

**Exercise 1. Tight-binding model**

Consider non-interacting particles on a lattice of  $N$  sites with periodic boundary condition, i.e. on a discrete ring. The position variable becomes a discrete variable  $\vec{r} \rightarrow x_i$  and the field operators with spin label  $s$ ,  $\Psi_s^{(\dagger)}(\vec{r})$ , become  $\Psi_{s,i}^{(\dagger)} \equiv \Psi_s^{(\dagger)}(x_i)$ .

- (a) Find the eigensolutions of the problem for the Hamiltonian

$$\mathcal{H} = -t \sum_s \sum_{j=0}^{N-1} \left( \Psi_{s,j+1}^\dagger \Psi_{s,j} + \Psi_{s,j}^\dagger \Psi_{s,j+1} \right), \quad (1)$$

by the use of the Fourier transform of the field operators

$$a_{s,k} = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{-ijk} \Psi_{s,j}, \quad k \in \left\{ \frac{2\pi}{N} \left( n - \left\lfloor \frac{N-1}{2} \right\rfloor \right) \mid n = 0, 1, 2, \dots, N-1 \right\}, \quad (2)$$

where  $[x]$  denotes the integer part of  $x$ . Write the result in occupation number basis of the eigenstates. How can the terms  $\Psi_{s,j+1}^\dagger \Psi_{s,j}$  be interpreted?

**Solution.** The interpretation of the term  $\Psi_{s,j+1}^\dagger \Psi_{s,j}$  is that a particle hops from site  $j$  to site  $j+1$ , from where the term *hopping model* arises.

Using the inverse transformation,

$$\Psi_{s,j} = \frac{1}{\sqrt{N}} \sum_k e^{ijk} a_{s,k} \quad (S.1)$$

gives

$$\mathcal{H} = -2t \sum_{s,k} \cos(k) a_{s,k}^\dagger a_{s,k} = -2t \sum_{s,k} \cos(k) n_{s,k}, \quad (S.2)$$

where  $n_{s,k}$  is the occupation number (operator) of the one-particle state labeled by quasi-momentum  $k$  and spin  $s$ .

- (b) Given the particles are fermionic, the transformation

$$b_{s,k} = \frac{1}{\sqrt{N}} \sum_j e^{-ijk} \Psi_{s,j}^\dagger \quad (3)$$

diagonalizes the Hamiltonian as well. Rewrite the problem in the occupation number basis of the  $b_k^{(\dagger)}$  operators. What is the difference between the two formulations, how are they related?

**Solution.** Repeating the calculation from above, we find

$$\mathcal{H} = 2t \sum_{s,k} \cos(k) b_{s,k}^\dagger b_{s,k} = 2t \sum_{s,k} \cos(k) \tilde{n}_{s,k}, \quad (S.3)$$

where  $\tilde{n}_{s,k}$  is the occupation number of the *one-hole* state labeled by quasi-momentum  $k$  and spin  $s$ .

The formulations differ by the interpretation of the particles corresponding to the operators  $a$  and  $b$ . In the first case we consider the fermionic particles we started with, in the second we consider the fermionic anti-particles of the initial fermions. Correspondingly, the vacuum associated with the occupation basis is

once the vacuum of having no particles in the system and once the vacuum of having no anti-particles in the system. Having no anti-particles is equivalent to having all states filled with particles.

There is a one-to-one correspondence of the eigensolutions to the problem in either formulation: the system has *particle-hole symmetry*.

- (c) Consider now a fixed number of  $M$  particles to be in the system. Calculate the leading order of the entropy in the high temperature expansion  $T \rightarrow \infty$ . Compare it to the case of free fermions. Can you recover the particle-hole symmetry in the result?

**Solution.** As usual, the entropy is given by

$$S = -\frac{\partial F}{\partial T}, \quad (\text{S.4})$$

with the free energy

$$F = -\frac{1}{\beta} \log Z. \quad (\text{S.5})$$

Unlike in the case of free particles, the spectrum is bounded. Therefore, in the high-temperature limit the partition sum can be approximated by

$$Z = \text{tr} e^{-\beta \mathcal{H}} = \text{tr} \left( \sum_{l=0}^{\infty} \frac{(-\beta \mathcal{H})^l}{l!} \right) = \text{tr}(\mathcal{H}^0) + \sum_{l=1}^{\infty} \frac{(-\beta)^l \text{tr} \mathcal{H}^l}{l!} = \frac{(2N)!}{(2N-M)!M!} + \mathcal{O}(T^{-1}), \quad (\text{S.6})$$

where  $2N$  corresponds to the total number of available states for spin-1/2 particles. From this follows that

$$S \approx k_B \log \frac{(2N)!}{(2N-M)!M!} \quad (\text{S.7})$$

in leading order. The entropy in this system is bounded and temperature independent in the high-temperature limit, while the entropy of a free Fermi gas is not. The origin of the difference lies within the (un)boundedness of the spectra.

The particle-hole symmetry can be seen by replacing the number of particles  $M$  by the number of holes  $2N - M$ , which leaves the expression for the entropy invariant.

- (d) Find the magnetic susceptibility using the fluctuation-dissipation theorem

$$\chi = \frac{1}{N} \frac{1}{k_B T} [\langle M_z^2 \rangle - \langle M_z \rangle^2], \quad (\text{4})$$

where the magnetization operator is defined by

$$M_z = \frac{g\mu_B}{\hbar} \sum_j S_j = \mu_B \sum_{j=0}^N \sum_{s=\pm 1} s \Psi_{s,j}^\dagger \Psi_{s,j}. \quad (\text{5})$$

Determine the result in the low-temperature limit by taking  $N \rightarrow \infty$ .

*Hint:* Rewrite the magnetization operator in occupation basis and use the Fermi-Dirac distribution.

**Solution.** We first observe that

$$\sum_{j=0}^N \Psi_{s,j}^\dagger \Psi_{s,j} = \sum_k a_{s,k}^\dagger a_{s,k} \quad (\text{S.8})$$

and hence, with  $\langle n_{1,k} \rangle = \langle n_{-1,k} \rangle$ ,

$$\langle M_z \rangle = \mu_B \sum_{k,s} s \langle n_{s,k} \rangle = 0. \quad (\text{S.9})$$

We are left with calculating  $\langle M_z^2 \rangle$ :

$$\langle M_z^2 \rangle = \mu_B^2 \sum_{s,s'} \sum_{k,k'} ss' \langle a_{s,k}^\dagger a_{s,k} a_{s',k'}^\dagger a_{s',k'} \rangle = \mu_B^2 \sum_{s,s'} \sum_{k,k'} ss' \langle n_{s,k} n_{s',k'} \rangle \quad (\text{S.10})$$

$$= \mu_B^2 \sum_{k,k'} [\langle n_{1,k} n_{1,k'} \rangle + \langle n_{-1,k} n_{-1,k'} \rangle - \langle n_{-1,k} n_{1,k'} \rangle - \langle n_{1,k} n_{-1,k'} \rangle] . \quad (\text{S.11})$$

As we are dealing with non-interacting fermions, we find

$$\langle n_{s,k} n_{s',k'} \rangle = \begin{cases} \langle n_{1,k} \rangle & k = k', \quad s = s' \\ \langle n_{s,k} \rangle \langle n_{s',k'} \rangle & \text{otherwise} \end{cases} \quad (\text{S.12})$$

and by using again that  $\langle n_{1,k} \rangle = \langle n_{-1,k} \rangle \equiv \langle n_k \rangle$ , we arrive at

$$\langle M_z^2 \rangle = \mu_B^2 2 \sum_k [\langle n_k \rangle - \langle n_k \rangle^2] . \quad (\text{S.13})$$

The states are occupied according to the Fermi-Dirac distribution and the susceptibility is therefore

$$\chi = \frac{1}{N} \frac{1}{k_B T} \mu_B^2 \sum_k \frac{1}{2 \cosh^2 \{\beta[-t \cos(k) - \mu/2]\}} . \quad (\text{S.14})$$

In the limit  $N \rightarrow \infty$  we can approximate the sum by an integral to obtain

$$\chi = \frac{1}{k_B T} \mu_B^2 \int_{-\pi}^{\pi} dk \frac{1}{2 \cosh^2 \{\beta[-t \cos(k) - \mu/2]\}} = \frac{1}{k_B T} \mu_B^2 \int_{-\infty}^{\infty} d\varepsilon N(\varepsilon) \frac{1}{4 \cosh^2 \{\beta[\varepsilon - \mu]/2\}} , \quad (\text{S.15})$$

where  $N(\varepsilon)$  denotes the density of states. In the low-temperature limit only energy values around the chemical potential, which in this case coincides with the Fermi energy, contribute. This allows us to approximate

$$\int_{-\infty}^{\infty} d\varepsilon N(\varepsilon) \frac{1}{4 \cosh^2 \{\beta[\varepsilon - \mu]/2\}} \approx \int_{-\infty}^{\infty} d\varepsilon N(\varepsilon_F) \frac{1}{4 \cosh^2 \{\beta[\varepsilon - \mu]/2\}} = k_B T N(\varepsilon_F) . \quad (\text{S.16})$$

The susceptibility in the low-temperature limit reads

$$\chi = \mu_B^2 N(\varepsilon_F) . \quad (\text{S.17})$$

Note that is exactly the same form as for the free Fermi gas in three dimensions (cf. script). Actually, this form holds for any non-interacting Fermi system. What changes is the density of states at the Fermi energy. Formulating the problem in second quantized form therefore simplifies the calculation significantly.

- (e\*) Restricting the problem to spinless Fermions and turning on a magnetic field (introduced in a specific gauge) perpendicular to the ring, changes the Hamiltonian to

$$\mathcal{H} = -t \sum_{j=0}^{N-1} \left( e^{-i\varphi} \Psi_{j+1}^\dagger \Psi_j + e^{i\varphi} \Psi_j^\dagger \Psi_{j+1} \right) . \quad (6)$$

In this case, calculate the expectation value of the current density operator

$$j = \frac{1}{N} \sum_n j_n , \quad j_n = -i \left( \Psi_{n+1}^\dagger \Psi_n - \Psi_n^\dagger \Psi_{n+1} \right) . \quad (7)$$

Interpret the current density operator in terms of particles hopping from site to site.

**Solution.** The Hamiltonian can still be diagonalized by the corresponding Fourier transform Eq. (2):

$$\mathcal{H} = -2t \sum_k \cos(k - \varphi) a_k^\dagger a_k = -2t \sum_k \cos(k - \varphi) n_k = -2t \sum_k \cos(k) n_{k+\varphi} . \quad (\text{S.18})$$

The phase factor in the hopping model leads to a shift in the dispersion relation.

For the expectation value of the current density operator we find

$$\langle j \rangle = \frac{-i}{N} \sum_n \frac{1}{N} \sum_{k,k'} \left[ e^{in(k-k')} e^{ik} \langle a_k^\dagger a_{k'} \rangle + h.c. \right] = \frac{1}{N} \sum_k 2 \sin(k) \langle n_k \rangle, \quad (\text{S.19})$$

where we used that

$$\Psi_{n+1}^\dagger \Psi_n = \frac{1}{N} \sum_{k,k'} e^{in(k-k')} e^{ik} a_k^\dagger a_{k'}. \quad (\text{S.20})$$

In the limit of  $N \rightarrow \infty$ , at fixed chemical potential  $\mu = 0$ , this becomes

$$\langle j \rangle \rightarrow \int_{-\pi}^{\pi} 2 \sin(k) \langle n_k \rangle = \int_{-\pi}^{\pi} dk 2 \sin(k + \varphi) \langle n_{k+\varphi} \rangle \quad (\text{S.21})$$

$$= \int_{-\pi}^{\pi} dk 2 [\sin(k) \cos(\varphi) + \sin(\varphi) \cos(k)] \frac{1}{e^{-2t\beta \cos(k)} + 1} \quad (\text{S.22})$$

$$= \sin(\varphi) \int_{-\pi}^{\pi} dk 2 \cos(k) \frac{1}{e^{-2t\beta \cos(k)} + 1}, \quad (\text{S.23})$$

and we arrive at the temperature dependence given in figure 1.

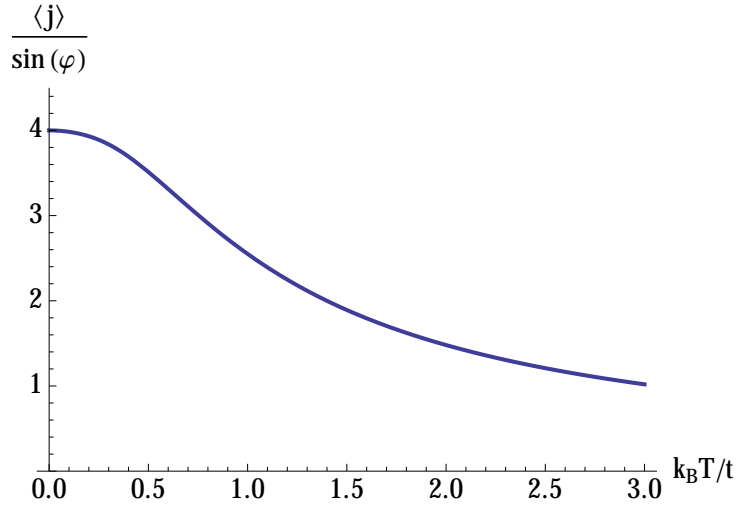


Figure 1: Temperature dependence of the current expectation value.

We conclude that a magnetic field induces an equilibrium persistent current in the ring.

In the limit of vanishing magnetic field (linearization about  $\varphi = 0$ ), the same result could directly be obtained from the fluctuation-dissipation theorem

$$\frac{\partial \langle j \rangle}{\partial \varphi} = \frac{Nt}{k_B T} (\langle j^2 \rangle - \langle j \rangle^2) = \frac{Nt}{k_B T} \langle j^2 \rangle, \quad (\text{S.24})$$

with

$$\langle j^2 \rangle = \frac{4}{N^2} \sum_{k,k'} \sin(k) \sin(k') \langle n_k n_{k'} \rangle = \frac{4}{N^2} \left[ \sum_{k,k'} \sin(k) \sin(k') \langle n_k \rangle \langle n_{k'} \rangle + \sum_k \sin^2(k) (\langle n_k \rangle - \langle n_k \rangle^2) \right] \quad (\text{S.25})$$

$$= \frac{4}{N^2} \left[ \left( \sum_k \sin(k) \langle n_k \rangle \right)^2 + \sum_k \sin^2(k) \langle n_k \rangle (1 - \langle n_k \rangle) \right] = \frac{4}{N^2} \sum_k \sin^2(k) \langle n_k \rangle (1 - \langle n_k \rangle) \quad (\text{S.26})$$

where we used that

$$\langle n_k n_{k'} \rangle = \begin{cases} \langle n_k \rangle \langle n_{k'} \rangle & k \neq k' \\ \langle n_k \rangle & k = k' \end{cases} \quad \text{and} \quad \langle n_k \rangle = \langle n_{-k} \rangle. \quad (\text{S.27})$$

Taking anew the limit  $N \rightarrow \infty$  gives, with the explicit form of  $\langle n_k \rangle$ ,

$$\langle j^2 \rangle \rightarrow \frac{4}{N} \int_{-\pi}^{\pi} dk \sin^2(k) \frac{e^{-2t\beta \cos(k)}}{(e^{-2t\beta \cos(k)} + 1)^2} = \frac{4}{N} \int_{-\pi}^{\pi} dk \sin(k) \frac{1}{-2t\beta} \frac{d}{dk} \frac{1}{(e^{-2t\beta \cos(k)} + 1)} \quad (\text{S.28})$$

$$= \frac{2k_B T}{tN} \int_{-\pi}^{\pi} dk \cos(k) \frac{1}{(e^{-2t\beta \cos(k)} + 1)}, \quad (\text{S.29})$$

and we recover

$$\frac{\partial \langle j \rangle}{\partial \varphi} = \int_{-\pi}^{\pi} dk 2 \cos(k) \frac{1}{(e^{\beta \cos(k)} + 1)}. \quad (\text{S.30})$$

### Exercise 2. *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)

$$\mathcal{H}_{N+1} = -J \sum_{i=1}^N \sigma_i \sigma_{i+1}, \quad \sigma_i = \pm 1. \quad (8)$$

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

(a) Compute the partition function  $Z_{N+1}$  using a recursive procedure.

**Solution.** We can split off the last spin in the Hamiltonian as follows:

$$\mathcal{H}_{N+1} = -J \sum_{i=1}^{N-1} \sigma_i \sigma_{i+1} - J \sigma_N \sigma_{N+1} \quad (\text{S.31})$$

$$= \mathcal{H}_N - J \sigma_N \sigma_{N+1}. \quad (\text{S.32})$$

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:

$$Z_{N+1} = \sum_{\{\sigma_i = \pm 1\}} \left[ e^{-\beta \mathcal{H}_N} \sum_{\sigma_{N+1} = \pm 1} e^{\beta J \sigma_N \sigma_{N+1}} \right] \quad (\text{S.33})$$

$$= \sum_{\{\sigma_i = \pm 1\}} e^{-\beta \mathcal{H}_N} \left( 2 \cosh(\beta J \sigma_N) \right) \quad (\text{S.34})$$

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

$$Z_{N+1} = \sum_{\{\sigma_i = \pm 1\}} e^{-\beta \mathcal{H}_{N-1}} \sum_{\sigma_N = \pm 1} e^{\beta J \sigma_{N-1} \sigma_N} \left( 2 \cosh(\beta J \sigma_N) \right) \quad (\text{S.37})$$

$$= \left( 2 \cosh \beta J \right) \sum_{\{\sigma_i = \pm 1\}} \left[ e^{-\beta \mathcal{H}_{N-1}} \left( 2 \cosh(\beta J \sigma_{N-1}) \right) \right], \quad (\text{S.38})$$

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

$$Z_{N+1} = \left( 2 \cosh \beta J \right)^{N-2} \sum_{\sigma_1, \sigma_2 = \pm 1} e^{\beta J \sigma_1 \sigma_2} \left( 2 \cosh(\beta J \sigma_2) \right) \quad (\text{S.39})$$

$$= \left( 2 \cosh \beta J \right)^{N-1} \sum_{\sigma_1 = \pm 1} \left( 2 \cosh(\beta J \sigma_1) \right) \quad (\text{S.40})$$

$$= 2 \left( 2 \cosh \beta J \right)^N \quad (\text{S.41})$$

<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:

$$Z_{N+1} = \sum_{\{\sigma_i = \pm 1\}} \underbrace{\exp(-\beta \mathcal{H}_N)}_{=Z_N} 2 \cosh \beta J \quad (\text{S.35})$$

$$= Z_2 (2 \cosh \beta J)^{N-1} = 2 (2 \cosh \beta J)^N. \quad (\text{S.36})$$

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

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

$$\mathcal{H} = -J \sum_{i=1}^N S_i \quad (\text{S.42})$$

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

$$Z = (2 \cosh \beta J)^N \quad (\text{S.43})$$

The additional factor 2 appearing in Eqs. (S.36) and (S.41) 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) 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.

**Solution.** The energy, entropy and response functions follow directly from the partition function  $Z_{N+1}$  as follows:

The free energy is given by

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

from which we can compute the entropy as

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

Next, the internal energy can be found via

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

Then the heat capacity can be found through computing

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

or

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

Both evaluate to

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

The heat capacity (see figure 2) shows no dependence on the sign of  $J$ , and is therefore identical for either a ferromagnet ( $J < 0$ ) or an antiferromagnet ( $J > 0$ ).

Comparing the results to the ideal paramagnet (see script), one sees that there is an exact correspondence if we set  $J = Hm$  (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) Calculate the magnetization density  $m = \langle \sigma_j \rangle$  where the spin  $\sigma_j$  is not close to either end of the chain. Which symmetries does the system exhibit? Interpret your result in terms of symmetry arguments.

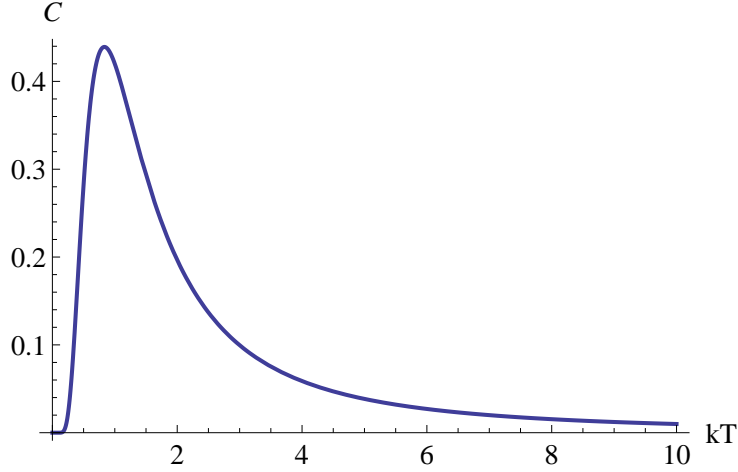


Figure 2: Heat capacity of the Ising chain.

**Solution.** 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\*) 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  $T \rightarrow 0$ .

**Solution.** 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

$$Z_{N+1} = 2 \prod_{k=1}^N (2 \cosh \beta J_k), \quad (\text{S.44})$$

while, using the property  $\sigma_k^2 = 1$ , the correlation function reads

$$\langle \sigma_i \sigma_j \rangle = \frac{1}{Z_{N+1}} \sum_{\{\sigma_k = \pm 1\}} (\sigma_i \sigma_{i+1}) (\sigma_{i+1} \sigma_{i+2}) \dots (\sigma_{j-1} \sigma_j) \exp \left( \sum_l \beta J_l \sigma_l \sigma_{l+1} \right) \quad (\text{S.45})$$

$$= \frac{1}{Z_{N+1}} \frac{1}{\beta^{j-i}} \left. \frac{\partial^{j-i} Z_{N+1}}{\partial J_i \dots \partial J_{j-1}} \right|_{J_k=J} = (\tanh \beta J)^{|j-i|} = e^{-|j-i|/\xi} \quad (\text{S.46})$$

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\*) Calculate the magnetic susceptibility in zero magnetic field using the fluctuation-dissipation relation of the form

$$\frac{\chi(T)}{N} = \frac{1}{k_B T} \sum_{j=-N/2}^{N/2} \Gamma_{0j}, \quad (9)$$

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  $N$ .

**Solution.** Using the result of d) we find

$$\sum_{j=-\infty}^{\infty} \langle \sigma_0 \sigma_j \rangle = \sum_{j=-\infty}^{\infty} (\tanh \beta J)^{|j|} = \frac{1 + \tanh \beta J}{1 - \tanh \beta J} = \exp(2\beta J). \quad (\text{S.47})$$

For the magnetic susceptibility at zero field we therefore find

$$\chi(T) = N \frac{e^{2J/k_B T}}{k_B T} \quad (\text{S.48})$$

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.

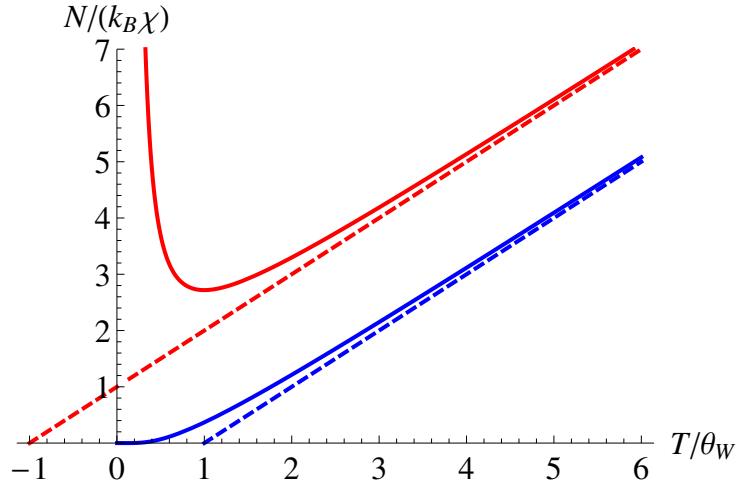


Figure 3: Inverse susceptibility (continuous line) with high-temperature extrapolation for the Weiss temperature (dashed line) for ferromagnetic coupling,  $J > 0$  (blue), and antiferromagnetic coupling,  $J < 0$  (red).

(f\*) 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.** Using the result from part (e), we write

$$\frac{1}{\chi(T)} = \frac{k_{\text{B}}T}{N} e^{-2\beta J} \quad (\text{S.49})$$

$$= \frac{k_{\text{B}}T}{N} [1 - 2\beta J + \mathcal{O}((2\beta J)^2)] \quad (\text{S.50})$$

$$\approx \frac{k_{\text{B}}}{N} \left( T - \underbrace{\frac{2J}{k_{\text{B}}}}_{=\Theta_{\text{W}}} \right). \quad (\text{S.51})$$

The Weiss temperature  $\Theta_{\text{W}} = 2J/k_{\text{B}}$  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 3.