Explicit thermalisation models II: Quantum master equations

Martin Fluder

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Outline

Introduction

I will be talking about:

- Quantum master equations in open and closed systems: first order differential equations for density matrices of a system
- Concept of quantum dynamical semigroup associated with quantum Markov systems
- Derivation of the general form of the Markovian master equation for a N-level system
- Example: Decay of a two-level system and relaxation into thermal equilibrium thereof

Closed systems

Definition

A closed quantum system is a system S, which is prepared in such a way that there is no interaction with the environment

If we thus have a closed system S, the state of such a system is then described by a state vector $|\psi\rangle \in \mathcal{H}_S$, where $\mathcal{H}_S$ is the Hilbert space corresponding to S, with inner product $\langle\psi \mid \varphi\rangle$. We therefore can use the technics studyied in our classes.

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Schrödinger equation and unitary time-evolution

$$\imath \frac{d}{dt} \mid \psi(t)\rangle = H(t) \mid \psi(t)\rangle \tag{1}$$

From which we know the solution:

$$\mid \psi(t)\rangle = U(t, t_0) \mid \psi(t_0)\rangle \tag{2}$$

where $U(t, t_0)$ is the *unitary time-evolution operator.*
If we plug (2) into (1) we get:

$$\imath \frac{d}{dt} U(t, t_0) = H(t) U(t, t_0) \tag{3}$$

with initial condition: $U(t_0, t_0) = id$

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Density matrices

Now, let us introduce the *density matrix* of the system S:

$$\rho(t) = \sum_{\alpha} \omega_{\alpha} \mid \psi_{\alpha}(t)\rangle\langle\psi_{\alpha}(t) \mid \quad (4)$$

where ω_{α} are the statistical weights.

With previous considerations we get:

$$\begin{aligned}\rho(t) &= \sum_{\alpha} \omega_{\alpha} U(t, t_0) \mid \psi_{\alpha}(t_0)\rangle\langle\psi_{\alpha}(t_0) \mid U^{\dagger}(t, t_0) \\ &= U(t, t_0)\rho(t_0)U^{\dagger}(t, t_0)\end{aligned} \quad (5)$$

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Liouville-von Neumann and master equation

Differentiate equation (5) on both sides by t and using equation (3) we get:

$$\frac{d}{dt}\rho(t) = -\imath(H(t)\rho(t) - \rho(t)H(t)) = -\imath\,[H(t), \rho(t)] \qquad (6)$$

Equation (6) is then called the *Liouville-von Neumann equation*.

Introduce the Liouville super-operator:

$$\mathcal{L}(t)\rho(t) = -\imath\,[H(t), \rho(t)] \qquad (7)$$

And we get another form of equation (6):

$$\frac{d}{dt}\rho(t) = \mathcal{L}(t)\rho(t) \qquad (8)$$

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Definition of an open system

Definition

- An *open quantum system* is the subsystem S, of a closed combined system S+B, where the B, represents the system corresponding to the *environment*.
- The subsystem S, being the system we are interested in, is then called the *reduced system*.

Denote by $\mathcal{H}_{\mathcal{S}}$, $\mathcal{H}_{\mathcal{B}}$ the Hilbert space of S, B respectively. We then know that the Hilbert space of the combined system S + B is: $\mathcal{H} = \mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{\mathcal{B}}$

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Hamiltonian of an open system

With the previous consideration, we can write the Hamiltonian of the total closed system S + B the following way:

$$H = H_S \otimes I_B + I_S \otimes H_B + H_I \tag{9}$$

where:

- H_S: the self-Hamiltonian of the reduced system S
- H_B: the free Hamiltonian of the environment
- H_I: the interaction Hamiltonian between S and B

Expectation values in the total and reduced system

- Recall: For any system described by a density matrix ρ and C an arbitrary observable of the system, we know, that the expectation value $\langle C \rangle$ of the observable C is given by:

$$\langle C \rangle = tr\{C\rho\} \tag{10}$$

  This follows immediately from the definition of the density matrix ρ.

- If A is an operator on $\mathcal{H}_S$ we get that $\tilde{A} = A \otimes I_B$ is an operator on $\mathcal{H}$ and the observable A acting on the open system's Hilbert space $\mathcal{H}_S$ is determined through the formula:

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  where $\rho_S = tr_B\rho$ is the reduced density matrix and $tr_B\{\cdot\}$ is the partial trace over the subsystem B.

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Master equation on the reduced system

From the derivation of the quantum master equation of a closed system we find for the density matrix of the reduced system:

$$\rho_S(t) = tr_B\{U(t,t_0)\rho(t_0)U^\dagger(t,t_0)\} \tag{12}$$

Taking these considerations into account, we can derive the *master equation on the reduced system S*, by taking the partial trace on both sides of the Liouville-von Neumann equation and we get:

$$\frac{d}{dt}\rho_S(t) = -\imath tr_B\{[H(t),\rho(t)]\} \tag{13}$$

We note that these two equations describe the reduced system exactly.

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Definition of the dynamical map on an arbitrary open system

Assume: At $t = 0$: total state uncorrelated $\Rightarrow \ \rho(0) = \rho_S(0) \otimes \rho_B$, and ρ_B some reference state.

Then:

- For $t > 0 : \rho_S(0) \mapsto \rho_S(t) = V(t)\rho_S(0)$ and

$$\rho_S(t) = V(t)\rho_S(0) = tr_B\{U(t,0)[\rho_S(0) \otimes \rho_B]U^\dagger(t,0)\} \quad (14)$$

- The map $V(t)$ is called a *dynamical map* acting on the space of density operators $\mathcal{S}(\mathcal{H}_s)$ on $\mathcal{H}_S$:

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Explicit form of the dynamical map

- **Spectral decomposition** of $\rho_B \;\Rightarrow\; \rho_B = \sum_\beta \lambda_\beta \mid \varphi_\beta\rangle\langle\varphi_\beta \mid$, where $\mid \varphi_\beta\rangle$ is an orthonormal basis of $\mathcal{H}_\mathcal{B}$ and $\lambda_\beta \geq 0$ such that $\sum_\beta \lambda_\beta = 1$

- **Then:**

$$V(t)\rho_S(0) = \sum_{\alpha,\beta} W_{\alpha\beta}(t)\rho_S(0)W^\dagger_{\alpha\beta}(t) \tag{15}$$

where $W_{\alpha\beta} = \sqrt{\lambda_\beta} \cdot \langle\varphi_\alpha \mid U(t,0) \mid \varphi_\beta\rangle$

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Definition of complete positivity of a map

Definition

A linear map $\Phi : \mathcal{A} \to \mathcal{B}$ is called *completely positive*, if the tensor product map $\Phi^{(n)} := \Phi \otimes I_n : \mathcal{A} \otimes \mathcal{M}(n) \to \mathcal{B} \otimes \mathcal{M}(n)$ is positive $\forall n \in \mathbb{N}$

Representation theorem for super-operators by Kraus

Let Φ be a super-operator then:

1. Φ is completely positive $\iff$ $\exists \Omega_k$, countable set of operators such that $\underline{\Phi(\rho) = \sum_k \Omega_k \rho \Omega_k^\dagger}$

Furthermore:

2. $tr(\Phi\rho) = tr(\rho)$ $\iff$ $\sum_k \Omega_k^\dagger \Omega_k = I$

$V(t)$ is completely positive and trace preserving

Applying the representation theorem to our result (15) we see that:

- V(t) is linear
- V(t) is completely positive
- V(t) is trace-preserving

Quantum Markov processes

Now, let us consider a *Markov system*: In such a system the time-evolution is „*Markovian*“, meaning local in time, so that memory effects are neglected.

Note:

- The Markovian assumption is often a brutal approximation to the time-evolution of the system, because $\rho_S(t+dt)$ normally not only depends on $\rho_S(t)$ but also on ρ_S at earlier times, since information that has left the system can be transferred back from the environment again.
- The condition underlying the Markovian approximation is: *timescale over which state of S varies appreciably* $= \tau_R \gg \tau_B =$ *timescale over which influence of S on B relaxes*

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If we assume S to be a Markov system, then:

The dynamical map takes on the following so called *semigroup property*:

$$V(t_1)V(t_2) = V(t_1 + t_2)$$

Because: $\rho_S(t_1 + t_2)$ is completely determined by $\rho_S(t_1)$ in a Markov system

Quantum dynamical semigroup

Define the continuous one-parameter family $V := \{V(t) \mid t \in \mathbb{R}_{\geq 0}\}$ of completely positive trace-preserving linear maps: $V(t) : \mathcal{S}(\mathcal{H}_{\mathcal{S}}) \to \mathcal{S}(\mathcal{H}_{\mathcal{S}})$, describing the whole future time evolution of the open system.

Definition

A continuous family of linear maps $V := \{V(t) \mid t \in \mathbb{R}_{\geq 0}\}$ is called a *quantum dynamical semigroup* if the following conditions are satisfied:

1. $V(0) = I$
2. $V(t)$ is completely positive $\forall t \in \mathbb{R}_{\geq 0}$
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The Markovian master equation

Assume: Semigroup property and sufficiently smooth evolution
Then: we can define a master equation for the Markovian evolution:

$$\begin{aligned}\frac{d}{dt}\rho_S(t) &= \lim_{\Delta t \to 0} \frac{\rho_S(t+\Delta t) - \rho_S(t)}{\Delta t} \\ &= \underbrace{\lim_{\Delta t \to 0} \left\{ \frac{V(\Delta t) - V(0)}{\Delta t} \right\}}_{\mathcal{L}} \cdot \underbrace{V(t)\rho_S(0)}_{\rho_S(t)} \\ &= \mathcal{L}\rho_S(t) \end{aligned} \tag{16}$$

(16) is the *Markovian master equation* and
$\mathcal{L} = \lim_{\Delta t \to 0} \frac{V(\Delta t) - V(0)}{\Delta t}$ is called the *generator* of the semigroup.

Generator of an N-level system

Consider now an N-level system with N-dimensional Hilbert space $\mathcal{H}_S \cong \mathbb{C}^N$. Then:

- The the Hilbert space of operators is N^2-dimensional. Therefore: $\mathcal{S}(\mathcal{H}_S) \subset \mathcal{M}(N) := \{(a_{ij})_{i,j=1}^N \mid a_{ij} \in \mathbb{C}\}$, with inner product: $(A, B) = tr(A^\dagger B)$
- Choose an orthonormal Basis $\{Fi\}_{i=1}^{N^2}$ of $\mathcal{M}(N)$ such that:
  1. $(F_i, F_j) = \delta_{ij}$
  2. $F_{N^2} = \sqrt{\frac{1}{N}} \cdot I_S$
  3. $tr(F_i) = 0, \quad \forall i \in \{1, \cdots, N^2 - 1\}$

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With the definitions from the previous slide we can now write $W_{\alpha\beta}(t)$ the following way:

$$W_{\alpha\beta}(t) = \sum_{i=1}^{N^2} Fi(Fi, W_{\alpha\beta}(t)) \tag{17}$$

And we get:

$$V(t)\rho_S = \sum_{i,j=1}^{N^2} c_{ij}(t) F_i \rho_S F_j^\dagger \tag{18}$$

where: $c_{ij} = \sum_{\alpha,\beta} (F_i, W_{\alpha\beta}(t))(F_j, W_{\alpha\beta}(t))^*$ is a Hermitean and positive matrix in $\mathcal{M}(N^2)$

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Use the Markovian master equation:

$$\frac{d}{dt}\rho_S = \mathcal{L}\rho_S = \lim_{\Delta t \to 0} \frac{V(\Delta t)\rho_S - \rho_S}{\Delta t} \tag{19}$$

And define:

$$\begin{aligned}
a_{ij} &= \lim_{\Delta t \to 0} \frac{c_{ij}(\Delta t)}{\Delta t}, && \text{if i,j} \in \{1, \cdots N^2 - 1\} \\
a_{iN^2} &= a_{N^2 i} = \lim_{\Delta t \to 0} \frac{c_{iN^2}(\Delta t)}{\Delta t}, && \text{if i} \in \{1, \cdots N^2 - 1\} \\
a_{N^2 N^2} &= \lim_{\Delta t \to 0} \frac{c_{N^2 N^2}(\Delta t) - N}{\Delta t} \\
F &= \frac{1}{\sqrt{N}} \cdot \sum_{i=1}^{N^2-1} a_{iN^2} F_i \\
G &= \frac{1}{2N} \cdot a_{N^2 N^2} I_S + \frac{1}{2} \cdot (F^\dagger + F) \\
H &= \frac{1}{2\imath} \cdot (F^\dagger - F)
\end{aligned}$$

With these definitions we get:

$$\mathcal{L}\rho_S = (-\imath)[H, \rho_S] + \{G, \rho_S\} + \sum_{i,j=1}^{N^2-1} a_{ij} F_i \rho_S F_j^\dagger \tag{20}$$

But since semigroup is tracepreserving, we have:

$$tr\{\mathcal{L}\rho_S\} = tr\{\frac{d\rho_S}{dt}\} = \frac{d}{dt}\underbrace{tr\{\rho_S\}}_{=1} = 0 \tag{21}$$

Now plug in (20) into (21) and use the fact that $tr\{AB\} = tr\{BA\}$:

$$\Rightarrow tr\Big\{(2G + \sum_{i,j=1}^{N^2-1} a_{ij} F_j^\dagger F_i)\rho_S\Big\} = 0 \qquad \forall \rho_S \in \mathcal{S}(\mathcal{H}_S) \tag{22}$$

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Generator of the N-level system

If we now use all our previous results and put them together we get the first standard form of the generator of an N-level open system:

$$\mathcal{L}\rho_S = -\imath[H, \rho_S] + \sum_{i,j=1}^{N^2-1} a_{ij}\left(F_i \rho_S F_j^\dagger - \frac{1}{2}\{F_j^\dagger F_i, \rho_S\}\right) \qquad (24)$$

Diagonal form of the generator of the N-level system

Using the fact that $\{a_{ij}\}_{i,j=1}^{N^2-1}$ is symmetric and positive, we can diagonalize it: $\exists$ unitary transformation $\mathbf{u}$ such that: $\gamma_i \in \mathbb{R}_{\geq 0}$ and:

$$\mathbf{u}\mathbf{a}\mathbf{u}^\dagger = \begin{pmatrix} \gamma_1 & 0 & \dots & 0 \\ 0 & \gamma_2 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & \gamma_{N^2-1} \end{pmatrix}$$

We get the *diagonal form* of the generator of the semigroup by defining A_k such that: $F_i = \sum_{k=1}^{N^2-1} u_{ki} A_k$:

$$\mathcal{L}\rho_S = -\imath[H, \rho_S] + \sum_{k=1}^{N^2-1} \gamma_k \left(A_k \rho_S A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S - \frac{1}{2} \rho_S A_k^\dagger A_k \right) \quad (25)$$

Diagonal form of the generator of the N-level system

Using the fact that $\{a_{ij}\}_{i,j=1}^{N^2-1}$ is symmetric and positive, we can diagonalize it: $\exists$ unitary transformation $\mathbf{u}$ such that: $\gamma_i \in \mathbb{R}_{\geq 0}$ and:

$$\mathbf{uau}^\dagger = \begin{pmatrix} \gamma_1 & 0 & \dots & 0 \\ 0 & \gamma_2 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & \gamma_{N^2-1} \end{pmatrix}$$

We get the *diagonal form* of the generator of the semigroup by defining A_k such that: $F_i = \sum_{k=1}^{N^2-1} u_{ki} A_k$:

$$\mathcal{L}\rho_S = -\imath[H, \rho_S] + \sum_{k=1}^{N^2-1} \gamma_k \left(A_k \rho_S A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S - \frac{1}{2} \rho_S A_k^\dagger A_k \right) \tag{25}$$

Notes:

- The diagonal form is the most general form of the generator of a quantum dynamical semigroup
- A_k are usually referred to as the *Lindblad operators* and $\frac{d}{dt}\rho_S = \mathcal{L}\rho_S$ as the *Lindblad equation*
- Lindblad proved in 1976 that (25) is the most general form for a bounded generator in a seperable Hilbert space if k is allowed over a countable set

Decay of two-level system

We consider now:

- A bound two-level quantum system (eg. atom), with energy-spacing $\Delta E = \omega_0$ ($\hbar = 1$) interacting with quantized radiation field
- The radiation field represents a reservoir of temperature T and the bound system is the reduced system

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- Hamiltonian H_S of atom
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Two-level system

The Hilbert space of the reduced system is: $\mathcal{H} = span\{|\, e\rangle, |\, g\rangle\}$, and $\mathcal{S}(\mathcal{H}) \subset \mathcal{M}(2)$.
Introduce *Pauli-operators* in basis $\{|\, e\rangle, |\, g\rangle\}$:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_2 = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix} \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

And the *raising/lowering operators*:

$$\sigma_+ = \frac{1}{2}(\sigma_1 + \imath\sigma_2) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \sigma_- = \frac{1}{2}(\sigma_1 - \imath\sigma_2) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Assume:

- $\tau_R \gg \tau_B \Rightarrow$ Markovian system
- weak-coupling
- interaction Hamiltonian in dipole approximation: $H_I = -\vec{D} \cdot \vec{E}$
- $H_S = \frac{1}{2}\omega_0\sigma_3$

Then: The quantum Markovian master equation for this system is:

$$\frac{d}{dt}\rho_S(t) = \gamma_0(N(\omega_0)+1)\left\{\sigma_-\rho_S(t)\sigma_+ - \frac{1}{2}\sigma_+\sigma_-\rho_S(t) - \frac{1}{2}\rho_S(t)\sigma_+\sigma_-\right\} + \gamma_0 N(\omega_0)\left\{\sigma_+\rho_S(t)\sigma_- - \frac{1}{2}\sigma_-\sigma_+\rho_S(t) - \frac{1}{2}\rho_S(t)\sigma_-\sigma_+\right\}$$

where $N(\omega_0) = N = \frac{1}{e^{\beta\hbar\omega_0}-1}$, $\quad \underbrace{\gamma_0 = \frac{4\omega_0^3|\vec{d}|^2}{3\hbar c}}_{\text{spontaneous emission rate}}$,

$\vec{d} = \langle e \mid \vec{D} \mid g \rangle$.

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To solve the Markovian master equation use the following ansatz for ρ_S:

$$\rho_S(t) = \frac{1}{2}(I + \langle \sigma(\vec{t}) \rangle \cdot \vec{\sigma}) = \begin{pmatrix} \frac{1}{2}(1 + \langle \sigma_3(t) \rangle) & \langle \sigma_-(t) \rangle \\ \langle \sigma_+(t) \rangle & \frac{1}{2}(1 - \langle \sigma_3(t) \rangle) \end{pmatrix}$$

where: $\langle \vec{\sigma}(t) \rangle = tr\{\vec{\sigma} \cdot \rho_S(t)\}$ and $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)^T$

Therefore we have the populations of the states $\mid e \rangle$ and $\mid g \rangle$:

$$p_e(t) = (\rho_S)_{11} = \frac{1}{2}(1 + \langle \sigma_3(t) \rangle)$$

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Plugging our ansatz into the Markovian master equation and using the commutation relations of the Pauli-Matrices we get:

$$\frac{d}{dt}\langle\vec{\sigma}(t)\rangle = \begin{pmatrix} -\frac{\gamma}{2}\langle\sigma_1(t)\rangle \\ -\frac{\gamma}{2}\langle\sigma_2(t)\rangle \\ -\gamma\langle\sigma_3(t)\rangle - \gamma_0 \end{pmatrix}, \quad \text{where } \underbrace{\gamma = \gamma_0 \cdot (2N+1)}_{\text{total emission rate}} \tag{26}$$

As we are interested in thermalisation, we need to find p_e^s and p_g^s: Set (26) $= (0,0,0)^T \Rightarrow \langle\sigma_3\rangle_S = -\frac{\gamma_0}{\gamma} = -\frac{1}{2N+1}$ and thus:

$$p_e^s = \frac{N}{2N+1} = \frac{1}{e^{\beta\hbar\omega_0}+1} \tag{27}$$

Choosing the initial state: $\rho_S(0) = | g\rangle\langle g |$ and solving (26) we find:

$$p_e(t) = p_e^s \cdot (1 - e^{-\gamma t}) \tag{28}$$

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Summary

- Exact master equations of closed quantum systems
- Open and Markovian quantum systems and its „exact“ master equations
- Quantum dynamical semigroup in relation with the Markovian quantum systems - and its generator
- General form of the generator and the master equation of a Markovian N-level system
- Application of the above theory to a thermalisation process of a two-level system