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Angular Momentum Distributions in the Thomas-Fermi and Thomas-Fermi-Dirac Models of the Atom

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The angular momentum distributions in the Thomas-Fermi and Thomas-Fermi-Dirac models of the atom are calculated by an improved method proposed previously. The maximum energy $(E_l)_{max}$ for a given orbital angular momentum state is not neglected and is treated as an eigenvalue by the WKB method.

The effective central field potentials in terms of the universal approximate Thomas-Fermi function proposed by Latter are utilized. The determination of the maximum energy $(E_l)_{max}$ and, therefore, the number of electrons n_l for a given angular momentum state l is greatly facilitated by the term values computed by Latter; The calculated angular momentum distributions are checked with the diagrams of term values against Z given in the Latter's paper to assure that our proposed method prouduces no appreciable error.

Comparing with the empirical data, we then find that the accuracy of the Thomas-Fermi-Dirac model is far better than that of the Thomas-Fermi model. The prediction of the first appearance of the s, p, d and f electrons by the Thomas-Fermi-Dirac model is almost perfectly exact.

I. INTRODUCTION

It has been believed that the problem of how many electrons of a given angular momentum $l\hbar$ are to be found in an atom of a given atomic number Z is not subject to treatment by the statistical model, because in this model the electrons have a continuous distribution in angular momentum. In the previous paper[1], however, we have shown that the problem can be almost exactly solved by the WKB method, once the exact form of potential $V(r)$ for the atom is given. The number of electrons n_l with a given angular momentum $l\hbar$ may be determined from the following equation:

$$n_l = \frac{2(2l+1)}{h}\left[2\int\sqrt{m[(E_l)_{max} - V(r)] - \frac{(l+\frac{1}{2})^2\hbar^2}{r^2}}\,dr + \frac{h}{2}\right], \tag{1}$$

where the maximum energy $(E_l)_{max}$ for a given angular momentum state involved in the WKB integral

1) J. L. Hwang, Chinese J. Phys. 1, 74 (1963)

$$2\int\sqrt{2m[(E_l)_{max}-V(r)]-\frac{(l+\frac{1}{2})^2\hbar^2}{r^2}}\,dr=(N-\frac{1}{2})h, \qquad (2)$$

N-1, 2, 3,·····,

should be determined as an eigenvalue. At a glance, it seems that the Eqn (1) spoils the statistical 'nature of the model. However, as mentioned in the footnote of the previous paper, the additional labor required in evaluating the Eqn (2) is practically limited within a small amount.

In the present paper an application of Eqn (1) will be made to the Fermi-Thomas model and also to the Fermi-Thomas-Dirac model of the atom.

II. ATOMIC POTENTIALS

The effective central held potentials used in the present calculation are cited below from the paper of Latter[2], in which he has made accurate fits to these potentials.

(a) The Thomas-Fermi Potential

$$V(r)=Zr\Phi(r/\mu)/r, \text{ if } V(r)>e/r.$$
$$V(r)=0, \text{ otherwise.} \qquad (3)$$

(b) The Thomas-Fermi-Dirac Potential

$$V_{ex}(r)=\frac{3\sqrt{2}}{4\pi}\frac{Z^{1/2}e}{a_0^{1/2}}\frac{[\Phi(r/\mu)]^{1/2}}{r^{1/2}}, \text{ for } V_{ex}(r)>e/r. \qquad (4)$$
$$V_{ex}(r)=e/r, \text{ otherwise.}$$

Here the universal Thomas-Fermi function $\Phi(r/\mu)$ is approximated to

$$\Phi(r/\mu)=[1+0.02747(r/\mu)^{1/2}+1.243(r/\mu)-0.1486(r/\mu)^{3/2}+0.2302(r/\mu)^2$$
$$\cdots\cdots+0.007298(r/\mu)^{5/2}+0.006944(r/\mu)^3]^{-1}, \qquad (5)$$

$\mu=0.8853a_0/Z^{1/3}$, and a_0 is the Bohr radius. The maximum error in Eqn (3) is less than 0.3 percent and that in Eqn (4) is within 5 percent.

III ANGULAR MOMENTUM DISTRIBUTIONS

The main reason for adopting the potentials Eqs (3) and (4) is that the eigenvalues of the Schrödinger equation with these potentials have been calculated by Latter with use of an electronic computer. These eigenvalues serve us the first guess for determining $(E_l)_{max}$ of Eqn (2), and facilitate us greatly when evaluating the integral. Furthermore, the diagrams of the term value *vs.* the atomic number Z furnish us with a good standard, for checking the calculated n_l's. The results are illustrated in Figs 1-4, where the angular momentum distributions for both models of the atom are compared with the exact one. The latter is determined from the empirical data of the ground state electron

2) R. Latter, Phys. Rev. 99, 510 (1955)

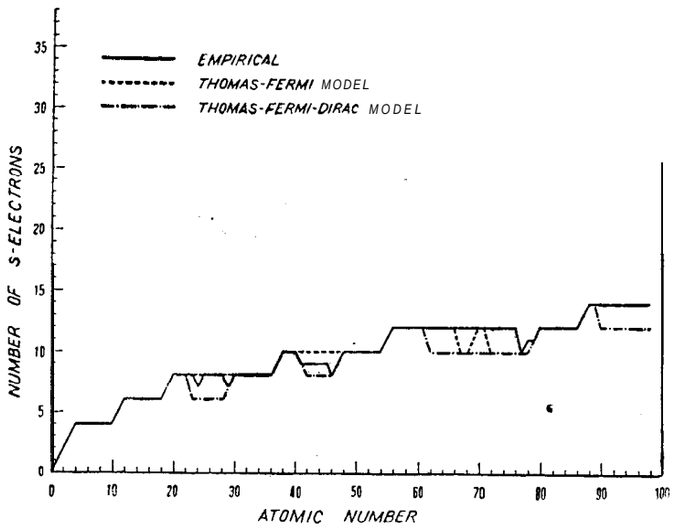

Fig. I. Number of *s* electrons in an atom of a given atomic number **Z.** In the Thomas-Fermi and **Thomas-Fermi-**Dirac Models, only the deviation from the empirical value is illustr-ated.

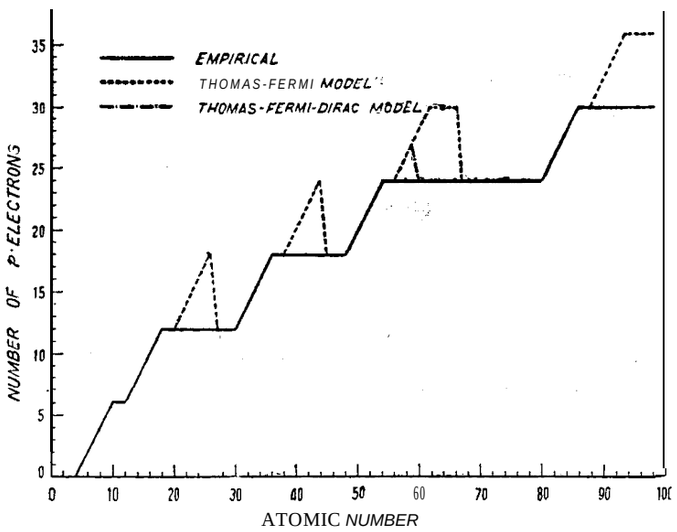

Fig. 2. Number of *p* electrons in an atom of a given atomic Number **Z. In the** Thomas-Fermi and **Thomas-**Fermi-Dirac Models, only the deviation from the empirical value is illustrated.

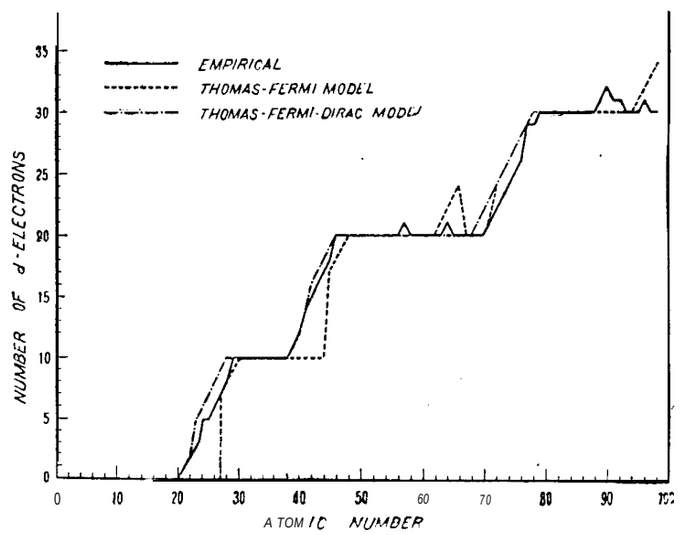

Fig. 3. Number of *d* electrons in an atom of a given atomic number **Z.** In the Thomas-Fermi and Thomas-Fermi-Dirac Models, only **thc** deviation from the empirical **valuc** is **illustratcd.**

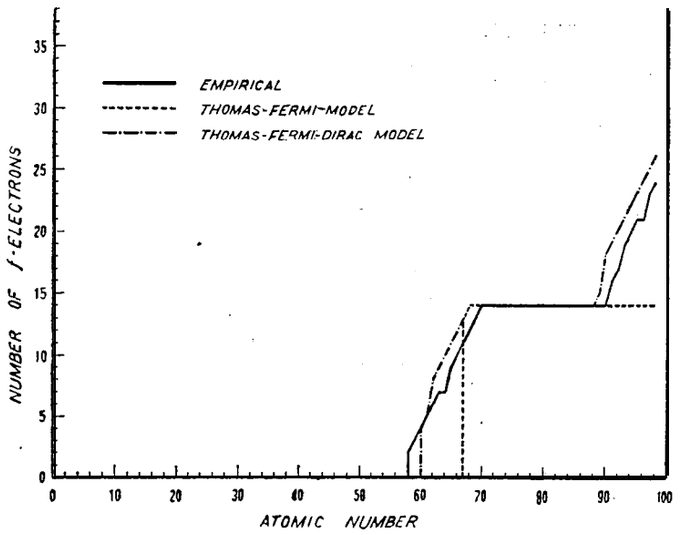

Fig. 4. Number of f electrons in an atom of a given atomic Number Z. In the Thomas-Fermi and Thomas-Fermi-Dirac Models, only the deviation from the empirical value is illustrated.

configuration of the elements given in the text of Condon and Shortley[3]. Since the calculated distributions agree exactly with those predicted from the Latter's diagrams over almost the whole range of Z, we can assure that the use of our proposed Eqn (1) does not yield any appreciable error. Therefore, the discrepancy existing between the calculated and empirical ones merely means the inherent defects in each model of the atom.

On viewing the Figs. 1—4 we readily notice that the accuracy of the Thomas-Fermi-Dirac model is far better than that of the Thomas-Fermi model. For the case of Thomas-Fermi model there are four spurious peaks in the distribution of p electrons. It is these peaks that make the appearence of $3d, 4d, 4f$ and $5f$ electrons lag behind the empirical values. On the other hand, for the case of Thomas-Fermi-Dirac model the distributions are all in good conformity with the empirical data, apart from a slight lead of appearence of $5d$ and $5f$ electrons and a slight lag of that of $4f$ and 7s electrons. This is the important result of the exchange effect among the electrons which Oliphant has attempted to show.[4]

ACKNOWLEDGMENT

A grant from the National Council on Science Development is gratefully acknowledged.

3) E. U. Condon and G. H. Shortley, The *Theory of Atomic Spectra* (University Press, Cambridge, 1935)

4) T. A. Oliphant, Jr. Phys. Rev. **104, 954 (1956)**