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Nonequilibrium Field Theories and Stochastic Dynamics
Sheet 10

Exercise 27 – Binodal Construction in Model B

In this exercise, we will analyze the conditions for two different phases (+ and −) to coexist, within one volume where the two phases "touch" each other at the interface. You can think of water and steam, where the liquid phase has a much higher density (ϕ_+) than the steam phase (ϕ_-). We assign the system the total free energy

$$F[\phi] = \int_V dx \left(f(\phi) + \frac{1}{2} D (\nabla \phi)^2 \right) , \tag{1}$$

with an interfacial penalty coefficient $D = \text{const.}$ and the local free energy $f(\phi)$ given by

$$f(\phi) = a\phi^2 + b\phi^4 \, . \tag{2}$$

with $a < 0$ and $b > 0$.

a) Sketch the free energy density $f(\phi)$ for $b = -a = 1$ and argue where the thermodynamically stable values of ϕ are located.

Suppose the system phase separates into two uniform regions (phases) with values ϕ_+ and ϕ_-, occupying fractions V_+ and V_- of the total volume V, respectively. Note that the total average density $\bar{\phi} = (V_+\phi_+ + V_-\phi_-)/V$ is constant throughout relaxational processes, due to mass conservation.

b) Write down an expression for the total free energy of the system, assuming that the interfaces between the two phases can be neglected compared to the bulk contributions. Formulate the problem of minimizing the free energy subject to the constraint of total mass conservation using a Lagrange multiplier.

c) By minimizing the total free energy with respect to ϕ_+, ϕ_-, and V_+, derive the two thermodynamic equilibrium conditions:

$$\mu(\phi_+) = \mu(\phi_-), \qquad \Pi(\phi_+) = \Pi(\phi_-), \tag{3}$$

where $\mu = df/d\phi$ and $\Pi = \phi\mu - f(\phi)$. Explain why, in a thermodynamic sense, the quantity μ can be understood as a chemical potential and Π as a pressure.

Hint: Recall the first law of termodynamics in differential form. Furthermore, the free energy is a thermodynamic potential, and thus it is extensive.

d) The dynamics of the mass-conserving field ϕ is determined by approaching the minima of its free energy:

$$\partial_t \phi(x,t) = -\nabla \cdot J \, , \tag{4}$$

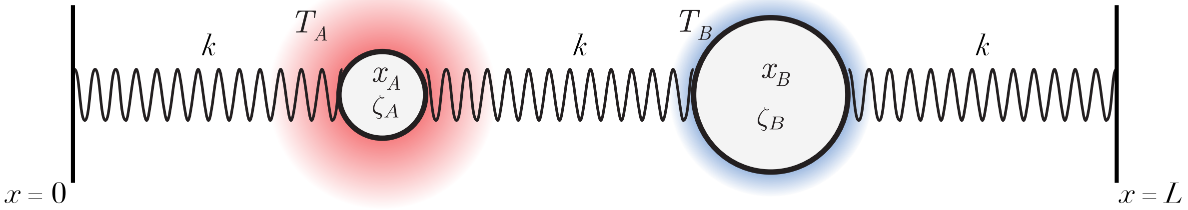
$$J = -\nabla \frac{\delta F}{\delta \phi(x,t)} \, . \tag{5}$$

Show that the same thermodynamic conditions are obtained from the steady-state solution of ϕ, i.e. from $\partial_t \phi = 0$. Interpret the resulting condition graphically and explain geometrically how it corresponds to phase coexistence.

Hint: You can simplify the analysis by only considering 1D space. Also, you do not have to solve for the steady-state density profile $\phi(x)$ to obtain the thermodynamic conditions that have to hold in steady state.

e) Using the form of $f(\phi)$ above, write the system of equations that must be solved to find the binodal points ϕ_+ and ϕ_-. Are these the same for the simple example form exercise part **a)**? What is special about the geometric construction you derived earlier for this particular choice of $f(\phi)$?

Exercise 28 – Brownian dynamics of two coupled particles at different temperatures



Consider a one-dimensional system which consists of two different, coupled particles A and B at positions x_A, x_B, respectively. Each of these particles has two properties, a friction constant $\zeta_{A/B}$ and an individual temperature $T_{A/B}$ (assume for the moment that "temperature" is now defined as a local quantity). The particles are coupled with identical springs (spring constant k) to each other and to the walls (see figure). All springs have the same rest length of $L/3$, where L is the distance between the walls.

a)

- Write down the Langevin equations for both particles in the overdamped limit.
- Make a transformation into the frame of eigenmodes $x_A, x_B \to y_A, y_B$ (i.e. diagonalize the system).
- Compute the correlation of the noises in this frame. When are they uncorrelated?
- Compute the power spectrum of the new variables y_A and y_B, $\langle \tilde{\mathbf{y}}(\omega)\, \tilde{\mathbf{y}}^*(\omega)\rangle$.
- How can you recover the correlation functions of $\mathbf{y}$ (you don't have to do the actual calculation)? What do you expect? Interpret your results.

Having gained some analytic intuition, we now turn towards simulations of a similar system. To this end, consider the case where both particles are coupled to each other but not to the walls.

b)

- Write a simulation in python to simulate this model in two dimensions.
- Plot some sample trajectories of the center of friction. This is defined as $R = \frac{\zeta_A T_B}{\zeta_A T_B + \zeta_B T_A} x_A + \frac{\zeta_B T_A}{\zeta_A T_B + \zeta_B T_A} x_B$.
- Compute the mean-square displacement of the center of friction with and without temperature difference. What do you find? Interpret your results.

Hint: To simulate the Gaussian noise terms, you can use the Euler method. Alternatively, you can also draw random numbers from a uniform distribution as described in the following paper: `http://www.damtp.cam.ac.uk/user/hinch/publications/JFM282_373.pdf` (pages 376-378).

Exercise 29 – Linear Stability of the Keller–Segel Model

Consider the Keller–Segel model for chemotaxis. This model describes a coarse-grained density living cells which produce a chemical they are themselves attracted towards (a *chemoattractant*). The chemoattractant can decay over time, but the total number of cells is assumed to be constant. Both the cells and the chemicals can diffuse in space, leading to the following set of equations:

$$\frac{\partial \rho(x,t)}{\partial t} = D\nabla\left(\nabla\rho(x,t) - \chi\rho(x,t)\nabla c(x,t)\right), \tag{6}$$

$$\frac{\partial c(x,t)}{\partial t} = \alpha\rho(x,t) - \beta c(x,t) + D_c\nabla^2 c(x,t), \tag{7}$$

where

- $\rho(x,t)$ is the density of cells,
- $c(x,t)$ is the concentration of a chemoattractant,
- D and D_c are the diffusion coefficients for the cells and chemoattractant, respectively,
- $\chi > 0$ is the chemotactic sensitivity,
- α is the production rate of chemoattractant,

- β is the decay rate of chemoattractant.

a) Show that the system admits a spatially homogeneous steady state given by

$$\rho(x,t) = \rho_0, \qquad c(x,t) = c_0 = \frac{\alpha}{\beta}\rho_0 \,. \tag{8}$$

b) Perform a linear stability analysis of the homogeneous steady state. Consider small perturbations:

$$\rho(x,t) = \rho_0 + \delta\rho(x,t), \qquad c(x,t) = c_0 + \delta c(x,t), \tag{9}$$

and linearize the equations to first order in $\delta\rho$ and δc.

c)

Assume solutions of the form

$$\delta\rho(x,t) \sim e^{\sigma t} e^{ikx} \,,\, \delta c(x,t) \sim e^{\sigma t} e^{ikx} \tag{10}$$

and derive the dispersion relation $\sigma(k)$.

d) Determine the condition under which the homogeneous state becomes linearly unstable. That is, find the values of ρ_0 and χ (in terms of other parameters) for which $\mathrm{Re}(\sigma(k)) > 0$ for some $k \neq 0$. Plot and interpret your dispersion relation.

e) Discuss the physical interpretation of this instability in terms of chemotactic aggregation.

Your solutions should be handed in by uploading them to Moodle by **Wednesday, 9$^{\text{th}}$ July 2025, 10:00 am**.