Turun yliopisto
University of Turku

Quantum World beyond Ensembles

Kalle-Antti Suominen

Department of Physics and Astronomy

University of Turku

Abstract

Quantum mechanics is a probabilistic theory, predicting phenomena for a large number of identical systems - or the outcome of a large number of identically applied measurements. Is it thus a theory that applies only to ensembles of quantum systems, unable to address the state or dynamics of single systems? One of the fathers of the theory, Erwin Schršdinger, doubted that one would ever observe single quantum systems such as atoms or molecules. Now such observations are basic tools for fundamental and applied research alike, and they encompass even photons, the quanta of light. In 2012 such pioneering work for atoms and photons was honoured with the Nobel Prize in Physics. I shall present examples of such observations and discuss their impact on our understanding of quantum mechanics and its random nature. One of the crucial aspects is looking how the environment of a quantum system and the subsequent decoherence phenomena connects the randomness in quantum mechanics to the randomness in classical world.
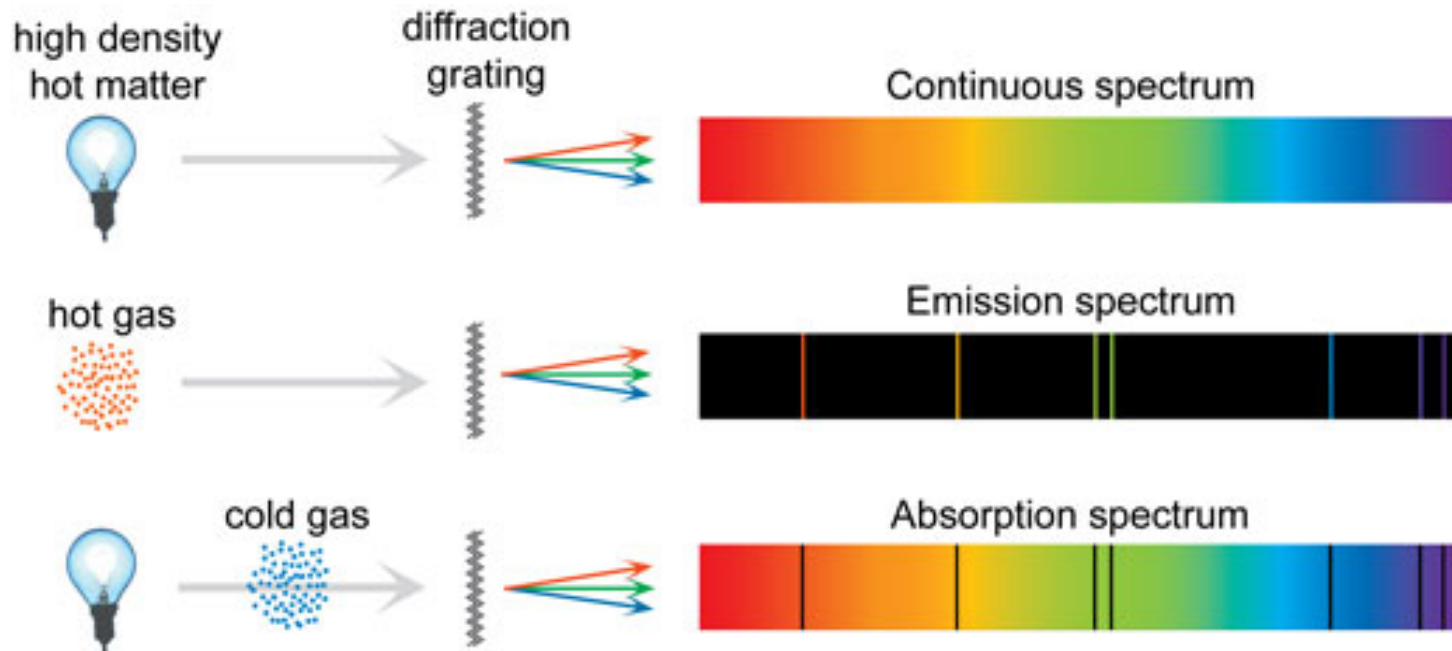
Niels Bohr and Atomic Model 1913 Centennial
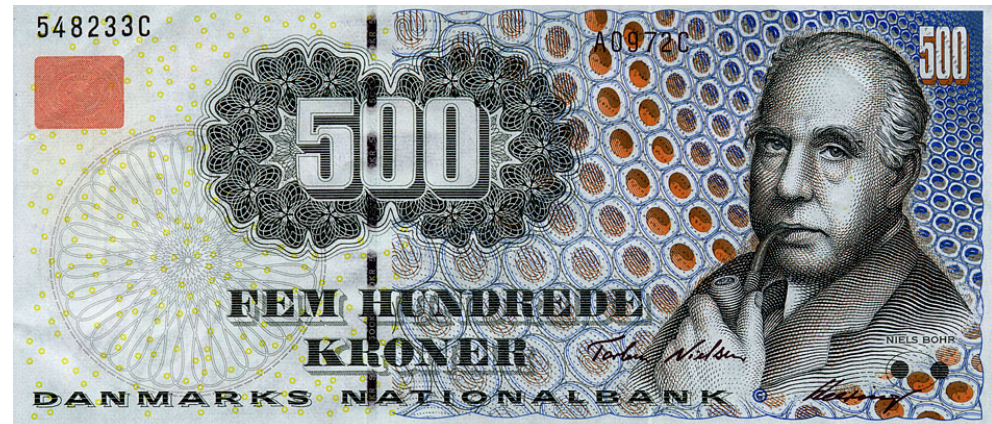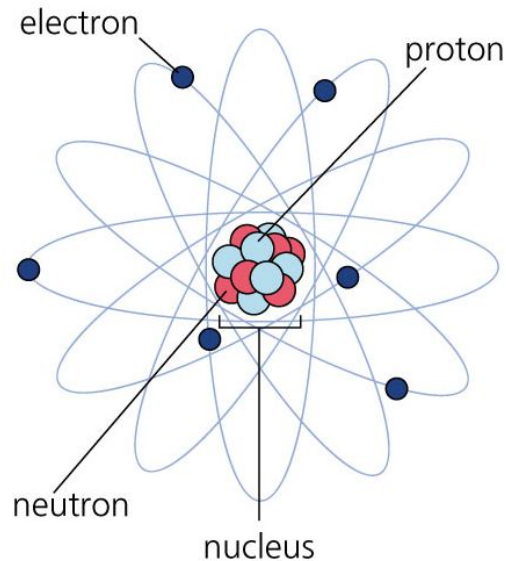
In 1913 Niels Bohr postulated a model for an atom that agreed with the observations. Negatively charged electrons are trapped by the positively charged nucleus and the excited states of these electrons can have only discrete values of energy.

Niels Bohr and Atomic Model 1913 Centennial

Bohr's model explained the discrete spectral lines observed in absorption and emission of light by atoms.

high density hot matter — diffraction grating — Continuous spectrum

hot gas — Emission spectrum

cold gas — Absorption spectrum

http://www.scienceinschool.org

Niels Bohr and Atomic Model 1913 Centennial

In Bohr's model

- Electrons change orbits suddenly, through a "*quantum jump*".

- The change is accompanied by emission or absorption of an energy quantum (later called a photon, in 1926 by Gilbert N. Lewis).

- Agrees conceptually well with Planck's description of black-body radiation (1900) and Einstein's description of the photoelectric effect (1905).

$n = 3$

$n = 2$

$n = 1$

$+Ze$

$\Delta E = h\nu$

http://en.wikipedia.org/wiki/File:Bohr-atom-PAR.svg
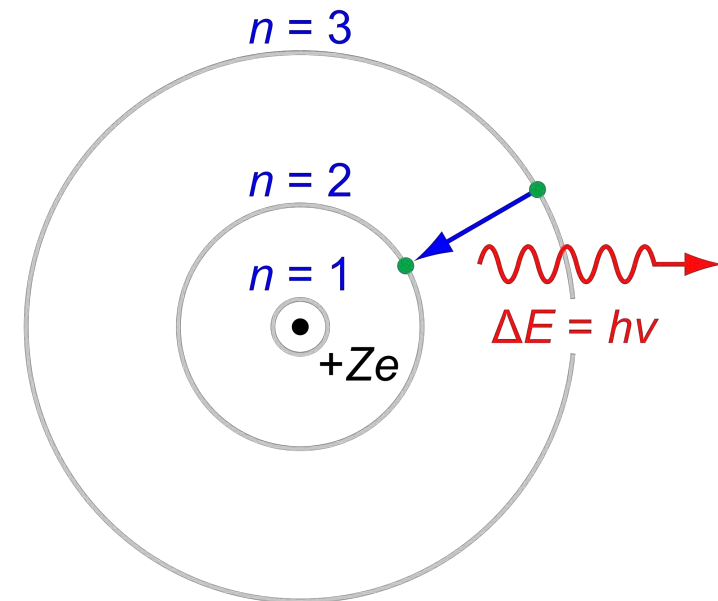
Niels Bohr and Atomic Model 1913 Centennial

- The life-time of an excited electronic state is only an *average*.

- Resembles radioactive decay: if we start with N_0 atoms in an excited state, then after time t, we have only

$$N = N_0 e^{-t/\tau}$$

  excited state atoms left. Here τ is the average life-time of the excited state.

- *For individual atoms the theory has no exact predictions, except the concept of an instantaneous quantum jump and absorption/emission of a single photon.*

$n = 3$

$n = 2$

$n = 1$

+Ze

$\Delta E = h\nu$

http://en.wikipedia.org/wiki/File:Bohr-atom-PAR.svg
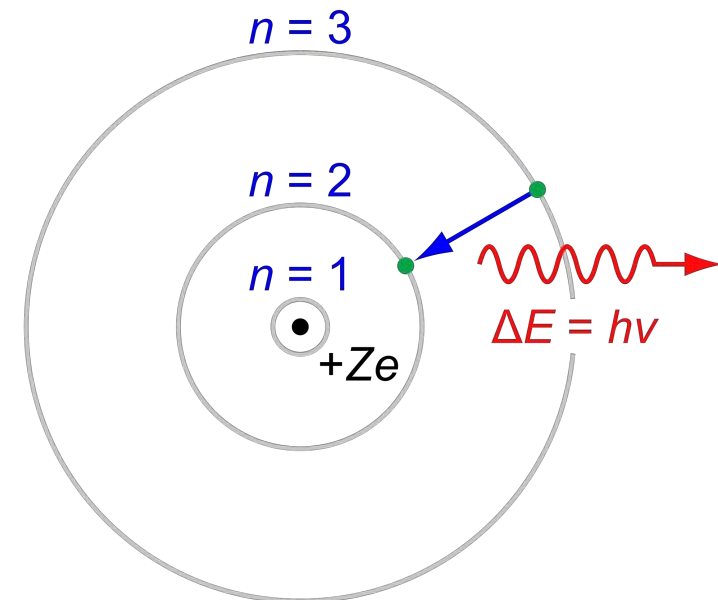
1920's: Modern quantum theory (non-relativistic)

A quantum system is characterized by a well-defined *quantum state* Ψ in a finite or infinite state space $\mathcal{H}$; $\Psi \rightarrow$ state vector $|\Psi>$.

Dynamics is given by the *time-dependent Schrödinger equation*,

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

where *H* is the Hermitean system Hamiltonian, and also the generator of unitary time evolution

$$|\Psi(t)\rangle = U(t,t_0)|\Psi(t_0)\rangle, \quad U(t,t_0) = \mathcal{T}e^{-i\int_{t_0}^{t} dt' H(t')/\hbar}$$

Discrete energy states and their respective wave functions are obtained from the *time-independent Schrödinger equation*. The Hamiltonian contains simply the kinetic energy term plus the potential term, e.g. moving electrons in the Coulomb field of the nucleus in an atom.

This time evolution is *deterministic and reversible*.

1920's: Modern quantum theory (non-relativistic)

The limits of quantum mechanics reside in the interpretation of the wave function, supplied by Max Born.

The probability for being in some state $|\Psi_i\rangle$ is

$$p_i = |\langle \Psi_i | \Psi \rangle|^2$$

i.e., we simply find out the portion of state *i* in the total wave function.

This also demonstrates a fundamental concept beyond the "old" quantum theory: *superposition of states.*

The fact that a quantum state can be "simultaneously" in a superposition of many states, for instance a ground state *g* and some excited state *e*

$$a|g\rangle + b|e\rangle \qquad P_g = |a|^2 \qquad P_e = |b|^2 \qquad |a|^2 + |b|^2 = 1$$

for electrons in an atom, poses conceptual problems for Bohr's quantum jumps.

1920's: Modern quantum theory (non-relativistic)

The issue became a heated debate between Niels Bohr and Erwin 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."

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

Quantum ensembles vs. single quantum systems

In the spirit of probability interpretation for the wave function on can arrive to the conclusion that quantum theory is strictly limited to predicting experimental results for infinitely large ensembles of 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
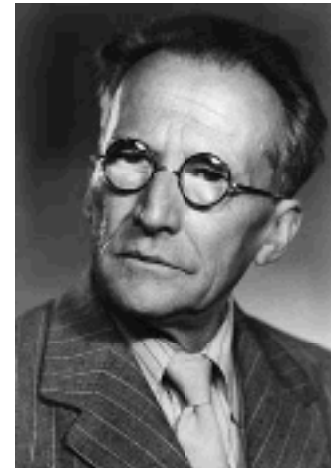
Non-unitary evolution

If we look at the evolution of a large number N of atoms in some excited state, we find that through spontaneous emission of photons their number reduces as

$$N = N_0 e^{-t/\tau}$$

and the number of atoms in the ground state increases accordingly.

But this evolution can not be described by the Schrödinger equation!

It is not unitary (even if the number of atoms on the whole is conserved) and
It is not reversible.

If we look only at the atoms, we are deliberately forgetting the photons. We simply need tools beyond the Schrödinger equation and wave function if we are considering only the atom.

Ensemble description of quantum mechanics

An equivalent way to describe a quantum system is *the density operator:*

$$\hat{\rho}(t) = |\Psi(t)\rangle\langle\Psi(t)|$$

for which the dynamics are given by the Liouville-von Neumann equation

$$i\hbar\frac{d\hat{\rho}}{dt} = [H, \hat{\rho}]$$

which is just 1-to-1 equivalent with the Schrödinger equation.

One can see that $\text{Tr}(\hat{\rho}) = \text{Tr}(\hat{\rho}^2) = 1$ which defines the concept of *a pure state*.

In some basis $\{|\varphi_m\rangle\}$ the density operator can be written in terms of its matrix elements, hence an alternative name *density matrix:*

$$\hat{\rho} = \hat{\mathbb{I}}\hat{\rho}\hat{\mathbb{I}} = \sum_{m,n} |\varphi_m\rangle\langle\varphi_m|\hat{\rho}|\varphi_n\rangle\langle\varphi_n| \equiv \sum_{m,n} \rho_{mn}|\varphi_m\rangle\langle\varphi_n|$$

Ensemble description of quantum mechanics

In the basis $\{|\varphi_m\rangle\}$ the pure state is written as a superposition

$$|\Psi(t)\rangle = \sum_m c_m(t)|\varphi_m\rangle$$

and thus we have

$$\rho_{mn} = c_m c_n^*$$

Clearly the diagonal elements (*m=n*) describe the probabilities, and the off-diagonal elements (*m≠n*) relate to the complex nature of the amplitudes. Thus they are often called *populations* and *coherences*, respectively.

Expectation values for observables are obtained as

$$\langle A \rangle = \mathrm{Tr}(\hat{\rho}\hat{A}) \quad = \quad \sum_m \langle \varphi_m|\hat{\rho}\hat{A}|\varphi_m\rangle$$
$$= \quad \sum_{m,n} \langle \varphi_m|\hat{\rho}|\varphi_n\rangle\langle \varphi_n|\hat{A}|\varphi_m\rangle = \sum_{m,n} \rho_{mn} A_{nm}$$

These expectation values have also variances, i.e., uncertainties, and for complementary observables (position/momentum, spatial components of angular momentum etc.) we have the *Heisenberg relations*.

Ensemble description of quantum mechanics

Let us generalize the concept of density operator/matrix.

Consider first an ensemble of quantum states, in which a particular state $|\Psi_i\rangle$ occurs with probability/weight p_i.

Then for an observable A we have

$$\langle A \rangle = \sum_i p_i \langle \Psi_i | \hat{A} | \Psi_i \rangle \equiv \mathrm{Tr}(\hat{\rho}\hat{A})$$

where the density operator is written in terms of states

$$\hat{\rho} = \sum_i |\psi_i\rangle \, p_i \langle \psi_i |$$

and we can consider it as an ensemble average of state projectors:

$$\hat{\rho} = \overline{|\Psi\rangle \langle \Psi|}$$

Ensemble description of quantum mechanics

Note that for a pure quantum state (a single eigenstate or a superposition) we had

$$\hat{\rho}(t) = |\Psi(t)\rangle\langle\Psi(t)|$$

But for the generalization we have

$$\hat{\rho} = \sum_i |\psi_i\rangle\, p_i \langle\psi_i|$$

This is an example of *a mixed state*, which is an ensemble of pure quantum states, and the pure state is the special case with only one p_i, which is equal to unity. Note that in general the mixed state can not be described by any wave function.

The generalization of the density operator provides e.g. a means to add temperature to the treatment of quantum systems. If the states correspond to energy eigenstates with energy E_i, then in thermal equilibrium p_i are simply

$$p_i = \frac{1}{N} e^{-E_i/k_b T}$$

where k_b is the Boltzmann constant, T is the temperature and N is normalization.

Open quantum systems

The generalized description applies for *an open quantum system*, i.e., the system has additional probabilistic nature beyond the standard probability amplitude description.

The wave function (pure state) description can be applied only to *a closed quantum system*.

In practice the open system description simply allows us to include to the description and dynamics of a quantum state the effect of additional degrees of freedom which we can not include to the Hilbert space in which we define our system.

It leads to the concepts of a system and its environment. Examples are an atom interacting with a continuum of electromagnetic modes, quantum dots and other systems in a solid material interacting with a multitude of phonon modes, or photons in a cavity with mirrors at non-zero temperature.

Atoms and photons

So far we have concentrated on atomic states, but let us look at the photons as well.

The electromagnetic field is a quantum field, with mode functions that arise from classical theory (boundary conditions), but the state of the field is given by quantum mechanics (photon numbers and their superpositions or incoherent classical mixtures).

An atom in free space is surrounded by a continuum of electromagnetic modes, and these modes interact with the atom, even those that have no photons (vacuum).

Quantum Electrodynamics, Quantum optics

Basics of open quantum systems

We assume that the system S and its environment E do not have overlapping state spaces, i.e.,

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$$

We can identify the Hamiltonian of the total system as

$$H = H_S \otimes \mathbb{I}_E + \mathbb{I}_S \otimes H_E + H_{SE}$$

The description of S (all our information about it) is now given by the *reduced density operator*

$$\hat{\rho}_S = \mathrm{Tr}_E \hat{\rho}$$

This reduced density operator corresponds to a mixed state, and thus by considering only a part of the quantum system we leave the pure world of Schrödinger's quantum mechanics behind.

The system and the environment can be interpreted as separated parts of the same quantum system, so their interaction actually *entangles* them.

Basics of open quantum systems

A very typical form for the system-environment coupling is

$$H_{SE} = \sum_k \hat{A}_k^S \otimes \hat{B}_k^E$$

The effect that the environment can have on the system is then given by the system operators $\hat{A}_k^S$

One can roughly consider two different effects:

Change of state in the system: For example, a change of an energy state. Typically energy dissipates into the environment, but in general, especially if the environment is in thermal equilibrium, the system is driven to a thermal equilibrium with the environment.
– example: spontaneous emission of photons by atoms

Pure decoherence: The populations of individual states are not affected, but the related coherences are affected (usually by loss of coherence)
– example: atomic collisions

Basics of open quantum systems

One can show that the time-evolution for the reduced density operator for the system S only is given by

$$i\hbar\frac{d\rho_S}{dt} = [H_S, \rho_S] + i\sum_{k=1}^{N^2-1}\gamma_k\left(A_k\rho_S A_k^\dagger - \frac{1}{2}A_k^\dagger A_k\rho_S - \frac{1}{2}\rho_S A_k^\dagger A_k\right)$$

where $N = \text{Dim}(\mathcal{H}_S)$, γ_k are non-negative, constant rates, and $\{A_k\}$ are specific quantum processes in $\mathcal{H}_S$

This is often called *master equation in Lindblad form.* Its validity requires that S and E are weakly coupled, and there is no memory of past history (Markovian process).

If the operator A_k describes the decay of an atomic state *k* and $A_k^\dagger$ its excitation, then one eventually finds that this equation leads to exponential decay of excited state populations.

Non-unitary evolution arises when we reduce our viewpoint to a quantum system which is fact is not isolated.

Quantum-to-classical transition

A clear advantage in the density operator description is that it can describe the loss of coherence. It means that there is a continuous transition from a pure quantum state

$$\hat{\rho}(t) = |\Psi(t)\rangle\langle\Psi(t)|$$

into a statistical mixture

$$\hat{\rho} = \sum_i |\psi_i\rangle\, p_i \langle\psi_i|$$

It provides one possible explanation why quantum superpositions can not be seen for macroscopic objects: the time for decoherence shortens quickly as the system size increases.

Let us now think about with single particles

"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
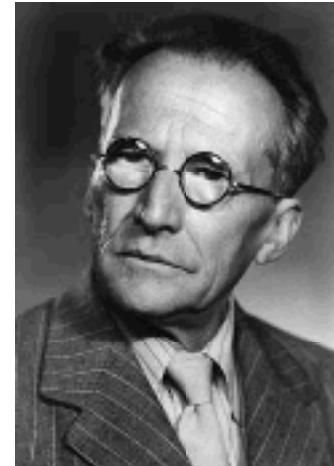
We know that considering e.g. an atom without including the photons is not possible by Schrödinger's formalism, but can be done with a density operator.

That description is nevertheless an ensemble approach.

Experimental development for the last 30-odd years has shown that at least experiments with single quantum systems are possible.
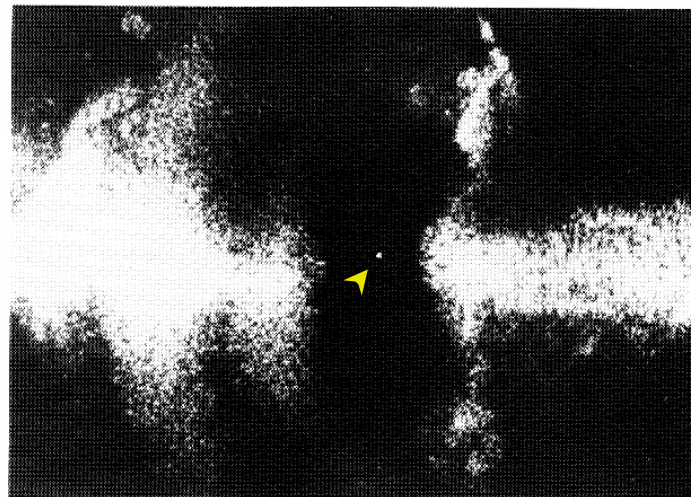
Experimenting with single ions

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.
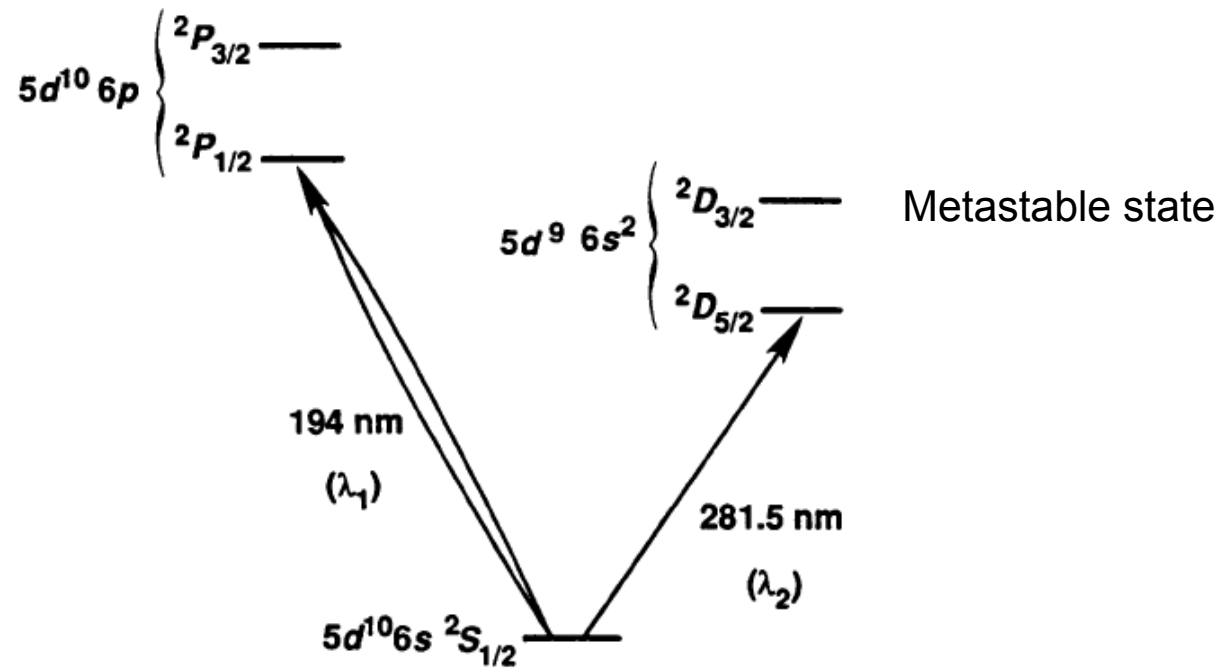
We "see" the ion!
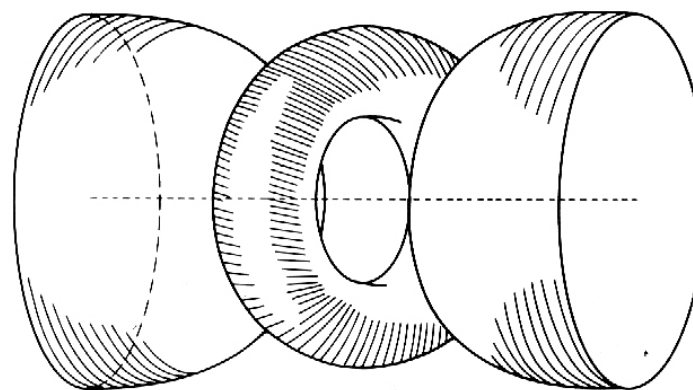
Possibility to see quantum jumps
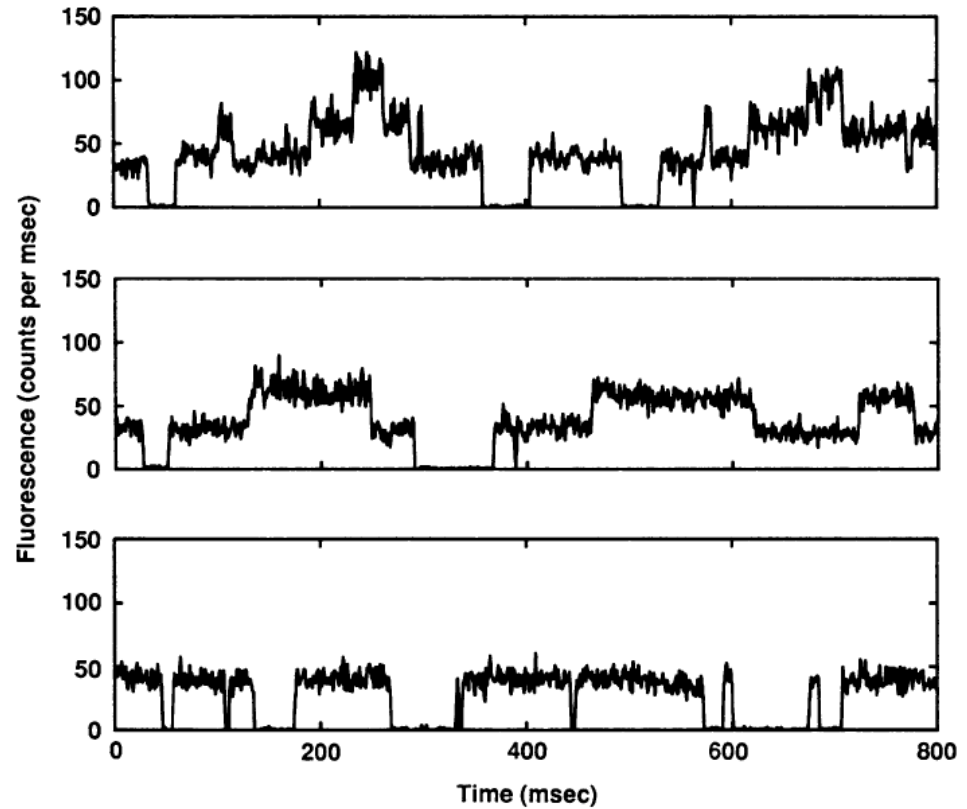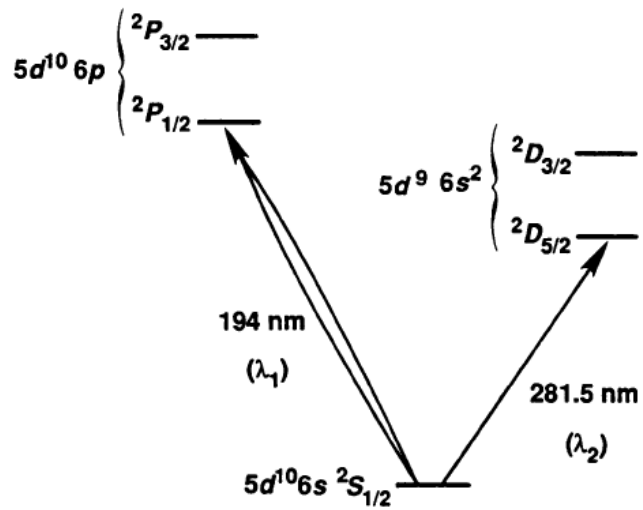
Fluorescent state

Mercury ion Hg$^+$

Metastable state

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

Observation of quantum jumps

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

Ensemble building from single events

Shelved Optical Electron Amplifier: Observation of Quantum Jumps

Warren Nagourney, Jon Sandberg, and Hans Dehmelt

Department of Physics, University of Washington, Seattle, Washington 98195
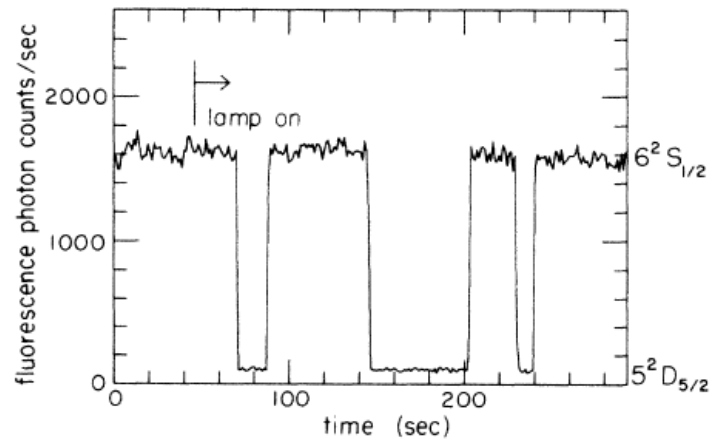(Received 5 May 1986)

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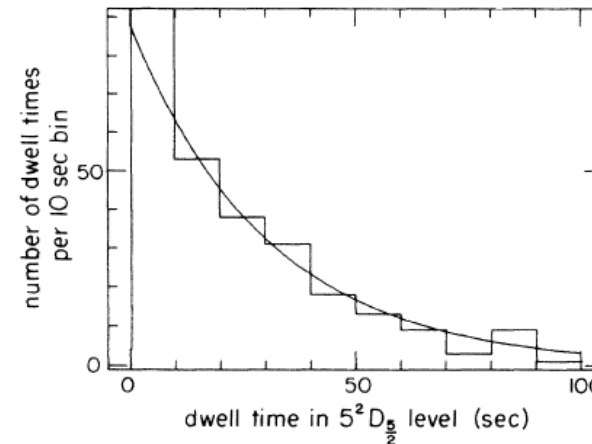
FIG. 3. Histogram of distribution of dwell times in the shelf level for 203 "off" times. A fitted theoretical (exponential) distribution for a metastable lifetime of 30 sec is superposed on the experimental histogram.

Ensemble building from single events

$$\frac{dN}{dt} = -\frac{1}{\tau}N \quad \rightarrow \quad N = N_0 e^{-t/\tau}$$
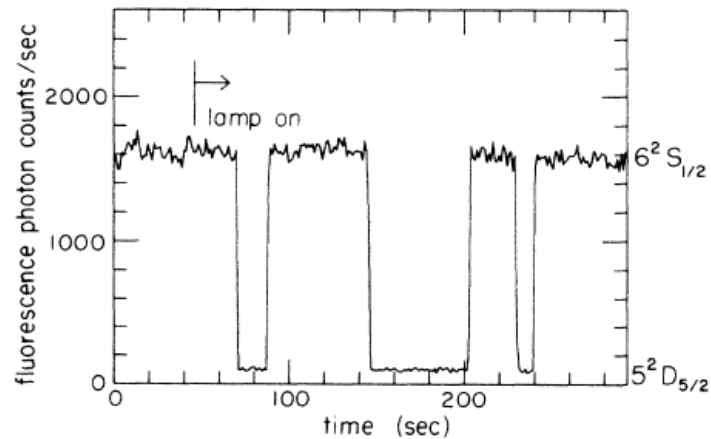
FIG. 2. A typical trace of the 493-nm fluorescence from the $6^2P_{1/2}$ level showing the quantum jumps after the hollow cathode lamp is turned on. The atom is definitely known to be in the shelf level during the low fluorescence periods.
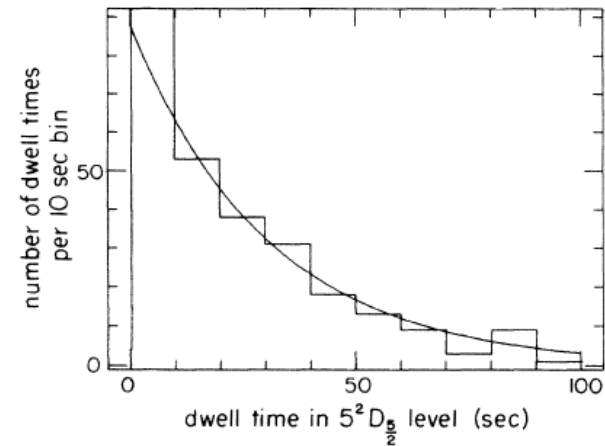
FIG. 3. Histogram of distribution of dwell times in the shelf level for 203 "off" times. A fitted theoretical (exponential) distribution for a metastable lifetime of 30 sec is superposed on the experimental histogram.
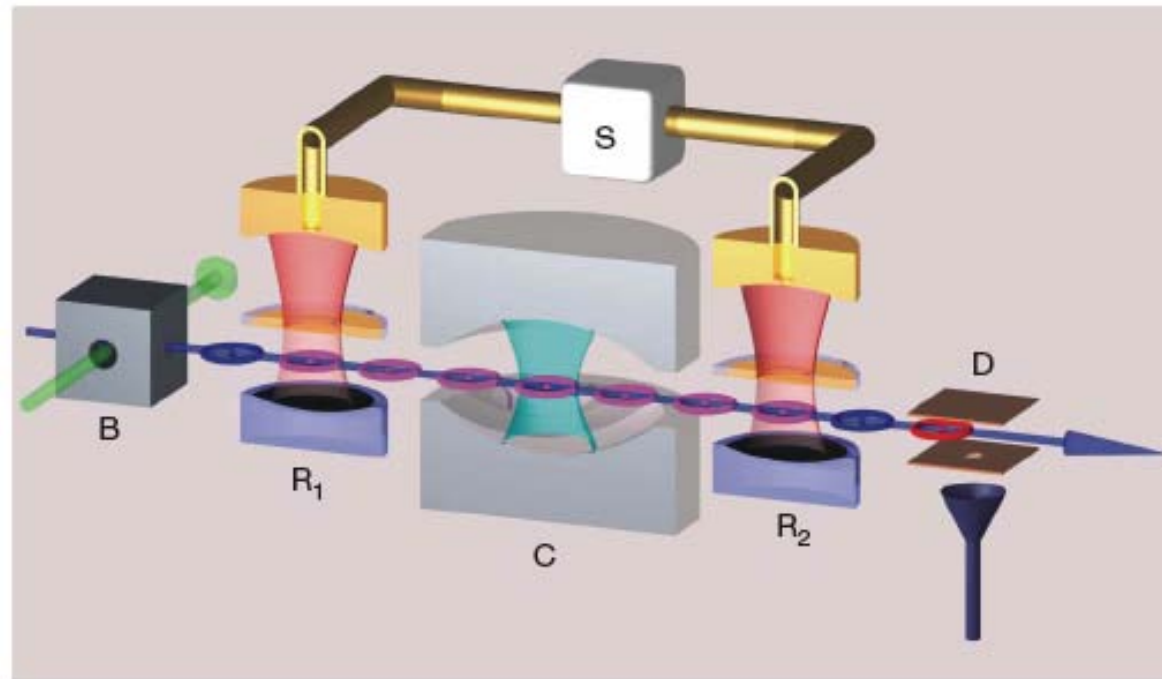
Jumping photons

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]

Jumping photons

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].

![University of Turku logo] Turun yliopisto
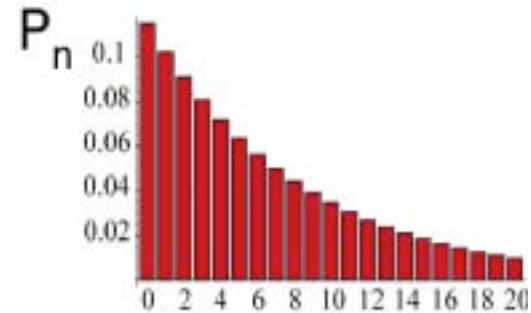University of Turku

Jumping photons

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 $<n> \ll 1$.

Only integral photon numbers can
be observed for single atoms.

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

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

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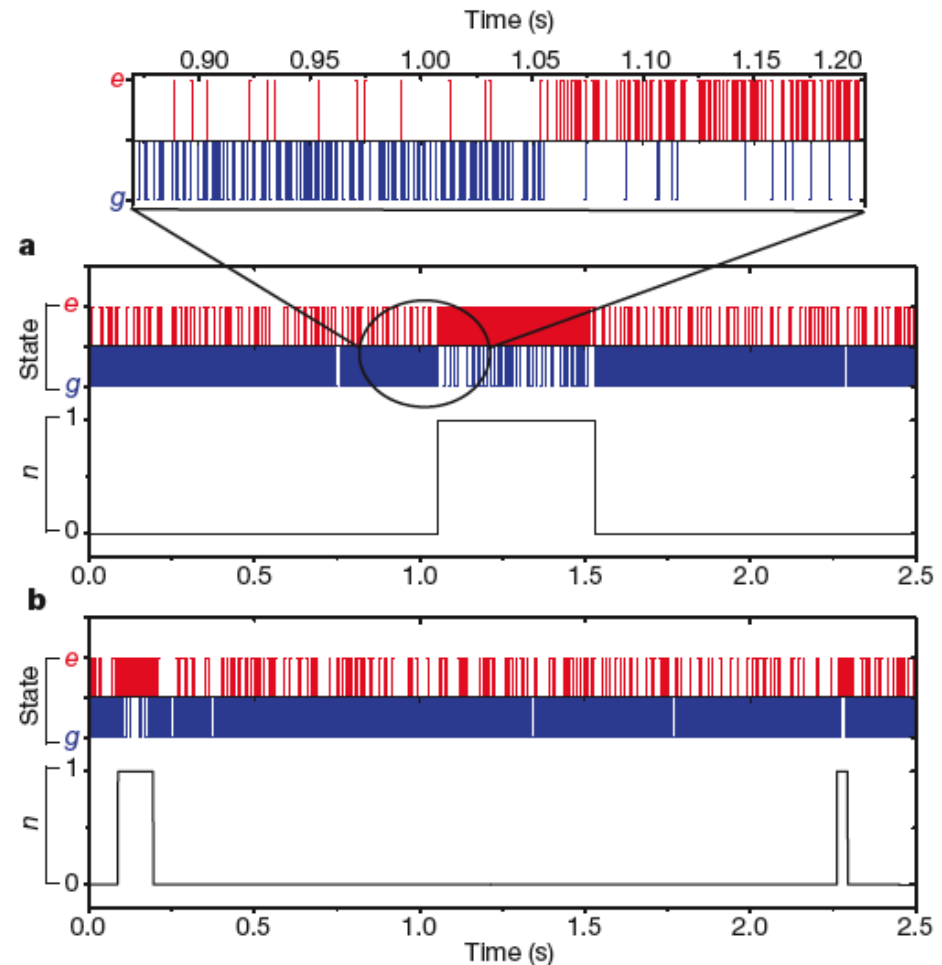
Can we see the birth and death of a thermal photon?

YES!

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

Jumping photons

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.

Further work: prepare n>1, observe the integer step decay into n=0, Guerlin et al., Nature 448, 889 (23 August 2007).
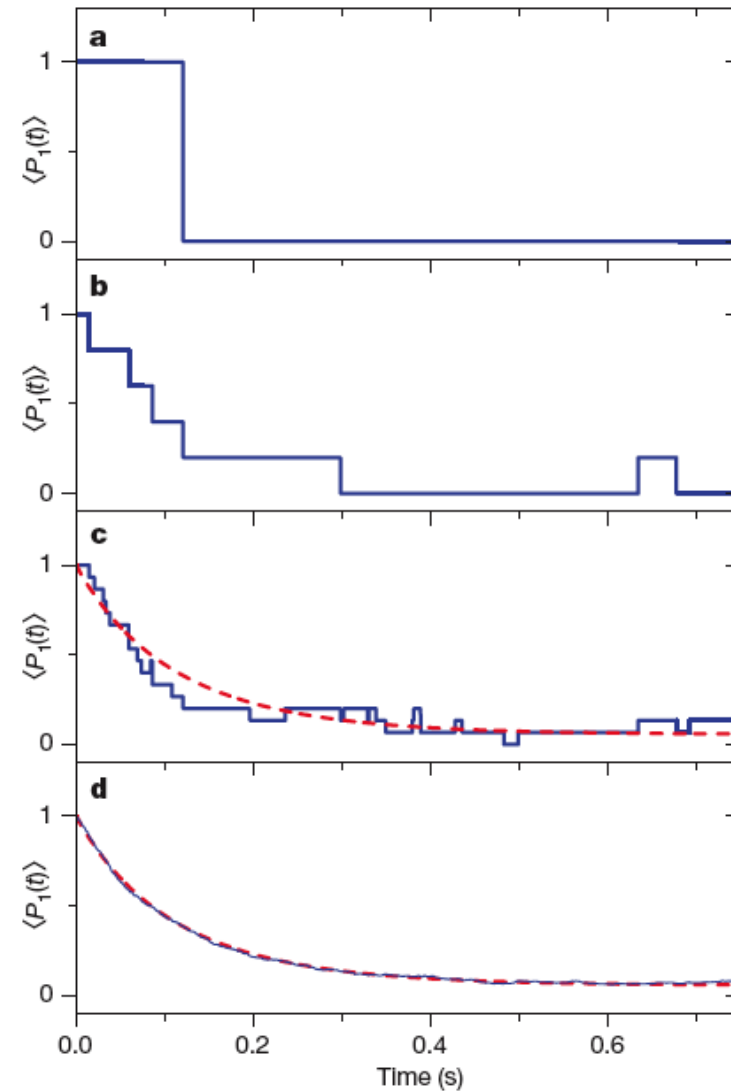
What the experiments tell us?

We see that

a) One can observe single system dynamics

b) Quantum jumps are an integral part of them

c) They are caused by the interaction of a small-scale system with an inifinite environment

d) An average of many such different and seemingly random "telegraphic" signals (histories or trajectories) produces the ensemble average predicted by ensemble quantum mechanics

But did we yet solve the dilemma between Niels and Erwin?

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."

How can a superposition state experience a jump, for example?

Unravelling a quantum system

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

d) The basis for the jump scheme is obtained from the master equation in Lindblad form

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

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

Unravelling a quantum system

Thus we can unravel the ensemble dynamics given by

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

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).

If we look into the "algorithm" we get one version of a solution for jumping superpositions

Monte Carlo Wave Function method

Solve the Schrödinger equation.

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

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.

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

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

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

$$P = \sum_m \delta p_m$$

The operators target only the excited states and ignore the ground state.

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

Monte Carlo Wave Function method
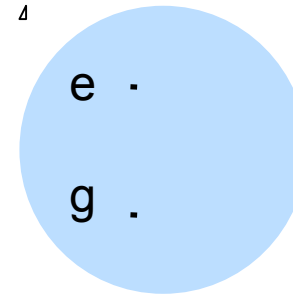
Jump operator

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

Non-Hermitian Hamiltonian

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

Jump probability (and change of norm)

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

e .

g .

Δ

Monte Carlo Wave Function method

1) We proceed by small time steps δt

2) For each step we compute the probability P for a jump
    and generate a random number ε between 0 and 1

3) If $\varepsilon < P$ then a jump happens and the system enters the ground state
    discontinuously

    If $\varepsilon > P$ then we evolve the system under the non-Hermitean
    Hamiltonian, but renormalize the probabilities to unity

4) We proceed to the next time step and repeat steps 2) and 3), and thus
    we generate one possible history for a single system.

5) In the end, we create an ensemble from these single systems, which are
    likely to be unique due to the random numbers.

Monte Carlo Wave Function method

Note the step:

- If $\varepsilon > P$ then we evolve the system under the non-Hermitean Hamiltonian, but renormalize the probabilities to unity.

Its role is easily shadowed by the jumps, but it is equally important in the process.

It states the effect of NOT observing a jump. The non-Hermitean evolution and renormalization correspond to a rotation of the state vector while preserving the sum of probabilities.

It increases the contribution of the ground state in the superposition, and reduces the one for excited states. In other words, if we see no jumps, then it is increasing likely that we were in the groung state in the first place.

Without it we would eventually always see a jump, even if there is a finite probability to have started on ground state.

Unravelling a quantum system

Example: A driven two-state atom + electromagnetic modes

single history **ensemble average**
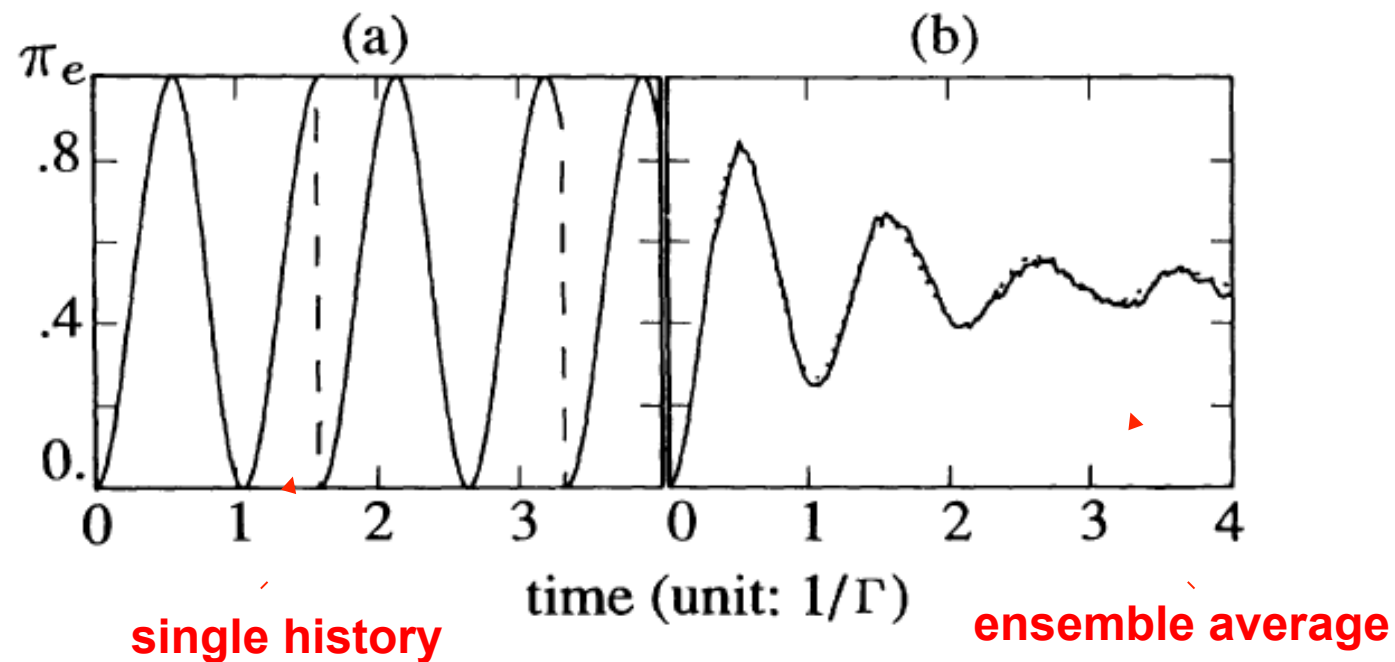
Dalibard, Castin & Mølmer, PRL 68, 580 (1992).

Unravelling a quantum system

- We can treat the open system dynamics as an ensemble of single wave vector histories, where the deterministic evolution (driven by a non-Hermitean Hamiltonian, though) is now perturbed by random jumps: *Piecewise Deterministic Process*.

- The method is very powerful and in some cases can be given a real measurement interpretation.

- It demonstrates how the concept of quantum jumps is not at odds with the concept of superpositions.

- There are other approaches as well, based on either jumps or incremental noise terms (Quantum State Diffusion method).

Summary

Quantum jumps are an integral part of modern quantum mechanics toolbox.

They demonstrate the limits of the theory, and our inability to predict everything exactly. There is always a random element involved.

The formalism required for handling open quantum systems and their dynamics has developed much over the years, and it has been partly fostered by the concept of jumps and single systems.

Open quantum system approach is also currently the best method that we know for handling the quantum-to-classical transition.

Much of the very recent advances have been motivated by quantum information studies and quantum computing, and the general interest in quantum entanglement and protecting quantum systems from decoherence (engineered environments etc.).
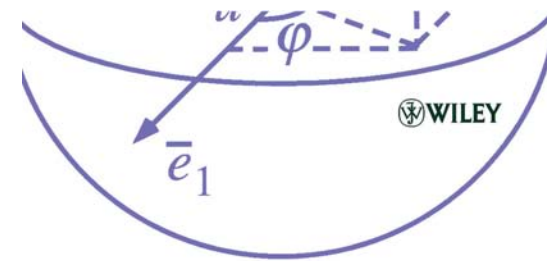
But is this the final word?

Summary

At least for this presentation.

Thank you.

C.G. Gerry and P.L. Knight:
Introductory Quantum Optics
Cambridge University Press, 2005
(ISBN 0-521-52735-X).

Stig Stenholm and Kalle-Antti Suominen:
Quantum Approach to Informatics
John Wiley and Sons, Inc., Hoboken NJ, 2005.
238 pages, ISBN: 0-471-73610-4.