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Nonequilibrium Field Theories and Stochastic Dynamics
Sheet 8

This sheet is intended to practice analyzing stochastic field theories exemplified in Model A, this time in the context of soft materials fluctuating in their shape.

Exercise 22 – Confined semiflexible polymer chain

Filamentous structures such as DNA stands, actin filaments and microtubules play a central role in cells to carry information, or give structural integrity to the cytoskeleton of eukaryotic cells, where they provide mechanical support, enable intracellular transport, and mediate force generation and shape changes. These biopolymers are semiflexible, meaning their mechanical response is governed by both bending elasticity and thermal fluctuations. A key question in understanding their behavior is how they fluctuate when confined—e.g., by narrow tubes, or the cellular cortex or molecular crosslinkers—and subjected to external forces or potentials. In this exercise, we explore the statistical properties of a simplified model: a polymer chain confined to a horizontal line.

Each position on the polymer's contour is parametrized by its projected position on the center line x (we assume that the polymer has no overhangs or loops, etc.). The distance of the polymer position to the central line at time t is denoted by $h(x, t)$ (see Fig. 1).

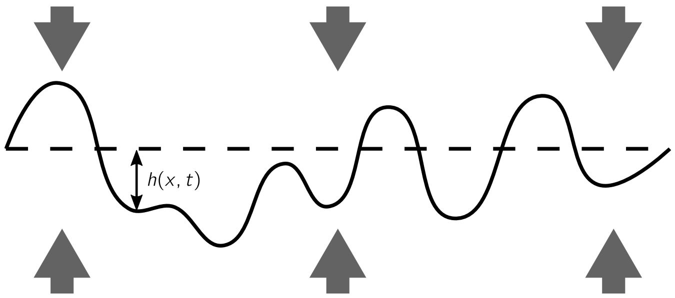

Figure 1: Sketch of a semi-flexible polymer in a harmonic potential. The distance from the minimum of the potential (dashed line) is given by $h(x, t)$, where x denotes the position along the center line.

The effective free energy functional $\mathcal{F}[h(x, t)]$ of the polymer is given by

$$\mathcal{F} = \int_{-\infty}^{\infty} \mathrm{d}x \left[\frac{\kappa}{2} \left(\frac{\partial^2 h(x,t)}{\partial x^2} \right)^2 + \frac{\gamma}{2} h(x,t)^2 \right], \tag{1}$$

we encourage you to confer Odijk, T.: *On the Statistics and Dynamics of Confined or Entangled Stiff Polymers*, Macromolecules, **16**, No. 8, (1983) ACS Publications.

a) Shortly explain the physical meaning of the two contributions in the free energy functional $\mathcal{F}$ and the effects they will have on a polymer. What is the meaning of γ? Briefly argue why Model A dynamics is sensible here (recall the connection between potential energy, force and velocity in the overdamped regime).

b) Write down the overdamped Langevin equation for the height field $h(x,t)$ in the form:

$$\partial_t h(x,t) = -\Gamma \frac{\delta \mathcal{F}}{\delta h(x,t)} + \eta(x,t), \tag{2}$$

where Γ is a kinetic (Onsager) coefficient and $\eta(x,t)$ is a stochastic noise term.

c) *Fluctuation–Dissipation Relation*

Determine the amplitude N of the correlator $\langle \eta(x,t)\eta(x',t')\rangle$ that ensures the system relaxes to thermal equilibrium at temperature T. Use the form $\langle \eta(x,t)\eta(x',t')\rangle = N\delta(t-t')\delta(x-x')$. Express the result in terms of Γ, k_B, and T.

d) *Scaling Argument for the Odijk Length*

Use a scaling argument for $\langle (\partial_x^2 h)^2\rangle$ to estimate the equilibrium deflection length λ, also known as the *Odijk length*, of the polymer, i.e., the distance over which the polymer bends under thermal fluctuations before being suppressed by the confining potential. To do so, balance the bending energy contribution in $\mathcal{F}$ and the harmonic confinement energy under the equipartition theorem to show that

$$\lambda \sim \left(\frac{\kappa}{\gamma}\right)^{1/4}. \tag{3}$$

e) *Fourier Representation of the Langevin Equation*

Expand $h(x,t)$ in Fourier modes:

$$h(x,t) = \int \frac{dk}{2\pi}\, \tilde{h}(k,t) e^{ikx},$$

and rewrite the Langevin equation in terms of $\tilde{h}(k,t)$. What is the equation of motion for each mode? Solve the resulting ODE. For a positive Γ, can you choose κ, γ of the sign you like?

f) *Dynamical Correlation Function*

Solve for the two-time correlation function:

$$C(k,k';t,t') = \langle \tilde{h}(k,t)\tilde{h}^*(k',t')\rangle - \langle \tilde{h}(k,t)\rangle\langle \tilde{h}^*(k',t')\rangle, \tag{4}$$

assuming the system is initially equilibrated, i.e. $\tilde{h}(k,0) = 0$. Express your result in terms of Γ, κ, γ, k, and T.

Hint: You should find:

$$C(k,k';t,t') = \frac{2\pi N}{2\lambda(k)} \left(e^{-\lambda(k)|t'-t|} - e^{-\lambda(k)(t'+t)}\right) \cdot \delta(k-k'). \tag{5}$$

g) *Equilibrium Limit*

Take the equal-time limit $t = t'$ of the correlation function above and consider it for $t = t' \to \infty$. Show that

$$\langle |\tilde{h}(k)|^2\rangle = 2\pi\delta(k-k') \frac{k_B T}{\kappa k^4 + \gamma}. \tag{6}$$

Comment on the behavior at small and large k.

h) *Limit of Vanishing Confinement*

Discuss what happens in the limit $\gamma \to 0$, i.e., the confinement is removed. How does the correlation function behave in this case, and what physical features of a free semiflexible filament does it reproduce?

Exercise 23 – Dynamics of phase boundaries

We continue our studies of height displacements of soft materials, this time, however, we consider the boundary between a liquid and a gas (either in 1 or 2D, so the dimension d is a parameter). The energy cost of deformations in the conformation of the boundary is due to the increased area and surface tension. Locally, it is given by

$$f_\sigma = \sigma\sqrt{1+\left(\nabla h\left(\boldsymbol{x},t\right)\right)^2} \tag{7}$$

with surface tension σ.

The total free energy is obtained by integrating the free energy density f_σ over the whole d-dimensional surface:

$$\mathcal{F}_\sigma = \int \mathrm{d}^d\boldsymbol{x} f_\sigma = \sigma\int \mathrm{d}^d\boldsymbol{x}\sqrt{1+\left(\nabla h\left(\boldsymbol{x},t\right)\right)^2}. \tag{8}$$

In the following we want to investigate the dynamics of such a water-air interface as sketched in figure 2 at finite temperatures.

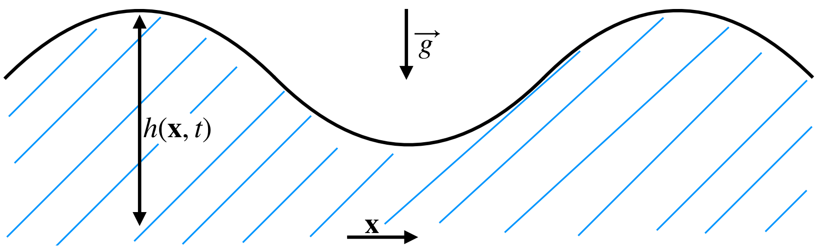

Figure 2: Sketch of the setup: $h(\boldsymbol{x},t)$ parametrizes the interface between water (bottom) and air (top). The zeroth order gravitational acceleration is perpendicular to the plane spanned by $\boldsymbol{x}$.

a) *Setting up the free energy*

To make the model more realistic, consider the effect of gravity and add a term, $\mathcal{E}_g$ which takes into account the gravitational potential energy. How does that term look like?

Furthermore, to ensure volume conservation of the water bulk, we need to add a Lagrange multiplier Λ, such that the resulting total free energy reads $\mathcal{F} = \mathcal{F}_\sigma + \mathcal{E}_g - \Lambda\int \mathrm{d}^d\boldsymbol{x}\; h\left(\boldsymbol{x},t\right)$.

Expand the total free energy $\mathcal{F}$ in orders of fluctuations of the height profile $\delta h\left(\boldsymbol{x},t\right) := h\left(\boldsymbol{x},t\right) - h_0$, where the fluctuations are assumed to be small, i.e. $|\delta h| \ll h_0$, and $|\nabla\delta h| \ll 1$.

The final free energy for the δh fluctuations up to including second order should read:

$$\mathcal{F} = \int \mathrm{d}^d\boldsymbol{x}\left[\frac{\sigma}{2}\left(\nabla\delta h\left(\boldsymbol{x},t\right)\right)^2 + P\delta h(\boldsymbol{x},t) + \frac{\rho g}{2}\delta h\left(\boldsymbol{x},t\right)^2\right] + \text{constant}, \tag{9}$$

where P is a parameter that you need to find, ρ is the density of water and g is the gravitational acceleration.

In the following, we are interested in the dynamics of $\delta h\left(\boldsymbol{x},t\right)$ only. As there is no danger of confusion, we will drop the δ to keep the notation clean.

b) *Deriving the Langevin equation*

We assume that the dynamics of the interface is governed by local restoring forces (gradient dynamics):

$$\partial_t h(\boldsymbol{x}, t) = -\Gamma \frac{\delta \mathcal{F}}{\delta h(\boldsymbol{x}, t)} + \xi(\boldsymbol{x}, t) \tag{10}$$

with Γ being a constant Onsager coefficient and $\xi(\boldsymbol{x}, t)$ a local stochastic force obeying:

$$\langle \xi(\boldsymbol{x}, t) \rangle = 0, \quad \langle \xi(\boldsymbol{x}, t)\, \xi(\boldsymbol{x'}, t') \rangle = 2D\delta(t - t')\, \delta^{(d)}(\boldsymbol{x} - \boldsymbol{x'}) \tag{11}$$

Show that the Langevin equation reads:

$$\partial_t h(\boldsymbol{x}, t) = -\Gamma \rho g\, h(\boldsymbol{x}, t) + \Gamma \sigma\, \nabla^2 h(\boldsymbol{x}, t) + \xi(\boldsymbol{x}, t) \tag{12}$$

Which value does the Lagrange multiplier Λ need to attain?
Hint: To infer the value of Λ, investigate the dynamics of the homogeneous solution $h(\boldsymbol{x}, t) = 0$ without noise.

c) *Solving the Langevin equation*

Since the Langevin equation is linear, it can be solved by Fourier analysis (also called a normal mode analysis). We again use the definition:

$$\tilde{g}(\boldsymbol{k}, t) = \int \mathrm{d}^d\boldsymbol{x}\, \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{x}} g(\boldsymbol{x}, t) \tag{13}$$

of the Fourier transform of a function $g(\boldsymbol{x}, t)$.
Show that:

$$\partial_t \tilde{h}(\boldsymbol{k}, t) = -\Gamma \left(\rho g + \sigma \boldsymbol{k}^2\right) \tilde{h}(\boldsymbol{k}, t) + \tilde{\xi}(\boldsymbol{k}, t) \tag{14}$$

with the noise amplitude in Fourier space obeying

$$\left\langle \tilde{\xi}(\boldsymbol{k}, t) \right\rangle = 0, \quad \left\langle \tilde{\xi}(\boldsymbol{k}, t)\, \tilde{\xi}(\boldsymbol{k'}, t') \right\rangle = 2D(2\pi)^d\, \delta(t - t')\, \delta^{(d)}(\boldsymbol{k} + \boldsymbol{k}') \tag{15}$$

For all further calculations, use an arbitrary initial condition $\tilde{h}(\boldsymbol{k}, 0)$.
Calculate the mean $\left\langle \tilde{h}(\boldsymbol{k}, t) \right\rangle$ and the variance $C_{\tilde{h}\tilde{h}}(\boldsymbol{k}, \boldsymbol{k}', t, t')$ of the fluctuations in Fourier space, where the variance $C_{\tilde{h}\tilde{h}}(\boldsymbol{k}, \boldsymbol{k}', t, t')$ is defined as:

$$C_{\tilde{h}\tilde{h}}(\boldsymbol{k}, \boldsymbol{k}', t, t') := \left\langle \left(\tilde{h}(\boldsymbol{k}, t) - \left\langle \tilde{h}(\boldsymbol{k}, t) \right\rangle\right) \left(\tilde{h}(\boldsymbol{k}', t') - \left\langle \tilde{h}(\boldsymbol{k}', t') \right\rangle\right) \right\rangle. \tag{16}$$

d) *Comparison to equilibrium system*

Find the value to which the equal-time variance $C_{\tilde{h}\tilde{h}}(\boldsymbol{k}, -\boldsymbol{k}, t, t)$ relaxes for $t \to \infty$.
Now, use the *equipartition theorem* on the correlator $\left\langle \tilde{h}(\boldsymbol{k}, \infty)\, \tilde{h}(\boldsymbol{k}', \infty) \right\rangle$ to relate the equilibrium value of $C_{\tilde{h}\tilde{h}}(\boldsymbol{k}, -\boldsymbol{k}, t, t)$ to the temperature and the inverse of the Gaussian kernel of the model.
This is the fluctuation dissipation theorem for the model. *Hint: rewrite the free energy in Fourier space and use that at equilibrium the probability of fluctuations is governed by the Boltzmann distribution $P\left(\tilde{h}(\boldsymbol{k}, t)\right) \propto \mathrm{e}^{-\beta\mathcal{F}}$ with the value of $\Lambda = \rho g h_0$.*

e) *Absence of gravity*

Now consider the time evolution of an interface in the absence of gravity ($g = 0$) starting from a flat interface in a system of size L in every dimension. The quantity we look at is again the average of the variance in real space, a measure for the interface width

$$w^2(L, t) := \frac{1}{L^d} \int \mathrm{d}^d\boldsymbol{x}\, \left(\langle h^2(\boldsymbol{x}, t) \rangle - \langle h \rangle^2\right). \tag{17}$$

Evaluate w^2 by going into Fourier-space and use the value of $C_{\tilde{h}\tilde{h}}(\boldsymbol{k}, -\boldsymbol{k}, t, t)$ obtained on part c). Specialize in the two limits for small time $t \ll t_\mathrm{s}$ and for large time $t \gg t_\ell$. How does the result scale with L depending on the dimension d? What does this tell you about the stability of interfaces? Interpret why the dimension $d = 2$ is special.

Note, to solve the integrals, you have to assume a minimal and a maximal wavelength that is allowed in the system. The minimal wavelength $2\pi/L$ is set by the system size, the upper limit is given by $2\pi/a$ where a is the minimal length scale in the system. You may think of it as of a lattice constant in solid state physics. In a more general sense, it is the length scale below which our field-theory does not hold anymore because other physical effects (like molecular dynamics) play a role. In any case $L \gg a$. Strictly, we would have to replace the Fourier transforms by Fourier series due to the finite domain. We assume that an approximate integral representation is still valid. We then only have to adapt the domain of integration to a shell restricting $|\boldsymbol{k}|$: $\int_{-\infty}^{\infty} k^{d-1}\, dk ... \rightarrow \int_{2\pi/L}^{2\pi/a} k^{d-1}\, dk ...$.

Your solutions should be handed in by uploading them to Moodle by **Wednesday,** $25^{\mathbf{th}}$ **June 2025, 10:00 am**.