Calculation of electron transport properties of hot metallic plasma using semiclassic average atom model

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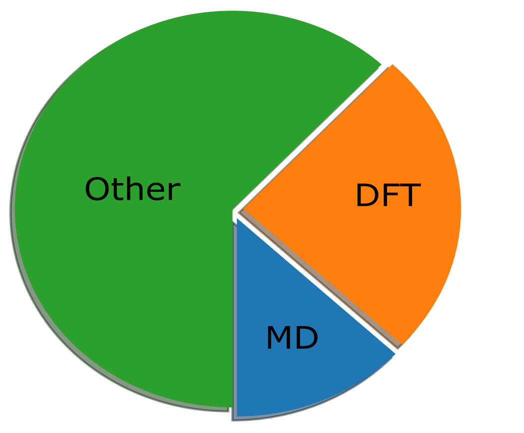
Introduction and motivation



Supercomputing time allocation, by area of research

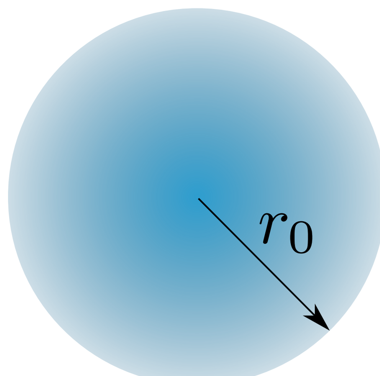
Interaction of intense laser pulses with metals in fusion experiments usually leads to the formation of hot plasma, so that the thermodynamic and transport properties of metals experience a dramatic change. To predict material response in such conditions an adequate wide-range model is required. Without these properties, it is impossible to calculate resistive heating, laser radiation absorption, heat transfer, and some other effects using only the continuum mechanics' approach.

Electron transport properties are usually defined in terms of Onsager theory [1]. Using the Boltzmann equation one can express Onsager coefficients via the electron relaxation time and the transport cross-section [2,3]. The latter can be expressed using phase shifts of electron wave functions in an atomic potential [4]. The present research provides calculations using a one-dimensional average atom model. Ab initio calculations such as DFT and Quantum molecular dynamic are not considered since the main aim of the study is developing a relatively simple and fast algorithm and mentioned above approaches are normally used only on supercomputers.

In this study, we calculate the electric and heat conductivity for electrons in copper and aluminium plasma using the semiclassical average atom model: the bound electron states are evaluated using semiclassic wave functions, while Thomas–Fermi model is used for accounting for the free electrons. The resulting self-consistent potential is used to obtain the transport cross-section and Onsager coefficients.

Semiclassic (SC) average atom model

single atom, spherical cell, electroneutrality



Poisson equation

$$\begin{cases} \frac{1}{r}\frac{d^2}{dr^2}(rU) = 4\pi n(r), \\ rU(r)|_{r=0} = Z,\ U(r_0) = 0,\ U'(r)|_{r=r_0} = 0 \end{cases}$$

Energy levels

Bohr-Sommerfeld (BS) quantization condition is used to get energy levels

$$S_{nl} = \int_{r_1}^{r_2} p_{nl}(r)dr = \pi\left(n - l - \frac{1}{2}\right) \to \varepsilon_{nl}$$

$$p_{nl}(r) = \sqrt{2\left[\varepsilon_{nl} - U(r) - \frac{(l+1/2)^2}{2r^2}\right]}$$

Electron density

$$n(r) = n_{discrete}(r) + n_{continuous}(r)$$

$$n_d(r) = \frac{1}{4\pi r^2}\sum_{\varepsilon<\varepsilon_0} N_{n,l} R^2_{n,l}(r)$$

$$n_c(r) = \frac{(2T)^{\frac{3}{2}}}{2\pi^2}\left[I_{\frac{1}{2}}\left(\frac{U(r)+\mu}{T}\right) - I^{inc}_{\frac{1}{2}}\left(\frac{U(r)+\mu}{T}, y^*\right)\right],$$

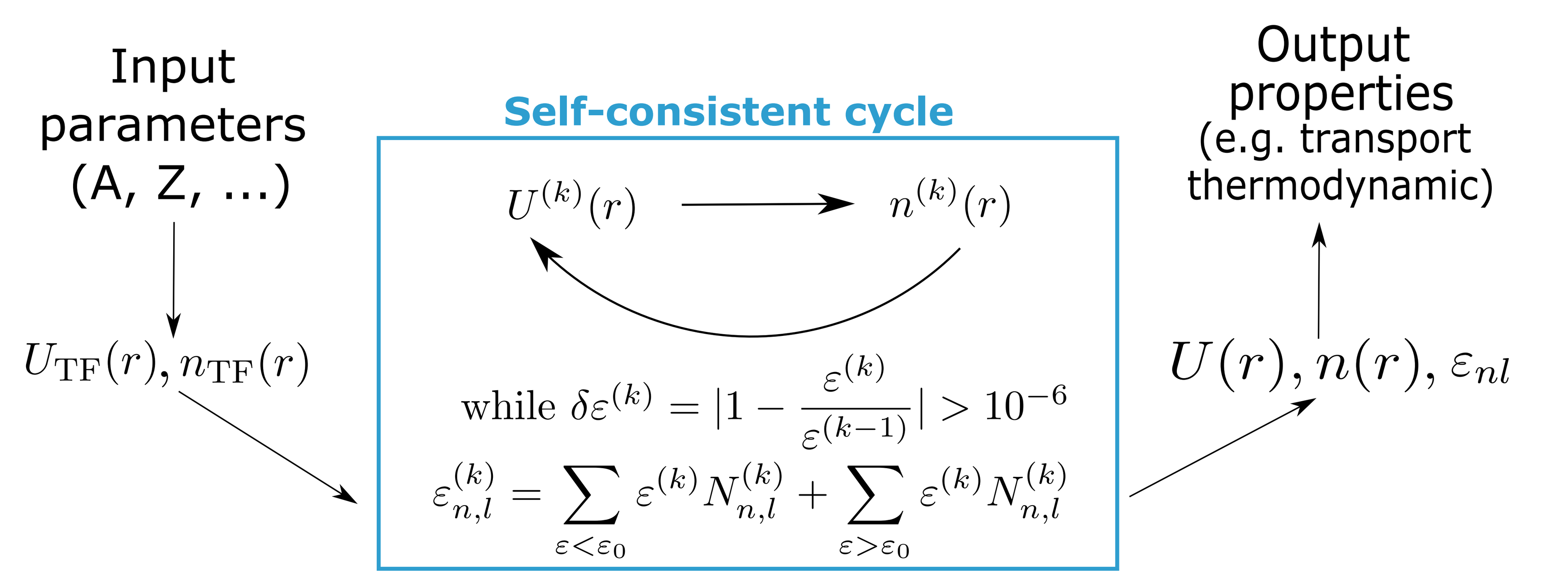
$$y* = \max\left(0, \frac{\varepsilon_0 + U(r)}{T}\right)$$

Energy levels broadening

Gaussian smoothing for discrete spectrum [5]

$$N_{n,l} = \frac{1}{\sigma\sqrt{2\pi}}\int_{\varepsilon_{n,l}-3\sigma}^{\varepsilon_{n,l}+3\sigma} \frac{2(2l+1)}{1+exp(\varepsilon-\mu)} exp\left(-\frac{(\varepsilon-\varepsilon_{n,l})^2}{2\sigma^2}\right) d\varepsilon$$

Self-consistent potential



Semiclassical (SC) wave functions

Starting from inner rotate point

$$R^{(i)}_{nl}(r) = \begin{cases} \frac{C_i}{\sqrt{3}}\sqrt{\frac{\xi_i}{|p|}} K_{1/3}(\xi_i) & (r \le r_i), \\ \frac{C_i}{\pi}\sqrt{\frac{\xi_i}{p}}\left[J_{-1/3}(\xi_i) + J_{1/3}(\xi_i)\right] & (r_i \le r < r_o), \end{cases}$$

$$\xi_i(r) = \left|\int_{r_i}^{r} |p_{nl}(r')| dr'\right|$$ - inner phase

Starting from outer rotate point

$$R^{(o)}_{nl}(r) = \begin{cases} \frac{C_o}{\pi}\sqrt{\frac{\xi_o}{p}}\left[J_{-1/3}(\xi_o) + J_{1/3}(\xi_o)\right] & (r_i < r \le r_o), \\ \frac{C_o}{\sqrt{3}}\sqrt{\frac{\xi_o}{|p|}} K_{1/3}(\xi_o) & (r \ge r_o), \end{cases}$$

$$\xi_o(r) = \left|\int_{r_o}^{r} |p_{nl}(r')| dr'\right|$$ - outer phase

Complete wave function [7]:

$$R_{nl}(r) = [1 - a(r)]R^{(i)}_{nl}(r) + a(r)R^{(o)}_{nl}(r), \qquad a(r) = \xi_i(r)/\xi_i(r_o).$$

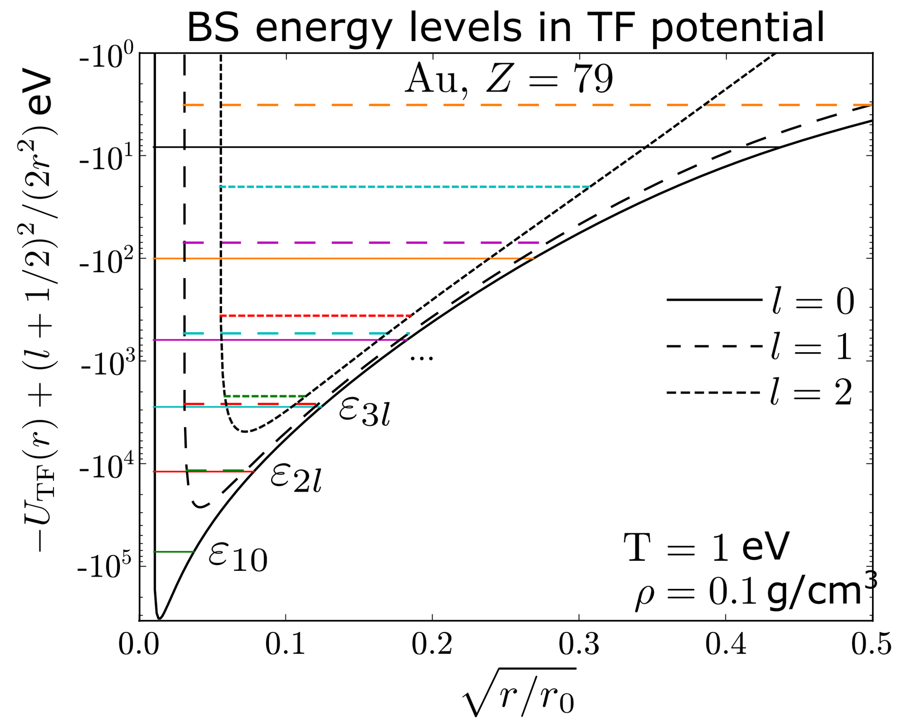
Bessel functions:

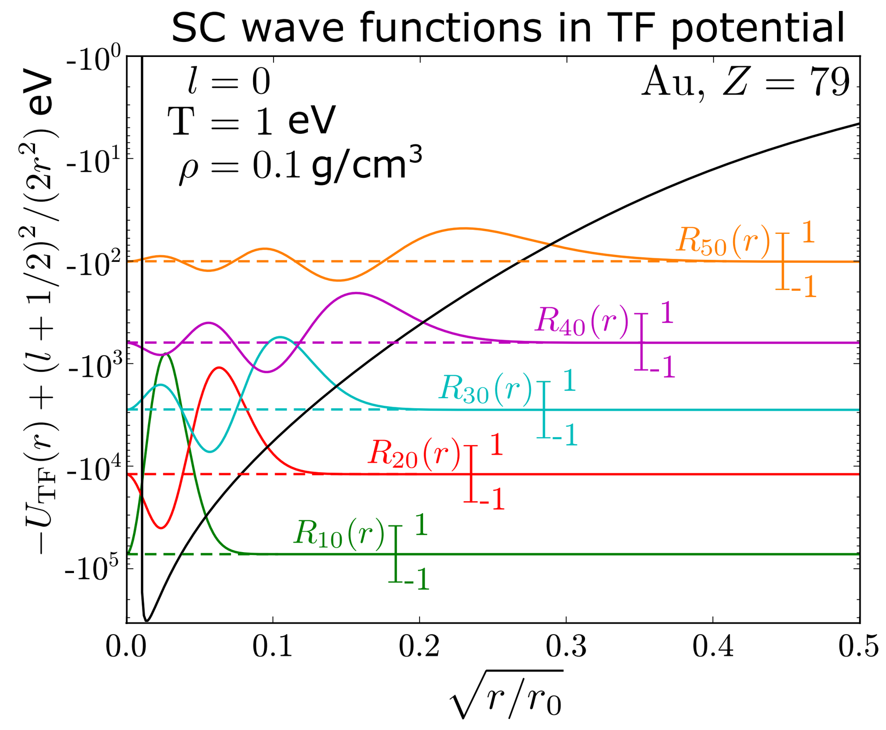
$$J_{-1/3}(x),\ J_{1/3}(x),\ K_{1/3}(x)$$

Normalization:

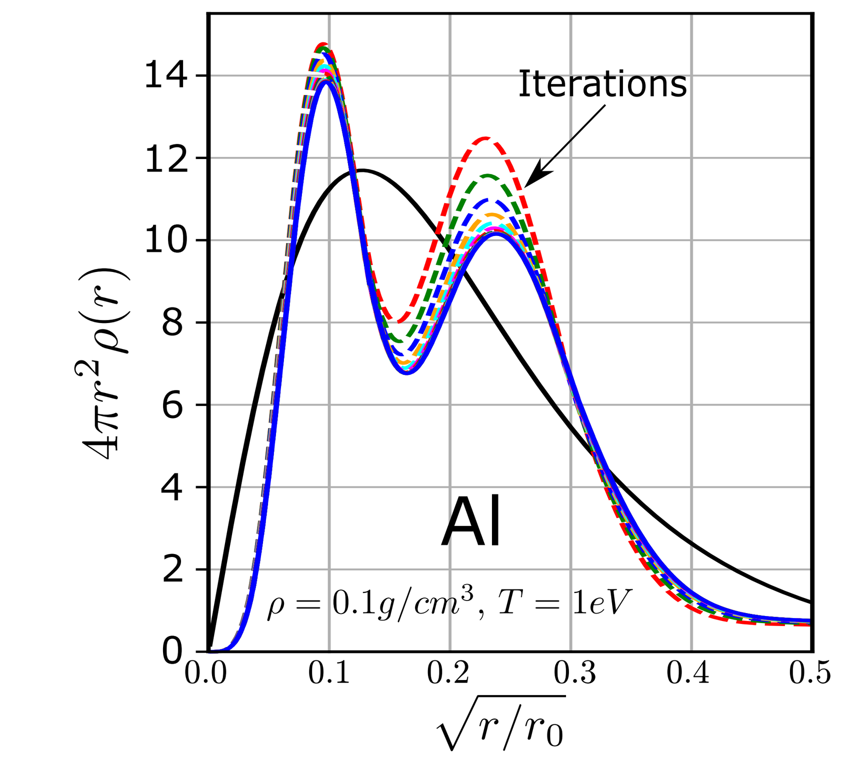
$$\int_0^{r_0} |R_{nl}(r)|^2 dr = 1.$$

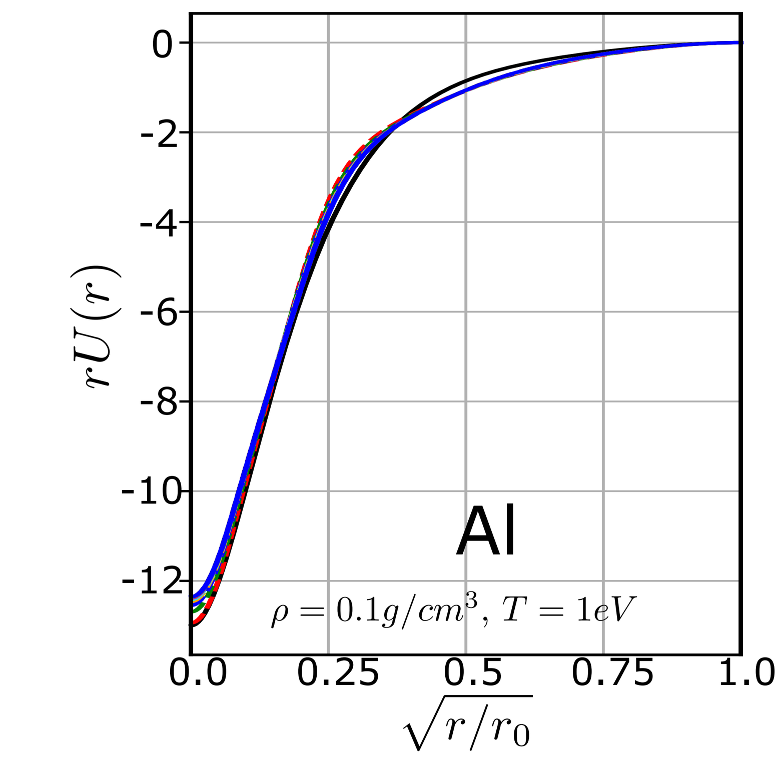
Examples:





Semiclassical electron density and potential





Specific oscillations in the semiclassic variant which correspond electron shells are absent in the Thomas–Fermi approximation. With the temperature growth these shells disappear sequentially starting from the outer ones.

Transport properties [3]

Electric and thermal conductivity: $\sigma = e^2 K_0$ $\quad K = \frac{1}{T}\left(1 - \frac{K_1^2}{K_0}\right)$

Kinetics approach: $K_n = -\tau_c \int \frac{\nu^2}{3}\varepsilon^n \frac{\partial f_0}{\partial \varepsilon}\frac{2d^3\mathbf{p}}{h^3}$ $\quad \frac{1}{\tau_c} = \frac{1}{\tau_{ei}} + \frac{1}{\tau_{en}}, \tau_{ei} = \frac{1}{n_i \nu \sigma_{ei}}, \tau_{en} = \frac{1}{n_0 \nu \sigma_{en}}$

Transport cross section: $\sigma_{ei} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(l+1)sin\left[\delta_l(k) - \delta_{l+1}(k)\right]$

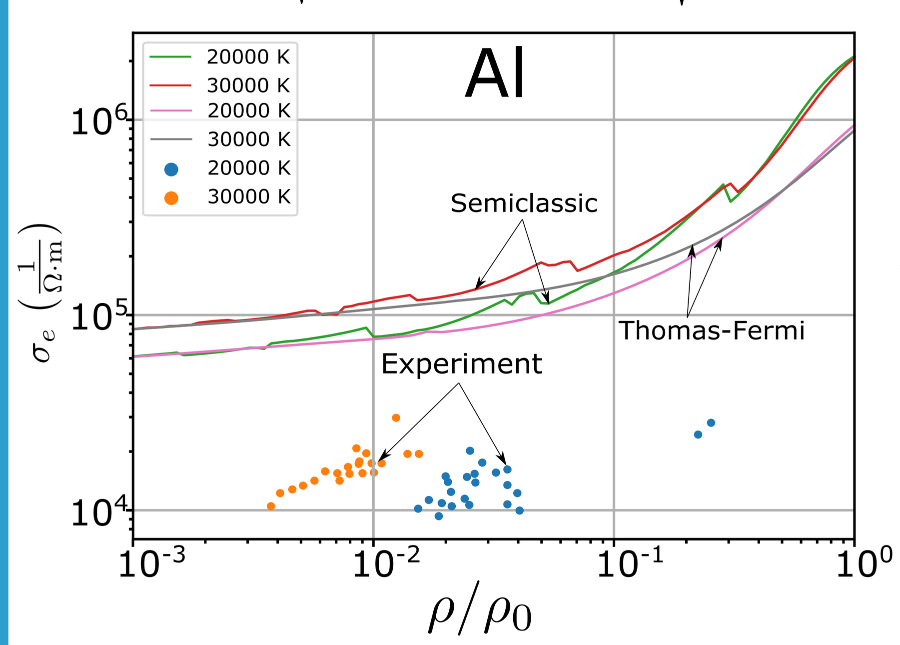
Phase shift equation [4]

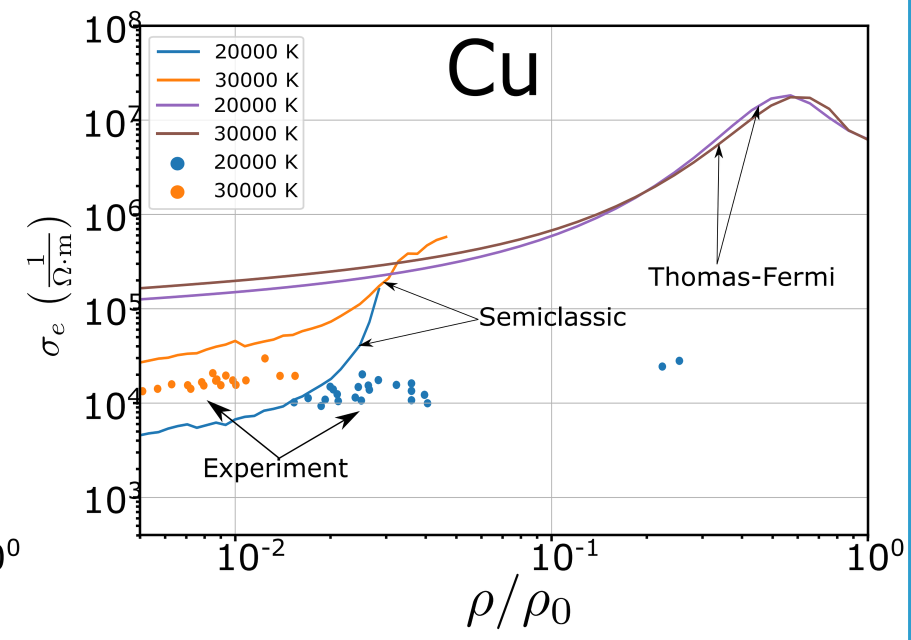
$$\frac{d\delta(r,k)}{dr} = -\frac{1}{k}V(r)|cos(\delta_l(r,k))j_l(kr) - sin(\delta_l(r,k))n_l(kr)|^2$$

$$\delta_l(0,k) = 0$$

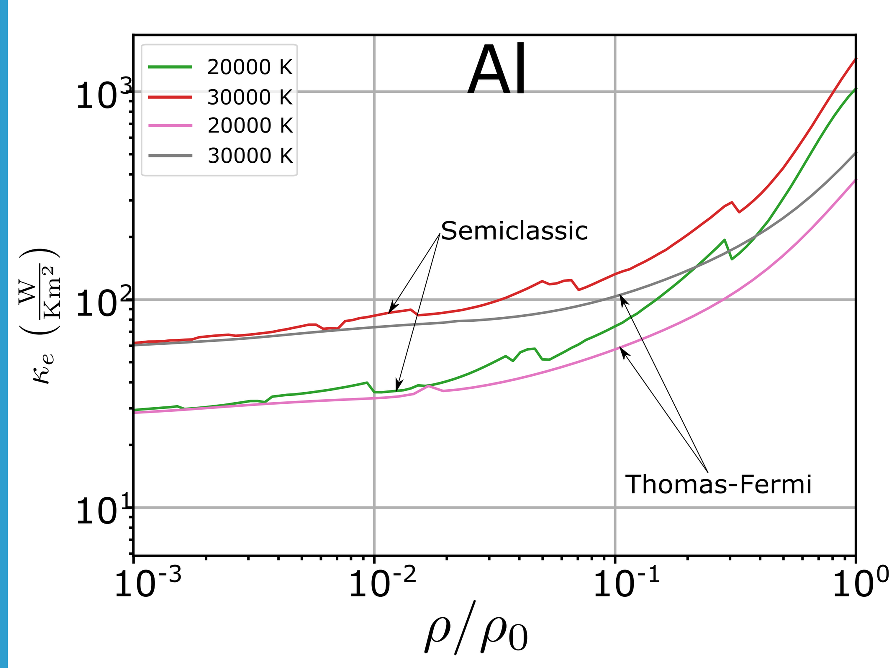
Bessel functions

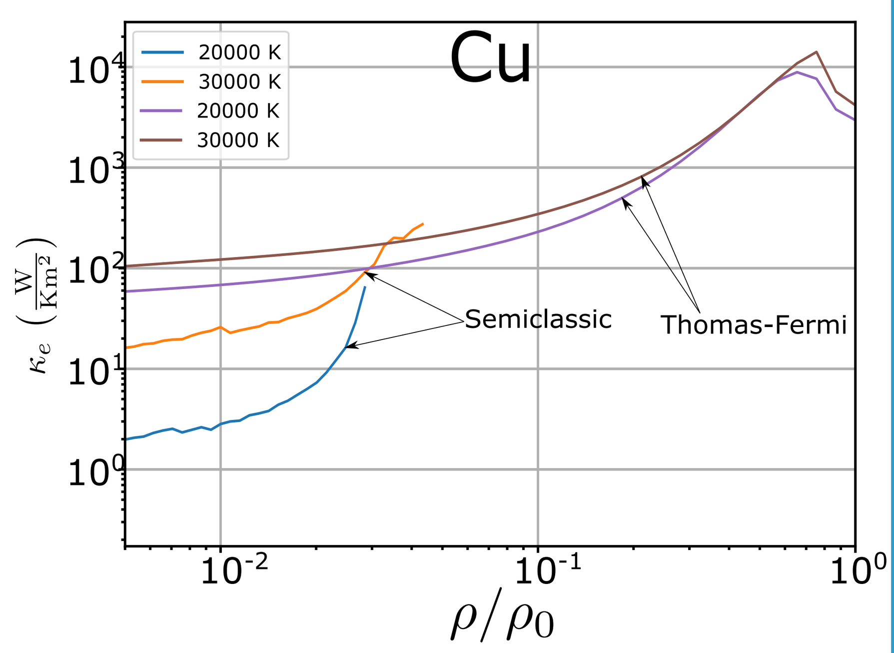
$$n_l(x) = \sqrt{\frac{\pi x}{2}}Y_{l+\frac{1}{2}}(x) \qquad j_l(x) = \sqrt{\frac{\pi x}{2}}J_{l+\frac{1}{2}}(x)$$





Comparison of electric conductivity of Al and Cu calculated using Thomas-Fermi and semiclassic self-consistent potentials with experimental results [6].





Plots of thermal conductivity for Al and Cu calculated using Thomas-Fermi and semiclassic model with self-consistent potential.

Our new semiclassic average atom model provides non-physical disturbances due to problems with convergence of self-consistent cycle. As a result, some points evaluated using atomic potential which is not converged with required precision. Nevertheless, one may notice better agreement with experiment for copper plasma with semiclassic potential, so that our approach seems promising.

Conclusion

We have developed an average atom model based on semiclassic evaluation of wave functions in a spherically symmetric potential. The algorithm for self-consistent field/density evaluation is implemented. Having the proper atomic potential it is possible to obtain Onsager coefficients by evaluating transport cross section for electrons using phase shifts of scattering electrons. As a result, we calculated transport properties of aluminum and copper plasma in wide range of densities. Our new approach seems promising in predicting plasma properties as demonstrated by comparison with experiment, but have unresolved issues with convergence of self-consistent cycle which temporary prevents us from massive computations in wide range of parameters with guaranteed precision.

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