

**Exercise 1. Classical ideal paramagnet**

We consider an ideal paramagnet of magnetic moments in a magnetic field. The magnetic moments have only two orientations, parallel and antiparallel to the magnetic field. The Hamiltonian of the system is given by

$$\mathcal{H} = - \sum_{i=1}^N m_i H, \quad (1)$$

with  $m_i = \pm m$ ,  $H$  as the magnetic field and  $N$  the number of magnetic moments.

- a) Calculate the internal energy, entropy, magnetization and magnetic susceptibility using the micro-canonical ensemble. *Hint:* Use combinatoric relation for binomial systems to determine the micro-canonical phase space count.

**Solution.** We define the magnetization  $M = nmH$ , with  $n = n_+ - n_-$  and  $N = n_+ + n_-$ , such that  $n_{\pm} = \frac{N \pm n}{2}$ . The (discrete) phase space area is then the number of combinations of moments that give the same magnetization, so  $\Omega(n) = \frac{N!}{n_+! n_-!}$ . We now use the Stirling's approximation  $\ln(N!) = N \ln N - N + \mathcal{O}(\ln N)$  and ignore terms of order  $\log N$ .

$$\begin{aligned} \log \Omega(n) &= \log(N!) - \log(n_+!) - \log(n_-!) \\ &\approx N(\log N - 1) - \frac{N+n}{2} \left( \log \left( \frac{N+n}{2} \right) - 1 \right) - \frac{N-n}{2} \left( \log \left( \frac{N-n}{2} \right) - 1 \right), \end{aligned}$$

where we neglected the term  $\frac{1}{2} \log(\pi^2(N^2 - n^2))$ . The entropy then reads:

$$S = k_B \log \Omega(n) = 2Nk_B \log(2) - \frac{Nk_B}{2} \left( \left(1 + \frac{n}{N}\right) \log \left(1 + \frac{n}{N}\right) + \left(1 - \frac{n}{N}\right) \log \left(1 - \frac{n}{N}\right) \right) \quad (S.1)$$

From the differential  $dS = (1/T)dU + (M/T)dH$  we can obtain the temperature, as follows. We insert  $n = -\frac{E}{Hm}$  to get  $S(E, H)$  and differentiate keeping  $n$  explicitly:

$$\begin{aligned} \frac{1}{T} &= \left( \frac{\partial S}{\partial E} \right)_H = \left( \frac{\partial n}{\partial E} \right)_H \frac{\partial S}{\partial n} = -\frac{1}{Hm} \frac{\partial S}{\partial n} \\ &= \frac{Nk_B}{2Hm} \left( \frac{1}{N} \log \left(1 + \frac{n}{N}\right) - \frac{1}{N} \log \left(1 - \frac{n}{N}\right) + \frac{1}{N} - \frac{1}{N} \right) = \frac{k_B}{2Hm} \log \left( \frac{N+n}{N-n} \right) \\ &= -\frac{k_B}{2Hm} \log \left( \frac{NHm + E}{NHm - E} \right). \end{aligned}$$

Inverting the above equation yields  $E = -NHm \tanh(\beta mH)$ , with  $\beta = 1/(k_B T)$ . In order to obtain the magnetization we first calculate the partial derivative

$$\left( \frac{\partial S}{\partial H} \right)_E = \left( \frac{\partial n}{\partial H} \right)_E \frac{\partial S}{\partial n} = -\frac{E}{H^2 m} \frac{\partial S}{\partial n} = \frac{Ek_B}{2H^2 m} \log \left( \frac{NHm + E}{NHm - E} \right),$$

and then

$$M = T \left( \frac{\partial S}{\partial H} \right)_E = -\frac{E}{H} = Nm \tanh(\beta mH). \quad (S.2)$$

The susceptibility reads:

$$\chi_H = \left( \frac{\partial M}{\partial H} \right) = \frac{Nm^2 \beta}{\cosh^2(\beta mH)}. \quad (S.3)$$

It is useful to study the magnetization and the susceptibility in the two regimes  $\beta mH \gg, \ll 1$  (see Fig. 1). When  $\beta mH \ll 1$  (small field and/or large temperature limit)  $\tanh x \approx x - \mathcal{O}(x^3)$  and  $\cosh x \approx 1 + \mathcal{O}(x^2)$  such that the magnetization grows linearly in the field, i.e., according to the Curie law of independent moments

$$M \approx Nm^2 \beta H = \chi_H \quad \text{with} \quad \chi_H \approx Nm^2 \beta = \chi. \quad (S.4)$$

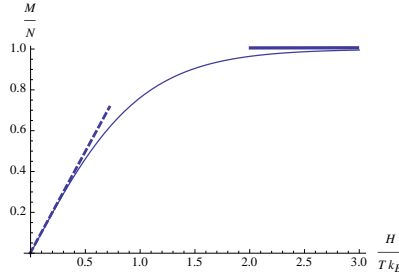


Figure 1: Magnetization (S.2) as a function of magnetic field strength  $H$  scaled to  $k_B T$ . The dashed (solid) line is the asymptote at small (large) field ( $m = 1$ ).

When  $\beta m H \gg 1$  (large field and/or small temperature limit)  $\tanh x \approx 1 - e^{-2x}$  and the magnetization tends to saturate, i.e.,

$$M \approx mN(1 - 2e^{-2\beta m H}). \quad (\text{S.5})$$

It is also interesting to consider the heat capacity for constant external field  $H$ . From  $dU = \left(\frac{\partial U}{\partial T}\right)_H dT + \left(\frac{\partial U}{\partial H}\right)_T dH$  and  $dM = \left(\frac{\partial M}{\partial T}\right)_H dT + \left(\frac{\partial M}{\partial H}\right)_T dH$  such that

$$\delta Q = dU - \delta W = dU - H dM = \left[ \left(\frac{\partial U}{\partial T}\right)_H - H \left(\frac{\partial M}{\partial T}\right)_H \right] dT + \left[ \left(\frac{\partial U}{\partial H}\right)_T - H \left(\frac{\partial M}{\partial H}\right)_T \right] dH. \quad (\text{S.6})$$

The heat capacity at fixed  $H$  is then given by:

$$C_H = \left(\frac{\partial U}{\partial T}\right)_H - H \left(\frac{\partial M}{\partial T}\right)_H = 2 \frac{Nk_B(\beta H m)^2}{\cosh^2(\beta m H)}, \quad (\text{S.7})$$

where we used  $\partial_T f(\beta) = -k_B \beta^2 \partial_\beta f(\beta)$ . Note that both the susceptibility and the heat capacity are exponentially suppressed at low temperature  $\sim T^{-\alpha} e^{-2Hm/k_B T}$  with  $\alpha = 1, 2$ , which is indicating a freezing of the degrees of freedom.

- b) Calculate the internal energy, entropy, magnetization and magnetic susceptibility using the canonical ensemble.

**Solution.** In order to determine the thermodynamics of the ideal paramagnet in the canonical ensemble, we calculate the partition function:

$$Z = \prod_{i=1}^N \left[ \sum_{\sigma=\pm} e^{-\beta H m \sigma} \right] = [2 \cosh(\beta m H)]^N = Z_m^N. \quad (\text{S.8})$$

We can now easily calculate all the thermodynamic functions, e.g, the free energy:

$$F(T, H, N) = -\frac{1}{\beta} \ln Z = -k_B T N \ln Z_m \quad (\text{S.9})$$

and the internal energy

$$U(T, H, N) = -\partial_\beta \ln Z = -N m H \tanh(\beta m H). \quad (\text{S.10})$$

From the free energy (S.9) we obtain the magnetization and the susceptibility, which are equal to the micro canonical case (S.2), (S.3).

## Exercise 2. Classical ideal lattice gas

We consider  $N_1$  particles on a lattice of  $N$  sites ( $N = N_1 + N_2$ ), which have the condition that only one particle can occupy a site at a time. We assume that the particles have the energy  $E_A$  on  $N_1$  sites and  $E_B$  on the other  $N_2$  sites. Consider the situation that  $N_1 < N_2$  and analyse the following situations in both the micro-canonical and canonical ensemble.

- a) The energies satisfy  $E_A < E_B$ .
- b) The energies satisfy  $E_A > E_B$ .
- c) Vary the energies continuously between case a) and b).

**Solution.** *Microcanonical case* We need to calculate the number of microscopic realizations that yields the same energy

$$E = N_A E_A + N_B E_B \quad (\text{S.11})$$

with  $N_{A(B)}$  the number of particles on the sites with energy  $E_{A(B)}$ . Note, that  $N_A \leq N_1$ , and

$$N_1 = N_A + N_B. \quad (\text{S.12})$$

At zero temperature, as  $N_1 \leq N_2$  we expect that when  $E_A < E_B$ ,  $N_A = N_1$  with zero entropy, as there is only one configuration possible (all atoms sitting on the  $N_A$  sites). On the other hand, when  $E_A > E_B$ , it will be favourable for the system to occupy the  $B$  sites, i.e.,  $N_A = 0$  and since  $N_2 > N_1$  the number of allowed configurations will be larger than 1 and the residual entropy non zero. More quantitatively,

$$\Omega = \Omega_A \Omega_B = \frac{N_1!}{(N_1 - N_A)! N_A!} \frac{N_2!}{(N_2 - N_B)! N_B!} = \frac{N_1!}{(N_1 - N_A)! N_A!} \frac{(N - N_1)!}{(N + N_A)! (N_1 - N_A)!}, \quad (\text{S.13})$$

where we used  $N = N_1 + N_2$  and  $N_1 = N_A + N_B$ . We immediately see that when  $N_A = N_1$ ,  $N_B = 0$  and  $\Omega = 1$ , while when  $N_A = 0$   $\Omega = \Omega_B > 1$ . The entropy reads:

$$S = k_B \ln \Omega = k_B [N_1 \ln N_1 + 2N_1 - 2(N_1 - N_A) \ln(N_1 - N_A) - N_A \ln N_A + (N - N_1) \ln(N - N_1) - (N + N_A) \ln(N + N_A)]. \quad (\text{S.14})$$

In order to obtain the temperature, we write

$$\frac{1}{T} = \frac{\partial S}{\partial E} = \frac{\partial N_A}{\partial E} \frac{\partial S}{\partial N_A} = \frac{1}{E_A - E_B} \frac{\partial S}{\partial N_A}, \quad (\text{S.15})$$

such that

$$\frac{1}{T} = \frac{k_B}{E_A - E_B} [2 \ln(N_1 - N_A) - \ln(N + N_A) - \ln N_A] \quad (\text{S.16})$$

which implies

$$\frac{(N_1 - N_A)^2}{N_A(N + N_A)} = e^{-\beta(E_B - E_A)}. \quad (\text{S.17})$$

At zero  $T$ , when  $E_A < E_B$  the R. H. S. of the equation above is zero and this can only be satisfied when  $N_1 = N_A$ . On the other hand, when  $E_A > E_B$  the R. H. S. diverges, implying  $N_A = 0$ . Therefore, the distribution  $N_A(E_A)$  goes from  $N_1$  when  $E_A < E_B$  to zero when  $E_A > E_B$  in a step-like fashion at zero temperature. For larger  $T$ , the step is smeared out over an energy interval  $\sim k_B T$ .

*Canonical case* It is straightforward to write the partition function in the following way:

$$Z = (1 + e^{-\beta(E_A - \mu)})^{N_1} (1 + e^{-\beta(E_B - \mu)})^{N_2} \quad (\text{S.18})$$

as each one among the  $N_{1,2}$  sites can be either occupied or empty. The quantity  $\mu$  fixes the particle number and results from the shifting of the Hamiltonian  $H = H_A + H_B \rightarrow H = H_A + H_B - \mu(N_A + N_B) = \tilde{H}_A + \tilde{H}_B$ . Therefore, the internal energy reads:

$$U = -\partial_\beta \ln Z = N_1 E_A \frac{z e^{-\beta E_A}}{1 + z e^{-\beta E_A}} + N_2 E_B \frac{z e^{-\beta E_B}}{1 + z e^{-\beta E_B}} = N_A E_A + N_B E_B, \quad (\text{S.19})$$

with  $z = \exp(\beta \mu)$ . From the last equivalence, we obtain

$$N_A = (N_1 - N_A) z e^{-\beta E_A} \quad \text{and} \quad N_B = (N_2 - N_B) z e^{-\beta E_B} \quad (\text{S.20})$$

such that

$$\frac{N_B(N_1 - N_A)}{N_A(N_2 - N_B)} = e^{-\beta(E_B - E_A)}. \quad (\text{S.21})$$

Again, at zero  $T$ , when  $E_A < E_B$  the R. H. S. of the equation above is zero and this implies  $N_1 = N_A$ , i.e., all particles are in the  $A$  sites. On the other hand, when  $E_A > E_B$  the R. H. S. diverges, implying  $N_A = 0$  or  $N_2 = N_B$ . Since  $N_1 < N_2$  it can only be  $N_A = 0$ . Alternatively, one could obtain the Boltzmann factors (S.20) by maximizing the phase space count (S.13) with respect to  $N_A$  with the energy (S.11) and particle number (S.12) constraints imposed through Lagrange multipliers. The multiplier  $\beta$  fixing the total energy can be shown to be equal to the inverse temperature via the thermodynamic relation

$$\frac{1}{T} = \frac{dS}{dE} = \frac{\partial S}{\partial N_A} \frac{\partial N_A}{\partial E} + \frac{\partial S}{\partial N_B} \frac{\partial N_B}{\partial E} = k_B \beta. \quad (\text{S.22})$$

**Exercise 3. Classical ideal gas in a harmonic trap**

We consider independent classical particles in a harmonic trap described by the Hamiltonian,

$$\mathcal{H} = \sum_i \left\{ \frac{\vec{p}_i^2}{2m} + a\vec{r}_i^2 \right\}. \quad (2)$$

a) Assume  $N$  particles and discuss the system in the micro-canonical ensemble.

**Solution.** In the microcanonical ensemble, the connection to thermodynamics is provided through the phase space volume

$$\Phi(E) = \Lambda_N \int_{H(p,q) \leq E} dp dq, \quad (S.23)$$

with

$$H(p, q) = \sum_{i=1}^N \left[ \frac{\vec{p}_i^2}{2m} + a\vec{q}_i^2 \right]. \quad (S.24)$$

We perform the rescaling,  $P_i = p_i/\sqrt{2m}$  and  $Q_i = q_i\sqrt{a}$ , such that the Hamiltonian is simplified

$$H(P, Q) = \sum_{i=1}^N \left[ \vec{P}_i^2 + \vec{Q}_i^2 \right] \quad (S.25)$$

as well as the phase space integral

$$\Phi(E) = \Lambda_N \left( \frac{2m}{a} \right)^{3N/2} \int_{H(P,Q) \leq E} dP dQ, \quad (S.26)$$

since  $dp = \prod_{i=1}^N d^3 p_i$  and  $dq = \prod_{i=1}^N d^3 q_i$ . We then need to calculate, as already explained in the lecture, the volume of a sphere in  $6N$  dimensional space, i.e.,

$$\Phi(E) = \Lambda_N \left( \frac{2m}{a} \right)^{3N/2} C_{6N} E^{3N}, \quad (S.27)$$

with

$$C_n = \frac{\pi^{n/2}}{\Gamma(\frac{n}{2} + 1)}. \quad (S.28)$$

In order to obtain the thermodynamics, we can then refer to the lecture, with the substitutions  $2m \rightarrow 2m/a$  and  $E^{3N/2} \rightarrow E^{3N}$ , i.e., the entropy

$$S(E, N) = Nk_B \ln \left[ \frac{1}{N} \left( \sqrt{\frac{2m}{a}} \frac{\pi E}{3Nh} \right)^3 \right] + 4Nk_B. \quad (S.29)$$

Inverting the above relation we find:

$$U(S, N) = E = \frac{3N^{4/3}h}{\pi} \sqrt{\frac{a}{2m}} \exp \left[ \frac{S}{3Nk_B} - 4/3 \right] \quad (S.30)$$

such that the equation of state can be obtained as follows,

$$T = \left( \frac{\partial U}{\partial S} \right)_N = \frac{U}{3Nk_B} \rightarrow U = 3Nk_B T, \quad (S.31)$$

which expresses the equipartition law.

b) Assume  $N$  particles and discuss the system in the canonical ensemble.

**Solution.** Within the canonical ensemble, we need again to calculate the partition function. It reads:

$$\begin{aligned}
Z &= \Lambda_N \int dp dq e^{-\beta H(p,q)} = \Lambda_N \left[ \prod_{i=1}^N \int d^3 p_i e^{-\beta \mathbf{p}_i^2 / 2m} \right] \left[ \prod_{i=1}^N \int d^3 q_i e^{-\beta a \bar{q}_i^2} \right] = \\
&= \Lambda_N \left[ \int dx dy dz e^{-\beta(x^2+y^2+z^2)/2m} \right]^N \left[ \int dx dy dz e^{-a\beta(x^2+y^2+z^2)} \right]^N = \\
&= \Lambda_N \left( \frac{2m}{a} \right)^{3N/2} [\pi k_B T]^{3N}.
\end{aligned} \tag{S.32}$$

We can then obtain all thermodynamic functions, as in Ex. 1, e.g., the free energy:

$$F(T, N) = -\frac{1}{\beta} \ln Z = -N k_B T \ln \left[ \frac{1}{N} \left( \sqrt{\frac{2m}{a}} \frac{\pi k_B T}{h} \right)^3 \right] - N k_B T \tag{S.33}$$

and the caloric equation of state,

$$U(T, N) = -\partial_\beta \ln Z = 3N k_B T. \tag{S.34}$$

- c) Assume a constant chemical potential  $\mu$  and discuss the system in the grand canonical ensemble. Note the differences. How would you determine/define compressibility?

**Solution.** In the grand-canonical ensemble, the thermodynamics for fixed chemical potential  $\mu$  and varying particle number  $N$  is given through the grand partition function,

$$\mathcal{Z} = \sum_{N=0}^{\infty} z^N Z_N, \tag{S.35}$$

with the fugacity  $z = \exp(\beta\mu)$ , while  $Z_N$  is the partition function of the corresponding canonical ensemble (S.32), i.e., with given  $N$ . We then obtain:

$$\begin{aligned}
\mathcal{Z} &= \sum_{N=0}^{\infty} \frac{1}{N! h^{3N}} e^{\beta\mu N} \left[ \sqrt{\frac{2m}{a}} \frac{\pi k_B T}{h} \right]^{3N} = \sum_{N=0}^{\infty} \frac{1}{N!} \left[ e^{\beta\mu} \left( \sqrt{\frac{2m}{a}} \frac{\pi k_B T}{h} \right)^3 \right]^N = \\
&= \exp \left[ e^{\beta\mu} \left( \sqrt{\frac{2m}{a}} \frac{\pi k_B T}{h} \right)^3 \right].
\end{aligned} \tag{S.36}$$

We are then able to calculate all thermodynamic functions, i.e., the grand potential

$$\Omega(T, V, \mu) = -pV = -\frac{1}{\beta} \ln \mathcal{Z} = -e^{\beta\mu} \left( \sqrt{\frac{2m}{a}} \frac{\pi}{h} \right)^3 (k_B T)^4. \tag{S.37}$$

In order to define compressibility, we exploit the Gibbs-Duhem relation

$$G(T, p, N) = \mu N \quad \rightarrow \quad SdT - Vdp + Nd\mu = 0, \tag{S.38}$$

where  $G$  is the Gibbs free energy. We can then write:

$$d\mu = vdp - \frac{S}{N}dT \quad \rightarrow \quad \left( \frac{\partial \mu}{\partial v} \right)_T = v \left( \frac{\partial p}{\partial v} \right)_T, \tag{S.39}$$

where  $v = V/N$ . One then obtains

$$\left( \frac{\partial \mu}{\partial v} \right)_T = \left( \frac{\partial N}{\partial v} \frac{\partial \mu}{\partial N} \right)_T = -\frac{N^2}{V} \left( \frac{\partial \mu}{\partial N} \right)_T \tag{S.40}$$

while for the R.H.S. of (S.39)

$$\left( \frac{\partial p}{\partial v} \right)_T = \left( \frac{\partial V}{\partial v} \frac{\partial p}{\partial V} \right)_T = N \left( \frac{\partial p}{\partial V} \right)_T \tag{S.41}$$

such that one can conclude:

$$-\frac{N^2}{V} \left( \frac{\partial \mu}{\partial N} \right)_T = V \left( \frac{\partial p}{\partial V} \right)_T \quad \rightarrow \quad N \left( \frac{\partial \mu}{\partial N} \right)_T = -vV \left( \frac{\partial p}{\partial V} \right)_T. \tag{S.42}$$

According to the definition of isothermal compressibility,

$$\kappa_T = -\frac{1}{V} \left( \frac{\partial V}{\partial p} \right)_T, \quad (\text{S.43})$$

that quantifies the normalized reduction in volume when changing the pressure at fixed temperature, we obtain:

$$\kappa_T = \frac{v}{N} \left( \frac{\partial N}{\partial \mu} \right)_T. \quad (\text{S.44})$$

In the grand-canonical ensemble, we replace  $N$  with  $\langle N \rangle$ , which can be calculated as follows:

$$\langle N \rangle = z \partial_z \ln \mathcal{Z} = \ln \mathcal{Z} = -\Omega \beta. \quad (\text{S.45})$$

Therefore,

$$\kappa_T = \frac{v}{\langle N \rangle} \left( \frac{\partial z}{\partial \mu} \frac{\partial \langle N \rangle}{\partial z} \right)_T = \frac{v}{z} \frac{\partial z}{\partial \mu} = v \beta. \quad (\text{S.46})$$

**Exercise 1. The Classical Ideal Paramagnet Reloaded.**

Consider a lattice of  $N$  noninteracting particles, each possessing a magnetic moment  $\vec{m}_i$  of fixed magnitude  $m$  which can point in any spacial direction. (This changes from last week's exercise, where  $m_i = \pm m$ .) The Hamiltonian is, as you might have guessed,

$$\mathcal{H} = - \sum_i \vec{m}_i \cdot \vec{H}, \quad (1)$$

where  $\vec{H}$  is the externally applied magnetic field, assumed homogeneous and in the Z direction.

- (a) Calculate the canonical partition function  $Z$  of the system.

**Solution.** All magnetic moments are independent, so we can calculate first the partition function  $Z_1$  of a single magnetic moment  $\vec{m}$ :

$$\begin{aligned} Z_1 &= \int \frac{d\Omega}{4\pi} e^{\beta \vec{m} \cdot \vec{H}} = \int \frac{d\Omega}{4\pi} e^{\beta m H \cos \theta} = \frac{1}{2} \int_0^\pi d\theta \sin \theta e^{\beta m H \cos \theta} \\ &= \frac{1}{2} \int_0^\pi d\theta \left( \frac{-1}{\beta m H} \right) \frac{\partial}{\partial \theta} e^{\beta m H \cos \theta} = -\frac{1}{2\beta m H} \left[ e^{\beta m H \cos \theta} \right]_0^\pi = \frac{\sinh \beta m H}{\beta m H}. \end{aligned} \quad (S.1)$$

The total partition function is then simply

$$Z = \left( \frac{\sinh \beta m H}{\beta m H} \right)^N. \quad (S.2)$$

- (b) Calculate the free energy  $F$ , internal energy  $U$  and heat capacity  $C$ . Discuss the limiting cases where  $k_B T \ll mH$  and  $k_B T \gg mH$ . Calculate the entropy  $S$  in those cases.

**Solution.** *Free Energy.* The free energy is given by

$$F = -\frac{1}{\beta} \ln Z = -N k_B T \ln \frac{\sinh \beta m H}{\beta m H}. \quad (S.3)$$

If  $k_B T \ll mH$  (i.e.  $\beta m H \rightarrow \infty$ ), we can approximate  $\sinh \beta m H \approx \frac{1}{2} e^{\beta m H}$  and

$$F \approx -N k_B T \ln \frac{e^{\beta m H}}{2\beta m H} = -N m H + N k_B T \ln (2\beta m H). \quad (S.4)$$

If  $k_B T \gg mH$  we have  $\beta m H \rightarrow 0$  and in this case

$$F \approx -N k_B T \ln \frac{\beta m H + \frac{(\beta m H)^3}{3!}}{\beta m H} = -N k_B T \ln \left( 1 + \frac{(\beta m H)^2}{3!} \right) \approx -N k_B T \frac{(\beta m H)^2}{3!} = -N k_B T \frac{1}{3!} \left( \frac{mH}{k_B T} \right)^2. \quad (S.5)$$

*Internal Energy.* It is given by

$$U = -\frac{\partial}{\partial \beta} N [\ln \sinh \beta m H - \ln \beta m H] = -N \left[ m H \coth \beta m H - \frac{m H}{\beta m H} \right] = N m H \left[ \frac{1}{\beta m H} - \coth \beta m H \right]. \quad (S.6)$$

*Heat Capacity.* The heat capacity is then

$$C = \frac{\partial U}{\partial T} = -\frac{1}{k_B T^2} \frac{\partial U}{\partial \beta} = -\frac{N m H}{k_B T^2} \left[ -\frac{1}{m H \beta^2} - \frac{-m H}{\sinh^2 \beta m H} \right] = N k_B \left( 1 - \frac{(\beta m H)^2}{\sinh^2 \beta m H} \right). \quad (S.7)$$

In the case  $k_B T \ll mH$ , i.e.  $\beta mH \rightarrow \infty$ , we have  $\sinh \beta mH \approx \frac{1}{2} e^{\beta mH}$ . Then  $\frac{\beta mH}{\sinh \beta mH} \approx 2\beta mH e^{-\beta mH} \rightarrow 0$ , such that  $C \rightarrow Nk_B$  like for an ideal gas (in violation of the third law of thermodynamics<sup>1</sup>). In the limit where  $k_B T \gg mH$ , we have  $\beta mH \rightarrow 0$ , in which case  $\sinh(\beta mH)/\beta mH \rightarrow 1$  and  $C \rightarrow 0$ .

*Entropy.* We have  $S - S_0 = -\left(\frac{\partial F}{\partial T}\right)_{H,N}$ . In the regime  $k_B T \ll mH$ ,

$$\begin{aligned} S - S_0 &= -Nk_B \ln(2\beta mH) - Nk_B T \left(\frac{\partial \beta}{\partial T}\right) \frac{\partial}{\partial \beta} \ln(2\beta mH) = -Nk_B \ln(2\beta mH) - Nk_B T \frac{-1}{k_B T^2} \frac{2mH}{2\beta mH} \\ &= -Nk_B \ln(2\beta mH) + Nk_B . \end{aligned} \quad (\text{S.8})$$

In the other regime,  $k_B T \gg mH$ , we have

$$S - S_0 = \frac{Nk_B}{3!} \left(\frac{mH}{k_B T}\right)^2 + \frac{Nk_B T}{3!} 2 \left(\frac{mH}{k_B T}\right) \frac{-mH}{k_B T^2} = -\frac{Nk_B}{3!} \left(\frac{mH}{k_B T}\right)^2 . \quad (\text{S.9})$$

(In case you had your doubts, you do indeed get the same expressions for the entropy in these limiting cases if you started off from (S.3), calculated the entropy in general and then looked at the limiting cases.)

(c) If  $M_z$  is the thermodynamic variable corresponding to magnetization, show that

$$M_z = -\left(\frac{\partial F}{\partial H_z}\right)_{T,N} . \quad (2)$$

*Hint.* Remember that in the thermodynamics of magnetic systems,  $H$  and  $M$  replace respectively variables  $p$  and  $V$  as conjugate variables.

**A Note: Which differential to use?**

In the beginning of the course “Theory of Heat” we derived the (correct) differential  $dU = TdS + HdM$ , which corresponds to fixing the (extensive) variable  $M$  (the magnetization). This relates well to the mechanical case with the analogies  $-p \leftrightarrow H$  and  $V \leftrightarrow M$ .

However, in “reality” it is much more convenient to fix the (intensive) external magnetic field  $H$ . This corresponds to the enthalpy  $H$ , which is the Legendre transform of the internal energy

$$dH = dU - d(HM) = TdS - MdH . \quad (\text{S.10})$$

That means, what we identify with the energy in the microcanonical treatment (when fixing the magnetic field) is in fact the *enthalpy*  $H$  (instead of the internal energy  $U$ ) and the canonical treatment technically leads to the *Gibbs free energy*  $G$  (instead of the Helmholtz free energy  $F$ ).

However, we do not want to change all these relations, so we just “redefine” the differential of the internal energy to

$$dU = TdS - MdH \quad (\text{S.11})$$

such that we swap  $H \leftrightarrow U$  and  $G \leftrightarrow F$ . Then we can keep the usual relations  $E = U$  (microcanonical) and  $F = k_B T \log(Z)$  (canonical).

**Solution.** We know from thermodynamics that the differential of the internal energy is given by

$$dU = TdS - MdH + \mu dN . \quad (\text{S.12})$$

(Here, we will write for short  $M \equiv M_z$  and  $H \equiv H_z$ .)

The differential  $-MdH$  should be chosen instead of  $HdM$  because  $H$  is the external parameter that can be varied, while the magnetization  $M$  is the system’s response. (This is like considering the enthalpy of a gas rather than its internal energy, in case we had control over the pressure and not the volume.)

The free energy is the Legendre transform  $F = U - TS$  and its differential is now

$$dF = -SdT - MdH + \mu dN , \quad (\text{S.13})$$

---

<sup>1</sup> The third law of thermodynamics states that the entropy must reach a finite value, conventionally zero, at zero temperature. This implies that the heat capacity must vanish. This is a well-known problem of the ideal gas model, for which the entropy diverges at zero temperature and also has a finite heat capacity.



from which we can now trivially read out

$$\left(\frac{\partial F}{\partial H}\right)_{T,N} = -M. \quad (\text{S.14})$$

(d) The magnetization in statistical mechanics is given by  $M_z = \sum_i m_i^z$ . Show explicitly that

$$\langle M_z \rangle = -\frac{\partial F}{\partial H_z}. \quad (3)$$

Calculate the value of  $\langle M_z \rangle$ . In which regime does the system obey Curie's law?

**Solution.** We have by definition

$$\langle M_z \rangle = \frac{1}{Z} \int d\Omega_1 \dots d\Omega_N M_z e^{-\beta \mathcal{H}(\vec{m}_1, \dots, \vec{m}_N, \vec{H})}. \quad (\text{S.15})$$

Because of the form of our Hamiltonian, we have  $\frac{\partial \mathcal{H}}{\partial H_z} = -\sum_i m_{i,z} = -M_z$  and thus  $\frac{\partial}{\partial H_z} e^{-\beta \mathcal{H}} = \beta M_z e^{-\beta \mathcal{H}}$ . Then

$$\begin{aligned} \langle M_z \rangle &= \frac{1}{Z} \int d\Omega' \text{'s} \cdot \frac{1}{\beta} \frac{\partial}{\partial H_z} e^{-\beta \mathcal{H}(\vec{m}' \text{'s}, \vec{H})} = \frac{1}{\beta} \frac{1}{Z} \frac{\partial}{\partial H_z} \int d\Omega' \text{'s} e^{-\beta \mathcal{H}(\vec{m}' \text{'s}, \vec{H})} \\ &= \frac{1}{\beta} \frac{\partial}{\partial H_z} \ln Z = -\frac{\partial F}{\partial H_z}, \end{aligned} \quad (\text{S.16})$$

recalling that  $F = -(1/\beta) \ln Z$ .

Now (with  $H \equiv H_z$ )

$$\begin{aligned} \langle M_z \rangle &= Nk_B T \frac{\partial}{\partial H} (\ln \sinh \beta m H - \ln \beta m H) = Nk_B T \left[ \frac{\cosh \beta m H}{\sinh \beta m H} \beta m - \frac{\beta m}{\beta m H} \right] \\ &= Nm \left[ \coth \beta m H - \frac{1}{\beta m H} \right]. \end{aligned} \quad (\text{S.17})$$

At small fields, or at high temperatures, we have  $\beta m H \rightarrow 0$ . Because of the series  $\coth x = x^{-1} + \frac{x}{3} + O(x^3)$ , we have

$$\langle M_z \rangle \approx Nm \left[ \frac{1}{\beta m H} + \frac{\beta m H}{3} - \frac{1}{\beta m H} \right] = \frac{Nm^2 H}{3k_B T}, \quad (\text{S.18})$$

which is Curie's law with the constant  $K = \frac{Nm^2}{3k_B}$ .

(e) Calculate the fluctuations  $\langle M_z^2 \rangle - \langle M_z \rangle^2$  and relate them to the magnetic susceptibility  $\chi_{zz} = (\partial M_z / \partial H_z)$ .

**Solution.** In order to calculate the fluctuations, we start off from the definition:

$$\langle M_z \rangle = \frac{1}{Z} \int d\Omega' \text{'s} M_z e^{-\beta \mathcal{H}(\vec{m}' \text{'s}, \vec{H})} = \int d\Omega' \text{'s} M_z e^{\beta(F - \mathcal{H}(\vec{m}' \text{'s}, \vec{H}))}, \quad (\text{S.19})$$

and notice that

$$0 = \int d\Omega' \text{'s} (\langle M_z \rangle - M_z) e^{\beta(F - \mathcal{H}(\vec{m}' \text{'s}, \vec{H}))}. \quad (\text{S.20})$$

Differentiating (S.20) by  $H_z$ ,

$$0 = \frac{\partial \langle M_z \rangle}{\partial H_z} + \int d\Omega' \text{'s} (\langle M_z \rangle - M_z) \frac{\partial}{\partial H_z} e^{\beta(F - \mathcal{H}(\vec{m}' \text{'s}, \vec{H}))} \quad (\text{S.21})$$

$$= \frac{\partial \langle M_z \rangle}{\partial H_z} + \int d\Omega' \text{'s} (\langle M_z \rangle - M_z) \beta (-\langle M_z \rangle + M_z) e^{\beta(F - \mathcal{H}(\vec{m}' \text{'s}, \vec{H}))} \quad (\text{S.22})$$

$$= \frac{\partial \langle M_z \rangle}{\partial H_z} - \beta \int d\Omega' \text{'s} (\langle M_z \rangle - M_z)^2 e^{\beta(F - \mathcal{H}(\vec{m}' \text{'s}, \vec{H}))} \quad (\text{S.23})$$

$$= \frac{\partial \langle M_z \rangle}{\partial H_z} - \beta \langle (\langle M_z \rangle - M_z)^2 \rangle. \quad (\text{S.24})$$

Eventually,

$$\langle M_z \rangle^2 - \langle M_z^2 \rangle = \langle (\langle M_z \rangle - M_z)^2 \rangle = k_B T \frac{\partial \langle M_z \rangle}{\partial H_z} = k_B T \chi_{zz} . \quad (\text{S.25})$$

Note that the higher the temperature, or the magnetic susceptibility, the higher the fluctuations.

Equation (S.25) is typical of a (dissipation-free) application of the fluctuation-dissipation theorem, which relates the fluctuation of a thermodynamic quantity to the response function of the system (in this case, the magnetic susceptibility).

## Exercise 2. *Rigid Pendulums.*

We will now consider a lattice of  $N$  classical rigid rotors. Each rotor is independent, is free to point in any spatial direction and has a moment of inertia  $I = mR^2$ . Its Hamiltonian is

$$\mathcal{H} = \frac{1}{2I} \left( p_\theta^2 + \frac{p_\varphi^2}{\sin^2 \theta} \right) . \quad (4)$$

First a note: how the Hamiltonian (4) is derived.

Let's start from the Lagrangian of the rotor in cartesian coordinates

$$\mathcal{L} = \frac{1}{2} m |\vec{v}|^2 , \quad \text{with} \quad \vec{v} = \frac{d\vec{r}}{dt} . \quad (\text{S.26})$$

In spherical coordinates with  $|\vec{r}| = R$ , we have

$$d\vec{r} = R (d\theta \vec{e}_\theta + \sin \theta d\varphi \vec{e}_\varphi) , \quad (\text{S.27})$$

and thus

$$\mathcal{L}(\theta, \varphi) = \frac{1}{2} m R^2 (\dot{\theta}^2 + \sin^2 \theta \dot{\varphi}^2) . \quad (\text{S.28})$$

The conjugate momenta are then

$$p_\theta = \frac{\partial \mathcal{L}}{\partial \dot{\theta}} = m R^2 \dot{\theta} \quad \Rightarrow \quad \dot{\theta} = \frac{p_\theta}{m R^2} ; \quad (\text{S.29})$$

$$p_\varphi = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}} = m R^2 \sin^2 \theta \dot{\varphi} \quad \Rightarrow \quad \dot{\varphi} = \frac{p_\varphi}{m R^2 \sin^2 \theta} . \quad (\text{S.30})$$

Then

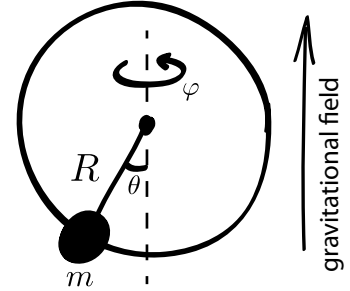
$$\mathcal{H} = \dot{\theta} p_\theta + \dot{\varphi} p_\varphi - \mathcal{L} = \frac{1}{2} \left[ \frac{p_\theta^2}{m R^2} + \frac{p_\varphi^2}{m R^2 \sin^2 \theta} \right] = \frac{1}{2I} \left[ p_\theta^2 + \frac{p_\varphi^2}{\sin^2 \theta} \right] . \quad (\text{S.31})$$

Also, for when we will calculate the partition function later, we need to determine the correct measure to integrate on the variables  $\theta$ ,  $\varphi$ ,  $p_\theta$  and  $p_\varphi$ . If you do the calculation explicitly (using in particular Eqs. (S.29) and (S.30)), one can see that the correct integration measure is simply  $d\theta d\varphi dp_\theta dp_\varphi$ .

- (a) Calculate the (canonical) partition function of the system of  $N$  rotors. Calculate the internal energy and the heat capacity. Study the regimes  $T \rightarrow 0$  and  $T \rightarrow \infty$ .

We now immerse the  $N$  rotors into a gravitational field with potential  $V = mg x_{i,z} = -mgR \cos \theta_i$ .

- (b) Determine the partition function and compare it with the partition function of Exercise 1. Calculate the free energy, internal energy and heat capacity of the system. Discuss the limits  $T \rightarrow 0$  and  $T \rightarrow \infty$ .



**Solution.** The solution to this exercise is attached on page 10.

**Exercise 3. Independent Dimers in a Magnetic Field. Quantum vs Ising.**

We consider a system of  $N$  independent dimers of two spins,  $s = 1/2$ , described by the Hamiltonian

$$\mathcal{H}_0^{\text{quantum}} = J \sum_i \left( \vec{S}_{i,1} \cdot \vec{S}_{i,2} \right), \quad (5)$$



where  $i$  is the dimer index and  $\vec{S}_{i,1}$  (resp.  $\vec{S}_{i,2}$ ) are the spin operators of the first (resp. second) particle of the dimer. Both particles have spin  $1/2$ . For simplicity, we use  $\hbar = 1$ . To this quantum system corresponds a classical Ising dimer, described by:

$$\mathcal{H}_0^{\text{Ising}} = \frac{1}{2} J \sum_i \left( \sigma_{i,1} \cdot \sigma_{i,2} - \frac{1}{2} \right), \quad (6)$$

where  $\sigma_{i,m} = \pm 1$ . The spins are aligned along the  $z$  axis. We will use eigenstates and eigenenergies to denote also the classical states and energies.

- (a) What are the eigenstates and the eigenenergies of a single dimer for the two cases?
- (b) For both cases consider the macroscopic system and determine the Helmholtz free energy, the entropy, the internal energy and the specific heat as a function of temperature and  $N$ . Discuss the limit  $T \rightarrow 0$  and  $T \rightarrow \infty$  for both signs of  $J$  (antiferromagnetic and ferromagnetic case).

Note: The following exercises are left for the fun of the interested reader.

- (c\*) We now apply a magnetic field along  $z$  direction leading to an additional term in the Hamiltonian,

$$\mathcal{H}_{\text{mag}}^{\text{quantum}} = -g\mu_B H \sum_{i,m} S_{i,m}^z \quad (7a)$$

$$\mathcal{H}_{\text{mag}}^{\text{Ising}} = -g\mu_B H \sum_{i,m} \frac{\sigma_{i,m}}{2}. \quad (7b)$$

How do the eigenenergies change? Sketch the energies with respect to the applied field  $H$ , the partition functions and determine the ground state for both cases. For the antiferromagnetic case you should notice a critical field. What differences do you notice between the classical and quantum system when the the critical field is reached? For the quantum case discuss in this context the entropy per dimer in the limit  $T \rightarrow 0$ .

- (d\*) Calculate the magnetization  $m$  for the two cases. In which limit are they the same? Moreover compute the magnetic susceptibility  $\chi$  for the quantum case and discuss its dependence on  $H$  for different temperatures.

**Solution.**

- (a) For the *Quantum case* we may write the Hamiltonian in terms of the total dimer spin  $\vec{S}_i = \vec{S}_{i,1} + \vec{S}_{i,2}$  as

$$\mathcal{H}_0^{\text{quantum}} = \frac{J}{2} \sum_i \left( \vec{S}_i^2 - \vec{S}_{i,1}^2 - \vec{S}_{i,2}^2 \right) = \frac{J}{2} \sum_i \left( \vec{S}_i^2 - \frac{3}{2} \right). \quad (\text{S.32})$$

Clearly, the eigenstates of a single dimer are the spin singlets and triplets:

- The singlet  $\Psi^s = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$  has total spin 0 and, thus, eigenvalue  $E^s = -\frac{3}{4}J$ .
- The triplet states are  $\Psi_0^t = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ ,  $\Psi_1^t = |\uparrow\uparrow\rangle$  and  $\Psi_{-1}^t = |\downarrow\downarrow\rangle$ . They have total spin 1,  $S_i^2 = 2$  and eigenvalue  $E^t = \frac{1}{4}J$ .

The *Ising case* has also four states:

- The doublet states  $\Phi_{up}^{anti} = |\uparrow\downarrow\rangle, \Phi_{down}^{anti} = |\downarrow\uparrow\rangle$  have total spin 0 and the eigenvalue  $E^s = -\frac{3}{4}J$ .
- The doublet state  $\Phi_1 = |\uparrow\uparrow\rangle, \Phi_{-1} = |\downarrow\downarrow\rangle$  have total spin magnitude 1 and the eigenvalue  $E^t = \frac{1}{4}J$ .

The two systems have the same eigenvalues but with different degeneracies.

(b) The partition function for the two cases is

$$Z^{\text{quantum}} = \left(3e^{-\frac{J}{4k_B T}} + e^{\frac{3J}{4k_B T}}\right)^N \quad (\text{S.33a})$$

$$Z^{\text{Ising}} = \left(2e^{-\frac{J}{4k_B T}} + 2e^{\frac{3J}{4k_B T}}\right)^N, \quad (\text{S.33b})$$

so we could write them as

$$Z = \left(ae^{-\frac{J}{4k_B T}} + be^{\frac{3J}{4k_B T}}\right)^N, \quad (\text{S.34})$$

where  $a = 3, b = 1$  for the quantum case and  $a = b = 2$  for the Ising one.

The connection to thermodynamics is made via the Helmholtz free energy:

$$F(T, N) = -\frac{1}{\beta} \ln Z = \frac{JN}{4} - \frac{N}{\beta} \ln(a + be^{\beta J}), \quad (\text{S.35})$$

where  $\beta = \frac{1}{k_B T}$ . The entropy is given by

$$\begin{aligned} S(T, N) &= -\frac{\partial F}{\partial T} = -\frac{\partial F}{\partial \beta} \cdot \frac{\partial \beta}{\partial T} = k_B \beta^2 \frac{\partial F}{\partial \beta} \\ &= k_B \beta^2 \left( \frac{N}{\beta^2} \ln(a + be^{\beta J}) - \frac{N}{\beta} \frac{bJ e^{\beta J}}{a + be^{\beta J}} \right) \\ &= Nk_B \ln(a + be^{\beta J}) - Nk_B \beta \frac{bJ e^{\beta J}}{a + be^{\beta J}}. \end{aligned} \quad (\text{S.36})$$

The internal energy is given by

$$U(T, N) = -\frac{\partial}{\partial \beta} \ln Z = JN \left( \frac{1}{4} - \frac{be^{\beta J}}{a + be^{\beta J}} \right), \quad (\text{S.37})$$

and, finally, the specific heat evaluates to

$$c(T, N) = \frac{1}{N} \frac{\partial U}{\partial T} = -\frac{k_B \beta^2}{N} \frac{\partial U}{\partial \beta} = abk_B J^2 \frac{\beta^2 e^{\beta J}}{(a + be^{\beta J})^2}. \quad (\text{S.38})$$

Note here that the specific heat vanishes in the limit of low and high temperatures independent of the sign of  $J$ . For the *quantum case* the internal energy vanishes for large temperatures (independent of the sign of  $J$ ) and reaches  $N$  times the ground state energy for  $T \rightarrow 0$  (for  $J > 0$  singlets are preferred and we get  $U \rightarrow -\frac{3}{4}JN$ , whereas for  $J < 0$  we get the triplets and  $U \rightarrow JN\frac{1}{4}$ ). On the other hand for the *Ising case*  $U \rightarrow -\frac{1}{4}JN$  for large temperature independent of the sign of  $J$ , while for  $T \rightarrow 0$  we get the minimum energy state ( $U \rightarrow -\frac{3}{4}JN$  for  $J > 0$  and  $U \rightarrow JN\frac{1}{4}$  for  $J < 0$ ).

- (c) The z-component of the magnetic moment vanishes for  $\Psi^s$  and  $\Psi_0^t$  and therefore their energy does not change. However, the  $\Psi_{\pm 1}^t$  do have a nonvanishing z-component of  $\pm g\mu_B$ , which leads to a new energy  $E_{\pm 1}^t = \frac{1}{4}J \mp g\mu_B H$  (Figure 1).

For the classical system the total magnetic moment for  $\Phi^{anti}$  is zero so the corresponding energy is unchanged when the magnetic field is applied, while for  $\Phi$  we have the same energy dependence like for the quantum case. Therefore only the energy for states with parallel spins is split, the other one remaining degenerate.

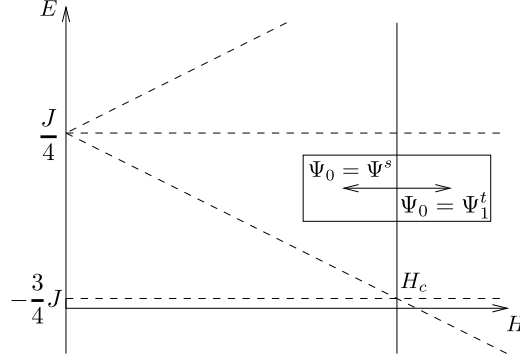


Figure 1: The energy for the four states of the quantum dimer as a function of the magnetic field for  $J > 0$  (the antiferromagnetic case).

To calculate the entropy per dimer for the quantum case (it is known as the von Neumann entropy<sup>2</sup>) we start with the thermal state (in the basis of its eigenstates) and the partition function (per dimer) is:

$$\rho = \frac{1}{Z} \begin{pmatrix} e^{\beta J} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{-\beta g \mu_B H} & 0 \\ 0 & 0 & 0 & e^{\beta g \mu_B H} \end{pmatrix} \quad \text{and} \quad (\text{S.39})$$

$$Z^{\text{quantum}} = \text{tr}(Z\rho) = e^{\beta J} + 1 + 2 \cosh(\beta g \mu_B H), \quad (\text{S.40})$$

where we have introduced an energy offset of  $\frac{J}{4}$  (the triplet and singlet energies become  $E_{\text{offset}}^s = -J, E_{\text{offset}}^t = 0$ ). Note that  $\rho$  is independent of the offset since we normalize it to  $\text{tr} \rho = 1$ . The von Neumann entropy per dimer is given by

$$\begin{aligned} \frac{s(T, H)}{k_B} &= -\text{tr}(\rho \log \rho) \\ &= \log Z - \frac{\beta}{Z} \frac{\partial Z}{\partial \beta} \\ &= \log(e^{\beta J} + 1 + 2 \cosh(\beta g \mu_B H)) - \frac{2\beta g \mu_B H \sinh(\beta g \mu_B H) + \beta J e^{\beta J}}{e^{\beta J} + 1 + 2 \cosh(\beta g \mu_B H)}. \end{aligned} \quad (\text{S.41})$$

The expression corresponds to the result we got in b) in the limit  $H \rightarrow 0$ .

Let us first consider the case  $J > 0$ . Here, the singlet state is preferable at low fields  $|H| < H_c$  and we get  $s(T; H) \rightarrow 0$  for  $T \rightarrow 0$ . At  $|H| = H_c$  we have a two-fold degeneracy in the ground state ( $s(T; H) \rightarrow k_B \log 2$  for  $T \rightarrow 0$ ) and with  $H > H_c$  the ground state is unique again ( $s(T; H) \rightarrow 0$  for  $T \rightarrow 0$ ). This is illustrated in Figure 1 and Figure 2.

If  $J < 0$  the triplet state is energetically favorable. If  $|H| = 0$  then the ground state is three-fold degenerate ( $s(T; H) \rightarrow k_B \log 3$  for  $T \rightarrow 0$ ). Finite fields break this symmetry and we get ( $s(T; H) \rightarrow 0$  for  $T \rightarrow 0$ ) if  $|H| > 0$ .

For the Ising case the partition function is given by:

$$Z^{\text{Ising}} = e^{-\frac{\beta J}{4}} \left( 2e^{\beta J} + 2 \cosh(\beta g \mu_B H) \right). \quad (\text{S.42})$$

For  $J > 0$  in the limit  $T \rightarrow 0$  the doublet state is the minimum one as long  $|H| < H_c$  and for  $|H| = H_c$  it has three-fold degeneracy while for  $|H| > H_c$  a unique state is obtained.

<sup>2</sup> This is equivalent to calculating the Helmholtz free energy per dimer and taking the derivative with regards to temperature as is done in (a). To see this, note that

$$\begin{aligned} s(T, H) &= -\frac{\partial F}{\partial T} = -k_B \beta^2 \frac{\partial}{\partial \beta} \frac{1}{\beta} \log Z = k_B \log Z - k_B \beta \frac{\partial}{\partial \beta} \log Z = k_B \log Z - \frac{k_B \beta}{Z} \frac{\partial}{\partial \beta} \text{tr} e^{-\beta \mathcal{H}} \\ &= k_B \log Z + \frac{k_B \beta}{Z} \frac{\partial}{\partial \beta} \text{tr} \rho Z = k_B \log Z - \frac{k_B \beta}{Z} \frac{1}{\beta} \text{tr}(\rho Z \log \rho Z) = k_B \log Z - k_B \text{tr}(\rho [\log \rho + \log Z]) \\ &= k_B \log Z - k_B \text{tr}(\rho \log \rho) - k_B \text{tr}(\rho) \log Z = -k_B \text{tr}(\rho \log \rho), \end{aligned}$$

where we used that  $\rho Z$  is of the form  $\rho Z = e^{-\beta \mathcal{H}}$  (and thus  $\frac{\partial}{\partial \beta}(\rho Z) = \frac{1}{\beta} \rho Z \log(\rho Z)$ ), and that  $\text{tr} \rho = 1$ . Don't forget also that  $Z$  is a scalar, not an operator.

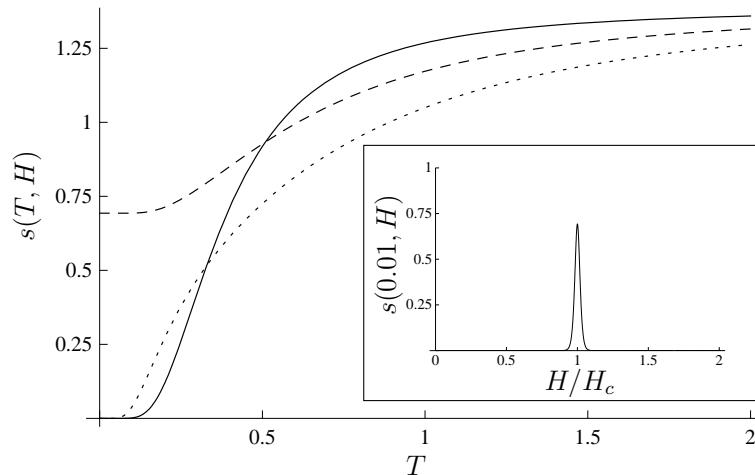


Figure 2: Entropy per dimer ( $J > 0$ ) as a function of temperature for zero field (solid line), critical field (dashed line) and for higher field (dotted line). The inset shows the entropy at low temperature as a function of the field, peaked around the critical field.

The description for  $J < 0$  is the same as for the quantum system.

- (d) For the quantum system using the free energy per dimer,

$$f(T, H) = -\frac{1}{\beta} \log Z = -\frac{1}{\beta} \log \left( e^{\beta J} + 1 + 2 \cosh(\beta g \mu_B H) \right) \quad (\text{S.43})$$

we find for the magnetization

$$m^{\text{quantum}}(T, H) = - \left( \frac{\partial f(T, H)}{\partial H} \right)_T = \frac{2g\mu_B \sinh(\beta g \mu_B H)}{e^{\beta J} + 1 + 2 \cosh(\beta g \mu_B H)} \quad (\text{S.44})$$

For the Ising system

$$m^{\text{Ising}}(T, H) = \frac{2g\mu_B \sinh(\beta g \mu_B H)}{2e^{\beta J} + 2 \cosh(\beta g \mu_B H)}, \quad (\text{S.45})$$

so for  $e^{\beta J} \sim 1$  it is the same with the one for the quantum case. This correspond to the high temperature limit  $\beta \rightarrow 0$ .

The susceptibility for the quantum case is given by:

$$\chi(T, H) = \frac{\partial m(T, H)}{\partial H} = 2\beta\mu_B^2 g^2 \frac{2 + (1 + e^{\beta J}) \cosh(\beta g \mu_B H)}{(1 + e^{\beta J} + 2 \cosh(\beta g \mu_B H))^2}. \quad (\text{S.46})$$

Let  $J > 0$ . If we plot the result for different temperatures (Figure 3), we see that for very small temperatures, the magnetization has a sudden increase at  $H_c$ , which follows directly from the fact that at this field strength, the ground-state of the system becomes magnetized. For higher temperatures,  $k_B T \sim J$ , the system behaves as if it was a simple paramagnet, i.e. we have a linear dependence on the magnetic field. In this regime, the relevant energy scale is given by the temperature and thus the system is not ordered anymore but fluctuations dominate.

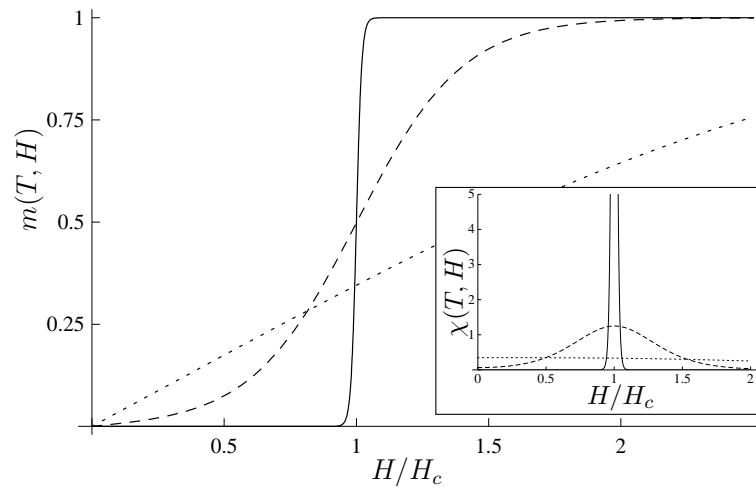


Figure 3: Magnetization as a function of applied field for small temperature (solid line), intermediate temperature (dashed line) and  $T \sim J$ . The inset shows the susceptibility for the corresponding temperatures. For  $T \rightarrow 0$ , the susceptibility diverges at  $H = H_c$ .

$$H = \frac{1}{2I} \left( p_\theta^2 + \frac{p_\phi^2}{\sin^2 \theta} \right) - mgR \cos \theta$$

Let's directly consider the case with the gravitational field. The case without can be obtained by setting  $g \rightarrow 0$ .

The partition function of an individual rotor is

$$\begin{aligned} Z_1 &= \int d\theta d\phi dp_\theta dp_\phi \exp \left\{ -\beta \left[ \frac{1}{2I} \left( p_\theta^2 + \frac{p_\phi^2}{\sin^2 \theta} \right) - mgR \cos \theta \right] \right\} \\ &= 2\pi \int dp_\theta e^{-\frac{\beta}{2I} p_\theta^2} \int d\theta e^{\beta mgR \cos \theta} \int dp_\phi e^{-\frac{\beta}{2I} \frac{p_\phi^2}{\sin^2 \theta}} \\ &= 2\pi \sqrt{\frac{2\pi I}{\beta}} \int d\theta e^{\beta mgR \cos \theta} \sqrt{\frac{2\pi I \sin^2 \theta}{\beta}} \\ &= \frac{4\pi^2 I}{\beta} \int_0^\pi d\theta \sin \theta e^{\beta mgR \cos \theta} = \frac{4\pi^2 I}{\beta} \int_{-1}^1 d(\cos \theta) e^{\beta mgR \cos \theta} \\ &= \frac{8\pi^2 I}{\beta} \frac{\sinh \beta mgR}{\beta mgR} \end{aligned}$$

Then the partition function of  $N$  rotors is

$$Z = \underbrace{\left( \frac{8\pi^2 I}{\beta} \right)^N}_{\text{"ideal gas" term}} \underbrace{\left( \frac{\sinh \beta mgR}{\beta mgR} \right)^N}_{\text{paramagnetic term (same as in ex 1!)}} = Z_0^N \cdot Z_g^N$$

Note: without gravity, we have  $g \rightarrow 0$  and  $Z_g \rightarrow 1$ , thus

$$Z = \left( \frac{8\pi^2 I}{\beta} \right)^N \quad (g \rightarrow 0)$$

The free energy is

$$F = -k_B T \ln Z = -N k_B T \left[ \ln \frac{8\pi^2 I}{\beta} + \ln \sinh \beta mgR - \ln \beta mgR \right]$$

(without gravity:  $F_0 = -N k_B T \ln \frac{8\pi^2 I}{\beta}$  )



The internal energy without gravity :

$$U_0 = -\frac{\partial}{\partial \beta} N \ln \frac{8\pi^2 I}{\beta} = -N \frac{\beta}{8\pi^2 I} \cdot \frac{8\pi^2 I}{-\beta^2} = \frac{N}{\beta} = \underline{k_B T \cdot N}$$

And the heat capacity :

$$C_0 = \frac{\partial U_0}{\partial T} = \underline{N \cdot k_B} \quad (\text{finite value, also if } T \rightarrow 0) \\ (\text{same as for an ideal gas})$$

Now, let's switch on gravity :

$$U = -\frac{\partial}{\partial \beta} \left[ \ln Z_0^N + N \ln \sinh \beta mgR - N \ln \beta mgR \right] \\ = N k_B T - N \frac{\cosh \beta mgR}{\sinh \beta mgR} \cdot mgR + N \frac{mgR}{\beta mgR} \\ = N k_B T - N mgR \coth \beta mgR + N k_B T \\ = \underline{2 N k_B T - N mgR \coth \frac{mgR}{k_B T}}$$

$$\left[ \frac{\partial}{\partial x} \coth x = \frac{-1}{\sinh^2 x} \right]$$

$$C = \frac{\partial U}{\partial T} = 2 N k_B - N mgR \frac{-1}{\sinh^2 \beta mgR} \left( \frac{mgR}{-k_B T^2} \right) \\ = N k_B \left( 2 - \left( \frac{\sinh \beta mgR}{\beta mgR} \right)^{-2} \right)$$

Limit :  $T \rightarrow 0$  i.e.  $\beta \rightarrow \infty$  :  $\sinh \beta mgR \approx \frac{1}{2} \exp(\beta mgR)$

$$\rightarrow \frac{\beta mgR}{\sinh \beta mgR} \approx \frac{2 \beta mgR}{\exp \beta mgR} = 2 \beta mgR e^{-\beta mgR} \rightarrow 0 \quad \text{as } \beta \rightarrow \infty$$

thus  $C \rightarrow 2 N k_B$ .

Note that in the limit  $T \rightarrow \infty$  ( $\beta \rightarrow 0$ ), we get the same limit as if  $g \rightarrow 0$  :

$$C \rightarrow N k_B \quad (\beta \rightarrow 0)$$

**Exercise 1. Quantum rotor in a magnetic field**

Consider a lattice of  $N$  quantum rotors. Each rotor is independent and has a momentum of inertia  $I = mR^2$ . It is described by the following Hamiltonian:

$$H = \frac{\mathbf{L}^2}{2mR^2} = \frac{\mathbf{L}^2}{2I}. \quad (1)$$

- (a) Calculate the (canonical) partition function of the system of  $N$  rotors. Determine the entropy, the internal energy, the projection of the angular momentum along the  $z$  direction and the heat capacity. Compute them numerically and study the high and low temperature limits. It is useful to define  $\theta_{\text{rot}}$  by  $k_B\theta_{\text{rot}} = 1/I$ .

*Hint.* If  $f^{(n)}(\infty) \rightarrow 0, \forall n \in \mathbb{N}$  then the Euler–Maclaurin formula could be simplified to:

$$\sum_{l=0}^{\infty} f(l) = \int_0^{\infty} dl f(l) + \frac{1}{2}f(0) - \sum_{k=2}^{\infty} \frac{(-1)^k b_k}{(k)!} f^{(k-1)}(0) + R_{\infty} \quad (2)$$

where  $R_{\infty}$  is a small correction and  $b_k$  are the Bernoulli numbers  $b_2 = 1/6, b_3 = 0, b_4 = -1/30, \dots$ .  
<http://people.csail.mit.edu/kuat/courses/euler-maclaurin.pdf>

**Solution.** Is it useful to work in the eigenbasis  $|l, m\rangle$  defined by  $\mathbf{L}^2|l, m\rangle = l(l+1)|l, m\rangle, L_z|l, m\rangle = m|l, m\rangle$  where  $l = 0 \dots \infty$  and  $m = -l \dots l$ . The partition function is  $Z = Z_1^N$  where

$$Z_1 = \sum_{l=0}^{\infty} \sum_{m=-l}^l e^{-\beta l(l+1)/(2I)} = \sum_{l=0}^{\infty} (2l+1) e^{-\beta l(l+1)/(2I)} = \sum_{l=0}^{\infty} (2l+1) e^{-l(l+1)\theta_{\text{rot}}/(2T)} \quad (S.1)$$

The high (low) temperature limits correspond to  $\frac{\theta_{\text{rot}}}{T} \rightarrow 0$  ( $\frac{\theta_{\text{rot}}}{T} \rightarrow \infty$ ). For low temperature limit we keep only first two terms in the sum. For the high temperature limit we use Euler-Maclaurin formula up to  $k = 4$  and collect the dominant terms.

$$\int_0^{\infty} dl (2l+1) e^{-l(l+1)\theta_{\text{rot}}/(2T)} = -\frac{2T}{\theta_{\text{rot}}} \int_0^{\infty} dl \frac{d}{dl} e^{-l(l+1)\theta_{\text{rot}}/(2T)} = \frac{2T}{\theta_{\text{rot}}} \quad (S.2)$$

In the two limits the results become:

$$Z_1 = \begin{cases} \frac{2T}{\theta_{\text{rot}}} + \frac{1}{3} + \frac{\theta_{\text{rot}}}{30T} & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow 0 \\ 1 + 3e^{-\theta_{\text{rot}}/T} & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow \infty \end{cases}. \quad (S.3)$$

The internal energy is:

$$U = -\frac{\partial \ln Z}{\partial \beta} = k_B T^2 \frac{\partial \ln Z}{\partial T} = \begin{cases} N k_B \left( \frac{2T^2}{\theta_{\text{rot}}} - \frac{\theta_{\text{rot}}}{30} \right) \left( \frac{2T}{\theta_{\text{rot}}} + \frac{1}{3} + \frac{\theta_{\text{rot}}}{30T} \right)^{-1} & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow 0 \\ 3N k_B \theta_{\text{rot}} e^{-\theta_{\text{rot}}/T} \left( 1 + 3e^{-\theta_{\text{rot}}/T} \right)^{-1} & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow \infty \end{cases} \quad (S.4)$$

$$\approx \begin{cases} N k_B \left( T - \frac{\theta_{\text{rot}}}{6} - \frac{\theta_{\text{rot}}^2}{180T} \right) & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow 0 \\ 3N k_B \theta_{\text{rot}} e^{-\theta_{\text{rot}}/T} & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow \infty \end{cases}. \quad (S.5)$$

The entropy is:

$$S - S_0 = -\frac{\partial F}{\partial T} = \frac{\partial k_B T \ln Z}{\partial T} = N k_B \left( \ln Z_1 + T \frac{\partial \ln Z_1}{\partial T} \right) = N k_B \ln Z_1 + \frac{U}{T} \quad (S.6)$$

$$\approx \begin{cases} Nk_B \left( \ln \left( \frac{2T}{\theta_{\text{rot}}} + \frac{1}{3} + \frac{\theta_{\text{rot}}}{30T} \right) + 1 - \frac{\theta_{\text{rot}}}{6T} - \frac{\theta_{\text{rot}}^2}{180T^2} \right) & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow 0 \\ Nk_B \left( \ln \left( 1 + 3e^{-\theta_{\text{rot}}/T} \right) + 3\frac{\theta_{\text{rot}}}{T} e^{-\theta_{\text{rot}}/T} \right) & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow \infty \end{cases} \quad (\text{S.7})$$

It is clear that  $S(T=0) = 0$ .

By symmetry, the projection of the angular momentum is 0.

The specific heat is:

$$C_V = \frac{\partial U}{\partial T} \approx \begin{cases} Nk_B \left( 1 + \frac{1}{180} \left( \frac{\theta_{\text{rot}}}{T} \right)^2 \right) & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow 0 \\ 3Nk_B \left( \frac{\theta_{\text{rot}}}{T} \right)^2 e^{-\theta_{\text{rot}}/T} & \text{if } \frac{\theta_{\text{rot}}}{T} \rightarrow \infty \end{cases} \quad (\text{S.8})$$

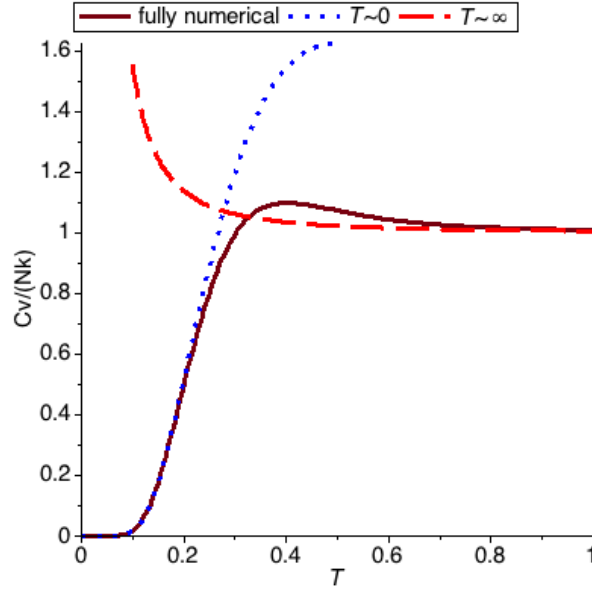


Figure 1: The two analytic approximations and the fully numerical solution for the specific heat as a function of temperature ( $\theta_{\text{rot}} = 1$ ).

Now add a magnetic field that couples to the angular momentum as:

$$H' = -\gamma \mathbf{B} \cdot \mathbf{L} . \quad (3)$$

- (b) What is the effect of the magnetic field? Determine the entropy, the internal energy, the projection of the angular momentum along the  $z$  direction and the heat capacity. Compute them numerically and study the high and low temperature limits. It is useful to define  $\theta_{\text{mag}}$  by  $k_B \theta_{\text{mag}} = \gamma B_z$ .

**Solution.**

$$H' = -\gamma \mathbf{B} \cdot \mathbf{L} = -\gamma B_z L_z . \quad (\text{S.9})$$

The magnetic field splits the  $2l + 1$  symmetry of  $H$ .

$$Z_1 = \sum_{l=0}^{\infty} \sum_{m=-l}^l e^{-\beta \{ l(l+1)/(2I) - \gamma B_z m \}} = \sum_{l=0}^{\infty} \left\{ e^{-\beta l(l+1)/(2I)} \sum_{m=-l}^l e^{\beta \gamma B_z m} \right\} = \sum_{l=0}^{\infty} \frac{\sinh(\beta \gamma B_z (2l+1)/2)}{\sinh(\beta \gamma B_z /2)} e^{-\beta l(l+1)/(2I)} \quad (\text{S.10})$$

where we used for the sum over  $m$  the result from the Lecture Notes 2.4.2 .

$$Z_1 = \frac{1}{\sinh\left(\frac{\theta_{\text{mag}}}{2T}\right)} \sum_{l=0}^{\infty} \sinh\left((2l+1)\frac{\theta_{\text{mag}}}{2T}\right) e^{-l(l+1)\theta_{\text{rot}}/(2T)} \quad (\text{S.11})$$

Using  $\lim_{x \rightarrow 0} \sinh x \approx x$  and  $\lim_{x \rightarrow \infty} \sinh x \approx \frac{e^x}{2}$  and assuming  $\theta_{\text{rot}} > \theta_{\text{mag}}$  we have:

$$Z_1 = \begin{cases} \frac{2T}{\theta_{\text{rot}}} + \frac{1}{3} - \frac{\theta_{\text{rot}}}{30T} & \text{if } \frac{1}{T} \rightarrow 0 \\ 1 + e^{\theta_{\text{mag}}/T} e^{-\theta_{\text{rot}}/T} & \text{if } \frac{1}{T} \rightarrow \infty \end{cases} = \begin{cases} \frac{2T}{\theta_{\text{rot}}} + \frac{1}{3} - \frac{\theta_{\text{rot}}}{30T} & \text{if } \frac{1}{T} \rightarrow 0 \\ 1 + e^{-\theta_{\text{eff}}/T} & \text{if } \frac{1}{T} \rightarrow \infty \end{cases}, \quad (\text{S.12})$$

where  $\theta_{\text{eff}} = \theta_{\text{rot}} - \theta_{\text{mag}}$ . In this approximation, for high temperature we recover the result from (a). In low temperature limit the effect of the magnetic field enters explicitly,  $\theta_{\text{rot}}$  being replaced by  $\theta_{\text{eff}}$  and the prefactor 3 is replaced by 1.

The internal energy is:

$$U \approx \begin{cases} Nk_B \left( T - \frac{\theta_{\text{rot}}}{6} - \frac{\theta_{\text{rot}}^2}{180T} \right) & \text{if } \frac{1}{T} \rightarrow 0 \\ Nk_B \theta_{\text{eff}} e^{-\theta_{\text{eff}}/T} & \text{if } \frac{1}{T} \rightarrow \infty \end{cases}. \quad (\text{S.13})$$

The entropy is:

$$S - S_0 \approx \begin{cases} Nk_B \left( \ln \left( \frac{2T}{\theta_{\text{rot}}} + \frac{1}{3} + \frac{\theta_{\text{rot}}}{30T} \right) + 1 - \frac{\theta_{\text{rot}}}{6T} - \frac{\theta_{\text{rot}}^2}{180T^2} \right) & \text{if } \frac{1}{T} \rightarrow 0 \\ Nk_B \left( \ln \left( 1 + e^{-\theta_{\text{eff}}/T} \right) + \frac{\theta_{\text{eff}}}{T} e^{-\theta_{\text{eff}}/T} \right) & \text{if } \frac{1}{T} \rightarrow \infty \end{cases}. \quad (\text{S.14})$$

The projection of the angular momentum is simply:

$$\langle L_z \rangle = -\frac{\partial F}{\partial(\gamma B_z)} = \frac{N}{\beta} \frac{\partial \ln Z_1}{\partial(\gamma B_z)} \approx \begin{cases} 0 & \text{if } \frac{1}{T} \rightarrow 0 \\ N e^{-\theta_{\text{eff}}/T} & \text{if } \frac{1}{T} \rightarrow \infty \end{cases}. \quad (\text{S.15})$$

The specific heat is:

$$C_V \approx \begin{cases} Nk_B \left( 1 + \frac{1}{180} \left( \frac{\theta_{\text{rot}}}{T} \right)^2 \right) & \text{if } \frac{1}{T} \rightarrow 0 \\ Nk_B \left( \frac{\theta_{\text{eff}}}{T} \right)^2 e^{-\theta_{\text{eff}}/T} & \text{if } \frac{1}{T} \rightarrow \infty \end{cases}. \quad (\text{S.16})$$

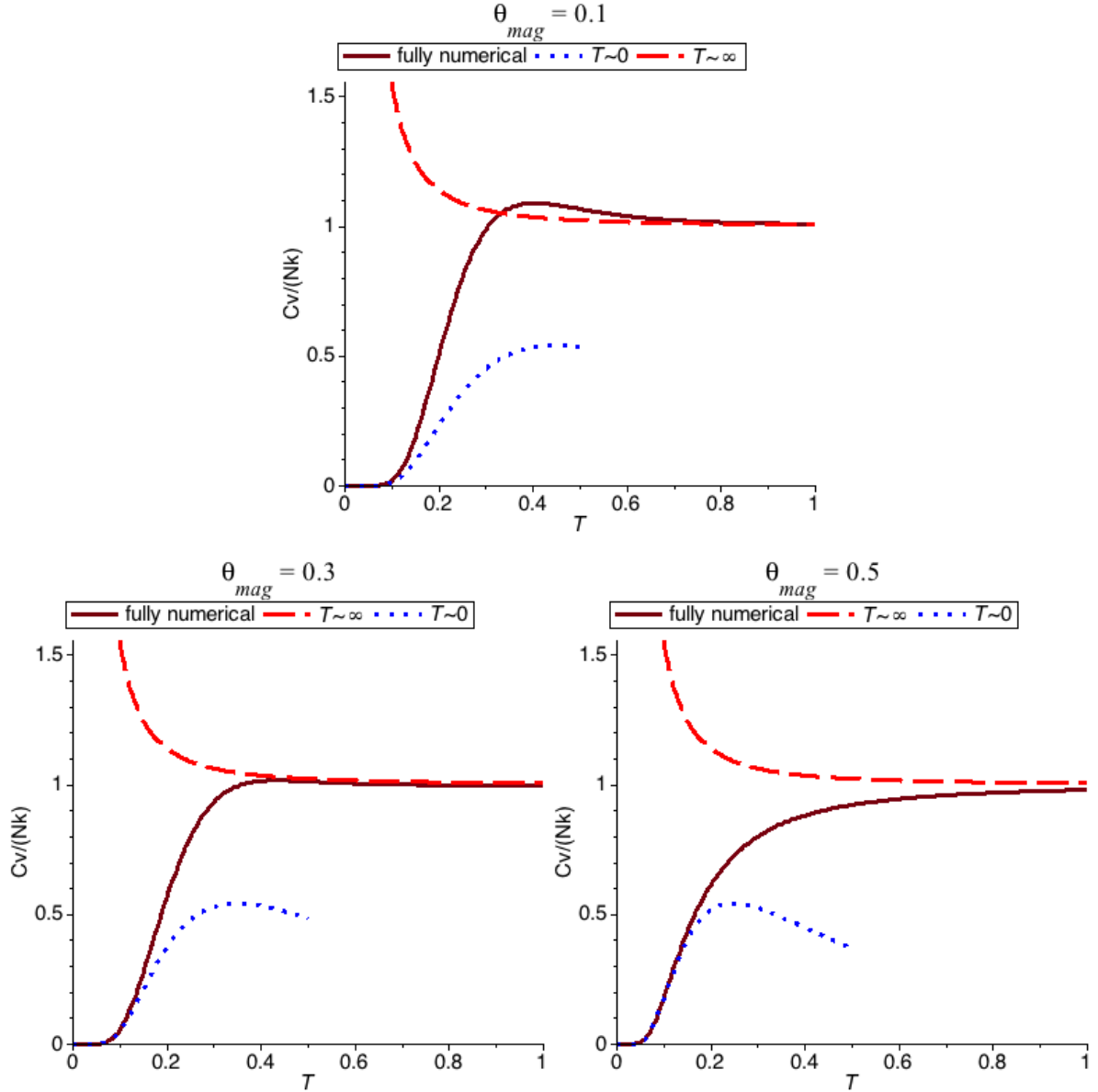


Figure 2: The two analytic approximations and the fully numerical solution for the specific heat as a function of temperature for different values of  $\theta_{\text{mag}} = 0.1, 0.3$  and  $0.5$  ( $\theta_{\text{rot}} = 1$ ).

### Exercise 2. *Ideal fermionic quantum gas in a harmonic trap*

In this exercise we study the fermionic spinless ideal gas confined in a three-dimensional harmonic potential and compare it with classical case (for the results of the classical case see Exercise Sheet 1). The energy states of the gas are given by

$$E_{\mathbf{a}} = \hbar\omega(a_x + a_y + a_z) \quad (4)$$

where we neglect the zero point energy  $E_0 = 3\hbar\omega/2$ . The occupation number of the oscillator modes of the state  $E_{\mathbf{a}}$  is given by  $n_{\mathbf{a}}$  where  $\mathbf{a} = (a_x, a_y, a_z)$  with  $a_i \in \{0, 1, 2, \dots\}$ .

- (a) Consider the high-temperature, low-density limit ( $z \ll 1$ ). Derive the grand canonical

partition function  $\mathcal{Z}_f$  of this system and compute the grand potential  $\Omega_f$ . Show that

$$\Omega_f \propto f_4(z), \quad (5)$$

where the function  $f_s(z)$  is defined as

$$f_s(z) = - \sum_{l=1}^{\infty} (-1)^l \frac{z^l}{l^s}. \quad (6)$$

**Solution.** We begin with the general definition of the grand canonical partition function within the occupation number formalism (section 2.5 of the lecture notes) and find

$$\mathcal{Z}_f = \prod_{\mathbf{a}} \sum_{n_{\mathbf{a}}} \left( z e^{-\beta E_{\mathbf{a}}} \right)^{n_{\mathbf{a}}} = \prod_{\mathbf{a}} (1 + z e^{-\beta E_{\mathbf{a}}}). \quad (S.17)$$

In order to compute the grand potential  $\Omega = -1/\beta \ln \mathcal{Z}$ , we use the series expansion

$$\ln(1+x) = - \sum_{\ell=1}^{\infty} \frac{(-x)^\ell}{\ell} \quad \text{for } -1 < x \leq 1. \quad (S.18)$$

This expansion is applicable for the logarithm of the partition function in (S.17) if  $z e^{-\beta E_{\mathbf{a}}} \leq 1$  (it is always positive). This certainly holds in the high-temperature limit  $z \ll 1$ .

Let us first consider the fermionic grand potential  $\Omega_f$ ,

$$\begin{aligned} \ln \mathcal{Z}_f &= \sum_{\mathbf{a}} \ln(1 + z e^{-\beta E_{\mathbf{a}}}) = - \sum_{\mathbf{a}} \sum_{\ell=1}^{\infty} (-1)^\ell \frac{z^\ell}{\ell} e^{-\ell \beta E_{\mathbf{a}}} = - \sum_{\ell=1}^{\infty} (-1)^\ell \frac{z^\ell}{\ell} \left( \sum_{\mathbf{a}=0}^{\infty} e^{-\ell \beta \hbar \omega a} \right)^3 \\ &= - \sum_{\ell=1}^{\infty} (-1)^\ell \frac{z^\ell}{\ell} \left( \frac{1}{1 - e^{-\ell \beta \hbar \omega}} \right)^3 = - \begin{cases} - \sum_{\ell=1}^{\infty} (-1)^\ell \frac{z^\ell}{\ell} \frac{1}{(\ell \beta \hbar \omega)^3} & \text{if } \beta \rightarrow 0 \\ - \sum_{\ell=1}^{\infty} (-1)^\ell \frac{z^\ell}{\ell} & \text{if } \beta \rightarrow \infty \end{cases} \\ &= \begin{cases} \frac{1}{(\beta \hbar \omega)^3} f_4(z) & \text{if } \beta \rightarrow 0 \\ f_1(z) & \text{if } \beta \rightarrow \infty \end{cases}. \end{aligned} \quad (S.19)$$

We obtained both the high and the low temperature limits. Otherwise, in the high temperature limit, we can approximate the sum over the oscillator modes by an integration with constant and normalized density of states,  $\sum_{a_k=0}^{\infty} \rightarrow \int_0^{\infty} da_k$ , for  $k = x, y, z$ .

$$\begin{aligned} \ln \mathcal{Z}_f &\approx - \int_0^{\infty} da_x \int_0^{\infty} da_y \int_0^{\infty} da_z \sum_{\ell=1}^{\infty} (-1)^\ell \frac{z^\ell}{\ell} e^{-\ell \beta \hbar \omega (a_x + a_y + a_z)} \\ &= \frac{-1}{(\beta \hbar \omega)^3} \sum_{\ell=1}^{\infty} \left[ (-1)^\ell \frac{z^\ell}{\ell^4} \right] = \frac{1}{(\beta \hbar \omega)^3} f_4(z). \end{aligned} \quad (S.20)$$

The fermionic grand potential is

$$\Omega_f = - \frac{1}{\beta} \frac{1}{(\beta \hbar \omega)^3} f_4(z). \quad (S.21)$$

- (b) Derive the internal energy  $U$  and the average particle number  $\langle N \rangle$ . In order to get  $U$  in terms of  $N$  (instead of dealing with the chemical potential), introduce the parameter

$$\rho \equiv \left( \frac{\hbar \omega N^{1/3}}{k_B T} \right)^3, \quad (7)$$

and relate it to  $z$  using the high-temperature, low-density expansion of  $\langle N \rangle$ . Interpret the condition  $\rho \ll 1$ .

Then, expand  $U$  up to second order in  $\rho$ , relating it to  $N$ .

**Solution.** First, we compute the internal energy of the system,

$$U_f = \left. \frac{\partial(\beta \Omega_f)}{\partial \beta} \right|_z, \quad (\text{S.22})$$

where the derivative has to be taken at constant fugacity  $z = e^{\beta\mu}$ . Starting from (S.21) we find

$$U_f = \frac{3}{\beta} \frac{1}{(\beta \hbar \omega)^3} f_4(z), \quad (\text{S.23})$$

which shows that the internal energy is proportional to the grand potential,  $U_f = -3 \Omega_f$ .

The average particle number can be computed in a similar way,

$$\langle N_f \rangle = z \frac{\partial}{\partial z} \ln \mathcal{Z}_f. \quad (\text{S.24})$$

We have

$$\langle N_f \rangle = z \frac{\partial}{\partial z} \frac{1}{(\beta \hbar \omega)^3} f_4(z) = \frac{1}{(\beta \hbar \omega)^3} f_3(z), \quad (\text{S.25})$$

where we used

$$z \frac{\partial}{\partial z} f_4(z) = f_3(z). \quad (\text{S.26})$$

In order to relate the internal energy to the particle number, we start with the high-temperature expansion of the particle number equation,

$$\langle N_f \rangle = \frac{1}{(\beta \hbar \omega)^3} f_3(z) \approx \frac{1}{(\beta \hbar \omega)^3} \left( z - \frac{z^2}{8} \right). \quad (\text{S.27})$$

The parameter  $\rho$  is given by (we are dropping the indices for readability)

$$\rho \equiv \left( \frac{\hbar \omega N^{1/3}}{k_B T} \right)^3. \quad (\text{S.28})$$

The condition  $z \ll 1$  also implies  $\rho \ll 1$ . Expanding in  $\rho$  allows us to deal with the particle number instead of the chemical potential. Solving  $\rho = z - z^2/8$ , we obtain  $z = 4 \pm 2\sqrt{4 - 2\rho}$ . Choosing the relevant solution and expanding  $\sqrt{1+x} \approx 1 + \frac{x}{2} - \frac{x^2}{8}$  we find

$$z = \rho + \frac{\rho^2}{8}. \quad (\text{S.29})$$

To interpret the condition  $\rho \ll 1$  we first note that for a system, in which every state up to a given maximal energy  $\epsilon_{\max} = \hbar \omega a_{\max}$  is singly occupied, the number of occupied states is proportional with  $a_{\max}^3$ . The characteristic energy scale of such a system is thus given by  $\hbar \omega N^{1/3}$  (for fermions  $\sim \epsilon_F$ ). Therefore, this condition requires that the characteristic energy scale of such a singly occupied system is much smaller than the thermal energy  $k_B T$  (*high-temperature* limit). This means that we consider temperatures at which the average occupation of the states is much smaller than one (*low-density* limit).

We write the internal energy up to second order in  $\rho$  as

$$\begin{aligned} U &= \frac{3}{\beta} \frac{1}{(\beta \hbar \omega)^3} f_4(z) = \frac{3}{\beta} \frac{1}{(\beta \hbar \omega)^3} \left( z - \frac{z^2}{16} \right) \\ &= \frac{3}{\beta} \frac{1}{(\beta \hbar \omega)^3} \left( \rho + \frac{\rho^2}{16} \right) \\ &= \frac{3}{\beta} \left( N + N^2 (\beta \hbar \omega)^3 \frac{1}{16} \right) = 3N k_B T \left( 1 + N \left( \frac{\hbar \omega}{k_B T} \right)^3 \frac{1}{16} \right), \end{aligned} \quad (\text{S.30})$$

where we recover the equipartition law in leading order and the positive first order quantum corrections  $\propto N(\hbar \omega/k_B T)^3 \ll 1$  distinguishing the fermions from the ideal classical gas.

- (c) Compute the specific heat  $C$ . Which quantity has to be fixed in order to do this?

**Solution.** Since our system does not really have a volume as thermodynamic variable we have to compute the specific heat  $C_N$  by fixing the number of particles. Hence, as a starting point we use the expression (S.30) for the inner energy, where we can keep  $N$  fixed:

$$C_N = \left( \frac{\partial U}{\partial T} \right)_N = 3Nk_B \left( 1 - \frac{1}{8} N \left( \frac{\hbar\omega}{k_B T} \right)^3 \right). \quad (\text{S.31})$$

(d) Compute the isothermal compressibility  $\kappa_T$ .

**Solution.** Be definition

$$\kappa_T = \frac{v}{N} \left( \frac{\partial N}{\partial \mu} \right)_T, \quad (\text{S.32})$$

where  $v = \frac{V}{N}$ . Therefore we have for our system

$$\kappa_T = \frac{v}{\langle N \rangle} \left( \frac{\partial z}{\partial \mu} \frac{\partial N}{\partial z} \right)_T = \frac{v}{N} \beta z \frac{1}{(\beta \hbar \omega)^3} \frac{\partial f_3(z)}{\partial z} = v \beta \frac{f_2(z)}{f_3(z)} \approx \frac{N}{V k_B T} \left( 1 - \frac{1}{8} N \left( \frac{\hbar\omega}{k_B T} \right)^3 \right). \quad (\text{S.33})$$

(e) Interpret your results for  $U$ ,  $C$ , and  $\kappa_T$  by comparing them with the corresponding results for the classical Boltzmann gas. How do the quantum corrections influence the fermionic system?

**Solution.** In summary we have found up to first order in  $\rho$ :

$$U = 3Nk_B T \left( 1 + N \left( \frac{\hbar\omega}{k_B T} \right)^3 \frac{1}{16} \right), \quad (\text{S.34})$$

$$C_N = 3Nk_B \left( 1 - \frac{1}{8} N \left( \frac{\hbar\omega}{k_B T} \right)^3 \right), \quad (\text{S.35})$$

$$\kappa_T = \frac{N}{V k_B T} \left( 1 - \frac{1}{8} N \left( \frac{\hbar\omega}{k_B T} \right)^3 \right), \quad (\text{S.36})$$

These results as a function of temperature are plotted in Fig. 3; each for the classical and the fermionic case. Note that our expansions up to first order in  $\rho$  are only valid for  $\rho \ll 1$ . We can still plot these expansions for larger values of  $\rho$  (that is, lower temperatures) to observe the trends, keeping in mind that these results are not exactly valid.

We see that

- In zeroth order in  $\rho$  the results for the classical (Boltzmann) gas in a harmonic trap are recovered.
- Due to quantum corrections, the internal energy  $U$  for fermions is higher than the ideal classical gas. This can be understood by taking quantum statistics into account. Fermions are not allowed to occupy the same state (Pauli). Lowering the temperature, the system tends to occupy low energy states with growing probability. While the classical system is not influenced at all by double occupancy, in the fermionic system the double occupancy is forbidden and occupation of low-energy states is thus reduced, increasing the inner energy  $U_f$  compared to the classical gas.



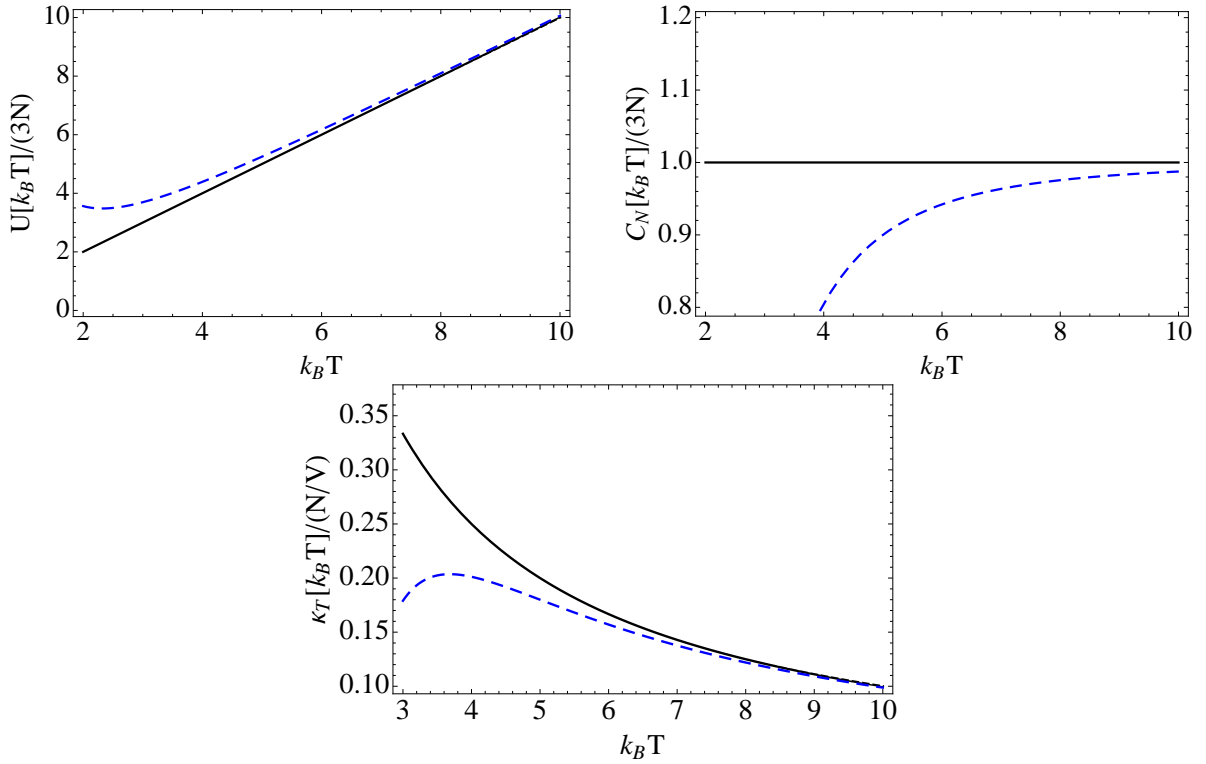


Figure 3: Thermodynamics of fermionic gas compared to the classical gas. Note that these quantities are computed within the high-temperature, low-density approximation and are therefore not exact results. Still, they can be used to observe trends. The dashed (blue) line is for the fermions and the continuous (black) line for the classical gas. We set  $N(\hbar\omega)^3 = 100$ .

**Exercise 1. *Ideal phonons in a harmonic trap.***

In this exercise we consider an ideal gas of phonons as an example of bosonic particles confined in a three-dimensional harmonic potential. Observe the differences to the cases of classical and fermionic particles in the same harmonic potential, which we discussed in Sheet 1, Exercise 3, and for Sheet 3, Exercise 2, respectively.

The energy states of the phonons are given by

$$E_{\mathbf{a}} = \hbar\omega(3/2 + a_x + a_y + a_z) , \quad (1)$$

including the zero point energy of  $E_0 = 3\hbar\omega/2$ . The occupation number of the oscillator modes of the state  $E_{\mathbf{a}}$  is given by  $\mathbf{a} = (a_x, a_y, a_z)$  with  $a_i \in \{0, 1, 2, \dots\}$ .

- (a) Consider the high-temperature, low-density limit ( $z \ll 1$ ). Derive the grand canonical partition function for the phonons,  $\mathcal{Z}_b$ , and compute the grand potential  $\Omega_b$ . Take into account also the zero-point energy of the harmonic oscillators. Show that

$$\Omega_b \propto g_4 \left( ze^{-\beta E_0} \right) , \quad (2)$$

where the function  $g_s(z)$  is defined as

$$g_s(z) = \sum_{l=1}^{\infty} \frac{z^l}{l^s} . \quad (3)$$

- (b) Derive the internal energy  $U$  and the average particle number  $\langle N \rangle$ . Follow the same approach as in Sheet 3, Exercise 2 in order to obtain  $U$  in terms of  $N$ .
- (c) Compute the specific heat  $C_N$  for constant particle number.  
Compute the thermal expansion coefficient  $\alpha$ . Use the average square displacement of the harmonic oscillator  $r_{\text{eff}}^2 = x_0^2 \langle a_x + a_y + a_z \rangle$  in order to define an effective volume  $V_{\text{eff}} = 4\pi/3 r_{\text{eff}}^3$ . Give an interpretation of  $V_{\text{eff}}$ .
- (d) Plot your results for  $U$ ,  $C$ , and  $\alpha$  for the classical, the fermionic, and the bosonic case and note the differences.
- (e) Find the critical temperature  $T_c$  at which Bose-Einstein condensation occurs. How can this be reconciled with the high-temperature, low-density limit?

*Hint. The chemical potential can not be larger than the lowest energy level of the particles.*

**Solution.**

- (a) We begin with the general definition of the grand canonical partition function within the occupation number formalism (section 2.5 of the lecture notes) and find

$$\mathcal{Z}_b = \prod_{\mathbf{a}} \sum_{n_{\mathbf{a}}=0}^{\infty} \left( ze^{-\beta E_{\mathbf{a}}} \right)^{n_{\mathbf{a}}} = \prod_{\mathbf{a}} (1 - ze^{-\beta E_{\mathbf{a}}})^{-1} \quad (\text{S.1})$$

In order to compute the grand potential  $\Omega = -1/\beta \log \mathcal{Z}$ , we use the series expansion

$$\log(1+x) = -\sum_{\ell=1}^{\infty} \frac{(-x)^\ell}{\ell} \quad \text{for } -1 < x \leq 1. \quad (\text{S.2})$$

This expansion is applicable for the logarithm of the partition function in (S.1) as  $0 < ze^{-\beta E_a} \leq 1$  (as  $\mu \leq E_{\min}$ ).

With this replacement we can exactly calculate  $\log(\mathcal{Z}_b)$  in the high-temperature limit ( $\beta \rightarrow 0$ ):

$$\begin{aligned} \log \mathcal{Z}_b &= -\sum_{\mathbf{a}} \log(1 - ze^{-\beta E_{\mathbf{a}}}) = \sum_{\mathbf{a}} \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell} e^{-\ell\beta E_{\mathbf{a}}} = \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell} \left( \sum_{\mathbf{a}=0}^{\infty} e^{-\ell\beta\hbar\omega/2} e^{-\ell\beta\hbar\omega\mathbf{a}} \right)^3 \\ &= \sum_{\ell=1}^{\infty} \frac{z^\ell}{\ell} \left( \frac{e^{-\ell\beta\hbar\omega/2}}{1 - e^{-\ell\beta\hbar\omega}} \right)^3 \stackrel{\beta \rightarrow 0}{\approx} \sum_{\ell=1}^{\infty} \frac{(ze^{-\beta E_0})^\ell}{\ell} \frac{1}{(\ell\beta\hbar\omega)^3} = \frac{1}{(\beta\hbar\omega)^3} g_4(ze^{-\beta E_0}) \end{aligned} \quad (\text{S.3})$$

The grand potential is then given by

$$\Omega_b = -\frac{1}{\beta} \frac{1}{(\beta\hbar\omega)^3} g_4(ze^{-\beta E_0}). \quad (\text{S.4})$$

(b) First, we compute the internal energy of the system,

$$U_b = \left. \frac{\partial(\beta\Omega_b)}{\partial\beta} \right|_z, \quad (\text{S.5})$$

where the derivative has to be taken at constant fugacity  $z = e^{\beta\mu}$ . Starting from (S.4) we find

$$U_b = \frac{3}{\beta} \frac{1}{(\beta\hbar\omega)^3} g_4(ze^{-\beta E_0}) + \frac{E_0}{(\beta\hbar\omega)^3} g_3(ze^{-\beta E_0}), \quad (\text{S.6})$$

which shows that the internal energy is proportional to the grand potential plus a term representing the zero-point energy of the harmonic oscillators.

The average particle number can be computed in a similar way,

$$\langle N_b \rangle = z \frac{\partial}{\partial z} \log \mathcal{Z}_b. \quad (\text{S.7})$$

We have

$$\langle N_b \rangle = z \frac{\partial}{\partial z} \frac{1}{(\beta\hbar\omega)^3} g_4(ze^{-\beta E_0}) = \frac{1}{(\beta\hbar\omega)^3} g_3(ze^{-\beta E_0}), \quad (\text{S.8})$$

where we used

$$z \frac{\partial}{\partial z} g_4(z) = g_3(z). \quad (\text{S.9})$$

We immediately see, that the second term in equation (S.6) is just given by  $\langle N_b \rangle E_0$ .

In order to simplify the following calculation, we define a renormalized fugacity

$$\tilde{z} = ze^{-\beta E_0} \quad (\text{S.10})$$

Now we want to relate the internal energy to the particle number and start with the high-temperature expansion of the particle number equation,

$$\langle N_b \rangle = \frac{1}{(\beta\hbar\omega)^3} g_3(\tilde{z}) \approx \frac{1}{(\beta\hbar\omega)^3} \left( \tilde{z} + \frac{\tilde{z}^2}{8} \right). \quad (\text{S.11})$$

The parameter  $\rho$  is given by

$$\rho \equiv \left( \frac{\hbar\omega N^{1/3}}{k_B T} \right)^3. \quad (\text{S.12})$$

The condition  $z \ll 1$  also implies  $\rho \ll 1$ . Expanding in  $\rho$  allows us to deal with the particle number instead of the chemical potential. Inverting the series  $\rho = z + z^2/8$ , we find

$$\tilde{z} = \rho - \frac{\rho^2}{8}. \quad (\text{S.13})$$

To interpret the condition  $\rho \ll 1$  we first note that for a system, in which every state up to a given maximal energy  $\epsilon_{\max} = \hbar\omega a_{\max}$  is singly occupied, the number of occupied states corresponds to  $a_{\max}^3/6$ . The characteristic energy scale of such a system is thus given by  $\hbar\omega N^{1/3}$ . Therefore, this condition requires that the characteristic energy scale of such a singly occupied system is much smaller than the thermal energy  $k_{\text{B}}T$  (*high-temperature* limit). This means that we consider temperatures at which the average occupation of the states is much smaller than one (*low-density* limit).

We write the internal energy up to second order in  $\rho$  as

$$\begin{aligned} U - NE_0 &= \frac{3}{\beta} \frac{1}{(\beta\hbar\omega)^3} g_4(\tilde{z}) = \frac{3}{\beta} \frac{1}{(\beta\hbar\omega)^3} \left( \tilde{z} + \frac{\tilde{z}^2}{16} \right) \\ &= \frac{3}{\beta} \frac{1}{(\beta\hbar\omega)^3} \left( \rho - \frac{\rho^2}{16} \right) \\ &= \frac{3}{\beta} \left( N - N^2 (\beta\hbar\omega)^3 \frac{1}{16} \right) = 3Nk_{\text{B}}T \left( 1 - N \left( \frac{\hbar\omega}{k_{\text{B}}T} \right)^3 \frac{1}{16} \right), \end{aligned} \quad (\text{S.14})$$

where we recover the equipartition law in leading order and the (negative) first order quantum corrections  $\propto N(\hbar\omega/k_{\text{B}}T)^3 \ll 1$  distinguishing the bosons from the ideal classical gas.

- (c) Since our system does not really have a volume as thermodynamic variable we have to compute the specific heat  $C_N$  by fixing the number of particles. Hence, as a starting point we use the expression (S.14) for the internal energy, where we can keep  $N$  fixed:

$$C_N = \left( \frac{\partial U}{\partial T} \right)_N = 3Nk_{\text{B}} \left( 1 + \frac{1}{8} N \left( \frac{\hbar\omega}{k_{\text{B}}T} \right)^3 \right). \quad (\text{S.15})$$

Finally, we compute the thermal expansion coefficient  $\alpha = V^{-1} (\partial V / \partial T)$  at fixed  $N$ . For this we have to define an effective volume of the system by introducing an effective radius  $r_{\text{eff}}^2 \equiv \langle r^2 \rangle$ . From basic quantum mechanics we know that  $r_{\text{eff}}^2 = x_0^2 \langle a_x + a_y + a_z \rangle$ , where  $x_0$  represents the characteristic length scale which we fix to unity. Hence, we can relate  $r_{\text{eff}}^2$  to the internal energy of the system via

$$\hbar\omega r_{\text{eff}}^2 N = U. \quad (\text{S.16})$$

Therefore, we find

$$V_{\text{eff}} \equiv \frac{4\pi}{3} r_{\text{eff}}^3 = \frac{4\pi}{3} \left( \frac{U}{\hbar\omega N} \right)^{3/2}. \quad (\text{S.17})$$

For the thermal expansion coefficient we obtain

$$\begin{aligned} \alpha &= U^{-3/2} \left( \frac{\partial U^{3/2}}{\partial T} \right)_N = \frac{3}{2} U^{-1} C_N \\ &= \frac{3}{2} U^{-1} 3k_{\text{B}}N \left( 1 + \frac{1}{8} N \left( \frac{\hbar\omega}{k_{\text{B}}T} \right)^3 \right) \\ &= \frac{3}{2} \frac{1}{T} \frac{1 + \frac{\rho}{8}}{1 - \frac{\rho}{16}} = \frac{3}{2} \frac{1}{T} \left( 1 + \frac{3}{16} \rho \right), \end{aligned} \quad (\text{S.18})$$

which agrees (in leading order) with the result for a classical gas in the harmonic trap ( $\alpha = 3/(2T)$ ).

- (d) In summary, in Sheet 3, Exercise 2 and in this exercise we have found up to first order in  $\rho$ :

$$U = 3Nk_{\text{B}}T \left( 1 \pm N \left( \frac{\hbar\omega}{k_{\text{B}}T} \right)^3 \frac{1}{16} \right), \quad (\text{S.19})$$

$$C_N = 3Nk_{\text{B}} \left( 1 \mp \frac{1}{8} N \left( \frac{\hbar\omega}{k_{\text{B}}T} \right)^3 \right), \quad (\text{S.20})$$

$$\alpha = \frac{3}{2} \frac{1}{T} \left( 1 \mp \frac{3}{16} N \left( \frac{\hbar\omega}{k_{\text{B}}T} \right)^3 \right), \quad (\text{S.21})$$

where the upper and lower sign corresponds to fermions and bosons, respectively. For the classical case, the corrections to 1 vanish for all three formulas.

These results as a function of temperature are plotted in Fig. 1; each for the classical, the fermionic, and the bosonic case. Note that our expansions up to first order in  $\rho$  are only valid for  $\rho \ll 1$ . We can still plot these expansions for larger values of  $\rho$  (that is, lower temperatures) to observe the trends, keeping in mind that these results are not exactly valid.

We see that

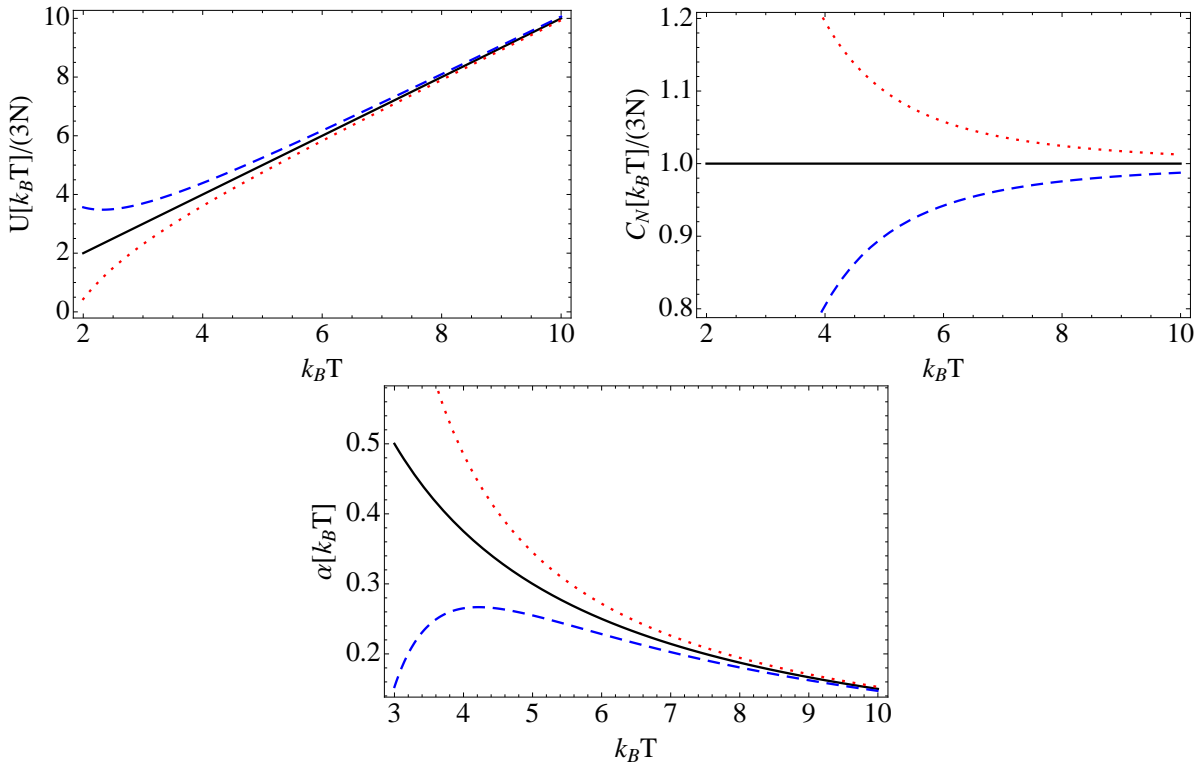


Figure 1: Thermodynamics of fermionic and bosonic gases compared to the classical gas. Note that these quantities are computed within the high-temperature, low-density approximation and are therefore not exact results. Still, they can be used to observe trends. The dashed (blue) line is for the fermions, the dotted (red) line for the bosons, and the continuous (black) line for the classical gas. We set  $N\hbar\omega = 100$ .

- In zeroth order in  $\rho$  the results for the classical (Boltzmann) gas in a harmonic trap are recovered.
- Due to quantum corrections the internal energy  $U$  for fermions (bosons) is higher (lower) than the ideal classical gas.

This can be understood by taking quantum statistics into account. Fermions are not allowed to occupy the same state (Pauli) while bosons tend to gather in the same quantum state. Lowering the temperature, the system tends to occupy low energy states with growing probability. While the classical system is not influenced at all by double occupancy, in the fermionic system the double occupancy is forbidden and occupation of low-energy states is thus reduced, increasing the internal energy  $U_b$  compared to the classical gas. In the bosonic case, the opposite happens: the probability of occupying low energy states is enhanced, reducing the internal energy  $U_b$ .

- The thermal expansion coefficient is lowered (enhanced) for fermions (bosons) compared to classical gas. This feature represents the fact that with decreasing temperature the bosons tend to occupy more low energy states than the fermions, thus reducing the effective volume  $V_{\text{eff}}$  more strongly with temperature which enhances the thermal expansion coefficient.
- (e) We now analyse the number equation (S.8) for the bosonic system in detail. If we decrease the temperature, in order to keep the particle number constant, the function  $g_3(z)$  has to increase. For a bosonic system, the chemical potential must always be smaller than the state with lowest energy. In this case, this corresponds to

$$z \leq e^{3\beta\hbar\omega/2} . \quad (\text{S.22})$$

The maximum of the monotonically increasing function  $g_3(\tilde{z})$  (see Fig. 2) is taken when  $z = e^{3\beta\hbar\omega/2}$ . Hence, the number equation cannot hold for arbitrary small temperature. There exists a critical temperature  $T_c$  at which the chemical potential is equal to the ground-state energy,  $\mu = E_0$ , and thus  $ze^{-\beta E_0} = 1$ . This temperature can easily be computed as

$$T_c = \frac{\hbar\omega N^{1/3}}{k_B} (g_3(1))^{-1/3} . \quad (\text{S.23})$$

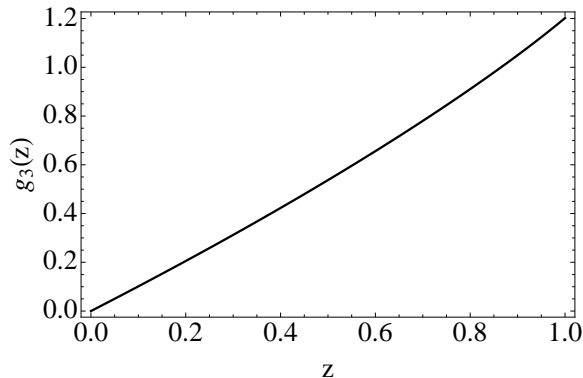


Figure 2: Plot of the function  $g_3(z)$  for values of  $z$  between 0 and 1.

The physical interpretation of this critical point is simple: For the derivation of the number equation, the zero energy state has been neglected. For temperatures above  $T_c$  this is a negligible error, but for temperatures below  $T_c$  it becomes energetically favorable to occupy this single state with a macroscopically large particle number. Hence, the approximation to neglect the occupation of the zero energy state becomes bad for temperatures below  $T_c$ . Macroscopically large occupation of a single quantum state, or equivalently a density matrix where a single eigenvalue is by far the dominant one, is a definition of a condensate. Hence,  $T_c$  represents the critical temperature for the bosonic gas to form a Bose-Einstein condensate.

With equation (S.23) we show that our high temperature approximation holds even until  $T_c$  if the number of particles  $N$  is large: when we compress enough particles, they will condense at a high temperature and we can use the instability of this approximation to find our  $T_c$ . Of course, at  $T_c$  itself the approximation breaks down.

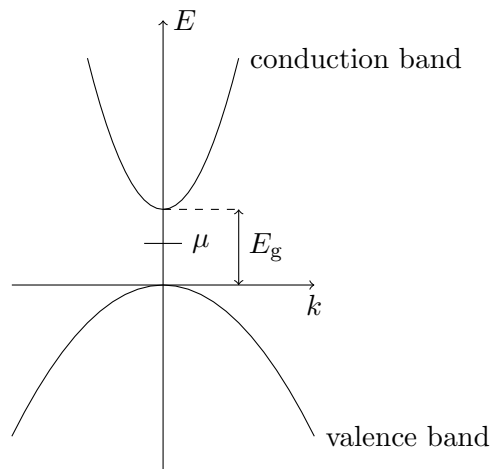
### Exercise 2. *Behavior of excitations in a semiconductor.*

In this exercise we analyze the properties and behavior of electron-excitations of a semiconductor at finite temperature. In solid state theory, electronic states  $|\mathbf{k}, \alpha\rangle$  are usually labeled by a *pseudomomentum*  $\mathbf{k} = (k_x, k_y, k_z)$  and a band-index  $\alpha \in \{1, 2, \dots\}$ . For a crystal with lattice constant  $a$ , the pseudomomentum takes values in the so-called *Brillouin zone*  $\{-\pi/a, \pi/a\}^3$ . Assuming a cubic crystal with side-length  $L$  there exist  $(L/a)^3$  equally distributed  $\mathbf{k}$ -vectors in this Brillouin zone. Each of the states is doubly degenerate due to the spin, such that there are in total  $2(L/a)^3$  states for each band.

In order to simplify the treatment, we only take into account two bands whose energies are approximated as parabolic,

$$\epsilon_v(\mathbf{k}) = -\frac{\hbar^2 \mathbf{k}^2}{2m_v} \quad \epsilon_c(\mathbf{k}) = E_g + \frac{\hbar^2 \mathbf{k}^2}{2m_c}, \quad (4)$$

as shown in the figure. Here the indices  $v$  and  $c$  stand for valence and conduction band, respectively. The parameters  $m_v$  and  $m_c$  which define the curvature of the two bands are called *effective masses* and can in general be different from one another and from the electron mass. The *bandgap*,  $E_g$ , is the energy difference between the bottom of the conduction band and the top of the valence band.



Assume for this exercise that the bandgap is much larger than the thermal energy and the chemical potential lies within the gap,  $\beta E_g \gg \beta \mu \gg 1$ .

- (a) Assume at first that the particle number is not fixed and calculate the grand potential  $\Omega$  of this system.

*Hint.* For large  $L$ , a sum over  $\mathbf{k}$  can be approximated by an integral:

$$\sum_{\mathbf{k}} \approx \int_{-\pi/a}^{\pi/a} d^3k \frac{L^3}{8\pi^3} \quad (5)$$

- (b) In a realistic system, the particle number is fixed, as every atom in the solid contributes a specific number of electrons. We assume here a particle number, such that the lower band is completely filled at zero temperature, i. e.  $N = 2(L/a)^3$ . Calculate the chemical potential  $\mu(T)$  at finite temperature.
- (c) Starting from your result for  $\Omega$ , calculate the internal energy  $U(T, N) - U(T = 0, N)$  (for  $N = 2(L/a)^3$ ), using a Legendre transform.

*Hint.* The final result is given by

$$U(T, N) - U(T = 0, N) = N \left( \frac{k_B T}{2\pi \hbar^3} \right)^{3/2} e^{-\beta E_g/2} (m_v m_c)^{3/4} (3k_B T + E_g) . \quad (6)$$

- (d) A picture that is frequently used in solid state theory is that of electrons and *holes*: When an electron is excited to the conduction band, it leaves an empty state in the valence band. This empty state now behaves like a particle itself and is called a *hole*. Therefore an excitation can be regarded as a creation of two particles, similar to the creation of particle-antiparticle pairs in particle physics.

Use this scheme to interpret the calculated internal energy in terms of the equipartition law for an ideal gas. How many electrons are in the conduction band?

### Solution.

- (a) In the grandcanonical ensemble, each of the states can be either occupied or empty, such that we can write the partition function in the occupation number formalism:

$$\begin{aligned} \mathcal{Z}(\beta, z) &= \left[ \prod_{\mathbf{k}} \prod_{\alpha=v,c} \sum_{n_{\mathbf{k},\alpha}=0}^1 \left( z e^{-\beta \epsilon_{\alpha}(\mathbf{k})} \right)^{n_{\mathbf{k},\alpha}} \right]^2 \\ &= \prod_{\mathbf{k}} \left[ \left( 1 + z e^{\beta \hbar^2 k^2 / 2m_v} \right) \left( 1 + z e^{-\beta(E_g + \hbar^2 k^2 / 2m_c)} \right) \right]^2 \end{aligned} \quad (S.24)$$

Here the exponent 2 is present due to the spin degeneracy. The grand potential is now given by

$$\Omega(\beta, z) = -1/\beta \log(\mathcal{Z}(\beta, z)) = 2 \sum_{\mathbf{k}} \left[ \log \left( 1 + z e^{\beta \hbar^2 k^2 / 2m_v} \right) + \log \left( 1 + z e^{-\beta(E_g + \hbar^2 k^2 / 2m_c)} \right) \right] . \quad (S.25)$$

Due to the assumption  $\beta E_g \gg \beta \mu \gg 1$  we know that

$$z e^{\beta \hbar^2 k^2 / 2m_v} \gg 1 \quad \text{and} \quad z e^{-\beta(E_g + \hbar^2 k^2 / 2m_c)} \ll 1 \quad (S.26)$$

for all  $\mathbf{k}$ , leading to the approximations

$$\begin{aligned} \log \left( 1 + z e^{\beta \hbar^2 k^2 / 2m_v} \right) &\approx \beta \left( \mu + \frac{\hbar^2 k^2}{2m_v} \right) + z^{-1} e^{-\beta \hbar^2 k^2 / 2m_v} \\ \log \left( 1 + z e^{-\beta(E_g + \hbar^2 k^2 / 2m_c)} \right) &\approx z e^{-\beta(E_g + \hbar^2 k^2 / 2m_c)} . \end{aligned} \quad (S.27)$$

At this point we can replace the sum over  $\mathbf{k}$  in (S.25) by an integral over  $\mathbf{k}$ . This leads to

$$\begin{aligned}\Omega &= -\frac{1}{\beta} \int_{-\pi/a}^{\pi/a} d^3k \frac{L^3}{4\pi^3} \left[ \beta\mu + \frac{\beta\hbar^2 k^2}{2m_v} + z^{-1} e^{-\beta\hbar^2 k^2/2m_v} + z e^{-\beta(E_g + \hbar^2 k^2/2m_c)} \right] \\ &\approx -2\mu(L/a)^3 - \frac{(L/a)^3 \hbar^2 \pi^2}{m_v} - \frac{(L/a)^3 (k_B T)^{5/2}}{\sqrt{2\pi^3/2}\hbar^3} \left( m_v^{3/2} e^{-\beta\mu} + m_c^{3/2} e^{\beta(\mu - E_g)} \right),\end{aligned}\quad (\text{S.28})$$

where we have replaced the integration interval  $[-\pi/a, \pi/a]^3$  by  $\mathbb{R}^3$  for the Gaussian integrals (last two terms in the integral).

(b) In the grandcanonical ensemble the average particle number is given by

$$\langle N \rangle = -\frac{\partial \Omega}{\partial \mu} . \quad (\text{S.29})$$

Here we assumed that  $\langle N \rangle = 2(L/a)^3$ . This leads to the equation

$$2(L/a)^3 = 2(L/a)^3 + \frac{(L/a)^3 (k_B T)^{5/2}}{\sqrt{2\pi^3/2}\hbar^3} \left[ -\beta m_v^{3/2} e^{-\beta\mu} + \beta m_c^{3/2} e^{\beta(\mu - E_g)} \right] . \quad (\text{S.30})$$

This is equivalent to

$$\left( \frac{m_v}{m_c} \right)^{3/2} = e^{\beta(2\mu - E_g)} , \quad (\text{S.31})$$

leading to the result

$$\mu = \frac{E_g}{2} + \frac{3}{4} k_B T \log \left( \frac{m_v}{m_c} \right) . \quad (\text{S.32})$$

(c) The internal energy is given by

$$U = \Omega + TS + \mu N . \quad (\text{S.33})$$

We already calculated  $\mu$  as a function of  $T$  and  $N$ . The entropy is given by the partial derivative

$$S = -\frac{\partial \Omega}{\partial T} = \frac{(L/a)^3 (k_B T)^{5/2}}{\sqrt{2\pi^3/2}\hbar^3} \left[ \frac{5}{2T} \left( m_v^{3/2} e^{-\beta\mu} + m_c^{3/2} e^{\beta(\mu - E_g)} \right) - \frac{1}{k_B T^2} \left( -\mu m_v^{3/2} e^{-\beta\mu} + (\mu - E_g) m_c^{3/2} e^{\beta(\mu - E_g)} \right) \right] \quad (\text{S.34})$$

where we used  $\frac{\partial}{\partial T} = -\frac{1}{k_B T^2} \frac{\partial}{\partial \beta}$ . Using equation (S.32), we find

$$\left( m_v^{3/2} e^{-\beta\mu} + m_c^{3/2} e^{\beta(\mu - E_g)} \right) = 2 e^{-\beta E_g/2} (m_v m_c)^{3/4} \quad (\text{S.35a})$$

$$\left( -\mu m_v^{3/2} e^{-\beta\mu} + (\mu - E_g) m_c^{3/2} e^{\beta(\mu - E_g)} \right) = E_g e^{-\beta E_g/2} (m_v m_c)^{3/4} , \quad (\text{S.35b})$$

and with  $N = 2(L/a)^3$

$$\frac{(L/a)^3 (k_B T)^{5/2}}{\sqrt{2\pi^3/2}\hbar^3} = N \left( \frac{k_B T}{2\pi\hbar^3} \right)^{3/2} k_B T . \quad (\text{S.35c})$$

Inserting equations (S.35) and (S.34) into equation (S.33), we now obtain the result

$$U(T, N) - U(T = 0, N) = N \left( \frac{k_B T}{2\pi\hbar^3} \right)^{3/2} e^{-\beta E_g/2} (m_v m_c)^{3/4} (3k_B T + E_g) . \quad (\text{S.36})$$

The zero-temperature energy

$$U(T = 0, N) = -\frac{N\hbar^2 \pi^2}{2m_v} \quad (\text{S.37})$$

that we subtracted is just the energy of the completely filled valence band.

(d) We call  $N_c$  the number of electrons in the conduction band. In the particle-hole picture this is also equal to the number of holes in the valence band. Assuming now the behavior of ideal gas particles for both electrons and holes, the internal energy of electrons and holes is given by

$$U_e = \frac{3}{2} N_c k_B T + N_c E_g \quad U_h = \frac{3}{2} N_c k_B T , \quad (\text{S.38})$$

where  $E_g$  describes the energy offset of the conduction band. The total internal energy is then

$$U = N_c (3k_B T + E_g) . \quad (\text{S.39})$$

By comparing this with equation (S.36) we find the number of electrons in the conduction band

$$N_c = N \left( \frac{k_B T}{2\pi\hbar^3} \right)^{3/2} e^{-\beta E_g/2} (m_v m_c)^{3/4} , \quad (\text{S.40})$$

which is exponentially suppressed by the size of the bandgap.



**Exercise 1. Canonical quantization of phonons**

We consider a chain of  $N$  atoms of mass  $m$  and coordinates  $x_n$ , with  $n = 1, \dots, N$ . The atoms interact through a potential  $V(x_n) = V(x_1, \dots, x_N)$  that can be written in the *harmonic approximation* as

$$V(u_1, \dots, u_N) = \frac{\lambda}{2} \sum_{n=1}^N (u_{n+1} - u_n)^2 + \frac{1}{2} m \Omega^2 \sum_{n=1}^N (u_n)^2, \quad (1)$$

where  $u_n = x_n - \bar{x}_n$ ,  $|u_n| \ll \bar{x}_n$  measures the (small) deviation from the equilibrium position of each atom  $\bar{x}_n = na$ ,  $a$  being the lattice constant. In (1)  $\lambda$  is the elastic constant of the chain and the  $\Omega$  term constrains each atom at its equilibrium position. The kinetic energy of the atoms is readily written as:

$$T(\dot{u}_1, \dots, \dot{u}_N) = \frac{1}{2} m \sum_{n=1}^N (\dot{u}_n)^2. \quad (2)$$

- a) After writing down the classical Lagrangian of the system and the corresponding equations of motion (Euler-Lagrange equations), solve for the normal modes by imposing periodic boundary conditions (PBC,  $u_n = u_{n+N}$ ). What are the symmetries of the system for  $\Omega = 0$ ? Comment on the resulting spectrum in the two cases  $\Omega \neq 0$  and  $\Omega = 0$ . In the latter case, how does the spectrum look like in the *long-wavelength* regime?

*Hint.* Solve the E-L equations with an exponential ansatz  $u_n \propto e^{i(kna - \omega t)}$  and impose PBC to obtain the normal modes  $\omega_l = \omega(k_l)$ . The general solution will look like:

$$u_n(t) = \sum_{l=1}^N [A_l e^{i(k_l n a - \omega_l t)} + c.c.], \quad (3)$$

where the  $A_l$  are fixed by the initial conditions. The long-wavelength regime is characterized by  $k_l \ll 1/a$ .

**Solution.** The classical Lagrangian is readily written as:

$$\mathcal{L}(u_1, \dots, u_N, \dot{u}_1, \dots, \dot{u}_N) \equiv \mathcal{L}(u_n, \dot{u}_n) = T - V = \frac{1}{2} \sum_{n=1}^N [m \dot{u}_n^2 - \lambda (u_{n+1} - u_n)^2 - m \Omega^2 u_n^2]. \quad (S.1)$$

Periodic boundary conditions endow the Lagrangian (S.1) with the *ring symmetry*, i.e.,  $\mathcal{L}(u_n, \dot{u}_n) = \mathcal{L}(u_{n+m}, \dot{u}_{n+m}) \forall m \in \mathbb{Z}$  and with translation invariance symmetry (only if  $\Omega = 0$ ), i.e.,  $\mathcal{L}(u_n, \dot{u}_n) = \mathcal{L}(u_n + ax, \dot{u}_n) \forall x \in \mathbb{R}$ . The associated Euler-Lagrange equations of motion are:

$$\begin{aligned} \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{u}_n} &= \frac{\partial \mathcal{L}}{\partial u_n} \quad n = 1, \dots, N \\ \rightarrow \quad m \ddot{u}_n &= \lambda (u_{n+1} + u_{n-1} - 2u_n) - m \Omega^2 u_n. \end{aligned} \quad (S.2)$$

The L.H.S. of the equation above is straightly derived from the Lagrangian. The R.H.S. requires a bit more calculation: for example, when  $n = 1$

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial u_1} &= \frac{1}{2} \partial_{u_1} [-\lambda (u_{N+1} - u_N)^2 - \lambda (u_2 - u_1)^2 - m \Omega^2 u_1^2] = \\ &= -\frac{1}{2} \partial_{u_1} [\lambda (u_1 - u_N)^2 + \lambda (u_2 - u_1)^2 + m \Omega^2 u_1^2] = \\ &= -[\lambda (u_1 - u_N) - \lambda (u_2 - u_1) + m \Omega^2 u_1] = -[\lambda (2u_1 - u_0 - u_2) + m \Omega^2 u_1], \end{aligned} \quad (S.3)$$

where we used  $u_n = u_{n+N}$  for  $n = 0, 1$ . The same calculation applies when  $n = 2, \dots, N$ . We have obtained a coupled system of differential equations, that can be solved inserting the exponential ansatz given in the hint,  $u_n = Ae^{i(kna - \omega t)}$  where  $A$  is some constant. We obtain:

$$-m\omega^2 Ae^{i(kna - \omega t)} = Ae^{i(kna - \omega t)} \left[ \lambda(e^{ika} + e^{-ika} - 2) - m\Omega^2 \right] \Leftrightarrow \omega^2 = 2\frac{\lambda}{m}(1 - \cos ka) + \Omega^2, \quad (\text{S.4})$$

i.e., the dispersion relation

$$\omega(k) = \sqrt{2\frac{\lambda}{m}(1 - \cos ka) + \Omega^2}. \quad (\text{S.5})$$

The resulting spectrum is plotted in Fig. 1. When  $\Omega \neq 0$  the spectrum has a gap, such that no propagation is allowed below the *cut-off frequency*  $\omega(k) = \Omega$ . When  $\Omega = 0$  the spectrum is gapless and lattice perturbations of arbitrarily small frequency can propagate. Imposing PBC on the lattice,  $u_n = u_{n+N}$  one is able to solve for the wave-number  $k$ , i.e.,

$$Ae^{i(kna - \omega t)} = Ae^{i(ka(n+N) - \omega t)} \Leftrightarrow e^{ikNa} = 1 = e^{2\pi l} \quad l \in \mathcal{Z} \rightarrow k = k_l = \frac{2\pi l}{Na}, \quad l = 1 \dots N \quad (\text{S.6})$$

The corresponding frequencies are usually called *normal modes*,  $\omega(k) = \omega(k_l)$ . The general solution of the E-L equations is then given by (3), as an expansion over normal modes. Specifying the initial conditions  $u_n(t=0)$  and  $\dot{u}_n(t=0) \forall n$  identifies a particular solution of the differential system (S.2).

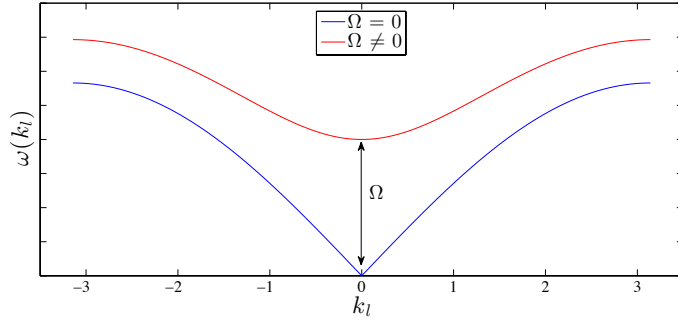


Figure 1: Phonon dispersion with and without pinning  $\Omega$  (we shifted  $l$  to the *first Brillouin zone*  $-N/2 \leq l < N/2$ ,  $a = 1$ ).

The long-wavelength regime is characterized by small wave-numbers,  $k_l \ll 1/a$ . Expanding the cosine contained in the dispersion relation for  $k_l \ll 1/a$ , one obtains a linear spectrum:

$$\omega(k_l) \approx \sqrt{\frac{\lambda}{m}k_l^2 a^2 + \Omega^2} \stackrel{\Omega=0}{=} \sqrt{\frac{\lambda}{m}}|k_l|a = c_p|k_l|a, \quad (\text{S.7})$$

such that  $c_p = \sqrt{\lambda/m}$  is associated to the velocity of propagation of sound waves in the lattice.

- b) Identify the conjugated momenta  $\pi_n(t)$  and write down the Hamiltonian for the system through a Legendre transformation.

**Solution.** According to the Hamiltonian formalism, the canonical momentum  $\pi_n$  conjugate to  $u_n$  reads:

$$\pi_n = \frac{\partial \mathcal{L}}{\partial \dot{u}_n} = m\dot{u}_n = -im \sum_{l=1}^N \omega_l [A_l e^{i(k_l n a - \omega_l t)} - \text{c.c.}] \quad n = 1, \dots, N. \quad (\text{S.8})$$

The Hamiltonian is obtained via a Legendre transformation, as follows:

$$\mathcal{H}(\pi_1, \dots, \pi_N, u_1, \dots, u_N) \equiv \mathcal{H}(\pi_n, u_n) = \sum_{n=1}^N \dot{u}_n \pi_n - \mathcal{L} = \frac{1}{2} \sum_{n=1}^N \left[ \frac{\pi_n^2}{m} + \lambda(u_{n+1} - u_n)^2 + m\Omega^2 u_n^2 \right]. \quad (\text{S.9})$$

- c) We set  $m = 1$  and introduce the dimensionless operators  $\hat{a}_l = \sqrt{N} \sqrt{\frac{2\omega_l}{\hbar}} \hat{A}_l$ , satisfying  $[\hat{a}_l, \hat{a}_l^\dagger] = \delta_{ll'}$ . Use them to elevate  $u_n(t), \pi_n(t)$  to quantum operators  $\hat{u}_n(t), \hat{\pi}_n(t)$ . Prove the equal-time canonical commutation relation  $[\hat{u}_n(t), \hat{\pi}_{n'}(t)] = i\hbar \delta_{nn'}$ .

**Solution.** Following the suggestion above, we write the position and momentum in terms of the dimensionless operators  $\hat{a}_l, \hat{a}_l^\dagger$ , as follows:

$$\begin{aligned}\hat{u}_n(t) &= \frac{1}{\sqrt{N}} \sum_{l=1}^N \sqrt{\frac{\hbar}{2\omega_l}} \left[ \hat{a}_l e^{i(k_l n a - \omega_l t)} + \text{h.c.} \right] \equiv \frac{1}{\sqrt{N}} \sum_{l=1}^N \sqrt{\frac{\hbar}{2\omega_l}} \left[ \hat{a}_l(t) e^{i k_l n a} + \text{h.c.} \right], \\ \hat{\pi}_n(t) &= -i \frac{1}{\sqrt{N}} \sum_{l=1}^N \sqrt{\frac{\hbar\omega_l}{2}} \left[ \hat{a}_l e^{i(k_l n a - \omega_l t)} - \text{h.c.} \right] \equiv -i \frac{1}{\sqrt{N}} \sum_{l=1}^N \sqrt{\frac{\hbar\omega_l}{2}} \left[ \hat{a}_l(t) e^{i k_l n a} - \text{h.c.} \right],\end{aligned}\tag{S.10}$$

We now prove the canonical commutation relation, making use of the postulated bosonic algebra  $[\hat{a}_l, \hat{a}_{l'}^\dagger] = \delta_{ll'}$ .

$$\begin{aligned}[\hat{u}_n(t), \hat{\pi}_{n'}(t)] &= \frac{1}{N} \frac{i\hbar}{2} \sum_{l, l'} \sqrt{\frac{\omega_{l'}}{\omega_l}} \left( [\hat{a}_l, \hat{a}_{l'}^\dagger] e^{i[(k_l n - k_{l'} n')a - (\omega_l - \omega_{l'})t]} - [\hat{a}_{l'}^\dagger, \hat{a}_l] e^{-i[(k_l n - k_{l'} n')a + (\omega_l - \omega_{l'})t]} \right) = \\ &= \frac{1}{N} \frac{i\hbar}{2} \sum_l \left( e^{i k_l (n - n')a} + e^{-i k_l (n - n')a} \right) = \frac{i\hbar}{N} \sum_{l=1}^N \cos[2\pi l (n - n')/N] = i\hbar \delta_{nn'}.\end{aligned}\tag{S.11}$$

The sum in the last passage is calculated as follows. If  $n = n'$  the sum gives  $N$ . If  $n \neq n'$  we exploit the algorithm:

$$S = \sum_{l=1}^N \mu^l \quad \rightarrow \quad S\mu = S - \mu + \mu^{N+1} \quad \rightarrow \quad S = \frac{\mu - \mu^{N+1}}{1 - \mu},\tag{S.12}$$

such that the sum in (S.11) becomes:

$$\sum_{l=1}^N \left( e^{i k_l (n - n')a} + e^{-i k_l (n - n')a} \right) = \frac{\cos[2\pi(n - n')/N] - \cos[2\pi(n - n')(N + 1)/N]}{1 - \cos[2\pi(n - n')/N]} \propto \sin[\pi(n - n')] = 0.\tag{S.13}$$

Note, that this is equivalent to the known completeness of the basis vectors of a Fourier series, i.e.,

$$\sum_{l=1}^N e^{2\pi i l (n - n')/N} = N \delta_{nn'}.\tag{S.14}$$

On the other hand, in order to preserve the commutation relations in Fourier (reciprocal) space,  $[\hat{a}_l, \hat{a}_{l'}^\dagger] = \delta_{ll'}$ , orthogonality is required, i.e.,

$$\sum_{n=1}^N e^{2\pi i n (l - l')/N} = N \delta_{ll'},\tag{S.15}$$

which is fully consistent with the equivalence of the two representations.

- d) Write the Hamiltonian in (c) in terms of the new operators  $\hat{a}_l, \hat{a}_l^\dagger$ . Write a general eigenstate. What is the ground state? What defines an excited state?

**Solution.** We calculate each term in (S.9) separately, starting from:

$$\begin{aligned}\frac{\hat{\pi}_n^2}{2} &= \sum_{l, l'} \frac{-\hbar\sqrt{\omega_l\omega_{l'}}}{4N} \left[ (\hat{a}_l \hat{a}_{l'})(t) e^{i(k_l + k_{l'})na} - (\hat{a}_l \hat{a}_{l'}^\dagger)(t) e^{i(k_l - k_{l'})na} - (\hat{a}_l^\dagger \hat{a}_{l'})(t) e^{i(k_{l'} - k_l)na} + (\hat{a}_l^\dagger \hat{a}_{l'}^\dagger)(t) e^{-i(k_l + k_{l'})na} \right] = \\ &= \sum_{l, l'} \frac{\hbar\sqrt{\omega_l\omega_{l'}}}{4N} \left[ 2(\hat{a}_l^\dagger \hat{a}_{l'})(t) e^{i(k_{l'} - k_l)na} - (\hat{a}_l \hat{a}_{l'})(t) e^{i(k_l + k_{l'})na} - (\hat{a}_l^\dagger \hat{a}_{l'}^\dagger)(t) e^{-i(k_l + k_{l'})na} \right] + \sum_l \frac{\hbar\omega_l}{4N}.\end{aligned}\tag{S.16}$$

From the first line to the second line we exchanged  $l, l'$  in the second summand and made use of the bosonic algebra of the operators. Exploiting (S.15) we can finally calculate:

$$\frac{1}{2} \sum_{n=1}^N \hat{\pi}_n^2 = \sum_l \frac{\hbar\omega_l}{4} \left[ 2\hat{a}_l^\dagger \hat{a}_l - \hat{a}_l \hat{a}_{-l} e^{-2i\omega_l t} - \hat{a}_l^\dagger \hat{a}_{-l}^\dagger e^{2i\omega_l t} \right] + \sum_l \frac{\hbar\omega_l}{4},\tag{S.17}$$

in which we used the parity property of the cosine, i. e.,  $\omega_l = \omega_{-l}$ . We are now following the most general approach in which  $l \in \mathbb{Z}$ , despite in the present case  $l \in \mathbb{N}$ . We will see that the two time-dependent

contributions above will be eliminated by the position terms in the Hamiltonian; in the present case of  $l \in \mathbb{N}$  those terms are immediately zero as  $l'$  cannot be equal to  $-l$ , but we decided to keep them in order to remain as general as possible. In the same way we obtain for the remaining terms in (S.9),

$$\begin{aligned} \frac{\Omega^2 \hat{u}_n^2}{2} &= \sum_{l'} \frac{\hbar \Omega^2}{4N \sqrt{\omega_l \omega_{l'}}} \left[ (\hat{a}_l \hat{a}_{l'})(t) e^{i(k_l + k_{l'})na} + (\hat{a}_l \hat{a}_{l'}^\dagger)(t) e^{i(k_l - k_{l'})na} + (\hat{a}_l^\dagger \hat{a}_{l'})(t) e^{i(k_{l'} - k_l)na} + (\hat{a}_l^\dagger \hat{a}_{l'}^\dagger)(t) e^{-i(k_l + k_{l'})na} \right] = \\ &= \sum_{l'} \frac{\hbar \Omega^2}{4N \sqrt{\omega_l \omega_{l'}}} \left[ 2(\hat{a}_l^\dagger \hat{a}_{l'})(t) e^{i(k_{l'} - k_l)na} + (\hat{a}_l \hat{a}_{l'})(t) e^{i(k_l + k_{l'})na} + (\hat{a}_l^\dagger \hat{a}_{l'}^\dagger)(t) e^{-i(k_l + k_{l'})na} \right] + \sum_l \frac{\hbar \Omega^2}{4N \omega_l}, \end{aligned} \quad (\text{S.18})$$

and

$$\frac{\Omega^2}{2} \sum_{n=1}^N \hat{u}_n^2 = \sum_l \frac{\hbar \Omega^2}{4\omega_l} \left[ 2\hat{a}_l^\dagger \hat{a}_l + \hat{a}_l \hat{a}_{-l} e^{-2i\omega_l t} + \hat{a}_l^\dagger \hat{a}_{-l}^\dagger e^{2i\omega_l t} \right] + \sum_l \frac{\hbar \Omega^2}{4\omega_l}. \quad (\text{S.19})$$

Finally,

$$\frac{\lambda}{2} \sum_{n=1}^N (\hat{u}_{n+1} - \hat{u}_n) = \sum_l \frac{2\hbar \lambda [1 - \cos(k_l a)]}{4\omega_l} \left[ 2\hat{a}_l^\dagger \hat{a}_l + \hat{a}_l \hat{a}_{-l} e^{-2i\omega_l t} + \hat{a}_l^\dagger \hat{a}_{-l}^\dagger e^{2i\omega_l t} \right] + \sum_l \frac{2\hbar \lambda [1 - \cos(k_l a)]}{4\omega_l}. \quad (\text{S.20})$$

Combining (S.19) with (S.20) and making use of the dispersion relation (S.5) one obtains:

$$(\text{S.19}) + (\text{S.20}) = \sum_l \frac{\hbar \omega_l}{4} \left[ 2\hat{a}_l^\dagger \hat{a}_l + \hat{a}_l \hat{a}_{-l} e^{-2i\omega_l t} + \hat{a}_l^\dagger \hat{a}_{-l}^\dagger e^{2i\omega_l t} \right] + \sum_l \frac{\hbar \omega_l}{4}, \quad (\text{S.21})$$

and finally the Hamiltonian  $\hat{\mathcal{H}} = (\text{S.17}) + (\text{S.21})$ , i.e.,

$$\hat{\mathcal{H}} = \sum_{l=1}^N \hbar \omega_l \left( \hat{a}_l^\dagger \hat{a}_l + \frac{1}{2} \right), \quad (\text{S.22})$$

which is explicitly time independent. The state

$$|N_p\rangle = |n_1, n_2, \dots, n_N\rangle = \prod_{l=1}^N \frac{1}{\sqrt{n_l!}} \left( \hat{a}_l^\dagger \right)^{n_l} |0\rangle, \quad (\text{S.23})$$

with  $N_p = \sum_{l=1}^N n_l$ , is an eigenstate of the Hamiltonian with energy

$$\hat{\mathcal{H}} |N_p\rangle = \sum_{l=1}^N \hbar \omega_l \left( n_l + \frac{1}{2} \right) |N_p\rangle = \sum_{l=1}^N \epsilon_l |N_p\rangle = \epsilon_p |N_p\rangle. \quad (\text{S.24})$$

In (S.23),  $|0\rangle$  is the unique ground state of the system, defined by  $\hat{a}_l |0\rangle = 0 \forall l = 1, \dots, N$ , with energy

$$\epsilon_0 = \frac{1}{2} \sum_{l=1}^N \hbar \omega_l. \quad (\text{S.25})$$

The state (S.23) is normalized to 1 and lives in the Fock space, which is a direct sum of the Hilbert spaces  $H_{N_p}$  of fixed total number of particles  $N_p$ . They in turn are symmetric tensor products of  $N_p$  single-particle Hilbert spaces. The occupation number  $n_l$  defines the number of excitations in the mode  $l$ . Excited states, i.e., with at least one non-zero  $n_l$ , obey Bose-Einstein statistics and are called *phonons*.

## Exercise 2. Planets as blackbodies?

The Stefan-Boltzmann law states that the emission power per unit surface area of a blackbody reads

$$P_{em} = \sigma T^4 \quad \text{with} \quad \sigma = \frac{\pi^2 k_B^4}{60 \hbar^3 c^2} \approx 5.6704 \cdot 10^{-8} \text{ Js}^{-1} \text{ m}^{-2} \text{ K}^{-4}. \quad (4)$$

- a) Making use of the Stefan-Boltzmann law, estimate the temperature of the Earth, Mars and Venus as if they were blackbodies.

*Hint.* The energy emitted and absorbed has to balance.

**Solution.** The Stefan-Boltzmann law gives a power per unit surface of emission. In order to estimate the temperature of the Earth as if it was a blackbody, we need to equate the energy emitted with the energy absorbed (Kirchoff's law). The Earth absorbs the radiation from the Sun, therefore we need to calculate the amount of solar energy that reaches us. In order to calculate the total power emitted by the Sun we need to integrate (4) over the Sun's surface, i.e.,

$$P_S = P_{em} \cdot 4\pi R_S^2 = \sigma T_S^4 \cdot 4\pi R_S^2, \quad (\text{S.26})$$

where  $T_S$  and  $R_S$  are the Sun surface temperature and radius, respectively. This power is spread all over the universe, and reaches the Earth after traveling the average distance  $a_0$  (also called *astronomical unit*). Therefore, the power per unit surface reaching the Earth is

$$p_{abs} = \frac{P_S}{4\pi a_0^2} \approx 1.4 \cdot 10^3 \text{ W}. \quad (\text{S.27})$$

In order to obtain the total power absorbed by the Earth we finally need to multiply the quantity above with the cross section of the Earth sphere, i.e.,

$$P_{abs} = \frac{P_S}{4\pi a_0^2} \cdot \pi R_E^2 = \frac{P_S R_E^2}{4a_0^2} \quad (\text{S.28})$$

where  $R_E$  is the Earth radius. The total power emitted by the Earth is still given by integrating (4) over the Earth surface,

$$P_E = P_{em} \cdot 4\pi R_E^2 = \sigma T_E^4 \cdot 4\pi R_E^2, \quad (\text{S.29})$$

where  $T_E$  is the temperature we want to estimate. We thus equate the emitted and absorbed power:

$$\sigma T_E^4 \cdot 4\pi R_E^2 = \frac{\sigma T_S^4 R_E^2 4\pi R_S^2}{4a_0^2} \Leftrightarrow T_E^4 = T_S^4 \frac{R_S^2}{4a_0^2} \Leftrightarrow T_E = T_S \sqrt{\frac{R_S}{2a_0}}, \quad (\text{S.30})$$

which is independent of the Earth radius. Using for  $T_S \approx 5778 \text{ K}$ , for  $R_S \approx 6.96 \cdot 10^8 \text{ m}$  and for  $a_0 \approx 1.496 \cdot 10^{11} \text{ m}$  we obtain

$$T_E \approx T_S \cdot 1.525 \cdot 10^{-3/2} \approx 279 \text{ K}. \quad (\text{S.31})$$

We can exploit the calculation above in the cases of the other planets, making use of  $a_M = 1.524a_0$  (average distance of Mars from the Sun) and  $a_V = 0.7233a_0$  (average distance of Venus from the Sun) to get:

$$\begin{aligned} T_M &\approx T_S \cdot 1.236 \cdot 10^{-3/2} \approx 226 \text{ K}, \\ T_V &\approx T_S \cdot 1.793 \cdot 10^{-3/2} \approx 328 \text{ K}. \end{aligned} \quad (\text{S.32})$$

- b) The correct results for the average temperatures are 288 K for the Earth, 218 K for Mars and 735 K for Venus. How do they compare with the estimates in (a)? What could be the reasons of the discrepancies?

**Solution.** There are many approximations in the calculation (a). There are mainly two effects, one lowering and one increasing the real temperature. First, all planets have albedo, such that part of the incoming solar radiation is scattered without absorption. This effect reduces the absorbed power and therefore the temperature. On the other hand, planets have an atmosphere, such that both the incoming and the emitted radiation suffer from reflection. The exact effect of the atmosphere is very complicated. For the Earth it turns out that the amount of radiation emitted from the surface (which, due to the lower temperature, has a higher wavelength) suffers more from reflection than the incoming Sun's radiation (mainly in the visible range of the electromagnetic spectrum), such that the resulting temperature of the Earth is slightly higher than the blackbody estimate. A similar reasoning is valid for the other planets, whose atmospheres are mainly composed of  $\text{CO}_2$ , with the important difference that the atmosphere of Mars is much thinner (therefore yielding a good estimate) while the one of Venus is much thicker (therefore yielding a bad estimate). Then, planets are not exactly spheres...:-)

**Exercise 1. Playing around with wave functions in second quantization.**

In the formalism of second quantization, a general state of  $N$  particles at positions  $\vec{r}_1, \vec{r}_2, \dots$  is given by

$$|\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N\rangle = \frac{1}{\sqrt{N!}} \hat{\Psi}^\dagger(r_N) \cdots \hat{\Psi}^\dagger(r_1) |0\rangle, \quad (1)$$

where  $|0\rangle$  is the vacuum state and the field operators  $\hat{\Psi}(\vec{r})$  are defined as

$$\hat{\Psi}(\vec{r}) = \sum_k \phi_k(\vec{r}) \hat{a}_k, \quad (2)$$

with  $\hat{a}_k$  the annihilator of mode  $k$  and  $\phi_k(\vec{r})$  the one-particle wave function of mode  $k$ .

Consider a state  $|\psi\rangle$  of three particles in modes  $k_1, k_2$ , and  $k_3$ . Consider its wave function

$$\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \langle \vec{r}_1, \vec{r}_2, \vec{r}_3 | \psi \rangle = \langle \vec{r}_1, \vec{r}_2, \vec{r}_3 | \hat{a}_{k_3}^\dagger \hat{a}_{k_2}^\dagger \hat{a}_{k_1}^\dagger |0\rangle. \quad (3)$$

(a) First calculate the vacuum expectation value

$$\langle 0 | \hat{a}_{\ell_1} \hat{a}_{\ell_2} \hat{a}_{\ell_3} \hat{a}_{k_3}^\dagger \hat{a}_{k_2}^\dagger \hat{a}_{k_1}^\dagger |0\rangle, \quad (4)$$

for bosons and for fermions.

**Solution.** Let's calculate using the usual (anti-)commutation relations (write for short  $\hat{a}_3 = \hat{a}_{k_3}$ ,  $\hat{a}_2 = \hat{a}_{k_2}$ ,  $\hat{a}_1 = \hat{a}_{k_1}$ ):

$$\begin{aligned} \hat{a}_l \hat{a}_m \hat{a}_n \hat{a}_3^\dagger \hat{a}_2^\dagger \hat{a}_1^\dagger &= \hat{a}_l \hat{a}_m [\delta_{nk_3} \pm \hat{a}_3^\dagger \hat{a}_n] \hat{a}_2^\dagger \hat{a}_1^\dagger = \hat{a}_l [\hat{a}_m \delta_{nk_3} \pm (\delta_{mk_3} \pm \hat{a}_3^\dagger \hat{a}_m) \hat{a}_n] \hat{a}_2^\dagger \hat{a}_1^\dagger \\ &= [\hat{a}_l \hat{a}_m \delta_{nk_3} \pm \hat{a}_l \delta_{mk_3} \hat{a}_n + \delta_{lk_3} \hat{a}_m \hat{a}_n] \hat{a}_2^\dagger \hat{a}_1^\dagger + \hat{a}^\dagger(\dots) \\ &= [(\hat{a}_l \delta_{mk_2} \pm \delta_{lk_2} \hat{a}_m) \delta_{nk_3} \pm \delta_{mk_3} (\hat{a}_l \delta_{nk_2} \pm \delta_{lk_2} \hat{a}_n) + \delta_{lk_3} (\hat{a}_m \delta_{nk_2} \pm \delta_{mk_2} \hat{a}_n)] \hat{a}_1^\dagger + \hat{a}^\dagger(\dots) \\ &= \delta_{lk_1} \delta_{mk_2} \delta_{nk_3} \pm \delta_{lk_2} \delta_{mk_1} \delta_{nk_3} \pm \delta_{lk_1} \delta_{mk_3} \delta_{nk_2} + \delta_{lk_2} \delta_{mk_3} \delta_{nk_1} + \delta_{lk_3} \delta_{mk_1} \delta_{nk_2} \pm \delta_{lk_3} \delta_{mk_2} \delta_{nk_1} + \hat{a}^\dagger(\dots) \\ &= \sum_{ijk} f_{ijk} \delta_{lk_i} \delta_{mk_j} \delta_{nk_k} + \hat{a}^\dagger(\dots), \end{aligned} \quad (S.1)$$

where the sum ranges over all sets of indices  $ijk$  which are all different, and where  $f_{ijk} = \epsilon_{ijk}$  is the fully antisymmetric tensor (Levi-Civita) for fermions and  $f_{ijk} = 1$  for bosons. We do not care about the terms which start by a creation operator (all symbolized above by  $\hat{a}^\dagger(\dots)$ ), because they will vanish once sandwiched between vacuum states. The vacuum expectation value is then

$$\langle 0 | \hat{a}_l \hat{a}_m \hat{a}_n \hat{a}_3^\dagger \hat{a}_2^\dagger \hat{a}_1^\dagger |0\rangle = \sum_{ijk} f_{ijk} \delta_{lk_i} \delta_{mk_j} \delta_{nk_k}. \quad (S.2)$$

For  $N$  particles, by similar procedure the expression generalizes to

$$\langle 0 | \hat{a}_{\ell_1} \dots \hat{a}_{\ell_N} \hat{a}_{k_N}^\dagger \dots \hat{a}_{k_1}^\dagger |0\rangle = \sum_{i_1 \dots i_N} f_{i_1 \dots i_N} \delta_{\ell_1 k_{i_1}} \dots \delta_{\ell_N k_{i_N}}. \quad (S.3)$$

(b) Determine  $\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3)$  for bosons and for fermions. What symmetries does the wave function possess?

**Solution.** The wave function is

$$\begin{aligned}\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) &= \frac{1}{\sqrt{N!}} \langle 0 | \hat{\Psi}_1 \hat{\Psi}_2 \hat{\Psi}_3 \hat{a}_3^\dagger \hat{a}_2^\dagger \hat{a}_1^\dagger | 0 \rangle = \frac{1}{\sqrt{N!}} \sum_{lmn} \phi_l^*(\vec{r}_1) \phi_m^*(\vec{r}_2) \phi_n^*(\vec{r}_3) \langle 0 | \hat{a}_l \hat{a}_m \hat{a}_n \hat{a}_3^\dagger \hat{a}_2^\dagger \hat{a}_1^\dagger | 0 \rangle \\ &= \frac{1}{\sqrt{N!}} \sum f_{ijk} \delta_{lk_i} \delta_{mk_j} \delta_{nk_k} \phi_l^*(\vec{r}_1) \phi_m^*(\vec{r}_2) \phi_n^*(\vec{r}_3) = \frac{1}{\sqrt{N!}} \sum f_{ijk} \phi_{k_i}^*(\vec{r}_1) \phi_{k_j}^*(\vec{r}_2) \phi_{k_k}^*(\vec{r}_3) .\end{aligned}\quad (\text{S.4})$$

Thus, the wave function is an explicit symmetrization (antisymmetrization) of  $\phi_{k_1}^*(\vec{r}_1) \phi_{k_2}^*(\vec{r}_2) \phi_{k_3}^*(\vec{r}_3)$  for bosons (fermions).

- (c) Determine the normalization of the wave function for fermions and for bosons. First consider the case where  $k_1$ ,  $k_2$  and  $k_3$  are all different, and then study the case where two or more modes are the same. What do you observe?

**Solution.** Recall the wave function is given by

$$\psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) = \frac{1}{\sqrt{3!}} \sum_{ijk} f_{ijk} \phi_{k_i}^*(\vec{r}_1) \phi_{k_j}^*(\vec{r}_2) \phi_{k_k}^*(\vec{r}_3) , \quad (\text{S.5})$$

and thus its normalization is

$$\begin{aligned}\int d^3\vec{r}_1 d^3\vec{r}_2 d^3\vec{r}_3 \psi^*(\vec{r}_1, \vec{r}_2, \vec{r}_3) \psi(\vec{r}_1, \vec{r}_2, \vec{r}_3) &= \frac{1}{3!} \sum f_{ijk} f_{i'j'k'} \int d^3\vec{r}_1 d^3\vec{r}_2 d^3\vec{r}_3 \phi_{k_i}^*(\vec{r}_1) \phi_{k_{i'}}(\vec{r}_1) \phi_{k_j}^*(\vec{r}_2) \phi_{k_{j'}}(\vec{r}_2) \phi_{k_k}^*(\vec{r}_3) \phi_{k_{k'}}(\vec{r}_3) \\ &= \frac{1}{3!} \sum f_{ijk} f_{i'j'k'} \int d^3\vec{r}_1 \phi_{k_i}^*(\vec{r}_1) \phi_{k_{i'}}(\vec{r}_1) \int d^3\vec{r}_2 \phi_{k_j}^*(\vec{r}_2) \phi_{k_{j'}}(\vec{r}_2) \int d^3\vec{r}_3 \phi_{k_k}^*(\vec{r}_3) \phi_{k_{k'}}(\vec{r}_3) \\ &= \frac{1}{3!} \sum f_{ijk} f_{i'j'k'} \delta_{k_i k_{i'}} \delta_{k_j k_{j'}} \delta_{k_k k_{k'}} .\end{aligned}\quad (\text{S.6})$$

This expression obviously generalizes to  $N$  particles as

$$\langle \psi | \psi \rangle = \frac{1}{N!} \sum_{\substack{i_1 \dots i_N, \\ i'_1 \dots i'_N}} f_{i_1 \dots i_N} f_{i'_1 \dots i'_N} \delta_{k_{i_1} k_{i'_1}} \dots \delta_{k_{i_N} k_{i'_N}} . \quad (\text{S.7})$$

Assuming that  $k_1, k_2, k_3$  are all different in (S.6), then all terms in the sum that don't satisfy  $i = i', j = j', k = k'$  vanish because of the orthogonality of the single-particle states, and thus

$$\langle \psi | \psi \rangle = \frac{1}{3!} \sum f_{ijk}^2 \delta_{k_i k_i} \delta_{k_j k_j} \delta_{k_k k_k} = \frac{1}{3!} \sum f_{ijk}^2 = 1 . \quad (\text{S.8})$$

Additionally, if two or more modes are equal (e.g.,  $k_1 = k_2$ ), then all possible permutations of matching modes must be included (e.g., if  $k_1 = k_2$ , then the term  $i = j', j = i', k = k'$  also needs to be counted in the above), multiplying the result by an additional factor  $N_n!$  for each repeated mode  $n$  ( $N_n$  then being the number of particles in mode  $n$ ):

$$\langle \psi | \psi \rangle = N_1! \dots = \prod_{\text{modes}} N_n! \quad (\text{S.9})$$

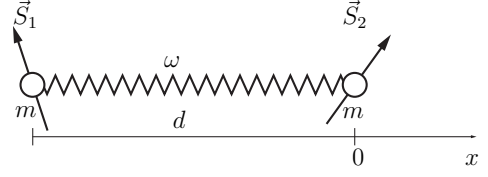
Of course, for fermions  $N_n$  is either zero or one, such that these factors do not contribute. However they must be included for bosons.

*Note: for the lazy, it is also possible to do the whole exercise with two particles only. For the motivated, calculate it for  $N$  particles.*

**Exercise 2. Magnetostriction in a Spin-Dimer-Model.**

As in Exercise 2.3, we consider a dimer consisting of two spin-1/2 particles with the Hamiltonian

$$\mathcal{H}_0 = J \left( \vec{S}_1 \cdot \vec{S}_2 + 3/4 \right) ,$$



with  $J > 0$  (note that the energy levels are shifted as compared to Ex. 2.3). This time, however, the distance between the two spins is not fixed, but they are connected to a spring. The spin-spin coupling constant depends on the distance between the two sites such that the Hamilton operator of the system is

$$\mathcal{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2} \hat{x}^2 + J(1 - \lambda \hat{x}) \left( \vec{S}_1 \cdot \vec{S}_2 + 3/4 \right) , \quad (5)$$

where  $\lambda \geq 0$ ,  $m$  is the mass of the two constituents,  $m\omega^2$  is the spring constant and where  $x$  denotes the displacement from the equilibrium distance  $d$  between the two spins (in the case of no spin-spin interaction).

- (a) Write the Hamiltonian (5) in second quantized form and calculate the partition sum, the internal energy, the specific heat and the entropy. Discuss the behavior of the entropy in the limit  $T \rightarrow 0$  for different values of  $\lambda$ .

*Hints.* Set  $\hbar = 1$ . Rewrite the Hamiltonian using the total spin as in Exercise 2.3, and bring it by completing the square to the form

$$\mathcal{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{X}^2 + \tilde{J} \hat{n}_t , \quad (6)$$

where  $\hat{n}_t$  is the projector on the triplet subspace, and  $\hat{X}$  and  $\tilde{J}$  are appropriately shifted quantities  $\hat{x}$  and  $J$  ( $\hat{X}$  may depend on  $\hat{n}_t$ ). Recall then the creation and annihilation operators of a harmonic oscillator.

- (b) Calculate the expectation value of the distance between the two spins,  $\langle d + \hat{x} \rangle$ , as well as the fluctuation,  $\langle (d + \hat{x})^2 \rangle$ . How are these quantities affected by a magnetic field in  $z$ -direction, i.e., by adding an additional term in (5) of the form

$$\mathcal{H}_m = -g\mu_B H \sum_i \hat{S}_i^z \quad ?$$

*Hints.* Write first those averages in terms of  $\langle \hat{n}_t \rangle$ , which you can calculate explicitly. Recall that for a harmonic oscillator,  $\langle \hat{X} \rangle$  vanishes, as well as  $\langle \hat{a} \rangle$ ,  $\langle \hat{a}^2 \rangle$  etc.

Recalculate the partition function adding the magnetic field term and see how this affects  $\langle \hat{n}_t \rangle$ .

- (c\*) If the two sites are oppositely charged, i.e.,  $\pm q$ , the dimer forms a dipole with moment  $P = q \langle d + \hat{x} \rangle$ . This dipole moment can be measured by applying an electric field  $E$  along the  $x$ -direction, resulting in the additional Hamiltonian term

$$\mathcal{H}_{el} = -q(d + \hat{x})E .$$

Calculate the susceptibility of the dimer at zero electric field,

$$\chi_0^{(el)} = - \left. \frac{\partial^2 F}{\partial E^2} \right|_{E=0} ,$$



and compare your result with the simple form of the fluctuation-dissipation theorem, which asserts that

$$\chi_0^{(\text{el})} \propto \langle (d + \hat{x})^2 \rangle - \langle d + \hat{x} \rangle^2 . \quad (7)$$

*Hint.* Proceeding as in Section 1.5.3 of the lecture notes or Exercise 2.1 (e), find out which step no longer applies. How should (7) be “corrected”?

Plot the susceptibility at zero electric field as a function of an applied magnetic field  $H$  and discuss your result.

**Solution.**

(a) As in Exercise 2.3, the Hamiltonian  $\mathcal{H}_0$  may be written in terms of the total spin operator  $\vec{S} = \vec{S}_1 + \vec{S}_2$ ,

$$\mathcal{H}_0 = J \frac{\vec{S}^2}{2} .$$

Let us set  $\hbar = 1$ . Then  $\langle \sigma | \vec{S}^2 | \sigma \rangle = \hbar^2 S(S+1) = S(S+1)$  with  $S = 0, 1$  for the singlet and a triplet state, respectively, so that  $\hat{n}_t := \vec{S}^2/2$  is just the projection operator onto the triplet subspace, satisfying

$$\langle \sigma | \hat{n}_t | \sigma \rangle = \begin{cases} 1 & \text{if } \sigma \text{ is a triplet} \\ 0 & \text{if } \sigma \text{ is a singlet} \end{cases}$$

Using this operator, the total Hamiltonian has the form

$$\begin{aligned} \mathcal{H} &= \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2} \hat{x}^2 + J(1 - \lambda \hat{x}) \hat{n}_t \\ &= \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2} \hat{X}^2 + \tilde{J} \hat{n}_t, \end{aligned}$$

where we have “completed the square” and introduced the shifted coordinate operator

$$\hat{X} = \hat{x} - \frac{J\lambda}{m\omega^2} \hat{n}_t , \quad (\text{S.10})$$

and the renormalized spin-spin coupling

$$\tilde{J} = J \left( 1 - \frac{J\lambda^2}{2m\omega^2} \right) \quad (\text{S.11})$$

and used the fact that  $\hat{n}_t^2 = \hat{n}_t$  (it is a projection operator).

We note that  $\hat{X}$  and  $\hat{p}$  satisfy the same commutation relation as  $\hat{x}$  and  $\hat{p}$ . Therefore we may introduce the corresponding raising and lowering operators

$$\begin{aligned} \hat{a} &= \sqrt{\frac{m\omega}{2}} \left( \hat{X} + \frac{i}{m\omega} \hat{p} \right) \\ \hat{a}^\dagger &= \sqrt{\frac{m\omega}{2}} \left( \hat{X} - \frac{i}{m\omega} \hat{p} \right) \end{aligned}$$

using which the Hamiltonian can be written as follows in second-quantized form:

$$\mathcal{H} = \omega \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right) + \tilde{J} \hat{n}_t . \quad (\text{S.12})$$

The canonical partition sum is

$$Z = \text{tr} e^{-\beta \mathcal{H}} = \sum_{n=0}^{\infty} \sum_{\sigma} \langle n, \sigma | e^{-\beta \mathcal{H}} | n, \sigma \rangle ,$$

where  $|n\rangle$  denotes the eigenstates of  $\hat{a}^\dagger \hat{a}$ . We observe that the harmonic oscillator term commutes with the spin dimer term in the Hamiltonian. Therefore, the partition function factorizes,

$$Z = Z_{\text{harmonic oscillator}} \cdot Z_{\text{spin dimer}} . \quad (\text{S.13})$$

The partition function of the harmonic oscillator is given by

$$Z_{\text{harmonic oscillator}} = \text{tr} e^{-\beta \mathcal{H}_{\text{harm. osc.}}} = \sum_n e^{-\beta \omega (n + \frac{1}{2})} = e^{-\beta \omega / 2} \frac{1}{1 - e^{-\beta \omega}}. \quad (\text{S.14})$$

The partition function of the dimer is simply given by

$$Z_{\text{spin dimer}} = \underbrace{1}_{\substack{\text{singlet state} \\ \hat{n}_t=0}} + \underbrace{3e^{-\beta \tilde{J}}}_{\substack{\text{triplet states} \\ \hat{n}_t=1}}.$$

We then finally have

$$Z = Z_{\text{harmonic oscillator}} \cdot Z_{\text{spin dimer}} = \frac{e^{-\beta \omega / 2}}{1 - e^{-\beta \omega}} (1 + 3e^{-\beta \tilde{J}}), \quad (\text{S.15})$$

It follows that the internal energy is given by

$$\begin{aligned} U &= -\frac{\partial}{\partial \beta} \log Z = -\frac{\partial}{\partial \beta} \log Z_{\text{harmonic oscillator}} - \frac{\partial}{\partial \beta} \log Z_{\text{spin dimer}} \\ &= \frac{\omega}{2} + \frac{\omega}{e^{\beta \omega} - 1} + \frac{3\tilde{J}}{e^{\beta \tilde{J}} + 3} = \frac{\omega}{2} \coth \frac{\beta \omega}{2} + \frac{3\tilde{J}}{e^{\beta \tilde{J}} + 3}. \end{aligned}$$

Therefore, specific heat, free energy and entropy are given by

$$\begin{aligned} C &= \frac{\partial U}{\partial T} = C_{\text{harmonic oscillator}} + C_{\text{spin dimer}} \\ &= \frac{\omega^2}{4k_B T^2} \frac{1}{\sinh^2(\beta \omega / 2)} + \frac{3\tilde{J}^2}{k_B T^2} \frac{e^{\beta \tilde{J}}}{(e^{\beta \tilde{J}} + 3)^2}, \\ F &= -k_B T \log Z = F_{\text{harmonic oscillator}} + F_{\text{spin dimer}} \\ &= \frac{\omega}{2} + k_B T \log(1 - e^{-\beta \omega}) - k_B T \log(1 + 3e^{-\beta \tilde{J}}), \\ S &= \frac{U - F}{T} = \frac{\omega}{T(e^{\beta \omega} - 1)} - k_B \log(1 - e^{-\beta \omega}) + \frac{3\tilde{J}}{T(e^{\beta \tilde{J}} + 3)} + k_B \log(1 + 3e^{-\beta \tilde{J}}). \end{aligned}$$

Note that the first two terms of the entropy always vanish in the limit  $T \rightarrow 0$ .

As long as  $\tilde{J}$  is positive, it is easy to see that  $\lim_{T \rightarrow 0} S = 0$ . In particular, this is the case for  $\lambda = 0$ , where  $\tilde{J} = J$ .

If we make  $\lambda$  large enough, namely  $\lambda > \lambda_c := \sqrt{2m\omega^2/J}$ , then  $\tilde{J}$  becomes negative and the entropy is in the limit  $T \rightarrow 0$  given by

$$\lim_{T \rightarrow 0} S = \lim_{T \rightarrow 0} \left( \frac{\tilde{J}}{T} + k_B \log 3e^{-\tilde{J}/k_B T} \right) = k_B \log 3.$$

For  $\lambda = \lambda_c$ ,  $\tilde{J}$  is equal to zero and  $\lim_{T \rightarrow 0} S = k_B \log 4$ .

This result corresponds, of course, to the number of degenerate ground-states for the spin configuration: For positive  $\tilde{J}$ , the ground-state is unique (the singlet) and thus the entropy has to vanish as  $T \rightarrow 0$ . For negative  $\tilde{J}$ , the ground-state is the triplet and thus three-fold degenerate. When there is no effective coupling between the spins then there are four degenerate ground-states, leading to an entropy of  $k_B \log 4$ .

(b) The mean distance between the two sites is given by

$$\langle d + \hat{x} \rangle = \left\langle d + \hat{X} + \frac{J\lambda}{m\omega^2} \hat{n}_t \right\rangle = d + \frac{J\lambda}{m\omega^2} \langle \hat{n}_t \rangle,$$

where we used (S.10) and the fact that the expectation value of the (shifted) position operator  $\hat{X}$  for the harmonic oscillator vanishes. The expectation value of the “number” operator  $\hat{n}_t$  is computed using the fact that the partition sum factorizes,

$$\langle \hat{n}_t \rangle = \frac{1}{Z_{\text{spin dimer}}} \sum_{\sigma} \langle \sigma | \hat{n}_t e^{-\beta \tilde{J} \hat{n}_t} | \sigma \rangle = \frac{3e^{-\beta \tilde{J}}}{Z_{\text{spin dimer}}} = \frac{3e^{-\beta \tilde{J}}}{1 + 3e^{-\beta \tilde{J}}}. \quad (\text{S.16})$$

Therefore, we find for the expectation value of the distance between the two spins

$$\langle d + \hat{x} \rangle = d + \frac{J\lambda}{m\omega^2} \frac{3}{e^{\beta \tilde{J}} + 3}.$$

To calculate the fluctuations of the distance, we write

$$\langle (d + \hat{x})^2 \rangle = \left\langle \left( d + \hat{X} + \frac{J\lambda}{m\omega^2} \hat{n}_t \right)^2 \right\rangle = d^2 + \langle \hat{X}^2 \rangle + \frac{J\lambda}{m\omega^2} \left( 2d + \frac{J\lambda}{m\omega^2} \right) \langle \hat{n}_t \rangle, \quad (\text{S.17})$$

where we have already omitted terms linear in  $\hat{X}$  and used that  $\hat{n}_t^2 = \hat{n}_t$ . For a harmonic oscillator,

$$\langle \hat{X}^2 \rangle = \left\langle \left( \frac{1}{\sqrt{2m\omega}} (\hat{a} + \hat{a}^\dagger) \right)^2 \right\rangle = \frac{1}{m\omega} \langle \hat{a}^\dagger \hat{a} + \frac{1}{2} \rangle = \frac{1}{m\omega} \left( \frac{1}{2} + \frac{1}{e^{\beta\omega} - 1} \right), \quad (\text{S.18})$$

because  $\hat{a}^\dagger \hat{a}$  is the bosonic number operator of the harmonic oscillator, and we know that its average gives the Bose statistics.<sup>1</sup> We thus find that

$$\langle (d + \hat{x})^2 \rangle = d^2 + \frac{1}{m\omega} \left( \frac{1}{2} + \frac{1}{e^{\beta\omega} - 1} \right) + \frac{J\lambda}{m\omega^2} \left( 2d + \frac{J\lambda}{m\omega^2} \right) \langle \hat{n}_t \rangle, \quad (\text{S.19})$$

with  $\langle \hat{n}_t \rangle$  given by (S.16).

In the presence of a magnetic field, the only change is in  $\langle \hat{n}_t \rangle$ . (Indeed, we did the calculation of the fluctuations without assuming anything about the density operator on the spin part of the dimer, and keeping the abstract averaging operation  $\langle \cdot \rangle$ .) We need to recalculate the partition function though:

$$\begin{aligned} Z_{\text{dimer with } H} &= \text{tr} e^{-\beta(\tilde{J} \hat{n}_t - g\mu_B H S_{\text{tot}}^z)} = 1 + e^{-\beta\tilde{J} \hat{n}_t} \left( e^{-\beta g\mu_B H} + 1 + e^{\beta g\mu_B H} \right) \\ &= 1 + e^{-\beta\tilde{J} \hat{n}_t} (1 + 2 \cosh(\beta g\mu_B H)). \end{aligned} \quad (\text{S.20})$$

It follows then that

$$\langle \hat{n}_t \rangle = \frac{1}{Z_{\text{dimer with } H}} \sum_{\sigma} \langle \sigma | \hat{n}_t e^{-\beta(\tilde{J} \hat{n}_t + \mathcal{H}_m)} | \sigma \rangle = \frac{e^{-\beta\tilde{J}} (1 + 2 \cosh(\beta g\mu_B H))}{1 + e^{-\beta\tilde{J}} (1 + 2 \cosh(\beta g\mu_B H))}. \quad (\text{S.21})$$

Note that  $\langle \hat{n}_t \rangle$  is a monotonously increasing function of  $|H|$ . Thus, by applying a magnetic field we can populate the triplet states and thereby increase the distance between the spins. This effect is called *magnetostriction*.

(c) We first consider the case without external magnetic field. Then the Hamiltonian is given by

$$\mathcal{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2} \hat{X}^2 + \tilde{J} \hat{n}_t - \frac{q^2 E^2}{2m\omega^2} - dqE, \quad (\text{S.22})$$

where now

$$\hat{X} = \hat{x} - \frac{J\lambda}{m\omega^2} \hat{n}_t - \frac{qE}{m\omega^2}, \quad (\text{S.23a})$$

$$\tilde{J} = J \left( 1 - \frac{J\lambda^2}{2m\omega^2} - \frac{\lambda qE}{m\omega^2} \right). \quad (\text{S.23b})$$

In the same way as in (a), we find that the partition sum is given by

$$Z = \frac{e^{-\beta\omega/2}}{1 - e^{-\beta\omega}} \left( 1 + 3e^{-\beta\tilde{J}} \right) e^{\beta(dqE + q^2 E^2 / (2m\omega^2))},$$

and the free energy is therefore

$$F = -dqE - \frac{q^2 E^2}{2m\omega^2} + \frac{\omega}{2} + k_B T \log(1 - e^{-\beta\omega}) - k_B T \log(1 + 3e^{-\beta\tilde{J}}).$$

<sup>1</sup> If you're not convinced, or if you forgot how to prove this:

$$\begin{aligned} \frac{1}{m\omega} \langle \hat{a}^\dagger \hat{a} + \frac{1}{2} \rangle &= \frac{1}{m\omega} \cdot Z_{\text{harm. osc.}}^{-1} \cdot \text{tr} \left[ \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right) e^{-\beta\omega(\hat{a}^\dagger \hat{a} + \frac{1}{2})} \right] \\ &= \frac{1}{m\omega} \cdot Z_{\text{harm. osc.}}^{-1} \cdot \left( -\frac{1}{\beta} \frac{\partial}{\partial \omega} \text{tr} \left[ e^{-\beta\omega(\hat{a}^\dagger \hat{a} + \frac{1}{2})} \right] \right) = -\frac{1}{m\omega} \frac{1}{\beta} \frac{\partial}{\partial \omega} \log Z_{\text{harm. osc.}} \\ &= -\frac{1}{m\omega} \frac{1}{\beta} \left( -\frac{\beta}{2} - \frac{1}{1 - e^{-\beta\omega}} \cdot (-e^{-\beta\omega}) \cdot (-\beta) \right) = \frac{1}{m\omega} \left( \frac{1}{2} + \frac{1}{e^{\beta\omega} - 1} \right). \end{aligned}$$

In order to compute the susceptibility, we have to differentiate the free energy twice with respect to the electric field  $E$ . Only for the last term this is somewhat non-obvious: the first differentiation yields

$$\frac{\partial}{\partial E} k_B T \log(1 + 3e^{-\beta\tilde{J}}) = \frac{3}{e^{\beta\tilde{J}} + 3} J \frac{\lambda q}{m\omega^2} = \frac{J\lambda q}{m\omega^2} \frac{3}{e^{\beta\tilde{J}} + 3}.$$

Taking one more derivative we find that

$$\frac{\partial^2}{\partial E^2} k_B T \log(1 + 3e^{-\beta\tilde{J}}) = \beta \left( \frac{J\lambda q}{m\omega^2} \right)^2 \frac{3e^{\beta\tilde{J}}}{(e^{\beta\tilde{J}} + 3)^2}.$$

For  $E = 0$ , this can simply be expressed in terms of the mean triplet number,

$$\left. \frac{\partial^2}{\partial E^2} k_B T \log(1 + 3e^{-\beta\tilde{J}}) \right|_{E=0} = \beta \left( \frac{J\lambda q}{m\omega^2} \right)^2 (\langle \hat{n}_t \rangle - \langle \hat{n}_t \rangle^2);$$

indeed, from (S.16), we have

$$\langle \hat{n}_t \rangle - \langle \hat{n}_t \rangle^2 = \frac{3e^{-\beta\tilde{J}} (1 + 3e^{-\beta\tilde{J}}) - (3e^{-\beta\tilde{J}})^2}{(1 + 3e^{-\beta\tilde{J}})^2} = \frac{3e^{-\beta\tilde{J}}}{(1 + 3e^{-\beta\tilde{J}})^2} = \frac{3e^{\beta\tilde{J}}}{(e^{\beta\tilde{J}} + 3)^2}. \quad (\text{S.24})$$

Therefore, the susceptibility at zero electric field is given by

$$\chi_0^{(\text{el})} = \frac{q^2}{m\omega^2} + \beta \left( \frac{J\lambda q}{m\omega^2} \right)^2 (\langle \hat{n}_t \rangle - \langle \hat{n}_t \rangle^2). \quad (\text{S.25})$$

If we try to use the fluctuation-dissipation theorem to calculate the susceptibility at zero electric field, we find that

$$\begin{aligned} \langle (d + \hat{x})^2 \rangle - \langle (d + \hat{x}) \rangle^2 &= d^2 + \langle \hat{X}^2 \rangle + \left( \frac{J\lambda}{m\omega^2} \right) \left( 2d + \frac{J\lambda}{m\omega^2} \right) \langle \hat{n}_t \rangle - d^2 - 2d \left( \frac{J\lambda}{m\omega^2} \right) \langle \hat{n}_t \rangle - \left( \frac{J\lambda}{m\omega^2} \right)^2 \langle \hat{n}_t \rangle^2 \\ &= \langle \hat{X}^2 \rangle + \left( \frac{J\lambda}{m\omega^2} \right)^2 (\langle \hat{n}_t \rangle - \langle \hat{n}_t \rangle^2). \end{aligned} \quad (\text{S.26})$$

Obviously, this is not proportional to the result found in (S.25).

This discrepancy is due to the fact that this simple form of the fluctuation-dissipation theorem is only valid for classical systems (or simple quantum systems).<sup>2</sup> In this case, the coupling does not commute with the rest of the Hamiltonian. However, it is still possible to apply the reasoning done in Section 1.5.3 of the lecture notes and Exercise 2.1 (e) by looking at the “correct” quantities. We will proceed with an analogous derivation here, and we will point out the step where the derivation fails for the “incorrect” choice of variables. There, the fluctuation-dissipation theorem is derived for magnetization  $M$  produced in response to a magnetic field  $H$  with some susceptibility  $\chi_M$ . Here, distance  $(d + \hat{x})$  is produced in response to an electric field  $E$  with some susceptibility  $\chi_0^{(\text{el})}$ . In both situations, we have added a linear coupling term to the Hamiltonian of the form  $-M \cdot H$ , respectively  $-q(d + \hat{x}) \cdot E$ . However, the “correct” degree of freedom of the Harmonic oscillator is  $\hat{X}$ , and not  $\hat{x}$ . The difference is that now  $\hat{x}$  is dependent on  $E$  and not  $\hat{X}$ . Proceeding as for the magnetization case, we write

$$0 = \text{tr} \left\{ \langle (d + \hat{x}) - (d + \hat{x}) \rangle e^{\beta(F - \mathcal{H})} \right\}, \quad (\text{S.27})$$

and we differentiate this equation by  $E$ . Here we notice a first few differences with the magnetization case. While we had  $M = -\frac{\partial \mathcal{H}}{\partial H}$ , if we calculate  $\frac{\partial \mathcal{H}}{\partial E}$  we obtain

$$\frac{\partial \mathcal{H}}{\partial E} = -q \left( \frac{qE}{m\omega^2} + d - \frac{J\lambda}{m\omega^2} \hat{n}_t \right) = -q (d + \hat{x} - \hat{X}), \quad (\text{S.28})$$

---

<sup>2</sup> To convince oneself, a simpler setup is to consider a harmonic oscillator with a charged particle in a uniform electric field, both in the classical and in the quantum case, which is a simplification of the current problem but which exhibits similar behavior. (Use  $\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - qx E$ )

where we used (S.23a) in the second equality. Note that this quantity is proportional to  $\hat{n}_t$  and commutes with original Hamiltonian (this will be relevant later). This gives us for the free energy<sup>3</sup>

$$\frac{\partial F}{\partial E} = \left\langle \frac{\partial \mathcal{H}}{\partial E} \right\rangle = -q \langle d + \hat{x} \rangle ; \quad (\text{S.29})$$

we also need the derivative of  $d + \hat{x}$ , given by

$$\frac{\partial}{\partial E} (d + \hat{x}) = \frac{\partial}{\partial E} \left( d + \hat{X} + \frac{Jq}{m\omega^2} \hat{n}_t + \frac{qE}{m\omega^2} \right) = \frac{q}{m\omega^2} .$$

Now, differentiating expression (S.27) by  $E$ ,

$$0 = \frac{\partial}{\partial E} \text{tr} \left\{ (\langle d + \hat{x} \rangle - (d + \hat{x})) e^{\beta(F-\mathcal{H})} \right\} = \text{tr} \left\{ \left( \frac{\partial \langle d + \hat{x} \rangle}{\partial E} - \frac{\partial}{\partial E} (d + \hat{x}) \right) e^{\beta(F-\mathcal{H})} \right\} \\ + \text{tr} \left\{ [\langle d + \hat{x} \rangle - (d + \hat{x})] e^{\beta(F-\mathcal{H})} \cdot \beta \cdot \left( -q \langle d + \hat{x} \rangle + q (d + \hat{x} - \hat{X}) \right) \right\} . \quad (\text{S.30})$$

But wait. The differentiation of the operators inside the second trace needs a little bit of justification here. First, we can rely on some basic differentiation rules for operators such as

$$\frac{\partial}{\partial E} \text{tr}(\dots) = \text{tr} \frac{\partial}{\partial E}(\dots) \quad \text{and} \quad \frac{\partial}{\partial E} (AB) = \frac{\partial A}{\partial E} B + A \frac{\partial B}{\partial E} .$$

Then, in general, for an operator  $A$  and a function  $f$ , one has that

$$\frac{\partial}{\partial E} f(A) = \sum_n c_n \frac{\partial}{\partial E} A^n = \sum_n c_n \left( \frac{\partial A}{\partial E} A^{n-1} + A \frac{\partial A}{\partial E} A^{n-2} + \dots \right) , \quad (\text{S.31})$$

where  $c_n$  are the coefficients of the Taylor expansion of  $f$  in terms of a power series.<sup>4</sup> Now, assuming that  $[A, \frac{\partial A}{\partial E}] = 0$ , we see that  $\frac{\partial A}{\partial E}$  commutes through the  $A$ 's and we can write

$$\frac{\partial}{\partial E} f(A) = \sum_n c_n n A^{n-1} \frac{\partial A}{\partial E} = f'(A) \frac{\partial A}{\partial E} . \quad (\text{S.32})$$

In our case, we have that  $\frac{\partial \mathcal{H}}{\partial E} \propto \hat{n}_t$  commutes with  $\mathcal{H}$ , and so

$$\frac{\partial}{\partial E} e^{-\beta \mathcal{H}} = -\beta e^{-\beta \mathcal{H}} \cdot \frac{\partial \mathcal{H}}{\partial E} .$$

Note, crucially, that had we chosen to work with the other degree of freedom  $\hat{x}$  (having  $\hat{X}$  depend on  $E$  and not  $\hat{x}$ ), we would have had  $\frac{\partial \mathcal{H}}{\partial E} = -q(d + \hat{x})$ , which obviously does not commute with  $\mathcal{H}$ .

The second term of (S.30) is then obtained by using

$$\frac{\partial}{\partial E} e^{\beta(F-\mathcal{H})} = \frac{\partial}{\partial E} e^{\beta F} e^{-\beta \mathcal{H}} = e^{\beta F} \beta \left( \frac{\partial F}{\partial E} \right) e^{-\beta \mathcal{H}} + e^{\beta F} (-\beta) e^{-\beta \mathcal{H}} \frac{\partial \mathcal{H}}{\partial E} = \beta e^{\beta(F-\mathcal{H})} \left( \frac{\partial F}{\partial E} - \frac{\partial \mathcal{H}}{\partial E} \right) ,$$

keeping in mind that  $F$  is a scalar, not an operator.

Continuing from (S.30), we find that

$$-\frac{1}{q} \frac{\partial^2 F}{\partial E^2} - \frac{q}{m\omega^2} = \beta \cdot q \cdot \left\langle \left[ \langle d + \hat{x} \rangle - (d + \hat{x}) \right]^2 + \hat{X} \left[ \langle d + \hat{x} \rangle - (d + \hat{x}) \right] \right\rangle \\ = \beta q \left\langle \left[ \langle d + \hat{x} \rangle - (d + \hat{x}) \right]^2 \right\rangle + \beta q \left\langle \hat{X} \left[ \hat{X} + \frac{J\lambda}{m\omega^2} \hat{n}_t + \frac{qE}{m\omega^2} \right] \right\rangle \\ = \beta q \left[ \langle (d + \hat{x})^2 \rangle - \langle d + \hat{x} \rangle^2 \right] + \beta q \langle \hat{X} \rangle$$

<sup>3</sup> In general, for an external parameter  $E$  the Hamiltonian can depend on, one has

$$\frac{\partial F}{\partial E} = -\frac{1}{\beta} \frac{\partial}{\partial E} \log Z = -\frac{1}{\beta} \frac{1}{Z} \frac{\partial}{\partial E} \text{tr} \left[ e^{-\beta \mathcal{H}} \right] = \frac{1}{Z} \text{tr} \left[ e^{-\beta \mathcal{H}} \frac{\partial \mathcal{H}}{\partial E} \right] = \left\langle \frac{\partial \mathcal{H}}{\partial E} \right\rangle ,$$

where the differentiation inside the trace can be justified by using the Taylor expansion of the exponential and using the cyclicity of the trace, without assuming that  $[\mathcal{H}, \frac{\partial \mathcal{H}}{\partial E}] = 0$ .

<sup>4</sup>Note that if we enclose Eq. (S.31) inside a trace, then we can use the cyclicity of the trace to prove the assertion in the previous footnote.

where we have used that  $\frac{\partial \langle d + \hat{x} \rangle}{\partial E} = -\frac{1}{q} \frac{\partial}{\partial E} \frac{\partial F}{\partial E} = -\frac{1}{q} \frac{\partial^2 F}{\partial E^2}$ , expressed  $\hat{x}$  as function of  $\hat{X}$  using (S.23a), repeatedly used  $\langle \hat{X} \rangle = 0$ , and noticed also  $\langle \hat{X} \hat{n}_t \rangle = \langle \hat{X} \rangle_{\text{H.O.}} \langle \hat{n}_t \rangle_{\text{spin}} = 0$  since  $\hat{X}$  and  $\hat{n}_t$  act on different subsystems. It follows that

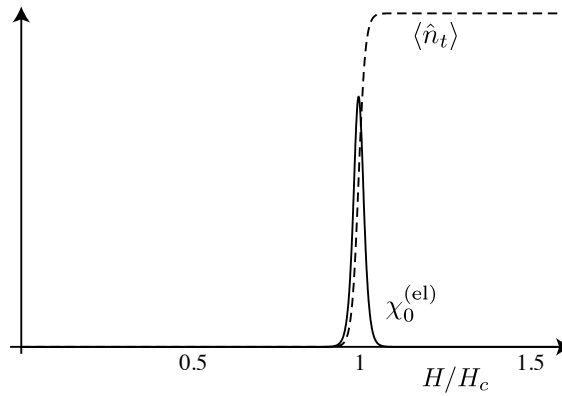
$$\frac{\chi_0^{(\text{el})}}{\beta q^2} - \frac{1}{\beta m \omega^2} = [\langle (d + \hat{x})^2 \rangle - \langle d + \hat{x} \rangle^2] + \langle \hat{X}^2 \rangle. \quad (\text{S.33})$$

This “corrected” fluctuation-dissipation theorem now agrees with the expressions (S.25) and (S.26).

Additionally, if for high temperatures we expand the expression we found for  $\langle \hat{X}^2 \rangle$  then

$$\langle (d + \hat{x})^2 \rangle - \langle d + \hat{x} \rangle^2 \approx \frac{1}{\beta m \omega^2} + \left( \frac{J\lambda}{m\omega^2} \right)^2 (\langle \hat{n}_t \rangle - \langle \hat{n}_t \rangle^2) = \frac{\chi_0^{(\text{el})}}{\beta q^2}.$$

The presence of a magnetic field again only affects the occupation number of the triplet state,  $\langle \hat{n}_t \rangle$ , from the expression in (S.16) to the one in (S.21). The second term in (S.25) then varies. The following plot shows the susceptibility at zero electric field (solid line) as well as the triplet occupation number at a low temperature (dashed line) in arbitrary units.



The susceptibility is largest when the triplet occupation number changes, i.e., when  $H = \pm H_c = \pm \tilde{J}/g\mu_B$ . This makes sense since in that case the system is most susceptible to an external influence like an electric field.

**Exercise 1. Pair correlation functions for fermions at finite temperature**

In this exercise we want to study the correlation functions for a system of free independent fermions at finite temperature, especially in the high temperature limit.

- (a) Evaluate the thermal average  $\langle \hat{O} \rangle = \frac{\text{tr}\{e^{-\beta H'} \hat{O}\}}{\text{tr} e^{-\beta H'}}$  for  $\hat{O} = \hat{n}_{\vec{k}}$  and  $\hat{O} = \hat{n}_{\vec{k}} \hat{n}_{\vec{q}}$  at  $T = 0$  and at  $T > 0$ , where  $H' = H - \mu \hat{N}$  and  $\beta = \frac{1}{k_B T}$ .

**Solution.** The  $T = 0$  is the ground state expectation value  $\langle \Phi_0 | \hat{O} | \Phi_0 \rangle$ .

$$\hat{n}_{\vec{k}} | \Phi_0 \rangle = \Theta(k_F - k) | \Phi_0 \rangle =: n_{\vec{k}} | \Phi_0 \rangle \quad (\text{S.1})$$

$$\hat{n}_{\vec{k}} \hat{n}_{\vec{q}} | \Phi_0 \rangle = \hat{n}_{\vec{k}} n_{\vec{q}} | \Phi_0 \rangle = n_{\vec{k}} n_{\vec{q}} | \Phi_0 \rangle, \quad (\text{S.2})$$

where  $k = |\vec{k}|$ ,  $\vec{k}_F$  is the Fermi wave vector and  $\Theta(x)$  is Heaviside step function:

$$\Theta(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{if } x \geq 0 \end{cases}. \quad (\text{S.3})$$

Therefore  $\langle \Phi_0 | \hat{n}_{\vec{k}} | \Phi_0 \rangle = n_{\vec{k}}$  and  $\langle \Phi_0 | \hat{n}_{\vec{k}} \hat{n}_{\vec{q}} | \Phi_0 \rangle = n_{\vec{k}} n_{\vec{q}} = \langle \Phi_0 | \hat{n}_{\vec{k}} | \Phi_0 \rangle \langle \Phi_0 | \hat{n}_{\vec{q}} | \Phi_0 \rangle$ .

For a non-interacting model

$$\begin{aligned} \langle \hat{n}_{\vec{k}} \rangle &= \frac{\left\{ \prod_{\vec{p} \neq \vec{k}} \sum_{\tilde{n}_{\vec{p}}=0,1} (ze^{-\beta \epsilon_{\vec{p}}})^{\tilde{n}_{\vec{p}}} \right\} \left\{ \sum_{\tilde{n}_{\vec{k}}=0,1} \tilde{n}_{\vec{k}} (ze^{-\beta \epsilon_{\vec{k}}})^{\tilde{n}_{\vec{k}}} \right\}}{\prod_{\vec{p}} \sum_{\tilde{n}_{\vec{p}}=0,1} (ze^{-\beta \epsilon_{\vec{p}}})^{\tilde{n}_{\vec{p}}}} = \frac{\sum_{\tilde{n}_{\vec{k}}=0,1} \tilde{n}_{\vec{k}} (ze^{-\beta \epsilon_{\vec{k}}})^{\tilde{n}_{\vec{k}}}}{\sum_{\tilde{n}_{\vec{k}}=0,1} (ze^{-\beta \epsilon_{\vec{k}}})^{\tilde{n}_{\vec{k}}}} \\ &= \frac{0 + ze^{-\beta \epsilon_{\vec{k}}}}{1 + ze^{-\beta \epsilon_{\vec{k}}}} = \frac{1}{1 + z^{-1} e^{-\beta \epsilon_{\vec{k}}}} = \frac{1}{1 + e^{-\beta(\epsilon_{\vec{k}} - \mu)}} =: n_{\vec{k}}, \end{aligned} \quad (\text{S.4})$$

where  $z = e^{\beta \mu}$ .

$$\begin{aligned} \langle \hat{n}_{\vec{k}} \hat{n}_{\vec{q}} \rangle &= \frac{\left\{ \prod_{\vec{p} \neq (\vec{k}, \vec{q})} \sum_{\tilde{n}_{\vec{p}}=0,1} (ze^{-\beta \epsilon_{\vec{p}}})^{\tilde{n}_{\vec{p}}} \right\} \left\{ \sum_{\tilde{n}_{\vec{k}}=0,1} \tilde{n}_{\vec{k}} (ze^{-\beta \epsilon_{\vec{k}}})^{\tilde{n}_{\vec{k}}} \right\} \left\{ \sum_{\tilde{n}_{\vec{q}}=0,1} \tilde{n}_{\vec{q}} (ze^{-\beta \epsilon_{\vec{q}}})^{\tilde{n}_{\vec{q}}} \right\}}{\prod_{\vec{p}} \sum_{\tilde{n}_{\vec{p}}=0,1} (ze^{-\beta \epsilon_{\vec{p}}})^{\tilde{n}_{\vec{p}}}} \\ &= \frac{\sum_{\tilde{n}_{\vec{k}}=0,1} \tilde{n}_{\vec{k}} (ze^{-\beta \epsilon_{\vec{k}}})^{\tilde{n}_{\vec{k}}} \sum_{\tilde{n}_{\vec{q}}=0,1} \tilde{n}_{\vec{q}} (ze^{-\beta \epsilon_{\vec{q}}})^{\tilde{n}_{\vec{q}}}}{\sum_{\tilde{n}_{\vec{k}}=0,1} (ze^{-\beta \epsilon_{\vec{k}}})^{\tilde{n}_{\vec{k}}} \sum_{\tilde{n}_{\vec{q}}=0,1} (ze^{-\beta \epsilon_{\vec{q}}})^{\tilde{n}_{\vec{q}}}} = \langle \hat{n}_{\vec{k}} \rangle \langle \hat{n}_{\vec{q}} \rangle = n_{\vec{k}} n_{\vec{q}}. \end{aligned} \quad (\text{S.5})$$

General remark: To obtain the correlation function at finite temperature (Section 3.6.1 from the Lecture Notes) we have to use the Fermi-Dirac distribution instead of the step function. Formally, the results written in terms of  $n_{\vec{k}}$  remain the same.

- (b) Show that the one-particle correlation function is

$$\frac{n}{2} g_s(\vec{R}) = \iiint \frac{d^3 k}{(2\pi)^3} n_{\vec{k}} e^{-i\vec{k} \cdot \vec{R}}, \quad (1)$$

where  $n_{\vec{k}}$  is the Fermi-Dirac distribution.

**Solution.** By definition:

$$\frac{n}{2} g_s(\vec{R}) = \langle \hat{\Psi}_s^\dagger(\vec{r} + \vec{R}) \hat{\Psi}_s^\dagger(\vec{r}) \rangle = \frac{1}{\Omega} \sum_{\vec{k}, \vec{k}'} e^{-i\vec{k} \cdot (\vec{r} + \vec{R}) + i\vec{k}' \cdot \vec{r}} \langle \hat{a}_{\vec{k}s}^\dagger \hat{a}_{\vec{k}'s} \rangle = \frac{1}{\Omega} \sum_{\vec{k}} n_{\vec{k}} e^{-i\vec{k} \cdot \vec{R}} = \iiint \frac{d^3 k}{(2\pi)^3} n_{\vec{k}} e^{-i\vec{k} \cdot \vec{R}}, \quad (\text{S.6})$$

where we used that  $n_{\vec{k}s} = n_{\vec{k}}$ .

(c) Show that in the high temperature limit

$$g_s(\vec{R}) \approx e^{-\frac{\pi \vec{R}^2}{\lambda^2}}, \quad (2)$$

where  $\lambda = \sqrt{\frac{\hbar^2}{2\pi m k_B T}}$  is the thermal wavelength. Compare this result with the one you know for  $T = 0$ .

*Hint.*  $\int_{-\infty}^{\infty} e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}} \quad \forall a \in \mathbb{R}_+, b \in \mathbb{C}.$

**Solution.** Using the thermal wavelength we have  $\beta \epsilon_{\vec{k}} = \frac{1}{4\pi} \frac{\hbar^2 \vec{k}^2}{2\pi m k_B T} = \frac{\lambda^2 \vec{k}^2}{4\pi}$ .

In the high temperature limit we could approximate  $n_{\vec{k}} \approx e^{-\beta(\epsilon_{\vec{k}} - \mu)}$ . Also,

$$\frac{n}{2} \approx \iiint \frac{d^3 k}{(2\pi)^3} e^{-\beta(\epsilon_{\vec{k}} - \mu)} = \frac{e^{\beta\mu}}{(2\pi)^3} \iiint d^3 k e^{-\frac{\lambda^2 \vec{k}^2}{4\pi}} = \frac{e^{\beta\mu}}{(2\pi)^3} \left( \frac{2\pi}{\lambda} \right)^3 = \frac{e^{\beta\mu}}{\lambda^3}. \quad (\text{S.7})$$

Replacing the chemical potential we obtain  $n_{\vec{k}} \approx \frac{n\lambda^3}{2} e^{-\frac{\lambda^2 \vec{k}^2}{4\pi}}$ .

The correlation functions becomes:

$$\begin{aligned} \frac{n}{2} g_s(\vec{R}) &\approx \iiint \frac{d^3 k}{(2\pi)^3} e^{-\beta(\epsilon_{\vec{k}} - \mu)} e^{-i\vec{k} \cdot \vec{R}} = \frac{n\lambda^3}{2} \frac{1}{(2\pi)^3} \left( \int_{-\infty}^{\infty} dk_x e^{-\frac{\lambda^2 k_x^2}{4\pi} - i k_x R_x} \right)^3 \\ &= \frac{n\lambda^3}{2} \frac{1}{(2\pi)^3} \left( \frac{2\pi}{\lambda} \right)^3 e^{-\frac{\pi \vec{R}^2}{\lambda^2}} = \frac{n}{2} e^{-\frac{\pi \vec{R}^2}{\lambda^2}}. \end{aligned} \quad (\text{S.8})$$

Therefore  $g_s(\vec{R}) \approx e^{-\frac{\pi \vec{R}^2}{\lambda^2}}$ . The oscillations from the  $T = 0$  case are no longer present.

(d) Show that in the high temperature limit

$$g(\vec{R}) = \frac{g_{\uparrow\uparrow}(\vec{R}) + g_{\uparrow\downarrow}(\vec{R})}{2} \approx 1 - \frac{e^{-\frac{2\pi \vec{R}^2}{\lambda^2}}}{2}. \quad (3)$$

Compare this result with the one you know for bosons.

**Solution.** The pair correlation function for fermions with different spins is  $g_{ss'}(\vec{R}) = 1$  while for equal-spin is  $g_{ss}(\vec{R}) = 1 - g_s(\vec{R})^2$ . Therefore

$$g(\vec{R}) \approx \frac{1 + 1 - e^{-\frac{2\pi \vec{R}^2}{\lambda^2}}}{2} = 1 - \frac{e^{-\frac{2\pi \vec{R}^2}{\lambda^2}}}{2}. \quad (\text{S.9})$$

For bosons the result is  $1 + e^{-\frac{2\pi \vec{R}^2}{\lambda^2}}$ . Therefore up to the prefactor  $\frac{1}{2}$  the two pair correlation functions are symmetric around  $g(R \rightarrow \infty) = 1$ . At  $R \rightarrow 0$ , fermions avoid each other  $g(R \rightarrow 0) = \frac{1}{2}$  ( $\frac{1}{2}$  comes from fermions with different spins) while bosons like to stay together  $g(R \rightarrow 0) = 2$ .

(e) How does the density depletion change? It is defined as  $n \iiint d^3 r (g(\vec{r}) - 1)$ .



**Solution.** The density depletion is just

$$n \iiint d^3r (g(\vec{r}) - 1) = -\frac{n}{2} \iiint d^3r g_s(\vec{r})^2 \approx -\frac{n}{2} \iiint d^3r e^{-\frac{2\pi\vec{r}^2}{\lambda^2}} = -\frac{n}{2} \left( \frac{\lambda}{\sqrt{2}} \right)^3 = -\frac{n}{4\sqrt{2}} \lambda^3, \quad (\text{S.10})$$

which decreases fast with the temperature  $\propto T^{-\frac{3}{2}}$ .

**Exercise 2. Single-particle correlation function for bosons**

Consider a homogeneous gas of free independent spin-0 bosons at  $T > T_c$ . The single-particle correlation function is given by

$$g(\vec{R}) = \iiint \frac{d^3k}{(2\pi)^3} n_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}}, \quad (4)$$

where  $\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$  and  $n_{\vec{k}} = \frac{1}{e^{\beta(\epsilon_{\vec{k}} - \mu)} - 1}$  (Section 3.7.2 from the Lecture Notes).

(a) Show that in the  $\vec{R} \rightarrow 0$  limit

$$g(\vec{R}) \approx n \left( 1 - \frac{\vec{R}^2}{6} \langle k^2 \rangle \right), \quad (5)$$

where  $n$  is the particle density.

**Solution.** Here we reused the notation from Section 3.7.2. If we normalize the value of the correlation function we have to do the following change  $g(\vec{R}) \rightarrow \frac{g(\vec{R})}{n}$ .

We have

$$e^{-i\vec{k}\cdot\vec{R}} \underset{\vec{R} \rightarrow 0}{\approx} 1 + (-i\vec{k}\cdot\vec{R}) + \frac{(-i\vec{k}\cdot\vec{R})^2}{2!} = 1 - i\vec{k}\cdot\vec{R} - \frac{(\vec{k}\cdot\vec{R})^2}{2}. \quad (S.11)$$

In this limit the correlation function becomes

$$g(\vec{R}) \approx \iiint \frac{d^3k}{(2\pi)^3} n_{\vec{k}} \left( 1 - i\vec{k}\cdot\vec{R} - \frac{(\vec{k}\cdot\vec{R})^2}{2} \right) = I_1 + I_2 + I_3, \quad (S.12)$$

with

$$I_1 = \iiint \frac{d^3k}{(2\pi)^3} n_{\vec{k}} = n \quad (S.13)$$

$$I_2 = \int \frac{d^3k}{(2\pi)^3} (-i\vec{k}\cdot\vec{R}) n_{\vec{k}} = \int_0^\infty \frac{dk}{(2\pi)^3} (-ikR) n_k \int_0^\pi d\phi \underbrace{\int_{-1}^1 d(\cos\theta) \cos\theta}_{1/2 - 1/2 = 0} = 0 \quad (S.14)$$

where we defined  $R = |\vec{R}|$ ,  $k = |\vec{k}|$  and we used  $\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 k^2}{2m} = \epsilon_k$ ,  $n_{\vec{k}} = n_k$ , and

$$\begin{aligned} I_3 &= \iiint \frac{d^3k}{(2\pi)^3} \frac{-(\vec{k}\cdot\vec{R})^2 n_{\vec{k}}}{2} = \int_0^\infty \frac{dk}{(2\pi)^3} \frac{-k^2 R^2 n_k}{2} \int_0^\pi d\phi \underbrace{\int_{-1}^1 d(\cos\theta) \cos^2\theta}_{1/3 + 1/3 = 2/3} \\ &= -\frac{R^2}{6} \int_0^\infty \frac{dk}{(2\pi)^3} k^2 n_k \int_0^\pi d\phi \underbrace{\int_{-1}^1 d(\cos\theta)}_{1+1=2} = -\frac{R^2}{6} \frac{\iiint \frac{d^3k}{(2\pi)^3} k^2 n_{\vec{k}}}{\iiint \frac{d^3k}{(2\pi)^3} n_{\vec{k}}} \iiint \frac{d^3k}{(2\pi)^3} n_{\vec{k}} \\ &= -n \frac{R^2}{6} \langle k^2 \rangle. \end{aligned} \quad (S.15)$$

Therefore  $g(\vec{R}) \approx n \left( 1 - \frac{\vec{R}^2}{6} \langle k^2 \rangle \right)$ .

(b) Study  $\langle k^2 \rangle$  in the low and high temperature limits and derive the correlation function  $g(\vec{R})$  in these limits. Express the result in terms of the thermal wave length  $\lambda = \sqrt{\frac{\hbar^2}{2\pi m k_B T}}$ .

*Hint.*  $\int_0^\infty dx x^{2n} e^{-ax^2} = \sqrt{\frac{\pi}{a}} \frac{1 \cdot 3 \cdots (2n-1)}{a^n 2^{n+1}} \quad \forall a \in \mathbb{R}_+, n \in \mathbb{N}.$

*Hint.*  $\zeta(x)\Gamma(x) = \int_0^\infty du \frac{u^{x-1}}{e^u - 1} \quad \forall x > 1.$

**Solution.** Using the thermal wavelength we have  $\beta\epsilon_{\vec{k}} = \frac{1}{4\pi} \frac{h^2 \vec{k}^2}{2\pi m k_B T} = \frac{\lambda^2 \vec{k}^2}{4\pi}$ . We define also the fugacity  $z = e^{\beta\mu}$ .

**Variant 1**

By symmetry

$$\langle \vec{k}^2 \rangle = \langle k_x^2 + k_y^2 + k_z^2 \rangle = 3 \langle k_z^2 \rangle. \quad (\text{S.16})$$

For the high temperature limit we have  $n_{\vec{k}} = \frac{1}{e^{\beta(\epsilon_{\vec{k}} - \mu)} - 1} \approx e^{-\beta(\epsilon_{\vec{k}} - \mu)}$ . Therefore

$$\begin{aligned} n \langle k_z^2 \rangle &\approx \iiint \frac{d^3 k}{(2\pi)^3} k_z^2 e^{-\beta(\epsilon_{\vec{k}} - \mu)} = \iint \frac{dk_x dk_y}{(2\pi)^3} \int_{-\infty}^{\infty} k_z^2 e^{-\frac{\lambda^2}{4\pi}(k_x^2 + k_y^2 + k_z^2) + \beta\mu} \\ &= \frac{1}{2} \frac{4\pi}{\lambda^2} \iint \frac{dk_x dk_y}{(2\pi)^3} \int_{-\infty}^{\infty} e^{-\frac{\lambda^2}{4\pi}(k_x^2 + k_y^2 + k_z^2) + \beta\mu} = \frac{2\pi}{\lambda^2} \iiint \frac{d^3 k}{(2\pi)^3} e^{-\beta(\epsilon_{\vec{k}} - \mu)} \\ &= \frac{2\pi}{\lambda^2} \iiint \frac{d^3 k}{(2\pi)^3} n_{\vec{k}} = \frac{2\pi}{\lambda^2} n, \end{aligned} \quad (\text{S.17})$$

where using the hint we conclude that  $\int_{-\infty}^{\infty} dx x^2 e^{-ax^2} = \frac{1}{2a} \int_{-\infty}^{\infty} dx e^{-ax^2}$ .

Therefore  $\langle \vec{k}^2 \rangle = \frac{6\pi}{\lambda^2}$ .

**Variant 2**

$$\langle k_z^2 \rangle = \frac{\iiint \frac{d^3 k}{(2\pi)^3} \vec{k}^2 n_{\vec{k}}}{\iiint \frac{d^3 k}{(2\pi)^3} n_{\vec{k}}} = \frac{4\pi \int_0^{\infty} dk k^4 n_k}{4\pi \int_0^{\infty} dk k^2 n_k} = \frac{G_4}{G_2}, \quad (\text{S.18})$$

where  $G_s = \int_0^{\infty} dk k^s n_k$ .

It is convenient to write  $G_s$  as

$$\begin{aligned} G_s &= \int_0^{\infty} dk k^s n_k = \int_0^{\infty} dk k^s \frac{1}{z^{-1} e^{\frac{\lambda^2 k^2}{4\pi}} - 1} = \int_0^{\infty} dy y^s \left( \frac{\sqrt{4\pi}}{\lambda} \right)^{s+1} \frac{1}{z^{-1} e^{y^2} - 1} \\ &= \left( \frac{\sqrt{4\pi}}{\lambda} \right)^{s+1} \int_0^{\infty} \frac{dx}{2} \frac{x^{\frac{s+1}{2}-1}}{z^{-1} e^x - 1} =: \left( \frac{\sqrt{4\pi}}{\lambda} \right)^{s+1} F_s(z). \end{aligned} \quad (\text{S.19})$$

For high temperature we could expand as

$$G_s = \left( \frac{\sqrt{4\pi}}{\lambda} \right)^{s+1} z \int_0^{\infty} dy \frac{y^s e^{-y^2}}{1 - ze^{-y^2}} = \left( \frac{\sqrt{4\pi}}{\lambda} \right)^{s+1} z \int_0^{\infty} dy y^s e^{-y^2} \left( 1 + ze^{-y^2} + (ze^{-y^2})^2 + \dots \right), \quad (\text{S.20})$$

where  $y = k \frac{\lambda}{\sqrt{4\pi}}$ ,  $x = y^2$ . Replacing this into (S.18) we have:

$$\begin{aligned} \langle k_z^2 \rangle &= \frac{4\pi F_4(z)}{\lambda^2 F_2(z)} = \frac{4\pi \int_0^{\infty} dy y^4 e^{-y^2} (1 + ze^{-y^2} + (ze^{-y^2})^2 + \dots)}{\lambda^2 \int_0^{\infty} dy y^2 e^{-y^2} (1 + ze^{-y^2} + (ze^{-y^2})^2 + \dots)} = \begin{cases} \frac{4\pi}{\lambda^2} \frac{\Gamma(5/2)\zeta(5/2)}{\Gamma(3/2)\zeta(3/2)} & \text{if } T \rightarrow 0 \\ \frac{4\pi}{\lambda^2} \frac{3}{2} & \text{if } T \rightarrow \infty \end{cases} \\ &= \begin{cases} \frac{4\pi}{\lambda^2} \frac{3\zeta(5/2)}{2\zeta(3/2)} & \text{if } T \rightarrow 0 \\ \frac{6\pi}{\lambda^2} & \text{if } T \rightarrow \infty \end{cases} = \begin{cases} \approx \frac{3\pi}{\lambda^2} & \text{if } T \rightarrow 0 \\ \frac{6\pi}{\lambda^2} & \text{if } T \rightarrow \infty \end{cases} \end{aligned} \quad (\text{S.21})$$

where we used that  $z \rightarrow 1$  for  $T \rightarrow 0$ ,  $\frac{\zeta(5/2)}{\zeta(3/2)} \approx 0.5$  and for high temperature we keep only first term in the expansion.

However, studying numerically  $F_4$  and  $F_2$  we could see that they are not so different (see Fig 1), therefore we could simply approximate  $\langle k_z^2 \rangle \approx \frac{4\pi}{\lambda^2}$ .

From (a) and the previous result we have

$$g(\vec{R}) \approx n \left( 1 - \frac{\vec{R}^2}{6} \langle \vec{k}^2 \rangle \right) \approx \begin{cases} n \left( 1 - \frac{\vec{R}^2}{2} \frac{\pi}{\lambda^2} \right) & \text{if } T \rightarrow 0 \\ n \left( 1 - \vec{R}^2 \frac{\pi}{\lambda^2} \right) & \text{if } T \rightarrow \infty \\ n \left( 1 - \frac{2\vec{R}^2}{3} \frac{\pi}{\lambda^2} \right) & \text{if } T \text{ in-between} \end{cases}. \quad (\text{S.22})$$

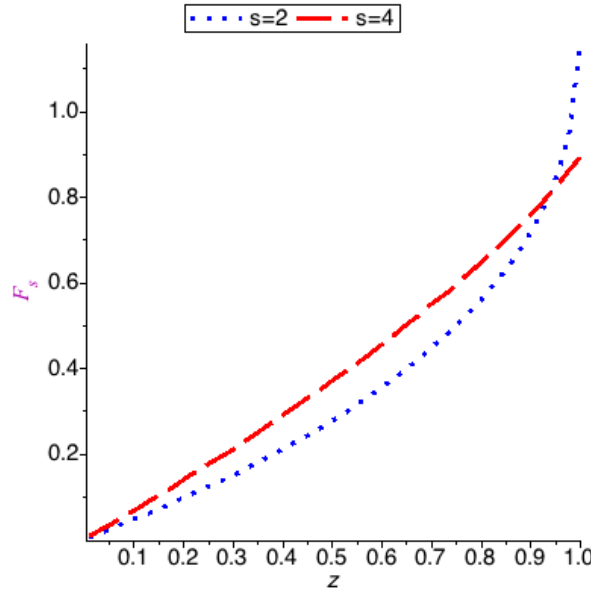


Figure 1:  $F_4$  and  $F_2$  as a function of  $z$ .

- (c) How would you modify the previous result for the correlation function to describe the Bose-Einstein condensate regime, too?

**Solution.** The total density  $n = n_0 + n_n$  is the sum of the macroscopic occupation at  $\vec{k} = 0$  and the remaining one. The previous treatment is valid for the  $n_n$  part of the density. Therefore we have:

$$g(\vec{R}) = n_0 + n_n \frac{g(\vec{R})}{n} . \quad (\text{S.23})$$

The normalization stays the same:  $g(\vec{R}) \rightarrow \frac{g(\vec{R})}{n}$ .

**Exercise 1. Exact solution of the Ising chain**

In this exercise we will investigate the physics of one of the few *exactly solvable interacting* models, the one-dimensional Ising model (Ising chain). Consider a chain of  $N + 1$  Ising-spins with free ends and nearest neighbor coupling  $-J$  ( $J > 0$  for ferromagnetic coupling)

$$\mathcal{H}_{N+1} = -J \sum_{i=1}^N \sigma_i \sigma_{i+1}, \quad \sigma_i = \pm 1. \quad (1)$$

In this exercise we will be interested in the thermodynamic limit of this system, i.e. we assume  $N$  to be very large.

- Compute the partition function  $Z_{N+1}$  using a recursive procedure.
- Find expressions for the free energy and entropy, as well as for the internal energy and heat capacity. Compare your results to the ideal paramagnet.
- Calculate the magnetization density  $m = \langle \sigma_j \rangle$  where the spin  $\sigma_j$  is far away from the ends. Which symmetries does the system exhibit? Interpret your result in terms of symmetry arguments.
- Show that the *spin correlation function*  $\Gamma_{ij} = \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle$  decays exponentially with increasing distance  $|j - i|$  on the scale of the so-called *correlation length*  $\xi$ , i.e.  $\Gamma_{ij} \sim e^{-|j-i|/\xi}$ . Show that  $\xi = -[\log(\tanh \beta J)]^{-1}$  and interpret your result in the limit  $T \rightarrow 0$ .
- Calculate the magnetic susceptibility in zero magnetic field using the fluctuation-dissipation relation of the form

$$\frac{\chi(T)}{N} = \frac{1}{k_B T} \sum_{j=-N/2}^{N/2} \Gamma_{0j}, \quad (2)$$

in the thermodynamic limit,  $N \rightarrow \infty$ . For simplicity we assume  $N$  to be even. Note that  $\chi(T)$  is defined to be extensive, such that we obtain the intensive quantity by normalization with  $N$ .

- Approximate  $1/\chi(T)$  up to first order in  $2\beta J$  in the high-temperature limit ( $\beta \rightarrow 0$ ). Use this result to calculate the *Weiss temperature*  $\Theta_W$ , which is defined by  $1/\chi(\Theta_W) = 0$ .

**Solution.**

- We can split off the last spin in the Hamiltonian as follows:

$$\mathcal{H}_{N+1} = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} - J \sigma_N \sigma_{N+1} \quad (S.1)$$

$$= \mathcal{H}_N - J \sigma_N \sigma_{N+1}. \quad (S.2)$$

Notice that  $\mathcal{H}_N$  now describes an identical system with one less spin, i.e. spin  $N$  is now the last on the chain. The Hamiltonian  $\mathcal{H}_N$  no longer depends on  $\sigma_{N+1}$ , and we therefore write the partition function as:

$$Z_{N+1} = \sum_{\{\sigma_i = \pm 1\}} \left[ e^{-\beta \mathcal{H}_N} \sum_{\sigma_{N+1} = \pm 1} e^{\beta J \sigma_N \sigma_{N+1}} \right] \quad (S.3)$$

$$= \sum_{\{\sigma_i = \pm 1\}} e^{-\beta \mathcal{H}_N} \left( 2 \cosh(\beta J \sigma_N) \right) \quad (S.4)$$

We can now repeat<sup>1</sup> splitting off the last spin  $\sigma_N$  to obtain

$$Z_{N+1} = \sum_{\{\sigma_i=\pm 1\}} e^{-\beta\mathcal{H}_{N-1}} \sum_{\sigma_N=\pm 1} e^{\beta J\sigma_{N-1}\sigma_N} \left( 2 \cosh(\beta J\sigma_N) \right) \quad (\text{S.7})$$

$$= \left( 2 \cosh \beta J \right) \sum_{\{\sigma_i=\pm 1\}} \left[ e^{-\beta\mathcal{H}_{N-1}} \left( 2 \cosh(\beta J\sigma_{N-1}) \right) \right], \quad (\text{S.8})$$

where we have used the fact that  $\cosh(x)$  is an even function. Continuing this sum, one finds

$$Z_{N+1} = \left( 2 \cosh \beta J \right)^{N-2} \sum_{\sigma_1, \sigma_2=\pm 1} e^{\beta J\sigma_1\sigma_2} \left( 2 \cosh(\beta J\sigma_2) \right) \quad (\text{S.9})$$

$$= \left( 2 \cosh \beta J \right)^{N-1} \sum_{\sigma_1=\pm 1} \left( 2 \cosh(\beta J\sigma_1) \right) \quad (\text{S.10})$$

$$= 2 \left( 2 \cosh \beta J \right)^N \quad (\text{S.11})$$

The same result can be obtained by mapping the problem to a *non-interacting* Ising paramagnet. The quantity  $S_i = \sigma_i\sigma_{i+1}$  might be viewed as a new *pseudo-spin* for which the Hamiltonian reads

$$\mathcal{H} = -J \sum_{i=1}^N S_i \quad (\text{S.12})$$

The partition sum of the system of  $N$  pseudo-spins (instead of  $N+1$  real spins  $\sigma$ ) is

$$Z = \left( 2 \cosh \beta J \right)^N \quad (\text{S.13})$$

The additional factor 2 appearing in Eqs. (S.6) and (S.11) comes from the fact that the mapping from the spin system to pseudo-spins is not unique but two-fold; inverting all real spins  $\sigma_i \rightarrow -\sigma_i$  produced the same state in pseudo-spin space.

- (b) The energy, entropy and response functions follow directly from the partition function  $Z_{N+1}$  as follows:

The free energy is given by

$$F = -k_B T \ln(Z_{N+1}) = -k_B T(N+1) \ln(2) - N k_B T \ln \left[ \cosh(\beta J) \right],$$

from which we can compute the entropy as

$$S = - \left( \frac{\partial F}{\partial T} \right) = k_B \left[ (N+1) \ln(2) + N \ln \left[ \cosh(\beta J) \right] - N \beta J \tanh(\beta J) \right].$$

Next, the internal energy can be found via

$$\begin{aligned} U &= - \frac{\partial}{\partial \beta} \ln(Z_{N+1}) \\ &= -N \frac{\partial}{\partial \beta} \ln \left[ \cosh(\beta J) \right] \\ &= -N J \tanh(\beta J). \end{aligned}$$

Then the heat capacity can be found through computing

$$C = T \frac{\partial S}{\partial T} = -T \frac{\partial^2 F}{\partial T^2}$$

---

<sup>1</sup>Alternatively, notice that the term  $\sigma_N\sigma_{N+1}$  is always equal to  $\pm 1$ , independent of the value of  $\sigma_N$ . Hence it will always evaluate to  $2 \cosh(\beta J)$ . This means we get:

$$Z_{N+1} = \underbrace{\sum_{\{\sigma_i=\pm 1\}} \exp(-\beta\mathcal{H}_N)}_{=Z_N} 2 \cosh \beta J \quad (\text{S.5})$$

$$= Z_2 (2 \cosh \beta J)^{N-1} = 2 (2 \cosh \beta J)^N. \quad (\text{S.6})$$

In the last line we used that  $Z_2 = \sum_{\{\sigma_1, \sigma_2\}} \exp(\beta J\sigma_1\sigma_2) = 4 \cosh \beta J$ .

or

$$C = \left( \frac{\partial U}{\partial T} \right).$$

Both evaluate to

$$C = Nk_B \frac{(\beta J)^2}{\cosh^2(\beta J)}.$$

The heat capacity (see figure 1) shows no dependence on the sign of  $J$ , and is therefore identical for either a ferromagnet ( $J < 0$ ) or an antiferromagnet ( $J > 0$ ).

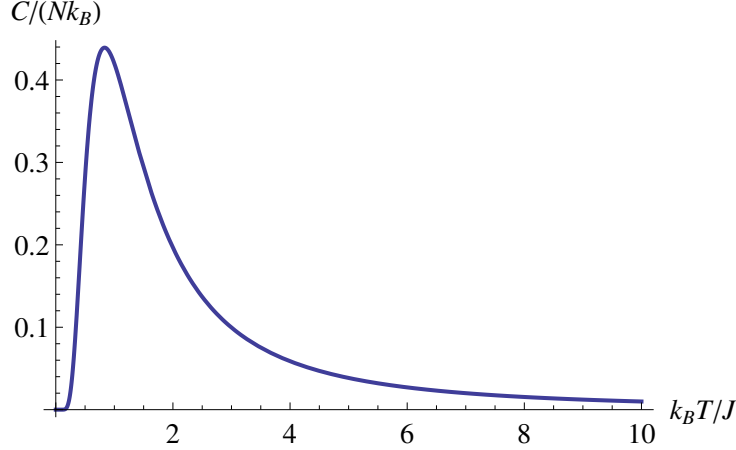


Figure 1: Heat capacity of the Ising chain.

Comparing the results to the ideal paramagnet (see script or exercise set 6), one sees that if we there is an exact correspondence if we let  $J = Hm$  (where  $H$  is the external field, and  $m$  is the magnetization of the paramagnet). Based on the mapping of this model to a non-interacting Ising paramagnet mentioned in part a), this was to be expected. Conversely, one may realize the possibility of this mapping given these identical results.

- (c) The magnetization density can be computed in a similar way:

$$\begin{aligned} \langle \sigma_j \rangle &= \frac{1}{Z_{N+1}} \sum_{\{\sigma_i = \pm 1\}} \sum_{\sigma_{N+1} = \pm 1} \sigma_j \exp \left( \beta J \sum_i \sigma_i \sigma_{i+1} \right) \\ &= \frac{(2 \cosh \beta J)^{N+1-j}}{Z_{N+1}} \sum_{\sigma_1 = \pm 1} \dots \sum_{\sigma_j = \pm 1} \sigma_j \exp \left( \beta J \sum_{k=1}^{j-1} \sigma_k \sigma_{k+1} \right) \\ &= \frac{(2 \cosh \beta J)^{N+1-j}}{Z_{N+1}} \sum_{\sigma_1 = \pm 1} \dots \sum_{\sigma_{j-1} = \pm 1} \exp \left( \beta J \sum_{k=1}^{j-2} \sigma_k \sigma_{k+1} \right) \underbrace{\sum_{\sigma_j = \pm 1} \sigma_j e^{\beta J \sigma_{j-1} \sigma_j}}_{\sigma_{j-1} (2 \sinh \beta J)} \\ &= \frac{(2 \cosh \beta J)^{N+1-j} (2 \sinh \beta J)^{j-2}}{Z_{N+1}} \underbrace{\sum_{\sigma_1 = \pm 1} \sum_{\sigma_2 = \pm 1} \sigma_2 \exp(\beta J \sigma_1 \sigma_2)}_{=0} = 0. \end{aligned}$$

This result can easily be interpreted in terms of symmetry. The Hamiltonian (1) on the exercise sheet is invariant under time-reversal, i.e.  $\sigma_i \mapsto -\sigma_i, \forall i \in \{1, \dots, N+1\}$ . Therefore, a finite magnetization, which breaks time-reversal invariance, cannot be found by means of analyzing the partition function (a weighted sum over all states respecting the symmetries of the system).

One could also have obtained this result by considering only the terms involved with spin  $\sigma_j$ .

- (d) Due to a vanishing magnetization  $\langle \sigma_i \rangle = 0$ , the spin correlation function simplifies to  $\Gamma_{ij} = \langle \sigma_i \sigma_j \rangle$ . We assume  $j > i$ . We will use a trick, namely to assume bond-dependent exchange constants  $J_k$ . In the end of the calculation  $J_k$  will be set to  $J$ . A generalization of a) leads to

$$Z_{N+1} = 2 \prod_{k=1}^N (2 \cosh \beta J_k), \quad (\text{S.14})$$

while, using the property  $\sigma_k^2 = 1$ , the correlation function reads

$$\langle \sigma_i \sigma_j \rangle = \frac{1}{Z_{N+1}} \sum_{\{\sigma_k = \pm 1\}} (\sigma_i \sigma_{i+1}) (\sigma_{i+1} \sigma_{i+2}) \dots (\sigma_{j-1} \sigma_j) \exp \left( \sum_l \beta J_l \sigma_l \sigma_{l+1} \right) \quad (\text{S.15})$$

$$= \frac{1}{Z_{N+1}} \frac{1}{\beta^{j-i}} \left. \frac{\partial^{j-i} Z_{N+1}}{\partial J_i \dots \partial J_{j-1}} \right|_{J_k = J} = (\tanh \beta J)^{|j-i|} = e^{-|j-i|/\xi} \quad (\text{S.16})$$

where the correlation length is

$$\xi = -[\log(\tanh \beta J)]^{-1} > 0.$$

In the limit  $T \rightarrow 0$ ,  $\xi$  diverges. This is an universal feature of systems undergoing a continuous phase transition.

(e) Using the result of d) we find

$$\sum_{j=-\infty}^{\infty} \langle \sigma_0 \sigma_j \rangle = \sum_{j=-\infty}^{\infty} (\tanh \beta J)^{|j|} = \frac{1 + \tanh \beta J}{1 - \tanh \beta J} = \exp(2\beta J). \quad (\text{S.17})$$

For the magnetic susceptibility at zero field we therefore find

$$\chi(T) = N \frac{e^{2J/k_B T}}{k_B T} \quad (\text{S.18})$$

which in the ferromagnetic case ( $J > 0$ ) diverges for  $T \rightarrow 0$  indicating that at low temperatures only an infinitesimal field is needed to produce saturation magnetization.

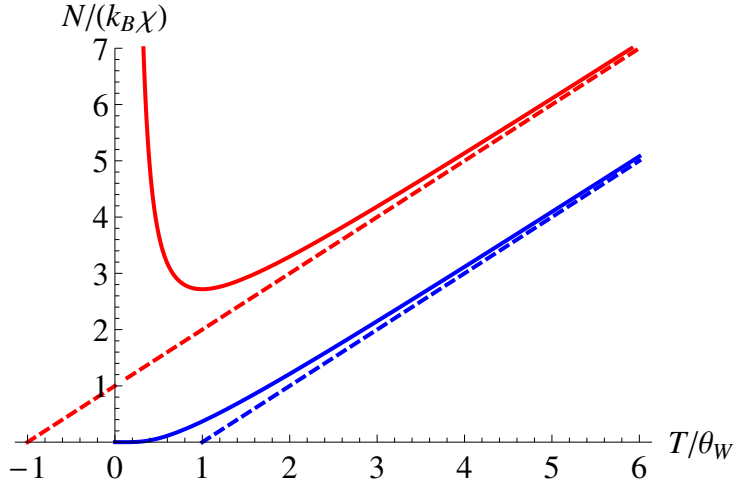


Figure 2: Inverse susceptibility (continuous line) with high-temperature extrapolation for the Weiss temperature (dashed line) for ferromagnetic coupling,  $J > 0$  (blue), and antiferromagnetic coupling,  $J < 0$  (red).

(f) Using the result from part (e), we write

$$\frac{1}{\chi(T)} = \frac{k_B T}{N} e^{-2\beta J} \quad (\text{S.19})$$

$$= \frac{k_B T}{N} [1 - 2\beta J + \mathcal{O}((2\beta J)^2)] \quad (\text{S.20})$$

$$\approx \frac{k_B}{N} \left( T - \underbrace{\frac{2J}{k_B}}_{=\Theta_W} \right). \quad (\text{S.21})$$

The Weiss temperature  $\Theta_W = 2J/k_B$  can be found by extrapolating the inverse susceptibility to low temperatures and finding the intersection with the temperature axis. It provides a possibility to determine the sign and the magnitude of the coupling  $J$  between neighboring spins. Refer to section 4.1.3 in the lecture notes for further details.

The full solution as well as the linear high-temperature approximation with an extrapolation for the Weiss temperature are shown in figure 2.



**Exercise 1. Ising Model: Variational Approach vs. Mean Field.**

Consider an Ising lattice in  $d$  dimensions, where each of the  $N$  spins takes values  $s_i = \pm s$  and has  $z$  nearest neighbors. In the presence of an external magnetic field  $H$ , the Hamiltonian is

$$\mathcal{H} = -J \sum_{\langle s_i, s_j \rangle} s_i s_j - \sum s_i H . \quad (1)$$

Let us also define the average magnetization of a spin as  $s \tilde{m} = M/N = s(N_+ - N_-)/N$ .

- (a) Calculate the configurational entropy of the system (or remember that we already did that in Exercise Sheet 1). Determine the internal energy by taking the average value of the Hamiltonian, by making the approximation that each of the spins  $s_i$  independently takes the value  $\pm 1$  with probability  $w_{\pm} = \frac{1}{2}(1 \pm \tilde{m})$ . Write your answers in terms of  $\tilde{m}$ .

*Hint.* If  $s_i$  and  $s_j$  are independent, their expectation factorizes:  $\langle s_i s_j \rangle = \langle s_i \rangle \langle s_j \rangle$ .

**Solution.** We calculated in Exercise Sheet 1 the entropy of the system by counting its possible configurations. In terms of  $n = N_+ - N_-$ , the entropy is given by

$$S(n) = \frac{1}{2} N k_B \left[ 2 \ln 2 - \left(1 + \frac{n}{N}\right) \ln \left(1 + \frac{n}{N}\right) - \left(1 - \frac{n}{N}\right) \ln \left(1 - \frac{n}{N}\right) \right] , \quad (S.1)$$

and with the average magnetization per spin,

$$S(\tilde{m}) = \frac{1}{2} N k_B [2 \ln 2 - (1 + \tilde{m}) \ln (1 + \tilde{m}) - (1 - \tilde{m}) \ln (1 - \tilde{m})] , \quad (S.2)$$

Now, each spin is  $\pm s$  with probability  $w_{\pm}$ , such that

$$\langle s_i \rangle = (-s) \cdot w_- + s \cdot w_+ = s(w_+ - w_-) = s \tilde{m} . \quad (S.3)$$

We thus have for the internal energy,

$$U = -J \sum_{\langle i, j \rangle} \langle s_i s_j \rangle - H \sum \langle s_i \rangle = -J \sum_{\langle i, j \rangle} \langle s_i \rangle \langle s_j \rangle - H \sum \langle s_i \rangle = -J \frac{Nz}{2} s^2 \tilde{m}^2 - H N s \tilde{m} , \quad (S.4)$$

where the number of bonds are calculated as  $z$  bonds per particle,  $N$  times, and correcting for the double counting of each bond by dividing by 2.

- (b) Determine the free energy of the system using the formula  $F = U - TS$ . Which variational principle determines the magnetization of the system? Derive the corresponding equation. Compare with (5.21) in the lecture notes, which was obtained with the mean field approximation.

**Solution.** The free energy is simply

$$\begin{aligned} F(\tilde{m}) &= U - TS \\ &= -J \frac{Nz}{2} s^2 \tilde{m}^2 - H N s \tilde{m} - \frac{1}{2} N k_B T [2 \ln 2 - (1 + \tilde{m}) \ln (1 + \tilde{m}) - (1 - \tilde{m}) \ln (1 - \tilde{m})] \end{aligned} \quad (S.5)$$

To find the magnetization that the system will spontaneously adopt, we have to minimize the free energy. Differentiation by  $\tilde{m}$  gives

$$\begin{aligned} 0 &\stackrel{!}{=} \frac{\partial F}{\partial \tilde{m}} = -J N z s^2 \tilde{m} - H N s - \frac{1}{2} N k_B T [ -(\ln(1 + \tilde{m}) + 1) - (-\ln(1 - \tilde{m}) - 1) ] \\ &= -J N z s^2 \tilde{m} - H N s + \frac{1}{2} N k_B T \ln \frac{1 + \tilde{m}}{1 - \tilde{m}} , \end{aligned}$$

thus obtaining

$$Jzs^2\tilde{m} + Hs = \frac{1}{2}k_B T \ln \frac{1 + \tilde{m}}{1 - \tilde{m}}, \quad (\text{S.6})$$

which can be expressed in terms of the effective magnetic field  $h_{\text{eff}} = Jzs\tilde{m} + H$  as

$$\frac{sh_{\text{eff}}}{k_B T} = \frac{1}{2} \ln \frac{1 + \tilde{m}}{1 - \tilde{m}}.$$

We can reorder this equation as

$$1 + \tilde{m} = \exp[2\beta sh_{\text{eff}}] (1 - \tilde{m}),$$

thus

$$\tilde{m} \left( 1 + e^{2\beta sh_{\text{eff}}} \right) = e^{2\beta sh_{\text{eff}}} - 1,$$

from which we deduce

$$\tilde{m} = \tanh[\beta sh_{\text{eff}}] = \tanh\left(\frac{Jzs^2\tilde{m} + Hs}{k_B T}\right). \quad (\text{S.7})$$

Equation (S.7) is exactly the same as the one obtained in the mean field approximation, cf. (5.21) in the lecture notes.

### Exercise 2. *Ising Model: Infinite-Range Forces and Mean Field.*

Consider an Ising model where now *all* spins interact between each other with the same strength  $J = 1/N$  (long-range forces). The Hamiltonian is given by

$$\mathcal{H} = -\frac{1}{2N} \sum_{i,k} s_i s_k - H \sum_i s_i. \quad (2)$$

The coupling constant is rescaled by  $N$  so that the total energy remains finite; also the factor one-half compensates the fact that in the sum, each index  $i$  and  $k$  ranges independently from 1 to  $N$ , and thus we counted each bond twice.

In this exercise, we'll show that the mean-field approach for this model is exact (at least for  $N \rightarrow \infty$ ).

- (a) In order to calculate the partition function for this model, we will introduce a little mathematical trick. Show that the Boltzmann factor which appears in the partition function can be written as

$$e^{-\beta\mathcal{H}} = \sqrt{\frac{N\beta}{2\pi}} \int_{-\infty}^{\infty} d\lambda \exp\left(-\frac{N\beta\lambda^2}{2} + \sum_i \beta(\lambda + H) s_i\right). \quad (3)$$

This is a particular case of the Gaussian transform method which will be seen in the lecture.

*Hint.* You should know the Gaussian integral by heart by now, but just in case:  $\int dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}$ .

**Solution.** To show that the Boltzmann term can be written as in Equation (3), one can first complete the square in the exponent (introducing  $M = \sum s_i$ ),

$$\begin{aligned} -\frac{N\beta\lambda^2}{2} + \sum_i \beta(\lambda + H)s_i &= -\frac{N\beta\lambda^2}{2} + \beta\lambda M + \beta HM = -\frac{N\beta}{2} \left[ \lambda^2 - \frac{2M}{N}\lambda - \frac{2HM}{N} \right] \\ &= -\frac{N\beta}{2} \left[ \left( \lambda - \frac{M}{N} \right)^2 - \frac{M^2}{N^2} - \frac{2HM}{N} \right] = -\frac{N\beta}{2} \left( \lambda - \frac{M}{N} \right)^2 + \frac{\beta M^2}{2N} + \beta HM \\ &= -\frac{N\beta}{2} \left( \lambda - \frac{M}{N} \right)^2 - \beta \mathcal{H} , \end{aligned}$$

where we have used that

$$\mathcal{H} = -\frac{M^2}{2N} - HM .$$

This allows us to compute the Gaussian integral in (3) as

$$\begin{aligned} \sqrt{\frac{N\beta}{2\pi}} \int d\lambda \exp \left( -\frac{N\beta\lambda^2}{2} + \sum_i \beta(\lambda + H)s_i \right) \\ = \sqrt{\frac{N\beta}{2\pi}} \int d\lambda \exp \left( -\frac{N\beta}{2} \left( \lambda - \frac{M}{N} \right)^2 \right) \exp(-\beta\mathcal{H}) = \sqrt{\frac{N\beta}{2\pi}} \sqrt{\frac{2\pi}{N\beta}} e^{-\beta\mathcal{H}} = e^{-\beta\mathcal{H}} . \end{aligned}$$

(b) Show that the partition function can be written as

$$Z = \sqrt{\frac{N\beta}{2\pi}} \int d\lambda e^{-N\beta A(\lambda)} , \quad A(\lambda) = \frac{\lambda^2}{2} - \frac{1}{\beta} \ln(2 \cosh[\beta(\lambda + H)]) \quad (4)$$

**Solution.** Let's calculate the partition function:

$$\begin{aligned} Z = \sum_{\text{configurations}} e^{-\beta\mathcal{H}} &= \sum \sqrt{\frac{N\beta}{2\pi}} \int d\lambda \exp \left\{ -\frac{N\beta\lambda^2}{2} + \sum_i \beta(\lambda + H)s_i \right\} \\ &= \sqrt{\frac{N\beta}{2\pi}} \int d\lambda e^{-\frac{N\beta\lambda^2}{2}} \sum e^{\beta \sum (\lambda + H)s_i} . \quad (\text{S.8}) \end{aligned}$$

We recognize the last sum as the partition function of an Ising paramagnet with noninteracting spins in a magnetic field  $\lambda + H$ . As a reminder:

$$\sum_{\{s_i\}} e^{\beta \sum_i (\lambda + H)s_i} = \sum_{\{s_i\}} \prod_i e^{\beta(\lambda + H)s_i} = \left( \sum_{s=\pm 1} e^{\beta(\lambda + H)s} \right)^N = (2 \cosh[\beta(\lambda + H)])^N ,$$

so that we eventually get from (S.8),

$$(\text{S.8}) = \sqrt{\frac{N\beta}{2\pi}} \int d\lambda e^{-\frac{N\beta\lambda^2}{2}} (2 \cosh[\beta(\lambda + H)])^N = \sqrt{\frac{N\beta}{2\pi}} \int d\lambda e^{-N\beta A(\lambda)} ,$$

where we now have defined

$$A(\lambda) = \frac{\lambda^2}{2} - \frac{1}{\beta} \ln(2 \cosh[\beta(\lambda + H)]) .$$

In order to determine the partition function, we will use the steepest descent method (a.k.a. Laplace method or saddle point approximation): the integral of the exponential is dominated by the maximum of the function in the exponential. Technically this is done by expanding the function in the exponent to second order at its maximum, and neglecting further orders.

- (c) Determine the equation that  $\lambda$  should satisfy in order for it to be the maximum of the argument of the exponential.

Show that the partition function can be written (for large  $N$ ) as

$$Z \approx e^{-N\beta f} ; \quad f = A(\lambda_0) + \frac{1}{2N\beta} \ln A''(\lambda_0) \approx A(\lambda_0) , \quad (5)$$

where  $f$  is the free energy per spin and  $\lambda_0$  is the minimum of the function  $A(\lambda)$ .

Show that  $\lambda_0$  is precisely the average magnetization of a spin,  $\lambda_0 = \langle s_i \rangle =: m$ . Deduce that your result coincides with the magnetization that you would get via mean field theory.

*Hint.* The average magnetization per spin can be obtained via the free energy per spin,  $m = -\frac{\partial f}{\partial H}$ .

**Solution.** In order to apply Laplace's method to the calculation of the partition function (4), we first need to determine the maximum of the argument of the exponential in the integral. This corresponds to finding the minimum of the function  $A(\lambda)$ . The condition of the minimum is

$$\frac{\partial A}{\partial \lambda} = 0 . \quad (S.9)$$

Differentiating the expression of  $A(\lambda)$  given by (4),

$$A'(\lambda) := \frac{\partial A}{\partial \lambda} = \lambda - \left\{ \frac{1}{\beta} \frac{1}{2 \cosh[\beta(\lambda + H)]} \times 2 \sinh[\beta(\lambda + H)] \times \beta \right\} = \lambda - \tanh[\beta(\lambda + H)] .$$

Thus the minimum condition (S.9) for  $A(\lambda)$  is simply

$$\lambda = \tanh[\beta(\lambda + H)] . \quad (S.10)$$

We can now apply Laplace's method to approximate the partition function, by expanding the argument of the exponential to second order and neglecting further orders. Of course the first order is zero because the expansion is done at a stationary point. Let  $\lambda_0$  be the minimum, satisfying Eq. (S.10).

$$Z \approx \sqrt{\frac{N\beta}{2\pi}} \int d\lambda e^{-N\beta A(\lambda_0) - \frac{N\beta}{2} A''(\lambda_0)(\lambda - \lambda_0)^2} = \sqrt{\frac{N\beta}{2\pi}} e^{-N\beta A(\lambda_0)} \sqrt{\frac{2\pi}{N\beta A''(\lambda_0)}} = \frac{e^{-N\beta A(\lambda_0)}}{\sqrt{A''(\lambda_0)}} = e^{-N\beta f} ,$$

where the free energy per spin  $f = F/N$  is given by

$$f = A(\lambda_0) - \frac{1}{2N\beta} \ln A''(\lambda_0) \approx A(\lambda_0) .$$

Now the magnetization is given by

$$m = -\frac{\partial f}{\partial H} = -\frac{\partial A}{\partial H} - \frac{\partial A}{\partial \lambda} \frac{\partial \lambda_0}{\partial H} = -\frac{\partial A}{\partial H} , \quad (S.11)$$

recalling that  $\lambda_0$  also depends on  $H$ , but that  $\frac{\partial A}{\partial \lambda}$  vanishes at its minimum, killing the second term in the expression above. Differentiating  $A(\lambda)$  in (4) by  $H$ ,

$$\frac{\partial A}{\partial H} = -\frac{1}{\beta} \frac{1}{2 \cosh[\beta(\lambda + H)]} \times 2 \sinh[\beta(\lambda + H)] \times \beta = -\tanh[\beta(\lambda + H)] ,$$

which, at  $\lambda = \lambda_0$ , is in virtue of Eq. (S.10) simply

$$\left. \frac{\partial A}{\partial H} \right|_{\lambda_0} = -\tanh[\beta(\lambda_0 + H)] = -\lambda_0 .$$

This now means that the magnetization is

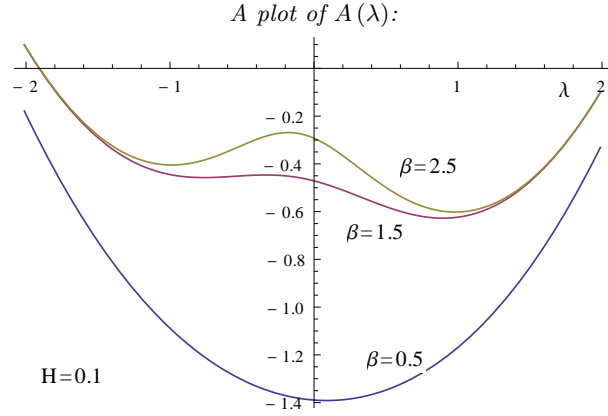
$$m = (S.11) = -\left. \frac{\partial A}{\partial H} \right|_{\lambda_0} = \lambda_0 . \quad (S.12)$$

Thus, the magnetization  $m$  obeys

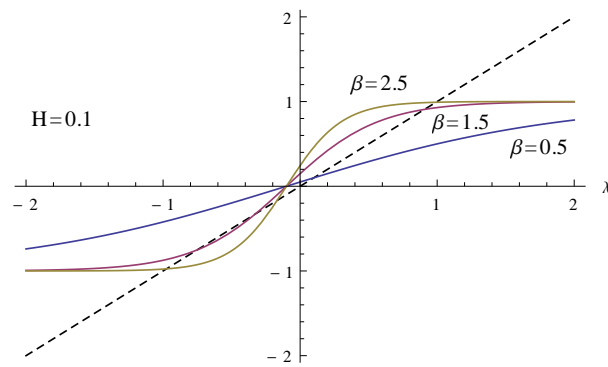
$$m = \tanh[\beta(m + H)] , \quad (S.13)$$

which is exactly the condition that mean field theory predicts. Indeed, mean field theory yields Equation (5.21) in the lecture notes, which for  $J = 1/N$  and  $z = N$  gives exactly (S.13).

*Note: when applying the Laplace method to calculate the partition function, the  $\lambda_0$  must be the global minimum of the function  $A(\lambda)$ . In general, the function will have one or two local minima, and if  $H \neq 0$ , one will be lower than the other (see Figure below). If the two are the same, the error done in the approximation for one of the minima is a factor 2, which is a constant in the free energy.*



The zeros of  $A(\lambda)$  can rather easily be found geometrically as the intersection of the lines  $y = \lambda$  and  $y = \tanh[\beta(\lambda + H)]$ :



**Exercise 1. Condensation and crystallization in the lattice gas model.**

The lattice gas model is obtained by dividing the volume  $V$  into microscopic cells which are assumed to be small such that they contain at most one gas molecule. The result is a square lattice in two dimensions and a cubic lattice in three dimensions. We neglect the kinetic energy of a molecule and assume that only nearest neighbors interact. The total energy is given by

$$H = -\lambda \sum_{\langle i,j \rangle} n_i n_j \quad (1)$$

where the sum runs over nearest-neighbor pairs and  $\lambda$  is the nearest-neighbor coupling. There is at most one particle in each cell ( $n_i = 0$  or  $1$ ). This model is a simplification of hard-core potentials, like the Lennard-Jones potential, characterized by an attractive interaction and a very short-range repulsive interaction that prevents particles from overlapping.

In order to study the case of a repulsive interaction,  $\lambda < 0$ , we divide the lattice into two alternating sublattices A and B. For square or cubic lattices, we find that all lattice sites A only have points in B as their nearest neighbors.

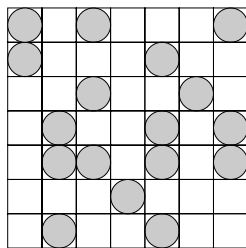


Figure 1: Schematic view of the lattice gas model.

- (a) First, show the equivalence of the grand canonical ensemble of the lattice gas model with the canonical ensemble of an Ising model in a magnetic field.

**Solution.** We consider the grand canonical Hamiltonian

$$H - \mu N = -\lambda \sum_{\langle i,j \rangle} n_i n_j - \mu \sum_i n_i. \quad (S.1)$$

By introducing Ising spins  $s_i$  through the relation

$$n_i = \frac{1}{2}(1 + s_i), \quad s_i = \pm 1, \quad (S.2)$$

we arrive at an Ising model

$$H - \mu N = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i - \left(h - \frac{\gamma}{2} J\right) N_L = H_I - \left(h - \frac{\gamma}{2} J\right) N_L \quad (S.3)$$

with

$$J = \frac{\lambda}{4}, \quad h = \frac{\lambda}{4} \gamma + \frac{\mu}{2}. \quad (S.4)$$

Here,  $\gamma$  denotes the coordination number (number of nearest neighbors) and  $N_L$  is the total number of lattice sites. The grand partition function  $\mathcal{Z} = \text{Tr}[\exp[-\beta(H - \mu N)]]$  of the lattice gas is thus related to the canonical partition function  $Z_I = \text{Tr}[\exp(-\beta H_I)]$  of the Ising model through

$$\mathcal{Z}_G = Z_I e^{\beta \left(\frac{\lambda}{8} \gamma + \frac{\mu}{2}\right) N_L} \quad (S.5)$$

with the relations (S.4) for the exchange coupling  $J$  and the magnetic field  $h$ .

- (b) Introduce two mean-field parameters  $m_A$  and  $m_B$  and adapt the mean-field solution of the Ising model discussed in Sec. 5.2 of the lecture notes for these two parameters. What are the self-consistency conditions for  $m_A$  and  $m_B$ ?

**Solution.** The Hamiltonian of the Ising model is

$$H_I = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_i s_i. \quad (\text{S.6})$$

We introduce the mean-field parameters  $m_A$  and  $m_B$ , which are defined as

$$m_A = \langle s_i \rangle_{i \in A}, \quad m_B = \langle s_j \rangle_{j \in B}. \quad (\text{S.7})$$

Now we can write for  $i \in A$

$$s_i = m_A + \delta_i := m_A + (s_i - m_A), \quad (\text{S.8})$$

where we assume  $\delta_i$  to be small. The case  $j \in B$  is analog.

Now we can expand the Hamiltonian

$$\begin{aligned} H_I &= -J \sum_{\langle i,j \rangle} (m_A + \delta_i)(m_B + \delta_j) - h \sum_i s_i \\ &= -J \sum_{\langle i,j \rangle} (m_A m_B + m_B \delta_i + m_A \delta_j + \delta_i \delta_j) - h \sum_i s_i \\ &\approx -J \sum_{\langle i,j \rangle} [m_A m_B + m_B (s_i - m_A) + m_A (s_j - m_B)] - h \sum_i s_i \\ &= \frac{\gamma N}{2} J m_A m_B - \gamma J \sum_{i \in A} m_B s_i - \gamma J \sum_{j \in B} m_A s_j - h \sum_i s_i \\ &= \frac{\gamma N}{2} J m_A m_B - \sum_{i \in A} (\gamma J m_B + h) s_i - \sum_{j \in B} (\gamma J m_A + h) s_j, \end{aligned} \quad (\text{S.9})$$

where we used that nearest neighbors always belong to different sublattices and neglected the product  $\delta_i \delta_j$ . We find that the two sublattices A and B behave as paramagnets in the effective fields

$$h_{\text{eff}}^A = \gamma J m_B + h, \quad h_{\text{eff}}^B = \gamma J m_A + h. \quad (\text{S.10})$$

The partition function of a paramagnet was already discussed previously, so the partition function of this mean-field Hamiltonian is

$$Z_I = \exp \left[ -\frac{1}{2} \beta \gamma N J m_A m_B \right] \cdot \left[ 2 \cosh \left( \beta h_{\text{eff}}^A \right) \right]^{N/2} \cdot \left[ 2 \cosh \left( \beta h_{\text{eff}}^B \right) \right]^{N/2}. \quad (\text{S.11})$$

This immediately leads to the Helmholtz free energy

$$F_I(\beta, h, N) = \frac{N}{2} \left( J \gamma m_A m_B - \frac{1}{\beta} \left\{ \log \left[ 2 \cosh(\beta h_{\text{eff}}^A) \right] + \log \left[ 2 \cosh(\beta h_{\text{eff}}^B) \right] \right\} \right). \quad (\text{S.12})$$

The self-consistent solutions are given by the local minima of the free energy. The conditions are therefore

$$\frac{\partial F_I}{\partial m_A} = 0 \quad \Leftrightarrow \quad m_B = \tanh \left[ \beta h_{\text{eff}}^A \right] \quad (\text{S.13a})$$

$$\frac{\partial F_I}{\partial m_B} = 0 \quad \Leftrightarrow \quad m_A = \tanh \left[ \beta h_{\text{eff}}^B \right]. \quad (\text{S.13b})$$

- (c) Use your results from parts (a) and (b) to calculate the grand potential for the lattice gas and determine the self-consistency relations for the two mean-field parameters  $\rho_A = \langle n_i \rangle_{i \in A}$  and  $\rho_B = \langle n_i \rangle_{i \in B}$ .

**Solution.** We use the mean-field approximation (S.12) derived in part (b) and the relations (S.4) in order to write the grand potential

$$\begin{aligned}\Omega(\beta, \mu, N_L) &= -\frac{1}{\beta} \log \mathcal{Z}_G = F_I(\beta, h, N_L) - \left(\frac{\lambda}{8}\gamma + \frac{\mu}{2}\right) N_L \\ &= \frac{N_L}{2} \left[ -\left(\frac{\lambda\gamma}{4} + \mu\right) + \frac{\lambda\gamma}{4}(2\rho_A - 1)(2\rho_B - 1) \right. \\ &\quad \left. - \frac{1}{\beta} \left\{ \log \left[ 2 \cosh \left( \frac{\beta}{2} (\lambda\gamma\rho_A + \mu) \right) \right] + \log \left[ 2 \cosh \left( \frac{\beta}{2} (\lambda\gamma\rho_B + \mu) \right) \right] \right\} \right],\end{aligned}\tag{S.14}$$

where we used the relation  $\rho = \frac{1}{2}(1 + m)$ . Here, the effective magnetic fields (S.10) are replaced by

$$h_{\text{eff}}^{A,B} \rightarrow \frac{1}{2}(\lambda\gamma\rho_{B,A} + \mu).\tag{S.15}$$

We can now reformulate the self-consistency equations (S.13) for the lattice gas by inserting the relations (S.15). Using  $\text{artanh } x = \frac{1}{2} \log[(1+x)/(1-x)]$  for  $x \in [-1, 1]$ , we obtain the two relations

$$\mu = \frac{1}{\beta} \log \frac{\rho_A}{1 - \rho_A} - \lambda\gamma\rho_B = \frac{1}{\beta} \log \frac{\rho_B}{1 - \rho_B} - \lambda\gamma\rho_A,\tag{S.16}$$

which can also be written in the form

$$\rho_A = \frac{1}{1 + e^{-\beta(\lambda\gamma\rho_B + \mu)}},\tag{S.17a}$$

$$\rho_B = \frac{1}{1 + e^{-\beta(\lambda\gamma\rho_A + \mu)}}.\tag{S.17b}$$

By inserting Eq. (S.17b) into Eq. (S.17a), we obtain the single condition

$$\rho_A = \left[ 1 + \exp \left( -\beta \left[ \frac{\gamma\lambda}{1 + \exp(-\beta(\lambda\gamma\rho_A + \mu))} + \mu \right] \right) \right]^{-1}.\tag{S.18}$$

In the following we will use the mean-field solution of the lattice gas model in order to discuss the liquid-gas transition for an attractive interaction  $\lambda > 0$ .

- (d) Argue, why in this case the mean-field results can be simplified as the two densities must be equal,  $\rho_A = \rho_B = \rho$ . Use your knowledge of the Ising model to define a critical temperature  $T_c$ , below which there are multiple solutions to the self-consistency equations, and discuss the solutions of  $\rho$  for temperatures above or below  $T_c$ . Define also the critical chemical potential  $\mu_0$  corresponding to  $h = 0$  in the Ising model and use this for a distinction of cases.

**Solution.** The two self-consistency equations (S.17) are of the mathematical form

$$a = \phi(b) \quad b = \phi(a),\tag{S.19}$$

where the function is given by

$$\phi(x) = \frac{1}{1 + e^{-\beta(\lambda\gamma x + \mu)}}.\tag{S.20}$$

It is easy to see that for  $\lambda > 0$  this function is monotonically increasing, while it is decreasing for  $\lambda < 0$ .

Now if we assume  $b > a$ , this implies  $f(b) > f(a)$ . This immediately leads to a contradiction, as  $a = f(b) \geq f(a) = b > a$ . The same contradiction follows for  $b < a$ . Therefore, for  $\lambda > 0$  there are only symmetric solutions  $\rho_A = \rho_B$  for the self-consistency equations and we can simplify the whole treatment by just omitting the second mean-field parameter altogether.

From Eq. (S.4) we see that  $h = 0$  corresponds to  $\mu = -\lambda\gamma/2 =: \mu_0$ . For this case we can use the knowledge about the magnetic transition in the zero-field Ising model. In particular, there is a critical temperature  $k_B T_c = \gamma\lambda/4 = -\mu_0/2$  below which there exist two degenerate solutions.



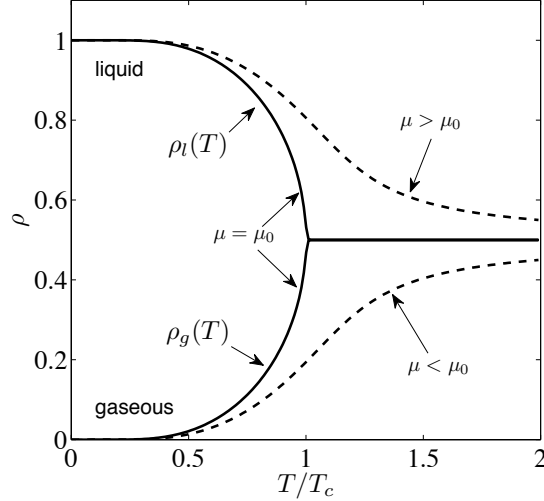


Figure 2: The density  $\rho$  as a function of temperature  $T$  for different values of the chemical potential  $\mu$ .

In the lattice gas, these solutions correspond to the liquid and to the gaseous phase and we will denote them by  $\rho_l(T)$  and  $\rho_g(T)$ , respectively (see Fig. 2). The third solution of Eq. (S.17) for  $\mu = \mu_0$ , namely  $\rho = 1/2$ , is only stable above  $T_c$ .

In the general case, there is a unique solution of Eq. (S.17) for  $T > T_c$  while for  $T \leq T_c$  there are three solutions in the neighborhood of  $\mu = \mu_0 = -2k_B T_c$  but only one minimizes  $\Omega$  (see Figs. 2 and 3). The solution with  $d\rho/d\mu > 0$  is stable or metastable while the solution with  $d\rho/d\mu < 0$  is unstable and corresponds to a local maximum of the grand potential  $\Omega$ . Thus, for  $T < T_c$ , the density  $\rho(T, \mu)$  jumps at  $\mu_0$  reflecting the first-order liquid-gas transition (see Fig. 3).

- (e) Find the equation of state  $p = p(T, \rho)$  or  $p = p(T, v)$  and discuss the liquid-gas transition in the  $p - v$  diagram. Thereby,  $v = 1/\rho$  is the specific volume. Compare with the van der Waals equation of state:

$$\left(p + \frac{\tilde{a}}{v^2}\right) (v - \tilde{b}) = k_B T.$$

*Hint.* For the lattice gas, the volume is given by the total number of lattice sites,  $N_L$ .

**Solution.** The pressure is given by

$$\begin{aligned} p(\beta, \mu) &= -\frac{\partial}{\partial N_L} \Omega(\beta, \mu, N_L) \\ &= \frac{\mu}{2} - \left( \frac{\lambda\gamma}{2} (\rho^2 - \rho) - \frac{1}{\beta} \log \left\{ 2 \cosh \left[ \beta \left( \frac{\lambda\gamma}{2} \rho + \frac{\mu}{2} \right) \right] \right\} \right), \end{aligned} \quad (\text{S.21})$$

where we used Eq. (S.14). For  $\rho(\beta, \mu) \leq \rho_g(\beta)$  and  $\rho(\beta, \mu) \geq \rho_l(\beta)$  we can simply insert Eq. (S.16) into the above equation and obtain

$$p(T, \rho) = -\frac{\lambda\gamma}{2} \rho^2 - \frac{1}{\beta} \log(1 - \rho) \quad (\text{S.22})$$

or in terms of the specific volume  $v = 1/\rho$

$$p(T, v) = -\frac{\lambda\gamma}{2} \frac{1}{v^2} - k_B T \log\left(1 - \frac{1}{v}\right). \quad (\text{S.23})$$

But for  $\rho_g(\beta) \leq \rho(\beta, \mu) \leq \rho_l(\beta)$  there is coexistence of the liquid and the gas. We have to set  $\mu = \mu_0$  and  $\rho = \rho_{g,l}(T)$  in Eq. (S.21) (this corresponds to the Maxwell construction) leading to a constant pressure! This is shown in the  $p - v$  diagram Fig. 4.

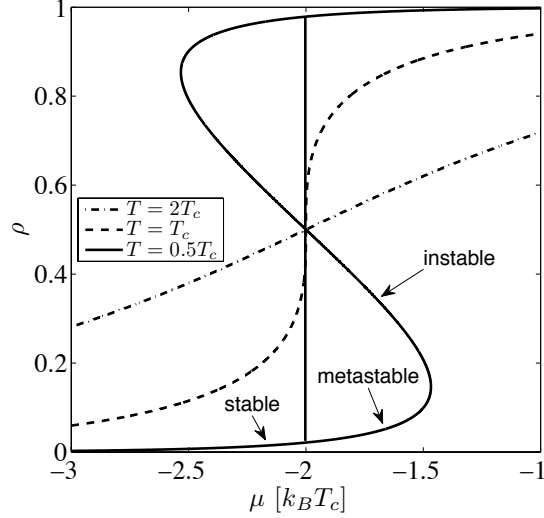


Figure 3: The density  $\rho$  as function of the chemical potential  $\mu$  for different temperatures. For  $T < T_c$  there is a jump in  $\rho$  at  $\mu = \mu_0 = -2k_B T_c$ .

We can rewrite the van der Waals equation of state as follows:

$$p(T, v) = -\frac{\tilde{a}}{v^2} + k_B T \frac{1}{v - \tilde{b}},$$

The elementary volume of the gas (hard core volume)  $\tilde{b}$  equals 1 in our model. Comparing this with Eq. (S.23), we see that the first term is identical (where  $\tilde{a} = \lambda\gamma/2$ ), whereas the second term diverges either linearly (van der Waals) or logarithmically (our model) with  $v \rightarrow 1$ . This different behavior is present in the limiting case of high density and can be attributed to the short-range difference of the potential for the discrete lattice gas model and the continuous van der Waals gas.

- (f) Find the phase diagram ( $T - p$  diagram). Determine the phase boundary ( $T, p_c(T)$ ) and, in particular, compute the critical point ( $T_c, p_c(T_c)$ ).

**Solution.** The critical pressure is given by Eq. (S.22) for  $\mu = \mu_0 = -2k_B T_c$  and  $\rho = \rho_{g,l}(T)$

$$p_c(T) = -2k_B T_c \rho_{g,l}^2(T) - k_B T \log(1 - \rho_{g,l}(T)), \quad (\text{S.24})$$

as shown in Fig. 5. In particular, for  $T = T_c$  we have  $\rho_{g,l}(T_c) = 1/2$  and

$$p_c(T_c) = \frac{k_B T_c}{2} (\log 4 - 1). \quad (\text{S.25})$$

Instead of the liquid-gas transition, which we have observed for an attractive interaction  $\lambda > 0$ , a crystallization transition (sublimation) can be observed for nearest-neighbor repulsion,  $\lambda < 0$ . In this case, we will find that the two mean-field parameters are different,  $\rho_A \neq \rho_B$ , below some critical temperature  $T_c$ .

- (g) Discuss the solutions above and below the critical temperature for  $\lambda < 0$ . Plot the densities  $\rho_A$  and  $\rho_B$ , as well as the average,  $(\rho_A + \rho_B)/2$  for both attractive and repulsive nearest-neighbor interaction at low temperature,  $T < T_c$ . Interpret the result in terms of compressibility.

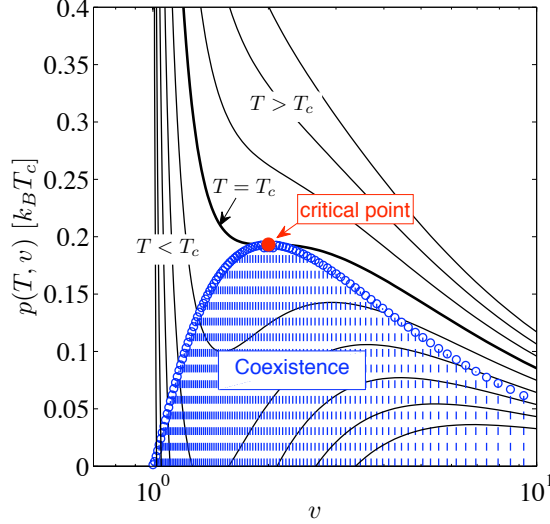


Figure 4: The isotherms  $p(T, v)$ . The shaded region denotes the region of liquid-gas phase coexistence.

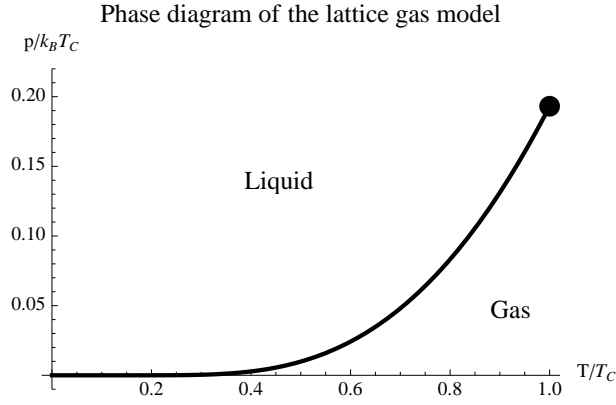


Figure 5:  $p$ - $T$  phase diagram of the lattice gas model. The two phases coexist when  $\mu = \mu_0$  and  $T < T_c$  (equilibrium line). Above  $T_c$  there is only one phase (a single density for a given pressure).

**Solution.** Below the same critical temperature  $k_B T_c = \gamma|\lambda|/4$  as for an attractive interaction and in a certain range  $\mu \in [\mu_0 - \Delta\mu, \mu_0 + \Delta\mu]$  around  $\mu_0 = \gamma\lambda/2$ , we find three different solutions for the self-consistency relations (S.17). There are two degenerate asymmetric solutions  $\rho_A \neq \rho_B$ , which are related by  $\rho_A \rightarrow \rho_B, \rho_B \rightarrow \rho_A$ , and one symmetric solution  $\rho_A = \rho_B$ .

The range is defined by the condition

$$\phi'(\rho)|_{\phi(\rho)=\rho} < -1 \quad (\text{S.26})$$

where  $\phi(\rho)$  is the function in the self-consistency equations defined in Eq. (S.20). This can be understood by looking at the plot of  $\phi(\rho_A)$  and  $\phi(\rho_B)$  shown in Fig. 6. As  $\phi(\rho) > 0$ , there have to be two asymmetric solutions whenever  $\phi'(\rho) < 1$  at the symmetric solution. By inserting  $\phi$  into Eq. (S.26) and solving for  $\mu$ , one obtains

$$\Delta\mu = \frac{\gamma\lambda}{2} \theta + \frac{1}{\beta} \log \left( \frac{1+\theta}{1-\theta} \right), \quad \theta = \sqrt{1 + \frac{4}{\beta\gamma\lambda}}. \quad (\text{S.27})$$

The asymmetric solutions, which are generally lower in energy, correspond to a crystal structure, where (at  $T = 0$ ) one of the sublattices is occupied while the other one is empty.

The densities for attraction and repulsion are shown in Fig. 7. While for a nearest-neighbor attraction the densities of the sublattices are identical, there is a symmetry-broken phase for nearest-neighbor repulsion.

The compressibility can be written as

$$\kappa_T = \frac{1}{\rho^2} \frac{\partial \rho}{\partial \mu}, \quad (\text{S.28})$$

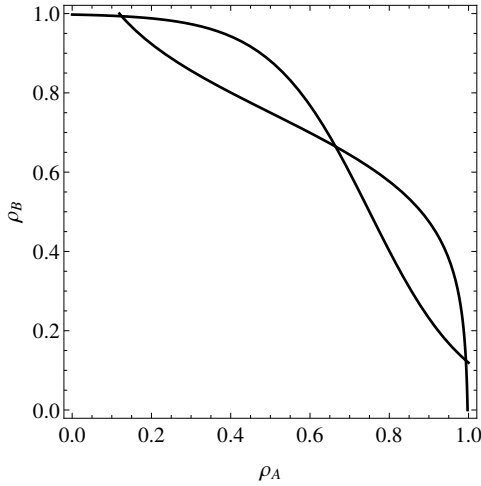


Figure 6: Plot of  $\phi(\rho_A)$  and  $\phi(\rho_B)$  for  $\mu \in [\mu_0 - \Delta\mu, \mu_0 + \Delta\mu]$ . The two graphs cross at the symmetric solution in a way that there must be two additional crossings. The condition is given in Eq. (S.26).

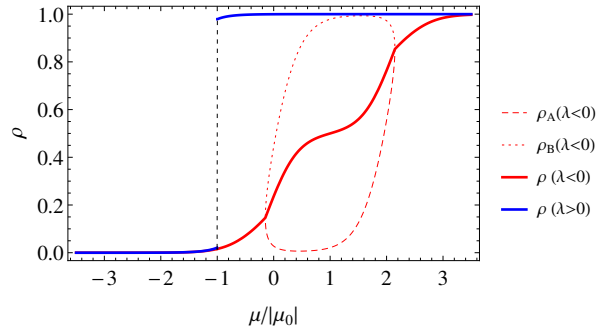


Figure 7: Densities on the two sublattices for attractive ( $\lambda > 0$ ) and repulsive ( $\lambda < 0$ ) nearest-neighbor interaction at  $T = 0.5 T_c$ . The thick lines show the average densities, the dashed and dotted lines the densities of the two sublattices.

see Sec. 1.5.2 in the lecture notes. The crystallization transition for  $\lambda < 0$  is of second order (except at  $T = 0$ , where it is of first order). For the average density, which is related to the total particle number, there exists a plateau around  $\mu_0$ . On this plateau the compressibility is small ( $\kappa_T = 0$  for  $T = 0$ ), see Fig. 8. This indicates that it costs a lot of energy to add additional particles, as one sublattice is almost completely filled (so no additional particles fit in) while it is very difficult to add particles to the second sublattice due to the repulsive interaction.

The liquid-gas transition for  $\lambda > 0$  is of first order. Therefore, there is a jump in the density (see Fig. 7) which is related to a diverging compressibility. The compressibility in the liquid phase is strongly reduced compared to the gaseous phase.

For both transitions, the compressibility vanishes for large chemical potentials, where the lattice is almost completely filled. In contrast, at low chemical potentials, the lattice is almost empty and the compressibility is large due to the factor  $\rho^{-2}$  in Eq. (S.28).

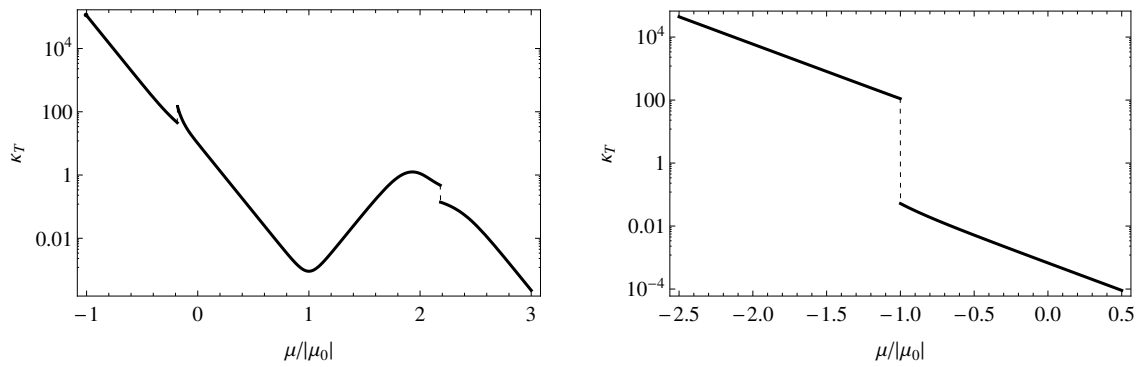


Figure 8: Compressibility for a nearest-neighbor repulsion  $\lambda < 0$  at  $T = 0.2 T_c$  (left) and for a nearest-neighbor attraction at  $T = 0.5 T_c$  (right). The second-order phase transitions for the crystallization are clearly visible as jumps in the compressibility. Around  $\mu_0$  there is a range where  $\kappa_T \approx 0$ , indicating the crystallization. The diverging compressibility at the condensation for  $\lambda > 0$  is not shown in the plot. However, the compressibility is decreased by a factor of 100 at the transition from gas to liquid.

**Exercise 1. *Magnetic domain wall.***

We want to calculate the energy of a magnetic domain wall in the framework of the Ginzburg-Landau (GL) theory. Assuming translational symmetry in the  $(y, z)$ -plane, the GL functional in zero field reads

$$F[m, m'] = F_0 + \int dx \left\{ \frac{A}{2} m(x)^2 + \frac{B}{4} m(x)^4 + \frac{\kappa}{2} [m'(x)]^2 \right\}. \quad (1)$$

(a) Solve the GL equation with boundary conditions

$$m(x \rightarrow \pm\infty) = \pm m_0, \quad m'(x \rightarrow \pm\infty) = 0, \quad (2)$$

where  $m_0$  is the magnetization of the uniform solution.

**Solution.** The Euler-Lagrange equation of the GL functional is

$$0 = \frac{\delta F}{\delta m} = \frac{\partial f}{\partial m} - \frac{d}{dx} \frac{\partial f}{\partial m'} = Am + Bm^3 - \kappa m''. \quad (S.1)$$

Assuming  $A < 0$  and  $B > 0$  the uniform solution is

$$m_0 := \sqrt{-\frac{A}{B}}. \quad (S.2)$$

By introducing rescaled variables  $s = x/\xi$  and  $u(s) = m(s\xi)/m_0$ , where

$$\xi = \sqrt{-\frac{\kappa}{A}}$$

is the correlation length, we arrive at the equation

$$u(s) - u(s)^3 + u''(s) = 0. \quad (S.3)$$

Multiplying the above equation by  $u'$  and integrating from  $-\infty$  to  $s$  we obtain

$$u'(s)^2 = \frac{1}{2} [1 - u(s)^2]^2$$

where we have used  $u(-\infty) = -1$  and  $u'(-\infty) = 0$ . The correct solution for  $u'$  is the positive root,

$$u'(s) = \frac{1}{\sqrt{2}} [1 - u(s)^2]$$

which can be integrated to give

$$u(s) = \tanh \left[ \frac{s - s_0}{\sqrt{2}} \right] \quad \implies \quad m(x) = m_0 \tanh \left[ \frac{x - x_0}{\sqrt{2}\xi} \right]. \quad (S.4)$$

Without loss of generality we set  $x_0 = s_0\xi = 0$  in the following.

(b) First, find the energy of the uniformly polarized solution (no domain walls). Next, compute the energy of the solution with a domain wall compared to the uniform solution. Use the coefficients  $A$ ,  $B$  and  $\kappa$  according to the expansion of the mean-field free energy of the Ising model (see Eqs. (5.78) and (5.83)). Finally, find the energy of a sharp step in the magnetization and compare it to the above results.

**Solution.** The free energy density of the uniformly polarized solution is  $f_u = f_0 + Am_0^2/4$ .

The energy of the domain wall as compared to the uniform solution is therefore

$$\begin{aligned}\Delta F &= \int dx \left\{ \frac{A}{2}m(x)^2 + \frac{B}{4}m(x)^4 + \frac{\kappa}{2}[m'(x)]^2 - \frac{A}{4}m_0^2 \right\} \\ &= \int dx \left\{ \frac{m(x)}{2} \left[ Am(x) + \frac{B}{2}m(x)^3 - \kappa m''(x) \right] - \frac{A}{4}m_0^2 \right\} \\ &= \int dx \left[ -\frac{B}{4}m(x)^4 - \frac{A}{4}m_0^2 \right] \\ &= -\frac{Am_0^2}{4} \int dx \left[ 1 - \frac{m(x)^4}{m_0^4} \right].\end{aligned}$$

In the second line we have used integration by parts and in the third line we have used the GL equation. Changing to the integration variable  $t = x/(\sqrt{2}\xi)$  yields

$$\Delta F = -\frac{Am_0^2}{4}\sqrt{2}\xi \int dt [1 - (\tanh t)^4], \quad (\text{S.5})$$

and by using  $\tanh' x = 1 - \tanh^2 x$  we find

$$\begin{aligned}\Delta F &= -\frac{Am_0^2}{4}\sqrt{2}\xi \int dt [1 - \tanh^2 t(1 - \tanh' t)] \\ &= -\frac{Am_0^2}{4}\sqrt{2}\xi \int dt \left[ (\tanh t)' + \frac{1}{3}(\tanh^3 t)' \right] \\ &= -\frac{2Am_0^2}{3}\sqrt{2}\xi.\end{aligned} \quad (\text{S.6})$$

Using the expressions of Chapter 5 (see Eqs. (5.78) and (5.83)) for the coefficients  $A$ ,  $B$  and  $\kappa$  (derived for an Ising model with coarse graining), we find that

$$\Delta F \sim Jm_0^2 \sqrt{1 - \frac{T}{T_c}} \rightarrow 0 \quad (T \rightarrow T_c). \quad (\text{S.7})$$

In contrast, a sharp step in the magnetization from  $-m_0$  to  $m_0$  costs an energy

$$E \sim Jm_0^2, \quad (\text{S.8})$$

(see Chap. 5.6), which for  $T \rightarrow T_c$  is less favorable.

1

Note that in the above energy discussions, the actual position of the domain wall (see entropy contribution in Chap. 5.6) was not taken into account.

## Exercise 2. *Gaussian Fluctuations in the Ginzburg-Landau Model.*

Consider the Ginzburg-Landau model of the  $d$ -dimensional Ising model in presence of a magnetic field  $H(\mathbf{r})$ , introduced in chapter 5.4 of the lecture notes. Here, we only consider temperatures above the critical temperature  $T_c$ . In order to make the model exactly tractable, we assume

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<sup>1</sup>Notice that (S.4) describes a sharp step in the magnetization if  $\xi \rightarrow 0$ . One might think then that (S.8) contradicts the expression (S.6), as the latter goes to zero if  $\xi \rightarrow 0$  while the former does not. However, one should keep in mind that the continuum model considered here is derived from a discrete model by coarse-graining. In particular,  $\xi$  depends on the lattice spacing  $a$  and the reduced temperature  $\tau$  according to

$$\xi \propto \frac{a}{\sqrt{\tau}}.$$

The correlation length  $\xi$  is thus always greater than  $a$  and can not be zero. The continuum limit keeps the information about the discreteness of the original model. A sharp step in the discrete case corresponds to a step of width  $a$ . At zero temperature, when the system is frozen and  $\xi = a$ , both expressions (S.8) and (S.7) agree.

that quartic fluctuations are negligible and ignore them. Therefore, the free energy functional for a given magnetization  $m$  and temperature  $T$  in  $d$  dimensions is given by

$$F(T, m, H) = \int d^d r \left\{ \frac{1}{2} A m(\mathbf{r})^2 - H(\mathbf{r}) m(\mathbf{r}) + \frac{1}{2} \kappa [\nabla m(\mathbf{r})]^2 \right\}, \quad (3)$$

where  $A = a\tau$ , with  $\tau = (T - T_c)/T_c$ . For the calculations we assume our system to be a cube of side length  $L$  with periodic boundary conditions on  $m$ .

(a) Use the Fourier transform of the magnetization field,

$$m(\mathbf{r}) = \frac{1}{\sqrt{L^d}} \sum_{\mathbf{q}} m_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}}, \quad (4)$$

and compute the energy functional  $F(T, m)$  in the transformed coordinates  $\{m_{\mathbf{q}}\}$ . Which values of  $\mathbf{q}$  are allowed in the sum and which values of  $\mathbf{q}$  are independent? Note that  $m(\mathbf{r})$  is real and interpret its implication on the  $m_{\mathbf{q}}$ .

(b\*) The calculation of the canonical partition function,

$$Z(T) = \int \mathcal{D}m e^{-F(T, m)/k_B T}, \quad (5)$$

is rather involved. If you have time to spare, show that  $Z(T)$  is equal to

$$Z(T) = \prod_{|\mathbf{q}| < \Lambda} \sqrt{\frac{2\pi}{\beta X_{\mathbf{q}}}} \exp \left\{ \frac{|H_{\mathbf{q}}|^2}{2k_B T (A + \kappa \mathbf{q}^2)} \right\}, \quad (6)$$

by using Gaussian integration. Otherwise, proceed directly to point (c) using this result.

*Hints.* Argue that the finite number of degrees of freedom (finite lattice spacing) of our Ising model introduces a momentum cutoff  $\Lambda$ , which is crucial to regulate the otherwise ill-defined integrals (cf. Debye wave vector for phonons).

Rewrite the functional measure  $\mathcal{D}m$  according to

$$\mathcal{D}m = \prod_{\mathbf{q}} dm_{\mathbf{q}} dm_{-\mathbf{q}}. \quad (7)$$

Why do we use  $dm_{\mathbf{q}} dm_{-\mathbf{q}}$ ?

You can also use the fact the measure  $\mathcal{D}m$  in Fourier space can be expressed as

$$\mathcal{D}m = dm_0 \cdot \prod_{\mathbf{q} \in \mathcal{A}^+} \sqrt{2d} dm'_{\mathbf{q}} \sqrt{2d} dm''_{\mathbf{q}}, \quad \text{with } m_{\mathbf{q}} = m'_{\mathbf{q}} + i m''_{\mathbf{q}}, \quad (8)$$

where  $\mathcal{A}^+$  is a choice of half the set of allowed momenta  $\mathbf{q} \neq 0$ , such that  $\mathbf{q} \in \mathcal{A}^+ \Leftrightarrow -\mathbf{q} \notin \mathcal{A}^+$ .

(c) Determine the free energy  $F(T) = -k_B T \log Z(T)$ .

Compute the specific heat  $c_V$  in the thermodynamic limit  $L \rightarrow \infty$  for vanishing external field ( $H(\mathbf{r}) \equiv 0$ ). Study its behavior for different dimensions  $d$  near the critical temperature where  $\tau = 0$ . Compare the critical exponent of  $c_V$  with the mean field result of section 5.4.2 of the lecture notes.

(d) Derive an expression for the magnetic susceptibility, defined as the negative second derivative of the free energy with respect to the external field  $H$  in the limit of vanishing field, i.e.

$$\chi(T) = - \left. \frac{\partial^2 F(T)}{\partial H^2} \right|_{H=0}. \quad (9)$$

What is the critical exponent of  $\chi$ ? Compare the result with the mean field result of section 5.2.2 of the lecture notes, Eq. (5.28).



**Solution.** Before we start with the solutions, we would like to stress that the form of the free energy, Eq. (1) on the exercise sheet, is only valid for temperatures above the critical temperature  $T_c$ . It corresponds to the second order expansion of the Ginzburg-Landau free energy (including quartic terms) in the expectation value of the magnetization  $\langle m \rangle = 0$ . This is of course only true in the disordered phase, i.e.  $T > T_c$ . A similar expansion up to second order in  $m$  is also possible in the phase with broken symmetry, but in that case the expansion is performed around the non-vanishing expectation value  $\langle m \rangle \neq 0$  which minimizes the free energy.

- (a) Periodic boundary conditions imply discretized momenta, i.e.  $\mathbf{q} \in \frac{2\pi}{L} \mathcal{Z}^d$ . As a consequence of the unitarity of the Fourier transform, we find that the integration over the absolute value of  $m$  equals the sum over the absolute value of its Fourier transform (Parseval-theorem). Hence, we immediately find

$$F(T, m, H) = \frac{1}{2} \sum_{\mathbf{q}} (A + \kappa \mathbf{q}^2) |m_{\mathbf{q}}|^2 + F_H, \quad (\text{S.9})$$

where  $F_H$  represents the coupling of  $m$  to the external field. The Fourier transform of  $H(\mathbf{r})$  is exactly the same as for  $m(\mathbf{r})$  and, thus, we obtain for the linear contribution the following term:

$$\begin{aligned} F_H &= -\frac{1}{L^d} \int d^d r \sum_{\mathbf{q}_1} \sum_{\mathbf{q}_2} e^{i\mathbf{q}_1 \cdot \mathbf{r}} e^{i\mathbf{q}_2 \cdot \mathbf{r}} m_{\mathbf{q}_1} H_{\mathbf{q}_2} \\ &= -\sum_{\mathbf{q}} m_{\mathbf{q}} H_{-\mathbf{q}} \\ &= -\sum_{\mathbf{q}} \frac{m_{\mathbf{q}} H_{-\mathbf{q}} + m_{-\mathbf{q}} H_{\mathbf{q}}}{2} \end{aligned} \quad (\text{S.10})$$

As a measurable value, the magnetization  $m(\mathbf{r})$  must be a real number and, hence, we find the condition

$$m_{\mathbf{q}} = m_{-\mathbf{q}}^*. \quad (\text{S.11})$$

This means that the set of independent coordinates for the magnetization field  $m$  is given by  $\{\text{Re } m_{\mathbf{q}}, \text{Im } m_{\mathbf{q}}\}$  and  $m_0$  (condition (S.11) implies that  $m_0$  is a real number), where  $\mathbf{q}$  lies in a half-space which we call  $\mathcal{A}^+$ . For  $\mathcal{A}^+$  any space can be chosen that fulfills the conditions

$$\mathbf{q} \in \mathcal{A}^+ \Leftrightarrow -\mathbf{q} \notin \mathcal{A}^+ \quad \text{for } \mathbf{q} \neq 0 \quad \text{and} \quad 0 \notin \mathcal{A}^+. \quad (\text{S.12})$$

- (b\*) By using the definition of the complex measure  $dz = d(\text{Re } z)d(\text{Im } z)$  we can define the functional measure of the magnetization field  $\mathcal{D}$  by introducing the variables  $m'$  and  $m''$  for real and imaginary parts of  $m$ ,

$$\mathcal{D}m = dm_0 \cdot \prod_{\mathbf{q} \in \mathcal{A}^+} \sqrt{2} d(m'_{\mathbf{q}}) \sqrt{2} d(m''_{\mathbf{q}}) \quad \text{with} \quad m_{\mathbf{q}} = m'_{\mathbf{q}} + im''_{\mathbf{q}}, \quad (\text{S.13})$$

where the factors of  $\sqrt{2}$  in front of the real differential  $m'_{\mathbf{q}}$  and  $m''_{\mathbf{q}}$  come from the Jacobian transformation of the differentials, cf. discussion in the framed inset below. Keep in mind that the set of independent variables is given by the  $m_{\mathbf{q}}$  with  $\mathbf{q} \in \mathcal{A}^+$  together with the real  $m_0$ . Alternatively, one could formulate the problem using complex Gaussian integration, but we will consider real variables here.

Now introduce the cutoff  $\Lambda$  and correspondingly interpret the half-space  $\mathcal{A}^+$  as the half-space of  $\mathbf{q}$ -vectors with  $|\mathbf{q}| < \Lambda$ , so that  $\mathcal{D}m$  becomes a well-defined finite-dimensional integral. The introduction of the cutoff  $\Lambda$  can be understood similar to the cutoff frequency within Debye theory of phonons and is a direct consequence of the finite lattice spacing. A finite lattice spacing of (in our case) spins directly implies a finite density of degrees of freedom, which means that the integral over the density of states must equal the number of degrees of freedom. This requires the introduction of a cutoff  $\Lambda$  for the product over the  $\mathbf{q}$ -vectors. The integrals over the real respectively imaginary part of  $m_{\mathbf{q}}$  run from  $-\infty$  to  $\infty$ .

$$\begin{aligned} Z(T) &= \int dm_0 \left( \prod_{\mathbf{q} \in \mathcal{A}^+} \int \sqrt{2} dm'_{\mathbf{q}} \sqrt{2} dm''_{\mathbf{q}} \right) \\ &\quad \times \exp \left\{ -\frac{\beta}{2} \sum_{|\mathbf{q}| < \Lambda} X_{\mathbf{q}} |m_{\mathbf{q}}|^2 - (H_{\mathbf{q}} m_{-\mathbf{q}} + H_{-\mathbf{q}} m_{\mathbf{q}}) \right\} \end{aligned} \quad (\text{S.14})$$

Here, we have defined  $X_{\mathbf{q}} \equiv X_{-\mathbf{q}} = (A + \kappa \mathbf{q}^2)$ . Now we can use  $|m_{\mathbf{q}}|^2 = (m'_{\mathbf{q}})^2 + (m''_{\mathbf{q}})^2$  and find for the partition sum

$$\int dm_0 \left( \prod_{\mathbf{q} \in \mathcal{A}^+} \int \sqrt{2} dm'_{\mathbf{q}} \sqrt{2} dm''_{\mathbf{q}} \right) \times \exp \left\{ -\frac{\beta}{2} \sum_{|\mathbf{q}| < \Lambda} X_{\mathbf{q}} (m'_{\mathbf{q}})^2 + X_{\mathbf{q}} (m''_{\mathbf{q}})^2 - (H_{\mathbf{q}}(m'_{-\mathbf{q}} + im''_{-\mathbf{q}}) + H_{-\mathbf{q}}(m'_{\mathbf{q}} + im''_{\mathbf{q}})) \right\}. \quad (\text{S.15})$$

Since the summand is completely invariant with respect to  $\mathbf{q} \rightarrow -\mathbf{q}$ , we can replace the sum by twice a sum with restriction to the half-space  $\mathcal{A}^+$  plus the contribution according to  $\mathbf{q} = 0$ . Then, we use the condition (S.11), we obtain

$$\begin{aligned} & \left( \prod_{\mathbf{q} \in \mathcal{A}^+} \int \sqrt{2} dm'_{\mathbf{q}} \sqrt{2} dm''_{\mathbf{q}} \right) \\ & \times \exp \left\{ -\beta \sum_{\mathbf{q} \in \mathcal{A}^+} X_{\mathbf{q}} (m'_{\mathbf{q}})^2 + X_{\mathbf{q}} (m''_{\mathbf{q}})^2 - (H_{\mathbf{q}}(m'_{-\mathbf{q}} + im''_{-\mathbf{q}}) + H_{-\mathbf{q}}(m'_{\mathbf{q}} + im''_{\mathbf{q}})) \right\} \\ & \times \int dm_0 e^{-\frac{\beta}{2}(X_0 m_0^2 - 2H_0 m_0)} \\ & = \left( \prod_{\mathbf{q} \in \mathcal{A}^+} \int \sqrt{2} dm'_{\mathbf{q}} e^{-\beta(X_{\mathbf{q}} (m'_{\mathbf{q}})^2 - 2(\text{Re } H_{\mathbf{q}}) m'_{\mathbf{q}})} \int \sqrt{2} dm''_{\mathbf{q}} e^{-\beta(X_{\mathbf{q}} (m''_{\mathbf{q}})^2 - 2(\text{Im } H_{\mathbf{q}}) m''_{\mathbf{q}})} \right) \\ & \times \int dm_0 e^{-\frac{\beta}{2}(X_0 m_0^2 - 2H_0 m_0)} \\ & = \left( \prod_{\mathbf{q} \in \mathcal{A}^+} \int \sqrt{2} dm e^{-\beta(X_{\mathbf{q}} m^2 - 2(\text{Re } H_{\mathbf{q}}) m)} \int \sqrt{2} dm e^{-\beta(X_{\mathbf{q}} m^2 - 2(\text{Im } H_{\mathbf{q}}) m)} \right) \\ & \times \int dm e^{-\frac{\beta}{2}(X_0 m^2 - 2H_0 m)}, \end{aligned} \quad (\text{S.16})$$

where in the last equality we did nothing but a relabeling of the real integration variables. We are left with three one-dimensional Gaussian integrals which we know explicitly how to integrate,

$$\int_{-\infty}^{\infty} dx e^{-ax^2 + bx + c} = \sqrt{\frac{\pi}{a}} \exp \left\{ \frac{b^2}{4a} + c \right\}. \quad (\text{S.17})$$

Therefore, noting that the condition (S.11) also holds in complete analogy to the magnetization for the Fourier components  $H_{\mathbf{q}}$  of the external field  $H(\mathbf{r})$ , we arrive at

$$\begin{aligned} & \left( \prod_{\mathbf{q} \in \mathcal{A}^+} \sqrt{\frac{2\pi}{\beta X_{\mathbf{q}}}} \exp \left\{ \frac{\beta(\text{Re } H_{\mathbf{q}})^2}{X_{\mathbf{q}}} \right\} \times \sqrt{\frac{2\pi}{\beta X_{\mathbf{q}}}} \exp \left\{ \frac{\beta(\text{Im } H_{\mathbf{q}})^2}{X_{\mathbf{q}}} \right\} \right) \times \sqrt{\frac{2\pi}{\beta X_0}} \exp \left\{ \frac{\beta H_0^2}{2 X_0} \right\} \\ & = \left( \prod_{\mathbf{q} \in \mathcal{A}^+} \frac{2\pi}{\beta X_{\mathbf{q}}} \exp \left\{ \frac{\beta |H_{\mathbf{q}}|^2}{X_{\mathbf{q}}} \right\} \right) \times \sqrt{\frac{2\pi}{\beta X_0}} \exp \left\{ \frac{\beta H_0^2}{2 X_0} \right\} \\ & = \prod_{|\mathbf{q}| < \Lambda} \sqrt{\frac{2\pi}{\beta X_{\mathbf{q}}}} \exp \left\{ \frac{\beta |H_{\mathbf{q}}|^2}{2 X_{\mathbf{q}}} \right\}, \end{aligned} \quad (\text{S.18})$$

where in the last equality we have replaced every term in the product by a product of the square root of the term and the square root of the term with  $\mathbf{q}$  replaced by  $-\mathbf{q}$  due to its invariance under this transformation. This enabled us then to transform the product over all  $\mathbf{q} \in \mathcal{A}^+$  into a product over all  $\mathbf{q}$  including the contribution  $\mathbf{q} = 0$ . Thus, the partition function is given by

$$Z(T) = \prod_{|\mathbf{q}| < \Lambda} \sqrt{\frac{2\pi k_B T}{A + \kappa \mathbf{q}^2}} \exp \left\{ \frac{|H_{\mathbf{q}}|^2}{2k_B T(A + \kappa \mathbf{q}^2)} \right\}. \quad (\text{S.19})$$

### Fourier Transformation of the Functional Differential $\mathcal{D}m$

In this part of the exercise we have introduced a discretized momentum space representation of  $\mathcal{D}m$ ,

$$\mathcal{D}m = dm_0 \cdot \prod_{\mathbf{q} \in \mathcal{A}^+} \sqrt{2} d(m'_\mathbf{q}) \sqrt{2} d(m''_\mathbf{q}) \quad \text{with} \quad m_\mathbf{q} = m'_\mathbf{q} + im''_\mathbf{q}. \quad (\text{S.13})$$

Here, we will briefly sketch how to derive the seemingly awkward factors of  $\sqrt{2}$  and how in principle such a transformation is performed explicitly. Note that we will only sketch the whole procedure so there is no claim made concerning mathematical exactness. For simplicity, we assume that our field  $m(\mathbf{r})$  is defined only on a given set of vectors  $\{\mathbf{r}_i\}$ , defining a lattice in real space. This assumption is always a good consistency check for any kind of low energy calculation in statistical physics. The continuum limit is achieved by smoothly taking the lattice spacing to zero. Here, we fix the lattice spacing  $a$  to one.

Starting with the discretized real space, the functional differential  $\mathcal{D}m$  is defined as

$$\mathcal{D}m = \prod_i dm(\mathbf{r}_i) = \prod_i dm_i. \quad (\text{S.20})$$

The Fourier transformation from real space to momentum space then simply corresponds to a change of variables from  $\{m_i\}$  to the  $\{m_{\mathbf{q}_l}\}$ , where the  $\mathbf{q}_l$  label the reciprocal lattice. First, as already discussed in part b) above, the momentum space variables are related via the condition

$$m_{\mathbf{q}_l} = m_{-\mathbf{q}_l}^*, \quad (\text{S.11})$$

which reduces the independent variables in momentum space to the  $m_{\mathbf{q}_l}$  with  $\mathbf{q}_l \in \mathcal{A}^+$  (for the purpose of this discussion, we will neglect the  $\mathbf{q}_l = 0$  contribution, which is real by definition). In the discretized real space picture, we are in the position to count the number of degrees of freedom in a simple way. In real space we have exactly  $N_r$  independent variables, where  $N_r$  is the number of lattice sites. In momentum space we have by definition of the Fourier transformation no loss of information, and consequently the same number of independent variables  $N_r$  which reduces the number of the independent *complex*  $m_{\mathbf{q}_l}$  to  $N_q = N_r/2$ .

Now in order to explicitly perform the transformation from real space to momentum space we have to calculate the Jacobian of this transformation. The Fourier transform of  $m_i$  is defined as

$$m_i = L^{-d/2} \sum_{\mathbf{q}_l} e^{i\mathbf{q}_l \mathbf{r}_i} m_{\mathbf{q}_l}. \quad (\text{S.21})$$

Consequently from Eqs. (S.11) and (S.21), the matrix elements of the Jacobian are given by

$$\frac{\partial m_i}{\partial m'_{\mathbf{q}_l}} = L^{-d/2} (e^{i\mathbf{q}_l \mathbf{r}_i} + e^{-i\mathbf{q}_l \mathbf{r}_i}) = \frac{2}{L^{d/2}} \cos(\mathbf{q}_l \mathbf{r}_i), \quad (\text{S.22})$$

$$\frac{\partial m_i}{\partial m''_{\mathbf{q}_l}} = iL^{-d/2} (e^{i\mathbf{q}_l \mathbf{r}_i} - e^{-i\mathbf{q}_l \mathbf{r}_i}) = -\frac{2}{L^{d/2}} \sin(\mathbf{q}_l \mathbf{r}_i), \quad (\text{S.23})$$

for the real and imaginary parts of  $m_{\mathbf{q}_l}$  respectively. Therefore, switching from the real space differentials to the  $m'_{\mathbf{q}_l}$  and  $m''_{\mathbf{q}_l}$  one has to multiply the entire product with the determinant of the Jacobian  $\mathbb{J}$ ,

$$\mathbb{J} = \begin{pmatrix} \vdots & \vdots & \vdots & \vdots & \vdots \\ \dots & 2L^{-d/2} \cos(\mathbf{q}_l \mathbf{r}_{i-1}) & 2L^{-d/2} \cos(\mathbf{q}_l \mathbf{r}_i) & 2L^{-d/2} \cos(\mathbf{q}_l \mathbf{r}_{i+1}) & \dots \\ \dots & -2L^{-d/2} \sin(\mathbf{q}_l \mathbf{r}_{i-1}) & -2L^{-d/2} \sin(\mathbf{q}_l \mathbf{r}_i) & -2L^{-d/2} \sin(\mathbf{q}_l \mathbf{r}_{i+1}) & \dots \\ \dots & 2L^{-d/2} \cos(\mathbf{q}_{l+1} \mathbf{r}_{i-1}) & 2L^{-d/2} \cos(\mathbf{q}_{l+1} \mathbf{r}_i) & 2L^{-d/2} \cos(\mathbf{q}_{l+1} \mathbf{r}_{i+1}) & \dots \\ \dots & -2L^{-d/2} \sin(\mathbf{q}_{l+1} \mathbf{r}_{i-1}) & -2L^{-d/2} \sin(\mathbf{q}_{l+1} \mathbf{r}_i) & -2L^{-d/2} \sin(\mathbf{q}_{l+1} \mathbf{r}_{i+1}) & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}, \quad (\text{S.24})$$

where  $l = 1, \dots, N_q$  and  $i = 1, \dots, N_r$ .

The matrix  $\mathbb{J}$  is a square matrix of size  $N_r$  (note that the number of  $\mathbf{q}_l$ -vectors equals half the number of lattice sites  $\mathbf{r}_i$ ). Due to special form with the trigonometric functions, the columns of  $\mathbb{J}$  represent an orthogonal basis.

Hence, the Jacobian determinant is given by the product of the norms of the basis vectors  $\mathbf{V}_i$ , which can be simply calculated.

$$\begin{aligned}
\|\mathbf{V}_i\|_2 &= \left\| \left( \dots, 2L^{-d/2} \cos(\mathbf{q}_i \mathbf{r}_i), -2L^{-d/2} \sin(\mathbf{q}_i \mathbf{r}_i), 2L^{-d/2} \cos(\mathbf{q}_{i+1} \mathbf{r}_i), -2L^{-d/2} \sin(\mathbf{q}_{i+1} \mathbf{r}_i) \right) \right\|_2 \\
&= \left( \sum_{l=1}^{N_q} \left\{ \left( 2L^{-d/2} \cos(\mathbf{q}_l \mathbf{r}_i) \right)^2 + \left( -2L^{-d/2} \sin(\mathbf{q}_l \mathbf{r}_i) \right)^2 \right\} \right)^{\frac{1}{2}} \\
&= \left( \sum_{l=1}^{N_q} 4L^{-d} \right)^{\frac{1}{2}} \\
&= \left( 4L^{-d} \times N_q \right)^{\frac{1}{2}} \tag{S.25}
\end{aligned}$$

The number  $N_q$  equals half the number  $N_r$  which, for a cubic system, can be given in terms of the dimension  $d$ , the system length  $L$  and the lattice spacing which we have fixed to one. Then, we find that there are exactly  $L^d$  lattice sites and consequently  $N_q = L^d/2$ , which renders the norm of each of the column vectors  $\mathbf{V}_i$  of  $\mathbb{J}$  to

$$\|\mathbf{V}_i\|_2 = \sqrt{2}. \tag{S.26}$$

The determinant  $\det \mathbb{J}$  is then given by

$$\det \mathbb{J} = (\|\mathbf{V}_i\|_2)^{N_r/2} = 2^{N_r/2} = 2^{N_q}, \tag{S.27}$$

and, therefore, every term  $dm'_{\mathbf{q}_l} dm''_{\mathbf{q}_l}$  in the product over all  $N_q$   $\mathbf{q}_l$ -vectors acquires a factor of 2. Thus, we finally have

$$\mathcal{D}m = dm_0 \det \mathbb{J} \prod_{\mathbf{q}_l \in \mathcal{A}^+} dm'_{\mathbf{q}_l} dm''_{\mathbf{q}_l} = dm_0 2^{N_q} \prod_{\mathbf{q}_l \in \mathcal{A}^+} dm'_{\mathbf{q}_l} dm''_{\mathbf{q}_l} = dm_0 \prod_{\mathbf{q}_l \in \mathcal{A}^+} \sqrt{2} dm'_{\mathbf{q}_l} \sqrt{2} dm''_{\mathbf{q}_l}, \tag{S.28}$$

where we have re-included the zero-wavevector contribution  $m_0$ .

(c) From (S.19) we get the free energy of the system as

$$F(T) = -k_B T \log Z(T) = -\frac{1}{2} k_B T \sum_{|\mathbf{q}| < \Lambda} \left[ \log(2\pi k_B T) - \log(A + \kappa \mathbf{q}^2) + \frac{|H_{\mathbf{q}}|^2}{k_B T (A + \kappa \mathbf{q}^2)} \right]. \tag{S.29}$$

First we note that the coefficient  $A$  is given by  $A = a(T - T_c)/T_c$ . The internal energy for vanishing external field is then given by

$$U(T) = k_B T^2 \frac{\partial}{\partial T} \log Z(T) = \frac{k_B T^2}{2} \sum_{|\mathbf{q}| < \Lambda} \left[ \frac{1}{T} - \frac{a/T_c}{a\tau + \kappa \mathbf{q}^2} \right]. \tag{S.30}$$

Therefore the specific heat is given by

$$c_V = \frac{1}{L^d} \frac{\partial U}{\partial T} = \frac{k_B T^2}{2L^d} \sum_{|\mathbf{q}| < \Lambda} \left[ -\frac{1}{T^2} + \frac{(a/T_c)^2}{(a\tau + \kappa \mathbf{q}^2)^2} \right] + 2 \frac{U(T)}{T} = A + B + C; \tag{S.31}$$

$$A = \text{constant} \quad ; \quad B \propto \sum_{|\mathbf{q}| < \Lambda} \frac{(a/T_c)^2}{(a\tau + \kappa \mathbf{q}^2)^2} \quad ; \quad C \propto \frac{U(T)}{T}.$$

In order to study the critical behavior of  $c_V$  at the phase transition, not all the terms in Eq. (S.31) are relevant. The term  $A$  gives a constant contribution which we ignore for the present analysis. The term  $B$  becomes in the thermodynamic limit

$$\frac{k_B T^2 (a/T_c)^2}{2(2\pi)^d} \int_{|\mathbf{q}| < \Lambda} d^d q \frac{1}{(a\tau + \kappa \mathbf{q}^2)^2}. \tag{S.32}$$

The behaviour in the vicinity of the critical temperature  $\tau = 0$  is therefore determined by the integral

$$\int_0^\Lambda dq \frac{q^{d-1}}{(a\tau + \kappa q^2)^2}. \tag{S.33}$$

Using the substitution  $s \mapsto \sqrt{\frac{\kappa}{a\tau}}q$  we find that the specific heat behaves like

$$\tau^{(d-4)/2} \int_0^{\Lambda(\tau)} ds \frac{s^{d-1}}{(1+s^2)^2}, \quad (\text{S.34})$$

where  $\Lambda(\tau) := \Lambda \sqrt{\kappa/(a\tau)}$ .

If  $d < 4$ , the integral above converges and we find

$$c_V \propto \tau^{(d-4)/2}. \quad (\text{S.35})$$

If  $d = 4$  the integral diverges logarithmically in  $\tau$  and we find

$$c_V \propto \log \tau. \quad (\text{S.36})$$

If  $d > 4$  the integral diverges proportionally to  $\tau^{-(d-4)/2}$ , so that

$$c_V \propto 1. \quad (\text{S.37})$$

Note that the term  $C$  is also divergent for  $d \leq 2$ , but it is less singular than term  $B$  ( $C$  diverges as  $\tau^{-1/2}$  for  $d = 1$  and as  $\log \tau$  for  $d = 2$ ).

With the results (S.35) to (S.37) we can summarize: The specific heat  $c_V$  of the  $d$ -dimensional Ising model, derived within the Ginzburg-Landau theory at the mean field level including Gaussian fluctuations is divergent in  $d \leq 4$  and at the critical temperature  $T_c$  and shows a cusp in for all higher dimensions.

Considering the case of three spacial dimensions ( $d = 3$ ), we find for the critical exponent of the specific heat (which in literature is called  $\alpha$ ) a value of  $1/2$ . Compared to the mean field result of  $\alpha = 0$ , we conclude that Gaussian fluctuations strongly renormalize the temperature dependence of the specific heat.

- (d) We are interested in the response of the system to a homogeneous external magnetic field, meaning that only the Fourier component with  $\mathbf{q} = 0$  survives. Hence, from the form of the free energy, Eq. (S.29), we can immediately read off the magnetic susceptibility,

$$\chi(T) = \frac{1}{a(T - T_c)/T_c} \propto \tau^{-1}, \quad (\text{S.38})$$

from which we find that at the phase transition, the susceptibility diverges with the critical exponent of  $\gamma = 1$ . This susceptibility has the exact same form as the one calculated in the lecture notes within mean field theory, Eq. (5.28). In other words, Gaussian fluctuations do not change the critical exponent of the magnetic susceptibility and, thus, do not contain non-trivial information about the magnetic correlations in the vicinity of the phase transition. The fact that Gaussian fluctuations do not qualitatively change the susceptibility can be understood by considering the correlation functions as second derivative of the free energy which is related to the curvature of the free energy around its minimum. In order to gain non-trivial (beyond mean-field) information about correlation functions, one has to take into account higher order terms such as the  $m^4$  term which we neglected in this exercise (cf. *Self-consistent field approximation*, chapter 5.5 of the lecture notes).

**Exercise 1. The Bogolyubov transformation.**

We consider a gas of weakly interacting bosonic particles at low temperatures. In this limit, the corresponding Hamiltonian can be approximated by

$$\mathcal{H} = \frac{1}{2}U\Omega n_0^2 - \mu\Omega n_0 + \frac{1}{2} \sum_{\mathbf{k} \neq 0} \left\{ (\epsilon_{\mathbf{k}} - \mu + 2Un_0) \left( \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{a}_{-\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}} \right) + Un_0 \left( \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}^\dagger + \hat{a}_{\mathbf{k}} \hat{a}_{-\mathbf{k}} \right) \right\}, \quad (1)$$

where  $\epsilon_{\mathbf{k}}$  is the free dispersion,

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}. \quad (2)$$

- (a) Introduce quasiparticle annihilation and creation operators  $\hat{\gamma}_{\mathbf{k}}$  and  $\hat{\gamma}_{\mathbf{k}}^\dagger$  which are defined by the relation

$$\hat{a}_{\mathbf{k}} = u_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}} - v_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}}^\dagger \quad \text{and} \quad \hat{a}_{-\mathbf{k}} = u_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}} - v_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}}^\dagger. \quad (3)$$

What is the condition for  $u_{\mathbf{k}}$  and  $v_{\mathbf{k}}$  in order to obtain bosonic commutation relations for these operators?

- (b) For real-valued  $u_{\mathbf{k}}$  and  $v_{\mathbf{k}}$  you can write the transformation coefficients as

$$u_{\mathbf{k}} = \frac{1}{\sqrt{1 - \chi_{\mathbf{k}}^2}} \quad \text{and} \quad v_{\mathbf{k}} = \frac{\chi_{\mathbf{k}}}{\sqrt{1 - \chi_{\mathbf{k}}^2}}. \quad (4)$$

Determine the function  $\chi_{\mathbf{k}}$  such that the Hamiltonian is diagonal in the quasiparticle operators,

$$\mathcal{H} = E_0 - \mu\Omega n_0 + \frac{1}{2} \sum_{\mathbf{k} \neq 0} E_{\mathbf{k}} \left( \hat{\gamma}_{\mathbf{k}}^\dagger \hat{\gamma}_{\mathbf{k}} + \hat{\gamma}_{-\mathbf{k}}^\dagger \hat{\gamma}_{-\mathbf{k}} \right). \quad (5)$$

- (c) Find the quasiparticle dispersion  $E_{\mathbf{k}}$ . Fix the chemical potential  $\mu$  in such a way that the energy spectrum is linear for  $\mathbf{k} \rightarrow 0$ . Approximate the dispersion for small ( $\mathbf{k} \rightarrow 0$ ) and large ( $\epsilon_{\mathbf{k}} \gg Un_0$ ) momenta and calculate the sound velocity for  $k \rightarrow 0$ .

**Solution.**

- (a) We can reverse the problem and start from bosonic commutation relations for the quasiparticles,

$$[\hat{\gamma}_{\mathbf{k}}, \hat{\gamma}_{\mathbf{k}'}^\dagger] = \delta_{\mathbf{k}, \mathbf{k}'} \quad \text{and} \quad [\hat{\gamma}_{\mathbf{k}}, \hat{\gamma}_{\mathbf{k}'}] = [\hat{\gamma}_{\mathbf{k}}^\dagger, \hat{\gamma}_{\mathbf{k}'}^\dagger] = 0. \quad (S.1)$$

We can use these to calculate the commutation relations for the original operators using the relation (3):

$$\begin{aligned} [\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k}}^\dagger] &= [u_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}} - v_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}}^\dagger, u_{\mathbf{k}}^* \hat{\gamma}_{\mathbf{k}}^\dagger - v_{\mathbf{k}}^* \hat{\gamma}_{-\mathbf{k}}] \\ &= |u_{\mathbf{k}}|^2 \underbrace{[\hat{\gamma}_{\mathbf{k}}, \hat{\gamma}_{\mathbf{k}}^\dagger]}_{=1} + |v_{\mathbf{k}}|^2 \underbrace{[\hat{\gamma}_{-\mathbf{k}}^\dagger, \hat{\gamma}_{-\mathbf{k}}]}_{=-1} - u_{\mathbf{k}} v_{\mathbf{k}}^* \underbrace{[\hat{\gamma}_{\mathbf{k}}, \hat{\gamma}_{-\mathbf{k}}]}_{=0} - u_{\mathbf{k}}^* v_{\mathbf{k}} \underbrace{[\hat{\gamma}_{-\mathbf{k}}^\dagger, \hat{\gamma}_{\mathbf{k}}^\dagger]}_{=0} \\ &= |u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2. \end{aligned} \quad (S.2)$$

As the original particles are bosons, we obtain the condition

$$|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1. \quad (\text{S.3})$$

It can be easily checked that all other commutation relations for  $\hat{a}_{\mathbf{k}}$  and  $\hat{a}_{\mathbf{k}}^\dagger$  are fulfilled.

(b) We write the Hamiltonian (1) as

$$\mathcal{H} = \frac{1}{2}U\Omega n_0^2 - \mu\Omega n_0 + \frac{1}{2} \sum_{\mathbf{k} \neq 0} h_{\mathbf{k}} \quad (\text{S.4})$$

and insert the definitions (3) to obtain

$$\begin{aligned} h_{\mathbf{k}} = & (\epsilon_{\mathbf{k}} - \mu + 2Un_0) \left[ \left( u_{\mathbf{k}}^* \hat{\gamma}_{\mathbf{k}}^\dagger - v_{\mathbf{k}}^* \hat{\gamma}_{-\mathbf{k}} \right) \left( u_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}} - v_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}}^\dagger \right) + \left( u_{\mathbf{k}}^* \hat{\gamma}_{-\mathbf{k}}^\dagger - v_{\mathbf{k}}^* \hat{\gamma}_{\mathbf{k}} \right) \left( u_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}} - v_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}}^\dagger \right) \right] \\ & + Un_0 \left[ \left( u_{\mathbf{k}}^* \hat{\gamma}_{\mathbf{k}}^\dagger - v_{\mathbf{k}}^* \hat{\gamma}_{-\mathbf{k}} \right) \left( u_{\mathbf{k}}^* \hat{\gamma}_{-\mathbf{k}}^\dagger - v_{\mathbf{k}}^* \hat{\gamma}_{\mathbf{k}} \right) + \left( u_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}} - v_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}}^\dagger \right) \left( u_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}} - v_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}}^\dagger \right) \right]. \end{aligned} \quad (\text{S.5})$$

Using the commutation relations, in particular  $\hat{\gamma}_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}}^\dagger = 1 + \hat{\gamma}_{\mathbf{k}}^\dagger \hat{\gamma}_{\mathbf{k}}$ , and collecting terms, we obtain

$$\begin{aligned} h_{\mathbf{k}} = & \left( \hat{\gamma}_{\mathbf{k}}^\dagger \hat{\gamma}_{\mathbf{k}} + \hat{\gamma}_{-\mathbf{k}}^\dagger \hat{\gamma}_{-\mathbf{k}} + 1 \right) \underbrace{\left[ (\epsilon_{\mathbf{k}} - \mu + 2Un_0) (|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2) - Un_0 (u_{\mathbf{k}}^* v_{\mathbf{k}}^* + u_{\mathbf{k}} v_{\mathbf{k}}) \right]}_{=E_{\mathbf{k}}} \\ & + \left( \hat{\gamma}_{\mathbf{k}}^\dagger \hat{\gamma}_{-\mathbf{k}}^\dagger \right) \left[ -2u_{\mathbf{k}}^* v_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu + 2Un_0) + Un_0 (u_{\mathbf{k}}^{*2} + v_{\mathbf{k}}^2) \right] \\ & + \left( \hat{\gamma}_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}} \right) \left[ -2u_{\mathbf{k}} v_{\mathbf{k}}^* (\epsilon_{\mathbf{k}} - \mu + 2Un_0) + Un_0 (u_{\mathbf{k}}^2 + v_{\mathbf{k}}^{*2}) \right]. \end{aligned} \quad (\text{S.6})$$

In order for this Hamiltonian to be diagonal, the condition

$$0 = -2u_{\mathbf{k}}^* v_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu + 2Un_0) + (u_{\mathbf{k}}^{*2} + v_{\mathbf{k}}^2) Un_0 \quad (\text{S.7})$$

must be fulfilled. Here we insert the relations (4), which leads to

$$0 = -\frac{2\chi_{\mathbf{k}}}{1 - \chi_{\mathbf{k}}^2} (\epsilon_{\mathbf{k}} - \mu + 2Un_0) + \frac{1 + \chi_{\mathbf{k}}^2}{1 - \chi_{\mathbf{k}}^2} Un_0. \quad (\text{S.8})$$

The result of this quadratic equation is given by

$$\begin{aligned} \chi_{\mathbf{k}} = & \frac{(\epsilon_{\mathbf{k}} - \mu + 2Un_0) - \sqrt{(\epsilon_{\mathbf{k}} - \mu + 2Un_0)^2 - (Un_0)^2}}{Un_0} \\ = & 2 + \frac{\epsilon_{\mathbf{k}} - \mu}{Un_0} - \sqrt{\left( 2 + \frac{\epsilon_{\mathbf{k}} - \mu}{Un_0} \right)^2 - 1}. \end{aligned} \quad (\text{S.9})$$

Here we can just choose the “-” sign, as the “+” would just correspond to exchanging  $u_{\mathbf{k}} \leftrightarrow v_{\mathbf{k}}$ .

(c) In order to determine the dispersion  $E_{\mathbf{k}}$ , we define

$$A := \epsilon_{\mathbf{k}} - \mu + 2Un_0, \quad B := Un_0, \quad \text{and} \quad Y = \frac{A}{B}. \quad (\text{S.10})$$

Using this definitions, we obtain

$$\chi_{\mathbf{k}} = Y - \sqrt{Y^2 - 1}, \quad (\text{S.11a})$$

$$\begin{aligned} \chi_{\mathbf{k}}^2 - 1 = & Y^2 - 2Y\sqrt{Y^2 - 1} + Y^2 - 2 \\ = & 2(Y^2 - 1) - 2Y\sqrt{Y^2 - 1} \\ = & 2\sqrt{Y^2 - 1} (\sqrt{Y^2 - 1} - Y). \end{aligned} \quad (\text{S.11b})$$

Also, the Eq. (S.8) can be written as

$$\frac{1 + \chi_{\mathbf{k}}^2}{1 - \chi_{\mathbf{k}}^2} = Y \frac{2\chi_{\mathbf{k}}}{1 - \chi_{\mathbf{k}}^2}. \quad (\text{S.12})$$

Now we can insert these results into Eq. (S.6) in order to calculate the dispersion relation

$$\begin{aligned} \frac{E_{\mathbf{k}}}{B} &= Y \frac{1 + \chi_{\mathbf{k}}^2}{1 - \chi_{\mathbf{k}}^2} - \frac{2\chi_{\mathbf{k}}}{1 - \chi_{\mathbf{k}}^2} \\ &= (Y^2 - 1) \frac{2\chi_{\mathbf{k}}}{1 - \chi_{\mathbf{k}}^2} \\ &= \frac{2(Y^2 - 1)(Y - \sqrt{Y^2 - 1})}{2\sqrt{Y^2 - 1}(Y - \sqrt{Y^2 - 1})} \\ &= \sqrt{Y^2 + 1}, \end{aligned} \quad (\text{S.13})$$

$$\Rightarrow E_{\mathbf{k}} = \sqrt{A^2 - B^2} = \sqrt{\epsilon_{\mathbf{k}}^2 + \epsilon_{\mathbf{k}}(4Un_0 - 2\mu) + (\mu^2 - 4\mu Un_0 + 3U^2 n_0^2)}. \quad (\text{S.14})$$

The occupation of the different quasiparticle states follows the Bose-Einstein distribution

$$n_{\mathbf{k}} = \frac{1}{e^{\beta E_{\mathbf{k}}} - 1}. \quad (\text{S.15})$$

If the energy of the state  $\mathbf{k} = 0$  is finite, the occupation will converge to 0 as  $T \rightarrow 0$ . So in order to have a fixed finite particle number at arbitrarily low temperatures, we need to have  $E_{\mathbf{k}=0} = 0$ , which leads to a linear dispersion. The condition for this is a vanishing constant term in the square-root. This fixes the chemical potential to

$$\mu \in \{Un_0, 3Un_0\}. \quad (\text{S.16})$$

For  $\mu > Un_0$  the discriminant becomes negative at either small or large momenta, such that we have to choose  $\mu = Un_0$ . In this case we obtain the dispersion

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + 2Un_0\epsilon_{\mathbf{k}}}. \quad (\text{S.17})$$

For  $k \rightarrow 0$ , we can neglect the quadratic term and approximate the dispersion relation by

$$E_{\mathbf{k}} \approx \sqrt{2Un_0\epsilon_{\mathbf{k}}} = \hbar k \sqrt{\frac{Un_0}{m}}. \quad (\text{S.18})$$

The sound velocity is defined as

$$c_s = \frac{\partial E_{\mathbf{k}}}{\partial(\hbar k)} = \sqrt{\frac{Un_0}{m}}. \quad (\text{S.19})$$

For large momenta we can write

$$E_{\mathbf{k}} = \epsilon_{\mathbf{k}} \sqrt{1 + \frac{2Un_0}{\epsilon_{\mathbf{k}}}} \approx \epsilon_{\mathbf{k}} \left(1 + \frac{Un_0}{\epsilon_{\mathbf{k}}}\right) = \epsilon_{\mathbf{k}} + Un_0. \quad (\text{S.20})$$



**Exercise 2. Temperature dependence of the superfluid fraction.**

In the lecture we calculated the number of condensed (superfluid) particles at zero temperature [Eq. (6.31)]. In this exercise we want to determine the temperature dependence of this fraction in the limit  $T \rightarrow 0$ .

- (a) Calculate the expectation value of the density of particles with momentum  $\mathbf{k}$ ,

$$n_{\mathbf{k}} := \frac{1}{\Omega} \langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \rangle. \quad (6)$$

*Hint. Use the fact that the Bogolyubov quasiparticles defined in Eq. (3) follow a Bose-Einstein distribution.*

- (b) Approximate the temperature dependence of this density,

$$\delta n_{\mathbf{k}}(T) := n_{\mathbf{k}}(T) - n_{\mathbf{k}}(T = 0), \quad (7)$$

in the limit  $T \rightarrow 0$ .

- (c) Calculate the temperature dependence of the density of condensed particles,

$$\delta n_0 = - \sum_{\mathbf{k}} \delta n_{\mathbf{k}}, \quad (8)$$

in the same limit. What happens in a two-dimensional system?

*Hint. Keep only the terms of lowest order in  $T$ .*

- (d) Calculate the expectation value  $\langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}^\dagger \rangle$ . What is the physical interpretation of this quantity?

**Solution.**

- (a) The Bose-Einstein distribution for the Bogolyubov quasiparticles reads

$$\langle \hat{\gamma}_{\mathbf{k}}^\dagger \hat{\gamma}_{\mathbf{k}} \rangle = \frac{1}{e^{\beta E_{\mathbf{k}}} - 1}. \quad (\text{S.21})$$

This allows us to easily calculate the particle number

$$\begin{aligned} \Omega n_{\mathbf{k}} &= \langle (u_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}}^\dagger - v_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}}) (u_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}} - v_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}}^\dagger) \rangle \\ &= u_{\mathbf{k}}^2 \langle \hat{\gamma}_{\mathbf{k}}^\dagger \hat{\gamma}_{\mathbf{k}} \rangle + v_{\mathbf{k}}^2 \langle \hat{\gamma}_{-\mathbf{k}}^\dagger \hat{\gamma}_{-\mathbf{k}} \rangle - u_{\mathbf{k}} v_{\mathbf{k}} (\langle \hat{\gamma}_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}} \rangle + \langle \hat{\gamma}_{-\mathbf{k}}^\dagger \hat{\gamma}_{\mathbf{k}}^\dagger \rangle) \\ &= u_{\mathbf{k}}^2 \langle \hat{\gamma}_{\mathbf{k}}^\dagger \hat{\gamma}_{\mathbf{k}} \rangle + v_{\mathbf{k}}^2 \langle \hat{\gamma}_{-\mathbf{k}}^\dagger \hat{\gamma}_{-\mathbf{k}} + 1 \rangle \\ &= (u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) \frac{1}{e^{\beta E_{\mathbf{k}}} - 1} + v_{\mathbf{k}}^2 \\ &= \frac{1 + \chi_{\mathbf{k}}^2}{1 - \chi_{\mathbf{k}}^2} \frac{1}{e^{\beta E_{\mathbf{k}}} - 1} + \frac{\chi_{\mathbf{k}}^2}{1 - \chi_{\mathbf{k}}^2}. \end{aligned} \quad (\text{S.22})$$

- (b) At  $T = 0$  the first term vanishes as  $\beta \rightarrow \infty$  and  $E_{\mathbf{k}} > 0$ , while the second term is independent from temperature. Therefore the density difference is given by

$$\Omega \delta n_{\mathbf{k}} = \frac{1 + \chi_{\mathbf{k}}^2}{1 - \chi_{\mathbf{k}}^2} \frac{1}{e^{\beta E_{\mathbf{k}}} - 1}. \quad (\text{S.23})$$

In the limit  $T \rightarrow 0$  we find  $\beta \rightarrow \infty$  such that the exponential  $e^{\beta E_{\mathbf{k}}}$  is strongly peaked around  $\mathbf{k} = 0$ . Therefore we can approximate  $\chi_{\mathbf{k}}$  for  $k \rightarrow 0$ . There we obtain

$$\begin{aligned} \chi_{\mathbf{k}} &= 1 + \frac{\hbar^2 k^2}{2mUn_0} - \sqrt{\left(1 + \frac{\hbar^2 k^2}{2mUn_0}\right)^2 - 1} \\ &= 1 + \frac{\hbar^2 k^2}{2mUn_0} - \sqrt{\frac{\hbar^2 k^2}{mUn_0} + \left(\frac{\hbar^2 k^2}{2mUn_0}\right)^2} \\ &\approx 1 - \frac{\hbar k}{\sqrt{mUn_0}}. \end{aligned} \quad (\text{S.24})$$

This leads to an approximation of the temperature-independent part of  $\delta n_{\mathbf{k}}$ :

$$\begin{aligned} \frac{1 + \chi_{\mathbf{k}}^2}{1 - \chi_{\mathbf{k}}^2} &\approx \frac{1 + 1 - \frac{2\hbar k}{\sqrt{mUn_0}} + \frac{\hbar^2 k^2}{Un_0 m}}{1 - 1 + \frac{2\hbar k}{\sqrt{mUn_0}} - \frac{\hbar^2 k^2}{Un_0 m}} \\ &\approx \frac{2 - \frac{2\hbar k}{\sqrt{mUn_0}}}{\frac{2\hbar k}{\sqrt{mUn_0}}} = \frac{\sqrt{mUn_0}}{\hbar k} - 1 \end{aligned} \quad (\text{S.25})$$

For finite  $\mathbf{k}$ , where  $\beta E_{\mathbf{k}} \gtrsim 1$ , we can approximate the Bose-Einstein distribution by the Boltzmann distribution

$$\frac{1}{e^{\beta E_{\mathbf{k}}} - 1} \approx e^{-\beta E_{\mathbf{k}}}, \quad (\text{S.26})$$

where we use the linear approximation for the energy,

$$E_{\mathbf{k}} \approx \sqrt{\frac{Un_0}{m}} \hbar k =: \hbar k c_s. \quad (\text{S.27})$$

Therefore, we obtain the approximation

$$\Omega \delta n_{\mathbf{k}} \approx \left(\frac{mc_s}{\hbar k} - 1\right) e^{-\beta \hbar k c_s}. \quad (\text{S.28})$$

- (c) In three dimensions, the density of condensed particles is given by

$$\delta n_0 = - \sum_{\mathbf{k}} \delta n_{\mathbf{k}} = - \int \frac{d^3 k}{(2\pi)^3} \delta n_{\mathbf{k}}. \quad (\text{S.29})$$

Here, we insert the approximation (S.28) and obtain

$$\begin{aligned} \Omega \delta n_0 &\approx - \int \frac{d^3 k}{(2\pi)^3} \left(\frac{mc_s}{\hbar k} - 1\right) e^{-\beta \hbar k c_s} \\ &= - \frac{1}{2\pi^2} \int dk \left(\frac{mc_s}{\hbar} k - k^2\right) e^{-\beta \hbar k c_s} \\ &= - \frac{1}{2\pi^2} \left(\frac{mc_s}{\hbar(\beta \hbar c_s)^2} - \frac{2}{(\beta \hbar c_s)^3}\right) \\ &\stackrel{T \rightarrow 0}{\approx} - \frac{mk_B^2}{2\pi^2 \hbar^3 c_s} T^2. \end{aligned} \quad (\text{S.30})$$

In two dimensions, a similar calculation would lead to a linear temperature-dependence,

$$\delta n_0 \propto T. \quad (\text{S.31})$$

However, in this calculation we underestimated the contributions for very small  $k$ : For  $\beta E_{\mathbf{k}} \lesssim 1$  we can approximate the Bose-Einstein distribution by

$$\frac{1}{e^{\beta E_{\mathbf{k}}} - 1} \approx \frac{1}{\beta E_{\mathbf{k}}} \approx \frac{1}{c_s \hbar k}. \quad (\text{S.32})$$

Due to the factor of  $k$  in the three-dimensional case, this contribution can be neglected. However, in two dimensions, the integral for  $\delta n_0$  diverges,

$$\Omega \delta n_0 \approx \int \frac{d^2 k}{(2\pi)^2} \frac{m c_s}{\hbar k} \frac{1}{c_s \hbar k} = \frac{m}{2\pi \hbar^2} \int \frac{dk}{k} \longrightarrow \infty, \quad (\text{S.33})$$

such that there exists no superfluid condensate at finite temperature.

(d) We can perform a similar calculation as in Eq. (S.22):

$$\begin{aligned} \langle \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{-\mathbf{k}}^\dagger \rangle &= \left\langle \left( u_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}}^\dagger - v_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}} \right) \left( u_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}}^\dagger - v_{\mathbf{k}} \hat{\gamma}_{\mathbf{k}} \right) \right\rangle \\ &= -u_{\mathbf{k}} v_{\mathbf{k}} \left( \langle \hat{\gamma}_{\mathbf{k}}^\dagger \hat{\gamma}_{\mathbf{k}} \rangle + \langle \hat{\gamma}_{-\mathbf{k}} \hat{\gamma}_{-\mathbf{k}}^\dagger \rangle \right) + u_{\mathbf{k}}^2 \langle \hat{\gamma}_{\mathbf{k}}^\dagger \hat{\gamma}_{-\mathbf{k}}^\dagger \rangle + v_{\mathbf{k}}^2 \langle \hat{\gamma}_{\mathbf{k}} \hat{\gamma}_{-\mathbf{k}} \rangle \\ &= -u_{\mathbf{k}} v_{\mathbf{k}} \left( \frac{2}{e^{\beta E_{\mathbf{k}}} - 1} + 1 \right) \\ &= -\frac{\chi_{\mathbf{k}}}{1 - \chi_{\mathbf{k}}^2} \frac{e^{\beta E_{\mathbf{k}}} + 1}{e^{\beta E_{\mathbf{k}}} - 1} \\ &= -\frac{\chi_{\mathbf{k}}}{1 - \chi_{\mathbf{k}}^2} \left[ \tanh \left( \frac{1}{2} \beta E_{\mathbf{k}} \right) \right]^{-1}. \end{aligned} \quad (\text{S.34})$$

This quantity can be physically understood as the rate at which particles are exchanged with the condensate.