Pressure and SPP's

Outline

1.) Active Brownian Particles
2.) Introduce the problem
3.) non-interacting part 1: Disks
4.) non-interacting part 2: Ellipsoid
5.) interactions < pictures
6.) outline my attempts (if time)

1] A B P's

- SPP - propelled by internal forces or external fuel source
- Most widely studied SPP's are Active Brownian Particles (ABP)
- Physical realizations include Teryx colloids, vibrated granular rods, bacteria, birds...

Model 1]

\[ \hat{\mathbf{u}} \text{ changes through brownian rotation} \]

\[ \frac{\partial \hat{\mathbf{u}}}{\partial t} = 2\nu \hat{\mathbf{u}} + \hat{\mathbf{u}} R(t) \]

\[ \frac{\partial \hat{\mathbf{0}}}{\partial t} = \gamma \hat{\mathbf{0}}(t) \]

0 mean and

\[ \langle \eta_i(t) \eta_j(t') \rangle = 2D_0 \delta(t-t') \]

\[ \langle \eta_i^2(t) \rangle = 2D_0 \delta(t-t') \]

all higher cumulants vanish (see Kabir, Bueke, Sunjib)
to get familiar

$$\langle r^2(t) \rangle = 2v_s^2 \left[ \frac{t}{Dr} - \frac{\exp(-D_t/t)}{Dr^2} \right] + 2D_t t$$  
(exercise for the professors)

Short times \( t \ll \frac{1}{Dr} \) \( \langle r^2(t) \rangle \rightarrow v_s^2 t^2 \)

Long times \( t \gg \frac{1}{Dr} \) \( \langle r^2(t) \rangle \rightarrow 2 \left( \frac{v_s^2}{Dr} + D_t \right) t \)

For \( t \gg \frac{1}{Dr} \), recover diffusive behavior (linear in \( t \)) but enhanced by \( \frac{v_s^2}{Dr} \)

Now we have the object so... what is pressure?

First work comes from A.P. Solon, Y. Fily, A. Baskaran, M.E. Cates, Y. Kafri, M. Kardar, J. Prost


SIP's are inherently out of equilibrium.

\( \Rightarrow \) we can ask simple question.

This talk:

(i) what is pressure for active particles?

(ii) is there an equation of state?

Answer: Generically no (depends on container/particle interaction) but sometimes yes

not true for passive
How to calculate pressure?

Definition: Pressure is the mechanical force per unit area that a confined system exerts on its container.

(i) For equilibrium systems, the above mechanical def is equivalent to the thermodynamic def \( \frac{\partial F}{\partial V} \) derivative of free energy w.r.t. volume.

(ii) Non-equilibrium: Thermodynamic concepts, such as temp, are known to be ill defined \( \Rightarrow \) let's use mechanical def.

Set up: 2D w/ spatial coord. \( \mathbf{r} = (x, y) \)

Assume periodic b.c. in \( \hat{y} \) \( \Rightarrow \) translational invariance.

System is confined by 2 walls \( \hat{z} \) specified positions that exert forces \( -\nabla V(\mathbf{r}) \) on particles \( \hat{x} \).

Take the origin at \( x = 0 \) (deep in the bulk) and place wall at \( x_w > 0 \).

\[
P = \int_{0}^{\infty} p(\mathbf{r}) \text{d}x \ V(\mathbf{r}) \text{d}x \quad \text{pressure on wall} \quad (\star)
\]

Forces have finite range and vanish in bulk \( \Rightarrow p(\mathbf{r}) \rightarrow 0 \) as \( x \rightarrow 0, \infty \).

The whole game is calculate \( \star \).
Non-interacting part 1: Disks

We have heard about trying to find \( \Psi(\mathbf{r}, \mathbf{\theta}, t) \) instead of dealing with coupled Langevin equations. In general, Langevin equations include forces and torques in general.

\[
\frac{\partial \mathbf{r}}{\partial t} = \mathbf{v}_r \mathbf{\hat{r}} - \mu \nabla V(\mathbf{r}) + \eta_r(t)
\]

\[
\frac{\partial \mathbf{\theta}}{\partial t} = \eta_\theta(t) + \mu_r \Gamma(x, \mathbf{\theta})
\]

May describe alignment of bacteria along wells.

In general, the Langevin equation for a set of variables \( x_i, \ldots, x_n \) is

\[
\frac{dx_i}{dt} = v_i(x_1, \ldots, x_n) + \eta_i(t)
\]

with \( \langle \eta_i(t), \eta_j(t') \rangle = 2B_{ij} \delta(t-t') \).

The associated Fokker-Planck is

\[
\frac{\partial}{\partial t} P(x_1, \ldots, x_n, t) = -\frac{\partial}{\partial x_i} \left[ v_i(x_1, \ldots, x_n) P(x_1, \ldots, x_n, t) \right] + \sum_{j \neq i} B_{ij} \frac{\partial}{\partial x_j} P(x_1, \ldots, x_n, t)
\]
In our case, we have

\[ \frac{\partial}{\partial t} \Psi(r, \theta, t) = -\nabla \cdot \left[ (v \nabla \cdot \mathbf{u}) \nabla \Psi + \mathbf{u} \nabla \Psi - \frac{D_t}{\rho} \nabla^2 \Psi \right] \]

both passive and active particles will experience a wall torque when not spherical.

So for it looks bad --- but let's carry it forward.

For convenience define

\[ m_0(x) = \int_{0}^{2\pi} d\theta \, \cos(\theta) \Psi(\theta) \]

Take moments and study state

\[ 0 = -\partial_x \left( v m_1 - \mu_t \rho \partial_x N - D_t \partial_x p \right) \quad (a) \]

\[ \partial_t m_1 = -\partial_x \left( v \frac{\rho + m_2}{2} \nabla \cdot \mathbf{u}_N - \mu_t \mathbf{m}_1 \cdot \nabla \mathbf{N} - D_t \partial_x m_1 \right) \quad (b) \]

\[ -\int_{0}^{2\pi} \sin \theta \mu_r \Gamma(x, \theta) \Psi(r, \theta) d\theta \]

where \( p = \int_{0}^{2\pi} \Psi(r, \theta) d\theta \) --- steady state density.

Notice (a) has form \( \partial_t p = -\partial_x J \) steady state \( \partial_x J = 0 \).
\[
\phi_{\text{Geyer}} = \int_0^{\infty} \frac{1}{\mu_t} \left[ \sum m_i - D_t \right] dx \rho \, dx
\]

Aside from torque, (6) is a total derivative \( \Rightarrow \) trivially integrate.

At \( x = 0 \) isotropic bulk conditions prevail \( \Rightarrow m_1 = m_2 = 0, \, \rho = \rho_0 \)

At \( x = \infty \) \( m_1 = m_2 = \rho = 0 \)

Restoring torque term

\[
P = \left[ \frac{v^2}{2\mu_t D_t} + \frac{D_t}{\mu_t} \right] \rho_0 - \frac{\mu_t \rho}{\mu_t D_t} \int_0^{2\pi} \int_0^\infty \Gamma(x, \theta) \psi(x, \theta) \sin \theta \, dx \, d\theta
\]

\( \Gamma \) depend on wall/particle
\( \psi \) depend on \( \Gamma, \psi \)

Clearly depends on wall/particle interactions

\( \psi \) depends on \( \Gamma \), \( v \)

\( \Rightarrow \) no eqn of state in general

Now special cases
\[ P = \frac{D_x}{M_k} P_0. \quad \text{Einstein} \rightarrow \frac{D_x}{M_k} = k_B T \]

\[ = P_0 k_B T \quad \text{ideal gas} \]

\[(ii) \text{ torque free} \]

\[ P = P_0 k_B T_{eff}, \quad k_B T_{eff} = \frac{V_o^2}{2M_k D_x} + \frac{D_t}{M_k} \]

We do get eqn. of state in this case.

You might think density has Boltzmann form \( (p(x) \propto e^{-\frac{V_0}{k_B T_{eff}}} ) \)

Given \( P = P_0 k_B T_{eff} \)

\[ \text{bad: only true if } \mu V(x) \ll V_0 \quad (\text{Cates, Tailleur}) \]

"Proof": One can show \( \dot{p} = -\nabla \cdot \left[ \frac{V_o}{D_r} \nabla p + \mu \nabla V p \right] \) \( (a) \)

\[ \dot{p} \text{ } \rightarrow \text{ } \frac{1}{D_r} \text{ and } \frac{1}{p} \ll \frac{D_r}{V_0} \]

(Gradients are small on the scale of the persistence length of particles motion \( \Rightarrow \) enables gradient expansion)

- has steady state solution of Boltzmann form

\[ \left( \frac{V_o}{D_r} \frac{\nabla p}{p} \right) \ll 1 \Rightarrow \frac{V_o}{D_r} \frac{\frac{\mu \nabla V}{V_0}}{\frac{\mu \nabla V}{V_0}} \ll 1 \]