

Exercise 10.1 Magnetostriction in a Spin-Dimer-Model

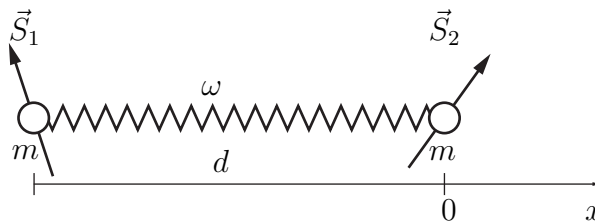
As in exercise 8.1, we again start with a dimer consisting of two (quantum) spins, $s = 1/2$, described by the Hamiltonian

$$\mathcal{H}_0 = J \left(\vec{S}_1 \cdot \vec{S}_2 + 3/4 \right), \quad (1)$$

with $J > 0$. This time, however, the distance between the spins is not fixed but they are connected by a spring (cf. Fig.) such that the Hamiltonian of the system reads

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

i.e., the spin-coupling constant depends on the distance between the two sites, where $\lambda \geq 0$.



In the above figure, m is the mass of the two constituents, $m\omega^2$ is the spring constant and d denotes the equilibrium distance between the two spins (in the case of no spin-spin interaction) from which the displacement x is measured.

- (a) Write the Hamiltonian (2) in second quantized form and calculate the partition sum, the internal energy, the specific heat and the entropy. In the limit $T \rightarrow 0$, discuss the entropy for different values of λ .

Hint: Set $\hbar = 1$ and introduce an operator \hat{n}_t defined through

$$\langle \sigma | \hat{n}_t | \sigma \rangle = \begin{cases} 1 & \sigma \text{ is a triplet,} \\ 0 & \sigma \text{ is the singlet,} \end{cases} \quad (3)$$

where $|\sigma\rangle$ denotes the spin-dependent part of the dimer state. Trace first over the spin-degrees of freedom.

- (b) Calculate the expectation value of the distance of the two spins, $\langle d + \hat{x} \rangle$, as well as the fluctuations $\langle (d + \hat{x})^2 \rangle$.

How are these quantities affected by a magnetic field in z -direction, i.e., by an additional term in (2) of the form

$$\mathcal{H}_m = -g\mu_B H \sum_{i,m} S_{i,m}^z \quad ? \quad (4)$$

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

$$\mathcal{H}_{el} = -q(d + \hat{x}) \cdot E. \quad (5)$$

Calculate the zero-field susceptibility of the dimer,

$$\chi_0^{(el)} = - \left. \frac{\partial^2 F}{\partial E^2} \right|_{E=0}, \quad (6)$$

and compare your result with the fluctuation-dissipation theorem which states

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

Plot the zero-field susceptibility as a function of the applied magnetic field H and discuss your result.

Exercise 10.2 The Ising Model in the High-Temperature Limit

Consider the Ising model with nearest neighbor interactions in the presence of a homogeneous magnetic field h ,

$$\mathcal{H} = -\frac{J}{2} \sum_{\langle i,j \rangle} S_i \cdot S_j - h \sum_i S_i, \quad J > 0, \quad (8)$$

where the spins assume the values $S_i = \pm S$ along the magnetic field and the sum $\sum_{\langle i,j \rangle}$ runs over nearest neighboring sites on the lattice. The number of spins is very large, $N \gg 1$, such that surface effects may be neglected.

- a) Determine the partition function in the high-temperature limit $\beta J \ll 1$.

Hint: Note that for $\beta J \ll 1$, one may neglect bond-bond correlations and the partition function simplifies to

$$Z \approx \sum_{\{S_i\}} e^{\beta h \sum_i S_i} \left(1 + \frac{\beta J}{2} \sum_j \sum_{m \in \Lambda_j} S_j \cdot S_m \right), \quad (9)$$

where Λ_j represents the set of nearest neighbors of site j such that $|\Lambda_j| = z$ with the coordination number z .

- b) Calculate the spin susceptibility at $h = 0$. In analogy to the lecture notes (Section 3.4.6), plot $1/\chi_0$ as a function of temperature and extrapolate the high- T limit to lower temperatures to find the intersection on the T -axis. What is the physical interpretation of the intersection temperature?

Office Hours: Monday, November 29, 10 – 12 am (HIT K 12.2, Adrien Bouhon)