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Quantum jumps and open systems
- from positive to negative probabilities
and back

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Supported by the Academy of Finland and the Finnish Academy of Science and Letters

TURUN YLIOPISTO

Quantum jumps

Old quantum mechanics & Niels Bohr (1910's):

– change of a quantum state by an instantaneous jump (e.g. photon absorption and emission).

Ensemble dynamics & Schrödinger (1920's):

– Superpositions and probability interpretation.

– Deterministic evolution of probability amplitudes.

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi$$

– Measurable with an infinite number of identical systems (ensemble).

Quantum jumps

Old quantum mechanics & Niels Bohr (1910's):

– change of a quantum state by an instantaneous jump (e.g. photon absorption and emission).

Ensemble dynamics & Schrödinger (1920's):

Traditional example: radioactive decay

$$\frac{dN}{dt} = -\frac{1}{\tau} N \quad \rightarrow N = N_0 e^{-t/\tau}$$

The same applies for the decay of electronic excitations in atoms by spontaneous emission of a photon.

Bohr vs. Schrödinger

Schrödinger:

"If all this damned quantum jumping were really to stay, I should be sorry I ever got involved with quantum theory."

Bohr:

"But we others are very grateful to you that you did, since your work did so much to promote the theory."

R.J. Cook: Quantum jumps, Prog. in Optics XXVIII, Elsevier, 1990

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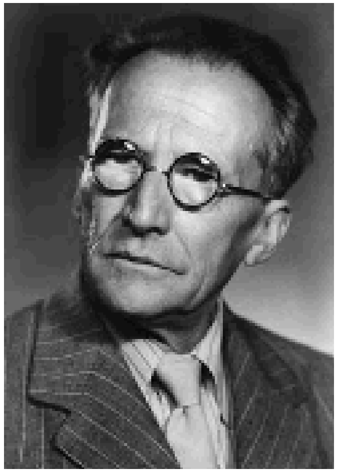
Single quantum systems

"We never experiment with just one electron or atom or (small) molecule. In thought experiments, we sometimes assume that we do; this invariably entails ridiculous consequences. In the first place it is fair to state that we are not experimenting with single particles any more than we can raise ichthyosauria in the zoo."

Erwin Schrödinger in 1952



Single quantum systems ?

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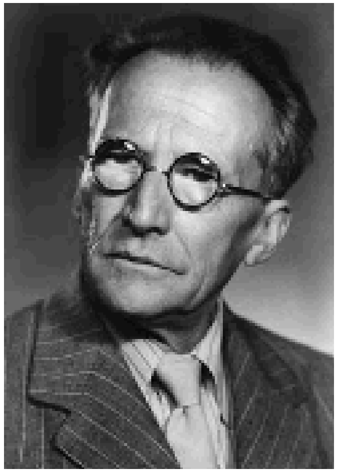


Superpositions and interference.
Probability amplitudes with deterministic dynamics.
Realised in ensembles.
Single system dynamics is not a meaningful concept (random future).

Single systems themselves are not meaningful?

Trapped ions

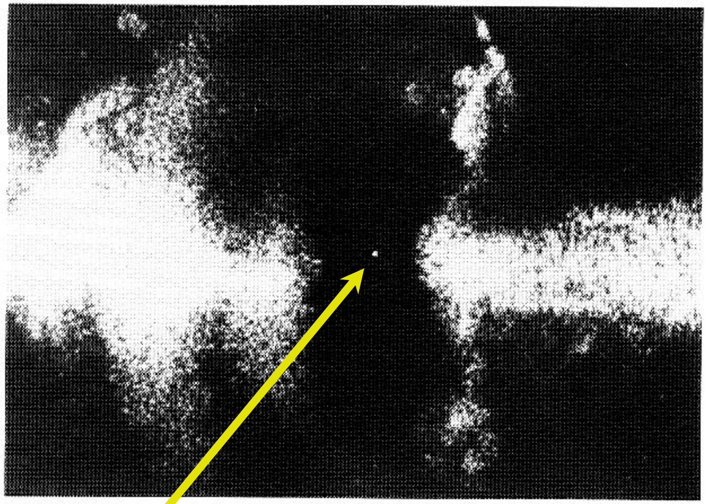
A photograph of a single ion in an electromagnetic trap

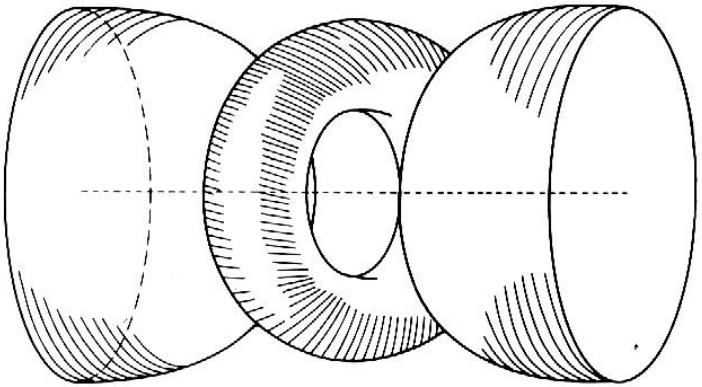
(Dehmelt & Toschek, Hamburg 1980)

The ion is excited by laser light from the electronic ground state to an excited state.

Excited ion returns to ground state by emitting a photon spontaneously.

We ”see” the ion!





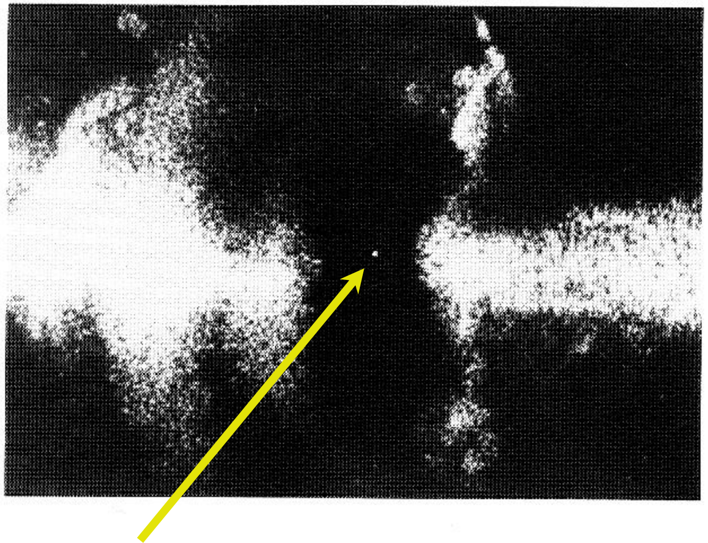
Single system ?

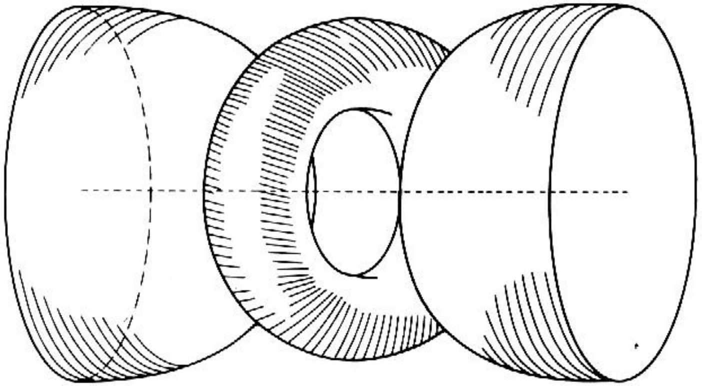
Excitation-emission happens with a nanosecond time scale: *continuous flow of light*.

Ion moves, broad-area picture.

How do we know that it is only a single ion and not a small ensemble?

By a detection scheme based on quantum jumps !





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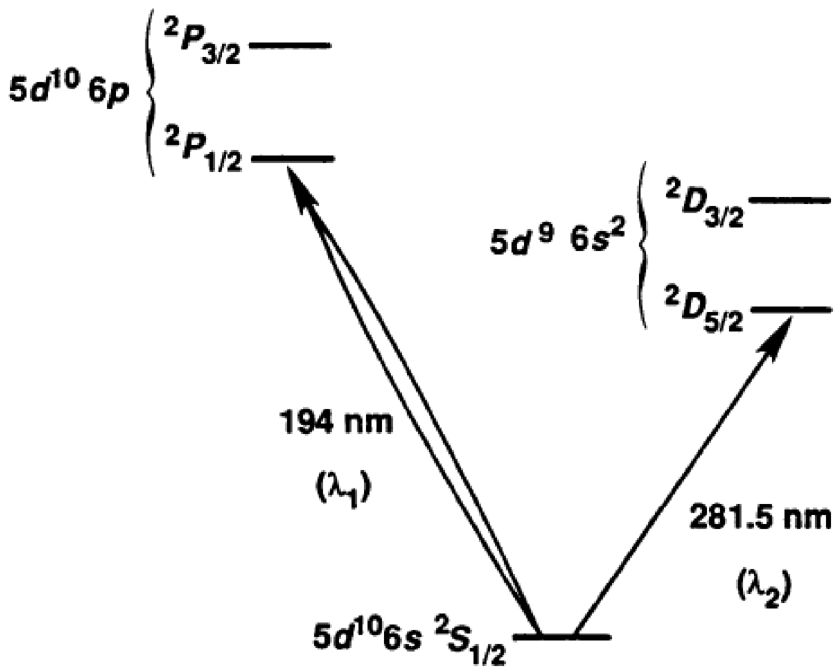
Detection by quantum jumps

Fluorescent state

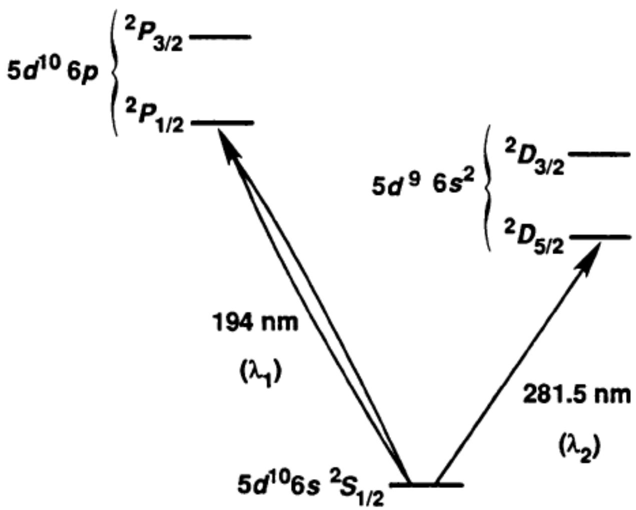
Mercury ion Hg^+

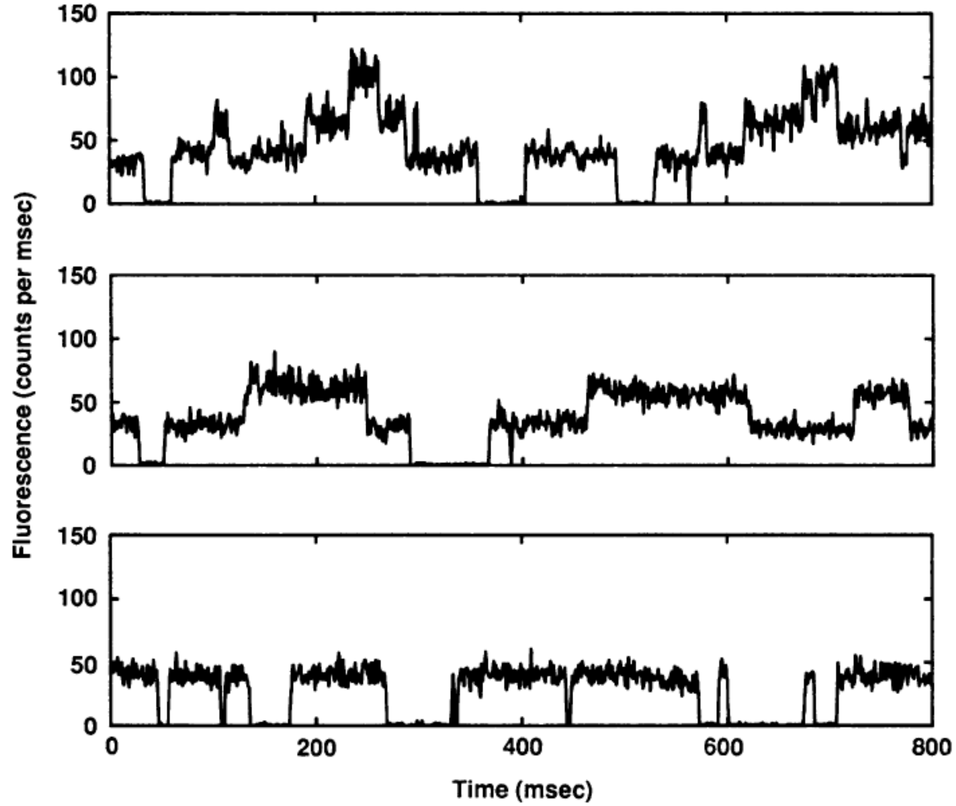


Metastable state

W.M. Itano, J.C. Bergquist, and D.J. Wineland, Science 37, 612 (1987)

One ion only or more?





W.M. Itano, J.C. Bergquist, and D.J. Wineland, Science 37, 612 (1987)

Detection by quantum jumps

Quantum Jumps

Recently, Cook and Kimble (*40*) theoretically investigated a three-level atom like the one considered by Dehmelt in his "shelved electron" proposal. Light at wavelengths λ_1 and λ_2 was assumed to be present at the same time. They predicted that one would observe the λ_1 fluorescence to turn off and on abruptly as the atom made transitions (quantum jumps) to and from the long-lived upper level. This paper generated a great deal of theoretical interest, and the problem was approached from various viewpoints (*41*). The novelty of this problem is that theorists are accustomed to calculating, and experimenters are accustomed to measuring, ensemble averages rather than following the development in time of a single quantum system.

W.M. Itano, J.C. Bergquist, and D.J. Wineland, Science 37, 612 (1987)

1st experiment in 1986 with Ba^+

VOLUME 56, NUMBER 26 — PHYSICAL REVIEW LETTERS — 30 JUNE 1986

Shelved Optical Electron Amplifier: Observation of Quantum Jumps

Warren Nagourney, Jon Sandberg, and Hans Dehmelt

Department of Physics, University of Washington, Seattle, Washington 98195

(Received 5 May 1986)

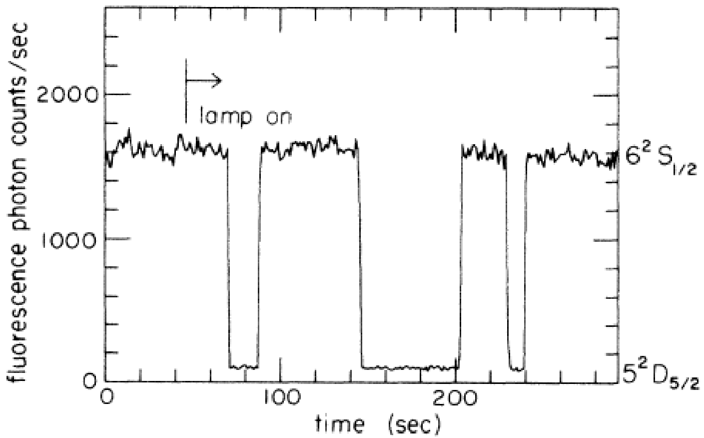


FIG. 2. A typical trace of the 493-nm fluorescence from the $6^2P_{1/2}$ level showing the quantum jumps after the hollow cathode lamp is turned on. The atom is definitely known to be in the shelf level during the low fluorescence periods.

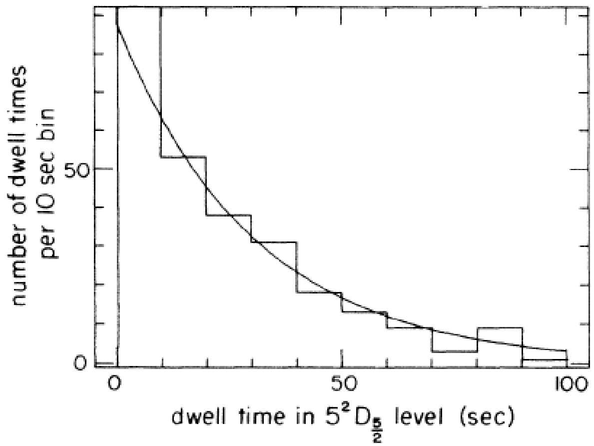


FIG. 3. Histogram of distribution of dwell times in the shelf level for 203 "off" times. A fitted theoretical (exponential) distribution for a metastable lifetime of 30 sec is superposed on the experimental histogram.

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1st experiment in 1986 with Ba^+

$$\frac{dN}{dt} = -\frac{1}{\tau} N \quad \rightarrow N = N_0 e^{-t/\tau}$$

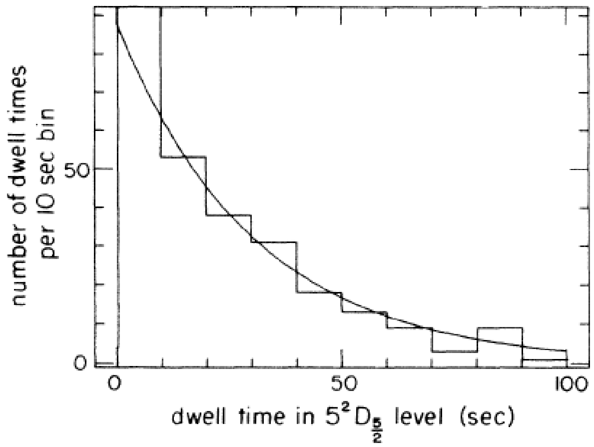


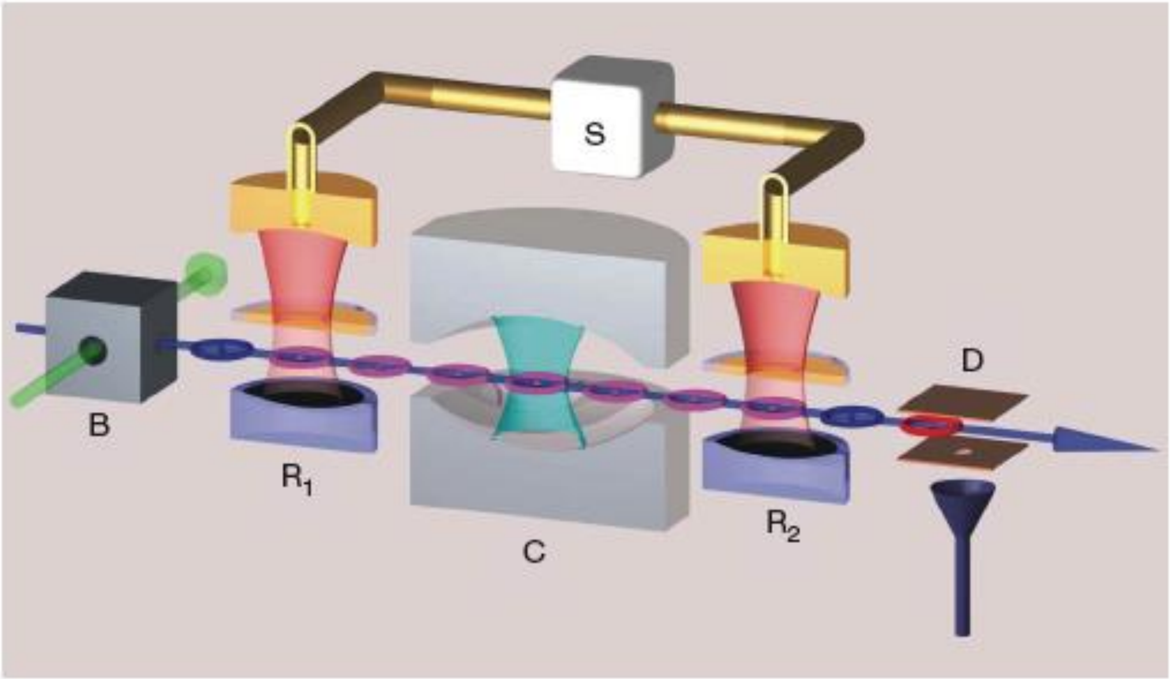
FIG. 3. Histogram of distribution of dwell times in the shelf level for 203 "off" times. A fitted theoretical (exponential) distribution for a metastable lifetime of 30 sec is superposed on the experimental histogram.

20 years later: Jumping photons

Quantum jumps of light recording the birth and death of a photon in a cavity

Nature 446, 297 (2007) - March 15

Sébastien Gleyzes[1], Stefan Kuhr[1]†, Christine Guerlin[1], Julien Bernu[1], Samuel Deléglise[1], Ulrich Busk Hoff[1], Michel Brune[1], Jean-Michel Raimond[1] & Serge Haroche[1,2]



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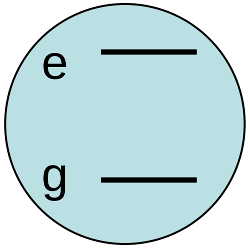
Cavity QED & QND



Rydberg state atoms are used to manipulate and detect the photon states in the cavity.

Only one cavity mode is near-resonant with the ”*e-g*” transition.

If the cavity is initially empty, i.e., photon number *n* = *0*, an atom comes out in state *g*.

If there is a photon, the atom comes out in state *e*.

– and the photon survives! QND

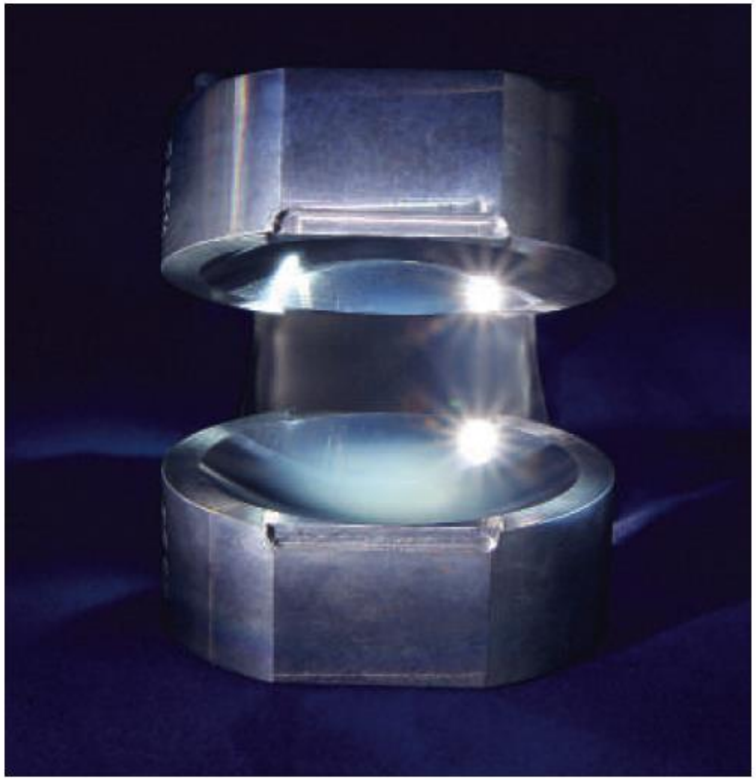


Figure 1 | They do it with mirrors. Gleyzes and colleagues' cavity for trapping photons[1].

Cavity QED

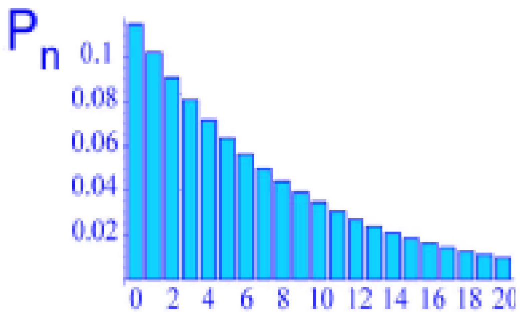
But the cavity is at a finite temperature *T= 0.8 K*.

Thermal occupation of cavity modes.

Excitation from *g* to *e* is possible.

For resonant mode <*n*> << *1*.

Only integral photon numbers can be observed for single atoms.



$$P_n = \frac{e^{-n\hbar\omega_0/k_BT}}{1-e^{-\hbar\omega_0/k_BT}}$$

$$<n>= \frac{1}{e^{\hbar\omega_0/k_BT}-1}$$

Jumping photons

Repeat: Only integral photon numbers can be observed for single atoms.

So, to obtain $\langle n \rangle \ll 1$ on average, we need to have 1 photon in the cavity for a finite and short time.

Can we see the birth and death of a thermal photon?

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Jumping photons

Repeat: Only integral photon numbers can be observed for single atoms.

So, to obtain <n> << 1 on average, we need to have 1 photon in the cavity for a finite and short time.

Can we see the birth and death of a thermal photon?

YES !

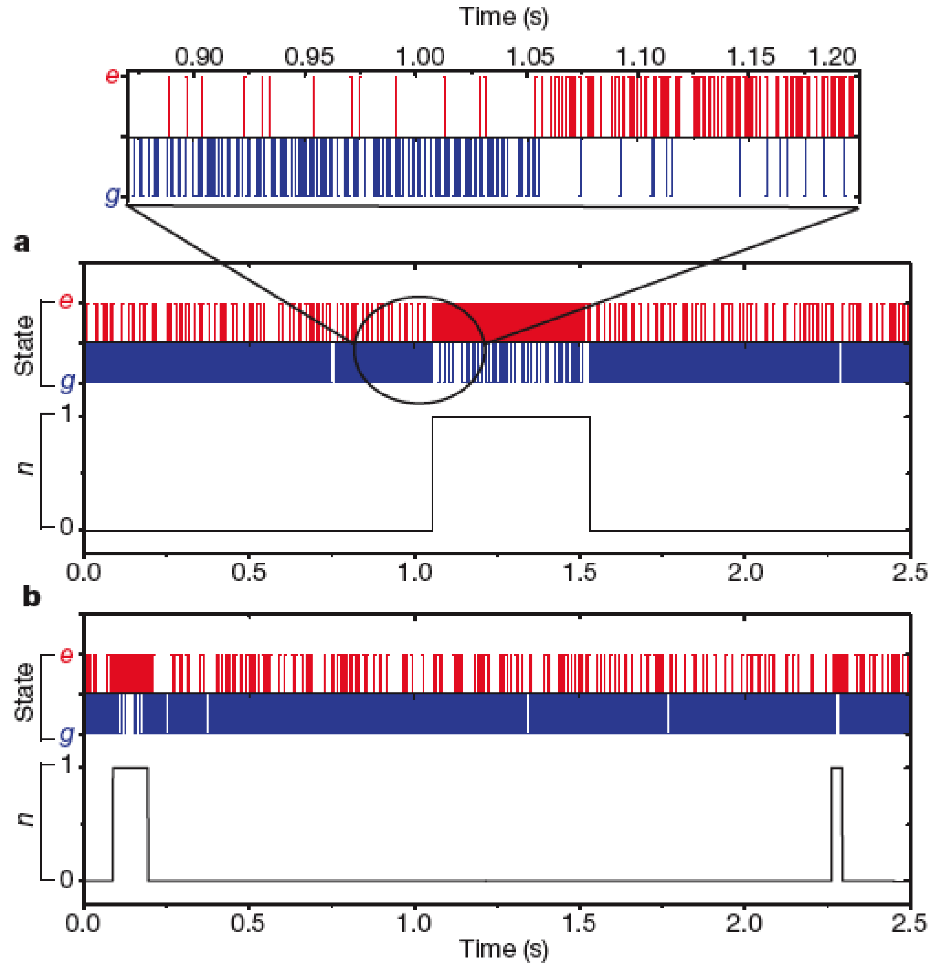
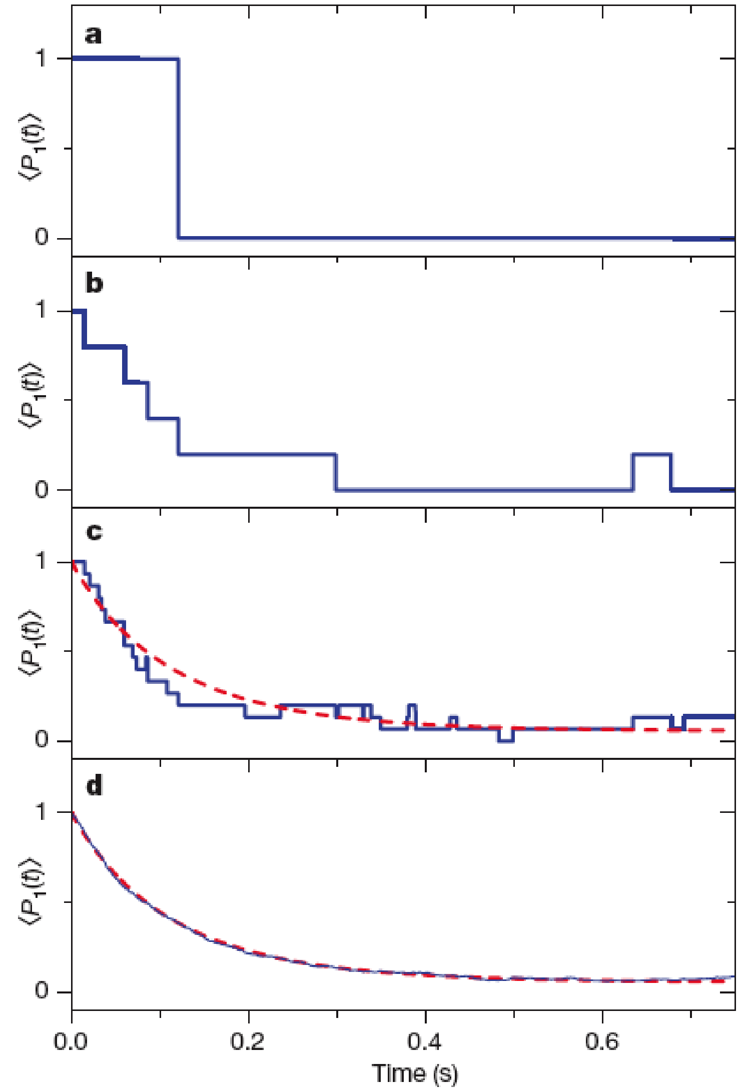


Figure 2 | Birth, life and death of a photon. a, QND detection of a single

Lifetime distribution

Figure 3 | Decay of the one-photon state. a, Measured value of $P_1 = |1\rangle\langle 1|$ as a function of time, in a single experimental realization; **b–d**, averages of 5, 15 and 904 similar quantum trajectories, showing the gradual transition from quantum randomness into a smooth ensemble average. Dotted red line in **c** and **d**, theoretical evolution of the probability of having one photon, $\langle P_1(t)\rangle$, obtained by solving the field master equation with the experimental values of T_c and n_0.



Key point:

We recover the ensemble result in the limit of (infinitely) many realisations as an average.

Recent work: prepare n>1, observe the integer step decay into n=0, Guerlin et al., Nature 448, 889 (23 August 2007).

Building the ensemble

We see that

a) One can observe single system dynamics

b) Quantum jumps are an integral part of them

c) An average of many such different and seemingly random ”telegraphic” signals produces the ensemble average

Unravelling the ensemble

We can turn the idea around:

a) We have a system that we want to study

b) The ensemble solution is difficult to calculate

c) Invent a fictitious quantum jump scheme to generate single system histories and build the directly unaccessible ensemble from them
   – and possibly obtain some insight as well

Now when would I need such an approach?

Unravelling the ensemble

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Now when would I need such an approach?

OPEN QUANTUM SYSTEMS

Open systems

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

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

This does not in fact yield exponential decay of excitations such as

$$\frac{dN}{dt} = -\frac{1}{\tau}N \quad \rightarrow N = N_0 e^{-t/\tau}$$

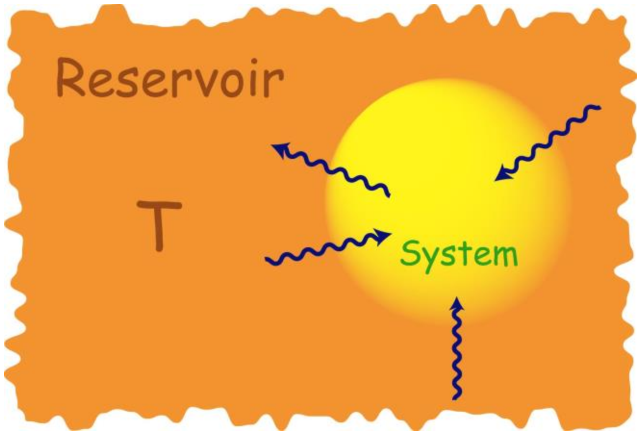
Usually what we perceive as a quantum system is actually much larger than we realize.

Excited states of atoms decay because they are coupled to surrounding electromagnetic field modes, usually nontractable.

If we ignore the modes and look at the atom only, the system evolves into a statistical mixture i.e. a mixed state.

Open systems

We can consider the system as coupled to a large reservoir.



State vector
-> density operator (matrix)

$$\rho = \rho_{system} = Tr_{reservoir}(\rho_{total}) = \sum_j \langle \varphi_j | \rho_{total} | \varphi_j \rangle$$

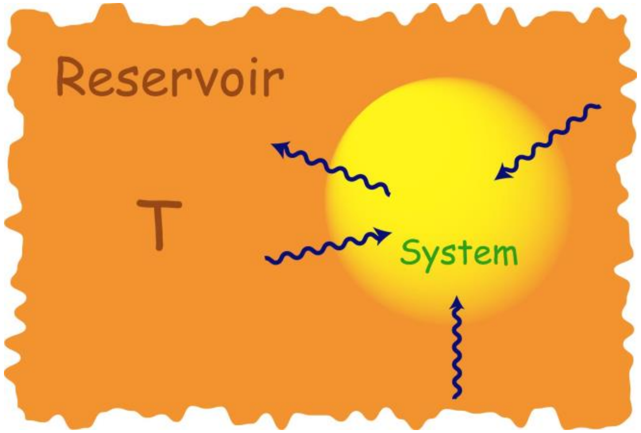
The time evolution of open quantum system:
Master equation for the density matrix in the Lindblad form.

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

Gorini, Kossakowski & Sudarshan, J. Math. Phys. 17, 821 (1976);
Lindblad, Commun. Math. Phys. 48, 119 (1976); Sudarshan PRA 46, 37 (1992)

Markovian open systems

To obtain the master equation we have made a few assumptions:



The system and the reservoir are weakly coupled (1st order).

The reservoir is large and its spectral structure is structureless:
No memory (Markovian approximation)

Result: The Γ_m -terms are positive constants.

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

Open systems and quantum jumps

A possible interpretation for the Master equation (Lindblad form)

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

The positive constants Γ_m are related to the probabilities to perform a quantum jump given by the operator C_m.

Note that the choice of the system basis or the set of operators C is not unique. It can correspond to a viable detection scheme but does not have to.

In quantum information one can actually consider measurements and interaction with a reservoir as the two sides of the same coin.

Open systems and quantum jumps

Thus we can unravel the ensemble dynamics given by

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

into a set of single system histories i.e. deterministic time evolution perturbed by random quantum jumps.

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

This leads to a very efficient simulation method.

Monte Carlo Wave Function (MCWF) method,

Dalibard, Castin & Mølmer, PRL 68, 580 (1992);
Mølmer, Castin & Dalibard, JOSA B 10, 527 (1993).

Simulations with quantum jumps

Why do we need simulations?

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

– single system histories can give more insight to system dynamics

– If the Hilbert space dimension for the system is n, the density matrix has n^2 components (ensemble size N is often such that N<<n)

Examples: laser cooling, cold collisions, molecular dynamics

Holland, Suominen & Burnett, PRL 72, 2367 (1994).

Castin & Mølmer, PRL 74, 3772 (1995).

Garraway & Suominen, Rep. Prog. Phys. 58, 365 (1995).

Piilo, Suominen & Berg-Sørensen, PRA 65, 033411 (2002).

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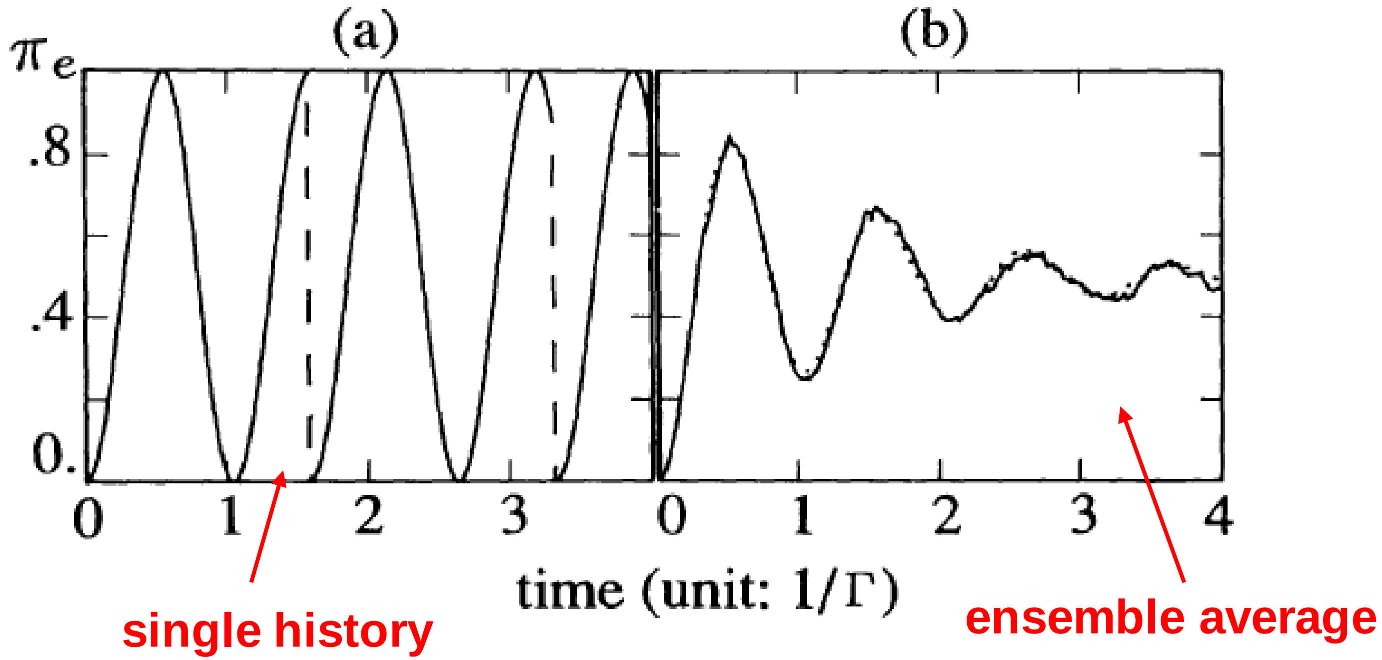
Simulations with quantum jumps

Example: A driven two-state atom + electromagnetic modes



Dalibard, Castin & Mølmer, PRL 68, 580 (1992).

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To generate an ensemble member

Solve the Schrödinger equation.

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

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

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

Jump operators C_m can be found from the dissipative part of the Master equation.

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

Effect of the non-Hermitian Hamiltonian: For each time step, the shrinking of the norm gives the jump probability *P*.

$$P = \sum_m \delta p_m$$

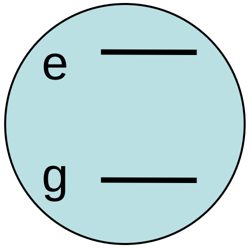
For each channel *m* the jump probability is given by the time step size, decay rate, and decaying state occupation probability.

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

Two-state atom: an example

Jump operator

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



Non-Hermitian Hamiltonian

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

Jump probability (and change of norm)

$$P = \delta p = \delta t \Gamma |c_e|^2$$

The algorithm

1. time-evolution over δt

2. generate random number, did quantum jump occur ?

$\delta p < \varepsilon$
no

$\delta p > \varepsilon$
yes

3. renormalize Ψ before new time step

3. apply jump operator C_j before new time step

4. At the end of time-evolution, take ensemble average

The equivalence

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

This gives comm. + anticomm. of m.e.

This gives "sandwich" term of the m.e.

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

Average

"No-jump" path weight

t-evol. and normalization

"Jump" path weight

Jump and normalization

Keeping in mind two things:

a) the time-evolved state is

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

b) the jump probability is

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

Non-Markovian systems

The reservoir may have a cutoff at high energies: short-time effects.

The spectral structure may be unusual, concentration around one or more energies (e.g. photonic bandgap materials).

We can think that there is a finite duration for any energy or information to spread inside the reservoir, and thus there is a possibility that some of it may come back to the system: **memory effect** .

Leads to non-Markovian dynamics. For some cases it can be handled with the time-convolutionless method (TCL).

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

Breuer & Petruccione, The theory of open quantum systems, Oxford 2002.

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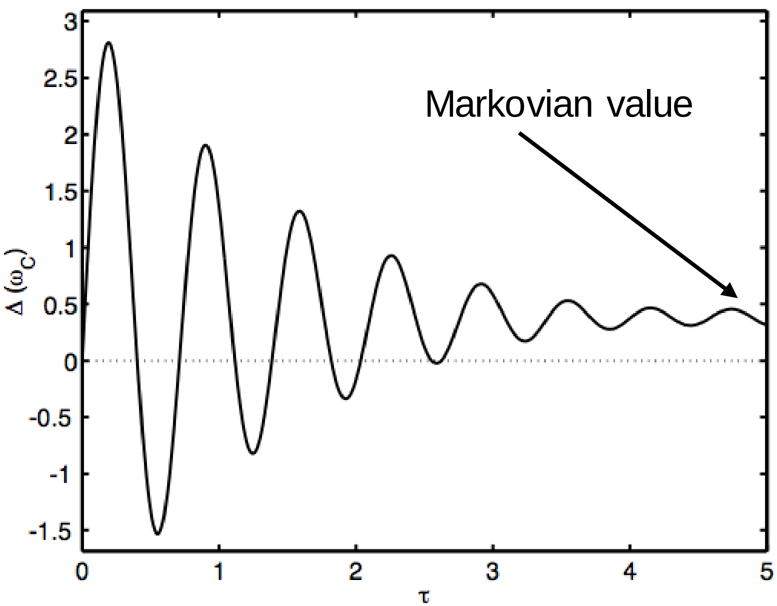
Non-Markovian systems

Non-Markovian effects lead to time dependent decay rates $\Delta_m(t)$.

$\Delta>0$: Lindblad-type
$\Delta<0$: non-Lindblad-type

Decay can have temporarily negative values but integral of decay over time has to be always positive.

And quantum jumps?



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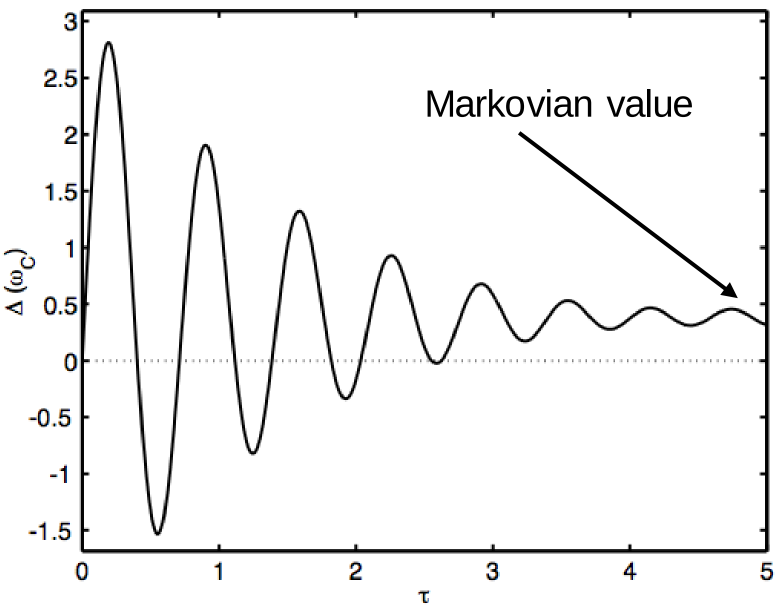


Decay can have temporarily negative values but integral of decay over time has to be always positive.

And quantum jumps?

Problems!

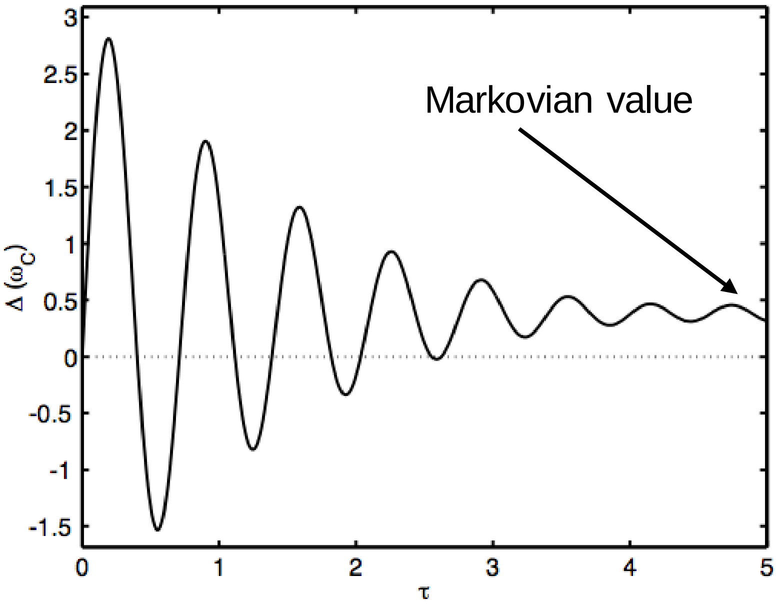
Non-Markovian systems

What happens when the decay rate is temporarily $\Delta(t)<0$?

The direction of information flow is reversed: for short periods of time information goes from the environment back to the system.

MCWF for Markovian system: since the jump probability is directly proportional to decay rate, we have

Negative jump probability !



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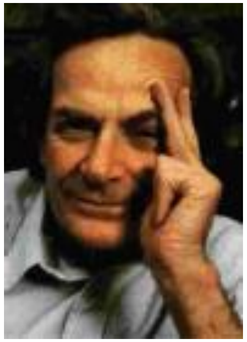
Feynman lecture on negative probabilities

R. Feynman, "Negative Probability" in "Quantum implications: Essays in Honour of David Bohm", eds. B. J. Hiley and F. D. Peat (Routledge, London, 1987) pp. 235-248

One of the assumptions was that the probability for an event must always be a positive number. Trying to think of negative probabilities gave me a cultural shock at first, but when I finally got easy with the concept I wrote myself a note so I wouldn't forget my thoughts. I

details. The idea of negative numbers is an exceedingly fruitful mathematical invention. Today a person who balks at making a calculation in this way is considered backward or ignorant, or to have some kind of mental block. It is the purpose of this paper to point out that we have a similar strong block against negative probabilities. By discussing a number of examples, I hope to show that they are entirely rational of course, and that their use simplifies calculations and thought in a number of applications in physics.

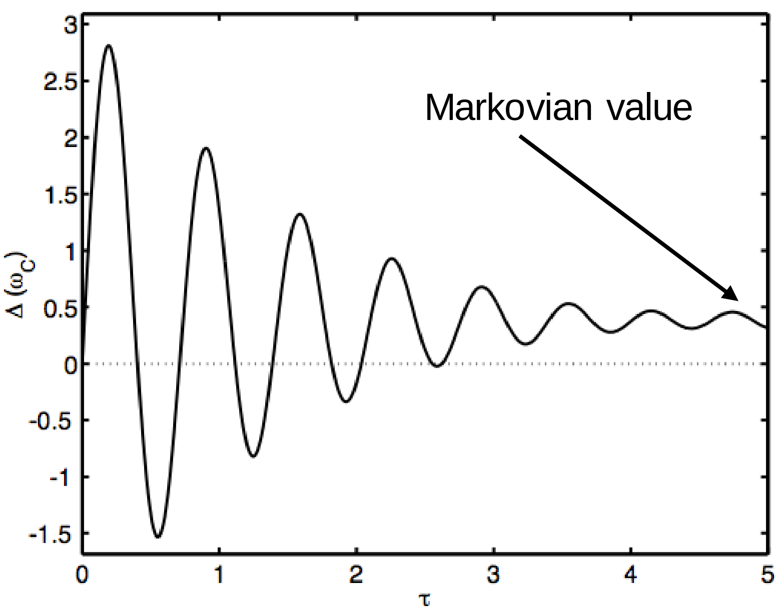


"...conditional probabilities and probabilities of imagined intermediary states may be negative in a calculation of probabilities of physical events or states."

Our solution for quantum jumps

In the region of $\Delta(t) < 0$ the system may recover the information it leaked to the environment earlier.

A quantum jump in the $\Delta(t) < 0$ region **reverses** an earlier jump which occured in the Δ (t) > 0 region.



Coherent reversal: original superposition is restored.

But if the jump destroyed the original superposition, where is the information that we restore?

And how do we calculate the probability for reversal?

Answer: Other ensemble members

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Our solution for quantum jumps

$$\rho(t) = \frac{N_0(t)}{N}\left|\Psi_0(t)\right\rangle\left\langle\Psi_0(t)\right| + \sum_i \frac{N_i(t)}{N}\left|\Psi_i(t)\right\rangle\left\langle\Psi_i(t)\right| + \sum_{i,j}\frac{N_{i,j}(t)}{N}\left|\Psi_{i,j}(t)\right\rangle\left\langle\Psi_{i,j}(t)\right| + \ldots$$

No jumps **1 jump (channel i)** **2 jumps (channels i, j)**

N: ensemble size
N_0, N_i, $N_{i,j}$: numbers of ensemble members in respective states

Here, the main quantities are similar as in original MCWF except:

P's: jump probabilities
D's: jump operators

$$P_{i\to 0} = \frac{N_0}{N_i}\,\delta t\left|\Delta\right|\left\langle\Psi_0\right|C^\dagger C\left|\Psi_0\right\rangle$$

$$D_{i\to 0} = \left|\Psi_0\right\rangle\left\langle\Psi_i\right|$$

What is the physical meaning of these ?

Our solution for quantum jumps

MCWF | **NMQJ**

jump operators

MCWF: C

Lindblad operator
from master equation

NMQJ: $D_{i\to 0} = |\Psi_0\rangle\langle\Psi_i|$

Transfers the state from 1 jump state to no jump state: cancels an earlier quantum jump (jump - reverse jump cycle)

jump probability

MCWF: $P = \delta t \Delta \langle \Psi | C^{\dagger} C | \Psi \rangle$

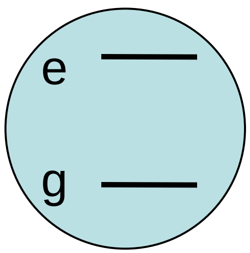
Histories independent
on each other

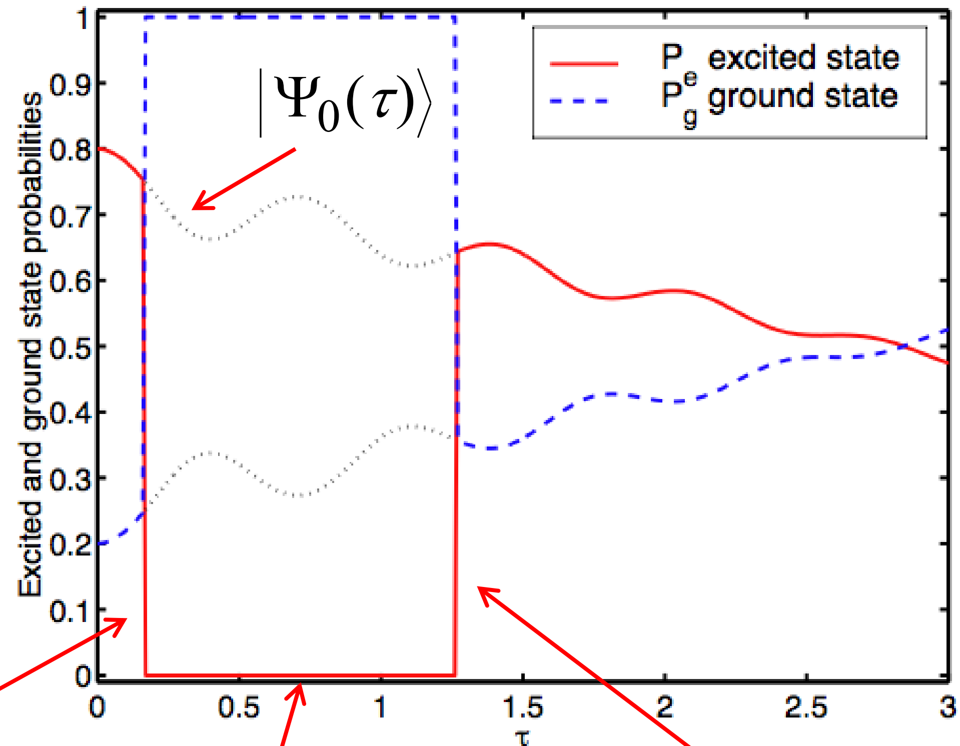
NMQJ: $P_{i\to 0} = \frac{N_0}{N_i} \delta t |\Delta| \langle \Psi_0 | D^{\dagger} D | \Psi_0 \rangle$

Histories depend on each other via jump probability.

Piilo, Maniscalco, Härkönen and Suominen, arXiv:0706.4438 [quant-ph] to appear in PRL.

Example: A two-state atom at zero T





$$P = \delta t \Delta \langle \Psi_0 | C^{\dagger} C | \Psi_0 \rangle$$

$$P_{i \to 0} = \frac{N_0}{N_i} \delta t |\Delta| \langle \Psi_0 | C^{\dagger} C | \Psi_0 \rangle$$

$$|\Psi_i(\tau)\rangle$$

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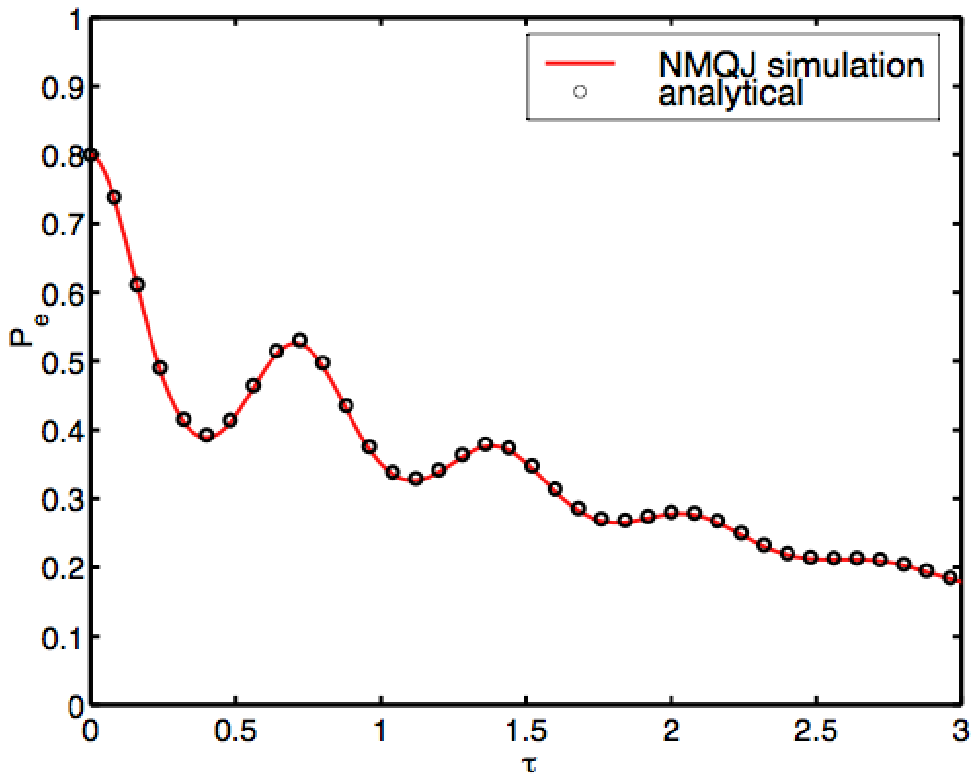
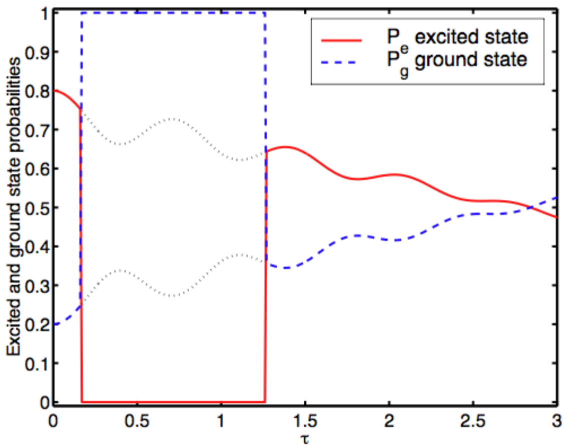
Example: A two-state atom at zero T





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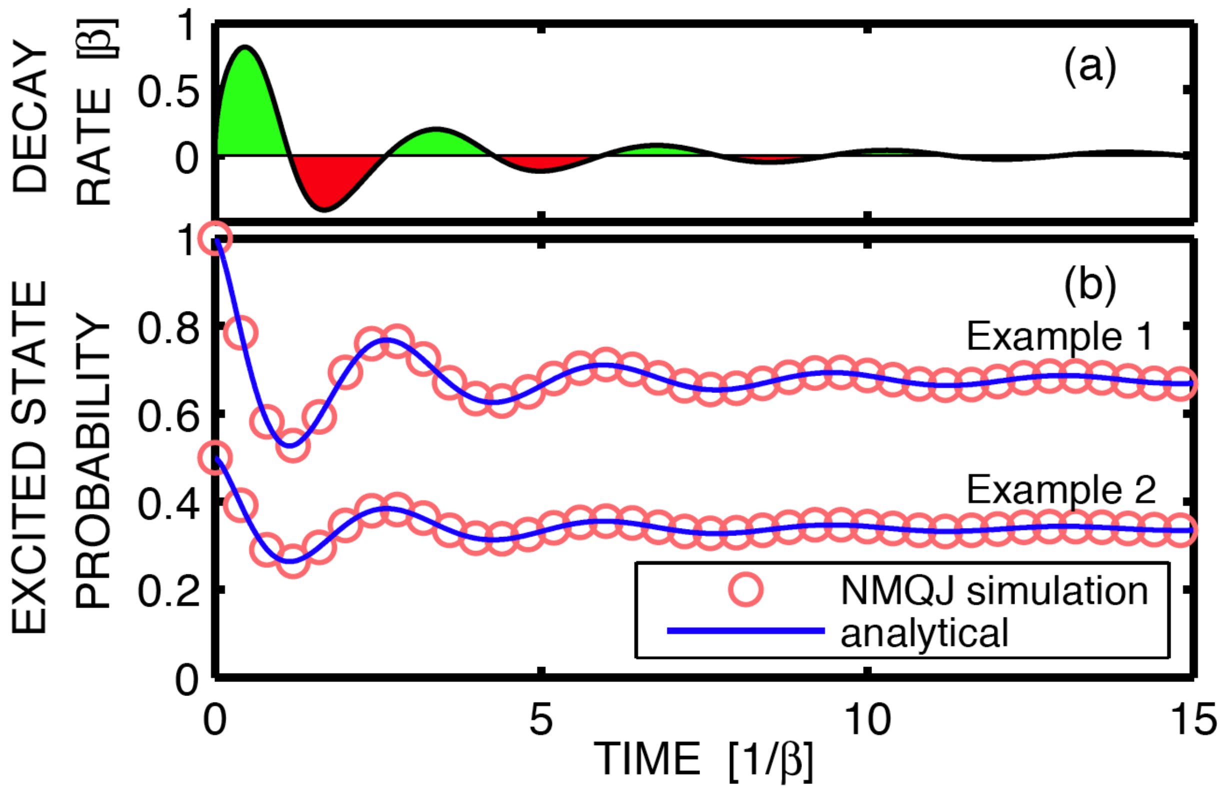
Example: Photonic bandgap material



Piilo, Maniscalco, Härkönen and Suominen, arXiv:0706.4438 [quant-ph] to appear in PRL.

Other methods

For many non-Markovian methods the crucial point is book-keeping of the alternative evolutions and the possibility to restore coherences.

For example (not an exhaustive list):

– Doubled Hilbert space

Breuer, Kappler and Petruccione, PRA 59, 1633 (1999)

– Pseudomodes

Garraway PRA 55, 2290 (1997)

Measurement scheme?

– an attempt to read the reservoir memory will alter it

– the restoration of coherences for $\Delta<0$ excludes the possiblity to ever find a measurement scheme?

Other methods, part 2

The Quantum State Diffusion/Stochastic Schrödinger Equation method has a non-Markovian version as well

Diosi, Gisin and Strunz, PRA 58, 1699 (1998)
Strunz, Diosi and Gisin, PRL 82, 1801 (1999)
Stockburger and Grabert, PRL 88, 170407 (2002)

– stochastic evolution, no jumps

– measurement scheme question also still unclear

Gambetta and Wiseman, PRA 2002, 2003
L. Diosi, quant-ph/0710.5489

Other methods vs. our method

We use the ensemble itself for book-keeping, and thus we do not introduce any additional artificial elements.
Cost: non-independent trajectories/histories

“Minimalistic model” -> physical implications? Positivity.

When decay rates are positive and eventually when the dynamics enters the Markovian region our method becomes equivalent with the standard MCWF method.

Easy to implement, numerically efficient.

Phenomenological extension to regions where one can not write the master equation directly?

Conclusions

Single systems and evolution with quantum jumps are practical aspects of modern quantum mechanics.

For open systems quantum jumps offer both an intuitive and experimentally relevant viewpoint, as well as an efficient simulation tool.

Non-Markovian evolution is becoming increasingly important with reservoir engineering.

The NM evolution can be used to implement Zeno and anti-Zeno effects:
S. Maniscalco, J. Piilo, and K.-A. Suominen, PRL 97, 130402 (2006).
Or to protect entanglement:
S. Maniscalco et al. PRL 100, 090503 (2008).

Conclusions

Single systems and evolution with quantum jumps are practical aspects of modern quantum mechanics.

For open systems quantum jumps offer both an intuitive and experimentally relevant viewpoint, as well as an efficient simulation tool.

Non-Markovian evolution is becoming increasingly important with reservoir engineering.

Within the jump description memory effects can lead to negative jump probabilities. These can be incorporated into the description by restoring alternative histories, and by collective decision-making.

Turku group

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Department of Physics

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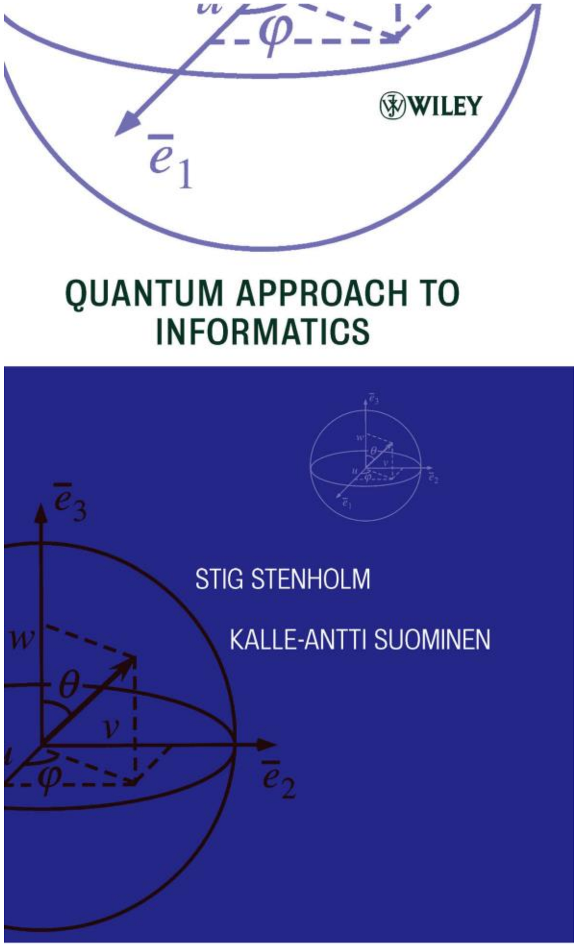

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