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

Problem sheet 7

Due date: December 12, 2012

Problem 21: Density matrices (1+1+1+1+1+1+1+1=8)

Let $\mathcal{H}$ be a d-dimensional Hilbert space and denote the set of linear operators on $\mathcal{H}$ by $\mathcal{B}(\mathcal{H}) := \{A : \mathcal{H} \to \mathcal{H} \mid A \text{ linear}\}$. A self-adjoint operator $A \in \mathcal{B}(\mathcal{H})$ is called *positive semi-definite* iff $\langle\psi| A |\psi\rangle \geq 0$ for all $|\psi\rangle \in \mathcal{H}$, which is denoted by $A \geq 0$.

a) Let $A^\dagger = A \in \mathcal{B}(\mathcal{H})$. Prove that $A \geq 0$ if and only if A has no negative eigenvalues.

The set of density matrices on $\mathcal{H}$ is

$$\mathcal{S}(\mathcal{H}) := \{\rho \in \mathcal{B}(\mathcal{H}) : \rho \geq 0,\ \mathrm{Tr}(\rho) = 1\}. \tag{1}$$

b) Let $\rho \in \mathcal{B}(\mathcal{H})$. Prove that ρ is a density matrix if and only if there is a probability vector $p \in [0,1]^n$ and normalized state vectors $(|\psi_j\rangle)_{j=1}^n \subset \mathcal{H}$ such that

$$\rho = \sum_{j=1}^{n} p_j\, |\psi_j\rangle\langle\psi_j|\,. \tag{2}$$

c) Let $A^\dagger = A \in \mathcal{B}(\mathcal{H})$, i.e, A is an observable. Prove for the decomposition (2) that

$$\mathrm{Tr}(\rho A) = \sum_{j=1}^{n} p_j\, \langle A\rangle_{\psi_j}, \tag{3}$$

i.e., that the expectation value of A in state ρ is the same as the expectation value w.r.t. p_j of the "pure state expectation values" $\langle A\rangle_{\psi_j} = \langle\psi_j| A |\psi_j\rangle$.

d) Consider the special case $\mathcal{H} = \mathbb{C}^2$. Show that the decomposition (2) is not unique, i.e., find pairwise different and normalized $|\psi_1\rangle, |\psi_2\rangle, |\phi_1\rangle, |\phi_2\rangle \in \mathbb{C}^2$ and probability vectors $p, q \in [0,1]^2$ such that

$$\sum_{j=1}^{2} p_j\, |\psi_j\rangle\langle\psi_j| = \sum_{j=1}^{2} q_j\, |\phi_j\rangle\langle\phi_j|\,. \tag{4}$$

e) Find a necessary condition on $(|\psi_j\rangle)_{j=1}^n$ in Eq. (2) such that n is the rank of ρ.

A state $\rho \in \mathcal{S}(\mathcal{H})$ is called *pure* if there is a vector $|\psi\rangle \in \mathcal{H}$ such that $\rho = |\psi\rangle\langle\psi|$ and *mixed* if no such a vector exists.

f) Prove that $\rho \in \mathcal{S}(\mathcal{H})$ is a pure state if and only if $\mathrm{Tr}(\rho^2) = 1$.

g) Prove that $\mathcal{S}(\mathcal{H})$ is a convex set, i.e.

$$\rho, \sigma \in \mathcal{S}(\mathcal{H}) \quad \Rightarrow \quad \lambda\rho + (1-\lambda)\sigma \in \mathcal{S}(\mathcal{H}) \quad \forall \lambda \in [0,1]. \tag{5}$$

Remark: This implies that a probability distribution over quantum states naturally defines again a quantum state.

A point $\rho \in \mathcal{S}$ of a convex set $\mathcal{S}$ is called an *extremal point* of $\mathcal{S}$ if it is impossible to write it as a non-trivial convex combination of two other points, i.e., for all $\rho_1, \rho_2 \in \mathcal{S}$ and $\lambda \in]0,1[$

$$\rho = \lambda\rho_1 + (1-\lambda)\rho_2 \quad \Rightarrow \quad \rho_1 = \rho_2. \tag{6}$$

h) Prove that the extremal points of $\mathcal{S}(\mathcal{H})$ are exactly the pure states.
Hint: First, conclude that the pure state are exactly the ones of rank one.

Problem 22: Tensor product (1+1+1+1+2)

Let $\mathcal{H}$ be a d-dimensional Hilbert space with basis $\{\,|j\,\rangle\}_{j=1}^{d}$. The dual space $\mathcal{H}^*$ has the basis $\{\,\langle j\,|\}_{j=1}^{d}$, satisfying the orthonormality relation $\langle j|k\rangle = \delta_{j,k}$.

Similarly, let $\mathcal{H}_i$ with $i = 1, 2$ be two other d_i-dimensional Hilbert space with basis $\{\,|j\,\rangle_i\}_{j=1}^{d_i}$. We will often use the common notation

$$|j,k\,\rangle \coloneqq |j\,\rangle\;|k\,\rangle \coloneqq |j\,\rangle \otimes |k\,\rangle \coloneqq |j\,\rangle_1 \otimes |k\,\rangle_2\,. \tag{7}$$

The vectors $\{\,|j,k\,\rangle\}_{j=1,\ldots,d_1;\,k=1,\ldots,d_2}$ are an orthonormal basis of the (tensor) product space $\mathcal{H}_1 \otimes \mathcal{H}_2$ and satisfy the orthogonality relations

$$\langle j,k|l,m\rangle = \langle j|l\rangle\,\langle k|m\rangle = \delta_{j,l}\,\delta_{k,m}. \tag{8}$$

The tensor product of two arbitrary vectors $|\psi\,\rangle \in \mathcal{H}_1$ and $|\phi\,\rangle \in \mathcal{H}_2$ can be defined via bilinear extension as

$$|\psi\,\rangle \otimes |\phi\,\rangle \coloneqq \sum_{j=1}^{d_1}\sum_{k=1}^{d_2} \langle j|\psi\rangle\,\langle k|\phi\rangle\;|j,k\,\rangle\,. \tag{9}$$

a) What is the Hilbert space dimension of the n-fold tensor product $\mathcal{H}^{\otimes n} = \mathcal{H} \otimes \ldots \otimes \mathcal{H}$?

b) For $|\psi\,\rangle \in \mathcal{H}_1$ and $|\phi\,\rangle\,, |\xi\,\rangle \in \mathcal{H}_2$ show that

$$|\psi\,\rangle \otimes |\phi\,\rangle + |\psi\,\rangle \otimes |\xi\,\rangle = |\psi\,\rangle\,(\,|\phi\,\rangle + |\xi\,\rangle)\,. \tag{10}$$

There are the natural isomorphisms

$$\mathcal{H} \otimes \mathcal{H}^* \to \mathcal{B}(\mathcal{H}), \qquad |j\,\rangle \otimes \langle k\,| \mapsto |j\,\rangle\langle k\,|\,, \tag{11}$$

$$\mathcal{H}_1 \otimes \mathcal{H}_2 \to \mathcal{H}_2 \otimes \mathcal{H}_1, \qquad |j\,\rangle \otimes |k\,\rangle \mapsto |k\,\rangle \otimes |j\,\rangle \tag{12}$$

and consequently

$$\mathcal{B}(\mathcal{H}_1) \otimes \mathcal{B}(\mathcal{H}_2) \to \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2), \qquad |j\,\rangle\langle k\,| \otimes |l\,\rangle\langle m\,| \mapsto |j,l\,\rangle\langle k,m\,| \qquad . \tag{13}$$

Therefore, one often writes, e.g., $|j\,\rangle\langle k\,|\otimes|l\,\rangle\langle m\,| = |j,l\,\rangle\langle k,m\,|$. Importantly, $|\psi\,\rangle\otimes|\phi\,\rangle \neq |\phi\,\rangle\otimes|\psi\,\rangle$ in general, even if $\mathcal{H}_1\otimes\mathcal{H}_2 \cong \mathcal{H}_2\otimes\mathcal{H}_1$. So one needs to be careful here: If one reorders basis elements during one calculation one needs to reorder *all* basis elements in the same way!
In terms of the basis (11) an operator $A \in \mathcal{B}(\mathcal{H})$ can be written as

$$A = \sum_{j,k=1}^{d} a_{j,k}\;|j\,\rangle\langle k\,|\,. \tag{14}$$

c) How can one calculate the $a_{j,k}$?

d) For the special case, where $A = \sigma_x \otimes \sigma_z$ find the basis expansion (14) of A explicitly, where σ_x, σ_y, and σ_z denote the Pauli matrices.

e) Show that for $A, C \in \mathcal{B}(\mathcal{H}_1)$ and $B, D \in \mathcal{B}(\mathcal{H}_2)$

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD). \tag{15}$$

Problem 23: Two indistinguishable particles (1+1+1+1+1)

a) Consider two state vectors $|\psi\rangle$ and $|\phi\rangle$ that represent indistinguishable states of a quantum system. Which mathematical relation between $|\psi\rangle$ and $|\phi\rangle$ is necessary and sufficient for indistinguishability? Explain your answer!

The swap operator $S \in \mathcal{B}(\mathcal{H} \otimes \mathcal{H})$ is defined via

$$S\,|j\rangle\,|k\rangle = |k\rangle\,|j\rangle\,, \tag{16}$$

where $\{|j\rangle\}_j$ is some orthonormal basis of the Hilbert space $\mathcal{H}$.

b) Show that the eigenvalues of S are $\operatorname{spec}(S) = \{-1, 1\}$.

From now on we consider the case, where the one-particle Hilbert space is two-dimensional, i.e., $\mathcal{H} \cong \mathbb{C}^2$.

c) Show that the famous *Bell states*

$$\left|\phi^+\right\rangle = (|0,0\rangle + |1,1\rangle)/\sqrt{2}, \qquad \left|\phi^-\right\rangle = (|0,0\rangle - |1,1\rangle)/\sqrt{2}, \tag{17}$$

$$\left|\psi^+\right\rangle = (|0,1\rangle + |1,0\rangle)/\sqrt{2}, \qquad \left|\psi^-\right\rangle = (|0,1\rangle - |1,0\rangle)/\sqrt{2} \tag{18}$$

are an orthonormal basis for our two-particle Hilbert-space.

d) For each eigenspace of S find a basis in terms of Bell states.

e) Now consider quantum state $|\psi\rangle$ of two indistinguishable particles, one of which is in state $|\psi_1\rangle \in \mathbb{C}^2$ and the other in state $|\psi_2\rangle \in \mathbb{C}^2$. Conclude that $|\psi\rangle$ is either symmetric or anti-symmetric under exchange of the two particles.
Remark: If $|\psi\rangle$ is symmetric the particles are called *bosons* and if $|\psi\rangle$ is anti-symmetric then they are called *fermions*.