Dynamics of Quantum Open Systems

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Seminar Structure

Dynamics of Pure States

In the quantum mechanics, for a physical system to be described in terms of a Hilbert space $\mathcal{H}$, one postulates that a state $\psi \in \mathcal{H}$ of the system evolves in time under the action of a one-parameter strongly continuous group of unitary operators.

Definition

A family of unitary maps $U_t \in \mathfrak{B}(\mathcal{H})$, $t \in \mathbf{R}^+$, sharing the two following properties

- $U_s U_t = U_{s+t}$, for $s, t \in \mathbf{R}^+$,
- $U_t \phi \to \phi$ as $t \to 0$ for $\phi \in \mathcal{H}$,

is called a *one-parameter strongly continuous semigroup of unitary operators*.

Although rather abstract, the definition appears to be sufficiently motivated by the following requirements.

- Since the Schrödinger equation is linear, the time evolution should be governed by a family of linear maps that preserve the norm of a vector in the Hilbert space.
- The continuity property assures that the evolution of all expectation values is continuous in time.
- The semigroup property seems to be self-explanatory.

The following deep result shows that a strongly continuous semigroup of unitary operators is fully described by its generator and can be extended to a group.

Stone's theorem

Let $U_t \in \mathfrak{B}(\mathcal{H})$ be a strongly continuous one-parameter semigroup of unitary operators. There exists a hermitian operator H, not necessary bounded, such that

$$U_t = e^{-itH}, \quad t \in \mathbf{R}^+,$$

and the semigroup has a strongly continuous extension to a group

$$U_t^{-1} = U_{-t} = e^{itH}.$$

Thus, the dynamics of a closed quantum system is reversible and can be completely described by the Hamiltonian.

General Hamiltonian Systems

In general, states of a quantum system are represented by so-called density matrices, i.e. positive linear operators of unit trace.

Reminder

- A linear operator $\rho \in \mathfrak{B}(\mathcal{H})$ is called *positive*, if for any $\phi \in \mathcal{H}$

$$(\phi, \rho\phi) \geq 0.$$

- We define the trace of a positive operator to be

$$\mathrm{tr}\rho = \sum_{n=1}^{N} (e_n, \rho e_n),$$

where $\{e_n\}_{n=1}^{N}$ is an orthonormal basis in $\mathcal{H}$ and $N = \dim \mathcal{H}$.

Once a strongly continuous group of unitary operators $U_t = e^{-itH}$ has been established, the evolution of the system can be seen from the two equivalent perspectives. Either a density matrix (a state) ρ changes in time while all the operators remain the same, or the dynamical group acts on the set of observables leaving the states unchanged.

The Schrödinger picture

$$\rho \longrightarrow \rho_t = U_t \rho U_t^* = e^{-itH} \rho e^{itH}.$$

The Heisenberg picture

$$A \longrightarrow A_t = U_t^* A U_t = e^{itH} A e^{-itH}.$$

Whichever picture we chose, the evolution of measurable quantities stays the same

$$\mathrm{tr} \rho_t A = \mathrm{tr} \rho A_t .$$

Quantum Dynamical Semigroups

- Let us use for a while the Heisenberg picture of a quantum dynamics.
- Let us denote by $\mathfrak{M} \subset \mathfrak{B}(\mathcal{H})$ the subset "generated by all relevant observables" [1], which actually constitutes the system.
- We are now able to generalise the definition of a strongly continuous semigroup of unitary operators in such a way, that it will include irreversible dynamics of quantum open systems.

[1] This rather vague notion has a precise mathematical realisation in the concept of a von Neumann algebra.

Definition

A family of maps $T_t : \mathfrak{M} \to \mathfrak{M}$, $t \in \mathbf{R}^+$ is called a *quantum dynamical semigroup*, if

- T_t is a positive linear map for every $t \in \mathbf{R}^+$,
- $T_t \to \mathbf{1}$, as $t \to 0$ in an appropriate sense, and $T_t(\mathbf{1}) = \mathbf{1}$,
- $T_s T_t = T_{s+t}$, $s, t \in \mathbf{R}^+$.

- A strongly continuous group of unitary operators is a special case of the above definition for $T_t A = U_t^* A U_t$.
- The definition provides the most general framework for studying time evolution of a quantum system interacting with its environment.

- Since the maps T_t are not necessary isometries, the Stone's theorem is no longer applicable and we may expect that dynamical semigroups are suitable to describe irreversible evolution of a quantum system.
- This time, there is no obvious reason, why a dissipative dynamics should satisfy the semigroup property.
  Indeed, let us consider a joint system consisting of a quantum system $(\mathcal{S})$ and its environment $(\mathcal{E})$.
  Since the compound system is genuinely quantum and closed, its time evolution should be governed by a Hamiltonian

$$H = H_{\mathcal{S}} \otimes \mathbf{1}_{\mathcal{E}} + \mathbf{1}_{\mathcal{S}} \otimes H_{\mathcal{E}} + H_I .$$

The time evolution of the reduced density matrix is then given by

$$\rho_t = \mathrm{tr}_{\mathcal{E}} \left(e^{-itH} (\rho_0 \otimes \omega_E) e^{itH} \right), \tag{1}$$

where $\mathrm{tr}_{\mathcal{E}}$ denotes the partial trace with respect to the environment degrees of freedom.

- In general, (1) is a hopeless integro-differential equation. It is often possible, however, to apply to it the so-called Markov approximation, which leads to a semigroup dynamics.

The Markov approximation is usually applied by assuming that the system is only weakly coupled to the environment. For this reason, the environment quickly "forgets" any internal self-correlations that result from the integration with the system and this gives rise to the semigroup dynamics

$$T_{s+t}A = T_t(T_s A).$$

Generators and Markovian Master Equation

Definition

Let $T_t : \mathfrak{M} \to \mathfrak{M}$, $t \in \mathbf{R}^+$ be a quantum dynamical semigroup. The operator S, defined on an appropriate domain $D(S) \subset \mathfrak{M}$ by the following relation

$$SA = \frac{d}{dt} T_t A \Big|_{t=0} \equiv \lim_{t \to 0} \frac{T_t A - A}{t},$$

is called *the generator* of the semigroup.

Example

Let $T_t A = e^{itH} A e^{-itH}$, then $SA = i[H, A]$, or in the Schrödinger picture $S\rho = -i[H, \rho]$.

Master Equation

Because $T_t S = S T_t$ for all $t \in \mathbf{R}^+$, the following equation holds true

$$\frac{d}{dt}\rho_t = S\rho_t,$$

which is called *the Markovian master equation*.

- In practice, the study of almost all real-life examples of quantum dynamical semigroups is reduced to the study of their generators derived from given master equations.
- Besides, it is possible (especially in Wrocław) to investigate general properties of dynamical semigroups in a mathematically precise fashion, their ergodic properties, existence of generators, various continuity requirements etc. (Cf. masterful [Bratelli, O.; Robinson, D.])

Decoherence

An open quantum system becomes in the course of the time evolution heavily, and in practice irreversibly, entangled with its environment. This may lead to the decay of the off-diagonal elements of a reduced density matrix representing the initial state of the system

$$\rho = \sum_{n,m} c_n c_m^* \psi_n \psi_m^* \longrightarrow \sum_n |c_n|^2 \psi_n \psi_n^*$$

- This effect of damping "quantum coherences" is usually assumed as the operational definition of decoherence.
- Observe, that a unitary dynamics cannot produce the effect of decoherence in the system.

Four Aspects of Decoherence

In general the effect of decoherence can manifest itself in four different ways.

- Dynamical appearance of superselection rules [Unruh, Zurek, 1989] [Twamley, 1993].
- Preferred basis of pointer states [Zurek, 1981].
- Classical behaviour as a result of quantum dynamical evolution [Frölich et al., 2002] [Gell-Mann, 1993].
- Entirely new quantum behaviour [Blanchard et al., 2003].

Examples of Decoherence Models (cf. [Schlosshauer])

In the Born-Markov approximation the most general form of a master equation is known as the Lindblad equation.

The Born-Markov approximation

- *The Born approximation*. The system-environment coupling is sufficiently weak and the environment is sufficiently large so the system-environment state remains approximately in the product state
$$\rho_t^{\mathcal{SE}} = \rho_t^{\mathcal{S}} \otimes \rho_t^{\mathcal{E}}.$$
- *The Markov approximation*. "Memory effects" of the environment are negligible.

Born-Markov Master Equation in the Lindblad form

$$\frac{d}{dt}\rho_t = -i[H'_{\mathcal{S}}, \rho_t] - \frac{1}{2}\sum_{\mu} \kappa_{\mu} \left[\hat{L}_{\mu}, [\hat{L}_{\mu}, \rho_t]\right],$$

where $H'_{\mathcal{S}}$ is a "Lamb-shifted" Hamiltonian $H_{\mathcal{S}}$ and $\hat{L}_{\mu}$ are Lindblad generators, directly dependent on the interaction part H_I of the Hamiltonian.

Many models of quantum systems displaying decoherence can be reduced to few "canonical" ones.

Quantum Brownian Motion

The model consists of a particle moving in one dimension and interacting linearly with an environment of independent harmonic oscillators in thermal equilibrium at the temperature T.

The Quantum Brownian Motion Master Equation

$$\frac{d}{dt}\rho_t = -i[H'_{\mathcal{S}}, \rho_t] - \\ - \int_0^\infty \mathrm{d}\tau \left\{ \nu(\tau) \left[\hat{X}, [\hat{X}(-\tau), \rho_t]\right] - i\eta(\tau) \left[\hat{X}, [\hat{X}(-\tau), \rho_t]\right] \right\}.$$

$$\hat{X}(\tau) = e^{i\tau H_{\mathcal{S}}} \hat{X} e^{-i\tau H_{\mathcal{S}}},$$

and $\nu(\tau)$, $\eta(\tau)$ are referred to as *the noise kernel* and *the dissipation kernel*.

Spin-Boson Model

The spin-boson model corresponds to a single qubit coupled to the environment of harmonic oscillators. The role of qubit systems in quantum computing has led to additional interest of the spin-boson model. Recently, the model has been used to analyse the role of quantum decoherence in biological systems [Gilmore et al.].

Spin-Boson Model Master Equation

$$\frac{d}{dt}\rho_t = -i[H'_{\mathcal{S}}, \rho_t] - \tilde{D}\,[\sigma_z, [\sigma_z, \rho_t]] + \zeta\sigma_z\rho_t\sigma_y + \zeta^*\sigma_y\rho_t\sigma_z,$$

where $\tilde{D}, \zeta$ are number coefficients related to the form of the interaction Hamiltonian H_I.

Summary

- The time reversible dynamics of closed quantum systems is by no means sufficient to describe various phenomena related to complex interactions between a quantum system and its environment.
- In the Markovian approximation, the study of the irreversible dynamics of quantum open systems employs tools such like quantum dynamical semigroups, their generators and master equations.

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Questions

- Do Markov equations have something in common with Markov processes in probability theory?
- What do people do with quantum dynamical semigroups and decoherence in Wrocław?
- Is decoherence a common phenomenon?
- I wasn't even listening, but I'm sure the whole idea is stupid anyway. What do you think about that?
- Do macroscopic Schrödinger's cat-like states exist?
- Is decoherence somehow related to the measurement problem?