A Thomas-Fermi Model

L. H. Thomas [58] and E. Fermi [59] obtained a simplified model of approximating the many-electron structure of atom as the free-electron gas around the nuclei. In free electron gas model, two electrons of opposed spin allow to be into a volume of wave number space equal to h^3, and in an atom, at a distance r from the nucleus, all momentum space up to $p_F(r)$ is occupied. Then the number of electrons per unit volume, $n_e(r)$, is given by

$$n_e(r) = \frac{2}{h^3} \cdot \frac{4}{3}\pi p_F(r)^3 = \frac{8\pi}{3h^3} p_F(r)^3. \tag{38}$$

If $V(r)$ is the electrostatic potential of the atom, the maximum kinetic energy at any distance r is $-eV(r)$, so that the maximum occupied energy level E_0 is

$$E_0 = \frac{p_F(r)^2}{2m_e} - eV(r) \tag{39}$$

The assumption that all negative states are bound would make E_0 zero. Using this equation, $p_F(r)$ of Eqn. (38) is eliminated, then,

$$n_e(r) = \frac{8\pi}{3h^3}(2m_e e)^{3/2} V(r)^{3/2}. \tag{40}$$

The $V(r)$ is satisfied with Poisson's equation since the potential is produced both by the nuclear charge and by the electron distribution:

$$\nabla^2 V(r) = -4\pi e n_e(r). \tag{41}$$

Eliminating $n_e(r)$ between Eqns.(40) and (41), we have

$$\nabla^2 V(r) = -\mu V(r)^{3/2} \tag{42}$$

where

$$\mu = \frac{32\pi^2 e}{3h^3}(2m_e e)^{3/2}. \tag{43}$$

We formulate the potential function $V(r)$ to

$$V(r) = -\frac{Ze}{r}\chi(x). \tag{44}$$

This means that we are screening the simple Coulomb field by the function $\chi(x)$. Suppose also that

$$x = \frac{r}{a_{TF}} \tag{45}$$

where

$$\begin{aligned} a_{TF} &= \left(\frac{3}{32\pi^2}\right)^{2/3} \frac{h^2}{2me^2 Z^{1/3}} \\ &\simeq \frac{0.88534 a_0}{Z^{1/3}} \end{aligned} \tag{46}$$

and a_0 is the Bohr radius:

$$a_0 = \frac{h^2}{4\pi^2 m e^2} \tag{47}$$

From Eqns. (refequ:poi2) and (44), the screening function $\chi(x)$ is obtained as a solution of a differential equation, Thomas-Fermi equation,

$$\frac{d^2\chi(x)}{dx^2} - \frac{\chi(x)^{3/2}}{\sqrt{x}} = 0. \tag{48}$$

The assumptions that the potential behaves like a simple Coulomb interaction in the extreme case as r approaches zero as r approaches infinity, yield the boundary conditions of the Thomas-Fermi function,

$$\chi(0) = 1 \tag{49}$$

and

$$\chi(\infty) = \chi'(\infty) = 0. \tag{50}$$