Molecular Dynamics Simulations of the Hydrodynamic Transport Coefficients

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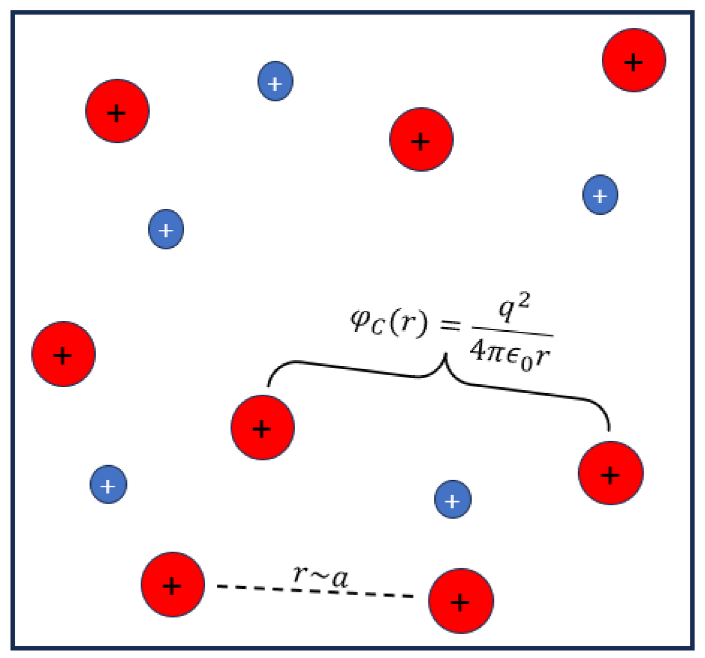
Motivation

- The Chapman-Enskog solution of the Boltzmann equation has yet to be thoroughly validated
- Results are needed in strong coupling to provide a testbed for theories
- Two-component systems are historically overlooked in favor of one-component systems

The Two-Component Plasma Model



- Repulsive two-component system
- Using open source code LAMMPS
- 5000 particles per species in 3D box with periodic boundary conditions
- Thermostat, then evolve particles in NVE ensemble

Electron coulomb coupling parameter:

$$\Gamma_e = \frac{q^2}{4\pi\epsilon_0 a_e k_B T} \qquad (1)$$

Non-Equilibrium Solutions

Transport coefficients are evaluated using the Green-Kubo relations:

$$\text{Electrical Conductivity: } \sigma = \frac{V}{3k_B T}\int_0^\infty dt\, \langle \mathbf{j}(t)\cdot\mathbf{j}(0)\rangle, \qquad (2a)$$

$$\text{Electrothermal Coefficient: } \varphi = -\frac{V}{3k_B T^2}\int_0^\infty dt\, \langle \mathbf{j}(t)\cdot\mathbf{q}(0)\rangle, \qquad (2b)$$

$$\text{Thermal Conductivity: } \lambda = \frac{V}{3k_B T^2}\int_0^\infty dt\, \langle \mathbf{q}(t)\cdot\mathbf{q}(0)\rangle, \qquad (2c)$$

$$\text{Thermoelectric Conductivity: } \phi = \frac{V}{3k_B T}\int_0^\infty dt\, \langle \mathbf{q}(t)\cdot\mathbf{j}(0)\rangle, \qquad (2d)$$

$$\text{Shear Viscosity: } \eta = \frac{V}{6k_B T}\sum_{i=1}^{3}\sum_{j\neq i}^{3}\int_0^\infty dt\, \langle \hat{P}_{ij}(t)\hat{P}_{ij}(0)\rangle, \qquad (2e)$$

with the microdynamics described using the Irving-Kirkwood procedure:

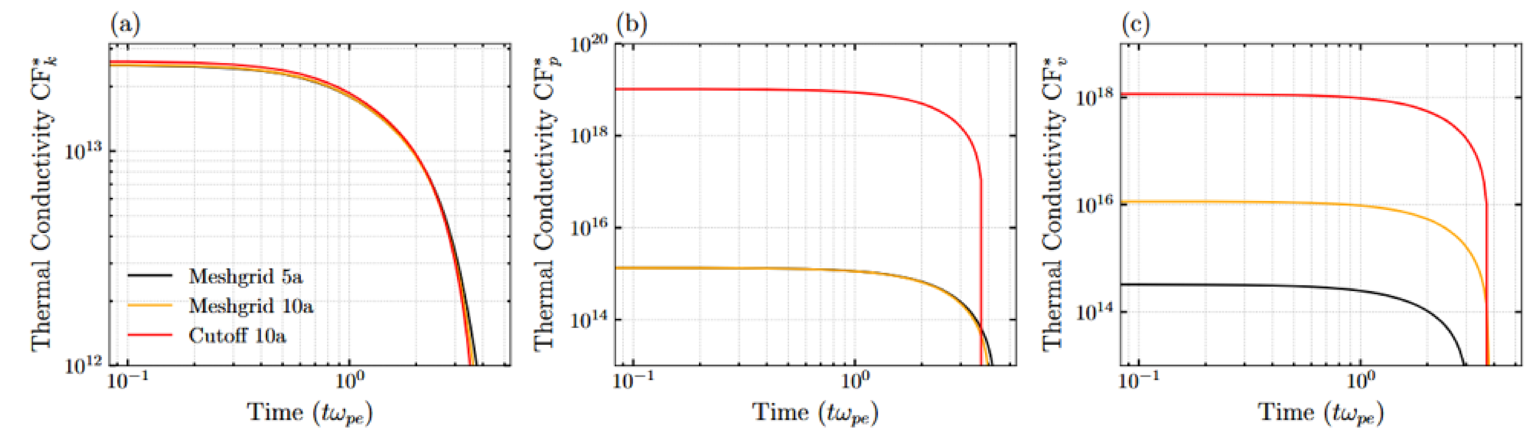
$$\mathbf{j} = \frac{1}{V}\sum_{i=1}^{N} q_i\mathbf{v}_i, \qquad (3a)$$

$$\mathbf{P} = \frac{1}{V}\sum_{i=1}^{N}\left(m_i\mathbf{v}_i\mathbf{v}_i + \frac{1}{2}\sum_{j\neq i}^{N}\mathbf{r}_{ij}\frac{\partial\phi_{ij}}{\partial\mathbf{r}_i}\right), \qquad (3b)$$

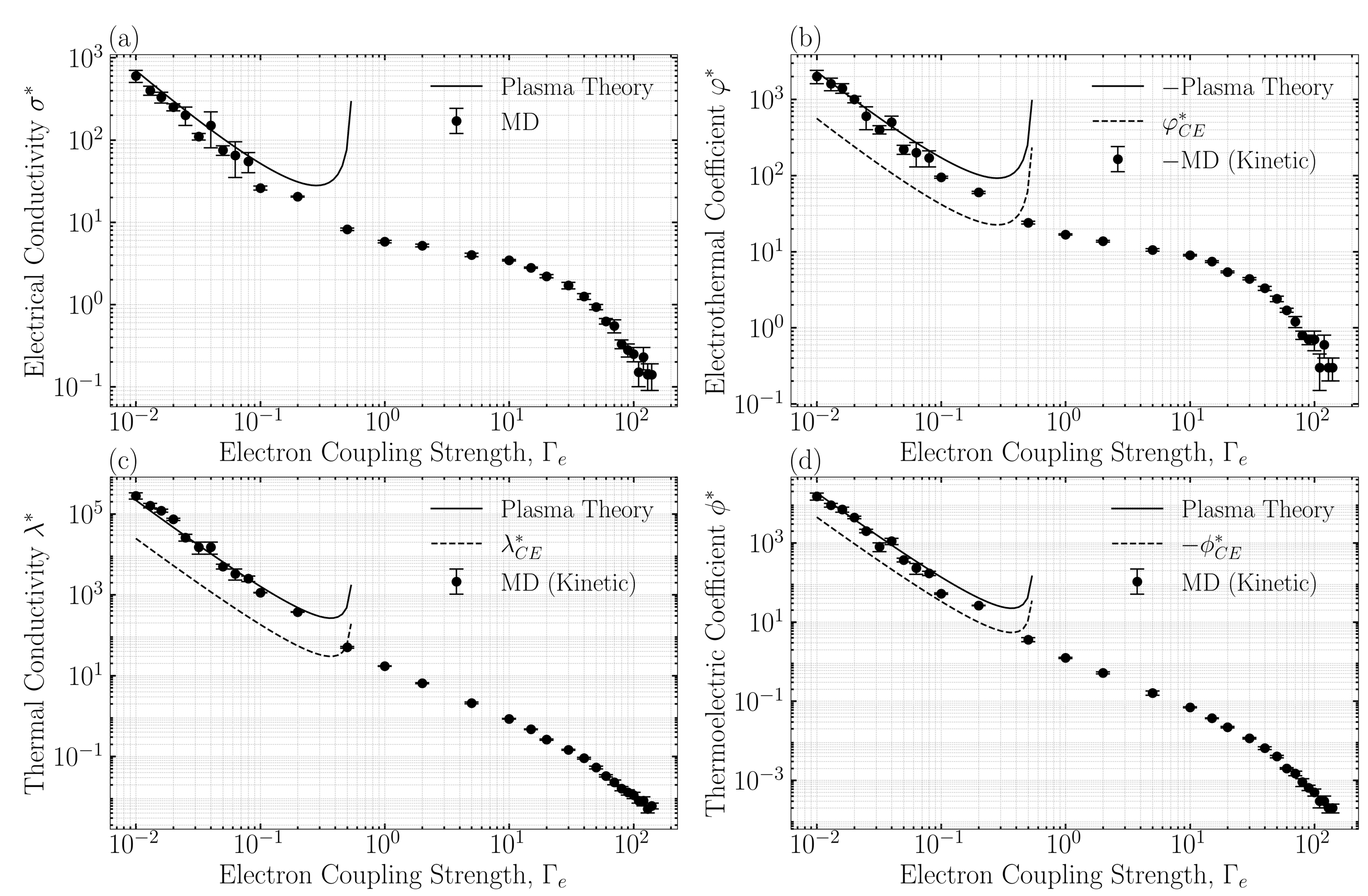
$$\mathbf{q} = \frac{1}{V}\sum_{i=1}^{N}\left[\underbrace{\mathbf{v}_i\frac{1}{2}m_i|\mathbf{v}_i|^2}_{\text{kinetic}} + \underbrace{\frac{1}{2}\mathbf{v}_i\sum_{j\neq i}^{N}\phi_{ij}}_{\text{potential}} + \underbrace{\frac{1}{2}\sum_{j\neq i}^{N}(\mathbf{r}_i\cdot\mathbf{v}_i)\frac{\partial\phi_{ij}}{\partial\mathbf{r}_i}}_{\text{virial}}\right]. \qquad (3c)$$

Separation of Heat Flux Components

- Potential is infinite in repulsive system $\implies$ heat flux is infinite
- Component significance:
  - Kinetic components dominate at weak coupling
  - OCP shows potential and virial components dominate when $\Gamma \geq 10$



Results



Chapman-Enskog Solution

The Chapman-Enskog solution is the textbook kinetic theory closure to the MHD equations and relate the transport coefficients to system parameters:

$$\sigma_{CE} = 1.93\frac{n_e q_e^2\tau_e}{2m_e}, \qquad (4a)$$

$$\varphi_{CE} = 0.78\frac{k_B n_e q_e\tau_e}{m_e}, \qquad (4b)$$

$$\lambda_{CE} = 1.02\frac{n_e k_B^2 T\tau_e}{m_e}, \qquad (4c)$$

$$\eta_{CE} = 0.96 n_i k_B T\sqrt{\frac{m_i}{2m_e}}\tau_e, \qquad (4d)$$

where

$$\tau_e = \frac{3}{2\sqrt{2\pi}}\frac{(4\pi\epsilon_0)^2\sqrt{m_e}(k_B T)^{3/2}}{n_e q_e^4\ln\Lambda} \qquad (5)$$

is the electron coulomb collision time.

Comparison of Linear Constitutive Relations

The fluxes in both theories are equivalent; however, the organization of the fluxes are different leading to different transport coefficients. After relating the fluxes, the following equations may be obtained:

$$\sigma = \sigma_{CE} = 1.93\frac{n_e q_e^2\tau_e}{2m_e} \qquad (6a)$$

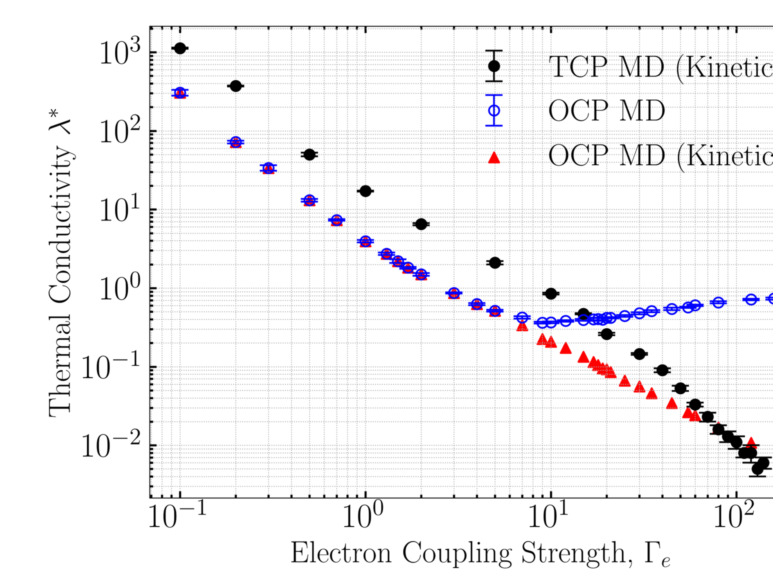
$$\varphi = -\varphi_{CE} - \frac{5k_B}{2q_e}\sigma_{CE} = -3.19\frac{k_B n_e q_e\tau_e}{m_e} \qquad (6b)$$

$$\phi = T\varphi_{CE} + \frac{5k_B T}{2q_e}\sigma_{CE} = 3.19\frac{k_B T n_e q_e\tau_e}{m_e} \qquad (6c)$$

$$\lambda = \lambda_{CE} + T\frac{\varphi_{CE}^2}{\sigma_{CE}} + \frac{5k_B T}{q_e}\varphi_{CE} + \frac{25k_B^2 T}{4q_e^2}\sigma_{CE} = 11.58\frac{n_e k_B^2 T\tau_e}{m_e} \qquad (6d)$$

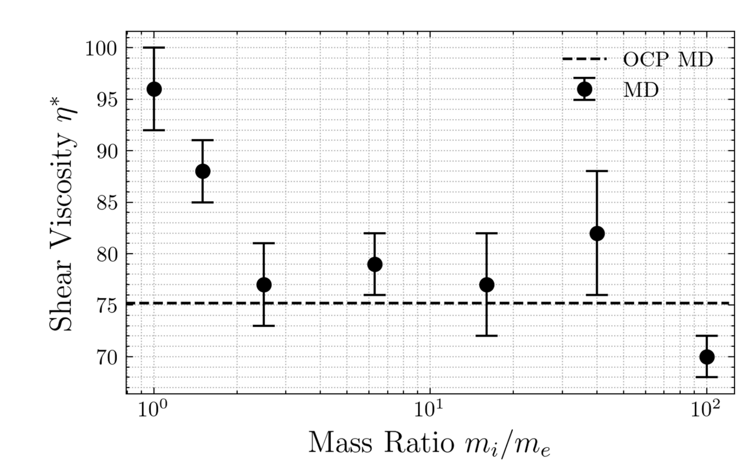
$$\eta = \eta_{CE} = 0.96 n_i k_B T\sqrt{\frac{m_i}{2m_e}}\tau_e. \qquad (6e)$$

Diffusive Contributions Dominate in the TCP

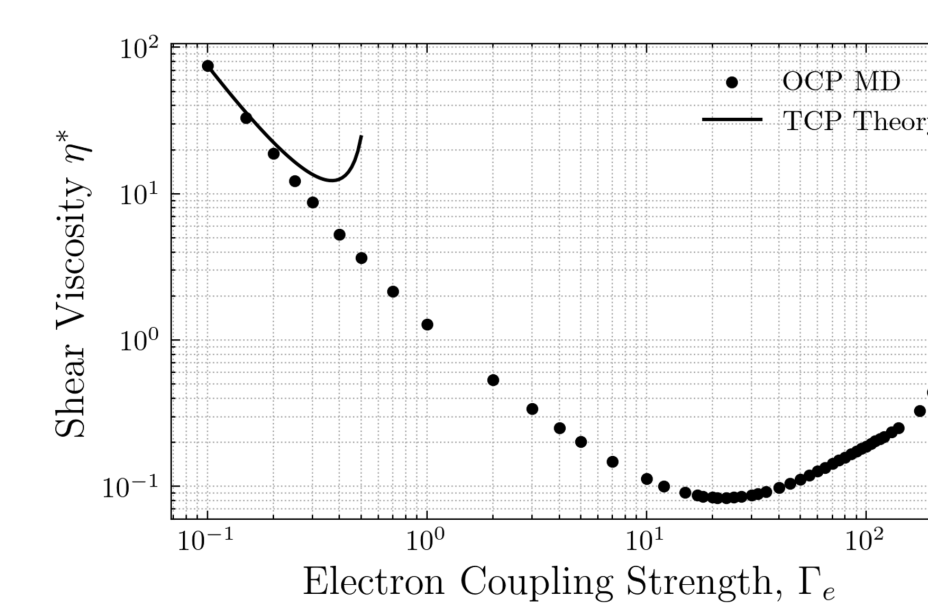


- One-component and two-component systems differ due to diffusive contributions
- Virial and potential components dominate at $\Gamma \geq 10$

Shear Viscosity Model



- MD Simulation of TCP Shear is intractable
- As mass ratio increases, TCP approaches OCP value
- Justifies using OCP as a model and we see good agreement with this comparison



References

[1] J. Daligault, and S. D. Baalrud. "Determination of the shear viscosity of the one-component plasma." Physical Review E 90: 033105 (2014).