

## Electrons in a Shell

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### **Abstract**

The spatial distribution of electrons inside an empty spherical shell with an impenetrable wall is considered. It is shown that with a large number  $N$  of non-relativistic electrons, the electrons are concentrated near the wall in a layer of thickness  $\delta \sim N^{-1/5} \cdot a^{2/5} \cdot a_B^{3/5}$ , where  $a$  is the radius of the shell, and  $a_B$  is the Bohr radius.

In this brief note, we consider the spatial distribution of  $N \gg 1$  non-relativistic electrons placed inside an empty spherical shell of radius  $a$  at zero temperature. This problem was offered as an exercise on the Thomas-Fermi (T-F) model (see, e.g., [1]) in an upper division class in atomic physics (Physics 138) at Berkeley.

First we note that this system can be described by the same T-F equation as an atom, which can be proven by tracing the steps made in the derivation of the T-F equation [1]. The boundary conditions are, of course, quite different than for an atom: here there is no nucleus at the center, and there is an infinitely high potential wall at  $r=a$ . Choosing the electrostatic potential  $\phi=0$  at the center of the sphere, we have  $\phi=Ne/a$  near

the boundary ( $e$  is the electron charge). The functions  $\varphi(r)$  and  $n(r)$  can be obtained by numerical integration of the T-F equation [2]. Instead of this, in what follows we prove that for sufficiently large  $N$ , the electron density is concentrated in a thin layer of characteristic thickness  $\delta$  near the wall (see Figure), and we give a rough estimate of  $\delta$ , showing how this parameter scales with  $N$  and  $a$ . In this estimate, we ignore all numerical factors as  $4\pi$ , which allows us to keep all expressions as simple as possible.

Since we are dealing with a large number of electrons, an appropriate concept to describe the problem is that of hydrostatic pressure. Let us define  $\delta$  as the thickness of the layer containing, say,  $1/2$  of all electrons (we will see that  $\delta \ll a$ ). This layer as a whole is pushed towards the wall by Coulomb repulsion from all other electrons. The corresponding force is

$$F_c \sim \frac{N^2 e^2}{a^2}. \quad (1.)$$

We define Coulomb pressure as this repulsion force per unit surface area of the layer:

$$P_c = \frac{F_c}{A} \sim \frac{N^2 e^2}{a^4}. \quad (2.)$$

This pressure acts to compress the layer. The compression, however, is limited by the Fermi pressure - the consequence of the Pauli exclusion principle forbidding more than one electron in a given quantum state. The number of available electron states per unit volume (which is equal to the electron density at zero temperature) is

$$\frac{p_0^3}{\hbar^3} \sim n, \quad (3.)$$

where  $p_0$  is the Fermi momentum. On the other hand, we have

$$n \sim \frac{N}{a^2 \delta}. \quad (4.)$$

Equating the two expressions for density, we get

$$p_0 \sim \left( \frac{N}{a^2 \delta} \right)^{1/3} \cdot \hbar. \quad (5.)$$

Now we can estimate the Fermi pressure. Consider electrons colliding with the wall. We have  $n \cdot p_0 / m$  such collisions per unit area per unit time. Here  $m$  is the electron mass. Each collision transfers momentum  $\sim p_0$  to the wall, so the Fermi pressure is

$$P_F \sim n \cdot p_0^2 / m = \left( \frac{N}{a^2 \delta} \right) \cdot \left( \frac{N}{a^2 \delta} \right)^{2/3} \cdot \hbar^2 / m = \left( \frac{N}{a^2 \delta} \right)^{5/3} \cdot \hbar^2 / m. \quad (6.)$$

Now consider the equilibrium condition for the layer as a whole. The layer is pushed by the wall with pressure  $P_F$ , while it pushes towards the wall with Coulomb pressure  $P_C$ . In equilibrium, the layer is stationary, and therefore we have  $P_F = P_C$ , or:

$$\frac{N^2 e^2}{a^4} \sim \left( \frac{N}{a^2 \delta} \right)^{5/3} \cdot \hbar^2 / m. \quad (7.)$$

Thus

$$\boxed{\delta \sim N^{-1/5} \cdot a^{2/5} \cdot a_B^{3/5}}, \quad (8.)$$

where  $a_B = \frac{\hbar^2}{m e^2}$  is the Bohr radius.

It is interesting to examine the range of values of  $N$  where this solution is valid. First, we find the critical number of electrons  $N^*$  at which the non-relativistic approximation used to obtain this result breaks down. This occurs when the Fermi

momentum  $p_0$  becomes of order  $mc$ , where  $c$  is the speed of light. From Equations (8) and (5), we find:

$$N^* \sim \left( \frac{a}{a_B} \right)^2 \cdot \alpha^{-5/2} \quad , \quad (9.)$$

where  $\alpha=1/137$  is the fine structure constant, and we have used the fact that  $\frac{\hbar}{mc} = \alpha \cdot a_B$ .

Second, the T-F approximation is valid when most electrons have large radial quantum numbers [<sup>1</sup>]. In order to see at which values of  $N$  high radial quantum numbers are excited, suppose that we gradually increase the number of electrons inside the shell [<sup>3</sup>]. At low densities, all electrons are in the lowest radial state, and in order to satisfy the Pauli principle, quantum states with orbital angular momentum  $l$  are excited. Suppose that  $L$  is the highest excited value of  $l$ . The overall number of states is equal to the number of particles:

$$N = \sum_{l=0}^L (2l+1) \sim L^2. \quad (10.)$$

In this regime, we can estimate the thickness of the layer containing the electrons by equating the Coulomb energy of the layer with the kinetic energy arising due to the uncertainty condition:

$$\frac{N^2 e^2 \delta}{a^2} \sim \frac{N \hbar^2}{m \delta^2} \quad , \quad (11.)$$

from which it follows that (cf. Equation (8)):

$$\delta \sim N^{-1/3} a^{2/3} a_B^{1/3}. \quad (12.)$$

An important difference with the T-F regime is that here the radial and orbital motion are of completely different character, and the concept of “hydrostatic” isotropic pressure that we used above is clearly inapplicable.

As we keep increasing  $N$ , at some point the centrifugal energy corresponding to electrons with angular momentum  $L$  becomes equal to the energy of radial motion:

$$\frac{\hbar^2 L^2}{ma^2} \sim \frac{\hbar^2}{m\delta^2}. \quad (13.)$$

At higher values of  $N$ , it becomes energetically beneficial to excite higher radial modes, which also corresponds to the transition to the T-F regime discussed above. From (13), and using Equations (10),(12), we obtain the boundary value of  $N$ :

$$N^{**} \sim \left( \frac{a}{a_B} \right)^2. \quad (14.)$$

It is curious to note that this corresponds to a surface density of electrons of about one per Bohr radius squared.

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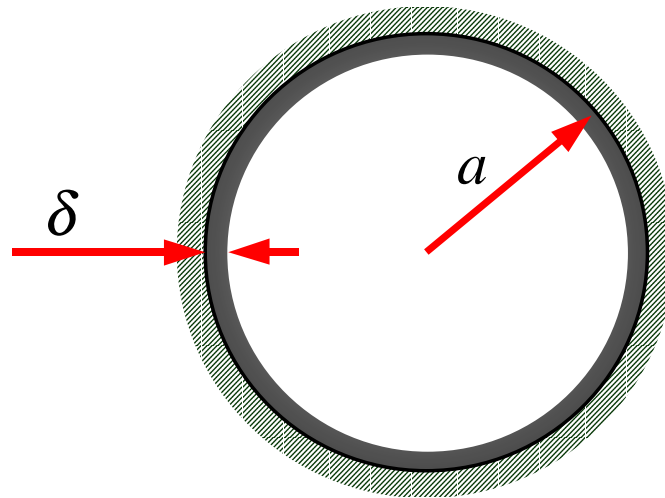


Figure 1. Electrons collect in a layer of thickness  $\delta$  near the wall.

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<sup>1</sup> L.D. Landau and E.M. Lifshitz, Quantum mechanics: non-relativistic theory, (Oxford, Pergamon Press, N.Y., 1991), 3d ed.

<sup>2</sup> E. D. Commins (private communication) has found a convenient parametrization of the T-F equation for the boundary conditions of this problem. The results of his numerical calculation are in qualitative agreement with the analytical estimate presented in this note.

<sup>3</sup> This argument was given by I. B. Khriplovich (private communication).