



Open Quantum Systems and Decoherence

Kalle-Antti Suominen

Turku Centre for Quantum Physics
Department of Physics and Astronomy
University of Turku
Finland

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About literature

There are some textbooks that can be mentioned:

- S. Stenholm & K.-A. Suominen: Quantum Approach to Informatics, Wiley, 2005
- H.-P. Breuer & F. Petruccione: The Theory of Open Quantum Systems, OUP, 2002
- H.M. Wiseman & G.J. Milburn: Quantum Measurement and Control, CUP, 2010
- C.C. Gerry & P.L. Knight: Introductory Quantum Optics, CUP, 2004
- H. Carmichael: Statistical Methods in Quantum Optics 1-2, Springer, 2003 & 2007
- C.W. Gardiner & P. Zoller: Quantum Noise, Springer, 2004

Some basics of closed quantum systems

- Characterized by a well-defined quantum state Ψ in a finite or infinite state space \mathcal{H} ; $\Psi \rightarrow$ state vector $|\Psi\rangle$.

- 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 Hermitian system Hamiltonian, and also the generator of unitary time evolution

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

- This time evolution is *deterministic and reversible*.
- Although the system is closed, external influence is still allowed (described classically, e.g. pulsed and chirped E and B fields) while H remains Hermitian.

Density operator

- An equivalent way to describe the 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*:

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

Populations and coherences

- 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 ($m \neq n$) relate to the complex nature of the amplitudes. Thus they are often called *populations* and *coherences*, respectively.

- Expectation values for observables are obtained as

$$\begin{aligned} \langle A \rangle &= \text{Tr}(\hat{\rho}\hat{A}) = \sum_m \langle\varphi_m|\hat{\rho}\hat{A}|\varphi_m\rangle \\ &= \sum_{m,n} \langle\varphi_m|\hat{\rho}|\varphi_n\rangle\langle\varphi_n|\hat{A}|\varphi_m\rangle = \sum_{m,n} \rho_{mn} A_{nm} \end{aligned}$$

Decoherence in a closed system

- Coherence is associated with the accuracy of the phase relations. Thus in a closed system there should not be any decoherence as a matter of principle.
- Consider a system that is initially (t=0) in a superposition of the energy eigenstates of its Hamiltonian:

$$H|\varphi_m\rangle = E_m|\varphi_m\rangle, \quad |\Psi(0)\rangle = \sum_m c_m(0)|\varphi_m\rangle$$

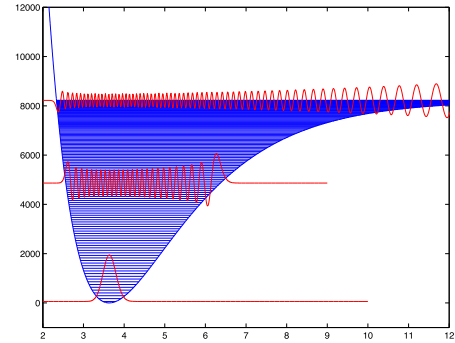
At a later time t we have

$$|\Psi(t)\rangle = \sum_m c_m(t)|\varphi_m\rangle, \quad c_m(t) = e^{-iE_m t/\hbar} c_m(0)$$

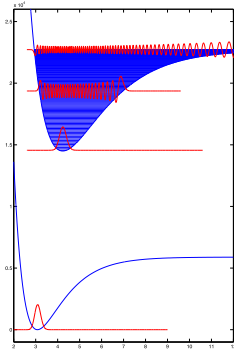
This phase evolution does not affect the populations of the energy states, and it is often called *the dynamical phase*.

- For multiterm superpositions and incommensurate values of eigenenergies we get phenomena labelled often as decoherence.

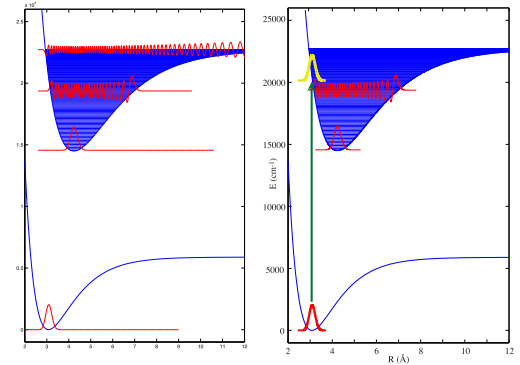
Oscillating wave packets



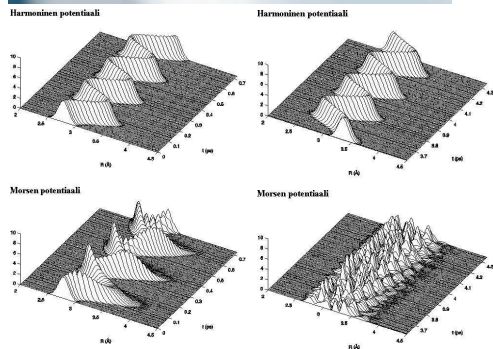
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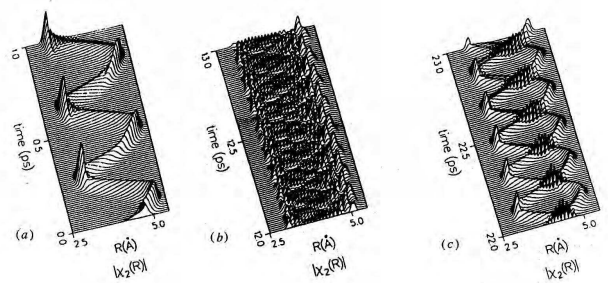
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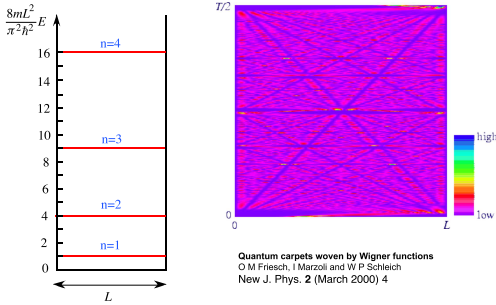
Oscillating wave packets



Oscillating wave packets: Revivals



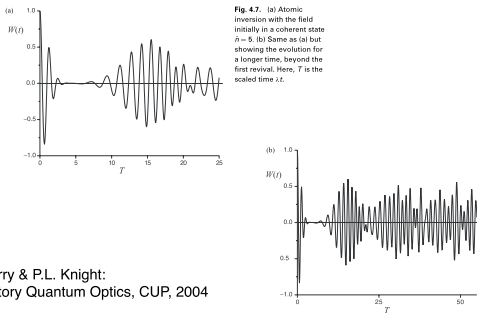
Quantum carpets in a square box



Decoherence in closed systems

- Loss of coherence is simply dephasing of oscillators that have initially the same phase, but due to different and incommensurate frequencies start to oscillate out of phase.
- For the wave packet the “measure of coherence” is e.g. $\langle x \rangle$, which first oscillates but soon settles to some mean value until oscillations might be revived.
- Other systems:
 - Jaynes-Cummings model: a two-level atom + a single cavity mode in a superposition of photon numbers: initially the atomic populations oscillate, then collapse to an apparent steady state, but can be revived partly or fully later.
 - Spin-echo: Ensemble of spins with slightly different precession frequencies around a B field. Leads to dephasing in time T, but by flipping the spins the time evolution is reversed, and at time 2T the spins are in-phase again.

Decoherence in closed systems



C.C. Gerry & P.L. Knight:
Introductory Quantum Optics, CUP, 2004

Composite (multipartite) systems

- In many cases we can partition the system into subsystems and consider them separately. A prime example is a quantum register made of several individually addressable and controllable quantum bits (qubits).
- Then quantum correlations such as entanglement between subsystems can then emerge.
- All knowledge about a subsystem is obtained by tracing out the other degrees of freedom (partial trace). Unless the subsystem is totally uncorrelated with the rest of the system, its description is now possible only through a density operator: we have a *mixed state* (even if the full system is closed and in a pure state).
- Now $\hat{\rho}_{\text{reduced}} = \text{Tr}_{\text{partial}} \hat{\rho}$ and $\text{Tr} \hat{\rho}_{\text{reduced}}^2 \leq 1 = \text{Tr} \hat{\rho}_{\text{reduced}}$

Open quantum systems

- Typically the quantum bits in a register, each in the general form

$$|\psi\rangle_m = e^{i\eta m} \left[\cos\left(\frac{\theta_m}{2}\right) |0\rangle + e^{i\varphi_m} \sin\left(\frac{\theta_m}{2}\right) |1\rangle \right]$$
 are initially in a product state at $t=0$, and then via logic operations involving one or two qubits they evolve into an entangled state for $t>0$.
- Even in a large register (N qubits) all degrees of freedom are in principle tractable.
- For our purposes we can define an open quantum system as such that the rest of the system is for all practical purposes too large to be tractable, but the subsystem at hand is something we can access and describe.
- The rest of the system is often called environment or reservoir and the subsystem is then called system.

Open quantum systems: Basics

- 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

$$\hat{\rho}_S = \text{Tr}_E \hat{\rho}$$
- It is important to note that if $\text{Dim}(\mathcal{H}_S) = D$, we will have $D^2 - 1$ independent density matrix elements. It means that a problem that may be tractable with a state vector is no longer so for density matrix.



About quantum ensembles

- Quantum mechanics is a probabilistic theory and embodied in the probabilities on being in some state $|\Psi_i\rangle$:

$$p_i = |\langle \Psi_i | \Psi \rangle|^2$$
- The advantage of the density operator description that we can generalize the description to include both quantum and other types of probabilities.
- One useful fact is that we can consider the mixed state as a probabilistic sum of pure states.
- There are two ways to approach this description.



About quantum ensembles

- 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

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

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:

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



About quantum ensembles

- Consider now an ensemble of N quantum systems, in which a particular ensemble member k is in a state $|\Psi^{(k)}\rangle$
- Then we have

$$\hat{\rho} = \frac{1}{N} \sum_k |\Psi^{(k)}\rangle \langle \Psi^{(k)}|$$

where the density operator is written in terms of the states of individual ensemble members.
- Thus we have either a sum over the occurrence of quantum states or sum over individual systems in the ensemble (ensemble members).
- If we consider that N_k ensemble members are in the same state as system k , we see that the two viewpoints are connected by writing

$$p_i = \frac{N_i}{N}$$



The effects of the environment

- 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: This usually means a change of an energy state and thus relates to energy exchange between S and E . 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 and molecules



The effects of the environment

- Pure decoherence:* The populations of individual states are not affected, but the related coherences are affected (usually by loss of coherence)
 – example: atomic collisions
- A typical effect is phase diffusion. Consider a quantum bit that goes through a transition

$$c_0|0\rangle + c_1|1\rangle \Rightarrow c_0|0\rangle + c_1 \exp(i\varphi)|1\rangle$$

Here φ is a random change in phase due to H_{SE} . This is equivalent to

$$\hat{\rho} \Rightarrow \begin{pmatrix} \rho_{00} & \exp(-i\varphi)\rho_{01} \\ \exp(i\varphi)\rho_{10} & \rho_{11} \end{pmatrix}$$



Phase diffusion

- For a distribution of random phases we must average: $\overline{\exp(i\varphi)} \equiv \alpha$
- If the distribution is Gaussian, we actually obtain

$$\alpha = 1 + i\overline{\varphi} - \frac{1}{2}\overline{\varphi^2} + \dots \sim \exp\left(-\frac{\overline{\varphi^2}}{2}\right)$$

and

$$\overline{\varphi^2} = \int_{-\infty}^{\infty} \varphi^2 W(\varphi, t) d\varphi = 2Dt$$

which simply states that

$$\hat{\rho} \Rightarrow \begin{pmatrix} \rho_{00} & \exp(-Dt)\rho_{01} \\ \exp(-Dt)\rho_{10} & \rho_{11} \end{pmatrix}$$

- Note that the coherences decay with time while populations are not affected. In the end we'll have only populations, i.e., a classical density matrix only.

Decoherence

- There is an important bias in the two mechanisms highlighted by the simple phase diffusion example:

Phases can erode without affecting state populations, but changes of state will always affect the coherence as well.

Thus in general we consider both mechanisms (state change and pure decoherence) as forms of decoherence.

- There is also a third type of mechanism, which is characterized by non-preservation of the norm (particle number) of the quantum system. Examples are e.g. in laser spectroscopy with a "truncated" set of levels, with decay out and pumping in of population, and multiparticle systems where particles can actually be removed or added.

Decoherence and quantum bits

- As we know already, a quantum bit (qubit) is just a two-state system, equivalent to a spin-1/2 particle in theoretical description.

- Operations affecting a qubit can be given in terms of the Pauli operators:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- These operators allow one to represent the state of a single qubit as

$$\hat{\rho} = \frac{1}{2} (1 + \vec{R} \cdot \vec{\sigma}) \quad \text{where} \quad \vec{\sigma} = \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix} \quad \text{and} \quad R_i \equiv \text{Tr}(\hat{\rho} \sigma_i)$$

- This gives the Bloch vector description of a qubit, applicable to both pure and mixed states.

Bloch sphere

- For pure states of a qubit we can write further that

$$R_x \equiv \langle \psi | \sigma_1 | \psi \rangle = c_0^* c_1 + c_0 c_1^* = \sin \theta \cos \varphi,$$

$$R_y \equiv \langle \psi | \sigma_2 | \psi \rangle = i(c_0 c_1^* - c_1 c_0^*) = \sin \theta \sin \varphi,$$

$$R_z \equiv \langle \psi | \sigma_3 | \psi \rangle = c_0 c_0^* - c_1 c_1^* = \cos \theta.$$

- Clearly the z-component of the Bloch vector gives population inversion, and x- and y-components are the coherences.
- The length of the vector is unity for a pure system and thus it resides on the surface of a unit sphere (Bloch sphere).
- For mixed systems, even though probabilities are conserved, the length of the Bloch vector is less than unity.

Bloch vector dynamics

- The Bloch vector was originally used to describe the dynamics of a spin in external magnetic fields.
- Usually one has a constant field in z-direction that separates the spin-up and spin-down energy states due to Zeeman effect, and then an applied (and weaker) coupling field. The latter field is often pulsed and oscillating or rotating in the xy-plane.
- Assuming a B-field, we can write the equation of motion for the Bloch vector for a pure state as

$$\frac{d\vec{R}}{dt} = \vec{B} \times \vec{R} \quad H = \begin{pmatrix} H_{00} & H_{01} \\ H_{10} & H_{11} \end{pmatrix}$$

where the effective field vector in terms of the qubit Hamiltonian is

$$\vec{B} = \{(H_{01} + H_{10}), i(H_{01} - H_{10}), (H_{00} - H_{11})\} = \text{Tr}(H\vec{\sigma})$$

Irreversible Bloch vector dynamics

- In NMR physics one can identify the two previous decoherence mechanisms as longitudinal and transverse relaxation, and write the full open quantum system equation of motion as

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

where $R_{z,0}$ is the equilibrium (infinite time) value of the population inversion and the time scales T_1 and T_2 are the longitudinal or energy relaxation time scale and transverse or phase relaxation time.

Typically $T_1 > T_2$ so that coherences are lost much faster than the populations are affected.

- We shall return to this equation again later with a more rigorous treatment of the reduced density operator dynamics.

Quantum channels

- The spin terminology has led to the terms such as σ_x and σ_z noise for change of state and pure decoherence.

In quantum information one often considers dynamical processes (especially transmission) as quantum channels that can be given the generalized measurement or Kraus operator description. The open system dynamics are mainly considered as channel-induced errors. Then the appropriate terms are bit flip error and phase flip error, respectively.

- We can define a set of POVM operators so that

$$\hat{\rho} \Rightarrow \sum_{\mu} p_{\mu} A_{\mu} \rho A_{\mu}^{\dagger} = \sum_{\mu} \tilde{A}_{\mu} \rho \tilde{A}_{\mu}^{\dagger}$$

$$\text{where} \quad \tilde{A}_{\mu} = \sqrt{p_{\mu}} A_{\mu}, \quad \sum_{\mu} \tilde{A}_{\mu}^{\dagger} \tilde{A}_{\mu} = 1$$

Physical environments

- The spin system is one example of a physical quantum system embedded in an environment.
- Another example is formed by the electronic states of atoms, molecules and even quantum dots that couple to the surrounding electromagnetic degrees of freedom, even to the vacuum (spontaneous emission).
- Many systems surrounded by solid state structures interact with the phonon excitations of the environment (spins, trapped charged particles, photons in a cavity).
- Thus it is convenient to assume that the system is coupled (weakly) to some quantised bosonic excitations (photons, phonons, magnons etc.) that have also some spectral density.

Some concepts for future use

- The bosonic field excitations are described by creation and annihilation operators for each mode of the field (labelled with wave vector \mathbf{k} , which corresponds to a frequency ω of the mode):

$$\hat{b}_{\mathbf{k}}^{\dagger}, \hat{b}_{\mathbf{k}}$$

- There may be other degrees of freedom such as polarization that add to the spectral density $J(\omega)$ (also known as $G(\omega)$ depending whether it also contains the frequency-dependence of the system-environment coupling).
- The operators change the field energy by $\pm\hbar\omega$ and they obey the bosonic commutation relations

$$[\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}^{\dagger}] = \delta_{\mathbf{k}, \mathbf{k}'}$$

More concepts for future use

- Quantum bits and other two-level systems are extensively treated with the Pauli matrices. A few relations and definitions are good to keep in mind:

$$[\sigma_i, \sigma_j] = 2i\sigma_k \quad \sigma_i^2 = 1$$

where indices i,j,k can be cyclically permuted.

- Also they are traceless but

$$\text{Tr}(\sigma_i \sigma_j) = 2\delta_{ij}$$

holds.

- Finally, we can define state change operators for the two level system in the form

$$\sigma^+ = \frac{1}{2}(\sigma_x + i\sigma_y), \quad \sigma^- = \frac{1}{2}(\sigma_x - i\sigma_y)$$

Example: Qubit and pure decoherence

- This model has been studied under variety of contexts, such as the spin-boson model, and double-well tunnelling model by Caldeira and Leggett.

- Here I follow the description given in G.M. Palma et al., Proc. R. Soc. Lond. A 452, 567 (1996)

- We assume a thermal reservoir of bosonic excitations (R_T) and write the total Hamiltonian as

$$H = \frac{1}{2}\sigma_z\omega_0 + \sum_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} \omega_{\mathbf{k}} + \sum_{\mathbf{k}} \sigma_x (g_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} + g_{\mathbf{k}}^* b_{\mathbf{k}})$$

- We also make the important assumption that the reservoir is large and its state is not affected by the system and initially to total system density operator is

$$\varrho(0) = \rho(0) \otimes \prod_{\mathbf{k}} R_{\mathbf{k}T}$$

Example: Qubit and pure decoherence

- As usual, it is best to move to *interaction picture* in which the time evolution becomes

$$U(t) = \exp \left\{ -i \int_0^t \sum_{\mathbf{k}} \sigma_x (g_{\mathbf{k}} b_{\mathbf{k}}^{\dagger} e^{i\omega_{\mathbf{k}} t'} + g_{\mathbf{k}}^* b_{\mathbf{k}} e^{-i\omega_{\mathbf{k}} t'}) dt' \right\}$$

$$= \exp \left\{ \sigma_x \frac{1}{2} \sum_{\mathbf{k}} (b_{\mathbf{k}}^{\dagger} \xi_{\mathbf{k}}(t) - b_{\mathbf{k}} \xi_{\mathbf{k}}^*(t)) \right\}$$

with

$$\xi_{\mathbf{k}}(t) = 2g_{\mathbf{k}} \frac{1 - e^{i\omega_{\mathbf{k}} t}}{\omega_{\mathbf{k}}}$$

Example: Qubit and pure decoherence

- Here $U(t)$ is a conditional displacement operator for the field, and the action depends now on the qubit state. For an unentangled pure state we get

$$U(t)|0\rangle \otimes |\Psi\rangle = |0\rangle \otimes \prod_{\mathbf{k}} D(-\frac{1}{2}\xi_{\mathbf{k}}(t)) |\Psi\rangle$$

$$U(t)|1\rangle \otimes |\Psi\rangle = |1\rangle \otimes \prod_{\mathbf{k}} D(+\frac{1}{2}\xi_{\mathbf{k}}(t)) |\Psi\rangle$$

with the displacement operator

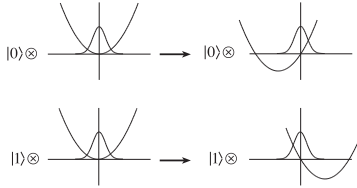
$$D(\xi_{\mathbf{k}}) = \exp \{ b_{\mathbf{k}}^{\dagger} \xi_{\mathbf{k}} - b_{\mathbf{k}} \xi_{\mathbf{k}}^* \}$$

Example: Qubit and pure decoherence

- This means simply that the time evolution entangles the qubit with the environment. For example, at $T = 0$ we have only vacuum and thus

$$(c_0|0\rangle + c_1|1\rangle) \otimes |0_k\rangle \xrightarrow{U(t)} c_0|0\rangle - \frac{1}{2}\xi_k(t) + c_1|1\rangle + \frac{1}{2}\xi_k(t)$$

where $|\frac{1}{2}\xi_k(t)\rangle$ is a coherent state of field.



Example: Qubit and pure decoherence

- Let us next look at the system density matrix elements, and especially the coherences as no bit flips are created by the interaction.

- We now have

$$\rho_{ij}(t) = \langle i | \text{Tr}_R U(t) \rho(0) U^{-1}(t) | j \rangle$$

and especially

$$\begin{aligned} \rho_{10}(t) &= \prod_k \text{Tr}_k \{ R_{kT} D(\xi_k(t)) \} \rho_{10}(0) \\ &= e^{-\Gamma(t)} \rho_{10}(0). \end{aligned}$$

- It is noteworthy that so far there has been no approximations, only the assumption of an initial product state.

Example: Qubit and pure decoherence

- It can be shown that for a harmonic oscillator in a thermal equilibrium

$$\text{Tr}_k \{ R_{kT} D(\xi_k) \} = \exp \left\{ -\frac{|\xi_k|^2}{2} \coth \left(\frac{\omega_k}{2T} \right) \right\}$$

when setting Boltzmann constant to unity.

- In the continuum limit we get finally

$$\begin{aligned} \Gamma(t) &\propto \int dk |g_k|^2 \coth \left(\frac{\omega_k}{2T} \right) \frac{1 - \cos \omega_k t}{\omega_k^2} \\ &\propto \int d\omega \frac{dk}{d\omega} G(\omega) |g(\omega)|^2 (1 + 2\langle n(\omega) \rangle_T) \frac{1 - \cos \omega t}{\omega^2} \end{aligned}$$

with

$$\langle n(\omega) \rangle_T = \exp(-\omega/2T) \text{cosech}(\omega/2T)$$

and $G(\omega)$ is the spectral density of the environment.

Example: Qubit and pure decoherence

- To get some results from the general expression we assume that

$$(dk/d\omega) G(\omega) |g(\omega)|^2 \propto \omega^n e^{-\omega/\omega_c}$$

- It is important to note that we have introduced a cut-off function to the spectrum, which effectively (as one will see) determines the limiting time scale with which the environment can affect the system.

- If we further set $n = 1$, we'll get

$$\Gamma(t) \propto \int d\omega e^{-\omega/\omega_c} \coth \left(\frac{\omega}{2T} \right) \frac{1 - \cos(\omega t)}{\omega}$$

leading to an analytical expression

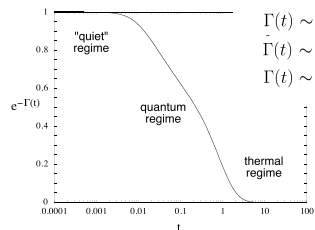
$$\Gamma(t) \propto \ln(1 + \omega_c^2 t^2) + 2 \ln \left[\frac{1}{\pi T t} \sinh(\pi T t) \right]$$

Example: Qubit and pure decoherence

- In general and especially with the expression

$$\Gamma(t) \propto \ln(1 + \omega_c^2 t^2) + 2 \ln \left[\frac{1}{\pi T t} \sinh(\pi T t) \right]$$

we can identify three regions of dynamics:

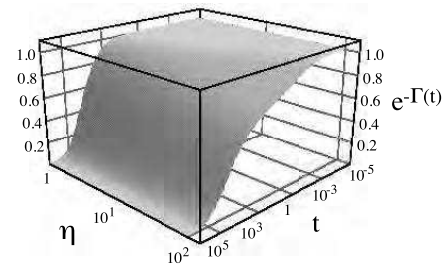


$$\begin{aligned} \Gamma(t) &\sim \omega_c^2 t^2 \text{ for } t < \omega_c^{-1} \\ \Gamma(t) &\sim 2 \ln \omega_c t \text{ for } \omega_c^{-1} < t < T^{-1} \\ \Gamma(t) &\sim T t \text{ for } t > T^{-1} \end{aligned}$$

$$\omega_c/T = 100$$

Example: Qubit and pure decoherence

- We can further define the scaled cut-off quantity $\eta = \omega_c/T$, and time in units of $1/T$, we get the following picture





General approach to open quantum systems

- Now we try to get a more general description for the open system dynamics when coupled to an environment described by a spectrum of bosonic excitations.

- Again, we assume as the initial state $\rho(0) = \rho_S(0) \otimes \rho_E$ (we omit the hats from operators).

- For the total system we assume unitary time evolution

$$\rho(t) = U(t, 0)[\rho_S(0) \otimes \rho_E]U^\dagger(t, 0)$$

and we also have

$$\rho_S(t) = \text{Tr}_E[\rho(t)]$$

as the reduced system density operator, that gives system-related expectation values via

$$\langle A_S \rangle = \text{Tr}_S(A_S \rho_S)$$



General approach to open quantum systems

- As a starting point we take the Liouville-von Neumann equation

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

which becomes now

$$i\hbar \frac{d\rho_S}{dt} = \text{Tr}_E([H, \rho])$$

and remembering that

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

- It can be shown that the above evolution is equivalent to a dynamical map $V(t)$

$$\rho_S(t) = V(t)\rho_S(0)$$



Dynamical maps and semigroups

- The *dynamical map* is important, because if we assume that the environment maintains no memory about its interaction with the system (Markovian approximation), then

$$V(t_1 + t_2) = V(t_1)V(t_2), \quad t_1, t_2 \geq 0$$

and the elements of the map for a *dynamical semigroup*.

- After some mathematical steps one eventually obtains the general form

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

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 (although Gorini, Kossakowski and Sudarshan published it in 1976).



Scattering approach to the Lindblad form

- Interestingly, there is an alternative way to view the irreversible dynamics. Let us consider the evolution as a series of scattering events, where a perturbative encounter lasts for a time Δt , and again, there is no memory carried in the environment between the events, nor relevant system evolution during the very short Δt .

- We describe the process via the scattering matrix \mathbf{S} :

$$\rho(t + \Delta t) = \mathbf{S}(\Delta t)\rho(t)\mathbf{S}^\dagger(\Delta t)$$

and the reaction matrix \mathbf{T} :

$$\mathbf{S} = \mathbf{1} + i\mathbf{T}$$

- Normalization is preserved during an event, thus we have

$$\mathbf{S}^\dagger \mathbf{S} = (\mathbf{1} - i\mathbf{T}^\dagger)(\mathbf{1} + i\mathbf{T}) = \mathbf{1}$$

which leads to

$$-i(\mathbf{T} - \mathbf{T}^\dagger) = 2\mathbf{T}_{imag} = \mathbf{T}^\dagger \mathbf{T}$$



Scattering approach to the Lindblad form

- Next we assume that there is a distinguishable set of events, characterized by \mathbf{T}_j and rate r_j .

- One can calculate the change in density matrix as an ensemble average

$$\begin{aligned} \Delta\rho &= \rho(t + \Delta t) - \rho(t) \\ &= \sum_j r_j \left[i(\mathbf{T}_j \rho - \rho \mathbf{T}_j^\dagger) + \mathbf{T}_j \rho \mathbf{T}_j^\dagger \right] \Delta t. \end{aligned}$$

- We can denote the ensemble average with an overbar as usual, take the system Hamiltonian H into account, and divide both sides with Δt , and take the limit $\Delta t \rightarrow \infty$:

$$\frac{d\rho}{dt} = -\frac{i}{\hbar} [H, \rho] + i(\overline{\mathbf{T}}\rho - \rho\overline{\mathbf{T}}^\dagger) + \overline{\mathbf{T}}\rho\overline{\mathbf{T}}^\dagger.$$



Scattering approach to the Lindblad form

- By writing $\mathbf{T} = \mathbf{T}_{real} + i\mathbf{T}_{imag}$ we get

$$\begin{aligned} \frac{d\rho}{dt} &= -\frac{i}{\hbar} [(H - \hbar\overline{\mathbf{T}}_{real}), \rho] - (\overline{\mathbf{T}}_{imag}\rho + \rho\overline{\mathbf{T}}_{imag}^\dagger) + \overline{\mathbf{T}}\rho\overline{\mathbf{T}}^\dagger \\ &= -\frac{i}{\hbar} [(H - \hbar\overline{\mathbf{T}}_{real}), \rho] - \frac{1}{2} (\overline{\mathbf{T}}^\dagger \mathbf{T} \rho + \rho \overline{\mathbf{T}}^\dagger \mathbf{T}) + \overline{\mathbf{T}}\rho\overline{\mathbf{T}}^\dagger, \end{aligned}$$

- We see that this approach gives even the dressing or renormalization of the system states by the environment interaction (e.g. Lamb shift).

- We now assume for \mathbf{T} the following decomposition into specific system state projections with specific project-related rate:

$$\mathbf{T} = \sum_k \lambda_k t_k, \quad t_k = |\chi_k\rangle\langle\psi_k|$$



Scattering approach to the Lindblad form

- If we assume that different reactions lack coherence, we have

$$\overline{\lambda_k \lambda_n} = \lambda_k^2 \delta_{kn}$$

which leads to the final form

$$\frac{d\rho}{dt} = -\frac{i}{\hbar} [H, \rho] - \frac{1}{2} \sum_k \lambda_k^2 \left(t_k^\dagger t_k \rho + \rho t_k^\dagger t_k - 2t_k \rho t_k^\dagger \right).$$

- Thus this alternative approach allows one to obtain the master equation in Lindblad form, describing the trace-preserving irreversible quantum dynamics of an open quantum system.



Complete positivity and the Lindblad form

- Let us consider the case when S and E are already entangled by the interaction. Now we assume a general linear operation on system only.

- The result must be a density operator that has only non-negative eigenvalues, otherwise the operation is non-physical.

- This is the requirement of *complete positivity (CP)*.

- It can be shown that an operation L is CP iff it can be written as

$$L(\rho) = \sum A_i^\dagger \rho A_i, \quad \sum A_i A_i^\dagger = 1$$

where we have again the Kraus operators, and the operation is trace-preserving.

- This is not quite the Lindblad form, but let us demand that the dynamics of the density operator is CP and trace preserving.



Complete positivity and the Lindblad form

- Let us add the operator X and demand that the trace of the system density operator is preserved (i.e., the trace of the time derivative is zero):

$$\frac{d}{dt} \rho = \sum_i A_i^\dagger \rho A_i - X \rho - \rho X$$

- It is clear that the above requirement sets

$$X = \frac{1}{2} \sum_i A_i A_i^\dagger$$

and we recover the Lindblad form.

- CP is a crucial component in showing that the Lindblad form is the most general form that one can obtain for Markovian (memoryless) evolution.



Microscopic perturbative description

- Consider again

$$H = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E + H_{SE}$$

and let's use the interaction picture so that

$$i\hbar \frac{d\rho}{dt} = [H_{SE}, \rho]$$

- Clearly we can take an iterative approach and write

$$\rho(t) = \rho(0) - \frac{i}{\hbar} \int_0^t dt' [H_{SE}(t'), \rho(t')]$$

- Next we insert this into the original equation and take the trace over the environment, obtaining (note that $\text{Tr}_E([H_{SE}(t), \rho(0)]) = 0$)

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



Microscopic perturbative description

- We stop iterations here, to the second order, and start making approximations. It means effectively that we assume a weak coupling between system and its environment.

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

- First we make *the Born approximation* by assuming that the environment is not affected by the interaction with the system so that we have

$$\rho(t) \simeq \rho_S(t) \otimes \rho_E$$

for all times t.

- The next step is a part of *the Markov approximation*. We assume that the past of the system does not affect the future (only the present density operator):

$$\rho_S(t') \rightarrow \rho_S(t)$$



Redfield equation

- By making these two approximations we get

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

This is *the Redfield equation*.

- To complete the Markov approximation we assume that any correlation between S and E induced by H_{SE} decays faster than the time scale of variation for $\rho_S(t)$

- It means that we can set $s = t - t'$ and extend the upper integration limit to infinity (if we do not, our eventual decay rates will not be constants ...)

Born-Markov master equation

- Thus we have arrived to the Born-Markov master equation

$$\frac{d\rho_S(t)}{dt} = -\frac{1}{\hbar^2} \int_0^\infty ds \text{Tr}_E ([H_{SE}(t), [H_{SE}(t-s), \rho_S(t) \otimes \rho_E]])$$

- This equation is local in time, i.e., it contains the system density operator at time t only on both sides.
- To solve it exactly for some particular problem may not be simple.
- It is not quite equivalent with the Lindblad form. It turns out that to derive the Lindblad form from Born-Markov master equation one still needs to make *the secular approximation*, which is similar to the rotating wave approximation in quantum optics.
- Let us approach this last issue through a specific example.

Two-state system with state change dynamics

- We continue with the Born-Markov master equation

$$\frac{d\rho_S(t)}{dt} = -\frac{1}{\hbar^2} \int_0^\infty ds \text{Tr}_E ([H_{SE}(t), [H_{SE}(t-s), \rho_S(t) \otimes \rho_E]])$$

and take the Hamiltonian

$$H_S = \frac{\hbar\omega_S}{2} \sigma_z \quad H_E = \sum_k \hbar\omega_k b_k^\dagger b_k$$

$$H_{SE} = \sum_k (g_k b_k + g_k b_k^\dagger) \overbrace{(\sigma^+ + \sigma^-)}^{\sigma_x}$$

Operator hats and vector markings from k have been omitted for simplicity.

Two-state system with state change dynamics

- Next we move to the interaction picture and obtain

$$H_{SE}(t) = \sum_k (g_k b_k e^{-i\omega_k t} + g_k^* b_k^\dagger e^{i\omega_k t}) (\sigma^+ e^{i\omega_S t} + \sigma^- e^{-i\omega_S t})$$

- At this point we make the assumption that the fast-oscillating terms in H_{SE} do not contribute to the final result. Thus we get the new Hamiltonian (only oscillations with frequency differences are kept)

$$H_{SE}(t) = \sum_k (g_k b_k e^{-i(\omega_k - \omega_S)t} \sigma^+ + g_k^* b_k^\dagger e^{i(\omega_k - \omega_S)t} \sigma^-)$$

- This often referred to also as taking away the non-energy-conserving terms.

Two-state system with state change dynamics

- As we are solving the Born-Markov equation

$$\frac{d\rho_S(t)}{dt} = -\frac{1}{\hbar^2} \int_0^\infty ds \text{Tr}_E ([H_{SE}(t), [H_{SE}(t-s), \rho_S(t) \otimes \rho_E]])$$

we need to evaluate

$$\text{Tr}_E ([H_{SE}(t), [H_{SE}(t-s), \rho_S(t) \otimes \rho_E]])$$

The result will have four terms:

$$\text{Tr}_E (H_{SE}(t) H_{SE}(t-s) \rho_S \rho_E - H_{SE}(t) \rho_S \rho_E H_{SE}(t-s) - H_{SE}(t-s) \rho_S \rho_E H_{SE}(t) + \rho_S \rho_E H_{SE}(t-s) H_{SE}(t))$$

Two-state system with state change dynamics

- Here the thermal equilibrium and independence of the environment modes comes to help: only terms with

$$\langle b_k^\dagger b_k \rangle \text{ and } \langle b_k b_k^\dagger \rangle = 1 + \langle b_k^\dagger b_k \rangle$$

will survive the trace over E and we need to keep only those terms. Let us also set $\hbar = 1$

$$H_{SE}(t) H_{SE}(t-s) = \sum_k |g_k|^2 (b_k b_k^\dagger \sigma^+ \sigma^- e^{-i(\omega_k - \omega_S)s} + b_k^\dagger b_k \sigma^- \sigma^+ e^{+i(\omega_k - \omega_S)s})$$

$$H_{SE}(t-s) H_{SE}(t) = \sum_k |g_k|^2 (b_k b_k^\dagger \sigma^+ \sigma^- e^{+i(\omega_k - \omega_S)s} + b_k^\dagger b_k \sigma^- \sigma^+ e^{-i(\omega_k - \omega_S)s})$$

Two-state system with state change dynamics

- For the sandwich terms we get

$$H_{SE}(t) \rho_S \rho_E H_{SE}(t-s) = \sum_k |g_k|^2 (b_k \sigma^+ \rho_S \rho_E b_k^\dagger \sigma^- e^{-i(\omega_k - \omega_S)s} + b_k^\dagger \sigma^- \rho_S \rho_E b_k \sigma^+ e^{+i(\omega_k - \omega_S)s})$$

$$H_{SE}(t-s) \rho_S \rho_E H_{SE}(t) = \sum_k |g_k|^2 (b_k \sigma^+ \rho_S \rho_E b_k^\dagger \sigma^- e^{+i(\omega_k - \omega_S)s} + b_k^\dagger \sigma^- \rho_S \rho_E b_k \sigma^+ e^{-i(\omega_k - \omega_S)s})$$

- Before proceeding let us assume that the k -sum can be transformed into a frequency integral:

$$\sum_k |g_k|^2 \rightarrow \int d\omega g^2(\omega) G(\omega) \quad \text{Tr}_E (b_k^\dagger b_k \rho_E) \rightarrow \langle n(\omega) \rangle$$

$$\text{Tr}_E (b_k b_k^\dagger \rho_E) \rightarrow \langle n(\omega) + 1 \rangle$$

Two-state system with state change dynamics

- We can see that we get integrals of the type

$$\Gamma_1^\pm = \int_0^\infty ds \int_0^\infty d\omega g^2(\omega) G(\omega) \langle n(\omega) \rangle e^{\pm i(\omega - \omega_S)s}$$

and

$$\Gamma_2^\pm = \int_0^\infty ds \int_0^\infty d\omega g^2(\omega) G(\omega) (n(\omega) + 1) e^{\pm i(\omega - \omega_S)s}$$

Due to the Markov approximation we extended the time integration to infinity and now these integrals can be evaluated (time integral gives the delta-function as real part and the prime value as imaginary part).

- We can write $\Gamma_1^\pm = \frac{1}{2}\gamma_1 \pm i\frac{1}{2}S_1$
 $\Gamma_2^\pm = \frac{1}{2}\gamma_2 \pm i\frac{1}{2}S_2$

Two-state system with state change dynamics

- Our four terms now become eight

$$\begin{aligned} & \Gamma_2^- (\sigma^+ \sigma^- \rho_S - \sigma^- \rho_S \sigma^+) \\ & + \Gamma_2^+ (\rho_S \sigma^+ \sigma^- - \sigma^- \rho_S \sigma^+) \\ & + \Gamma_1^+ (\sigma^- \sigma^+ \rho_S - \sigma^+ \rho_S \sigma^-) \\ & + \Gamma_1^- (\rho_S \sigma^- \sigma^+ - \sigma^+ \rho_S \sigma^-) \end{aligned}$$

and can be eventually cast into the form

$$\begin{aligned} & \frac{1}{2}\gamma_1 (\sigma^- \sigma^+ \rho_S + \rho_S \sigma^- \sigma^+ - 2\sigma^+ \rho_S \sigma^-) \\ & \frac{1}{2}\gamma_2 (\sigma^+ \sigma^- \rho_S + \rho_S \sigma^+ \sigma^- - 2\sigma^- \rho_S \sigma^+) \\ & + i\frac{1}{2}S_1 [\sigma^- \sigma^+, \rho_S] + i\frac{1}{2}S_2 [\sigma^+ \sigma^-, \rho_S] \end{aligned}$$

Two-state system with state change dynamics

- We can see from

$$\begin{aligned} & \frac{1}{2}\gamma_1 (\sigma^- \sigma^+ \rho_S + \rho_S \sigma^- \sigma^+ - 2\sigma^+ \rho_S \sigma^-) \\ & \frac{1}{2}\gamma_2 (\sigma^+ \sigma^- \rho_S + \rho_S \sigma^+ \sigma^- - 2\sigma^- \rho_S \sigma^+) \\ & + i\frac{1}{2}S_1 [\sigma^- \sigma^+, \rho_S] + i\frac{1}{2}S_2 [\sigma^+ \sigma^-, \rho_S] \end{aligned}$$

that the first two lines give us the irreversible Lindblad form, and the two terms on the last line provide a shift to the system energies (renormalization, Lamb shift) and are usually ignored.

Two-state system with state change dynamics

- Finally, we can write

$$\begin{aligned} i\hbar \frac{d\rho_S}{dt} = & [H'_S, \rho_S] \\ & - \frac{i\hbar\gamma_0}{2} n(\omega_S) (\sigma^- \sigma^+ \rho_S + \rho_S \sigma^- \sigma^+ - 2\sigma^+ \rho_S \sigma^-) \\ & - \frac{i\hbar\gamma_0}{2} [n(\omega_S) + 1] (\sigma^+ \sigma^- \rho_S + \rho_S \sigma^+ \sigma^- - 2\sigma^- \rho_S \sigma^+) \end{aligned}$$

Here $\gamma_0 = g^2(\omega_S)G(\omega_S)$ is clearly a rate related to vacuum processes, i.e., it is the rate for spontaneous emission at $T = 0$.

- We can see that the first Lindblad term disappears at $T = 0$ and is related to the system absorbing energy from the environment. The second term relates to emission of energy into the environment, which can happen at $T = 0$ (spontaneous emission) and at $T \neq 0$ (stimulated emission).

Two-state system with state change dynamics

- The rate $\gamma_0 = g^2(\omega_S)G(\omega_S)$ contains the spectral density and the coupling evaluated at the exact resonance. This is due to the Markov approximation.
- In that sense the approach is similar to the Fermi Golden rule, which also gives transition rates that are proportional to the density of states at resonance.
- The Lindblad form allows one to identify clear processes in the system that happen with a certain rate due to the coupling to the environment. When combined with the concept of building quantum ensembles from single members it opens possibilities for unravelling the master equation dynamics.