

# PHYSICS OF COMPLEX SYSTEMS

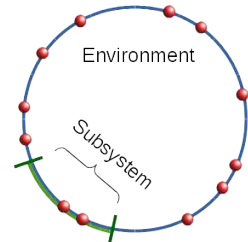
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## SAMPLE SOLUTIONS EXERCISE 9

### EXERCISE 9.1: THERMALIZATION

(7P)

In this exercise we consider again the symmetric exclusion process in 1D. The chain as a whole is considered as a closed thermodynamic system isolated from the environment, i.e., the number of particles is conserved. The aim of this exercise is to show that a small section of this chain, regarded as a subsystem, thermalizes in a grand-canonical ensemble since the complement of the section acts like a reservoir.



Let us consider a 1-dimensional chain with  $L$  sites, periodic boundary conditions, and symmetric rates  $w_L = w_R = 1$ . Assume that the system is populated with  $N < L$  particles. Consider a section of  $K$  consecutive sites. The aim is to approximate the stationary probability distribution  $P_s^{\text{stat}}$  in the subsystem, where  $s$  denotes the microscopic configuration of the particles in the subsystem.

- Find an exact expression for  $P_s^{\text{stat}}$  in the stationary state (correctly normalized).  
*Hint:* It will depend on  $M_s$ , the number of particles in the subsection. (3P)
- Use Stirling's formula  $n! \approx \sqrt{2\pi n} \left(\frac{n}{e}\right)^n$  in order to derive a simpler approximation for probability distribution  $P_s^{\text{stat}}$ . (2P)
- Take this approximation to compute the thermodynamic limit of an infinitely long chain ( $L \rightarrow \infty$ ), keeping the particle density  $\rho = N/L$  as well as the size of the section  $K$  constant. (1P)
- How do we have to choose the density  $\rho$  in order to get a grand-canonical distribution  $P_s^{\text{stat}} \propto e^{-\mu M_s}$ , where  $M_s$  denotes the number of particles of the subsystem in the configuration  $s$ ? How does the chemical potential  $\mu$  depend on  $\rho$ ? (1P)

### SAMPLE SOLUTION

- Since the whole chain can be regarded as a closed system, all possible configurations of the  $N$  particles on the chain with  $L$  sites have to occur with the same probability in the stationary state (microcanonical equilibrium). This means that we have to determine the number of possibilities for distribution  $N$  particles on  $L$  sites. This is just the binomial distribution:

$$|\Omega_{N,L}| = \binom{L}{N} = \frac{L!}{N!(L-N)!}$$

The (constant) probability of each configuration is just the reciprocal of this expression.

Now let us consider the section of the first  $K$  sites (only observationally, we do not manipulate or alter the physical system). The total number of

configurations  $c$ , which are compatible with a given configuration  $s$  of  $M$  particles in the subsystem, equals

$$\binom{L-K}{N-M} = \frac{(L-K)!}{(N-M)!(L-K-N+M)!}$$

In order to determine  $P_s^{\text{stat}}$ , this number has to be multiplied by the (constant) probability of finding the total system in a certain configuration:

$$P_s^{\text{stat}} = \frac{\binom{L-K}{N-M}}{\binom{L}{N}} = \frac{(L-K)! N! (L-N)!}{(N-M)!(L-K-N+M)! L!}.$$

Another binomial factor which would take the different arrangements of particles in the subsystem into account is not needed here since we are asking for a *particular* configuration  $s$  in the subsystem.

- (b) Substituting Stirling's formula  $n! \approx \sqrt{2\pi n} \left(\frac{n}{e}\right)^n$  we get

$$P_s^{\text{stat}} \approx \tilde{P}_s^{\text{stat}} = L^{-L-\frac{1}{2}} N^{N+\frac{1}{2}} (L-K)^{-K+L+\frac{1}{2}} (L-N)^{L-N+\frac{1}{2}} \times \\ \times (N-M)^{M-N-\frac{1}{2}} (-K+L+M-N)^{K-L-M+N-\frac{1}{2}}$$

- (c) Finally we set  $N = \rho L$  and get

$$\lim_{L \rightarrow \infty} \tilde{P}_s^{\text{stat}} = \rho^M (1-\rho)^{K-M}.$$

- (d) The subsystem (i.e., the section of sites  $1 \dots K$ ) is now allowed to exchange particles with the almost infinite reservoir of particles in the rest of the chain, keeping the total number of particles constant. We therefore expect to find a canonical distribution of the form  $P_s^{\text{stat}} \approx e^{-\mu M}$ , where  $\mu$  denotes the chemical potential. Comparing the expressions we find that such an exponential characteristics is obtained for particle densities  $\rho < 1/2$ . In this case the chemical potential is given by

$$\mu = \ln \left( \frac{1}{\rho} - 1 \right) \approx -\ln \rho.$$

Hence, the smaller the particle density in the reservoir, the larger is the chemical potential  $\mu$ .

## EXERCISE 9.2: ISING MEANFIELD THEORY (5P)

In the mean field approximation of the Ising model, the average magnetization of a spin  $\langle s \rangle$  is given by the implicit equation (see lecture notes)

$$\langle s \rangle = \tanh(\beta \bar{H}) = \tanh[2dJ\beta \langle s \rangle + \beta h]. \quad (1)$$

The aim of this exercise is to compute the partition sum as well as the critical exponents within the mean field approximation.

- (a) Compute the partition sum  $Z(\beta, h)$ , keeping  $\bar{H}$  (a function that implicitly depends on  $\beta$  and  $h$ ) in your calculation as it is. (1P)

(b) Show that the partition sum can be written in the form

$$Z(\beta, h) = \left( \frac{2}{\sqrt{1 - \langle s \rangle^2}} \right)^N$$

and give an expression for the thermodynamic potential  $\mathcal{V} = \ln Z$ . (1P)

(c) Show that the heat capacity can be expressed as (1P)

$$C = N\beta^2 \bar{H}^2 (1 - \langle s \rangle^2).$$

(d) Expand and solve the implicit equation (1) in a suitable manner that allows you to determine the exponents  $\tilde{\beta}$  as well as  $\delta$  (please avoid confusing the exponent  $\tilde{\beta}$  with the inverse temperature  $\beta$ ). (2P)

### SAMPLE SOLUTION

(a) The partition sum can be computed as follows: (1P)

$$\begin{aligned} Z(\beta, h) &= \sum_s \exp \left( \beta \sum_i \underbrace{(2dJ\langle s \rangle + h)}_{=\bar{H}} s_i \right) = \prod_i \sum_{s_i=\pm 1} \exp(\beta \bar{H} s_i) \\ \Rightarrow Z(\beta, h) &= \left( e^{\beta \bar{H}} + e^{-\beta \bar{H}} \right)^N = (2 \cosh(\beta \bar{H}))^N. \end{aligned}$$

(b) The given expression can be derived by the following identity: (1P)

$$\begin{aligned} \cosh x &= 1/\sqrt{1 - \tanh^2 x} \\ \Rightarrow Z(\beta, h) &= \left( \frac{2}{\sqrt{1 - \tanh^2(\beta \bar{H})}} \right)^N = \left( \frac{2}{\sqrt{1 - \langle x \rangle^2}} \right)^N \end{aligned}$$

Then the potential (aka free energy  $-\beta F$ ) is given by

$$\mathcal{V} = N \left( \ln 2 - \frac{1}{2} \ln[1 - \langle x \rangle^2] \right).$$

(c) The heat capacity can be computed via

$$C = \beta^2 \frac{\partial^2 \ln Z}{\partial \beta^2}$$

When taking the derivative we have to keep  $\bar{H}$  as it is (although it depends implicitly on  $\beta$ ) since otherwise we do not get the right expression. Starting with (a) we get (1P)

$$C = \frac{N\beta^2 \bar{H}^2}{\cosh^2(\beta \bar{H})} = N\beta^2 \bar{H}^2 (1 - \tanh^2(\beta \bar{H})) = N\beta^2 \bar{H}^2 (1 - \langle s \rangle^2)$$

(d1) The exponent  $\tilde{\beta}$  is defined as

$$m(\beta, 0) \sim (\beta_c - \beta)^{\tilde{\beta}},$$

where we used a tilde in  $\tilde{\beta}$  in order to avoid confusion with the inverse temperature  $\beta = 1/T$ . In this formula,  $\beta_c = 1/2Jd$  denotes the critical point where the transition takes place. Note that we have set  $h = 0$ . With  $m = \langle x \rangle$  we are led to the implicit equation

$$m = \tanh(2dJ\beta m).$$

Near the transition, where  $m$  is very small, we can expand the hyperbolic function:  $\tanh x \approx x - \frac{1}{3}x^3 + \dots$ . This expansion leads us to the equation

$$m = 2dJ\beta m - \frac{1}{3}(2dJ\beta m)^3$$

with the solution (1P)

$$m = \sqrt{\frac{3}{8} \frac{\sqrt{2dJ\beta - 1}}{(dJ\beta)^{3/2}}} = \sqrt{6dj(\beta - \beta_c)} + \mathcal{O}(\beta - \beta_c).$$

Because of the square root, we get the exponent  $\tilde{\beta} = 1/2$ .

(d2) For getting the critical exponent  $\delta$ , we have to vary  $h$  around 0 precisely at the critical point. More specifically,  $\delta$  is defined by

$$m(\beta_c, h) \sim h^{1/\delta},$$

where  $\beta_c = \frac{1}{2dJ}$  is the critical point within the mean field approximation. With  $m = \langle x \rangle$  this leads us to the relation

$$m = \tanh(m + \beta_c h).$$

Since both  $m$  and  $h$  are very small, we can expand it by  $\tanh x \approx x - \frac{1}{3}x^3 + \dots$ . Our equation thus reduces to

$$(m = (m + \beta_c h) - \frac{1}{3}(m + \beta_c h)^3$$

with the real-valued solution (1P)

$$m = (3\beta_c h)^{1/3} - \beta_c h.$$

Here the first term vanishes, hence  $m \sim h^{1/3} \Rightarrow \delta = 3$ .

( $\Sigma = 12P$ )