



Lecture II

Non-Markovian Quantum Jumps

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TCQP

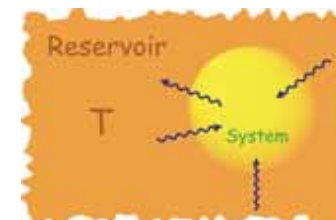
Turku Centre for Quantum Physics
Non-Markovian Processes and Complex Systems Group



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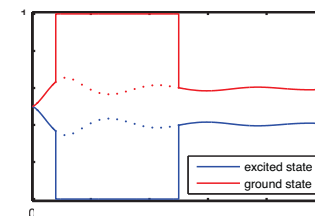
Lecture I

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



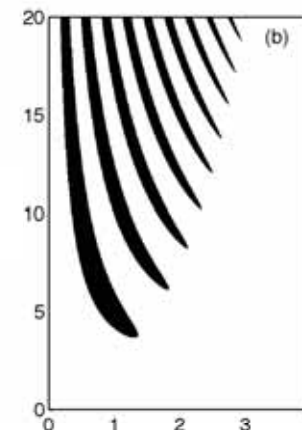
Lecture II

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

$$\frac{d\rho_S(t)}{dt} = \mathcal{L}_S \rho_S(t) \quad \text{Semigroup iff generator } \mathcal{L}_S \text{ in Lindblad form}$$

$$\frac{d\rho_S(t)}{dt} = \int_0^t ds \mathcal{K}_S(t-s) \rho_S(s) \quad \text{Memory kernel } \mathcal{K}_S(t-s)$$

$$\frac{d\rho_S(t)}{dt} = \mathcal{L}_S(t) \rho_S(t) \quad \text{Time-dependent generator } \mathcal{L}_S(t)$$

General form of the local in time (TCL) equation

$$\begin{aligned} \frac{d\rho_S(t)}{dt} = & -i[H_S, \rho_S] + \sum_k (C_k(t) \rho_S(t) D_k(t)^\dagger + D_k(t) \rho_S(t) C_k(t)^\dagger) \\ & - \frac{1}{2} \left\{ D_k^\dagger(t) C_k(t) + C_k^\dagger(t) D_k(t), \rho_S(t) \right\} \end{aligned}$$

Operators may depend on time

Lindblad-like structure if $D_k(t) = C_k(t)$



Density matrix and state vector ensemble

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

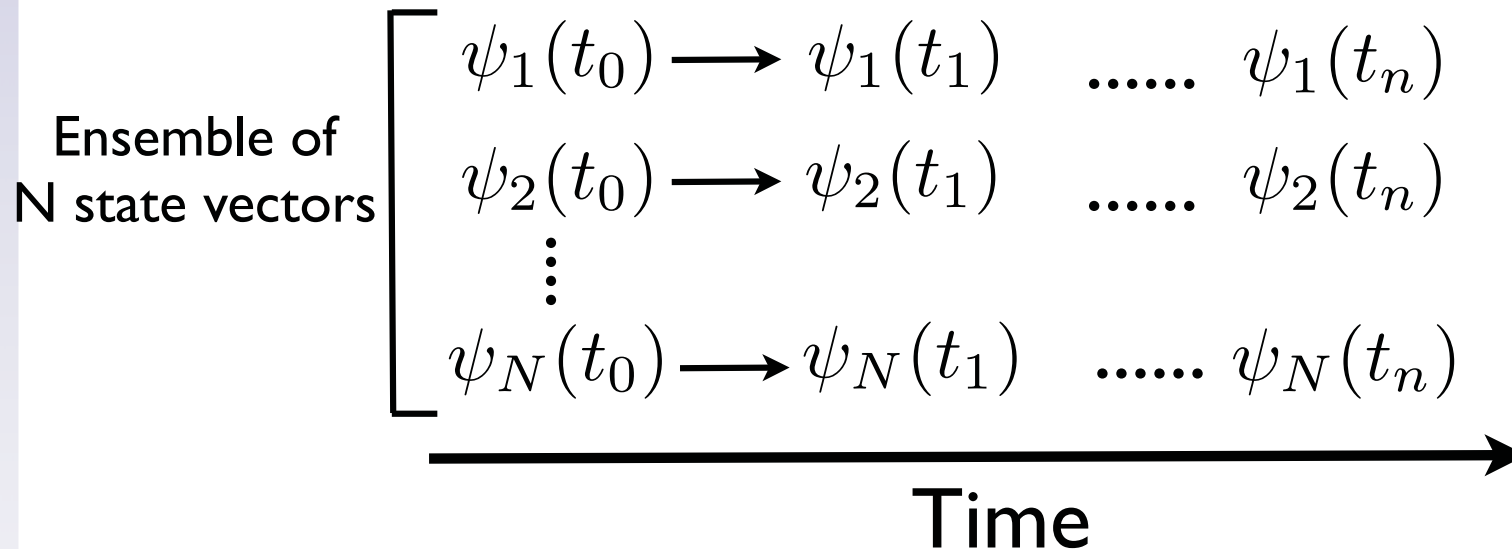
$$\frac{d\rho(t)}{dt} = -i[H, \rho_S] + \sum_k \gamma_k \left(A_k \rho_S A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S - \frac{1}{2} \rho_S A_k^\dagger A_k \right)$$



Basics of stochastic state vector evolution

Monte Carlo wave function method (Markovian)

(Dalibard, Castin, Molmer, PRL 1992)



At each point of time, density matrix ρ as average of state vectors Ψ_i :

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

The time-evolution of each Ψ_i contains stochastic element due to random quantum jumps.



Jump probability, example

Time-evolution of state vector Ψ_i :

At each point of time: decide if quantum jump happened.

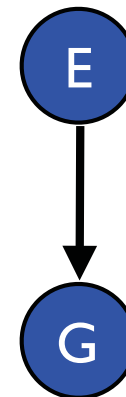
P_j : probability that a quantum jump occurs in a given time interval δt :

$$P_j = \delta t \Gamma p_e$$

time-step decay rate occupation probability of excited state

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”.

W. Heisenberg: “The development of the interpretation of quantum theory”, in “Niels Bohr and the development of physics: Essays dedicated to the Niels Bohr on the occasion of his seventieth birthday”, eds. W. Pauli, L. Rosenfeld, and V. Weisskopf, Pergamon Press, London, 1955.

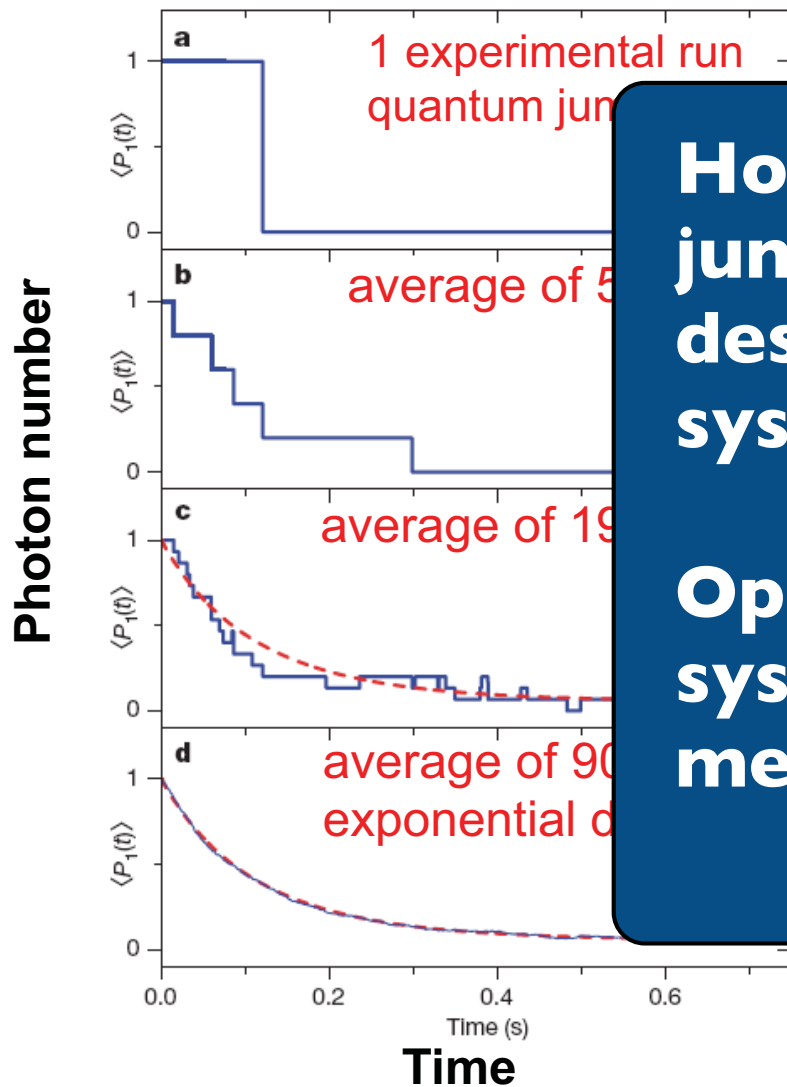
Are quantum jump “real”?



Quantum jumps in experiments

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

Jump methods:

Markovian

MCWF
(Dalibard, Castin, Molmer)
Quantum Trajectories
(Zoller, Carmichael)

non-Markovian

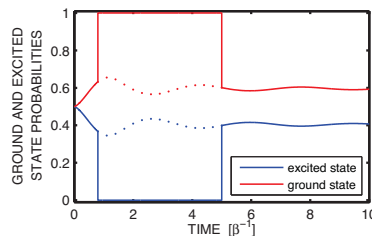
Fictitious modes (Imamoglu)
Pseudo modes (Garraway)
Doubled H-space (Breuer, Petruccione)
Triple H-space (Breuer)
Non-Markovian Quantum Jump (Piilo et al)

Diffusion methods:

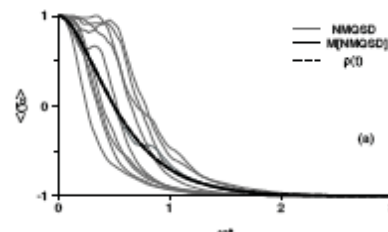
QSD
(Diosi, Gisin, Percival...)

Non-Markovian QSD
(Strunz, Diosi, Gisin)
Stochastic Schrödinger equations
(Bassi)

Jump



Diffusion



Plus: Wiseman, Gambetta, Budini, Gaspard, Lacroix...and others
(not comprehensive list, apologies for any omissions)



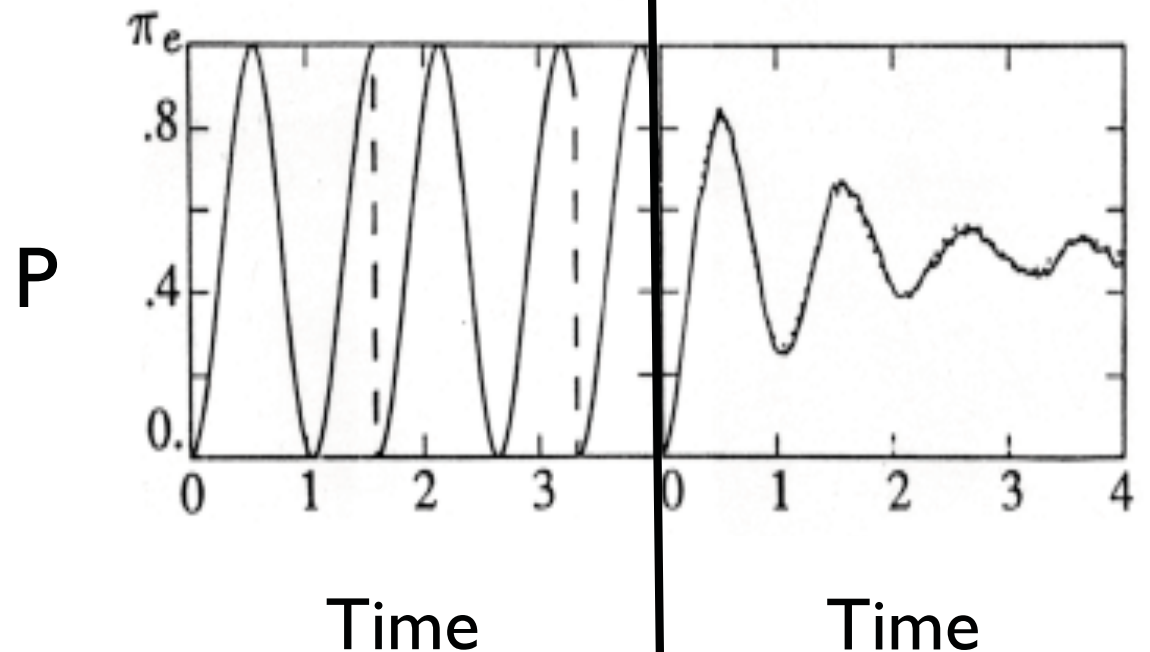
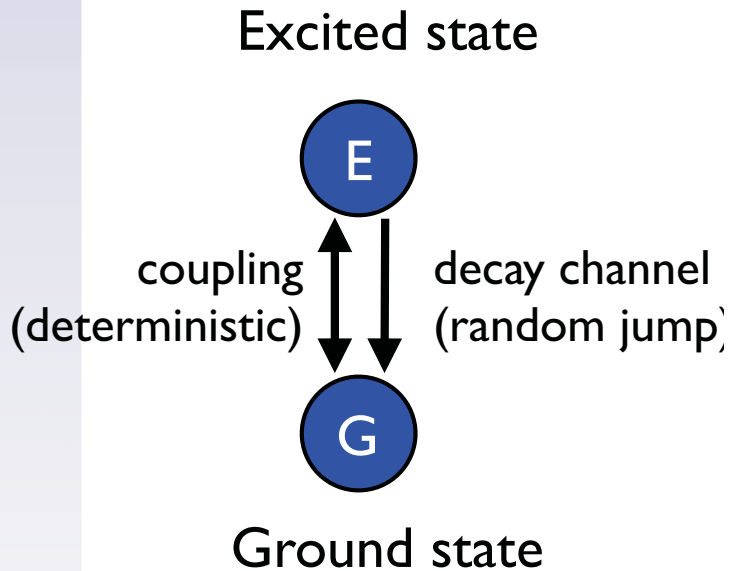
Example: driven 2-state system, Markovian

Quantum jump: Discontinuous stochastic change of the state vector.

Excited state probability P for a driven 2-level atom

Markovian Monte Carlo

single realization ensemble average



damped Rabi oscillation
of the atom

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

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



Markovian Monte Carlo wave function method

Master equation to be solved:

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

For each ensemble member ψ :

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H |\Psi(t)\rangle$$

Solve the time dependent Schrödinger equation.

$$H = H_s + H_{dec}$$

Use non-Hermitian Hamiltonian H which includes the decay part H_{dec} .

$$H_{dec} = -\frac{i\hbar}{2} \sum_m \Gamma_m C_m^\dagger C_m$$

Key for non-Hermitian Hamiltonian: Jump operators C_m can be found from the dissipative part of the master equation.

$$\delta p_m = \delta t \Gamma_m \langle \Psi | C_m^\dagger C_m | \Psi \rangle$$

For each channel m the jump probability is given by the time step size, decay rate, and decaying state occupation probability.



Algorithm:

1. Time evolution over time step δt
2. Generate random number, did jump occur?

No

Yes

3. Renormalize ψ before new time step

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

3. Apply jump operator C_j before new time step

$$|\psi_i(t + \delta t)\rangle = \frac{C_j |\psi_i(t)\rangle}{\|C_j |\psi_i(t)\rangle\|}$$

4. Ensemble average over ψ :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)

This gives comm. + anticom. of m.e. This gives "sandwich" term of the m.e.

$$\overline{\sigma(t + \delta t)} = (1 - P) \frac{|\phi(t + \delta t)\rangle\langle\phi(t + \delta t)|}{1 - P} + P \frac{C|\Psi(t)\rangle\langle\Psi(t)|C^\dagger}{\langle\Psi(t)|C^\dagger C|\Psi(t)\rangle}$$

Average \rightarrow "No-jump" path weight \rightarrow t-evol. and normalization \rightarrow "Jump" path weight \rightarrow Jump and normalization

Keeping in mind two things:

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

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

b) the jump probability is:

$$P = \delta t \Gamma \langle\Psi|C^\dagger C|\Psi\rangle$$

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

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



Measurement scheme interpretation

Two-level atom in vacuum

Two-level atom MC evolution by

$$C = \sqrt{\Gamma} |g\rangle\langle e| \quad \text{Jump operator}$$

$$H_{dec} = -\frac{i\hbar\Gamma}{2} |e\rangle\langle e| \quad \text{Non-Hermitian Hamiltonian}$$

$$P = \delta t \Gamma |c_e|^2 \quad \text{Jump probability}$$

Total system evolution

Measurement scheme:
continuous measurement of
photons in the environment.

$$(c_g |g\rangle + c_e |e\rangle) \otimes |0\rangle \rightarrow (c'_g |g\rangle + c'_e |e\rangle) \otimes |0\rangle + \sum_{\lambda} c_{\lambda} |g\rangle \otimes |1_{\lambda}\rangle$$

- 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?

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

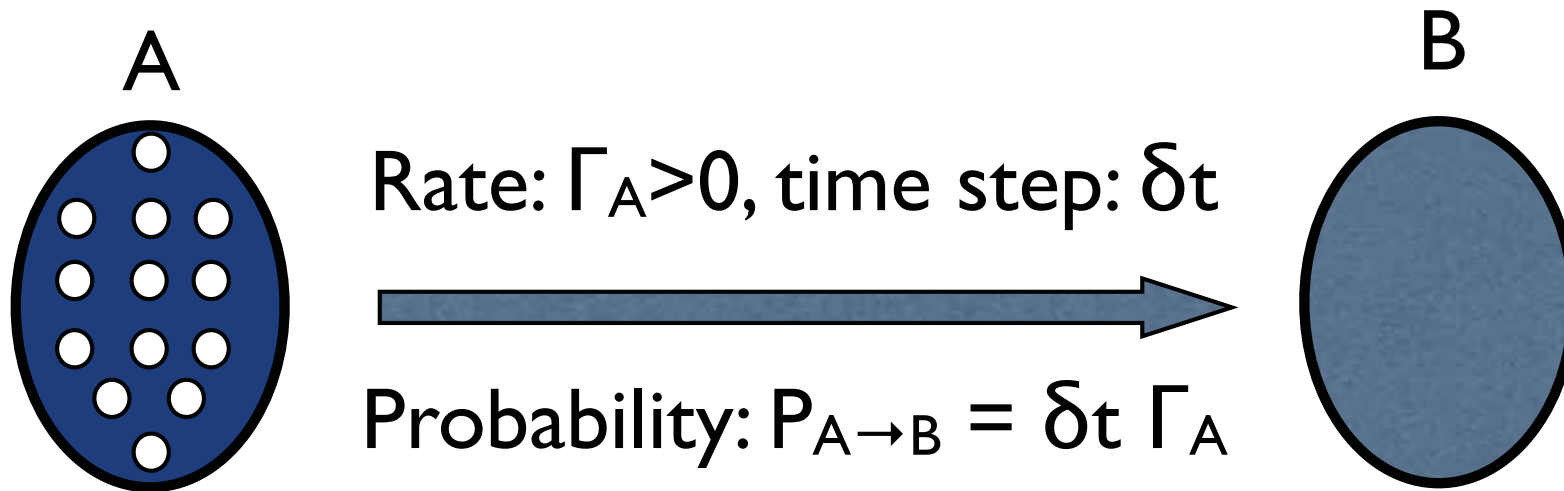
Piilo, Maniscalco, Härkönen, Suominen:
Phys. Rev. Lett. 100, 180402 (2008)

Piilo, Härkönen, Maniscalco, Suominen:
Phys. Rev. A 79, 062112 (2009)



Cartoon of the motivation

Transfer from A to B. Ensemble initially in state 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

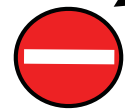
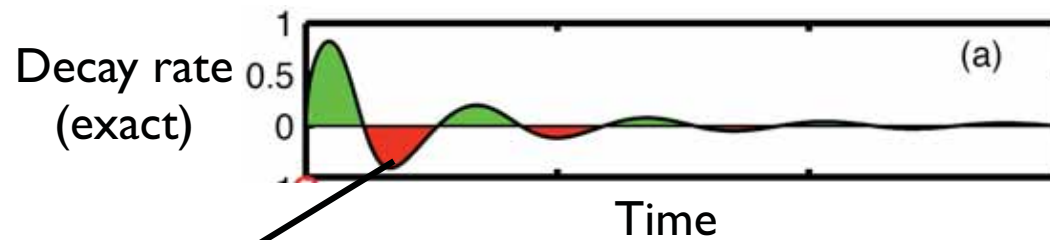


Markovian vs. non-Markovian evolution (1)

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)

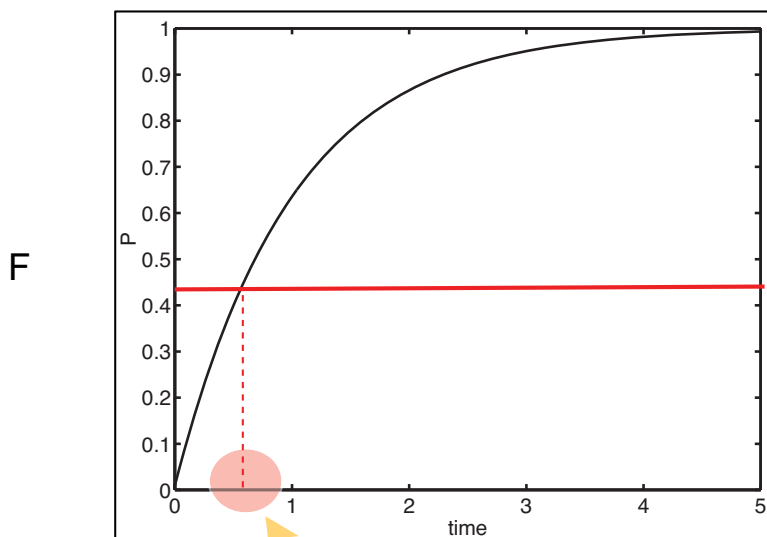
Waiting time distribution (2-level atom): $F(t) = 1 - \exp \left[- \int_0^t dt' \Delta(t') \right]$

decay rate

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

At which point of time atom emits photon ?

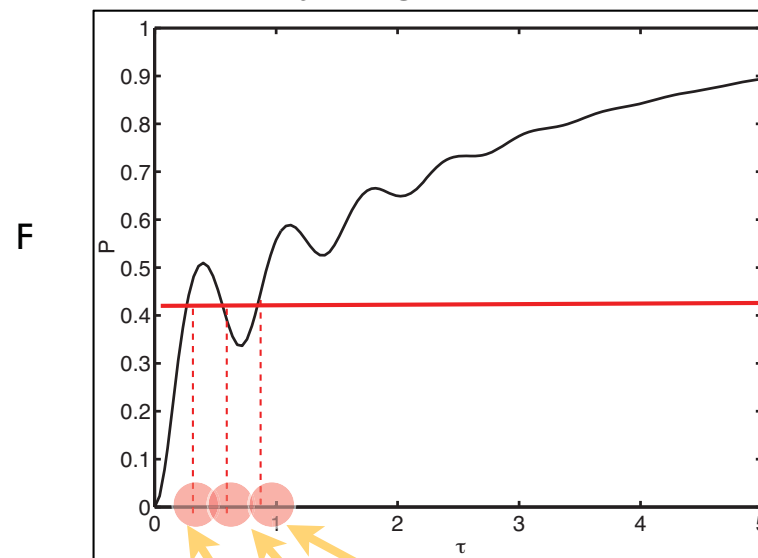
Markovian: constant rate



Time

photon emission here

non-Markovian:
temporary negative rate



Time

photon emission here, here and here ?

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:

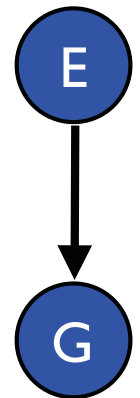
General non-Markovian master equation local-in-time:

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

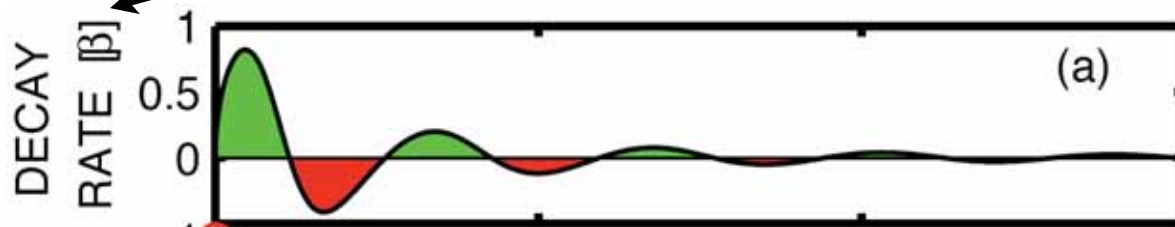
- Jump operators C_m
- Time dependent decay rates $\Delta_m(t)$.
- Decay rates have temporarily negative values.

Example: 2-level atom in photonic band gap.

Jump operator C for positive decay: $\sigma_- = |g\rangle\langle e|$



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



Time



Non-Markovian quantum jump (NMQJ) method

Quantum jump in negative decay region:
The direction of the jump process reversed

$$|\psi\rangle \xrightarrow{\text{green}} |\psi'\rangle = \frac{C_m |\psi\rangle}{\|C_m |\psi\rangle\|}, \quad \Delta_m(t) > 0$$

$$|\psi\rangle \xrightarrow{\text{red}} |\psi'\rangle = \frac{C_m |\psi\rangle}{\|C_m |\psi\rangle\|}, \quad \Delta_m(t) < 0$$

Negative rate process creates coherences

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

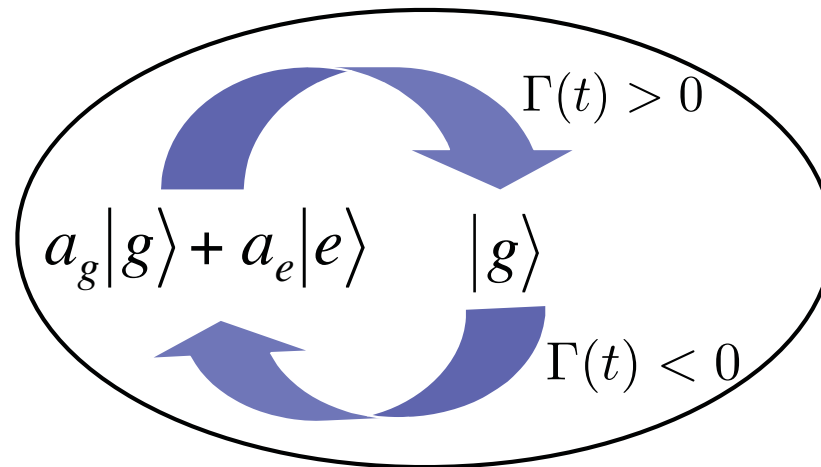
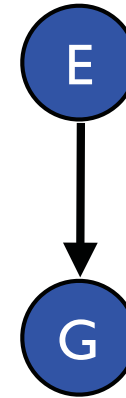
The probability proportional to the target state!



NMQJ example

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.**



NMQJ: general algorithm

$$\begin{aligned}\frac{d}{dt}\rho &= -i[H(t), \rho] \\ &+ \sum_k \Delta_k^+(t) \left[C_k(t)\rho C_k^\dagger(t) - \frac{1}{2} \{C_k^\dagger(t)C_k(t), \rho\} \right] \\ &- \sum_l \Delta_l^-(t) \left[C_l(t)\rho C_l^\dagger(t) - \frac{1}{2} \{C_l^\dagger(t)C_l(t), \rho\} \right]\end{aligned}$$

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

Deterministic evolution and positive channel jumps as before...

Negative channel with jumps

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

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

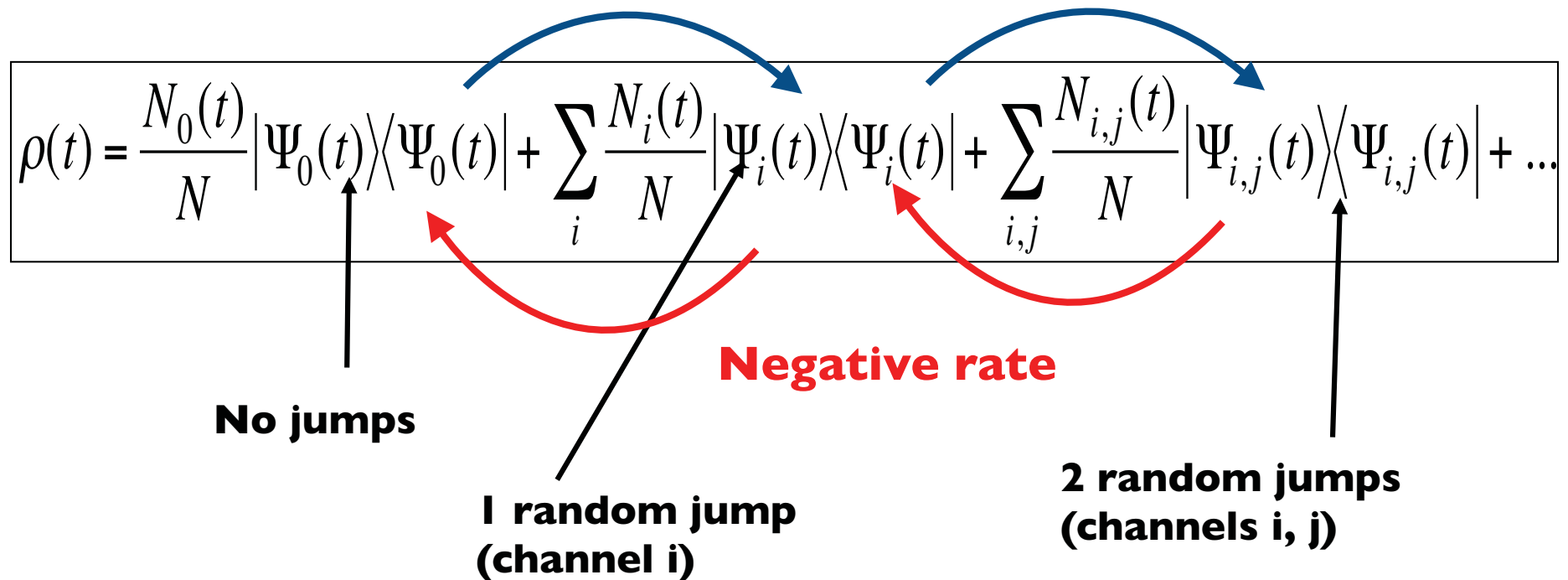
$$P_{\alpha \rightarrow \alpha'}^{j-}(t) = \frac{N_{\alpha'}(t)}{N_{\alpha}(t)} |\Delta_{j-}(t)| \delta t \langle\psi_{\alpha'}(t)| C_{j-}^\dagger(t) C_{j-}(t) |\psi_{\alpha'}(t)\rangle.$$



Non-Markovian quantum jumps

In terms of probability flow in Hilbert space:

Positive rate



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 dt is

$$\overline{\sigma(t + \delta t)} =$$

$\frac{N_0(t) \Phi_0(t + \delta t)\rangle\langle\Phi_0(t + \delta t) }{N \quad 1 + n_0}$	←	0 jumps earlier, no jumps to be cancelled
$+ \sum_i \frac{N_i(t)}{N} (1 - P_{i \rightarrow 0}) \frac{ \Phi_i(t + \delta t)\rangle\langle\Phi_i(t + \delta t) }{1 + n_i}$	←	1 jump earlier, does not cancel jump at this time
$+ \sum_i \frac{N_i(t)}{N} P_{i \rightarrow 0} \frac{D_{i \rightarrow 0} \Phi_i(t + \delta t)\rangle\langle\Phi_i(t + \delta t) D_{i \rightarrow 0}^\dagger}{n_{i \rightarrow 0}} + \dots$	←	1 jump earlier, cancels jump

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

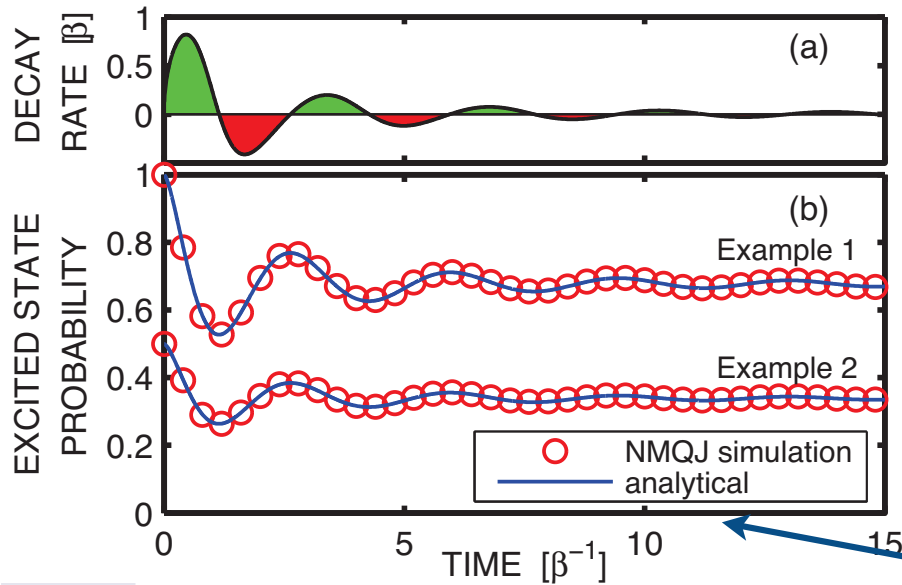
P's: jump probabilities

D's: jump operators

By plugging in the appropriate quantities gives the match with the master equation !



Example: 2-level atom in photonic band gap



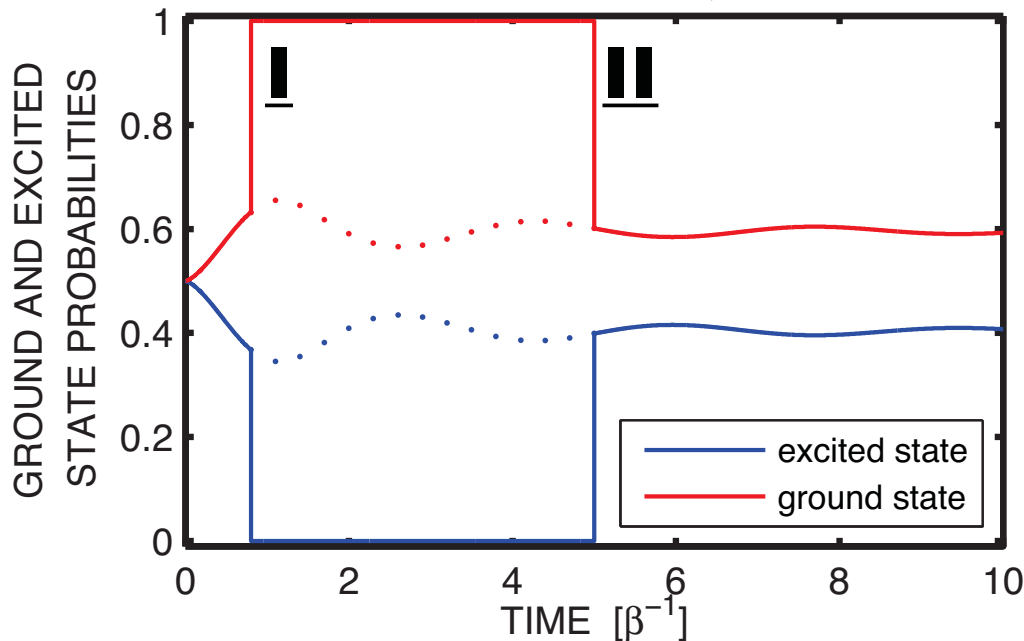
The simulation and exact results match.

Typical features of photonic band gap:

- Population trapping
- Atom-photon bound state.

Density matrix: average over the ensemble

Single state vector history



Example of one state vector history:

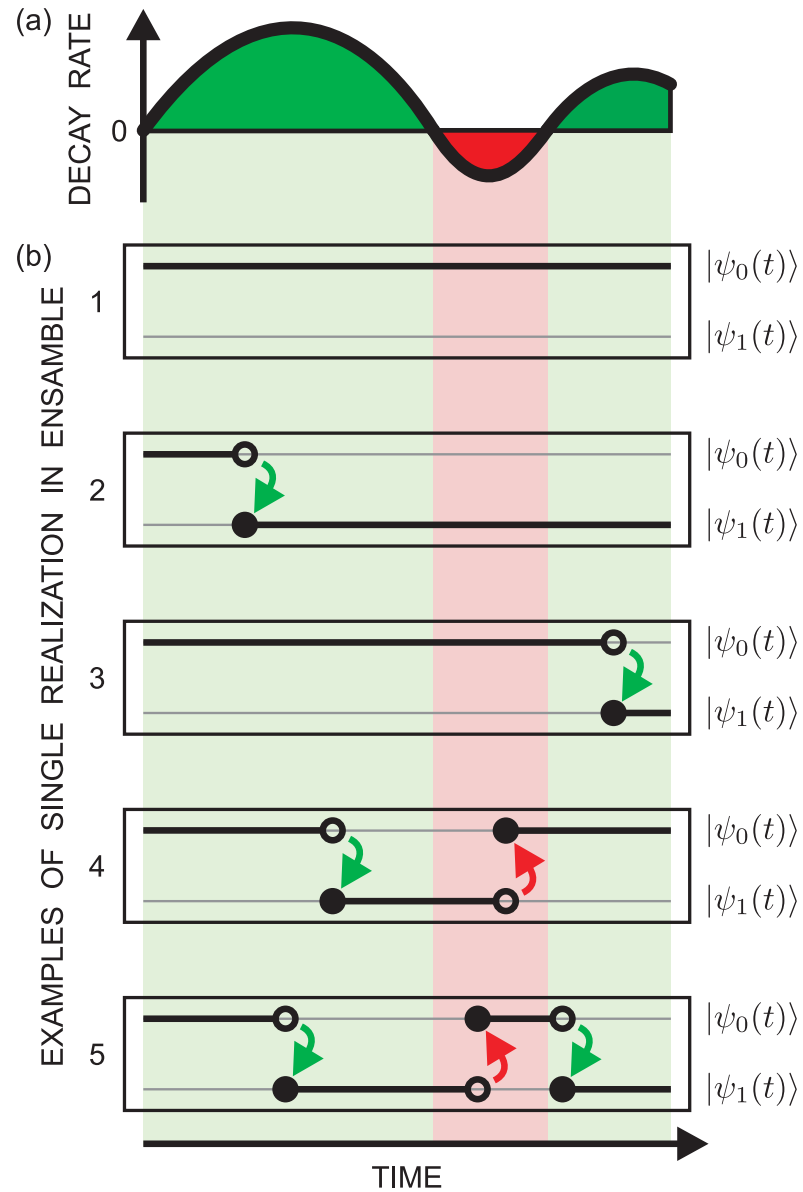
I: Quantum jump at positive decay region destroys the superposition.

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



2-level atom

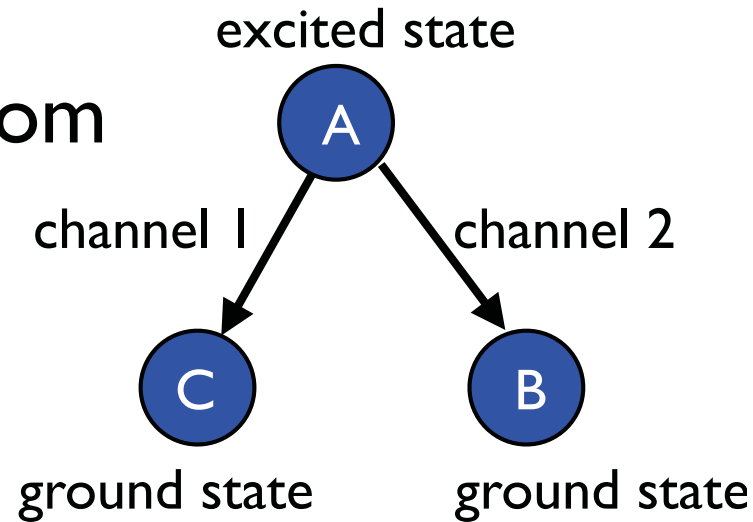
Examples of realizations:





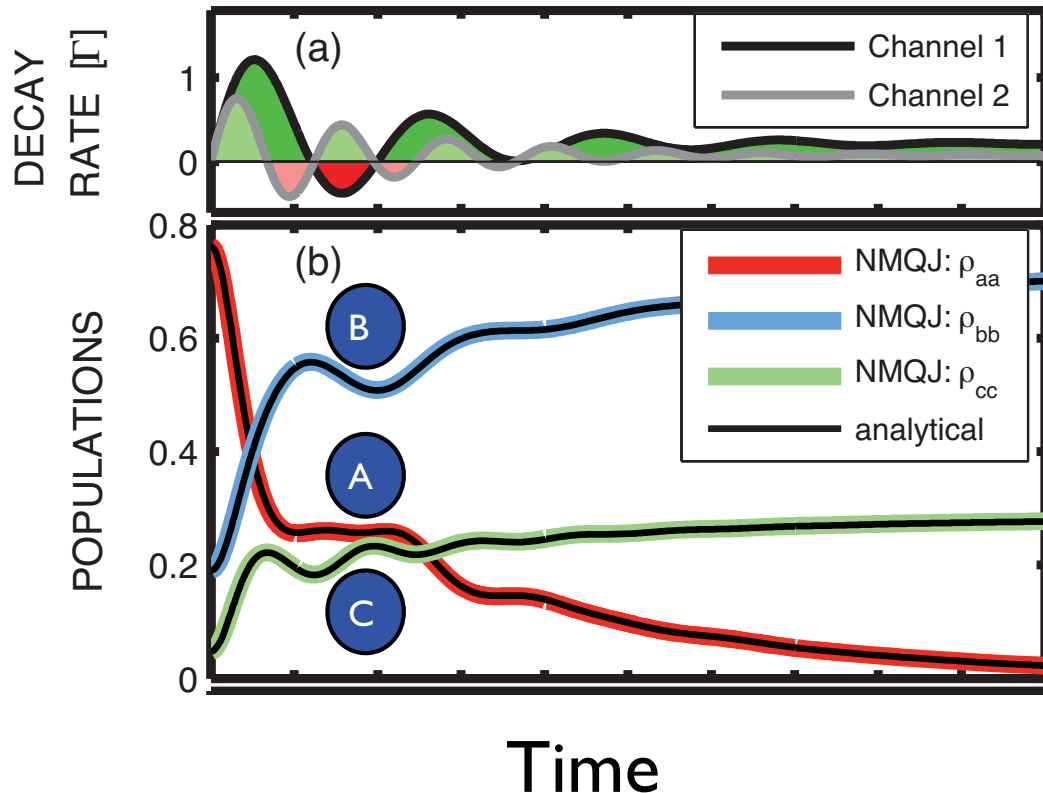
Simultaneous positive and negative rates

3-level atom



Two channels which can have different sign of the decay rate

$$\dot{\rho}(t) = \frac{1}{i}\lambda_1(t)[|a\rangle\langle a|, \rho(t)] + \frac{1}{i}\lambda_2(t)[|a\rangle\langle a|, \rho(t)] + \Delta_1(t) \times \left[|b\rangle\langle a| \rho(t) |a\rangle\langle b| - \frac{1}{2}\{\rho(t), |a\rangle\langle a|\} \right] + \Delta_2(t) \left[|c\rangle\langle a| \rho(t) |a\rangle\langle c| - \frac{1}{2}\{\rho(t), |a\rangle\langle a|\} \right]$$

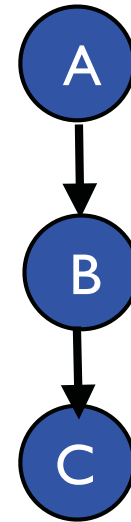


- Positive channel generates new random jumps
- Negative channel undoes the random jumps
- Total probability flow consists of positive and negative components
- Temporary plateau in the excited state A probability.

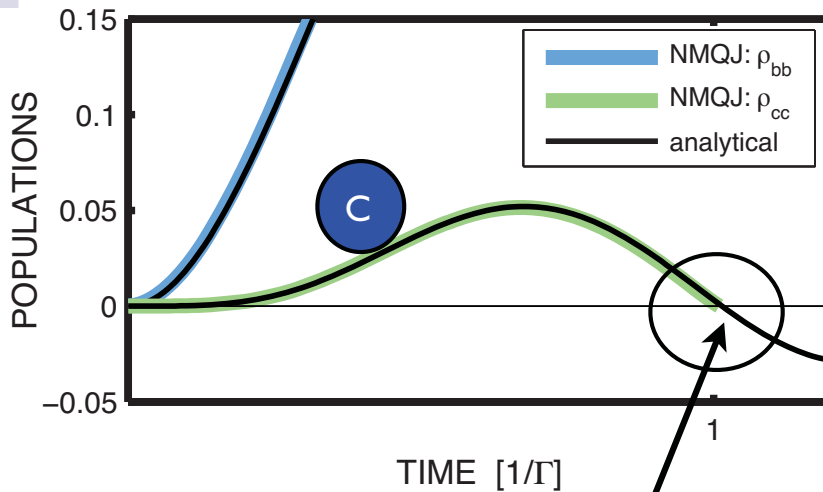
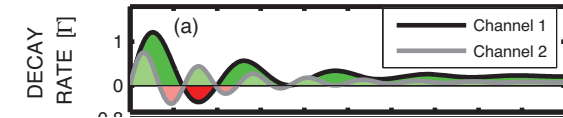


Examples of identification of positivity violation

3-level ladder atomic system:



Decay rates



Breakdown of positivity

$$\begin{aligned} \dot{\rho}(t) = & \frac{1}{i}\lambda_1(t)[|a\rangle\langle a|, \rho(t)] + \frac{1}{i}\lambda_2(t)[|a\rangle\langle a|, \rho(t)] + \Delta_1(t) \\ & \times \left[|b\rangle\langle a| \rho(t) |a\rangle\langle b| - \frac{1}{2}\{\rho(t), |a\rangle\langle a|\} \right] \\ & + \Delta_2(t) \left[|c\rangle\langle a| \rho(t) |a\rangle\langle c| - \frac{1}{2}\{\rho(t), |a\rangle\langle a|\} \right]. \end{aligned}$$

- Initial state **A**
- 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.



Application of NMQJ: energy transfer in bacteria

- 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

THE JOURNAL OF CHEMICAL PHYSICS 131, 184102 (2009)

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.

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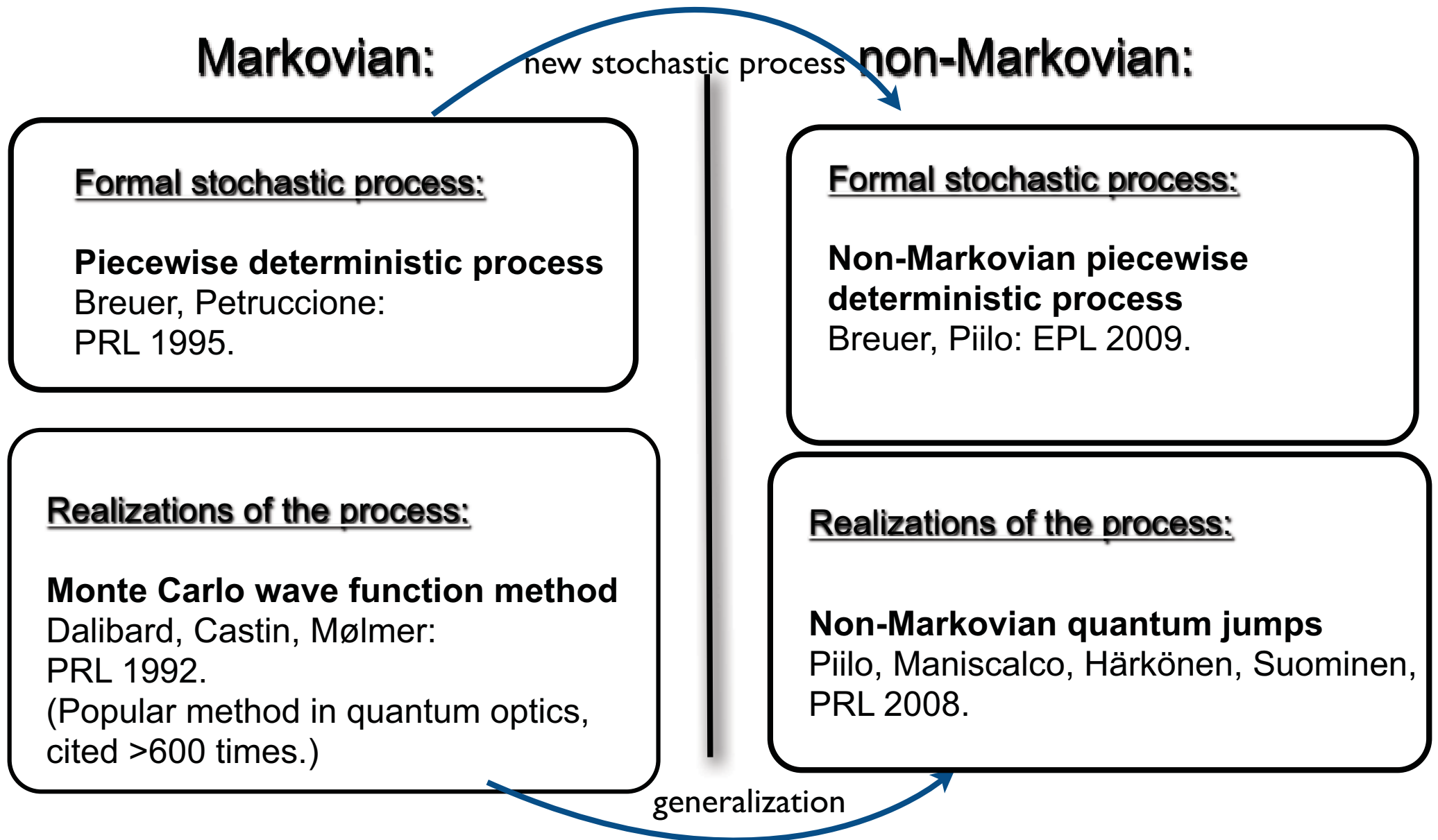
Formal stochastic process description

Non-Markovian piecewise deterministic process



Stochastic processes and probability theory view

For open quantum systems: state vector is random variable.





Stochastic process description

Non-Markovian piecewise deterministic process.

Stochastic Schrödinger equation for non-Markovian open system:

$$d|\psi(t)\rangle = -iG(t)|\psi(t)\rangle dt \quad \leftarrow \text{Deterministic evolution}$$

Positive channels

$$+ \sum_k \left[\frac{C_k(t)|\psi(t)\rangle}{\|C_k(t)|\psi(t)\rangle\|} - |\psi(t)\rangle \right] dN_k^+(t)$$

Negative channels

$$+ \sum_l \int d\psi' [|\psi'\rangle - |\psi(t)\rangle] dN_{l,\psi'}^-(t).$$

Poisson increments for positive and negative channels

Negative channel jump rate:

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

Possibility for singularity?



Stochastic process description

Negative channel jump rate:

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

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.



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Open system dynamics with non-Markovian quantum jumps

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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.

How to understand and quantify the information flow...



End of lecture II

Next lecture: measures of non-Markovianity