Problem set 5

5.1 Density operators

A density operator of a two-level system can be represented by a 2×2 density matrix in the form

$$\hat{\rho} = \frac{1}{2}(\mathbb{1} + \mathbf{r} \cdot \boldsymbol{\sigma}) \,, \quad |\mathbf{r}| \leq 1 \tag{1}$$

where $\mathbb{1}$ is the 2×2 identity matrix, $\mathbf{r}$ is a vector in three dimensions and $\boldsymbol{\sigma}$ is a vector operator with the Pauli matrices as the Cartesian components.

a) Show that $\mathbf{r} = \langle \boldsymbol{\sigma} \rangle$.

b) If

$$\hat{\rho}_1 = \frac{1}{2}(\mathbb{1} + \mathbf{r}_1 \cdot \boldsymbol{\sigma}) \qquad \text{and} \qquad \hat{\rho}_2 = \frac{1}{2}(\mathbb{1} + \mathbf{r}_2 \cdot \boldsymbol{\sigma})$$

are two density matrices, show that the statistical mixture

$$\hat{\rho} = p_1 \hat{\rho}_1 + p_2 \hat{\rho}_2 = \frac{1}{2}(\mathbb{1} + \mathbf{r} \cdot \boldsymbol{\sigma})$$

with $\mathbf{r} = p_1 \mathbf{r}_1 + p_2 \mathbf{r}_2$.

c) Explain why this means that geometrically the set of all density matrices form of a sphere in three dimensions, with the pure states $|\mathbf{r}| = 1$ as the surface of the sphere (the Bloch sphere), and the mixed states as the interior of the sphere.

d) The density operator can also be expressed in bra-ket formulation as

$$\hat{\rho} = \rho_{11} \, |+\rangle\langle+| \; + \; \rho_{12} \, |+\rangle\langle-| \; + \; \rho_{21} \, |-\rangle\langle+| \; + \; \rho_{22} \, |-\rangle\langle-| \tag{2}$$

with $|\pm\rangle$ defined by $\sigma_z |\pm\rangle = \pm |\pm\rangle$.

What are the coefficients $\rho_{ij}, \; i, j = 1, 2$, expressed in terms of the Cartesian components x, y, z of $\mathbf{r}$?

e) Assume a spin-half system is prepared in a mixed state, with equal probability for *spin up* in the (positive) directions of the three coordinate axes x, y and z . Find the corresponding density matrix, expressed in the form (1). What is the von Neumann entropy of the state?

f) The above mixed state was realized as an ensamble of three different pure states (spin up along each of the three coordinate axes). Find at least one different ensamble of two or more pure states which gives the same density matrix.

5.2 Entropy of a thermal state

A thermal state is described by a temperature dependent density operator of the form

$$\hat{\rho} = N(\beta) \, e^{-\beta \hat{H}} \tag{3}$$

where $\beta = 1/(k_B T)$ with T as the temperature, k_B as the Boltzmann constant, and $N(\beta)$ as a normalization factor. This factor is given by

$$N(\beta)^{-1} = \mathrm{Tr}(e^{-\beta\hat{H}}) = \sum_k e^{-\beta E_k} \tag{4}$$

with E_k as the energy eigenvalues.

a) Show that the temperature dependent von Neumann entropy of this state can be expressed in terms of the normalization factor as

$$S(\beta) = \beta\frac{d}{d\beta}\log N(\beta) - \log N(\beta) \tag{5}$$

b) For a one-dimensional harmonic oscillator, with Hamiltonian

$$\hat{H} = \hbar\omega\sum_{n=0}^{\infty}(n+\frac{1}{2})|n\rangle\langle n| \tag{6}$$

what is the expression for the temperature dependent entropy $S(\beta)$?

c) Plot S as a function of temperature, with $x = 2k_BT/(\hbar\omega)$ as the dimensionless temperature coordinate on the horizontal axis, for example in the interval $(0, 5)$. What are the asymptotic expressions for S in the limits $T \to 0$ ($\beta \to \infty$) and $T \to \infty$ ($\beta \to 0$). Comment on these results with reference to what we know about the values of the entropy for pure states and maximally mixed states. (Assume *log* in the definition of S to mean the natural logarithm.)

5.3 Tensor products of matrices

Assume $|a\rangle = \sum_{i=1}^{2} a_i\,|i\rangle_A$ is a vector in an 2-dimensional Hilbert space $\mathcal{H}_A$ and $|b\rangle = \sum_{j=1}^{2} b_j\,|j\rangle_B$ is a vector in another 2-dimensional Hilbert space $\mathcal{H}_B$, with $\{|i\rangle_A\}$ as an orhonormal basis set in $\mathcal{H}_B$ and $\{|j\rangle_B\}$ as a similar vector set in $\mathcal{H}_B$. The composite vector $|c\rangle = |a\rangle \otimes |b\rangle$ is 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 $|c\rangle = \sum_{ij} a_i b_j\,|ij\rangle$ with $|ij\rangle = |i\rangle_A \otimes |j\rangle_B$.

We consider the matrix representation of the vectors

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \tag{7}$$

a) Show that the 2×2 matrix $\mathbf{c}$, with matrix elements $c_{ij} = a_i b_j$, can be written as the matrix product

$$\mathbf{c} = \mathbf{a}\,\mathbf{b}^T \tag{8}$$

where T denotes transposition of the matrix.

An alternative representation of the vector $|c\rangle$ is as a single column matrix of dimension 4. We define the matrix elements $\tilde{c}_k, k = 1, ..., 4$, of such a matrix by the following relation

$$\tilde{c}_{j+2(i-1)} = c_{ij} \tag{9}$$

b) Express 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

$$\tilde{\mathbf{c}} = \begin{pmatrix} a_1\,\mathbf{b} \\ a_2\,\mathbf{b} \end{pmatrix} \tag{10}$$

What are the corresponding expressions for the four basis vectors $|ij\rangle$?

We consider next operators $\hat{A}$, $\hat{B}$ and $\hat{C} = \hat{A} \otimes \hat{B}$, which 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 representation is as a 4-index tensor

$$C_{ij,i'j'} = A_{ii'}B_{jj'} \tag{11}$$

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

$$\tilde{C}_{j+2(i-1),j'+2(i'-1)} = C_{ij,i'j'} \tag{12}$$

similar to the column matrix $\tilde{c}_i$, defined in (9).

c) 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. Write them in a form similar to (10). It is sufficient to do this for three different choices of the Pauli matrices.