Active Matter

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Active matter: Biological, but also synthetic systems

- **Biological Swimmers**
  - Spermatozoa
  - *E. coli*

- **Artificial Swimmers**
  - Janus rods
  - Janus spheres
  - Chiral particles
  - Vesicles
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Active matter

- A large numbers of active "agents", each of which consumes energy in order to move.
- Due to the energy consumption, these systems are intrinsically out of thermal equilibrium.
- Every particle in an active matter system is out of equilibrium, in contrast to 'boundary driven' systems, like a strip of metal heated at one end, that are locally equilibrated.
- Schools of fish, flocks of birds, bacteria, artificial self-propelled particles, and self-organising bio-polymers such as microtubules and actin.
- Analytical approaches include hydrodynamics, kinetic theory, and non-equilibrium statistical physics. Numerical studies mainly involve self-propelled-particles models, making use of agent-based techniques and molecular dynamics algorithms.
Self Propulsion in Berg’s Run and tumble non-interacting model

- **Run**: straight line (velocity $v \simeq 20 \mu m.s^{-1}$)
- **Tumble**: change of direction (rate $\alpha \simeq 1 s^{-1}$, duration $\tau \simeq 0.1 s$)

**Diffusion at large scale**
- **Run-and-Tumble** $D = \frac{v^2}{\alpha(1+\alpha \tau)} \sim 100 \mu m^2.s^{-1}$
- **Brownian Motion** $D_{col} = \frac{kT}{6\pi \eta r} \sim 0.2 \mu m^2.s^{-1}$
Run and Tumble and Active Brownian particles models

Cells alternate periods of smooth forward swimming (runs) with abrupt reorientations (tumbles).

Active Brownian

\[ \dot{x}_i(t) = v_0 e_i(t) + \frac{F_i}{\gamma}, \quad \dot{\theta}_i(t) = \sqrt{D_r} \eta_i^\theta(t), \quad D = \frac{v_0^2}{2D_r} \]

Gaussian colored noise model

\[ \dot{x}_i(t) = u_i(t) + \frac{F_i}{\gamma}, \quad \dot{u}_i(t) = -\frac{1}{\tau} u_i(t) + \frac{D^{1/2}}{\tau} \eta_i(t) \]
Interacting active systems

Overdamped dynamics of $N$ of degrees of freedom ($x_1, \ldots, x_N$):

$$\frac{dx_i}{dt} = -\frac{\partial U}{\partial x_i} + \eta_i(t)$$  \hfill (1)

$U(x_1, \ldots, x_N)$ is a potential energy and $\eta_i(t)$ is an exponentially correlated colored noise satisfying

$$\langle \eta_i(t) \rangle = 0, \quad \langle \eta_i(t) \eta_j(t') \rangle = \delta_{ij} \frac{D}{\tau} e^{-|t-t'|/\tau}.$$  \hfill (2)
The exponentially correlated colored noise $\eta_i(t)$ can be interpreted as resulting from an Ornstein-Uhlenbeck process,

$$\frac{d\eta_i}{dt} = -\frac{\eta_i}{\tau} + \frac{1}{\tau}\xi_i(t)$$  \hspace{1cm} (3)

where $\xi_i(t)$ is a white noise satisfying

$$\langle \xi_i(t) \rangle = 0, \quad \langle \xi_i(t)\xi_j(t') \rangle = 2T\delta_{ij}\delta(t-t')$$  \hspace{1cm} (4)

$$T = D\gamma$$

Taking the time derivative of Eq. (1) and combining the resulting equation with Eq. (3), one obtains

$$\tau \frac{d^2x_i}{dt^2} + \sum_j \left( \delta_{ij} + \tau \frac{\partial^2 U}{\partial x_i \partial x_j} \right) \frac{dx_i}{dt} = -\frac{\partial U}{\partial x_i} + \xi_i(t).$$  \hspace{1cm} (5)

The Unified Colored Noise Approximation consists in neglecting the second derivative term in Eq. (5) The approximation is assumed to be valid both for $\tau \to 0$ and for $\tau \to \infty$.
Dropping the second order time derivative (analogous to Kramers → Smoluchowski reduction)

\[
\frac{dx_i}{dt} = - \sum_j (M^{-1})_{ij} \frac{\partial U}{\partial x_j} + \sum_j (M^{-1})_{ij} \xi_j(t) \tag{6}
\]

which is a multiplicative Langevin equation, to be interpreted in the Stratonovich sense.

\[
M_{ij} = \delta_{ij} + \tau \frac{\partial^2 U}{\partial x_i \partial x_j} \tag{7}
\]
Distribution of positions of $N$ interacting persistent random walkers

For the $N$ interacting particles, the probability distribution $P(x_1, \ldots, x_N, t)$ is ruled by the following Fokker-Planck equation,

$$\frac{\partial P}{\partial t} = \sum_i \frac{\partial J_i}{\partial x_i}$$

(8)

where the probability current $J_i(x_1, \ldots, x_N, t)$ is given by

$$J_i = \sum_j (M^{-1})_{ij} \frac{\partial U}{\partial x_j} P + T \sum_{j,k} (M^{-1})_{ij} \frac{\partial}{\partial x_k} [(M^{-1})_{jk} P].$$

(9)

Consider the stationary solution of Eq. (8) with vanishing current, $J_i = 0$. Jacobi’s formula

$$\frac{\partial}{\partial x_i} \ln |\det M| = \text{Tr} \left( M^{-1} \frac{\partial M}{\partial x_i} \right),$$

(10)
The condition of vanishing probability current \( J_i = 0 \) leads to

\[
\frac{\partial P}{\partial x_i} = \left( -\frac{1}{T} \sum_j M_{ij} \frac{\partial U}{\partial x_j} + \frac{\partial}{\partial x_i} \ln |\det M| \right) P. \tag{11}
\]

Recalling the definition (7) of the matrix \( M \), the stationary distribution \( P(x_1, \ldots, x_N) \) is obtained as

\[
P = \frac{1}{Z} |\det M| \exp \left[ -\frac{U}{T} - \frac{\tau}{2T} \sum_i \left( \frac{\partial U}{\partial x_i} \right)^2 \right] \tag{12}
\]

with \( Z \) a normalization constant. Eq. (12) generalizes the Boltzmann-Gibbs probability distribution, and reduces to it in the limiting case \( \tau = 0 \).

Detailed balance is satisfied by UCNA...

Notice Many body nature of the effective potential, even when \( U \) is a sum of pairwise potentials.

Consequence: Attraction out of repulsion.
The conditional distribution of velocity at fixed positions $\Pi(v|x)$

At order $\tau$ is a Gaussian distribution

$$\Pi((\{v_i\}|\{x_i\})) = (\frac{\tau}{2\pi D})^{N/2} \sqrt{\det M} \exp\left(-\frac{\tau}{2D_a} \sum_{ij} v_i M_{ij}(\{x\}) v_j \right) \quad (13)$$

Using the Gaussianity of the distribution we can immediately write the averages of the velocity as

$$< v_i v_j > = \int d^N x \overline{v_i v_j} P_N(\{x_i\}) = \frac{D_a}{\tau} \int d^N x M_{ij}^{-1}(\{x_i\}) P_N(\{x_i\}) \quad (14)$$
Two nearby particles have correlated velocities

\[
\overline{x_1 x_2}(\Delta x) = \int d\dot{x}_1 d\dot{x}_2 \dot{x}_1 \dot{x}_2 \Pi = \frac{D}{\tau} \frac{\tau \phi''(\Delta x)}{1 + 2\tau \phi''(\Delta x)}
\]
Testing the $\Pi(v)$ only

$$\langle \dot{x}^2 \rangle = N^{-1} \left\langle \int d\mathbf{x} \dot{x} \cdot \dot{x} \mathcal{N}^{-1} e^{-\tau/(2D)\dot{x} \cdot [\mathbf{I} + \tau \nabla \nabla \phi] \cdot \dot{x}} \right\rangle_{\text{num confs}}$$

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How do we interpret the normalisation factor $Z$: Free energy?

$$F \equiv -T \ln Z$$

$$\mathcal{F}[P] = \text{Tr} P (\mathcal{H} + T \ln P)$$

for all normalised distribution one has the following H-theorem

$$\frac{d\mathcal{F}}{dt} \leq 0.$$  \hspace{1cm} (15)

How the $-T \ln Z$ is related to thermodynamic observables? Pressure:

$$p \equiv T \frac{\partial \ln Z}{\partial V}$$

Does it coincides with the mechanical pressure: force on a wall? Virial pressure. To first order in $\tau$, yes, virial and ”thermodynamic” pressure coincide.
\[ \partial_t P_N(r_1, \ldots, r_N; t) = \mathcal{L}_{FP} P_N(r_1, \ldots, r_N; t) \]  

\[ \frac{d\langle O(t) \rangle}{dt} = \int d^N r P_N \sum_{\alpha i} \sum_{\beta k} M_{\alpha i, \beta k}^{-1} \left( \frac{1}{\gamma} F_{\beta k} \frac{\partial}{\partial r_{\alpha i}} + D \frac{\partial}{\partial r_{\alpha i}} \sum_{\gamma j} M_{\gamma j, \beta k}^{-1} \frac{\partial}{\partial r_{\gamma j}} \right) O \]  

\[ O = \sum_{\alpha i} \left( \frac{r_{\alpha i}^2}{2} + \frac{\tau}{\gamma} \frac{\partial}{\partial r_{\alpha i}} r_{\alpha i} \right) - \frac{\tau}{\gamma} \]  

\[ \sum_i \langle (F_{i}^{ext} + F_{i}^{int}) \cdot r_i \rangle + D \gamma \sum_{\alpha i} \langle M_{\alpha i, \alpha i}^{-1} \rangle = 0 \]  

The forces exerted by the bounding walls of the container, represented by the first term are macroscopically described as external pressure: each oriented area element \( dA \) exerts a force \( -p_v(r) dA \) (the subscript ”v” stands for virial) so that

\[ \sum_i \langle F_{i}^{ext} \cdot r_i \rangle = - \int p_v(r) r \cdot dA = -\bar{p}_v V d, \]
Pressure at a circular wall

...but very similar pressure again! Do we see this in experiments?

I. D. Vladescu et al. PRL 113, 268101 (2014)
Future directions

Understand phase behaviour and phase transitions (if any) between stationary bulk phases.
Recall mechanism of attraction out of repulsion.
So far, only numerical results.
Mean field theory is possible, but the range of effective interactions is so short that it cannot be trusted quantitatively.
Explore non stationary regime.
Go beyond the Unified color approximation.