Webnucleo Technical Report: Screening Example with libstatmech

Tianhong Yu

August 25, 2009

This technical report describes some details of the screening example in the libstatmech distribution.

1 Thomas Fermi Screening

The Thomas-Fermi model is a quantum mechanical theory for the electronic structure of many-body systems. For simplicity, we will just apply a Yukawa potential to the electrons in an atom to describe the screening effect. The example demonstrates how to add a user-defined potential to the integrand.

The Yukawa potential is a function of radius away from a charge:

$$\phi(r) = \frac{Ze}{r} e^{-r/r_0}$$

where Z is the atomic number, e is the proton charge, r_0 is a parameter to describe how the potential drops with radius. Because the potential contributes to the energy of an electron, the number density integral for electrons in the presence of the charge becomes a function of the radius:

$$n(r) = \frac{(mc^2)^3 g}{2\pi^2(\hbar c)^3\gamma^3} \int_0^\infty (x+\gamma)\sqrt{x^2 + 2\gamma x} \left[\frac{1}{1 + \exp(x - \mu'/kT - e\phi(r)/kT)} \right] dx$$

To find the chemical potential, we consider that the nuclei are separated by a distance $2R$ and thus associate a sphere of radius R with each nucleus. Because of charge neutrality, we then have the constraint

$$\int_0^R n(r) e \, dr = Z.$$

We root find on this equation to get the chemical potential (μ'/kT in the integral).

We use $e^2 = \alpha\hbar c$ in the example, where α is the fine-structure constant, $\hbar$ is Planck's constant divided by 2π, and c is the speed of light in vacuum. We use the GNU Scientific Library values for these constants (in cgs units).

2 Example

The figure below shows how the electron number density drops with radius under the Yukawa potential. The curves with different r_0 shows that the electrons penetrate deeper with smaller r_0.

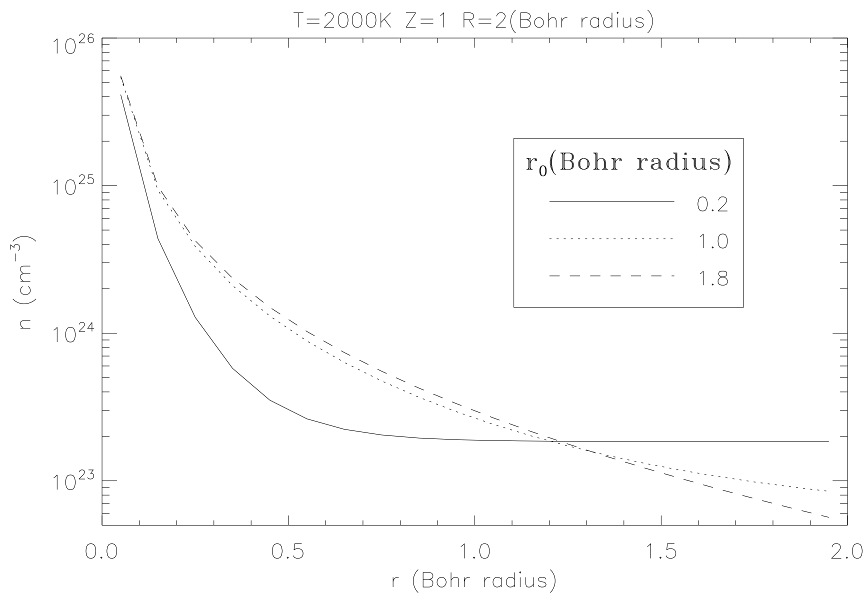

Figure 1: Number densities vs radius. For atomic number = 1 and atomic radius = 2 (Bohr radius), the electron densities get larger at smaller radius.