Statistical Physics
Exercise 10

Exercise 10.1 Magnetostriction in a Spin-Dimer-Model

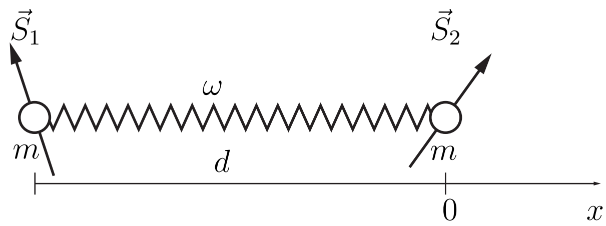
As in exercise 8.1, we again start with a dimer consisting of two (quantum) spins, $s = 1/2$, described by the Hamiltonian

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

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

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

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 $T \to 0$, discuss the entropy for different values of λ.
Hint: Set $\hbar = 1$ and introduce an operator $\hat{n}_t$ defined through

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

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

$$\mathcal{H}_m = -g\mu_B H \sum_i S_i^z \quad ? \tag{4}$$

(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,

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

Calculate the zero-field susceptibility of the dimer,

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

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

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

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,

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

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

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

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 27, 9 – 11 am (HIT K 23.3, David Oehri)