HEAVY ATOM IN AN ULTRASTRONG MAGNETIC FIELD

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The Hartree-Thomas-Fermi approximation for a heavy atom in an ultrastrong magnetic field appreciably exceeding 10^{10} Oe is considered, when a complete rearrangement of the electron shells occurs. It is shown that spherical symmetry is preserved, and the radius of the atom decreases with magnetic field in a certain range of its variation. The problem of the excitation levels of such an atom is discussed.

1. INTRODUCTION

THE discovery of quasars and pulsars has put on the agenda the possibility of observing matter in very strong magnetic fields, which are not yet attainable under laboratory conditions. Fields in the range 10^9 to 10^{10} Oe or even in the range 10^{12} to 10^{14} Oe, which appear in contemporary astrophysics,[1-3] make an examination of the question of the behavior of ordinary matter (not plasmas) in fields above 10^{10} Oe, at which the interaction of the atomic electrons with the external magnetic field begins to become larger than their Coulomb interaction, even if not expedient at least not entirely unjustified. First of all it is of interest to analyze the problem of the behavior of individual atoms in ultrastrong magnetic fields. For the hydrogen atom or, more precisely, for hydrogen-like systems of the type of excitons in semiconductors, for which the corresponding field is substantially smaller in virtue of the smallness of the effective mass and the presence of a dielectric medium, this question has been studied at length.[4-8] Here we consider the problem of the ground state of a very heavy atom, when the more simple Hartree-Fock and Thomas-Fermi approximations can be used.

2. THE SELF-CONSISTENT FIELD APPROXIMATION

Let us consider a heavy atom with atomic number $Z \gg 1$ in a strong homogeneous magnetic field. In the Hartree-Fock approximation it is sufficient for us to consider the motion of the individual electrons in a self-consistent electric field, and then to determine the field itself. The Schrödinger equation for an electron with a wave function $\psi \sim e^{-im\theta}$ in a cylindrical system of coordinates ρ, θ, and z has the form

$$\frac{1}{2}\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right)-\frac{1}{2}\frac{\partial^2\psi}{\partial z^2}+\left(\frac{m^2}{2\rho^2}-\frac{mB}{2}+\frac{B^2}{8}\rho^2+B\sigma\right)\psi-\varphi\psi=E\psi, \tag{1}$$

where φ denotes the potential of the electric field and σ is the spin. All quantities in (1) are expressed in atomic units, in particular, the magnetic field is expressed in units of $m^2e^3c\hbar^{-3} = 2.35 \times 10^9$ Oe.

For $B \gg \varphi \sim Z$ one can use the approximation of a strong magnetic field.[4-8] For this, the expression inside the round brackets of the third term in Eq. (1) is expanded near the minimum at

$$\rho=\rho_m=\sqrt{2m/B} \tag{2}$$

in terms of a small deviation $\xi = \rho - \rho_m$ from the minimum point (we assume that $m > 0$). For $m \gg 1$ which we require later on, it is sufficient to restrict our attention to the quadratic term in ξ, and in the first term of (1) one can keep only the chief term containing the second derivative with respect to ξ. To this approximation we obtain a simple harmonic oscillator with respect to the variable ρ, and as $B \to \infty$ it is necessary for us to choose the ground state of the oscillator with the wave function

$$\psi=\psi(z)\exp(-\xi^2/2B), \tag{3}$$

i.e., the very lowest Landau level. Here one should also assume that $\sigma = -1/2$, i.e., all magnetic moments are turned with the field. After separation of these variables we obtain a simple one-dimensional equation

$$-\frac{1}{2}\frac{\partial^2\psi}{\partial z^2}-\varphi(\rho,z)\psi=E\psi, \tag{4}$$

in which $\rho = \rho_m$ should be considered as a parameter labeling the levels with respect to m.

Thus, we arrive at a natural picture in which as $B \to \infty$ each individual electron moves in a narrow cylindrical shell of radius ρ_m, undergoing oscillations with respect to z. Since at very large values of B the width of a shell may be arbitrarily small, then the ψ-functions of the individual electrons do not overlap as $B \to \infty$, i.e., the exchange interaction is not present. This means that in the limiting case $B \to \infty$ one can use the simple Hartree approximation instead of the more accurate but at the same time more cumbersome Hartree-Fock approximation.

Let ψ be a solution of Eq. (4) which is normalized to unity and depends on ρ as a parameter. Then the density of the electrons can be represented in the form

$$n=n_\rho\psi^2, \tag{5}$$

where n_ρ denotes the number of electrons occurring in a column of unit cross section: $n_\rho = \int n\,dz$.

The potential φ of the self-consistent field is determined by Poisson's equation

$$\Delta\varphi=4\pi n \tag{6}$$

with the boundary condition $r\varphi \to Z$ as $r \to 0$. Equations (4)–(6) determine the stationary state of a heavy atom in the self-consistent field approximation as $B \to \infty$.

The function n_ρ for the ground state must be found from the condition for a minimum of the energy of the stationary state. Before going on to a discussion of this rather complicated problem, let us consider the simpler case of the Thomas-Fermi approximation.

3. THE THOMAS-FERMI MODEL

Let us assume that B, although large, still cannot be regarded as infinite in comparison with the atomic number Z in the units adopted by us. Physically this means that the Larmor frequency is not infinitely large in comparison with $I/\hbar$, where I denotes the ionization potential. As is seen from Eq. (3) the width of the ψ-function with respect to ξ, i.e., with respect to ρ, is of the order of magnitude of $B^{-1/2}$. If this value is not very small, then the ψ-functions of the neighboring levels in m will overlap strongly, and the occupation of several levels in z with comparatively small values $m \ll Z$ will be energetically favored. Thus, there exists a definite range of variation of B (we shall subsequently define it more precisely) in which one can use the Thomas-Fermi approximation with respect to the variable z, and at the same time one can assume that the higher Landau levels are not occupied. Since $\rho = \sqrt{2m/B}$ then dm states with respect to m correspond to $d\rho = \sqrt{2/mB}\,dm = (\rho B)^{-1}dm$, but with respect to the variable z in virtue of the one-dimensional nature of the motion $dN = p_z dz/2\pi$ electrons with a given m occur in the interval dz, where p_z denotes the maximum momentum, which is equal to $\sqrt{2\varphi}$. From here we obtain

$$dmdN = p_z B\rho d\rho dz / 2\pi = n 2\pi\rho d\rho dz, \tag{7}$$

i.e., the density n of the electrons is given by

$$n = B\sqrt{2\varphi} / 4\pi^2. \tag{8}$$

If this expression is substituted into Eq. (8), then we obtain the equation

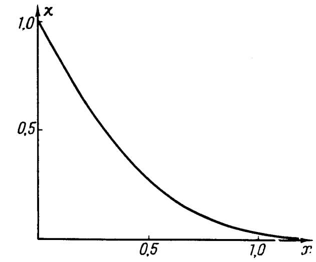
$$\Delta\varphi = B\sqrt{2\varphi} / \pi, \tag{9}$$

which is similar to the Thomas-Fermi equation.

Equation (9) is spherically symmetric so that its solution only depends on r—the distance from the nucleus. The solution of Eq. (9) must go over into Z/r as $r \to 0$ and must tend to zero faster than r^{-1} as $r \to \infty$. In terms of the variables χ and x defined by the relations $\chi(x) = r\varphi/Z$ and $x = r(2B^2/\pi^2 Z)^{1/5}$, it takes the form

$$\chi'' = \sqrt{x\chi} \tag{10}$$

with the boundary conditions $\chi = 1$ for $x = 0$ and $\chi = 0$ for $x \to \infty$. The result of a numerical solution of Eq. (10) is shown in the figure.



The density of electrons (8) can be expressed in terms of the function χ in the following way:

$$n = 2^{-7/5}\pi^{-11/5}(B^3 Z)^{2/5}\sqrt{\chi / x}. \tag{11}$$

From here it is seen that, just as in the ordinary Thomas-Fermi model, the density distribution remains similar upon a change of Z and B, where the characteristic size of the atom varies like $Z^{1/5}B^{-2/5}$. In other words, the application of a field decreases the size of the atom.

Now we can determine the conditions for validity of the approximation under consideration. Within the framework of the Thomas-Fermi approximation, electrons with $\sigma = 1/2$ or in the first excited Landau level can appear only in the region $\varphi > (1/2)B$ or $\varphi > B$, respectively. Therefore, for the validity of the approximation under consideration it is necessary that the potential φ in the fundamental region should be appreciably smaller than B, that is, $B \gg Z^{4/3}$. On the other hand, from the condition that even if several electrons occur in each level m, it follows that $d\rho/dm \gg r_0/Z$, where $r_0 \sim (Z/B^2)^{1/5}$ denotes the atom's radius. Taking it into account that $d\rho/dm \sim 1/r_0 B$, we get $B \ll Z/r_0^2$, i.e., $B \ll Z^3$. Thus, the range of applicability of the approximation under consideration is rather broad:

$$Z^{4/3} \ll B \ll Z^3. \tag{12}$$

Now let us turn to an examination of the case $B \to \infty$, i.e., $B > Z^3$.

4. The Case $B > Z^3$

For $B > Z^3$ not more than one electron remains in each level m; therefore the distribution of the electron density with respect to z should be determined by the square of the ψ-function of a single electron, which is the solution of Eq. (4) for the ground state. Correspondingly the use of the density of the Thomas-Fermi model given by Eqs. (7) and (8) instead of (5) undoubtedly must lead to quantitative deviations. However, if great accuracy is not required, then one can approximately use the approximation $\psi^2 \sim p_z = \sqrt{2\varphi}$, which is utilized in the Thomas-Fermi model. By the same token we assume that ψ^2 is large in the region near the median plane and tends to zero, where $\varphi = 0$. If this approximation for the electronic density is also extended in regard to the variable ρ, then we arrive at an expression of the type (8):

$$n = B_0\sqrt{2\varphi} / 4\pi^2, \tag{13}$$

with the only difference being that now the quantity B_0 is simply a certain arbitrary constant which one should choose from the condition that the energy of the ground state be a minimum. This energy is composed of the kinetic energy which, under conditions when all electrons "sit" in the lower z-levels, is of the order of magnitude of Z/r_0^2 for all electrons, and the potential $\sim -Z^2/r_0$. The minimum of the energy occurs at $r_0 \sim Z^{-1}$. But the value $r_0 \approx Z^{-1}$ is reached exactly at the limit of validity (12) of the Thomas-Fermi model, $B = Z^3$. This means that for the ground state of the atom the constant B_0 in (13) should be of the order of Z^3.

Thus, for $B > Z^3$ there exists a complete set of spherically-symmetric states of the atom, out of which only one with $B_0 \sim Z^3$ corresponds to the ground state. The radius of the atom in the ground state, $r_0 \sim Z^{-1}$, ceases to depend on B for $B > Z^3$. In this connection the average number of occupied m levels turns out to be less than unity, as is not difficult to see. This means that the electrons do not at all tend to fill all lower levels—their Coulomb repulsion leads to a "swelling" of the atom so that for $B \gg Z^3$ many lower levels remain unoccupied. As B increases the width of each shell in ρ, $\Delta\rho \sim 1/\sqrt{B}$, continues to decrease and for $B > Z^4$ it becomes smaller than the average distance between the shells which is $\sim r_0/Z \sim Z^{-2}$. Thus, for $B > Z^4$ the ψ-functions of the individual electrons cease to overlap, i.e., the conditions for the Hartree approximation are satisfied.

The qualitative arguments presented here actually do not depend on the approximation (13), but rest only on the fact of the occupation of a lower state by each electron. Using similar qualitative considerations, one can reach the conclusion that the ground state should not deviate strongly from spherical symmetry, since upon deformation of the electron shells (or $\psi^2(z)$) the energy associated with the Coulomb repulsion of the electrons increases.

The effect of occupying only part of the lower m-m-levels for $B \gg Z^3$ leads to the result that near the ground level of a heavy atom there must be a band of weakly excited states, which correspond to a superposition of states with one and the same macroscopic distribution of the electron density, but with different occupation numbers with respect to the neighboring m-levels. This band is separated by an appreciable energy gap from the similar band where one of the z-levels of the longitudinal motion of the electrons is excited. And, finally, the excitations of the Landau levels lie very high. Since the excitation of the Landau levels for the individual electrons has very little effect on the distribution of the electron density, then both for $B > Z^3$ and in the region $Z^{4/3} < B < Z^3$, the corresponding state will be Z-fold degenerate. One can say that such an excitation is analogous to an exciton in a crystal—it will be passed on from electron to electron, and therefore the corresponding z-levels will correspond to different interference states with the excitation of one of the electrons. Correspondingly, a reversal of one of the spins will correspond to a spin wave in a ferromagnetic.

5. CONCLUSION

Thus, we have shown that for very strong magnetic fields, $B \gg 10^9 Z^{4/3}$ Oe, a substantial change of the electronic states occurs in a heavy atom with atomic number $Z \gg 1$. In this case all electrons undergo motion in comparatively thin cylindrical shells with the axis directed along the magnetic field, oscillating along the field and precessing around the nucleus. If $B \ll 10^9 Z^3$ Oe, then several electrons are found in each shell m, and in order to determine the distribution of the electron density in the atom one can use the modified Thomas-Fermi model in the appropriate manner. According to this model an atom in a strong magnetic field retains spherical symmetry, and its radius r_0 changes like $(Z/B^2)^{1/5}$, i.e., the atom is compressed with increasing B. For a field $B > 10^9 Z^3$ Oe the compression of the atom stops and its radius in the ground state ceases to depend on the field. In this connection the m-shells in the ground state turn out to be incompletely filled, and for $B \gg 10^9 Z^4$ Oe the ψ-functions of the individual electrons do not even overlap. The spectrum of the excited states of an atom in an ultrastrong field consists of equidistant Landau levels and levels corresponding to a reversal of the spins, with a wide band around each level of excitations of the longitudinal motion. For $B \gg 10^9 Z^3$ Oe weak excitations still appear, corresponding to a change of the occupation numbers in the shells with a weak excitation of the averaged distribution of the density.

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