

Workshop 11 - questions

1. By taking the trace of both sides and simplifying, show that Liouville – von Neumann equation

$$\frac{\partial \rho}{\partial t} = -i[\mathbf{H}, \rho]$$

conserves the trace (sum of diagonal elements) of the density matrix. What does this conservation law physically correspond to?

2. Prove that the density matrix is Hermitian (its conjugate-transpose is equal to itself) and explain why this is important in quantum mechanics. Use the following facts from mathematics:

$$|\psi\rangle^\dagger = \langle\psi|, \quad (\mathbf{AB})^\dagger = \mathbf{B}^\dagger \mathbf{A}^\dagger$$

in the construction of your proof.

3. Can a density matrix have:

- (a) zero eigenvalues?
- (b) negative eigenvalues?
- (c) complex eigenvalues?
- (d) complex elements?

Provide formal proofs where necessary.

4. Using the same method as in the lecture, derive the general solution to the equation describing concentration dynamics under a network of first-order chemical reactions:

$$\frac{d\mathbf{c}}{dt} = \mathbf{K}\mathbf{c}$$

where $\mathbf{c}$ is the concentration vector and $\mathbf{K}$ is the time-independent chemical reaction rate matrix. Which method is easier for numerical calculations – the one used in the chemistry textbooks (solving a system of differential equations with calculus) or the one you have just derived?