Active matter – Week 3: Active scalar field theory
DRSTP Advanced Topics in Theoretical Physics (Spring 2025)

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This lecture is largely based on the lecture "Active field theories"[1] by Michael E. Cates [1].

I. FIELD THEORIES

Our goal is to construct a *field theory* for some order parameter $\psi(\boldsymbol{r}, t)$, which corresponds to the coarse-graining of some microscopic quantity such as density $\delta(\boldsymbol{r} - \boldsymbol{r}_i(t))$, polarisation $\boldsymbol{p}_i(t)$, or nematic tensor $(\boldsymbol{u}_i(t) \otimes \boldsymbol{u}_i(t) - \frac{1}{d}\mathbb{1})$, and which takes the generic form of a stochastic differential equation

$$\dot{\psi}(\boldsymbol{r}, t) = \dots \tag{1}$$

which can be determined either from the formal coarse-graining of our microscopic degrees of freedom (bottom-up approach) [2] or from general symmetry considerations (top-down approach) [3, 4]. While the first route enables to link microscopic and coarse-grained parameters it is often the most technically involved. The second path is often more straightforward however some parameters are unknown, especially in active matter systems where relations like the fluctuation-dissipation theorem are unavailable.

While field theories correspond to the treatment of a stochastic system at the coarse-grained or hydrodynamic level, these differ from Fokker-Planck equations in two important ways. First, these theories describe the evolution of a given quantity in space and time and not of its probability distribution. Second, these theories will include stochastic terms while Fokker-Planck equations are deterministic.

I.A. Model B

We will focus here on a single *conserved scalar field* ρ, the density[2], whose evolution does not need to satisfy momentum conservation[3]. According to the classification introduced by Hohenberg and Halperin [5], this corresponds to "Model B". This model is described by a conservation equation,

$$\dot{\rho}(\boldsymbol{r}, t) = -\nabla \cdot \boldsymbol{J}(\boldsymbol{r}, t), \tag{2a}$$

where $\nabla \equiv \partial/\partial \boldsymbol{r}$ and $\boldsymbol{J}$ is a flux written as

$$\boldsymbol{J} = -M[\rho]\,\nabla\mu + \boldsymbol{J}^{\mathrm{N}}, \tag{2b}$$

where $M[\rho]$ is a mobility, written as a functional[4] of the density field ρ, μ is a chemical potential, and $\boldsymbol{J}^{\mathrm{N}}$ is a noise term. It is noteworthy that noise appears as a divergence term $-\nabla \cdot \boldsymbol{J}^{\mathrm{N}}$ in the equation of evolution of ρ (2a) since the latter quantity must be conserved.

At thermodynamic equilibrium, there exists a free energy functional $F[\rho]$ from which the chemical potential derives,

$$\mu = \frac{\delta F}{\delta \rho}, \tag{3}$$

where $\delta/\delta\rho$ is a functional derivative[5]. According to Fick's law [7] (§ 2 – Linear thermodynamics of irreversible processes [6.2. Diffusion coefficient]) we write the mobility

$$M[\rho] = \beta\rho D[\rho], \tag{6}$$

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[1] Videos from the lectures at Les Houches summer school on "Active Matter and Nonequilibrium Statistical Physics" (2018) can be found at `https://www.youtube.com/playlist?list=PLo9ufcrEqwWFT3RoHoynyoYEcwBTQdEwy`.

[2] Density is conserved in the sense that there is no creation or deletion of particles.

[3] Momentum conservation would be achieved by coupling our scalar field to a momentum-conserving solvent, following for example the Navier-Stokes equation (see "Model H" [5]).

[4] We will denote functionals f of fields ρ as $f[\rho]$ (with square brackets) throughout this lecture.

[5] Considering a functional

$$F[\rho] = \int \mathrm{d}\boldsymbol{r}\, f(\boldsymbol{r}, \rho(\boldsymbol{r}), \nabla\rho(\boldsymbol{r})), \tag{4}$$

we write its functional derivative [6]

$$\frac{\delta F}{\delta \rho} = \frac{\partial f}{\partial \rho} - \nabla \cdot \frac{\partial f}{\partial \nabla \rho}. \tag{5}$$

where $\beta = (k_B T)^{-1}$ with k_B the Boltzmann constant and T the temperature, and where we will furthermore assume, for simplicity, that the diffusion constant only depends locally on the density $D(\rho)$. At equilibrium the system must follow the Boltzmann distribution,

$$\mathrm{Prob_B}[\rho] = \frac{1}{Z}\exp(-\beta F[\rho]), \tag{7}$$

where Z is the partition function. The role of the noise flux $\boldsymbol{J}^{\mathrm{N}}$ is to enable this sampling of the Boltzmann distribution, this means that the amplitude and functional form of the noise must be dictated by the fluctuation-dissipation theorem[6]. We have here

$$\boldsymbol{J}^{\mathrm{N}}(\boldsymbol{r},t) = \sqrt{2\rho D(\rho)}\,\boldsymbol{\Lambda}(\boldsymbol{r},t), \tag{8a}$$

where $\boldsymbol{\Lambda}(\boldsymbol{r},t)$ is a Gaussian white noise with mean and variance

$$\langle \boldsymbol{\Lambda}(\boldsymbol{r},t)\rangle = 0, \tag{8b}$$

$$\langle \boldsymbol{\Lambda}(\boldsymbol{r},t)\otimes\boldsymbol{\Lambda}(\boldsymbol{r},t)\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}')\,\delta(t-t')\,\mathbb{1}. \tag{8c}$$

I.B. Equilibrium phase separation

I.B.1. Free energy functional

An example of a free energy functional may be

$$\beta F[\rho] = \int \mathrm{d}\boldsymbol{r}\,\rho(\boldsymbol{r},t)(\log\rho(\boldsymbol{r},t)-1) + \beta\int \mathrm{d}\boldsymbol{r}_1\int \mathrm{d}\boldsymbol{r}_2\,\rho(\boldsymbol{r}_1)\,\rho(\boldsymbol{r}_2)\,w(|\boldsymbol{r}_1-\boldsymbol{r}_2|), \tag{9}$$

where the first term corresponds to the ideal gas free energy[7], and the second term includes the energy cost of a soft interaction potential w. In the case where w is attractive in the middle-to-short range[8], there is an inherent competition between the entropy, which is maximised for homogeneous density fields, and the energy, which is minimised for closely packed particles. This competition may dictate phase transitions.

At the level of the scalar field theory, we can make analytical progress in the description of such transitions through the approximation of the free energy (10) by its Taylor expansion in weak gradients[9] of $\phi = \rho - \rho_0$,

$$F[\phi] = \int \mathrm{d}\boldsymbol{r}\, f(\phi,\nabla\phi) = \int \mathrm{d}\boldsymbol{r}\,\left[\frac{a}{2}\phi^2 + \frac{b}{3}\phi^3 + \frac{c}{4}\phi^4 + \frac{\kappa}{2}(\nabla\phi)^2\right], \tag{14a}$$

where ρ_0 is some reference density[10] and f is the free energy density, which leads to the chemical potential

$$\mu = \frac{\delta F}{\delta\phi} = a\phi + b\phi^2 + c\phi^3 - \kappa\nabla^2\phi. \tag{14b}$$

We will determine the stability of homogeneous phases ($\nabla\phi = 0$) at the mean-field level (without fluctuations, $\boldsymbol{J}^{\mathrm{N}} = 0$). To this effect, we write the homogeneous free energy

$$f^h = \frac{a}{2}\phi^2 + \frac{b}{3}\phi^3 + \frac{c}{4}\phi^4, \tag{15a}$$

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[6] See problem III.A.

[7] With the ideal gas free energy,

$$\beta F_{\mathrm{free}}[\rho] = \int \mathrm{d}\boldsymbol{r}\,\rho(\boldsymbol{r},t)(\log\rho(\boldsymbol{r},t)-1), \tag{10}$$

we obtain the ideal gas chemical potential,

$$\mu_{\mathrm{free}} = \frac{\delta F_{\mathrm{free}}}{\delta\rho} = \frac{1}{\beta}\log\rho(\boldsymbol{r},t), \tag{11}$$

and the flux (2b) reduces to

$$\boldsymbol{J} = -D(\rho)\nabla\rho + \boldsymbol{J}^{\mathrm{N}}, \tag{12}$$

leading to the diffusion equation with conserved noise

$$\dot{\rho} = \nabla\cdot(D(\rho)\nabla\rho) - \nabla\cdot\boldsymbol{J}^{\mathrm{N}}. \tag{13}$$

[8] You may think of a Lennard-Jones potential $w(r) = 4\varepsilon[(r/\sigma)^{-12} - (r/\sigma)^{-6}]$ where ε is an energy scale and σ is a length scale.

[9] This approximation leads to the Landau ϕ^4 free energy.

[10] There is no linear term in ϕ in (14a) since its integral would be proportional to the volume of the system, which is assumed constant, and it would thus not affect the variations of the free energy. It is also noteworthy that ρ may be chosen so as to cancel the cubic ϕ^3 term in (14a).

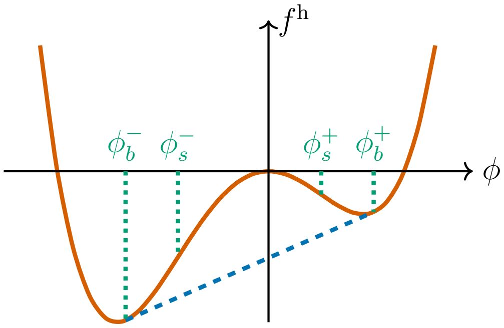

FIG. 1. Common-tangent construction. We represent the free energy for a homogeneous density field f^h (15a) as the orange solid line ($a = -20$, $b = 3$, $c = 4$), and the common tangent construction as the blue dashed line. Densities $\phi_b^\pm$ are the bionodal densities and densities $\phi_s^\pm$ are the spinodal densities.

which we plot in Fig. 1, and the chemical potential

$$\mu^{\mathrm{h}} = \frac{\partial f^h}{\partial \phi} = a\phi + b\phi^2 + c\phi^3. \tag{15b}$$

In the case where f^h has several local minima, the system may be able to lower its free energy by phase separating.

I.B.2. Global instability: binodal region and common-tangent construction

Would the system phase separates, thermodynamic equilibrium dictates that coexisting phases, at densities ϕ_1 and ϕ_2, should have equal chemical potentials,

$$\mu^h(\phi_1) = \mu^h(\phi_2) \Leftrightarrow \frac{\partial f^h}{\partial \phi}(\phi_1) = \frac{\partial f^h}{\partial \phi}(\phi_2), \tag{16a}$$

which translates to equal slope of tangents at ϕ_1 and ϕ_2 in the graph of the free energy density. Thermodynamic equilibrium also dictates that coexisting phases should also have equal pressures,

$$\begin{aligned} p_1 = p_2 &\Leftrightarrow \phi_1\mu^h(\phi_1) - f^h(\phi_1) = \phi_2\mu^h(\phi_2) - f^h(\phi_2) \\ &\Leftrightarrow \phi_1\frac{\partial f^h}{\partial \phi}(\phi_1) - f^h(\phi_1) = \phi_2\frac{\partial f^h}{\partial \phi}(\phi_2) - f^h(\phi_2), \end{aligned} \tag{16b}$$

where the first equivalence derives from the thermodynamic relation between pressure, density, free energy density, and chemical potential, and which relation translates to equal intercept of tangents at ϕ_1 and ϕ_2 in the graph of the free energy density. We identify in Fig. 1 the densities $\phi_1 = \phi_b^-$ and $\phi_2 = \phi_b^+$ which satisfy conditions (16) and which delimit the *binodal region*, where the system is *globally unstable* to phase separation. Within this region $\phi \in [\phi_1, \phi_2]$, the system is able to minimise its free energy by forming phases at densities ϕ_1 and ϕ_2 with volumes V_1 and V_2, where conservation of matter dictates

$$V_1 + V_2 = V, \tag{17a}$$

$$V_1\phi_1 + V_2\phi_2 = V\phi, \tag{17b}$$

which leads to the following coexistence free energy density[11]

$$\begin{aligned} \tilde{f}(\phi) &= f^h(\phi_1)\frac{V_1}{V} + f^h(\phi_2)\frac{V_2}{V} \\ &= f^h(\phi_1) + (f^h(\phi_2) - f^h(\phi_1))\frac{\phi - \phi_1}{\phi_2 - \phi_1} \leq f^h(\phi), \end{aligned} \tag{18}$$

which corresponds to the line which satisfies (16) and plotted in Fig. 1. This construction is known as *common-tangent construction.*

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[11] We have neglected the energy cost of maintaining the interface. This cost grows with the area between the phases and is thus subextensive in the volume, compared to the free energy of bulk phases which are extensive in the volume. Therefore, while there is a free energy cost to nucleating phase interfaces, this cost becomes relatively small for large systems.

I.B.3. Local instability: spinodal region

We may rewrite our field theory (2) using the mobility (6),

$$\dot{\phi} = -\nabla \cdot \left(-\beta\rho D(\rho) \nabla \frac{\partial f}{\partial \phi} \right) = \nabla \cdot \left(\beta\rho D(\rho) \frac{\partial^2 f}{\partial \phi^2} \nabla \phi \right), \tag{19}$$

where fluctuations of ϕ are amplified rather than damped if the free energy is concave,

$$\frac{\partial^2 f}{\partial \phi^2} = \frac{\partial \mu}{\partial \phi} < 0, \tag{20}$$

such that the system is *locally unstable*. This identifies the *spinodal region*, denoted $[\phi_s^-, \phi_s^+]$ in Fig. 1, where the system spontaneously demixes with no thermodynamic cost.

II. FIELD THEORY OF ACTIVE BROWNIAN PARTICLES

II.A. Active Model B

We consider an ensemble of active Brownian particles[12], equipped with unitary self-propulsion directions $\hat{\boldsymbol{u}}_i(t)$ which diffuse with diffusion coefficient $1/\tau$, and propelled at self-propulsion velocities $v_0(\boldsymbol{r}_i, [\rho]))$ which is a functional of the density field ρ.

Refs. [1, 2] coarse-grain the equations of motion of these particles when their self-propulsion directions follow independent processes and where particles interact through a *quorum-sensing interaction*, whose effect is to decrease self-propulsion velocity in regions of large density. This choice of interaction is more analytically tractable than the *repulsive interaction* potential between self-propelled particles introduced in the previous lecture. These two interactions are however closely related: self-propelled particles move slower in crowded environments because propulsion forces compete with crowding effects emerging from repulsions [8].

Since there are no interactions between self-propulsion directions, there is no mesoscopic polarisation of the system, and the latter is described at the coarse-grained level by the evolution of its density field. Moreover there is no creation or deletion of particles, therefore the density field is conserved, as in Model B. We report the field theory derived in Refs. [1, 2],

$$\dot{\rho}(\boldsymbol{r}, t) = -\nabla \cdot \boldsymbol{J}(\boldsymbol{r}, t), \tag{22a}$$

$$\boldsymbol{J} = -\rho \frac{\tau v_0[\rho]}{d} \nabla v_0[\rho] - D[\rho] \nabla \rho + \sqrt{2D[\rho]\rho}\, \boldsymbol{\Lambda}, \tag{22b}$$

$$D[\rho] = \frac{v_0[\rho]^2 \tau}{d}, \tag{22c}$$

where d is the dimension, $\boldsymbol{\Lambda}$ is a zero-mean unit-variance Gaussian white noise (8), and the relation (22c) between the diffusion D, self-propulsion velocity v_0 and persistence time τ is consistent with our derivation of the mean-squared displacement of active Brownian particles in the previous lecture.

We recognise the last two terms in the right-hand-side of (22b) as the usual diffusive flux with diffusivity D. In addition to this, the quorum-sensing interaction leads to the first term in the right-hand-side of (22b) which indicates that there is a flux of density towards regions with lesser self-propulsion velocities. This can be understood microscopically by considering two repulsive self-propelled particles at contact with opposite self-propulsion direction and different self-propulsion velocities: in this case, both particles will move in the direction from the particle with the largest to the particle with the smallest self-propulsion velocity.

We can rewrite (22b) with an effective chemical potential,

$$\boldsymbol{J} = -\beta\rho D[\rho] \nabla \mu + \sqrt{2\rho D[\rho]}\, \boldsymbol{\Lambda}, \tag{22d}$$

$$\beta\mu = \log v_0[\rho] + \log \rho, \tag{22e}$$

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[12] In the absence of interaction, we can see the dynamics of these active Brownian particles as following

$$\dot{\boldsymbol{r}}_i = v_0(\boldsymbol{r}_i, [\rho])\, \hat{\boldsymbol{u}}_i, \tag{21a}$$

$$\dot{\hat{\boldsymbol{u}}}_i = \sqrt{2/\tau}\, \hat{\boldsymbol{u}}_i \times \boldsymbol{\eta}_i, \tag{21b}$$

where $\boldsymbol{r}_i$ and $\hat{\boldsymbol{u}}_i$ are the position and self-propulsion directions of particle i, and $\boldsymbol{\eta}_i$ is a zero-mean unit-variance Gaussian white noise.

where we have introduced β for consistency of notations but there is *no thermal phenomenon* in the system and thus these factors cancel. At the mean-field level (without fluctuations, and homogeneous density thus $v_0[\rho] = v_0(\rho)$), we can assess the local instability condition (20),

$$\beta \frac{\partial \mu}{\partial \rho} = \frac{1}{\rho} + \frac{1}{\rho} \frac{\partial v_0}{\partial \rho} < 0, \tag{23}$$

which may be verified if $v_0(\rho)$ decreases sufficiently steeply with increasing density ρ, rendering homogeneous density fields unstable and possibly leading to phase separation. We should not be fooled however by the seemingly equilibrium-like formulation of (22d): while the system indeed phase separates (spoiler), we will find that the chemical potential does not derive from a free energy $\mu \neq \delta F/\delta\rho$ (as should be expected for an active system) and thus describing the global instability criterion needs a more elaborate construction.

II.B. Motility-induced phase separation

II.B.1. Breakdown of equilibrium in the chemical potential

In order to make analytical progress, we first need to give an expression for the self-propulsion velocity functional $v_0[\rho]$, and in particular we will aim for a local function of the density

$$v_0[\rho] = v_0(\overline{\rho}(\boldsymbol{r})), \tag{24a}$$

which we achieve by introducing a coarse-grained density $\overline{\rho}(\boldsymbol{r})$ with means of a normalised kernel function K,

$$\begin{aligned}
\overline{\rho}(\boldsymbol{r}) &= \int \mathrm{d}\boldsymbol{r}'\, K(\boldsymbol{r} - \boldsymbol{r}')\, \rho(\boldsymbol{r}') \\
&= \int \mathrm{d}\boldsymbol{s}\, K(\boldsymbol{s}) \left[\rho(\boldsymbol{r}) - \boldsymbol{s}\cdot\nabla\rho(\boldsymbol{r}) + \frac{1}{2}|\boldsymbol{s}|^2 \nabla^2 \rho(\boldsymbol{r})\right] \\
&= \rho(\boldsymbol{r}) - \left(\int \mathrm{d}\boldsymbol{s}\, K(\boldsymbol{s})\boldsymbol{s}\right)\cdot\nabla\rho(\boldsymbol{r}) + \left(\int \mathrm{d}\boldsymbol{s}\, K(\boldsymbol{s})\, \frac{1}{2}|\boldsymbol{s}|^2\right)\nabla^2\rho(\boldsymbol{r}) \\
&= \rho(\boldsymbol{r}) + c_2 \nabla^2 \rho(\boldsymbol{r}),
\end{aligned} \tag{24b}$$

where the term linear in $\nabla\rho$ cancels for K an even function, and where we have neglected higher gradients of the density fields in its Taylor expansion. We use this first expression to Taylor-expand the self-propulsion velocity for low c_2,

$$v_0(\overline{\rho}(\boldsymbol{r})) = v_0(\rho(\boldsymbol{r})) + c_2 \frac{\partial v_0}{\partial \rho}(\rho(\boldsymbol{r}))\, \nabla^2 \rho(\boldsymbol{r}), \tag{24c}$$

which is now a purely local function of the density, and we use this second expression to Taylor-expand the effective chemical potential (22e),

$$\begin{aligned}
\beta\mu &= \log\left(v_0(\rho)\left(1 + \frac{1}{v_0(\rho)} c_2 \frac{\partial v_0}{\partial \rho}(\rho)\nabla^2\rho\right)\right) + \log\rho \\
&= \log\rho + \log v_0(\rho) + \frac{1}{v_0(\rho)} c_2 \frac{\partial v_0}{\partial \rho}(\rho)\nabla^2\rho \\
&= \mu_0(\rho) - \kappa(\rho)\nabla^2\rho,
\end{aligned} \tag{25a}$$

where we have dropped the position-dependence for ease of notation and where we have introduced

$$\mu_0(\rho) = \log\rho + \log v_0(\rho), \tag{25b}$$

$$\kappa(\rho) = -\frac{1}{v_0(\rho)} c_2 \frac{\partial v_0}{\partial \rho}(\rho). \tag{25c}$$

Our effective chemical potential (25a) has a gradient term which is reminiscent of the chemical potential we have derived from our equilibrium free energy (14b). An important different however is that our parameter $\kappa(\rho)$ (25c) now also depends on the density. Therefore if we were to introduce a free energy similar to (14a) from which the gradient term in the chemical potential may derive,

$$\beta F[\rho] = \int \mathrm{d}\boldsymbol{r}\, \left[f_0(\rho) + \frac{\kappa(\rho)}{2} (\nabla\rho)^2 \right], \tag{26a}$$

$$\frac{\partial f_0}{\partial \rho}(\rho) = \mu_0(\rho), \tag{26b}$$

we would obtain the following equilibrium chemical potential

$$\mu^{\mathrm{eq}}(\rho) = \frac{\delta F}{\delta \rho} = \mu_0(\rho) + \frac{1}{2}\kappa'(\rho)(\nabla\rho)^2 - \nabla\cdot(\kappa(\rho)\nabla\rho) = \mu_0(\rho) - \frac{\kappa'(\rho)}{2}(\nabla\rho)^2 - \kappa(\rho)\nabla^2\rho, \tag{26c}$$

which, compared to (25a), has an additional $\kappa' \equiv \partial\kappa/\partial\rho$ term. We conclude that our effective chemical potential does not derive from a free energy $\mu \neq \delta F/\delta\rho$ and our system remains *out of equilibrium* at the field-theory level.

II.B.2. Generalisation of the common-tangent construction

There is no free energy from which the steady state behaviour of our system may be described, therefore we cannot use the properties of the free energy to derive the binodal region from the common-tangent construction as we did in Sec. I.B.2. Refs. [1, 2] provide a way to nonetheless determine phase-separation conditions in steady states from a mapping of the density to an other scale.

At the mean-field level (without fluctuations), we rewrite our field theory (22) as following

$$\dot\rho = \nabla\cdot(M\nabla\mu), \tag{27a}$$

$$\mu = \mu_0(\rho) + \lambda(\rho)(\nabla\rho)^2 - \kappa(\rho)\nabla^2\rho. \tag{27b}$$

At equilibrium, we have shown that (26c)

$$2\lambda(\rho) + \kappa'(\rho) = 0, \tag{28}$$

while in our active Model B (25a) we have $\lambda(\rho) = 0$ and $\kappa'(\rho) \neq 0$. We will solve (27) for two steady-state coexisting phases, at densities ρ_1 and ρ_2, along a one-dimensional profile (with coordinate x) represented in Fig. 2: this solution should only exist if ρ_1 and ρ_2 are possible coexisting densities, and this will enable us to map our coexistence binodal region.

We are looking for a current-free steady state, which from (27a) must thus satisfy $\nabla\mu = 0$. Therefore our effective chemical gradient is constant over space and in particular between the coexisting phases,

$$\mu(\rho_1) = \mu(\rho_2) = \overline{\mu}, \tag{29}$$

similarly to the "equal-slope" equilibrium condition (16a).

Contrarily to the homogeneous chemical gradient (with $\nabla\rho = 0$) considered at equilibrium (15b), we have kept the gradient terms in our effective nonequilibrium chemical gradient (27b). In the one-dimensional profile we are

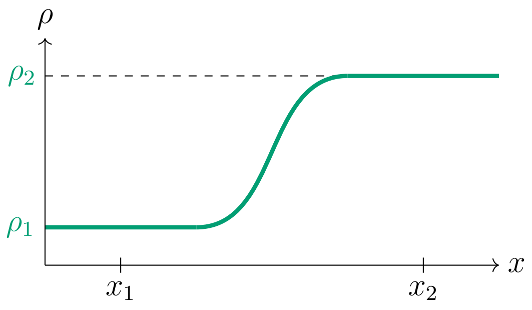

FIG. 2. One-dimensional coexisting phases density profile.

considering (Fig. 2) these gradient terms only contribute close to the interface. To get rid of this dependence on the specific shape of the interface, we introduce a mapping $R(\rho)$ of the density which satisfies

$$\kappa(\rho)R''(\rho) = -(2\lambda(\rho) + \kappa'(\rho))R'(\rho). \tag{30}$$

At equilibrium, $R''(\rho) = 0$ (28), and this mapping amounts to an affine rescaling of the density ρ. This mapping is introduced to derive the following relation

$$\left[\lambda(\rho)\left(\frac{\partial\rho}{\partial x}\right)^2 - \kappa(\rho)\frac{\partial^2\rho}{\partial x^2}\right]\frac{\partial R(\rho)}{\partial x} = \frac{\partial}{\partial x}\left(-\frac{\kappa(\rho)}{2}R'(\rho)\left(\frac{\partial\rho}{\partial x}\right)^2\right), \tag{31a}$$

$$\frac{\partial R(\rho)}{\partial x} = R'(\rho)\frac{\partial\rho}{\partial x}, \tag{31b}$$

which will come in handy below. We will now use this map to build a new relation between the pseudo density $R(\rho)$, the effective chemical potential μ, and a pseudo free energy $\Phi(R(\rho))$ which satisfies

$$\frac{\partial\Phi(R(\rho))}{\partial R} = \mu_0(\rho). \tag{32}$$

To this effect we compute on the one hand,

$$\int_{x_1}^{x_2} \mathrm{d}x\,\mu(\rho)\,\frac{\partial R(\rho)}{\partial x} = \int_{x_1}^{x_2} \mathrm{d}x\,\overline{\mu}\,\frac{\partial R(\rho)}{\partial x} = \overline{\mu}\,(R(\rho_2) - R(\rho_1)), \tag{33a}$$

where x_α ($\alpha = 1, 2$) are chosen such that $\rho(x_\alpha) = \rho_\alpha$ and $\partial\rho(x_\alpha)/\partial x = 0$, and on the other hand

$$\begin{aligned}\int_{x_1}^{x_2} \mathrm{d}x\,\mu(\rho)\,\frac{\partial R(\rho)}{\partial x} &= \int_{x_1}^{x_2} \mathrm{d}x\,\mu_0(\rho)\frac{\partial R(\rho)}{\partial x} + \int_{x_1}^{x_2} \mathrm{d}x\left[\lambda(\rho)\left(\frac{\partial\rho}{\partial x}\right)^2 - \kappa(\rho)\frac{\partial^2\rho}{\partial x^2}\right]\frac{\partial R(\rho)}{\partial x}\\ &= \int_{x_1}^{x_2} \mathrm{d}x\,\frac{\partial\Phi(R(\rho))}{\partial R}\frac{\partial R(\rho)}{\partial x} + \int_{x_1}^{x_2} \mathrm{d}x\,\frac{\partial}{\partial x}\left(-\frac{\kappa(\rho)}{2}R'(\rho)\left(\frac{\partial\rho}{\partial x}\right)^2\right)\\ &= \Phi(R(\rho_2)) - \Phi(R(\rho_1)),\end{aligned} \tag{33b}$$

where we have used (31) and (32) in the first to second line, and where the second integral cancels from the second to the third line since the gradients $\partial\rho/\partial x$ cancel at x_1 and x_2 by construction. We put (33a) and (33b) together to write

$$\overline{\mu}\,(R(\rho_2) - R(\rho_1)) = \Phi(R(\rho_2)) - \Phi(R(\rho_1)) \Leftrightarrow R(\rho_1)\mu(\rho_1) - \Phi(R(\rho_1)) = R(\rho_2)\mu(\rho_2) - \Phi(R(\rho_2)), \tag{34}$$

which is similar to the “equal-intercept” equilibrium condition (16b).

This concludes our demonstration that current-free steady-state phase separation spontaneous emerges in our field theory of self-propelled particles (22), provided that densities ρ_1 and ρ_2 satisfy the generalised common-tangent construction given by (29) and (34). This phase separation emerges solely from the competition between the self-propulsion of individual agents and the decrease of their velocity in crowded environment (via repulsive or quorum-sensing interactions), and is termed *motility-induced phase separation* (MIPS) [2].

III. PROBLEMS

III.A. Fluctuation-dissipation theorem

We will consider two scalar field theories, first for a non-conserved field ψ ("Model A"),

$$\dot{\psi} = -\Gamma \frac{\delta F}{\delta \psi} + \nu \Lambda, \tag{35}$$

and second for a conserved field ρ ("Model B"),

$$\dot{\rho} = -\nabla \cdot \boldsymbol{J}, \tag{36a}$$

$$\boldsymbol{J} = -\beta \rho D \nabla \frac{\delta F}{\delta \rho} + \nu \boldsymbol{\Lambda}, \tag{36b}$$

where $\boldsymbol{\Lambda}$ is a zero-mean unit-variance Gaussian white noise, such that the probability of a given spatial and temporal realisation of this noise, *forward* in time between time t_1 and time t_2, is

$$\mathrm{Prob}_{\rightarrow}[\boldsymbol{\Lambda}] = \mathcal{N}_{\Lambda} \exp\left(-\frac{1}{2}\int \mathrm{d}\boldsymbol{r} \int_{t_1}^{t_2} \mathrm{d}t\, |\boldsymbol{\Lambda}(\boldsymbol{r},t)|^2\right), \tag{37}$$

and Λ is the one-dimensional version of vector $\boldsymbol{\Lambda}$.

1. Show that the probability of a given *forward* realisation of ψ in Model A (35) is given by

$$\mathrm{Prob}_{\rightarrow}[\psi] = \mathcal{N}_{\psi} \exp\left(-\frac{1}{2\nu^2}\int \mathrm{d}\boldsymbol{r} \int_{t_1}^{t_2} \mathrm{d}t\, \left(\dot{\psi}(\boldsymbol{r},t) + \Gamma \frac{\delta F}{\delta \psi}(\boldsymbol{r},t)\right)^2\right). \tag{38}$$

2. Under time reversal ($t \rightarrow -t$), time derivatives are negated while field variables remain unchanged. Show that the probability of a given *backward* realisation of ψ (*i.e.* under time reversal) in Model A (35) is given by

$$\mathrm{Prob}_{\leftarrow}[\psi] = \mathcal{N}_{\psi} \exp\left(-\frac{1}{2\nu^2}\int \mathrm{d}\boldsymbol{r} \int_{t_1}^{t_2} \mathrm{d}t\, \left(-\dot{\psi}(\boldsymbol{r},t) + \Gamma \frac{\delta F}{\delta \psi}(\boldsymbol{r},t)\right)^2\right). \tag{39}$$

3. We assume detailed balance thus, with ψ_1 and ψ_2 the initial and final states in the forward realisation of ψ, we have

$$\mathrm{Prob}_{\mathrm{B}}[\psi_1]\, \mathrm{Prob}_{\rightarrow}[\psi] = \mathrm{Prob}_{\mathrm{B}}[\psi_2]\, \mathrm{Prob}_{\leftarrow}[\psi], \tag{40}$$

where $\mathrm{Prob}_{\mathrm{B}}$ is the Boltzmann distribution (7). Using this relation, show that, in Model A (35),

$$\frac{\mathrm{Prob}_{\mathrm{B}}[\psi_2]}{\mathrm{Prob}_{\mathrm{B}}[\psi_1]} = \exp\left(-\frac{2\Gamma}{\nu^2}\int \mathrm{d}\boldsymbol{r} \int_{t_1}^{t_2} \mathrm{d}t\, \dot{\psi}(\boldsymbol{r},t) \frac{\delta F}{\delta \psi}(\boldsymbol{r},t)\right) = \exp(-\beta\,(F[\psi_2] - F[\psi_2])), \tag{41}$$

where $F[\psi_1]$ and $F[\psi_2]$ are the free energy at the initial and final states of the forward realisation of ψ.

4. Using (41) and the following relation

$$\int \mathrm{d}\boldsymbol{r}\, \dot{\psi}(\boldsymbol{r},t) \frac{\delta F}{\delta \psi}(\boldsymbol{r},t) = \frac{\mathrm{d}F}{\mathrm{d}t}, \tag{42}$$

show that the amplitude ν of the noise in Model A (35) satisfies the following fluctuation-dissipation theorem

$$\nu = \sqrt{2\Gamma/\beta}. \tag{43}$$

5. Show, using the same procedure as above, that the noise amplitude in Model B (36) satisfies the following fluctuation-dissipation theorem

$$\nu = \sqrt{2\rho D}, \tag{44}$$

as we have assumed in the lecture (8a).

III.B. Entropy production rate

We define the entropy production rate of a process ψ from the ratio of probabilities of its forward and backward realisations over a time $\tau = t_2 - t_1$ (using the notations of problem III.A),

$$\dot{s} = \frac{1}{\tau} \log \frac{\mathrm{Prob}_{\rightarrow}[\psi]}{\mathrm{Prob}_{\leftarrow}[\psi]}, \tag{45a}$$

and its steady state value

$$\dot{\sigma} = \lim_{\tau\to\infty} \langle \dot{s} \rangle \,. \tag{45b}$$

This definition translates the idea that the entropy indicates the arrow of time: when $\dot{s} > 0$ then the forward process is more probable and its backward counterpart. It also translates that equilibrium phenomena, where $\dot{s} = 0$, are statistically identical when looked forward or backward.

1. Under the assumptions of (i) detailed balance (40), (ii) the system obeying the Boltzmann distribution (7), and (iii) the free energy F being bounded, show that the entropy production rate cancels $\dot{\sigma} = 0$.

2. Consider a single particle, with equation of motion

$$\zeta \boldsymbol{v} = -\nabla U + \boldsymbol{F}_{\mathrm{ext}} + \nu\, \boldsymbol{\eta}, \tag{46}$$

where ζ is a drag coefficient, $\boldsymbol{v}$ the velocity of the particle, U a potential energy, $\boldsymbol{F}_{\mathrm{ext}}$ an external force, ν a noise amplitude, and $\boldsymbol{\eta}$ is a zero-mean unit-variance Gaussian white noise. Show that the steady state entropy production rate of this process depends only on the steady state mechanical power generated by the external force,

$$P = \lim_{\tau\to\infty} \left\langle \frac{1}{\tau} \int_t^{t+\tau} \mathrm{d}t\, \boldsymbol{v}(t) \cdot \boldsymbol{F}_{\mathrm{ext}}(t) \right\rangle . \tag{47}$$

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IV. SOLUTIONS

IV.A. Fluctuation-dissipation theorem

1. We rewrite (35) as

$$\Lambda = \frac{1}{\nu}\left[\dot{\psi} + \Gamma\frac{\delta F}{\delta\psi}\right], \tag{48}$$

and subsequently (37) as

$$\begin{aligned}\mathrm{Prob}_{\rightarrow}[\Lambda] &= \mathcal{N}_\Lambda\,\exp\left(-\frac{1}{2}\int \mathrm{d}\boldsymbol{r}\int_{t_1}^{t_2}\mathrm{d}t\,|\Lambda(\boldsymbol{r},t)|^2\right)\\ &= \mathcal{N}_\Lambda\,\exp\left(-\frac{1}{2\nu^2}\int \mathrm{d}\boldsymbol{r}\int_{t_1}^{t_2}\mathrm{d}t\,\left[\dot{\psi}(\boldsymbol{r},t) + \Gamma\frac{\delta F}{\delta\psi}(\boldsymbol{r},t)\right]^2\right).\end{aligned} \tag{49}$$

Since the trajectory of ψ is uniquely determined by the realisation of the noise, (49) also corresponds to the probability of the trajectory and we write

$$\mathrm{Prob}_{\rightarrow}[\psi] = \mathcal{N}_\psi\,\exp\left(-\frac{1}{2\nu^2}\int \mathrm{d}\boldsymbol{r}\int_{t_1}^{t_2}\mathrm{d}t\,\left[\dot{\psi}(\boldsymbol{r},t) + \Gamma\frac{\delta F}{\delta\psi}(\boldsymbol{r},t)\right]^2\right). \tag{50}$$

2. Computing the probability of the backward trajectory is computing the probability that our realisation of the noise leads to the same spatial trajectory but with negated temporal derivatives. We should thus note that $\Gamma(\delta F/\delta\psi)$ only depends on the instantaneous spatial profile of ψ, while $\dot{\psi}(\boldsymbol{r},t)$ is a time-derivative of this profile. We then compute the probability of the backward trajectory from (50) by negating the first term in squared brackets and keeping the second one identical,

$$\mathrm{Prob}_{\leftarrow}[\psi] = \mathcal{N}_\psi\,\exp\left(-\frac{1}{2\nu^2}\int \mathrm{d}\boldsymbol{r}\int_{t_1}^{t_2}\mathrm{d}t\,\left[-\dot{\psi}(\boldsymbol{r},t) + \Gamma\frac{\delta F}{\delta\psi}(\boldsymbol{r},t)\right]^2\right). \tag{51}$$

3. We compute the ratio of (50) and (51),

$$\begin{aligned}\frac{\mathrm{Prob}_{\rightarrow}[\psi]}{\mathrm{Prob}_{\leftarrow}[\psi]} &= \exp\left(-\frac{1}{2\nu^2}\int \mathrm{d}\boldsymbol{r}\int_{t_1}^{t_2}\mathrm{d}t\,\left(\left[\dot{\psi}(\boldsymbol{r},t) + \Gamma\frac{\delta F}{\delta\psi}(\boldsymbol{r},t)\right]^2 - \left[-\dot{\psi}(\boldsymbol{r},t) + \Gamma\frac{\delta F}{\delta\psi}(\boldsymbol{r},t)\right]^2\right)\right)\\ &= \exp\left(-\frac{1}{2\nu^2}\int \mathrm{d}\boldsymbol{r}\int_{t_1}^{t_2}\mathrm{d}t\,4\Gamma\,\dot{\psi}(\boldsymbol{r},t)\frac{\delta F}{\delta\psi}(\boldsymbol{r},t)\right),\end{aligned} \tag{52}$$

and from detailed balance (40) and the definition of the Boltzmann distribution (7),

$$\frac{\mathrm{Prob}_{\rightarrow}[\psi]}{\mathrm{Prob}_{\leftarrow}[\psi]} = \frac{\mathrm{Prob}_{\mathrm{B}}[\psi_2]}{\mathrm{Prob}_{\mathrm{B}}[\psi_1]} = \exp(-\beta(F[\psi_2] - F[\psi_1])). \tag{53}$$

4. We use relations (42) and (52) to write

$$\frac{\mathrm{Prob}_{\rightarrow}[\psi]}{\mathrm{Prob}_{\leftarrow}[\psi]} = \exp\left(-\frac{2\Gamma}{\nu^2}\int_{t_1}^{t_2}\mathrm{d}t\,\frac{\mathrm{d}F}{\mathrm{d}t}\right) = \exp\left(-\frac{2\Gamma}{\nu^2}(F(t_2) - F(t_1))\right) = \exp\left(-\frac{2\Gamma}{\nu^2}(F[\psi_2] - F[\psi_1])\right), \tag{54}$$

which by comparison with (53) leads to

$$\frac{2\Gamma}{\nu^2} = \beta, \tag{55}$$

which is equivalent to (43).

5. In order to adapt the above procedure to Model B (36), we write the equivalent of (48),

$$\mathbf{\Lambda} = \frac{1}{\nu}\left(\boldsymbol{J} + \beta\rho D\nabla\frac{\delta F}{\delta\rho}\right), \tag{56}$$

therefore we have the forward trajectory probability

$$\mathrm{Prob}_{\rightarrow}[\rho] = \mathcal{N}_\rho\,\exp\left(-\frac{1}{2\nu^2}\int \mathrm{d}\boldsymbol{r}\int_{t_1}^{t_2}\mathrm{d}t\,\left|\boldsymbol{J} + \beta\rho D\nabla\frac{\delta F}{\delta\rho}\right|^2\right). \tag{57}$$

Under time reversal, $t \to -t$, the time derivative of the order parameter $\dot\rho$ is negated, thus its flux $\boldsymbol{J}$ is also negated. On the contrary, the gradient of the chemical potential $\nabla(\delta F/\delta\rho)$ only depends on the instantaneous spatial profile of ρ and thus keeps the same sign. We thus write

$$\mathrm{Prob}_{\leftarrow}[\rho] = \mathcal{N}_\rho\,\exp\left(-\frac{1}{2\nu^2}\int \mathrm{d}\boldsymbol{r}\int_{t_1}^{t_2}\mathrm{d}t\,\left|-\boldsymbol{J} + \beta\rho D\nabla\frac{\delta F}{\delta\rho}\right|^2\right). \tag{58}$$

We take the ratio of (58) and (58),

$$\frac{\mathrm{Prob}_{\rightarrow}[\rho]}{\mathrm{Prob}_{\leftarrow}[\rho]} = \exp\left(-\frac{2\beta\rho D}{\nu^2}\int \mathrm{d}\boldsymbol{r}\int_{t_1}^{t_2}\mathrm{d}t\,\boldsymbol{J}\cdot\nabla\frac{\delta F}{\delta\rho}\right), \tag{59}$$

in which we compute

$$\int \mathrm{d}\boldsymbol{r}\int_{t_1}^{t_2}\mathrm{d}t\,\boldsymbol{J}\cdot\nabla\frac{\delta F}{\delta\rho} = -\int \mathrm{d}\boldsymbol{r}\int_{t_1}^{t_2}\mathrm{d}t\,(\nabla\cdot\boldsymbol{J})\frac{\delta F}{\delta\rho} = \int \mathrm{d}\boldsymbol{r}\int_{t_1}^{t_2}\mathrm{d}t\,\dot\rho\frac{\delta F}{\delta\rho} = F(t_2) - F(t_1) = F[\rho_2] - F[\rho_1], \tag{60}$$

where we have integrated by part in space while assuming that the flux $\boldsymbol{J}$ cancels at infinity, and where we have also used (42). The ratio of forward and backward probabilities using detailed balance remains identical. Therefore, by comparing (53) and (59) using (60), we obtain

$$\frac{2\beta\rho D}{\nu^2} = \beta, \tag{61}$$

which is equivalent to (44).

IV.B. Entropy production rate

1. We have shown from detailed balance and the definition of the Boltzmann distribution that the ratio of forward and backward trajectory probabilities is related to the variation of free energy (53), therefore

$$\dot s = \frac{1}{\tau}\log\exp(-\beta(F(t+\tau) - F(t))) = \frac{\beta}{\tau}(F(t) - F(t+\tau)). \tag{62}$$

We assume that the free energy is bounded, therefore

$$|F(t) - F(t+\tau)| < C, \tag{63}$$

where C is some constant. This means that

$$|\dot\sigma| = \left|\lim_{\tau\to\infty}\frac{\beta}{\tau}(F(t) - F(t+\tau))\right| < \lim_{\tau\to\infty}\frac{C}{\tau} = 0, \tag{64}$$

and thus the steady state entropy production rate cancels $\dot\sigma = 0$.

2. We rewrite the equation of motion (46) as

$$\boldsymbol{\eta} = \frac{1}{\nu}\left(\zeta\boldsymbol{v}(t) + \nabla U(t) - \boldsymbol{F}_{\mathrm{ext}}(t)\right). \tag{65}$$

Using (37), and similarly to (50) and (58), we write the forward trajectory probability

$$\mathrm{Prob}_{\rightarrow} = \mathcal{N}\,\exp\left(-\frac{1}{2\nu^2}\int_t^{t+\tau}\mathrm{d}t\,\left(\zeta\boldsymbol{v}(t)+\nabla U(t)-\boldsymbol{F}_{\mathrm{ext}}(t)\right)^2\right). \tag{66}$$

Under time reversal, $t \to -t$, the velocity is negated but the force deriving from the potential and the external force are not, therefore we write the backward trajectory probability

$$\mathrm{Prob}_{\leftarrow} = \mathcal{N}\,\exp\left(-\frac{1}{2\nu^2}\int_t^{t+\tau}\mathrm{d}t\,\left(-\zeta\boldsymbol{v}(t)+\nabla U-\boldsymbol{F}_{\mathrm{ext}}(t)\right)^2\right). \tag{67}$$

We can now compute the entropy production rate,

$$\begin{aligned}\dot{s} &= \frac{1}{\tau}\log\exp\left(-\frac{1}{2\nu^2}\int_t^{t+\tau}\mathrm{d}t\,\left[\left(\zeta\boldsymbol{v}(t)+\nabla U(t)-\boldsymbol{F}_{\mathrm{ext}}(t)\right)^2-\left(-\zeta\boldsymbol{v}(t)+\nabla U(t)-\boldsymbol{F}_{\mathrm{ext}}(t)\right)^2\right]\right)\\ &= -\frac{1}{\tau}\frac{2\zeta}{\nu^2}\int_t^{t+\tau}\mathrm{d}t\,\boldsymbol{v}(t)\cdot\left(\nabla U(t)-\boldsymbol{F}_{\mathrm{ext}}(t)\right)\end{aligned} \tag{68a}$$

where we note that $\boldsymbol{v}(t)\cdot\nabla U(t) = \mathrm{d}U/\mathrm{d}t$ since U is a potential energy and thus only depends on time through its dependence on the position, therefore

$$\begin{aligned}\dot{s} &= -\frac{2\zeta}{\tau\nu^2}\left[\int_t^{t+\tau}\mathrm{d}t\,\frac{\mathrm{d}U(t)}{\mathrm{d}t}-\int_t^{t+\tau}\mathrm{d}t\,\boldsymbol{v}(t)\cdot\boldsymbol{F}_{\mathrm{ext}}(t)\right]\\ &= \frac{1}{\tau}\frac{2\zeta}{\nu^2}\left(U(t)-U(t+\tau)\right)+\frac{1}{\tau}\frac{2\zeta}{\nu^2}\int_t^{t+\tau}\mathrm{d}t\,\boldsymbol{v}(t)\cdot\boldsymbol{F}_{\mathrm{ext}}(t),\end{aligned} \tag{68b}$$

where the first term cancels in the limit $\tau \to \infty$ if the variations of U are bounded, and thus

$$\dot{\sigma} = \frac{2\zeta}{\nu^2}\lim_{\tau\to\infty}\left\langle\frac{1}{\tau}\int_t^{t+\tau}\mathrm{d}t\,\boldsymbol{v}(t)\cdot\boldsymbol{F}_{\mathrm{ext}}(t)\right\rangle = \frac{2\zeta}{\nu^2}P. \tag{69}$$