The Thomas-Fermi Equation

Consider a heavy nucleus of atomic number $Z \gg 1$, with Z corresponding to the number of electrons of mass m and charge $-e$ around the nucleus. If Z is large enough, then most of the electrons will be in excited states with energies close to 0. In this regime, we might expect a quasi-classical treatment to provide a decent description of the behavior of the electrons.

At a very crude level, we can treat the electrons as a simple gas of fermions with number density (in position space) n.[1] Fermi-Dirac statistics tells us that ignoring thermal effects, all electrons will condense into the lowest possible energy states without violating the Pauli exclusion principle. Approximate that we can partition classical (Hamiltonian) phase space into cells of size $(2\pi\hbar)^3$, and remember that each electron can have spin up or spin down.

(a) Let p_0 be the maximum allowed value of momentum at a given point in space. Show that this is related to n by the equation

$$n = \frac{p_0^3}{3\pi^2\hbar^3}.$$

Now consider an electron with energy E. If $E > 0$, then the electron can escape and this would ionize the atom: thus, we only want to consider states where $E \le 0$. Let φ be the electrostatic potential caused by both the electrons and the nucleus, and assume that the charge density of the nucleus is entirely concentrated at the origin.

(b) Show that if all electrons are non-relativistic and at each point in space, the maximum number of electrons possible is present, then Poisson's equation becomes

$$\nabla^2\varphi = \kappa\varphi^{3/2}$$

and find the expression for κ in terms of Z, m, e, $\hbar$ and ϵ_0.

This is the **Thomas-Fermi equation**, and it is a very basic starting point for studying nuclear physics. Although this equation does not have an analytic solution, we will still be able to explore some of its basic properties. For starters, let's assume that the nucleus is rotationally invariant, so that the potential φ is a function only of distance r from the nucleus. Furthermore, define the following dimensionless parameters:

$$y \equiv \left(\frac{Ze\kappa^2}{4\pi\epsilon_0}\right)^{1/3} r,$$
$$\chi(y) \equiv \frac{4\pi\epsilon_0 r}{Ze}\varphi(r).$$

(c) Show that

$$\frac{\mathrm{d}^2\chi}{\mathrm{d}y^2} = \frac{\chi^{3/2}}{y^{1/2}}.$$

(d) What are the boundary conditions on χ? Show that $\chi(y)$ is independent of Z, and discuss the implication of this result.

[1] In a volume element $\mathrm{d}V$, there are thus $n\mathrm{d}V$ electrons.

(e) Using a computer program, solve for and plot $\chi(y)$.

(f) Show that the electron density is

$$n(r) = Z^2 e f\left(\frac{r}{Z^{1/3}}\right).$$

Thus, the characteristic size of a nucleus should grow as $Z^{1/3}$.

(g) Now, suppose that we look at a singly ionized atom: i.e., there are only $Z-1$ electrons. Discuss how this modifies the boundary conditions, and solve numerically the differential equation of part (c) under these new boundary conditions.