FYS 4110 Non-relativistic Quantum Mechanics, Fall Semester 2008

Problem set 6

6.1 Density matrices

a) Show that a density operator $\hat{\rho}$ represents a *pure* quantum state if and only if it satisfies

$$\hat{\rho}^2 = \hat{\rho} \tag{1}$$

We have the following set of 8 2×2 matrices,

$$\hat{\rho}_1 = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \quad \hat{\rho}_2 = \begin{pmatrix} 1 & \frac{i}{2} \\ -\frac{i}{2} & 0 \end{pmatrix}, \quad \hat{\rho}_3 = \begin{pmatrix} \frac{1}{2} & 1 \\ 1 & \frac{1}{2} \end{pmatrix}, \quad \hat{\rho}_4 = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$
$$\hat{\rho}_5 = \frac{1}{4}\begin{pmatrix} 3 & 1 \\ 1 & 1 \end{pmatrix}, \quad \hat{\rho}_6 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \hat{\rho}_7 = \frac{1}{2}\begin{pmatrix} 3 & 1 \\ 1 & -1 \end{pmatrix}, \quad \hat{\rho}_8 = \frac{1}{4}\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \tag{2}$$

b) Check which of the 8 matrices that satisfy the conditions for being a density matrix.

c) For those matrices that satisfy the conditions, decide which ones that represent pure states and which ones that represent mixed states.

d) Calculate the von Neumann entropy S of the density matrices and arrange them according to decreasing entropy. (Use here natural logarithm in the definition of S.)

6.2 Convexity

Density operators do not satisfy the superposition principle like the state vectors. They do however satisfy a *convexity criteria* in the following form. If $\hat{\rho}_1$ and $\hat{\rho}_2$ are two density operators, also the following linear combination is a density operator,

$$\hat{\rho} = \alpha\hat{\rho}_1 + (1-\alpha)\hat{\rho}_2 \tag{3}$$

with α as a real number in the interval $0 \leq \alpha \leq 1$. Show this. Why do we call a set that satisfies a condition of the form (3) a *convex* set?

Can the density operator of a *pure* state be written as a combination (3) of two other density operators?

6.3 Tensor products of matrices

Assume $|a\rangle = \sum_i a_i |i\rangle_A$ is a vector in an 2-dimensional Hilbert space $\mathcal{H}_A$ and $|b\rangle = \sum_j b_j |j\rangle_B$ is a vector in another 2-dimensional Hilbert space $\mathcal{H}_B$. The composite vector $|c\rangle = |a\rangle \otimes |b\rangle$ is then a product vector in the tensor product space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Expanded in the product basis it has the form $|c\rangle = \sum_{ij} c_{ij} |ij\rangle$ with $|ij\rangle = |i\rangle_A \otimes |j\rangle_B$.

We consider the matrix representation of the vectors

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \tag{4}$$

a) Write the 2×2 matrix $\mathbf{c}$ with matrix elements c_{ij} and show that it can be written as the matrix product

$$\mathbf{c} = \mathbf{a}\,\mathbf{b}^T \tag{5}$$

where T denotes transposition of the matrix.

An alternative representation of the vector $|c\rangle$ is as a single column matrices of of dimension 4. We define the matrix elements $\tilde{c}_k$ of such a matrix by the following relation

$$\tilde{c}_{i+2(j-1)} = c_{ij} \tag{6}$$

b) Write the column matrix $\tilde{\mathbf{c}}$ (4×1 matrix) in terms of the matrix elements of $\mathbf{a}$ and $\mathbf{b}$ and show that it can be written in a compact form as

$$\tilde{\mathbf{c}} = \begin{pmatrix} \mathbf{a}\,b_1 \\ \mathbf{a}\,b_2 \end{pmatrix} \tag{7}$$

We consider next operators $\hat{A}$, $\hat{B}$ and $\hat{C} = \hat{A} \otimes \hat{B}$ that act in $\mathcal{H}_A$, $\mathcal{H}_B$ and $\mathcal{H}$ respectively. The corresponding 2×2 matrix $\mathbf{A}$ represents $\hat{A}$ in the basis $\{|i\rangle_A\}$ and the 2×2 matrix $\mathbf{B}$ represents $\hat{B}$ in the basis $\{|j\rangle_B\}$. The tensor product of the operators, in a similar way as the vectors, can be represented in two ways. The first one is to represent it as a 4-index tensor

$$C_{ij,i'j'} = A_{ii'} B_{jj'} \tag{8}$$

and the second one is to represent it as a 4×4 matrix with two indices $\tilde{C}_{kl}$, so that

$$\tilde{C}_{i+2(j-1),i'+2(j'-1)} = C_{ij,i'j'} \tag{9}$$

in the similar way as for the matrix $\tilde{c}_i$, as discussed above.

c) Use the second representation ($\tilde{c}, \tilde{C}$) for vectors and operators, and show what the matrix representation of the four basis vectors $|ij\rangle$ are.

Also find the 4×4 matrix representations of the tensor products $\sigma_k \otimes \sigma_l$, where $\sigma_k, k = 1, 2, 3$ are the Pauli matrices.