

8. Open Quantum Systems

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We now proceed to the next step of our program of understanding the behavior of one part of a bipartite quantum system. We have seen that a pure state of the bipartite system may behave like a mixed state when we observe subsystem A alone. What if we want to know the dynamics of A only? Can we describe its evolution even if we don't have full knowledge of B? (the bath) We assume that the state of the bipartite system undergoes unitary evolution: how do we describe the evolution of A alone?

8.1 Combined evolution of system and bath

We will first start introducing the evolution of an open quantum system by considering it as a part of a larger (closed) system undergoing the usual unitary evolution. The total Hilbert space is thus $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$ and we assume the initial state is represented by the separable density matrix $\rho = \rho_S \otimes |0\rangle\langle 0|_B$ ²³. The evolution of the total system is then

$$\rho(t) = U_{SB}(\rho_S \otimes |0\rangle\langle 0|_B)U_{SB}^\dagger$$

If we are only interested in the evolution of the system S we can at this point perform a partial trace on B

$$\rho_S(t) = \text{Tr}_B \{\rho(t)\} = \sum_k \langle k| U_{SB}(\rho_S \otimes |0\rangle\langle 0|_B)U_{SB}^\dagger |k\rangle = \sum_k \langle k| U_{SB}|0\rangle \rho_S(0) \langle 0| U_{SB}^\dagger |k\rangle$$

where $\{|k\rangle\}$ is an orthonormal basis for \mathcal{H}_B . As the result of $\langle k| U_{SB}|0\rangle = \text{Tr}_B \{|0\rangle\langle k| U_{SB}\}$ we obtain an operator M_k that acts only on the S Hilbert space. For example, in a matrix representation the elements of M_k are simply $M_k^{i,j} = \langle i| M_k |j\rangle$ (with $|i\rangle, |j\rangle$ defined on \mathcal{H}_S); that is, we have $M_k^{i,j} = \text{Tr} \{|j, 0\rangle \langle i, k| U_{SB}\} = \langle i, k| U_{SB} |j, 0\rangle$. Now we can write the evolution of the system only density matrix as

$$\rho_S(t) = \mathcal{M}(\rho_S(t)) = \sum_k M_k \rho_S(0) M_k^\dagger$$

²³ Here we only assume that the system B is in a pure state that we indicate as $|0\rangle$, we are not assuming that B is a TLS.

Since the propagator U_{SB} is unitary, we have that

$$\sum_k M_k^\dagger M_k = \mathbb{1}_S$$

? Question: Prove the above.

Inserting the definition for M_k we have $\sum_k M_k^\dagger M_k = \sum_k \langle 0|U_{SB}^\dagger |k\rangle \langle k|U_{SB}|0\rangle = \langle 0|U_{SB}^\dagger (\sum_k |k\rangle \langle k|) U_{SB}|0\rangle = \mathbb{1}_S$. \square

The properties of the system density matrix are preserved by the map:

1. $\rho_S(t)$ is hermitian: $\rho_A(t)^\dagger = (\sum_k M_k \rho_S(0) M_k^\dagger)^\dagger = \sum_k M_k \rho_S(0)^\dagger M_k^\dagger = \rho_S(t)$.
2. $\rho_S(t)$ has unit trace. (since $\text{Tr} \left\{ \sum_k M_k \rho_S M_k^\dagger \right\} = \text{Tr} \left\{ \rho_S \sum_k M_k M_k^\dagger \right\} = \text{Tr} \{ \rho_S \mathbb{1} \}$)
3. $\rho_S(t)$ is positive.

In the special case where there is only one term in the sum, we revert to the unitary evolution of the density matrix. In that case, a pure state, for example, would remain pure. If that is not the case, that is, the evolution is not unitary, it means that in the course of the evolution the system S and bath B became *entangled*, so that ρ_A is in a mixed state after partial trace. Because of the loss of unitarity, superoperators are in general not invertible and thus there is a specific arrow of time.

A. Ancillary Bath

In many cases it is not possible to fully calculate the evolution of the total system ($S + B$) as either it is too large or we have imperfect knowledge of the bath. However, if we have a description of the system dynamics in terms of the operator sum, it is possible to always *augment* the system and find a larger, composite system that evolves unitarily and yields the operator sum upon partial trace. The ancillary system might however not have all the characteristic of the (unknown) physical bath. What we are looking for is in fact a minimal description for the bath.

We choose as ancillary Hilbert space \mathcal{H}_B a space of dimensions at least equal to the number of terms in the operator sum. This space will have then a set of orthonormal vectors $\{|k\rangle\}$, and we can define a normalized state $|0\rangle_B$ on \mathcal{H}_B . Then the unitary evolution operator of the combined system is defined by imposing the relationship:

$$U_{SB}(|\psi\rangle_S \otimes |0\rangle_B) = \sum_k (M_k \otimes \mathbb{1})(|\psi\rangle_S \otimes |k\rangle_B), \quad \forall |\psi\rangle_S \in \mathcal{H}_S$$

This ensures that the evolution of the reduced system is given by the Kraus map. The total system evolution is:

$$U_{SB}(\rho_S \otimes |0\rangle\langle 0|_B)U_{SB}^\dagger = \sum_{k,h} (M_k \otimes \mathbb{1}) |\psi_S, k\rangle \langle \psi_S, h| (M_h^\dagger \otimes \mathbb{1})$$

and upon taking the partial trace:

$$\begin{aligned} \rho_S(t) &= \text{Tr}_B \{ \rho(t) \} = \sum_j \langle j| \left(\sum_{k,h} (M_k \otimes \mathbb{1}) |\psi_S, k\rangle \langle \psi_S, h| (M_h^\dagger \otimes \mathbb{1}) \right) |j\rangle \\ &= \sum_j \langle j|k\rangle \langle h|j\rangle (M_k^\dagger |\psi\rangle \langle \psi| M_h) \\ \rho_S(t) &= \sum_j M_j^\dagger |\psi\rangle \langle \psi| M_j \end{aligned}$$

Although this relationship doesn't fully define the operator on the full Hilbert space, we can extend the operator as desired. In particular we want it to be unitary (and this imposes added constraints). As the operator U_{SB} as defined above preserves the inner product on the full Hilbert space, a unitary extension of it to the full space does indeed exist. Furthermore, we can check that upon taking a partial trace on B we retrieve the operator sum as desired, for an initial pure state on S . But any density matrix can be expressed as an ensemble of pure states, hence this property is true for any general state on S . \square

B. Non-uniqueness of the sum representation

The operator sum is of course not unique, since the choice of the set $\{|k\rangle\}$ was quite arbitrary and not unique. If we had chosen another set $\{|h\rangle\}$ we would have arrived to a different sum

$$\rho_S(t) = \sum_h N_h \rho_S(0) N_h^\dagger$$

? Question: What is the relationship between the operators M and N ?

They are related by the simple unitary transformation that connects the two sets of orthonormal vectors $N_h = U_{hk} M_k$ with $|h\rangle = \sum_k U_{hk} |k\rangle$. \square

8.2 Superoperators

We want to describe the quantum evolution of systems in the most general case, when the system evolves non-unitarily due to the presence of an environment²⁴. As we have seen, the states need to be described by density operators. Therefore, the evolution is to be represented by a map connecting the initial density matrix to the evolved one $\rho(t) = \mathcal{M}[\rho(0)]$. The most general characteristics of this map will be determined by the fact that the properties of the density matrix should be in general maintained (such as unit trace). As the map \mathcal{M} is an operator acting on operators, it is called a superoperator.

Most generally, we can define a quantum operator describing the time evolution law for density matrices as a map $\mathcal{M} : \rho \rightarrow \rho'$ with the following properties

1. Linear
2. Trace preserving
3. Hermiticity preserving
4. Positive
- 4' (Completely positive)

A. Linearity

Although a non-linear map could also always map a density matrix to another density matrix, if we impose linearity we arrive at results that are more physical. Specifically, the linearity property retains the ensemble interpretation of the density matrix. What we mean is the following. Suppose we can write a density operator as a linear superposition of two densities, $\rho = a\rho_1 + (1-a)\rho_2$. The meaning of this expression is that with probability a we have a system described by ρ_1 and with probability $1-a$ by ρ_2 . If the map describing the time evolution law is linear, this probabilistic interpretation is valid also for the evolved state. Assume now that the map is not linear, for example it depends on the trace of the density matrix: $\mathcal{M}(\rho) = e^{iA\text{Tr}\{\rho M\}} \rho e^{-iA\text{Tr}\{\rho M\}}$, where M is an operator in the Hilbert space of ρ and A an Hermitian operator. We now consider a density operator ρ_1 such that $\text{Tr}\{\rho_1 M\} = 0$. We assume that we do not know exactly how we prepared the system, but with 50% probability is in ρ_1 . Assume then the density matrix $\rho = \frac{1}{2}(\rho_1 + \rho_\perp)$, such that $\text{Tr}\{\rho_\perp M\} = 0$. Then, $\mathcal{M}(\rho) = \rho$ as the traces are zero. If we now instead consider the initial density matrix $\rho = \frac{1}{2}(\rho_1 + \rho_\parallel)$ (that is, still a 50% probability of being in ρ_1), where $\text{Tr}\{M\rho_\parallel\} > 0$ we obtain an evolution for ρ_1 . That means, that in the two scenarios, the system behaves differently, even if we had prepared it in the state ρ_1 (remember the probabilistic interpretation), so that the evolution of a potential state of a system ρ_1 depends on another potential state (ρ_\perp or ρ_\parallel), even if this second state never occurred.

²⁴ This presentation in this section and the following examples are taken from J. Preskill's notes at <http://www.theory.caltech.edu/people/preskill/ph229/>

B. The superoperator preserves trace and hermiticity

Since the density matrix trace has the property to describe the sum of the probabilities of all possible states in the ensemble, it is important that the trace be preserved. An exception can be made for operators that describe measurement (and not time evolution). In that case $0 \leq \text{Tr}\{\rho\} \leq 1$. In this case, $\text{Tr}\{\rho\}$ represent the probability that the measurement outcome described by the map \mathcal{M} has occurred and the normalized final state is $\rho/\text{Tr}\{\rho\}$. As more than one outcome of the measurement is possible, the probability of obtaining ρ might be less than one.

The superoperator preserves the hermiticity of the density matrix: $[\mathcal{M}(\rho)]^\dagger = \mathcal{M}(\rho)$ if $\rho^\dagger = \rho$

C. Positivity and complete positivity

The property of positivity means that the map is such that $\mathcal{M}(\rho)$ is non-negative if ρ is. Although this condition is enough to obtain a valid density matrix, it leads to a contradiction when we consider composite systems. Let's take a valid map \mathcal{M}_1 on system 1. Then, if we consider a bipartite system and we apply the map $\mathcal{M}_1 \otimes \mathbb{1}$ we would like to still obtain a density matrix on the composite system. Unfortunately, if the map is simply positive, this is not always the case. Thus, we require it to be *completely* positive. A map is completely positive if $\mathcal{M}_1 \otimes \mathbb{1}_2$ is positive for any extension \mathcal{H}_2 of the Hilbert space \mathcal{H}_1 .

8.3 The Kraus Representation Theorem

We have seen in the preceding sections two different ways of describing the evolution of an open system.

The first description started from the evolution of a composite system (including the system of interest and a bath) and by tracing over arrived at a description of the open evolution via the operator sum.

The second description was instead quite abstract, and only defined the properties of the linear map describing the evolution in order to arrive at an acceptable (physical) evolved state (that still possess the characteristics of a density operator). The Kraus representation theorem reconciles these two description, by stating that they are equivalent.

■ **Theorem:** Any operator $\rho \rightarrow S(\rho)$ in a space of dimensions N_S^2 that obeys the properties 1-3,4' (Linearity, Trace preservation, Hermiticity preservation, complete positivity) can be written in the form:

$$S(\rho) = \sum_{k=1}^K M_k \rho M_k^\dagger, \quad \text{with} \quad \sum_{k=1}^K M_k^\dagger M_k = \mathbb{1}$$

where $K \leq N_S^2$ is the Kraus number (with N_S the dimension of the system). As seen above, the Kraus representation is not unique²⁵.

We consider three important examples of open quantum system evolution that can be described by the Kraus operators. To simplify the description we consider just a TLS that is coupled to a bath.

8.3.1 Amplitude-damping

The amplitude-damping channel is a schematic model of the decay of an excited state of a (two-level) atom due to spontaneous emission of a photon. By detecting the emitted photon (“observing the environment”) we can get information about the initial preparation of the atom.

We denote the atomic ground state by $|0\rangle_A$ and the excited state of interest by $|1\rangle_A$. The “environment” is the electromagnetic field, assumed initially to be in its vacuum state $|0\rangle_E$. After we wait a while, there is a probability p that the excited state has decayed to the ground state and a photon has been emitted, so that the environment has made a transition from the state $|0\rangle_E$ (“no photon”) to the state $|1\rangle_E$ (“one photon”). This evolution is described by a unitary transformation that acts on atom and environment according to

$$\begin{aligned} |0\rangle_S |0\rangle_E &\rightarrow |0\rangle_S |0\rangle_E \\ |1\rangle_S |0\rangle_E &\rightarrow \sqrt{1-p} |1\rangle_S |0\rangle_E + \sqrt{p} |0\rangle_S |1\rangle_E \end{aligned}$$

(Of course, if the atom starts out in its ground state, and the environment is at zero temperature, then there is no transition.)

By evaluating the partial trace over the environment, we find the Kraus operators

$$M_0 = \langle 0|U_{SE}|0\rangle = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}, \quad M_1 = \langle 1|U_{SE}|0\rangle = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix}$$

The operator M_1 induces a “quantum jump”, the decay from $|1\rangle_A$ to $|0\rangle_A$, and M_0 describes how the state evolves if no jump occurs. The density matrix evolves as

$$\begin{aligned} S(\rho) &= M_0 \rho M_0^\dagger + M_1 \rho M_1^\dagger = \\ &= \begin{pmatrix} \rho_{00} & \sqrt{1-p} \rho_{01} \\ \sqrt{1-p} \rho_{10} & (1-p) \rho_{11} \end{pmatrix} + \begin{pmatrix} p \rho_{11} & 0 \\ 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} \rho_{00} + p \rho_{11} & \sqrt{1-p} \rho_{01} \\ \sqrt{1-p} \rho_{10} & (1-p) \rho_{11} \end{pmatrix}. \end{aligned}$$

²⁵ The proof can be found in Prof. Preskill [online notes](#).

If we apply the channel n times in succession, the ρ_{11} matrix element decays as $\rho_{11} \rightarrow \rho_{11}(1-p)^n$ so if the probability of a transition in time interval δt is $\Gamma\delta t$, then the probability that the excited state persists for time t is $(1-\Gamma\delta t)^{t/\delta t} \approx e^{-\Gamma t}$, the expected exponential decay law. Also we have $\rho_{12} \rightarrow \rho_{12}(1-p)^{n/2} \approx \rho_{12}e^{-\Gamma t/2}$. As $t \rightarrow \infty$, the decay probability approaches unity, so

$$S(\rho) = \begin{pmatrix} \rho_{00} + \rho_{11} & 0 \\ 0 & 0 \end{pmatrix}$$

The atom always winds up in its ground state. This example shows that it is sometimes possible for a superoperator to take a mixed initial state to a pure state.

In the case of the decay of an excited atomic state via photon emission, it may not be impractical to monitor the environment with a photon detector. The measurement of the environment prepares a pure state of the atom, and so in effect prevents the atom from decohering. Returning to the unitary representation of the amplitude-damping channel, we see that a coherent superposition of the atomic ground and excited states evolves as

$$(a|0\rangle_S + b|1\rangle_S) |0\rangle_E \rightarrow (a|0\rangle_S + b\sqrt{1-p}|1\rangle_S) |0\rangle_E + \sqrt{p}|0\rangle_A |1\rangle_E$$

If we detect the photon (and so project out the state $|1\rangle_E$ of the environment), then we have prepared the state $|0\rangle_A$ of the atom. In fact, we have prepared a state in which we know with certainty that the initial atomic state was the excited state $|1\rangle_A$ as the ground state could not have decayed. On the other hand, if we detect no photon, and our photon detector has perfect efficiency, then we have projected out the state $|0\rangle_E$ of the environment, and so have prepared the atomic state

$$a|0\rangle_S + b\sqrt{1-p}|1\rangle_S$$

(or more precisely, if we normalize it: $(a|0\rangle_S + b\sqrt{1-p}|1\rangle_S)/\sqrt{1-pb^2}$). Then $p(0) = |a|^2 \rightarrow \frac{|a|^2}{1-p|b|^2} > |a|^2$.

The atomic state has evolved due to our failure to detect a photon, it has become more likely that the initial atomic state was the ground state!

8.3.2 Phase-damping

Phase damping describes a process where the system interacts with a large environment composed of many small subsystems. The interaction of the system with each of the environment subsystems is weak (compared to the system energy, but strong compared to the subsystem energy). Therefore the system is unchanged, while the environment subsystem is changed. Since there will be many of these interactions with the environment subsystem, their combined action does have an effect on the system, however it will not be enough to change its energy.

An example is the interaction of a dust particle with photons. Collision of the particle with one photon is not going to change the particle state. However, if the particle was in the ground or excited state, the photon will acquire more or less energy in the collision, thus being excited to its first or second excited state. We now formalize this model.

When looking at the unitary evolution of this process, only the environment changes:

$$|0\rangle_S |0\rangle_E \rightarrow \sqrt{1-p}|0\rangle_S |0\rangle_E + \sqrt{p}|0\rangle_S |1\rangle_E = |0\rangle_S (\sqrt{1-p}|0\rangle_E + \sqrt{p}|1\rangle_E)$$

$$|1\rangle_S |0\rangle_E \rightarrow \sqrt{1-p}|1\rangle_S |0\rangle_E + \sqrt{p}|1\rangle_S |2\rangle_E = |1\rangle_S (\sqrt{1-p}|0\rangle_E + \sqrt{p}|2\rangle_E)$$

Thus a possible unitary is

$$U = \begin{pmatrix} \sqrt{1-p} & \sqrt{p} & 0 & 0 & 0 & 0 \\ \sqrt{p} & \sqrt{1-p} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{1-p} & 0 & \sqrt{p} \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \sqrt{p} & 0 & \sqrt{1-p} \end{pmatrix}$$

The Kraus operator are found by operating the partial trace of the operator above:

$$M_0 = \langle 0|U|0\rangle = \sqrt{1-p}\mathbb{1} \quad M_1 = \langle 1|U|0\rangle = \sqrt{p}|0\rangle\langle 0| \quad M_2 = \langle 2|U|0\rangle = \sqrt{p}|1\rangle\langle 1|$$

The state evolution is then

$$S(\rho) = \sum_{k=1}^3 M_k \rho M_k^\dagger = (1-p)\rho + p|0\rangle\langle 0|\rho|0\rangle\langle 0| + p|1\rangle\langle 1|\rho|1\rangle\langle 1|$$

In matrix form:

$$S(\rho) = \begin{pmatrix} \rho_{00} & (1-p)\rho_{01} \\ (1-p)\rho_{10} & \rho_{11} \end{pmatrix}$$

Considering the Bloch vector: $[n_x, n_y, n_z] \rightarrow [(1-p)n_x, (1-p)n_y, n_z]$ (that is, the transvers component are reduced. For $p = 1$ the state becomes diagonal). Assume $p = p(\Delta t) = \Gamma \Delta t$ is the probability of one such scatter events during the time Δt . Then if we have n such events in a time $t = n\Delta t$ the off-diagonal terms become $\propto (1-p)^n = (1 - \Gamma \Delta t)^{t/\Delta t} \approx e^{-\Gamma t}$:

$$S(\rho, t) = \begin{pmatrix} \rho_{00} & e^{-\Gamma t} \rho_{01} \\ e^{-\Gamma t} \rho_{10} & \rho_{11} \end{pmatrix}$$

Consider for example an initial pure state $\alpha|0\rangle + \beta|1\rangle$. At long times, this state reduces to:

$$S(\rho, t) = \begin{pmatrix} |\alpha|^2 & e^{-\Gamma t} \alpha \beta^* \\ e^{-\Gamma t} \alpha^* \beta & |\beta|^2 \end{pmatrix} \xrightarrow{t \rightarrow \infty} \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix}$$

thus any phase coherence is lost and the state reduces to a classical, incoherent superposition of populations. Because in this process phase coherence is lost (but the energy/population is conserved) the process is called dephasing and the time constant $1/\Gamma$ is usually denoted by T_2 . Then we have a representation of the superoperator, by expressing ρ as a linear vector: $S(\rho, t) = S(t)\rho$, where $S = \text{diag}([1, e^{-\Gamma t}, e^{-\Gamma t}, 1])$.

8.3.3 Depolarizing process

The depolarizing channel is a model of a decohering qubit that has particularly nice symmetry properties. We can describe it by saying that, with probability $1 - p$ the qubit remains intact, while with probability p an “error” occurs. The error can be of any one of three types, where each type of error is equally likely. If $\{|0\rangle|1\rangle\}$ is an orthonormal basis for the qubit, the three types of errors can be characterized as:

1. Bit-flip error: $|\psi\rangle \rightarrow \sigma_x |\psi\rangle$ or $|0\rangle \rightarrow |1\rangle$ & $|1\rangle \rightarrow |0\rangle$.
2. Phase-flip error: $|\psi\rangle \rightarrow \sigma_z |\psi\rangle$ or $|0\rangle \rightarrow |0\rangle$ & $|1\rangle \rightarrow -|1\rangle$.
3. Both errors: $|\psi\rangle \rightarrow \sigma_y |\psi\rangle$ or $|0\rangle \rightarrow i|1\rangle$ & $|1\rangle \rightarrow -i|0\rangle$.

If an error occurs, then $|\psi\rangle$ evolves to an ensemble of the three states $\sigma_x |\psi\rangle, \sigma_y |\psi\rangle, \sigma_z |\psi\rangle$.

The depolarizing channel can be represented by a unitary operator acting on $\mathcal{H}_{SE} = \mathcal{H}_S \otimes \mathcal{H}_E$, where \mathcal{H}_E has dimension 4. The unitary operator U_{SE} acts as

$$U_{SE} |\psi\rangle_S \otimes |0\rangle_E \rightarrow \sqrt{1-p} |\psi\rangle_S \otimes |0\rangle_E + \sqrt{\frac{p}{3}} [\sigma_x |\psi\rangle_S \otimes |1\rangle_E + \sigma_y |\psi\rangle_S \otimes |2\rangle_E + \sigma_z |\psi\rangle_S \otimes |3\rangle_E]$$

The environment evolves to one of four mutually orthogonal states that “keep a record” of what transpired; if we could only measure the environment in the basis $\{|\mu\rangle, \mu = 0, 1, 2, 3\}$, we would know what kind of error had occurred (and we would be able to intervene and reverse the error).

Kraus representation: To obtain an operator-sum representation of the channel, we evaluate the partial trace over the environment in the $\{|\mu\rangle_E\}$ basis. Then

$$M_\mu = \langle \mu | U_{SE} | 0 \rangle_E$$

$$M_0 = \sqrt{1-p} \mathbb{1}, \quad M_1 = \sqrt{\frac{p}{3}} \sigma_x, \quad M_2 = \sqrt{\frac{p}{3}} \sigma_y, \quad M_3 = \sqrt{\frac{p}{3}} \sigma_z$$

A general initial density matrix ρ_S of the qubit evolves as

$$\rho \rightarrow \rho' = (1-p)\rho + \frac{p}{3}(\sigma_x\rho\sigma_x + \sigma_y\rho\sigma_y + \sigma_z\rho\sigma_z)$$

It is also instructive to see how the depolarizing channel acts on the Bloch sphere. An arbitrary density matrix for a single qubit can be written as $\rho = \frac{1}{2}(\mathbb{1} + \vec{n} \cdot \vec{\sigma})$, where \vec{n} is the Bloch vector (with $P = |\vec{n}|$ the polarization of the spin). Suppose we rotate our axes so that $\vec{n} = \vec{z}$ and $\rho = \frac{1}{2}(\mathbb{1} + P_z\sigma_z)$. Then since $\sigma_z\sigma_z\sigma_z = \sigma_z$ and $\sigma_x\sigma_z\sigma_x = \sigma_y\sigma_z\sigma_y = -\sigma_z$, we find

$$\rho' = \left(1 - p + \frac{p}{3}\right) \frac{1}{2}(\mathbb{1} - P_z\sigma_z) + \frac{2p}{3} \frac{1}{2}(\mathbb{1} - P_z\sigma_z) = \frac{1}{2} \left[\mathbb{1} + \left(1 - \frac{4}{3}p\right)P_z\sigma_z \right]$$

or $P'_z = \left(1 - \frac{4}{3}p\right)P_z$. From the rotational symmetry, we see that $P' = \left(1 - \frac{4}{3}p\right)$ irrespective of the direction in which P points. Hence, the Bloch sphere contracts uniformly under the action of the channel; the spin polarization is reduced by the factor $\left(1 - \frac{4}{3}p\right)$ (which is why we call it the depolarizing process). This result was to be expected in view of the observation above that the spin is totally “randomized” with probability $\frac{4}{3}p$.

Why do we say that the superoperator is not invertible? Evidently we can reverse a uniform contraction of the sphere with a uniform inflation. But the trouble is that the inflation of the Bloch sphere is not a superoperator, because it is not positive. Inflation will take values of $P \leq 1$ to values $P > 1$, and so will take a density operator to an operator with a negative eigenvalue. Decoherence can shrink the ball, but no physical process can blow it up again! A superoperator running backwards in time is not a superoperator.

8.4 The Master Equation

8.4.1 Markov approximation

In the case of coherent evolution, we find it very convenient to characterize the dynamics of a quantum system with a Hamiltonian, which describes the evolution over an infinitesimal time interval. The dynamics is then described by a differential equation, the Schrödinger equation, and we may calculate the evolution over a finite time interval by integrating the equation, that is, by piecing together the evolution over many infinitesimal intervals. It is often possible to describe the (not necessarily coherent) evolution of a density matrix, at least to a good approximation, by a differential equation. This equation, the master equation, will be our next topic. In fact, it is not at all obvious that there need be a differential equation that describes decoherence. Such a description will be possible only if the evolution of the quantum system is “Markovian,” or in other words, local in time. If the evolution of the density operator $\rho(t)$ is governed by a (first-order) differential equation in t , then that means that $\rho(t + dt)$ is completely determined by $\rho(t)$.

In general the density operator $\rho_A(t + dt)$ can depend not only on $\rho_A(t)$, but also on ρ_A at earlier times, because the environment (reservoir) retains a memory of this information for a while, and can transfer it back to system. An open system (whether classical or quantum) is dissipative because information can flow from the system to the reservoir. But that means that information can also flow back from reservoir to system, resulting in non-Markovian fluctuations of the system.

Still, in many contexts, a Markovian description is a very good approximation. The key idea is that there may be a clean separation between the typical correlation time of the fluctuations and the time scale of the evolution that we want to follow. Crudely speaking, we may denote by δt_E the time it takes for the reservoir to “forget” information that it acquired from the system. After time δt_E we can regard that information as forever lost, and neglect the possibility that the information may feed back again to influence the subsequent evolution of the system. Our description of the evolution of the system will incorporate “coarse-graining” in time; we perceive the dynamics through a filter that screens out the high frequency components of the motion, with $\omega \gg 1/\delta t_{coarse}$. An approximately Markovian description should be possible, then, if $\delta t_E \ll \delta t_{coarse}$; we can neglect the memory of the reservoir, because we are unable to resolve its effects. This “Markovian approximation” will be useful if the time scale of the dynamics that we want to observe is long compared to δt_{coarse} , e.g., if the damping time scale δt_{damp} satisfies

$$\delta t_{damp} \gg \delta t_{coarse} \gg \delta t_E$$

8.4.2 Lindblad equation

Our goal is to generalize the Liouville equation $\dot{\rho} = -i[\mathcal{H}, \rho]$ to the case of Markovian but non-unitary evolution, for which we will have $\dot{\rho} = \mathcal{L}[\rho]$. The linear operator \mathcal{L} , which generates a finite superoperator in the same sense that a Hamiltonian \mathcal{H} generates unitary time evolution, will be called the Lindbladian.

We can derive the Lindblad equation from an infinitesimal evolution described by the Kraus sum representation, with the following steps:

1. From the Kraus sum we can write the evolution of ρ from t to $t + \delta t$ as: $\rho(t + \delta t) = \sum_k M_k(\delta t)\rho(t)M_k^\dagger(\delta t)$.
2. We now take the limit of infinitesimal time, $\delta t \rightarrow 0$. We only keep terms up to first order in δt , $\rho(t + \delta t) = \rho(t) + \delta t \delta\rho$. This implies that the Kraus operator should be expanded as $M_k = M_k^{(0)} + \sqrt{\delta t}M_k^{(1)} + \delta t M_k^{(2)} + \dots$. Then there is one Kraus operator such that $M_0 = \mathbb{1} + \delta t(-i\mathcal{H} + K) + O(\delta t^2)$ with K hermitian (so that $\rho(t + \delta t)$ is hermitian), while all others have the form: $M_k = \sqrt{\delta t}L_k + O(\delta t)$, so that we ensure $\rho(t + \delta t) = \rho(t) + \delta\rho\delta t$:

$$\begin{aligned} \rho(t + \delta t) &= M_0\rho(t)M_0^\dagger + \sum_{k>0} M_k\rho M_k^\dagger \\ &= [\mathbb{1} + \delta t(-i\mathcal{H} + K)]\rho[\mathbb{1} + \delta t(i\mathcal{H} + K)] + \delta t \sum_k L_k\rho L_k^\dagger \\ &= \rho - i\delta t[\mathcal{H}, \rho] + \delta t(K\rho + \rho K) + \delta t \sum_k L_k\rho L_k^\dagger \end{aligned}$$

3. K and the other operators L_k are related to each other, since they have to respect the Kraus sum normalization condition,

$$K = -\frac{1}{2} \sum_{k>0} L_k^\dagger L_k.$$

4. Finally we substitute K in the equation above and take the limit $\delta \rightarrow 0$: $\rho(t + dt) = \rho(t) + dt\dot{\rho}$. We thus obtain the Lindblad equation

$$\dot{\rho}(t) = \mathcal{L}[\rho] = -i[\mathcal{H}, \rho(t)] + \sum_{k=1}^M \left(L_k \rho(t) L_k^\dagger - \frac{1}{2} L_k^\dagger L_k \rho(t) - \frac{1}{2} \rho(t) L_k^\dagger L_k \right)$$

The first term in $\mathcal{L}[\rho]$ is the usual Schrödinger term that generates unitary evolution (thus we identify the hermitian operator \mathcal{H} with the usual Hamiltonian). The other terms describe the possible transitions that the system may undergo due to interactions with the reservoir. The operators L_k are called Lindblad operators or quantum jump operators. Each $L_k \rho L_k^\dagger$ term induces one of the possible quantum jumps, while the $-\frac{1}{2} L_k^\dagger L_k \rho - \frac{1}{2} \rho L_k^\dagger L_k$ terms are needed to normalize properly the case in which no jumps occur.

If we recall the connection between the Kraus representation and the unitary representation of a superoperator, we clarify the interpretation of the master equation. We may imagine that we are continuously monitoring the reservoir, projecting it in each instant of time onto the $|\mu\rangle_E$ basis. With probability $1 - O(\delta t)$, the reservoir remains in the state $|0\rangle_E$, but with probability of order δt , the reservoir makes a quantum jump to one of the states $|\mu\rangle_E$. When we say that the reservoir has “forgotten” the information it acquired from the system (so that the Markovian approximation applies), we mean that these transitions occur with probabilities that increase linearly with time.

This is equation is also called the Kossakowski-Lindblad equation²⁶.

The Lindblad equation above is expressed in the Schrödinger picture. It is possible to derive the Heisenberg picture Lindblad equation, which has the form:

$$\frac{dx}{dt} = i[\mathcal{H}, x] + \sum_k L_k^\dagger x L_k - \frac{1}{2} L_k^\dagger L_k x + x L_k^\dagger L_k \quad ,$$

where x is the observable under study.

Another way to express the Lindblad equation is for a “vectorized” density matrix: $\dot{\rho} = (\mathbf{H} + \mathcal{G})\rho$, with the generator \mathcal{G} :

$$\mathcal{G} = \sum_{m=0}^M \bar{L}_m \otimes L_m - \frac{1}{2} \mathbb{1} \otimes (L_m^\dagger L_m) - \frac{1}{2} (\bar{L}_m^\dagger \bar{L}_m) \otimes \mathbb{1}$$

and the Hamiltonian part will be given by $\mathbf{H} = -i(\mathcal{H} \otimes \mathbb{1} - \mathbb{1} \otimes \mathcal{H})$. In this form, the Lindblad equation becomes a linear equation (a matrix multiplying a vector, if we are considering e.g. discrete systems). Thus it is “easy” to solve the differential equation, finding:

$$\rho(t) = \exp [(\mathbf{H} + \mathcal{G})t] \rho(0),$$

where we identify the superoperator $S = \exp [(\mathbf{H} + \mathcal{G})t]$. More details on how to convert from Kraus sum, to Lindblad to superoperator description of the open quantum system dynamics can be found in T. F. Havel, *Robust procedures for converting among Lindblad, Kraus and matrix representations of quantum dynamical semigroups*, *J. Math. Phys.* **44**, 534 (2003).

A. Example: spin-1/2 dephasing

Dephasing, or transverse relaxation, is the phenomenon associated with the decay of the coherence terms (off-diagonals) in the density matrix. In NMR, since the signal is due to the ensemble of spins, a coherence term which lasts forever would require all the same spins of the different molecules to precess about the magnetic field at exactly the same rate. As previously mentioned, the frequency of a single spin depends on the local magnetic field, which depends on the external field, and on the field created by the surrounding spins. Due to rapid tumbling, the average

²⁶ Andrzej Kossakowski *On quantum statistical mechanics of non-Hamiltonian systems*, Rep. Math. Phys. **3** 247 (1972)
Göran Lindblad *On the generators of quantum dynamical semigroups*, Commun. Math. Phys. **48** 119 (1976)).

field over time is the same, but does vary across the sample at a particular given time. This instantaneous variation causes the identical spins of all the molecules to slowly desynchronize and therefore lose coherence across the sample. Another example of dephasing was already presented when we described phase-damping for a dust particle interacting with many photons.

The dephasing noise can be thought as arising from random z rotation across the sample, so that the state of the system can be described by a statistical average over a distribution of rotation angles $q(\vartheta)$:

$$S_d(\rho) = \int d\vartheta q(\vartheta) e^{-i\vartheta/2\sigma_z} \rho(0) e^{i\vartheta/2\sigma_z}$$

Consider an initial density operator

$$\rho(0) = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix}$$

The evolution under a propagator $U_\vartheta = e^{-i\vartheta/2\sigma_z}$ gives

$$\rho(\vartheta) = \begin{pmatrix} \rho_{00} & \rho_{01} e^{-i\vartheta} \\ \rho_{10} e^{i\vartheta} & \rho_{11} \end{pmatrix}$$

Taking the integral over the angle distribution we find

$$\rho(\vartheta) = \begin{pmatrix} \rho_{00} & \rho_{01} \Gamma \\ \rho_{10} \Gamma^* & \rho_{11} \end{pmatrix},$$

where $\Gamma = \langle e^{-i\vartheta} \rangle = \int q(\vartheta) e^{-i\vartheta} d\vartheta$. If $q(\vartheta) = q(-\vartheta)$ (as given by an isotropic environment) we obtain $\langle e^{-i\vartheta} \rangle = \langle \cos \vartheta \rangle$. For a non-Markovian environment where memory effects are present, we can describe the distribution $q(\vartheta)$ as a Gaussian stochastic process, so that $\Gamma = \langle \cos \vartheta \rangle \approx e^{-\langle \vartheta^2 \rangle / 2} = e^{-t^2 / T_2^2}$. For a Markovian process instead we have an exponential decay $\Gamma = e^{-t/T_2}$.

We can also explicitly evaluate S_d :

$$\begin{aligned} S_d(\rho) &= \int d\vartheta q(\vartheta) [\cos(\vartheta/2)\mathbb{1} - i \sin(\vartheta/2)\sigma_z] \rho(0) [\cos(\vartheta/2)\mathbb{1} + i \sin(\vartheta/2)\sigma_z] = \\ &= \int d\vartheta q(\vartheta) [\cos^2(\vartheta/2)\rho(0) + \sin^2(\vartheta/2)\sigma_z \rho(0) \sigma_z - i \cos(\vartheta/2) \sin(\vartheta/2) (\sigma_z \rho(0) - \rho(0) \sigma_z)] \end{aligned}$$

By evaluating the integral, and assuming again a symmetric distribution, we have:

$$S_d(\rho) = (1 - p)\rho(0) + p\sigma_z \rho(0) \sigma_z$$

where $p = \int d\vartheta q(\vartheta) \sin^2(\vartheta/2)$. By comparison with the previous result we find $p = \frac{1-\Gamma}{2}$. From the superoperator, we can find the corresponding Kraus sum decomposition:

$$M_0 = \sqrt{1-p}\mathbb{1}, \quad M_1 = \sqrt{p}\sigma_z$$

We want now to describe this same evolution under a dephasing environment by a Lindblad equation. Notice that this is going to be possible only if we have a Markovian environment, $\Gamma = e^{-t/T_2}$.

Consider the action of the superoperator $S_d(\rho) = \frac{1+\Gamma}{2}\rho(0) + \frac{1-\Gamma}{2}\sigma_z \rho(0) \sigma_z$. If we consider a small time $\Gamma = e^{-\delta t/T_2} \approx 1 - \delta t/T_2$ and we obtain:

$$S_d(\rho, \delta t) = \rho - \frac{\gamma \delta t}{2} \rho + \frac{\gamma \delta t}{2} \sigma_z \rho \sigma_z$$

where $\gamma = 1/T_2$. Then, taking the difference $\rho(\delta t) - \rho(0)$ in the limit $\delta t \rightarrow 0$ we have

$$\frac{\partial \rho}{\partial t} = \frac{\gamma}{2} (\sigma_z \rho \sigma_z - \rho) = \frac{\gamma}{2} (\sigma_z \rho \sigma_z - \frac{1}{2} \{\sigma_z \sigma_z, \rho\})$$

where we used the fact $\sigma_z^2 = \mathbb{1}$. Thus $\sqrt{\frac{\gamma}{2}} \sigma_z$ is the Lindblad operator for dephasing.

Assume now that we had considered a non-Markovian environment, for which $\Gamma = e^{-(t/T_2)^2}$. Then if we tried to find the infinitesimal time evolution, we cannot define a differential equation, since $\rho(\delta t) - \rho(0)$ is not $\propto \delta t$. For this type of environment, the Lindblad equation cannot be defined.

8.4.3 Redfield-Born theory of relaxation

Consider a system \mathcal{S} coupled to an environment \mathcal{E} (the heat bath) such that

$$\mathcal{H} = \mathcal{H}_0 + V = \mathcal{H}_S + \mathcal{H}_E + V,$$

and V describes the interaction between the system and the environment. Most generally it will take the form $V = \sum_k A_k \otimes B_k(t)$, with A acting on the system and B on the environment (and we have even allowed for a time-dependence of the random environment field). In the Schrödinger picture, the time evolution of the density matrix is given by the Liouville equation, $i\hbar \frac{d\rho(t)}{dt} = [\mathcal{H}, \rho(t)]$. Define the interaction picture density matrix

$$\rho_I(t) \equiv e^{\frac{i}{\hbar}(\mathcal{H}_S + \mathcal{H}_E)t} \rho(t) e^{-\frac{i}{\hbar}(\mathcal{H}_S + \mathcal{H}_E)t},$$

and similarly the interaction-picture system-environment interaction

$$V_I(t) \equiv e^{\frac{i}{\hbar}(\mathcal{H}_S + \mathcal{H}_E)t} V e^{-\frac{i}{\hbar}(\mathcal{H}_S + \mathcal{H}_E)t}.$$

Then the evolution in the interaction picture is given by

$$i\hbar \frac{d\rho_I(t)}{dt} = e^{\frac{i}{\hbar}\mathcal{H}_0 t} ([\mathcal{H}, \rho(t)] - [\mathcal{H}_0, \rho(t)]) e^{-\frac{i}{\hbar}\mathcal{H}_0 t} = e^{\frac{i}{\hbar}\mathcal{H}_0 t} [V, \rho(t)] e^{-\frac{i}{\hbar}\mathcal{H}_0 t} = [V_I(t), \rho_I(t)].$$

This has the formal solution

$$\rho_I(t) = \rho_I(0) + \frac{1}{i\hbar} \int_0^t dt_1 [V_I(t_1), \rho_I(t_1)]$$

(Note that this is the same equation as above, except in integral form).

Expanding once (by inserting the same equation at the place of $\rho_I(t)$) we obtain,

$$\rho_I(t) = \rho_I(0) + \frac{1}{i\hbar} \int_0^t dt_1 [V_I(t_1), \rho_I(0)] + \frac{1}{(i\hbar)^2} \int_0^t \int_0^{t_1} dt_1 dt_2 [V_I(t_1), [V_I(t_2), \rho_I(t_2)]]$$

We could repeat this process to obtain an infinite series (the Dyson series we already saw).

Let us concentrate instead on the evolution of the (interaction picture) reduced density matrix $\rho_S = \text{Tr}_{\mathcal{E}} \{\rho_I\}$, obtained by tracing over the environment. To obtain the average density operator, we also need to take an ensemble average over the random fluctuating environment:

$$\rho_S(t) = \rho_S(0) + \frac{1}{i\hbar} \int_0^t dt_1 \langle \text{Tr}_{\mathcal{E}} \{[V_I(t_1), \rho_I(0)]\} \rangle + \frac{1}{(i\hbar)^2} \int_0^t \int_0^{t_1} dt_1 dt_2 \langle \text{Tr}_{\mathcal{E}} \{[V_I(t_1), [V_I(t_2), \rho_I(t_2)]]\} \rangle.$$

We want to find an explicit expression for the system evolution only (in the form of a differential equation). To do this, we will make a number of approximations.

A. Simplification: Separability and energy shift

We first assume that at time $t = 0$ the system and environment are in a separable state:

$$\rho(0) = \rho_S(0) \otimes \rho_E(0).$$

(this can always be obtained by choosing $t = 0$ appropriately).

This condition helps simplifying the second term in the LHS of the expression above. We have

$$\text{Tr}_{\mathcal{E}} \{[V_I(t_1), \rho_I(0)]\} = \sum_k [A_I(t_1), \rho_S(0)] \text{Tr}_{\mathcal{E}} \{B_k(t) \rho_E\},$$

that is, we consider the expectation value of the operators B_k . In general we will also need to take an ensemble average over the random fluctuating field $\langle B_k(t) \rangle$, as we look at expectation values for the density operator.

We can now make the assumption that $\langle B_{\mathcal{E}} \rangle_{\mathcal{E}} = 0$, which implies $\langle V_I(t) \rangle_{\mathcal{E}} \sim \text{Tr}_{\mathcal{E}} \{V_I(t) \rho_{\mathcal{E}}(0)\} = 0$. This is not restrictive, since, if V is of the form $V = A_S \otimes B_{\mathcal{E}}$ with $\langle B_{\mathcal{E}} \rangle_{\mathcal{E}} \neq 0$ we can replace V with $V = A_S \otimes (B_{\mathcal{E}} - \langle B_{\mathcal{E}} \rangle_{\mathcal{E}})$, and simultaneously add $A_S \langle B_{\mathcal{E}} \rangle_{\mathcal{E}}$ to \mathcal{H}_S . With this condition, $\langle V \rangle_{\mathcal{E}} = 0$ and since $\rho_{\mathcal{E}}(0)$ has the same form in both Schrödinger and interaction pictures, the result holds in the interaction picture also. The same argument can be made if $V = \sum_{\alpha} A_{S,\alpha} \otimes B_{\mathcal{E},\alpha}$. Then the second term in the equation above vanishes and we have

$$\rho_S(t) = \rho_S(0) + \frac{1}{(i\hbar)^2} \int_0^t \int_0^{t_1} dt_1 dt_2 \langle \text{Tr}_{\mathcal{E}} \{ [V_I(t_1), [V_I(t_2), \rho_I(t_2)]] \} \rangle.$$

B. Assumption 1: Born approximation

We can always write (in any picture) $\rho(t) = \rho_S(t) \otimes \rho_{\mathcal{E}}(t) + \rho_{\text{correlation}}(t)$, which may be taken as a definition of $\rho_{\text{correlation}}$. Let us assume (as done in the previous section) that the interaction is turned on at time $t = 0$, and that prior to that the system and environment are not correlated ($\rho_{\text{correlation}}(0) = 0$). This assumption is not very restrictive, since we can always find a time prior to which the system and environment did not interact. Now however we make a stronger assumption.

We will assume that the coupling between the system and the environment is weak, so that $\rho(t) \approx \rho_S(t) \otimes \rho_{\mathcal{E}}(t)$, for timescales over which perturbation theory remains valid. Furthermore, we will assume that the correlation time $\tau_{\mathcal{E}}$ (and thus the relaxation time) of the environment is sufficiently small that $\rho_{\mathcal{E}}(t) \approx \rho_{\mathcal{E}}(0)$ if $t \gg \tau_{\mathcal{E}}$.

Note that since we assume that the environment is in a thermal equilibrium, it has a thermal density matrix

$$\rho_{\mathcal{E}}(0) = \frac{1}{Z_{\mathcal{E}}} \sum_n e^{-\frac{E_n}{k_B T}} |n_{\mathcal{E}}\rangle \langle n_{\mathcal{E}}|,$$

which is a stationary state, i.e., $[\rho_{\mathcal{E}}(0), \mathcal{H}_{\mathcal{E}}] = 0$, so that $\rho_{\mathcal{E}}(0)$ has the same form in both the interaction picture and Schrödinger picture. Then

$$\rho_S(t) = \rho_S(0) + \frac{1}{(i\hbar)^2} \int_0^t \int_0^{t_1} dt_1 dt_2 \langle \text{Tr}_{\mathcal{E}} \{ [V_I(t_1), [V_I(t_2), \rho_S(t_2) \otimes \rho_{\mathcal{E}}(0)]] \} \rangle.$$

We can also go further and explicitly write the partial trace:

$$\langle \text{Tr}_{\mathcal{E}} \{ [V_I(t_1), [V_I(t_2), \rho_S(t_2) \otimes \rho_{\mathcal{E}}(0)]] \} \rangle = \sum_{k,h} \langle B_k(t_1) B_h(t_2) \rangle [A_k^I(t_1), [A_h^I(t_2), \rho_S(t_2)]]$$

where $\langle B_k(t_1) B_h(t_2) \rangle = G_{k,h}(t_1, t_2)$ is the correlation function for the environment.

Differentiating, we get

$$\frac{d}{dt} \rho_S(t) = \frac{1}{(i\hbar)^2} \int_0^t ds \langle \text{Tr}_{\mathcal{E}} \{ [V_I(t), [V_I(s), \rho_S(s) \otimes \rho_{\mathcal{E}}(0)]] \} \rangle.$$

or

$$\frac{d}{dt} \rho_S(t) = \frac{1}{(i\hbar)^2} \int_0^t ds \sum_{k,h} \langle B_k(t) B_h(s) \rangle [A_k^I(t), [A_h^I(s), \rho_S(s)]].$$

This should properly be considered a difference equation, since we have assumed that $t \gg \tau_{\mathcal{E}}$.

C. Assumption 2: Markov approximation

We will also assume that we are working over timescales that are shorter than the gross timescale over which the system evolves, so that $\rho_S(s) \approx \rho_S(t)$. Thus we can replace $\rho_S(s)$ in the integral with $\rho_S(t)$. We finally get the Redfield equation:

$$\frac{d}{dt} \rho_S(t) = \frac{1}{(i\hbar)^2} \int_0^t ds \text{Tr}_{\mathcal{E}} \{ [V_I(t), [V_I(s), \rho_S(t) \otimes \rho_{\mathcal{E}}(0)]] \}$$

or

$$\frac{d}{dt}\rho_S(t) = \frac{1}{(i\hbar)^2} \int_0^t ds \sum_{k,h} \langle B_k(t)B_h(s) \rangle [A_k^I(t), [A_h^I(s), \rho_S(t)]] .$$

We can change variables from $s \rightarrow s' = t - s$ (so that we change the integrals as: $\int_0^t ds \rightarrow \int_t^0 d(t-s) = -\int_0^t ds' = \int_0^t ds'$). Then

$$\frac{d}{dt}\rho_S(t) = \frac{1}{(i\hbar)^2} \int_0^t ds \sum_{k,h} \langle B_k(t)B_h(t-s) \rangle [A_k^I(t), [A_h^I(t-s), \rho_S(t)]] .$$

The correlation time of the thermal bath \mathcal{E} is assumed to be very short, so that the correlation function $\langle B_k(t_1 - t_2)B_h(0) \rangle_{\mathcal{E}}$ differs only significantly from zero when $t_1 \approx t_2$. We can therefore extend the limit of integration to ∞ (and call $t - s = \tau$):

$$\frac{d}{dt}\rho_S(t) = \frac{1}{(i\hbar)^2} \int_0^\infty d\tau \sum_{k,h} \langle B_k(t)B_h(\tau) \rangle [A_k^I(t), [A_h^I(\tau), \rho_S(t)]] .$$

D. Spectral densities

The next step in the simplification program is to take the expectation values with respect to the eigenstates of the system and then Fourier transform. We will write $A_k(t) = \sum_p A_k^p e^{-i\omega_p t}$:

$$\frac{d}{dt}\rho_S(t) = \frac{1}{(i\hbar)^2} \sum_{k,h} \sum_{p,q} \int_0^\infty d\tau G_{kh}(\tau) [A_k^p e^{-i\omega_p t}, [A_h^q e^{-i\omega_q(t-\tau)}, \rho_S(t)]] .$$

Here we used the fact that $G(t, \tau)$ is stationary, and thus depend only on the difference $t - \tau$, $G(t, \tau) = G(t - \tau)$. We then changed variables from $\tau \rightarrow t - \tau$. We can rewrite the equation as

$$\frac{d}{dt}\rho_S(t) = \frac{1}{(i\hbar)^2} \sum_{k,h} \sum_{p,q} [A_k^p, [A_h^q, \rho_S(t)]] e^{-i(\omega_p + \omega_q)t} \int_0^\infty d\tau G_{kh}(\tau) e^{i\omega_q \tau} .$$

Thus we have the integral $\int_0^\infty e^{i\omega\tau} G(\tau) = J(\omega)$, where the Fourier transform of the correlation function $G(\tau)$ is the the spectral function $J(\omega)$. With some simplifications (due to statistical properties of the bath operators and to the fact that we only take terms resulting in an Hermitian operator), we finally arrive at the master equation:

$$\frac{d}{dt}\rho_S(t) = - \sum_k \sum_p J_k(\omega_p) [A_{-k}^p, [A_k^p, \rho_S(t)]]$$

We can also write the master equation as the Redfield equation (subscripts indicate matrix elements):

$$\frac{d}{dt}\rho_{a,a'} = \sum_{b,b'/b-b'=a-a'} R_{aa',bb'} \rho_{b,b'}$$

8.5 Other description of open quantum system dynamics

8.5.1 Stochastic Liouville equation and cumulants

Stochastic Liouville theory is based on a semiclassical model of decoherence, in which the Hamiltonian at any instant in time consists of a deterministic and a stochastic part, which represents the effects of a random noise. In the simplest case of NMR T_2 relaxation, this typically takes the form

$$\mathcal{H}_{tot}(t) = \mathcal{H}_{det}(t) + \mathcal{H}_{st}(t) = \mathcal{H}_{det}(t) + \omega(t)\mathcal{H}_N,$$

where \mathcal{H}_{det} is the static deterministic Hamiltonian, and we separated the stochastic time dependence described by the coefficient $\omega(t)$ from the noise generator \mathcal{H}_N . $\omega(t)$ is a random variable due to stochastic, time-dependent fluctuating fields and \mathcal{H}_N is an operator which describes how these classical fields are coupled to the quantum system. We now introduce a superoperator $\mathcal{L}(t)$ defined on Liouville (operator) space via

$$\mathcal{L}(t) = \mathcal{H}_{tot}^*(t) \otimes \mathbb{1} - \mathbb{1} \otimes \mathcal{H}_{tot}(t) = \mathcal{L}_{det}(t) + \omega(t)\mathcal{L}_N$$

where $\mathcal{L}_N = \mathcal{H}_N^* \otimes \mathbb{1} - \mathbb{1} \otimes \mathcal{H}_N$. This superoperator is the generator of motion for density operator $\hat{\rho}$, meaning

$$\rho(t) = \mathcal{U}\hat{\rho}(0) = \mathcal{T} \exp\left(-i \int_0^t dt' \mathcal{L}(t')\right) \hat{\rho}(0)$$

where \mathcal{T} is the usual Dyson time ordering operator. Since what is actually observed in an experiment is the statistical average over the microscopic trajectories of the system $\langle \hat{\rho}(t) \rangle$, we have to take the ensemble average superpropagator to obtain $\langle \hat{\rho}(t) \rangle = \langle \mathcal{U} \rangle \hat{\rho}(0)$. The problem of calculating the average of the exponential of a stochastic operator has been solved by Kubo²⁷ using the cumulant expansion.

First, expand the time-ordered average exponential $S = \langle \mathcal{T} \exp(-i \int_0^t dt' \mathcal{H}(t')) \rangle$ via the Dyson series:

$$\begin{aligned} S &= \mathbb{1} - i \int_0^t dt' \langle \mathcal{H}(t') \rangle + \frac{(-i)^2}{2!} \mathcal{T} \int_0^t dt_1 \int_0^t dt_2 \langle \mathcal{H}(t_1) \mathcal{H}(t_2) \rangle + \dots \\ &\quad + \frac{(-i)^n}{n!} \mathcal{T} \int_0^t dt_1 \dots \int_0^t dt_n \langle \mathcal{H}(t_1) \dots \mathcal{H}(t_n) \rangle + \dots \end{aligned}$$

The term $\langle \mathcal{H}(t_1) \dots \mathcal{H}(t_n) \rangle$ is called the n -th moment of the distribution. We want now to express this same propagator in terms of the cumulant function $K(t)$, defined by:

$$S = e^{K(t)}$$

The cumulant function itself can most generally be expressed as a power series in time:

$$K(t) = \sum_{n=1}^{\infty} \frac{(-it)^n}{n!} K_n = -itK_1 + \frac{(-it)^2}{2!} K_2 + \dots$$

Expanding now the exponential using the expression above we have:

$$S = \mathbb{1} + K(t) + \frac{1}{2!} (K(t))^2 + \dots = \mathbb{1} - itK_1 + \frac{(-it)^2}{2!} (K_2 + K_1^2) + \dots$$

By equating terms of the same order in the two expansions we obtain the cumulants K_n in terms of the moments of order at most n . For example:

$$\begin{aligned} K_1 &= \frac{1}{t} \int_0^t dt' \langle \mathcal{H}(t') \rangle \\ K_2 &= \frac{1}{t^2} \mathcal{T} \int_0^t dt_1 \int_0^t dt_2 \langle \mathcal{H}(t_1) \mathcal{H}(t_2) \rangle - K_1^2 \end{aligned}$$

The propagator can therefore be expressed in terms of the cumulant averages:

$$\begin{aligned} \langle \mathcal{H}(t') \rangle_c &= \langle \mathcal{H}(t') \rangle \\ \langle \mathcal{H}(t_1) \mathcal{H}(t_2) \rangle_c &= \mathcal{T} \langle \mathcal{H}(t_1) \mathcal{H}(t_2) \rangle - \langle \mathcal{H}(t_1) \rangle \langle \mathcal{H}(t_2) \rangle \end{aligned}$$

The propagator can therefore be written as:

$$S = \exp\left(-i \int_0^t dt' \langle \mathcal{H}(t') \rangle_c - \int_0^t dt_1 \int_0^t dt_2 \langle \mathcal{H}(t_1) \mathcal{H}(t_2) \rangle_c + \dots\right)$$

²⁷ R. Kubo, *Generalized Cumulant Expansion Method*, [Journal of the Physical Society of Japan](#), **17**, 1100-1120 (1962)

Note that if \mathcal{H} is a deterministic function of time, the ensemble averages can be dropped and $\langle \mathcal{H}(t) \rangle_c = \int_0^t dt' \mathcal{H}(t')$ becomes the time-average Hamiltonian, which is the first term in the Magnus expansion. The second term in the cumulant expansion, on the other hand, becomes

$$\begin{aligned} & \mathcal{T} \int_0^t dt_1 \int_0^{t_1} dt_2 \mathcal{H}(t_1) \mathcal{H}(t_2) - \left(\int_0^t dt' \mathcal{H}(t') \right)^2 \\ &= 2 \int_0^t dt_1 \int_0^{t_1} dt_2 \mathcal{H}(t_1) \mathcal{H}(t_2) - \int_0^t dt_1 \int_0^t dt_2 \mathcal{H}(t_1) \mathcal{H}(t_2) \\ &= \int_0^t dt_1 \int_0^{t_1} dt_2 \mathcal{H}(t_1) \mathcal{H}(t_2) - \int_0^t dt_1 \int_{t_1}^t dt_2 \mathcal{H}(t_1) \mathcal{H}(t_2) \\ &= \int_0^t dt_1 \int_0^{t_1} dt_2 [\mathcal{H}(t_1), \mathcal{H}(t_2)], \end{aligned}$$

where we have used the fact that the time-ordering operator \mathcal{T} symmetrizes its argument with respect to permutation of the time points. This is the second term in the Magnus expansion for the “average” (effective) Hamiltonian. Proceeding in this fashion one can in principle derive average Hamiltonian theory²⁸ from the Dyson and cumulant expansions.

In terms of the so-called “cumulant averages” $\langle \dots \rangle_c$, the superpropagator is given by:

$$\langle \mathcal{U} \rangle = \exp \left(-i \int_0^t dt' \langle \mathcal{L}(t') \rangle_c - \frac{1}{2} \mathcal{T} \int_0^t dt_1 \int_0^t dt_2 \langle \mathcal{L}(t_1) \mathcal{L}(t_2) \rangle_c + \dots \right)$$

Provided $\| \int_0^t dt' \mathcal{L}(t') \| \ll 1$ for all $t > 0$, we can safely neglect high order terms in the exponential’s argument.

8.5.2 Stochastic Wavefunctions

The Monte Carlo wavefunction was derived simultaneously in the 1990s by two groups interested in very different questions. A group of scientists in France, Dalibard, Castin, and Mølmer, wanted to simulate laser cooling of atoms quantum mechanically in three dimensions. Their numerical solution required discretizing space into a grid of $40 \times 40 \times 40$ positions; to implement the master equation on such a space would have required a density matrix with $O(40^6) \sim 10^9$ entries such calculations are beyond the scope of even modern computers. However, simulating a wavefunction with $O(40^3)$ entries is quite feasible. Consequently the group sought to convert the master equation to something more like the Schrödinger equation²⁹.

At the same time, Carmichael was interested in the effects that continuous monitoring would have on a system³⁰. For example, a two-level atom prepared in an equal superposition of states can decay by emitting a photon; if that photon is detected, the experimenter knows with certainty that the atom is in its ground state. But what happens 50% of the time when a photon is not detected? Certainly, after a long time has passed, the atom must be in its ground state, but how does that happen? To study these and similar questions, Carmichael wanted to incorporate the effects of continuous monitoring, and understand how a measurement can cause the system state to suddenly jump into a different state.

The description on which both groups converged begins with the most general form of the master equation,

$$\frac{d\rho}{dt} = -i[\mathcal{H}, \rho] + \mathcal{L}(\rho),$$

with the Lindbladian

$$\mathcal{L}(\rho) = - \sum_k \frac{\gamma_k}{2} (L_k^\dagger L_k \rho + \rho L_k^\dagger L_k - 2L_k \rho L_k^\dagger).$$

²⁸ See for example Haeberlen, *High Resolution NMR in Solids: Selective Averaging*, Academic Press Inc., New York (1976)

²⁹ Jean Dalibard, Yvan Castin and Klaus Mølmer *Wave-function approach to dissipative processes in quantum optics*, *Phys. Rev. Lett.* **68**, 580583 (1992)

³⁰ H. J. Carmichael *Quantum trajectory theory for cascaded open systems* *Phys. Rev. Lett.* **70**, 22732276 (1993)

Using this explicit expression and rearranging the terms we have

$$\begin{aligned}\frac{d\rho}{dt} &= -i \left[(\mathcal{H} - i \sum_k \frac{\gamma_k}{2} L_k^\dagger L_k) \rho - \rho (\mathcal{H} + \sum_k \frac{\gamma_k}{2} L_k^\dagger L_k) \right] + \sum_k \gamma_k L_k \rho L_k^\dagger \\ &= -i \mathcal{H}_{\text{eff}} \rho - \rho \mathcal{H}_{\text{eff}}^\dagger + \sum_k \gamma_k L_k \rho L_k^\dagger,\end{aligned}$$

where we have defined an effective *Hamiltonian*

$$\mathcal{H}_{\text{eff}} = \mathcal{H} - i \sum_k \frac{\gamma_k}{2} L_k^\dagger L_k$$

(notice that this is not a valid Hamiltonian in the usual sense, since it is not Hermitian, so its eigenvalues are not the energy, since they could be imaginary numbers).

Expanding the density matrix in terms of an ensemble of pure states, $\rho = \sum_j p_j |\psi_j\rangle \langle \psi_j|$, we can rewrite the master equation in a suggestive form:

$$\frac{d\rho}{dt} = \sum_j p_j \left[-i(\mathcal{H}_{\text{eff}} |\psi_j\rangle \langle \psi_j| - |\psi_j\rangle \langle \psi_j| \mathcal{H}_{\text{eff}}^\dagger) + \sum_k \gamma_k L_k |\psi_j\rangle \langle \psi_j| L_k^\dagger \right]$$

Now we can interpret the first two terms of this equation as a Schrödinger evolution for each of the pure states in the density matrix expansion:

$$\frac{d}{dt} |\psi_j\rangle = -i \mathcal{H}_{\text{eff}} |\psi_j\rangle$$

while we interpret the last term as a *quantum jump* operator that changes $|\psi_j\rangle$ into $|\varphi_{j,k}\rangle = L_k |\psi_j\rangle$ with some probability.

We can then have a probabilistic picture of the pure state evolution. After an infinitesimal time, in the absence of *jumps*, the state will have evolved to

$$|\psi_j(t + \delta t)\rangle = (1 - i \mathcal{H}_{\text{eff}}) |\psi_j\rangle / \sqrt{1 - \delta p_j},$$

where we have introduced a normalization factor, which is needed since the Hamiltonian is not hermitian:

$$\delta p_j = \sum_k \delta p_{j,k} = \delta t \sum_k \gamma_k \langle \psi_j | L_k^\dagger L_k | \psi_j \rangle$$

If instead a jump has occurred, the state would have evolved to

$$|\varphi_{j,k}\rangle = \sqrt{\frac{\gamma_k \delta t}{\delta p_{j,k}}} L_k |\psi_j\rangle$$

Thus the evolution of the density matrix is given by

$$\rho(t + \delta t) = \sum_j p_j \left[(1 - \delta p_j) |\psi_j(t + \delta t)\rangle \langle \psi_j(t + \delta t)| + \sum_k \delta p_{j,k} |\varphi_{j,k}\rangle \langle \varphi_{j,k}| \right]$$

This expression leads us to the following interpretation: the system undergoes a dynamics that yields two possible outcomes:

1. with probability $1 - \delta p_j$ the system evolves to the state $|\psi_j(t + \delta t)\rangle$, according to the operator \mathcal{H}_{eff} with an appropriate normalization
2. with probability δp_j the system jumps to another state. There are many possible states the system can jump to, each one with a probability $\delta p_{j,k}$.

This probabilistic picture is of course a coarse graining of the continuous time evolution. However, by discretizing time it becomes easier to devise a simulation procedure to reproduce the desired dynamics, with a wavefunction Montecarlo procedure.

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Fall 2012

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