Lecture II
Non-Markovian Quantum Jumps

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Lecture I
1. General framework: Open quantum systems
2. Local in time master equations

Lecture II
3. Solving local in time master equations:
   Markovian and non-Markovian quantum jumps

Lecture III
4. Measures of non-Markovianity
5. Applications of non-Markovianity
3. Markovian and non-Markovian quantum jumps

- General local in time master equation
- Density matrix as an ensemble of state vectors
- Markovian case: Monte Carlo wave function method
- Generalization: Non-Markovian quantum jumps
- What do non-Markovian jumps tell about the memory
General local in time master equation

\[ \frac{d\varrho_S(t)}{dt} = \mathcal{L}_S \varrho_S(t) \]

- Semigroup iff generator \( \mathcal{L}_S \) in Lindblad form

\[ \frac{d\varrho_S(t)}{dt} = \int_0^t ds \mathcal{K}_S(t - s) \varrho_S(s) \]

- Memory kernel \( \mathcal{K}_S(t - s) \)

\[ \frac{d\varrho_S(t)}{dt} = \mathcal{L}_S(t) \varrho_S(t) \]

- Time-dependent generator \( \mathcal{L}_S(t) \)

General form of the local in time (TCL) equation

\[ \frac{d\varrho_S(t)}{dt} = -i[H_S, \varrho_S] + \sum_k \left( C_k(t) \rho_S(t) D_k(t)^\dagger + D_k(t) \rho_S(t) C_k(t)^\dagger \right) \]

\[ - \frac{1}{2} \left\{ D_k^\dagger(t) C_k(t) + C_k^\dagger(t) D_k(t), \rho_S(t) \right\} \]

- Operators may depend on time
- Lindblad-like structure if \( D_k(t) = C_k(t) \)
Q: How to solve the master equation?

- Few exact models and analytical solutions
- Can we find the solution by evolving an ensemble of state vectors instead of directly solving the density matrix?

Generally, we can decompose the density matrix as

$$\rho(t) = \sum_i P_i(t) |\psi_i(t)\rangle \langle \psi_i(t)|$$

Suppose now we want to solve the semigroup, Markovian, Lindblad equation

$$\frac{d\rho(t)}{dt} = -i[H, \rho_S] + \sum_k \gamma_k \left( A_k \rho_S A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S - \frac{1}{2} \rho_S A_k^\dagger A_k \right)$$
Monte Carlo wave function method (Markovian)  
(Dalibard, Castin, Mølmer, PRL 1992)

Ensemble of $N$ state vectors

\[
\begin{align*}
\psi_1(t_0) &\rightarrow \psi_1(t_1) \quad \ldots \quad \psi_1(t_n) \\
\psi_2(t_0) &\rightarrow \psi_2(t_1) \quad \ldots \quad \psi_2(t_n) \\
&\quad \vdots \\
\psi_N(t_0) &\rightarrow \psi_N(t_1) \quad \ldots \quad \psi_N(t_n)
\end{align*}
\]

Time

At each point of time, density matrix $\rho$ as average of state vectors $\Psi_i$:  
\[
\rho(t) = \frac{1}{N} \sum_{i=1}^{N} |\psi_i(t)\rangle\langle\psi_i(t)|
\]

The time-evolution of each $\Psi_i$ contains stochastic element due to random quantum jumps.
At each point of time: decide if quantum jump happened.

\[ P_j = \delta_t \Gamma p_e \]

For example: 2-level atom

Probability for atom being transferred from the excited to the ground state and photon emitted.
Historical remark on quantum jumps: Schrödinger vs. Bohr

**Schrödinger:**
“If we are going to stick to this damned quantum-jumping, then I regret that I ever had anything to do with quantum theory.”

**Bohr:**
“But the rest of us are thankful that you did, because you have contributed so much to the clarification of quantum theory”.


Are quantum jump “real”? 
Are quantum jump “real”? Observed in experiments.

Haroche group @ ENS: “Quantum jumps of light recording the birth and death of a photon in a cavity”, Nature 446, 297 (2007).

How to use quantum jumps in theoretical descriptions of physical systems?

Open quantum systems, Monte Carlo methods...
### Simple classification of Monte Carlo/stochastic methods

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<td><strong>QSD</strong> (Diosi, Gisin, Percival...)</td>
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<td>MCWF (Dalibard, Castin, Molmer)</td>
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**Jump**

**Diffusion**

![Ground and excited state probability over time graphs](image)
Example: driven 2-state system, Markovian

Quantum jump: Discontinuous stochastic change of the state vector.

Excited state probability \( P \) for a driven 2-level atom

Excited state

\( E \)

coupling (deterministic)

decay channel (random jump)

Ground state

\( G \)

\[
\frac{d\rho}{dt} = -i[H, \rho] + \Gamma \left[ \sigma_- \rho \sigma_+ - \frac{1}{2} \{ \sigma_+ \sigma_- , \rho \} \right]
\]

\[
\rho(t) = \frac{1}{N} \sum_{i=1}^{N} |\psi_i(t)\rangle \langle \psi_i(t)|
\]

Markovian Monte Carlo

single realization

ensemble average

P

Time

Time

damped Rabi oscillation of the atom
Markovian Monte Carlo wave function method

Master equation to be solved:

\[
\frac{d\rho(t)}{dt} = \frac{1}{\hbar} [H_S, \rho] + \sum_m \Gamma_m C_m \rho C_m^\dagger - \frac{1}{2} \sum_m \Gamma_m \left( C_m^\dagger C_m \rho + \rho C_m C_m^\dagger \right)
\]

For each ensemble member \( \psi \):

- Solve the time dependent Schrödinger equation.
- Use non-Hermitian Hamiltonian \( H \) which includes the decay part \( H_{\text{dec}} \).
- Key for non-Hermitian Hamiltonian: Jump operators \( C_m \) can be found from the dissipative part of the master equation.
- For each channel \( m \) the jump probability is given by the time step size, decay rate, and decaying state occupation probability.

Markovian Monte Carlo wave function method

Algorithm:

1. Time evolution over time step $\delta t$

2. Generate random number, did jump occur?

   No

   3. Renormalize $\psi$ before new time step

   \[
   |\psi_i(t + \delta t)\rangle = \frac{e^{-iH_{\text{eff}}\delta t}|\psi_i(t)\rangle}{\sqrt{1 - \delta p}}
   \]

   Yes

   3. Apply jump operator $C_j$ before new time step

   \[
   |\psi_i(t + \delta t)\rangle = \frac{C_j|\psi_i(t)\rangle}{||C_j|\psi(t)\rangle||}
   \]

4. Ensemble average over $\psi$'s gives the density matrix and the expectation value of any operator $A$

   \[
   \langle A\rangle(t) = \frac{1}{N} \sum_i \langle \psi_i(t)|A|\psi_i(t)\rangle
   \]
Markovian Monte Carlo wave function method

Equivalence with the master equation:

The state of the ensemble averaged over time step:
(for simplicity here: initial pure state and one decay channel only)

\[
\frac{\sigma(t + \delta t)}{\delta t} = (1 - P) \left| \phi(t + \delta t) \rightangle \left\langle \phi(t + \delta t) \right|  + P \frac{\left| \Psi(t) \rightangle \left\langle \Psi(t) \right| C^\dagger}{1 - P} C \frac{\left\langle C | \Psi(t) \right\rangle \left\langle \Psi(t) | C^\dagger \right|}{\left\langle \Psi(t) | C^\dagger C | \Psi(t) \right\rangle}
\]

Keeping in mind two things:

a) the time-evolved state is (1st order in \(dt\), before renormalization):

\[
\left| \phi(t + \delta t) \rightangle = \left( 1 - \frac{iH_s \delta t}{\hbar} - \frac{\Gamma \delta t}{2} C C^\dagger \right) \left| \Psi(t) \right\rangle
\]

b) the jump probability is:

\[
P = \delta t \Gamma \left\langle \Psi | C^\dagger C | \Psi \right\rangle
\]

it is relatively easy to see that the ensemble average corresponds to master equation

\[
\frac{d\rho(t)}{dt} = -i[H, \rho_S] + \sum_k \gamma_k \left( A_k \rho_S A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S - \frac{1}{2} \rho_S A_k^\dagger A_k \right)
\]
Markovian Monte Carlo wave function method

Measurement scheme interpretation

Two-level atom in vacuum

Two-level atom MC evolution by

\[
C = \sqrt{\Gamma} |g\rangle \langle e| \]

Jump operator

\[
H_{dec} = -\frac{i\hbar \Gamma}{2} |e\rangle \langle e| \]

Non-Hermitian Hamiltonian

\[
P = \delta t \Gamma |c_e|^2 \]

Jump probability

Total system evolution

Measurement scheme:
continuous measurement of photons in the environment.

\[
\left( c_g |g\rangle + c_e |e\rangle \right) \otimes |0\rangle \rightarrow \\
\left( c'_g |g\rangle + c'_e |e\rangle \right) \otimes |0\rangle + \sum_\lambda c_\lambda |g\rangle \otimes |\lambda\rangle 
\]

- Continuous measurement of the environmental state gives conditional pure state realizations for the open system
- The open system evolution is average of these realizations
Non-Markovian quantum jumps

Questions:
- What happens when the decay rates depend on time? (time-dependent generator)
- What happens when the decay rates turn temporarily negative?

\[
\frac{d\rho(t)}{dt} = -i[H, \rho_S] + \sum_k \gamma_k(t) \left( A_k \rho_S(t) A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S(t) - \frac{1}{2} \rho_S A_k^\dagger A_k \right)
\]

Piilo, Maniscalco, Härkönen, Suominen:  

Piilo, Härkönen, Maniscalco, Suominen:  
Transfer from A to B. Ensemble initially in state A.

Rate: $\Gamma_A > 0$, time step: $\delta t$

Probability: $P_{A \rightarrow B} = \delta t \Gamma_A$

What about the transfer $A \rightarrow B$ with negative rate $\Gamma_A < 0$?

Claim: stochastic processes with negative rates appear in nature. Essential feature: memory
Markovian vs. non-Markovian evolution (1)

Markovian dynamics: Decay rate constant in time.
Non-Markovian dynamics: Decay rate depends on time, obtains temporarily negative values.

Example: 2-level atom in photonic band gap.

\[ P_j = \delta t \Gamma p_e < 0 \]

Markovian description of quantum jumps fails, since gives negative jump probability. For example: negative probability that atom emits a photon.
Markovian vs. non-Markovian evolution (2)

Waiting time distribution (2-level atom): \( F(t) = 1 - \exp \left[-\int_0^t dt' \Delta(t') \right] \)

Gives the probability that quantum jump occurred in time interval between 0 and \( t \).

At which point of time atom emits photon?

Markovian: constant rate

non-Markovian: temporary negative rate

1. It is not possible to emit the same photon 3 times.
2. Includes negative increment of probability.
3. What is the process that has positive probability and corresponds to negative probability quantum jump?
Non-Markovian master equation

Starting point:
General non-Markovian master equation local-in-time:

\[
\frac{d\rho(t)}{dt} = \frac{1}{i\hbar} [H_S, \rho] + \sum_m \Delta_m(t) C_m \rho C_m^\dagger - \frac{1}{2} \sum_m \Delta_m(t) \left( C_m^\dagger C_m \rho + \rho C_m C_m^\dagger \right)
\]

- Jump operators \( C_m \)
- Time dependent decay rates \( \Delta_m(t) \).
- Decay rates have temporarily negative values.

Example: 2-level atom in photonic band gap.
Jump operator \( C \) for positive decay: \( \sigma_- = |g\rangle \langle e| \)

\[
\frac{d\rho(t)}{dt} = \frac{1}{i\hbar} [H_S, \rho] + \Gamma(t) |g\rangle \langle e| \rho \langle e| \langle g| - \frac{1}{2} \Gamma(t) (|e\rangle \langle e| \rho + \rho |e\rangle \langle e|)
\]

![Graph](a)
Quantum jump in negative decay region:
The direction of the jump process reversed

$$|\psi\rangle \rightarrow |\psi'\rangle = \frac{C_m |\psi\rangle}{||C_m |\psi\rangle||}, \quad \Delta m(t) > 0$$

$$|\psi\rangle \leftarrow |\psi'\rangle = \frac{C_m |\psi\rangle}{||C_m |\psi\rangle||}, \quad \Delta m(t) < 0$$

Jump probability:

$$P = \frac{N}{N'} \delta t |\Delta m(t)| \langle \psi | C_m^\dagger C_m |\psi(t)\rangle$$

N: number of ensemble members in the target state
N': number of ensemble members in the source state

The probability proportional to the target state!
For example: two-level atom

\[ \sigma_- = |g\rangle \langle e| \]

Jump probability:

\[ P = \frac{N_0}{N_g} \delta t |\Gamma(t)| |\langle \psi_0 | e \rangle|^2 \]

The essential ingredient of non-Markovian system: memory. Recreation of lost superpositions.
$$\frac{d}{dt}\rho = -i[H(t), \rho]$$

$$+ \sum_k \Delta_k^+(t) \left[ C_k(t) \rho C_k^\dagger(t) - \frac{1}{2} \{ C_k^\dagger(t) C_k(t), \rho \} \right]$$

$$- \sum_l \Delta_l^-(t) \left[ C_l(t) \rho C_l^\dagger(t) - \frac{1}{2} \{ C_l^\dagger(t) C_l(t), \rho \} \right]$$

$$\rho(t) = \sum_{\alpha} \frac{N_{\alpha}(t)}{N} |\psi_\alpha(t)\rangle \langle \psi_\alpha(t)| \quad \text{ensemble}$$

Deterministic evolution and positive channel jumps as before...

Negative channel with jumps

$$D_{\alpha \to \alpha'}^-(t) = |\psi_{\alpha'}(t)\rangle \langle \psi_\alpha(t)|$$

where the source state of the jump is

$$|\psi_\alpha(t)\rangle = C_{j^-}(t) |\psi_{\alpha'}(t)\rangle / ||C_{j^-}(t) |\psi_{\alpha'}(t)\rangle||$$

...and jump probability for the corresponding channel

$$P_{\alpha \to \alpha'}^j(t) = \frac{N_{\alpha'}(t)}{N_{\alpha}(t)} |\Delta_{j^-}(t)| \delta t \langle \psi_{\alpha'}(t) | C_{j^-}^\dagger(t) C_{j^-}(t) | \psi_{\alpha'}(t) \rangle.$$
In terms of probability flow in Hilbert space:

Positive rate

\[ \rho(t) = \frac{N_0(t)}{N} |\psi_0(t)\rangle\langle \psi_0(t)| + \sum_i \frac{N_i(t)}{N} |\psi_i(t)\rangle\langle \psi_i(t)| + \sum_{i,j} \frac{N_{i,j}(t)}{N} |\psi_{i,j}(t)\rangle\langle \psi_{i,j}(t)| + \ldots \]

No jumps

1 random jump (channel i)

2 random jumps (channels i, j)

Memory in the ensemble: no jump realization carries memory of the 1 jump realization; 1 jump realization carries the memory of 2 jumps realization...

Negative rate: earlier occurred random events get undone.
Basic steps of the proof

Basic idea:
Weighting jump path with jump probability and deterministic path with no-jump probability gives the master equation (as in MCWF)

The ensemble averaged state over $\Delta t$ is

\[
\sigma(t + \Delta t) =
\begin{array}{c}
\frac{N_0(t)}{N} \langle \Phi_0(t + \Delta t) \rangle \langle \Phi_0(t + \Delta t) \rangle \\
1 + n_0 \\
+ \sum_i \frac{N_i(t)}{N} (1 - P_{i\rightarrow 0}) \langle \Phi_i(t + \Delta t) \rangle \langle \Phi_i(t + \Delta t) \rangle \\
1 + n_i \\
+ \sum_i \frac{N_i(t)}{N} P_{i\rightarrow 0} \frac{D_{i\rightarrow 0}}{n_i} \langle \Phi_i(t + \Delta t) \rangle \langle \Phi_i(t + \Delta t) \rangle \left| D_{i\rightarrow 0} \right|^* \end{array} + ...
\]

Here, other quantities are similar as in original MCWF except:

**P’s:** jump probabilities

**D’s:** jump operators

By plugging in the appropriate quantities gives the match with the master equation!
The simulation and exact results match.

**Typical features of photonic band gap:**
- Population trapping
- Atom-photon bound state.

**Single state vector history**

Example of one state vector history:

**I:** Quantum jump at positive decay region destroys the superposition.

**II:** Due to memory, non-Markovian jump recreates the superposition.

Piilo, Maniscalco, Härkönen, Suominen: PRL 100, 180402 (2008)
Examples of realizations:
Simultaneous positive and negative rates

3-level atom

- A: excited state
- C: ground state
- B: ground state

Two channels which can have different sign of the decay rate

\[
\dot{\rho}(t) = \frac{1}{i}{\lambda}_1(t)[|a\rangle\langle a|,\rho(t)] + \frac{1}{i}{\lambda}_2(t)[|a\rangle\langle a|,\rho(t)] + \Delta_1(t)
\]

\[
\times \left[ |b\rangle\langle a|\rho(t)|a\rangle\langle b| - \frac{1}{2}\{\rho(t),|a\rangle\langle a|\} \right]
\]

\[
+ \Delta_2(t) \left[ |c\rangle\langle a|\rho(t)|a\rangle\langle c| - \frac{1}{2}\{\rho(t),|a\rangle\langle a|\} \right]
\]

- Positive channel generates new random jumps
- Negative channel undoes the random jumps
- Total probability flow consists of positive and negative components
- Temporary plateau in the excited state A probability.

Examples of identification of positivity violation

3-level ladder atomic system:

Breakdown of positivity

Initial state

Positivity broken when the stochastic process hits singularity - master equation has formal solution beyond this point.

Implies that some of the approximations in deriving the master equation breaks down.

\[ \dot{\rho}(t) = \frac{1}{i} \lambda_1(t) \langle a | a \rangle \rho(t) + \frac{1}{i} \lambda_2(t) \langle a | a \rangle \rho(t) + \Delta_1(t) \]
\[ \times \left[ \langle b | b \rangle \rho(t) \langle a | a \rangle - \frac{1}{2} \{\rho(t), \langle a | a \rangle\} \right] \]
\[ + \Delta_2(t) \left[ \langle c | c \rangle \rho(t) \langle a | a \rangle - \frac{1}{2} \{\rho(t), \langle a | a \rangle\} \right]. \]
Our NMQJ description originally developed in the context of quantum optics and open quantum systems. Recently used to simulate Fenna-Matthews-Olson complex: energy transfer wire in green sulphur bacteria *Chlorobium tebidum*

Harvard group:
P. Rebentrost, R. Chakraborty, A. Aspuru-Guzik

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**Non-Markovian quantum jumps in excitonic energy transfer**

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We utilize the novel non-Markovian quantum jump (NMQJ) approach to stochastically simulate exciton dynamics derived from a time-convolutionless master equation. For relevant parameters and time scales, the time-dependent, oscillatory decoherence rates can have negative regions, a signature of non-Markovian behavior and of the revival of coherences. This can lead to non-Markovian population beatings for a dimer system at room temperature. We show that strong exciton-phonon coupling to low frequency modes can considerably modify transport properties. We observe increased exciton transport, which can be seen as an extension of recent environment-assisted quantum transport concepts to the non-Markovian regime. Within the NMQJ method, the Fenna-Matthew-Olson protein is investigated as a prototype for larger photosynthetic complexes.

Formal stochastic process description

Non-Markovian piecewise deterministic process
For open quantum systems: state vector is random variable.

**Markovian:**

*Formal stochastic process:*
Piecewise deterministic process  

*Realizations of the process:*
Monte Carlo wave function method  
(Popular method in quantum optics, cited >600 times.)

**non-Markovian:**

*Formal stochastic process:*
Non-Markovian piecewise deterministic process  

*Realizations of the process:*
Non-Markovian quantum jumps  
Non-Markovian piecewise deterministic process. Stochastic Schrödinger equation for non-Markovian open system:

\[
\begin{align*}
    d|\psi(t)\rangle &= -iG(t)|\psi(t)\rangle dt \\
    \text{Positive channels} &+ \sum_k \left[ \frac{C_k(t)|\psi(t)\rangle}{||C_k(t)|\psi(t)\rangle||} - |\psi(t)\rangle \right] dN_k^+(t) \\
    \text{Negative channels} &+ \sum_l \int d\psi' \left[ |\psi'\rangle - |\psi(t)\rangle \right] dN_{l,\psi'}^-(t).
\end{align*}
\]

Negative channel jump rate:

\[
\Gamma_- = \Delta_l P \frac{||\psi'\rangle\rangle d\psi'}{P[|\psi\rangle] d\psi} \langle \psi' | C_l^t C_l | \psi' \rangle \delta \left( |\psi\rangle - \frac{C_l |\psi'\rangle}{||C_l |\psi'\rangle||} \right) d\psi.
\]

Possibility for singularity?
Negative channel jump rate:

$$\Gamma_- = \Delta_l \frac{P[|\psi'\rangle]}{P[|\psi\rangle]} \frac{d\psi'}{d\psi} \langle \psi' | C_l^\dagger C_l | \psi' \rangle \delta \left( |\psi\rangle - \frac{C_l |\psi'\rangle}{||C_l |\psi'\rangle||} \right) d\psi.$$

Probability to be in the source state of negative rate jump

- Possible to prove: Whenever the dynamics breaks positivity, the stochastic process has singularity.
- The system is trying to undo something which did not happen.

Stochastic process identifies the point where the description loses physical validity. Master equation does not do this.

In memoryless Markovian open systems, the environment acts as a sink for the system information. Due to the system-reservoir interaction, the system of interest loses information on its state into the environment and this lost information does not play any further role in the system dynamics. However, if the environment has a nontrivial structure, then the seemingly lost information can return to the system at a later time leading to non-Markovian dynamics with memory. This memory effect is the essence of non-Markovian dynamics.
End of lecture II

Next lecture: measures of non-Markovianity