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APPROXIMATE ANALYTICAL SOLUTION OF THE THOMAS-FERMI-AMALDI EQUATION FOR NEGATIVE IONS IN A SUPERSTRONG MAGNETIC FIELD

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Abstract: An approximate analytical solution of the Thomas-Fermi-Amaldi equation for negative ions in a superstrong magnetic field is obtained by making use of an equivalent variational principle. It is possible because the TFA model for these ions is expressed by a differential equation of the same form as these of the Thomas-Fermi model for neutral atoms in a superstrong magnetic field. Then we can use the same variational principle for the TFA equation for negative ions as that used in obtaining an approximate analytical solution of the TF equation for neutral atoms. The approximate analytical solutions obtained through this model are then used to calculate total energies for several negative ions and a comparison with the TF model is made.

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I.- INTRODUCTION

The existence of magnetic fields amounting to 10 G caused great interest in the investigation of electron-binding energy for atoms and molecules in strong magnetic fields (1). Properties of matter at the surface of a neutron star, where superstrong magnetic fields exist, should be very different from those of ordinary matter since energies associated with the magnetic motion of electrons become much larger than their Coulomb energies (2).

We get a great increase in the binding energy because the electrons are much more likely to be found near the binding nucleus. The usual shell structure of heavier atoms dissapears, and the minimum ionization energy of the neutral atoms decreases slowly and monotonically with increasing atomic number Z.

The statistical theory of atoms in a magnetic field, developed by Kadomtsev (3), offers the simplest way to investigate these quantities. The TFA model (4) differs from the TF model (5) by the Fermi-Amaldi correction (4). One of the shortcomings of the TF theory is the fact that one electron interacts not only with the remaining electrons but also with itself. The FA correction is an attempt to remove this self-interaction from the TF theory. As a consequence, the TFA equation has a solution for singly charged negative ions, while the TF equation has no such solution. In a recent work, an approximate analytical solution of the TF differential equation for atoms in a superstrong magnetic field have been found (6), by making use of an equivalent variational principle.

It is the aim of this article, to obtain approximate analytical solutions of the TFA equation for singly charged negative ions in a superstrong magnetic field by making use of the same equivalent variational principle. This is possible by the fact that the TFA model for the ions that we are going to study can be expressed by a differential equation of the same form as that which describes the TF model for neutral atoms mentioned above. The solutions are then used to calculate total energies of those negative ions and a comparison with the TF model is made.

II.- THEORY

The physical idea behind the FA correction lies in the fact that in an N-electron atom described by an electron density ρ, each electron is assigned a density of ρ / N. If this choice is valid, the potential resulting from (N - 1) electrons at the position of the nth electron is of the form

$$V_{ee}^{*}(r) = -(N-1)\, e \int \rho(r') / |r - r'|\, dV \qquad (1)$$

$$V_{ee}^{*}(r) = ((N-1)/N)\ V_{ee}(r) \qquad (2)$$

where Vee(r) is the potential at the position r in the TF theory, and e is the magnitude of the electron charge. Then, the FA correction would be more significant for lighter atoms than for heavier ones, because from Eq. (2), it is seen that when N increases, V_{ee}^{*} goes to Vee.

In Reference (6), the steps involved in the derivation of the TF equation are described in detail, and when the same steps are redone with Eq. (2), the result is the TFA equation in a superstrong magnetic field

$$\varphi'' = (x\,\varphi)^{1/2} \qquad (3)$$

where the primes refer to the second derivatives of φ with respect to the variable x, that is defined by (6)

$$r = ao\,\beta^{*} x \tag{4}$$

and r stands for the distance from the nucleus of an atom of atomic number Z.

In Eq. (4), ao is the Bohr radius and β^{*} is a constant defined by

$$\beta^{*} = (N/(N-1))^{2}\,\beta \tag{5}$$

where β is another constant given by

$$\beta = 2^{-1/5}\,\pi^{2/5}\,(B/Bo)^{2/5}\,Z^{1/5} \tag{6}$$

In Eq. (6), B is the magnetic field under study and Bo is a reference magnetic field

$$Bo = \hbar\,c\,/\,2\,e\,ao^{2} = 1.17 \times 10^{9}\ G \tag{7}$$

In terms of φ, the total potential within an atom is given by

$$V = (Ze/r)\,\varphi + Vo \tag{8}$$

where Vo is a constant defined by

$$Vo = (Z-N+1)\, e / ro \tag{9}$$

with ro denoting the "radius" of the atom.

The electron density within an atom is given, in terms of φ, by

$$\rho = (Z/3\, L^{5}\, ao\, \beta^{*})^{1/2}\; (N/(N-1))\; (\varphi(x)/x)^{1/2} \tag{10}$$

where L is related with the magnetic field B through

$$L^{5} = (8\, \pi^{4}/3)\; ao^{5}\; (B/Bo)^{2} \tag{11}$$

The boundary conditions for Eq. (2) are given by

$$\varphi(0) = 1 \tag{12}$$

$$\varphi(xo) = 0 \tag{13}$$

and the subsidiary condition

$$xo\, \varphi'(xo) = -\,(Z-N+1)/Z \tag{14}$$

where xo is a constant defined by

$$r_0 = ao\, \beta^{*}\, x_0 \tag{15}$$

For a singly charged ion we have Z = N - 1, and Eqs. (13) and (14) become

$$\varphi(\infty) = 0 \qquad (16)$$

and

$$\varphi'(\infty) = 0 \qquad (17)$$

In Ref. (2) and (6), the TF equation for atoms in a strong magnetic field is given by

$$\psi'' = (y\psi)^{1/2} \qquad (18)$$

where the variable y is defined by

$$r = a_0\beta y \qquad (19)$$

The boundary conditions for Eq. (18) are given by

$$\psi(0) = 1 \qquad (20)$$

$$\psi(y_0) = 0 \qquad (21)$$

and

$$y_0\,\psi'(y_0) = -(Z-N)/Z \qquad (22)$$

where yo is defined by Eq. (19) with $\beta^{\bullet}$ replaced by β.

We see that Eqs. (18), (20) and (21) are independent of the magnetic field, and the same equations and Eq. (22) will also be independent of Z for neutral atoms (N = Z), and then we get a universal solution for all such atoms when yo $\rightarrow \infty$.

Therefore, Eqs. (21) and (22), become

$$\psi(\infty) = 0 \tag{23}$$

and

$$\psi'(\infty) = 0 \tag{24}$$

The boundary conditions for the TF differential equation for neutral atoms in a superstrong magnetic field, given by Eqs. (20), (23) and (24) are identical with the boundary conditions for a singly charged negative TFA ion, defined by Eqs. (12), (16) and (17).

This implies that the TFA electron density of a singly charged negative ion runs out to infinity, and shows the same behaviour as that of the electron density of a neutral atom in a superstrong magnetic field.

In Ref. (6) Equation (18) has been solved aproximately by an equivalent variational principle, that for the present TF case can be stated as

$$L(\psi) = \int_0^\infty F(\psi, \psi', y)\, dy \qquad (25)$$

where the prime on ψ refers to the derivative of ψ with respect to y.

If we choose for F the expression

$$F(\psi, \psi', y) = (1/2)(\psi')^2 + (2/3)\, \psi^{3/2}\, y^{1/2} \qquad (26)$$

and then substituing Eq. (26) into the Euler-Lagrange equation given by

$$\frac{\partial}{\partial y}(\partial F / \partial \psi') - \partial F / \partial \psi = 0 \qquad (27)$$

results in Eq. (18), the TF equation for neutral atoms in a superstrong magnetic field.

The trial function has the form

$$\psi = (1 - p\, y + q\, y^2)^2\, e^{-0.57\, y^2} \qquad (28)$$

where the parameters appearing in Eq. (28) are given by

$$P = 0.466427 \qquad Q = 0.04991447 \qquad (29)$$

With this considerations, one realizes that Eq. (3) can also be solved approximately by making use of Eq. (27) if instead of Eq. (28), one uses the trial solution

$$\varphi = (1 - p\,x + q\,x^2)^2\, e^{-0.5\,P x^2} \qquad (30)$$

which upon consideration of Eqs. (4) and (5), can also be written as

$$\varphi = (1 - p\,h + q\,h^2)^2\, e^{-0.5\,P h^2} \qquad (31)$$

with $h = ((N-1)/N)^2\ (r/ao\beta)$.

Equation (31) is to be contrasted with Eq. (28), which by means of Eq. (19) can also be written as

$$\psi = (1 - p\,j + q\,j^2)^2\, e^{-0.5\,P J^2} \qquad (32)$$

with $j = r/ao\beta$.

Comparison of Eq. (21) with Eq. (32) shows that the FA correction manifests itself in the appearance of the factor $((N-1)/N)^2$, or powers of it, multiplying the variational parameters P and Q.

As N increases, this factor tends to unity, and the importance of the TFA correction diminishes with increasing N.

III.- DISCUSSION

Having obtained approximate analytical solutions of the

TFA equation for singly charged negative ions, we now want to calculate total energies for several ions and to compare these results with those which belong to the same ions in the TF model.

The virial theorem for the Thomas-Fermi model for atoms in a superstrong magnetic field is given by the following relationship:

$$3\,K = (-1/2)\,(V_{en} + V_{ee}) \tag{33}$$

$$K = (-1/9)\,V_{en} \qquad V_{ee} = (-1/3)\,V_{en} \tag{34}$$

where K is the kinetic energy of the electrons, Ven is the electron-nucleus potential energy and Vee is the electron-electron potential energy.

The total energy is

$$E = K + V_{en} + V_{ee} = (-1/9 + 1 - 1/3)\,V_{en} = (5/9)\,V_{en} \tag{35}$$

From Ref. (2) and (6), it has been shown that

$$V_{en} = -\,2^{6/5}\,\pi^{-2/5}\,Z^{9/5}\,(B/B_o)^{2/5}\,E_o\,f(N,Z) \tag{36}$$

where $E_o = \epsilon^2/2\,a_o = 13.6$ eV and

$$f\,(N,Z) = (\psi'(0) + (1 - N/Z)^2/x_o) \tag{37}$$

For xo running to ∞, the total energy is then

$$E = -2^{6/5}\pi^{-2/5}Z^{9/5}(B/Bo)^{2/5}\,Eo\,\epsilon \qquad (38)$$

where

$$\epsilon = -(5/9)\,\psi'(0) \qquad (39)$$

Considering Eq. (2), we can write the total energy in the TFA model as follows

$$E = \left[-1/9 + 1 - 1/3\,((N-1)/N)\right] Ven \qquad (40)$$

and from Eq. (31)

$$\varphi'(0) = -2\,p\,((N-1)/N)^2 \qquad (41)$$

Then

$$E = -2^{6/5}\pi^{-2/5}Z^{6/5}(B/Bo)^{2/5}\,Eo\,\epsilon' \qquad (42)$$

with

$$\epsilon' = \left[8/9 - 1/3\,((N-1)/N)\right] 2\,p\,((N-1)/N)^2 \qquad (43)$$

Results for total energies for several ions according to this model are shown in Table I.

We cannot estimate in detail the accuracy of the expressions obtained for lack of exact data. Nevertheless, we can point several trends like the great increase in total energy with the magnetic field and that this energy increases with increasing atomic number Z.

Due to the fact that the description of negative ions in a strong magnetic field have not been reported up to date, and taking into account that we cannot make comparison with other theoretical results, then we can say that the analytical approximations quoted here to the TFA model are not the last word.

Possibilities for further theoretical work, as an alternative to the present model , are now being done in our laboratories and results will be published elsewhere in a forthcoming paper.

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TABLE I - TOTAL ENERGIES (KeV) FOR SEVERAL IONS IN A SUPERSTRONG MAGNETIC FIELD ACCORDING TO THE THOMAS-FERMI-AMALDI MODEL.

$B(10^{12}\,G)$	0.1	0.5	1	5	10	50
$-E(F^-)$	2.72	5.18	6.83	13.01	17.16	32.67
$-E(Cl^-)$	9.17	17.47	23.05	43.87	57.90	110.2
$-E(Br^-)$	35.09	66.80	88.15	167.8	221.4	421.5
$-E(I^-)$ p	75.10	142.9	188.6	358.9	473.6	901.6

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6.- M. D. Glossman and E. A. Castro (to be published).