1 Ensambles of quantum states

This note closely follows the presentation in Section 2.4.2 of Nielsen and Chuang [1]. The probablity density operator (or matrix) is used to characterize quantum systems whose state is not completely known. Suppose a quantum system is in one of a number of states $\psi_i \in \mathbb{C}^N$ with respective probablility p_i, for $i \in [1, N]$. We call $\{p_i, \psi_i\}$ an ensamble of pure states. The density matrix for the quantum system is defined by the $N \times N$ complex matrix

$$\rho = \sum_{i=1}^{N} p_i \psi_i \psi_i^\dagger, \quad p_i \geq 0.$$

From the definition follows immediately that the density matrix is Hermitian (self-adjoint),

$$\rho^\dagger = \sum_{i=1}^{N} p_i \psi_i \psi_i^\dagger = \rho,$$

because the probabilities p_i are real non-negative numbers.

Consider the evolution of a closed quantum system that is described by the unitary operator U. Let the system initially be in the state ψ_i, with probablitity p_i, corresponding to the density matrix $\rho(0)$. After the evolution (at time T) the system will then be in the state $U\psi_i$ with probability p_i. Thus, the evolution of the density matrix is described by

$$\rho(T) = \sum_{i=1}^{N} p_i U \psi_i \psi_i^\dagger U^\dagger = U \rho(0) U^\dagger.$$

A quantum system whose state is known exactly is said to be in a pure state. Let the state be represented by the unit vector $\psi \in C^N$. Because the system is in this state with certainty (probability 1), the density matrix is represented by the rank-1 matrix

$$\rho = \psi \psi^\dagger \in \mathbb{C}^{N \times N}.$$

In this case, the density matrix is a projection,

$$\rho^2 = \psi \psi^\dagger \psi \psi^\dagger = \psi \psi^\dagger = \rho.$$

If the state of the quantum system is *not* known exactly, the density operator is in a mixed state, meaning that it is in an ensemble of pure states that result in a density matrix that is not a projection.

Definition 1. *Consider a quantum system that is in a pure or a mixed state. Let $\psi_i \in \mathbb{C}^N$ be the state vector for the ith state and let the quantum system be in this state with probability $p_i \geq 0$, for $i \in [1, N]$. Also assume $\sum_{i=1}^{N} p_i = 1$. The Hermitian $N \times N$ probability density matrix for the quantum system is defined by*

$$\rho = \sum_{i=1}^{N} p_i \psi_i \psi_i^\dagger, \quad p_i \geq 0, \quad \rho^\dagger = \rho, \quad tr(\rho) = 1.$$

Conversely, $\rho \in \mathbb{C}^{N \times N}$ is the probability density matrix associated with an ensamble of quantum states, if and only if:

$$\rho^\dagger = \rho, \quad tr(\rho) = 1, \quad \phi^\dagger \rho \phi \geq 0, \quad \text{for all } \phi \in \mathbb{C}^N.$$

A simple criteria for determining whether a state is pure or mixed is:

$$\begin{cases} tr(\rho^2) = 1, & \text{pure state} \\ tr(\rho^2) < 1, & \text{mixed state} \end{cases}$$

It is easy to see that the statement is true for a pure state, because then the quantum system is described by the state vector ψ with certainty. The corresponding density matrix becomes

$$\rho = \psi\psi^\dagger, \quad \Rightarrow \quad \rho^2 = \psi\psi^\dagger\psi\psi^\dagger = \psi\psi^\dagger = \rho,$$

because $\psi^\dagger\psi = |\psi|^2 = 1$. Thus, $tr(\rho^2) = tr(\rho) = 1$.

Freedom of ensambles. In this example, it is shown that two different ensambles of quantum states can result in the same density matrix. Let $\mathbf{e}_k$ be the kth unit vector, i.e., $\mathbf{e}_0 = [1, 0, 0, \ldots, 0]^\dagger$, $\mathbf{e}_1 = [0, 1, 0, \ldots, 0]^\dagger$, etc., and consider a quantum system with the density matrix

$$\rho = \frac{3}{4}\mathbf{e}_0\mathbf{e}_0^\dagger + \frac{1}{4}\mathbf{e}_1\mathbf{e}_1^\dagger.$$

Clearly, this density matrix arises if the quantum system is in the state $\mathbf{e}_0$ with probability $3/4$ and in state $\mathbf{e}_1$ with probability $1/4$. Now define the states

$$\mathbf{a} = \sqrt{\frac{3}{4}}\mathbf{e}_0 + \sqrt{\frac{1}{4}}\mathbf{e}_1, \tag{1}$$

$$\mathbf{b} = \sqrt{\frac{3}{4}}\mathbf{e}_0 - \sqrt{\frac{1}{4}}\mathbf{e}_1, \tag{2}$$

and let the quantum system be in the state $\mathbf{a}$ with probability $1/2$ and in the state $\mathbf{b}$ with probability $1/2$. Then the corresponding density matrix becomes

$$\rho = \frac{1}{2}\mathbf{a}\mathbf{a}^\dagger + \frac{1}{2}\mathbf{b}\mathbf{b}^\dagger = \frac{1}{2}\begin{bmatrix} \frac{3}{4} & \frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & \frac{1}{4} \end{bmatrix} + \frac{1}{2}\begin{bmatrix} \frac{3}{4} & -\frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{4} & \frac{1}{4} \end{bmatrix} = \begin{bmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{bmatrix}.$$

Thus, two different ensambles of quantum states can result in the same density matrix! In general, the eigenvectors and eigenvalues of a density matrix only indicate one of many possible ensambles that result in the same density matrix. It is possible to further characterize the freedom of ensambles that result in the same density operator, see [1].

2 The Lindblad master equation

Interactions with the environment in a quantum system can be modeled by considering the evolution of the Hermitian density matrix,

$$
\rho = \begin{bmatrix} \rho_{11} & \rho_{12} & \cdots & \rho_{1N} \\ \rho_{21} & \rho_{22} & \cdots & \rho_{2N} \\ \vdots & \vdots & & \vdots \\ \rho_{N1} & \rho_{N2} & \cdots & \rho_{NN} \end{bmatrix} = \rho^\dagger.
$$

For a closed quantum system, the density matrix evolves according to

$$
\dot{\rho} = -i\left(H\rho - \rho H\right), \quad t \geq 0, \quad \rho(0) = \rho_0, \quad \mathrm{tr}(\rho_0) = 1, \quad \rho_0^\dagger = \rho_0. \tag{3}
$$

Here, $H = H(t)$ is the Hamiltonian matrix, $H \in \mathbb{C}^{N \times N}$ and $H^\dagger = H$. Thus, the expression on the right hand side satisfies

$$
\left(-i\left(H\rho - \rho H\right)\right)^\dagger = +i\left(\rho^\dagger H^\dagger - H^\dagger \rho^\dagger\right) = +i\left(\rho H - H\rho\right),
$$

because both H and ρ are Hermitian. We conclude that the right hand side of (3) is anti-Hermitian (skew-symmetric). The evolution of the density matrix is therefore oscillatory in time.

The above equation is called the Liouville-von Neumann (LvN) equation and is a special case of the Lindblad master equation,

$$
\dot{\rho} = -i\left(H\rho - \rho H\right) + \sum_j \gamma_j \left(\mathcal{L}_j \rho \mathcal{L}_j^\dagger - \frac{1}{2}\left(\mathcal{L}_j^\dagger \mathcal{L}_j \rho + \rho \mathcal{L}_j^\dagger \mathcal{L}_j \right) \right), \tag{4}
$$

where γ_j are constants and $\mathcal{L}_j$ are collapse operators. One example of a collapse operator is $\mathcal{L}_j = a$, which lowers the energy level. It is called a jump operator. Another example is $\mathcal{L}_j = a^\dagger a$. It is called a de-phasing operator. From the grouping of the collapse operators in (4), we immediately see that each term in the sum on the right hand side is Hermitian,

$$
\left(\mathcal{L}_j \rho \mathcal{L}_j^\dagger - \frac{1}{2}\left(\mathcal{L}_j^\dagger \mathcal{L}_j \rho + \rho \mathcal{L}_j^\dagger \mathcal{L}_j \right) \right)^\dagger = \mathcal{L}_j \rho^\dagger \mathcal{L}_j^\dagger - \frac{1}{2}\left(\rho^\dagger \mathcal{L}_j^\dagger \mathcal{L}_j + \mathcal{L}_j^\dagger \mathcal{L}_j \rho^\dagger \right)
$$

$$
= \mathcal{L}_j \rho \mathcal{L}_j^\dagger - \frac{1}{2}\left(\mathcal{L}_j^\dagger \mathcal{L}_j \rho + \rho \mathcal{L}_j^\dagger \mathcal{L}_j \right),
$$

because $\rho^\dagger = \rho$. Thus, the collapse operators act as damping or source terms in the evolution of the density matrix.

2.1 Vectorizing the density matrix

The right hand sides of the LvN (3) and Lindblad equations (4) involve the dependent variable ρ in matrix form. To utilize the sparse structure of the Hamiltonian matrix

and use standard solvers for systems of ordinary differential equations, we reorder ρ by stacking its columns into one column vector with N^2 elements and use Kronecker products to reformulate the equations. For the LvN equation, we get

$$\frac{d}{dt}\text{vec}(\rho) = -i\left(I_N \otimes H - H^T \otimes I_N\right)\text{vec}(\rho), \quad \text{vec}(\rho) = \begin{bmatrix} \rho_{11} \\ \vdots \\ \rho_{N1} \\ \vdots \\ \vdots \\ \rho_{1N} \\ \vdots \\ \rho_{NN} \end{bmatrix}. \tag{5}$$

Here, I_N denotes the $N \times N$ identity matrix. Note that H is transposed in the second term on the right hand side (without complex conjugation). Because H is Hermitian, the terms in the matrix on the right hand side satisfy

$$(I_N \otimes H)^\dagger = I_N \otimes H^\dagger = I_N \otimes H, \quad (H^T \otimes I_N)^\dagger = \bar{H} \otimes I_N = \bar{H}^\dagger \otimes I_N = H^T \otimes I_N.$$

Because of the factor i in front of the matrix in (5), it satisfies

$$\left(-i\left(I_N \otimes H - H^T \otimes I_N\right)\right)^\dagger = +i\left(I_N \otimes H - H^T \otimes I_N\right).$$

This verifies that the skew-symmetric property of the LvN equation was retained after ρ was reordered into a column vector.

2.2 Test problem 1

Consider the LvN equation (3) when the Hamiltonian matrix and the initial data for the density matrix are

$$H(t) = f(t)\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad f(t) = \frac{1}{4}\left(1 - \cos(\omega t)\right), \quad \rho_0 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

After vectorizing the problem, we get the system

$$\frac{d}{dt}\text{vec}(\rho) = -if(t)\begin{bmatrix} 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & -1 \\ -1 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 \end{bmatrix}\text{vec}(\rho) \tag{6}$$

Note that the matrix on the right hand side is skew-symmetric. Thus all eigenvalues are purely imaginary and the solution is oscillatory in time. An exact solution can be

constructed from the Schrodinger equation with the same Hamiltonian matrix. It is solved by the state vector

$$\Psi(t) = \begin{bmatrix} \cos(\phi(t)) \\ -i\sin(\phi(t)) \end{bmatrix}, \quad \phi(t) = \frac{1}{4}\left(t - \frac{1}{\omega}\sin(\omega t)\right)$$

The solution of (6) follows as the corresponding density matrix,

$$\rho(t) = \Psi(t)\Psi^{\dagger}(t) = \begin{bmatrix} \cos^2(\phi(t)) & i\cos(\phi(t))\sin(\phi(t)) \\ -i\cos(\phi(t))\sin(\phi(t)) & \sin^2(\phi(t)) \end{bmatrix}$$

To further utilize standard routines for solving ordinary differential equations, we further re-formulate the problem in terms of real-valued vectors and matrices,

$$\text{vec}(\rho) = \mathbf{u} + i\mathbf{v}, \quad -i\left(I_N \otimes H(t) - H^T(t) \otimes I_N\right) =: A(t) + iB(t).$$

This leads to the equivalent system,

$$\frac{d}{dt}\begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix} = \begin{bmatrix} A(t) & -B(t) \\ B(t) & A(t) \end{bmatrix}\begin{bmatrix} \mathbf{u} \\ \mathbf{v} \end{bmatrix}$$

Because the system (5) is skew-symmetric, $(A + iB)^{\dagger} = -(A + iB)$. Thus, $A^T = -A$ and $B^T = B$. As expected, the real-valued formulation is also skew-symmetric. Since ρ is Hermitian, not all off-diagonal elements are unique,

$$\rho_{jk} = \bar{\rho}_{kj}, \quad \Rightarrow \quad u_{jk} = u_{kj}, \quad v_{jk} = -v_{kj}.$$

Hence, only the lower triangular part of the density matrix needs to be stored for the real part of ρ. Further savings can be realized for the imaginary part of ρ, because it is zero along the diagonal, $v_{jj} = 0$.

References

[1] M. Nielsen and I. Chuang. *Quantum computation and quantum information.* Cambridge University Press, 2000.