Open Quantum Systems and Decoherence

Kalle-Antti Suominen

Turku Centre for Quantum Physics
Department of Physics and Astronomy
University of Turku
Finland
Contents of Part II

1. Relaxation of a quantum oscillator
2. Decoherence of a quantum register
3. Unravelling the master equation: Quantum jumps
4. Non-Markovian dynamics: Master equation approach
5. Unravelling non-Markovian dynamics: NMQJ method
6. Non-Markovian dynamics and pseudomodes
7. Summary
Relaxation of a harmonic oscillator

• We have derived the Lindblad master equation for a two-level system:

\[ i\hbar \frac{d\rho_S}{dt} = [H'_S, \rho_S] \]

\[ - \frac{i\hbar \gamma_0}{2} n(\omega_S)(\sigma^- \sigma^+ \rho_S + \rho_S \sigma^- \sigma^+ - 2\sigma^+ \rho_S \sigma^-) \]

\[ - \frac{i\hbar \gamma_0}{2} [n(\omega_S) + 1](\sigma^+ \sigma^- \rho_S + \rho_S \sigma^+ \sigma^- - 2\sigma_- \rho_S \sigma^+) \]

\[ \gamma_0 = g^2(\omega_S)G(\omega_S) \]

• Alternatively, one can consider the relaxation of a quantised harmonic oscillator. This is sometimes called the Quantum Brownian Motion problem. Instead of starting from the microscopic derivation (which follows similar lines as the two-level atom derivation), let us just state the final result and then some aspects related to it.
Relaxation of a harmonic oscillator

- If the oscillator is described by operators $a$, $a^\dagger$ then we have

$$H_S = \hbar\omega a^\dagger a$$

and if the interaction with the reservoir causes a lowering or raising the oscillator state by one quantum, then we get eventually

$$\frac{d}{dt}\rho = -i\omega [a^\dagger a, \rho]$$

$$= -\frac{A}{2} (a^\dagger a\rho - 2a\rho a^\dagger + \rho a^\dagger a)$$

$$- \frac{C}{2} (aa^\dagger \rho - 2a^\dagger \rho a + \rho a a^\dagger)$$

which is similar to the two-level atom (both lowering and raising appear as their own Lindblad terms).
Relaxation of a harmonic oscillator

As a next step we can look at the dynamics of the expectation value

\[
\frac{d}{dt} \langle a \rangle = \text{Tr} \left( a \frac{d}{dt} \rho \right)
\]

\[
= -i\omega \text{Tr} \left( [a, a \dagger a] \rho \right)
\]

\[
- \frac{C}{2} \text{Tr} \left( [a, a \dagger a] \rho \right) - \frac{A}{2} \text{Tr} \left( [aa \dagger, a] \rho \right)
\]

\[
= \left( -i\omega - \frac{(C - A)}{2} \right) \langle a \rangle.
\]

where one has used the relation

\[
\text{Tr}(A[B, C]) = \text{Tr}([A, B]C)
\]
Relaxation of a harmonic oscillator

- The solution to the equation is simple:

\[
\langle a(t) \rangle = \exp \left[ - \left( i \omega + \frac{(C - A)}{2} \right) t \right] \langle a(0) \rangle.
\]

- This shows that, as long as C>A, the amplitude is damped in the way expected from a classical solution. This behavior relates to the expectation value only. The operator cannot be damped as this would violate the commutation rules. The correct behavior of the operator is restored by the quantum fluctuations of the environment effecting the damping.

- If C<A, the equations describe a quantum amplifier. This description is, however, incomplete, because the exponential growth can continue for a limited period only. After that nonlinear saturation effects must set in and limit the growth.
Relaxation of a harmonic oscillator

- Let us next consider the expectation value of a proper observable:

\[
\frac{d}{dt} \langle a^\dagger a \rangle = Tr \left( a^\dagger a \frac{d}{dt} \rho \right) = A(\langle a^\dagger a \rangle + 1) - C\langle a^\dagger a \rangle.
\]

which is the same as

\[
\frac{d}{dt} \bar{n} = -(C - A) \bar{n} + A.
\]

- For $C > A$ this agrees with the damping of the amplitude but the inhomogeneous term displays the effects of the fluctuations deriving from the environment providing the damping. In steady state, we have

\[
\bar{n} = \frac{A}{C - A}
\]
Relaxation of a harmonic oscillator

• From

\[ \bar{n} = \frac{A}{C - A} \]

we see that for a reservoir providing no amplification, \( A=0 \), the oscillator relaxes to its ground state. With a thermal reservoir, however, we expect the steady state to be of thermal character

\[ \bar{n} = n_B = \frac{1}{\exp \left( \frac{\hbar \omega}{k_B T} \right) - 1} \]

• This implies the detailed balance condition

\[ \frac{C}{A} = \exp \left( \frac{\hbar \omega}{k_B T} \right) \]

and thus

\[ A = \Gamma n_B, \quad C = \Gamma (n_B + 1), \]

with

\[ \Gamma = \lim_{T \to 0} C \]
Two-level system revisited

- For the two-level system with Bloch vector description we have earlier given the equation

\[
\frac{d}{dt} \vec{R} = \vec{B} \times \vec{R} - \frac{1}{T_1} (R_z - R_{z,0}) \hat{e}_z - \frac{1}{T_2} (R_x \hat{e}_x + R_y \hat{e}_y)
\]

- One the other hand, we have derived for longitudinal noise (change of state) the microscopic master equation. The transverse noise can be added easily and thus we get

\[
\frac{d}{dt} \rho = -i \frac{\omega}{2} [\sigma_z, \rho] - \frac{\gamma}{2} (\rho - \sigma_z \rho \sigma_z)
\]

\[
- \frac{C}{2} (\sigma^+ \sigma^- \rho - 2 \sigma^- \rho \sigma^+ + \rho \sigma^+ \sigma^-)
\]

\[
- \frac{A}{2} (\sigma^- \sigma^+ \rho - 2 \sigma^+ \rho \sigma^- + \rho \sigma^- \sigma^+).
\]
Two-level system revisited

• So now in the equation

\[
\frac{d}{dt} \vec{R} = \vec{B} \times \vec{R} - \frac{1}{T_1} (R_z - R_{z,0}) \hat{e}_z - \frac{1}{T_2} (R_x \hat{e}_x + R_y \hat{e}_y)
\]

we have

\[
\frac{1}{T_1} = A + C,
\]

\[
\frac{1}{T_2} = \gamma + \frac{A + C}{2},
\]

\[
R_{z,0} = \frac{A - C}{A + C}.
\]

where A and C depend on the temperature of the environment (Remember: C is for damping, A for gain). For T = 0 we have only damping and \( R_{z,0} = -1 \), otherwise

\[
R_{z,0} = -\tanh \left( \frac{\hbar \omega}{2 k_B T} \right)
\]
Two-level system revisited

- The master equation is actually a very robust way to describe dynamics. We can e.g. add to the system Hamiltonian terms that couple the original states.

- Another situation occurs frequently in laser spectroscopy. We often use some truncated set of energy eigenstates, but can still have decay out of the system. This is described by adding simply to the relevant energy states decay terms that reduces the population, i.e., we give their energy some imaginary contribution. In atomic collision physics these are called optical potentials as they may depend on position.

- We can also add simply a constant to the right-hand side of the master equation. In laser spectroscopy this stands for pumping the truncated state. Together with the decay terms they usually lead to a steady state for the system.
Decoherence in quantum registers

• Let us consider again the case of pure decoherence for a quantum bit. Qubits can form a register and we can ask the crucial question: how does the decay of coherences scale with the number of qubits?

• We start with a system of two qubits. Now we need to assign them positions as well

\[ H = \frac{1}{2} \sigma_z^a \omega_0^a + \frac{1}{2} \sigma_z^b \omega_0^b + \sum_k b_k^\dagger b_k \omega_k \]

\[ + \sum_k \left( \sigma_z^a (g_k^a b_k^\dagger + g_k^{a*} b_k) + \sigma_z^b (g_k^b b_k^\dagger + g_k^{b*} b_k) \right) \]

• In the interaction picture we get

\[ U(t) = \exp \left\{ \frac{1}{2} \sum_k b_k^\dagger \left[ \sigma_z^a \xi_k^a (t) + \sigma_z^b \xi_k^b (t) \right] - b_k^\dagger \left[ \sigma_z^a \xi_k^{a*} (t) + \sigma_z^b \xi_k^{b*} (t) \right] \right\} \]
Decoherence in quantum registers

- Let us for simplicity assume that $T = 0$. In addition, we select two different initial states

\[
|\Phi^-(\cdot)\rangle = (c_{10}|1_a, 0_b\rangle + c_{01}|0_a, 1_b\rangle) \otimes |0_k\rangle
\]

\[
|\Phi^+(\cdot)\rangle = (c_{00}|0_a, 0_b\rangle + c_{11}|1_a, 1_b\rangle) \otimes |0_k\rangle
\]

- The time evolution of these states is then

\[
|\Phi^-(\cdot)|t\rangle = c_{10}|1_a, 0_b\rangle \pm \frac{1}{2}(\xi^a_k - \xi^b_k) + c_{01}|0_a, 1_b\rangle \pm \frac{1}{2}(\xi^a_k - \xi^b_k),
\]

\[
|\Phi^+(\cdot)|t\rangle = c_{00}|0_a, 0_b\rangle - \frac{1}{2}(\xi^a_k + \xi^b_k) + c_{11}|1_a, 1_b\rangle \pm \frac{1}{2}(\xi^a_k + \xi^b_k).
\]

- This shows an interesting result: as the two qubits approach each other, the decoherence is removed for the first state and enhanced by factor of 2 for part of the second state.

- This leads to the idea of using a subspace of a two-qubit system as a qubit. It is an example of Decoherence-Free Subspaces (DFS).
Decoherence in quantum registers

- Let us continue with some general reduced density matrix for the two-qubit system:
  \[ \rho_{i_a j_a, i_b j_b}(t) = \langle i_a, i_b | T R \{ \varrho(t) \} | j_a, j_b \rangle \]

- Using again the displacement operators one can show that
  \[ \rho_{i_a j_a, i_b j_b}(t) = \rho_{i_a j_a, i_b j_b}(0) \prod_k T R_k \{ R_k T D[(i_a - j_a) \xi_k^a] D[(i_b - j_b) \xi_k^b] \} \]

- The interesting case is that if \( i_a \neq j_a, i_b \neq j_b \), we see collective decay
  \[ \rho_{10,10}(t) = \rho_{10,10}(0) \prod_k T R_k \{ R_k T D(\xi_k^a + \xi_k^b) \} \]
  \[ = e^{-\Gamma^+(t)} \rho_{10,10}(0) \]
  \[ \rho_{10,01}(t) = \rho_{10,01}(0) \prod_k T R_k \{ R_k T D(\xi_k^a - \xi_k^b) \} \]
  \[ = e^{-\Gamma^-(t)} \rho_{10,01}(0) \]

  \[ g_k^a = g_k e^{i k \cdot r_a} \quad \text{and} \quad g_k^b = g_k e^{i k \cdot r_b} \]

  \[ \Gamma(\mathbf{R}, t) \propto \int d\mathbf{k} |g_k|^2 \coth \left( \frac{\omega_k}{2T} \right) \frac{1 - \cos \omega_k t}{\omega_k^2} [1 \pm \cos(\mathbf{k} \cdot \mathbf{R})] \]

  \[ \mathbf{R} = \mathbf{r}_a - \mathbf{r}_b \]
Decoherence in quantum registers

- We can define a transit time between the qubits as $t_s \left( \omega t_s = k \cdot R \right)$.
  Then the two decay rates for finite temperature, normalised to cutoff frequency, $\eta = \omega_c / T$, look like:

![Graph 1](image1)

$e^{-\Gamma^-_{1D}(t)}$

![Graph 2](image2)

$e^{-\Gamma^+_{1D}(t)}$
Decoherence in quantum registers

• The two-qubit situation can be extended into the general L-qubit case. For

\[ \rho_{i_n,j_n}(t) = \langle i_{L-1}, i_{L-2}, \ldots, i_0 | Tr_R \{ \rho(t) \} | j_{L-1}, j_{L-2}, \ldots, j_0 \rangle \]

it turns out that in the limiting case of all qubits at the same position we get

\[ \rho_{1_n,0_n} = \rho_{1_n,0_n}(0) e^{-L^2 \Gamma(t)} \]

whereas for qubits having independent environments the decay rate scales linearly with L.

• Thus the case of having the same environment for all qubits is a double-edged sword: a) in general the decoherence rates scale badly, but b) one can have also very slowly decohering state combinations.
Decoherence in quantum computing: example

- Let us just briefly consider a basic quantum computing operation such as the Discrete Fourier Transformation.

\[
U = \begin{pmatrix}
1 & 1 & 1 & \cdots & 1 \\
1 & \omega & \omega^2 & \cdots & \omega^{2^L-1} \\
1 & \omega^2 & \omega^4 & \cdots & \omega^{2(2^L-1)} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & \omega^{2^L-1} & \omega^{2(2^L-1)} & \cdots & \omega^{(2^L-1)^2}
\end{pmatrix}
\]

\[
\omega = e^{i\pi/2^L}
\]

Original register content

Quality factor \( Q = \text{sum of the red areas} \)
Network for DFT

\[
|a\rangle \quad \longrightarrow \quad |a'\rangle \\
|0\rangle \quad \longrightarrow \quad (|0\rangle + |1\rangle) / \sqrt{2} \\
|1\rangle \quad \longrightarrow \quad (|0\rangle - |1\rangle) / \sqrt{2}
\]

\[
|a_i\rangle a_j \quad \longrightarrow \quad |a'_i a'_j\rangle \\
|0\rangle \quad \longrightarrow \quad |0 \ 0\rangle \\
|0\rangle \quad \longrightarrow \quad |0 \ 1\rangle \\
|1\rangle \quad \longrightarrow \quad |1 \ 0\rangle \\
|1\rangle \quad \longrightarrow \quad |1 \ 1\rangle \times e^{i 2\pi j / 3}
\]
Noise in DFT

• We introduce after each computational step a phase kick that has a random strength given by a Gaussian distribution with a width delta.

• This introduces noise that affects the quality factor Q. How does this noise scale for a fixed delta as a function of the qubit number L?

Noise in DFT

\[ Q \frac{2L}{T} \]

\[ \delta = 0.01, 0.02, 0.03 \]
Noise in approximate DFT
Unravelling of the master equation

• As mentioned before, the system dynamics may become difficult to calculate even if the master equation is known, since if the state space dimension is D, the density matrix has $D^2-1$ a priori independent elements.

• Example: for a wave packet $|\Psi(x, t)\rangle \rightarrow \rho(x, x', t)$ so that the density matrix now contains correlations between positions.

• Such situations arise e.g. in laser cooling of atoms, or laser-assisted ultracold collisions between atoms.

• On the other hand, if we consider the density matrix as representing an ensemble of single quantum systems, we can ask if the time evolution can be regarded as an ensemble of single system histories (or trajectories).

• There is a physical justification to this view: Quantum jumps
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).
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
Bohr vs. Schrödinger

"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

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 ion

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!
Detection scheme

Fluorescent state

Mercury ion Hg$^+$

Metastable state

W.M. Itano, J.C. Bergquist, and D.J. Wineland, Science 37, 612 (1987)
Trapping to the metastable states

W.M. Itano, J.C. Bergquist, and D.J. Wineland, Science 37, 612 (1987)
Ensemble behaviour: exponential decay

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.
Jumping photons

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

Nature 446, 297 (2007) - March 15

Sébastien Gleyzes¹, Stefan Kuhr¹†, Christine Guerlin¹, Julien Bernu¹, Samuel Delégisé¹, Ulrich Busk Hoff¹, Michel Brune¹, Jean-Michel Raimond¹ & Serge Haroche¹²
Rydberg states and microwave cavities

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 thermodynamics

But the cavity is at a finite temperature $T = 0.8 \text{ K}$.

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.
Photon state change by jumps

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

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

This is seen in experimental data

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

**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).
Summary

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 infinite environment

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

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

\[
\frac{d\rho(t)}{dt} = \frac{1}{i\hbar}[H_s,\rho] + \sum_m \Gamma_m C_m \rho C_m^\dagger - \frac{1}{2} \sum_m \Gamma_m \left( C_m^\dagger C_m \rho + \rho C_m^\dagger C_m \right)
\]
Master equation and jump processes

A possible interpretation for the Master equation (Lindblad form)

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

The positive constants \( \Gamma_m \) 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.
Monte Carlo Wave Function Method

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.

$$
\rho(t) = \sum_i P_i(t) \left| \Psi_i(t) \right> \left< \Psi_i(t) \right|
$$

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).
Monte Carlo Wave Function Method

Example: A driven two-state atom + electromagnetic modes

To generate an ensemble member

Solve the Schrödinger equation.

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

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 $P$.

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

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

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

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

$$P = \sum_m \delta p_m$$

$$\delta p_m = \delta t \Gamma_m \langle \psi | C_m^\dagger C_m | \psi \rangle$$
Two-state atom example

Jump operator

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

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 $\delta t$

2. generate random number, did quantum jump occur?  
   - $\delta p < \varepsilon$ no  
   - $\delta p > \varepsilon$ yes

3. renormalize $\Psi$ before new time step

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

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

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

This gives comm. + anticommm. of m.e.
This gives ”sandwich” term of the m.e.
\[
\rho(t + \delta t) = (1 - P) \left(1 - P \right) \frac{\phi(t + \delta t) \langle \phi(t + \delta t) \rangle}{1 - P} + P \frac{C | \Psi(t) \rangle \langle \Psi(t) | C^\dagger}{\langle \Psi(t) | C^\dagger C | \Psi(t) \rangle}
\]

”No-jump” path weight
”Jump” path weight
Jump and normalization
Average
T-evol. 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
\[
P = \delta t \Gamma \langle \Psi | C^\dagger C | \Psi \rangle
\]
Unravelling of master equation: Summary

- 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.

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

- Non-Markovianity implies that there are memory effects.

- Basic treatment is the Nakajima-Zwanzig projection method, which produces an integral involving the density matrix and a memory kernel. Problem: usually not easy to solve, and even harder to simulate.

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

- 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.

- This leads to non-Markovian dynamics. For some cases it can be handled with the time-convolutionless method (TCL).
Microscopic view on non-Markovian dynamics

• Consider the Redfield equation again

\[ \frac{d\rho_S(t)}{dt} = -\frac{1}{\hbar^2} \int_0^t dt' \text{Tr}_E ([H_{SE}(t), [H_{SE}(t'), \rho_S(t) \otimes \rho_E]]) \]

• It was obtained by assuming initially uncorrelated system and environment, an unchanging environment (Born) and replacing

\[ \rho_S(t') \rightarrow \rho_S(t) \]

• The last action formed a part of the Markov approximation. But we do not have the take the integration limit to infinity. Without going into details we see that we will get decay rates that depend on time.

• The key issue is that the more advanced methods (TCL) show that this “partially Markovian” approach gives a consistent master equation up to the second order.
Microscopic view on non-Markovian dynamics

Thus the non-Markovian are given by the *time-local master equation*

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

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 (to obtain CP).

And quantum jumps?
Microscopic view on non-Markovian dynamics

- Thus the non-Markovian dynamics is given by the master equation

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

with

\[
\Delta_\omega(t) = 2 \int_0^t ds \int_0^\infty d\nu J(\nu) \cos[(\nu - \omega)s].
\]

- Examples of physical systems are e.g. and atom coupled with a single but leaky cavity mode:

\[
J_{\text{Lorentz}}(\nu) = \frac{\alpha^2}{2\pi} \frac{\Gamma}{(\nu - \omega_{\text{cav}})^2 + (\Gamma/2)^2},
\]
Microscopic view on non-Markovian dynamics

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

This is possible e.g. if cavity mode and atom are well off-resonance.

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 probabilities*. 
Feynman view on non-Markovian dynamics


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.”
Non-Markovian 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 occurred in the $\Delta(t) > 0$ 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
Non-Markovian quantum jumps

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

No jumps 1 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:

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

P’ s: jump probabilities
D’ s: jump operators

What is the physical meaning of these?
Non-Markovian quantum jumps

<table>
<thead>
<tr>
<th><strong>MCWF</strong></th>
<th><strong>NMQJ</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>( C ) jump operators</td>
<td>( D_{i \rightarrow 0} =</td>
</tr>
<tr>
<td>Lindblad operator</td>
<td>Transfers the state from 1 jump state to no jump state: cancels an earlier quantum jump (jump - reverse jump cycle)</td>
</tr>
</tbody>
</table>

Jump probability

\[
P = \delta t \Delta \langle \Psi | C \, \dagger C | \Psi \rangle
\]

Histories independent on each other

\[
P_{i \rightarrow 0} = \frac{N_0}{N_i} \delta t \Delta \langle \Psi_0 | D \, \dagger D | \Psi_0 \rangle
\]
Example: Decaying two-level system

\[ P = \delta t \Delta \langle \Psi_0 | C^\dagger C | \Psi_0 \rangle \]

\[ P_{\text{g} \rightarrow 0} = \frac{N_0}{N_i} \delta t \Delta \langle \Psi_0 | C^\dagger C | \Psi_0 \rangle \]

\[ |\Psi_0(\tau)\rangle \]

\[ |\Psi_i(\tau)\rangle \]
Example: Decaying two-level system
Non-Markovian quantum jumps: Summary

- The NMQJ method allows the unravelling of the non-Markovian time-local master equation even for negative rates/jump probabilities.

- The method is a straightforward extension of the normal Monte Carlo Wave Function (MCWF) method, and becomes equivalent with it for positive rates. Equivalence to the master equation can be shown.

- It does not correspond to some measurement scheme such as detecting spontaneously emitted photons. In fact, it implies that one can not find such schemes for non-Markovian dynamics.

- The method is already finding its applications in various physical systems, including “quantum biology”.

- The method is based on ideas developed mainly by Jyrki Piilo and it is reported in two articles: J. Piilo at al., PRL 100, 180402 (2008); PRA 79, 062112 (2009).
Alternative approach: Pseudomodes

• An alternative method to consider dynamics for spectral densities which have a pole in complex plane (such as the Lorentzian one) is the pseudomode approach by B.M. Garraway, PRA 55, 2290 (1997)

• We start with the state change Hamiltonian

\[ H = \hbar \omega_0 \sigma_+ \sigma_- + \sum_{\lambda} \hbar \omega_{\lambda} a_{\lambda}^{\dagger} a_{\lambda} + \sum_{\lambda} (\hbar g_{\lambda}^{*} a_{\lambda} \sigma_+ + \text{H.c.}) \]

and assume a state with either zero or one excitations.

\[ |\psi(t)\rangle = c_0 |g, 0_{\lambda}\rangle + c_1(t) |e, 0_{\lambda}\rangle + \sum c_{\lambda}(t) |g, 1_{\lambda}\rangle \]

• It can be shown that a pole \( z_1 = \omega_{c}^{\lambda} - i\Gamma / 2 \) in spectral distribution appears as an extra mode for the system:

\[
\frac{d\rho}{dt} = -i[H_0, \rho] - \frac{\Gamma}{2}[a^{\dagger} a \rho - 2a \rho a^{\dagger} + \rho a^{\dagger} a]
\]

\[ H_0 = \omega_0 \sigma_+ \sigma_- + \omega_c a^{\dagger} a + \Omega_0[a^{\dagger} \sigma_- + a \sigma_+] \]
Alternative approach: Pseudomodes

- The system is now such that the atom and pseudomode form a new system that undergoes normal Markovian decay.

\[
\frac{d\rho}{dt} = -i[H_0, \rho] - \frac{\Gamma}{2}[a^\dagger a\rho - 2a\rho a^\dagger + \rho a^\dagger a]
\]

\[
H_0 = \omega_0 \sigma_+ \sigma_- + \omega_c a^\dagger a + \Omega_0[a^\dagger \sigma_- + a\sigma_+]
\]

- If we write the pseudomode amplitude as \( b_1(t) \) we get the equations of motion for the system:

\[
i \frac{d}{dt} c_1 = \omega_0 c_1 + \Omega_0 b_1, \quad i \frac{d}{dt} b_1 = z_1 b_1 + \Omega_0 c_1
\]

Thus we have the excited state of the atom and the pseudomode coupled, and the pseudomode population can decay out of the system because \( z_1 = \omega_c - i\Gamma/2 \)

- Sum of atomic populations is conserved but not the pseudomode.
Alternative approach: Pseudomodes

- Thus, for all spectral densities with poles we can write a model with a system of an atom+pseudomodes, and the pseudomode population decays in a Markovian fashion.

- We are limited by the need of having one or more poles, but then the approach is not limited to weak couplings between the system (atom) and its environment.
Alternative approach: Pseudomodes

- More poles means more pseudomodes. However, let us consider a special Lorentzian with a dip at the centre (photonic bandgap model):

\[
D(\omega) = \frac{W_1 \Gamma_1}{(\omega - \omega_c)^2 + (\Gamma_1/2)^2} - \frac{W_2 \Gamma_2}{(\omega - \omega_c)^2 + (\Gamma_2/2)^2}
\]

- We get two pseudomodes with constant decay and

\[
H_0 = \omega_0 \sigma_+ \sigma_+ + \omega_c a_1^\dagger a_1 + \omega_c a_2^\dagger a_2 + \Omega_0 [a_2^\dagger \sigma_- + a_2 \sigma_+] \\
+ V(a_1^\dagger a_2 + a_1 a_2^\dagger),
\]

which shows that also the pseudomodes are coupled,

\[
V = \sqrt{W_1 W_2 (\Gamma_1 - \Gamma_2)/2}
\]

but only one of the pseudomodes is coupled to the atom.
Alternative approach: Pseudomodes
Alternative approach: Pseudomodes

• One can actually show that the pseudomode approach and the time-local master equation with time-dependent rates are equivalent.

It turns out that the pseudomode rate of change relates to the time-dependent rates in the time-local non-Markovian master equation:

\[
\frac{d|b_1(t)|^2}{dt} + \Gamma|b_1(t)|^2 = \gamma(t)|c_1(t)|^2
\]

With this, the pseudomode approach becomes also equivalent to the NMQJ method.

• For more details, see L. Mazzola et al., PRA 80, 012104 (2009)

• We can turn this around as well: if a system is coupled to some mode or modes, which then decay in a Markovian way, we have a non-Markovian system.
Summary

• In these lectures I have dwelled into the concepts and dynamics of open quantum systems & decoherence from various directions.

• Non-Markovian dynamics has recently become a popular topic in research due to the existence of spectrally non-trivial environments, or due to the possibility to engineer them (reservoir engineering).

• The drive to construct quantum computers using various e.g. solid state systems challenges some of the traditional quantum optics viewpoints. For instance, one can not assume that the secular approximation is valid in such systems.

• In quantum information (and other fields as well) decoherence is usually considered as a problem. Sometimes, as in energy transport, its presence may actually be necessary, in order to avoid localisation effects (see e.g. recent work by Plenio, Huelga & coworkers).