Non-Markovian Open Quantum Systems

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Open Quantum Systems

The theory of open quantum systems describes the interaction of a quantum system with its environment.

Quantum Mechanics
- closed systems
- unitary dynamics
- reversible dynamics

Schrödinger Equation
\[ i\hbar \frac{d}{dt} |\Psi\rangle = \hat{H} |\Psi\rangle \]

Liouville – von Neumann Equation
\[ i\hbar \frac{d\hat{\rho}}{dt} = [\hat{H}, \hat{\rho}] \]

Open quantum systems
- reduced density operator
  \[ \hat{\rho}_s(t) = Tr_E[\hat{\rho}_T(t)] \]
- master equation
  \[ \frac{d\hat{\rho}}{dt} = L\hat{\rho} \]
- non-unitary and irreversible dynamics
Motivation

**Fundamentals of Quantum Theory**

**Quantum Measurement Theory**

Border between quantum and classical descriptions

**Quantum Technologies**

**Decoherence**

Entanglement between the degrees of freedom of the system and those of the environment

**PROBLEM:** All new quantum technologies rely on quantum coherence

- quantum computation
- quantum cryptography
- quantum communication

**Qubit**
Approaches to the dynamics of open quantum systems

1 Derivation of an equation of motion for the reduced density matrix of the system of interest: The master equation

- **Microscopic approach**
  - Microscopic Hamiltonian for the total closed system (model of environment and interaction)
  - Trace over the environmental degrees of freedom
- **Phenomenological approach**
  - Approximations

2 Solution of the master equation

- **Analytical methods**
  - Damping basis method\(^1\)
  - Green function
  - Algebraic superoperatorial methods\(^2\)
- **Numerical methods**
  - Monte Carlo wave function (and variants)\(^3,4\)
  - Influence functional – path integral\(^5\)

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Approximations

**weak coupling approximation**
weak coupling between system and environment

- perturbative approaches
  (expansions in the coupling constant)

**Markovian approximation**

assumes that the reservoir correlation time is much smaller than the relaxation time of the open system

- coarse-graining in time

changes in the reservoir due to the interaction with the system do not feed back into the system
Lindblad master equation \(^1, ^2\)

Weak coupling + Markovian approximation + RWA or secular approx.

\[
\frac{d\rho}{dt} = -i[H, \rho] + \sum_j \left( V_j \rho V_j^\dagger - \frac{1}{2} \{ \rho, V_j V_j^\dagger \} \right)
\]

\(\rho\) density matrix of the reduced system

ADVANTAGES

- Semigroup property: \(\Lambda_{t+t'}[\rho] = \Lambda_t \circ \Lambda_{t'}[\rho]\)
- Positivity: \(\Lambda_t : \text{iff } \rho(0) \succeq 0 \Rightarrow \Lambda_t[\rho(0)] \succeq 0, \forall \rho \in B(H)\)

\[
\rho(t) = \Lambda_t \rho(0)
\]

dynamical map

\[
\Lambda_t = e^{Lt}
\]
Markovian dynamical map

Positivity and Complete positivity

**Positivity**

\[ \langle \Psi | \rho | \Psi \rangle \geq 0, \ \forall \Psi \]

**Complete Positivity**

\[ \Lambda_t : B(H) \rightarrow B(H) \text{ completely positive iff} \]

\[ \Lambda_t \otimes I_n : B(H \otimes H_n) \rightarrow B(H \otimes H_n) \text{ is positive } \forall n \in \mathbb{N} \]

Less intuitive property!

Violation of CP incompatible with the assumption of a total closed system (for factorized initial condition)

Complete positivity of the dynamical map \( \Lambda_t \) guarantees that the eigenvalues of any *entangled state* \( \rho_{S+S_n} \) of \( S + S_n \) remain positive at any time.
A consistent physical description of an open quantum system must be not only positive but also completely positive. The Lindblad form of the master equation is the only possible form of first-order linear differential equation for a completely positive semigroup having bounded generator.

This is valid whenever

\[ \rho_{TOT} = \rho \otimes \rho_{ENV} \]

What about non-Lindblad-type master equations?

CP is not guaranteed and unphysical situations, showing that the model we are using is not appropriate, may show up in the dynamics.

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Non-Markovian master equations

Non-Markovian master equations need not be in the Lindblad form, and usually they are not.

Why to study them?

- photonic band-gap materials \(^1\)
- quantum dots
- atom lasers \(^2\)
- non-Markovian quantum information processing \(^3\)

Non-Lindblad ME

No man’s land

QUANTUM NANOTECHNOLOGIES \(^4,5,6,7\)


Damped harmonic oscillator
or Quantum Brownian Motion in a harmonic potential

Paradigmatic model of the theory of open quantum systems

Ubiquitous model may be solved exactly

Quantum Optics, Quantum Field Theory, Solid State Physics

**System**

\[ H_{sys} = \hbar \omega_0 \left( a^\dagger a + \frac{1}{2} \right) \]

**Microscopic model**

\[ H_{tot} = H_{sys} + H_{res} + H_{int} \]

**Environment**

\[ H_{res} = \sum_n \hbar \omega_n b_n^\dagger b_n \]

**Coupling**

\[ H_{int} = \alpha \sum_n k_n \sqrt{\frac{\hbar}{2m_n \omega_n}} \left( b_n + b_n^\dagger \right) \left( a + a^\dagger \right) \]

**Spectral density of the reservoir**

\[ J(\omega) = \sum_n \frac{k_n^2}{2m_n \omega_n} \delta(\omega - \omega_n) \]
Two approaches: microscopic and phenomenologic

GOAL: To study the dynamics of the system oscillator, in presence of coupling with the reservoir beyond the Markovian approximation

Exact Master Equation
Time-convolutionless approach

Phenomenological master equation containing a memory kernel

generalized master equation
local in time

\[ \frac{d\rho(t)}{dt} = L(t)\rho(t) \]

generalized master equation
non-local in time

\[ \frac{d\rho(t)}{dt} = \int_0^t K(t-t')L\rho(t')dt' \]

Exact Master Equation \(^1,\,^2\)  
(time convolutionless approach)

\[
\frac{d\rho(t)}{dt} = \left[ -i\bar{H}_S^s - \Delta(t)X^s - \Pi(t)X^sP^s + \gamma(t)(N + 2) \right] \rho(t) \\
= L(t)\rho(t)
\]

Time dependent coefficients have the form of series in the coupling constant \(\alpha\)

- \(\Delta(t) = \int_0^t \kappa(\tau) \cos(\omega_0\tau) d\tau\)
- \(\Pi(t) = \int_0^t \kappa(\tau) \sin(\omega_0\tau) d\tau\)

Noise kernel

To the second order in the coupling constant we have

- \(\gamma(t) = \int_0^t \mu(\tau) \sin(\omega_0\tau) d\tau\)

Damping term (dissipation)

Dissipation kernel


Secular approximated master equation (and applications)

\[
\frac{d\rho(t)}{dt} = -\frac{\Delta(t) + \gamma(t)}{2}[a^\dagger a\rho - 2a\rho a^\dagger + \rho a^\dagger a] \\
- \frac{\Delta(t) - \gamma(t)}{2}[aa^\dagger \rho - 2a^\dagger \rho a + \rho aa^\dagger]
\]

Trapped ions


Linear amplifier

The Quantum Characteristic Function (QCF)\(^2\)

\[
\chi(\xi) = Tr[\rho D(\xi)] = Tr[\rho \exp(\xi a^\dagger - \xi^* a)] = \rho(t) = \frac{1}{2\pi} \int \chi(\xi, t) D(\xi) d\xi d\xi^*
\]

\[
\chi(\xi, t) = e^{-\Delta \Gamma(t) \xi^2} \chi_0 \left[ e^{-\Gamma(t)/2} e^{-i\omega_0 t} \xi \right]
\]

\[
\Gamma(t) = 2 \int_0^t \gamma(t') dt' \quad \Delta \Gamma(t) = e^{-\Gamma(t)} \int_0^t e^{\Gamma(t')} \Delta(t') dt'
\]

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Example of non-Markovian dynamics

The risks of working with non-Lindblad Master Equations
Master equation with memory kernel

**EXAMPLE:** Phenomenological non-Markovian master equation describing an harmonic oscillator interacting with a zero T reservoir

\[
\frac{d\rho(t)}{dt} = \int_0^t K(t-t')L\rho(t')dt' \quad \text{Markovian Liouvillian}
\]

\[
L\rho = 2a\rho a^\dagger - a^\dagger a\rho - \rho a^\dagger a
\]

Exponential memory kernel

\[
K(t-t') = g^2 e^{-\gamma|t-t'|}
\]

g coupling strength

g decay constant of system-reservoir correlations

Non-Lindblad Master Equation: CP and positivity are not guaranteed!
Solution using the QCF

What is the QCF?

\[ \chi(\xi, p) = Tr[\rho D(\xi)] \left| \xi \right|^2 / 2 \]

Fourier transform

\( p = 1 \)  
P function

\( p = 0 \)  
Wigner function

\( p = -1 \)  
Q function

Quantum Characteristic Function

\[ \chi(\xi) = \chi(\xi, p = 0) \]

defining properties

\[ \chi(\xi = 0) = 1 \]

\[ |\chi(\xi)| \leq 1 \]

useful property

\[ \langle a^+^m a^-^n \rangle = \left( \frac{d}{d\xi} \right)^m \left( -\frac{d}{d\xi^*} \right)^n \chi(\xi) \]
Solution using the QCF

Example: \( g / g = 1 \)\n\( t = g t \)

\[
\chi(\xi, \tau) = \left[ 1 - |\xi|^2 \right] e^{-\tau/2} \left( \cos(1.32\tau) + 0.37 \sin(1.32\tau) \right) e^{-|\xi|^2/2}
\]

defining properties

\[
\chi(\xi = 0) = 1 \quad |\chi(\xi)| \leq 1
\]

The defining properties are always satisfied

No problem with the dynamics
Density matrix solution

The quantum characteristic function contains all the information necessary to reconstruct the density matrix, and therefore is an alternative complete description of the state of the system\(^1\).

\[
\rho(t) = \frac{1}{2\pi} \int \chi(\xi, t) D(\xi) d\xi d\xi^* 
\]

we look at the time evolution of the population of the initial state \(|n = 1\rangle\)

\[
\rho_{11}(t) = \langle n = 1 | \rho(t) | n = 1 \rangle 
\]

\[
\rho_{11}(t) = e^{-\gamma t/2} \left( \cos \Omega t + \frac{\gamma}{2\Omega} \sin \Omega t \right) 
\]

Example: \(g / g = 1\)

\[
t = g t 
\]

Problem of positivity firstly noted by Barnett & Stenholm\(^2\).

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The QCF and the density matrix are not “operatively” equivalent descriptions of the dynamics, in the sense that the QCF may fail in discriminating when non-physical conditions (negativity of the density matrix eigenvalues) show up.

The defining properties of the QCF are only necessary conditions

\[ \chi(\xi = 0) = 1 \]
\[ |\chi(\xi)| \leq 1 \]

The additional condition to be imposed on the QCF in order to ensure the positivity of the density matrix does not seem to have a simple form

Non-Markovian dynamics of a qubit

Phenomenological model: Non-Markovian master equation with exponential memory

\[
\frac{d\rho}{dt} = \int_0^t dt' k(t') L \rho(t-t')
\]

memory kernel
\[
k(t) = \gamma e^{-\gamma t}
\]

Markovian Liouvillian
\[
L \rho = \gamma_0 (N+1) \left( \sigma_- \rho \sigma_+ - \frac{1}{2} \sigma_+ \sigma_- \rho - \frac{1}{2} \rho \sigma_+ \sigma_- \right) + \gamma_0 N \left( \sigma_+ \rho \sigma_- - \frac{1}{2} \sigma_- \sigma_+ \rho - \frac{1}{2} \rho \sigma_- \sigma_+ \right)
\]

Solution in terms of the Bloch vector
\[
\rho(t) = \frac{1}{2} \left[ I + \vec{w}(t) \cdot \vec{\sigma} \right]
\]

Bloch vector
\[
\Phi : \vec{w}(0) \rightarrow \vec{w}(t) = \Lambda \vec{w}(0) + \vec{T}
\]

\[
\xi(R, \tau) = e^{-\tau/2} \left[ 1 - 4R \right]^{1/2} \sinh \left[ \sqrt{1 - 4R} \tau/2 \right] + \cosh \left[ \sqrt{1 - 4R} \tau/2 \right]
\]

\[
\tau = \gamma t \quad R = \gamma_0 / \gamma
\]
Positivity and Complete Positivity

THE BLOCH SPHERE

\[
\left( \frac{w_x}{\xi(R/2, t)} \right)^2 + \left( \frac{w_y}{\xi(R/2, t)} \right)^2 + \left( \frac{w_z - (2N + 1) \xi(R, t) - 1}{\xi(R, t)} \right)^2 = 1
\]

Condition for positivity: The dynamical map \( \Phi \) maps a density matrix into another density matrix if and only if the Bloch vector describing the initial state is transformed into a vector contained in the interior of the Bloch sphere, i.e. the Bloch ball.

\[ 4R \leq 1 \]

**THIS RESULT PROVIDES THE EXPLICIT CONDITIONS OF VALIDITY OF A PARADIGMATIC PHENOMENOLOGICAL MODEL OF THE THEORY OF OPEN QUANTUM SYSTEMS, NAMELY THE SPIN-BOSON MODEL WITH EXPONENTIAL MEMORY.**

we have derived for our model, we have proved that, in the case of exponential memory and for the non-Markovian model here considered **positivity is a necessary and sufficient condition for complete positivity [2]**


**Summary**

Open quantum systems

- **Markovian master equation**
  - Lindblad form

- **Non-Markovian master equation**
  - Non-Lindblad form

**Beyond the Lindblad form**

- Two approaches: *microscopic* and *phenomenological*
  - Paradigmatic model: QBM or damped harmonic oscillator

**TCL (microscopic exact approach)**

- Generalized master equation
- Solution based on algebraic method
- Applications: trapped ions, linear amplifier

**Memory kernel**

- QCF and density matrix solutions
- Positivity violation
- Limits in the use of the QCF
References

Quantum Brownian Motion

Trapped ion simulator

Lindblad non-Lindblad border and the existence of a continuous measurement interpretation for non-Markovian stochastic processes

Non-Markovian wavefunction method

Positivity and complete positivity
S. Maniscalco “Complete positivity of the spin-boson model with exponential memory”, submitted for publication