

Exercise 1.1 Statistical Polarization

a) The general master equation is

$$\dot{N}_\nu(t) = -N_\nu(t) \sum_{\nu' \neq \nu} \Gamma_{\nu\nu'} + \sum_{\nu' \neq \nu} \Gamma_{\nu'\nu} N_{\nu'}(t). \quad (1)$$

As we only allow hopping to neighboring directions (at rate Γ), only $\Gamma_{\nu, \nu \pm 1}$ are non-vanishing (and equal to Γ), and the master equation reduces to

$$\dot{N}_\nu(t) = \Gamma (N_{\nu+1}(t) + N_{\nu-1}(t) - 2N_\nu(t)), \quad (2)$$

where the indices are taken modulo z . The entropy function of the system is simply

$$H(t) = - \sum_{\nu} \frac{N_\nu(t)}{N} \log \frac{N_\nu(t)}{N}. \quad (3)$$

At equilibrium we have $\dot{H} = 0$, which implies detailed balance, i.e., $N_\nu = N_{\nu'}$ for all ν, ν' . One finds $N_\nu/N = 1/z$ for all directions ν .

b) The initial distribution corresponds to

$$N_\nu = \begin{cases} 2N/z & 0 \leq \nu < z/2 \\ 0 & \text{else} \end{cases} \quad (4)$$

Therefore, the initial entropy is

$$H_{\text{initial}} = - \sum_{\nu} \frac{N_\nu}{N} \log \frac{N_\nu}{N} = \log \frac{z}{2}. \quad (5)$$

Since the equilibrium corresponds to $N_\nu = N/z$ for all ν , the (equilibrium) entropy is simply $H_{\text{final}} = \log z$ and we find for the difference

$$H_{\text{final}} - H_{\text{initial}} = \log(2) = \log \frac{V_{\text{final}}}{V_{\text{initial}}} \quad (6)$$

where we denote by V_{\dots} the number of directions (i.e., the discrete phase space volume) occupied in the initial and final distribution. If we identify V with the volume of an ideal gas, then this corresponds directly to the ideal gas, where $\Delta S = Nk_B \log(V_{\text{final}}/V_{\text{initial}})$.

c) To find the time evolution of the system, we first need to solve the master equation (2) which can easiest be done in Fourier space, where

$$N_\nu(t) = \sum_{k=-z/2}^{z/2-1} \tilde{N}_k(t) e^{-i \frac{2\pi}{z} k \nu} \quad \text{and} \quad \tilde{N}_k(t) = \frac{1}{z} \sum_{\nu=0}^{z-1} N_\nu(t) e^{i \frac{2\pi}{z} k \nu}. \quad (7)$$

Using this in (2), we find

$$\dot{\tilde{N}}_k(t) = -2\Gamma \left(1 - \cos \frac{2\pi k}{z} \right) \tilde{N}_k(t) \quad (8)$$

with the solution

$$\tilde{N}_k(t) = e^{-t/\tau_k} \tilde{N}_k(0), \quad \tau_k^{-1} = 2\Gamma \left(1 - \cos \frac{2\pi k}{z}\right). \quad (9)$$

We thus see that for every $k \neq 0$, the corresponding distortion away from the equilibrium \tilde{N}_0 has its own decay time τ_k . Note that $\tau_i > \tau_j$ for $|i| < |j|$ ($i, j \in \{-z/2, \dots, z/2 - 1\}$), i.e., the slowest decaying modes are $k = \pm 1$ with characteristic timescale $\tau_1 = \tau_{-1}$.

If we now start with the initial state as given on the exercise sheet, we see that $\tilde{N}_k(0) = N/z$ for all k . Hence, the time evolution of the polarization is

$$P(t) = \frac{1}{N} \sum_{\nu} N_{\nu}(t) \cos \frac{2\pi\nu}{z} \quad (10)$$

$$= \frac{1}{N} \sum_{\nu} \sum_k \tilde{N}_k(t) e^{i\frac{2\pi}{z}k\nu} \cos \frac{2\pi\nu}{z} \quad (11)$$

$$= \frac{z}{2N} (\tilde{N}_1(t) + \tilde{N}_{-1}(t)) = e^{-t/\tau_1}, \quad (12)$$

where we used that

$$\sum_{\nu=0}^{z-1} e^{i\frac{2\pi\nu}{z}k} = z \sum_{m=-\infty}^{\infty} \delta_{k,mz} \quad \forall k \in \mathbb{Z}.$$

In our situation where $k \in \{-z/2, \dots, z/2 - 1\}$ the right hand side of the above equation simplifies to $z\delta_{k,0}$. The result in (12) shows that the polarization decays with the characteristic timescale τ_1 .

Looking at the entropy function for times $t \gg z^2/\Gamma$, only the constant and slowest decaying modes ($k = 0, \pm 1$) need to be taken into account and we can approximate N_{ν} by

$$N_{\nu}(t) \approx \frac{N}{z} + \frac{2N}{z} \cos \frac{2\pi\nu}{z} e^{-t/\tau_1} = \frac{N}{z} (1 + \delta_{\nu}(t)), \quad (13)$$

where the error term $\delta_{\nu}(t) := 2 \cos \frac{2\pi\nu}{z} e^{-t/\tau_1}$ was introduced. Therefore, we find

$$\begin{aligned} H(t) &= - \sum_{\nu} \frac{N_{\nu}(t)}{N} \log \frac{N_{\nu}(t)}{N} \\ &\approx - \sum_{\nu} \frac{1}{z} [1 + \delta_{\nu}(t)] \log \left\{ \frac{1}{z} [1 + \delta_{\nu}(t)] \right\} \\ &\approx - \sum_{\nu} \frac{1}{z} [1 + \delta_{\nu}(t)] \left[-\log(z) + \delta_{\nu}(t) \right] \end{aligned} \quad (14)$$

$$= \log(z) - \frac{1}{z} \sum_{\nu} \delta_{\nu}(t)^2, \quad (15)$$

since $\sum_{\nu} \delta_{\nu}(t) = 0$. Hence, the entropy relaxes to its equilibrium value $H_{\text{final}} = \log(z)$ as $H_{\text{final}} - H(t) \propto e^{-2t/\tau_1}$. As was also seen in the script for the two level system, the H -function approaches its equilibrium value twice as fast as the polarization.

d) Using the same initial distribution and the results of c), the occupation of direction ν is

$$N_{\nu}(t) = \frac{N}{z} \sum_{k=-z/2}^{z/2-1} e^{-i\frac{2\pi}{z}k\nu} e^{2\Gamma t(\cos \frac{2\pi k}{z} - 1)}. \quad (16)$$

We now use the Jacobi–Anger expansion as given on the exercise sheet to substitute

$$e^{2\Gamma t \cos \frac{2\pi k}{z}} = \sum_{n=-\infty}^{\infty} I_n(2\Gamma t) e^{in \frac{2\pi k}{z}}. \quad (17)$$

Using the relation

$$\frac{1}{z} \sum_{k=-z/2}^{z/2-1} e^{-i \frac{2\pi k}{z} (\nu-n)} = \sum_{m=-\infty}^{\infty} \delta_{n, \nu+mz}, \quad (18)$$

we find

$$N_\nu(t) = N e^{-2\Gamma t} \sum_{m=-\infty}^{\infty} I_{\nu+mz}(2\Gamma t) \quad (19)$$

$$\xrightarrow{z \rightarrow \infty} N e^{-2\Gamma t} I_\nu(2\Gamma t). \quad (20)$$

- e) We can go to a continuum description by letting a go to zero and z to infinity while keeping $L = za$ constant. The master equation in $N_\nu(t) = N(x_\nu, t)$ is

$$\begin{aligned} \dot{N}(x_\nu, t) &= \Gamma a^2 \frac{[N(x_{\nu+1}, t) - N(x_\nu, t)] - [N(x_\nu, t) - N(x_{\nu-1}, t)]}{a^2} \\ \implies \dot{\rho}(x, t) &= D \partial_x^2 \rho(x, t) \end{aligned} \quad (21)$$

where $\rho(x, t) = N(x, t)/a$ is the density and $D = \Gamma a^2$ is the diffusion constant. Note that this implies that $\Gamma \propto \frac{1}{a^2}$ in the continuum limit.

In the limit $L \rightarrow \infty$ our ring loses its periodic boundary, i.e. we can assume that $x \in \mathbb{R}$. We can solve the above equation in Fourier space, which yields

$$\tilde{\rho}(k, t) = e^{-Dk^2 t} \tilde{\rho}(k, 0). \quad (22)$$

The initial condition corresponding to c) is $\rho(x, 0) = N\delta(x)$ and thus, $\tilde{\rho}(k, 0) = N$ for all k . With this, we find for the density in real space

$$\rho(x, t) = N \int \frac{dk}{2\pi} e^{-Dk^2 t} e^{ikx} = \frac{N e^{-\frac{x^2}{4Dt}}}{\sqrt{4\pi Dt}}, \quad (23)$$

which is a Gaussian wave packet spreading in time. We can now calculate the time-dependent H -function:

$$H(t) = - \int dx \frac{\rho(x, t)}{N} \log \frac{\rho(x, t)}{N} \quad (24)$$

$$= \int dx \frac{e^{-\frac{x^2}{4Dt}}}{\sqrt{4\pi Dt}} \left(\frac{x^2}{4Dt} + \log \sqrt{4\pi Dt} \right) \quad (25)$$

$$= \frac{1}{2} [1 + \log(4\pi Dt)]. \quad (26)$$

This function diverges, implying that the system never reaches equilibrium. We can again interpret the result with respect to the ideal gas. In b), we have seen that the entropy grows logarithmically with the volume the gas occupies. Here, we can define the volume by $\sqrt{\langle x^2 \rangle}$ (note that $\langle x \rangle$ vanishes because of symmetry):

$$\langle x^2 \rangle = \int dx x^2 \frac{N e^{-\frac{x^2}{4Dt}}}{\sqrt{4\pi Dt}} = 2NDt \propto t. \quad (27)$$

Thus we could have expected that the entropy diverges proportionally to $\log(t)$.

Exercise 1.2 Particle Current and Entropy Production

a) The master equation for this system is

$$\dot{N}_\nu(t) = \Gamma[N_{\nu+1}(t) + N_{\nu-1}(t) - 2N_\nu(t)] \quad (28)$$

for $\nu = 1, \dots, z-1$, and the stationary state is reached when $\dot{N}_\nu = 0$ for all ν . From this we can find recursively

$$\left. \begin{aligned} N_2 &= 2N_1 - N_L \\ \vdots \\ N_z = N_R &= zN_1 - (z-1)N_L \end{aligned} \right\} \implies N_1 = N_L + \frac{N_R - N_L}{z}. \quad (29)$$

and thus

$$N_\nu = N_L + \frac{\nu}{z}(N_R - N_L). \quad (30)$$

In the steady state, all occupation numbers are constant. Therefore the currents across all bonds in the interior of the chain are equal, and using the boundary we find that

$$J_1 = \dots = J_z = \frac{\Gamma}{z}(N_L - N_R), \quad (31)$$

since $\dot{N}_0 = J_0 + \Gamma(N_1 - N_0) = J_0 - J_1$.

b) Since N_ν as given by (30) is a stationary state, $\dot{N}_\nu = 0$, the H -function for the chain does not change with time.

On the other hand,

$$\frac{dH(t)}{dt} = \frac{1}{2} \sum_{\nu, \nu'} \Gamma_{\nu\nu'} \left(\ln \frac{N_\nu}{N} - \ln \frac{N_{\nu'}}{N} \right) \left(\frac{N_\nu}{N} - \frac{N_{\nu'}}{N} \right) \quad (32)$$

$$= \frac{\Gamma}{N} \sum_{\nu=0}^{z-1} \left(\ln \frac{N_\nu}{N_{\nu+1}} \right) (N_\nu - N_{\nu+1}) \quad (33)$$

$$= \frac{\Gamma}{Nz} (N_L - N_R) \sum_{\nu=0}^{z-1} \ln \frac{N_\nu}{N_{\nu+1}} \quad (34)$$

$$= \frac{\Gamma}{Nz} (N_L - N_R) \ln \frac{N_L}{N_R}. \quad (35)$$

shows that the entropy production is manifestly positive

$$\frac{dS(t)}{dt} = Nk_B \frac{dH(t)}{dt} = \frac{\Gamma k_B}{z} (N_L - N_R) \ln \frac{N_L}{N_R}. \quad (36)$$

There is no contradiction, because the master equation used to derive (32) is the one where

$$\dot{N}_0 = \Gamma(N_1 - N_0), \quad \dot{N}_z = \Gamma(N_{z-1} - N_z), \quad (37)$$

which are non-zero in the stationary state.

The entropy increase can be understood as follows: even though the occupation number for each N_ν is a constant over time in the steady state, we still have a flow of “particles” from the higher reservoir to the lower one, i.e. we do not have detailed balance between two neighbouring micro-states ν and $\nu+1$. This system does not reach thermal equilibrium.

c) Using the formula (31) for the current and the assumption that $N_L - N_R = \epsilon$, we find that

$$J = \frac{\Gamma}{z}(N_L - N_R) = \frac{\Gamma}{z}\epsilon \propto \epsilon. \quad (38)$$

On the other hand, the entropy production can be approximated by

$$\dot{S}(t) = \frac{\Gamma k_B}{z} \epsilon \ln \frac{N_R + \epsilon}{N_R} \quad (39)$$

$$\approx \frac{\Gamma k_B}{z N_R} \epsilon^2 \propto \epsilon^2. \quad (40)$$

This has a very important consequence: The fact that the response (here a current) is still proportional while the entropy only grows with ϵ^2 means, that even though we are strictly speaking not in the equilibrium, it's still a good starting point to calculate the response as if we were in the equilibrium.