Thomas-Fermi model

Simple approximate mode for calculation of EoS and mean ion charge in strongly coupled plasma

R_0 – radius of ion sphere (Wigner-Seitz radius)

$$\lambda_D \le R_0$$

Debye screening takes place inside ion sphere

Poisson equation for potential inside ion sphere + Fermi-Dirac distribution for electron density (Integral of electron charge over sphere = - charge of nucleus)

Boundary condition

$$\left.\frac{\partial \phi}{\partial r}\right|_{R_0} = 0$$

$$\Delta \phi(r) = \frac{e\, n_e(r)}{\varepsilon_0} - \frac{e Z_{nuc}\, \delta(r)}{\varepsilon_0}$$

$$n_e(r) = \frac{8\pi}{h^3} \int_0^\infty \frac{p_e^2\, dp_e}{\exp[(-\mu - e\phi(r) + \varepsilon_e)/k_B T_e] + 1}$$

$$\varepsilon_e = \frac{p_e^2}{2m_e} \qquad x = \frac{\varepsilon_e}{k_B T_e}$$

$$\Rightarrow n_e(r) = \frac{4\pi (2 m_e k_B T_e)^{3/2}}{h^3} \int_0^\infty \frac{\sqrt{x}\, dx}{\exp[x - (\mu + e\phi(r))/k_B T_e] + 1}$$

$$Z_{nuc} = 4\pi \int_0^{R_0} n_e(r)\, r^2\, dr \quad \rightarrow$$

defines μ

Usually one sets $\Phi(R_0) = 0$ (the choice influences μ)

Mean ion charge can be calculated – $n_e(R_0)$ contains only free electrons $\Rightarrow$

$$Z = \frac{4\pi R_0^3}{3} n_e(R_0)$$

One can also calculate parameters of state

$$p_e = p_e(R_0) = \frac{8\pi (2m_e)^{3/2}(k_B T_e)^{5/2}}{3h^3} \int_0^\infty \frac{x^{3/2}\,dx}{\exp[x-\mu/k_B T_e]+1}$$

Kinetic energy of electrons

$$K_e = \frac{4\pi (2m_e)^{3/2}(k_B T_e)^{5/2}}{h^3} \int_0^{R_0} dr \int_0^\infty \frac{x^{3/2}\,dx}{\exp[x-(\mu+e\phi(r))/k_B T_e]+1}$$

Potential energy

$$U_{en} = -\frac{Z_{nuc}^2 e^2}{\varepsilon_0} \int_0^{R_0} n_e(r)\, r\, dr$$

$$U_{ee} = \frac{1\, e^2}{4\pi 2 \varepsilon_0} \int_0^{R_0} d^3r \int d^3r' \, \frac{n(r)\, n(r')}{|\vec{r}-\vec{r}'|}$$

Total energy per unit mass

$$\epsilon_m = \frac{K_e + U_{en} + U_{ee}}{A m_p} \qquad (J/kg)$$

For comparison with other approaches – energy of complete ionization of atom must be added

Conceptually simple approach, but it needs complicated numerical calculations
∃ many various amendments of the method
TF is predecessor of modern “density functional” methods

Universal EoS

e.g. QEOS – approximate EOS that connects various limits (models), so that it can describe solid matter + strongly coupled plasmas + weakly coupled plasmas
Table EoS – e.g. SESAME (developed and managed by Los Alamos) – data for low Z materials are in principle accessible