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The Atomic Radius of the Thomas-Fermi-Dirac Atom*

By

Kwai UMEDA

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Using the accurate table of the Thomas-Fermi-Dirac function published recently, the atomic radius of the Thomas-Fermi-Dirac atom has been calculated as a function of the atomic number. The discrepancy from that of the Thomas-Fermi atom is of the order of several %.

The atomic radius, i.e. the radius for the maximum radial density in an atom is a primary quantity in the treatment of the screening effect. For example, in the case of the Bremsstrahlung Bethe(1) has taken an approximate value for the Thomas-Fermi atom

$$a \sim Z^{-\frac{1}{3}} a_{H} . \qquad (1)$$

For the Thomas-Fermi-Dirac atom, the atomic radius measured in the Fermi unit, x_a (T.F.D.), is the root of the following equation obtained by the differentiation of $D(r)$, eq. (25a)(2a),

$$3x\psi' + \psi + 4\beta\sqrt{x\psi} = 0, \qquad (2)$$

where ψ is the Thomas-Fermi-Dirac function and β is the Thomas-Fermi-Dirac parameter. We have evaluated it for the neutral atoms by the use of our accurate table of the Thomas-Fermi-Dirac function(2). The obtained values decrease slowly as the atomic number increases, as plotted in Fig. 1, while the Thomas-Fermi atom has for any atomic number a constant value

$$x_a \text{ (T.F.)} = 0.3857653 \text{ (Matsukuma}^{(3)}), \qquad (3)$$

* Physical Quantities of the Thomas-Fermi-Dirac Atom, No. 2.

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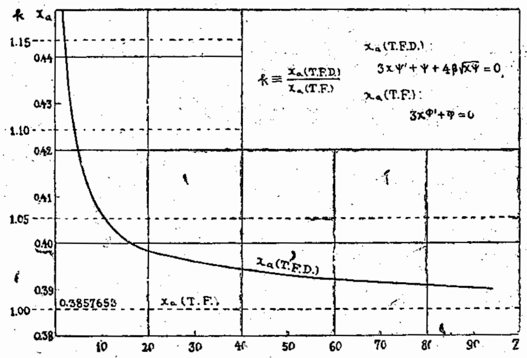

Fig. 1 Atomic radius of the Thomas-Fermi-Dirac atom in the Fermi unit as a function of the atomic number.

which is the root of the equation containing the Thomas-Fermi function φ

$$3\,x\,\varphi' + \varphi = 0 \qquad (4)$$

and is to be naturally the asymptotic value of x_a (T.F.D.) in the limit $Z = \infty$.

Conveniently we can write down

$$a\,(\text{T.F.D.}) = k \cdot a\,(\text{T.F.}) = k \cdot 0.34153 \cdot Z^{-\frac{1}{3}} \cdot a_{\text{H}}, \qquad (5)$$

where $k = x_a\,(\text{T.F.D.}) / x_a\,(\text{T.F.}) = 1.24 \sim 1.01$ for $Z = 1 \sim 92$.

The discrepancy factor k predominates only for lighter elements and makes a (T.F.D.) approach slightly more to that of the Hartree model in comparison to a (T.F.), as seen from the extrem case given in the following table.

TABLE I *Atomic radii a of the lightest atoms in the unit of the Bohr radius a_{H}.*

Atom	T.F.	T.F.D	Hartree
H	0.342	0.425	1
He	0.271	0.314	0.6 [4]

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References

(1) H. A. BETHE: *Proc. Camb. Phil. Soc.*, **30** (1934), 524.

(2) K. UMEDA: *Journ. of the Fac. of Sci., Hokkaidô Univ., Ser.* II, **3** (1942), 171.

(2a) K. UMEDA: *Journ. of the Fac. of Sci., Hokkaidô Univ., Ser*, II, **3** (1949), 245.

(3) New calculation by Prof. MATSUKUMA in Tôhoku University. We are indebted to his private communication. At first we have obtained the value 0.386 by the use of Miranda's table of the Thomas-Fermi function.

(4) D. R. HARTREE: *Proc. Camb. Phil. Soc.*, **24** (1928), 89.

Institute of Theoretical Physics,
Faculty of Science, Hokkaidô University.