Prof. Igor Lesanovsky
Gabriele Perfetto
Albert Cabot

Advanced Statistical Physics
Problem Class 4
Tübingen 2022

10/05/2022

Please encircle the questions you have solved and are able to present/discuss in class.

4.1(a)	4.1(b)	4.1(c)	4.1(d)	4.2(a)	4.2(b)

Problem 4.1 (5 points)

In this exercise we start discussing the *quantum-classical mapping*. This topic will be addressed in more detail in the next tutorial sheet. Here, we consider a simplified, yet instructive, case where all the calculations can be performed exactly: the classical Ising model in one spatial dimension $d = 1$. We will show that it can be mapped into a quantum spin Hamiltonian in zero dimension $d = 0$ (a single spin). We have already seen the one-dimensional classical Ising model, whose Hamiltonian (energy function) with the usual notation adopted in the script reads as follows

$$E = -\epsilon \sum_{i=1}^{N} s_{ia} s_{(i+1)a} - H \sum_{i=1}^{N} s_{ia}. \tag{1}$$

We assume in this exercise periodic boundary conditions $s_{aN+a} = s_a$. For brevity we will also denote $h = \beta H$ and $k = \beta\epsilon$. Note an important point: in Eq. (1) we reintroduced the lattice spacing a, which in the lectures was set to 1. The volume (length) of the chain in dimensionful units is therefore $L = Na$, where N is the total number of spins.
The quantum-classical mapping is constructed by making use of the transfer matrix, which allows to draw a connection between the Feynmann imaginary path integral and the partition function of a classical system. The partition function Z with the transfer matrix T can be written as

$$Z = \sum_{s_1=\pm1} \sum_{s_2=\pm1} \cdots \sum_{s_N=\pm1} \langle s_1| T |s_2\rangle \langle s_2| T |s_3\rangle \dots \langle s_n| T |s_1\rangle = \mathrm{Tr}(T^N). \tag{2}$$

Here we have introduced a 2-dimensional Hilbert space on each lattice site

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \sum_{s=\pm1} |s\rangle \langle s| = \mathbb{I}, \tag{3}$$

and $\mathbb{I}$ denotes the 2×2 identity matrix. The transfer matrix T is the same as in the first exercise sheet. We recall also the definition of the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4}$$

In this sheet we want to write T as

$$T = e^{-aH}, \tag{5}$$

which allows to write Eq. (2) as

$$Z = \mathrm{Tr}(T^N) = \mathrm{Tr}(e^{-aNH}) = \mathrm{Tr}(e^{-LH}). \tag{6}$$

The latter equation provides a deep and clear physical interpretation of Eq. (2). The original one-dimensional lattice can be interpreted as the "temporal axis" along which the dynamics under the quantum Hamiltonian H proceeds. The transfer matrix, from Eq. (6), then plays the role of the imaginary-time evolution operator for a time step of length a. The total time evolution for a time interval $L = Na$ is split into the time evolution over N time steps a upon inserting N resolutions of the identity in Eq. (3) into Eq. (2). Note that this is exactly the construction that you have for the Feynmann path integral in the Lagrangian formulation of quantum mechanics (and more generally in quantum field theory). Identifying the Hamiltonian operator H in Eq. (6) is usually infeasible in full generality and one has to consider a particular scaling for the coupling constants of the model and/or the lattice spacing a. The case of the classical $1d$ Ising model in Eq. (1) is, however, special as it allows for a completely general derivation of the Hamiltonian H. This is what we are going to do next.

(a) Show that the transfer matrix T of the $1d$ Ising model in Eq. (1) can be written as follows

$$\begin{aligned} T &= (e^k \cosh(h))\mathbb{I} + e^{-k}\sigma_1 + (e^k \sinh(h))\sigma_3 \\ &= C \exp(c_1\sigma_1 + c_2\sigma_2 + c_3\sigma_3), \end{aligned} \tag{7}$$

with the coefficients fixed as

$$C = \sqrt{2\sinh(2k)}, \tag{8}$$
$$c_2 = 0, \tag{9}$$
$$c_3 = c_1 e^{2k}\sinh(h), \tag{10}$$

and c_1 the solution of the equation

$$\tanh\left(c_1\sqrt{1+e^{4k}\sinh^2(h)}\right) = \frac{\sqrt{1+e^{4k}\sinh^2(h)}}{e^{2k}\cosh(h)}. \tag{11}$$

(**1 point**)
Hint: Expand the exponential in the second line of Eq. (7) in a power series and then use the following useful identities

$$(c_1\sigma_1 + c_2\sigma_2 + c_3\sigma_3)^{2n} = r^{2n}, \tag{12}$$
$$(c_1\sigma_1 + c_2\sigma_2 + c_3\sigma_3)^{2n+1} = (c_1\sigma_1 + c_2\sigma_2 + c_3\sigma_3)r^{2n}, \tag{13}$$

with $r = \sqrt{c_1^2 + c_2^2 + c_3^2}$. The coefficients C, c_1, c_2, c_3 are then fixed by matching the result of the expansion with the first line in Eq. (7).

(b) Using the result of the previous point, identify the quantum Hamiltonian H defined by Eq. (5). In the following points, to simplify the calculations, we will set the magnetic field to zero $h = 0$. (**1 point**)

(c) Write the Hamiltonian H for zero magnetic field $h = 0$. Which Hamiltonian do you obtain? Diagonalize it and find its eigenvalues and eigenvectors. Compute the energy difference

$$m = E_1 - E_0, \tag{14}$$

between the first excited state E_1 and the ground state E_0. What is the relation between m and the correlation length ξ (derived in the lecture script and in the first sheet)? Comment and interpret the result physically. (**2 points**)

(d) Compute the ground state energy E_0 of the quantum Hamiltonian for zero magnetic field $h = 0$. What is the relation between E_0 and the free energy density $f = F/L$ of the one-dimensional classical Ising model in Eq. (1)? Comment and interpret the result physically. (**1 point**)

Problem 4.2 (5 points)

We consider a dimer consisting of two quantum spin-$1/2$ particles with the Hamiltonian

$$H_s = J\left(\vec{S}_1\cdot\vec{S}_2 + \frac{3}{4}\right), \tag{15}$$

with $J > 0$ and $\vec{S}_i = \left(\frac{\sigma_i^x}{2}, \frac{\sigma_i^y}{2}, \frac{\sigma_i^z}{2}\right)$ and $i = 1, 2$. The distance between the two spins is not fixed and they are connected

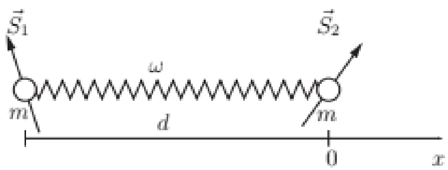

Figure 1: System of two quantum spins of mass m, whose interaction is mediated by a spring and equilibrium elongation d.

to each other by a spring. The spin–spin coupling constant depends on the distance between the two spins such that the Hamiltonian of the system is

$$H_{so} = H_o + (1 - \lambda x)H_s,$$
$$H_o = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2. \tag{16}$$

Here H_o is the usual Hamiltonian of the quantum harmonic oscillator in one spatial dimension, m is the mass of the two spin particles, $m\omega^2$ is the spring constant, and x denotes the displacement from the equilibrium distance d between the two spins as shown in Fig. 1. In this exercise we assume that the coupling constant λ between the spins and the harmonic oscillator is non-negative $\lambda \geq 0$.

(a) Calculate the canonical partition function, the internal energy, the specific heat and the entropy for the Hamiltonian H_{so} in Eq. (16). Discuss the behavior of the entropy in the limit $T \to 0$ for different values of λ. Is there a violation of the third law of thermodynamics ? (**3 points**)

Hint: You can decouple the spin and the oscillator degrees of freedom in H_{so} in Eq. (16) by rewriting the Hamiltonian in terms of the total spin operator $\vec{S} = \vec{S}_1 + \vec{S}_2$. Rewrite the Hamiltonian H_{so} in the form

$$H_{so} = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 X^2 + Jn_t - \frac{\lambda^2 J^2 n_t^2}{2m\omega^2}, \tag{17}$$

with $n_t = \vec{S}^2/2$ and $X = x - \frac{\lambda J n_t}{m\omega^2}$.

Hint: Remember that the spectrum of the Hamiltonian of the harmonic oscillator H_o is given by

$$H_o|n\rangle = E_n|n\rangle, \quad \text{with} \quad E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad \text{with} \quad n = 0, 1, 2...\infty. \tag{18}$$

(b) Calculate the expectation value of the distance between the two spins, $\langle d + x\rangle$, as well as $\langle (d + x)^2\rangle$. (**2 points**)