Indian Journal of Pure & Applied Physics
Vol. 40, June 2002, pp. 393-395

Thomas-Fermi calculations for atoms in high magnetic field using realistic model

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Received 3 October 2001; accepted 10 April 2002

An approximate solution of the Thomas-Fermi equation for positive ions in a high magnetic field is obtained by making use of the variational principle. The radial wavefunctions of the hydrogen-like atom are used as the trial function that contains some variational parameters and satisfies the appropriate boundary and the normalization conditions. These parameters are determined by extemalizing the variational expression with respect to the parameters. These parameter values are then used to obtain the desired physical quantities. The initial slope of the variational trial function for several ions is obtained from which the energy and the ionization energy can be found. The results of the present calculation are in good agreement with those available in literature.

1 Introduction

The Thomas-Fermi model has proved to be useful in the study of atoms and molecules, specially for those with numerous electrons. The model has also been applied to atoms in external fields and dense plasma. In particular, it has been studied extensively for high magnetic field[1-7] because of possible astrophysical implications connected with the emission of electrons and ions from pulsars.

The dimensionless Thomas-Fermi equation in a strong magnetic field is:

$$\Phi(x)'' = (x\Phi)^{1/2} \qquad \ldots(1)$$

$$r = \sigma x = a_0 2^{-3/5}\pi^{2/5}\beta^{4/5}Z^{1/5}L^{-2/5}x \qquad \ldots(2)$$

where β is the fine-structure constant, $L = eB/m^2 = B/B_c$, $B_c = 4.4\times10^{13}$ G and B is the magnetic field. Eq. (1) must be solved for a positive ion subject to the subsidiary conditions:

$$N = \int n\,dv \qquad \ldots(3)$$

which becomes:

$$\Phi(x_0) - x_0\Phi'(x_0) = 1 - \frac{N}{Z} \qquad \ldots(4)$$

and

$$\Phi(0) = 1 \qquad \ldots(5)$$

Here N is the number of electrons and x_0 is the finite radius of the ion that can be approximated by[7]:

$$x_0\left(\frac{N}{Z}\right) = \left(\frac{N}{Z}\right)^k \sum_{n=0}^{\infty} a_{on}\left(\frac{N}{Z}\right)^n \qquad \ldots(6)$$

where $k = \frac{2}{5}$. Eq. (6), after truncating the summation at $n = 5$, has been used in[7] as a basis of a fit to the numerical results in Table 1.

Table 1 — a_{mn} Coefficients of Eq. (6)

n	a_{0n}	a_{1n}	a_{2n}
0	2.87489	-1.40287	1.56067
1	-5.99637	4.329990	-6.9774
2	15.45998	-6.22789	13.60648
3	-16.65557	4.40984	-12.29400
4	7.00010	-1.22091	4.20405

For a free state:

$$\Phi(x_0) = 0 \qquad \ldots(7)$$

The Thomas-Fermi energy in this case is:

$$E_{TF}(Z,N,B) = -2^{8/5}\pi^{-2/5}\beta^{-4/5}Z^{9/5}L^{2/5}\Sigma(Ry)$$

$$= -98.2215\,Z^{9/5}L^{2/5}\Sigma(Ry) \qquad \ldots(8)$$

where Σ is expressed in terms of the slope at the origin as:

Table 2 — Values of the variational parameters and the initial slope of the potential $\Phi'(0)$ for the present work and that of Ref. [2] with $N = Z-1$

Z,N	α	a	b	c	$\Phi'_B(0)$	$-\Phi'(0)$	x_0
2,1	0.133	11.380575	-0.380575	0		1.064528	589426
3,2	0.1254	-4.607553	5.607553	0		1.003221	1.867362
4,3	0.1234	-5.875527	6.875527	0		0.987084	2.016265
5,4	0.116	-23.67647	24.57647	0.171	0.9420177	0.927164	2.114369
6,5	0.116	-24.28203	25.28203	0.173	0.9409322	0.9270449	2.185827
7,6	0.116	-24.92332	25.92332	0.176	0.9403313	0.9269436	2.24082
8,7	0.115	-26.53282	27.53282	0.1845	0.9399638	0.9188281	2.284666
9,8	0.1148	-27.25937	28.25937	0.1886	0.9397284	0.9171476	2.320522
10,9	0.1146	-28.0398	29.03980	0.11936	0.939565	0.9154705	2.350423

Table 3 — Values of the variational parameters and the initial slope of the potential $\Phi'(0)$ for the present work and that of Ref. [2] with $N=Z-2$

Z,N	α	a	b	c	$\Phi'_B(0)$	$\Phi'(0)$	x_0
5,3	0.11516	-20.22497	21.22479	0.1794598	0.9575471	0.9209874	1.754516
6,4	0.11655	-20.33035	21.33035	0.16678	0.9501936	0.9319674	1.867362
7,5	0.11652	-21.35922	22.35922	0.16638	0.946438	0.9315977	1.950834
8,6	0.11668	-21.85503	22.85503	0.16517	0.944276	0.9327824	2.016265
9,7	0.11618	-22.93527	23.93527	0.16898	0.942920	0.9286819	2.069631
10,8	0.116	-23.5731	24.5731	0.1709599	0.942017	0.9271637	2.114369

$$\Sigma = -\frac{5}{9}\left(\Phi'(0) + \frac{\left(1-\frac{N}{Z}\right)^2}{x_0}\right) \qquad \ldots(9)$$

The electron density is obtained from the zero-field Thomas-Fermi equation as:

$$n(r) = a_0^{-3} 2^{-1/5} \pi^{-11/5} \beta^{12/5} Z^{2/5} L^{6/5} [\Phi(x)/x]^{3/2} \qquad \ldots(10)$$

which is used to obtain some of the atomic properties such as the ionization energy, the expectation values, $< r^j >$, (j is an integer) and the magnetic susceptibilities. In section 2, the variational principle is made use of, to obtain an equivalent solution to Eq. (1). The radial wavefunctions of the hydrogen-like ions are used as the trial wavefunctions, where an approximate $\Phi(x)$ is formed. Using this method, one can study the properties of positive ions. In section 3, the results are listed and discussed.

2 The Model

Instead of solving Eq. (1) exactly with the boundary conditions (4) and (5), the variational principle is made use of as:

$$\delta L(\Phi) = \delta \int_0^\infty F(\Phi, \Phi', x)\mathrm{d}x = 0 \qquad \ldots(11)$$

where

$$F(\Phi, \Phi', x) = \frac{1}{2}\Phi'^2 + \frac{2}{3}\Phi(x\Phi)^{1/2} \qquad \ldots(12)$$

The variational principle in Eq. (11) is equivalent to the differential equation [Eq. (1)] as can be seen[8] by substituting F into the Euler-Lagrange equation:

$$\frac{\partial}{\partial \Phi}F - \frac{\partial}{\partial x}\frac{\partial}{\partial \Phi'}F = 0 \qquad \ldots(13)$$

where, from Eq. (13) the TF equation results.

It is known that, the electron density has a decaying exponential behaviour at large distances, so the problem is to select a trial function, which assures this behaviour and at the same time satisfies

the boundary conditions. A large class of functions is admissible; therefore in choosing one, a form is resorted to, which permits simplicity in calculations. The choice of the radial wavefunctions of hydrogen-like ions as the trial function seems to satisfy this criterion.

The density of a hydrogen-like ion is of the form:

$$n(r) = \sum_{n=1}^{N} R_{nl}(r)^2 \qquad \ldots(14)$$

where

$$R_{1s}(r) = \sqrt{a}e^{-\alpha r}, R_{2s}(r)\sqrt{b}(1-\alpha r)e^{-\alpha r},$$
$$R_{2p}(r) = \sqrt{c}re^{-\alpha r} \qquad \ldots(15)$$

with $\alpha, a, b, c...$ as the variational parameters of the variational principle described by Eq. (11), subject to the restrictions imposed by the boundary conditions.

Eq. (10) can be rewritten as:

$$\Phi(x) = \gamma n x n(r)^2 \qquad \ldots(16)$$

Instead of using the exact form of $\Phi(x)$ as in Eq. (16) an approximate solution will be used, which permits simplicity in calculations:

$$\Phi(x) = n(x, \alpha, a, b, c, ...)^2 \qquad \ldots(17)$$

Using the trial functions in Eq. (17) one calculates $F(\Phi, \Phi', x)$ by means of Eq. (13).

3 Results and Discussion

The TF equation was solved using the variational principle for $N = Z - 2$ and $N = Z - 1$ in the range of $1 < Z < 10$. The results are given in Tables 2 and 3. They contain all the information needed for calculating the energies and the atomic sizes, using Eqs (8-9) and (2). The variational principle requires L of Eq. (12) to be extremum. The parameters which satisfy this condition together with the initial slope, $\Phi'(0)$, are listed in the tables. For the purpose of comparison, $\Phi'_B(0)$ have also been listed which is the initial slope[2]. The comparison shows that, $\Phi'(0)$ and $\Phi'_B(0)$ are in good agreement and the percentage error is between 1.5 and 3.5. To simplify the calculation, one can take $c = 0$ in Eq. (15). For more accurate results, one can take it into consideration. The universal solution corresponding to neutral atoms $(N = Z)$ is found to be 0.906700.

To conclude, in this work, a method has been proposed for solving the Thomas-Fermi equation for positive ions in a high magnetic field using the variational principle. The high point of approach in this paper is, application of the radial wavefunction of hydrogen-like ions as the trial wavefunction, which ensures that the electronic density is finite at the origin, decays exponentially with r and incorporates the shell structure. A comparison of the present results with earlier calculations shows that, the proposed method is simple and promising.

Acknowledgement

The authors are grateful to their colleague Prof I Ahmad for his valuable remarks and for checking the manuscript.

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