Calculating Transport Coefficients in Warm Dense Matter with the Strongly Coupled Transport (SCOUT) Code

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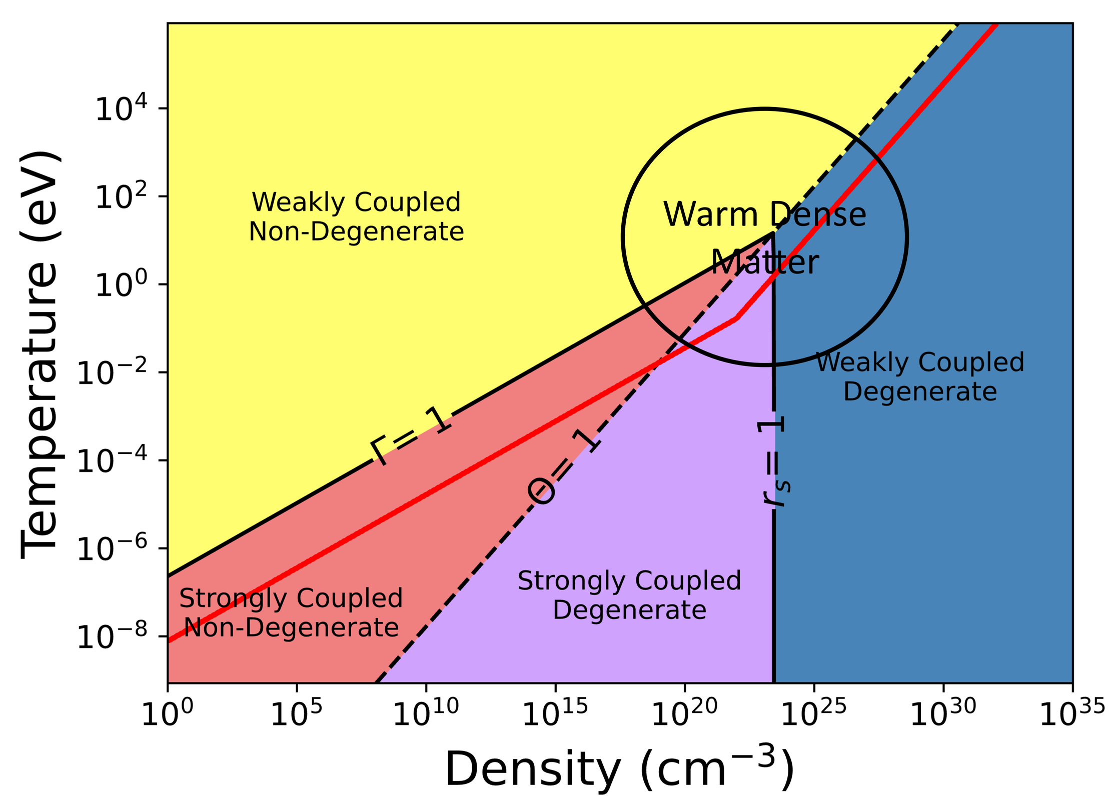
Warm Dense Matter is a state between condensed matter and plasmas

- Plasmas can be characterized by various parameters
  - Coulomb Coupling Parameter: $\Gamma = \frac{\phi(a)}{k_b T} \sim \frac{n^{1/3}}{T}$,
  - Degeneracy Parameter: $\Theta = \frac{k_b T}{E_f} \sim \frac{T}{n^{2/3}}$
  - Degenerate Coupling Parameter: $r_s = \frac{\phi(a)}{E_f} \sim \frac{1}{n^{2/3}}$
- Classical plasma physics: $\Gamma \ll 1, \Theta \gg 1$
- Condensed matter physics: $\Gamma \gg 1, \Theta \ll 1$
- Warm Dense Matter (WDM): $\Gamma \sim 1, \Theta \sim 1$



Motivation and goal of SCOUT is to reduce computation times of transport

- Current state of the art -> Density Functional Theory Molecular Dynamics (DFTMD)
  - Takes days for single point
- Analytic solutions are fast, not accurate
- Kinetic theory is somewhere in the middle

Analytic Formulas | Kinetic Theory (SCOUT) | PseudoAtom MD | DFTMD

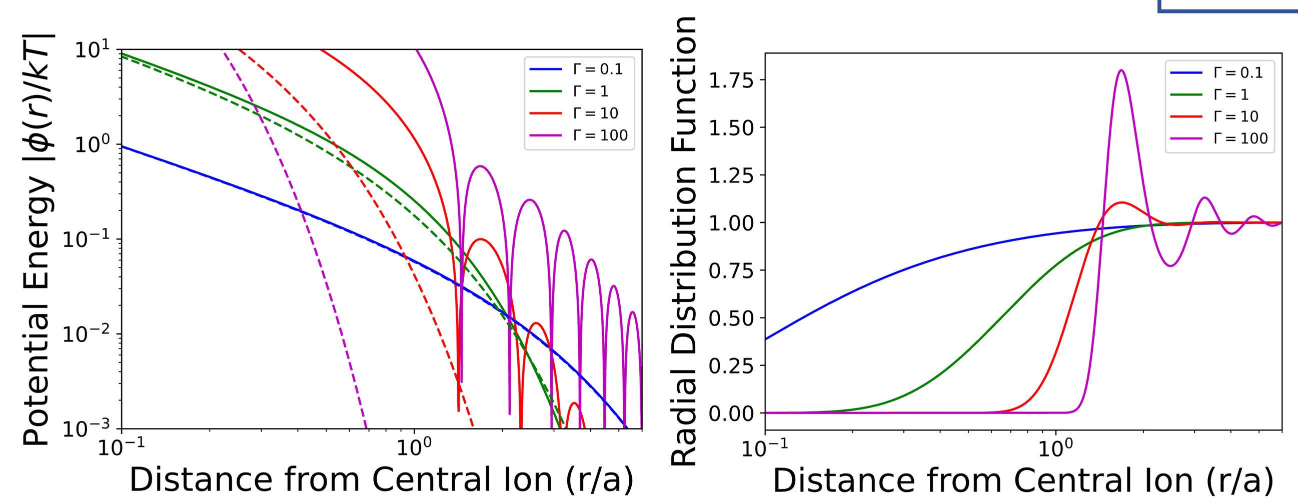
Less time, less accuracy ⟷ More time, more accuracy

- Want to create code (SCOUT) to evaluate the kinetic theory
  - Allows controlled accuracy to quickly fill out tables
- SCOUT workflow:

Input: Density, Temperature, Material → Use atomic and statistical physics to determine interaction potentials → Use potentials in a kinetic theory → **Output:** Transport Coefficients

Mean Force Kinetic Theory extends the Boltzmann Equation to higher coupling

- Usual Boltzmann theory assumes $\Gamma \ll 1$
- Expand on deviations from equilibrium -> Mean Force Kinetic Theory (MFKT) [1]
- Interactions occur via the Potential of Mean Force (PMF)
- PMF determined by Radial Distribution Function, $\phi_{MF}(r) = -k_b T \ln(g(r))$
- Works for $\Gamma \lesssim 30$

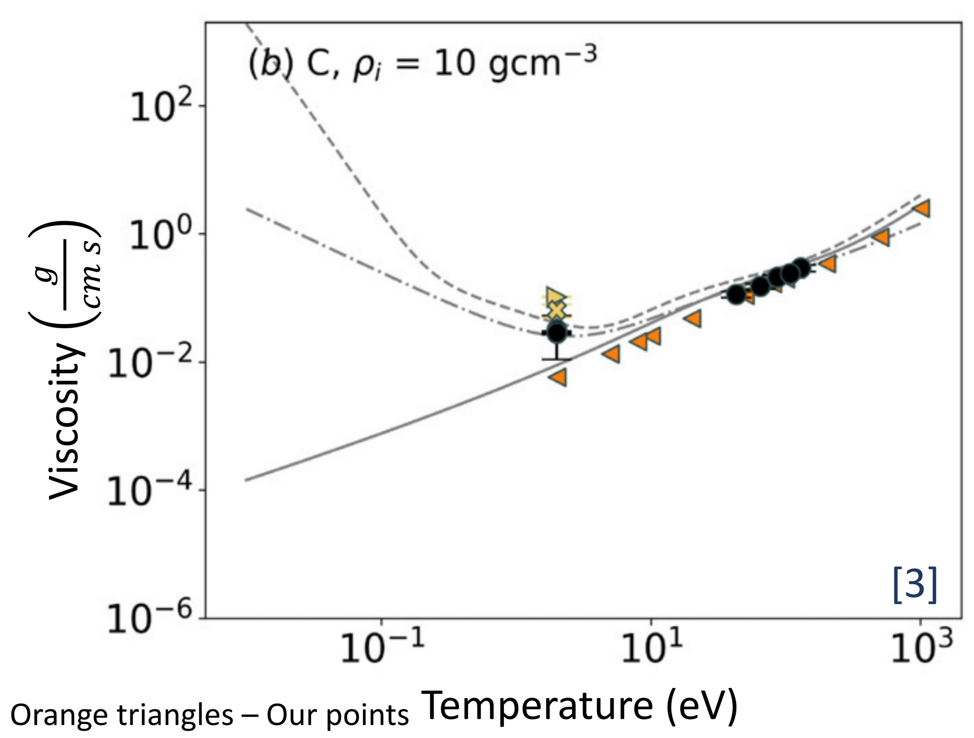


$$\frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{r}} + \frac{\vec{F}}{m} \cdot \frac{\partial f}{\partial \vec{v}} = \int d^3 v_2 \, d\Omega \, \frac{d\sigma}{d\Omega} u (f_1' f_2' - f_1 f_2)$$

Differential Scattering Cross Section, uses PMF | Post collision distribution functions | Pre collision distribution functions

The Potential of Mean Force in WDM includes degenerate electron screening

- WDM is strongly coupled $\Gamma \approx 1$, and degenerate $\Theta \approx 1$
- MFKT takes care of the coupling, need average atom for degeneracy
- Use Average Atom – Two Component Plasma (AA-TCP) model by Starrett and Saumon [2]
  - SCOUT implements Thomas-Fermi version
- Use AA-TCP potentials in MFKT



Orange triangles – Our points
Black circles – Quantum MD
Yellow triangle/cross – Classical MD
Solid line – Stanton Murillo Theory
Dashed/Dotted line – Yukawa Viscosity Model
Dashed line – Yukawa plasma with Gibbs- Bogolyubov Inequality

BUU Equation can be used to model degenerate electrons

- Electrons degenerate -> Boltzmann Uehling-Uhlenbeck equation [4]

$$\frac{\partial f}{\partial t} + \frac{\vec{p}}{m} \cdot \frac{\partial f}{\partial \vec{r}} + \vec{F} \cdot \frac{\partial f}{\partial \vec{p}} = \int d^3 p_2 \, d\Omega \, \frac{d\sigma}{d\Omega} u (f_1' f_2' (1 + \delta_1 \theta_1 f_1)(1 + \delta_2 \theta_2 f_2) - f_1 f_2 (1 + \delta_1 \theta_1 f_1')(1 + \delta_2 \theta_2 f_2'))$$

Differential Scattering Cross Section, uses PMF from [5], full Quantum cross section | Need to couple pre and post collision distribution functions to satisfy particle statistics | Phase space volume per particle | Determining the particle statistics

$$\theta_i = \frac{(2\pi\hbar)^3}{g_i} \qquad \delta_i = \begin{cases} 1 & \text{Boson} \\ 0 & \text{Classical} \\ -1 & \text{Fermion} \end{cases}$$

- PMF used without rigorous proof here [5]
- BUU equilibrium is a Fermi-Dirac/ Bose-Einstein distribution

$$f^{(0)}(\vec{p}) = \frac{1}{\theta} \frac{1}{\exp\left(\frac{p^2}{2mk_B T} - \frac{\mu}{k_B T}\right) - \delta}$$

Linearizing the BUU equation gives us explicit expressions for electron transport

- Chapman-Enskog expansion allows us to calculate transport
- Coefficients written explicitly in terms of "Bracket Integrals"

Thermal Conductivity

$$[\lambda]_2 \sim \frac{\Lambda^{22}}{\Lambda^{11}\Lambda^{22} - (\Lambda^{12})^2}$$

Bracket Integrals

$$\Lambda^{ij} \sim \int d^3 p_1 \, d^3 p_2 \, d\Omega \, \frac{d\sigma}{d\Omega} u f_1^{(0)} f_2^{(0)} \left(1 + \delta_1 \theta_1 f_1^{(0)}\right) \left(1 + \delta_2 \theta_2 f_2^{(0)}\right) G_1^{(i)} \left(F_1^{(j)} + F_2^{(j)} - F_1^{(j)\prime} - F_2^{(j)\prime}\right)$$

Arbitrary functions of momenta, primes indicate post collision momentum

- This integral is difficult/ high dimensional
  - For electron-electron collisions
- Simpler for ion-electron collisions
  - $\delta_1 = 0, \delta_2 = -1$
  - Take mass ratio expansion

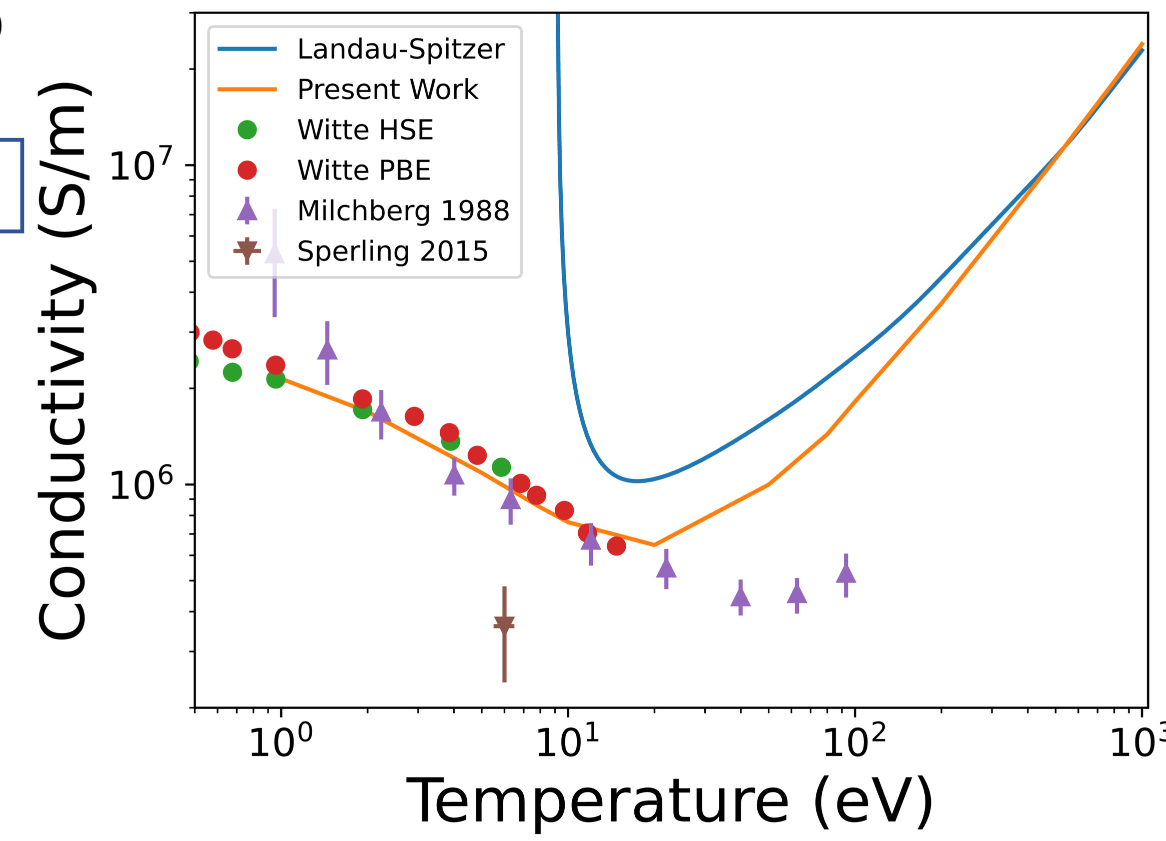
$$\Lambda^{ij} \sim \int \frac{e^{u^2 - \frac{\mu_e}{k_B T}}}{\left(e^{u^2 - \frac{\mu_e}{k_B T}} + 1\right)^2} u^{2(i+j+1)+3} \sigma_p \, du$$

Momentum Transfer Cross section, solved with Quantum scattering

$$\sigma_p = \int d\Omega \frac{d\sigma}{d\Omega} (1 - \cos(\chi))$$

SCOUT can calculate conductivity in Warm Dense Aluminum

- Simplified bracket integral + Quantum cross section -> conductivity in Aluminum at solid density (2.7g/cc)



Witte points are QMD results using Heyd-Scuseria-Ernzerhof (HSE) and Perdew-Burke-Ernzerhof (PBE) exchange correlation functionals [6], Landau-Spitzer is the classical result [7], Milchberg [8] and Sperling [9] are experimental measurements

Conclusions

- SCOUT is planned to be an open-sourced code which can calculate transport coefficients in WDM
- The Mean Force Kinetic Theory can be used for ions with the degenerate screening of electrons provided by the AA-TCP model
- Degenerate electron transport can be modeled by the BUU equation with the PMF
- A Chapman-Enskog expansion has been done on the BUU equation, but the resulting expressions are complicated
- Taking a mass ratio expansion, ion-electron conductivities can be calculated
- Electron-electron contributions are still a work in progress and will involve the full Chapman-Enskog solution

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