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Exercise 11.1 (von Neumann equation and time evolution with density operators)

(a) Based on the Schrödinger equation (cf. tutorial 3), derive the following *von Neumann equation* for a density matrix $\rho(t) = \sum_j p_j \, |\psi_j(t)\rangle \langle\psi_j(t)|$:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = [H, \rho(t)].$$

Here $[\cdot,\cdot]$ is the matrix commutator.

Hint: Use the product rule for computing the time derivative of each term $|\psi_j(t)\rangle \langle\psi_j(t)|$.

(b) What is the formal solution for $\rho(t)$ expressed in terms of the time evolution operator $U(t) = \mathrm{e}^{-iHt/\hbar}$?

(c) We consider the specific single-qubit Hamiltonian operator

$$H = JX$$

with parameter $J \in \mathbb{R}$. Compute the time-dependent density matrix $\rho(t)$ starting from the initial state $\rho_0 = \begin{pmatrix} 2/3 & 0 \\ 0 & 1/3 \end{pmatrix}$ at $t = 0$. For simplicity, you can set $\hbar = 1$.

(d) Since the map $\rho \mapsto [H, \rho]$ is linear, we can represent it as matrix-vector multiplication after "vectorizing" ρ, i.e., collecting its entries in a vector, denoted $\vec{\rho}$ in the following. For the commutator, this leads to

$$\vec{\rho} \mapsto \mathrm{vec}([H, \rho]) = \left(H \otimes I - I \otimes H^T\right)\vec{\rho},$$

where the identity matrix has the same dimension as H. Thus we can represent the von Neumann equation equivalently in the "superoperator" form

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\vec{\rho}(t) = \mathcal{H}\vec{\rho}(t), \quad \mathcal{H} = H \otimes I - I \otimes H^T.$$

Write down the formal solution of this differential equation, and determine $\mathcal{H}$ for the Hamiltonian from (c).

Solution

(a) By the product rule,

$$\begin{aligned} i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\rho(t) &= i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \sum_j p_j \, |\psi_j(t)\rangle \langle\psi_j(t)| = \sum_j p_j \left(\frac{i\hbar \, \mathrm{d}\,|\psi_j(t)\rangle}{\mathrm{d}t} \langle\psi_j(t)| + |\psi_j(t)\rangle \frac{i\hbar \, \mathrm{d}\,\langle\psi_j(t)|}{\mathrm{d}t} \right) \\ &= \sum_j p_j \Big(\big(H\,|\psi_j(t)\rangle\big) \langle\psi_j(t)| - |\psi_j(t)\rangle \big(\langle\psi_j(t)|\, H^\dagger\big) \Big) = H\rho(t) - \rho(t)H = [H, \rho(t)]. \end{aligned}$$

Here we have used that the Hamiltonian H is Hermitian, that is, $H^\dagger = H$. The minus sign stems from taking the conjugate-transpose of the Schrödinger equation.

(b) The formal solution for a pure state is $|\psi(t)\rangle = U(t)\,|\psi(0)\rangle$, and thus

$$\rho(t) = U(t)\rho_0 U(t)^\dagger = U(t)\rho_0 U(-t).$$

This $\rho(t)$ indeed solves the von Neumann equation, since $\frac{\mathrm{d}}{\mathrm{d}t}U(t) = -\frac{i}{\hbar}H$.

(c) We first determine the unitary time evolution operator $U(t)$, using the formula for the R_x rotation operator:

$$U(t) = \mathrm{e}^{-iHt} = \mathrm{e}^{-iJXt} = \cos(Jt)I - i\sin(Jt)X = \begin{pmatrix} \cos(Jt) & -i\sin(Jt) \\ -i\sin(Jt) & \cos(Jt) \end{pmatrix}.$$

Inserted into the equation from (b) leads to

$$\begin{aligned} \rho(t) = U(t)\rho_0 U(-t) &= \begin{pmatrix} \cos(Jt) & -i\sin(Jt) \\ -i\sin(Jt) & \cos(Jt) \end{pmatrix} \begin{pmatrix} \frac{2}{3} & 0 \\ 0 & \frac{1}{3} \end{pmatrix} \begin{pmatrix} \cos(Jt) & i\sin(Jt) \\ i\sin(Jt) & \cos(Jt) \end{pmatrix} \\ &= \begin{pmatrix} \frac{2}{3}\cos^2(Jt) + \frac{1}{3}\sin^2(Jt) & \frac{i}{3}\cos(Jt)\sin(Jt) \\ -\frac{i}{3}\cos(Jt)\sin(Jt) & \frac{1}{3}\cos^2(Jt) + \frac{2}{3}\sin^2(Jt) \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{3} + \frac{1}{3}\cos^2(Jt) & \frac{i}{6}\sin(2Jt) \\ -\frac{i}{6}\sin(2Jt) & \frac{1}{3} + \frac{1}{3}\sin^2(Jt) \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2} + \frac{1}{6}\cos(2Jt) & \frac{i}{6}\sin(2Jt) \\ -\frac{i}{6}\sin(2Jt) & \frac{1}{2} - \frac{1}{6}\cos(2Jt) \end{pmatrix} = \frac{1}{2}\left(I - \frac{1}{3}\sin(2Jt)Y + \frac{1}{3}\cos(2Jt)Z \right). \end{aligned}$$

(d) The superoperator differential equation can be identified with a Schrödinger equation, with analogous formal solution

$$\vec{\rho}(t) = \mathrm{e}^{-i\mathcal{H}t/\hbar}\,\vec{\rho}_0.$$

For the Hamiltonian from (c), we note that $X^T = X$, and obtain

$$\mathcal{H} = J(X \otimes I - I \otimes X) = J \begin{pmatrix} 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \end{pmatrix}.$$