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The Mean Excitation Energy of the THOMAS-FERMI-DIRAC Atom*

By

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As a test of the validity of the THOMAS-FERMI-DIRAC atom the mean excitation energy of the neutral atom was calculated as a function of the atomic number, on using the recently published table of the TFD function. The TFD atom did not much improve the accord with the experimental values in comparison to the TF atom.

According to BETHE[1] and SOMMERFELD[2], the mean excitation energy† $\bar{E}$ of an atom of atomic number Z based on the statistical model, is defined by the formula:

$$Z \log \bar{E} = \int \log |E(r)| \cdot D(r)\, dr\,, \qquad (1)$$

where $D(r)$ and $E(r)$ are the radial electron density and the mean total energy per electron respectively in the shell dr.

On the basis of experiments of energy loss of α particle in matter, BLOCH[3] has given a semiempirical formula

$$\bar{E} = 13.5\, Z \ \text{eV}\,, \qquad (2)$$

which is valid not only for heavy atoms but also for light ones and even for hydrogen. On the other hand, the geometrical means of the ionisation energies of each atomic shell derived from X-ray spectra are, however, according to BETHE[4] far lower than the values given by Eq. (2).

Theoretically, SOMMERFELD has obtained for the THOMAS-FERMI atom by means of his asymptotic formula for the TF function

* Physical Quantities of the THOMAS-FERMI-DIRAC Atom, No. 3.

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† Notation: E (BETHE[1]), $\bar{E}$ (BETHE[4], SOMMERFELD[2]), J (SOLOMON[5]).

$$\bar{E}_{\mathrm{TF,asymptotic}} = 1.78\, Z^{4/3}\ \mathrm{eV}\ . \qquad (3)$$

This is in not satisfactory accord with the experimental values. Expecting to improve the discrepancy, we have now calculated $\bar{E}$ for the THOMAS-FERMI-DIRAC atom in order to test at the same time its validity.

In the TFD atom, $D(r)$ is expressed by Eq. (25a) in reference (7) as

$$D(r)\,dr = Zx^2\,(\beta + \sqrt{\psi(x)/x})^3\,dx\ , \qquad (4)$$

$\psi(x)$ denoting the TFD function. As shown by SLATER and KRUTTER[6], $E(r)$ for the TFD atom is composed from the following three parts:

i. the mean kinetic energy: $(3/5)\ (P^2/2m)$

ii. the Coulomb potential energy due to the nucleus and the electron cloud: $(-e)\,V = -Ze^2/\mu\cdot\psi/x$,

iii. the mean exchange energy: $(-3e^2/h)\,P$,

where P is the maximum momentum in the shell considered dx:

$$P = \frac{2me^2}{h} + \sqrt{2m}\sqrt{\frac{Ze^2}{\mu}}\,\frac{\psi}{x}\ ,$$

so that on account of the relation $(2me^4/\hbar^2)/(Ze^2/\mu) = \beta^2$ we get

$$E(x) = -\frac{2}{5}\,\frac{Ze^2}{\mu}\left(\frac{\psi}{x} + \frac{9}{2}\beta\sqrt{\frac{\psi}{x}} + 6\beta^2\right) \qquad (5)$$

and finally, on inserting Eqs. (4) and (5) into Eq. (1),

$$\bar{E}_{\mathrm{TFD}} = \frac{2}{5}\,\frac{Ze^2}{\mu}\exp\int_0^{x_0}\log\left(\frac{\psi}{x} + \frac{9}{2}\beta\sqrt{\frac{\psi}{x}} + 6\beta^2\right)\cdot x^2\left(\beta + \sqrt{\frac{\psi}{x}}\right)^3 dx, \qquad (6)$$

which is further expressed by the reduced quantities $\bar{\beta}$, $\bar{x}$, $\bar{\psi}$ as follows, for the convenience of the numerical evaluation by the use of the table of the TFD function published recently by us[7]

$$\bar{E}_{\mathrm{TFD}} = 576.6^{(\mathrm{eV})}\exp_{10}\frac{1}{\bar{\psi}_0}\int_0^{\bar{x}_0}\log_{10}\left(\frac{\bar{\psi}}{\bar{x}} + \frac{9}{2}\bar{\beta}\sqrt{\frac{\bar{\psi}}{\bar{x}}} + 6\bar{\beta}^2\right)$$
$$\cdot\,\bar{x}^2\left(\bar{\beta} + \sqrt{\frac{\bar{\psi}}{\bar{x}}}\right)^3 d\bar{x}\ , \qquad (7)$$

adopting the value of the ionization potential of H atom $e^2/2a_0 = 13.53\,\mathrm{eV}$. The integrand converges fortunately in such a way as $\lim x^{1/2}\log x \to 0$ at $x = 0$, while $\log|E(x)|$ alone is in its turn singular there. The dependence of $\bar{E}_{\mathrm{TFD}}$ on atomic number Z is given in TABLE I as well as in Fig. 1.

TABLE I. *Dependence of the mean excitation energy of the* TFD *atom* $\bar{E}_{\mathrm{TFD}}$ *in* eV *on atomic number* Z *for* $Z=1$ *to* 92, *Eq.* (7).

Z	$\bar{E}_{\mathrm{TFD}}$	Z	$\bar{E}_{\mathrm{TFD}}$	Z	$\bar{E}_{\mathrm{TFD}}$	Z	$\bar{E}_{\mathrm{TFD}}$	Z	$\bar{E}_{\mathrm{TFD}}$
1	11.8	21	136.3	41	280.9	61	441.2	81	614.2
2	17.9	22	143.1	42	288.6	62	449.6	82	623.2
3	23.8	23	149.9	43	296.3	63	458.0	83	632.1
4	29.5	24	156.8	44	304.0	64	466.4	84	641.1
5	35.3	25	163.8	45	311.8	65	474.9	85	650.1
6	41.2	26	170.8	46	319.7	66	483.3	86	659.2
7	47.2	27	177.8	47	327.5	67	491.8	87	668.2
8	53.1	28	184.8	48	335.4	68	500.3	88	677.3
9	59.2	29	191.9	49	343.4	69	508.9	89	686.4
10	65.3	30	199.0	50	351.3	70	517.5	90	695.6
11	71.5	31	206.2	51	359.3	71	526.1	91	704.8
12	77.7	32	213.5	52	367.4	72	534.9	92	714.1
13	84.0	33	220.8	53	375.5	73	543.6		
14	90.2	34	228.2	54	383.6	74	552.3		
15	96.5	35	235.6	55	391.7	75	561.1		
16	102.9	36	243.1	56	399.9	76	569.9		
17	109.5	37	250.6	57	408.1	77	578.7		
18	116.2	38	258.1	58	416.3	78	587.5		
19	122.9	39	265.7	59	424.6	79	596.4		
20	129.6	40	273.3	60	432.9	80	605.3		

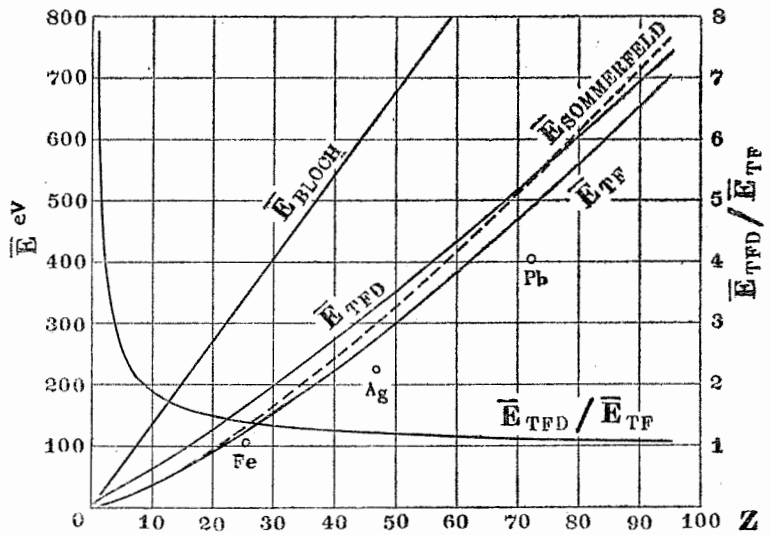

Fig. 1. The mean excitation energy of the TFD atom, $\bar{E}_{\mathrm{TFD}}$, Eq. (7), as a function of atomic number Z, compared with that of the TF one $\bar{E}_{\mathrm{TF}}$ Eqs. (2) and (8). ○'s are that calculated from the X-ray spectra by SOMMERFELD for Fe, Ag and Pb.

The 4/3–power of Z in Eq. (3) is arising directly from Z/μ, so that the exp-part in Eq. (6) represents the additional Z-dependence of $\bar{E}_{\mathrm{TFD}}$ in comparison to $\bar{E}_{\mathrm{TF}}$, i. e. the discrepancy of the TFD atom from the TF one, which is embodied by the $\bar{E}_{\mathrm{TFD}}/\bar{E}_{\mathrm{TF}}$ vs. Z curve given in Fig. 1. The discrepancy is more conspicuous in the limit $Z\to 0$, where the $\bar{E}$ vs. Z curve is tangent for the TFD atom to the $\bar{E}$ axis, as seen from TABLE II or Fig. 2, and for the TF atom

TABLE II. *Dependence of the mean excitation energy of the* TFD *atom* $\bar{E}_{\mathrm{TFD}}$ *in* eV *on atomic number* Z *at small values of* Z.

Z	$\bar{E}_{\mathrm{TFD}}$
0.00182	3.45
0.00715	3.76
0.02004	4.07
0.04711	4.50
0.1001	5.13
0.2007	6.11
0.3896	7.63
0.7479	10.13

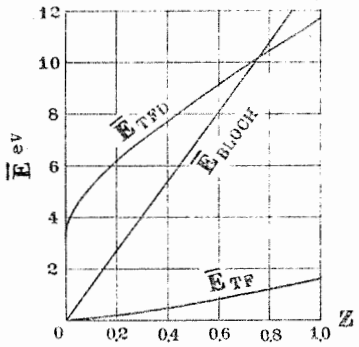

Fig. 2. Characteristic discrepancy of the mean excitation energy of the TFD atom from that of the TF one at small values of atomic number.

to the Z axis as it follows from Eq. (3). This is a characteristic difference between these two models. Since β vanishes in the limit $Z\to\infty$, the $\bar{E}_{\mathrm{TFD}}$ curve has to run asymptotically into the $\bar{E}_{\mathrm{TF}}$ curve. This is the case, however, not for Eq. (3) which cut the $\bar{E}_{\mathrm{TFD}}$ curve at a finite value of Z, as shown by the broken line in Fig. 1, but for the alternative formula

$$\bar{E}_{\mathrm{TF,exact}} = 1.621\, Z^{4/3}\,\mathrm{eV}\,, \qquad (8)$$

which was reevaluated by us exactly by the use of the MIRANDA[8] table of the TF function.

Now we see that the TFD atom does not much improve the accord with the experimental values calculated from the X-ray spectra by SOMMERFELD, in comparison to the TF one. It may be due to that the finite extension of the TFD atom is not effective since the mean excitation energy is contributed principally from the inner atomic shells in contrary to the case of the diamagnetic susceptibility[9].

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