Webnucleo Technical Report: Screening Example with libstatmech

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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:

$$\begin{aligned} n(r) &= \frac{(mc^2)^3 g}{2\pi^2(\hbar c)^3\gamma^3} \int_0^\infty (x+\gamma)\sqrt{x^2+2\gamma x}\left[\frac{1}{1+\exp(x-\mu'/kT-e\phi(r)/kT)}\right] dx \\ &\equiv \int_0^\infty n(r,x)\,dx \\ &\equiv n(r,T,\mu_{eff}/kT) \end{aligned}$$

where the effective chemical potential is

$$\frac{\mu_{eff}}{kT} = \frac{\mu'}{kT} + \frac{e\phi(r)}{kT}.$$

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, the average number density is

$$\langle n_e \rangle = \frac{3Z}{4\pi R^3}.$$

We similarly have the constraint

$$\int_0^R 4\pi r^2 n(r)\, dr = Z.$$

We can thus define a number density

$$n_e(T, \mu'/kT) = \frac{3Z}{R^3} \int_0^R dr\, r^2 n_e(r, T, \mu_{eff}/kT)\, dx.$$

We use the integrand for $n_e(T, \mu'/kT)$ in the example. $n_e(T, \mu'/kT)$ needs to equal the average number density $\langle n_e \rangle$.

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. In general, the electrons are concentrated towards the nucleus because of the Coulomb attraction. The smaller the r_0 value, the more the Coulomb potential from the nucleus is screened. The electron number density then flattens in the outer radii.

In running the examples, we found some cases, particularly at small temperature, where the calculation did not converge. Decreasing the integral accuracy can solve this problem. Commented code in the example shows how to do this.

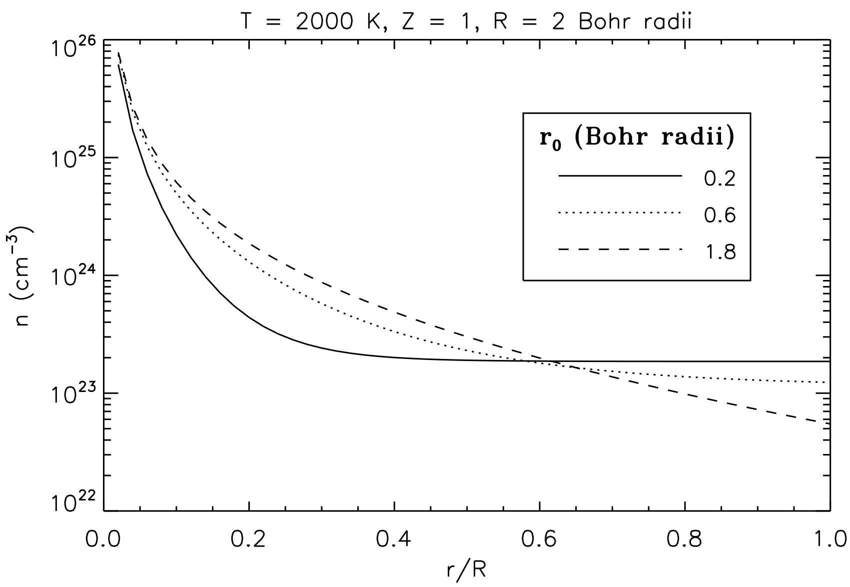

Figure 1: Number densities vs radius. For atomic number = 1 and atomic radius = 2 (Bohr radius), the electron densities get larger at smaller radius where the Coulomb pull from the nucleus is higher.