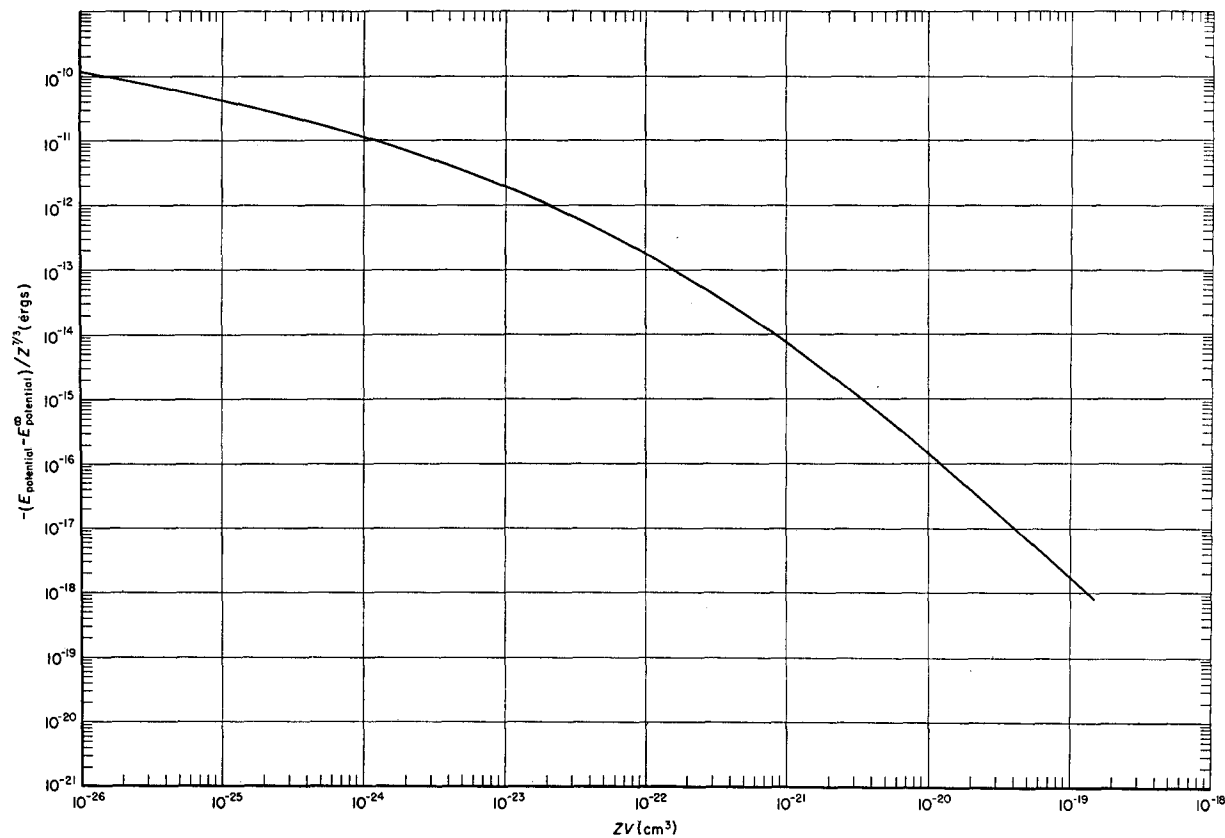


FIG. 5. Kinetic energy *versus* volume.

TABLE III.

	Present Calculation		Slater and Krutter		Feynman, Metropolis and Teller		March	
$r_0/\mu$	$-\frac{1}{r_0/\mu} \frac{d\phi(x)}{dx^2} \Big _{x=0}$	$\frac{1}{\phi(0)}$	$-\frac{1}{r_0/\mu} \frac{d\phi(x)}{dx^2} \Big _{x=0}$	$\frac{1}{\phi(0)}$	$-\frac{1}{r_0/\mu} \frac{d\phi(x)}{dx^2} \Big _{x=0}$	$\frac{1}{\phi(0)}$	$-\frac{1}{r_0/\mu} \frac{d\phi(x)}{dx^2} \Big _{x=0}$	$\frac{1}{\phi(0)}$
1.190	1.0026	1.4492	1.00					
1.690	1.3815	.94091	1.38					
2.200	1.4999	.66628	1.50					
2.800	1.5500	.47667	1.55				1.55	.4767
3.043	1.5601	.42262					1.56	.4226
3.285	1.5671	.37751					1.567	.3775
3.704	1.5746	.31483					1.5748	.3148
4.230	1.5803	.25570	1.58					
4.330	1.5809	.24633					1.581	.2463
5.229	1.5849	.18058					1.5849	.1806
5.401	1.5853	.17095					1.5853	.1710
5.850	1.5862	.14899	1.586					
6.206	1.5866	.13433						
7.385	1.5874	.098098			1.58806	.07799	1.5866	.1343
7.790	1.5876	.088823					1.58756	.0888
8.015	1.5876	.084193					1.58764	.0842
8.588	1.5876	.073821			1.58842	.07395		
8.590	1.5876	.073789	1.588					
9.565	1.5879	.059868			1.58856	.05990		
10.804	1.5880	.046934			1.58865	.04701		
11.300	1.5880	.042832	1.58803					
11.963	1.5880	.038086			1.58870	.03813		
15.870	1.5881	.020825			1.58874	.02086		
16.000	1.5881	.020454						

Hartree theory. It may be anticipated that, though the equation of state of the model is unsatisfactory, the potential distribution for compressed atomic states may be fairly realistic.

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