



OPEN QUANTUM SYSTEMS WITH MEMORY

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In collaboration with:

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1. Intro:

Open quantum systems: Jumps vs. Diffusion.
Markovian Monte Carlo Wave Function method

2. Non-Markovian Quantum Jump (NMQJ) method

Piilo, Maniscalco, Härkönen, Suominen:

Phys. Rev. Lett. 100, 180402 (2008), Phys. Rev A 79, 062101 (2009)

3. Measure for non-Markovianity of quantum processes

Breuer, Laine, Piilo:

Phys. Rev. Lett. 103, 210401 (2009), arXiv:1002.2583 [quant-ph]



4. Witness for initial system-environment correlations

Laine, Piilo, Breuer:

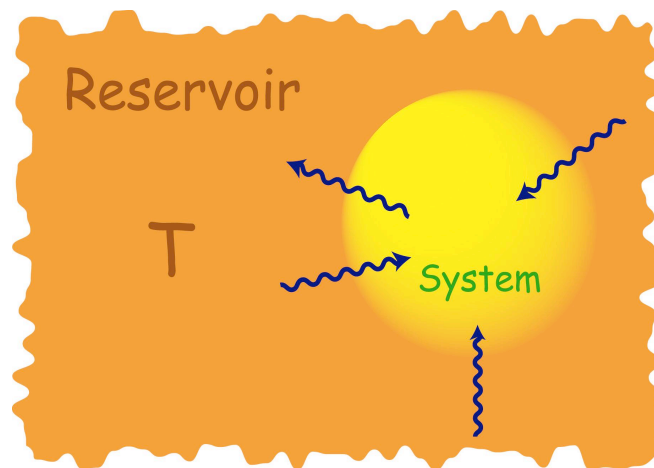
preprint arXiv:1004.2184 [quant-ph]



Open quantum systems

The time evolution of closed quantum system:
Schrödinger equation and the state vector.

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



The time evolution of open quantum system:
Master equation and the density matrix.

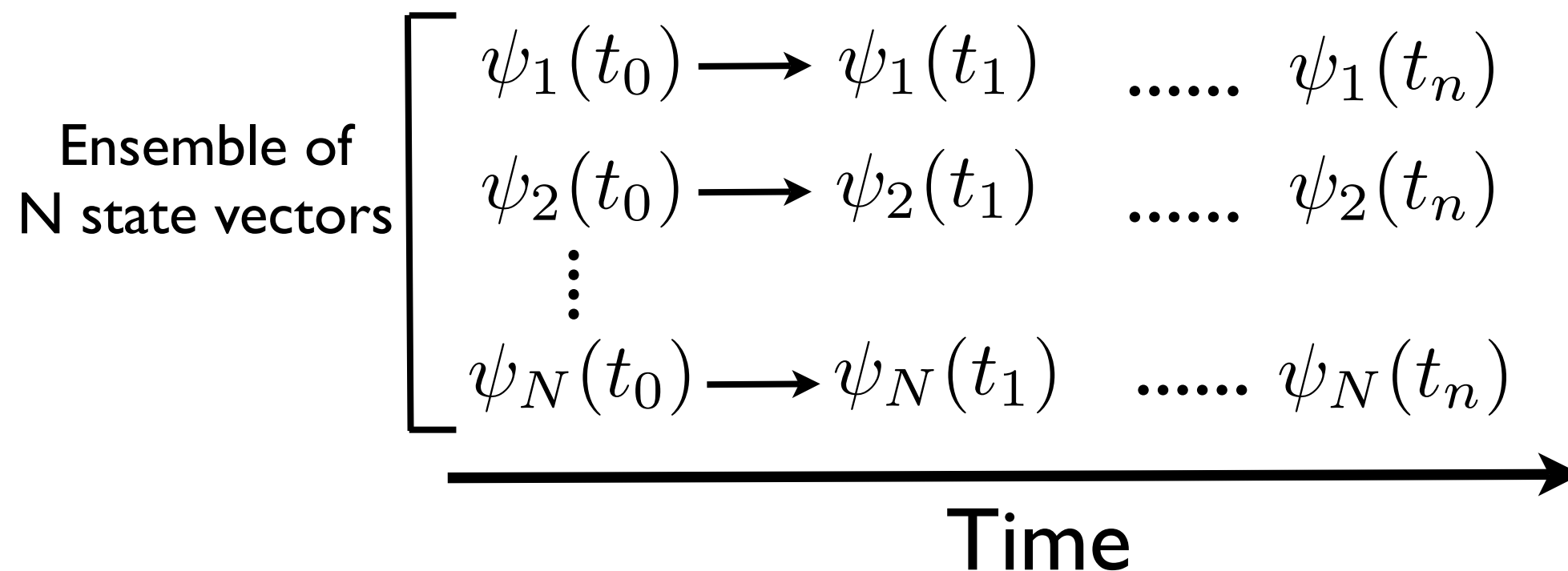
$$\frac{d\rho(t)}{dt} = \frac{1}{i\hbar} [H_S, \rho] + \sum_m \Gamma_m C_m \rho C_m^\dagger - \frac{1}{2} \sum_m \Gamma_m (C_m^\dagger C_m \rho + \rho C_m^\dagger C_m)$$

Density matrix as an ensemble of state vectors:

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



Monte Carlo methods in quantum optics: basic idea



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 continuous or discontinuous stochastic element.



Simple classification of Monte Carlo/stochastic methods

	Markovian	non-Markovian
Jump methods:	MCWF (Dalibard, Castin, Molmer) Quantum Trajectories (Zoller, Carmichael)	Fictitious modes (Imamoglu) Pseudo modes (Garraway) Doubled H-space (Breuer, Petruccione) Triple H-space (Breuer) NMQJ
Diffusion methods:	QSD (Diosi, Gisin, Percival...)	Non-Markovian QSD (Strunz, Diosi, Gisin) Stochastic Schrödinger equations (Bassi)

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

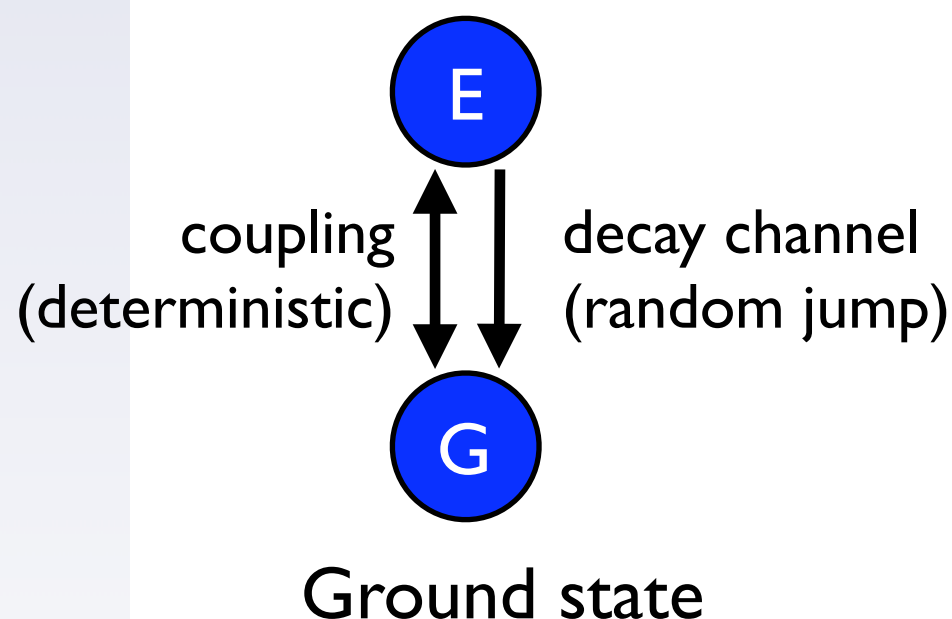


Markovian Monte Carlo wave function method, example

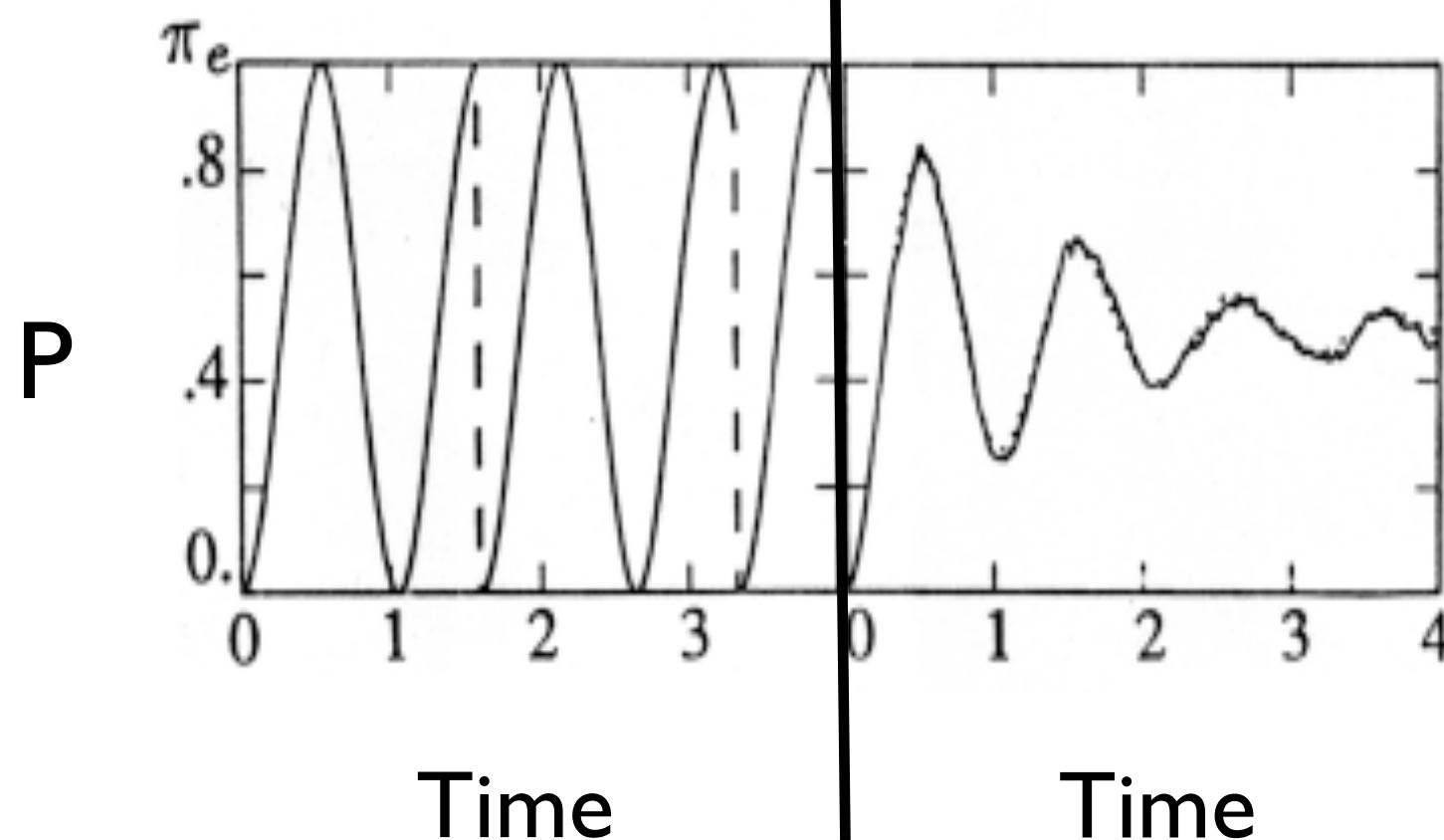
Quantum jump: Discontinuous stochastic change of the state vector.

Example: excited state probability P
for a driven 2-level atom

Unstable excited state



Markovian Monte Carlo
single realization | **ensemble average**



damped Rabi oscillation
of the atom



Jump probability, example

Time-evolution of state vector Ψ_i :

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

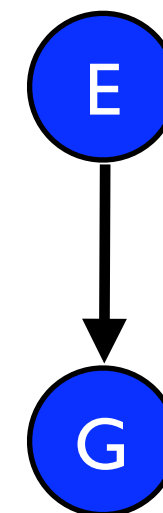
P_j : probability that a quantum jump occurs in a given time interval δt :

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

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.





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.



General algorithm:

1. Time evolution over time step δt

2. Generate random number, did jump occur?

No

Yes

3. Renormalize ψ before new time step

3. Apply jump operator C_j before new time step

4. Ensemble average over ψ :s gives the density matrix



2. Markovian vs. non-Markovian evolution: Non-Markovian quantum jump method (NMQJ)

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

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

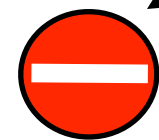
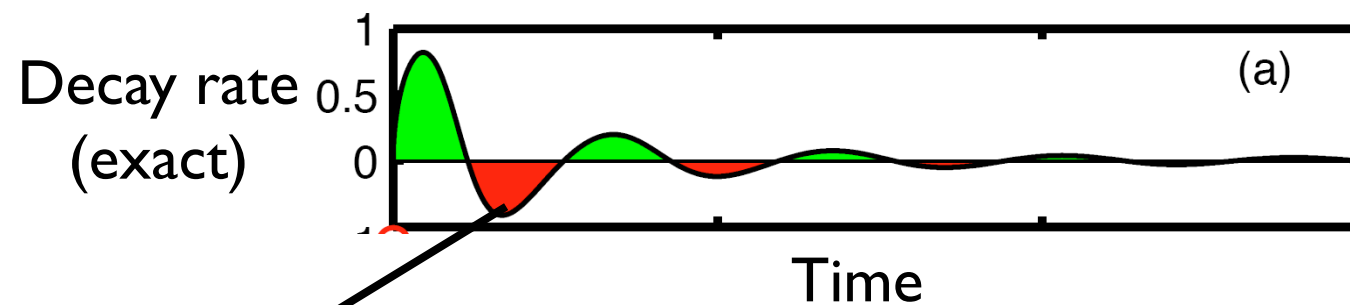


Markovian vs. non-Markovian evolution (1)

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)

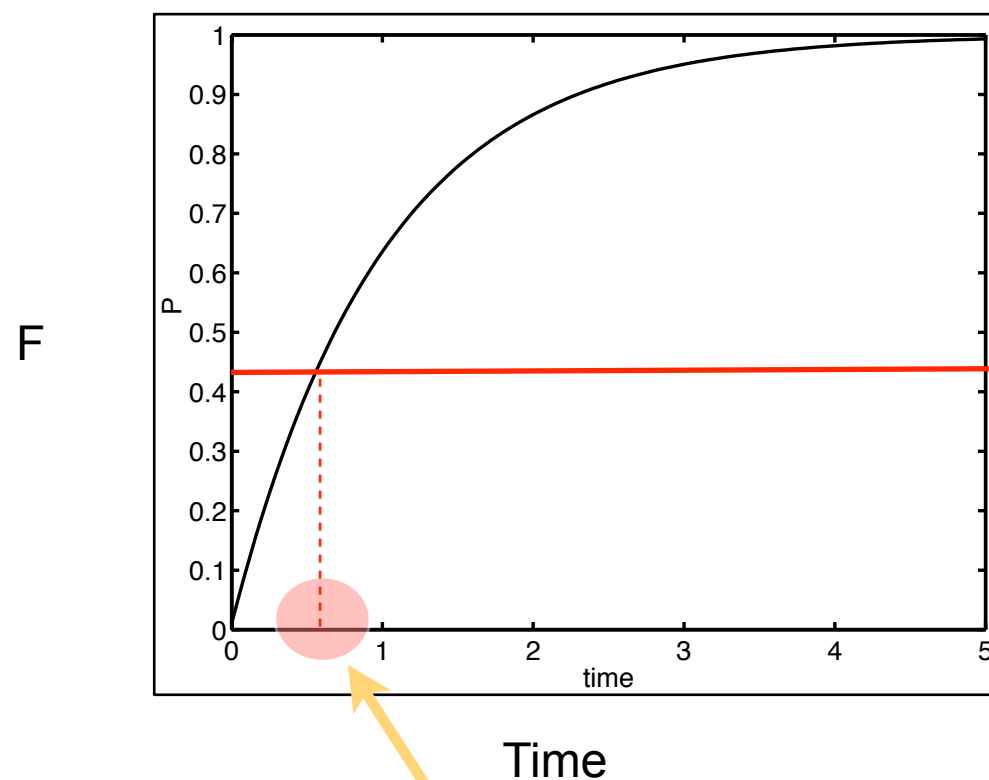
Waiting time distribution (2-level atom): $F(t) = 1 - \exp \left[- \int_0^t dt' \Delta(t') \right]$

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

decay rate

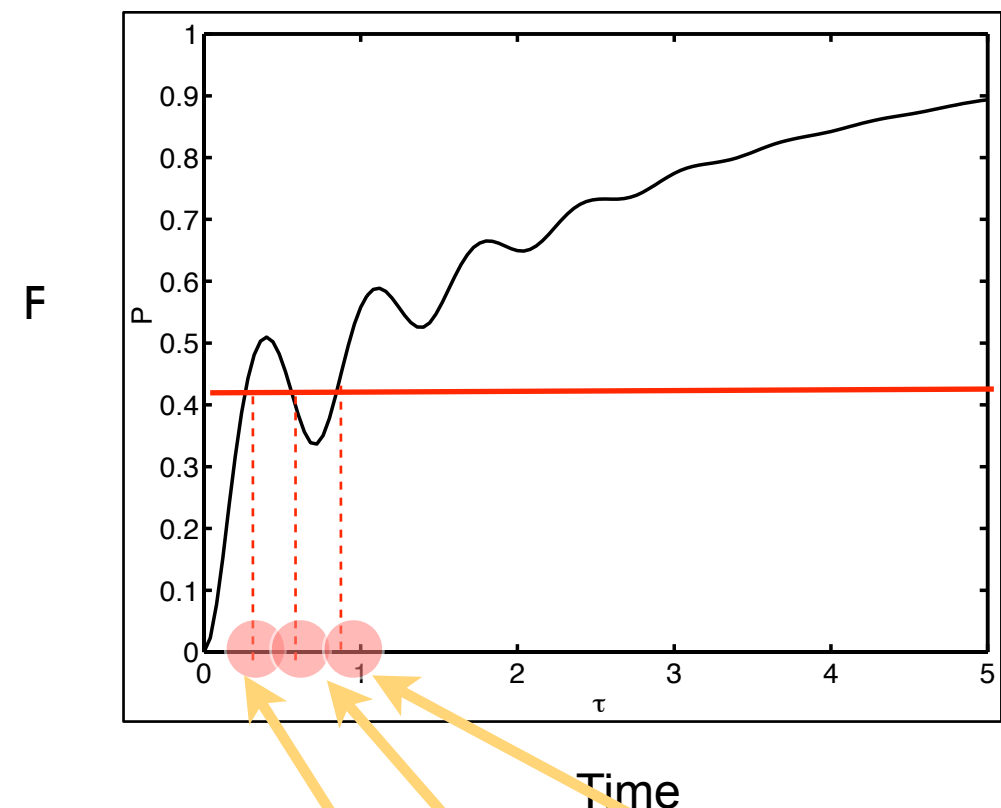
At which point of time atom emits photon ?

Markovian: constant rate



photon emission here

non-Markovian:
temporary negative rate



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:

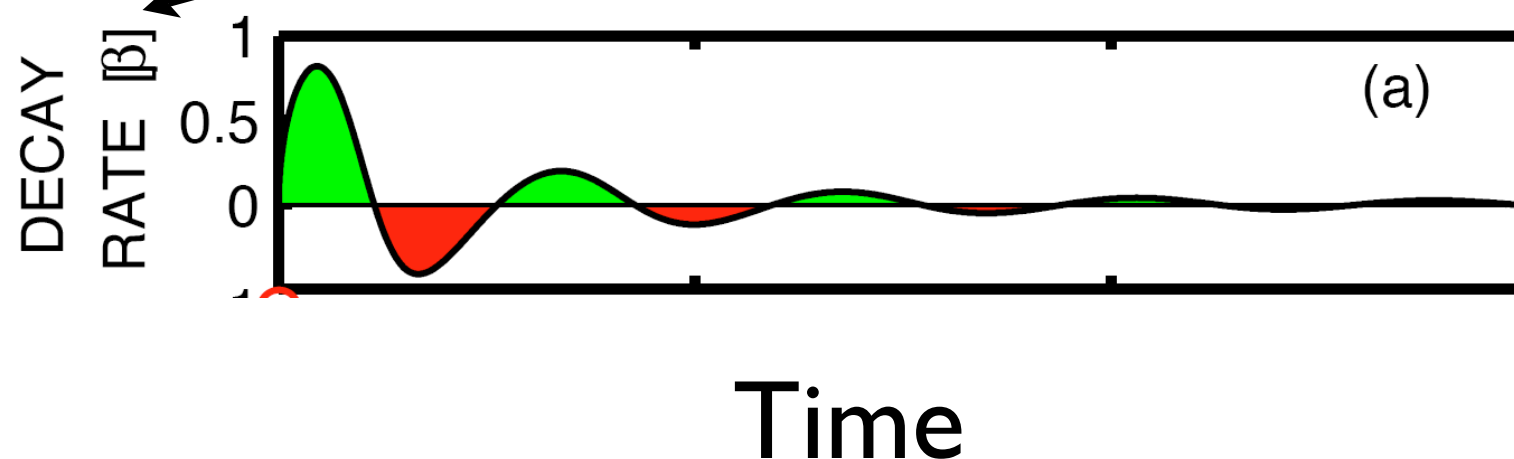
$$\frac{d\rho(t)}{dt} = \frac{1}{i\hbar} [H_S, \rho] + \sum_m \Delta_m(t) C_m \rho C_m^\dagger - \frac{1}{2} \sum_m \Delta_m(t) (C_m^\dagger C_m \rho + \rho C_m^\dagger C_m)$$

- 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: $\sigma_- = |g\rangle\langle e|$

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





Non-Markovian quantum jump (NMQJ) method

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

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

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

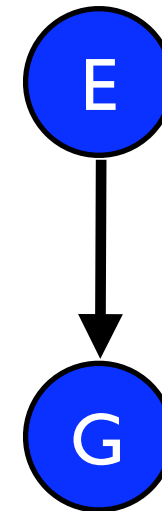
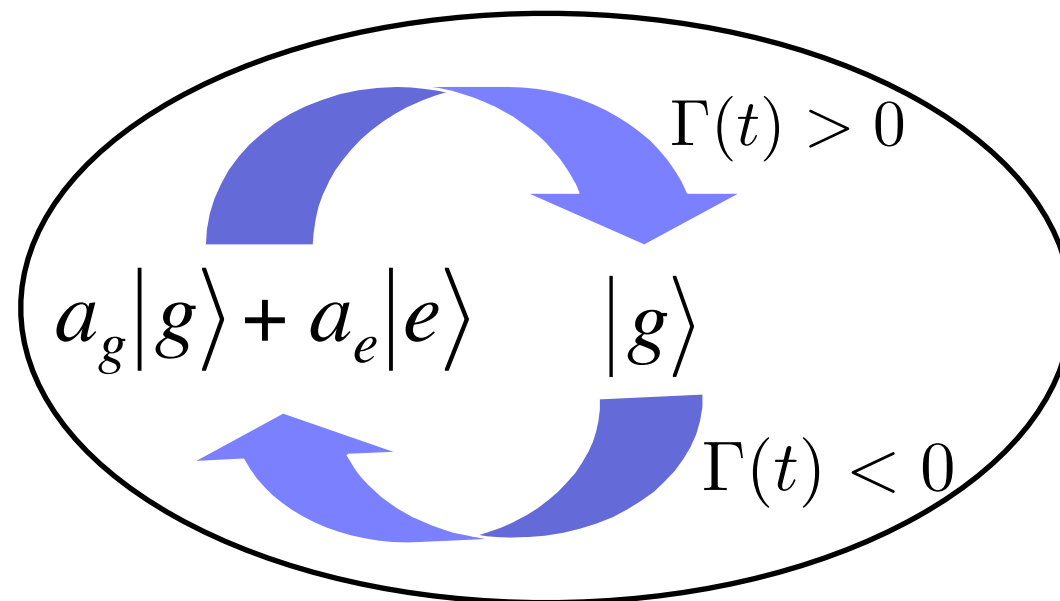
The probability proportional to the target state!



NMQJ example

For example: two-level atom

$$\sigma_- = |g\rangle\langle e|$$



Jump probability:
$$P = \frac{N_0}{N_g} \delta t |\Gamma(t)| |\langle \psi_0 | e \rangle|^2$$

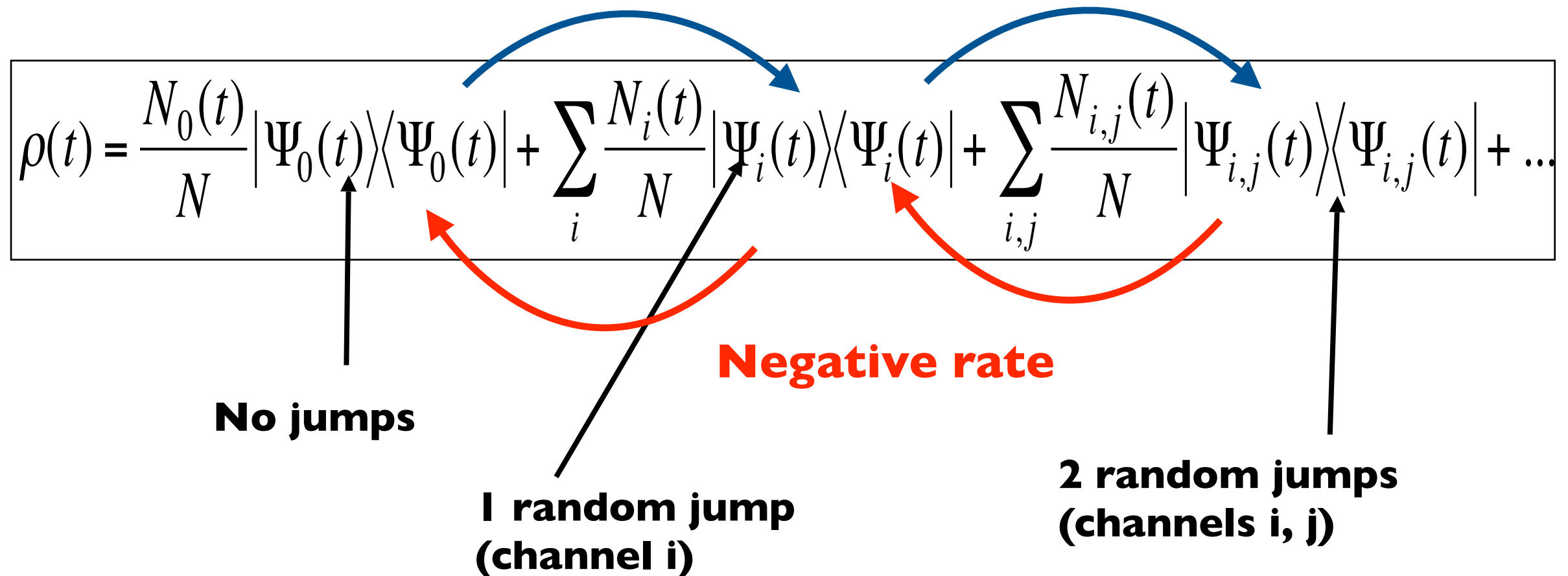
**The essential ingredient of non-Markovian system: memory.
Recreation of lost superpositions.**



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.



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

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



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

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

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

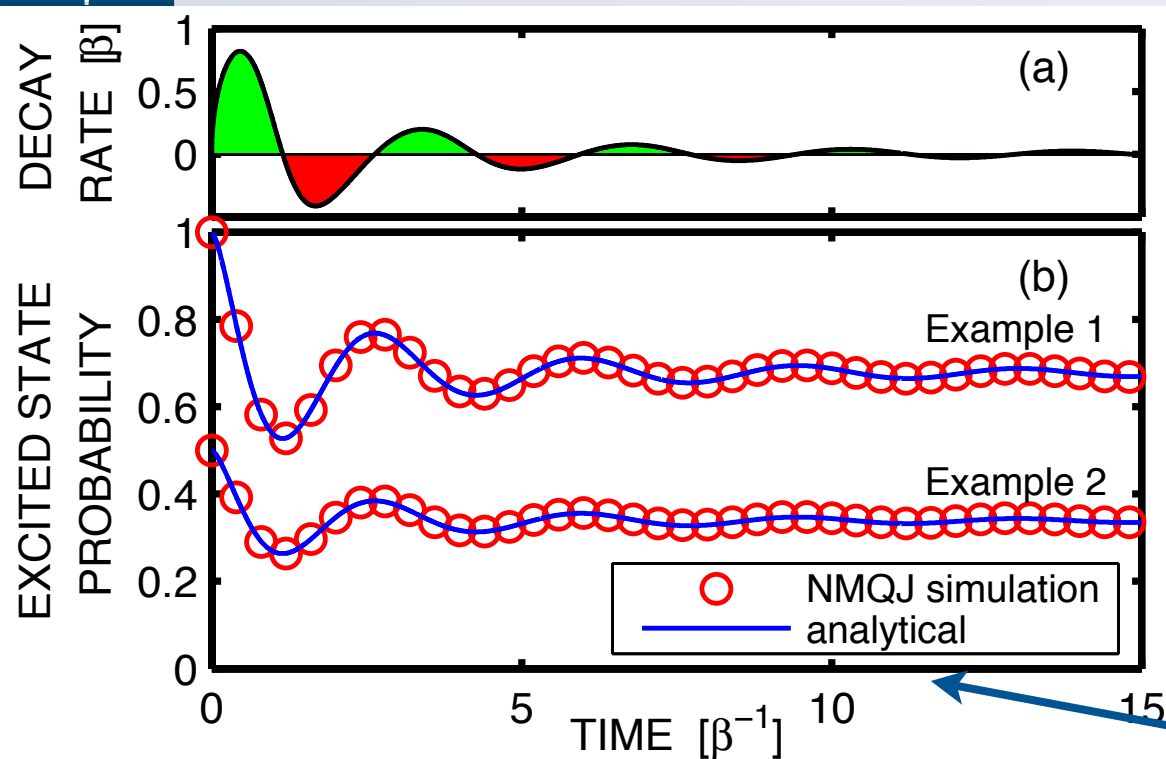
P's: jump probabilities

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

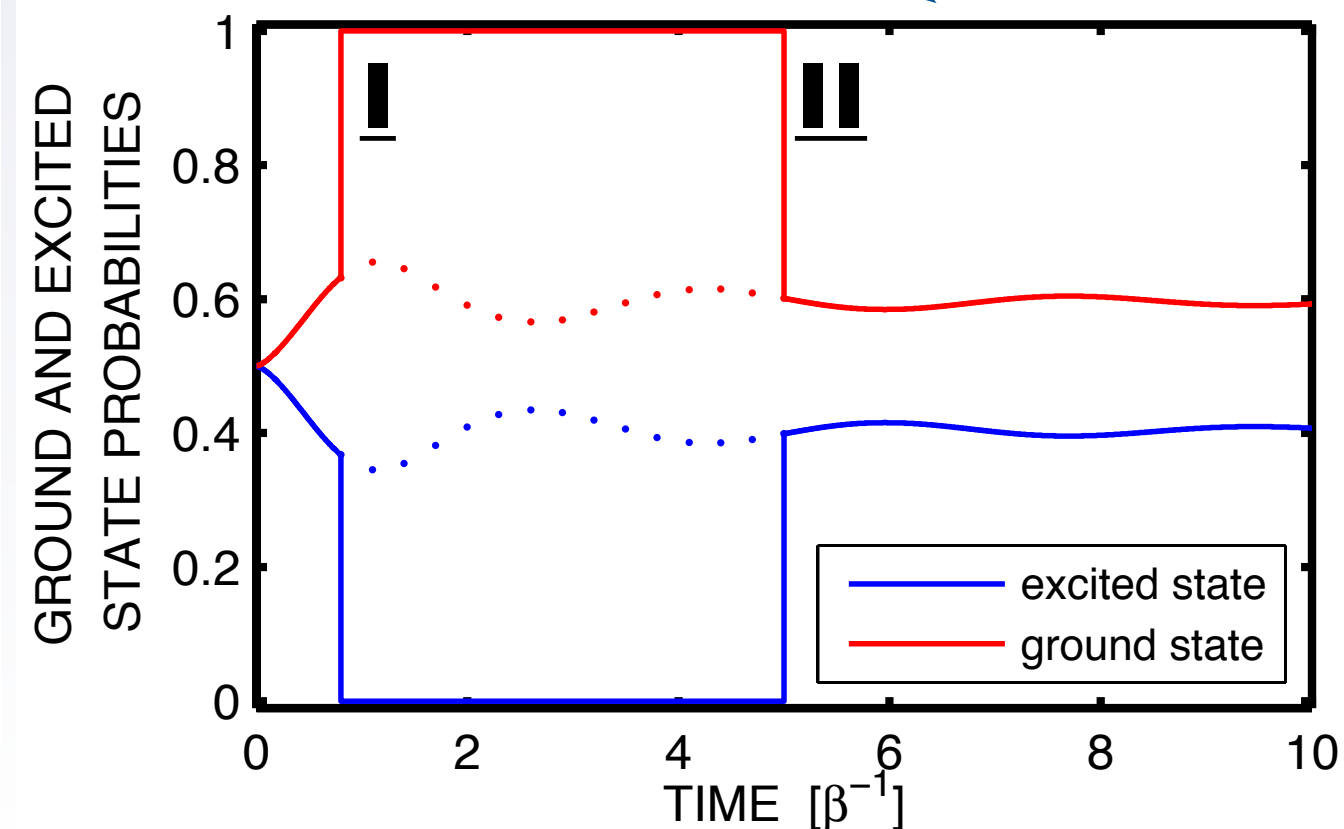


The simulation and exact results match.
Typical features of photonic band gap:

- Population trapping
- Atom-photon bound state.

Density matrix: average over the ensemble

Single state vector history



Example of one state vector history:

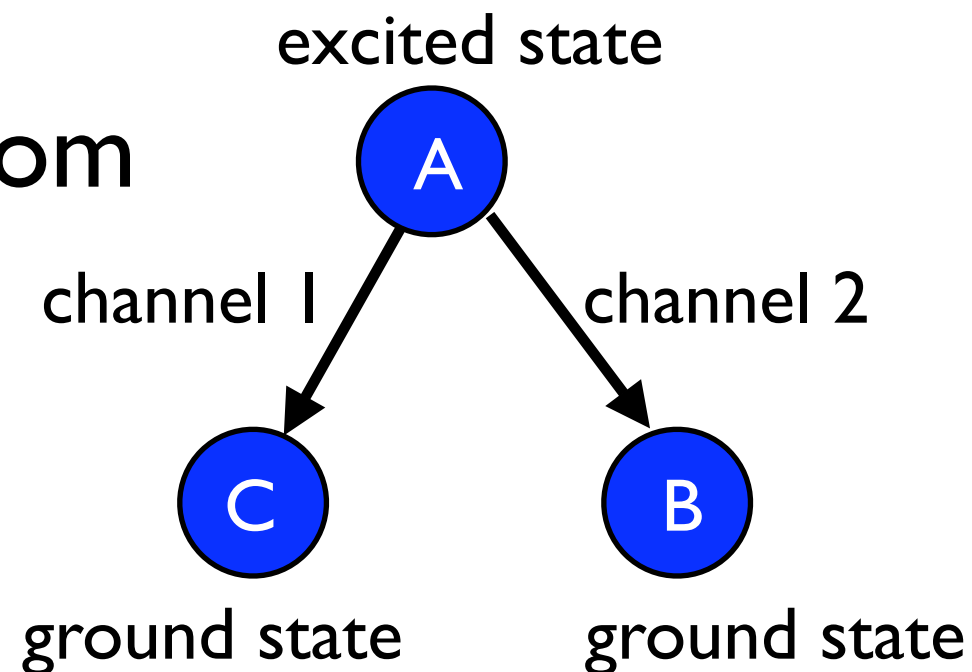
I: Quantum jump at positive decay region destroys the superposition.

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

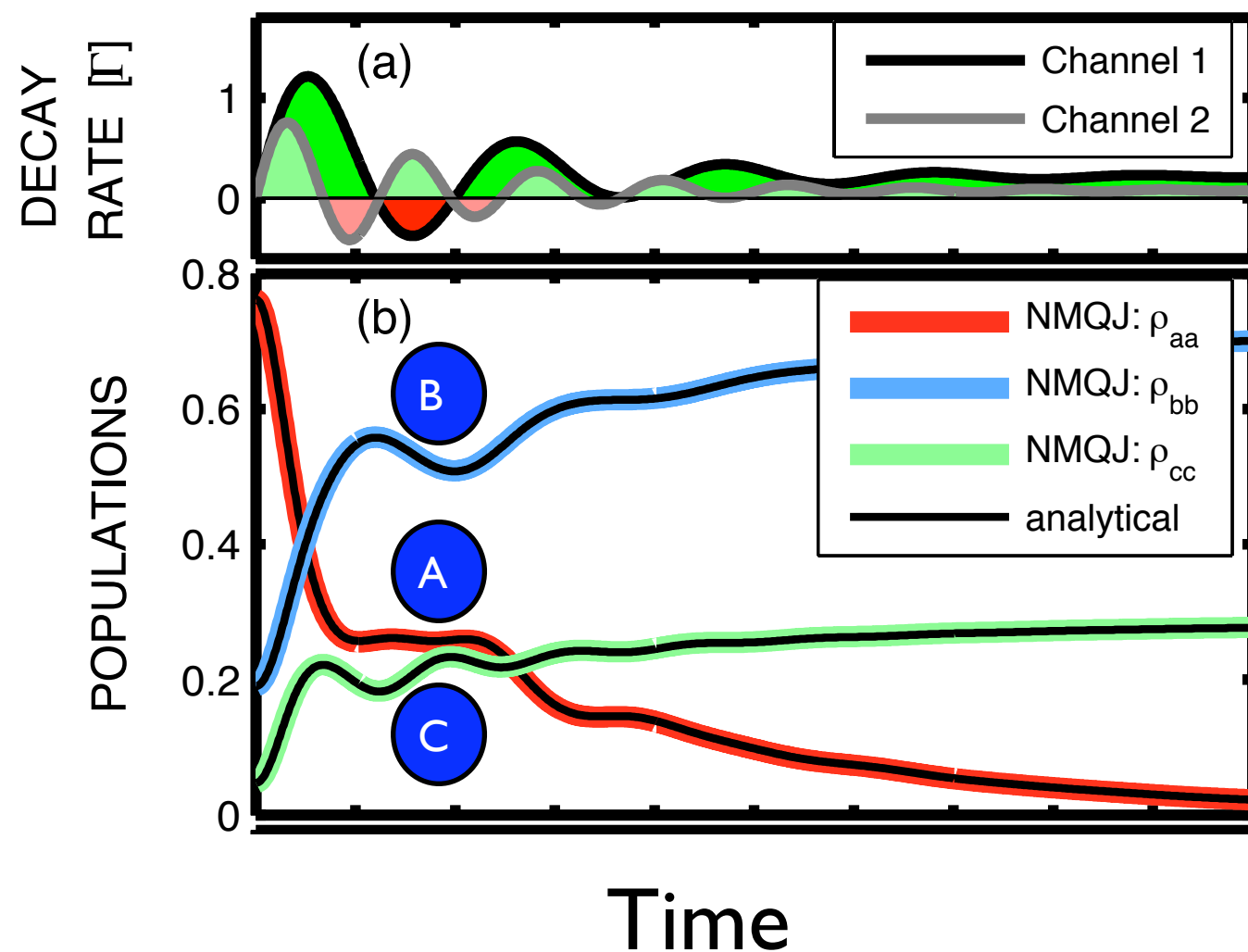


Simultaneous positive and negative rates

3-level atom



Two channels which can have different sign of the decay rate



- 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.



Application of NMQJ: excitonic energy transfer

- 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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(Received 13 August 2009; accepted 19 October 2009; published online 9 November 2009)

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.

© 2009 American Institute of Physics. [doi:[10.1063/1.3259838](https://doi.org/10.1063/1.3259838)]



Stochastic process description

Non-Markovian piecewise deterministic process.

Stochastic Schrödinger equation for non-Markovian open system:

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

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:

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

Probability to be in the source state
of negative rate jump

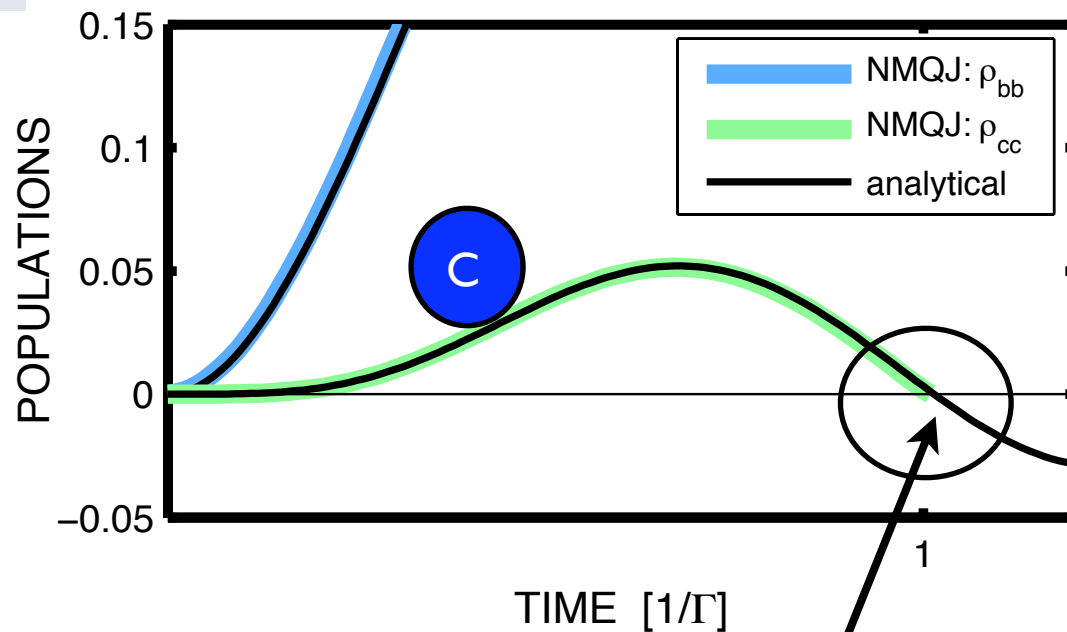
- Possible to prove: Whenever the dynamics breaks positivity, the stochastic process has singularity.
- The system is trying to undo something which did not happen.

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

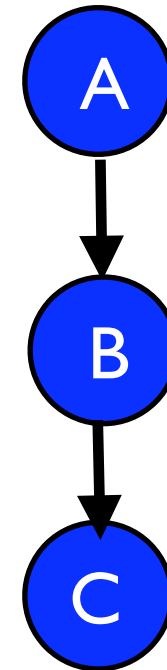


Examples of identification of positivity violation

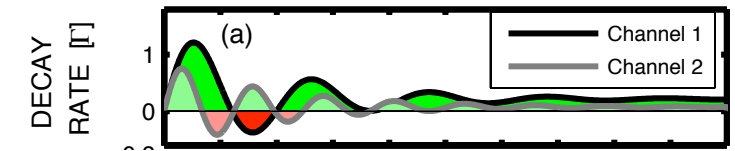
3-level ladder atomic system:



Breakdown of positivity



Decay rates



- 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.



3. Measure for non-Markovianity

Breuer, Laine, Piilo:
Phys. Rev. Lett. 103, 210401 (2009)

Laine, Piilo, Breuer:
arXiv:1002.2583 [quant-ph]

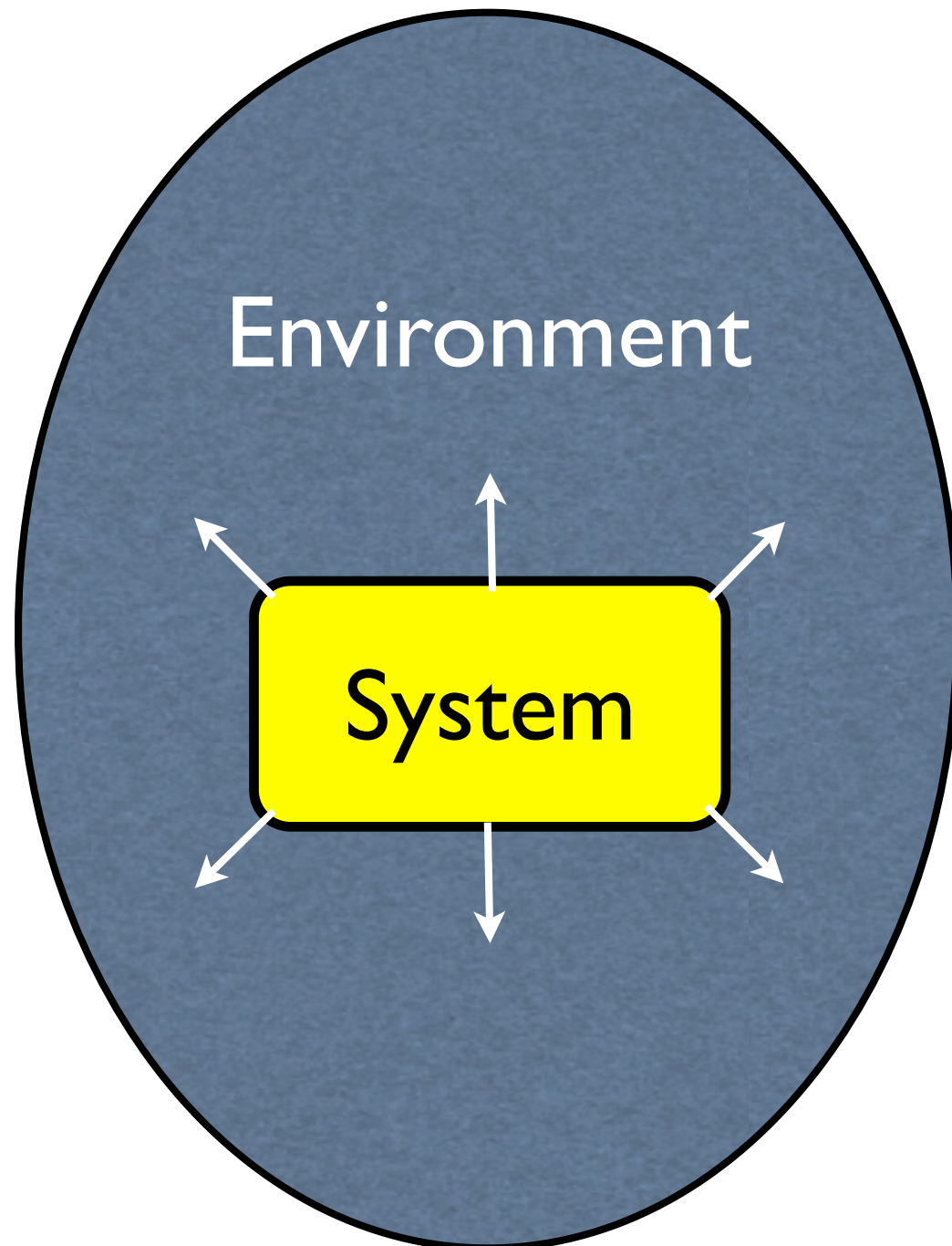


Information flow: Markovian case

Cartoon of the information flow: Markovian case (no memory).

“Small” system.

“Large” environment.



System-environment interaction



System reaches steady state

Any initial state of the system
leads to same steady state



The system loses information
on its initial state.

**Markovian system:
Information flow from the
system to the environment.**



Information flow and distinguishability of states (1)

Distance measure for two states ρ_1 and ρ_2 (density matrices):
Trace distance D :

$$D(\rho_1, \rho_2) = 1/2 \operatorname{tr} |\rho_1 - \rho_2|$$

$0 \leq D \leq 1$, identical states $D=0$, orthogonal states $D=1$

The physical interpretation:

The probability to distinguish the two states is equal to
 $1/2 (1+D)$

Notation: the change of the trace distance:

$$\sigma(t) = dD(t)/dt$$



Information flow and distinguishability of states (2)

In terms of the information flow:

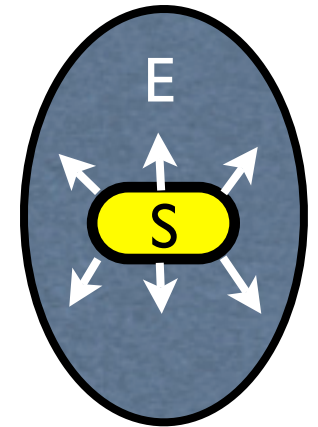
$$\sigma(t) < 0$$

Decreasing trace distance:

More and more difficult to distinguish the different states.



The information flows from the system to the environment.



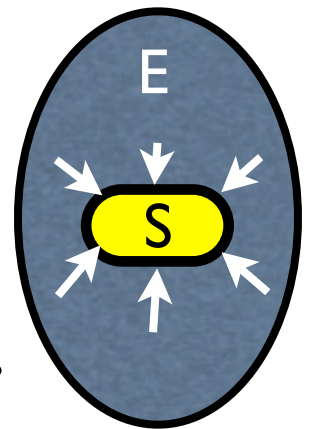
$$\sigma(t) > 0$$

Increasing trace distance:

More and more easy to distinguish the different states.



The information flows from the environment to the system.



The aim: quantify memory by calculating the reverse flow of information from the environment to the system.



Measure for non-Markovianity

Allows to define a measure for non-Markovianity:

$$\mathcal{N}(\Phi) = \max_{\rho_{1,2}(0)} \int_{\sigma > 0} dt \sigma(t, \rho_{1,2}(0)).$$

- Gives the total increase of the trace distance during the time evolution
- The total amount of information that has flown from the environment to the system during the time evolution.

General definition, independent of the used formalism to solve the open system dynamics*.

*Property of the map Φ : $\rho(t) = \Phi(t,0) \rho(0)$
(map takes the initial state to final state)



Measure for non-Markovianity

$$\mathcal{N}(\Phi) = \max_{\rho_{1,2}(0)} \int_{\sigma > 0} dt \sigma(t, \rho_{1,2}(0)).$$

For Markovian systems: $\mathcal{N}=0$

The information flows always from the system to the environment.

For non-Markovian system with memory: $0 < \mathcal{N} \leq \infty$

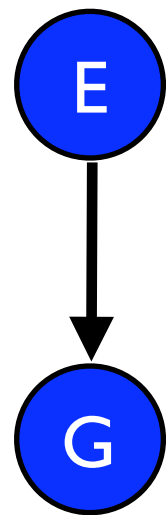
Periods of time when the information flow direction reversed, the system regains information it earlier leaked

- All divisible* maps contractive in trace distance - info flows always out
- Master equation description:
Map divisible if and only if all the rates positive.
- Master equations with negative rates include info flow component from the environment to the system
- Deciding if system has memory does not require information about the environment structure - relevant for experiments

*Divisibility of the map: $\Phi(t,0) = \Phi(t,t') \Phi(t',0)$



Example: 2-level atom



+ electromagnetic environment with Lorentzian spectral density

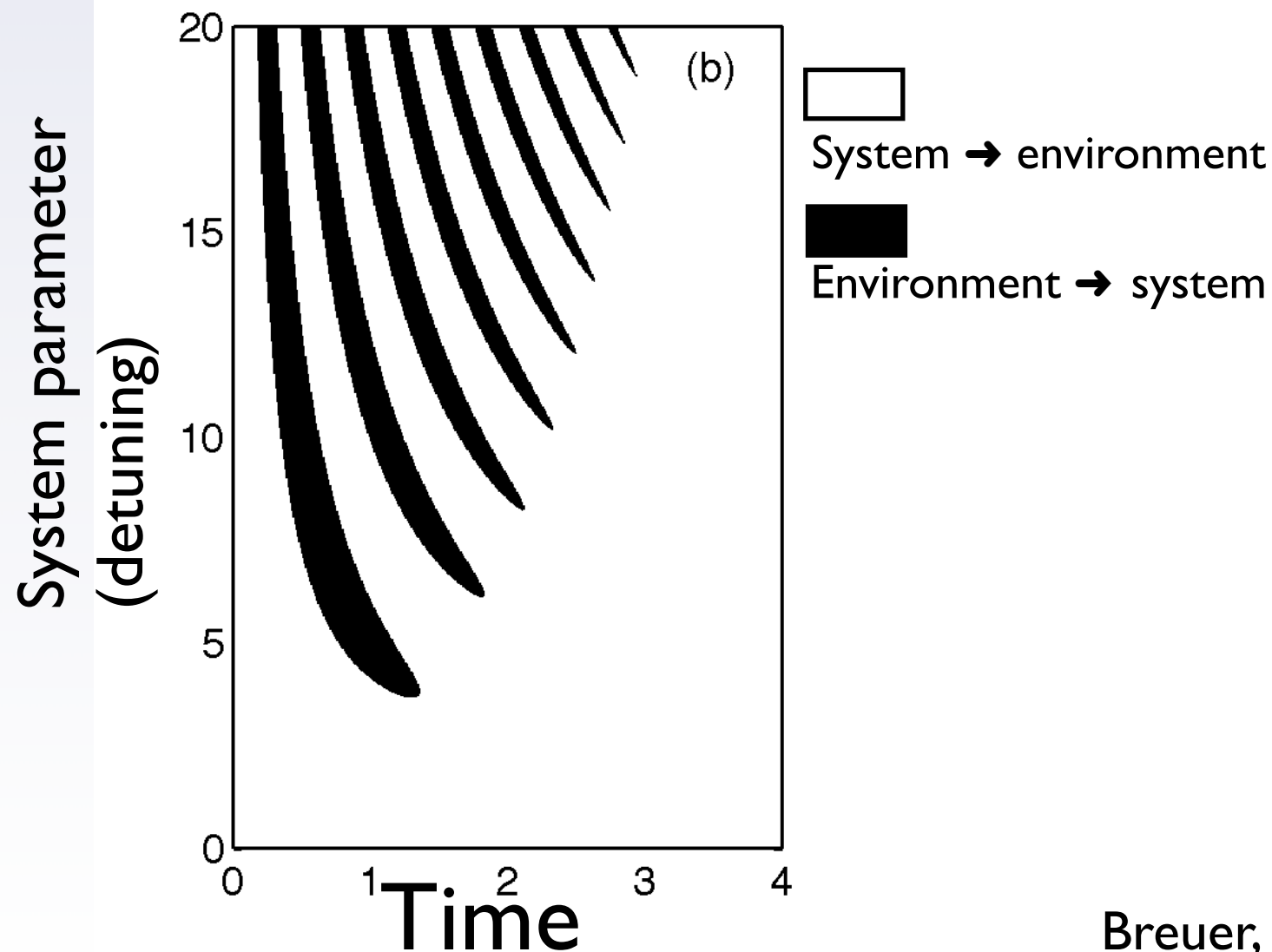
Change of the trace distance

$$\sigma(t, \rho_{1,2}(0)) = -\gamma(t) \exp[-\Gamma(t)],$$

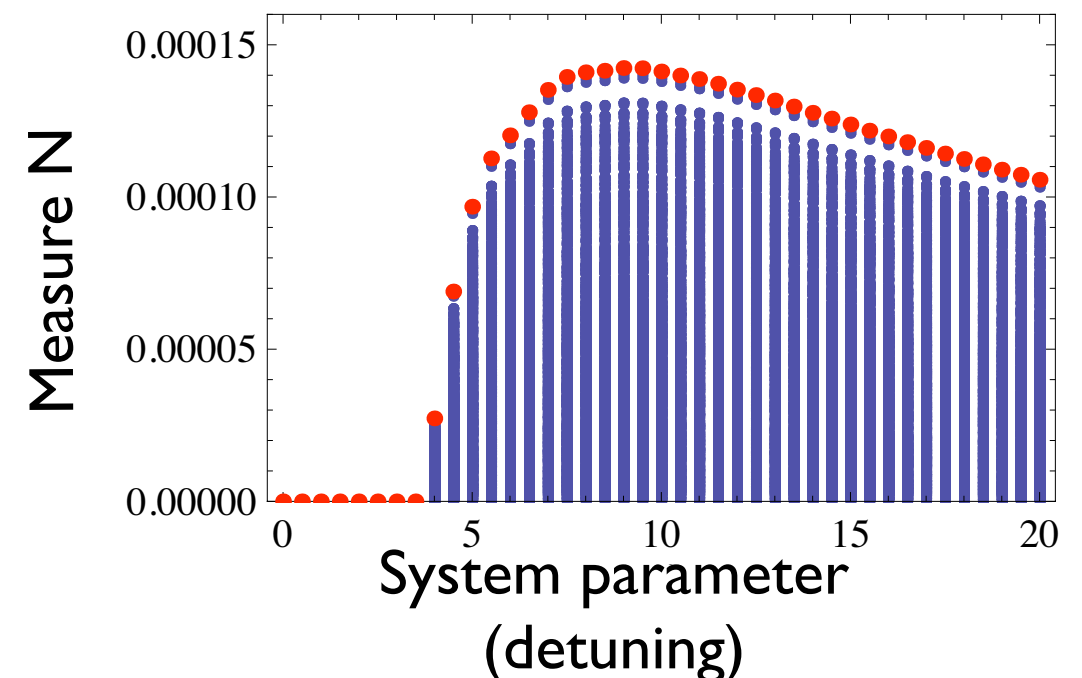
decay rate

The sign of the decay rate gives directly the direction of the information flow.

Information flow



For which system parameter strongest memory?





Measure for non-Markovianity

Other measures:

Wolf, Eisert, Cubitt, Cirac: Phys. Rev. Lett. 2008

- Markovianity vs non-Markovianity from a snapshot of the evolution.

Rivas, Huelga, Plenio: arXiv:0911.4270

- Measure for non-divisibility of the process.
- We conjecture: there also exists non-divisible Markovian processes

Our view (Phys. Rev. Lett. 2009):

- Reversed information allows system to “remember” its earlier state and this affects what happens at the current point of time
- Memory is a feature of a system dynamics which has physical origin instead of being a mathematical property of the equation of motion

Also: do all phenomenological memory-kernel equations describe backflow of info or memory? No.

Mazzola, Laine, Breuer, Maniscalco, Piilo, arXiv:1003.3817 (quant-ph)



4. Witness for initial system-environment correlations

Laine, Piilo, Breuer:
arXiv:1004.2184 [quant-ph]



Initial product state

$$\rho_{SE}(0) = \rho_S(0) \otimes \rho_E(0)$$



Dynamics is described by
a CP-map between the system states

$$\Phi(t, 0) : \rho_S(0) \mapsto \rho_S(t)$$

Contractivity of the trace distance

$$D(\Phi\rho_1, \Phi\rho_2) \leq D(\rho_1, \rho_2)$$



Initially correlated system-reservoir state

$$\begin{aligned} & D \left(\text{Tr}_E [U_t \rho_{SE}^1 U_t^\dagger], \text{Tr}_E [U_t \rho_{SE}^2 U_t^\dagger] \right) - D(\rho_S^1, \rho_S^2) \\ & \leq D(\rho_{SE}^1, \rho_{SE}^2) - D(\rho_S^1, \rho_S^2) \equiv I(\rho_{SE}^1, \rho_{SE}^2) \end{aligned}$$

The increase of the the trace of the reduced system states bounded above by the initial information outside the reduced system.

Take ρ_{SE}^2 to be ρ_{SE}^1 without correlations: $\rho_{SE}^2 = \rho_S^1 \otimes \rho_E^1$

$$\begin{aligned} & D \left(\text{Tr}_E [U_t \rho_{SE}^1 U_t^\dagger], \text{Tr}_E [U_t \rho_S^1 \otimes \rho_E^1 U_t^\dagger] \right) \\ & \leq D(\rho_{SE}^1, \rho_S^1 \otimes \rho_E^1) \end{aligned}$$

The maximum amount of information, the system can recover from the environment is the amount of information flowed out from the system since the initial time plus the amount of information in the initial correlations.



Initially correlated system-reservoir state

$$D \left(\text{Tr}_E \left[U_t \rho_{SE}^1 U_t^\dagger \right], \text{Tr}_E \left[U_t \rho_S^1 \otimes \rho_E^1 U_t^\dagger \right] \right) \\ \leq D(\rho_{SE}^1, \rho_S^1 \otimes \rho_E^1)$$

The increase of trace distance of the system states above the initial value is a witness of initial correlations:

$$D(\text{Tr}_E [U \rho_{SE} U^\dagger], \text{Tr}_E [U \rho_S \otimes \rho_E U^\dagger]) > 0$$



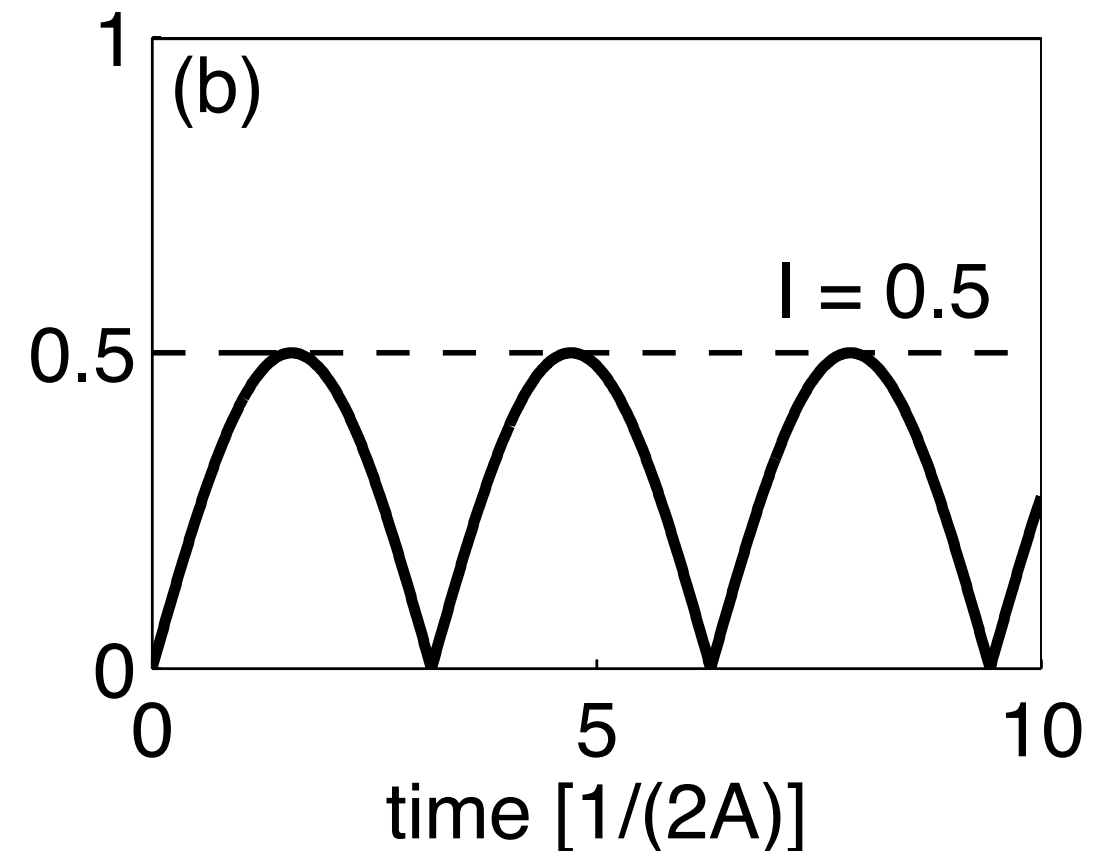
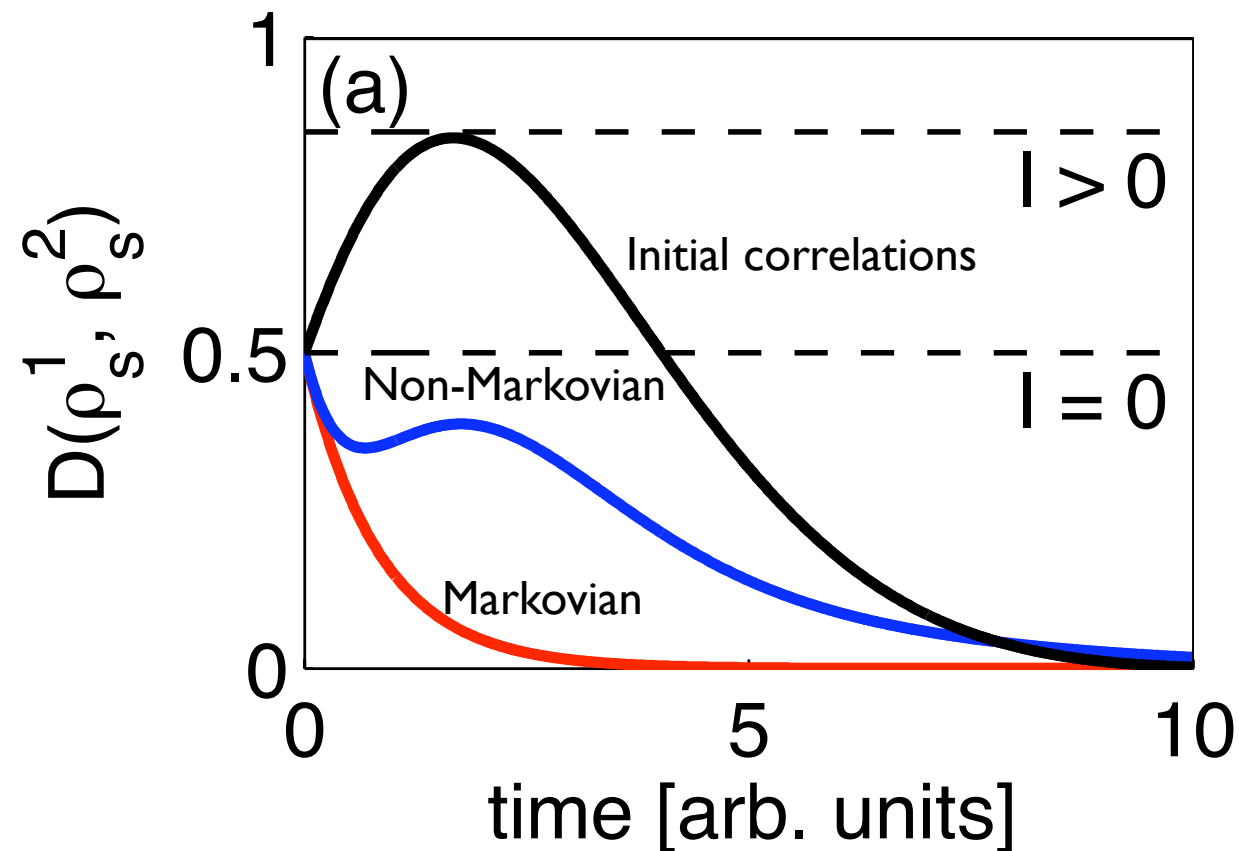
ρ_{SE} is initially correlated



Examples

Schematic view on various cases

Central spin in N-spin bath for initially correlated system-bath state



Central spin in N-spin bath:

$$H = A_0 \sum_{k=1}^N (\sigma_+ \sigma_-^{(k)} + \sigma_- \sigma_+^{(k)})$$

$$\rho_{SE}^1 = |\Psi\rangle\langle\Psi|, \quad |\Psi\rangle = \alpha |-\rangle \otimes |\chi_+\rangle + \beta |+\rangle \otimes |\chi_-\rangle$$

$$\rho_{SE}^2 = |\alpha|^2 |-\rangle\langle-| \otimes |\chi_+\rangle\langle\chi_+| + |\beta|^2 |+\rangle\langle+| \otimes |\chi_-\rangle\langle\chi_-|$$

$$|\chi_+\rangle = |++\cdots+\rangle$$

$$|\chi_-\rangle = \frac{i}{\sqrt{N}} \sum_k |k\rangle$$

$$D\left(\text{Tr}_E[U_t \rho_{SE}^1 U_t^\dagger], \text{Tr}_E[U_t \rho_{SE}^2 U_t^\dagger]\right) = |\Re(\alpha^* \beta) \sin(2At)|$$

$$A = \sqrt{N} A_0$$



1: Non-Markovian quantum jump (NMQJ) method for open systems:

Negative rate random events undo the earlier random events.

Piilo, Maniscalco, Härkönen, Suominen:

Phys. Rev. Lett. 100, 180402 (2008), Phys. Rev. A 79, 062112 (2009).

2: General measure for memory in open systems:

Connection between the information flow and memory:

Breuer, Laine, Piilo:

Phys. Rev. Lett. 103, 210401 (2009)



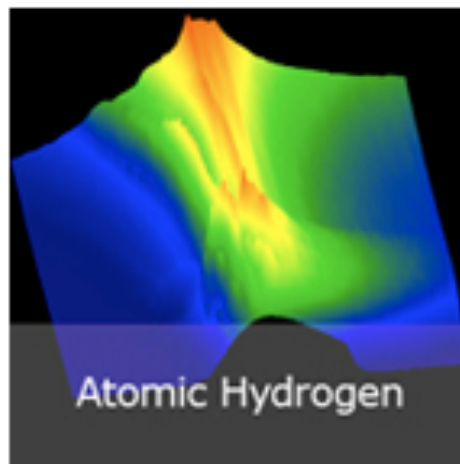
3: Witness for initial system-environment correlations

Bound for info flow into open system.

Laine, Piilo, Breuer: arXiv:1004.2184 [quant-ph]

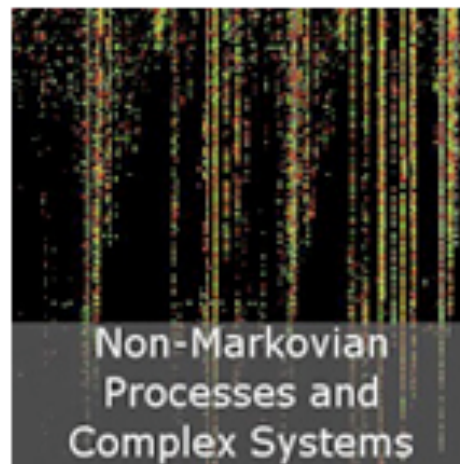


Turku Centre for Quantum Physics



Atomic Hydrogen

Vasiliev

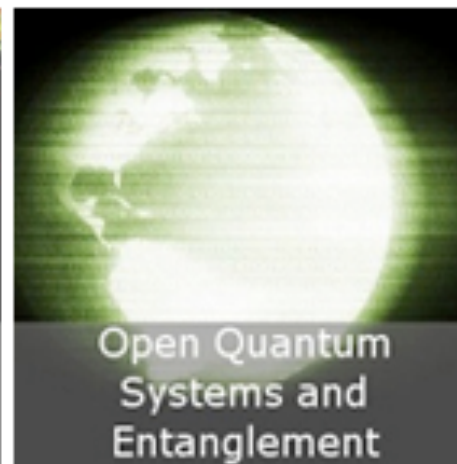


Non-Markovian
Processes and
Complex Systems

Piilo

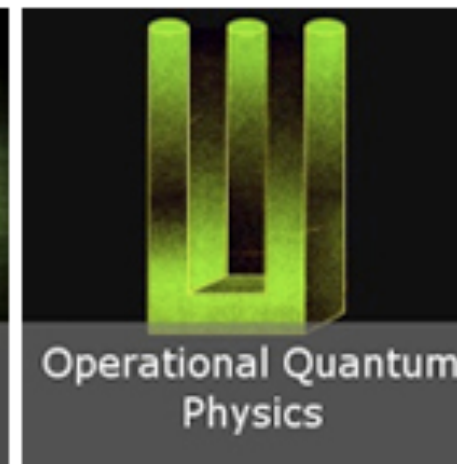


Non-Markovian Processes and Complex Systems Group



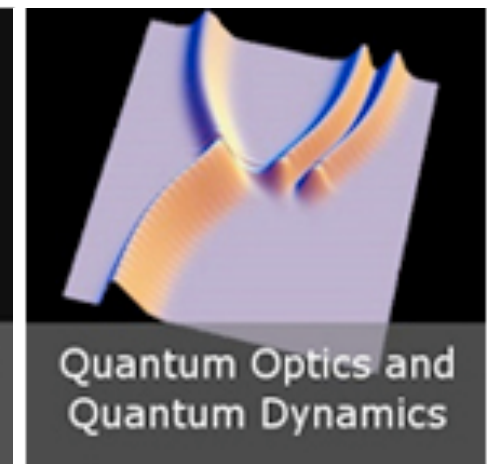
Open Quantum
Systems and
Entanglement

Maniscalco



Operational Quantum
Physics

Lahti



Quantum Optics and
Quantum Dynamics

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Markovian:

Constant info flow rate from the system to the environment.

Time-dependent Markovian:

Time dependent info flow rate from the system to the environment.

Non-Markovian:

Reverse flow of info from the environment to the system.