Advanced Statistical Mechanics

Exercises

Theoretical Physics track, ICFP Master 2 program

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The sequence of sections follows the chapters of the lectures. Some of the problems will not be presented during the tutorials : 1.2, 2.6, 2.8, 6.1, 7.1, 7.2, 7.3. In addition, the October 2022 homework can be found in Sec. 8 and the January 2023 exam in Sec. 9 (neither will be solved in class). Solutions to the problems will be posted at the end of each chapter.

1 Statistical Dynamics and Markov Processes

1.1 Path statistics, Crooks and Jarzynski theorems

The physical picture you should have in mind here is the following: consider, for instance, a colloidal particle in some solvent. The particle is trapped at some location x_0 by optical tweezers. That location x_0 is controlled by an external operator. And now this external operator decides to shift x_0 in the course of time between $t = 0$ and $t = t_p$ (x_0 thus becomes time dependent). A protocol is simply the whole function $x_0(t)$, which varies from some initial value x_0^i to some final value x_0^f between 0 and t_p. Before $t = 0$ the system is in equilibrium around some value x_0^i. After $t = t_p$ the system will relax to equilibrium at a new value x_0^f. We want to unravel some interesting properties of the work done by the operator on the colloidal particle as the particle is dragged from x_0^i to x_0^f. At this stage, we do not want to enter the details of the practical applications. We adopt a rather a general approach based on a master equation for a system whose states are labeled by $\mathscr{C}$ (think of $\mathscr{C}$ as being the position of the colloidal particle). This problem is based on two papers by G. Crooks [12, 13] that shed a clear light on the result derived by C. Jarzynski [26] the year before within the framework of deterministic dynamics.

Consider a Markov process whose states are labeled by $\mathscr{C}$ and whose rates are $W(\mathscr{C} \to \mathscr{C}')$. We assume the system is initially in equilibrium with the distribution $P_{\text{eq}}(\mathscr{C}) = \mathrm{e}^{-\beta H(\lambda,\mathscr{C})+\beta F(\lambda)}$. Here λ refers to an external parameter that enters the energy $H(\lambda, \mathscr{C})$.

1. Show that the choice $W(\mathscr{C} \to \mathscr{C}') = \gamma \mathrm{e}^{-\frac{\beta}{2}(H(\lambda,\mathscr{C}')-H(\lambda,\mathscr{C}))}$ is consistent with detailed balance and is thus synonymous for equilibrium dynamics.

We now vary λ in the course of time (starting from the equilibirum state with $\lambda_i = \lambda_0 = \lambda(0)$ at time $t = 0$ and reaching $\lambda_f = \lambda_K$ before time t). We assume the rates take the same functional form as before, but the time dependence of λ renders these rates time dependent as well.

The system visits the sequence of states $\mathscr{C}_0, \mathscr{C}_1, \ldots, \mathscr{C}_K$ up until time t (this time t is sufficiently large for the protocol to have reached its final value at t_K at the latest). It stays in each of these states times $\tau_0, \tau_1, \ldots, \tau_K$. The system thus leaves state j for state $j+1$ at a time $t_{j+1} = \sum_{\ell=0}^{j} \tau_\ell$. We write λ_{j+1} the value of λ over the time interval $[t_j, t_{j+1}]$, and we define $r_j(\mathscr{C}_j)$ to be the corresponding escape rate from state $\mathscr{C}_j$.

2. Justify that the probability of a such a trajectory reads

$$\begin{aligned}\mathscr{P}[\text{traj}] =& P_{\text{eq}}(\mathscr{C}_0, \lambda_0) \prod_{j=0}^{K} \mathrm{d}\tau_j \mathrm{e}^{-\sum_{j=0}^{K} r_j(\mathscr{C}_j)\tau_j} \delta(t - \tau_0 - \ldots - \tau_K) \\ & \times \gamma^K \mathrm{e}^{-\frac{\beta}{2}\sum_{j=0}^{K-1}(H(\lambda_{j+1},\mathscr{C}_{j+1})-H(\lambda_{j+1},\mathscr{C}_j))}\end{aligned} \tag{2}$$

3. Consider now a time reversed trajectory in which one samples the initial state $\mathscr{C}_K$ from the same equilibrium distribution and one applies the time-reversed protocol (this means that one starts from an equilibrated system with λ_f). Show that

$$\begin{aligned}\mathscr{P}[\text{traj}^{\text{R}}] =& P_{\text{eq}}(\mathscr{C}_K,\lambda_K)\prod_{j=0}^{K}\text{d}\tau_j \text{e}^{-\sum_{j=0}^{K} r_j(\mathscr{C}_j)\tau_j}\delta(t-\tau_0-\ldots-\tau_K) \\ &\times \gamma^K \text{e}^{-\frac{\beta}{2}\sum_{j=0}^{K-1}(H(\lambda_{j+1},\mathscr{C}_j)-H(\lambda_{j+1},\mathscr{C}_{j+1}))}\end{aligned} \tag{4}$$

4. Let $\bar{Q}[\text{traj}] = \ln\frac{\mathscr{P}[\text{traj}]}{\mathscr{P}[\text{traj}^{\text{R}}]}$. Show that

$$\bar{Q}[\text{traj}] = \beta(F(\lambda(0)-F(\lambda(t))+\beta(H(\lambda(t),\mathscr{C}_K)-H(\lambda(0),\mathscr{C}_0))-\beta\sum_{j=0}^{K-1}\left[H(\lambda_{j+1},\mathscr{C}_{j+1})-H(\lambda_{j+1},\mathscr{C}_j)\right] \tag{8}$$

5. We split the energy difference $H(\lambda_K,\mathscr{C}_K)-H(\lambda_0,\mathscr{C}_0)$ into

$$H(\lambda(t),\mathscr{C}_K)-H(\lambda(0),\mathscr{C}_0) = \sum_{j=0}^{K-1}(H(\lambda_{j+1},\mathscr{C}_{j+1})-H(\lambda_{j+1},\mathscr{C}_j))+\sum_{j=0}^{K-1}(H(\lambda_{j+1},\mathscr{C}_j)-H(\lambda_j,\mathscr{C}_j)) \tag{10}$$

After you have checked this identity, what physical meaning would you endow each of these sums with? Which of these would you call the work W exerted by the operator on the system?

6. Why do we have that $W[\text{traj}] = -W[\text{traj}^{\text{R}}]$?

7. Using the Evans-Searles theorem, namely that $P(\bar{Q}) = P(-\bar{Q})\text{e}^{\bar{Q}}$, show that $P(W) = P(-W)\text{e}^{\beta W-\beta\Delta F}$, where ΔF is the free-energy variation between equilibrium states with $\lambda(0)$ and $\lambda(t)$ (you can also prove this identity directly). This is Crooks' theorem.

8. In standard thermodynamics one knows that for an isothermal process $T\Delta S = \Delta U - \Delta F$, with $\Delta U = Q+W$. Idendify trajectory-dependent quantities ΔS, Q and W that somehow extend this thermodynamic identity to the level of individual trajectories.

9. In an actual experiment, it is possible to measure W and by repeating the experiment again and again, one can access a histogram of W, and a similar one for the time-reversed protocol. In practice, one plots $P(W)$ (from the direct protocol) and $P(-W)$ (from the time reversed protocol). These curves cross at some specific value W. Which?

10. Prove Jarzynski's equality: $\langle \text{e}^{-\beta W}\rangle = \text{e}^{-\beta\Delta F}$ by using Crook's theorem.

11. Show that this implies that $\langle W\rangle \geq \Delta F$. What is the physical meaning of this inequality?

1.2 A solvable master equation and dynamical complexity

A physical system with states $\mathscr{C}$ has its time evolution described by a master equation. The rate of hopping from configuration $\mathscr{C}$ to configuration $\mathscr{C}'$ is $W(\mathscr{C} \to \mathscr{C}')$ and we define $r(\mathscr{C}) = \sum_{\mathscr{C}'} W(\mathscr{C} \to \mathscr{C}')$.

1. What is the meaning of $r(\mathscr{C})$?

2. Write the master equation for the probability $P(\mathscr{C}, t)$ that the system is in state $\mathscr{C}$ at time t. What is the equation verified by the stationary distribution $Q(\mathscr{C})$?

3. The system is assumed to be in its stationary state. Let a history of the system taking place over the time interval $[0, t]$ during which the system visits K states $\mathscr{C}_1, \ldots, \mathscr{C}_K$ starting from $\mathscr{C}_0$. These are not necessarily distinct. What is the probability to observe that history?

4. Prove that the Shannon entropy per unit time h_{KS} for the probability over histories is given by $h_{\text{KS}} = -\sum_{\mathscr{C},\mathscr{C}'} W(\mathscr{C} \to \mathscr{C}') \ln \frac{W(\mathscr{C}\to\mathscr{C}')}{r(\mathscr{C})} Q(\mathscr{C})$.

5. For the very specific choice $W(\mathscr{C} \to \mathscr{C}') = Q(\mathscr{C}')$ is Q an equilibrium distribution? Give the corresponding expression for h_{KS} and comment upon your result.

6. The evolution operator for the master equation has elements $\mathbb{W}_{\mathscr{C},\mathscr{C}'} = W(\mathscr{C}' \to \mathscr{C}) - r(\mathscr{C})\delta_{\mathscr{C},\mathscr{C}'}$. Rewrite the master equation with the choice of rates proposed in question 5 and solve for $P(\mathscr{C}, t)$ using a given initial distribution $P(\mathscr{C}, 0) = P_{\text{init}}(\mathscr{C})$. What are the eigenvalues of $\mathbb{W}$? Can you say anything about their multiplicity?

7. Let $A(\mathscr{C})$ be an arbitrary observable. Express $\langle A\rangle(t)$ in terms of the initial average $\langle A\rangle_0$, of the final stationary average $\langle A\rangle_Q$, and of time t.

8. Think of $\mathscr{C}$ as a spin configuration in an Ising ferromagnet (in space dimension $d = 3$). And let $A(\mathscr{C})$ stand for the magnetization in that configuration $\mathscr{C}$. And of course $Q(\mathscr{C}) = Z^{-1}\mathrm{e}^{-\beta E(\mathscr{C})}$ is the canonical distribution. As the critical temperature is approached, do you think that the dynamics in question 5 would lead to a critical slowing down?

1.3 On the number of hops of a Markov process

Over a given time window $[0, t_{\text{obs}}]$ a time-realization of Markov process (whose evolution is governed by a master equation with rates $W(\mathscr{C} \to \mathscr{C}')$) changes configuration K times. The number $K(t_{\text{obs}})$ is itself a random variable. We will discuss a few properties of the distribution of K.

1. Denoting by $\langle \ldots \rangle$ an average in the steady-state of the process, show that $\lim_{t\to+\infty} \frac{\langle K(t)\rangle}{t} = \langle f(\mathscr{C})\rangle$, where f is a configuration-dependent quantity that will be specified.

2. Write a master equation for the probability $P(\mathscr{C}, K, t)$ that the system is in state $\mathscr{C}$ at time t and that it has witnessed K hops up until that time.

3. Let $\hat{P}(\mathscr{C}, z, t) = \sum_K \mathrm{e}^{-zK} P(\mathscr{C}, K, t)$. Show that $\hat{P}$ evolves according to

$$\partial_t \hat{P} = \mathbb{W}(z)\hat{P} + \boldsymbol{\lambda}(z)\hat{P} \tag{29}$$

where $\boldsymbol{\lambda}(z)$ is a diagonal matrix with elements $\lambda(\mathscr{C}, z) = (\mathrm{e}^{-z}-1)r(\mathscr{C})$, and where $\mathbb{W}(z)$ is a *stochastic* operator whose elements will be given. While $\hat{P}$ is not a probability, its evolution equation can nevertheless be interpreted in terms of population dynamics. Explicitly phrase that interpretation. Is there any practical consequence?

4. Consider a random walker on a one-dimensional lattice with L sites (and a unit lattice spacing), hopping left or right with unit rate. Its initial condition is uniform on the lattice. Show that $P(K, t)$ is a Poisson distribution?

5. Find a simple model for which $P(K, t)$ is not a Poisson distribution.

2 Stochastic dynamics

2.1 Recipe for a Gaussian white noise

This is an exercise from Van Kampen's book [41]. The goal of this exercise is to show that a Gaussian white noise can be seen as the limiting process of a family of continuous time random signals. We consider a Poisson distribution of time points t_i over some time interval with density ν. Each t_i is a uniform random variable over the time axis. Let the c_i be identically distributed independent random numbers, with zero average and finite moments, associated to each t_i. Finally, let $\psi(t)$ be a nonnegative function such that $\int \mathrm{d}x \psi(x) = 1$. We consider the random process

$$x(t) = \frac{1}{\sqrt{\nu}} \sum_i c_i \frac{1}{\tau} \psi\left(\frac{t - t_i}{\tau}\right) \tag{32}$$

1. Let ξ be a Gaussian white noise with zero mean and correlations $\langle \xi(t)\xi(t') \rangle = \sigma^2 \delta(t - t')$. Recall the expression of the generating functional $Z[h] = \langle \mathrm{e}^{-\int \mathrm{d}t h(t)\xi(t)} \rangle$ for an arbitrary function h.

2. Prove that in the

$$\tau \to 0, \qquad \nu \to \infty \tag{34}$$

limit, the process $x(t)$ is a Gaussian white noise. It may be useful to first determine the generating functional of $x(t)$.

2.2 Differential calculus likes Stratonovich discretization

Consider a Langevin equation $\frac{\mathrm{d}x}{\mathrm{d}t} = A + B\xi$, where ξ is a Gaussian white noise with correlations $\langle \xi(t)\xi(t')\rangle = \delta(t-t')$. The multiplicative noise B is understood with the α discretization rule, namely according to

$$\Delta x = x(t+\Delta t)-x(t) = A(x(t)+\alpha\Delta x)\Delta t + B(x(t)+\alpha\Delta x)\Delta\xi,\ \Delta\xi = \int_t^{t+\Delta t} \mathrm{d}t'\xi(t') \quad (40)$$

In the above equation, in the rhs, the first term is of order Δt while the second one is of order $\sqrt{\Delta t}$.

1. Justify the above statement and show that an equivalent discretization reads

$$\Delta x = B(x(t))\Delta\xi + (A(x(t)\Delta t + \alpha B'(x(t))B(x(t))\Delta\xi^2) + \mathcal{O}(\Delta t^{3/2}) \qquad (41)$$

2. Let $x \mapsto f(x)$ be an arbitrary function. Let $F(t) = f(x(t))$. Show that $\Delta F = F(t+\Delta t) - F(t)$ can be expressed as

$$\Delta F = B\Delta\xi f'(x(t)) + (A(x(t))\Delta t + \alpha B'(x(t))B(x(t))\Delta\xi^2)f'(x(t)) + \frac{1}{2}B^2(x(t))\Delta\xi^2 f''(x(t)) \qquad (46)$$

up to $\mathcal{O}(\Delta t^{3/2})$ terms.

3. If regular differential calculus was allowed, one could actually write that $\frac{\mathrm{d}F}{\mathrm{d}t} = f'\frac{\mathrm{d}x}{\mathrm{d}t}$, and hence that $\frac{\mathrm{d}F}{\mathrm{d}t} = f'A + f'B\xi$. Assuming this Langevin equation is written with an α' discretization rule, show that

$$\Delta F = f'B\Delta\xi + f'A\Delta t + \alpha'(f'B)'B\Delta\xi^2 + \mathcal{O}(\Delta t^{3/2}) \qquad (49)$$

where all functions are evaluated at time t.

4. What are the conditions on α and α' for the two expressions found in **2** and **3** for ΔF to match, irrespective of the function f?

5. Why is it legitimate to use differential calculus when working with the Stratonovich convention?

2.3 How "natural" is Stratonovich calculus?

In physics, a Langevin equation is always the result of a series of approximations. An obvious approximation is the existence of a diffusive limit, in which the typical length scale governing the evolution of the system is larger than the scale involved in its various changes throughout time (the size of the jump is smaller than the typical size of the process). But even before that diffusive limit, lies the Markov approximation, which is based on the separation of time scales between the (fast) ones characterizing the bath and entering the source of noise, and the (slow) ones related to the system of interest whose degrees of freedom are modeled. In the limit where memory effects induced by the time-correlations of the bath can be discarded, one gets a Markov approximation. In this exercise, we want to explore how an evolution equation with a noise displaying time correlations naturally leads, in the limit where these correlations are short-ranged, to a Langevin equation expressed in the Stratonovich discretization. This exercise echoes Sec. **IX.7** of Van Kampen's book [41].

1. Let $\mathit{\Delta}(t) = \frac{1}{2\tau}\mathrm{e}^{-|t|/\tau}$. Show that $\mathit{\Delta}$ converges to the δ distribution when $\tau \to 0$. It may be useful to consider $\int \mathrm{d}t \mathit{\Delta}(t) f(t)$ for an arbitrary function f in the $\tau \to 0$ limit.

2. Determine $\int_{t_0}^{t_0+\Delta t} \mathrm{d}s\mathrm{d}s' \mathit{\Delta}(s-s')$ at finite τ for t_0 and $\Delta t > 0$ that are fixed. Determine the asymptotic behavior of that quantity in the $\tau \to 0$ and $\Delta t \to 0$ limits. Discuss the importance of the order of limits.

   Let $x(t)$ be a function evolving according to the following equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = A(x(t)) + B(x(t))\eta(t) \tag{57}$$

   where η is a Gaussian process with time correlations $\langle \eta(t)\eta(t')\rangle = \mathit{\Delta}(t-t')$. Here A and B are arbitrary smooth functions of x.

3. Let $\Delta x = x(t_0+\Delta t) - x(t_0)$ for $\Delta t > 0$, t_0 and $x(t_0) = x_0$ being given. Explain why, at fixed $\tau > 0$, the process $x(t)$ remains a smoothly differentiable function (a physicist's argument would be to show that Δx is of order Δt, instead of being of order $\sqrt{\Delta t}$ in a standard Langevin equation).

4. Prove that $\lim_{\Delta t \to 0} \lim_{\tau \to 0} \frac{\langle \Delta x\rangle}{\Delta t} = A(x_0) + \frac{1}{2}B'(x_0)B(x_0)$.

5. Consider the α discretized Langevin equation $\dot{x} = A + B\eta$ where η is a white (delta correlated) noise. How should we choose α in order to recover the predictions of Eq. (57) in the $\tau \to 0$ limit?

2.4 Particle in contact with a thermostat

Our interest goes to a particle with unit mass in contact with a thermostat at temperature T and with friction coefficient γ. The velocity v of the particle evolves according to a Langevin equation

$$\frac{\mathrm{d}v}{\mathrm{d}t} = F \tag{60}$$

where the force F reads $F = -\gamma v + \sqrt{2\gamma T}\xi$, with ξ a Gaussian white noise with correlations $\langle \xi(t)\xi(t')\rangle = \delta(t-t')$. Let $E(t) = \frac{1}{2}v^2(t)$ be the particle's kinetic energy.

1. Write the evolution equation for the probability $p(v,t)$ that the particle has velocity v at time t.

2. Write a Langevin equation for $E(t)$ that couples to ξ.

3. Let t_0 be a given time at which the energy is $E(t_0)$ and let Δt be an infinitesimal time duration. Find $\frac{\langle E(t_0+\Delta t)-E(t_0)\rangle}{\Delta t}$ as a function of γ and of T.

4. What's the stationary value of $\langle v^2\rangle = T$? Was that expected?

5. We define $W(t)=\int_0^t \mathrm{d}t\sqrt{2\gamma T}\xi v$ (the integral is understood in the Stratonovich sense). Can you endow W with some physical meaning? In the evolution equation for E found in **2**, not only does $\frac{\mathrm{d}W}{\mathrm{d}t}$ appear, but also some additional contribution the physical meaning of which will be given.

6. We set out to determine the large time behavior of the pdf of W. Write an evolution equation for the probability $p(v,W,t)$ that the particle has velocity v at time t, and that $W(t)=W$.

7. Fourier transform the equation found in question 6 with respect to W, and prove that $\hat{p}(v,\lambda,t)=\int \mathrm{d}W \mathrm{e}^{-\lambda W} p(v,W,t)$ evolves according to

$$\partial_t \hat{p} = \text{part with no explicit dependence in } \lambda + \gamma T(\lambda^2 v^2-\lambda)\hat{p} + 2\gamma T\lambda\partial_v(v\hat{p}) \quad (84)$$

Here the parameter λ lives in a region of the complex plane such that $\hat{p}$ remains well-defined.

8. Prove that $\hat{p}(v,\lambda,t)=\mathrm{e}^{t\psi(\lambda)}\mathrm{e}^{-av^2}$ is a solution. Express both a and ψ in terms of T, γ and λ.

9. Justify that the probability to get a value W at large times behaves as $P(W,t)\simeq \mathrm{e}^{t\pi(W/t)}$, where the function $\pi(w)$ will be related to $\psi(\lambda)$.

10. Qualitatively plot $\pi(w)$ as a function of w. Does this function possess any remarkable symmetry property? Comment on your finding.

2.5 Playing around with stochastic calculus

We consider an overdamped Langevin particle with position $\mathbf{r}$ evolving under the action of an external force field $\mathbf{F}(\mathbf{r})$ in contact with a thermal bath at temperature T:

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mu\mathbf{F} + \sqrt{2T\mu}\boldsymbol{\eta} \tag{100}$$

where the space components $\eta^\mu(t)$ of $\boldsymbol{\eta}$ are independent white noises with unit variance: $\langle\eta^\mu(t)\eta^\nu(t')\rangle = \delta^{\mu\nu}\delta(t-t')$. The particle's mobility has been set to unity for convenience. In what follows the mobility μ will be set to unity.

1. Let $W(t) = \int_0^t \mathrm{d}t\mathbf{F}\cdot\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}$. What is the direct physical meaning of W? Explain in what sense W is the work exerted by the particle on its surrounding thermostat.

2. Write a stochastic evolution for W (aka Langevin equation) that couples to $\mathbf{r}$. If you did it right, this equation features a multiplicative noise. Write the equation in both the Ito and the Stratonovich forms.

3. Let $\mathscr{V} = \frac{\mathbf{r}^2}{2}$. Write a stochastic evolution for $\mathscr{V}$ that couples to $\mathbf{r}$. Write the equation in both the Itō and the Stratonovich forms. From this equation deduce that the pressure of an ideal gas of N identical Langevin particles is $P = NT/V$. (Hint: Think of the particle being trapped in a closed box of volume V and of $\mathbf{F}$ as being the force exerted by the wall.

4. First consider the conservative case where we have $\mathbf{F} = -\boldsymbol{\nabla}v$ (here v depends on $\mathbf{r}$ only). Write a stochastic evolution for v that couples to $\mathbf{r}$. Write the equation in both the Itō and the Stratonovich forms.

5. Second, consider $\mathbf{F} = -\boldsymbol{\nabla}v + \mathbf{f}$, where the force $\mathbf{f}$ stands for a (possibly time dependent) additional force (like that of an operator performing some action on the system). Between t and $t+\mathrm{d}t$, v varies by $\mathrm{d}v = v(\mathbf{r}(t+\mathrm{d}t)) - v(\mathbf{r}(t))$. Show that it is possible to write $\mathrm{d}v = \delta W + \delta Q$, where $\delta W = \mathbf{f}\cdot\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\mathrm{d}t$. What is the microscopic mechanical meaning of δQ? Does this relationship ring any bell?

2.6 Dean-Kawasaki dynamics from a microscopic approach

Consider N Brownian colloidal particles with mobility μ in a solvent acting as a thermostat at temperature T. These particles interact via a two body potential $v(\mathbf{r})$, so that the individual dynamics of particle i reads

$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = \mu\mathbf{F}_i + \sqrt{2\mu T}\boldsymbol{\eta}_i \tag{117}$$

where $\mathbf{F}_i = -\sum_{j\neq i}\boldsymbol{\nabla}v(\mathbf{r}_i - \mathbf{r}_j)$ is the force exerted by the $N-1$ particles on particle i, and $\boldsymbol{\eta}_i$ is a Gaussian white noise vector with correlations $\langle\eta_i^\alpha(t)\eta_j^\beta(t')\rangle = \delta^{\alpha\beta}\delta_{ij}\delta(t-t')$.

Particles (labeled by $i, j = 1, \ldots, N$) and space directions (labeled by $\alpha, \beta = 1, \ldots, d$) are independent. Our interest goes to the following random variable $\rho(\mathbf{x}, t)$ defined by

$$\rho(\mathbf{x}, t) = \sum_{i=1}^{N} \delta^{(d)}(\mathbf{x} - \mathbf{r}_i(t)) \tag{118}$$

Let us also introduce $\rho'(\mathbf{x}, t) = \ell^{-d} \int_{||\mathbf{x}-\mathbf{y}|| \leq \ell} \mathrm{d}^d y \rho(\mathbf{y}, t)$ where ℓ is a yet unspecified length scale.

1. Given the definition of ρ, explain why $\partial_t \rho(\mathbf{x}, t) = -\boldsymbol{\nabla}_{\mathbf{x}} \cdot \sum_i \frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} \delta^{(d)}(\mathbf{x} - \mathbf{r}_i)$. This would be true if the $\mathbf{r}_i(t)$'s were differentiable functions, which they are not. Is there a sense in which this is nevertheless still true?

2. Explain why $\mathbf{r}_i$ is not differentiable. To do so, assume that $\mathbf{r}_i(t_0)$ is given, and explain why $\Delta \mathbf{r}_i = \mathbf{r}_i(t_0 + \Delta t) - \mathbf{r}_i(t_0)$ is typically of order $\sqrt{\Delta t}$ as $\Delta \to 0$. It may be useful to introduce $\Delta \eta^\alpha = \int_{t_0}^{t_0 + \Delta t} \mathrm{d}\tau \eta^\alpha(\tau)$ and to determine its variance.

3. Determine $\lim_{\Delta t \to 0} \frac{\langle \Delta r_i^\alpha \rangle}{\Delta t}$ and $\lim_{\Delta t \to 0} \frac{\langle \Delta r_i^\alpha \Delta r_j^\beta \rangle}{\Delta t}$ in terms of μ, T and of the potential v evaluated at the positions at time t_0.

4. What is the physical meaning of $\mathbf{J}(\mathbf{x}, t) = \sum_i \frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} \delta^{(d)}(\mathbf{x} - \mathbf{r}_i)$?

5. Let $\Delta \rho(\mathbf{x}) = \rho(\mathbf{x}, t_0 + \Delta t) - \rho(\mathbf{x}, t_0)$ and let $\Delta J^\alpha(\mathbf{x}) = \int_{t_0}^{t_0 + \Delta t} \mathrm{d}\tau J^\alpha(\mathbf{x}, \tau)$. What is the relationship between $\langle \Delta \rho(\mathbf{x}) \rangle$ and $\langle \Delta J^\alpha(\mathbf{x}) \rangle$? And between $\langle \Delta \rho(\mathbf{x}) \Delta \rho(\mathbf{x}') \rangle$ and $\langle \Delta J^\alpha(\mathbf{x}) \Delta J^\beta(\mathbf{x}') \rangle$?

6. Explain carefully why $\lim_{\Delta t \to 0} \frac{\langle \Delta J^\alpha(\mathbf{x}) \Delta J^\beta(\mathbf{x}') \rangle}{\Delta t} = 2\mu T \rho(\mathbf{x}, t_0) \delta^{\alpha\beta} \delta^{(d)}(\mathbf{x} - \mathbf{x}')$.

7. Explain even more carefully why $\lim_{\Delta t \to 0} \frac{\langle \Delta J^\alpha(\mathbf{x}) \rangle}{\Delta t} = -\mu T \frac{\partial \rho(\mathbf{x}, t_0)}{\partial x^\alpha} - \mu \rho(\mathbf{x}, t_0) \int_{\mathbf{y}} \frac{\partial v(\mathbf{x}-\mathbf{y})}{\partial x^\alpha} \rho(\mathbf{y}, t_0)$.

8. Give the physical meaning of each of the two terms in $\lim_{\Delta t \to 0} \frac{\langle \Delta J^\alpha(\mathbf{x}) \rangle}{\Delta t}$.

9. Determine $\lim_{\Delta t \to 0} \frac{\langle \Delta \rho(\mathbf{x}_1) \ldots \Delta \rho(\mathbf{x}_n) \rangle}{\Delta t}$ for $n \geq 3$.

10. If we assume that the statistics of ρ can be encoded in a Langevin equation of the form

$$\partial_t \rho = -\boldsymbol{\nabla} \cdot \mathbf{J} \tag{129}$$

with $\mathbf{J} = \ldots(1) + \boldsymbol{\xi}(\mathbf{x}, t)$, and with $\langle \xi^\alpha(\mathbf{x}, t) \xi^\beta(\mathbf{x}', t) \rangle = \ldots(2) \delta^{\alpha\beta} \delta(t - t')$ a Gaussian white noise, fill in the dots (1) and (2) with the corresponding expressions in terms of ρ, μ and T.

11. Find the *simplest* argument acccounting for the fact that the dynamics of ρ is an equilibrium one.

12. We now want to address the dynamics of $\rho'(\mathbf{x}, t)$, a coarse-grained version of $\rho(\mathbf{x}, t)$ (the latter being fully microscopic). We also postulate that ρ' evolves according to a Langevin equation. Why can we assert that the dynamics of ρ' takes the form $\partial_t \rho' = -\boldsymbol{\nabla} \cdot \mathbf{J}'$? And which argument allows to assert that $\mathbf{J}' = -\mu T \boldsymbol{\nabla} \rho' + \ldots$, where $\ldots$ stand for noise and nonlinear contributions.

13. We write the nonlinear part in $\mathbf{J}'$ in the form

$$\mathbf{J}' = -\rho'(\mathbf{x}, t) T \left[\int_{\mathbf{y}} \boldsymbol{\nabla}_{\mathbf{x}} c^{(2)}(\mathbf{x}, \mathbf{y}) \rho'(\mathbf{y}, t) + \int_{\mathbf{y},\mathbf{z}} \boldsymbol{\nabla}_{\mathbf{x}} c^{(3)}(\mathbf{x}, \mathbf{y}, \mathbf{z}) \rho'(\mathbf{y}, t) \rho'(\mathbf{z}, t) + \ldots \right] \tag{132}$$

Is there any *a priori* reason for the expansion to vanish to order 2 (*i.e.* $c^{(n)} = 0$ for $n \geq 3$)?

14. For the field ρ' to make physical sense, what condition would you impose on the coarse-graining scale ℓ that is used to define it?

2.7 Ornstein-Uhlenbeck process

In this tutorial, we study the Ornstein-Uhlenbeck (OU) process which is a one-dimensional stochastic process $x(t)$ that evolves via the Langevin equation

$$\dot{x}(t) = -\mu\, x(t) + h(t) + \zeta(t)\ , \tag{133}$$

starting from an initial position (at time t_0) $x(t_0) = x_0$. In Eq. (133)), $\mu > 0$, $h(t)$ is a (small) external field which is used here to probe the response of the process and $\zeta(t)$ is a Gaussian white (thermal) noise with zero mean, i.e. $\langle \zeta(t) \rangle = 0$ and $\langle \zeta(t)\zeta(t') \rangle = 2T\delta(t-t')$ where $T > 0$ is the temperature. For $\mu = 0$, one recovers the standard Brownian motion. The OU process was initially introduced to describe the velocity $x(t) \equiv v(t)$ of a massive Brownian particle under the influence of friction. Since then, the OU process has become a fundamental stochastic process to describe noisy relaxation in various situations. As such, it has found various applications in statistical mechanics but also in financial mathematics (*e.g.* to model interest rates), biology (*e.g.* to model neuronal activity) or computer science (*e.g.* in queuing theory).

The goal of this tutorial is to compute, from the dynamical action of the OU process, the two-time correlation $C(t, t')$

$$C(t, t') = \langle x(t) x(t') \rangle \Big|_{h=0} \tag{134}$$

and the response function $R(t, t')$

$$R(t, t') = \left\langle \frac{\delta x(t)}{\delta h(t')} \right\rangle \Big|_{h=0} \tag{135}$$

where in Eqs. (134) and (135) the notation $\langle \cdots \rangle$ denotes an average over the thermal noise ζ.

2.7.1 A direct approach without path integrals

The equation of motion Eq. (133) can be integrated. This exact solution, which we derive here, will serve as a guideline for later computations with the dynamical action.

1. Compute explicitly $x(t)$, the solution of Eq. (133) at time t, for a single realization of the noise $\zeta(t')$, for $t_0 \leq t' \leq t$.

2. From this explicit solution, compute the correlation function $C(t,t')$ and the response function $R(t,t')$ for a fixed initial condition x_0.

3. In the limit $t_0 \to -\infty$ show that these averaged observables are: i) independent of x_0, ii) stationary (i.e. time-translation invariant) with $C(t,t') \to C_{\rm st}(t-t')$ and $R(t,t') \to R_{\rm st}(t-t')$ and iii) that they are related by the relation

$$R_{\rm st}(\tau) = -\frac{1}{T}\frac{dC_{\rm st}(\tau)}{d\tau} \;, \quad \text{for } \tau \geq 0 \;, \tag{141}$$

   which is called the "Fluctuation Dissipation Theorem" (FDT). What about the existence of this FDT regime in the Brownian limit $\mu \to 0$?

2.7.2 Computation of $C(t,t')$ and $R(t,t')$ using the dynamical action

We consider the limit $t_0 \to -\infty$ where we have seen that the correlation and response are independent of x_0. We thus set $x_0 = 0$. We recall that the dynamical action corresponding to the stochastic equation that governs the OU process in Eq. (133) on the time interval $]-\infty, +\infty[$ with $h = 0$, denoted as $S_{\rm OU}[\hat{x}, x] \equiv S_{\rm OU}[\{\hat{x}(t'), x(t')\}, -\infty < t' < +\infty]$, reads

$$S_{\rm OU}[\hat{x}, x] = \int_{-\infty}^{+\infty} dt'\, \hat{x}(t')\left[\dot{x}(t') + \mu\, x(t')\right] - T\int_{-\infty}^{+\infty} dt'\, \hat{x}^2(t') \;, \tag{147}$$

where $x(t')$ and $-i\hat{x}(t')$ are real scalar fields, such that $x(t' \to \pm\infty) = -i\hat{x}(t' \to \pm\infty) = 0$.

4. It is thus useful to introduce a two-component vector $\phi(t)$

$$\phi(t) = \begin{pmatrix} x(t) \\ \hat{x}(t) \end{pmatrix} \tag{148}$$

   such that $S_{\rm OU}$ in Eq. (147) can be written in a matrix form as

$$S_{\rm OU} = \frac{1}{2}\phi : G^{-1} : \phi = \frac{1}{2}\int_{-\infty}^{+\infty} {\rm d}t_1 \int_{-\infty}^{+\infty} {\rm d}t_2\, \phi(t_1) G^{-1}(t_1, t_2)\phi(t_2) \;. \tag{149}$$

   Show that G^{-1} has the following block structure

$$G^{-1}(t,t') = \begin{pmatrix} 0 & \delta(t-t')\,(-\partial_{t'} + \mu) \\ \delta(t-t')\,(\partial_{t'} + \mu) & -2T\delta(t-t') \end{pmatrix} \tag{150}$$

5. We now introduce the sources $\hat{J}(t')$ and $J(t)$ coupled respectively to the field $x(t)$ and to the response field $\hat{x}(t)$, and we define the generating functional $Z[\hat{J}, J] \equiv Z[\{\hat{J}(t'), J(t')\}, -\infty < t' < +\infty]$ as

$$Z[\hat{J}, J] = \int \mathcal{D}\hat{x}\mathcal{D}x \; \mathrm{e}^{-S_{\mathrm{OU}}[\hat{x},x]+\int_{-\infty}^{+\infty} \mathrm{d}t' \hat{J}(t')x(t')+\int_{-\infty}^{+\infty} \mathrm{d}t' \hat{x}(t')J(t')} \; . \tag{154}$$

Show that the correlation function $C(t, t')$ defined in Eq. (134) and the response function $R(t, t')$ defined in Eq. (135) are obtained from $Z[\hat{J}, J]$ as

$$C(t, t') = \left. \frac{\delta^2 Z}{\delta \hat{J}(t')\delta \hat{J}(t)} \right|_{J=\hat{J}=0} , \tag{155}$$

$$R(t, t') = \left. \frac{\delta^2 Z}{\delta J(t')\delta \hat{J}(t)} \right|_{J=\hat{J}=0} , \tag{156}$$

and comment on the terminology “response field” given to $\hat{x}(t)$.

6. Show that the matrix $G(t, t')$ encodes the correlation and response functions of the process and has the following form:

$$G(t, t') = \begin{pmatrix} C(t, t') & R(t, t') \\ R(t', t) & D(t, t') \end{pmatrix} . \tag{157}$$

Show that $C(t, t')$ and $R(t, t')$ are solutions of

$$\partial_t R(t, t') + \mu \, R(t, t') = \delta(t - t') \, , \tag{158}$$

$$\partial_t C(t, t') + \mu \, C(t, t') = 2T R(t', t) \, , \tag{159}$$

and that $D(t, t') = 0$.

7. Show that the stationary solution $C(t, t') = C_{\mathrm{st}}(t - t')$, $R(t, t') = R_{\mathrm{st}}(t - t')$ found above in question 3 is solution of this coupled set of equations (158) and (159).

8. (*Optional*) In the case where t_0 is finite, how will these equations (158)-(159) get modified?

9. In the case of an OU process, the generating functional $Z[\hat{J}, J]$ can in fact be evaluated explicitly. Show that it reads:

$$Z[\hat{J}, J] = \mathrm{e}^{-\int_{-\infty}^{+\infty} \mathrm{d}t_1 \int_{-\infty}^{+\infty} \mathrm{d}t_2 \left(\frac{T}{2\mu} \mathrm{e}^{-\mu |t_1 - t_2|} J(t_1)J(t_2) - i\,\theta(t_2 - t_1)\, \mathrm{e}^{-\mu(t_2 - t_1)} \hat{J}(t_1)J(t_2) \right)} \tag{172}$$

10. Using Eqs. (155) and (156), compute $C(t, t')$ and $R(t, t')$ from $Z[\hat{J}, J]$ and check that you recover the expression of $C_{\mathrm{st}}(\tau)$ and $R_{\mathrm{st}}(\tau)$ found above.

11. (*Optional*) We now consider t_0 finite. Compute $Z[J, \hat{J}]$ in this case and extract from it the correlation $C(t, t')$ and the response $R(t, t')$ for an arbitrary t_0 and $x(t_0) = x_0$.

2.8 First passage by the origin of an Ornstein-Uhlenbeck process

We consider an Ornstein-Uhlenbeck process $x(t)$ evolving according to

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\mu x + \sqrt{2\mu}\xi(t) \tag{174}$$

with $\mu > 0$ and ξ a Gaussian white noise with correlations $\langle \xi(t)\xi(t')\rangle = \delta(t'-t)$. The goal of this problem is to find the probability that the random process x has remained on the same side of the $x = 0$ axis over a prescribed time window.

1. What is the probability $G(x, t; x_0, 0)$ the find the process at position x at time t given its starting position x_0 at $t = 0$?
2. What is the time correlation function $C(t, t') \equiv \langle x(t)x(t')\rangle - \langle x(t)\rangle\langle x(t')\rangle$ of the process?
3. What is the equilibrium distribution $P_{\mathrm{eq}}(x)$? How long does it (typically) take for the process to forget about its initial position?
4. Use P_{eq} and G to determine the probability $P(y, t; x, 0)$ to be at x at time 0 and at y at time $t > 0$.
5. What is the probability $P_+(y, t; x, 0)$ to find the process at $x > 0$ at time $t = 0$ and at $y > 0$ at time t, without ever having visited the negative position side?
6. Find the probability $\mathcal{P}(t)$ that he process has always remained on the positive side between 0 and t (the leading behavior at large t is enough). How can this result be used to determine the same probability for a one-dimensional Brownian motion (instead of an Ornstein-Uhlenbeck process)?

3 Time reversal and its consequences

3.1 On a family of equilibrium Langevin processes

Consider the n-dimensional Langevin process $\mathbf{X}(t) = \sum_{i=1}^{n} X_i(t)\mathbf{e}_i$ whose time evolution is governed by the following Langevin equation

$$\frac{\mathrm{d}\mathbf{X}}{\mathrm{d}t} = -(M + A)\partial_{\mathbf{X}} H + \boldsymbol{\eta} \tag{184}$$

where $M = M^T$ is a constant symmetric, positive semidefinite matrix, $A = -A^T$ is a constant skew symmetric matrix, and $\boldsymbol{\eta}$ is a Gaussian white noise with correlations

$$\langle \eta_i(t)\eta_j(t')\rangle = 2TM_{ij}\delta(t - t') \tag{185}$$

The function $H(\mathbf{X})$ is for the moment arbitrary. The exercise rests on the introduction of the following article W. Mou, Y.-A. Ma, M. J. Wainwright, P. L. Bartlett, M. I. Jordan, Journal of Machine Learning Research **22**, 1 (2021), *High-Order Langevin Diffusion Yields an Accelerated MCMC Algorithm*.

1. Show that the distribution $P_{\rm ss}(\mathbf{X}) \propto \mathrm{e}^{-H(\mathbf{X})/T}$ is indeed the stationary distribution.

2. Find a condition on M, A and $\partial_{\mathbf{X}} H$ for the stationary distribution $P_{\rm ss}(\mathbf{X}) \propto \mathrm{e}^{-H(\mathbf{X})/T}$ to actually be equilibrium one (temporarily assume that M is positive-definite).

3. Verify that the choice $A = 0$, $M = \mu I_d$ (I_d is the $d \times d$ identity matrix), $\mathbf{X} = \mathbf{r}$, $H(\mathbf{X}) = V(\mathbf{r})$ leads to an overdamped Langevin equation for a particle with position $\mathbf{r} \in \mathbb{R}^d$ in an external potential $V(\mathbf{r})$ with mobility μ.

4. We now consider a vector $\mathbf{X}$ with $2d$ components $\mathbf{X} = (\mathbf{r}, \mathbf{p})$. Find an explicit choice of A and M such that the evolution equation for $\mathbf{X}$ results in an underdamped Langevin equation for a particle with position $\mathbf{r}$, momentum $\mathbf{p} = m\dot{\mathbf{r}}$ and with energy $H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r})$. Verify that the dynamics is reversible (beware, M has no inverse).

5. Write the corresponding second order stochastic differential equation for the process $\mathbf{r}(t)$ when $V(\mathbf{r}) = k\frac{\mathbf{r}^2}{2}$ is a harmonic well and identify the typical time it takes for the process to equilibrate.

6. Finally, consider the vector $\mathbf{X} = (\mathbf{r}, \mathbf{p}, \mathbf{u})$ with $n = 3d$ components, with $M = \gamma \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & I_d \end{pmatrix}$ and $A = \begin{pmatrix} 0 & -I_d & 0 \\ I_d & 0 & -\gamma' I_d \\ 0 & \gamma' I_d & 0 \end{pmatrix}$. Check first that the dynamics is reversible. Write the corresponding third order stochastic differential equation for the process $\mathbf{r}(t)$ for $H(\mathbf{X}) = V(\mathbf{r}) + \frac{\mathbf{p}^2}{2m} + \frac{\mathbf{u}^2}{2m'}$.

7. Is there a physical reasoning that could lead to such a Langevin equation for the process $\mathbf{r}(t)$? Read the reference given in the introduction to find out why, whether physically motivated or not, such a third-order stochastic equation can actually be relevant.

3.2 Glauber dynamics and the fluctuation-dissipation theorem

The one-dimensional Ising model can be endowed with Glauber's dynamical evolution rules: a spin configuration $\boldsymbol{\sigma} = \{\sigma_i(t)\}_{i=1,\dots,N}$ is a Markov variable whose evolution, in the absence of any magnetic field, is governed by the following transition rates,

$$\begin{array}{lccccccccl} \text{at } t: & i-1 & i & i+1 & \longrightarrow & \text{at } t+\mathrm{d}t: & i-1 & i & i+1 & \text{rate}: w_i(\sigma_i) \\ & \uparrow & \uparrow & \uparrow & & & \uparrow & \downarrow & \uparrow & \frac{1}{2}-\frac{1}{2}\tanh 2K \\ & \uparrow & \downarrow & \uparrow & & & \uparrow & \uparrow & \uparrow & \frac{1}{2}+\frac{1}{2}\tanh 2K \\ & \uparrow & \uparrow & \downarrow & & & \uparrow & \downarrow & \downarrow & \frac{1}{2} \end{array} \tag{219}$$

These transition rates can be cast in the synthetic form

$$W(\boldsymbol{\sigma} \to \boldsymbol{\sigma'}) = \sum_i \prod_{j\neq i} \delta_{\sigma_j,\sigma'_j} \times \delta_{\sigma_i,-\sigma'_i} w_i(\sigma_i) \tag{220}$$

$$w_i(\sigma_i) \equiv \frac{1}{2}\left(1 - \frac{1}{2}\sigma_i(\sigma_{i-1}+\sigma_{i+1})\mathrm{th}2K)\right) \tag{221}$$

The initial condition is left unspecified. In short, at time t a site i is drawn at random and its spin σ_i is flipped at a rate $w_i(\sigma_i)$.

Our goal is to explicitly obtain the fluctuation-dissipation theorem related to the global magnetization. In the first part of the exercise, some properties of the average magnetization and of its fluctuations are established, without any magnetic field. In the second part, a time-dependent magnetic field is introduced and the system's response is investigated. The system is made of a large number N of spins; all extensive quantities will be expressed to leading order in N.

3.2.1 Without a magnetic field

1. Verify that the transition rates of table (219) indeed lead the system to converge to an equilibrium state with the following Hamiltonian:

$$\mathcal{H} = -J\sum_i \sigma_i\sigma_{i+1}, \quad \beta J = K \tag{222}$$

   Write the evolution equation of the local average magnetization $m_n(t) \equiv \langle\sigma_n(t)\rangle$. We define $S(t) \equiv \sum_i \sigma_i(t)$. Write the evolution equation for the total average magnetization $M(t) \equiv \langle S(t)\rangle$. Solve the latter equation for a fixed initial condition $S(0)$.

2. The spin-spin correlation function is introduced

$$c_{i,i+\ell}(t) \equiv \langle\sigma_i(t)\sigma_{i+\ell}(t)\rangle \tag{229}$$

   What are the conditions under which the $c_{i,i+\ell}(t)$'s are independent of i? The latter function will now be denoted by $c_\ell(t)$. Write an evolution equation for $c_\ell(t)$ and solve it in the stationary state.

3. We sit in equilibrium. Using the previous question, find the variance $\langle S^2\rangle$. What is the pdf of S?

4. Assume the system is in equilibrium at $t = 0$, and consider an arbitrary time t ($t > 0$ or $t < 0$). Determine the correlation function

$$C_{\text{eq}}(t) \equiv \langle S(0)S(t)\rangle$$

   along with its Fourier transform $\tilde{C}_{\text{eq}}(\omega) \equiv \int_{-\infty}^{+\infty} \mathrm{d}t\ \mathrm{e}^{i\omega t}C_{\text{eq}}(t)$.

3.2.2 With a magnetic field

5. An external magnetic field $h(t)$ is now applied. The additional magnetic energy of a spin σ_i is $-h\sigma_i$. We begin with a constant field. The transition rates have to be modified so that the system samples the new equilibrium distribution in the presence of the field. These new rates are written in the form

$$w_i'(\sigma_i) = w_i(\sigma_i)(1-\alpha\sigma_i)$$

What is α? Is that formula still valid when h depends on time? In the latter case, is the process $\{\sigma_i(t)\}$ still Markovian?

6. At $t_{\text{initial}} = -\infty$ the system is prepared in a given magnetization state. Write the evolution equation for the local average magnetization $m_i(t) \equiv \langle \sigma_i(t) \rangle$ ($c_{i\pm 1}(t)$ will be involved). Find the evolution equation for the total average magnetization $M(t)$. Simplify that equation in the limit of a vanishingly small field to first order in h. We'll stick to that approximation in the sequel.

7. Assuming that $h(t) = h_0 \mathrm{e}^{-i\omega t}$, identify $\chi(\omega)$ such that

$$M(t) = \chi(\omega) h(t) \tag{243}$$

What is $\chi(0)$? Is there an alternative method leading to $\chi(0)$?

8. Prove that

$$\tilde{C}_{\text{eq}}(\omega) = \frac{2k_{\text{B}}T}{\omega} \text{Im}\chi(\omega) \tag{246}$$

Discuss this identity.

4 Metastability and rare events

4.1 Kramers' escape problem for a self-propelled particle

Self-propelled particles are micron-sized entities (whether bacteria or synthetic colloids) that use energy from their environment to convert it into motion. Energy is then dissipated instead of being returned to the environment (as would be the case for a passive colloid undergoing Brownian motion). There are various ways of modelling the motion of such a particle. One of them is to describe it by means of an overdamped Langevin equation with a colored noise,

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\boldsymbol{\nabla} V(\mathbf{r}) + \sqrt{2T}\boldsymbol{\eta} \tag{247}$$

where $\boldsymbol{\eta}$ is a Gaussian noise whose spatial components η^μ have correlations $\langle \eta^\mu(t)\eta^\nu(t')\rangle = \delta^{\mu\nu}\frac{\mathrm{e}^{-|t-t'|/\tau}}{2\tau}$ where τ is a time scale expressing the persistent nature of the motion. A natural question that arises is whether such a particle hops over a potential barrier faster or slower than its equilibrium counterpart. We will explore this question in one space dimension in the limit where T is small with respect to the relevant potential energy scale. This is based on [28, 6, 43, 42].

1. Show that as $\tau \to 0$ one recovers an equilibrium process. In physics, it is meaningless to write $\tau \to 0$, as one should instead write $\tau \ll \tau'$ where τ' is some other time scale. What is the physical meaning and physical origin of τ'?

2. In the absence of the external potential V, determine the mean-square displacement of the particle after a duration t in terms of T, t and τ. Briefly discuss the various regimes that are observed.

3. Henceforth we work in one space dimension and we consider a potential landscape displaying a minimum V_m at x_m and a maximum V_M at x_M. We denote by $\Delta V = V_M - V_m$ and we ask about the typical time it take a particle starting from x_m to reach x_M. Do you see a way of casting this question within a Fokker-Planck equation form?

4. Write the Janssen-De Dominicis action for the path $x(t)$ and its conjugate path $\bar{x}(t)$.

5. What are, at low temperature, for a trajectory starting from x_m and ending at x_M, the evolution equations for $x(t)$ and $\bar{x}(t)$? Check that in the $\tau \to 0$ limit the equations actually match those of the equilibrium dynamics (and recall the corresponding solution $x_0(t)$ and $\bar{x}_0(t)$ in terms of $V'(x_0(t))$).

6. While such equations are hard to solve for an arbitrary value of τ, we attempt to find how a small but finite value of τ alters the standard Kramers trajectory. Rewrite the equations of question 5 to their first nontrivial order in τ in the form $x = x_0 + \tau^\alpha \dots x_1 + \dots$ and a similar expansion for $\bar{x}$. Find the power α. Check that $x_1 = 2\,V'(x_0)\,V''(x_0)$ and find the corresponding expression for $\bar{x}_1$ (as a functional of x_0).

7. Show that the energy barrier is effectively increased.

5 The mean-field approximation

5.1 The contact process

The contact process is the crudest model describing the propagation of an epidemic. Its purpose is to described the growth of a spatially extended population of individuals (agents, particles, chemicals, *etc.*) subjected to competing processes: if an individual is present at some location it has a (unit) rate of disappearing. However, an empty location can become occupied at a rate λ further proportional to the local population around it. This process has (and still is) extensively studied in the mathematical literature (see [32] or [8] for a formulation in terms of a directed percolation process) but a version of it emanating from chemical physics [35] has led to field-theoretic developments (based on the Reggeon field theory) [22, 9, 25] connecting this problem to the Gribov process of particles physics [23] (dealing with the scattering of partons (hadrons)). Parts of this problem are excerpts from [15].

1. In a one dimensional version of the contact process, the sites i of a lattice are either empty (with local occupation number $n_i = 0$) or occupied ($n_i = 1$). Each occupied site can become empty at a unit rate (this fixes our time units). Each site i can become occupied at a rate $\frac{1}{2}\lambda(n_{i+1} + n_{i-1})(1 - n_i)$ provided at least either $i + 1$ or $i - 1$ are occupied (the factor $(1-n_i)$ ensures this can happen only if site i is empty). In a mean-field version defined on a fully-connected graph with N vertices, the total number n of occupied sites can increase by one unit (with a rate $W_+(n \to n + 1)$) or decrease by one unit (with a rate $W_-(n \to n - 1)$). What would you suggest for W_-? We choose $W_+(n \to n + 1) \propto n(N - n)$: how would you write the prefactor?

2. What is the master equation for the probability $P(n,t)$ to find n particles in the system at time t? Write an evolution equation for $\langle n \rangle$.

3. Let $\rho = \frac{\langle n \rangle}{N}$. Plot ρ as a function of λ in the steady-state for $N \gg 1$. What are the typical relaxation times $\tau_{\text{relax}}(\lambda)$ to the steady-state ($\lambda \to 1^{\pm}$)?

4. Let $\nu = \frac{n}{N}$. Argue why, for $N \gg 1$, $\nu(t)$ evolves according to a Langevin equation

$$\frac{\mathrm{d}\nu}{\mathrm{d}t} \stackrel{0}{=} f(\nu) + g(\nu)\eta \tag{260}$$

where $\langle \eta(t)\eta(t') \rangle = \delta(t-t')$. What is the function f?

5. Find the function g.

6. Let $P_{\text{ss}}(n)$ be the steady-state distribution. What is P_{ss} at any finite N? Let $\pi(\nu) = \lim_{N\to+\infty} \frac{1}{N} \ln P_{\text{ss}}(\nu N)$. Determine $\pi(\nu)$ directly from the master equation for $P_{\text{ss}}(n)$, and plot it.

7. What is the typical time $\tau_{\text{abs}}(\lambda, N)$ it takes the process to reach its true, finite-size, steady-state? Work out the $\lambda \to 1^+$ limiting expression.

8. Could you recover the expression of $\tau_{\text{abs}}(\lambda, N)$ by an instanton calculation based on the Janssen-De Dominicis action related to Eq. (260)?

9. Our goal is to build an exact field-theoretic representation of the initial process without resorting to the Janssen-De Dominicis procedure, which itself is based on an approximate Langevin equation. Let $\Delta n = n(\Delta t) - n(0)$ and consider, as a first step towards a field theory, the average of a physical quantity $A(n)$ at time Δt, $\langle A \rangle(\Delta t)$. The initial value $n(0)$ is assumed to be fixed. Show that

$$\langle A \rangle(\Delta t) = \int \frac{\mathrm{d}\hat{\rho}(0)}{2\pi i} \mathrm{d}\rho(0)\mathrm{d}\rho(\Delta t) A(\rho(0) + \Delta\rho) \langle \mathrm{e}^{\hat{\rho}(0)(\Delta n - \Delta\rho)} \rangle \delta(\rho(0) - n(0)) \tag{271}$$

where the brackets $\langle \dots \rangle$ denote an average with respect to the possible values of $\Delta n = n(\Delta t) - n(0)$.

10. Determine the expression of $\langle \mathrm{e}^{\hat{\rho}(0)\Delta n} \rangle$ as a function of $\hat{\rho}(\Delta t)$, λ, N, Δt and $\rho(0)$ (or $n(0)$).

11. Explain in what sense one can actually write that, for an initial distribution P_{init} of the particle number $n(0)$, we have

$$\langle A(t_{\text{obs}}) \rangle = \int \mathscr{D}\hat{\rho}\mathscr{D}\rho A(\rho(t_{\text{obs}})) \mathrm{e}^{-\int_0^{t_{\text{obs}}} \mathrm{d}t \left[\hat{\rho}\partial_t \rho + \frac{\lambda}{N}(1-\mathrm{e}^{\hat{\rho}})\rho(N-\rho) + (1-\mathrm{e}^{-\hat{\rho}})\rho\right] - \delta S_{\text{init}}} \tag{278}$$

where δS_{init} refers to a contribution involving fields at the initial time $t = 0$.

12. Show that an instanton calculation based on Eq. (278) leads to the correct $\tau_{\rm abs}(\lambda, N)$.

13. Could you write an exact field theory for the one-dimensional process defined on a lattice (as described in the introduction to this problem)?

14. For this final more speculative question, we work on a hypercubic lattice. Finite connectivity fluctuations will certainly shift the critical value of λ. Will the real critical λ be larger or smaller than 1? Can you guess an upper critical dimension above which the mean-field scaling (say for the relaxation to the steady-state, or the λ dependence of ρ) applies?

5.2 Bistability out of equilibrium, from 1972 to 2022

Our interest goes to a model introduced by Schlögl [35] (*Chemical reaction models for non-equilibrium phase transitions*) fifty years ago, also studied by Janssen [24] (*Stochastic reaction model for a non-equilibrium phase transition*. This model was revived by Tănase-Nicola and Lubensky [39] (*Exchange of stability as a function of system size in a nonequilibrium system*) ten years ago, and revisited in 2022 by Zakine and Vanden-Eijnden [45] (*Minimum Action Method for Nonequilibrium Phase Transitions*). Another recent reference is the work of Nguyen and Seifert [33] (*Exponential volume dependence of entropy-current fluctuations at first-order phase transitions in chemical reaction networks*) where the authors discuss the behavior of entropy production in a bistable system far from equilibrium. This text is taken from an exam. Beware, questions 16 to 22 are ahead of the lectures; you can get back to these at the end of the term. Questions 23 and 24, however, can be answered independently.

The model involves a species A undergoing the various reactions

$$\emptyset \underset{k_1}{\overset{k_0}{\rightleftharpoons}} A,\ A+A \underset{k_3}{\overset{k_2}{\rightleftharpoons}} A+A+A \tag{284}$$

Species A is diffusive and its diffusion constant is D. It is useful to think in terms of particles hopping on a lattice with N lattices sites labeled by $\mathbf{x}$, where each lattice site $\mathbf{x}$ can host an arbitrary integer number $n_{\mathbf{x}}$ of particles.

A preliminary lemma for a generic Markov process

1. We begin by three questions that apply to a generic Markov process with configurations denoted by $\mathscr{C}$ and characterized by transition rates $W(\mathscr{C} \to \mathscr{C}')$. In the steady-state, we consider a trajectory over a given time window $[0, t_{\rm obs}]$ that visits K configurations:

$$\mathscr{C}_0 \to \mathscr{C}_1 \to \ldots \to \mathscr{C}_{K-1} \to \mathscr{C}_K \tag{285}$$

where $\mathscr{C}_0$ is sampled from the steady-state distribution $P_{\rm ss}$. Determine the corresponding trajectory-dependent observable $\overline{Q}[\text{traj}] = \ln \frac{\mathscr{P}[\text{traj}]}{\mathscr{P}[\text{traj}^{\rm R}]}$ in terms of the transition rates $W(\mathscr{C}_i \to \mathscr{C}_{i+1})$, $j = 0, \ldots, K-1$, and in terms of $P_{\rm ss}(\mathscr{C}_0)$ and $P_{\rm ss}(\mathscr{C}_K)$ ($\mathscr{P}$[traj] refers to the probability of observing the trajectory "traj").

2. Simplify the above expression for a trajectory whose final state coincides with the initial one $\mathscr{C}_K = \mathscr{C}_0$.

3. Show that, for a trajectory whose final state coincides with the initial one, if the dynamics further satisfies the detailed balance condition then one has $\overline{Q}[\text{traj}] = 0$.

Mean-field approximation

In this set of questions, we forget about space: the system is assumed to be well mixed at all times. We are interested in the number n of A particles in the system. This number n is assumed to be extensive, namely proportional to the total number of lattice sites N (and this total number of sites N is very large). Under these conditions, the rate W_+ at which this total number of particles increases by one unit is

$$W_+(n \to n+1) = k_0 N + k_2 \frac{n(n-1)}{2N} \tag{288}$$

where the appearance of N is designed to keep n a typically extensive observable.

4. Express the rate $W_-(n \to n-1)$ at which the total number of particles decreases by one unit in terms of k_1, k_3, n and N.

5. Let $P(n,t)$ be the probability that the system contains n particles at time t. Write the master equation for $P(n,t)$ in the form $\frac{\mathrm{d}P(n,t)}{\mathrm{d}t} = J_{n-1\to n} - J_{n\to n+1}$ where $J_{n\to n+1}$ is the mean-probability flow between a state with n particles and a state with $n+1$ particles. Express $J_{n\to n+1}$ in terms of $P(n,t)$, $P(n+1,t)$, and of the rates W_+ and W_-.

6. At this global level of description (in terms of the total particle number n), what is the condition on $J_{n\to n+1}$ for the steady-state distribution $P_{\text{eq}}(n)$ to be an equilibrium one? Make sure this condition leads to a nontrivial acceptable equilibrium steady-state distribution.

7. Show that $\frac{\mathrm{d}\langle n\rangle}{\mathrm{d}t} = \langle W_+(n \to n+1) - W_-(n \to n-1)\rangle$.

8. We write the random variable $\rho = \frac{n}{N}$ in the form $\rho = \frac{n}{N} = \frac{\langle n\rangle}{N} + \chi$? What is the order in N of the variance of the random variable χ? Show that, up to a negligible fluctuating part (as $N \gg 1$), we have

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -f'(\rho),\; f(\rho) = -k_0\rho + \frac{1}{2}k_1\rho^2 - \frac{1}{3!}k_2\rho^3 + \frac{1}{4!}k_3\rho^4 \tag{293}$$

Could you have written this equation from the beginning based on heuristic arguments?

9. Within this mean-field approach in which there is no underlying space, we expect that for large N the equilibrium distribution behaves as $P_{\text{eq}}(n) \sim \mathrm{e}^{-Nh(n/N)}$ where h is an intensive function of the intensive parameter $\rho = n/N$. If one plugs this form of $P_{\text{eq}}(n)$ into the master equation, show that, as $N \to +\infty$, this leads to the following equation for $h(\rho)$:

$$0 = \left(k_0 + k_2 \frac{\rho^2}{2}\right)\left(\mathrm{e}^{h'} - 1\right) + \left(k_1 \rho + k_3 \frac{\rho^3}{3!}\right)\left(\mathrm{e}^{-h'} - 1\right), \; h' = \frac{\mathrm{d}h}{\mathrm{d}\rho} \tag{297}$$

Do not explicitly solve for h (the explicit h will be given further down).

10. Show that the extremas of h correspond to $f' = 0$.

11. The expression for h reads

$$\begin{aligned} h(\rho) = &- \underbrace{\ln \frac{k_0}{k_1}}_{\text{physical meaning?}} \rho + \underbrace{\rho \ln \rho - \rho}_{\text{physical meaning?}} \\ &- 2\sqrt{\frac{k_0}{k_2}} \arctan\left(\sqrt{\frac{k_2}{k_0}}\rho\right) + 2\sqrt{\frac{k_3}{k_1}} \arctan\left(\sqrt{\frac{k_3}{k_1}}\rho\right) \\ &- \rho \ln\left(\frac{1 + k_2\rho/k_0}{1 + k_3\rho^2/k_1}\right) \end{aligned} \tag{301}$$

What are the respective physical interpretations of the two terms in Eq. (301) above the braces?

12. It is of course possible to rewrite the evolution equation Eq. (293) in terms of h:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -m(\rho)h'(\rho) + \text{a noise term negligible in the } N \to +\infty \text{ limit} \tag{302}$$

where $m(\rho) = \frac{f'(\rho)}{h'(\rho)}$. Explain in simple qualitative terms what the noise term should be in Eq. (302). Express its variance in terms of $m(\rho)$ and of N. This is a multiplicative noise (its variance depends on ρ), but why is it nevertheless irrelevant to specify the underlying discretization of the stochastic equation Eq. (302)?

13. For the sake of discussion, up to changing the time and density units, two of the constants can be fixed. We choose $k_2 = 3$ and $k_3 = 1$, while k_0 and k_1 are yet unspecified. In Fig. 1 we show a plot of $f'(\rho) + k_0$ for various values of k_1: Discuss the number of possible steady-state values of ρ in terms of k_0 and k_1 whenever $k_1 \geq 3$.

14. Consider now the $k_1 \leq 3$ situation. If there exist several possible values of the density, discuss their stability. If ρ_- and ρ_+ are, respectively, the smallest and the largest possible steady-state values, discuss the state of the system in terms of $f(\rho_\pm)$ and $h(\rho_\pm)$. Could you draw an analogy with a familiar physical phenomenon that occurs in equilibrium?

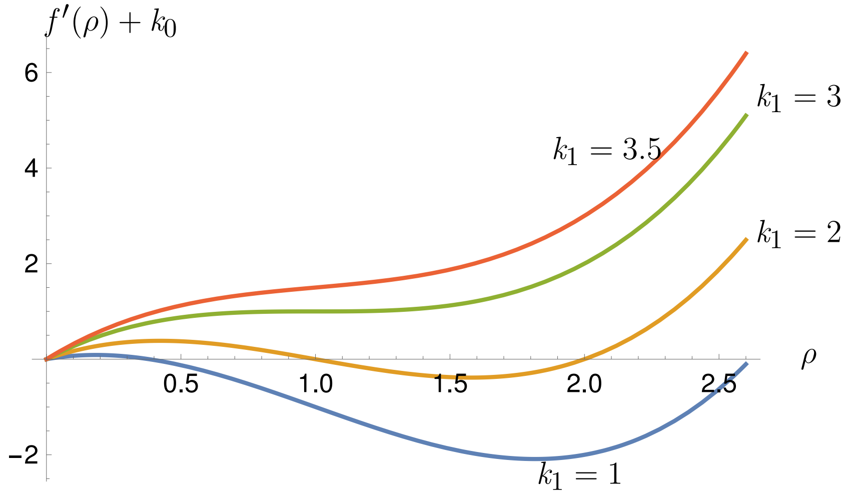

Figure 1: For $k_1 \geq 3$ the function is monotonous.

15. In their 2012 article, Tănase-Nicola and Lubensky find that in the original microscopic model described in the introduction, the density picked by the system in its stationary state can actually depend on the value of the diffusion constant (hor hopping rate) D. How can this be?

Mesoscopic approach in terms of a stochastic partial differential equation

We take our inspiration from the above mean-field approach, in which space is forgotten because a strong homogeneization is assumed, to come back to the original problem, defined in an extended space with diffusion, and our goal is to capture fluctuations by postulating a Langevin equation for the local fluctuating density of particles, which we denote by $\rho(\mathbf{r}, t)$. Here $\rho(\mathbf{r}, t)$ is the coarse grained-version of the local fluctuating occupation number $n_{\mathbf{x}}(t)$, where $\mathbf{r}$ is the coarse-grained position built from the lattice site $\mathbf{x}$. We postulate that

$$\partial_t \rho(\mathbf{r}, t) = -f'(\rho(\mathbf{r}, t)) + \underset{\text{deterministic part}}{\ldots} + \underset{\text{some noise with zero mean}}{\xi(\mathbf{r}, t)} \tag{304}$$

16. What expression (in terms of $\rho(\mathbf{r}, t)$) would you suggest for the missing deterministic part?

17. Assume that the noise is white with correlations $\langle \xi(\mathbf{r}, t)\xi(\mathbf{r}', t')\rangle = 2\gamma(\rho(\mathbf{r}, t))\delta^{(d)}(\mathbf{r} - \mathbf{r}')\delta(t - t')$. Why is $\gamma(0)$ necessarily nonzero?

18. Now we approximate the noise amplitude $\gamma(\rho(\mathbf{r}, t))$ with the constant $\Gamma = \gamma(0)$. Explain why the dynamics Eq. (304) is an equilibrium one, and determine the functional $\mathscr{F} = \int \mathrm{d}^d r \, [\ldots]$ such that $P_{\text{eq}}[\rho] \sim \mathrm{e}^{-\frac{1}{\Gamma}\mathscr{F}[\rho]}$.

19. Let ρ_{ss} the homogeneous mean-field steady-state value picked by the system and let $\psi(\mathbf{r}, t) = \rho(\mathbf{r}, t) - \rho_{\text{ss}}$. For small fluctuations around ρ_{ss}, one can write that the Fourier

modes $\tilde{\psi}_{\mathbf{q}}(t)$ evolve according to

$$\partial_t \tilde{\psi}_{\mathbf{q}} = -\lambda_{\mathbf{q}} \tilde{\psi}_{\mathbf{q}} + \sqrt{2\Gamma}\tilde{\xi}_{\mathbf{q}}(t),\ \langle \tilde{\xi}_{\mathbf{q}}(t)\tilde{\xi}_{\mathbf{q}'}(t')\rangle = (2\pi)^d \delta^{(d)}(\mathbf{q}+\mathbf{q}')\delta(t-t') \tag{306}$$

Express $\lambda_{\mathbf{q}}$ in terms of $f''(\rho_{\rm ss})$, $\mathbf{q}$ and D.

20. In the steady-state, determine the dots in $\langle \tilde{\psi}_{\mathbf{q}}(t)\tilde{\psi}_{\mathbf{q}'}(0)\rangle = (2\pi)^d \delta^{(d)}(\mathbf{q}+\mathbf{q}') \times \ldots$ in terms of t, Γ and of $\lambda_{\mathbf{q}}$.

21. Prove that $\langle \rho(\mathbf{r},t)^2\rangle = \rho_{\rm ss}^2 + \langle \psi(\mathbf{r},t)^2\rangle$. Use this to make a statement on how fluctuations effectively affect some of the reaction rates k_i.

22. What have you learnt that would allow you to answer question 15 more precisely?

Back to the microscopic model

23. Consider now a spatially extended system on a lattice (at the microscopic level) where each lattice site $\mathbf{x}$ has $n_{\mathbf{x}} = 0, 1, 2\ldots$ particles. Consider two nearest neighbor lattice sites $\mathbf{x}$ and $\mathbf{y}$, each of them being initially occupied by two particles. Our interest goes to the sequence of states:

$$\mathscr{C}_0 = (n_{\mathbf{x}}, n_{\mathbf{y}}) = (2,2) \to \mathscr{C}_1 = (1,3) \to \mathscr{C}_2 = (1,2) \to \mathscr{C}_0 = (2,2) \tag{309}$$

where the initial state with two particles in $\mathbf{x}$ and $\mathbf{y}$ is sampled from the steady-state distribution. Express the corresponding $\overline{Q}[\text{traj}]$ for this sequence of states in terms of the rates k_i, $i = 0, 1, 2, 3$ and of the hopping rate D. For the change of the local particle number $n_{\mathbf{x}}$ use the mean-field rates $W_\pm(n_{\mathbf{x}} \to n_{\mathbf{x}} \pm 1)$ after setting $N = 1$.

24. Show that the steady-state of the original microscopic model cannot be an equilibrium state (it may be useful to use the results of questions 1, 2 and 3).

25. Would you be able to construct a field theory describing the microscopic dynamics?

6 Exactly solvable models

6.1 Quantum formulation of classical stochastic dynamics

A single site can be either occupied ($n = 1$) or empty ($n = 0$). The transition rates between the two possible states are $w(0 \to 1) = \alpha$ and $w(1 \to 0) = \gamma$.

1. Write the master equation for the probability $P(n,t)$ that the site is in state n at time t.

2. Find the stationary solution $P_{\rm ss}(n)$ as a function of n, α and γ. Show that the stationary solution can be cast in the form $P_{\rm ss}(n) = \frac{1}{Z}\mathrm{e}^{-\beta\mathcal{H}}$ where $\mathcal{H} = -h\sigma$, with $\sigma = 2n-1$ (connect β and h to α and γ).

3. After writing an envolution equation for $\langle n(t)\rangle$, check that in the stationary state $\langle n\rangle = \frac{z}{1+z}$ with $z = \alpha/\gamma$. What is the typical time it takes to relax to that stationary value? Express $\langle\sigma\rangle$ in terms of β and h.

4. Is the detailed balance condition satisfied (is $P_{\rm ss}$ a genuine equilibrium distribution)?

5. Using the spin language, we denote by $|\sigma = -1\rangle$ and $|\sigma = +1\rangle$ the empty and occupied states and we define $|\psi(t)\rangle = P(1, t)|1\rangle + P(-1, t)|-1\rangle$ (where $P(\pm 1, t)$ stand for the probability to find a $|\pm 1\rangle$ state at time t. Show that $\frac{\mathrm{d}|\psi\rangle}{\mathrm{d}t} = -\hat{H}|\psi\rangle$ with $\hat{H} = \alpha(1-\sigma^x)\frac{1-\sigma^z}{2} + \gamma(1-\sigma^x)\frac{1+\sigma^z}{2}$ where the operators σ^α acting in the $|\pm 1\rangle$ space are the standard Pauli matrices.

6. Let $\langle p| = \langle -1| + \langle +1|$. Show that $\langle p|$ is a left eignevector of $\hat{H}$. What is its eigenvalue? What is the physical meaning of this property?

7. What is the right eigenvector associated to the same eigenvalue as in question6? Write it in the $|\pm 1\rangle$ basis.

8. What is the other eigenvalue of $\hat{H}$. Could you have guessed it?

6.2 Current distribution in a TASEP with periodic boundary conditions

A set of N mutually excluding particles perform a biased random walk on a one-dimensional lattice with L sites and with periodic boundary condititions. The probability that, between t and $t+\mathrm{d}t$, a particle hops to the nearest neighbor to its right is $\mathrm{d}t$ (provided the target set is empty), while it is simply zero to the left. This is the Totally Asymmetric Simple Exclusion Process (TASEP). We denote by σ_i the state of site i, $i = 1, \ldots, L$, with the convention that an occupied site has $\sigma_i = +1$ and an empty site has $\sigma_i = -1$.

The steady-state phase diagram of this model is rather trivial (by contrast to its open-ended version), which led Derrida and Lebowitz [16] to believing that it would be possible to characterize such a dynamical property as the particle current flowing through the system over a large time window. They managed to determine the distribution of this time-integrated current, showing that atypical trajectories harboring a less-than-typical current were markedly different from their counterparts with a larger-than-typical current. This can be considered as the first explicit example, in a many body system, of an emergent dynamical phase transition. Though we will stay away from the technicalities of the original article, we will show that some of the results in [16] can be recovered by means of an analogy with a problem of free fermions.

1. What does quantity $\frac{1}{2}\sum_{i=1}^{L}(1+\sigma_i(t))$ represent? Does it depend on time?

2. Write an evolution equation for $\langle\sigma_i\rangle$ at time t in terms of the local averages $\langle\sigma_i\rangle$ and $\langle\sigma_i\sigma_{i\pm 1}\rangle$ at time t. Check the consistency of your equation with the result of question

1. It may be useful to introduce $J_{j+1} = \langle \frac{1+\sigma_j}{2}\frac{1-\sigma_{j+1}}{2}\rangle$ the physical meaning of which will be explained.

3. Let $P(\sigma_1, \ldots, \sigma_L, t)$ the probability to observe a given configuration of the lattice specified by $\sigma_1, \ldots, \sigma_L$. A tired professor finds that P evolves according to

$$\partial_t P(\sigma_1, \ldots, \sigma_L, t) = \sum_j \left[\frac{1+\sigma_j}{2}\frac{1-\sigma_{j+1}}{2} P(\sigma_1, \ldots, -\sigma_j, -\sigma_{j+1}, \ldots, \sigma_L, t) \right. \\ \left. - \frac{1+\sigma_j}{2}\frac{1-\sigma_{j+1}}{2} P(\sigma_1, \ldots, \sigma_j, \sigma_{j+1}, \ldots, \sigma_L, t) \right] \tag{321}$$

Explain the meaning of each of the two terms in the right hand side. Locate, and then correct the two sign mistakes (explain your correction). Keep the discussion to a few words. This is not an essay.

4. Either using the (corrected) master equation of question 3 or a less technical reasoning, show that $\frac{\mathrm{d}}{\mathrm{d}t}\langle \sigma_i \sigma_{i+1}\rangle$ actually involves not only two-point but also three-point correlations.

5. Show that in the steady-state, $P_{\text{ss}}(\sigma_1, \ldots, \sigma_L) = \frac{1}{\binom{L}{N}}$ is the solution of the master equation. Does this configuration-independent solution verify the detailed balance condition? Is P_{ss} an equilibrium distribution?

6. Show that in the steady-state, J_j as defined in question 2 is independent of j in the steady-state and give its expression J in terms of N and L.

7. We construct a vector space with the configurations $\boldsymbol{\sigma} = \{\sigma_1, \ldots, \sigma_L\}$, and we denote its basis vectors by $|\boldsymbol{\sigma}\rangle = |\sigma_1, \ldots, \sigma_L\rangle$. Let $|\psi(t)\rangle = \sum_{\boldsymbol{\sigma}} P(\boldsymbol{\sigma}, t)|\boldsymbol{\sigma}\rangle$. Show that

$$\frac{\mathrm{d}|\psi\rangle}{\mathrm{d}t} = -\hat{H}|\psi\rangle \tag{327}$$

where

$$\hat{H} = \sum_j (1 - \sigma_j^x \sigma_{j+1}^x)\frac{1+\sigma_j^z}{2}\frac{1-\sigma_{j+1}^z}{2} \tag{328}$$

where the σ_j^α's are the Pauli matrices ($\alpha = x, y, z$).

8. Let $Q(t)$ be the total number of particle hops that have occurred between 0 and t (this is the total, space-integrated, particle current). Express the steady-state average $\langle Q\rangle$ in terms of J, t and L (the initial state is sampled from the steady-state distribution).

9. Write the master equation for the probability $P(\sigma_1, \ldots, \sigma_L, Q, t)$ that the system is in configuration $\boldsymbol{\sigma}$ at time t having accumulated a value Q for $Q(t)$.

10. Let $\tilde{P}(\boldsymbol{\sigma}, \lambda, t) = \sum_Q \mathrm{e}^{-\lambda Q} P(\boldsymbol{\sigma}, Q, t)$. What is the evolution equation satisfied by $\tilde{P}$?

11. Show that $|\psi(t)\rangle = \sum_{\boldsymbol{\sigma}} \tilde{P}(\boldsymbol{\sigma}, \lambda, t)|\boldsymbol{\sigma}\rangle$ evolves according to $\frac{\mathrm{d}|\psi\rangle}{\mathrm{d}t} = -\hat{H}(\lambda)|\psi\rangle$. How is the operator $\hat{H}(\lambda)$ modified (by λ-dependent factors) with respect to the expression given in Eq. (328).

12. Let $\mu(\lambda)$ be the smallest eigenvalue of $\hat{H}(\lambda)$. What is $\mu(0)$? Explain why, at large times, $\langle \mathrm{e}^{-\lambda Q(t)}\rangle \sim \mathrm{e}^{-t\mu(\lambda)}$. If $\mu(\lambda)$ were known, how could we then extract the pdf of $Q(t)$ at large time?

We would like to determine $\mu(\lambda)$ as a function of λ. This is in general rather difficult, but at least the $\lambda \to -\infty$ regime is accessible at reasonable mathematical cost. To make progress we resort to a trick exploited by Jordan and Wigner [27] to convert a problem of interacting spins into one of interacting fermions (the trick can be valid beyond spin $\frac{1}{2}$, see [1]), at least in one space dimension. On a more formal level, this is also a trick that converts a problem of strongly interacting bosons into one of weakly interacting fermions, and as such it stands as one of the simplest examples of dual quantum field theories. This being said, the Jordan-Wigner transformation is mostly used in hard-condensed matter problems in one space dimension [18]. Attempts in higher space dimension have been proposed (see chapter 8 in [17]).

13. Let $\sigma_j^\pm = \frac{\sigma_j^x \pm i\sigma_j^y}{2}$ and let $c_j = \sigma_j^- \left(\prod_{i<j}(-\sigma_i^z)\right)$. Show that $\{c_n, c_m^\dagger\} = \delta_{nm}$ along with $\{c_n, c_m\} = \{c_n^\dagger, c_m^\dagger\} = 0$. Here $\{A, B\} = AB + BA$ refers to the anticommutator.

14. Express σ_i^- in terms of c_i and of the $\hat{n}_j = c_j^\dagger c_j$ for $j < i$.

15. Express $\sigma_i^- \sigma_{i+1}^+$ in terms of the fermionic operators.

16. Using the Jordan-Wigner transformation to fermionic operators, show that

$$\hat{H}(\lambda) = \sum_j \left[-\mathrm{e}^{-\lambda} c_{j+1}^\dagger c_j + c_j^\dagger c_j - c_j^\dagger c_j c_{j+1}^\dagger c_{j+1}\right] \tag{341}$$

17. We now take $L \gg 1$ and discard any potential issue related to boundary conditions (leading to subleading corrections in $L \gg 1$). Show that for $\lambda \to -\infty$, and $L \gg 1$, we can write that $\hat{H}(\lambda) \simeq -L\mathrm{e}^{-\lambda} \int_{-\pi}^{\pi} \frac{\mathrm{d}q}{2\pi} \mathrm{e}^{iq} \hat{n}_q$, where $\hat{n}_q = a_q^\dagger a_q$, $a_q = \sum_j \mathrm{e}^{iqj} c_j$.

18. For $\rho = N/L < 1/2$ we introduce κ such that $\int_{-\kappa}^{\kappa} \frac{\mathrm{d}q}{2\pi} = \rho$. Give the expression, for $\lambda \to -\infty$, of $\mu(\lambda)$ as a function of λ, L and κ.

19. In light of question 12, is there a regime of Q in which you can state the asymptotic behavior of $P(Q, t)$?

7 Critical Dynamics and Mesoscopic Descriptions

7.1 Kawasaki dynamics

An Ising model on a d-dimensional lattice is characterized by the Hamiltonian $\mathcal{H} = -\sum_{\langle i,j\rangle} \sigma_i \sigma_j$. The system is in contact with a thermostat at inverse temperature β. It is endowed with the following evolution rules: at time t a bond $\langle i,j\rangle$ connecting nearest neighbor sites is picked at random. With a probability $w(\sigma_i, \sigma_j \to \sigma_j, \sigma_i)\mathrm{d}t$, the spins σ_i and σ_j are swapped. This means that, denoting with a prime the spins after the change, $\sigma'_i = \sigma_j$ and $\sigma'_j = \sigma_i$.

1. These dynamical rules possess a conservation law. Which?

2. How would you tune $w(\sigma_i, \sigma_j \to \sigma_j, \sigma_i)$ so that the stationary distribution is the equilibrium one $P_{\mathrm{eq}} = \mathrm{e}^{-\beta\mathcal{H}}/Z$? Propose one possible explicit expression (among plenty of choices) for that rate. This will be assumed to hold for the following questions.

3. Close to the critical point, it is legitimate to replace σ_i with some coarse grained field $\phi(\mathbf{x}, t)$ living in continuous space and taking continuous values. Under the assumption that the dynamics of ϕ can be approximated with a Langevin equation, we write it in the form

$$\partial_t \phi = -\boldsymbol{\nabla} \cdot \mathbf{J} \tag{348}$$

   where $\mathbf{J}$ is some fluctuating field and noise dependent vector field. Why does the evolution of ϕ necessarily take up that form?

4. One can actually prove that $\mathbf{J} = -\boldsymbol{\nabla}\frac{\delta F}{\delta\phi} + \sqrt{2}\boldsymbol{\xi}(\mathbf{x}, t)$, where $\boldsymbol{\xi}$ is a Gaussian white random field and where $F[\phi] = \int \mathrm{d}^d x \left[\frac{1}{2}(\boldsymbol{\nabla}\phi)^2 + \frac{r}{2}\phi^2 + \frac{g}{4!}\phi^4\right]$. We want to prove this assertion when $g = 0$. To begin with, write the explicit expression of $\mathbf{J}$ in terms of ϕ.

5. Introducing the Fourier modes $\phi(\mathbf{q}, t)$ of the field, show that each of them evolves according to

$$\partial_t \phi(\mathbf{q}, t) = -\kappa_{\mathbf{q}}\phi(\mathbf{q}, t) + \sqrt{2} i\mathbf{q} \cdot \boldsymbol{\xi}(\mathbf{q}, t) \tag{350}$$

   where the expression of $\kappa_{\mathbf{q}}$ will be given in terms of $\mathbf{q}$ and of r. Note that this equation also means that the modes are independent.

6. Write a Fokker-Planck equation for the probability $P(\varphi(\mathbf{q}), t)$ that $\phi(\mathbf{q}, t)$ takes the value $\varphi(\mathbf{q})$ at time t.

7. Solve it in the long time limit and check that the assertion of question 4 is correct, at least for $g = 0$.

7.2 Critical dynamics of model C

Two fluctuating fields $\phi(\mathbf{x},t)$ and $\varepsilon(\mathbf{x},t)$ evolve according to the following coupled Langevin equations,

$$\partial_t\phi = -\Gamma\frac{\delta F}{\delta\phi} + \sqrt{2\Gamma}\xi(\mathbf{x},t),\ \partial_t\varepsilon = \Gamma'\boldsymbol{\nabla}^2\frac{\delta F}{\delta\varepsilon} + \sqrt{2\Gamma'}\boldsymbol{\nabla}\cdot\boldsymbol{\eta} \tag{352}$$

where $F[\phi,\varepsilon]$ is a functional of the two fields ϕ and ε, Γ and Γ' are positive constants, and finally $\xi(\mathbf{x},t)$, $\eta^\alpha(\mathbf{x},t)$ stand for Gaussian white noises with unit variance:

$$\langle\xi(\mathbf{x},t)\xi(\mathbf{x}',t')\rangle = \delta^{(d)}(\mathbf{x}-\mathbf{x}')\delta(t-t'),\ \langle\eta^\alpha(\mathbf{x},t)\eta^{\alpha'}(\mathbf{x}',t')\rangle = \delta^{\alpha\alpha'}\delta^{(d)}(\mathbf{x}-\mathbf{x}')\delta(t-t') \tag{353}$$

The indices $\alpha = 1,\ldots,d$ refer to the d space dimensions the system lives in.

We first wish to establish that at large times, ϕ and ε are sampled from the equilibrium distribution $P_{\rm eq}[\phi,\varepsilon] = Z^{-1}\mathrm{e}^{-F[\phi,\varepsilon]}$, irrespective of the explicit form of F.

1. One of the two fields is said to be conserved. Which is it, and what does it mean?
2. Let $\zeta = \boldsymbol{\nabla}\cdot\boldsymbol{\eta}$. Explain why one has $\langle\zeta(\mathbf{x},t)\zeta(\mathbf{x}',t')\rangle = -\boldsymbol{\nabla}^2_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{x}')\delta(t-t')$.
3. Starting from the fact that $\mathcal{P}[\xi,\zeta] \propto \mathrm{e}^{-\frac{1}{2}\int \mathrm{d}t\mathrm{d}^dx(\xi^2+\zeta(-\boldsymbol{\nabla}^2)^{-1}\zeta)}$, explain why a realization of the fields over the time interval $[0,t_{\rm obs}]$ has a weight

$$\mathcal{P}[\phi,\varepsilon] \propto \mathrm{e}^{-\frac{1}{4\Gamma}\int_{\mathbf{x}}\int_0^{t_{\rm obs}}\mathrm{d}t\left[\partial_t\phi+\Gamma\frac{\delta F}{\delta\phi}\right]^2 - \frac{1}{4\Gamma'}\int_{\mathbf{x}}\int_0^{t_{\rm obs}}\mathrm{d}t\left(\partial_t\varepsilon-\Gamma'\boldsymbol{\nabla}^2\frac{\delta F}{\delta\varepsilon}\right)(-\boldsymbol{\nabla}^2)^{-1}\left(\partial_t\varepsilon-\Gamma'\boldsymbol{\nabla}^2\frac{\delta F}{\delta\varepsilon}\right)} \tag{355}$$

   where the initial value of the fields is fixed to $\phi(\mathbf{x},0)$ and $\varepsilon(\mathbf{x},0)$. Here the notation $(-\boldsymbol{\nabla}^2)^{-1}$ refers to the Green's functions of the Laplacian : formally one should actually write $(-\boldsymbol{\nabla}^2)^{-1}(\mathbf{x},\mathbf{x}') = G(\mathbf{x},\mathbf{x}')$ and $G(-\boldsymbol{\nabla}^2) = 1$ actually means $-\boldsymbol{\nabla}^2_{\mathbf{x}}G(\mathbf{x},\mathbf{x}') = \delta^{(d)}(\mathbf{x}-\mathbf{x}')$. Do not bother to be too explicit here (the idea is not to be rigorous with Green's functions).

4. By changing t into $t_{\rm obs}-t$ one obtains the weight of a time-reversed realization of the two fields. Show that

$$\sigma = \frac{1}{t_{\rm obs}}\ln\frac{\mathcal{P}[\phi,\varepsilon,\text{forward in time}]}{\mathcal{P}[\phi,\varepsilon,\text{backward in time}]} = -\frac{1}{t_{\rm obs}}\int_0^{t_{\rm obs}}\mathrm{d}t\int_{\mathbf{x}}\left[\partial_t\phi\frac{\delta F}{\delta\phi}+\partial_t\varepsilon\frac{\delta F}{\delta\varepsilon}\right] \tag{357}$$

5. What is the physical meaning of σ?
6. If now the initial and final fields (at $t=0$ and at $t=t_{\rm obs}$) are sampled from $\mathrm{e}^{-F[\phi,\varepsilon]}$, $\mathcal{P}[\phi,\varepsilon,\text{forward in time}]$ picks up an additional prefactor $\mathrm{e}^{-F[\phi(\mathbf{x},0),\varepsilon(\mathbf{x},0)]}$ and $\mathcal{P}[\phi,\varepsilon,\text{backward in time}]$ picks up a similar $\mathrm{e}^{-F[\phi(\mathbf{x},t_{\rm obs}),\varepsilon(\mathbf{x},t_{\rm obs})]}$ prefactor. What's the new simplified value of σ? What does it teach us regarding the stationary distribution of the fields?

We now specialize our analysis to the case in which

$$F[\phi,\varepsilon] = \int \mathrm{d}^d x \left[\frac{1}{2}(\boldsymbol{\nabla}\phi)^2 + \frac{r}{2}\phi^2 + \frac{g}{4!}\phi^4 + \frac{1}{2}\varepsilon^2 + \frac{u}{2}\varepsilon\phi^2\right] \tag{359}$$

7. Show that partially integrating the partition function over energies, $\int \mathcal{D}\varepsilon \mathrm{e}^{-F[\phi,\varepsilon]}$, leads to an effective standard ϕ^4 theory in which g has been changed into g' (give the connection between g, g' and u, and assume that $g' > 0$). What does it teach you regarding the equilibrium phase diagram of ϕ alone?

8. From a purely static point of view, would you say the coupling u is relevant when it comes to affecting the critical behavior of the magnetization field ϕ below 4 space dimensions? It may be useful to find the scaling dimension of u.

When interested in dynamical properties in the vicinity of the critical point for the field ϕ, we know that the typical relaxation time τ and the correlation length ξ are related by a scaling relation of the form $\tau \sim \xi^z$, where z is a dynamical exponent.

9. Based on your intuition or on a simple analysis, what will the value of z be in a mean-field approximation?

10. To investigate the z exponent a little further, we write the Martin-Siggia-Rose-Janssen-De Dominicis action for the fields ϕ and ε, and for the related response fields $\bar{\phi}$ and $\bar{\varepsilon}$. You are asked to write on your exam sheet the three *missing terms* only (do not copy the full expression). The dynamical action reads

$$\begin{aligned} S[\bar{\phi},\bar{\varepsilon},\phi,\varepsilon] = \int \mathrm{d}t\mathrm{d}^d x \Big[&\bar{\phi}\partial_t\phi + \mathit{\Gamma}\boldsymbol{\nabla}\bar{\phi}\cdot\boldsymbol{\nabla}\phi + \mathit{\Gamma} r\bar{\phi}\phi + \mathit{\Gamma}\frac{g}{3!}\bar{\phi}\phi^3 \\ &-\mathit{\Gamma}\times\left\{\text{missing term 1, involving only } \bar{\phi}\right\} \\ &+\bar{\varepsilon}\partial_t\varepsilon + \mathit{\Gamma}'\boldsymbol{\nabla}\bar{\varepsilon}\cdot\boldsymbol{\nabla}\varepsilon - \mathit{\Gamma}'(\boldsymbol{\nabla}\bar{\varepsilon})^2 \\ &+\mathit{\Gamma} u\bar{\phi}\times\{\text{missing term 2, involving } \phi \text{ and } \varepsilon\} \\ &-\mathit{\Gamma}' u\boldsymbol{\nabla}^2\bar{\varepsilon}\times\{\text{missing term 3, involving only } \phi\}\Big] \end{aligned} \tag{361}$$

11. Show that $S[\bar{\phi},\bar{\varepsilon},\phi,\varepsilon+c]$, where c is an arbitrary real number, is the same as $S[\bar{\phi},\bar{\varepsilon},\phi,\varepsilon]$ up to a redefinition of one of the couplings. Which is the concerned coupling and how is it changed? By couplings, we mean either of the various constants appearing in the dynamical action ($\mathit{\Gamma}$, $\mathit{\Gamma}'$, r, g, or u).

12. There are techniques for exploiting a continuous symmetry of an action. When implemented for this particular invariance under a shift of ε, they lead to equalities between correlation functions which, in turn, enforce the condition $z = 2 + \frac{\alpha}{\nu}$. This is of course the mathematical translation of a physical property of the system. Which one are we talking about?

7.3 Critical dynamics of a lattice gas

Consider an Ising spin system where a spin σ_i labels the presence ($\sigma_i = +1$) or absence ($\sigma_i = -1$) of a particle at lattice site i. The chemical potential is adjusted so that there is, in the equivalent Ising model, no magnetic field. The energy of a configuration $\{\sigma_i\}_{i=1,\ldots,N}$ is

$$E[\{\sigma_i\}] = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{363}$$

where the brackets $\langle i,j \rangle$ refer to distinct pairs of nearest neighbor sites. The spins are endowed with the following update rule: At time t, a bond of nearest neighbors $\langle i,j \rangle$ is picked at random. With a probability $\gamma \mathrm{d}t$ the two spins are exchanged between t and $t+\mathrm{d}t$ on condition that the energy E of the system remains constant, in the sense that $\sigma_i(t), \sigma_j(t) \to \sigma'_i(t+\mathrm{d}t) = \sigma_j(t), \sigma'_j(t+\mathrm{d}t) = \sigma_i(t)$ if the move is allowed by the condition

$$E = E(\ldots, \sigma_i(t), \sigma_j(t), \ldots] = E(\ldots, \sigma_j(t), \sigma_i(t), \ldots] \tag{364}$$

Else, no update is implemented. This model was introduced by Kadanoff and Swift [29] in 1968 (*Transport Coefficients near the Critical Point: A Master-Equation Approach*) in an effort to investigate the role of conservation laws in dynamical processes.

1. We label a configuration of the spins by $\mathscr{C}(t) = \{\sigma_i(t)\}$. If there is a change of configuration between t and $t+\mathrm{d}t$ from $\mathscr{C}$ to $\mathscr{C}'$, what is the value of the ratio $\frac{W(\mathscr{C}\to\mathscr{C}')}{W(\mathscr{C}'\to\mathscr{C})}$, where $W(\mathscr{C}\to\mathscr{C}')$ is the rate at which the system hops from configuration $\mathscr{C}$ to configuration $\mathscr{C}'$?

2. Throughout a time interval $[0, t_{\mathrm{obs}}]$ the system will visit a sequence of states $\mathscr{C}_0, \ldots, \mathscr{C}_K$ (where K is an integer). Determine $\sum_{k=0}^{K} \ln \frac{W(\mathscr{C}_k\to\mathscr{C}_{k+1})}{W(\mathscr{C}_{k+1}\to\mathscr{C}_k)}$. Is the stationary state an equilibrium one?

3. What is the stationary probability $P(\{\sigma_i\})$ of observing a given configuration $\{\sigma_i\}$ of the N spins making up the system?

4. What are the two conservation laws that these proposed dynamical evolution rules respect?

5. We assume that there is a regime (of the total energy) in which the system develops long range correlations. In this regime a coarse grained description of the system is possible. We use $\phi(\mathbf{x}, t)$ and $\varepsilon(\mathbf{x}, t)$ to refer to the local magnetization and to the local energy density. They are respectively coarse-grained versions of σ_i and of $-J\sum_{j \text{ a nn of } i} \sigma_i \sigma_j + 2E/N$ (ε is actually a local fluctuating deviation with respect to the average energy density). The energy of the system in terms of these fields is postulated to be

$$H[\phi(\mathbf{x}), \varepsilon(\mathbf{x})] = \int \mathrm{d}^d x \left[\frac{1}{2}(\boldsymbol{\nabla}\phi)^2 + \frac{r}{2}\phi^2 + \frac{g_1}{4!}\phi^4 + \frac{1}{2}\varepsilon^2 + \frac{g_2}{2}\varepsilon\phi^2\right] \tag{365}$$

Write and solve the stationary mean-field equations for ϕ and ε (discuss your result according to the sign of the phenomenological parameter r). We further assume that $g = g_1 - 3g_2^2 > 0$.

6. We now want that ϕ and ε evolve in time respectfully of the original symmetries and conservation laws of the microscopic model. We *a priori* write

$$\partial_t \phi = -\boldsymbol{\nabla} \cdot \mathbf{j},\ \partial_t \varepsilon = -\boldsymbol{\nabla} \cdot \mathbf{q} \tag{368}$$

where $\mathbf{j}(\mathbf{x}, t)$ and $\mathbf{q}(\mathbf{x}, t)$ are flucuating vector fields whose physical meanings will be given. Why do we write a first-order-in-time differential equation for ϕ and ε? Why do we write an evolution equation with the divergence of a vector field in the right-hand side?

7. We suggest that $\mathbf{j} = -\Gamma \boldsymbol{\nabla} \frac{\delta H}{\delta \phi} + \sqrt{2\Gamma'} \boldsymbol{\xi}$, with the spatial components of $\boldsymbol{\xi}$ being Gaussian white noises: $\langle \xi^\alpha(\mathbf{x}, t) \xi^\beta(\mathbf{x}', t') \rangle = \delta^{\alpha\beta} \delta^{(d)}(\mathbf{x} - \mathbf{x}') \delta(t - t')$. Explain why $\boldsymbol{\nabla} \cdot \boldsymbol{\xi}(\mathbf{x}, t)$ is a Gaussian white noise and give its correlations $\langle \boldsymbol{\nabla} \cdot \boldsymbol{\xi}(\mathbf{x}, t) \boldsymbol{\nabla}' \cdot \boldsymbol{\xi}(\mathbf{x}', t') \rangle$.

8. We postulate that $\mathbf{q} = -\Gamma'' \boldsymbol{\nabla}(\ldots) + \sqrt{2\Gamma'''} \boldsymbol{\zeta}$, where the spatial components of $\boldsymbol{\zeta}$ are Gaussian white noises: $\langle \zeta^\alpha(\mathbf{x}, t) \zeta^\beta(\mathbf{x}', t') \rangle = \delta^{\alpha\beta} \delta^{(d)}(\mathbf{x} - \mathbf{x}') \delta(t - t')$. Fill in the ... with a sensible expression.

9. Given a fixed initial configuration $\phi(\mathbf{x}, 0)$ and $\varepsilon(\mathbf{x}, 0)$ and a final configuration $\phi(\mathbf{x}, t_{\text{obs}})$ and $\varepsilon(\mathbf{x}, t_{\text{obs}})$ after a time t_{obs}, we are interested in the probability $\mathscr{P}[\phi(\mathbf{x}, t), \varepsilon(\mathbf{x}, t); 0 \to t_{\text{obs}}]$ of a realization of boths fields connecting their initial value to their value at t_{obs}. Show that

$$\frac{\mathscr{P}[\phi(\mathbf{x}, t), \varepsilon(\mathbf{x}, t); 0 \to t_{\text{obs}}]}{\mathscr{P}[\phi(\mathbf{x}, t_{\text{obs}} - t), \varepsilon(\mathbf{x}, t_{\text{obs}} - t); 0 \to t_{\text{obs}}]} = \mathrm{e}^{-(a) \int \mathrm{d}t \int \mathrm{d}^d x \partial_t \phi \frac{\delta H}{\delta \phi} - \frac{\Gamma''}{\Gamma'''} \int \mathrm{d}t \int \mathrm{d}^d x (b)} \tag{369}$$

Express (a) in terms of the various phenomenological constants involved in the dynamics and express (b) in terms of the fields.

10. What is(are) the condition(s) on the various phenomenological coefficients for the dynamics to be an equilibrium one?

11. We now sit in the disordered phase with $r > 0$ and we truncate to quadratic order. Write the Langevin equations for the spatial Fourier modes $\phi_{\mathbf{k}}(t)$ and $\varepsilon_{\mathbf{k}}(t)$ in the form

$$\partial_t \phi_{\mathbf{k}}(t) = -\lambda_{\mathbf{k}} \phi_{\mathbf{k}} - \lambda'_{\mathbf{k}} \varepsilon_{\mathbf{k}} + \sqrt{2\Gamma'} i\mathbf{k} \cdot \boldsymbol{\xi}_{\mathbf{k}}(t),\ \partial_t \varepsilon_{\mathbf{k}}(t) = -\kappa_{\mathbf{k}} \varepsilon_{\mathbf{k}} - \kappa'_{\mathbf{k}} \phi_{\mathbf{k}} + \sqrt{2\Gamma'''} i\mathbf{k} \cdot \boldsymbol{\zeta}_{\mathbf{k}}(t) \tag{370}$$

Express $\lambda_{\mathbf{k}}, \lambda'_{\mathbf{k}}, \kappa_{\mathbf{k}}, \kappa'_{\mathbf{k}}$ in terms of $\mathbf{k}$ and of the phenomenological constants.

12. Determine $\langle \phi_{\mathbf{k}}(t) \phi_{-\mathbf{k}}(t') \rangle$ in the stationary state. Use that expression to argue that a field fluctuation over a length scale $L \gg 1$ is smoothened out over a typical time τ_L to be specified. Show that for $r \to 0$, $\tau_L \propto L^z$ where the value of z will be given.

7.4 Coarsening dynamics of the $O(N)$ model in the limit $N \to \infty$

The goal of this tutorial is to study the phase ordering kinetics or "coarsening dynamics" following a quench from a homogeneous (high temperature) phase to a (low temperature) phase with broken symmetry. Systems quenched from a disordered phase into an ordered phase do not order instantaneously. Instead, the length scale of ordered regions grows with time as the different broken symmetry phases compete to select the equilibrium state [7, 4]. To fix our ideas, it is helpful to consider the simplest, and most familiar, system: the ferromagnetic Ising model. At time $t = 0$, the system is quenched from an initial temperature T_i above the critical point T_c to a final temperature T_f below T_c. At T_f, there are two equilibrium phases, with magnetization $\pm M_0$. Immediately after the quench however, the system is in an unstable disordered state corresponding to equilibrium at temperature T_i. The theory of phase ordering kinetics is concerned with the dynamical evolution of the system from the initial disordered state to the final equilibrium state.

A useful model to study such ferromagnetic systems is the continuous Ginzburg-Landau $O(N)$ model defined, in d spatial dimensions, by the Hamiltonian

$$\mathcal{H}[\boldsymbol{\phi}] = \int_V d^d x \left[\frac{1}{2}(\nabla\boldsymbol{\phi})^2 + \frac{r}{2}\boldsymbol{\phi}^2 + \frac{g}{4N}(\boldsymbol{\phi}^2)^2\right] \tag{373}$$

where $\boldsymbol{\phi} = (\phi_1, \phi_2, \cdots, \phi_N)$ is a N-component vector field and V is the volume of the system (and we consider periodic boundary conditions). In Eq. (373), we used the shortcut $\boldsymbol{\phi} = \boldsymbol{\phi}(\mathbf{x})$ where $\mathbf{x} \in \mathbb{R}^d$ and we denote $\boldsymbol{\phi}^2 = \sum_{a=1}^N \phi_a^2$ as well as $(\nabla\boldsymbol{\phi})^2 = \sum_{a=1}^N (\nabla\phi_a)^2$ while r and g denote respectively the distance from the critical temperature ($r < 0$ corresponding to the ferromagnetic phase) and the coupling constant. These models with different finite values of $N = 1, 2, 3$ correspond respectively to the Ising, XY or Heisenberg universality classes. We focus here on the purely relaxational dynamics which is described by the Langevin equation

$$\gamma\frac{\partial\phi_a}{\partial t} = -\frac{\delta\mathcal{H}}{\delta\phi_a} + h_a(\mathbf{x}, t) + \eta_a(\mathbf{x}, t) \tag{374}$$

for $a = 1, 2, \cdots, N$ and where γ is the friction coefficient, and we set $\gamma = 1$ in the following. In Eq. (374), $\eta_a(\mathbf{x}, t)$ are independent Gaussian white noises of zero mean $\langle\eta_a(\mathbf{x}, t)\rangle = 0$ and short-ranged diagonal correlations

$$\langle\eta_a(\mathbf{x}, t)\eta_b(\mathbf{x}', t)\rangle = 2k_{\mathrm{B}} T\delta_{a,b}\,\delta^d(\mathbf{x}-\mathbf{x}')\delta(t-t')\;, \tag{375}$$

with $a, b = 1, 2, \cdots, N$ and where T is the temperature of the bath (and in the following we will set the Boltzmann constant $k_{\mathrm{B}} = 1$, for convenience). In Eq. (374) we have added an infinitesimal external field $\mathbf{h}$ to compute response functions. The dynamical evolution of the system is fully specified by Eq. (374) together with the initial condition at $t = 0$. Since we are interested in the coarsening dynamics, we choose random initial conditions that are uncorrelated in the N-dimensional space and in the real space and have a Gaussian distribution (mimicking an infinite temperature initial condition) given by

$$P[\boldsymbol{\phi}(\mathbf{x}, 0)] \propto \exp\left(-\frac{1}{2\varDelta^2}\sum_{a=1}^N \int d^d x\,\phi_a^2(\mathbf{x}, 0)\right) \tag{376}$$

and in the following the average brackets always include an average over the initial condition, according to the Gaussian weight in Eq. (376).

7.4.1 General framework in the limit $N \to \infty$

1. Show that the equation of motion Eq. (374) for $\phi_a = \phi_a(x,t)$ reads explicitly, for the $O(N)$ model in Eq. (373)

$$\frac{\partial}{\partial t}\phi_a = \nabla^2\phi_a - \left(\frac{g}{N}\boldsymbol{\phi}^2 + r\right)\phi_a + h_a(\mathbf{x},t) + \eta_a(\mathbf{x},t)\ . \tag{377}$$

For any finite N, solving the dynamics in arbitrary dimension d is a challenging task. It turns out, however, that both the statics and the dynamics of the $O(N)$ model are exactly solvable in the limit $N \to \infty$, and for any d.

2. In the large N limit explain qualitatively why we can replace $\boldsymbol{\phi}^2$ with its average value $\langle \boldsymbol{\phi}^2(\mathbf{x},t)\rangle$ (the average brackets $\langle \ldots \rangle$ denote an average with respect to the initial distribution and over the time realizations of the noise)? Hereafter we thus denote

$$z(\mathbf{x},t) = \frac{g}{N}\boldsymbol{\phi}^2 + r \approx z(t) = \frac{g}{N}\langle \boldsymbol{\phi}^2\rangle + r\ . \tag{381}$$

   Why is $z(t)$ independent of x ?

The study of the statics of the $O(N)$ model Eq. (373) in the limit $N \to \infty$ reveals that it has a transition from a paramagnetic to a ferromagnetic phase—the low temperature phase being characterized by a condensation phenomenon, signalling ordering. The upper critical dimension is $d = 4$ and the lower critical dimension is $d = 2$, i.e. in dimension $d = 1, 2$, the critical temperature vanishes ($T_c = 0$) [11].

3. With the following conventions for Fourier transforms

$$\hat{f}(\mathbf{k}) = \int d^d x f(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{x}}\ ,\ f(\mathbf{x}) = \int \frac{d^d k}{(2\pi)^d}\hat{f}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{x}}\ , \tag{383}$$

   show that the Fourier transform $\hat{\phi}_a(\mathbf{k},t)$ satisfies, in the $N \to \infty$ limit, the following Langevin equation

$$\frac{\partial \hat{\phi}_a}{\partial t} = -k^2\hat{\phi}_a - z(t)\hat{\phi}_a + \hat{h}_a + \hat{\eta}_a\ , \tag{384}$$

   where $\hat{\eta}_a$ are independent Gaussian white noises.

4. Give a "strategy" to solve this set of equations (384). In particular, how will you compute $z(t)$?

7.4.2 Zero temperature coarsening dynamics

Here, we focus on the zero temperature limit $T = 0$, which captures the main features of the coarsening process in the ferromagnetic phase—this is expected since the ordered phase is described by a zero temperature fixed point, in the renormalization group sense. Note that at $T = 0$ the average brackets $\langle \ldots \rangle$ refer only to an average over the initial state defined in Eq. (376) which is the only source of stochasticity (there is no average over the thermal noise).

5. Compute $\hat{\phi}_a(\mathbf{k}, t)$ explicitly in terms of $\hat{h}_a(\mathbf{k}, t)$ and $z(t)$ as

$$\hat{\phi}_a(\mathbf{k}, t) = \hat{R}(\mathbf{k}, t, 0)\, \hat{\phi}_a(\mathbf{k}, 0) + \int_0^t dt' \hat{R}(\mathbf{k}, t, t')\, \hat{h}_a(\mathbf{k}, t') \tag{387}$$

   where

$$\hat{R}(\mathbf{k}, t, t') = \theta(t - t')\, \frac{Y(t')}{Y(t)} e^{-k^2(t-t')} \;,\;\; Y(t) = \exp\left(\int_0^t z(t')\, dt'\right) \tag{388}$$

   where $\theta(x) = 1$ if $x \geq 0$ and $\theta(x) = 0$ and where $z(t)$ is defined in Eq. (381).

6. Show that $\hat{R}(\mathbf{k}, t, t')$ is the response function, *i.e.*

$$\frac{\delta \langle \hat{\phi}_a(\mathbf{k}, t) \rangle}{\delta \hat{h}_b(-\mathbf{k}', t')}\Big|_{\mathbf{h}=0} = \delta_{a,b} \delta^{(d)}(\mathbf{k} + \mathbf{k}') \hat{R}(\mathbf{k}, t, t') \; . \tag{392}$$

7. Show that the two-point two-time correlation function (in Fourier space), and in the absence of external field $\mathbf{h} = \mathbf{0}$, is given by

$$\langle \hat{\phi}_a(\mathbf{k}, t) \hat{\phi}_b(\mathbf{k}', t') \rangle = \delta_{a,b} (2\pi)^d \delta^{(d)}(\mathbf{k} + \mathbf{k}') \hat{C}(\mathbf{k}, t, t') \;,\;\; \hat{C}(\mathbf{k}, t, t') = \frac{\Delta^2}{Y(t)\, Y(t')} e^{-k^2(t+t')} \tag{394}$$

At this stage, we know the response Eq. (388) and correlation Eq. (394) functions both in terms of $Y(t)$ but the function $Y(t)$ itself is still undetermined. We thus still need to compute it using Eq. (381).

8. Show that

$$\langle \phi_a^2(\mathbf{x}, t) \rangle = \frac{\Delta^2}{Y^2(t)} (8\pi t)^{-d/2} \;, \tag{401}$$

   and deduce from Eq. (381) the following equation for $Y(t)$

$$\frac{\mathrm{d}}{\mathrm{d}t} Y^2(t) = 2r Y^2(t) + 2g\, \Delta^2 (8\pi t)^{-d/2} \; . \tag{402}$$

9. In the ferromagnetic phase, where $r < 0$, obtain the large time behavior of $Y(t) \sim (t/t_0)^{-\nu}$ and determine the exponent ν as well as t_0.

10. Show finally that the response $\hat{R}(\mathbf{k}, t, t')$ and the correlation $\hat{C}(\mathbf{k}, t, t')$ behave, for large t and t' (with $t > t'$), as

$$\hat{R}(\mathbf{k}, t, t') \sim \left(\frac{t}{t'}\right)^{d/4} e^{-k^2(t-t')} \tag{412}$$

$$\hat{C}(\mathbf{k}, t, t') \sim \Delta^2 \left(\frac{t\,t'}{t_0^2}\right)^{d/4} e^{-k^2(t+t')} \,. \tag{413}$$

11. Coming back to real space, show that the two-point two-time correlation function $\langle \phi_a(\mathbf{x}, t)\phi_b(\mathbf{x}', t')\rangle$ is given by

$$\langle \phi_a(\mathbf{x}, t)\phi_b(\mathbf{x}', t')\rangle = \delta_{a,b} \int \frac{\mathrm{d}^d k}{(2\pi)^d} e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \hat{C}(\mathbf{k}, t, t') \,. \tag{415}$$

12. Using the asymptotic behavior in Eq. (413), show that $\langle \phi_a(\mathbf{x}, t)\phi_a(\mathbf{x}', t')\rangle$ takes the scaling form for $t \gg 1$, $t' \gg 1$, $|\mathbf{x} - \mathbf{x}'| \gg 1$ keeping $|\mathbf{x} - \mathbf{x}'|/L(t)$ as well as $L(t)/L(t')$ fixed, with $L(t) \sim t^{1/2}$

$$\langle \phi_a(\mathbf{x}, t)\phi_a(\mathbf{x}', t')\rangle \sim \mathcal{F}\left(\frac{|\mathbf{x} - \mathbf{x}'|}{L(t)}, \frac{L(t)}{L(t')}\right) \,, \tag{416}$$

and explicitly compute the scaling function $\mathcal{F}(u, v)$. What is the physical meaning of $L(t)$? Such a scaling form Eq. (416), which we have demonstrated here explicitly for the $O(N \to \infty)$ model is believed to hold for a wide class of coarsening processes, albeit with different growth laws $L(t)$ and different scaling functions $\mathcal{F}(u, v)$.

7.5 Dynamics of the roughening transition

Our goal is to describe the interface between the two phases of a ferromagnetic crystal, say on a cubic lattice. The horizontal directions are labeled by $\mathbf{r} = (x, y)$ and z denotes the orthogonal direction. The interface at time t is described by its height function: $z/a = h(\mathbf{r}, t)$. The lattice spacing is denoted by a. It is important to note that both x/a, y/a and z/a (or h) assume integer values. This text rests on [40, 10]. It deals with the so-called solid-on-solid model. Connections will appear in the course of the problem with canonical statistical mechanical models [31, 34].

Since our interest goes to the modeling of the interface, we wish to build a Hamiltonian $\mathcal{H}_0$ that captures the thermal fluctuations of the interface when it is in equilibrium at a given temperature. However the fact the $h(\mathbf{r}, t)$ is integer-valued makes our mathematical life rather cumbersome. We shall therefore take the liberty to allow $h(\mathbf{r}, t)$ to take real values while adding a penalty, in the Hamiltonian, for non-integer values of h:

$$\mathcal{H}_0 = J\sum_{\mathbf{r}}\sum_{\mathbf{e}=\mathbf{e}_x,\mathbf{e}_y}(h(\mathbf{r}+a\mathbf{e})-h(\mathbf{r}))^2 + Jg^2\sum_{\mathbf{r}}h^2(\mathbf{r}) - 2yJ\sum_{\mathbf{r}}\cos 2\pi h(\mathbf{r}) \tag{418}$$

where J, y and g are positive constants.

1. There are three contributions in the Hamiltonian. Explain in a few qualitative words the physical and/or mathematical role of each of them.

2. To begin with we take $y = 0$. Determine the $C(\mathbf{r}) \equiv \langle (h(\mathbf{r}) - h(\mathbf{0}))^2\rangle$ correlation at a given temperature T and let $g^2 \to 0$ whenever possible in the calculation. Show that $C(\mathbf{r})$ has a logarithmic divergence at $r \to \infty$. The interface is then said to be rough.

From here on, the notation $\sum_{\mathbf{r}}$ will be replaced with a continuous integral. The original lattice will appear through a lower cut-off in spatial integrals that exhibit a short-distance divergence (this is of the order of the lattice spacing a, hence the UV cut-off is a^{-1}). We now study the dynamics of the interface under the action of a driving field $\mu(\mathbf{r}, t)$ that modifies the Hamiltonian into

$$\mathcal{H} = \mathcal{H}_0 - \sum_{\mathbf{r}}\mu(\mathbf{r}, t)h(\mathbf{r}) \tag{422}$$

The postulated dynamical evolution is

$$\partial_t\, h(\mathbf{r}, t) = -\frac{\Gamma}{T}\frac{\delta\mathcal{H}}{\delta h(\mathbf{r}, t)} + \eta(\mathbf{r}, t) \tag{423}$$

where η is a Gaussian white noise with correlations

$$\langle \eta(\mathbf{r}, t)\eta(\mathbf{r}, t')\rangle = 2\Gamma\,\delta^{(2)}(\mathbf{r}-\mathbf{r}')\delta(t'-t) \tag{424}$$

3. Explain why at large time the probability to observe an interface profile $h(\mathbf{r})$ is given by $P_{\text{eq}}[h] \sim \mathrm{e}^{-\beta\mathcal{H}[h]}$.

4. For $g^2 = 0$ and for a constant drive $\mu(\mathbf{r}, t) = \mu_0$, what is the expected limiting behavior of the interface?

5. Returning to an arbitrary drive $\mu(\mathbf{r}, t)$, write the Janssen-De Dominicis dynamical action $S[\bar{h}, h]$.

6. The response function χ is defined by $\chi(\mathbf{x}-\mathbf{y}, ; t'-t) = \left.\frac{\delta\langle h(\mathbf{x},t')\rangle}{\delta\mu(\mathbf{y},t)}\right|_{\mu=0}$. Express χ as a function average over the two fields $\bar{h}$ and h weighted by $\mathrm{e}^{-S[\bar{h},h]}$.

7. We work in the steady-state. We now expand χ in powers of y. Can you see an argument explaining why the expansion contains even powers of y only?

8. Let $h(\mathbf{q},t) = a^{-2}\int \mathrm{d}^2r\ \mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}}h(\mathbf{r},t)$. Find the height autocorrelation $C(\mathbf{k}\,;t-t')$ such that $\langle h(\mathbf{k},t)h(\mathbf{k}',t')\rangle = (2\pi)^2\delta^{(2)}(\mathbf{k}+\mathbf{k}')\,C(\mathbf{k}\,;t-t')$ in equilibrium when $\mu = 0$, $g^2 = 0$, $y = 0$.

9. Let $h(\mathbf{q},\omega) = a^{-2}\int \mathrm{d}t\mathrm{e}^{-i\omega t}h(\mathbf{q},t)$. To second order in y, and to the lowest non trivial order in $\mathbf{q}$ and ω, a tedious calculation shows that $\chi(\mathbf{q},\omega) = \int \mathrm{d}^2r\mathrm{d}t\mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}-i\omega t}\chi(\mathbf{r},t)$ has the expression

$$\begin{aligned}\chi^{-1}(\mathbf{q},\omega) =& \mathbf{q}^2\left(K^{-1}+\pi^3K^{-2}\tilde{y}^2\int_a^\infty a^{-1}\mathrm{d}r\ (r/a)^{3-2\pi K}\right)\\ &- i\omega\left(\varGamma^{-1}+\varGamma^{-1}\pi^4\frac{\tilde{y}^2}{\pi K-1}\int_a^\infty a^{-1}\mathrm{d}r\ (r/a)^{3-2\pi K}\right)+\mathcal{O}(y^4)\end{aligned} \tag{432}$$

with $\tilde{y} = y\mathrm{e}^{-\pi^2K/2}$ and $K = T/2J$. Upon separating length scales between a and $ba > a$ and ba and $+\infty$, what are the effective couplings K_b, $\tilde{y}_b$ and $\varGamma_b$ that describe the system at scale b in terms of the couplings at the scale of the original lattice?

10. Using an infinitesimal rescaling from scale b to scale $b+\mathrm{d}b$ show that the recursion relations of the previous question take the form

$$\frac{\mathrm{d}K}{\mathrm{d}\ell} = f_1(K(\ell),\tilde{y}(\ell),\varGamma(\ell)) \tag{438}$$

$$\frac{\mathrm{d}\tilde{y}^2}{\mathrm{d}\ell} = f_2(K(\ell),\tilde{y}(\ell),\varGamma(\ell)) \tag{439}$$

$$\frac{\mathrm{d}\varGamma}{\mathrm{d}\ell} = f_3(K(\ell),\tilde{y}(\ell),\varGamma(\ell)) \tag{440}$$

where $\ell = \ln b$. What are the explicit expressions of the f_i's, $i = 1,2,3$?

11. What are the fixed points of the renormalization group flow in the $(K,\tilde{y})$ plane? Sketch the flow lines in that subspace (show that they are hyperboles). How would you define the critical temperature?

12. Show that the $\varGamma(\ell)/(\pi K(\ell)-1)$ ratio remains a constant along the flow. How does the relaxation time governing the decay of the height autocorrelation function behave in the vicinity of the critical temperature?

13. Could you predict, above the critical temperature, the behavior of $C(\mathbf{r},t)$ as a function of r and t (both r and t are large)? How about below the critical temperature?

8 Homework 24/10/2022 – Emergent long range correlations in a one-dimensional diffusive system

We want to describe a system of partially excluding particles moving on a one-dimensional lattice. We begin with a single site.

1. A single site can harbor at most M particles ($M \in \mathbb{N}^*$ is a parameter) and its occupation number n can increase by one unit at a rate $\alpha(M-n)$ or decrease by one unit at a rate γn. Write the master equation for the probability $P(n,t)$ to find n particles at time t.

2. What is the stationary solution $P_{\text{ss}}(n)$ of this master equation?

3. The average of a quantity $A(n)$ can be expressed in a path integral form as

$$\langle A(n)\rangle(t) = \int \mathscr{D}\hat{\rho}\mathscr{D}\rho A(\rho(t))\mathrm{e}^{-S[\hat{\rho},\rho]} \tag{462}$$

where the action $S[\hat{\rho},\rho] = \int_0^{+\infty} \mathrm{d}\tau \ldots$ up to terms involving the fields at the initial time. Fill in the dots in terms of the fields $\hat{\rho}(\tau)$ and $\rho(\tau)$ and in terms of α and γ and M.

We now consider the L sites of a one dimensional lattice, each of which can harbor $n_i = 0, 1, \ldots, M$ particles at most. A particle at site i can hop to its right/left nearest neighbor with a rate $\frac{1}{M} n_i (M - n_{i\pm 1})$. At site $i = 1$, a particle can be injected and n_1 increases by one at a rate $\alpha(M - n_1)$. At $i = 1$ a particle can be removed and n_1 decreases by one at a rate γn_1. Similarly at site L, a particle can be injected or removed (n_L increases or decreases by one at a rate $\delta(M - n_L)$ or βn_L).

4. Write an evolution equation for $\langle n_i\rangle(t)$ (for $i = 2, \ldots, L-1$) in terms of the $\langle n_j\rangle$'s. Comment on how remarkable, or not, this equation is.

5. Let $Q_{i+1}(t_{\text{obs}})$, $i = 0, \ldots, L$ be the total particle current integrated over the time window $[0, t_{\text{obs}}]$ flowing from site i to site $i+1$. Sites $i = 0$ and $i = L+1$ respectively refer to the left and right reservoirs injecting/removing particles at rates α and γ or δ and β. Express the variation of the total number of particles in the lattice $\Delta N(t_{\text{obs}})$ in terms of Q_1 and of Q_{L+1}.

6. In the particular case $M = 1$, express the total average entropy production $\langle Q_S\rangle$ in the steady-state in terms of α, β, γ, δ and $\langle Q_1\rangle$. Under what constraints on the injection/removal rates is the steady-state an equilibrium one?

7. Because of the additional hopping mechanism, and because we are now dealing with L sites, the action found in question 3 becomes an action for a set of field $\{\hat{\rho}_i(\tau), \rho_i(\tau)\}_{i=1,\ldots,L}$. The action splits into several contributions:

$$S[\{\hat{\rho}_i(\tau), \rho_i(\tau)\}_{i=1,\ldots,L}] = \int \mathrm{d}\tau \sum_{i=1}^{L} \hat{\rho}_i \partial_\tau \rho_i + S_{\text{left reservoir / site } i=1} + S_{\text{right reservoir / site } i=L} + S_{\text{hopping}} \tag{465}$$

Write the contribution specific to the hopping mechanism in the bulk of the system ($i = 2, \ldots, L-1$) by filling in the dots:

$$S_{\text{hopping}}[\{\hat{\rho}_i(\tau), \rho_i(\tau)\}_{i=1,\ldots,L} = \int \mathrm{d}\tau \left(\underbrace{\sum_{i=1}^{L-1} [\ldots]}_{\text{hops to the right}} + \underbrace{\sum_{i=2}^{L} [\ldots]}_{\text{hops to the left}} \right) \tag{466}$$

8. We now define a field ϕ by $\rho_i(\tau) = M\phi(x,t)$ where $t = \tau/L^2$ and $x = \frac{i}{L}$. Similarly we also introduce $\hat{\phi}(x,t) = \hat{\rho}_i(\tau)$. There is *a priori* no reason for ϕ or $\hat{\phi}$ to be smoothly varying fields. Argue in a few simple words why this must be true in the $M \gg 1$ and $L \gg 1$ limits.

9. Express the action S_{hopping} in terms of the ϕ and $\hat{\phi}$ fields for large L to leading order (don't bother about boundary terms at $x = 0$ and $x = 1$, feel free to simplify things using integration by parts if that makes the formulas any nicer).

10. Consider the following Langevin equation for a field $\phi(x,t)$:

$$\partial_t \phi = -\partial_x j,\; j = -\frac{\sigma(\phi)}{2}\partial_x \frac{\delta F}{\delta \phi} + \sqrt{\frac{\sigma(\phi)}{ML}}\xi(x,t) \tag{470}$$

where $\sigma(\phi)$ is a local function of $\phi(x,t)$ and $F[\phi] = \int_0^1 \mathrm{d}x f(\phi)$ where f is a local function of $\phi(x,t)$. The noise ξ is Gaussian and white, $\langle \xi(x,t)\xi(x',t')\rangle = \delta(x-x')\delta(t-t')$. Find the two functions f and σ that ensure the statistical equivalence between the Langevin process of Eq. (470) and the dynamical action found in question 9.

11. When looking at Eq. (470) we see that the noise is multiplicative. How come we did not bother to discuss discretization issues?

12. From Eq. (470) one can see that, if boundary conditions allow for it, the equilibrium distribution for $\phi(x)$ will be given by $P_{\text{eq}}[\phi] \simeq \mathrm{e}^{-ML(F[\phi]-F[\phi_c])}$. Briefly explain one possible strategy to justify this statement (just explain what sort of calculation would give you the answer).

In the remaining questions, we'll take Eq. (470) as our starting point and the equilibrium or nonequilibrium nature of the dynamics will be entirely controled by the boundary conditions for ϕ at $x = 0$ and $x = 1$. The regime $M \gg 1$ and $L \gg 1$ is assumed to hold.

13. We expect the scaled fluctuation $\delta\phi(x,t) = \sqrt{ML}(\phi(x,t) - \phi_c(x))$ to be finite as M and L become large. Can you support this assertion by a qualitative argument?

14. In equilibrium, show, using question 12, that $\delta\phi(x,t)$ has equal time fluctuations given by
$$\langle \delta\phi(x,t)\delta\phi(y,t)\rangle = \delta(x-y)/f''(\phi_c) \tag{475}$$
where $\phi_c = \rho_a = \rho_b$ is uniform in space.

15. Given the boundary conditions $\phi(0,t) = \rho_a = \frac{\alpha}{\alpha+\gamma}$ and $\phi(1,t) = \rho_b = \frac{\delta}{\delta+\beta}$, find the mean profile $\phi_c(x) = \langle \phi(x,t)\rangle_{\text{ss}}$ in the steady-state.

16. In general, for a generic function f, Eq. (470) for ϕ takes the form $\partial_t\phi = \partial_x(D(\phi)\partial_x\phi) + \frac{1}{\sqrt{ML}}\partial_x(\sqrt{\sigma}\xi)$. Show that $D(\phi) = f''(\phi)\sigma(\phi)/2$. Explain the qualitative physical meaning of σ/D (a handwaving argument can do).

17. Let $\Gamma(x;x';t)$ be the Green's function verifying
$$(\partial_t - \partial_x^2)\Gamma(x;x';t) = \delta(t)\delta(x-x'),\ \Gamma(0 \text{ or } 1; y; t) = 0 \tag{478}$$
Explain why, in the steady-state of our specific model, and for M and L large, we can write that $C(x,y) = \langle \delta\phi(x,t)\delta\phi(y,t)\rangle_{\text{ss}}$ has the integral expression
$$C(x,y) = \int_0^1 \mathrm{d}x'\mathrm{d}y' \int_0^{+\infty} \mathrm{d}t\Gamma(x;x';t)\Gamma(y;y';t)\partial_{x'}\partial_{y'}\left(\sigma(\phi_c(x'))\delta(x'-y')\right) \tag{479}$$

With a few more manipulations on Green's functions, one arrives at
$$C(x,y) = \frac{1}{2}\sigma(\phi_c(x))\delta(x-y) - (\rho_a-\rho_b)^2 G(x,y) \tag{491}$$
where $G(x,y)$ is the Green's function verifying $-\partial_x^2 G(x,y) = \delta(x-y)$ with $G(0 \text{ or } 1, y) = 0$.

18. Show how the first contribution $\frac{1}{2}\sigma(\phi_c(x))\delta(x-y)$ to C can be obtained from Eq. (479) (beware, $\int_0^{+\infty}\mathrm{d}u\delta(u) = 1/2$).

19. Express G as a function of x and y.

20. Let $\Delta N(t) = \int_0^1 \delta\phi(x,t)$ denote the (rescaled) fluctuation of the total number of particles in $[0,1]$ with respect to its average. The variance of ΔN can be written as
$$\langle \Delta N^2\rangle = \langle \Delta N^2\rangle_{\text{loc. eq}} + c(\rho_a-\rho_b)^2 \tag{500}$$
where c is a numerical constant and where $\langle \Delta N^2\rangle_{\text{loc. eq}}$ refers to the result one would obtain if at each location the system were in equilibrium at a density $\phi_c(x)$. In that sense the additional contribution $c(\rho_a-\rho_b)^2$ genuinely reflects the nonequilibrium nature of the dynamics. Find c, and comment on its sign.

21. In which regime of x and y can G be thought of as the usual Coulomb potential? In what sense does it illustrate the title of this homework?

9 Exam 06/01/2023

9.1 Coupled oscillators and heat conduction

This problem considers one, and then several coupled oscillators in one space dimension, thus forming a chain. The system is eventually driven out of equilibrium by connecting the chain at both ends to thermostats imposing unequal temperatures.

Consider first a single harmonic oscillator with position $x(t)$ in contact with one thermostat evolving according to the overdamped Langevin equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -\mu x + \sqrt{2\mu T}\eta \tag{501}$$

where the mobility μ and the temperature T are given, and η refers to a Gaussian white noise with correlations $\langle \eta(t)\eta(t')\rangle = \delta(t-t')$.

1. Let t_0 be some arbitrary time and $\Delta t > 0$. Let $\Delta\eta = \int_{t_0}^{t_0+\Delta t} \mathrm{d}t\eta(t)$. Determine $\langle \Delta\eta\rangle$ and $\langle \Delta\eta^2\rangle$ as functions of Δt.
2. Given an initial value $x(t_0)$, we study the process $x(t)$ over the $[t_0, t_0+\Delta t]$ time interval. We denote by $\Delta x = x(t_0+\Delta t) - x(t_0)$. Express the $\langle \Delta x\rangle$ and $\langle \Delta x^2\rangle$ averages in terms of $x(t_0)$ and Δt to leading order in $\Delta t \to 0$.
3. Deduce the Fokker-Planck equation for the probability density $p(x,t)$ ($p(x,t)\mathrm{d}x = \mathrm{Prob}\{x \le x(t) \le x + \mathrm{d}x\}$).
4. Determine $\langle x\rangle$ and $\langle x^2\rangle$ in the steady-state.
5. What is the steady-state probability density $p_{\mathrm{ss}}(x)$?
6. Explain why $p_{\mathrm{ss}}(x)$ is actually an equilibrium distribution.
7. Consider now the local fluctuating elastic energy $\varepsilon(t) = \frac{x^2}{2}$ stored in the oscillator. The Langevin equation for ε can be written in the form

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}t} = -2\mu\varepsilon + \mu T + 2\sqrt{\mu T\varepsilon}\eta \tag{505}$$

   This is a Langevin equation with multiplicative noise. Explain why there is an ambiguity, and specify the correct way of understanding Eq. (505). Determine $\langle \varepsilon\rangle$ in equilibrium.

We now consider L coupled oscillators indexed by $i = 1, \ldots, L$. Each position x_i evolves according to

$$i = 2, \ldots, L-1,\ \frac{\mathrm{d}x_i}{\mathrm{d}t} \overset{1/2}{=} x_{i+1}\xi_{i,i+1} - x_{i-1}\xi_{i-1,i} \tag{508}$$

along with

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} \overset{1/2}{=} -x_1/2 + x_2\xi_{1,2} - \sqrt{T_a}\xi_{0,1},\ \frac{\mathrm{d}x_L}{\mathrm{d}t} \overset{1/2}{=} -x_L/2 + \sqrt{T_b}\xi_{L,L+1} - x_{L-1}\xi_{L-1,L} \tag{509}$$

where the independent $L+1$ white Gaussian noises have correlations $\langle \xi_{i,i+1}(t)\xi_{j,j+1}(t')\rangle = \delta_{ij}\delta(t-t')$, $i = 0, \dots, L$. The index 0 refers to the left thermostat imposing temperature T_a while site $L+1$ refers to the right thermostat imposing temperature T_b.

8. Show that the local energy $\varepsilon_i(t) = \frac{1}{2}x_i(t)^2$ stored in oscillator i evolves according to

$$\forall i = 1, \dots, L,\ \frac{\mathrm{d}\varepsilon_i}{\mathrm{d}t} = J_i - J_{i+1} \tag{510}$$

   with $J_{i+1} \overset{1/2}{=} -2\sqrt{\varepsilon_i\varepsilon_{i+1}}\xi_{i,i+1}$, for $i = 1, \dots, L-1$. The $i = 1$ and $i = L$ sites will be dealt with further down.

9. Show that $J_{i+1} \overset{0}{=} \varepsilon_i - \varepsilon_{i+1} - 2\sqrt{\varepsilon_i\varepsilon_{i+1}}\xi_{i,i+1}$, for $i = 1, \dots, L-1$.

10. In Eq. (510), give the expressions of the quantities J_1 and J_{L+1} in terms of ε_1, ε_2 and T_a, and ε_{L-1}, ε_L and T_b, respectively (make sure the discretization being used is specified).

11. Based on your intuition, on what condition is the chain of oscillators in equilibrium?

We now make the assumption that for $L \gg 1$, on condition that we work with a properly rescaled time $t' = t/L^2$, the set of energies $\varepsilon_i(t)$ can be seen as a smoothly varying function of $t' = t/L^2$ and of $x = i/L$: $\varepsilon_i(t) = \varepsilon(x, t')$ where we have kept the same notation ε for the field $\varepsilon_i(t)$ on the lattice $i = 1, \dots, L$ and the field $\varepsilon(x, t')$ in the continuum $x \in [0, 1]$. At $x = 0$ and $x = 1$ the contact with the thermostats is expressed through the boundary conditions $\varepsilon(0, t) = T_a/2$ and $\varepsilon(1, t) = T_b/2$.

12. We postulate that $\varepsilon(x, t')$ evolves according to a Langevin equation. For $0 < x < 1$ the equation looks like

$$\partial_{t'}\varepsilon(x, t') = -\partial_x j(x, t'),\ j(x, t') = -\partial_x\varepsilon + \sqrt{\frac{\sigma(\varepsilon(x, t'))}{L}}\eta(x, t') \tag{518}$$

   where η is a Gaussian white noise with correlations $\langle \eta(x_1, t_1)\eta(x_2, t_2)\rangle = \delta(t_1 - t_2)\delta(x_1 - x_2)$. What would you suggest to use for the function $\varepsilon \mapsto \sigma(\varepsilon)$? Is there any good reason not to specify the discretization used in Eq. (518)?

13. Express the energy profile $\varepsilon_c(x) = \langle \varepsilon(x, t')\rangle$ in the steady-state as a function of x, T_a and T_b.

14. Find the local functional $F[\varepsilon] = \int_0^1 \mathrm{d}x f(\varepsilon(x))$ such that $j = -\frac{\sigma}{2}\partial_x\frac{\delta F}{\delta\varepsilon} + \sqrt{\frac{\sigma(\varepsilon)}{L}}\eta$ (find the function $\varepsilon \mapsto f(\varepsilon)$).

15. Let $\delta\varepsilon(x,t') = \sqrt{L}(\varepsilon(x,t') - \varepsilon_c(x))$. What is the linear Langevin equation governing the evolution of $\delta\varepsilon(x,t')$ for L large?

After some manipulations one can show that, in the stationary state the equal time correlations of $\delta\varepsilon$ are given by

$$\langle \delta\varepsilon(x,t')\delta\varepsilon(y,t')\rangle = \sigma(\varepsilon_c(x))\delta(x-y) + \frac{1}{2}(T_b - T_a)^2 G(x,y) \tag{520}$$

where $G(x,y)$ is the Green's function of the Laplacian, $\partial_x^2 G(x,y) = -\delta(x-y)$ with absorbing boundary conditions at $x=0$ and $x=1$.

16. Let $\Delta E(t') = \int_0^1 \delta\varepsilon(x,t')\mathrm{d}x$ denote the (rescaled) fluctuation of the total energy contained in the system. In the steady-state, the variance of ΔE can be written as $\langle \Delta E\rangle^2 = \langle \Delta E^2\rangle_{\text{loc. eq.}} + c(T_b - T_a)^2$, where c is a numerical constant and where $\langle \Delta E^2\rangle_{\text{loc. eq.}}$ refers to the result one would obtain if at each location the system were in equilibrium with an average energy $\varepsilon_c(x)$. In that sense the additional contribution $(T_b - T_a)^2$ genuinely reflects the nonequilibrium nature of the dynamics. Find c, and comment on its sign.

9.2 An epidemic process

The sites i of a lattice can be in either of three states: healthy, infected or empty. Between t and $t+\mathrm{d}t$, a site can change from infected to healthy with probability $\gamma\mathrm{d}t$ (this is recovery). And the probability that a healthy site possessing an infected nearest neighbor becomes contaminated over $\mathrm{d}t$ is $k\mathrm{d}t$. In a mean-field picture, the rate at which the total population of infected individuals, denoted by $I(t)$, decreases by one unit is γI while the rate at which I increases by one unit is kSI/N. The total number of occupied sites is N_0 ($\rho_0 = N_0/N$ is the fraction of occupied sites).

1. In a mean-field picture, and for $N \gg 1$, write a deterministic evolution equation for $\rho_I(t) = \frac{\langle I(t)\rangle}{N}$ in terms of ρ_I, γ, k and ρ_0.
2. Show that in the stationary state ρ_I can take two possible values. Discuss the value chosen by the system depending on whether $\rho_0 > \rho_c$ or $\rho_0 < \rho_c$, where $\rho_c = \frac{\gamma}{k}$. Plot ρ_I in the steady state as a function of ρ_0.
3. Show that the typical time it takes to relax to either of the possible steady-states diverges as $|\rho_0 - \rho_c|^{-1}$ as $\rho_0 \to \rho_c^{\pm}$.
4. Let $\psi(t) = \frac{I}{N}$. Choose α such that $N^\alpha(\psi - \rho_I)$ has nontrivial statistical properties independent of N. Explain your choice in a few words.
5. For $N \gg 1$ we write a Langevin equation for ψ in the form

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} \stackrel{0}{=} k(\rho_0 - \rho_c)\psi - k\psi^2 + \frac{1}{\sqrt{N}}\sqrt{f(\psi(t))}\xi(t) \tag{521}$$

where ξ is a Gaussian white noise with correlations $\langle \xi(t)\xi(t') \rangle = \delta(t-t')$ and where the function f is for the moment undetermined. Why is the 0 index above the equal sign superfluous?

6. As $\psi \to 0$ we expand the function f as follows: $f(\psi) = f(0) + f'(0)\psi + \ldots$. Why do we necessarily have $f(0) = 0$? In what follows, we shall use $f(\psi) = k'\psi$, where $k' > 0$ is a phenomenological coefficient.

7. In a finite system with N sites, there is always a finite probability to visit a state with $I = 0$ infected individuals, out of which the system cannot escape. Starting from a stationary state in which $\rho_I > 0$, the time needeed to fall into the state with $I = 0$ is denoted by τ_N. Why does τ_N grow exponentially with N? Sketch a possible calculation leading to that result.

Of course, mean-field ignores the existence of an underlying space which we now want to restore. Assuming diffusive motion of the infected and healthy individuals, we consider the local coarse-grained fluctuating density $\psi(\mathbf{r}, t)$ of infected individuals, along with the local density $\rho(\mathbf{r}, t)$ of individuals (such that $\rho - \psi$ stands for the local density of healthy individuals). We postulate that we can write

$$\partial_t \psi = D\partial_{\mathbf{r}}^2 \psi - D(m^2 + g''\phi)\psi - g\psi^2 + \xi(\mathbf{r}, t) \tag{523}$$

where $\langle \xi(\mathbf{r}, t)\xi(\mathbf{r}', t') \rangle = 2g'\psi(\mathbf{r}, t)\delta^{(d)}(\mathbf{r} - \mathbf{r}')\delta(t - t')$, where ξ has Gaussian statistics, and the (positive) coefficients D, m^2, g, g', g'' are phenomenological. Here $m^2 \propto (\rho_c - \rho_0)$ controls the nature of the steady-state.

8. Justify the presence of the ϕ field in Eq. (523) right next to the m^2 coefficient.

9. In fact ϕ too is a fluctuating field. If we wanted to write a Langevin equation for ϕ it would read
$$\partial_t \phi = \ldots + \text{noise} \tag{524}$$
Can you suggest a contribution to fill in the $\ldots$?

10. The noise itself in Eq. (524) is assumed to be Gaussian and white. What other property should it be endowed with?

11. It is technically difficult to deal with both the ψ and ϕ fields. Assuming one can simply forget about ϕ (which is henceforth set to 0), write the Janssen-De Dominicis action for ψ and its companion response field $\bar{\psi}$.

12. What is the upper critical dimension d_c above which the mean-field scaling will apply? In your opinion, will the fluctuations of ϕ affect d_c?

13. What is, at the mean-field level, the dynamical exponent z that controls the way the relaxation time τ is connected to the correlation length ξ via $\tau \sim \xi^z$? If the ϕ field is omitted from the analysis, one finds that the value of z in space dimension $d < d_c$ is actually lower than in mean-field. Will this property survive if the fluctuations of ϕ are included in the analysis?

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