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Angular Momentum Distributions in the Thomas-Fermi Model

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We reinvestigate the problem of how many electrons (protons and neutrons) of a given orbital angular momentum $l\hbar$ are to be found in an atom (a neuclens) of a given atomic number Z (proton number Z or neutron number A-Z). We point out the sources of errors inherent to this problem including the arbitrariness in selecting the manner of angnlar momentum assignment, and further show that the problem is essentially equivalent to the evaluation of WKB integral if we want the exact result. The maximum energy $(E_l)_{max}$ of a given angular momentum state l should be determined as an eigenvalue. In this sense the present freatment strictly considers the quantized nature of angular momentum.

Two hypothetical 'models of nuclei with an average potential of the harmonic oscillator and of the square well obeying the previously reported rules of nuclear radii are treated both by an improved method and the original Fermi's method. The results are compared with the exact values to show the superiority of the new method.

I INTRODUCTION

THE problem of how many electrons of a given orbital angular momentum $l\hbar$ are to be found in an atom of a given atomic number Z was first treated by Fermi.[1] Later, Yang[2] made an application of this problem to the atomic nuclei to find the relation between the shell structure and the first appearence of particle of higher angular momentum. Since then several authors[3),4),5),6)] have reinvestigated this problem and discussed the reliability of the calculation. They found that there is some arbitrariness in selecting the manner of angular momentum assignment and also that in order to find the best manner to fit the empirical data reasonably well we must rely upon a sufficient "juggling".

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[2] L. M. Yang, Proc. Phys. Soc. (London) 64, 632 (1951)

[3] J. H. D. Jensen and J. M. Luttinger, Phys. Rev. 86, 907 (1952)

[4] W. R. Theis, Z. Physik **140,** 1 (1955)

[5] D. Ivanenko and S. Larin, Doklady Akad. Nauk (S. S. S. R.), 88, 45 (1953); S. I. Larin, J. Exptl. Theoret Phys. (U. S. S. R.) **28,** 498 (1955)

[6] T. A. Oliphant, Jr. Phys. Rev. **104, 954** (1956)

In this paper we point out the sources of errors inherent to this problem including the above mentioned arbitrariness, and further show that the problem is essentially equivalent to the evaluation of WKB integral. The problem can be exactly solved without use of juggling if we evaluate the integral. Two hypothetical models of neucleus with an average potential of the harmonic oscillator well and also of the square well are treated both with an improved method and the original Fermi's method. The results are then compared with the theoretically predicted values to show the superiority of the improved' method.

II FORMULATION AND APPROXIMATIONS

In order to obtain a deeper insight into the problem and in turn to obtain clues for improving the methods we reformulate the theory in a way somewhat different from the earlier work. Let us take the independent particle picture for the atom or for the atomic nucleus. A partide moving in an average field $V(r)$ in the spherical polar coordinates has the energy for a given orbital angular momentum state I:

$$E_l = \frac{p^2}{2m} + V(r) = \frac{1}{2m}(p_{\rho l}^2 + p_{\theta l}^2) + V(r),$$

where the kinetic energy is divided into two parts, the "radial kinetic energy $p_{\rho l}^2/2m$" and the "kinetic energy of rotation $p_{\theta l}^2/2m = l^2\hbar^2/2mr^2$." Solving for the "radial momentum $P_{\rho l}$", we get

$$p_{\rho l} = \sqrt{2m[E_l - V(r)] - \frac{l^2\hbar^2}{r^2}} = \sqrt{p_l^2 - \frac{l^2\hbar^2}{r^2}}.$$

Since in the latter arguments only the state of maximum energy or of maximum momentum will concern us, $p_{\rho l}$ will be used throughout in the following sense:

$$p_{\rho l} = \sqrt{2m[(E_l)_{max} - V(r)] - \frac{l^2\hbar^2}{r^2}} = \sqrt{(P_l)_{max} - \frac{l^2\hbar^2}{r^2}}.$$

The particle density $\rho(r)$ at a point of the ordinary space is obtained by dividing the volume in momentum space into cells of volume h^3, namely,

$$\rho(r) = \frac{8\pi}{h^3}\int_0^{l_{max}\hbar/r} p_{\rho l}\, p_{\theta l}\, dp_{\theta l} \tag{1}$$

$$= \frac{8\pi}{h^3}\int_0^{l_{max}\hbar/r} \sqrt{(P_l)_{max} - p_{\theta l}^2}\cdot p_{\theta l}\, dp_{\theta l}. \tag{2}$$

The earlier methods started from the latter Eqn. (2);

$$\rho(r) = \frac{8\pi}{h^3}\sum_{l=0}^{l_{max}}\int_{l\hbar/r}^{(l+1)\hbar/r} \sqrt{(P_l)_{max} - p_{\theta l}^2}\, p_{\theta l}\, dp_{\theta l} \tag{3}$$

$$= \frac{8\pi}{h^3}\sum_{l=0}^{l_{max}}\left[\left((P_l)^2_{max} - \frac{l^2\hbar^2}{r^2}\right)^{3/2} - \left((P_{l+1})^2_{max} - \frac{(l+1)^2\hbar^2}{r^2}\right)^{3/2}\right]. \tag{3}$$

The maximum momentum $(P_l)_{max}$ depends in general on l. If. we neglect this fact

and let

$$(P_l)_{max} = P_0 \text{ for any } l, \tag{4}$$

then p(r) becomes the familiar expression

$$\rho(r) = (8\pi/3h^3)\, P_0^3(r). \tag{5}$$

Multiplying Eqn (3) by $4\pi r^2 dr$ and integrating over the appropriate space, we have the number of particles having the given angular momentum $l\hbar$,

$$n_l = \frac{8\pi}{h^3}\int\left[\left(P_0^2 - \frac{l^2\hbar^2}{r^2}\right)^{3/2} - \left(P_0^2 - \frac{(l+1)^2\hbar^2}{r^2}\right)^{3/2}\right]4\pi r^2\, dr. \tag{6}$$

Fermi[1] and Theis[4] used this form of angular momentum assignment. However, Jensen and Luttinger[3] replaced l by $\{[l(l+1)]^{1/2}+[l(l-1)]^{1/2}\}/2$, and Oliphant[6] l^2 by $l(l+1)$. While, Yang[2] and Ivanenko and Larin[5] both used $l+{}^1/_2$ instead of l.

The following approximations made in the above treatment have spoiled the precision of calculation:

(i) The approximation Eqn. (4) is most sensitive to the calculation. $(P_l)_{max}$ variates l by l. As will be seen latter for the case of square well potential, the extent of variation sometimes becomes different by a factor 2.

(ii) Replacement of l^2 is also sensitive, especially to the case of small l.

(iii) The use of $P_0(r)$ determined from $\rho(r)$ in Eqn (5), i.e. the use of

$$P_0(r) = \sqrt{2m(E_l)_{max} - V(r)} = (3\hbar^3/8\pi)^{1/3}\rho(r)^{1/3} \tag{7}$$

should be done with a precaution. The usual omission of $(E_l)_{max}$ in Eqn (7) may produce considerable errors.

III WKB INTEGRAL AND IMPROVED METHOD

We would rather start from Eqn (1) than from Eqn **(2).** Eqn (1) becomes

$$\rho(r) = \frac{8\pi}{h^3}\sum_{l=0}^{l_{max}} p_{\rho l}\int_{l\hbar/r}^{(l+1)\hbar/r} p_{\theta l}\, dp_{\theta l} = \frac{4\pi}{h^3}\sum_{l=0}^{l_{max}}(2l+1)\frac{\hbar^2}{r^2}p_{\rho l},$$

and thus the number of particles within a thin spherical shell of radius r and thickness dr is given by

$$dn = 4\pi r^2\rho(r)dr = 4\pi r^2 dr\,\frac{4\pi}{h^3}\sum_{l=0}^{l_{max}}(2l+1)\,\frac{\hbar^2}{r^2}\,p_{\rho l}.$$

Integrating over the space yields the total number of particles

$$n = \sum_{l=0}^{l_{max}}\frac{2(2l+1)}{h}\cdot 2\int p_{\rho l}\, dr$$

$$= \sum_{l=0}^{l_{max}}\frac{2(2l+1)}{h}\cdot 2\int\sqrt{2m[(E_l)_{max} - V(r)] - \frac{l^2\hbar^2}{r^2}}\; dr. \tag{8}$$

The individual term in the summation of Eqn (8),

$$n_l = \frac{2(2l+1)}{h}\oint p_{\rho l}\, dr, \tag{9}$$

represents the number of particles with angular momentum $l\hbar$. The integral is the

well known WKB integral. Thus the calculation of n_l is essentially equivalent to the evaluation of WKB integral. $(E_l)_{max}$ should be found beforehand from the condition

$$\oint p_{\rho l}\, dr = (N - \frac{1}{2})\, h, \qquad (10)$$
$$N = 1, 2, 3, \cdots,$$

that is, $(E_l)_{max}$ should be treated as the eigenvalue. Following the advice of Langer we had better replace l^2 in- the square root by $(l+{}^1/_2)^2$. On observing the condition Eqn (10), we notice that Eqn (9) will not give the exact value of n_l; we should add the correction term $h/2$ to the right side of Eqn (9), namely

$$n_l = \frac{2(2l+1)}{h}\left[2\int\sqrt{2m[(E_l)_{max} - V(r)] - \frac{(l+{}^1/_2)^2\hbar^2}{r^2}}\, dr + \frac{h}{2}\right] \qquad (11)$$

Therefore, once if the eigenvalue $(E_l)_{max}$ and in the same time N are found[7], the exact value of n_l may be readily obtained from

$$n_l = 2(2l+1)\ N. \qquad (11)'$$

Since N is an integer, Eqn (11) or (11)' is correct only when all the energy levels are completely filled up to constitute the lowest energy state as permitted by the Pauli exclusion principle. However, the maximum lnergy level or the top level is not always completely occupied. Even for such case Eqn (11) or (11)' still gives the values as if the imcomplete level is completely occupied. Therefore the number of particles on the maximum energy level should be determined by checking the calculated total number Σn_l with the known value which has already given prior to the calculation.

Now the approximations mentioned in the last paragraph of the previous section have been improved in Eqn (11). In some problems in which the form of potential is not given, such as in the case of atoms, we have no alternative but to use the particle density and the relation

$$-V(r) = (3h^3/8\pi)^{2/3}\rho^{2/3}(r)/2m. \qquad (7)'$$

However, no serious error will arise when it is used in the Eqn (11) as far as $(E_l)_{max}$ is treated as an eigenvalue.

IV ILLUSTRATIVE EXAMPLES

(a) Harmonic Oscillator Well

We suggest a set of hypothetical nuclei in which nucleons move in an average potential of the harmonic oscillator

$$V(r) = -V_0 + \frac{1}{2}m\omega^2 r^2.$$

For simplicity we let $V_0 = 42$ Mev for all nuclei and determine ω from the relation

$$\hbar\omega = (2\nu/R^2)\hbar^2/2m,$$

where ν denotes the number of protons (or neutrons) and R the equivalent uniform

[7] **Practically very accurate evaluation of $(E_l)_{max}$ and the integral is not necessary. What we need is only the order for which we can guess the integer N.**

radius. We assume further that ν and R obey the rules proposed previously by the present author.*)

Table 1. Number of protons (or neutrons) with a given orbital angular momentum $l\hbar$ moving in a hypothetical nuclear potential of the harmonic oscillator

Number of protons ν	radius (fm)	$\hbar\omega$ (Mev)	l	$n_l=2(2l+1)n_p$ (improved)	$v_0=V_0/\hbar\omega$ (V_0=42Mev)	$n_l=2(2l+1)n_p$ (original)	$n_l=2(2l+1)n_p$ (exact)
2	2.500	16.72	0(s)	1×2	2.512	1.506×2	1x2
8	3.500	12.80	0(s)	1×2	3.281	1.891 x2	1x2
			1(P)	1×6		1.391 x6	1x6
20	4.509	10.32	0(s)	2×2	4.070	2.285 x 2	2x2
			1(p)	1×6		1.785×6	1x6
			2(d)	1×10		1.285×10	1x10
40	5.542	8.508	0(s)	2×2	4.937	2.719x2	2x2
			1(P)	2×6		2.219x6	2x6
			2(d)	1×10		1.719×10	1x10
			3(f)	1×14		1.219x 14	1x14
70	6.625	7.144	0(s)	3×2	5.879	3.190×2	3x2
			1(P)	2×6		2.690 x6	2x6
			2(d)	2x10		2.190×10	2x10
			3(f)	1x14		1.590×14	1x14
			4(g)	1x18		1.190×18	1x18
112	7.685	6.194	O(s)	3x2	6.781	3.641 x2	3x2
			1 (P)	3x6		3.141 x6	3x6
			2(d)	2x10		2.641 x 10	2x10
			3(f)	2x14		2.141 x14	2x14
			4(g)	1x18		1.541 x 18	1x18
			5(h)	1x22		1.041 x22	1x22

Now the WKB integral can be evaluated analytically, if considering that

$$E=\left(\Omega+\frac{3}{2}\right)h\omega. \quad \Omega=0,1,2,3\cdots.$$

It becomes

$$\oint p_{rl}\,dr=\pi\left[\frac{(\Omega+\frac{3}{2})h\omega}{\omega}-\left(l+\frac{1}{2}\right)\hbar\right]=\frac{h}{2}(\Omega-l+1).$$

8) J.L. Hwang, Chinese J. Phys. 1, 24 (1963) and also 1, 30 (1963)

Since, as is well known, $\Omega = 2n_p + l - 2$, where $n_p = 1, 2, 3 \cdots$ is the radial quantum number, we have $n_l = 2\,(2l+1)\,n_p$.

If we let $(E_l)_{max} = 0$ as was done in the earlier work, then we have

$$n_l = 2\,(2l+1)\left(\frac{v_0}{2} - \frac{l}{2} + \frac{1}{4}\right) \text{ with } v_0 = \frac{V_0}{\hbar\omega}.$$

As shown in Table 1, this approximation produces larger values of n_l.

(b) Square Well

As an example for the case of utilizing particle density p(r), we suppose another set of hypothetical nuclei of uniform density

$$\begin{cases} \mathrm{p(r)} = \nu / \frac{4}{3}\pi R^3 = \text{const.}, & r < R \\ \rho(r) = 0, & r > R. \end{cases}$$

The number of particle ν and the equivalent uniform radius R again obey our proposed rules. Then, by the relation Eqn. (7)′, we have

$$\begin{cases} V(r) = -(9\pi/4)^{2/3}(\hbar^2/2mR^2)\,\nu^{2/3} = \text{const.}, & r < R \\ V(r) = 0, & r > R. \end{cases} \tag{12}$$

The WKB integral may also be evaluated analytically for this case;

$$\frac{1}{h}\oint p_{\rho l}\,dr = \frac{1}{\pi}\,\frac{1}{\sqrt{\delta}}\left[\sqrt{(E_l)_{max} - V - \zeta} - \sqrt{\zeta}\cos^{-1}\left(\frac{\zeta}{E-V}\right)^{1/2}\right],$$

$$\text{where } \delta = \hbar^2/2mR^2 \text{ and } \zeta = (l + {}^1/_2)^2\delta.$$

$(E_l)_{ma.2}$ should be found from the solutions of the transcendental equation obtained by letting the right hand side equal to (N- $^1/_2$). For convenience sake, however, we adopt the readings from the diagram of Green's paper[9] as their substitutes. In this diagram only two or three significant figures are available Neverthless, as listed in Table 2, where the values for (l/h) $\oint p_{\rho l}\,dr + {}^1/_2$ are listed instead of n_l, the results are all in the neighbourhood of the exact values.

Finally we illustrate the result of approximation $(E_l)_{max} = 0$ for each l. As in our potential Eqn. (12) the maximum energy level cannot come just to its top, we lessen the depth of potential so as to make the maximum energy $(E_l)_{max}$ be zero. Calculations with the usual omission of $(E_l)_{max}$ are made and again listed in Table 2. Even with the above modification of potential, the results are still disappointing.

The application to realistic nuclei and to the case of atom with use of solutions of Thomas-Fermi equation will be reported in another paper.

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[9] A. E. S. Green, and K. Lee, Phys. Rev. 99, 772 (1955)

Table 2. Number of protons (or neutrons) with a given orbital angular momentum $l\hbar$ moving in a hypothetical nuclear potential of square well

Number of protons ν	radius (fm)	V_0 (Mev)	$(E_l)_{max}-V_0$ (Mev)	l	$n_l=2(2l+1)n_p$ (improved)	$(E_l)_{max}-V_0$ (V_0 modified)	$n_l=2(2l+1)n_p$ (original)	$n_l=2(2l+1)n_p$ (exact)
2	2.50	19.56	16.7	O(s)	0.980×2	16.7	0.980 x 2	1x2
8	3.50	25.14	10.2	0(s)	1.05 x2	20.5	1.36 x2	1x2
			20.5	1(p)	0.958x6		0.958x6	1x6
18	4.33	28.17	7.46	O(s)	1.09 x2	24.3	1.75 x2	1x2
			15.0	1(P)	1.02 x6		1.31 x6	1x6
			24.3	2(d)	0.954 x 10		0.954 x 10	1 x 10
34	5.27	29.07	20.9	0(s)	1.94 x2	26.0	2.13 x2	2x2
			11.0	1(P)	1.10 x6		1.73 x6	1x6
			18.0	2(d)	1.01 x10		1.29 ×10	1×10
			26.0	3(f)	0964x14		0.964x 14	1x14
58	6.25	29.54	16.0	0(s)	2.00 x2	26.8	2.51 x2	2x2
			23.5	1(P)	1.91 x6		2.05 x6	2x6
			13.5	2(d)	1.05 ×10		1.64 ×10	1x10
			19.8	3(f)	1.02 xl4		1.28 x14	1x14
			26.8	4(g)	0.974 x 18		0.974 x 18	1x18
90	7.18	29.98	27.2	O(s)	2.86 x.2	27.7	2.89 x2	3x2
			18.8	1(P)	1.97 x6		2.43 x6	2x6
			25.7	2(d)	1.91 ×10		2.00 x10	2x10
			15.6	3(f)	1.05 xl4		1.62 x14	1x14
			21.3	4(g)	1.02 x18		1.22 x18	1x18
			27.7	5(h)	0.989 x 22		0.989 x 22	1x22
132	8.10	30.40	22.6	O(s)	2.94 x2	28.3	3.20 x2	3x2
			15.4	1(P)	2.01 x6		2.79 x6	2x6
			21.0	2(d)	1.96 ×10		2.36 ×10	2x10
			27.2	3(f)	1.91 xl4		1.99 x 14	2x14
			17.3	4(g)	1.05 x 18		1.60 x18	1x18
			22.5	5(h)	1.02 x22		1.28 x22	1x22
			28.3	6(i)	0.999×26		0.999 x 26	1x26
28	5.00	28.34	22.6	0(s)	191 x2	23.2	2.11 x2	2x2
			12.1	1(P)	1.06 x6		1.66 x 6	1x6
			19.5	2(d)	0.998 x 10		1.27 ×10	1×10
			28.2	3(f)	0.945 x 14		0.945x14	8*

* This is determined by checking the calculated total number $\Sigma n_l \approx 34$ with the given value 28.

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