Dynamics of Open Quantum Systems

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June 8, 2010

Abstract

The basic introduction to the theory of open quantum systems has been presented, following the brief overview of standard Hamiltonian systems typically encountered in quantum mechanics. The rudimentary facts concerning open systems have been explained and empirically justified together with a few examples focused on the applications to the description of decoherence.

1 Dynamics of Quantum Hamiltonian Systems

1.1 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 1. *A family of unitary maps $U_t \in \mathfrak{B}(\mathcal{H})$, $t \in \mathbf{R}^+$ (the set of non-negative reals), 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 the 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 [1].

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.

Theorem 1 (Stone)**.** *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 the strongly continuous extension to the group

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

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

The proof of the theorem can be found in [2].

1.2 General Quantum Hamiltonian Systems

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

Definition 2. *A linear operator $\rho \in \mathfrak{B}(\mathcal{H})$ is called* positive*, if for any $\phi \in \mathcal{H}$*

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

or, equivalently, if it is self-adjoint and its spectrum is a subset of $\mathbf{R}^+$.

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. Thus, in *the Schrödinger picture*

$$\rho \to \rho_t = U_t \rho U_t^* = e^{-itH} \rho e^{itH},$$

whereas *the Heisenberg picture* describes the evolution by

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

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

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

2 The Irreversible Dynamics of Open Quantum Systems

2.1 Quantum Dynamical Semigroups

Let us adopt the Heisenberg picture of a quantum dynamics and denote by $\mathfrak{M} \subset \mathfrak{B}(\mathcal{H})$ the subset "generated by all relevant observables" [1], which actually

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

Definition 3. *Let $\mathfrak{M}$ be a subalgebra of $\mathfrak{B}(\mathcal{H})$ and let $\mathfrak{M}'$ be its commutant*

$$\mathfrak{M}' = \{y \in \mathfrak{B}(\mathcal{H}) : xy = yx, x \in \mathfrak{M}\}.$$

We say that $\mathfrak{M}$ is a von Neumann algebra*, if $\mathfrak{M} = \mathfrak{M}''$.*

This particular type of operator algebras has many desired properties, e.g. if $\mathfrak{M}$ contains a hermitian operator x, then all the projections that constitute the spectral decomposition of x belong to $\mathfrak{M}$ as well. Of course, $\mathfrak{B}(\mathcal{H})$ is a perfect example of a von Neumann algebra.

For more information about von Neumann algebras and their application to mathematical physics, see for example [2].

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.

Definition 4. *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 the 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 the Hamiltonian

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

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

$$\rho_t = \mathrm{tr}_{\mathcal{E}} \left(e^{-itH} (\rho_0 \otimes \omega_E) e^{itH} \right), \tag{2}$$

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

In general, (2) 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 resulting from the integration with the system, which gives rise to the semigroup dynamics

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

2.2 Generators and Markovian Master Equation

Since, by definition, a quantum dynamical semigroup is in a sense continuous with respect to the parameter $t \in \mathbf{R}^+$, one may expect the semigroup to possess a generator. It is in fact true that the generator defined below always exists and its domain is a dense subspace of $\mathcal{H}$.

Definition 5. *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 T_t.*

The paper by Kossakowski [3] was among the first ones addressing the issue of quantum dynamical semigroups and their generators.

As an example, let $T_t A = e^{itH} A e^{-itH}$. Then

$$\frac{d}{dt} e^{itH} A e^{-itH} \Big|_{t=0} = iHe^{itH} A e^{-itH} - e^{itH} A e^{-itH}(-iH) \Big|_{t=0} = i[H, A].$$

Thus, $SA = i[H, A]$, or in the Schrödinger picture $S\rho = -i[H, \rho]$.

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

$$\frac{d}{dt} \rho_t = S\rho_t, \tag{3}$$

which is called *the Markovian master equation*. One may expect the approach to the dynamical description of a open quantum system given by a Markovian master equation to be largely equivalent to the one employing a semigroup of operators. In practice, the study of almost all real-life examples of quantum dynamical semigroups is reduced to the study of their generators derived from the given master equations.

2.3 The Born-Markov Master Equation

The most important type of the Markovian master equation, a type used extensively in applications, is the so-called Born-Markov master equation. Let us formulate the two basic assumptions that lead to this particular type of dynamics.

- *The Markov approximation.* The assumption already mentioned above which states that an open quantum system is sufficiently weakly coupled to its environment, so that the "memory effects" of the environment are negligible in the long run.
- *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

  $$\rho_t^{\mathcal{SE}} = \rho_t^{\mathcal{S}} \otimes \rho_t^{\mathcal{E}},$$

  and the state of the environment, $\rho_t^{\mathcal{E}}$, remains approximately constant over the course of time.

By imposing the above approximations to the dynamics given by the Hamiltonian (1) with the interaction part of the form

$$H_I = \sum_\alpha \hat{S}_\alpha \otimes \hat{E}_\alpha, \tag{4}$$

where $\hat{S_\alpha}$ and $\hat{E_\alpha}$ are unitary operators acting on the state space and the environment space respectively, we are able to derive the general form of the Born-Markov equation

$$\frac{d}{dt}\rho_t^{\mathcal{S}} = -i[H_{\mathcal{S}}, \rho_t^{\mathcal{S}}] - \sum_\alpha \left\{ [\hat{S_\alpha}, \hat{B_\alpha}\rho_t^{\mathcal{S}}] + [\rho_t^{\mathcal{S}}\hat{C_\alpha}, \hat{S_\alpha}] \right\}. \tag{5}$$

The operators $\hat{B_\alpha}$ and $\hat{B_\alpha}$ are defined as

$$\hat{B_\alpha} \equiv \int_0^\infty \sum_\alpha \mathcal{C}_{\alpha\beta}(\tau)\hat{S_\alpha^I}(-\tau)\mathrm{d}\tau,$$

$$\hat{C_\alpha} \equiv \int_0^\infty \sum_\beta \mathcal{C}_{\alpha\beta}(-\tau)\hat{S_\beta^I}(-\tau)\mathrm{d}\tau,$$

where $\mathcal{C}_{\alpha\beta}$ are scalar functions and the superscript 'I' denotes the so-called interaction picture. For the detailed explanation of the above formulae together with the derivation of (5), see [4].

The particularly simple form of the quantum dynamics given by the Born-Markov master equation (5) allows many models to be solved exactly. Among other features the dynamics determined by this type of equation can display, one of the most interesting is decoherence.

3 Decoherence

In the course of the time evolution, an open quantum system becomes heavily, and in practice irreversibly, entangled with its environment. This may lead to the decay of the off-diagonal elements of the 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 coherence is usually assumed as the operational definition of decoherence. Let us observe that a unitary dynamics cannot result in the system displaying decoherence.

Four Aspects of Decoherence In general, the effect of decoherence can manifest itself in four different ways. Perhaps the most important one is the appearance of the classical properties in a quantum system as a result of the irreversible dynamical evolution [5], [6].

Other aspects include the dynamical appearance of superselection rules [7], [8] and preferred basis of pointer states [9]. It is even possible for an open quantum system to exhibit entirely new and purely quantum behaviour after decoherence takes place [10].

3.1 Examples of Decoherence Models

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

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

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 [4].

Many models of quantum systems displaying decoherence can be reduced to only 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 master equation for the quantum Brownian motion takes the form

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

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

and $\nu(\tau)$, $\eta(\tau)$ are referred to as *the noise kernel* and *the dissipation kernel* respectively [4].

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 [11]. The spin-boson model master equation takes the following form

$$\frac{d}{dt}\rho_t = -i[H'_{\mathcal{S}}, \rho_t] - \tilde{D}\left[\sigma_z, [\sigma_z, \rho_t]\right] + \zeta\sigma_z\rho_t\sigma_y + \zeta^*\sigma_y\rho_t\sigma_z, \tag{6}$$

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

Spin-Environment Models The central system of this model consists of a two-level quantum system (e.g. a spin-$\frac{1}{2}$ particle) linearly coupled to the environment being a collection of other spins.

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As a summary, let us remark once again that the time reversible dynamics of closed quantum systems is by no means sufficient to describe various phenomena related to the complex interactions between a quantum system and its environment. In the Markovian approximation, an approximation concerning a quantum system weakly coupled to its environment, the study of the irreversible dynamics of open quantum systems employs tools such as quantum dynamical semigroups, their generators and master equations. In this formalism, one is able to prove the appearance of decoherence in many models of particular physical interest.

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