Classical Simulation Methods

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One-component plasma models

- reduced description of strongly correlated plasmas → single species
- include effect of background species (e.g., electrons) in effective pair potential
- simplest approximation: Yukawa potential

$$v(r) = q^2 \exp(-r/\lambda)/r$$

screening parameter

$$\kappa = \frac{a}{\lambda}$$

$$\Gamma = \frac{q^2}{4\pi\epsilon_0 a_{\rm ws}} \frac{1}{k_{\rm B}T} \sim \frac{U_{\rm int}}{E_{\rm kin}}$$

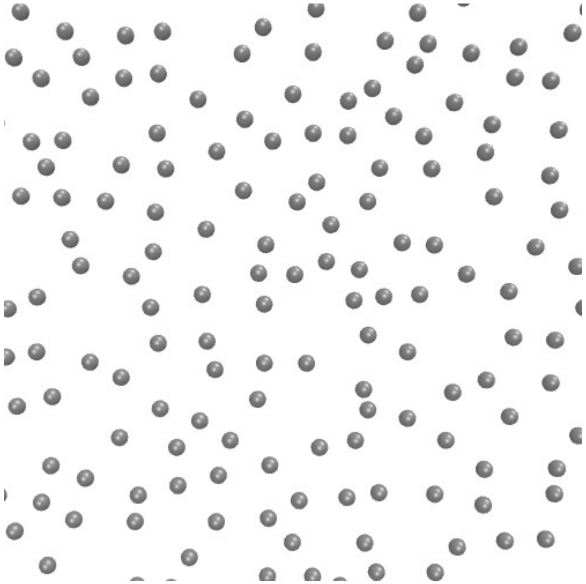
coupling parameter

$$\frac{4}{3}\pi n\, a_{\rm ws}^3 = 1$$

Wigner-Seitz radius

Molecular dynamics:

Applications



Molecular dynamics (MD) simulation

$$m\ddot{\boldsymbol{r}}_i = \sum_{j\neq i}^{N} \boldsymbol{F}_{ij}$$

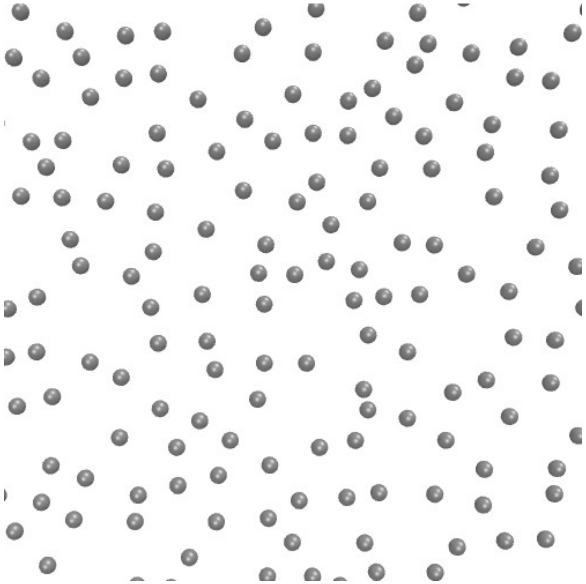
→ complete microscopic information { $\mathbf{r}_i(t)$, $\mathbf{p}_i(t)$ }

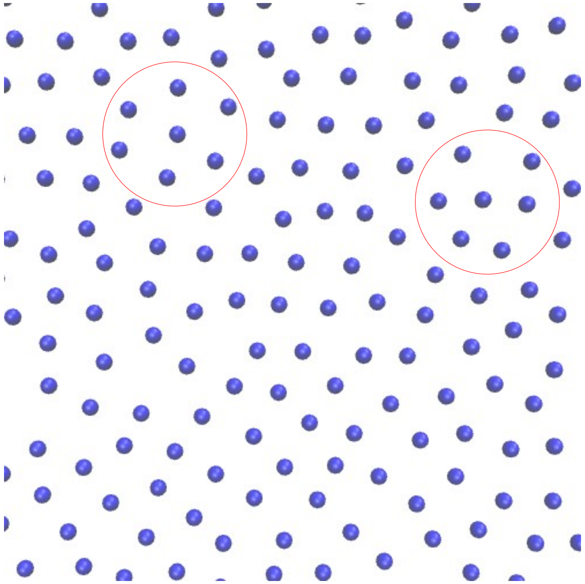
weak coupling

$\Gamma << 1$

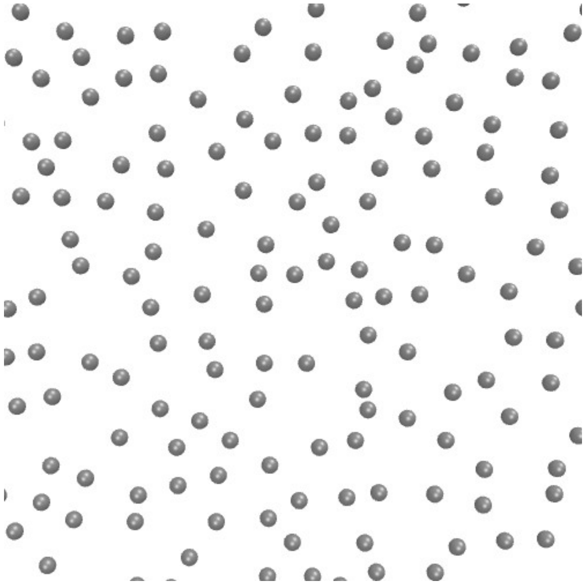
gas-like
no order

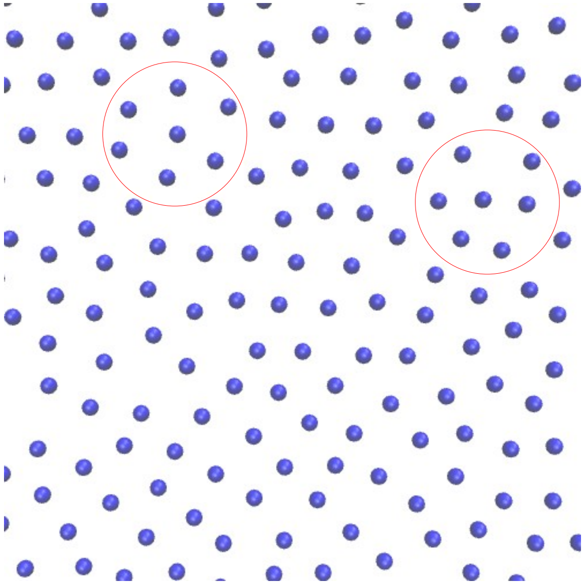
Strong coupling

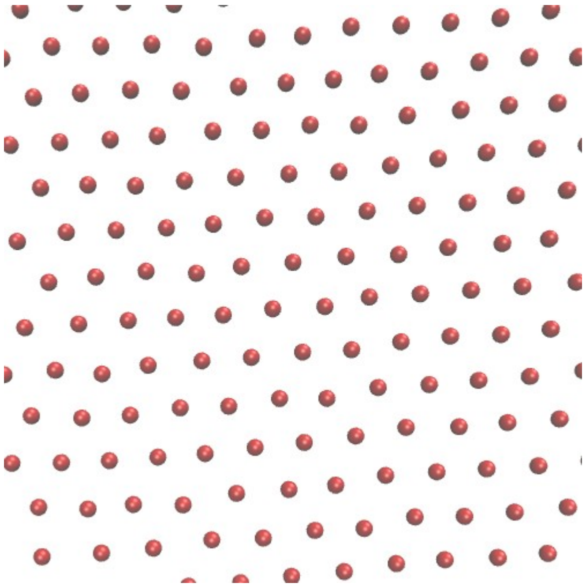




weak coupling	**strong coupling**
$\Gamma << 1$	$\Gamma > 1$
gas-like no order	liquid-like short-range order







weak coupling

$\Gamma << 1$

gas-like
no order

strong coupling

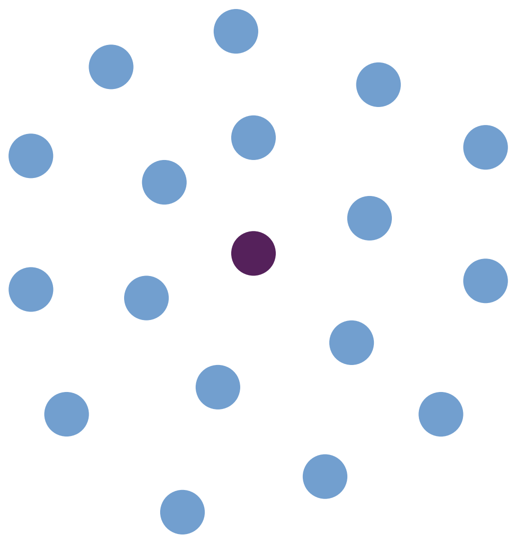
$\Gamma > 1$

liquid-like
short-range order

$\Gamma > \Gamma_s$

crystal
long-range order

Distribution functions



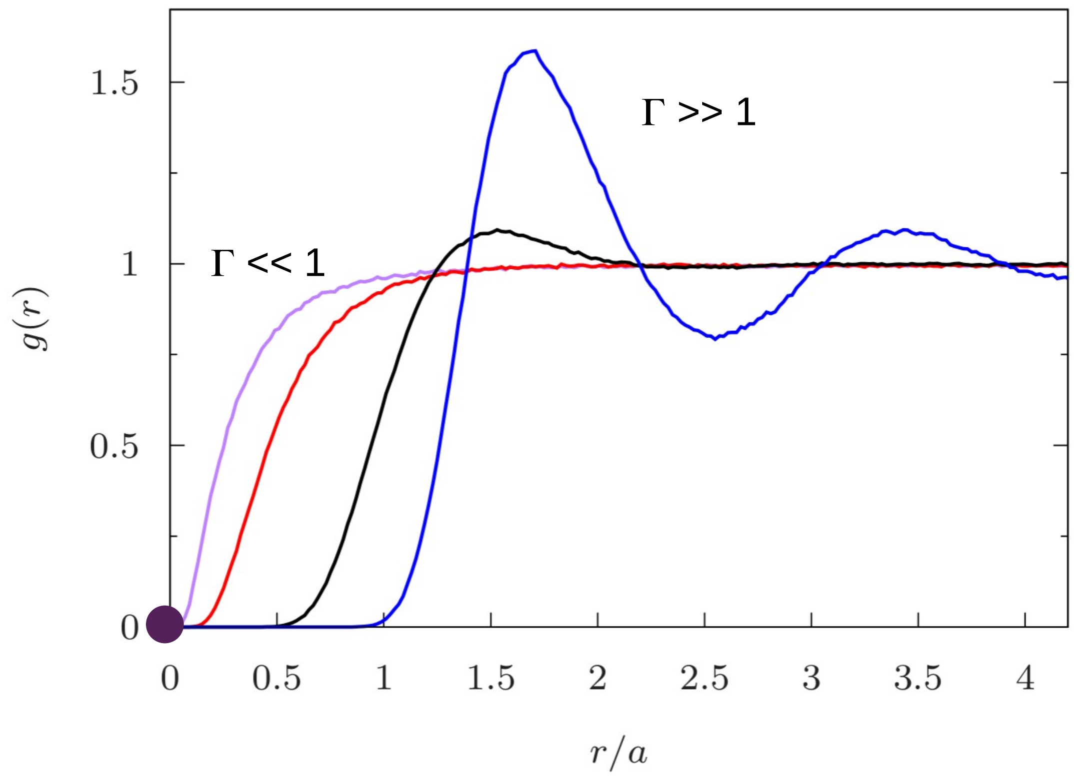
$g(r) = n_1(r) / n_0$

density profile around fixed particle

uniform density $n_0 = N / V$

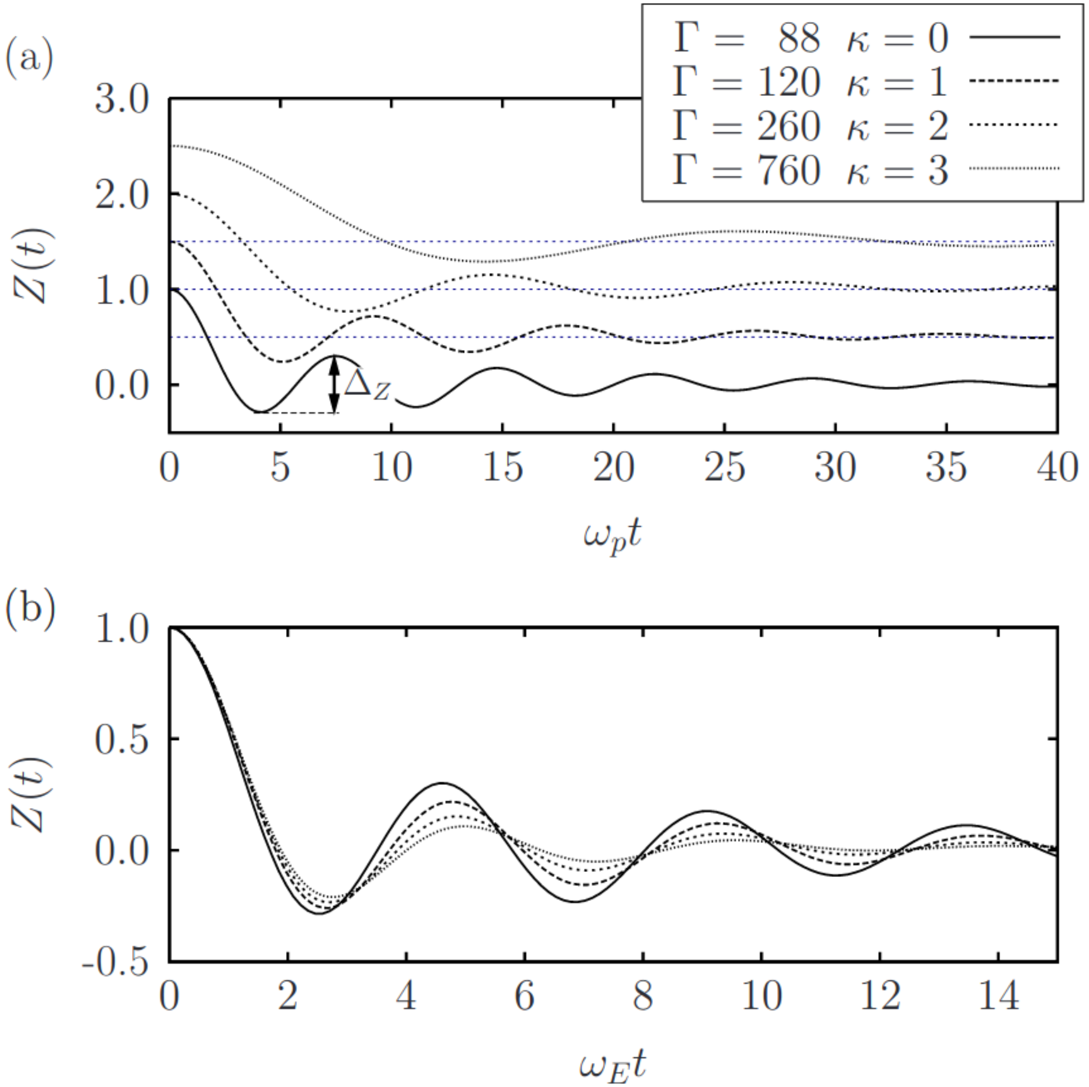
Pair distribution function

→ two-particle distribution function



Velocity autocorrelation function

$$Z(t) = \frac{\langle \boldsymbol{v}(t) \cdot \boldsymbol{v}(0) \rangle}{\langle |\boldsymbol{v}(0)|^2 \rangle}$$



frequency of oscillations ~ Einstein frequency

Ott, Stanley, and Bonitz, Phys. Plasmas (2011)

Transport coefficients

$$P_{xy}(t) = \sum_{i=1}^{N} \left[m v_{ix} v_{iy} - \frac{1}{2} \sum_{j \neq i}^{N} \frac{x_{ij} y_{ij}}{r_{ij}} \frac{\partial \Phi(r_{ij})}{\partial r_{ij}} \right]$$

$$C_s(t) = \langle P_{xy}(t) P_{xy}(0) \rangle,$$

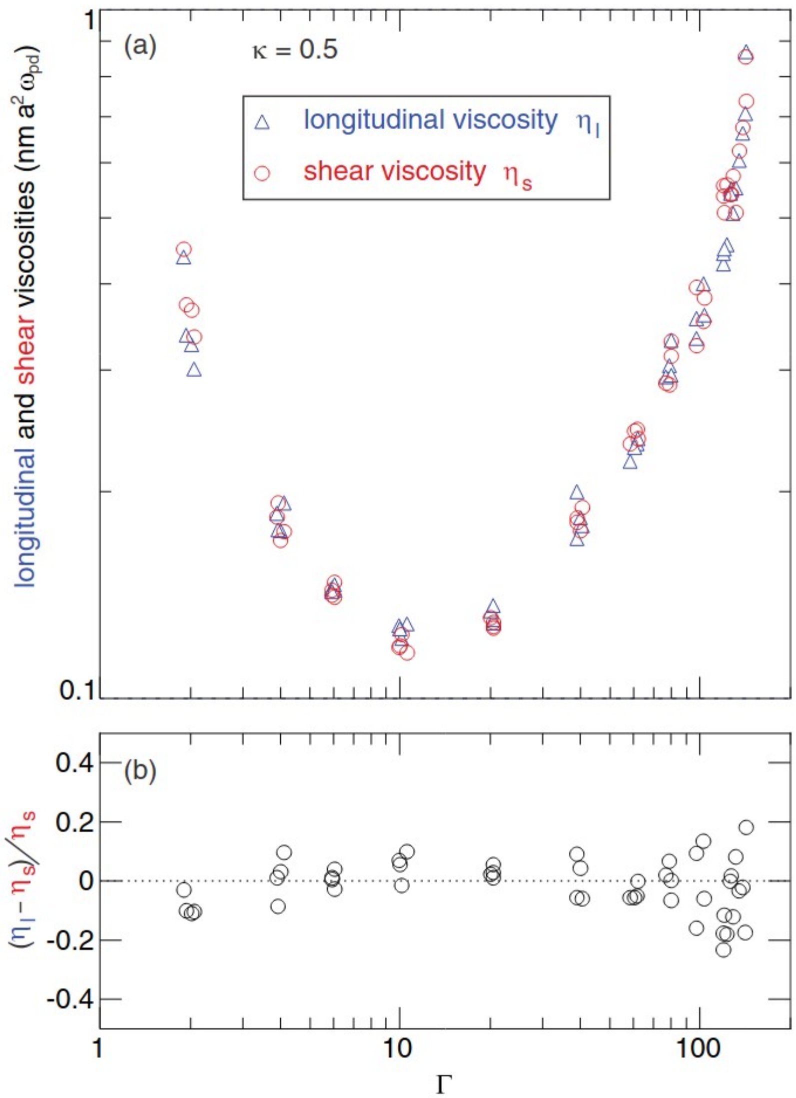
off-diagonal pressure tensor

$$\eta_s = \frac{1}{A k_B T} \int_0^\infty C_s(t) dt$$

Shear viscosity

Green-Kubo relation:

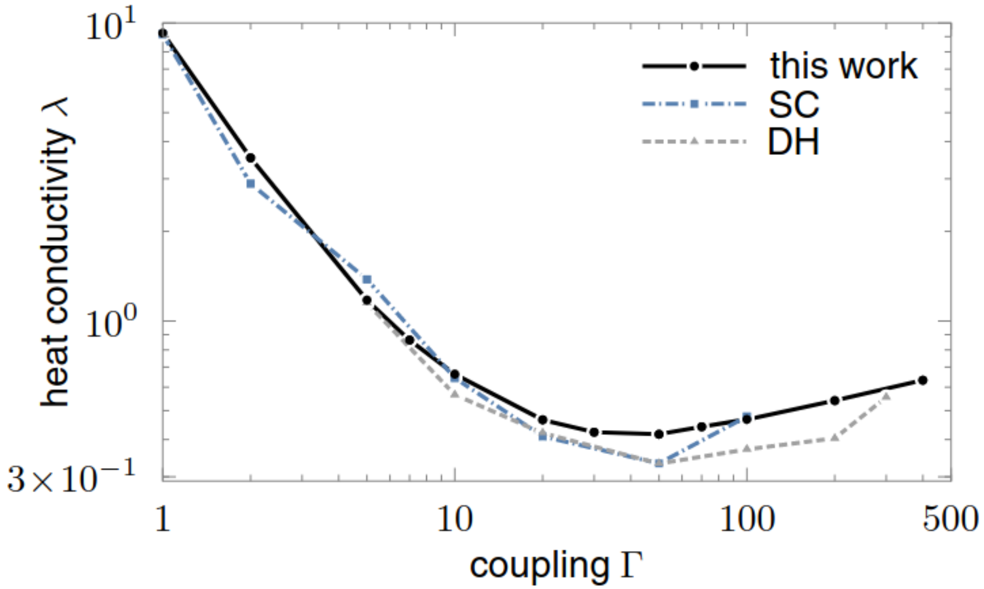
microscopic correlation function
↔
macroscopic transport coefficient



Feng, Goree, and Liu, PRE (2013)

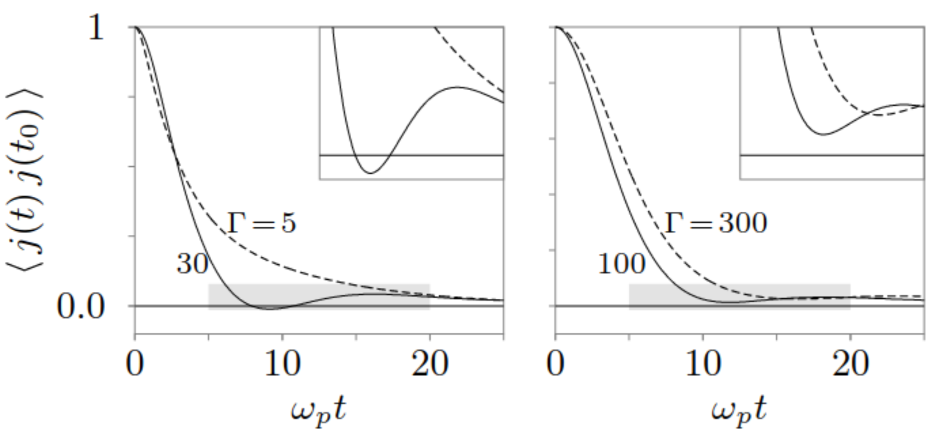
heat flux

$$\mathbf{j} = \sum_{i=1}^{N} \mathbf{v}_i \left[\frac{1}{2} m |\mathbf{v}_i|^2 + \frac{1}{2} \sum_{j \neq i}^{N} \phi(r_{ij}) \right] + \frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} (\mathbf{r}_{ij} \cdot \mathbf{v}_i) \mathbf{F}_{ij},$$



Heat conductivity

$$\lambda_{\mu\nu} = \lim_{\tau \to \infty} \frac{1}{V k_B T^2} \int_0^{\tau} \langle j_\mu(t) j_\nu(0) \rangle dt$$



Ott and Bonitz, and Donkó, PRE (2015)

density autocorrelation function

$$F(\boldsymbol{k},t) = \frac{1}{N}\langle n(\boldsymbol{k},t)n^*(\boldsymbol{k},0)\rangle$$

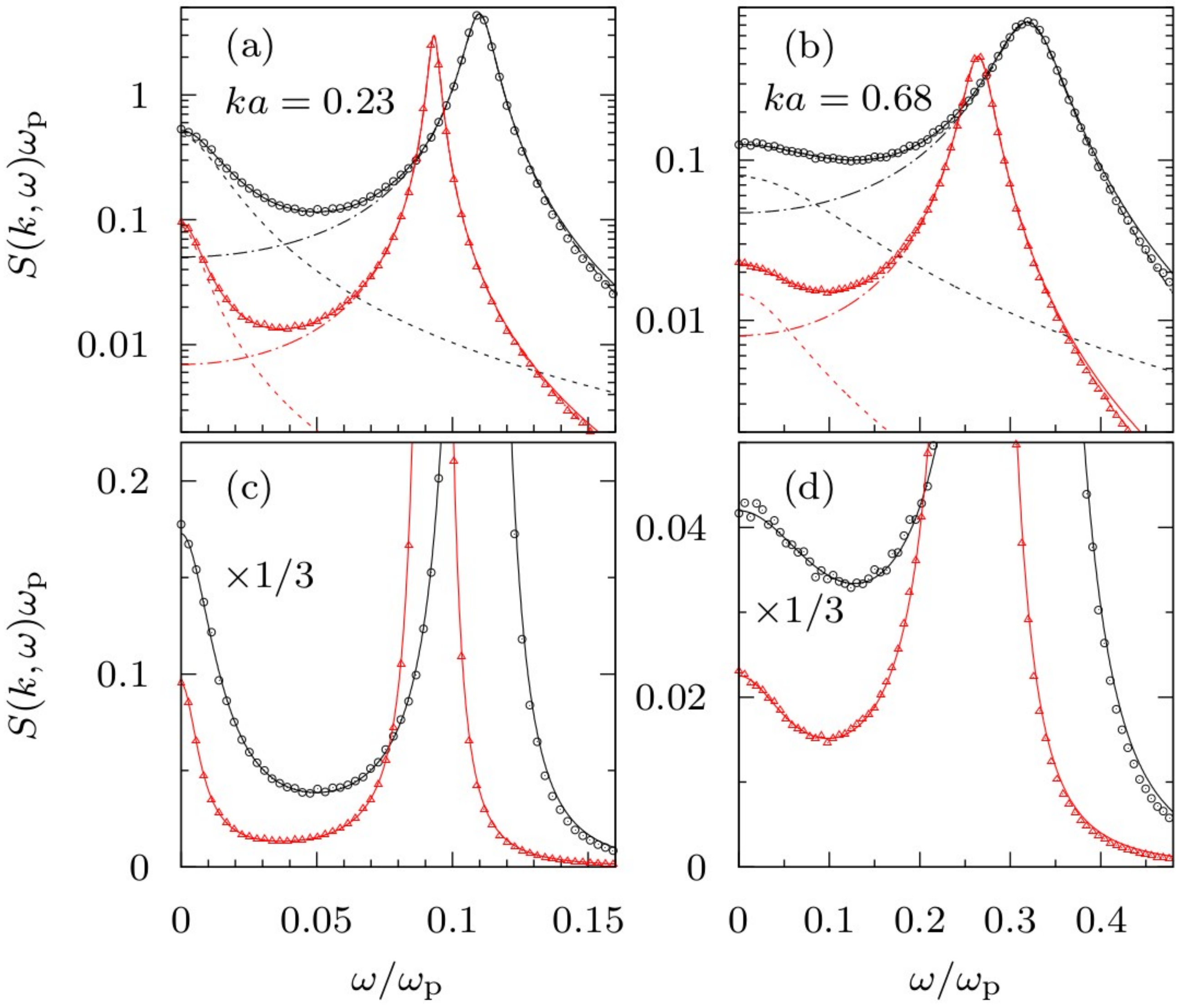
Fourier spectrum →

dynamic structure factor

$$S(\boldsymbol{k},\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\omega t}F(\boldsymbol{k},t)\,\mathrm{d}t$$

$$n(\boldsymbol{k},t) = \sum_{i=1}^{N} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i(t)}$$

Dynamic structure factor



coupling

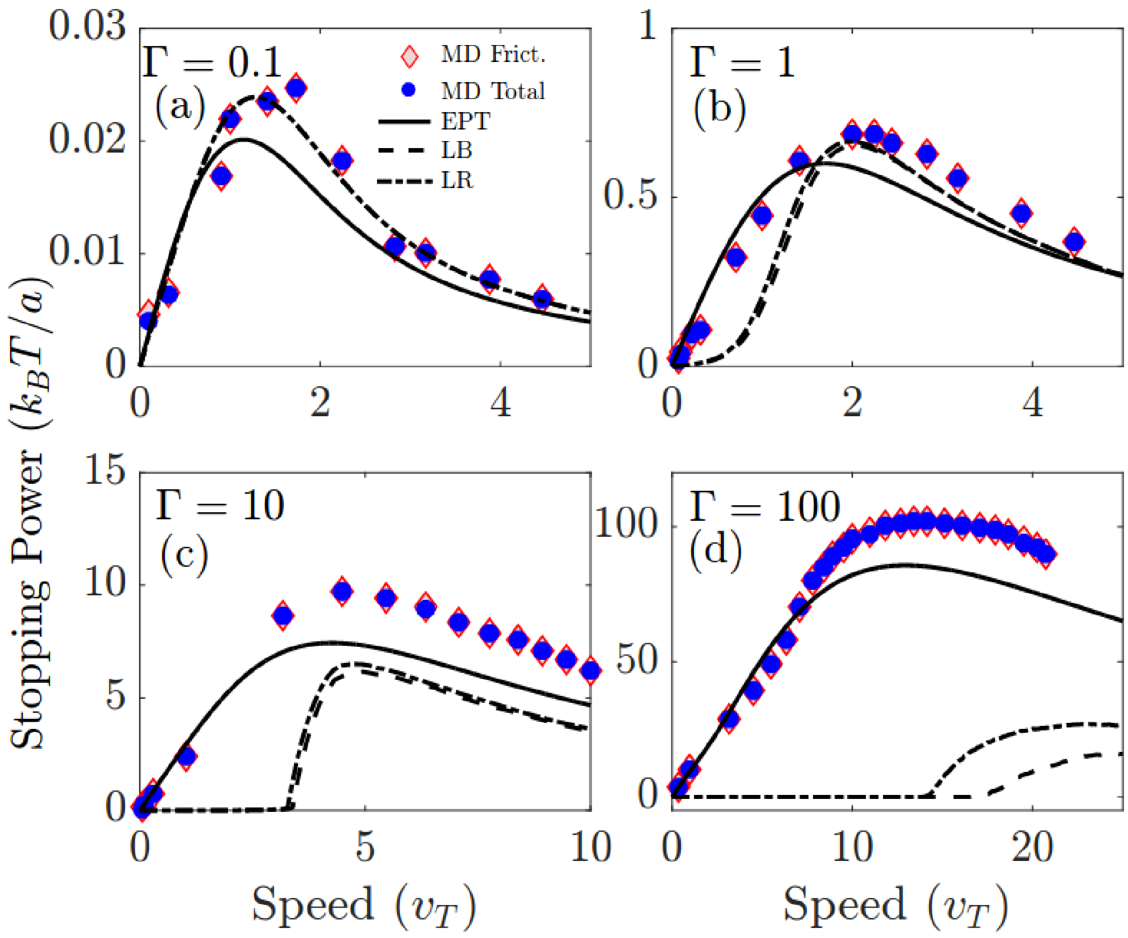
black: Γ = 10
red: Γ = 50

screening: κ = 2

symbols: MD simulation, lines: theoretical model

Kählert, PRR (2020)

Stopping power: (negative) energy loss of a particle in a medium per unit length



One-component plasma:

MD simulation results (symbols) compared with theory

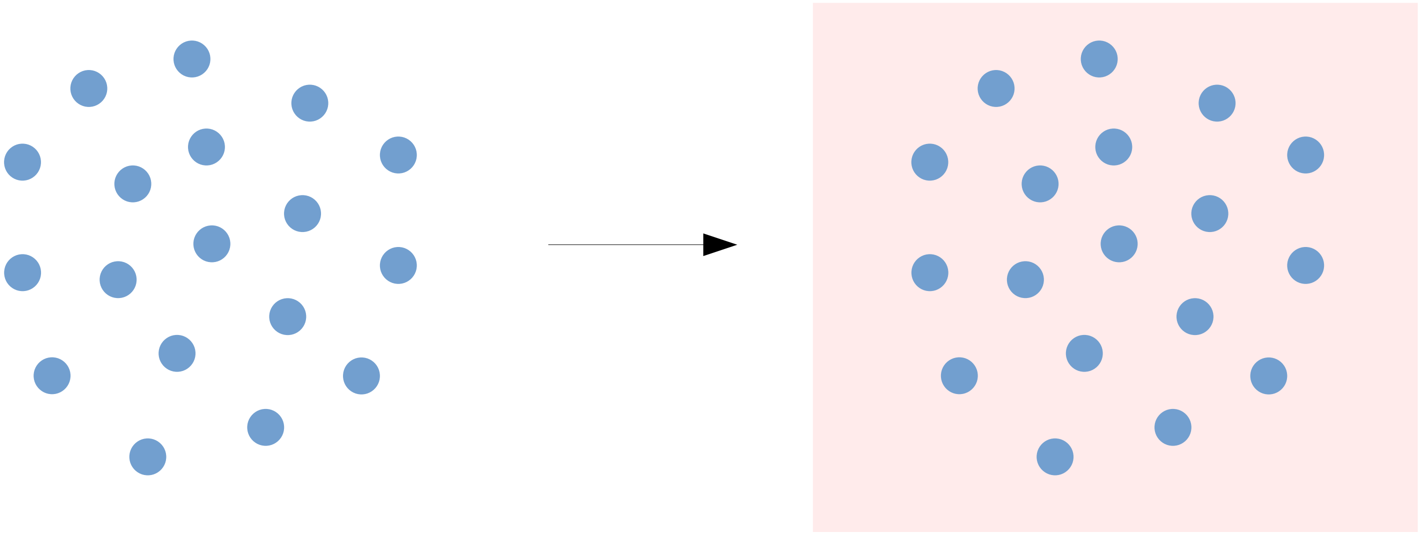
Bernstein, Baalrud, and Daligault, Phys. Plasmas (2019)

Langevin dynamics to account for dissipation

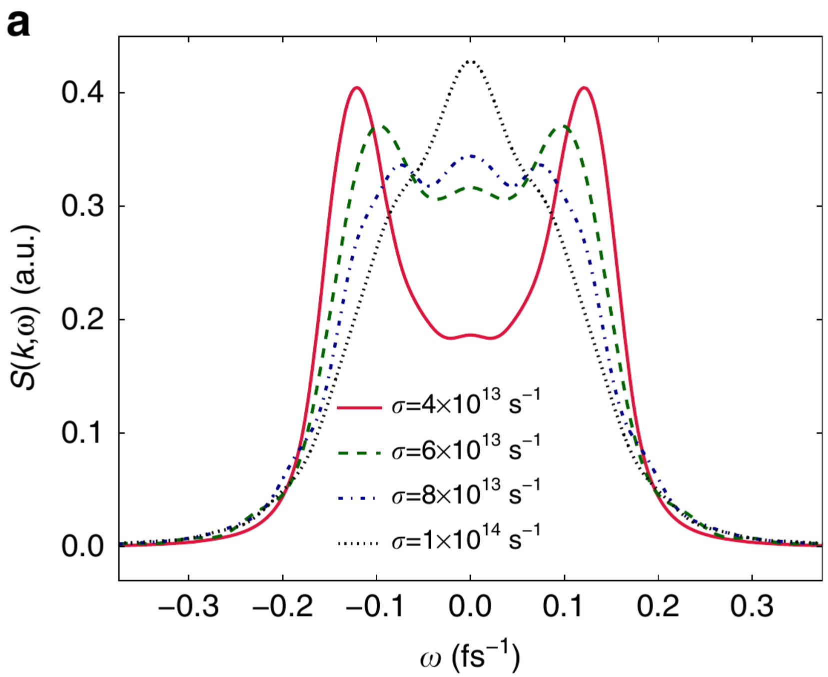
random force

$$m\ddot{\boldsymbol{r}}_i = \sum_{j\neq i}^{N} \boldsymbol{F}_{ij} - \nu m\dot{\boldsymbol{r}}_i + \boldsymbol{f}_i(t)$$

- friction with light background species



DFT-MD simulation of warm dense Al
→ friction leads to strong diffusive mode



Mabey *et al.*, Nat. Commun. (2017)

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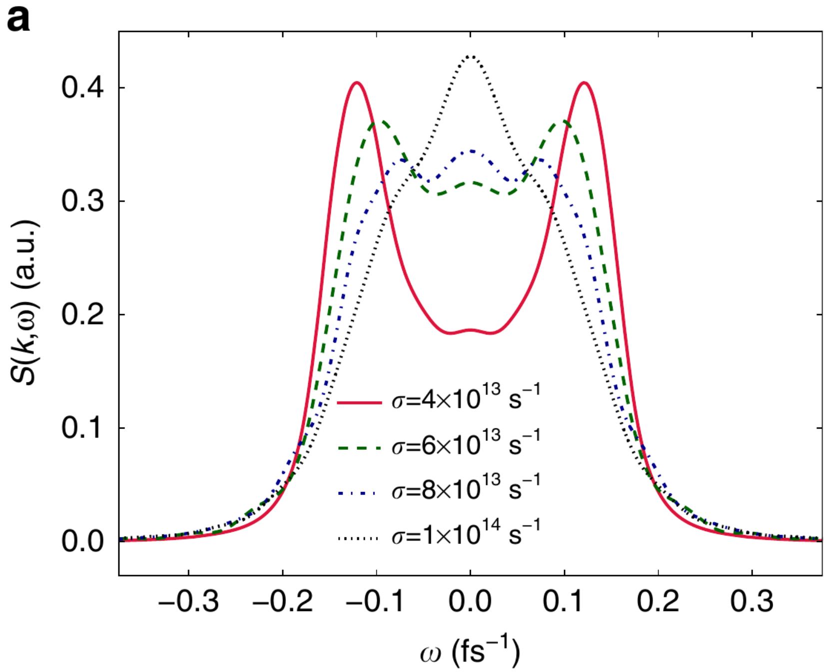
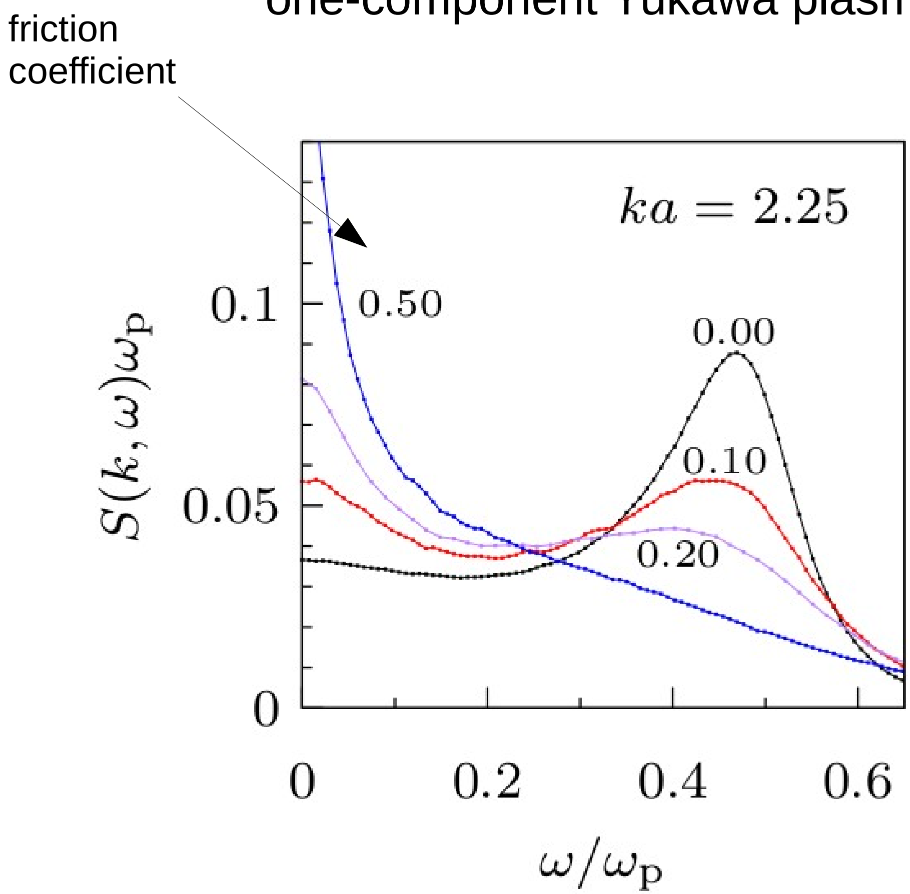


Mabey *et al.*, Nat. Commun. (2017)

analogous behavior in
one-component Yukawa plasma



Kählert, Phys. Plasmas (2019)