Dynamic Structure Factor and Transport Coefficients of a Homogeneously Driven Granular Fluid in Steady State

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March 24, 2011

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Goal: Dynamics of Granular Fluid in Non-Equilibrium Steady State

Outline:

- Simulations
- Theory: Fluctuating Hydrodynamics
- Comparison for Dynamic Structure Factor $S(q, \omega)$
- Transport Coefficients

Model

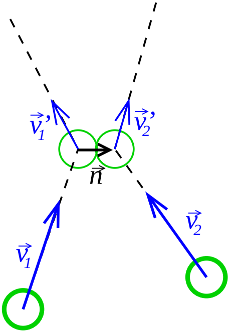
- Hard Spheres, 3 dim.
- Dissipation

$$\vec{n} \cdot \left(\vec{v_1}' - \vec{v_2}'\right) = -\epsilon \vec{n} \cdot (\vec{v_1} - \vec{v_2})$$

$\epsilon =$ coefficient of normal restitution

- Nonequilibrium Steady State
- Volume Driving
  - $\frac{\mathrm{d}}{\mathrm{d}t}\vec{v_i} = \left(\frac{\mathrm{d}}{\mathrm{d}t}\vec{v_i}\right)_{\text{coll}} + \vec{\xi_i}(t)$ [van Noije et al. 1999]
  - $\xi_i(t)$ Gaussian white noise with

$$\langle\vec{\xi} = 0\rangle \text{ and } \langle\xi_{i\alpha}(t)\xi_{j\beta}(t')\rangle = \xi_0^2\delta_{ij}\delta_{\alpha\beta}\delta(t-t')$$



Model & Simulation

- Hard Spheres, 3 dim.
- Dissipation

  $$\vec{n} \cdot \left(\vec{v_1}' - \vec{v_2}'\right) = -\epsilon \vec{n} \cdot \left(\vec{v_1} - \vec{v_2}\right)$$

  $\epsilon =$ coefficient of normal restitution
- Nonequilibrium Steady State
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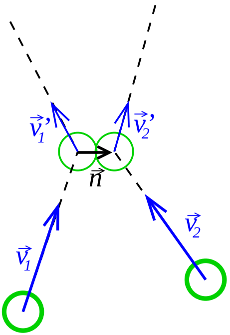
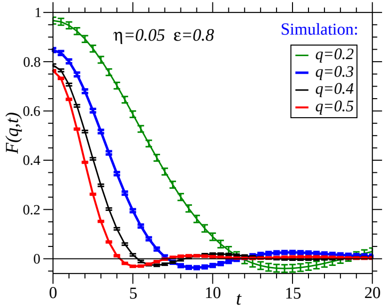
    $\langle\vec{\xi} = 0\rangle$ and $\langle\xi_{i\alpha}(t)\xi_{j\beta}(t')\rangle = \xi_0^2\delta_{ij}\delta_{\alpha\beta}\delta(t-t')$
  - to conserve total momentum globally fixed pairs with opposite kicks
- Event Driven Simulations
  - $N = 10000$
  - $\epsilon = 0.9,\ 0.8$
  - Volume Fractions $\eta = 0.05, 0.1, 0.2$
  - each 100 independent simulation runs



Definition of Dynamic Structure Factor

Intermediate Coherent Scattering Function

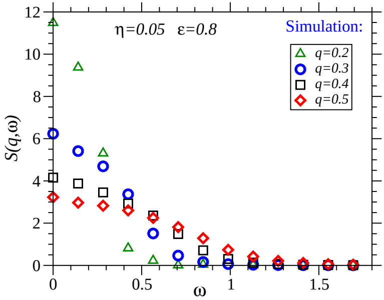
$$F(q,t) = \langle \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} e^{i\vec{q}\cdot(\vec{r}_i(t)-\vec{r}_j(0))} \rangle$$
$$= \langle n(\vec{q},t)n(-\vec{q},0)\rangle$$



⟶ damped sound wave

Dynamic Structure Factor

$$S(q,\omega) = \langle n(\vec{q},\omega)n(-\vec{q},\omega)\rangle$$



Theory: Fluctuating Hydrodynamics

$$\partial_t \delta n = -iqn_0 u$$

$$\partial_t u = -\frac{iq}{\rho_0}\left(\frac{\partial p}{\partial n}\delta n + \frac{\partial p}{\partial T}\delta T\right) - \nu_l\, q^2 u + \xi_l$$

$$\partial_t \delta T = -D_T q^2 \delta T - \frac{3\Gamma_0}{2T_0}\delta T - iq\frac{2p_0}{dn_0}u - \Gamma_0\left(\frac{1}{n_0} + \frac{1}{\chi}\frac{\mathrm{d}\chi}{\mathrm{d}n}\right)\delta n + \theta$$

fluctuating number density $\delta n(\vec{q}, t) = n - n_0$
longitudinal flow velocity $u(\vec{q}, t) = \vec{u} \cdot \frac{\vec{q}}{q}$
fluctuating temperature $\delta T = T - T_0$

[Noije et al., PRE **59**, 4326 (1999)]

Theory: Fluctuating Hydrodynamics

conservation of mass and momentum, driving, collisional dissipation

$$\begin{aligned} \partial_t \delta n &= -iqn_0 u \\ \partial_t u &= -\frac{iq}{\rho_0}\left(\frac{\partial p}{\partial n}\delta n + \frac{\partial p}{\partial T}\delta T\right) - \nu_l q^2 u + \xi_l \\ \partial_t \delta T &= -D_T q^2 \delta T - \frac{3\Gamma_0}{2T_0}\delta T - iq\frac{2p_0}{dn_0}u - \Gamma_0\left(\frac{1}{n_0} + \frac{1}{\chi}\frac{\mathrm{d}\chi}{\mathrm{d}n}\right)\delta n + \theta \end{aligned}$$

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Approximate Solution of Hydrodynamic Eqs. for $S(q,\omega)$

$$
\begin{aligned}
\partial_t \delta n &= -iqn_0 u \\
\partial_t u &= -\frac{iq}{\rho_0}\left(\frac{\partial p}{\partial n}\delta n + \frac{\partial p}{\partial T}\delta T\right) - \nu_{\mathsf{l}}\, q^2 u + \xi_{\mathsf{l}} \\
\partial_t \delta T &= \cancel{-D_T q^2 \delta T} - \frac{3\Gamma_0}{2T_0}\delta T - iq\frac{2p_0}{dn_0}u - \Gamma_0\left(\frac{1}{n_0} + \frac{1}{\chi}\frac{d\chi}{dn}\right)\delta n + \theta
\end{aligned}
$$

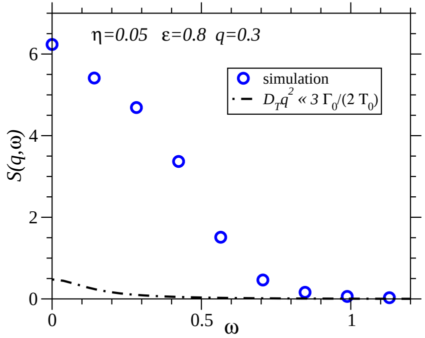
Dissipative Regime: $D_T q^2 \ll \frac{3\Gamma_0}{2T_0}$

Poles of $S(q,\omega)$:

$$
\begin{aligned}
\omega_T &= \pm i\frac{3\Gamma_0}{2T_0} \\
\omega_s &= \pm cq \pm i\gamma q^2
\end{aligned}
$$

sound mode with sound velocity

$$
c^2 = \frac{1}{m}\left(\frac{\partial p}{\partial n}\right)_T - \frac{2p_0}{3mn_0}\left(1 + \frac{n_0}{\chi}\frac{\partial \chi}{\partial n}\right)
$$



Approximate Solution of Hydrodynamic Eqs. for $S(q,\omega)$

$$\partial_t \delta n = -iqn_0 u$$

$$\partial_t u = -\frac{iq}{\rho_0}\left(\frac{\partial p}{\partial n}\delta n + \frac{\partial p}{\partial T}\delta T\right) - \nu_l\, q^2 u + \xi_l$$

$$\partial_t \delta T = -D_T q^2 \delta T - \frac{3\Gamma_0}{2T_0}\delta T - iq\frac{2p_0}{dn_0}u - \Gamma_0\left(\frac{1}{n_0} + \frac{1}{\chi}\frac{d\chi}{dn}\right)\delta n + \theta$$

Diffusive Regime: $D_T q^2 \gg \frac{3\Gamma_0}{2T_0}$

Poles of $S(q,\omega)$:

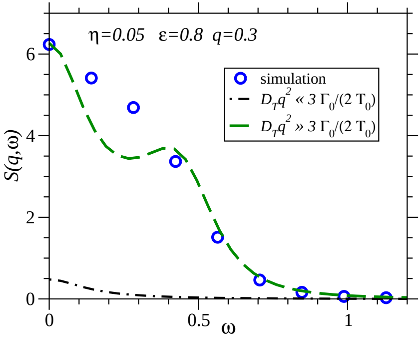
$$\omega_T = \pm i D_T q^2 \frac{v_{th}^2}{v_s^2}$$

$$\omega_s = \pm cq \pm i\gamma q^2$$

sound mode with sound velocity

$$c^2 = v_s^2 = v_{th}^2 + \frac{2p_0^2}{dmT_0 n_0^2}$$

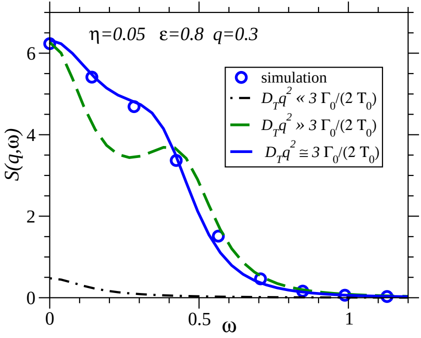
where $v_{th}^2 = \frac{1}{m}\left(\frac{\partial p}{\partial n}\right)_T$



Full Solution of Hydrodynamic Eqs. for $S(q,\omega)$

$$
\begin{aligned}
\partial_t \delta n &= -iqn_0 u \\
\partial_t u &= -\frac{iq}{\rho_0}\left(\frac{\partial p}{\partial n}\delta n + \frac{\partial p}{\partial T}\delta T\right) - \nu_\mathsf{l}\, q^2 u + \xi_\mathsf{l} \\
\partial_t \delta T &= -D_T q^2 \delta T - \frac{3\Gamma_0}{2T_0}\delta T - iq\frac{2p_0}{dn_0}u - \Gamma_0\left(\frac{1}{n_0} + \frac{1}{\chi}\frac{\mathrm{d}\chi}{\mathrm{d}n}\right)\delta n + \theta
\end{aligned}
$$

$$
S(q,\omega) = n_0 q^2 \left(\frac{\left[\omega^2 + \left(\frac{3\Gamma_0}{2T_0} + D_T q^2\right)^2\right]\left[\frac{\xi_0^2}{n_0} + \frac{2\nu_\mathsf{l} T_0 q^2}{m n_0}\right] + q^2\left(\frac{p_0}{m n_0 T_0}\right)^2\left[\frac{4mT_0\xi_0^2}{dn_0} + \frac{4D_T T_0^2 q^2}{dn_0}\right]}{|\det M|^2} \right),
$$

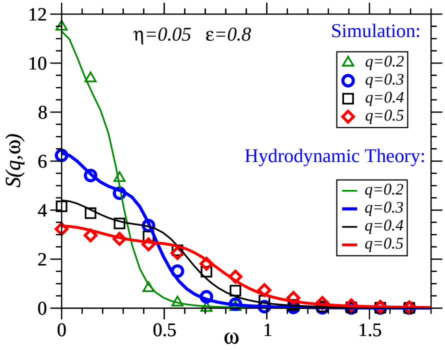


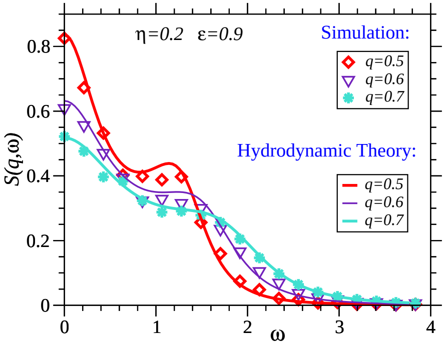
$$D_T q^2 \approx \frac{3\Gamma_0}{2T_0}$$

$\longrightarrow$ full solution necessary

Dynamic Structure Factor $S(q,\omega)$ (Full Solution)

$$S(q,\omega) = \langle n(q,\omega) n(-q,-\omega) \rangle$$





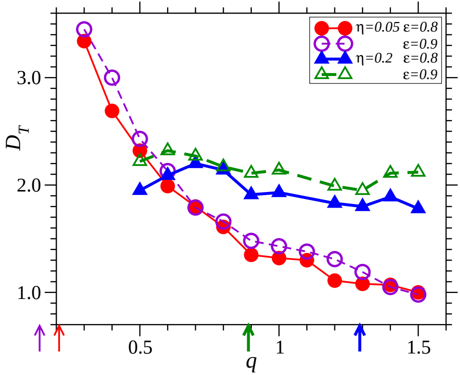
$\Longrightarrow$ $S(q,\omega)$ is well approximated

Transport Coefficient: Thermal Diffusivity D_T

$$\partial_t \delta n = -iqn_0 u$$

$$\partial_t u = -\frac{iq}{\rho_0}\left(\frac{\partial p}{\partial n}\delta n + \frac{\partial p}{\partial T}\delta T\right) - \nu_l q^2 u + \xi_l$$

$$\partial_t \delta T = -D_T q^2 \delta T - \frac{3\Gamma_0}{2T_0}\delta T - iq\frac{2p_0}{dn_0}u - \Gamma_0\left(\frac{1}{n_0} + \frac{1}{\chi}\frac{d\chi}{dn}\right)\delta n + \theta$$



Kinetic Theory for $D_T = \frac{2\kappa}{3n}$:

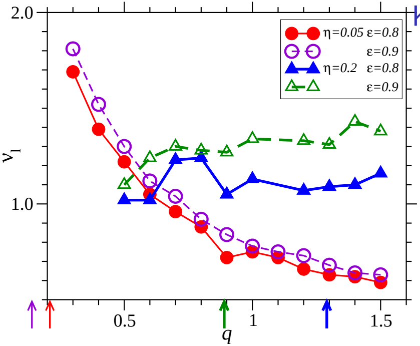
$\eta = 0.05$		
	$\varepsilon = 0.8$	$\varepsilon = 0.9$
Fit Results: $q = 0.2$	4.72	4.63
$q = 0.3$	3.34	3.45
Brilliantov et al. 2004	3.19	3.54
Dufty et al. 1997	4.71	4.07
Garzó et al. 2007	5.62	5.06
Garzó et al. 2002	3.57	3.93

$\eta = 0.2$		
	$\varepsilon = 0.8$	$\varepsilon = 0.9$
Fit Results: $q = 0.5$	1.95	2.22
$q = 0.6$	2.09	2.32
Brilliantov et al. 2004	0.52	0.57
Dufty et al. 1997	2.03	2.01
Garzó et al. 2007	1.40	1.26
Garzó et al. 2002	0.89	0.98

κ = heat conductivity

Transport Coefficient: Longitudinal Viscosity ν_l

$$
\begin{aligned}
\partial_t \delta n &= -iqn_0 u \\
\partial_t u &= -\frac{iq}{\rho_0}\left(\frac{\partial p}{\partial n}\delta n + \frac{\partial p}{\partial T}\delta T\right) - \nu_l q^2 u + \xi_l \\
\partial_t \delta T &= -D_T q^2 \delta T - \frac{3\Gamma_0}{2T_0}\delta T - iq\frac{2p_0}{dn_0}u - \Gamma_0\left(\frac{1}{n_0} + \frac{1}{\chi}\frac{d\chi}{dn}\right)\delta n + \theta
\end{aligned}
$$



Kinetic Theory for $\nu_l = \frac{1}{\rho}\left(\frac{4}{3}\eta_{\text{shear}} + \zeta\right)$:

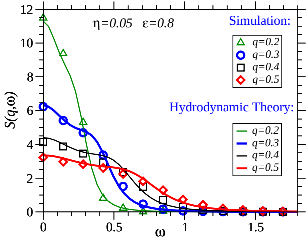
$\eta = 0.05$		
	$\varepsilon = 0.8$	$\varepsilon = 0.9$
Fit Results: $q = 0.2$	2.55	3.23
$q = 0.3$	1.69	1.81
Brilliantov et al. 2004	2.26	2.25
Dufty et al. 1997	2.82	2.77
Garzó et al. 2007	2.78	2.67
Garzó et al. 2002	2.56	2.55

$\eta = 0.2$		
	$\varepsilon = 0.8$	$\varepsilon = 0.9$
Fit Results: $q = 0.5$	1.02	1.10
$q = 0.6$	1.02	1.24
Brilliantov et al. 2004	0.83	0.85
Dufty et al. 1997	1.63	1.72
Garzó et al. 2007	1.15	1.15
Garzó et al. 2002	1.10	1.12

η_{shear} = shear viscosity $\quad$ ζ = bulkviscosity

Summary

- Damped Sound Waves
- Fluctuating Hydrodynamic Theory:
  - $D_T q^2 \approx \frac{3\Gamma_0}{2T_0}$ (full solution)
  - $S(q,\omega)$ well approximated
  - transport coefficients agree with kinetic theory



[KVL, T. Aspelmeier, A. Zippelius,PRE **83**, 011301 (2011)]

Acknowledgments:

Support from Institute of Theoretical Physics, University Göttingen