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Behavior of positive ions in extremely strong magnetic fields

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The Thomas-Fermi statistical theory yields a total energy for positive ions with N electrons and atomic number Z in a very strong magnetic field B of the form $E_{\rm TF}(Z,N,B) = -Z^{9/5}B^{2/5}f(N/Z)$. It is first shown that for small N/Z, $f(N/Z)$ is proportional to $(N/Z)^{3/5}$. The Coulomb field energy is also calculated in the statistical limit as $E_{\rm TF}^{\rm Coulomb}(Z,N,B) = {\rm const}\times Z^{9/5}B^{2/5}(N/Z)^{3/5}$, and the constant is obtained. Finally, the relation to the $1/Z$ expansion for ions in very strong magnetic fields is established.

INTRODUCTION

Considerable interest has been shown in the properties of atoms in very strong magnetic fields because of possible astrophysical implications concerned with the emission of electrons and ions from the surface of pulsars, the abundances of the elements in cosmic radiation, and the properties of condensed matter forming the outer crust of magnetic neutron stars.

This has led to extensive studies of the statistical model of an atom, with or without exchange, in the limit of very high magnetic fields.[1-5] In this note, we wish to examine

(a) the form of the Thomas-Fermi energy $E_{\rm TF}(Z,N,B)$ of a positive ion of atomic number Z, with N electrons ($N\leq Z$), in a very strong magnetic field B,

(b) the connection of $E_{\rm TF}$ with the Z^{-1} expansion,[6] which is so valuable for atoms in zero magnetic field.

SELF-CONSISTENT STATISTICAL ATOM

We begin with the statistical model without exchange, where we can write,[2,3] using natural units $\hbar=c=1$ throughout,

$$E_{\rm TF}(Z,N,B) = -2^{8/5}\pi^{-2/5}\alpha^{-4/5}Z^{9/5}L^{2/5}\epsilon \ ({\rm Ry}), \tag{1}$$

where α is the fine-structure constant, $L=eB/m^2$, $=B/B_c$, with $B_c=4.4\times10^{13}$ G, and the energy is measured in the Rydberg unit $\frac{1}{2}m\alpha^2$. In (1), ϵ is expressed in terms of the slope at the origin $\phi'(0)$ of the solution of the appropriate dimensionless Thomas-Fermi equation

$$\phi'' = (x\phi)^{1/2}, \qquad r=\mu' x = a_0 2^{-3/5}\pi^{2/5}\alpha^{4/5}Z^{1/5}L^{-2/5}x \tag{2}$$

in the strong-field case. Clearly, we must solve (2) for a positive ion, in which case the ion has a finite (dimensionless) radius x_0, while to ensure N electrons the solution of (2) must satisfy

$$\phi(x_0) - x_0\phi'(x_0) = 1 - N/Z, \tag{3a}$$

and if the ion is in a free state

$$\phi(x_0) = 0. \tag{3b}$$

Then

$$\epsilon = -\frac{5}{9}\left[\phi'(0) + \frac{1}{x_0}\left(1-\frac{N}{Z}\right)^2\right].$$

It is a straightforward matter to show that a solution of (2) satisfying (3) can be expanded around x_0 as

$$\phi(x) = \left(\frac{x_0 - x}{x_0}\right)\left(1-\frac{N}{Z}\right) + a_5(x_0-x)^{5/2} + \text{higher order terms}, \tag{4}$$

where

$$a_5 = \frac{4}{15}\left(1-\frac{N}{Z}\right)^{1/2}.$$

In the limit of small N/Z, (4) is valid also into $x=0$, and from the condition $\phi(0)=1$ it can be demonstrated that, for small N/Z,

$$x_0 \sim {\rm const}\times\left(\frac{N}{Z}\right)^{2/5} + \text{higher-order terms}. \tag{5}$$

Furthermore, evaluating $\phi'(0)$ from (4) in the limit of small N/Z, it can be shown that

$$\epsilon \sim {\rm const}\times\left(\frac{N}{Z}\right)^{3/5} + \cdots. \tag{6}$$

Hence, the conclusion is that for small N/Z, (1) and (6) yield

$$E_{\rm TF}(N,Z,B) \sim Z^{9/5}\left(\frac{N}{Z}\right)^{3/5}L^{2/5} \tag{7}$$

in the high-field regime.

Developing ϵ to higher order shows that the next term in (6) is $O(N/Z)$ higher. We note that Mueller *et al.*[2] used a variational trial function within the Thomas-Fermi framework which yielded the energy of the neutral atom $\sim B^{2/5}Z^{9/5}$, which agrees with (1) when $N/Z=1$.

COULOMB ENERGY FROM STATISTICAL THEORY

Next we establish the Coulomb energy $E^{\rm TF}_{\rm Coulomb}\,(Z,N,B)$ from the statistical theory by noting that the Thomas-Fermi density $\rho_{\rm TF}(r)$ is given by[1,2]

$$\rho(r)=\frac{m^{1/2}(eB)}{2^{1/2}\pi^2}\left(\frac{Ze^2}{r}-\mu\right)^{1/2}. \tag{8}$$

Writing $\mu=Ze^2/r_0$, where $r_0=\mu' x_0$, and using $\int\rho(r)d\vec{r}=N$ yields

$$\mu=\frac{Ze^2}{r_0}=\frac{Ze^2}{(N\pi)^{2/5}}2^{3/5}m^{1/5}(eB)^{2/5}C^{2/5}(Ze^2)^{1/5}=\frac{Z^{6/5}L^{2/5}}{\alpha^{4/5}N^{2/5}}\,[\mathrm{Ry}], \tag{9}$$

where

$$C=\int_0^1 S^2\left(\frac{1}{S}-1\right)^{1/2}dS=\frac{\pi}{16}.$$

Furthermore, the electron-nuclear potential energy V, related to E by the virial theorem,[2,3] is given by

$$E_{\rm Coulomb}=\tfrac{5}{6}V=-\tfrac{5}{6}Ze^2\int\frac{\rho(\vec{r})d\vec{r}}{r}=-\frac{5}{6}\frac{(Ze^2)^{3/2}}{\pi}\frac{2^{3/2}m^{1/2}(eB)(N\pi)^{3/5}D}{2^{9/10}m^{3/10}(eB)^{3/5}C^{3/5}(Ze^2)^{3/10}}=-\tfrac{5}{3}\alpha^{-4/5}Z^{6/5}L^{2/5}N^{3/5}\,[\mathrm{Ry}], \tag{10}$$

where

$$D=\int_0^1 S\left(\frac{1}{S}-1\right)^{1/2}dS=\frac{\pi}{8}.$$

Clearly, (10) is simply $\sim\mu N$ using Eq. (9) which is evidently correct.

RELATION TO Z^{-1} EXPANSION

We now generalize the well-known Z^{-1} expansion[6] in zero magnetic field to the high-field regime by writing formally the exact nonrelativistic energy as

$$E(Z,N,B)=E_{\rm Coulomb}(Z,N,B)+\frac{1}{Z}E_1(Z,N,B)+\cdots+\frac{1}{Z^n}E_n(Z,N,B)+\cdots; \tag{11}$$

the idea is to correct the Coulomb term by electron shielding effects in higher-order terms. The implication of the $1/Z$ expansion is that one can factor out the remaining Z dependence, and in particular, in the statistical theory without exchange, (11) becomes

$$E_{\rm TF}(Z,N,B)=Z^{9/5}L^{2/5}\left(\frac{N}{Z}\right)^{3/5}\left[\epsilon_0+\frac{N}{Z}\epsilon_1+\cdots+\left(\frac{N}{Z}\right)^n\epsilon_n+\cdots\right]. \tag{12}$$

It is now readily demonstrated from Eqs. (1), (7), and (10) that ϵ_n is independent of N for large N. Explicitly, $\epsilon_0=-\frac{5}{3}\alpha^{-4/5}=-85.364$. From Table I of Ref. 3, ϵ and thus $E_{\rm TF}$ can be obtained for several N/Z values. We have thereby estimated ϵ_1 and ϵ_2 by a least-squares method as 36.9 and −2.78, respectively. It should be noted that since $\phi'(0)$ and x_0 are independent of L or B, these quantities are pure numbers to be contrasted with the zero-field result given earlier by March and White.[7] The asymptotic N dependence of E_n in Eq. (11) for large N is thereby established.

In summary, we have demonstrated the way in which $E_{\rm TF}(Z,N,B)$ behaves for small N/Z and have thereby been able to determine the asymptotic N dependence of the coefficients of the $1/Z$ expansion in the limit of large N in the high-field limit and in a nonrelativistic framework.

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