Quantum Information Theory

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Classical vs Quantum systems

1 Overview of quantum mechanics

1.1 Axioms of quantum mechanics

(a) Quantum states are represented by normalized vectors, i.e, $\psi \in H : ||\psi||^2 = 1$

(b) Quantum observables are represented by Hermitian operators, i.e,

$$A : H \longrightarrow H \ \text{ such that } \ \langle Ax, y \rangle = \langle x, Ay \rangle \ \forall \ x, y \in H$$

(c) Let $A : H \longrightarrow H$ be a quantum observable. Experimentally, we can only observe its eigenvalues.

(Assumption: Observables have non degenerate eigenvalues, i.e, $\lambda_k \neq \lambda_m$ for all $k \neq m$).

Born postulate: Given a state ψ and a quantum observable A, the probability of observing the eigenvalue λ_j is
$$P_\psi(A = \lambda_j) = |\langle \psi, e_j \rangle|^2$$
where e_j is the eigenvector of A corresponding to λ_j.

1.2 Schrödinger physical quantization

On subspaces of the infinite Hilbert space of square integrable functions $H = L_2(\mathbb{R})$, Schrödinger defined the position and momentum operators:

$$q \colon L_2(\mathbb{R}) \longrightarrow L_2(\mathbb{R}) \ , \quad p \colon L_2(\mathbb{R}) \longrightarrow L_2(\mathbb{R})$$

$$f \longmapsto xf \qquad\qquad f \longmapsto \tfrac{h}{i}\dot{f}$$

where h is Planck's constant. We then find that $[p, q]f(x) = \frac{h}{i}f(x) \Rightarrow [p, q] = \frac{h}{i}I$, i.e, p and q do not commute.

1.3 Uncertainty principle

Robertson's inequality for two given Hermitian operators A and B is

$$\sigma_A \sigma_B \geq \frac{1}{2}|\langle [A, B] \rangle|$$

and when applied to the position and momentum operators yields

$$\sigma_q \sigma_p \geq \frac{h}{2}$$

which is known as the Heisenberg uncertainty relation. The dispersion of both position and momentum cannot be zero and hence, both position and momentum cannot be determined simultaneously. This is a direct consequence of the non-commutativity of the two corresponding operators.

1.4 Representation of quantum states by density operators

Pure states can be represented by projection operators (state vectors or wavefunctions)

$$P_\psi : H \longrightarrow H$$

$$\varphi \longmapsto P_\psi(\varphi)$$

where $P_\psi(\varphi)$ is the projection of φ onto ψ. More generally, a mixed state can be represented by any operator ρ satisfying the following properties:

- ρ is positive definite, i.e, $\langle \rho(\varphi), \varphi \rangle \geq 0$ for all $\varphi \in H$.

- ρ is Hermitian

- $\text{Tr}(\rho) = \sum_{k=1}^n \langle \rho(e_k), e_k \rangle = 1$ where $\{e_k\}_{k=1}^n$ are the eigenvectors of ρ (and therefore a basis for H).

An operator ρ satisfying the above properties is called a density operator. For any Hermitian operator A we can then use Born's rule to compute the probability of observing e_k

$$P(A = e_k) = \langle \rho(e_k), e_k \rangle$$

and the average

$$\langle A \rangle_\rho = \text{Tr}(\rho A).$$

The main particularity of a pure state is that its corresponding operator is idempotent, i.e, $P_\psi^2 = P_\psi$ since projecting two times yields the same vector as projecting only once.

2 Evolution in time of a classical system vs a quantum system

2.1 Hamiltonian equations and Liouville equation

In Hamiltonian mechanics, the state of a particle is determined by the position and momentum at a time $t = t_0$ in phase space $(q(t_0), p(t_0))$. The evolution in time of the particle is described by taking into consideration the Hamiltonian formulation of Newton's 2nd law, $\dot{p} = f(q)$ where $f(q) = -\frac{\partial V}{\partial q}$ is a potencial force, combined with the complete energy of the system

$$\mathcal{H}(q, p) = \frac{p^2}{2m} + V(q).$$

These yield the Hamiltonian equations

$$\begin{cases} \dot{q} = \frac{\partial \mathcal{H}}{\partial p} \\ \dot{p} = -\frac{\partial \mathcal{H}}{\partial q} \\ (q(t_0), p(t_0)) \end{cases}$$

and imply that the energy of the system is preserved along trajectories for any Hamiltonian dynamics, i.e, $\mathcal{H}(q(t), p(t)) = \mathcal{H}(q_0, p_0)$ for all $t \geq 0$.

From this fact it is proven that the probability density function $\rho(t, q(t), p(t))$, which, when integrated in some domain V of the phase space gives the probability of finding particles in V, is also preserved along each trajectory. This result is reflected in Liouville's equation, which given an initial density $\rho_0(q, p)$ and a Hamiltonian function $\mathcal{H}(p, q)$ finds the probability density $\rho(t, q, p)$ for future $t \geq 0$,

$$\begin{cases} \frac{\partial \rho}{\partial t} = \{\mathcal{H}, \rho\} \\ \rho(0) = \rho_0 \end{cases}$$

where, for simplicity, the Poisson bracket $\{f, g\} = \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial q}$ is used.

2.2 Schrödinger's equation

In quantum mechanics, the state of a system is represented by a time dependent complex vector $\psi(t) \in H$. By setting Planck's constant $h = 1$, and considering the energy Hamiltonian operator $\mathcal{H}$, Schrödinger came up with the equation

$$\begin{cases} i\frac{\partial \psi}{\partial t}(t) = \mathcal{H}\psi(t) \\ \psi(0) = \psi_0 \end{cases}$$

which was motivated to ensure that every state $\psi(t) \in H$ would preserve its norm in the process of evolution,

$$||\psi(t)||^2 = 1 \text{ for all } t \geq 0 \Leftrightarrow \langle \psi(t), \psi(t) \rangle = 1 \text{ for all } t \geq 0.$$

Example

Consider the Hamiltonian

$$\mathcal{H}(q, p) = \frac{p^2}{2} + q^2$$

Denote $\hat{q}$ and $\hat{p}$ the operators of Schrödinger's quantization procedure and let $H = L_2(\mathbb{R})$. Then,

$$\begin{cases} \hat{q}^2\psi(x) = x^2\psi(x) \\ \hat{p}^2\psi(x) = (-i)^2\psi''(x) \end{cases}$$

So, from

$$\mathcal{H}(\hat{q}, \hat{p}) = \frac{\hat{p}^2}{2} + \hat{q}^2$$

we obtain the energy operator

$$\mathcal{H}(\hat{q}, \hat{p})\psi(x) = -\frac{\partial^2\psi(x)}{2\partial x^2} + x^2\psi(x)$$

and the Schrödinger equation

$$\begin{cases} i\frac{\partial \psi}{\partial t}(t, x) = -\frac{\partial^2\psi}{2\partial x^2}(t, x) + x^2\psi(t, x) \\ \psi(0, x) = \psi_0(x) \end{cases}$$

2.3 Von Neumann's equation

The evolution in time of a mixed state (represented by a density operator ρ) is described by the equation

$$\begin{cases} \frac{\partial \rho}{\partial t}(t) = -i[\mathcal{H}, \rho(t)] \\ \rho(0) = \rho_0 \end{cases} \tag{1}$$

where the brackets denote the commutator operator. An important realization is that the entropy of an isolated quantum system is not changed with time, i.e,

$$S(\rho(t)) = S(\rho(0)) \text{ for all } t \geq 0.$$

3 Classical vs Quantum entropy

3.1 Boltzmann Entropy

Given a classical isolated system comprised of a set Ω of microstates and a set $\Lambda = \{M_1, ..., M_n\} \subset \Omega$ of disjoint macrostates, the Boltzmann entropy of the macrostate M is defined as

$$S(M) = K_B \ln(N_M)$$

where K_B is the Boltzmann constant and N_M is the number of microstates in M. Hence, if the size of M increases, so does the entropy, which results in the 2$^{\text{nd}}$ law of thermodynamics.

3.2 Shannon Entropy

If $p = (p_j)$ is a discrete probability distribution followed by a random variable, Shannon's entropy is defined as

$$S(p) = -\sum_j p_j \ln(pj) \tag{2}$$

and measures the average level of uncertainty inherent in the variable's possible outcomes.

Example

Given a biased coin with probability $p_1 = x$ of landing on heads and probability $p_2 = 1 - x$ of landing on tails for $x \in [0, 1]$ the entropy looks as follows:
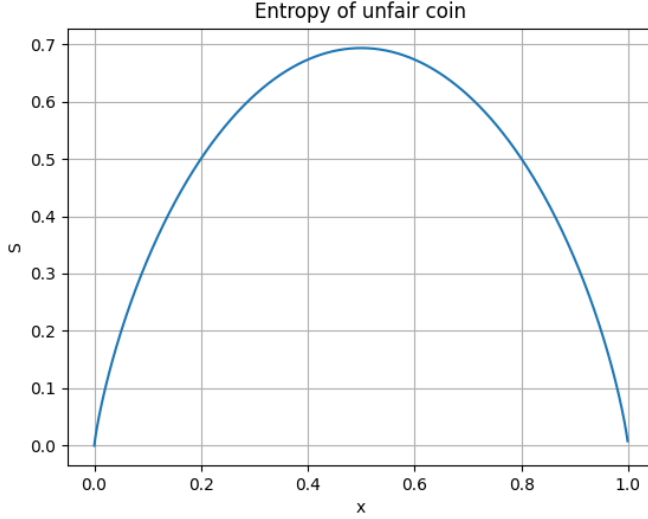
3.3 Von Neumann Entropy

For a quantum system described by a density operator ρ, the von Neumann entropy is defined as

$$S(\rho) = -\mathrm{Tr}(\rho) \ln(\rho)$$

where the logarithm is defined such that $e^{\ln(\rho)} = \rho$ and

$$e^\rho = \sum_{n=0}^{\infty} \frac{\rho^n}{n!}$$

Moreover, if $\{p_j\}$ are the eigenvalues of ρ, then in the basis $\{e_j\}$ of eigenvectors of ρ, the entropy reduces to the sum of its diagonal entries and then coincides with Shannon's formula (2).

The von Neumann entropy satisfies the following conditions:

- $\mathcal{S}(\rho) = 0$ if and only if ρ is a pure quantum state ($\rho^2 = \rho$).

- Let N be the dimension of the state space. Then the maximum entropy is approached on the state

$$\rho_{disorder} = \frac{1}{N} I$$

and $\mathcal{S}(\rho_{disorder}) = \ln N$.

- In contrast with classical entropy, the entropy of a quantum system is not changed with time (see von Neumann equation (1)).

Examples

1. Consider the state represented by the density operator

$$\rho = \begin{pmatrix} \frac{1}{2} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{2} \end{pmatrix}$$

with eigenvalues $p_1 = 0.625$ and $p_2 = 0.375$. If we take as basis the orthonormal eigenvectors e_1 and e_2 of ρ then the Von Neumann entropy of this state is given by

$$\mathcal{S}(\rho) = -\mathrm{Tr}(\rho)\ln(\rho) = -p_1 \ln p_1 - p_2 \ln p_2 \approx 0.662$$

2. Let $\alpha, \beta \in \mathbb{C}$ such that $|\alpha|^2 + |\beta|^2 = 1$ and consider the state represented by the density operator

$$\rho = \begin{pmatrix} |\alpha|^2 & \alpha\overline{\beta} \\ \overline{\alpha}\beta & |\beta|^2 \end{pmatrix}$$

From the identity $z \cdot \overline{z} = |z|^2$ it is easy to verify that $\rho^2 = \rho$, so in particular, ρ is a pure quantum state. By the first property of the Von Neumann entropy we have that $\mathcal{S}(\rho)=0$.

4 Conclusion

In classical systems,

- Dynamics are perfectly determined in the phase space as position q and momentum p by the Hamiltonian equations of the system.

- The energy of the system is preserved along individual trajectories (Hamiltonian dynamics).

- Since the energy is carried by particles, the probability density function for a collection of particles is also preserved (Liouville equation).

- The 2nd law of thermodynamics states that the entropy inside a classical isolated system increases with time and thereby there is an eventual destruction of order (Boltzmann entropy).

In quantum systems,

- It is impossible to determine the position and momentum of a particle (Heisenberg uncertainty principle). Instead, the notion of states as normalized vectors and observables as Hermitian operators in a Hilbert space are introduced. Given a state ψ and an observable A, only the probability of observing an eigenvalue λ of A can be computed via Born's rule.

- State normalization for pure states is preserved in the process of evolution (Schrödinger equation).

- The dynamics of a pure state (represented by a projection operator) are described by Schrödinger's equation whereas the dynamics of a mixed state (represented by a density operator) are described by von Neumann's equation.

- The entropy of an isolated quantum system is not changed with time (von Neumann entropy).