Rheology and linear response of sheared granular flows

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Kinetic theory — elastic hard spheres

- Velocity distribution
  \[ f(x, u) \, dx \, du. \]
- Fluctuating velocity
  \[ c = u - U \]

\[
\begin{align*}
\text{Boltzmann eq } & \quad \frac{\partial(\rho f)}{\partial t} + \frac{\partial(\rho c_i f)}{\partial x_i} + \frac{\partial(\rho a_i f)}{\partial c_i} - \frac{\partial U_i}{\partial x_j} \frac{\partial(\rho c_j f)}{\partial c_i} = \frac{\partial_c(\rho f)}{\partial t} \\
\end{align*}
\]
Collision integral — molecular chaos approximation.

Boltzmann equation: \[
\frac{\partial (\rho f)}{\partial t} + \frac{\partial (\rho c_i f)}{\partial x_i} - \frac{\partial U_i}{\partial x_j} \frac{\partial (\rho c_j f)}{\partial x_i} = \frac{\partial_c (\rho f)}{\partial t}
\]

Equilibrium (no gradients)

\[
\frac{\partial_c f}{\partial t} = 0
\]

Solution — Maxwell-Boltzmann distribution

\[
f = (2\pi T)^{-3/2} \exp\left(-m u^2 / 2T\right)
\]
Non-equilibrium — Chapman-Enskog procedure:

\[
\frac{\partial (\rho f)}{\partial t} + \frac{\partial (\rho c_i f)}{\partial x_i} - \frac{\partial U_i}{\partial x_j} \frac{\partial (\rho c_j f)}{\partial c_i} = \frac{\partial c(\rho f)}{\partial t}
\]

\[
\frac{T^{1/2} \rho f}{L} - G_{xy} \rho f - \frac{T^{1/2} \rho (f - f_{eq})}{\lambda}
\]

Asymptotic expansion in parameter \( \epsilon = (\lambda/L) \); \( f = f_0 + \epsilon f_1 + \ldots \)

Leading order \( \frac{\partial c(\rho f)}{\partial t} = 0 \rightarrow f = f_{MB} \).

First correction

\[
\frac{\partial (\rho f_0)}{\partial t} + \frac{\partial (\rho c_i f_0)}{\partial x_i} - \frac{\partial U_i}{\partial x_j} \frac{\partial (\rho c_j f_0)}{\partial c_i} = \frac{\partial c(\rho f_1)}{\partial t}
\]
Moments of Boltzmann equation

- Other ‘fast’ moments decay over time scales $\sim$ collision time.

Linear response

- $f(c) = f_0(c) + \tilde{f}(c)e^{(st+i\kappa x)}$
- Linearised Boltzmann equation
  \[ \left[ s + i\kappa c_x - G_{ij} \frac{\partial c_i}{\partial c_j} \right] \tilde{f} = L[\tilde{f}] \]
- $\tilde{f}(c) = \sum_{i=1}^{N} A_i \psi_i(c)$
- $(sI_{ij} + i\kappa X_{ij} - G_{ij} - L_{ij}) A_j = 0$
Hydrodynamic modes for elastic system

- Number of eigenvalues depends on number of basis functions chosen.
- For \( k \to 0 \),
  Transverse momenta \( s_t = -\frac{(\mu/\rho)}{k^2} \).
  Energy \( s_e = -D_T k^2 \).
  Mass & longitudinal mom.
  \( s_l = \pm i k \sqrt{p \rho} - \rho^{-1}(\mu_b + 4\mu/3)k^2 \).
- All other modes with negative eigenvalues, indicating that other transients decay.
Calculation of Transport coefficients (dilute):

\[ \sigma_{xy} = -\rho \langle u_x u_y \rangle \]
\[ = -\rho \int d\mathbf{u} f_1(\mathbf{u}) u_x u_y \]
\[ = \eta G_{xy} \]

Beyond molecular chaos — incorporate correlated collisions.

Two dimensions \( \sigma_{xy} = \eta G_{xy} + \eta' G_{xy} \log (G_{xy}) \)

Three dimensions \( \sigma_{xy} = \eta G_{xy} + \eta' G_{xy} |G_{xy}|^{1/2} \)
Green-Kubo formula (shear viscosity):

\[
\eta = \frac{\beta}{V} \lim_{k \to 0} \int_0^\infty dt \langle \sigma_{xy}(k, t) \sigma_{xy}(-k, 0) \rangle
\]

Microscopic stress:

\[
\sigma_{xy}(k) = \int_{k'} u_x(k - k') u_y(k')
\]

Velocity fluctuations:

\[
\partial_t u_x(k) = -\eta k^2 u_x(k)
\]

\[
u_x(k, t) = \exp(-\eta k^2) u_x(k, 0)
\]

Viscosity

\[
\eta = \frac{\beta}{V} \int d\mathbf{k}' \int_0^\infty dt \langle u_x(k', t) u_x(-k', 0) \rangle \langle u_y(-k', t) u_y(k', 0) \rangle
\]

\[
\log(<u_x(k, t) u_x(k, 0)>)
\]
Time correlation — long time tail:

\[
\int d\mathbf{k} \langle u_x(\mathbf{k}, t) u_x(-\mathbf{k}, 0) \rangle \\
\sim \int d\mathbf{k} \exp (-\eta k^2 t) \\
\sim t^{-d/2}
\]

Sheared system:

\[
(\partial_t + G_{xy} k_x \frac{\partial}{\partial k_y}) u_x = -\eta k^2 u_x
\]

\[
u_x(t) = u_x(0) \exp \left[ -Dt \left( k^2 - G_{xy} tk_xk_y + \frac{1}{3} G_{xy}^2 t^2 k_x^2 \right) \right]
\]

\[
u_x(t) \sim \exp (-1/3 G_{xy}^2 k_x^2 t^3)
\]
‘Turning’ of wave vector due to shear:
‘Turning’ of wave vector due to shear:
Green-Kubo relation:

\[ \eta = \frac{\beta}{V} \int d\mathbf{k}' \int_0^{G_{xy}^{-1}} dt \ t^{-d/2} \]

Two dimensions:

\[ \eta = \eta_0 + \eta_1 \log (G_{xy}) \]

Three dimensions:

\[ \eta = \eta_0 + \eta_1 |G_{xy}|^{1/2} \]
Beyond the Boltzmann equation:

One particle distribution
\( f_\alpha(x_\alpha, u_\alpha) \).

Two-particle distribution:
\( f_{\alpha\beta}(x_\alpha, u_\alpha, x_\beta, u_\beta) \)

Molecular chaos truncation:
\( f_{\alpha\beta} = f_\alpha f_\beta \).

Ring kinetic truncation:
\( f_{\alpha\beta} = f_\alpha f_\beta (1 + g_{\alpha\beta}) \).

\[ f_{\alpha\beta\gamma} = f_\alpha f_\beta f_\gamma (1 + g_{\alpha\beta} + g_{\alpha\gamma} + g_{\beta\gamma}) \]

Single particle distribution
\[ \frac{\partial(c_{\alpha i} f_\alpha)}{\partial x_{\alpha i}} - G_{ij} c_{\alpha j} \frac{\partial f_\alpha}{\partial x_{\alpha i}} = \frac{\partial c f_\alpha}{\partial t} \]

Ring kinetic equation:
\[ \partial_t f_{\alpha\beta} - G_{ij} x_{\alpha\beta j} \frac{\partial f_{\alpha\beta}}{\partial x_i} + c_{\alpha\beta i} \frac{\partial f_{\alpha\beta}}{\partial x_i} - G_{ij} \left( c_{\alpha j} \frac{\partial f_{\alpha\beta}}{\partial c_{\alpha i}} + c_{\beta j} \frac{\partial f_{\alpha\beta}}{\partial c_{\beta i}} \right) = \frac{\partial c f_{\alpha\beta}}{\partial t} \]
Propagator in ring kinetic equation:
Steady homogeneous shear flow of inelastic particles:

\[-G_{ij} \frac{\partial (\rho c_j f)}{\partial c_i} = \frac{\partial_c (\rho f)}{\partial t}\]

Nearly elastic collisions:

\[e_n \ll 1 \rightarrow \text{Dissipation} \ll \text{Particle energy}\]

Expand in \(\varepsilon_n = (1 - e_n)^{1/2}\).

Leading order \(\frac{\partial_c (\rho f_0)}{\partial t} = 0 \rightarrow f = f_{MB}\).

Rate of energy production \(\sim \mu G_{xy}^2 \sim (T^{1/2} / d^2) G_{xy}^2\).

Rate of energy dissipation \(\sim \rho^2 T^{3/2} (1 - e_n^2)^{1/2}\).

\(\rightarrow G_{xy} \sim (1 - e_n^2)^{1/2} T^{1/2} \sim \varepsilon_n T^{1/2}\).
Hydrodynamic modes for smooth inelastic spheres

- Energy *not conserved*.
- Source of energy.
- Rate of conduction \((\lambda_M T^{1/2}/L^2)\).
- Rate of dissipation \(((1 - e)T^{1/2}/\lambda_M)\).
- Conduction length \(L_c = (\lambda_M/(1 - e)^{1/2})\).
- Energy conserved \(L \ll L_c\).
- *Adiabatic approx.* \(L \gg L_c\).
  Local balance between source and dissipation.
Smooth nearly elastic particles

\[
\sigma_{ij} = -p(\phi, S_{ij}, G_{ii})\delta_{ij} + 2\mu(\phi, S_{ij} G_{ii})S_{ij} + \mu_b(\phi, S_{ij}, G_{ii})\delta_{ij} G_{kk} + (A(\phi)(S_{ik} S_{kj} - (\delta_{ij} / 3) S_{kl} S_{lk}) + B(\phi)\delta_{ij} G_{kk}^2 + C(\phi) S_{ij} G_{kk})
+ D(\phi)(S_{ik} A_{kj} + S_{jk} A_{ki}) + F(\phi)(A_{ik} A_{kj} - (\delta_{ij} / 3) A_{kl} A_{lk})
- \frac{D(\phi)}{2} \left( \frac{\partial}{\partial x_i} \left( \frac{1}{\rho} \frac{\partial p}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \frac{1}{\rho} \frac{\partial p}{\partial x_i} \right) - \frac{2\delta_{ij}}{3} \frac{\partial}{\partial x_k} \left( \frac{1}{\rho} \frac{\partial p}{\partial x_k} \right) \right)
\]

\[
p = \rho T (1 + (4 - 2\epsilon^2)\phi \chi(\phi))
\]

\[
\mu(\phi) = \frac{5T^{1/2}}{16\sqrt{\pi} \chi(\phi)} \left( 1 + \frac{8\phi \chi(\phi)}{5} \right)^2 + \frac{48\phi^2 \chi(\phi) T^{1/2}}{5\pi^{3/2}}
\]

\[
\mu_b(\phi) = \frac{16\phi^2 \chi T^{1/2}}{\pi^{3/2}}
\]

Coefficients $A - G$ identical to Burnett expansion for $\epsilon_n \to 0$. 
Linear response \( L \ll L_c \)

- Number of eigenvalues depends on number of basis functions chosen.
- For \( k \to 0 \),
  Transverse momenta \( s_t = -\frac{\mu}{\rho}k^2 \).
  Energy \( s_e = -D_Tk^2 \).
  Mass \& longitudinal mom.
  \( s_l = \pm i k \sqrt{p_\rho} - \rho^{-1} (\mu_b + 4\mu/3)k^2 \).
- All other modes with negative eigenvalues, indicating that other transients decay.
Linear response

Infinite sheared granular material

- Mean flow \( \bar{u}_x = \bar{G} y, \bar{u}_y = 0, \bar{u}_z = 0. \)
- Small dissipation \( \epsilon = (1 - e_n)^{1/2} \ll 1. \)
- Macroscopic length \( L \gg L_c. \)
- Mass conservation
  \( \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0. \)
- Momentum conservation
  \( \rho(\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}) = \nabla \cdot \sigma. \)
- Perturbations
  \[
  \begin{pmatrix}
    \rho(x, t) \\
    \mathbf{u}(x, t)
  \end{pmatrix} = \begin{pmatrix}
    \tilde{\rho}(t) \\
    \tilde{\mathbf{u}}(t)
  \end{pmatrix} \exp(ikx + ily + imz)
  \]
Linear response

- Infinite shear flow not homogeneous.

- Time dependent wave vector
  \( k = k_0, l = l_0 - k_0 \tilde{G} t, m = m_0. \)

- ‘Linear’ response equations

\[
\partial_t \begin{pmatrix} \tilde{\rho}(t) \\ \tilde{u}(t) \end{pmatrix} + (\mathcal{L}_0 + t \mathcal{L}_1 + t^2 \mathcal{L}_2) \begin{pmatrix} \tilde{\rho}(t) \\ \tilde{u}(t) \end{pmatrix} = 0
\]

\[
\begin{pmatrix} \tilde{\rho}(t) \\ \tilde{u}(t) \end{pmatrix} = \exp \left( -t \mathcal{L}_0 - (t^2/2) \mathcal{L}_1 - (t^3/3) \mathcal{L}_2 \right) \begin{pmatrix} \tilde{\rho}(0) \\ \tilde{u}(0) \end{pmatrix}
\]

For \( k_0 = 0, \mathcal{L}_1 = 0, \mathcal{L}_2 = 0. \)
Linear response — flow plane
Linear response — flow plane transverse mode

Perturbations to $\tilde{u}_z$:

$$\tilde{u}_z(t) = \tilde{u}_z(0) \exp (s_{0z} t + (s_{1z} t^2 / 2) + (s_{2z} t^3 / 3))$$

$$s_{0z} = -\frac{(\bar{\mu} + \bar{G} \bar{G}^2 / 8) (k_0^2 + l_0^2)}{\bar{\rho}}$$

$$s_{1z} = \left( \frac{\bar{A} \bar{G}^2 k_0^2}{2} + \frac{2 \bar{G} k_0 l_0}{\bar{\rho}} (\bar{\mu} + (\bar{G} \bar{G}^2 / 8)) \right)$$

$$s_{2z} = -\frac{\bar{G}^2 k_0^2}{\bar{\rho}} (\bar{\mu} + (\bar{G} \bar{G}^2 / 8))$$

For $t \ll \bar{G}^{-1}$, $\tilde{u}_z \sim \exp (-\bar{\mu} k_0^2 t)$.

For $t \gg \bar{G}^{-1}$, $\tilde{u}_z \sim \exp (-\bar{\mu} \bar{G}^2 k_0^2 t^3)$.
Linear response — flow plane

Short time \( t \ll \tilde{G}^{-1} \):

\[
\begin{pmatrix}
\tilde{\rho}(t) \\
\tilde{u}_x(t) \\
\tilde{u}_y(t)
\end{pmatrix} = \exp(\mathbf{s}_{\rho xy})
\begin{pmatrix}
\tilde{\rho}(0) \\
\tilde{u}_x(0) \\
\tilde{u}_y(0)
\end{pmatrix}
\]

where

\[
s_{\rho xy}^3 = -\tilde{G}^2 k_0^2 \left( \bar{\rho}_\rho + \frac{\tilde{G}^2 \bar{\mathcal{E}}}{8} \right) + k_0 l_0 \tilde{G} \left( \bar{p}_\rho - \frac{\tilde{G}^2}{4}(\bar{A}_\rho + 2\bar{\mathcal{C}}_\rho) \right)
\]

- Three solutions — two propagating, one diffusive.
- For \( l_0 = 0 \), \( s_{\rho xy} \propto -(-1, (-1)^{1/3}, (-1)^{2/3}) \tilde{G}^{2/3} k_0^{2/3} \bar{p}_\rho^{1/3} \).
- For \( l_0 \neq 0 \), \( s_{\rho xy} \propto (-1, (-1)^{1/3}, (-1)^{2/3}) k_0^{1/3} l_0^{1/3} \bar{p}_\rho^{1/2} \).
Linear response — flow plane

\[ s_{\rho xy} \ddot{\rho} + \bar{\rho} i k_0 \ddot{u}_x + \bar{\rho} i l_0 \ddot{u}_y = 0 \]

\[ \bar{\rho}(s_{\rho xy} \ddot{u}_x + \bar{G} \ddot{u}_y) = 0 \]

\[ \bar{\rho} s_{\rho xy} \ddot{u}_y - (i \bar{G} k_0 \bar{\mu}_\rho \ddot{\rho} + i l_0 \bar{\rho}_\rho) \ddot{\rho} = 0 \]
Summary — Flow direction:

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<th>$k \ll \epsilon$</th>
<th>$k \gg \epsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Propagating</td>
<td>$s_{pr}$</td>
<td>$-k^{2/3}$</td>
</tr>
<tr>
<td></td>
<td>$s_{pi}$</td>
<td>$\pm k^{2/3}$</td>
</tr>
<tr>
<td>Diffusive</td>
<td>$s_d$</td>
<td>$+k^{2/3}$</td>
</tr>
<tr>
<td>Transverse</td>
<td>$s_z$</td>
<td>$-k^2$</td>
</tr>
<tr>
<td>Energy</td>
<td>$s_T$</td>
<td>$-k^0$</td>
</tr>
</tbody>
</table>
Linear response — flow plane

$\epsilon = 0.01$

- $s_{pr}$
- $|s_{pi}|$
- $\pm s_d$
- $s_z$
- $s_T$
Linear response — flow plane

Long time $t \gg \bar{G}^{-1}$:

$$
\begin{pmatrix}
\tilde{u}_x(t) \\
\tilde{u}_y(t)
\end{pmatrix} = \exp \left( -s_{xy} t^3 / 3 \right) \begin{pmatrix}
\tilde{u}_x \\
\tilde{u}_y
\end{pmatrix}
$$

$$
s_{xy} = -\frac{\bar{G}^2 k_0^2}{\bar{\rho}} \left( \frac{5\bar{\mu}}{3} + \frac{\bar{\mu}_b}{2} + \frac{\bar{\rho} \bar{R}}{\bar{G}} \right)
$$

$$
\pm \left( \frac{1}{9} \left( \bar{\rho} - \frac{3\bar{\mu}_b}{2} \right)^2 + \frac{4\bar{\rho} \bar{\rho} \bar{R}}{3\bar{G}} + \frac{\bar{\mu}_b \bar{\rho} \bar{R}}{\bar{G}} + \frac{\bar{\rho}^2 \bar{R}^2}{\bar{G}^2} \right)^{1/2}
$$

$$
s_{xy1} = (-2k_0^2 \bar{G} \bar{\rho} \bar{R} / \bar{\rho})
$$

$$
s_{xy2} = (-\bar{G}^2 k_0^2 \bar{\mu} / \bar{\rho}).
$$
Linear response — gradient direction
Linear response — gradient direction

- Diffusive mode correct to $O(\epsilon^3)$

\[
s_d = \frac{8\bar{\mu}\bar{p}_\rho - 8\bar{p}\bar{\mu}_\rho + 2\bar{G}^2\bar{\mu}_\rho(\bar{A} + 2\bar{C}) - 2\bar{G}^2\bar{\mu}(\bar{A}_\rho + 2\bar{C}_\rho)}{-4\bar{p}\bar{p}_\rho - 8\bar{p} + 2\bar{G}^2(\bar{A} + 2\bar{C}) + \bar{p}\bar{G}^2(\bar{A}_\rho + 2\bar{C}_\rho)} l^2
\]

\[
\approx \frac{2(\bar{p}\bar{\mu}_\rho - \bar{\mu}\bar{p}_\rho)}{2\bar{p} + \bar{p}\bar{p}_\rho} l^2
\]

Qualitative difference — $(\bar{p}\bar{\mu}_\rho - \bar{\mu}\bar{p}_\rho) = 0$ at low and high density.

- Propagating modes

\[
s_{pi} = \pm u l \sqrt{\bar{p}_\rho + (2\bar{p}/\bar{\rho})} - l^2 \left( \frac{\bar{p}_\rho(\bar{G}(4\bar{\mu} + 3\bar{\mu}_b) + 6\bar{p}\bar{R}) + 6\bar{G}\bar{\mu}_\rho\bar{p}}{6\bar{G}(2\bar{p} + \bar{p}\bar{p}_\rho)} + \frac{5\bar{\mu}}{3\bar{\rho}} + \frac{\bar{\mu}_b}{2\bar{\rho}} + \frac{\bar{p}\bar{R}}{\bar{G}\bar{\rho}} \right)
\]
Linear response — gradient direction

$\epsilon = 0.01$

- $s_{pr}$
- $|s_{pi}|$
- $s_d$
- $s_z$
- $s_T$
Linear response — vorticity direction
Linear response — vorticity direction

Decoupling $\rho - z$ and $x - y$.

\[
s_{\rho z} = \pm im \sqrt{\bar{p}_\rho - (\bar{C}_\rho \bar{G}^2 / 2)} - \frac{m^2}{2\bar{\rho}} \left( \frac{4\bar{\mu}}{3} + \bar{\mu}_b + \frac{2\bar{p}\bar{R}}{\bar{G}} \right)
\]

For $\phi \ll 1$, $\bar{p}_\rho < 0 \rightarrow$ unstable. For $\phi \rightarrow \phi_c$, $\bar{p}_\rho > 0 \rightarrow$ stable.

\[
s_{xy} = \pm m \sqrt{\frac{\bar{A}\bar{G}}{4\bar{\rho}}} - m^2 \frac{\bar{\mu}}{\bar{\rho}}
\]

One stable and one unstable mode.
<table>
<thead>
<tr>
<th>Summary</th>
<th>Vorticity Direction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$m \ll \epsilon$</td>
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<tr>
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Linear response — vorticity direction

$\epsilon = 0.01$

- $s_{pr}$
- $|s_{pi}|$
- $|s_{pz1}|$
- $s_{pz2}$
- $s_{T}$
Linear response — vorticity direction

\[ \pm s_{d2}^*, - s_{d4}^* \]

\( m^* \)

\( \epsilon = 0.01 \)

- \( |s_{xy1}| \)
- \( -s_{xy2} \)
Time correlation functions:

\[ \log(\langle u_x(k,t)u_x(-k,0)\rangle) \]

- \( k \gg \varepsilon \)
  \[ \int_k \langle u_x(k,t)u_x(-k,0)\rangle \sim t^{-d/2} \]
  \[ \sigma_{xy} = \eta G_{xy} + \eta' G_{xy} \log(|G_{xy}|) \]

- \( k \ll \varepsilon \)
  \[ \int_k \langle u_x(k,t)u_x(-k,0)\rangle \]
  \[ \sim \int dk \exp(-\eta k^{2/3} t) \]
  \[ \sim t^{-3d/2} \]
  \[ \sigma_{xy} = \eta G_{xy} + \eta' G_{xy}^3 + \ldots \]
Conclusions

Linear response for shear flow:

- Perturbations grow at short times, decay at long times in the flow directions. Growth rate $\propto k^{2/3}, (kl)^{1/3}$ at short times, $\propto k^{2/3}$ at long times.

- Perturbations stable in gradient direction. Diffusive mode $s_d \propto -l^2$, propagating modes $\propto \pm ul - l^2$.

- Diffusive mode in gradient direction not adequately described by Navier-Stokes approximation.

- Perturbations in vorticity directions $\propto \pm m$ at low density, $\propto \pm m - m^2$ at high density.

- Not adequately described by Navier-Stokes approximation.
Conclusions

- **Cautious conclusion:** transport coefficients do not diverge in two dimensions, regular in three dimensions.
- **However:** transport coefficients could be different from their microscopic values.