

The Thomas-Fermi Equation

By: Joe Chenard

Where does the equation come from?

The Thomas-Fermi Model

- A model for describing the density of electrons around an atom
- Made classically in the early twentieth century
- Arose from the schrödinger equation
- Llewellyn Thomas
- Enrico Fermi



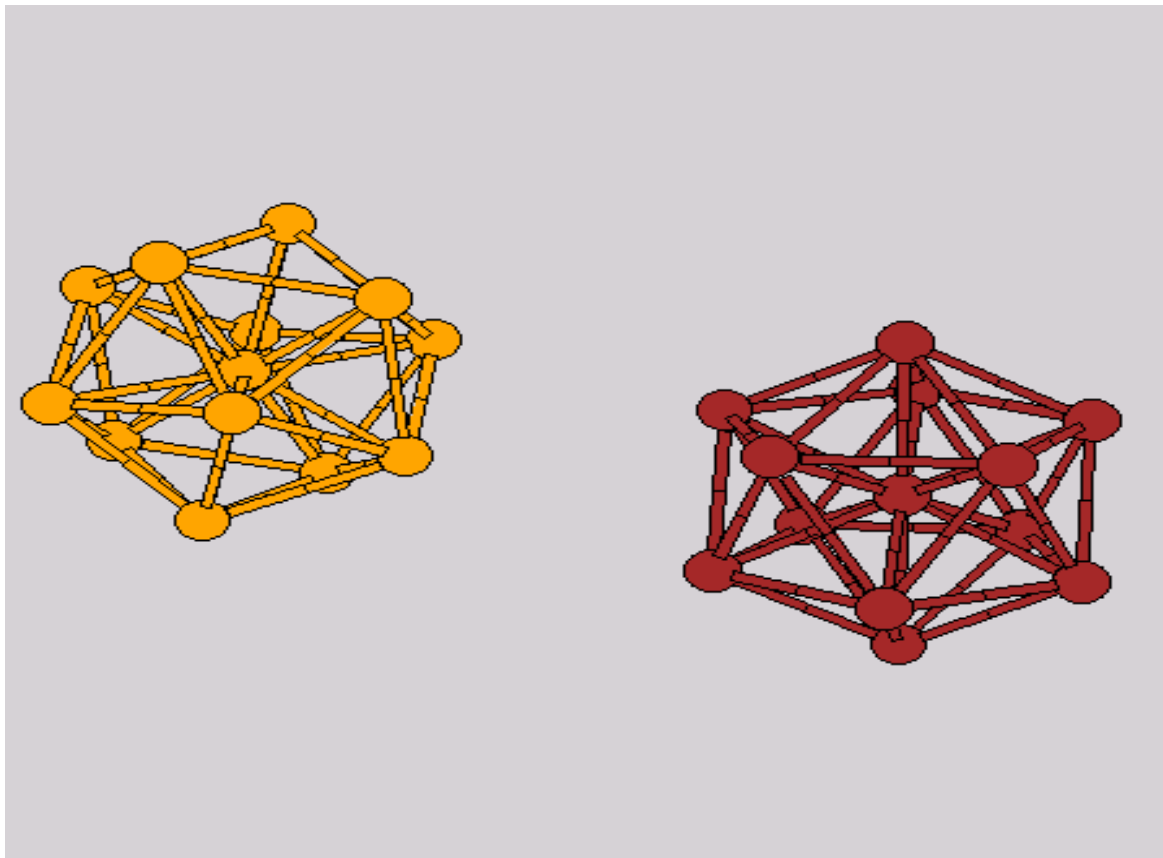
Derivation

$$\begin{aligned}
 \mathcal{E}(\rho) := & \frac{3}{5} \int_{\mathbb{R}^3} |\nabla \psi|^2 d^3\mathbf{x} + \frac{1}{2} \int_{\mathbb{R}^3} \frac{d^2 y}{dx^2} = \frac{1}{\sqrt{x}} y^{3/2} d^3\mathbf{x} \\
 & + \frac{1}{2} \int_{\mathbb{R}^3} V(\mathbf{x}) \rho(\mathbf{x}) d^3\mathbf{x}
 \end{aligned}$$

subject to the boundary conditions

$$y(0) = 1 \quad ; \quad y(+\infty) = 0$$

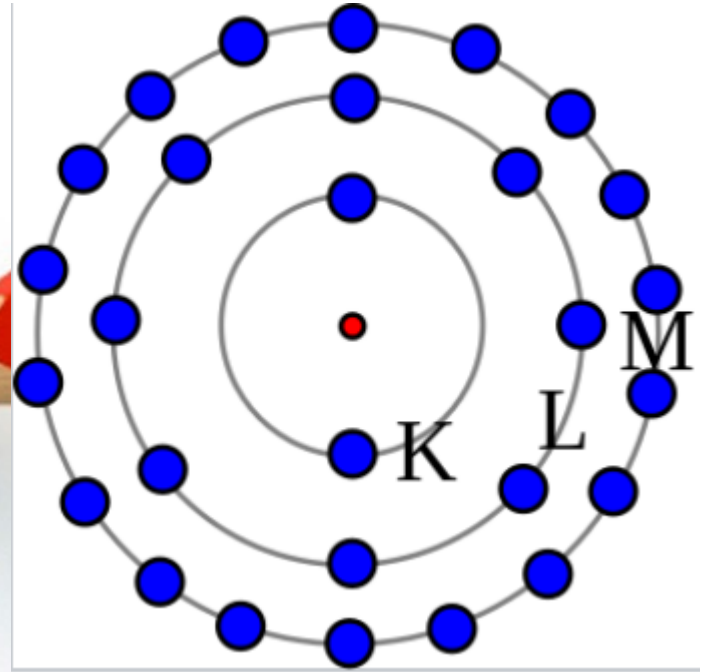
JOHANNES W. K. 2010



What does the equation describe?

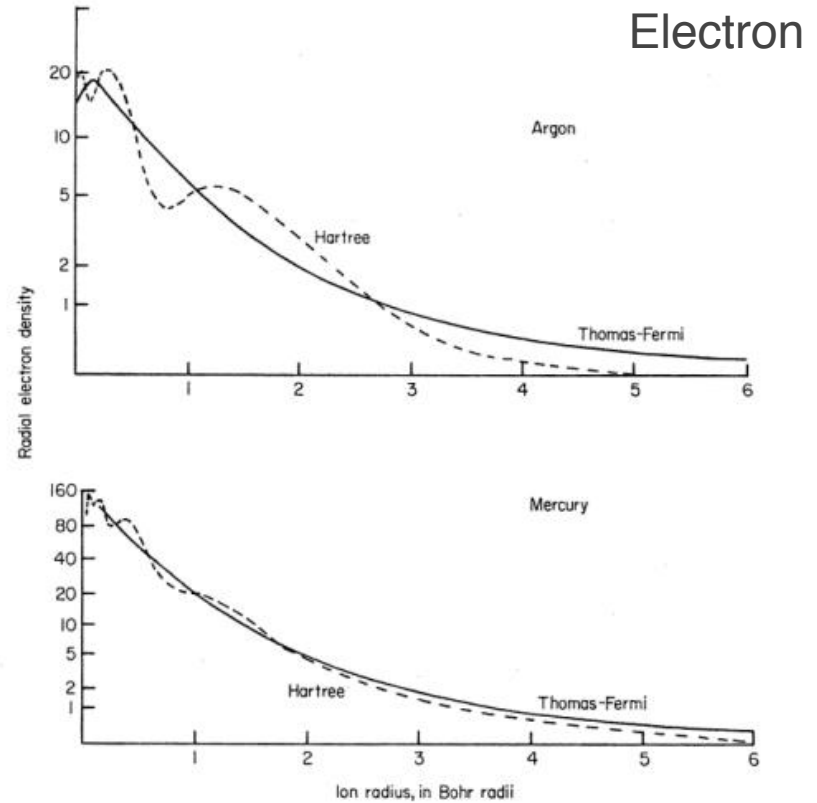
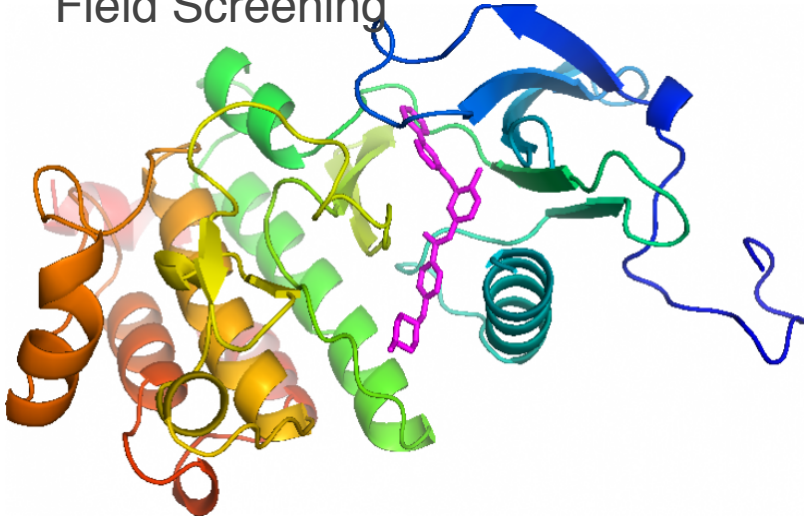
Is it accurate?

No!



Uses for the Thomas-Fermi Equation

Computational Chemistry
Field Screening



Improvements to the Differential Equation

- The von Weizsäcker correction
- Thomas-Fermi-Dirac Equation

$$(\text{const.}) \int_{\mathbb{R}^3} |\nabla \sqrt{\rho(\mathbf{x})}|^2 d^3\mathbf{x}$$

$$-(\text{const.}) \int_{\mathbb{R}^3} \rho(\mathbf{x})^{4/3} d^3\mathbf{x}$$



Sources

- <https://www.theory.nipne.ro/CMP/movies/movies/atomic/node4.html>
- https://en.wikipedia.org/wiki/Thomas%E2%80%93Fermi_model
- https://en.wikipedia.org/wiki/Thomas%E2%80%93Fermi_equation
- <http://physics.nyu.edu/LarrySpruch/Lieb.pdf>
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- <http://www.physlink.com/Education/askexperts/ae329.cfm>

