

## Thomas-Fermi Theory for Atoms in a Strong Magnetic Field

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Along the general scheme of Sondheimer and Wilson, the kinetic energy density of an electron gas under constant magnetic field is expressed as a functional of the electron density at absolute zero of temperature. On this basis, the statistical theory for atoms in a magnetic field is formulated, which includes the theory developed by Banerjee et al. as an extreme of high magnetic field. Some numerical results on the atomic radius, the total energy etc. are also shown for free neutral Ne atom.

### § 1. Introduction

Since it became a widely accepted hypothesis that magnetic fields of the order  $10^{12}\sim 10^{13}G$  exist on the surface of pulsars, the properties of atoms under high magnetic field attract a great attention of many physicists. While the problem is rather clear, that is, the Hamiltonian is clearly given, solving the Schrödinger equation seems to be a fairly difficult task. Even for the Hydrogen atom under magnetic field we do not yet know its exact solution.

For many electron atoms, only some preliminary calculations<sup>1),2)</sup> were reported on the basis of the statistical atom model. Recently, Banerjee, Constantinescu and Reháč<sup>3)</sup> have developed a statistical theory of the atom in a fairly complete form. However, their expression of the kinetic energy as a functional of electron density is still based on the adiabatic hypothesis. In other words it is assumed that the electrons move in Landau orbitals in the direction perpendicular to the magnetic field and the Coulomb field due to nucleus has an effect only on the motion parallel to the magnetic field. Although the Thomas-Fermi equation they obtained is very simple and shows many elegant characters, we cannot help wondering how exact the adiabatic hypothesis holds.

On the other hand, Sondheimer and Wilson,<sup>4)</sup> in their elegant article concerning the diamagnetism of free electrons, developed a general and exact scheme of the calculation of the density matrix, the partition function, the free energy, etc. Although they retained only the leading terms for their purpose, if one performs the calculation without any neglect of small terms, one could get an exact relation between the kinetic energy density and the electron density, on which the statistical theory of atoms is constructed.

Along the line stated above, we will here show an alternative form of the

statistical theory of atoms. The theory should include the one developed by Banerjee et al. and the usual non-magnetic Thomas-Fermi theory as an extreme of high magnetic field and that of zero magnetic field, respectively.

In § 2, we will calculate the kinetic energy density as a functional of the electron density on the general scheme of Sondheimer and Wilson. The Thomas-Fermi theory is developed in § 3, where it is also proved that the equation derived by Banerjee et al. is the limiting case of high magnetic field. The numerical calculation is carried out for free neutral Ne atom. These results are discussed in § 4.

## § 2. The density functional formula of the kinetic energy

In order to construct the statistical theory of an atom under magnetic field, we should first of all have an expression of the kinetic energy density as a functional of the electron density. We can follow the procedure given by Sondheimer and Wilson.<sup>4)</sup> They retained only the leading terms in calculating the susceptibility of free electron gas, but now we should obtain the energy density and the electron density without any neglect. The reason for this will become clear by later discussion.

The Hamiltonian of a free electron in a uniform magnetic field  $\mathbf{H}$  directed to the  $z$ -axis is given by

$$\mathcal{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{e\hbar}{imc}\mathbf{A}\cdot\nabla + \frac{e^2}{2mc^2}\mathbf{A}^2, \quad (2.1)$$

where  $\mathbf{A} = (-Hy/2, Hx/2, 0)$  is the vector potential,  $-e$  the electronic charge,  $m$  the electron mass. Throughout this paper, we use the atomic unit  $e = m = \hbar = 1$ , and the most commonly used unit for  $H$ ;  $\mu_0 H / \text{Ry} = \gamma$  ( $\mu_0 = \text{Bohr magneton}$ ,  $H = 2.3478 \times 10^9$  Gauss for  $\gamma = 1$ ). Then Eq. (2.1) becomes simply

$$\mathcal{H} = -\frac{1}{2}\nabla^2 + \frac{\gamma}{2}L_z + \frac{1}{8}\gamma^2(x^2 + y^2). \quad (2.2)$$

Using this Hamiltonian, Sondheimer and Wilson calculated the free energy per unit volume of a free electron gas, which is expressed as follows:

$$F - n\zeta = \int_0^\infty z(E) \frac{\partial f_0}{\partial E} dE, \quad (2.3)$$

where  $n$  is the electron density,  $\zeta$  Fermi energy,  $f_0$  Fermi-Dirac distribution function

$$f_0 = \frac{1}{\exp[(E - \zeta)/kT] + 1}, \quad (2.4)$$

and  $z(E)$  is the inverse Laplace transform of the partition function

$$z(E) = \left(\frac{1}{2\pi}\right)^{3/2} \left\{ \frac{8}{15\sqrt{\pi}} E^{5/2} - \frac{1}{3\sqrt{\pi}} \left(\frac{\gamma}{2}\right)^2 E^{1/2} \right\}$$

$$\begin{aligned}
 & + \frac{1}{\pi} \left(\frac{\gamma}{2}\right)^{5/2} \int_0^\infty \left(\frac{1}{y^{7/2}} - \frac{1}{6y^{3/2}} - \frac{1}{y^{5/2} \sinh y}\right) e^{-2yE/\gamma} dy \\
 & - 2 \left(\frac{\gamma}{2}\right)^{5/2} \sum_{k=1}^\infty \frac{(-1)^k}{(k\pi)^{5/2}} \cos\left(\frac{2k\pi E}{\gamma} - \frac{\pi}{4}\right) \Big\}. \tag{2.5}
 \end{aligned}$$

It should be noted that the spin degeneracy is not taken into account in Eq. (2.3).

Now, at absolute zero of temperature,  $\partial f_0/\partial E = -\delta(E - \zeta)$ , then Eq. (2.3) becomes

$$F - n\zeta = -\frac{2^{3/2}}{15\pi^2} \zeta^{5/2} \left\{ 1 - \frac{5}{8} \xi^{-2} + \frac{15}{8\sqrt{\pi}} \xi^{-5/2} F_2(\xi) - \frac{15}{4\pi^2} \xi^{-5/2} G_2(\xi) \right\}, \tag{2.6}$$

where

$$F_2(\xi) = \int_0^\infty \left[ \frac{1}{y^{7/2}} - \frac{1}{6y^{3/2}} - \frac{1}{y^{5/2} \sinh y} \right] e^{-\xi y} dy, \tag{2.7}$$

$$G_2(\xi) = \sum_{k=1}^\infty \frac{(-1)^k}{k^{5/2}} \cos\left(k\pi\xi - \frac{1}{4}\pi\right) \tag{2.8}$$

and

$$\xi = 2\zeta/\gamma. \tag{2.9}$$

Differentiating Eq. (2.6) with respect to  $\zeta$ , and using the condition  $\partial F/\partial \zeta = 0$ , we obtain the electron density expression:

$$n = \frac{1}{6\pi^2} \gamma^{3/2} \xi^{3/2} f(\xi), \tag{2.10}$$

where

$$f(\xi) = 1 - \frac{1}{8} \xi^{-2} - \frac{3}{4\sqrt{\pi}} \xi^{-3/2} F_1(\xi) + \frac{3}{2\pi} \xi^{-3/2} G_1(\xi), \tag{2.11}$$

$$F_1(\xi) = \int_0^\infty \left[ \frac{1}{y^{5/2}} - \frac{1}{6y^{1/2}} - \frac{1}{y^{3/2} \sinh y} \right] e^{-\xi y} dy \tag{2.12}$$

and

$$G_1(\xi) = \sum_{k=1}^\infty \frac{(-1)^k}{k^{3/2}} \sin\left(k\pi\xi - \frac{1}{4}\pi\right). \tag{2.13}$$

Since  $F$  in Eq. (2.6) gives just the kinetic energy density  $\varepsilon_k$  at  $T=0$ , we have from Eqs. (2.6) and (2.10)

$$\varepsilon_k = \frac{1}{20\pi^2} \gamma^{5/2} \xi^{5/2} g(\xi), \tag{2.14}$$

$$\begin{aligned}
 g(\xi) = & 1 + \frac{5}{24} \xi^{-2} - \frac{5}{4\sqrt{\pi}} \xi^{-3/2} F_1(\xi) - \frac{5}{4\sqrt{\pi}} \xi^{-5/2} F_2(\xi) \\
 & + \frac{5}{2\pi} \xi^{-3/2} G_1(\xi) + \frac{5}{2\pi^2} \xi^{-5/2} G_2(\xi). \tag{2.15}
 \end{aligned}$$

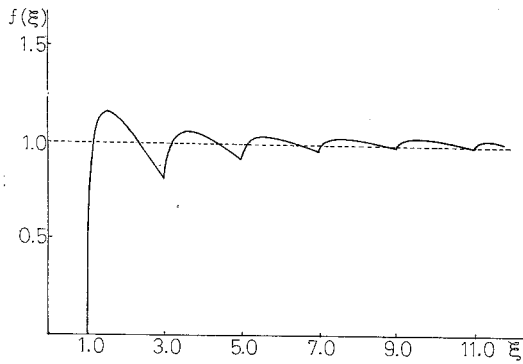


Fig. 1. The behavior of  $f(\xi)$ .

Equations (2.10) and (2.14) are the required relation which connects the kinetic energy density  $\varepsilon_k$  and the electron density  $n$ , through the parameter  $\xi$ .

Since the minimum eigenvalue of the Hamiltonian (2.2) is  $\gamma/2$ ,<sup>5)</sup>  $\xi$  varies from 1 to  $\infty$ . The behavior of  $f(\xi)$  is shown in Fig. 1. It is clear from Eq. (2.11) that  $f(\xi)$  tends to 1 as  $\xi \rightarrow \infty$ . Also we see in Appendix A that  $f(\xi)$  approaches zero as  $3\sqrt{\xi}-1$  for  $\xi \rightarrow 1$ . The

wavy character of the variation of  $f(\xi)$ , which is also found in  $g(\xi)$ , is the origin of the de Haas-van Alphen effect.

For  $\gamma \rightarrow 0$ ,  $\xi$  becomes infinity, so that  $f(\xi)$  and  $g(\xi)$  tend to 1. Eliminating  $\xi$  from Eqs. (2.10) and (2.14),  $\varepsilon_k$  is rewritten as

$$\varepsilon_k = \frac{3}{10} (3\pi^2)^{2/3} 2^{2/3} n^{5/3}. \quad (2.16)$$

We have the well-known relation for a degenerate electron gas, on which the usual Thomas-Fermi theory is based. The factor  $2^{2/3}$  originates from the fact that here the spin degeneracy is not taken into account.

On the other hand, for  $\gamma \rightarrow \infty$ ,  $\xi$  tends to 1. Using the relations

$$\frac{d\varepsilon_k}{dn} = \frac{d\varepsilon_k/d\xi}{dn/d\xi} = \frac{\gamma}{2} \xi \quad (2.17)$$

and

$$n \rightarrow \frac{\sqrt{2}}{\pi^2} \left( \frac{\gamma}{2} \right)^{3/2} (\xi - 1)^{1/2} \quad \text{for } \xi \rightarrow 1 \quad (\text{see Appendix A}), \quad (2.18)$$

we have

$$\varepsilon_k = \frac{\gamma}{2} \int_0^n \xi dn = \frac{\gamma}{2} n + \frac{2\pi^4}{3\gamma^2} n^3. \quad (2.19)$$

The first term is the zero point energy of  $n$  electrons and the second is just the same expression given by Banerjee et al.

### § 3. The Thomas-Fermi equation

Let us take an atom with the atomic number  $Z$  and the electron number  $N$ , and let it be in a uniform magnetic field of strength  $\gamma$  directed to the  $z$ -axis. All electron spins are assumed to be antiparallel to the magnetic field, and the

energy due to spin magnetic moments is omitted in the following calculation as a constant. In accordance with Banerjee et al., we define the energy of the atom  $E$  as  $E = E_t - \gamma N/2$ ,  $E_t$  being the total energy of the system and  $\gamma N/2$  the zero point energy. In other words,  $E$  is defined as the energy of all the electrons bound together by the nucleus minus their energy when they are free but still in the magnetic field. In the realm of the Thomas-Fermi approximation it is given by

$$E = E_k + E_n + E_e, \tag{3.1}$$

$$E_k = \int \left\{ \varepsilon_k - \frac{\gamma}{2} n(\mathbf{r}) \right\} d\mathbf{r}, \tag{3.1a}$$

$$E_n = - \int \frac{Zn(\mathbf{r})}{r} d\mathbf{r}, \tag{3.1b}$$

$$E_e = \frac{1}{2} \iint \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' d\mathbf{r}, \tag{3.1c}$$

where  $E_k$  is the total kinetic energy of the electrons subtracted by the zero point energy,  $E_n$  the potential energy due to the nucleus,  $E_e$  the electron-electron interaction energy.  $\varepsilon_k$  and  $n$  are the kinetic energy density and the number density of electrons given by Eqs. (2.14) and (2.10), where  $\xi$  or  $\zeta$  should be dependent on position  $\mathbf{r}$ . The present form of  $E_k$  is adopted simply because of the convenience for comparison with the results of Banerjee et al.

$E$  should be minimum with respect to the variation of  $n(\mathbf{r})$ , subject to the subsidiary condition

$$N = \int n(\mathbf{r}) d\mathbf{r} = \text{constant}. \tag{3.2}$$

The variational condition

$$\delta(E + V_0 N) = 0, \tag{3.3}$$

$V_0$  being the Lagrange multiplier, gives

$$\frac{\delta \varepsilon_k(\mathbf{r})}{\delta n(\mathbf{r})} - \frac{\gamma}{2} - V(\mathbf{r}) + V_0 = 0, \tag{3.4}$$

where

$$V(\mathbf{r}) = \frac{Z}{r} - \int \frac{n(\mathbf{r}')^{\frac{1}{2}}}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' \tag{3.5}$$

is the total electrostatic potential at position  $\mathbf{r}$ .

By the use of Eq. (2.17), Eq. (3.4) can be written as

$$\hat{\xi} = 1 + \frac{V(\mathbf{r}) - V_0}{\gamma/2}. \tag{3.6}$$

Equation (3.6) and the Poisson equation

$$\nabla^2 V(\mathbf{r}) = 4\pi n = \frac{2}{3\pi} \gamma^{3/2} \xi^{3/2} f(\xi) \quad (3.7)$$

are the basic equations for determining  $V(\mathbf{r})$ .

In the following, we assume that the solution  $V(\mathbf{r})$  of Eqs. (3.6) and (3.7), then  $n(\mathbf{r})$  too, is spherically symmetric\*<sup>1)</sup> because there are no quantities explicitly dependent on the direction of the magnetic field. If we put

$$V(r) - V_0 = \frac{Z}{r} \varphi(r), \quad (3.8)$$

Eqs. (3.7) and (3.6) are transformed as follows:

$$\frac{d^2 \varphi}{dr^2} = \frac{2\gamma^{3/2}}{3\pi Z} r \xi^{3/2} f(\xi), \quad (3.9)$$

where

$$\xi = 1 + \frac{2Z}{\gamma r} \varphi(r). \quad (3.10)$$

Equation (3.9) is the Thomas-Fermi equation for an atom in a magnetic field.

#### Determination of $V_0$

Although  $V_0$  might be determined by the normalization condition (3.2), it can be given by the following physical considerations. We assume that the electron distribution is confined in a sphere of radius  $r_0$ , then

$$E = \int_0^{r_0} \left\{ \varepsilon_k(r) - \frac{\gamma}{2} n(r) \right\} 4\pi r^2 dr - \int_0^{r_0} V_n(r) n(r) 4\pi r^2 dr - \frac{1}{2} \int_0^{r_0} V_e(r) n(r) 4\pi r^2 dr, \quad (3.11)$$

where

$$V_n(r) = \frac{Z}{r} \quad (3.11a)$$

and

$$V_e(r) = - \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'. \quad (3.11b)$$

After a slight manipulation,<sup>9)</sup> we have

\*<sup>1)</sup> As will be shown later, by assuming the spherical symmetry of  $V$  and  $n$ , we can set up the boundary condition consistent to the atom in free state. This means that in the Thomas-Fermi model the minimum energy of a free atom is realized by the spherically symmetric electron distribution as was pointed out by Mueller et al.,<sup>2)</sup> while the other model gives the electron distribution elongated in the direction of external magnetic field.

$$\begin{aligned} \frac{dE}{dr_0} &= 4\pi r_0^2 \left( \varepsilon_k - \frac{\gamma \xi}{2} n \right)_{r=r_0} \\ &= \frac{2}{\pi} r_0^2 \gamma^{5/2} [\xi^{5/2} h(\xi)]_{r=r_0}, \end{aligned} \tag{3.12}$$

$$h(\xi) = -\frac{1}{15} + \frac{1}{24} \xi^{-2} - \frac{1}{8\sqrt{\pi}} \xi^{-5/2} F_2(\xi) + \frac{1}{4\pi^2} \xi^{-5/2} G_2(\xi). \tag{3.13}$$

If the atom is in free state, the surface pressure or  $dE/dr_0$  should be zero and this is realized by putting  $\xi=1$  in Eq. (3.13) (see Appendix A). That is, from Eq. (3.6)

$$V_0 = V(r_0) = \frac{Z-N}{r_0}. \tag{3.14}$$

*Boundary conditions*

At  $r=0$ , from Eq. (3.8) we have as usual

$$\varphi(0) = 1. \tag{3.15}$$

For  $r \rightarrow 0$ ,  $\varphi(r) \rightarrow 1$ , then  $\xi \rightarrow 2Z/\gamma r \rightarrow \infty$ ,  $f(\xi) \rightarrow 1$ . Therefore Eq. (3.9) can be transformed into the usual Thomas-Fermi equation

$$\frac{d^2\varphi}{dx^2} = \frac{1}{2} \frac{\varphi^{3/2}}{x^{1/2}}, \tag{3.16}$$

where the unit of length is taken as  $r = \mu x$ ,  $\mu = (1/4) (9\pi^2/2Z)^{1/3}$ . The factor 1/2 on the right-hand side of Eq. (3.16) is due to the neglect of the spin degeneracy. As is apparent from Eq. (2.16), Eq. (3.16) gives also the limiting case  $\gamma \rightarrow 0$ .

At  $r=r_0$ , on the other hand,  $(dV/dr)_{r=r_0} = -(Z-N)/r_0^2$ , from which we have

$$\varphi(r_0) - r_0 \varphi'(r_0) = \frac{Z-N}{Z}. \tag{3.17}$$

In free state of the atom, owing to Eqs. (3.8) and (3.14),

$$\varphi(r_0) = 0 \tag{3.18}$$

and

$$\varphi'(r_0) = -\frac{Z-N}{Zr_0}. \tag{3.19}$$

For  $r \rightarrow r_0$ ,  $\varphi(r) \rightarrow 0$ , then  $\xi \rightarrow 1$  and  $f(\xi) \rightarrow 3\sqrt{\xi} - 1$ . Therefore Eq. (3.9) takes the form

$$\frac{d^2\varphi}{dr^2} = \frac{2^{3/2}\gamma}{\pi Z^{1/2}} (r\varphi)^{1/2}. \tag{3.20}$$

This equation allows  $\varphi$  being expanded in a power series of  $(r_0-r)$  near the

outer boundary. For neutral atoms,

$$\varphi = \frac{\gamma^2}{18\pi^2 Z} r_0 (r_0 - r)^4 + \dots \quad (3.21)$$

and the conditions (3.18) and (3.19) will be satisfied for finite  $r_0$ . The fact that the atomic radius is finite even for neutral free atom makes a sharp contrast with the usual Thomas-Fermi atom.

For positive ions,  $\varphi$  can be expanded as

$$\begin{aligned} \varphi &= b_2 (r_0 - r) + b_5 (r_0 - r)^{5/2} + \dots, \\ b_2 &= \frac{Z - N}{r_0 Z}, \quad b_5 = -\frac{2^{7/2} \gamma}{15\pi Z^{1/2}} r_0^{1/2} b_2^{1/2}, \dots \end{aligned} \quad (3.22)$$

We should notice that Eq. (3.20) is also the limiting equation for  $\gamma \rightarrow \infty$ . This may be somewhat apparent from Eq. (2.19). Changing the unit of length as  $r = \mu' x$ ,  $\mu' = (\pi^2 Z / 8\gamma^2)^{1/5}$ , we have the equation derived by Banerjee et al.

$$\frac{d^2 \varphi}{dx^2} = (x\varphi)^{1/2}. \quad (3.23)$$

Therefore it becomes clear that Eq. (3.23) is only valid for extremely large values of  $\gamma$ .

#### § 4. Numerical results and discussions

We have solved the Thomas-Fermi equation and calculated the total electronic energy of neutral Ne atom ( $Z=10$ ) for several values of  $\gamma$ . The results will be summarized here.

The equation to be solved and the boundary conditions are written as

$$\frac{d^2 \varphi}{dr^2} = \frac{2\gamma^{3/2}}{3\pi Z} r \left(1 + \frac{2Z}{\gamma r} \varphi\right)^{3/2} f \left(1 + \frac{2Z}{\gamma r} \varphi\right), \quad (4.1)$$

$$\varphi(0) = 1, \quad (4.2)$$

$$\varphi(r) \rightarrow \frac{\gamma^2}{18\pi^2 Z} r_0 (r_0 - r)^4 \quad \text{for } r \rightarrow r_0. \quad (4.3)$$

Equation (3.23) derived by Banerjee et al. does not include  $Z$  and  $\gamma$  explicitly. This means that one solution can express the solution for arbitrary  $Z$  and  $\gamma$  just by changing the unit of length. Furthermore Eq. (3.23) allows the application of the scaling method (see Appendix B), so that from an arbitrary solution which is obtained by starting from an arbitrary  $r_0$  and integrating inward, we can get the required solution just by scaling.

Equations (4.1), (4.2) and (4.3), however, could not be transformed into the form independent of  $Z$  and  $\gamma$ , and do not allow the application of the scaling method. Therefore we must solve the equation independently for each  $Z$  and  $\gamma$ .



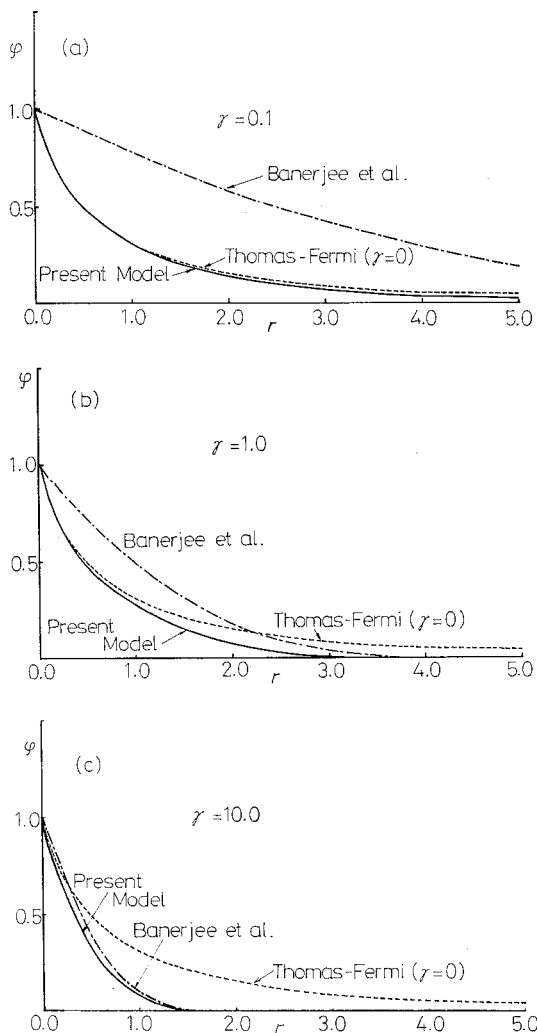


Fig. 2. The Thomas-Fermi function  $\varphi(r)$  for Ne atom. For comparison, the result of Banerjee et al. as well as the non-magnetic Thomas-Fermi function is also plotted.

(a)  $\gamma=0.1$  (b)  $\gamma=1.0$  (c)  $\gamma=10.0$

Using the value of  $\varphi$ , Eqs. (3.10) and (2.10), we can calculate the electron density  $n$ . The behavior of  $n$  against  $r$  is shown in Figs. 3(a), (b), (c). For comparison, we have solved Eq. (3.23) derived by Banerjee et al. and calculated  $n$  anew. The present results show quite a big difference from those by Banerjee et al., and also from simple Thomas-Fermi results. What is very remarkable in the present model is the wavy variation of the electron density distribution which is a reflection of that of  $f(\xi)$ . It is not so significant for smaller values of  $\gamma$  but is

Table I. Atomic radius  $r_0$  in a.u. ( $Z=10$ ).

$\gamma$	Present	Banerjee et al.
0.0	$\infty$	$\infty$
0.05	11.936	16.913
0.1	9.6314	12.818
0.5	5.7389	6.7334
1.0	4.5375	5.1029
5.0	2.5541	2.6806
10.0	1.9686	2.0315
50.0	1.0549	1.0672
100.0	0.80181	0.80876
500.0	0.42216	0.42485
1000.0	0.32003	0.32197

Starting from arbitrary  $r_0$ , we integrate Eq. (4.1) inward. If  $\varphi(0)$  is not equal to 1, we adjust  $r_0$  and solve Eq. (4.1) again until  $\varphi(0) = 1$  is satisfied.

Figures 2 (a), (b), (c) show the solution  $\varphi$  compared with those of Banerjee et al. and simple non-magnetic Thomas-Fermi, and in Table I, the values of  $r_0$  for various  $\gamma$  are tabulated. As was mentioned before, it is one of the most remarkable effects due to the magnetic field that the atomic radius becomes finite even for a neutral free atom. Although the atomic radius for the present model is a little bit smaller than that of Banerjee's model ( $r_0 = 3.2197 \cdot (Z/\gamma^2)^{1/5}$ , see Appendix B), the former approaches the latter as  $\gamma$  increases as is expected.

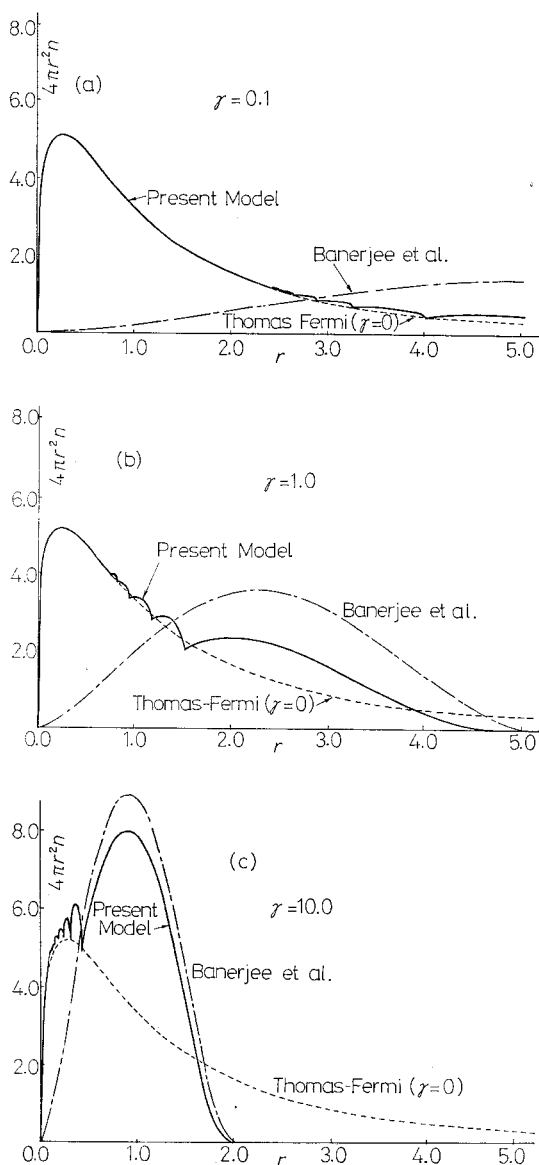


Fig. 3. The values of  $4\pi r^2 n$  for Ne atom.

For comparison, the results of Banerjee et al. as well as the non-magnetic Thomas-Fermi results are also plotted.

(a)  $\gamma=0.1$  (b)  $\gamma=1.0$  (c)  $\gamma=10.0$

amplified more and more with increasing  $\gamma$ . Also the following two features should be noticed.

(a) The electron density distribution becomes more and more similar to that of the model of Banerjee et al. as  $\gamma$  increases, while it becomes similar to that of the simple Thomas-Fermi model as  $\gamma$  decreases.

(b) For a given value of  $\gamma$ , the electron density distribution is similar to that of the simple Thomas-Fermi model near the origin, while it is similar to that of Banerjee's near the outer boundary. This can be understood from the limiting forms of the basic equation, that is, Eqs. (3.16) and (3.23).

In both usual Thomas-Fermi atom and the atom model by Banerjee et al., there exists a simple relation between the energy  $E$  and the values of  $\varphi'(0)$ . In the present model of the atom, however, we could not find any such relations, so that we have to calculate  $E$  directly by using Eq. (3.1) and the values of  $\varphi$  and  $n$  obtained above. Those values are listed in Table II.

Referring to Table II, one can recognize that the energy  $E$  of the present model and its components  $E_k$  and  $E_n$  are very large in their absolute values compared to those of Banerjee et al., while the former approaches the latter as the value of  $\gamma$  increases. This

originates from the big difference of the electron density near the nucleus in both models. As far as the ionization energy is concerned, however, we could expect that the present model would give similar results as those of Banerjee et al.

Table II. Energy values [Eq. (3.1)] ( $Z=10$ ).

$\gamma$	$E$		$E_k$		$E_n$		$E_e$	
	Present	Banerjee et al.	Present	Banerjee et al.	Present	Banerjee et al.	Present	Banerjee et al.
0.0	-104.33	0	104.33	0	-243.45	0	34.78	0
0.05	-104.57	- 9.52	104.11	1.90	-243.70	-17.14	35.02	5.71
0.1	-104.78	-12.56	103.91	2.51	-243.92	-22.62	35.23	7.54
0.5	-106.43	-23.92	102.61	4.78	-245.78	-43.05	36.74	14.35
1.0	-108.24	-31.56	101.29	6.31	-247.88	-56.81	38.35	18.94
5.0	-119.46	-60.08	95.60	12.02	-262.82	-108.14	47.76	36.05
10.0	-130.12	-79.27	91.97	15.86	-278.35	-142.69	56.26	47.56
50.0	-182.67	-150.91	83.90	30.18	-360.35	-271.64	93.78	90.55
100.0	-223.61	-199.13	83.28	39.83	-428.36	-358.43	121.47	119.48
500.0	-392.13	-379.07	99.25	75.81	-719.27	-682.33	227.89	227.44
1000.0	-509.72	-500.19	116.60	100.04	-926.64	-900.34	300.32	300.11

because the electron distribution near the outer boundary is similar to each other.

In both models the energy  $E$  and its components  $E_n$  and  $E_e$  vary monotonically with increasing  $\gamma$ . In particular, it is interesting to notice that the atomic binding energy,  $-E$ , increases with increasing magnetic field strength. The non-monotonic behavior of  $E_k$  disappears if we add the zero point energy to it.

Finally in Table III, we tabulate the total energy of the atom  $E_t$ , which exhibits a sharp contrast between both models. For Banerjee's model it can be proved that  $E_t$  has a minimum at  $\gamma=4.6814$ , while

for our model  $E_t$  increases monotonically with increasing magnetic field strength. Because we can expect from the quantum mechanical perturbation theory that the energy of the atom increases with increasing  $\gamma$  when  $\gamma$  is small, the behavior of  $E_t$  in the present model is more reasonable.

The relation between the energy variation against  $\gamma$  and the magnetic property of the atom is still an open problem, because in this model the magnetic effect is taken into account only through the local kinetic energy density. Furthermore, it is assumed at the outset that the spin orientation is fixed antiparallel to the direction of the magnetic field. Since this assumption would not be valid for small values of  $\gamma$ , the model should be improved in order to include the spin degeneracy effect. These physically interesting problems will be discussed in succeeding papers.

Table III. The total energy  $E_t$  ( $Z=10$ ):  $E_t=E+\gamma N/2$ .

$\gamma$	Present	Banerjee et al.
0.0	-104.33	0
0.05	-104.32	- 9.27
0.1	-104.28	-12.06
0.5	-103.93	-21.42
1.0	-103.24	-26.56
5.0	-94.46	-35.08
10.0	-80.12	-29.27
50.0	67.33	99.09
100.0	276.39	300.87
500.0	2107.87	2120.93
1000.0	4490.28	4499.81

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**Appendix A**

To evaluate  $f(1)$  [Eq. (2·11)],  $g(1)$  [Eq. (2·15)] and  $h(1)$  [Eq. (3·13)], we need to calculate  $F_1(1)$ ,  $F_2(1)$ ,  $G_1(1)$  and  $G_2(1)$ . Take the contour integral,

$$\int_c (-y)^{-5/2} e^{-y} dy - \frac{1}{6} \int_c (-y)^{-1/2} e^{-y} dy + 2^{3/2} \int_c \frac{(-2y)^{-3/2}}{e^{2y} - 1} d(2y), \quad (A.1)$$

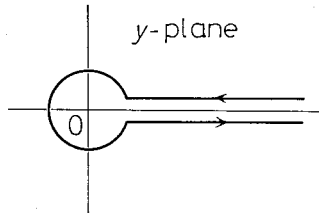


Fig.4. Contour  $C$  in Eq. (A.1).

where contour  $C$  being shown in Fig. 4. By definition of  $\Gamma$ - and  $\zeta$ -functions, (A.1) can be written as

$$\frac{2\pi}{i} \left[ \frac{1}{\Gamma(5/2)} - \frac{1}{6\Gamma(1/2)} + 2^{3/2} \frac{\zeta(-1/2)}{\Gamma(3/2)} \right]. \quad (A.2)$$

Since the contribution to the integral (A.1) from an infinitesimal circle around the origin cancels out, (A.1) can be expressed by the integral on positive real axis,

$$-2i \int_0^\infty \left[ \frac{1}{y^{5/2}} - \frac{1}{6y^{1/2}} - \frac{1}{y^{3/2} \sinh y} \right] e^{-y} dy. \quad (A.3)$$

Equating (A.2) and (A.3), we have

$$F_1(1) = \frac{7}{6} \sqrt{\pi} - \sqrt{\frac{2}{\pi}} \zeta\left(\frac{3}{2}\right). \quad (A.4)$$

Similarly

$$F_2(1) = -\frac{1}{5} \sqrt{\pi} + \frac{1}{\pi} \sqrt{\frac{2}{\pi}} \zeta\left(\frac{5}{2}\right). \quad (A.5)$$

And from the definition of  $\zeta$ -function, we have

$$G_1(1) = -\frac{1}{\sqrt{2}} \zeta\left(\frac{3}{2}\right), \quad (A.6)$$

$$G_2(1) = \frac{1}{\sqrt{2}} \zeta\left(\frac{5}{2}\right). \tag{A.7}$$

By using (A.4) ~ (A.7), we can show

$$f(1) = g(1) = h(1) = 0. \tag{A.8}$$

Behavior  $f(\xi)$  near  $\xi=1$ .

We put

$$f(1 + \delta^2) = \left(\frac{df}{d\delta}\right)_{\delta=0} \delta + \dots, \tag{A.9}$$

$$\left(\frac{df}{d\delta}\right)_{\delta=0} = \lim_{\delta \rightarrow 0} 2\delta \left(\frac{df(\xi)}{d\xi}\right)_{\xi=1+\delta^2}. \tag{A.10}$$

The non-vanishing term in (A.10) is only from the derivative of  $G_1$ , so that

$$\begin{aligned} \left(\frac{df}{d\delta}\right)_{\delta=0} &= \frac{3}{\pi} \lim_{\delta \rightarrow 0} \delta \cdot G'(1 + \delta^2) \\ &= \frac{3}{\sqrt{2}} \lim_{\delta \rightarrow 0} \delta \sum_{k=1}^{\infty} \frac{1}{k^{1/2}} (\cos k\pi\delta^2 + \sin k\pi\delta^2) \\ &= \frac{3}{\sqrt{2}} \int_0^{\infty} \frac{1}{\sqrt{x}} (\cos \pi x + \sin \pi x) dx \\ &= 3. \end{aligned} \tag{A.11}$$

Therefore

$$f(\xi) = 3\sqrt{\xi-1} + \dots \quad \text{for } \xi \rightarrow 1. \tag{A.12}$$

### Appendix B

Scaling method is given for Eq. (3.23):

$$\frac{d^2\varphi}{dx^2} = (x\varphi)^{1/2}. \tag{B.1}$$

If we put

$$\varphi(x) = \lambda \tilde{\varphi}(\tilde{x}), \quad x = \lambda^{1/5} \tilde{x}, \tag{B.2}$$

then

$$\frac{d^2\tilde{\varphi}}{d\tilde{x}^2} = (\tilde{x}\tilde{\varphi})^{1/2}. \tag{B.3}$$

The outer boundary condition

$$\varphi(x_0) = 0 \quad \text{and} \quad \varphi'(x_0) = -\frac{1}{x_0} \frac{Z-N}{Z} \tag{B.4}$$

becomes

$$\tilde{\varphi}(\tilde{x}_0) = 0 \quad \text{and} \quad \tilde{\varphi}'(\tilde{x}_0) = -\frac{1}{\lambda \tilde{x}_0} \frac{Z-N}{Z}. \quad (\text{B}\cdot 5)$$

For neutral atoms, (B·4) and (B·5) have the same form.

Here we notice that  $\varphi$  and  $\tilde{\varphi}$  satisfy the same type of differential equation and also the same outer boundary conditions. Therefore once we have a solution of (B·3) under the boundary condition  $\tilde{\varphi}(\tilde{x}_0) = 0$  and  $\tilde{\varphi}'(\tilde{x}_0) = 0$ , we can get a desired solution  $\varphi$  which satisfies  $\varphi(0) = 1$  besides the condition (B·4), by taking  $\lambda = [\tilde{\varphi}(0)]^{-1}$ .

We have calculated Eq. (B·1) anew, and obtained

$$x_0 = 3.08730. \quad (\text{B}\cdot 6)$$

By changing the unit of length as stated above (3·23), we have

$$\gamma_0 = \mu' x_0 = 3.2197 Z^{1/5} \gamma^{-2/5}. \quad (\text{B}\cdot 7)$$

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