Advanced statistical mechanics
(WS 12/13, FU Berlin)

Problem sheet 8

Due date: December 19, 2012

Problem 24: Partial trace and reduced states (1+1+1+1+1+2*+1+1+1)

For $i = 1, 2$ let $\mathcal{H}_i$ be two Hilbert spaces of dimension d_i. We use the notation introduced in Problem 22, e.g., $\{|j\rangle_i\}_{j=1}^{d_i}$ denotes an orthonormal basis of $\mathcal{H}_i$, where we usually just write $|j\rangle$ instead of $|j\rangle_i$. The partial trace over $\mathcal{H}_2$ is the linear map

$$\mathrm{Tr}_2 : \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_1) \tag{1}$$

that acts on all product operators as

$$\mathrm{Tr}_2(A \otimes B) = A\,\mathrm{Tr}(B), \tag{2}$$

where $A \in \mathcal{B}(\mathcal{H}_1)$ and $B \in \mathcal{B}(\mathcal{H}_2)$ and Tr denotes the usual trace. The partial trace Tr_1 over $\mathcal{H}_1$ is defined similarly.

a) What is $\mathrm{Tr}_2(|j,k\rangle\langle l,m|)$?

b) Let $\mathbb{1} \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ be the identity operator. What is $\mathrm{Tr}_2(\mathbb{1})$?

c) Let $A \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ be some operator. Then it can be written as

$$A = \sum_{j,l=1}^{d_1} \sum_{k,m=1}^{d_2} a_{j,k,l,m}\, |j,k\rangle\langle l,m| \tag{3}$$

with $a_{j,k,l,m} = \langle l,m|\, A\, |j,k\rangle$. Show that

$$\mathrm{Tr}_2(A) = \sum_{j,l}^{d_1} a_{j,l}^{(1)}\, |j\rangle\langle l| \quad \text{with} \quad a_{j,l}^{(1)} = \sum_{k=1}^{d_2} a_{j,k,l,k}. \tag{4}$$

d) Show that

$$\mathrm{Tr}(\mathrm{Tr}_2(A)) = \mathrm{Tr}(A) \tag{5}$$

for all $A \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$.

e) Let $\mathcal{H}_3$ be another finite dimensional Hilbert space and $A \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3)$. Show that

$$\mathrm{Tr}_3(\mathrm{Tr}_2(A)) = \mathrm{Tr}_2(\mathrm{Tr}_3(A)). \tag{6}$$

f) *Bonus question:* Prove that a reduced state is indeed a state, i.e., that $\mathrm{Tr}_2(\rho) \in \mathcal{S}(\mathcal{H}_1)$ for all states $\rho \in \mathcal{S}(\mathcal{H}_1 \otimes \mathcal{H}_2)$.
Hint: Results from Problem 21 and from part 24i) can be used.

The maximally mixed state on a d-dimensional Hilbert space $\mathcal{H}$ is $\mathbb{1}/d \in \mathcal{S}(\mathcal{H})$.

g) Let $\rho \in \mathcal{S}(\mathcal{H}_1)$ and $\sigma \in \mathcal{S}(\mathcal{H}_2)$ be two states. Prove that

$$\mathrm{Tr}_2(\rho \otimes \sigma) = \rho \tag{7}$$

and conclude that the reduced maximally mixed state $\mathrm{Tr}_2(\mathbb{1}/d_1 d_2)$ is the maximally mixed state on $\mathcal{H}_1$.

h) Now we consider the Bell state $\phi^+ = |\phi^+\rangle\langle\phi^+|$ with $|\phi^+\rangle = (|0,0\rangle + |1+1\rangle)/\sqrt{2}$ on the Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$. Calculate it's reduced state $\mathrm{Tr}_2(\phi^+)$ and compare it with the maximally mixed state on the Hilbert space $\mathbb{C}^2$.

Let $A_1 \in \mathcal{B}(\mathcal{H}_1)$ be an observable on $\mathcal{H}_1$. Then its *extension* to the composite system $\mathcal{H}_1 \otimes \mathcal{H}_2$ is defined to be $A_1 \otimes \mathbb{1} \in \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$.

i) Prove that for $A = A_1 \otimes \mathbb{1}$

$$\mathrm{Tr}(\rho A) = \mathrm{Tr}(\mathrm{Tr}_2(\rho) A_1) \tag{8}$$

for all states $\rho \in \mathcal{S}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ on the composite system.
Remark: This also implies that $\mathrm{Tr}_2(\rho) \in \mathcal{B}(\mathcal{H}_1)$ is indeed the reduced state, i.e., all expectation values on $\mathcal{H}_1$ can be calculated from it!

Problem 25: 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

$$H := H_S \otimes \mathbb{1}_B + \mathbb{1}_B \otimes H_B + H_I \tag{9}$$

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 ρ 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.,

$$\forall k : \exists l, m : \qquad |E_k\rangle \approx |E_l^S\rangle \otimes |E_m^B\rangle \qquad \text{and} \qquad E_k \approx E_l^S + E_m^B, \tag{10}$$

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 (10) to argue that

$$\rho_S \approx \frac{1}{Z} \sum_{l=1}^{d_S} |E_l^S\rangle\langle E_l^S| \, \Omega_B(E - E_l^S, \Delta), \tag{11}$$

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, Δ sufficiently small, and B sufficiently large, $\Omega_B(E, \Delta)$ is very well approximated by a Gaussian of the form

$$\Omega_B(E, \Delta) \approx \Xi_B(E, \Delta) = C\, \Delta\, \mathrm{e}^{-(E - \mathrm{Tr} H_B)^2/(2\sigma^2)} \tag{12}$$

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

We now think of Δ as fixed and small enough such that the approximation (12) 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

$$\Omega_B(E - E_l^S, \Delta) \approx \mathrm{e}^{S(E) - E_l^S (\mathrm{Tr} H_B - E)/\sigma^2}. \tag{13}$$

d) Use Eqs. (11) and (13) to show that we have

$$\rho_S \approx \mathrm{e}^{-\beta H_S} / \mathrm{Tr}(\mathrm{e}^{-\beta H_S}), \tag{14}$$

i.e., ρ_S is approximately a Gibbs state and determine β in terms of H_B and E and σ.

Problem 26: Density of states (1+2+1)

A crucial ingredient in the argument of Problem 25 was that the density of states of the bath is approximately given by

$$\Omega_B(E, \Delta) \approx \Xi_B(E, \Delta) = C\, \Delta\, \mathrm{e}^{-(E - \mathrm{Tr} H_B)^2/(2\sigma^2)}. \tag{15}$$

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

$$H_B = \sum_{i=1}^{n} \sigma_z^{(i)} + \frac{1}{2} \sum_{i=1}^{n-1} \sigma_x^{(i)}\, \sigma_x^{(i+1)} \tag{16}$$

where σ_x and σ_z are the Pauli matrices and the superscript indicates on which site they act, i.e.,

$$\sigma_z^{(i)} := \underbrace{\mathbb{1}_{2\times 2} \otimes \cdots \otimes \mathbb{1}_{2\times 2}}_{i-1 \text{ times}} \otimes \sigma_z \otimes \underbrace{\mathbb{1}_{2\times 2} \otimes \cdots \otimes \mathbb{1}_{2\times 2}}_{n-i \text{ times}}, \tag{17}$$

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 (15) and approximately determine C and σ 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.