Open Quantum Systems: Exercise session 1

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Exercise 1

- (a) Prove that the trace of an operator A, $\operatorname{Tr} A = \sum_n u_n^{\dagger} A u_n$ is independent of the orthonormal basis $\{u_n\}$ chosen for its evaluation. 1pt
- (b) Show that $Tr(Avv^{\dagger}) = v^{\dagger}Av$. 1pt

Exercise 2

(Ballentine, exercise 1.3)

Consider the vector space $M_2(\mathbb{C})$, show that the Pauli matrices form a basis for this vector space:

$$\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

3pts

Exercise 3: Hilbert-Schmidt product

(Ballentine, exercise 1.4)

- (a) If A, B and C are matrices of the same shape, show that $(A, B) = \text{Tr}(A^{\dagger}B)$ has all the properties of an inner product. I.e. show that
 - 1. $(A, B) = \overline{(B, A)}$, where denotes the complex conjugate. 0.5pts
 - 2. (A + C, B) = (A, B) + (C, B) and for $c \in \mathbb{C}$, (A, cB) = c(A, B). 0.5pts
 - 3. (A, A) > 0 for A not the zero-matrix. 0.5pts

This inner product is called the HIlbert-Schmidt product.

(b) Show that the Pauli matrices (see exercise 3) are orthogonal with respect to the inner product (A, B). 1.5pts

Exercise 4

Prove that for $X \in M_n(\mathbb{C})$, the $n \times n$ -dimensional complex matrices, the following statements are equivalent

a. X is of the form $B^{\dagger}B$, with $B \in M_n(\mathbb{C})$.

- b. $\phi^{\dagger} X \phi \geq 0 \ \forall \phi \in \mathbb{C}^n$.
- c. $X = X^{\dagger}$ and every eigenvalue is non-negative.

(show for example $a \Rightarrow b, b \Rightarrow c, c \Rightarrow a$) 3pts

Exercise 5

- (a) Show that for $A, B \in M_n(\mathbb{C})$ the trace is cyclic i.e. Tr(AB) = Tr(BA). 1pt
- (b) Consider $X, Y \in M_n(\mathbb{C})$ and $X, Y \geq 0$, show that $Tr(XY) \geq 0$. 1pt
- (c) Is XY a positive matrix? 1pt

hint: for (b) use (a) and Exercise 4

Exercise 6

The exponential of a matrix A is defined as

$$\exp(A) = \sum_{n=0}^{\infty} \frac{1}{n!} A^n$$

Show that

- a. Let A be fully diagonalisable, i.e. $A = \sum_i a_i v_i v_i^{\dagger}$ for $a_i \in \mathbb{C}$ and $\{v_i\}$ and orthonormal basis. Then $\exp(A) = \sum_i \exp(a_i) v_i v_i^{\dagger}$. 1pt
- b. Let σ_i be one of the Pauli matrices, show that $\exp(i\sigma_i t) = \cos(t)\mathbb{I} + i\sin(t)\sigma_i$ for $t \in \mathbb{R}$ and \mathbb{I} the identity matrix. 1pt
- c. Show that $\frac{d}{dt} \exp(At) = A \exp(At)$. 1pt

Exercise 7: BBGKY hierarchy

Consider an system of N identical particles with the probability density functional $f_N(\mathbf{q}_1 \dots \mathbf{q}_N, \mathbf{p}_1 \dots \mathbf{p}_N)$, where \mathbf{q}_i and \mathbf{p}_i are 3-dimensional vectors for the position and momentum coordinates respectively. The probability density function satisfies the Liouville equation

$$\frac{\partial f_N}{\partial_t} + \sum_{i=1}^N \frac{\mathbf{p}_i}{m} \cdot \frac{\partial f_N}{\partial \mathbf{q}_i} + \sum_{i=1}^N \mathbf{F}_i \cdot \frac{\partial f_N}{\partial \mathbf{p}_i} = 0$$

with the net force acting on the i-th particle

$$\mathbf{F}_{i} = -\sum_{j=1, j \neq i}^{N} \frac{\partial \Phi_{ij}}{\partial \mathbf{q}_{i}} - \frac{\partial \Phi^{ext}}{\partial \mathbf{q}_{i}}$$

where Φ_{ij} is the pair interaction between particles and Φ^{ext} an external potential. We define the *n*-particle density functional

$$f_n(\mathbf{q}_1 \dots \mathbf{q}_n, \mathbf{p}_1 \dots \mathbf{p}_n) = \int f_N(\mathbf{q}_1 \dots \mathbf{q}_N, \mathbf{p}_1 \dots \mathbf{p}_N) d\mathbf{q}_{n+1} \dots d\mathbf{q}_N d\mathbf{p}_{n+1} \dots d\mathbf{p}_N$$

1. Show that the one-particle density function satisfies

$$\frac{\partial f_1}{\partial t} + \frac{\mathbf{p}_1}{m} \cdot \frac{\partial f_1}{\partial \mathbf{q}_1} - \frac{\partial \Phi^{ext}}{\partial \mathbf{q}_1} = (N-1) \int \frac{\partial \Phi_{12}}{\partial \mathbf{q}_1} \frac{\partial f_2}{\partial \mathbf{p}_1} d\mathbf{q}_2 d\mathbf{p}_2$$

2pts

2. Find the corresponding equation for the n-particle density function. 2pts