Shear Viscosity and Shear Thinning in Two-Dimensional Yukawa Liquids

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Transport coefficients of Yukawa liquids

**Motivation:**

1) There is an increasing interest in transport phenomena in strongly coupled plasmas: diffusion, viscosity, thermal conductivity have been studied both experimentally and via simulations. → Calculate shear viscosity for strongly-coupled 2D Yukawa liquids.

2) Various systems exhibit dependence of the viscosity on shear rate (non-Newtonian behavior), usually shear thinning. → Check whether this effect exists in dusty plasmas?
## Transport coefficients of Yukawa liquids

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<th>Authors</th>
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<tr>
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Molecular dynamics calculation of shear viscosity

Equilibrium MD for Yukawa systems

Short – range interaction makes it possible to find cutoff radius

Periodic boundary conditions avoid edge effects

Force calculation:

\[ \mathbf{F}_i(t) = \sum_{r_{ij} < r_{\text{cutoff}}} \mathbf{F}_{ij}(t) \]

“Neighbors” must be searched for in image cells, too.

... and integrate equation of motion
Molecular dynamics calculation of shear viscosity

**Equilibrium MD for Yukawa systems**

\[ P^{xy}(t) = \sum_{i=1}^{N} m v_{x_i} v_{y_i} - \sum_{j<i} x_{ij} v_{ij} \frac{d}{d\mathbf{r}_{ij}} \phi(r_{ij}) \]

The shear viscosity is obtained through the Green-Kubo relation:

\[ \eta = \frac{1}{V k T} \int_0^\infty C(t) dt \]

\[ C(t) = \left\langle P^{xy}(t) P^{xy}(0) \right\rangle \]


Nonequilibrium MD for determination of shear viscosity

Constitutive relation for shear viscosity:
(Shear flow $\Rightarrow$ momentum transport)

$$j_{px}(y) = -\eta \frac{dv_x(y)}{dy}$$

FLUX = - TRANSPORT COEFF. X FIELD

The idea of nonequilibrium simulation:

to determine transport coefficient:
apply FIELD (some kind of perturbation) and measure FLUX

BUT NEXT WE'LL DO SOMETHING TOTALLY DIFFERENT
METHOD #1: "Reverse Molecular Dynamics"

- F. Müller-Plathe, *Phys. Rev. E* 59. 4894 (1999): "Reverse Molecular Dynamics" exchanges the cause and the consequence:
  - Exchanging $p_x$ momenta of particles in cells A and B in a way that $< p_x > (A) < 0$ and $< p_x > (B) > 0$
  - we (artificially) induce a flux and a velocity field builds up as a consequence.
- Measure velocity profile $v_x(y)$
- Shear viscosity is calculated as:

$$\eta = \frac{\Delta P_x}{\Delta T} \frac{1}{2L} \frac{\Delta v_x(x)}{\Delta y}$$
Shear viscosity of 2D Yukawa liquids

Velocity profiles at different rates of momentum exchange

\[ \Gamma = 100, \ \kappa = 1.0 \]

\[ \frac{v_x(y)}{v_0} \]

\[ y / L_y \]

Shear viscosity as a function of coupling parameter

\[ \eta / \eta_0 = \frac{n \omega_P a^2}{\eta_0} \]

\[ \Gamma \]

\[ \kappa \]

\[ N \]

\[ \text{IOWA EMD} \]

\[ k = 800 \]

\[ k = 400 \]

\[ k = 250 \]

\[ k = 125 \]

\[ \text{IOWA EMD} \]

\[ \kappa = 0.5 \]

\[ \kappa = 0.56 \]

\[ \kappa = 1.0 \]

\[ \kappa = 2.0 \]

\[ N = 1600 \]

\[ N = 1024 \]

\[ N = 990 \]

\[ N = 3960 \]

\[ N = 990 \]

\[ N = 3960 \]
Shear viscosity of 2D Yukawa liquids

Scaling property of the viscosity:

\[ \frac{\eta_{eq}}{\eta_E} \]

\[ \begin{array}{c|c|c} \kappa & N \\ \hline 0.5 & 1600 \\ 1.0 & 990 \\ 1.0 & 3960 \\ 2.0 & 990 \\ 2.0 & 3960 \end{array} \]

\[ \eta_E = m n \omega_E a^2 \]

\[ \omega_E : \text{Einstein frequency} \]

\[ \frac{\eta_{eq}}{\eta_E} = a T' + \frac{b}{T'} + c \]

\[ T' = T / T_{\text{melting}} \]

Similar as found by T. Saigo and S. Hamaguchi, *Phys. Plasmas* 9, 1210 (2002); for 3D case.
Method #2: Homogeneous shear algorithm

\[ \langle v_x \rangle = \gamma \left( y - \frac{L}{2} \right) \]

Shear rate

Sliding (Lees-Edwards) boundary conditions

Equations of motion

\[
\frac{d\mathbf{r}_i}{dt} = \frac{d\mathbf{p}_i}{m} + \gamma y \hat{x}
\]

\[
\frac{d\mathbf{p}_i}{dt} = \mathbf{F}_i - \gamma \mathbf{p}_y \hat{x} - \alpha \mathbf{p}_i
\]

[Evans & Morris: “Statistical physics of nonequilibrium liquids”]
Shear viscosity of 2D Yukawa liquids

Example: $\Gamma = 140$, $\kappa = 1$,
Shear rate: $\gamma = 0.1$

Measure off-diagonal element of pressure tensor:

$$P^{xy}(t) = \sum_{i=1}^{N} \left[ m v_{i} v_{iy} + \sum_{j>i}^{N} \frac{x_{ij} y_{ij}}{r_{ij}} \frac{d}{d r_{ij}} \phi(r_{ij}) \right]$$

... and calculate:

$$\eta = \lim_{t \to \infty} \frac{-\langle P^{xy}(t) \rangle}{\gamma}$$
The results obtained from methods #1 and #2 agree well in the limit of small shear rates. BUT: What happens at high shear rates? Is Newtonian behavior violated?
Shear viscosity of 2D Yukawa liquids

At high shear rates: non-Newtonian behavior:
shear thinning: decrease of viscosity
with increasing stress

Dependence of kinetic and potential contributions to the viscosity on the shear rate

\[ \bar{y} = \frac{d v_x}{d y} \frac{a}{v_{th}} \]

A real life example of shear thinning: “The ketchup mystery”

Shear Mystery

Some fluids have a mysterious property: one moment they’re thick, the next they’re thin. Physicists aim to find out why with the aid of an experiment in space.

Listen to this story via streaming audio, a downloadable file, or get help.

“Shake and shake the ketchup bottle. None’ll come, and then a lot’ll.” --Richard Armour

June 7, 2002: Everyone has fallen prey to the ketchup bottle at one time or another.

After struggling to dislodge a meager few drops of the red liquid, an avalanche suddenly gushes out and buries your perfectly cooked burger. With suspiciously perfect timing, the ketchup changes from a thick paste to a runny liquid.

If you find yourself splattered and wondering "why?", you’re in good company. Theoretical physicists are puzzled, too.

Above: The sudden surge of ketchup from a bottle typifies an important and puzzling property of many liquids: shear thinning. Credit: MackKingShow.com.
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Summary

• Shear viscosity of 2D Yukawa liquids has been calculated for a wide range of coupling and screening parameters. Minimum of viscosity is found at intermediate coupling, similarly to 3D.

• In the limit of small shear rates two independent NEMD methods gave results in agreement with each other

• The shear viscosity was found to exhibit universality: $\frac{\eta_{eq}}{\eta_E} = f\left(\frac{T}{T_m}\right)$

• At high shear rates the homogeneous shear algorithm indicated the existence of shear thinning

THANK YOU FOR YOUR ATTENTION