[Journal of the Faculty of Science, Hokkaidô University, Japan, Ser. II, Vol. III, No. 7, 1949.]

The Diamagnetic Susceptibility of the Thomas-Fermi-Dirac Atom*

By

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(Received February 15, 1949)**

As a test of the validity of the Thomas-Fermi-Dirac atom the diamagnetic susceptibility of the neutral atom has been evaluated as a function of the atomic number, on using the recently published accurate table of the Thomas-Fermi-Dirac function. The results are in better accord with the experimental values.

The atomic diamagnetic susceptibility χ_{at} is given by the well-known formula of Langevin and Pauli[1]

$$\chi_{at} = -\frac{Le^2}{6mc^2}\sum \overline{r^2} = -2.832 \cdot 10^{10} \sum \overline{r^2}, \tag{1}$$

This is sensibly influenced by the charge distribution. As shown by Sommerfeld[2], the Thomas-Fermi atom results too large values, which can be easily understood by the infinite extension of the Thomas-Fermi function. Taking the Amaldi-Fermi correction into account, Jensen[3] has obtained remarkably better values. For the Thomas-Fermi-Dirac atom, however, it is to be expected that the theoretical values may give a much better agreement with the experimental ones, because the Thomas-Fermi-Dirac function has only a finite domain[4]. Recently an accurate table of the Thomas-Fermi-Dirac function[5] has been published. By the use of it we have calculated the expression (1). Referring to the equations (17) and (27a) given in the table for $\sum \overline{r^2}$, χ_{at} becomes for the Thomas-Fermi-Dirac atom with the atomic number $Z=18\overline{\varphi}_0$

* Physical Quantities of the Thomas-Fermi-Dirac Atom, No. 1.

** Presented in part at the semiannual meeting of The Institute of Physical and Chemical Research in Tokyo, June 14, 1940, and at the annual Hiroshima meeting of The Physico-Mathematical Society of Japan, April 4, 1941. The publication was delayed owing to the wartime external conditions.

TABLE I. *Diamagnetic susceptibility of the Thomas-Fermi-Dirac atom in* 10^{-6} cm^3

Z	$-\chi_{at}$	Z	$-\chi_{at}$	Z	$-\chi_{at}$	Z	$-\chi_{at}$	Z	$-\chi_{at}$
1	1.77	21	23.41	41	36.24	61	46.16	81	54.45
2	3.50	22	24.16	42	36.79	62	46.60	82	54.83
3	5.09	23	24.89	43	37.33	63	47.04	83	55.20
4	6.56	24	25.62	44	37.86	64	47.48	84	55.58
5	7.92	25	26.33	45	38.39	65	47.92	85	55.96
6	9.21	26	27.03	46	38.91	66	48.35	86	56.33
7	10.42	27	27.72	47	39.43	67	48.78	87	56.70
8	11.57	28	28.39	48	39.94	68	49.20	88	57.07
9	12.67	29	29.04	49	40.45	69	49.62	89	57.44
10	13.73	30	29.69	50	40.95	70	50.04	90	57.80
11	14.75	31	30.33	51	41.45	71	50.46	91	58.16
12	15.73	32	30.96	52	41.94	72	50.86	92	58.52
13	16.68	33	31.58	53	42.42	73	51.27		
14	17.60	34	32.19	54	42.90	74	51.68		
15	18.50	35	32.80	55	43.38	75	52.08		
16	19.37	36	33.38	56	43.85	76	52.48		
17	20.21	37	33.97	57	44.32	77	52.88		
18	21.04	38	34.55	58	44.79	78	53.28		
19	21.85	39	35.12	59	45.25	79	53.67		
20	22.64	40	35.68	60	45.71	80	54.06		

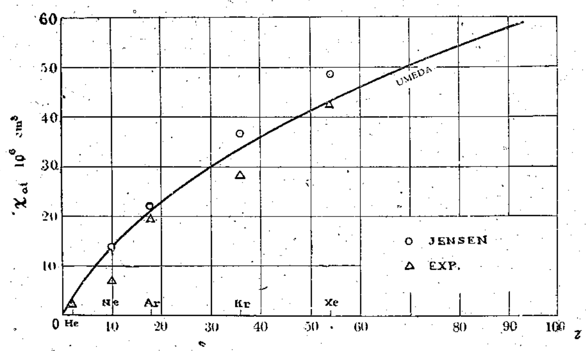

Fig. 1. *Diamagnetic susceptibility of the Thomas-Fermi-Dirac atom in* 10^{-6} cm^3.

$$\chi_{at} = -\frac{Le^2}{6mc^2} \, 6 Z \mu^2 \int_0^{x_0} x \, \psi \, dx \,,$$

$$= -9.738 \cdot 10^{-6} \int_0^{\bar{x}_0} \bar{x} \, \bar{\psi} \, d\bar{x} \quad cm^3. \qquad (2)$$

The numerical values for all elements are tabulated in TABLE I. Fig. 1. shows their dependence on the atomic number. The direct comparison with the experimental data is limited only for the

TABLE II.

Atomic diamagnetic susceptibility of inert gases in 10^{-6} cm^3.

Atomic number / Inert gas	2 He	10 Ne	18 Ar	36 Kr	54 Xe
Thomas-Fermi (Sommerfeld(2))		−67	−81	−102	−117
Thomas-Fermi-Amaldi (Jensen(3))		−13.7	−22.0	−36.5	−48.5
Thomas-Fermi-Dirac (Umeda, Eq. 2)	−3.51	−13.73	−21.04	−33.38	−42.90
Experiment (Mann(6))	−1.9	−6.75	−19.54	−28.0	−42.4

All the other theoretical values are collected in Mann's paper.

inert gases for which several different theoretical values and the experimental ones are given in TABLE II. So far as the diamagnetic susceptibility is concerned, the Thomas-Fermi-Dirac atomic model seems to be primarily one of the best.

In conclusion, The Department of Education and The Foundation for the Promotion of Scientific and Industrial Research of Japan (Gakujutsushinkôkai) are for the financial supports gratefully acknowledged.

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