Suspensions of active particles

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Outline

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1. *Systems with two different temperatures*

2. *Interaction between a cold and a hot colloidal particle*
   - Langevin dynamics
   - Equipartition of energy

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1. *Systems with two different temperatures*

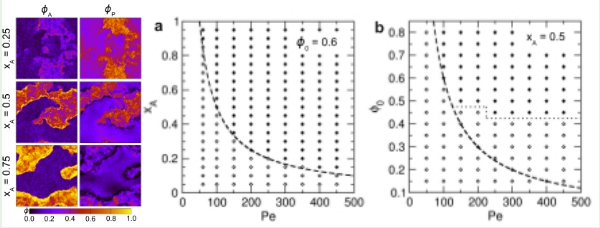
2. *Interaction between a cold and a hot colloidal particle*
   - Langevin dynamics
   - Equipartition of energy

3. *Non-equilibrium phase transitions*
   - Dilute solutions of hot and cold particles
   - Phase diagram
   - Beyond second virial approximation

4. *Ornstein-Uhlenbeck particles*
   - Dilute solutions
   - Physics of small systems

Phase separation between active and non-active particles

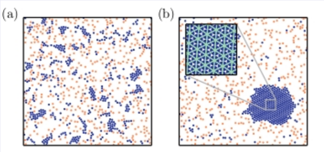
Active Brownian particles and passive particles Stenhammar



Particles with different diffusivities Weber et al.

Binary Mixtures of Particles with Different Diffusivities Demix

Simon N. Weber,[1,*] Christoph A. Weber,[2] and Erwin Frey[1,†]



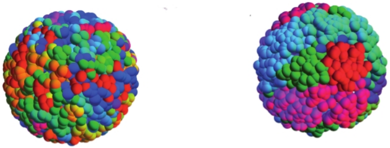
Effective temperature

- Active particles: velocity v_0, rotational diffusion constant D_r
- Effective diffusion constant $D_{eff} = D + v_0^2/(6D_r)$
- Passive particles $T_p = D\zeta$
- Active particles $T_a = T_p + \zeta v_0^2/(6D_r)$

Phase separation in systems with two temperatures

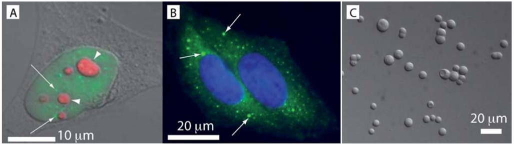
Gene activity and nuclear domains Ganai et al

- Coarse grain genome into a 1μm beads
- Active versus non-active beads with different $T_a = 20T_{eq}$



Other examples

- Granules in cells T. Hyman, F. Julicher
- Molecular motors and diffusible particles on a filament
- Multiphase Interstellar Medium F. Combes



Outline

Langevin Equations

$$\zeta_{\mathcal{A}}\dot{x}_{\mathcal{A}} = -\partial_{\mathcal{A}} u^{\mathcal{AB}} + (2T_{\mathcal{A}}\zeta_{\mathcal{A}})^{1/2}\xi_{\mathcal{A}}(t)$$
$$\zeta_{\mathcal{B}}\dot{x}_{\mathcal{B}} = -\partial_{\mathcal{B}} u^{\mathcal{AB}} + (2T_{\mathcal{B}}\zeta_{\mathcal{B}})^{1/2}\xi_{\mathcal{B}}(t)$$

- Each particle in contact with a reservoir at a fixed temperature
- $\xi_{\mathcal{A},\mathcal{B}}$ are Gaussian white noises of unit variance

Relative motion

- Equation for the relative distance $r = x_{\mathcal{A}} - x_{\mathcal{B}}$

$$\zeta_r\dot{r} = f(r) + (2\zeta_r\overline{T})^{1/2}\xi_r$$

- Relative mobility $\mu_r = \mu_{\mathcal{A}} + \mu_{\mathcal{B}}$
- Mobility averaged temperature $\overline{T} = (\mu_{\mathcal{A}} T_{\mathcal{A}} + \mu_{\mathcal{B}} T_{\mathcal{B}})/(\mu_{\mathcal{A}} + \mu_{\mathcal{B}})$
- Boltzmann distribution $P(r) \sim \exp -u^{\mathcal{AB}}(r)/\overline{T}$

Non equilibrium effects

Center of diffusion motion

- Center of diffusion $R = \frac{D_{\mathcal{A}} x_{\mathcal{A}} + D_{\mathcal{B}} x_{\mathcal{B}}}{D_{\mathcal{A}} + D_{\mathcal{B}}}$
- Langevin equation

$$(\zeta_{\mathcal{A}} + \zeta_{\mathcal{B}})\,\dot{R} = \frac{T_{\mathcal{B}} - T_{\mathcal{A}}}{\bar{T}} f(r) + \sqrt{2\,(\zeta_{\mathcal{A}} + \zeta_{\mathcal{B}})\,\frac{T_{\mathcal{A}} T_{\mathcal{B}}}{\bar{T}}}\,\xi_R(t)$$

- Effective temperature $\frac{T_{\mathcal{A}} T_{\mathcal{B}}}{\bar{T}}$
- Diffusion constant $D_R = \frac{1}{1/D_{\mathcal{A}} + 1/D_{\mathcal{B}}} + \frac{1}{2}\frac{(T_{\mathcal{A}} - T_{\mathcal{B}})^2}{\bar{T}}\frac{\zeta_{\mathcal{A}}\zeta_{\mathcal{B}}}{(\zeta_{\mathcal{A}} + \zeta_{\mathcal{B}})^3}$
- Non-equilibrium contribution

Energy flux

- Energy flux from $\mathcal{B}$ particle to $\mathcal{A}$ particle $w_{\mathcal{B}\to\mathcal{A}} = \left\langle -\dot{x}_{\mathcal{A}} \partial_{\mathcal{A}} u^{\mathcal{A}\mathcal{B}} \right\rangle = \left\langle +\dot{x}_{\mathcal{B}} \partial_{\mathcal{B}} u^{\mathcal{A}\mathcal{B}} \right\rangle$
- $w_{\mathcal{B}\to\mathcal{A}} = \frac{T_{\mathcal{B}} - T_{\mathcal{A}}}{\bar{T}(\zeta_{\mathcal{A}} + \zeta_{\mathcal{B}})} \langle (\partial_r u^{\mathcal{A}\mathcal{B}}(r))^2 \rangle$

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Violation of equipartition of energy

Inertial effects and kinetic energy

$$m_\mathcal{A}\ddot{x}_\mathcal{A} + \zeta_\mathcal{A}\dot{x}_\mathcal{A} = -\partial_\mathcal{A} u^{\mathcal{AB}} + (2T_\mathcal{A}\zeta_\mathcal{A})^{1/2}\xi_\mathcal{A}(t)$$
$$m_\mathcal{B}\ddot{x}_\mathcal{B} + \zeta_\mathcal{B}\dot{x}_\mathcal{B} = -\partial_\mathcal{B} u^{\mathcal{AB}} + (2T_\mathcal{B}\zeta_\mathcal{B})^{1/2}\xi_\mathcal{B}(t)$$

- Finite kinetic energy $\langle \frac{1}{2} m_A \dot{x}_\mathcal{A}^2 \rangle = \frac{1}{2} T_\mathcal{A}^{eff}$

Effective kinetic temperature

- Harmonic interaction $u^{\mathcal{AB}} = \frac{1}{2}\kappa r^2$, elastic time $\tau_e = 1/(\kappa\mu_r)$, $\tau = m_\mathcal{A}/\zeta_\mathcal{A} = m_\mathcal{B}/\zeta_\mathcal{B}$

$$T_\mathcal{A}^{eff} = T_\mathcal{A} + \frac{2\tau}{\tau + \tau_e}(T_\mathcal{B} - T_\mathcal{A})\frac{\mu_\mathcal{A}\mu_\mathcal{B}}{\mu_r^2}$$

- Energy conservation for particle A

$$w_{\mathcal{B}\to\mathcal{A}} = -\langle \zeta v^2 \rangle + \langle v\xi \rangle$$

- Effective temperature

$$w_{\mathcal{B}\to\mathcal{A}} = \frac{T_A}{\tau_A} - \frac{T_A^{eff}}{\tau_A}$$

Outline

Fokker Planck equation

Fokker Planck Equation of a solution

- Pair potential interactions
  $U = \frac{1}{2}\sum_{i\neq j}^{N_{\mathcal{A}}} u^{\mathcal{AA}}\left(\mathbf{r}_i^{\mathcal{A}} - \mathbf{r}_j^{\mathcal{A}}\right) + \sum_i^{N_{\mathcal{A}}}\sum_j^{N_{\mathcal{B}}} u^{\mathcal{AB}} + \frac{1}{2}\sum_{i\neq j}^{N_{\mathcal{B}}} u^{\mathcal{BB}}$
- Fokker Planck equation $\dot{P} = \sum_i \partial_i\left(\partial_i U\, P/\zeta_i + T_i\partial_i P/\zeta_i\right)$

Concentration correlations

- Hierarchy of equations for the cumulants of the concentration

$$\begin{aligned}\frac{\partial c^{\mathcal{A}}(\mathbf{r})}{\partial t} &= \frac{1}{\zeta_{\mathcal{A}}}\partial_{\mathbf{r}}\left[\int \frac{\partial u^{\mathcal{AA}}}{\partial \mathbf{r}} G_2^{\mathcal{AA}}\left(\mathbf{r},\mathbf{r}'\right) d\mathbf{r}'\right] \\ &+ \frac{1}{\zeta_{\mathcal{A}}}\partial_{\mathbf{r}}\left[\int \frac{\partial u^{\mathcal{AB}}}{\partial \mathbf{r}} G_2^{\mathcal{AB}}\left(\mathbf{r},\mathbf{r}'\right) d\mathbf{r}'\right] + \frac{T_{\mathcal{A}}}{\zeta_{\mathcal{A}}}\nabla_{\mathbf{r}}^2 c^{\mathcal{A}}(\mathbf{r})\end{aligned}$$

- Pair correlation functions
  $G_2^{\mathcal{AB}}(\mathbf{r},\mathbf{r}') = \sum_i^{N_{\mathcal{A}}}\sum_j^{N_{\mathcal{B}}}\int \delta\left(\mathbf{r}_i^{\mathcal{A}} - \mathbf{r}\right)\delta\left(\mathbf{r}_j^{\mathcal{B}} - \mathbf{r}'\right) P\left(\{\mathbf{r}\}\right) d\{\mathbf{r}\} =$
  $c^{\mathcal{A}}(\mathbf{r})c^{\mathcal{B}}(\mathbf{r}') \quad g^{\mathcal{AB}}(\mathbf{r},\mathbf{r}')$
- Depend on 3 body correlation functions

Dilute solution: effective thermodynamics

Conservation equations

- Low density limit $g^{\mathcal{AA}} = \exp -u^{\mathcal{AA}}/T_{\mathcal{A}}$, $g^{\mathcal{BB}} = \exp -u^{\mathcal{BB}}/T_{\mathcal{B}}$, $g^{\mathcal{AB}} = \exp -u^{\mathcal{AB}}/\overline{T}$
- Conservation equation with short range interactions

$$\frac{\partial c^{\alpha}(\mathbf{r})}{\partial t} = \frac{1}{\zeta_i}\frac{\partial}{\partial \mathbf{r}}\left(c^{\alpha}\frac{\partial \mu^{\alpha}}{\partial \mathbf{r}}\right) = -\frac{\partial \mathbf{j}_{\alpha}}{\partial \mathbf{r}}$$

- Particle currents $\mathbf{j}_{\mathcal{A},\mathcal{B}} = -\frac{1}{\zeta_{\mathcal{A},\mathcal{B}}}\frac{\partial \mu_{\mathcal{A},\mathcal{B}}}{\partial \mathbf{r}}$

Effective thermodynamics

- Chemical potentials derive from an effective free energy
  $f = T_{\mathcal{A}}c^{\mathcal{A}}\ln\left(c^{\mathcal{A}}/e\right) + T_{\mathcal{B}}c^{\mathcal{B}}\ln\left(c^{\mathcal{B}}/e\right) + (1/2)T_{\mathcal{A}}B_{\mathcal{A}}c_{\mathcal{A}}^2 + (1/2)T_{\mathcal{B}}B_{\mathcal{B}}c_{\mathcal{B}}^2 + \overline{T}B_{\mathcal{AB}}c^{\mathcal{A}}c^{\mathcal{B}}$
- Nonequilibrium virial coefficients $B_{\alpha\beta} = \int\left[1 - e^{-u^{\alpha\beta}(\mathbf{r})/T_{\alpha\beta}}\right]d^3\mathbf{r}$
- Different temperatures for different virial coefficients $T_{\mathcal{AB}} = \overline{T}$
- Osmotic pressure can be calculated from the effective free energy

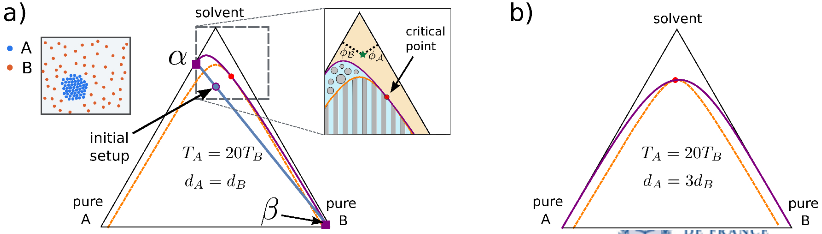
Phase diagram E. Ilker

Spinodal instability

- Volume fractions $\phi_\alpha = c^\alpha B^\alpha/8$, physical excluded volume condition $\phi_\mathcal{A} + \phi_\mathcal{B} \leq 1$
- Spinodal stability limit $\frac{8\phi_\mathcal{A}}{1+8\phi_\mathcal{A}} \frac{8\phi_\mathcal{B}}{1+8\phi_\mathcal{B}} > \frac{T_\mathcal{A} T_\mathcal{B}}{T^2} \frac{B^2_{\mathcal{AB}}}{B_\mathcal{A} B_\mathcal{B}}$

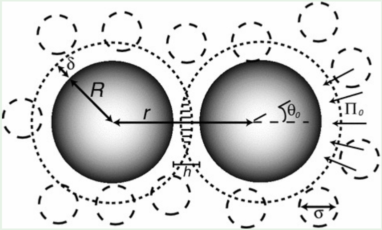
Triangular Phase diagram

- Same equilibrium conditions as thermodynamic phase diagram
- If $B_{\mathcal{AA}} = B_{\mathcal{AB}} = B_{\mathcal{BB}} = B$ phase separation exists only if $T_\mathcal{B}/T_\mathcal{A} > 4$



Depletion interactions in hard sphere solutions Akasura and Oosawa

Depletion interaction

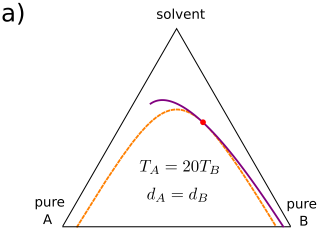


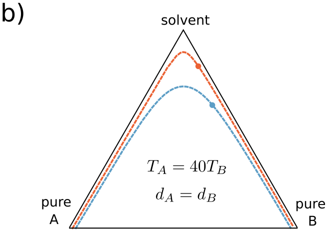
- Force between the two spheres $f = P_{ext} S$
- Using the ideal gas pressure, this gives the exact three body interactions for hard spheres
- Potential of mean force $w(r)$ obtained by integration of the force
- Pair distribution function $g_{\alpha\beta} = \exp -\frac{w_{\alpha\beta}(r)}{T_{\alpha\beta}}$

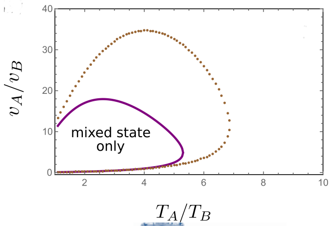
Conservation equations

- Go back to the dynamic equations and insert the pair distribution function
- Particle currents $\mathbf{j}_{\mathcal{A},\mathcal{B}} = -\frac{c_{\mathcal{A},\mathcal{B}}}{\zeta_{\mathcal{A},\mathcal{B}}} M_{\mathcal{A},\mathcal{B}}$
- No well defined chemical potential, no equivalent thermodynamic
- Phase diagram directly obtained from the dynamic equation

Non-equilibrium steady state, Phase diagram







- Smaller region of phase separation
- Spinodal line and critical point
- No complete determination of steady state phases.
- Beyond third virial coefficient Cates and Mao

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Langevin Equation with colored noise

Ornstein-Uhlenbeck particles

- Langevin Equation $\zeta \frac{dx}{dt} = f(x) + \eta(t)$
- Colored noise $\langle \eta(0)\eta(t) \rangle = kT\zeta/\tau \exp -|t|/\tau$
- Persistent random walk with a velocity v_0, $kT = \zeta v_0^2 \tau$
- Run length $v_0\tau$

Two parameters description

- Position and random force

$$
\begin{aligned}
\zeta \frac{dx}{dt} &= f(x) + \eta(t) \\
\tau \frac{d\eta}{dt} + \eta &= \xi(t)
\end{aligned}
$$

- White noise $\langle \xi(0)\xi(t) \rangle = 2kT\zeta\delta(t)$
- Analogy with a particle with inertia $\tau\zeta \frac{d^2x}{dt^2} + (\zeta - \tau \frac{df}{dx}) \frac{dx}{dt} - f(x) = \xi(t)$

Stress tensor and pressure

Fokker-Planck equation

$$\partial_t P(x,\eta) = -\frac{1}{\zeta}\partial_x \left[(\eta + f(x))\, P(x,\eta)\right] + \frac{1}{\tau}\partial_\eta \left[\eta P(x,\eta)\right] + \frac{\zeta T}{\tau^2}\partial_\eta^2 \left[P(x,\eta)\right]$$

- Advection in x and η, Diffusion in η
- Current loops in (x,η) space

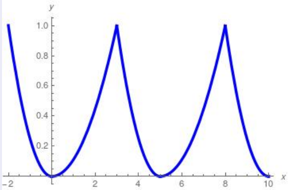
Moment expansion

- Particle density $\rho = \int d\eta P(x,\eta)$
- First moment $f_i(\vec{x}) = -\langle \eta_i \rangle (\vec{x})$
- Second moment $f_j(\vec{x})\rho(\vec{x}) = \frac{\tau}{\zeta}\partial_{x_i}\left[\left(\langle \eta_i \eta_j \rangle - \langle \eta_i \rangle \langle \eta_j \rangle\right)\rho(\vec{x})\right]$

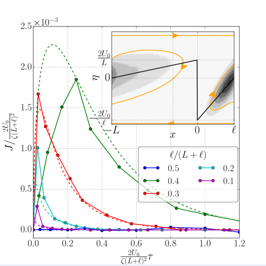
Stress tensor

- Local force balance
- Stress tensor $\sigma_{ij} = -\frac{\rho\tau}{\zeta}\langle \delta\eta_i \delta\eta_j \rangle$
- Pressure $\Pi = \frac{1}{3}\frac{\rho\tau}{\zeta}\langle \vec{\delta\eta}^2 \rangle$
- No external force : Ideal gas $\langle \vec{\delta\eta}^2 \rangle = \frac{3kT\zeta}{\tau}$, pressure $\Pi = kT\rho$ Solon et al.

Pumping by an asymmetric periodic potential



- Finite flux



- Penetration length in the harmonic potential $U = U_0(\frac{x}{L})^2 = \frac{1}{2}\kappa x^2$,
  $l_{OUP} = \left(\frac{kT}{\kappa(\kappa\tau/\zeta+1)}\right)^{1/2}$
- Crossing a potential barrier
  - $\tau = 0$ energy dominated, Boltzmann factor
  - $\kappa\tau/\zeta \gg 1$, force dominated $\eta \geq 2U_0/L$
- Asymmetry in the force dominated regime

- Non-equilibrium phase separation due to temperature (activity) contrast
  - Energy fluxes between hot and cold thermal bath
  - Effective thermodynamics with a well defined free energy at low concentration
  - No effective thermodynamics at higher concentration
  - Other examples of phase separation in active systems
    - Non homogeneous solutions, surface tension between two phases E. Ilker
    - Polymers and copolymers with monomers at different temperatures Hsuan Yi Chen
    - Self-diffusion in a mixture of active and passive particles E. Ilker, M. Castellana

- Ornstein-Uhlenbeck Particles
  - Strongly non-equilibrium effects in small systems
  - Curvature effects in a 2d system
  - Repulsive depletion forces C. Sanford