# Advanced statistical mechanics II

(SS 16, FU Berlin)

**Problem sheet 7**

Due date: June 14th, 2016

## Problems

**19. Two Spins (1+1+1+2+1+2+1)**

We first consider the Hilbert-space of one spin 1/2 particle, $\mathcal{H} = \mathbb{C}^2$. A *basis for the operators* on $\mathcal{H}$ is given by $\{\mathbb{1}, \sigma_x, \sigma_y, \sigma_z\}$ where the Pauli-matrices are defined as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1}$$

a) Show $\sigma_j^2 = \mathbb{1}$ for $j \in \{x, y, z\}$.

b) What is $\mathrm{Tr}_2\,(\sigma_j \otimes \sigma_k)$ for all $j, k \in \{x, y, z\}$?

We now consider two spins, whose interaction is described by the Hamiltonian

$$H = \gamma \sigma_x \otimes \sigma_x, \tag{2}$$

where $\gamma$ is some constant. We define the basis vectors $|0\rangle = (1,0)^\top$, $|1\rangle = (0,1)^\top$.

c) Write out $H$ in matrix form in the ordered basis $(|0\rangle \otimes |0\rangle, |1\rangle \otimes |0\rangle, |0\rangle \otimes |1\rangle, |1\rangle \otimes |1\rangle)$.

d) Show that $\exp(-\mathrm{i}Ht) = \cos(t\gamma)\mathbb{1} - \mathrm{i}\sin(t\gamma)\sigma_x \otimes \sigma_x$.

e) Calculate $|\Psi(t)\rangle = \exp(-\mathrm{i}Ht)\,|\Psi(0)\rangle$ with $|\Psi(0)\rangle = |0\rangle \otimes |0\rangle$.

f) Compute $\rho = \mathrm{Tr}_2\,(|\Psi(t)\rangle\langle\Psi(t)|)$

g) Are there times for which $|\Psi(t)\rangle$ is maximally entangled?

**20. From microcanonical to canonical (1+2+2+2)**

Consider a bipartite quantum system consisting of two parts $S$ (subsystem) and $B$ (bath) with Hilbert spaces $\mathcal{H}_S$ and $\mathcal{H}_B$ (both finite dimensional). The Hamiltonian of the system is

$$H := H_S \otimes \mathbb{1}_B + \mathbb{1}_B \otimes H_B + H_I \tag{3}$$

where $H_S \in \mathcal{B}(\mathcal{H}_S)$, $H_B \in \mathcal{B}(\mathcal{H}_B)$ and $H_I \in \mathcal{B}(\mathcal{H})$, with $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$ are all assumed to be non-degenerate. Let $E_k$ and $|E_k\rangle$ be the eigenvalues and eigenvectors of $H$.

a) Assume all we know about the joint system is that its energy is in the interval $[E, E + \Delta]$, i.e., we make a microcanonical ansatz. What is the density matrix $\rho$ of the joint system?

The interaction Hamiltonian $H_I$ is assumed to be sufficiently "weak" such that the energy eigenstates $|E_k\rangle$ of $H$ are close to product states and the energy close to additive, i.e.,

$$\forall k : \exists l, m : \qquad |E_k\rangle \approx |E_l^S\rangle \otimes |E_m^B\rangle \qquad \text{and} \qquad E_k \approx E_l^S + E_m^B, \tag{4}$$

where $E_l^S$, $|E_l^S\rangle$, and $E_m^B$ $|E_m^B\rangle$ are the eigenvalues and eigenstates of $H_S$ and $H_B$ respectively.

Our aim is to show that under these conditions the reduced density matrix on $S$, i.e., $\rho_S = \mathrm{Tr}_B \rho$ is close to a canonical state.

b) Use (4) to argue that

$$\rho_S \approx \frac{1}{Z} \sum_{l=1}^{d_S} |E_l^S\rangle\langle E_l^S|\, \Omega_B(E - E_l^S, \Delta), \tag{5}$$

where $d_S = \dim(\mathcal{H}_S)$ and $\Omega_B(E, \Delta)$ is the number of eigenstates of $H_B$ in the interval $[E, E + \Delta]$ and $Z$ is some normalization constant.

It turns out that for many realistic many body Hamiltonians with short range interactions, $\Delta$ sufficiently small, and $B$ sufficiently large, $\Omega_B(E,\Delta)$ is very well approximated by a Gaussian of the form

$$\Omega_B(E,\Delta) \approx \Xi_B(E,\Delta) = C\,\Delta\,\mathrm{e}^{-(E-\mathrm{Tr}H_B)^2/(2\sigma^2)} \tag{6}$$

where $C > 0$ and $\sigma > 0$ depend on the specific model, but are independent of $E$.

We now think of $\Delta$ as fixed and small enough such that the approximation (6) is applicable and assume that $E \leq \mathrm{Tr}H_B$.

Define $S(E) := \ln(\Xi_B(E,\Delta))$.

c) Approximate $S(E - E_l^S)$ by a Taylor expansion to first order around $E$ to show that

$$\Omega_B(E - E_l^S, \Delta) \approx \mathrm{e}^{S(E) - E_l^S(\mathrm{Tr}H_B - E)/\sigma^2}. \tag{7}$$

d) Use Eqs. (5) and (7) to show that we have

$$\rho_S \approx \mathrm{e}^{-\beta H_S}/\mathrm{Tr}(\mathrm{e}^{-\beta H_S}), \tag{8}$$

i.e., $\rho_S$ is approximately a Gibbs state and determine $\beta$ in terms of $H_B$ and $E$ and $\sigma$.

**21. Density of states (1+2+1)**

A crucial ingredient in the argument of Problem 20 was that the density of states of the bath is approximately given by

$$\Omega_B(E,\Delta) \approx \Xi_B(E,\Delta) = C\,\Delta\,\mathrm{e}^{-(E-\mathrm{Tr}H_B)^2/(2\sigma^2)}. \tag{9}$$

Consider a quantum system that consists of $n$ subsystem with Hilbert space $\mathbb{C}^2$ described by the Hamiltonian

$$H_B = \sum_{i=1}^{n} \sigma_z^{(i)} + \frac{1}{2}\sum_{i=1}^{n-1} \sigma_x^{(i)}\,\sigma_x^{(i+1)} \tag{10}$$

where $\sigma_x$ and $\sigma_z$ are the Pauli matrices and the superscript indicates on which site they act, i.e.,

$$\sigma_z^{(i)} := \underbrace{\mathbb{1}_{2\times 2} \otimes \cdots \otimes \mathbb{1}_{2\times 2}}_{i-1 \text{ times}} \otimes \sigma_z \otimes \underbrace{\mathbb{1}_{2\times 2} \otimes \cdots \otimes \mathbb{1}_{2\times 2}}_{n-i \text{ times}}, \tag{11}$$

a) Numerically diagonalize $H_B$ with your favorite programming language or computer algebra system. Up to which $n$ can you do this in a reasonable time?

For the remaining questions use this maximal feasible $n$.

b) Plot $\Omega_B(E,1)$.

c) Compare with the functional form of $\Xi_B(E,\Delta)$ given in (9) and approximately determine $C$ and $\sigma$ for this model by fitting (either least squares or simply by hand).

*Hint:* Numerically the tensor product is usually implemented using the so called Kronecker Product. Mathematica and MATLAB come with implementations of this function.