Theory of Open quantum systems

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1 Fundamentals

Hilbert space

For every quantum system there is an associated vector space, the so-called Hilbert space $\mathcal{H}$.

For our purpose a vector space is defined by a set of d-dimensional vectors

$$\vec{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} \quad \text{with } v_k \in \mathbb{C}$$

- Dirac notation:

standard basis: $|k\rangle = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \leftarrow k^{th}$ position

Any vector can be expanded as

$$|v\rangle = \sum_{k=1}^{d} v_k |k\rangle \quad \text{with } v_k \in \mathbb{C}.$$

The coefficients v_k are called probability amplitudes, since the probability for being in the state $|k\rangle$ is $|v_k|^2$

- Scalar product (inner product):

„bra" vector: $\langle v| = |v\rangle^+$ ← transpose & complex conjugation

$$\langle v|w\rangle = (v_1^*, \dots, v_d^*) \begin{pmatrix} w_1 \\ \vdots \\ w_d \end{pmatrix} = \sum_{k=1}^{d} v_k^* w_k$$

- normalisation condition:

$$\underbrace{1 = \sum_{k=1}^{d} |v_k|^2}_{\text{probabilities sum up to 1}} = \sum_{k=1}^{d} v_k^* v_k = \langle v|v\rangle = \| |v\rangle \|^2$$

i.e. every vector in $\mathcal{H}$ shall be normalised

- outer product:

The outer product of two vectors in the same Hilbert space is defined as

$$|v\rangle\langle w| = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} (w_1^* \dots w_d^*) = \begin{pmatrix} v_1 w_1^* & \dots & v_1 w_d^* \\ \vdots & & \vdots \\ v_d w_1^* & \dots & v_d w_d^* \end{pmatrix}$$

Time evolution

The state vector of a quantum system satisfies the Schrödinger equation

$$\frac{\partial}{\partial t}|\psi(t)\rangle = -iH|\psi(t)\rangle,$$

where H is the Hamiltonian of the system.

There exists a unitary operator $U(t)$ which evolves the state in time:

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$

For time-independent Hamiltonians:

$$U(t) = \exp(-itH) = \sum_{m=0}^{\infty} \frac{(-itH)^m}{m!}.$$

For time-dependent Hamiltonians:

$$U(t) = \mathcal{T} \exp\left(-i \int_0^t d\tau\, H(\tau)\right)$$

$\uparrow$ time-ordering operator

Spectral decomposition

- Spectral theorem: A linear operator $A: \mathcal{H} \to \mathcal{H}$ obeys $A^\dagger A = A A^\dagger$ ($[A^\dagger, A] = 0$), i.e. it is a normal operator, if and only if $A = \sum_{a=1}^{d} \lambda_a |a\rangle\langle a|$ for a set of orthonormal basis vectors $\{|a\rangle\}$ for $\mathcal{H}$, which are also eigenvectors of A with respective eigenvalues $\{\lambda_a\}$.

Hermitean operators are normal: $H = H^\dagger$

$\hookrightarrow H H^\dagger = H^\dagger H$.

The Hamiltonian can be spectrally decomposed:

$$H = \sum_{n=1}^{d} E_n |E_n\rangle\langle E_n|$$

($|E_n\rangle$: energy eigenstate; E_n: eigenenergy $\in \mathbb{R}$)

- functions of normal operators:

defined as $f(A) = \sum_{a=1}^{d} f(\lambda_a) |a\rangle\langle a|$

example: time-evolution operator

$$U = \exp(-itH) = \sum_{n=1}^{d} \exp(-it E_n) |E_n\rangle\langle E_n|$$

Measurement postulate

The measurement postulate has two parts

i) measuring states: Quantum measurements are described by a set $\{M_k\}_{k=1}^N$ of measurement operators, satisfying the constraint $\sum_{(k)} M_k^\dagger M_k = \mathbb{1}$ ← $N \times N$ - dimensional identity matrix

(k) ← we omit the summation boundaries

Given a state $|\psi\rangle \in \mathcal{H}$, it instantaneously after the measurement becomes

$$|\psi\rangle \mapsto \frac{M_k|\psi\rangle}{\sqrt{p_k}} \equiv |\psi_k\rangle$$

with probability

$$p_k = \langle\psi|M_k^\dagger M_k|\psi\rangle = \|M_k|\psi\rangle\|^2.$$

Note, that probability / norm conservation is ensured by the above constraint

$$1 = \sum_k p_k = \sum_k \langle\psi|M_k^\dagger M_k|\psi\rangle = \langle\psi|\underbrace{\sum_k M_k^\dagger M_k}_{\mathbb{1}}|\psi\rangle$$

$$= \langle\psi|\psi\rangle$$

ii) Observables: To every measurable physical quantity is associated an observable, i.e. a hermitean operator A. A has a spectral decomposition

$$A = \sum_a \lambda_a |a\rangle\langle a| \quad \text{with } \lambda_a \in \mathbb{R}.$$

($|a\rangle$: orthonormal)

The eigenvalues λ_a are the outcomes of the measurement.

- projective measurement:

The measurement operators M_k are projectors (onto the eigenstates of A).

$$M_k = |k\rangle\langle k|, \quad M_k^2 = |k\rangle\langle k|k\rangle\langle k| = |k\rangle\langle k| = M_k \quad (\langle k|k\rangle = 1)$$

They satisfy the constraint

$$\mathbb{1} = \sum_k M_k = \sum_k |k\rangle\langle k|$$

If a system is in the state $|\psi\rangle$ before the observable A is measured, the probability of the outcome λ_a is

$$p_a = \langle\psi| M_a^\dagger M_a |\psi\rangle = \langle\psi|a\rangle\langle a|\psi\rangle = |\langle\psi|a\rangle|^2$$

Moreover, the state after the measurement with outcome λ_a is performed, is

$$|\psi_a\rangle = \frac{M_a|\psi\rangle}{\sqrt{p_a}} = \frac{\langle a|\psi\rangle}{|\langle a|\psi\rangle|}|a\rangle = e^{i\theta}|a\rangle,$$

where $e^{i\theta}$ is the phase of the complex number $\langle a|\psi\rangle$.

Example: Qubit (spin $\frac{1}{2}$ particle) in state

$$|\psi\rangle = c_0|0\rangle + c_1|1\rangle$$

- Measurement operators: $M_0 = |0\rangle\langle 0|$, $M_1 = |1\rangle\langle 1|$

$$|\psi\rangle \mapsto \begin{cases} \frac{M_0|\psi\rangle}{|c_0|} & \text{with probability } p_0 = |c_0|^2 \\ \frac{M_1|\psi\rangle}{|c_1|} & p_1 = |c_1|^2 \end{cases}$$

This example corresponds to measuring the magnetisation of the spin / qubit in z-direction. The corresponding observable is the Pauli z-matrix.

$$Z = \underbrace{(+1)}_{\lambda_0}\underbrace{|0\rangle\langle 0|}_{M_0} + \underbrace{(-1)}_{\lambda_1}\underbrace{|1\rangle\langle 1|}_{M_1} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z$$

Pauli z-matrix

We measure a magnetisation of $+1\,(-1)$ with probability $|c_0|^2\,(|c_1|^2)$.

- energy measurement under Hamiltonian

$= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ ← Pauli x-matrix

$$H = \omega_x \sigma_x + \omega_z \sigma_z$$

$$= E_- |E_-\rangle\langle E_-| + E_+ |E_+\rangle\langle E_+|$$

projector on energy eigenstate

with $E_\pm = \pm\sqrt{\omega_x^2 + \omega_z^2} = \pm |\vec{\omega}|^2$

and $|E_+\rangle = \begin{pmatrix} \cos\alpha \\ -\sin\alpha \end{pmatrix}$, $|E_-\rangle = \begin{pmatrix} \sin\alpha \\ \cos\alpha \end{pmatrix}$

with $\alpha = \frac{1}{2}\operatorname{atan}\left(\frac{\omega_x}{\omega_z}\right)$

probability for measuring spin with state $|\downarrow\rangle$ in the ground state is

$$p_- = |\langle E_-|\downarrow\rangle|^2 = |c_0^* \sin\alpha + c_1^* \cos\alpha|^2$$

can show non-trivial behaviour as α is varied

↳ interference

2 The density operator

We motivate the introduction of the density operator by considering ensembles of pure states. Instead of having a single pure state, we only know that the system is in the pure state $|\psi_i\rangle$ with a probability q_i.

$$\text{pure state ensemble: } \{q_i, |\psi_i\rangle\}_{i=1}^{N}$$

When measuring with a set of measurement operators $\{M_k\}$ we find for each state

$$|\psi_i\rangle \mapsto \frac{M_k|\psi_i\rangle}{\sqrt{p_{k|i}}} = |\psi_i^k\rangle$$

where $p_{k|i} = \langle\psi_i|M_k^\dagger M_k|\psi_i\rangle$ is the probability to obtain outcome k given a state $|\psi_i\rangle$.

Let us now assume that we didn't know what the state was but only that it came from the ensemble $\{q_i, |\psi_i\rangle\}_{i=1}^{N}$.

The probability to obtain measurement outcome k is then

$$p_k = \sum_{i=1}^{N} p_{k|i} q_i = \sum_{i=1}^{N} q_i \langle \psi_i | M_k^\dagger M_k | \psi_i \rangle$$

$$= \sum_{i=1}^{N} q_i \langle \psi_i | \underbrace{\sum_\alpha |\alpha\rangle\langle\alpha|}_{\text{complete set of states}} M_k^\dagger M_k | \psi_i \rangle$$

$$= \sum_\alpha \sum_{i=1}^{N} q_i \langle \alpha | M_k^\dagger M_k | \psi_i \rangle\langle \psi_i | \alpha \rangle$$

$$= \mathrm{Tr}\left[M_k^\dagger M_k \underbrace{\sum_{i=1}^{N} q_i |\psi_i\rangle\langle\psi_i|}_{\text{density operator/matrix}} \right]$$

Using the density matrix $\rho = \sum_{i=1}^{N} q_i |\psi_i\rangle\langle\psi_i|$ is equivalent to using the pure state ensemble $\{q_i, |\psi_i\rangle\}_{i=1}^{N}$, but has the advantage of being directly useful for calculations

<u>state after a measurement:</u>

Suppose that outcome k is observed when measuring the initial state

$$\rho = \sum_i q_i |\psi_i\rangle\langle\psi_i| .$$

probability of being in state $|4_i\rangle$ given the measurement outcome is k

probability of having measurement outcome k given the state is $|4_i\rangle$

probability of having state $|4_i\rangle$

$$p_{i|k}\, p_k = p_{k|i}\, q_i$$

probability of having measurement outcome k

We need to sum over all possible states compatible with the outcome.

$$\rho \mapsto \rho_k = \sum_i p_{i|k} |\psi_i^k\rangle\langle\psi_i^k| = \sum_i p_{i|k} \frac{M_k |\psi_i\rangle\langle\psi_i| M_k^+}{p_{k|i}}$$

we used $p_{i|k} p_k = p_{k|i} q_i$ Bayes' rule

$$= \sum_i \frac{q_i}{p_k} M_k |\psi_i\rangle\langle\psi_i| M_k^+$$

$$= \frac{M_k \rho M_k^+}{p_k} = \frac{M_k \rho M_k^+}{\mathrm{Tr}[\rho M_k^+ M_k]}$$

(q_i = a priori probability for having state $|\psi_i\rangle$;

p_k = probability for measurement outcome k)

pure state: $|\psi\rangle \mapsto \frac{M_k|\psi\rangle}{\sqrt{p_k}}$

density matrix: $\rho \mapsto \frac{M_k \rho M_k^+}{p_k}$

Properties of the density operator

- unit trace: $\mathrm{Tr}[\rho] = \sum_i q_i \mathrm{Tr}[|\psi_i\rangle\langle\psi_i|] = \sum_i q_i = 1$

- Hermiticity: $\rho^+ = \sum_i q_i^* (|\psi_i\rangle\langle\psi_i|)^+ = \sum_i q_i |\psi_i\rangle\langle\psi_i| = \rho$

Since $q_i \in \mathbb{R}$ and $|\psi\rangle^+ = \langle\psi|$

- positive semi-definite: For all vectors $|v\rangle \in \mathcal{H}$ the density matrix ρ has the property $\langle v|\rho|v\rangle \geq 0$: $\langle v|\rho|v\rangle = \sum_i \underbrace{q_i}_{\geq 0} \underbrace{\langle v|\psi_i\rangle\langle\psi_i|v\rangle}_{\geq 0} \geq 0$

↳ eigenvalues of ρ are either positive or 0

Dynamics of the density operator

The evolution of pure states is given by the Schrödinger equation

$$\frac{\partial}{\partial t}|\psi(t)\rangle = -iH|\psi(t)\rangle \quad \longleftrightarrow \quad |\psi(t)\rangle = U(t)|\psi(0)\rangle$$

For the density matrix we thus find

$$\rho(t) = \sum_i q_i |\psi_i(t)\rangle\langle\psi_i(t)| = \sum_i q_i U(t)|\psi_i(0)\rangle\langle\psi_i(0)|U^\dagger(t)$$

$$= U(t)\sum_i q_i |\psi_i(0)\rangle\langle\psi_i(0)| U^\dagger(t) = U(t)\rho(0)U^\dagger(t)$$

or, in differential form,

$$\frac{\partial}{\partial t}\rho(t) = \sum_i q_i \left\{ \left(\frac{\partial}{\partial t}|\psi_i(t)\rangle\right)\langle\psi_i(t)| + |\psi_i(t)\rangle\left(\frac{\partial}{\partial t}\langle\psi_i(t)|\right)\right\}$$

$$= \sum_i q_i \left\{ -iH|\psi_i(t)\rangle\langle\psi_i(t)| + i|\psi_i(t)\rangle\langle\psi_i(t)|H\right\}$$

$$= -i(H\rho(t) - \rho(t)H) = -i[H, \rho(t)]$$ von Neumann equation

- Calculation of expectation values:

  The expectation value of an observable A is calculated as $\langle A \rangle = \mathrm{Tr}(A\rho)$

- pure vs. mixed states:

  The purity P of a state is defined as $P = \mathrm{Tr}\,\rho^2$. If $P=1$ ρ is pure and can be represented as $\rho = |\psi\rangle\langle\psi|$. In general $P \leq 1$. States with $P<1$ are called mixed states.

- unitary equivalence of ensembles:

  Consider the two ensembles

i) $\{q_i, |\psi_i\rangle\} = \{(\frac{3}{4}, \frac{1}{4}), (|0\rangle, |1\rangle)\}$ (biased classical coin)

ii) $\{q_i, |\psi_i\rangle\} = \{(\frac{1}{2}, \frac{1}{2}), (\sqrt{\frac{3}{4}}|0\rangle + \sqrt{\frac{1}{4}}|1\rangle, \sqrt{\frac{3}{4}}|0\rangle - \sqrt{\frac{1}{4}}|1\rangle)\}$.

Both represent, in fact, the same density matrix. I.e. a density matrix can be „unravelled" in different ways.

In general two ensembles of pure states $\{q_i, |\psi_i\rangle\}_{i=1}^{n}$, $\{r_j, |\phi_j\rangle\}_{j=}^{\wedge}$ correspond to the same density operator if and only if there exists a unitary U with entries U_{ij} such that $\sqrt{q_i}|\psi_i\rangle = \sum_j U_{ij}\sqrt{r_j}|\phi_j\rangle$.

i) $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$

$= \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|$

ii) $\rho = \frac{1}{2}\left(\sqrt{\frac{3}{4}}|0\rangle + \sqrt{\frac{1}{4}}|1\rangle\right)\left(\sqrt{\frac{3}{4}}\langle 0| + \sqrt{\frac{1}{4}}\langle 1|\right)$

$+ \frac{1}{2}\left(\sqrt{\frac{3}{4}}|0\rangle - \sqrt{\frac{1}{4}}|1\rangle\right)\left(\sqrt{\frac{3}{4}}\langle 0| - \sqrt{\frac{1}{4}}\langle 1|\right)$

$= \frac{1}{2}\left(\frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1| + \sqrt{\frac{3}{4}}\left(|0\rangle\langle 1| + |1\rangle\langle 0|\right)\right)$

$+ \frac{1}{2}\left(\frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1| - \sqrt{\frac{3}{4}}\left(|0\rangle\langle 1| + |1\rangle\langle 0|\right)\right)$

$= \frac{3}{4}|0\rangle\langle 0| + \frac{1}{4}|1\rangle\langle 1|$

$$\sqrt{q_i}\,|\psi_i\rangle = \sum_j u_{ij}\sqrt{r_j}\,|\varphi_j\rangle$$

$$\rho = \sum_i q_i |\psi_i\rangle\langle\psi_i| = \sum_i \sqrt{q_i}\,|\psi_i\rangle\langle\psi_i|\sqrt{q_i}$$

$$= \sum_i \sum_j \sum_k u_{ij}\sqrt{r_j}\,|\varphi_j\rangle\langle\varphi_k|\sqrt{r_k}\,u^*_{ik}$$

$$= \sum_j \sum_k \sqrt{r_j}\,|\varphi_j\rangle\langle\varphi_k|\sqrt{r_k} \underbrace{\sum_i u^*_{ik} u_{ij}}_{\sum_i (u^\dagger)_{ki} u_{ij}}$$

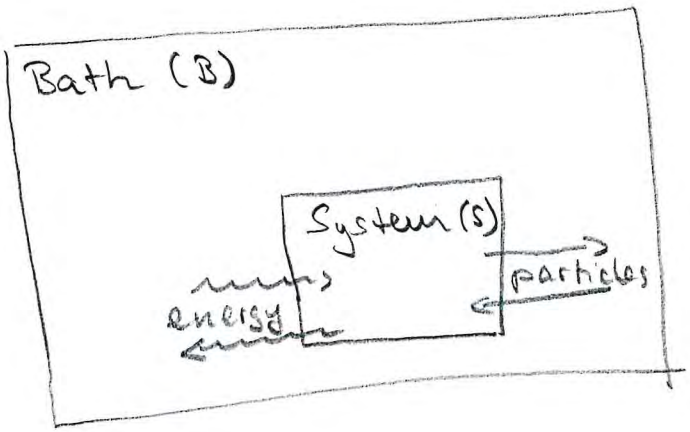
$$= \delta_{kj}$$

$$= \sum_j \sum_k \sqrt{r_j}\,|\varphi_j\rangle\langle\varphi_k|\sqrt{r_k}\,\delta_{kj}$$

$$= \sum_j r_j |\varphi_j\rangle\langle\varphi_j|$$

11 Composite systems

Combining a system and a bath



Consider a two component system where we have the subsystem of interest, S, and another subsystem, B, which we call bath.

The total system evolves according to the Schrödinger equation.

The Hilbert spaces of the system and the bath are, respectively,

$$\mathcal{H}_S = \text{span}\{|i\rangle_S\}\ , \ i = 1, \dots, d_S$$

$$\mathcal{H}_B = \text{span}\{|\mu\rangle_B\}\ , \ \mu = 1, \dots, d_B .$$

Usually the dimension of the bath, d_B, is much larger than d_S.

The Hilbert space of the two systems combined is the tensor product of the individual spaces.

$$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B = \text{span}\{|i\rangle_S \otimes |\mu\rangle_B\}$$

Partial trace

Our primary interest is in the System S. Ideally we would thus like to find a way to remove the bath B from our description. This is achieved by the partial trace which averages out the components of B from the combined system-bath state.

Consider a (simple) operator $O = M_S \otimes N_B$ with acts on $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$.

Then $$\mathrm{Tr}_B (M_S \otimes N_B) = M_S \, \mathrm{Tr}(N_B) = M_S \sum_\mu \langle \mu | N_B | \mu \rangle$$
$$= \sum_\mu \langle \mu | M_S \otimes N_B | \mu \rangle .$$

For a general operator $O = \sum_{kj} l_{kj} M_S^k \otimes N_B^j$ we then find due to linearity

$$\mathrm{Tr}_B O = \sum_{kj} l_{kj} \mathrm{Tr}_B (M_S^k \otimes N_B^j) = \sum_{kj} l_{kj} M_S^k \sum_\mu \langle \mu | N_B^j | \mu \rangle .$$

State of a quantum subsystem

The density matrix of the subsystem S is given by taking the partial trace of the total density matrix ρ:

$$\rho_S = \mathrm{Tr}_B \rho$$

Examples:

- product state

$$\rho = \rho_S \otimes \rho_B$$

$$\hookrightarrow \mathrm{Tr}_B \rho = \rho_S \underbrace{\mathrm{Tr}_B \rho_B}_{=1} = \rho_S$$

- maximally entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle_S |0\rangle_B + |1\rangle_S |1\rangle_B \right)$$

$$\hookrightarrow \mathrm{Tr}_B |\psi\rangle\langle\psi| = \frac{1}{2} \mathrm{Tr}_B \Big[\underset{S}{|0\rangle\langle 0|} \otimes \underset{B}{|0\rangle\langle 0|} + \underset{S}{|0\rangle\langle 1|} \otimes \underset{B}{|0\rangle\langle 1|} + \underset{S}{|1\rangle\langle 0|} \otimes \underset{B}{|1\rangle\langle 0|} + \underset{S}{|1\rangle\langle 1|} \otimes \underset{B}{|1\rangle\langle 1|} \Big]$$

$$= \frac{1}{2} \Big[\underset{S}{|0\rangle\langle 0|} \cdot 1 + \underset{S}{|0\rangle\langle 1|} \cdot 0 + \underset{S}{|1\rangle\langle 0|} \cdot 0 + \underset{S}{|1\rangle\langle 1|} \cdot 1 \Big]$$

$$= \frac{1}{2} \Big[\underset{S}{|0\rangle\langle 0|} + \underset{S}{|1\rangle\langle 1|} \Big] = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$\hookrightarrow$ the reduced state of the system S is completely mixed $\left\{ \left(\frac{1}{2}, \frac{1}{2}\right), (|0\rangle, |1\rangle) \right\}$

Kraus operator representation

The joint unitary evolution of a system S plus bath B is given by $U(t) = \exp(-itH)$, where H is the total Hamiltonian.

The total density matrix thus evolves as

$$\rho(t) = U(t)\,\rho(0)\,U^{+}(t)$$

($\rho(0)$ ← initial state)

The reduced density matrix of S is thus

$$\rho_S(t) = \mathrm{Tr}_B\,\rho(t) = \sum_{\mu} \langle\mu|\,U(t)\,\rho(0)\,U^{+}(t)\,|\mu\rangle$$

To simplify things we assume that initially the system and the bath are decoupled, that is $\rho(0) = \rho_S(0) \otimes \rho_B(0)$.

We further make use of the fact that the density matrix of the bath can be written in its spectral decomposition:

$$\rho_B(0) = \sum_{\nu} \lambda_\nu\,|\nu\rangle\langle\nu|$$

Then $\rho_S(t) = \sum_\mu \langle\mu| U(t)\, \rho_S(0) \otimes \sum_\nu \lambda_\nu |\nu\rangle\langle\nu| U^+(t) |\mu\rangle$

$$= \sum_{\mu\nu} \sqrt{\lambda_\nu}\, \langle\mu|U(t)|\nu\rangle_B\, \rho_S(0)\, \sqrt{\lambda_\nu}\, \langle\nu|U^+(t)|\mu\rangle_B$$

$$= \sum_{\mu\nu} K_{\mu\nu}(t)\, \rho_S(0)\, K^+_{\mu\nu}(t) .$$

In the last step we have introduced the Kraus operators

$$K_{\mu\nu}(t) = \sqrt{\lambda_\nu}\, \langle\mu|U(t)|\nu\rangle ,$$

which only act on the system.

> Kraus operator sum representation (OSR)
>
> $$\rho_S(t) = \sum_\alpha K_\alpha(t)\, \rho_S(0)\, K^+_\alpha(t)$$

Since $1 = \mathrm{Tr}\, \rho_S(t) = \mathrm{Tr}\left[\sum_\alpha K_\alpha(t) \rho(0) K^+_\alpha(t)\right]$

$= \mathrm{Tr}\left[\sum_\alpha K^+_\alpha(t) K_\alpha(t)\, \rho(0)\right]$ for any $\rho(0)$,

we find that the Kraus operators satisfy the identity $\sum_\alpha K^+_\alpha(t) K_\alpha(t) = \mathbb{1}$.

special case: Schrödinger evolution under unitary operator U

$$\rho_S(t) = U \rho_S(0) U^\dagger \rightarrow K = U$$

Connection to measurements

The OSR does not only represent dynamics, but also captures measurements. Consider the measurement operator set $\{M_k\}$ with $\sum_k M_k^\dagger M_k = \mathbb{1}$. Provided that we measure outcome k, the density matrix becomes

$$\rho \mapsto \rho_k = \frac{M_k \rho M_k^\dagger}{\mathrm{Tr}[M_k^\dagger M_k \rho]}.$$

Now suppose we measure, but do not learn about the outcome. In this case the density matrix will be the sum over all outcomes weighted by the corresponding probability:

$$\rho \mapsto \sum_k p_k \rho_k = \sum_k M_k \rho M_k^\dagger.$$

Such non-selective measurement is represented by a OSR

OSR as a map

It is useful to think of the OSR as a map (synonyms often used are "process" or "channel"), i.e.

$$\rho(t) = \Phi[\rho(0)] \quad \text{or} \quad \Phi : \rho(0) \to \rho(t)$$

with $\Phi[X] \equiv \sum_\alpha K_\alpha X K_\alpha^\dagger$. The operator Φ is often called superoperator as it acts on operators.

Properties of the (Kraus) map:

1) Trace preservation:

$$\mathrm{Tr}\,\Phi[\rho] = \mathrm{Tr} \sum_\alpha K_\alpha \rho K_\alpha^\dagger = \mathrm{Tr} \underbrace{\sum_\alpha K_\alpha^\dagger K_\alpha}_{\mathbb{1}} \rho = \mathrm{Tr}\,\rho$$

2) Linearity:

$$\Phi[a\rho_1 + b\rho_2] = a\Phi[\rho_1] + b\Phi[\rho_2]$$

3a) Positivity: Using the spectral decomposition $\rho = \sum_i \lambda_i |i\rangle\langle i|$, with $\lambda_i \geq 0$, we find

$$\langle v|\Phi[\rho]|v\rangle = \sum_\alpha \langle v|K_\alpha \rho K_\alpha^\dagger|v\rangle = \sum_{\alpha i} \lambda_i \langle v|K_\alpha|i\rangle\langle i|K_\alpha^\dagger|v\rangle$$

$$= \sum_{\alpha i} \lambda_i |\langle v|K_\alpha|i\rangle|^2 \geq 0$$

↳ $\Phi[\rho]$ is positive, i.e. it maps positive operators on positive operators

3b) The Kraus map Φ is in fact a <u>completely positive (PT)</u> map. This means that it does not only map positive operators into positive operators, but that it maintains positivity also when acting on a subspace of a larger Hilbert space.

Consider the map $\Phi \otimes \mathbb{1}_X$ which acts on the Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_X$, then

$$\langle v| \Phi \otimes \mathbb{1}_X [\rho] |v\rangle = \sum_{\alpha i} \lambda_i \langle v| K_\alpha \otimes \mathbb{1}_X |i\rangle\langle i| K_\alpha^\dagger \otimes \mathbb{1}_X |v\rangle$$

$$= \sum_{\alpha i} \lambda_i |\langle v| K_\alpha \otimes \mathbb{1}_X |i\rangle|^2 \geq 0$$

$\hookrightarrow \Phi$ is completely positive

Why is it important to demand complete positivity? Not all positive maps are completely positive.

<u>Example:</u> transposition T

$T\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$, Eigenvalues of a matrix are invariant under transposition. Therefore the transpose of a positive matrix is positive.

Now lets extend T in the sense that it acts on a subspace of a larger system

This is called partial transpose.

$$T^P = T \otimes \mathbb{1}_x, \quad T^P(|i\rangle\langle j| \otimes |\mu\rangle\langle\nu|) = |j\rangle\langle i| \otimes |\mu\rangle\langle\nu|$$

Consider now a 2 qubit system in the state $|\psi\rangle = \frac{1}{\sqrt{2}}\left[|0\rangle_s|0\rangle_x + |1\rangle_s|1\rangle_x\right]$. Then

$$|0\rangle_s|0\rangle_x\langle 0|_s\langle 0|_x$$

$$T^P(|\psi\rangle\langle\psi|) = \frac{1}{2}(T \otimes \mathbb{1})\left[|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|\right]$$

$$= \frac{1}{2}\left[|00\rangle\langle 00| + |10\rangle\langle 01| + |01\rangle\langle 10| + |11\rangle\langle 11|\right]$$

$$= \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The eigenvalues of the partially transposed density matrix are $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$.

↳ This is not a positive operator and thus T^P is not CP. Remark: T^P can be used as entanglement measure.

Definition of a quantum map

A map that is:

1) trace preserving
2) linear
3) completely positive

Quantum maps of a qubit

- Bloch sphere:

The density matrix of a qubit can be parameterised as follows:

Bloch vector

$$\rho = \frac{1}{2}\left(\mathbb{1} + \sum_i v_i \sigma_i\right) = \frac{1}{2}\left(\mathbb{1} + \vec{v}\cdot\vec{\sigma}\right)$$

Here we used the Pauli matrices

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

so that

$$\rho = \frac{1}{2}\begin{pmatrix} 1+v_z & v_x - iv_y \\ v_x + iv_y & 1-v_z \end{pmatrix}.$$

The trace of ρ is by construction 1, but we need to require that $\|\vec{v}\| \leq 1$ for ρ to be positive.

To calculate the purity, we use that

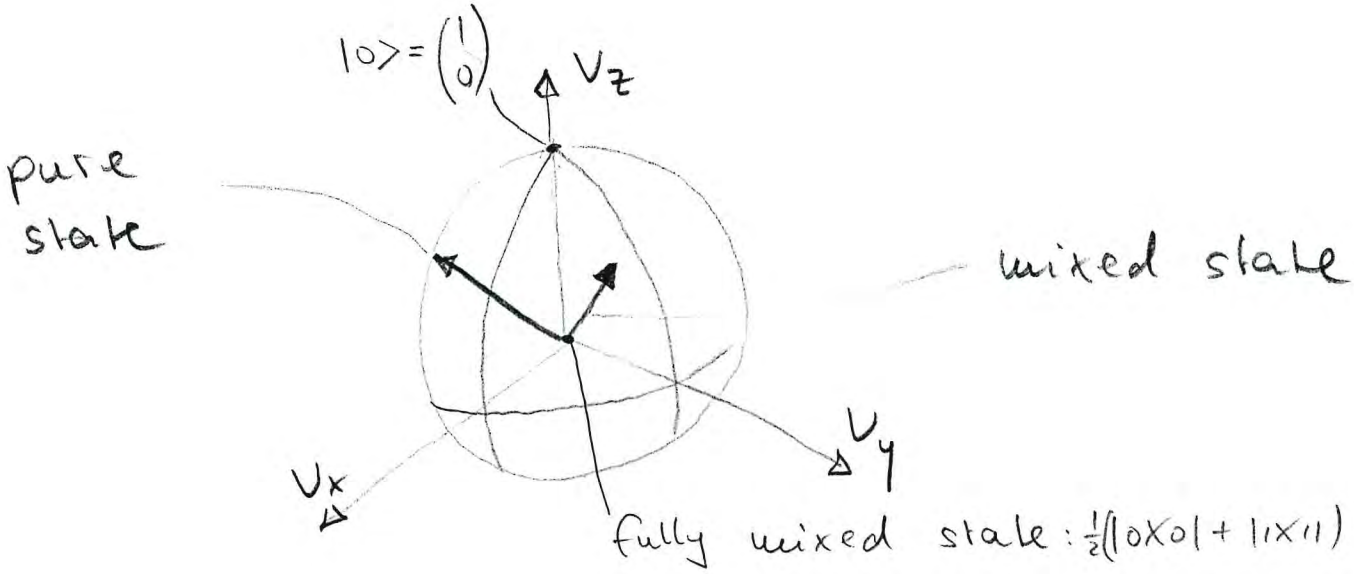
$$\rho^2 = \frac{1}{4}\left(\mathbb{1} + \vec{v}\cdot\vec{\sigma}\right)\left(\mathbb{1} + \vec{v}\cdot\vec{\sigma}\right) = \frac{1}{4}\left(\mathbb{1} + 2\vec{v}\cdot\vec{\sigma} + (\vec{v}\cdot\vec{\sigma})^2\right)$$

$$\hookrightarrow \operatorname{Tr}\rho^2 = \frac{1}{4}\Big(\underbrace{\operatorname{Tr}\mathbb{1}}_{2} + 2\sum_k v_k \underbrace{\operatorname{Tr}\sigma_k}_{=0} + \sum_{km} v_k v_m \underbrace{\operatorname{Tr}(\sigma_k\sigma_m)}_{2\delta_{km}}\Big)$$

$$= \frac{1}{4}\left(2 + 2\sum_k v_k^2\right) = \frac{1}{2}\left(1 + \|\vec{v}\|^2\right)$$

$\hookrightarrow \rho$ is only pure if $\|\vec{v}\| = 1$.

The vector $\vec{v}$ is called the Bloch vector and allows the visualisation of the density matrix on the Bloch sphere.



- Phase damping map:

$$\Phi(\rho) = p\rho + (1-p)\sigma_z \rho \sigma_z = \sum_{\alpha=0}^{1} K_\alpha \rho K_\alpha^\dagger$$

- the two Kraus operators are

$$K_0 = \sqrt{p}\,\mathbb{1}, \quad K_1 = \sqrt{1-p}\,\sigma_z$$

- the map can be understood as follows

$$\rho \longmapsto \rho' = \begin{cases} \rho & \text{with probability } p \\ \sigma_z \rho \sigma_z & \text{with probability } 1-p \end{cases}$$

In order to see what happens to the Bloch vector under this transformation we write

$$\rho' = \sum_\alpha K_\alpha \rho K_\alpha^+ = \frac{1}{2}\sum_\alpha K_\alpha (\mathbb{1} + \vec{v}\cdot\vec{\sigma}) K_\alpha^+$$

$$= \frac{1}{2}\left(\sum_\alpha K_\alpha K_\alpha^+ + \sum_{\alpha j} v_j K_\alpha \sigma_j K_\alpha^+\right)$$

$$\overset{!}{=} \frac{1}{2}(\mathbb{1} + \vec{v}'\cdot\vec{\sigma})$$

To get the components of $\vec{v}'$ we use:

$$\mathrm{Tr}(\rho'\sigma_i) = \frac{1}{2}\left(\mathrm{Tr}\,\sigma_i + \sum_j v_j' \mathrm{Tr}\,\sigma_i\sigma_j\right) = v_i'$$

and $\mathrm{Tr}(\rho'\sigma_i) = \underbrace{\frac{1}{2}\mathrm{Tr}\left(\sum_\alpha K_\alpha K_\alpha^+ \sigma_i\right)}_{c_i} + \sum_j v_j \underbrace{\frac{1}{2}\mathrm{Tr}(K_\alpha \sigma_j K_\alpha^+ \sigma_i)}_{M_{ij}}$

↳ the Kraus map performs an affine transformation of the Bloch vector: $\vec{v} \mapsto \vec{v}' = M\vec{v} + \vec{c}$

For the dephasing map we find

$$\vec{c} = 0\,; \quad M = \begin{pmatrix} 2p-1 & 0 & 0 \\ 0 & 2p-1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

↳ rescaling of sphere of pure states from ⊖ to ⊖

↳ the pure states $\binom{0}{1}$ and $\binom{0}{-1}$ are fixed points

- amplitude damping map (spontaneous emission):

We want to find a map that accomplishes: $|0\rangle \longmapsto |0\rangle$ with probability 1

$|1\rangle \longmapsto |0\rangle$ with probability p

One Kraus operator is obviously

$$K_1 = \sqrt{p}\,|0\rangle\langle 1| = \sqrt{p}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

but what is the other Kraus operator K_0, so that the map satisfies the condition $K_0^\dagger K_0 + K_1^\dagger K_1 = \mathbb{1}$?

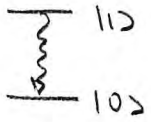
Ansatz: $K_0 = \begin{pmatrix} 1 & a \\ b & c \end{pmatrix}$

$$\hookrightarrow K_0^\dagger K_0 + K_1^\dagger K_1 = \begin{pmatrix} 1+|b|^2 & a+b^*c \\ a^*+bc^* & |a|^2+|c|^2 \end{pmatrix} + p\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \overset{!}{=} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

with $a = b = 0$ and $c = \sqrt{1-p}$ this equation is satisfied

$$\hookrightarrow K_0 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}$$

$$\Phi(\rho) = \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}\rho\begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}}_{\text{"no-jump evolution"}} + \underbrace{p\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\rho\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}}_{\text{spin flip / spontaneous emission}}$$



Decomposition into jump and no-jump term is characteristic for quantum maps. We will see more later when discussing quantum jump trajectories.

affine transformation of the Bloch vector:

$$M = \begin{pmatrix} \sqrt{1-p} & & \\ & \sqrt{1-p} & \\ & & 1-p \end{pmatrix}, \quad \vec{c} = \begin{pmatrix} 0 \\ 0 \\ p \end{pmatrix}$$

↳ sphere of pure states is compressed along x & y direction.

Centre of sphere is shifted.

When $p=1$ the Bloch sphere is compressed to a single point, which is the north pole and represents a fixed point of the map.

$$\Phi(|0\rangle\langle 0|) = \underbrace{K_0|0\rangle\langle 0|K_0^\dagger}_{|0\rangle\langle 0|} + \underbrace{K_1^\dagger|0\rangle\langle 0|K_1}_{0} = |0\rangle\langle 0|$$

IV A qubit coupled to a bath – exactly solvable models

Phase damping

Let's now illustrate the rather abstract preceeding discussions with a specific model. The model will describe a qubit whose coherences decay. It can be regarded as a physical realisation of phase damping and allows us to understand, e.g., the involved time scales.

Hamiltonian:

$$H = \underbrace{\frac{\omega_0}{2}\sigma_z}_{\text{spin Hamiltonian } H_S} + \underbrace{\sum_k \omega_k b_k^\dagger b_k}_{\text{free Hamiltonian of the bath } H_B} + \underbrace{\sum_k \sigma_z (g_k b_k^\dagger + g_k^* b_k)}_{\text{spin-bath coupling Hamiltonian } H_{SB}}$$

- ω_0: level spacing of qubit $\left.\begin{matrix}|1\rangle \\ |0\rangle\end{matrix}\right\} \omega_0$
- $b_k^\dagger$: creation operator of the bosonic bath mode k, satisfying $[b_k, b_{k'}^\dagger] = \delta_{kk'}$
- ω_k: frequency of the k-th bath mode
- g_k: spin–bath mode coupling constants

The first step is to transform in the interaction picture, by applying the unitary

$$U(t) = \exp(-it(H_S + H_b))$$

to the Schrödinger equation:

$$i\partial_t |\psi\rangle = (H_S + H_b + H_{Sb})|\psi\rangle$$

↳ with $|\psi\rangle = U(t)|\varphi\rangle$ we have

$$\underbrace{i U^\dagger(t)\partial_t U(t)|\varphi\rangle}_{} = \underbrace{U^\dagger(t)[H_S + H_b + H_{Sb}]U(t)|\varphi\rangle}_{}$$

$$\underbrace{iU^\dagger(\partial_t U)|\varphi\rangle}_{} + i\partial_t|\varphi\rangle = [H_S + H_b + U^\dagger H_{Sb} U]|\varphi\rangle$$

$(H_S + H_b)|\varphi\rangle$

↳ $i\partial_t|\varphi\rangle = U^\dagger H_{Sb} U|\varphi\rangle$ Schrödinger equation in the interaction picture

- interaction picture Hamiltonian:

$$H_I = U^\dagger H_{Sb} U = \sum_k \underbrace{U^\dagger \sigma_z U}_{=\sigma_z} (g_k U^\dagger b_k^\dagger U + g_k^* U^\dagger b_k U)$$

using $U^\dagger b_k^\dagger U = e^{it(H_S+H_b)} b_k^\dagger e^{-it(H_S+H_b)} = e^{itH_b} b_k^\dagger e^{-itH_b}$

$$= e^{it\sum_m \omega_m b_m^\dagger b_m} b_k^\dagger e^{-it\sum_m \omega_m b_m^\dagger b_m} = e^{it\omega_k b_k^\dagger b_k} b_k^\dagger e^{it\omega_k b_k^\dagger b_k} = b_k^\dagger e^{i\omega_k}$$

$$e^{it\omega b^+b}\, b^+\, e^{-it\omega b^+b} = b^+ + \underbrace{[it\omega b^+b,\, b^+]}_{it\omega\,[b^+b,\,b^+]} + \frac{1}{2!}\underbrace{[it\omega b^+b,\, \underbrace{[it\omega b^+b,\, b^+]}_{it\omega b^+}]}_{\frac{1}{2!}(it\omega)^2 b^+} + \frac{1}{3!}\underbrace{[it\omega b^+b,\, \underbrace{[it\omega b^+b,\, \underbrace{[it\omega b^+b,\, b^+]}_{it\omega b^+}]}_{(it\omega)^2 b^+}]}_{(it\omega)^3 b^+} + \dots$$

$$[b^+b,\, b^+] = b^+[b, b^+] + [b, b^+]b^+ = b^+ \underbrace{[b, b^+]}_{=1} = b^+$$

$$= \sum_{n=0}^{\infty} \frac{(it\omega)^n}{n!}\, b^+ = b^+ \sum_{n=0}^{\infty} \frac{(it\omega)^n}{n!} = b^+ e^{it\omega}$$

we find:

$$H_I = \sum_k \sigma_z \left(g_k b_k^+ e^{i\omega_k t} + g_k^* b_k e^{-i\omega_k t} \right)$$

$$= H_I(t)$$

To find the time evolution operator we use the Magnus expansion:

$$U_I(t) = \exp \sum_{k=1}^{\infty} \Omega_k(t)$$

with $\Omega_1(t) = \int_0^t d\tau \left(-i H_I(\tau) \right)$

$$\Omega_2(t) = \frac{1}{2} \int_0^t d\tau \int_0^\tau d\tau' \left[-i H_I(\tau), -i H_I(\tau') \right]$$

$$\Omega_3(t) = \frac{1}{6} \int_0^t d\tau \int_0^\tau d\tau' \int_0^{\tau'} d\tau'' \Big(\left[-i H_I(\tau), \left[-i H_I(\tau'), -i H_I(\tau'') \right] \right]$$

$$+ \left[-i H_I(\tau''), \left[-i H_I(\tau'), -i H_I(\tau) \right] \right] \Big)$$

$$\vdots$$

Since $\left[H_I(\tau), H_I(\tau') \right] = \sum_{km} \Big\{ g_k g_m^* e^{i\omega_k \tau - i\omega_m \tau'} \overbrace{\left[b_k^+, b_m \right]}^{-\delta_{km}}$

$$+ g_k^* g_m e^{-i\omega_k \tau + i\omega_m \tau'} \overbrace{\left[b_k, b_m^+ \right]}^{\delta_{km}} \Big\}$$

$$= \sum_k \left\{ -|g_k|^2 e^{i\omega_k(\tau - \tau')} + |g_k|^2 e^{-i\omega_k(\tau - \tau')} \right\}$$

$$= -2i \sum_k |g_k|^2 \sin\left[\omega_k (\tau - \tau') \right]$$

is a c-number, $\Omega_3(t)$ and higher terms vanish.

One thus finds that

$$U_I(t) = \underbrace{\exp\left[i \int_0^t d\tau \int_0^\tau d\tau' \sum_k |g_k|^2 \sin\left[\omega_k(\tau-\tau')\right]\right]}_{\exp(i\varphi(t))} \cdot \underbrace{\exp\left[-i\int_0^t d\tau\, H_I(\tau)\right]}_{U_I(t)}$$

with $\int_0^t d\tau\, e^{i\omega_k\tau} = \frac{i(e^{i\omega_k t}-1)}{\omega_k}$

$$U_I(t) = \exp\left[i\sigma_z \sum_k \left(g_k \frac{i(e^{i\omega_k t}-1)}{\omega_k} b_k^\dagger + g_k^* \frac{(-i)(e^{-i\omega_k t}-1)}{\omega_k} b_k \right)\right]$$

abbreviating $\alpha_k = \frac{g_k}{\omega_k}(e^{i\omega_k t}-1)$

$$= \exp\left[\sigma_z \sum_k (\alpha_k b_k^\dagger - \alpha_k^* b_k)\right]$$

introducing the displacement operator $D(x) = e^{xb^\dagger - x^* b}$

$$= \prod_k D(\sigma_z \alpha_k)$$

$$= |0\rangle\langle 0| \prod_k D(-\alpha_k) + |1\rangle\langle 1| \prod_k D(\alpha_k)$$

$$= |0\rangle\langle 0| \prod_k D^\dagger(\alpha_k) + |1\rangle\langle 1| \prod_k D(\alpha_k)$$

- decay of coherences

Let us suppose that the initial state of the total system is given by

$$\rho(0) = \rho_S(0) \otimes \rho_B \quad \text{with} \quad \rho_B = \frac{1}{Z_B} e^{-\beta H_B}$$

Z_B: partition function of the bath

the bath is in a thermal state with temperature $k_B T = \frac{1}{\beta}$

The spin density matrix we write with the help of the Bloch vector as

$$\rho_S(0) = \frac{1}{2}\left(\mathbb{1} + \vec{v}(0)\cdot\vec{\sigma}\right).$$

Our goal is now to calculate the reduced density matrix of the spin at time t: (note, that we are still in the interaction picture)

$$\rho_S(t) = \mathrm{Tr}_B\left[U_I(t)\,\rho(0)\,U_I^+(t)\right]$$

$$= \frac{1}{2}\Big[\underbrace{\mathrm{Tr}_B\left(U_I(t)\,\rho_B\,U_I^+(t)\right)}_{=\mathrm{Tr}_B\rho_B=\mathbb{1}} + v_z\,\overbrace{\mathrm{Tr}_B\left(U_I(t)\,\sigma_z\,\rho_B\,U_I^+(t)\right)}^{=\mathrm{Tr}_B\left(U_I(t)\rho_B U_I^+(t)\right)\sigma_z=\sigma_z}$$

$$+ v_y\,\mathrm{Tr}_B\left(U_I(t)\,\sigma_y\,\rho_B\,U_I^+(t)\right)$$

$$+ v_x\,\mathrm{Tr}_B\left(U_I(t)\,\sigma_x\,\rho_B\,U_I^+(t)\right)\Big]$$

$$= \frac{1}{2}\Big[\mathbb{1} + v_z\sigma_z + (v_x - iv_y)\,\mathrm{Tr}_B\left(U_I(t)\,\sigma^+\rho_B\,U_I^+(t)\right)$$

$$+ (v_x + iv_y)\,\mathrm{Tr}_B\left(U_I(t)\,\sigma^-\rho_B\,U_I^+(t)\right)\Big]$$

↳ z-component of Bloch vector does not change → populations do not change

Let us now investigate the evolution of the coherences through analysing the term

$$\mathrm{Tr}_B\left(U_I(t)\,\sigma^-\rho_B\,U_I^+(t)\right) = \mathrm{Tr}_B\left(\prod_k D^+(\alpha_k)\,\rho_B\,D^+(\alpha_k)\right)\sigma^-$$

$$\mathrm{Tr}\left[D^+(2\alpha)\, e^{-\beta\omega b^+ b}\right]$$

$$= \sum_n e^{-\beta\omega n} \underbrace{\langle n|D^+(2\alpha)|n\rangle}$$

$$\exp\left(-\frac{|2\alpha|^2}{2}\right) L_n(|2\alpha|^2)$$

$$= \exp\left(-\frac{|2\alpha|^2}{2}\right) \sum_n e^{-\beta\omega n} L_n(|2\alpha|^2)$$

generating function of Laguerre polynomials

$$\sum_{n=0}^{\infty} t^n L_n(x) = \frac{1}{1-t}\, e^{-x\frac{t}{1-t}}$$

$$= e^{-\frac{|2\alpha|^2}{2}} \cdot \frac{1}{1-e^{-\beta\omega}}\, e^{\left(-|2\alpha|^2 \frac{e^{-\beta\omega}}{1-e^{-\beta\omega}}\right)}$$

$$= \underbrace{\frac{1}{1-e^{-\beta\omega}}}_{Z} \exp\left[-|2\alpha|^2 \underbrace{\left(\frac{1}{2} + \frac{e^{-\beta\omega}}{1-e^{-\beta\omega}}\right)}\right]$$

$$\frac{1 - e^{-\beta\omega} + 2e^{-\beta\omega}}{2(1-e^{-\beta\omega})}$$

$$\frac{1}{2}\,\frac{1+e^{-\beta\omega}}{1-e^{-\beta\omega}} = \frac{1}{2}\coth\left(\frac{\beta\omega}{2}\right)$$

$$= Z \cdot \exp\left[-2|\alpha|^2 \coth\left(\frac{\beta\omega}{2}\right)\right], \quad |\alpha|^2 = 2\frac{|g|^2}{\omega^2}(1-\cos\omega t)$$

$$= \sigma^- \prod_k \mathrm{Tr}_B \left[D^+(2\alpha_k) \frac{e^{-\beta\omega_k b_k^+ b_k}}{Z_k} \right]$$

$$= \sigma^- \prod_k \left\langle \exp\left(2\alpha_k^* b_k - 2\alpha_k b_k^+\right) \right\rangle_B$$ ← average with respect to thermal distribution

$$= \sigma^- \prod_k \exp\left[-2|\alpha_k|^2 \left\langle \{b_k, b_k^+\} \right\rangle_B \right]$$

$$= \sigma^- \exp\left[-\sum_k \frac{4|g_k|^2}{\omega_k^2} \coth\left(\frac{\beta\omega_k}{2}\right)\left(1-\cos\omega_k t\right) \right] = \sigma^- e^{\Gamma(t)}$$

In order to make progress we have to deal with the summation. To this end we introduce the density $f(\omega)$ of oscillator modes such that $\sum_k \frac{|g_k|^2}{\omega_k^2} \to \int_0^\infty d\omega\, f(\omega)\, |g(\omega)|^2 \frac{1}{\omega^2}$

Furthermore, we introduce the spectral mode density: $J(\omega) = 4 f(\omega) |g(\omega)|^2$.

$$\hookrightarrow \Gamma(t) = -\int_0^\infty d\omega\, J(\omega) \coth\left(\frac{\beta\omega}{2}\right) \frac{1-\cos\omega t}{\omega^2}$$

In order to finish the calculation we require an explicit expression for the spectral mode density.

We use $J(\omega) = \omega \exp\left(-\frac{\omega}{\Omega}\right)$ where Ω is a cut-off frequency.

We thus obtain

$$\Gamma(t) = \underbrace{-\int_0^\infty d\omega\, \omega e^{-\frac{\omega}{\Omega}} \frac{1-\cos\omega t}{\omega^2}}_{\Gamma_{vac}(t) \ldots \text{vacuum contribution}} + \underbrace{\int_0^\infty d\omega\, \omega e^{-\frac{\omega}{\Omega}} \left(1-\coth\left(\frac{\beta\omega}{2}\right)\right) \frac{1-\cos\omega t}{\omega^2}}_{\Gamma_{th}(t) \ldots \text{thermal contribution}}$$

The temperature-independent vacuum contribution yields $\Gamma_{vac}(t) = -\frac{1}{2}\ln(1+\Omega^2 t^2)$.

It describes how vacuum fluctuations of the bath affect coherence and depends on the cut off frequency Ω.

In order to evaluate the thermal part we rewrite it as

$$\Gamma_{th}(t) = -\frac{1}{\beta}\int_0^t ds \int_0^\infty dx \, e^{-\frac{x}{\Omega\beta}} \left[\coth\left(\frac{x}{2}\right)-1\right] \sin\left(\frac{sx}{\beta}\right).$$

We assume now that the temperature is much smaller than the cut off frequency, i.e. $\frac{1}{\Omega\beta} = \frac{T}{\Omega} \ll 1$.

With this assumption we obtain

$$\Gamma_{th}(t) \approx -\frac{1}{\beta}\int_0^t ds \underbrace{\int_0^\infty dx \left[\coth\left(\frac{x}{2}\right)-1\right]\sin\left(\frac{sx}{\beta}\right)}_{\pi\coth\left(\frac{s}{\beta}\pi\right)-\frac{\beta}{s}}$$

$$= \ln(t) + \ln\left(\frac{\pi}{\beta}\right) - \ln\left(\sinh\left(\frac{t\pi}{\beta}\right)\right)$$

$$= -\ln\left[\frac{\sinh\left(\frac{\pi}{\beta}t\right)}{\frac{\pi}{\beta}t}\right] = -\ln\left[\frac{\sinh\left(t/\tau_{th}\right)}{t/\tau_{th}}\right].$$

Here we have introduced the thermal correlation time $\tau_{th} = \frac{\beta}{\pi} = \frac{1}{\pi T} = 2.4\cdot 10^{-12}\,\frac{s}{T[K]}$.

Our final result for the reduced density matrix of the spin is thus:

$$\rho_s(t) = \frac{1}{2}\left[\mathbb{1} + v_z\sigma_z + (v_x+iv_y)\sigma^- e^{\Gamma(t)} + (v_x-iv_y)\sigma^+ e^{\Gamma^*(t)}\right]$$

$$= \frac{1}{2}\left[\mathbb{1} + (v_x\sigma_x + v_y\sigma_y)e^{\Gamma(t)} + v_z\sigma_z\right]$$

with $\Gamma(t) \simeq -\frac{1}{2}\ln(1+\Omega^2t^2) - \ln\left[\frac{\sinh\left(\frac{t}{\tau_{th}}\right)}{t/\tau_{th}}\right]$.

↳ While the populations are unchanged the coherences (off-diagonal terms) decay.

The corresponding affine transformation of the Bloch vector is

$$\vec{v} \longmapsto \vec{v}' = \begin{pmatrix} e^{\Gamma(t)} & & \\ & e^{\Gamma(t)} & \\ & & 1 \end{pmatrix} \vec{v}$$

which corresponds to the phase damping map with $p = \frac{1+e^{\Gamma(t)}}{2}$.

Let us finally have a look at the time scale at which the coherences decay. We can identify three regimes:

1) short time regime, i.e. $t \ll \Omega^{-1}$:

Here $\Gamma(t) \approx -\frac{1}{2}\Omega^2 t^2$. This quadratic dependence is characteristic for a quantum dynamics in the sense that one typically obtains this from expanding the time-evolution operator.

2) vacuum regime, i.e. $\Omega^{-1} \ll t \ll \tau_{th}$

Here $\Gamma(t) \approx -\ln \Omega t$ and decoherence effects are mainly due to the vacuum fluctuations of the bath.

3) thermal regime, i.e. $\tau_{th} \ll t$

Here $\Gamma(t) \approx -\frac{t}{\tau_{th}}$. Due to the linear dependence with time one calls this also the Markovian regime. Coherences decay exponentially. This dynamics in this regime can be captured by a Markovian Lindblad Master equation.

Radiative decay - spontaneous emission

It is well-known that an atom in an excited state $|e\rangle$ is not stationary. It will eventually decay into the ground state $|g\rangle$ under the emission of a photon into the electromagnetic field.

Lets assume that initially the atom-field system is in the state

$$|\psi(0)\rangle = |e, \{0\}\rangle = |e\rangle \otimes |\{0\}\rangle$$

($|e\rangle$: excited state of atom; $|\{0\}\rangle$: vacuum state of the electromagnetic field)

The state will evolve under the Hamiltonian

$$H = \omega_0 |e\rangle\langle e| \; \Big\{ \text{Hamiltonian of a two-level atom } \omega_0 \begin{cases} |e\rangle \\ |g\rangle \end{cases}$$

$$+ \sum_{\vec{k},s} \omega_k a^\dagger_{\vec{k}s} a_{\vec{k}s} \; \Big\} \text{Hamiltonian of the electromag field } (\vec{k},s \text{ label wavevector and polarisation}); \; \omega_k = \omega_{|\vec{k}|} = c|\vec{k}|$$

$$\underbrace{- \sum_{\vec{k},s} \left(g_{\vec{k}s} |e\rangle\langle g| a_{\vec{k}s} + g^*_{\vec{k}s} |g\rangle\langle e| a^\dagger_{\vec{k}s} \right)}$$

coupling between electromag. field and atom (de-excitation of atom creates photon)

coupling constant: $g_{\vec{k}s} = i \sqrt{\frac{\omega_k}{2\varepsilon_0 V}} (\vec{d} \cdot \vec{\varepsilon}_{\vec{k}s})$

- $\vec{d}$ ... dipole moment of the atomic transition
- $\vec{\varepsilon}_{\vec{k}s}$ .. polarisation vector of photons
- V ... volume of space (results will not depend on that)

Under the action of the Hamiltonian the state $|\psi(0)\rangle$ will evolve into

$$|\psi(t)\rangle = \alpha(t)\, e^{-i\omega_0 t}\, \underbrace{|e, \{0\}\rangle}_{\text{initial state}} + \underbrace{\sum_{\vec{k},s} \beta_{\vec{k}s}(t)\, e^{-i\omega_k t}\, |g, 1_{\vec{k}s}\rangle}_{\substack{\text{final state can only contain one} \\ \text{photon with wave} \\ \text{vector } \vec{k} \text{ and polarisation } s}}$$

In the next step we plug this wave function into the Schrödinger equation $i\partial_t |\psi(t)\rangle = H|\psi(t)\rangle$

$$H|\psi\rangle = \alpha(t)\, e^{-i\omega_0 t}\, \omega_0 |e\,\{0\}\rangle + \sum_{\vec{k}s} \beta_{\vec{k}s}(t)\, e^{-i\omega_k t}\, \omega_k |g\, 1_{\vec{k}s}\rangle$$
$$- \sum_{\vec{k}s} \beta_{\vec{k}s}(t)\, g_{\vec{k}s}\, e^{-i\omega_k t} |e\,\{0\}\rangle - \alpha(t)\, e^{-i\omega_0 t} \sum_{\vec{k}s} g^*_{\vec{k}s} |g, 1_{\vec{k}s}\rangle$$

$$i\partial_t |\psi(t)\rangle = i\left(\dot{\alpha}(t) - i\omega_0 \alpha(t)\right) e^{-i\omega_0 t} |e\,\{0\}\rangle + i \sum_{\vec{k}s} \left(\dot{\beta}_{\vec{k}s}(t) - i\omega_k \beta_{\vec{k}s}(t)\right) e^{-i\omega_k t} |g, 1_{\vec{k}s}\rangle$$

Comparing the coefficients leads to

$$\dot{\alpha}(t) = i \sum_{\vec{k}s} g_{\vec{k}s}\, e^{-i(\omega_k - \omega_0)t}\, \beta_{\vec{k}s}(t), \quad \dot{\beta}_{\vec{k}s}(t) = i g^*_{\vec{k}s}\, e^{i(\omega_k - \omega_0)t}\, \alpha(t).$$

We formally integrate the equation for the $\beta_{\vec{k}s}$'s using the initial condition $\beta_{\vec{k}s}(0) = 0$:

$$\beta_{\vec{k}s}(t) = i g^*_{\vec{k}s} \int_0^t dt' \, e^{i(\omega_k - \omega_0)t'} \alpha(t')$$

Plugging this back into the equation for $\alpha(t)$, yields:

$$\dot{\alpha}(t) = -\sum_{\vec{k}s} |g_{\vec{k}s}|^2 \int_0^t dt' \, e^{-i(\omega_k - \omega_0)(t-t')} \alpha(t')$$

(memory kernel)

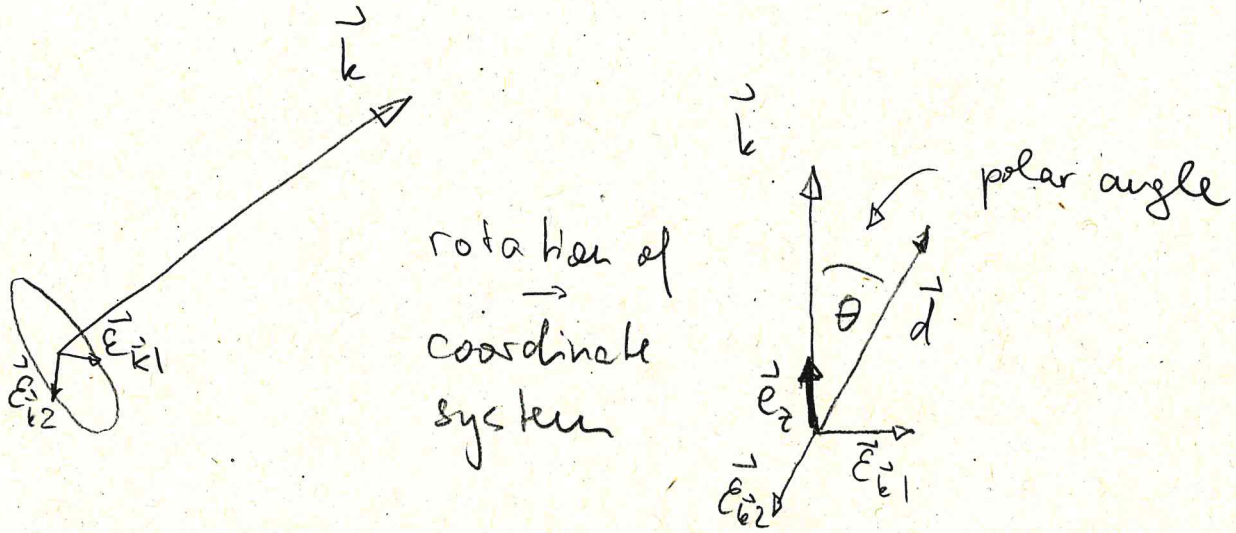
This type of integro-differential equation is very typical when dealing with open quantum systems. In order to solve it we need to make some simplifications / approximations. The first step is to go from the sum over $\vec{k}$ to an integral:

$$\sum_{\vec{k}s} \to \sum_{s=1}^{2} \frac{V}{(2\pi)^3} \int_0^\infty dk \, k^2 \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\varphi$$

One then has:

$$\sum_{\vec{k}s} |g_{\vec{k}s}|^2 = \int_0^\infty dk \, k^2 \frac{\omega_k}{2(2\pi)^3 \varepsilon_0} \left[\sum_{s=1}^{2} \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\varphi \, (\vec{d} \cdot \vec{\varepsilon}_{\vec{k}s})^2 \right]$$

Using $(\vec{d} \cdot \vec{\varepsilon}_{\vec{k},1})^2 + (\vec{d} \cdot \vec{\varepsilon}_{\vec{k},2})^2 = |\vec{d}|^2 (1 - \cos^2\theta) = |\vec{d}|^2 \sin^2\theta$ one finds:



$$\hookrightarrow \quad (\vec{d}\cdot\vec{e}_z)^2 + (\vec{d}\cdot\vec{\varepsilon}_{k1})^2 + (\vec{d}\cdot\vec{\varepsilon}_{k2})^2 = |\vec{d}|^2$$

with $\quad \vec{d}\cdot\vec{e}_z = |\vec{d}|\cos\theta$

$$\hookrightarrow \quad (\vec{d}\cdot\varepsilon_{k1})^2 + (\vec{d}\cdot\varepsilon_{k2})^2 = |\vec{d}|^2(1-\cos^2\theta)$$

$$\int_0^t dt'\, e^{-i(\omega_k-\omega_0)(t-t')}\,\alpha(t') \;=\; -\int_t^0 d\tau\, e^{-i(\omega_k-\omega_0)\tau}\,\alpha(t-\tau)$$

(inbodnce $\tau = t-t'$ $\hookrightarrow$ $d\tau = -dt'$)

$$= \int_0^t d\tau\, e^{-i(\omega_k-\omega_0)\tau}\,\alpha(t-\tau)$$

$$\sum_{s=1}^{2} \int_0^{\pi} d\theta \sin\theta \int_0^{\pi} d\varphi \, (\vec{d}\cdot\vec{\varepsilon}_{\vec{k}s})^2 = \frac{8\pi}{3} |\vec{d}|^2$$

$$\hookrightarrow \sum_{\vec{k}s} |g_{\vec{k}s}|^2 = \frac{|\vec{d}|^2}{6\pi^2\varepsilon_0 c^3} \int_0^{\infty} d\omega_k \, \omega_k^3 \qquad (\text{We used } \omega_k = c|\vec{k}|.)$$

With this we can write for the excited state amplitude:

$$\dot{\alpha}(t) = -\frac{|\vec{d}|^2}{6\pi^2\varepsilon_0 c^3} \int_0^{\infty} d\omega_k \, \omega_k^3 \int_0^{t} dt' \, e^{-i(\omega_k-\omega_0)(t-t')} \alpha(t')$$

$\int_0^t d\tau \, e^{-i(\omega_k-\omega_0)\tau} \alpha(t-\tau)$

In the next step we assume that $\alpha(t)$ evolves on a time scale that is much slower than the inverse of the frequency ω_0. Therefore $\alpha(t')$ is hardly changing its value over the time before the integral over the exponential is averaging out to zero.

$$\hookrightarrow \dot{\alpha}(t) \approx -\frac{|\vec{d}|^2}{6\pi^2\varepsilon_0 c^3} \left[\int_0^{\infty} d\omega_k \, \omega_k^3 \int_0^{t} d\tau \, e^{-i(\omega_k-\omega_0)\tau} \right] \alpha(t)$$

This makes the equation local in time, i.e. $\dot{\alpha}(t)$ does not depend on the past, but only on $\alpha(t)$.

The final approximation is to extend the upper limit of the integration to infinity. This is justified because $\alpha(t)$ varies on a time scale $t \gg \frac{1}{\omega_0}$. Hence for the times of interest we can as well assume $t \to \infty$.

$$\hookrightarrow \int_0^t dt' e^{-i(\omega_k-\omega_0)(t-t')} \to \int_0^\infty d\tau\, e^{-i(\omega_k-\omega_0)\tau}$$

$$= \pi \delta(\omega-\omega_0) - i \mathcal{P}\left\{ \frac{1}{\omega_k-\omega_0} \right\}$$

where $\mathcal{P}$ stands for Cauchy principal part.

We thus obtain

$$\dot{\alpha}(t) = \left[i\Delta\omega - \frac{\Gamma}{2} \right] \alpha(t)$$

where $\Gamma = \dfrac{\omega_0^3 |\vec{d}|^2}{3\pi\varepsilon_0 c^3}$ is the decay rate

and $\Delta\omega = \dfrac{|\vec{d}|^2}{6\pi^2\varepsilon_0 c^3} \mathcal{P}\left\{ \int_0^\infty d\omega_k \dfrac{\omega_k^3}{\omega_k-\omega_0} \right\}$ is the so-called Lamb-shift.

$$\int_0^\infty dt\, e^{-at}\, e^{-i\omega t} = \frac{1}{a + i\omega}$$

$$= \frac{a}{a^2 + \omega^2} - i\,\frac{\omega}{a^2 + \omega^2}$$

$$\lim_{a \to 0} \frac{a}{a^2 + \omega^2} = \pi\,\delta(\omega)$$

$$\lim_{a \to 0} \frac{\omega}{a^2 + \omega^2} = \frac{1}{\omega} \longrightarrow \mathcal{P}\left\{\frac{1}{\omega}\right\}$$

both expressions are distributions that appear under an integral

Within this treatment the Lamb-shift diverges, which we ignore here (the integral must be properly regularized). Nevertheless we can calculate now the probability for the atom being in the excited state, which is given by $|\alpha(t)|^2$. Since, $\alpha(t) = \alpha(0)\, e^{(i\Delta\omega - \frac{\Gamma}{2})t}$ we find $|\alpha(t)|^2 = |\alpha(0)|^2 e^{-\Gamma t}$.

- At the level of the Bloch vector $\vec{v}$ this dynamics corresponds to the affine map

$$\vec{v}' = M\vec{v} + \vec{c}$$

with (assuming $\Delta\omega = 0$, i.e. neglecting Lamb-shift)

$$M = \begin{pmatrix} e^{-\Gamma/2 t} & 0 & 0 \\ 0 & e^{-\Gamma/2 t} & 0 \\ 0 & 0 & e^{-\Gamma t} \end{pmatrix}, \quad \vec{c} = \begin{pmatrix} 0 \\ 0 \\ 1 - e^{-\Gamma t} \end{pmatrix}$$

(see also page 27)

- This is amplitude damping
- The stationary state is given by $\lim_{t\to\infty} \vec{v}' = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ which corresponds to the stationary density matrix $\rho_{ss} = |g\rangle\langle g|$

V The Lindblad master equation

Our goal is to find a more general procedure that allows us to obtain an equation of motion for the density matrix of the system.

We consider a situation where the system is weakly coupled to the bath. The total Hamiltonian is assumed to have the form

$$H = H_S + H_b + H_{sb}.$$

H_S: system, H_b: bath, H_{sb}: interaction

In the next step we transform into the interaction picture, using the unitary transformation $U_I = \exp\left[-it(H_S + H_b)\right]$.

The density matrix ρ of the total system, i.e. system + bath, then evolves in time according to the von Neumann equation

$$\frac{\partial}{\partial t}\rho(t) = -i\left[H_I(t), \rho(t)\right], \quad \text{with } H_I(t) = U_I^\dagger H_{sb} U_I.$$

Formally integrating this equation yields

$$\rho(t) = \rho(0) - i \int_0^t ds \, [H_I(s), \rho(s)] \,,$$ and after

inserting this result into the differential equation, we obtain:

$$\frac{\partial}{\partial t} \rho(t) = -i \, [H_I(t), \rho(0)] - \int_0^t ds \, [H_I(t), [H_I(s), \rho(s)]] \,.$$

In the next step we take the trace over the bath degrees of freedom and assume that $\mathrm{Tr}_b \, [H_I(t), \rho(0)] = 0$ (this can be achieved when the state of the bath and system factorise at $t = 0$, which we assume - see below).

The density matrix of the system then evolves according to

$$\frac{\partial}{\partial t} \rho_S(t) = \frac{\partial}{\partial t} \mathrm{Tr}_b (\rho(t)) = - \int_0^t ds \, \mathrm{Tr}_b \left\{ [H_I(t), [H_I(s), \rho(s)]] \right\}.$$

- Born approximation: We assume that the coupling between the system and the reservoir is weak. Thus the density matrix of the reservoir is only negligibly affected by the interaction.

The total density matrix at time t may then be approximated by a tensor product:

$$\rho(t) = \rho_S(t) \otimes \rho_b .$$

This yields a closed integro-differential equation:

$$\frac{\partial}{\partial t}\rho_S(t) = -\int_0^t ds\, Tr_b \left\{ [H_I(t), [H_I(s), \rho_S(s)\otimes\rho_b]] \right\} .$$

- Markov approximation: We replace $\rho_S(s)$ by $\rho_S(t)$, which will be justified by the fact that bath correlations / excitations decay on a much shorter timescale than that of any relevant dynamics of the system. In some sense this is equivalent to a coarse-graining over a time scale which is long for the bath, but short for the system.

This yields the Redfield equation:

$$\frac{\partial}{\partial t}\rho_S(t) = -\int_0^t ds\, Tr_b \left\{ [H_I(t), [H_I(s), \rho_S(t)\otimes\rho_b]] \right\} .$$

The final step is to perform the change of variable $s \to t - s$ and to shift the upper integration boundary to infinity. This is justified when the integrand vanishes sufficiently fast (we justify this a posteriori). This leads to the Markovian quantum master equation:

$$\frac{\partial}{\partial t} \rho_S(t) = - \int_0^\infty ds \; \mathrm{Tr}_b \left\{ [H_I(t), [H_I(t-s), \rho_S(t) \otimes \rho_b]] \right\}.$$

- Secular approximation: Ultimately, this approximation entails an averaging over rapidly oscillating terms. It will allow us to bring the master equation into a convenient shape, which is called the Lindblad form.

The starting point is the following general decomposition of the system-bath interaction.

$$H_{sb} = \sum_\alpha A_\alpha \otimes B_\alpha \,, \text{ with } A_\alpha = A_\alpha^\dagger, \; B_\alpha = B_\alpha^\dagger.$$

A_α: system operator; B_α: bath operator

As a first step towards the envisaged averaging procedure we introduce the operators

$$A_\alpha(\omega) = \sum_{\varepsilon'-\varepsilon=\omega} \Pi(\varepsilon) A_\alpha \Pi(\varepsilon'),$$

where the $\Pi(\varepsilon)$ are projectors onto the energy eigenspaces (with energy ε) of H_S.

They obey $\sum_\varepsilon \Pi(\varepsilon) = \mathbb{1}$, such that

$$H_S = \sum_{\varepsilon\varepsilon'} \Pi(\varepsilon) H_S \Pi(\varepsilon') = \sum_\varepsilon \varepsilon\, \Pi(\varepsilon)$$

and hence $A_\alpha = \sum_{\varepsilon\varepsilon'} \Pi(\varepsilon) A_\alpha \Pi(\varepsilon') = \sum_\omega \sum_{\varepsilon'-\varepsilon=\omega} \Pi(\varepsilon) A_\alpha \Pi(\varepsilon') = \sum_\omega A_\alpha(\omega)$.

We thus find that

$$[H_S, A_\alpha(\omega)] = -\omega A_\alpha(\omega)$$

and $$[H_S, A_\alpha^\dagger(\omega)] = \omega A_\alpha^\dagger(\omega).$$

↳ The $A_\alpha(\omega)$ & $A_\alpha^\dagger(\omega)$ are eigenoperators of H_S and as a consequence their time evolution in the interaction picture is

$$e^{iH_S t} A_\alpha(\omega) e^{-iH_S t} = e^{-i\omega t} A_\alpha(\omega)$$

$$e^{iH_S t} A_\alpha^\dagger(\omega) e^{-iH_S t} = e^{i\omega t} A_\alpha^\dagger(\omega)$$

The interaction picture representation of the system - bath interaction then becomes:

$$H_I = \sum_{\alpha\omega} e^{-i\omega t} A_\alpha(\omega) \otimes B_\alpha(t)$$

$$\text{with } B_\alpha(t) = e^{iH_b t} B_\alpha e^{-iH_b t}.$$

Note, that with this decomposition the condition $Tr_b [H_I(t), \rho(0)] = 0$ can be reformulated as

$\langle B_\alpha(t) \rangle = Tr_b \{ B_\alpha(t) \rho_b \} = 0$, i.e. the average of $B_\alpha(t)$ is zero. This can be always achieved be a redefinition of the system bath coupling (a possible constant part will simply be absorbed in the system Hamiltonian).

The master equation becomes now

$$\frac{\partial}{\partial t} \rho_s(t) = \int_0^\infty ds \, Tr_b \{ H_I(t-s) \rho_s(t) \rho_b H_I(t) - H_I(t) H_I(t-s) \rho_s(t) \rho_b \} + h.c.$$

$$= \sum_{\omega\omega'} \sum_{\alpha\beta} e^{i(\omega'-\omega)t} \Gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_s(t) A_\alpha^\dagger(\omega') - A_\alpha^\dagger(\omega') A_\beta(\omega) \rho_s(t) \right)$$

$$+ h.c.$$

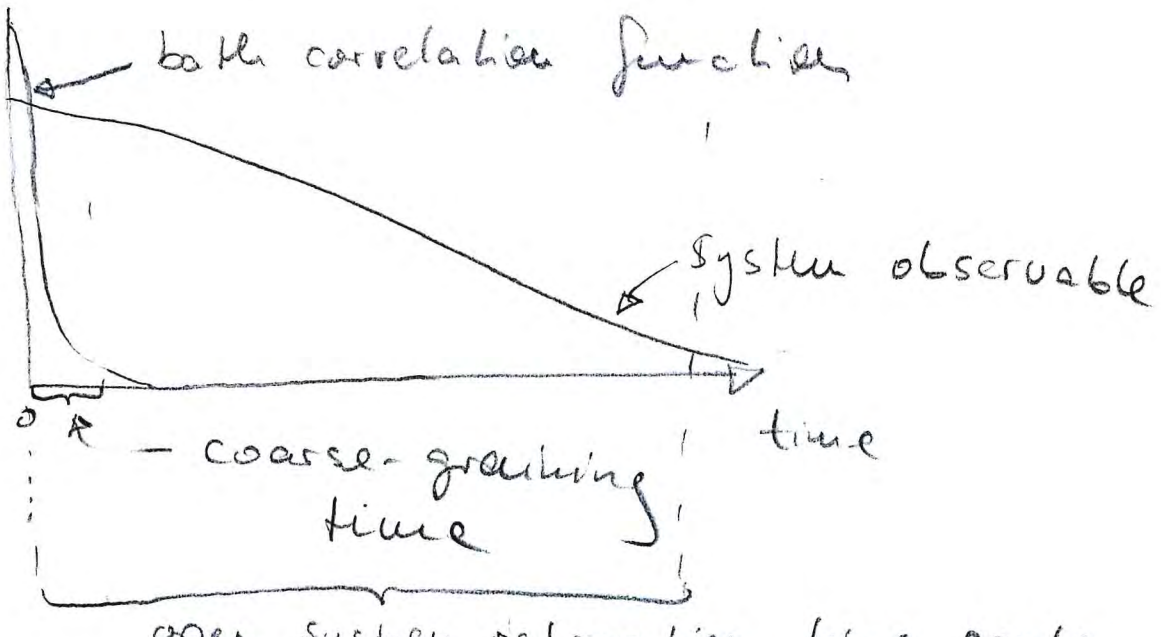
with $\Gamma_{\alpha\beta}(\omega) = \int_0^\infty ds\, e^{i\omega s}\, Tr_b\{ B_\alpha^+(t)\, B_\beta(t-s)\, \rho_b \}$

$= \int_0^\infty ds\, e^{i\omega s} \langle B_\alpha^+(t)\, B_\beta(t-s) \rangle$, which is the Fourier transform of the bath two-time correlation function.

When the bath is in a stationary state (which we assume), this correlation function does not depend on the absolute time t, but only on the time differences

$$\langle B_\alpha^+(t)\, B_\beta(t-s) \rangle = \langle B_\alpha^+(s)\, B_\beta(0) \rangle .$$

The assumption underlying the Markov approximation was that this correlation function decays sufficiently fast.



a posteriori justification of Markov approximation

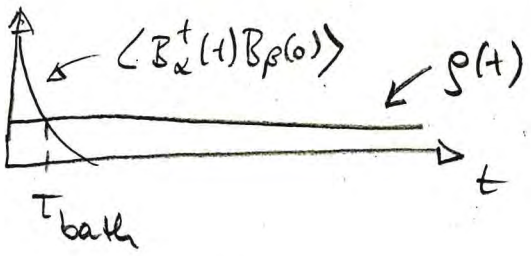
$$\int_0^t ds\, Tr_b \left\{ \left[H_I(t), \left[H_I(s), \rho_s(s) \otimes \rho_b \right] \right] \right\}$$

$\tau = t - s \;;\; d\tau = -ds$

$$\hookrightarrow \int_0^t d\tau\, Tr_b \left\{ \left[H_I(t), \left[H_I(t-\tau), \rho(t-\tau) \right] \right] \right\}$$

$$\sim \dots \int_0^t d\tau \, \langle B_\alpha^+(t)\, B_\beta(t-\tau) \rangle A_\beta(\omega)\, \rho_s(t-\tau)\, A_\alpha(\omega') \dots$$

$$\sim \dots \int_0^t d\tau \, \langle B_\alpha^+(\tau)\, B_\beta(0) \rangle A_\beta(\omega)\, \rho_s(t-\tau)\, A_\alpha(\omega') \dots$$



- density matrix hardly changes over correlation time, τ_{bath}, of the bath

$\rho_s(t-\tau) \approx \rho_s(t)$

$$\hookrightarrow \sim \dots \int_0^t d\tau \, \langle B_\alpha^+(\tau)\, B_\beta(0) \rangle A_\beta(\omega)\, \rho_s(t) A_\alpha(\omega')$$

- we are interested in times much longer than τ_{bath} (coarse graining)

$$\hookrightarrow \sim \dots \int_0^\infty d\tau \, \langle B_\alpha^+(\tau)\, B_\beta(0) \rangle A_\beta(\omega)\, \rho_s(t) A_\alpha(\omega')$$

When the relaxation time scale of the open system is much larger than the intrinsic timescale (typical values of $|\omega-\omega'|^{-1}$) we can perform the secular approximation: "$e^{i(\omega-\omega')t} \to \delta_{\omega\omega'}$"

[in q. optics: $|\omega-\omega'| \sim 10^{15}$ Hz, decay rate $\sim 10^9$ Hz]

$$\hookrightarrow \frac{\partial}{\partial t}\rho_S(t) = \sum_{\omega\alpha\beta} \Gamma_{\alpha\beta}(\omega)\left[A_\beta(\omega)\rho_S(t)A_\alpha^\dagger(\omega) - A_\alpha^\dagger(\omega)A_\beta(\omega)\rho_S(t)\right] + \text{h.c.}$$

In a final step we decompose

$$\Gamma_{\alpha\beta}(\omega) = \frac{1}{2}\gamma_{\alpha\beta}(\omega) + i S_{\alpha\beta}(\omega)$$

decay rates ↑ ← energy shifts (Lamb shift)

(Kossakowski matrix)

$$\gamma_{\alpha\beta}(\omega) = \Gamma_{\alpha\beta}(\omega) + \Gamma^*_{\beta\alpha}(\omega) = \int_{-\infty}^{\infty} ds\, e^{i\omega s}\langle B_\alpha^\dagger(s) B_\beta(0)\rangle$$

Fourier transform of the bath correlation function

The final result is the Lindblad-Kossakowski master equation:

$$\frac{\partial}{\partial t}\rho_S(t) = -i\left[H_{LS}, \rho_S(t)\right] + \mathcal{D}(\rho_S(t))$$

with the Lamb-shift Hamiltonian

$$H_{LS} = \sum_{\omega\alpha\beta} S_{\alpha\beta}(\omega) A_\alpha^\dagger(\omega) A_\beta(\omega)$$

and the dissipator

$$\mathcal{D}(\rho_S) = \sum_{\omega\alpha\beta} \gamma_{\alpha\beta}(\omega)\left(A_\beta(\omega)\rho_S A_\alpha^\dagger(\omega) - \frac{1}{2}\left\{A_\alpha^\dagger(\omega)A_\beta(\omega), \rho_S\right\}\right)$$

In the final step let us make one further simplification of the dissipator. We introduce the eigenvalues and eigenvectors of the Kossakowski matrix

$$\underline{\underline{\gamma}}(\omega) = \sum_\alpha \gamma_\alpha(\omega)\, V_\alpha(\omega)\, V_\alpha^+(\omega)$$

This allows us to write

$$\mathcal{D}(\rho_S) = \sum_{\omega\alpha} \gamma_\alpha(\omega) \left(L_\alpha(\omega) \rho_S L_\alpha^+(\omega) - \frac{1}{2} \{ L_\alpha^+(\omega) L_\alpha(\omega), \rho_S \} \right)$$

The $\gamma_\alpha(\omega)$ are the decay rates and

the $L_\alpha(\omega) = \sum_j V_{\alpha,j}(\omega)\, A_j(\omega)$

are the so-called jump operators.

This takes the master equation to the

Lindblad form

$$\frac{\partial}{\partial t}\rho = -i\,[H,\rho] + \sum_j \gamma_j \left(L_j \rho L_j^+ - \frac{1}{2} \{ L_j^+ L_j, \rho \} \right)$$

In the following we will see that the master equation can be derived through a short-time expansion of a quantum map.

To see this we note that the evolution of an initial state $\rho(0)$ over an infinitesimally small time interval dt is given by

$$\rho(dt) = \rho(0) + \dot{\rho}(0)\, dt + \mathcal{O}(dt^2).$$

On the other hand we should have

$$\rho(dt) = \sum_\alpha K_\alpha(dt)\, \rho(0)\, K_\alpha^+(dt).$$

Let us now try to find Kraus operators that make those two equations agree up to order dt. Clearly, in order to get the $\rho(0)$-term one Kraus operator has to contain the identity. We thus attempt

$$K_0 = \mathbb{1} + L_0\, dt,$$

so that

$$K_0 \rho(0) K_0^+ = \rho(0) + [L_0 \rho(0) + \rho(0) L_0^+]\, dt + \mathcal{O}(dt^2).$$

These must be further Kraus operators, since having only one would correspond to unitary evolution. So we choose

$$K_\alpha = \sqrt{dt}\, L_\alpha \quad , \quad \alpha \geq 1$$

such that $K_\alpha \rho(0) K_\alpha^\dagger = L_\alpha \rho(0) L_\alpha^\dagger \, dt$.

Enforcing the normalisation condition yields

$$\mathbb{1} = K_0^\dagger K_0 + \sum_{\alpha \geq 1} K_\alpha^\dagger K_\alpha = \mathbb{1} + dt \left(L_0 + L_0^\dagger + \sum_{\alpha \geq 1} L_\alpha^\dagger L_\alpha \right) + \mathcal{O}(dt^2)$$

We can now decompose into an hermitean and an anti-hermitean part: $L_0 = A - iH$, with $A = A^\dagger$ and $H = H^\dagger$. Thus, in order to fulfill the normalisation condition up to order dt, we need to choose

$$A = -\frac{1}{2} \sum_{\alpha \geq 1} L_\alpha^\dagger L_\alpha .$$

We thus have:

$$\begin{aligned}
\rho(dt) &= K_0 \rho(0) K_0^\dagger + \sum_{\alpha \geq 1} K_\alpha \rho(0) K_\alpha^\dagger \\
&= \rho(0) + (A - iH)\rho(0)\, dt + \rho(0)(A + iH)\, dt \\
&\qquad + \sum_{\alpha \geq 1} L_\alpha \rho(0) L_\alpha^\dagger \, dt + \mathcal{O}(dt^2) \\
&= \rho(0) - i[H, \rho(0)]\, dt + \{A, \rho(0)\}\, dt + \sum_{\alpha \geq 1} L_\alpha \rho L_\alpha^\dagger \, dt + \mathcal{O}(dt^2) \\
&= \rho(0) - i[H, \rho(0)]\, dt + \sum_{\alpha \geq 1} \left(L_\alpha \rho L_\alpha^\dagger - \frac{1}{2} \{ L_\alpha^\dagger L_\alpha, \rho(0) \} \right) dt + \mathcal{O}(dt^2)
\end{aligned}$$

Finally, we obtain:

$$\dot{\rho}(0) = \lim_{dt\to 0} \frac{\rho(dt)-\rho(0)}{dt} = -i[H,\rho(0)] + \sum_{\alpha\geq 1}\left(L_\alpha \rho(0) L_\alpha^\dagger - \frac{1}{2}\{L_\alpha^\dagger L_\alpha, \rho(0)\}\right),$$
$$= \mathcal{L}(\rho(0))$$

which is the Lindblad master equation.

• <u>Semi-group property:</u>

The formal solution of the master equation $\dot{\rho}(t) = \mathcal{L}\rho$ is

$$\rho(t) = e^{\mathcal{L}t}\rho(0) = \Lambda_t \rho(0),$$

where Λ_t is called the Markovian evolution operator. The set $\{\Lambda_t\}_{t\geq 0}$ forms a one-parameter semi-group, because it satisfies three out of four properties of a group:

1. Identity operator: $\Lambda_0 = \mathbb{1}$
2. Closed under multiplication:
$$\Lambda_t \Lambda_s = e^{\mathcal{L}t} e^{\mathcal{L}s} = e^{\mathcal{L}(t+s)} = \Lambda_{t+s}$$
3. Associativity: $(\Lambda_t \Lambda_s)\Lambda_r = \Lambda_t(\Lambda_s \Lambda_r)$.

However, not every element has an inverse. The map Λ_t is contractive, corresponding to exponential decay. I.e. Λ_∞ has at least one zero eigenvalue, so that it does not possess an inverse.

The relation between state changes of the open system and the unitary dynamics of the total system, including the bath, can be visualised as follows:

$$\rho(0) = \rho_S(0) \otimes \rho_b(0) \xrightarrow[\text{evolution}]{\text{unitary}} \rho(t) = U(t)\left[\rho_S(0) \otimes \rho_b(0)\right] U^\dagger(t)$$

$$\downarrow \mathrm{tr}_b \qquad\qquad\qquad\qquad \downarrow \mathrm{tr}_b$$

$$\rho_S(0) \xrightarrow[\text{"dynamical map"}]{e^{\mathcal{L}t}} \rho_S(t) = e^{\mathcal{L}t}\rho_S(0)$$

The master equation $\dot{\rho} = \mathcal{L}\rho$ is a linear equation, which has the solution $\rho(t) = e^{\mathcal{L}t}\rho(0)$ (provided that $\mathcal{L}$ is not explicitly time-dependent). This is formally equivalent to solving, e.g. the Schrödinger equation. However, a complication arises since $\mathcal{L}$ involves terms in which operators are multiplied to both sides of the density matrix.

The idea behind the Choi - Jamiołkowski isomorphism is to bring the master equation into a form, where $\mathcal{L}$ is an $N^2 \times N^2$ matrix (assuming the dimension of the system Hilbert space is N), and ρ is represented by an N^2-dimensional vector.

The procedure is often referred to "vectorisation" and becomes tremendously helpful when solving master equations in practice, e.g. on a computer.

The isomorphism is given by the relation $|i\rangle\langle j| \longrightarrow |j\rangle \otimes |i\rangle$, i.e. the outer product is turned into a direct product. The density matrix $\rho = \sum_{ij} \rho_{ij} |i\rangle\langle j|$ then becomes a vector in a "doubled space", which has dimension N^2.

$$\rho \longrightarrow \underbrace{\vec{\rho} = \sum_{ij} \rho_{ij} |j\rangle \otimes |i\rangle}_{\text{vectorised density matrix}}$$

For example, if $M = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, $\vec{M} = \begin{pmatrix} a \\ c \\ b \\ d \end{pmatrix}$.

A first convenient property of the isomorphism is that it turns the Hilbert-Schmidt inner product of operators into the standard inner product for its vectorised forms:

$$\mathrm{tr}\,(A^\dagger B) = \vec{A}^\dagger \cdot \vec{B}.$$

With the vectorisation of the identity operator

$$\mathbb{1} = \sum_i |i\rangle\langle i| \longrightarrow \vec{\mathbb{1}} = \sum_i |i\rangle \otimes |i\rangle$$

we can thus write the normalization condition of the density matrix as

$$\mathrm{tr}\,\rho = \mathrm{tr}\,\mathbb{1}^{+}\rho = \vec{\mathbb{1}}^{+}\vec{\rho} = 1 .$$

A second useful property of the isomorphism concerns the product of three matrices:

$$\overrightarrow{ABC} = (C^{T}\otimes A)\,\vec{B} .$$

In order to see that this is true we write both sides explicitely:

$$ABC = \sum_{ijklmn} (A_{ij}\,|i\rangle\langle j|)\,(B_{kl}\,|k\rangle\langle l|)\,(C_{mn}\,|m\rangle\langle n|) = \sum_{ijmn} A_{ij}\,B_{jm}\,C_{mn}\,|i\rangle\langle n| .$$

$$\hookrightarrow \overrightarrow{ABC} = \sum_{ijmn} A_{ij}\,B_{jm}\,C_{mn}\,|n\rangle\otimes|i\rangle ;$$

$$(C^{T}\otimes A)\,\vec{B} = \Big(\sum_{mnij} C_{mn}A_{ij}\,|n\rangle\langle m|\otimes|i\rangle\langle j|\Big)\sum_{kl} B_{lk}\,|k\rangle\otimes|l\rangle$$

$$= \sum_{mnij} C_{mn}\,A_{ij}\,B_{jm}\,|n\rangle\otimes|i\rangle = \overrightarrow{ABC} .$$

Let us now apply these rules to the master equation in Lindblad form:

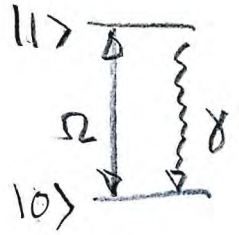
$$\dot{\rho} = -i\,[H,\rho] + \sum_{\alpha}\Big(L_{\alpha}\rho L_{\alpha}^{+} - \frac{1}{2}\{L_{\alpha}^{+}L_{\alpha},\rho\}\Big)$$

$$\hookrightarrow \frac{\partial}{\partial t}\vec{\rho} = -i\,\overrightarrow{H\rho\mathbb{1}} + i\,\overrightarrow{\mathbb{1}\rho H} + \sum_\alpha \left(\overrightarrow{L_\alpha \rho L_\alpha^\dagger} - \frac{1}{2}\overrightarrow{L_\alpha^\dagger L_\alpha \rho \mathbb{1}} - \frac{1}{2}\overrightarrow{\mathbb{1}\rho L_\alpha^\dagger L_\alpha} \right)$$

$$= \underbrace{\left[-i\,\mathbb{1}\otimes H + iH^T\otimes\mathbb{1} + \sum_\alpha \left(L_\alpha^*\otimes L_\alpha - \frac{1}{2}\mathbb{1}\otimes L_\alpha^\dagger L_\alpha - \frac{1}{2}(L_\alpha^\dagger L_\alpha)^T\otimes\mathbb{1} \right) \right]}_{\hat{\mathcal{L}}} \vec{\rho}$$

The master operator $\mathcal{L}$ has now been turned into a matrix $\hat{\mathcal{L}}$, which can be analysed and manipulated with the standard tools (spectral decomposition, etc.).

Example. Resonantly driven two-level atom with decay



Hamiltonian: $H = \Omega\sigma_x$, with Ω being the so-called Rabi frequency (∝ electric field strength of the laser)

Decay: $L = \sqrt{\gamma}\,\sigma^-$, with γ being the decay rate

$$\hat{\mathcal{L}} = -i\Omega \underbrace{\mathbb{1}\otimes\sigma_x}_{\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix}} + i\Omega \underbrace{\sigma_x\otimes\mathbb{1}}_{\begin{pmatrix}0&0&1&0\\0&0&0&1\\1&0&0&0\\0&1&0&0\end{pmatrix}} + \gamma\Big[\underbrace{\sigma^-\otimes\sigma^-}_{\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&0\\1&0&0&0\end{pmatrix}} - \frac{1}{2}\underbrace{\mathbb{1}\otimes(\sigma^+\sigma^-)}_{\begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&1&0\\0&0&0&0\end{pmatrix}} - \frac{1}{2}\underbrace{(\sigma^+\sigma^-)\otimes\mathbb{1}}_{\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix}}\Big]$$

$$= \begin{pmatrix} -\gamma & -i\Omega & i\Omega & 0 \\ -i\Omega & -\frac{\gamma}{2} & 0 & i\Omega \\ i\Omega & 0 & -\frac{\gamma}{2} & -i\Omega \\ \gamma & i\Omega & -i\Omega & 0 \end{pmatrix}$$

This is a non-hermitean matrix (opposed to a Hamiltonian). In order to proceed we decompose it into its spectral representation:

$$\hat{\mathcal{L}} = \lambda_0 \vec{r}_0 \vec{l}_0^{\,+} + \sum_{\alpha=1}^{3} \lambda_\alpha \vec{r}_\alpha \vec{l}_\alpha^{\,+}, \quad \text{with } \vec{l}_\alpha^{\,+}\vec{r}_\beta = \delta_{\alpha\beta}.$$

Here, λ_α are the eigenvalues and $\vec{r}_\alpha$ and $\vec{l}_\alpha$ are the corresponding right and left eigenvectors, respectively. Note, that $\mathrm{Tr}\, r_0 = 1$ & $\mathrm{Tr}\, r_{\alpha>0} = 0$.
For all master operators the following holds:

1) $\lambda_0 = 0$, is the eigenvalue with the largest real part (unless there are oscillating solutions or degeneracies). All other eigenvalues have a real part that is negative.

2) $\vec{r}_0$ is the stationary state:

$$\hat{\mathcal{L}}\,\vec{r}_0 = \lambda_0 \vec{r}_0 \underbrace{\left(\vec{l}_0^{+} \cdot \vec{r}_0\right)}_{1} + \sum_\alpha \lambda_\alpha \vec{r}_\alpha \underbrace{\left(\vec{l}_\alpha^{+} \cdot \vec{r}_0\right)}_{\delta_{\alpha 0}}$$

$$= \lambda_0 \vec{r}_0 = 0$$

3) $\vec{l}_0$ is the identity operator:

$$1 = \vec{l}_0^{+} \vec{r}_0 = \mathrm{Tr}\left(l_0^{+} r_0\right) = \mathrm{Tr}\left(r_0\right)$$

r_0: stationary state density matrix (not vectorised)

4) time evolution operator:

$$e^{\hat{\mathcal{L}}t} = \underbrace{e^{\lambda_0 t}}_{1} \vec{r}_0 \vec{l}_0^{+} + \sum_\alpha e^{\lambda_\alpha t} \vec{r}_\alpha \vec{l}_\alpha^{+}$$

$$\hookrightarrow \lim_{t\to\infty} e^{\hat{\mathcal{L}}t} = \underbrace{\vec{r}_0 \vec{l}_0^{+}}$$

projector on stationary state

Let us come back to the two-level atom and set for simplicity $\Omega = 0$ (pure decay). We then have

$$\hat{\mathcal{L}} = 0 \cdot \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}(1001) - \frac{\gamma}{2}\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}(0100) - \frac{\gamma}{2}\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}(0010) - \gamma\begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}(1000)$$

$$= \begin{pmatrix} -\gamma & 0 & 0 & 0 \\ 0 & -\gamma/2 & 0 & 0 \\ 0 & 0 & -\gamma/2 & 0 \\ \gamma & 0 & 0 & 0 \end{pmatrix}$$

The time evolution is hence given by the operator

$$e^{\hat{\mathcal{L}}t} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}(1001) + e^{-\frac{\gamma}{2}t}\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}(0100) + e^{-\frac{\gamma}{2}t}\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}(0010) + e^{-\gamma t}\begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}(1000).$$

This allows us to calculate the evolution of an atom, that is initially in the excited state. Its density matrix is:

$$\rho(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \longrightarrow \vec{\rho}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$e^{\hat{\mathcal{L}}t}\vec{\rho}(0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} + e^{-\gamma t}\begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix} = \begin{pmatrix} e^{-\gamma t} \\ 0 \\ 0 \\ 1-e^{-\gamma t} \end{pmatrix}$$

$$\hookrightarrow \rho(t) = \begin{pmatrix} e^{-\gamma t} & 0 \\ 0 & 1-e^{-\gamma t} \end{pmatrix} = \frac{1}{2}\left[\mathbb{1} - (1-2e^{-\gamma t})\sigma_z\right]$$

The stationary state is $|0\rangle$, with Bloch vector $\vec{v}_\infty = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix}$.

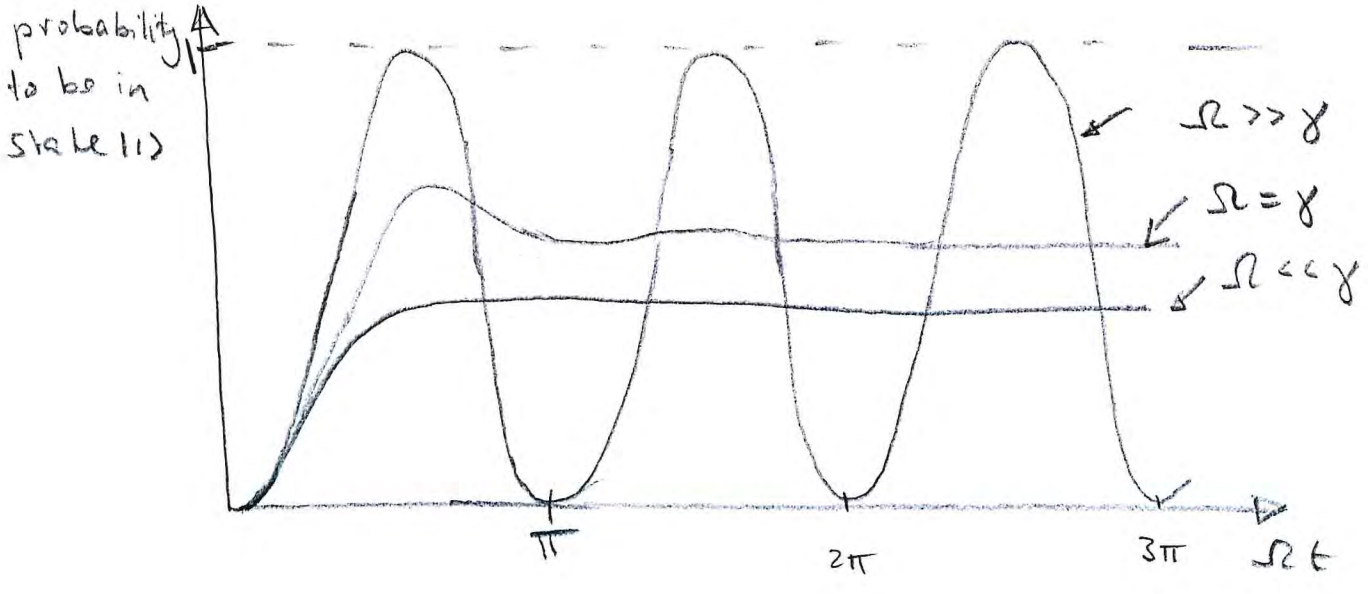
Performing the calculation for $\Omega \neq 0$ is significantly more involved. The stationary state is

$$\rho(\infty) = \frac{1}{\gamma^2 + 8\Omega^2} \begin{pmatrix} 4\Omega^2 & 2i\gamma\Omega \\ -2i\gamma\Omega & \gamma^2 + 4\Omega^2 \end{pmatrix}.$$

For the time-dependent state, starting from $\rho(0) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$, we obtain.

$$\rho(t) = \begin{pmatrix} \frac{1}{2}\frac{\gamma^2 - \Gamma^2}{\Gamma^2 - 9\gamma^2}\left(1 + \left\{\cosh\left(\frac{\Gamma}{4}t\right) + 3\frac{\gamma}{\Gamma}\sinh\left(\frac{\Gamma}{4}t\right)\right\}e^{-\frac{3}{4}\gamma t}\right) & * \\ -\frac{i}{4}\frac{\sqrt{\gamma^2 - \Gamma^2}}{\Gamma}\left(\frac{8\gamma\Gamma}{9\gamma^2 - \Gamma^2} + e^{-\frac{3}{4}\gamma t}\left\{\frac{(\gamma+\Gamma)e^{\frac{\Gamma}{4}t}}{\Gamma - 3\gamma} + \frac{(\gamma-\Gamma)e^{-\frac{\Gamma}{4}t}}{\Gamma + 3\gamma}\right\}\right) & * \end{pmatrix}$$

with $\Gamma = \sqrt{\gamma^2 - 64\Omega^2}$.



- When $\Omega \gg \gamma$, the probability of being in the excited state is oscillating in time with a frequency $2\pi\Omega$ (Rabi oscillations).
- When $\Omega \approx \gamma$ the oscillations are damped
- For $\Omega < \frac{\gamma}{8}$ the oscillations are overdamped.

VIII Quantum jump trajectories

Generally, we can write the Markovian evolution operator $\mathcal{L}$ as a sum of two parts: $\mathcal{L} = \mathcal{L}_0 + \mathcal{J}$, with

$$\mathcal{L}_0 \rho = -i[H,\rho] - \frac{1}{2}\sum_k^N \gamma_k \{L_k^+ L_k, \rho\} \quad \text{and}$$

$$\mathcal{J}\rho = \sum_k^N \gamma_k L_k \rho L_k^+ .$$ The first term we can rewrite as

$$\mathcal{L}_0 \rho = -i\left(H - \frac{i}{2}\sum_k^N \gamma_k L_k^+ L_k\right)\rho + i\rho\left(H + \frac{i}{2}\sum_k^N \gamma_k L_k^+ L_k\right)$$

$$= -i H_{eff}\rho + i\rho H_{eff}^+ ,$$

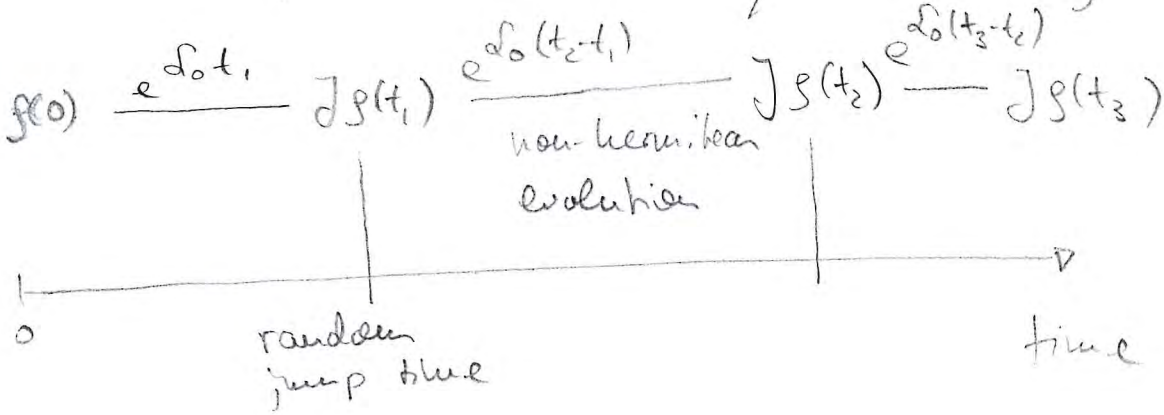
with $H_{eff} = H - \frac{i}{2}\sum_k^N \gamma_k L_k^+ L_k$ being the so-called effective Hamiltonian. Note, that H_{eff} is not hermitean. However, it evolves the quantum state ρ in a similar way as an ordinary Hamiltonian.

$$\partial_t \rho = \mathcal{L}_0 \rho \quad \rightarrow \quad \rho(t) = e^{-it H_{eff}} \rho(0)\, e^{it H_{eff}^+}$$

$$= e^{\mathcal{L}_0 t}\rho(0)$$

The term $\mathcal{J}\rho$ can be interpreted as a "jump term" as its action on the quantum state causes transitions of the kind $\rho \to L_k \rho L_k^+$ at a rate γ_k.

The evolution of an open quantum system can indeed be regarded as proceeding via a non-unitary dynamics under H_{eff}, which is interspersed with quantum jumps:



This picture can be formalised by expanding the master equation evolution into a Dyson series: Our starting point is to consider the evolution of the object

$$\bar{\rho}(t) = e^{-\mathcal{L}_0 t} \rho(t)$$

where $\rho(t)$ is the density matrix obeying $\partial_t \rho(t) = (\mathcal{L}_0 + \mathcal{J})\rho(t)$

We find that

$$\partial_t \bar{\rho}(t) = -\mathcal{L}_0 e^{-\mathcal{L}_0 t} \rho(t) + e^{-\mathcal{L}_0 t} \partial_t \rho(t)$$

$$= -\mathcal{L}_0 e^{-\mathcal{L}_0 t} \rho(t) + e^{-\mathcal{L}_0 t} (\mathcal{L}_0 + \mathcal{J}) \rho(t)$$

$$= e^{-\mathcal{L}_0 t} \mathcal{J} \rho(t).$$

Integrating this equation yields

$$\bar{\rho}(t) = \bar{\rho}(0) + \int_0^t d\tau\, e^{-\mathcal{L}_0 \tau} \mathcal{J} \rho(\tau)$$

and hence (using $\bar{\rho}(t) = e^{-\mathcal{L}_0 t} \rho(t)$)

$$\rho(t) = e^{\mathcal{L}_0 t} \rho(0) + \int_0^t d\tau\, e^{\mathcal{L}_0 (t-\tau)} \mathcal{J} \rho(\tau).$$

We can iterate this expression, which yields

$$\rho(t) = e^{\mathcal{L}_0 t} \rho(0) + \int_0^t d\tau\, e^{\mathcal{L}_0 (t-\tau)} \mathcal{J} e^{\mathcal{L}_0 \tau} \rho(0)$$

$$+ \int_0^t d\tau \int_0^\tau d\tau'\, e^{\mathcal{L}_0 (t-\tau)} \mathcal{J} e^{\mathcal{L}_0 (\tau-\tau')} \mathcal{J} \rho(\tau')$$

$$= e^{\mathcal{L}_0 t} \rho(0) +$$

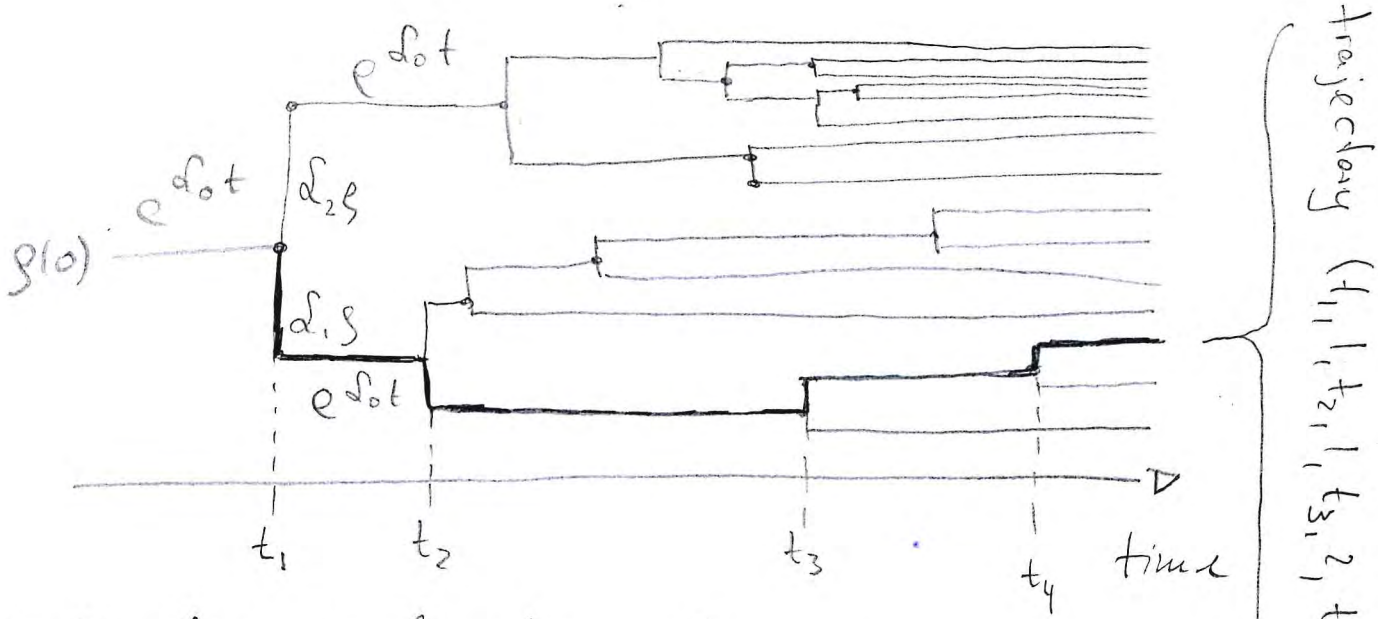
$$+ \sum_{n=1}^{\infty} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \cdots \int_0^{t_2} dt_1\, e^{\mathcal{L}_0 (t-t_n)} \mathcal{J} e^{\mathcal{L}_0 (t_n - t_{n-1})} \mathcal{J} \cdots e^{\mathcal{L}_0 (t_2 - t_1)} \mathcal{J} e^{\mathcal{L}_0 t_1} \rho(0),$$

The latter expression is the Dyson expansion and indeed one sees here that the state at time t is given by a sum of "trajectories" which correspond to repeated actions of the operator $\mathcal{J}$ and a time evolution under H_{eff} in between.

We now rewrite the operator $\mathcal{J}$ as

$$\mathcal{J}\rho = \sum_k \gamma_k L_k \rho L_k^\dagger = \sum_k \mathcal{L}_k \rho$$

in order to explicitly account for the different possible jump events.



A particular realisation of n jump events is specified by a sequence of the form $R_n^t = (t_1, k_1, t_2, k_2, \ldots, t_n, k_n)$

jump time ↑ ↑ jump type

The jump times satisfy $0 < t_1 < t_2 < \dots < t_n$ and $k_j \in \{1, \dots, N\}$. We call R_n^t a quantum jump trajectory. The time evolution of the quantum state can now be written as

$$\rho(t) = e^{\mathcal{L}_0 t}\rho(0) + \sum_{n=1}^{\infty} \underbrace{\sum_{\{R_n^t\}}}_{\text{contains integral over jump times}} \overbrace{e^{\mathcal{L}_0(t-t_n)}\mathcal{L}_{k_n} e^{\mathcal{L}_0(t_n - t_{n-1})}\mathcal{L}_{k_{n-1}} \dots \mathcal{L}_{k_1} e^{\mathcal{L}_0 t_1}\rho(0)}^{K_{R_n^t}}$$

$\sum_{n=1}^{\infty}$: sum over number of jumps

$\sum_{\{R_n^t\}}$: sum over all possible quantum jump trajectories with n jumps and length t

The probability of no jump occurring over a time period t is given by the trace of the first term, which represents the quantum jump trajectory containing zero jumps: $P(R_0^t | \rho(0)) = \mathrm{tr}\left(e^{\mathcal{L}_0 t}\rho(0)\right)$.

Analogously the probability for a particular trajectory R_n^t to occur, given the initial state $\rho(0)$, is $P(R_n^t, \rho(0)) = \mathrm{tr}\left(K_{R_n^t}\rho(0)\right)$, with

$$K_{R_n^t} = e^{\mathcal{L}_0(t-t_n)}\mathcal{L}_{k_n} e^{\mathcal{L}_0(t_n - t_{n-1})}\mathcal{L}_{k_{n-1}} \dots \mathcal{L}_{k_1} e^{\mathcal{L}_0 t_1}.$$

The quantum state at time t can then be written as

$$\rho(t) = \underbrace{\mathrm{tr}\left(K_{R_0^t}\rho(0)\right)}_{\text{probability to have zero jumps}} \underbrace{\rho_{R_0^t}}_{\text{state, conditioned on zero jumps}} + \sum_{n=1}^{\infty} \underbrace{\sum_{\{R_n^t\}}}_{\text{contains sum over } k_n \text{ and } t_n} \mathrm{tr}\left(K_{R_n^t}\rho(0)\right) \underbrace{\rho_{R_n^t}}_{\text{state, conditioned on a specific quantum jump trajectory}}$$

The quantum state conditioned to a specific trajectory R_n^t is given as

$$\rho_{R_n^t} = \frac{K_{R_n^t}\,\rho(0)}{\mathrm{tr}\left(K_{R_n^t}\,\rho(0)\right)}.$$

However, since we can write

$$K_{R_n^t}\,\rho = \underbrace{e^{-iH_{\mathrm{eff}}(t-t_n)} L_{k_n} e^{-iH_{\mathrm{eff}}(t_n-t_{n-1})} L_{k_{n-1}} \cdots L_{k_1} e^{-iH_{\mathrm{eff}}t_1}}_{M_{R_n^t}} \rho \underbrace{e^{iH_{\mathrm{eff}}^\dagger t_1} L_{k_1}^\dagger \cdots L_{k_n}^\dagger e^{+iH_{\mathrm{eff}}^\dagger(t-t_n)}}_{M_{R_n^t}^\dagger}$$

this establishes immediately a connection to the transformation of a quantum state under a measurement:

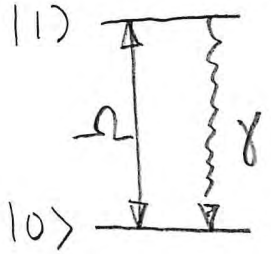
$$\rho_{R_n^t} = \frac{M_{R_n^t}\,\rho(0)\,M_{R_n^t}^\dagger}{\mathrm{tr}\left(M_{R_n^t}^\dagger M_{R_n^t}\,\rho(0)\right)}$$

with the compound measurement operator

$$M_{R_n^t} = e^{-iH_{\mathrm{eff}}(t-t_n)} L_{k_n} \cdots L_{k_2} e^{-iH_{\mathrm{eff}}(t_2-t_1)} L_{k_1} e^{-iH_{\mathrm{eff}}t_1}.$$

This shows that one can view the open system dynamics generated by $\mathcal{L}$ to emerge from a continuous monitoring of the system by the environment.

Example: two-level atom



The Master equation is given by

$$\dot{\rho} = -i\Omega[\sigma_x, \rho] + \gamma \sigma^- \rho \sigma^+ - \frac{\gamma}{2}\{\sigma^+\sigma^-, \rho\},$$

and we can read off the effective Hamiltonian:

$$H_{\text{eff}} = \Omega\sigma_x - i\frac{\gamma}{2}\sigma^+\sigma^- = \begin{pmatrix} -i\frac{\gamma}{2} & \Omega \\ \Omega & 0 \end{pmatrix}.$$

We also can see that

$$J\rho = \gamma \sigma^- \rho \sigma^+ = \gamma \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \rho \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

Let us now assume that the atom is initially prepared in the ground state $|0\rangle$. We can now use the formalism developed before in order to calculate how much time one needs to wait on average before a photon is emitted, i.e. a jump event takes place. To this end we first start by calculating the no-jump probability.

This is given by

$$p_{nojump}(t) = \mathrm{tr}\left(e^{\mathcal{L}_0 t}\rho(0)\right), \text{ with}$$

$$\mathcal{L}_0\rho = -iH_{eff}\rho + i\rho H_{eff}^{+}.$$

Since $\rho(0) = |0\rangle\langle 0|$, we have $e^{\mathcal{L}_0 t}\rho(0) = e^{-iH_{eff}t}|0\rangle\langle 0|e^{+iH_{eff}^{+}t}$.

Using $e^{-iH_{eff}t}|0\rangle = -\frac{4i\Omega}{\bar{\gamma}} e^{-\frac{\gamma}{4}t}\sinh\left(\frac{\bar{\gamma}t}{4}\right)|0\rangle$

$$+ e^{-\frac{\gamma}{4}t}\left(\cosh\left(\frac{\bar{\gamma}t}{4}\right) + \frac{\gamma}{\bar{\gamma}}\sinh\left(\frac{\bar{\gamma}t}{4}\right)\right)|1\rangle$$

with $\bar{\gamma} = \sqrt{\gamma^2 - 16\Omega^2}$, we obtain

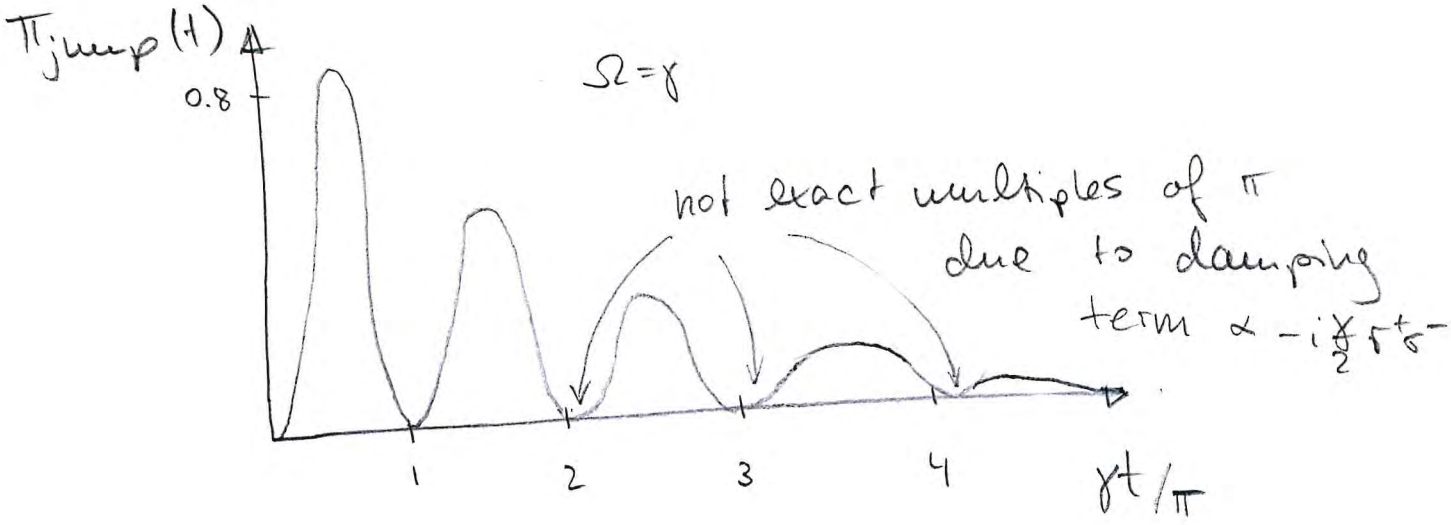
$$p_{nojump}(t) = e^{-\frac{\gamma}{2}t}\left(\frac{16\Omega^2}{\bar{\gamma}^2}\sinh^2\left(\frac{\bar{\gamma}t}{4}\right) + \left[\cosh\left(\frac{\bar{\gamma}t}{4}\right) + \frac{\gamma}{\bar{\gamma}}\sinh\left(\frac{\bar{\gamma}t}{4}\right)\right]^2\right)$$

$$= e^{-\frac{\gamma}{2}t}\left(\frac{\gamma^2}{\bar{\gamma}^2}\cosh\left(\frac{\bar{\gamma}t}{2}\right) + \frac{\gamma}{\bar{\gamma}}\sinh\left(\frac{\bar{\gamma}t}{2}\right) - 16\frac{\Omega^2}{\bar{\gamma}^2}\right).$$

Hence, the probability for a jump event to take place before time t is given by $p_{jump}(t) = 1 - p_{nojump}(t)$, which can be written also in terms of a probability density

$$p_{jump}(t) = \int_0^t d\tau\, \pi_{jump}(\tau)$$

with $\Pi_{jump}(t) = 16\gamma \frac{\Omega^2}{\gamma^2} e^{-\frac{\gamma t}{2}} \sinh\left(\frac{\gamma t}{4}\right)$. This probability density is oscillating, which is a consequence of the fact that the atom is performing „Rabi oscillations" under the effective Hermitian, and that there cannot be an emission/jump event, when the atom was rotated back to it's ground state, $|0\rangle$.



The average time to the jump event is calculated as $\langle t \rangle = \int_0^\infty d\tau\, \tau\, \Pi_{jump}(\tau) = \frac{2}{\gamma} + \frac{\gamma}{4\Omega^2}$, and the fluctuations of the jump time are

$$\Delta t = \left[\langle t^2 \rangle - \langle t \rangle^2\right]^{1/2} = \left[\frac{4}{\gamma^2} - \frac{1}{2\Omega^2} + \frac{\gamma^2}{16\Omega^4}\right]^{1/2}.$$

In the limit of large decay rate γ, we find $\langle t \rangle \to \frac{\gamma}{4\Omega^2}$ and $\Delta t \to \frac{\gamma}{4\Omega^2}$, i.e. the fluctuations become equal to the mean. The probability density of the jump-time assumes a particularly simple form, $\pi_{jump}(t) \overset{\gamma \gg \Omega}{=} \frac{4\Omega^2}{\gamma} e^{-\frac{4\Omega^2}{\gamma} t}$, ($\Omega$ also needs to be large) and so does the no-jump probability:

$$p_{no\,jump}(t) = e^{-\frac{4\Omega^2}{\gamma} t}.$$

Let us now investigate more generally the statistics of the jump events. The probability for the occurrence of n events before time t is given by

$$p_n(t) = \mathrm{tr} \int_0^t dt_n \cdots \int_0^{t_2} dt_1 \, e^{\mathcal{L}_0 (t - t_n)} \mathcal{J} e^{\mathcal{L}_0 (t_n - t_{n-1})} \mathcal{J} \cdots \mathcal{J} e^{\mathcal{L}_0 t_1} \rho(0).$$

Using the fact that $\rho(0) = |0\rangle\langle 0|$, and that

J can be written as

$$J\rho = \gamma \sigma^- \rho \sigma^+ = \gamma\, |0\rangle\langle 1|\rho|1\rangle\langle 0|,$$

this expression simplifies to

$$\rho_n(t) = \mathrm{tr} \int_0^t dt_n \cdots \int_0^{t_2} dt_1 \gamma^n e^{-iH_{\mathrm{eff}}(t-t_n)} |0\rangle\langle 1| \cdots |0\rangle\langle 1| \underbrace{\langle 1| e^{-iH_{\mathrm{eff}}t_1} |0\rangle\langle 0| e^{iH_{\mathrm{eff}}^\dagger t_1}}_{q(t_1)/\gamma} |1\rangle\langle 0| \cdots |1\rangle\langle 0| e^{iH_{\mathrm{eff}}^\dagger (t-t_n)}$$

Introducing $q(t) = \gamma |\langle 1| e^{-iH_{\mathrm{eff}}t} |0\rangle|^2$, we can write

$$\rho_n(t) = \mathrm{tr} \int_0^t dt_n \cdots dt_1\; e^{-iH_{\mathrm{eff}}(t-t_n)} |0\rangle\langle 0|\, q(t_n - t_{n-1}) q(t_{n-1} - t_{n-2}) \cdots q(t_1) \langle 0| e^{iH_{\mathrm{eff}}^\dagger (t-t_n)}$$

$$= \int_0^t dt_n \cdots dt_1\; \underbrace{\mathrm{tr}\left[e^{-iH_{\mathrm{eff}}(t-t_n)} |0\rangle\langle 0| e^{iH_{\mathrm{eff}}^\dagger (t-t_n)} \right]}_{p_{\mathrm{nojump}}(t-t_n)} q(t_n - t_{n-1}) q(t_{n-1} - t_{n-2}) \cdots q(t_1)$$

$$= \int_0^t dt_n \cdots \int_0^{t_2} dt_1\; p_{\mathrm{nojump}}(t-t_n)\, q(t_n - t_{n-1})\, q(t_{n-1} - t_{n-2}) \cdots q(t_1)$$

An explicit calculation shows, that in fact

$$q(t) = \pi_{\mathrm{jump}}(t) \quad \longleftrightarrow \quad p_{\mathrm{nojump}}(t) = 1 - \gamma \int_0^t dt\, |\langle 1| e^{-iH_{\mathrm{eff}}t} |0\rangle|^2,$$

so that

$$p_n(t) = \int_0^t dt_n \cdots \int_0^{t_2} dt_1\; p_{\mathrm{nojump}}(t-t_n)\, \pi_{\mathrm{jump}}(t_n - t_{n-1}) \pi_{\mathrm{jump}}(t_{n-1} - t_{n-2}) \cdots \pi_{\mathrm{jump}}(t_1).$$

The interpretation of this equation is rather straight-forward, e.g.

$$p_1(t) = \int_0^t dt_1\, p_{\text{nojump}}(t-t_1)\, \pi_{\text{jump}}(t_1)$$

} probability for the occurrence of only one jump event up to time t

is the integral over the probability of all trajectories that contain one jump event at time t_1 that then is followed by an evolution without jumps up to time t.

In general, there is no closed form for $p_n(t)$, but we can obtain one in the case where $\gamma \gg \Omega$ and Ω also being large. Here we have $p_{\text{nojump}}(t) = e^{-\frac{4\Omega^2}{\gamma}t}$ and $\pi_{\text{jump}}(t) = \frac{4\Omega^2}{\gamma} e^{-\frac{4\Omega^2}{\gamma}t}$.

Taking the Laplace transform of $p_n(t)$, yields

$$\bar{p}_n(s) = \mathcal{L}\{p_n(t)\}(s) = \int_0^\infty dt\, e^{-st} p_n(t)$$

$\overset{\text{convolution theorem}}{=}$

$$\mathcal{L}\{p_{\text{nojump}}(t)\}(s) \cdot \left[\mathcal{L}\{\pi_{\text{jump}}(t)\}(s)\right]^n$$

$$= \frac{1}{s + \frac{4\Omega^2}{\gamma}} \cdot \left(\frac{4\Omega^2}{\gamma}\right)^n \cdot \left[\frac{1}{s+\frac{4\Omega^2}{\gamma}}\right]^n = \left(\frac{4\Omega^2}{\gamma}\right)^n \left[\frac{1}{s+\frac{4\Omega^2}{\gamma}}\right]^{n+1}$$

Inverting the Laplace transform results in

$$p_n(t) = \mathcal{L}^{-1}\{\bar{p}_n(s)\}(t) = \left(\frac{4\Omega^2}{\gamma}\right)^n \mathcal{L}^{-1}\left\{\left(\frac{1}{s+\frac{4\Omega^2}{\gamma}}\right)^{n+1}\right\}(t)$$

$$= \left(\frac{4\Omega^2}{\gamma}\right)^n \frac{t^n}{n!} e^{-\frac{4\Omega^2}{\gamma}t} = \frac{\left(\frac{4\Omega^2}{\gamma}t\right)^n}{n!} e^{-\frac{4\Omega^2}{\gamma}t}.$$

This is a Poisson distribution $P_\lambda(n) = \frac{\lambda^n}{n!} e^{-\lambda}$ with the parameter $\lambda = \frac{4\Omega^2}{\gamma}t$. Since λ is the mean and also the variance, the average number of jump events, but also the number fluctuations, increase linearly with observation time t.

The trajectory picture allows to derive an elegant approach for simulating the dynamics of an open quantum system, via so-called quantum jump Monte Carlo.

To see this let us come back to the integral equation

$$\rho(t) = e^{\mathcal{L}_0 t}\rho(0) + \int_0^t d\tau\, e^{\mathcal{L}_0(t-\tau)} \mathcal{J}\, \rho(\tau).$$

This equation tells us that the density matrix at time t is given by the no-jump evolution plus all other evolution paths that contain at least one jump.

Now, let us assume the trajectory view point, and instead of looking at the density matrix, which is the „superposition" of all paths, we consider the instantaneous state of the system.

To this end, let us assume that at time $t=0$, the state is pure: $|\psi_0\rangle$.

The probability to undergo a quantum jump up to time t_{jump} is then given by:

$$p_{jump}(t_{jump}) = 1 - p_{nojump}(t_{jump})$$

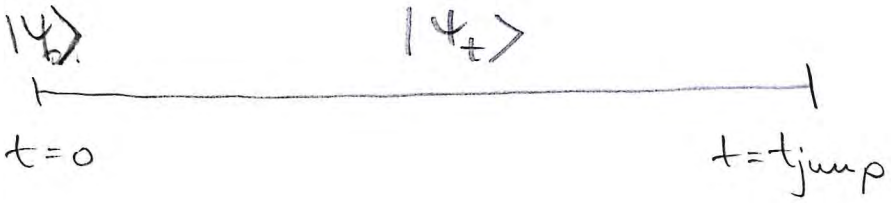
$$= 1 - \mathrm{tr}\left(e^{\mathcal{L}_0 t_{jump}} |\psi_0\rangle\langle\psi_0|\right)$$

$$= 1 - \| e^{-iH_{eff} t_{jump}} |\psi_0\rangle \|^2$$

The jump time is of course random, and in order to obtain a value for a single realisation, we have to draw a uniform distributed random number $r \in [0,1]$ and solve the equation

$$r = 1 - p_{nojump}(t_{jump}).$$

Up to this point in time the state is $|\psi_t\rangle = \dfrac{e^{-iH_{eff}t}|\psi_0\rangle}{\| e^{-iH_{eff}t}|\psi_0\rangle \|}$



At $t = t_{jump}$ the state becomes

$$\rho(t_{jump}) = \sum_k p_k \frac{L_k |\psi_{t_{jump}}\rangle\langle\psi_{t_{jump}}| L_k^+}{\sqrt{p_k}\sqrt{p_k}},$$

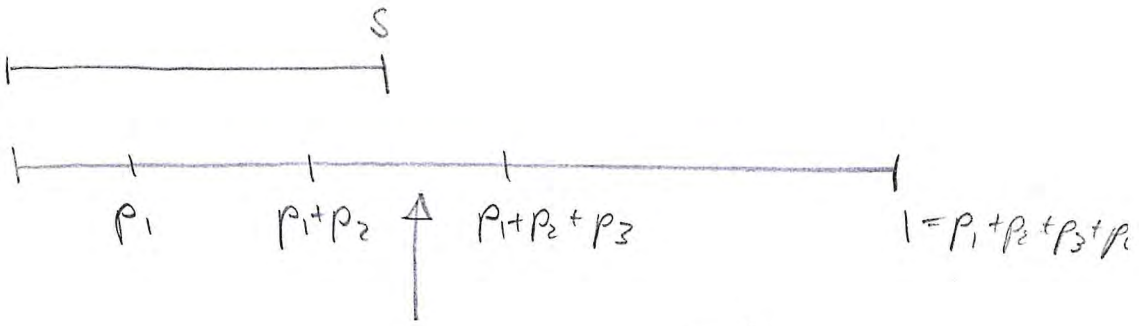
with $p_k = \langle \psi_{t_{jump}} | L_k^\dagger L_k | \psi_{t_{jump}} \rangle$.

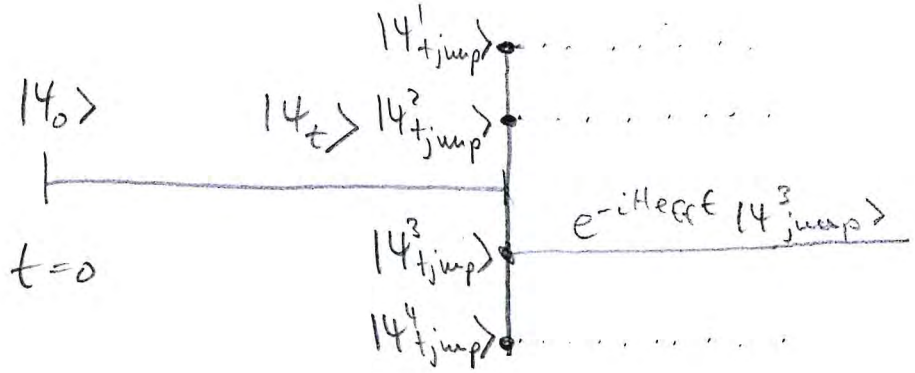
Therefore, with probability p_k, the system is in the state $|\psi^k_{t_{jump}}\rangle = \frac{L_k |\psi_{t_{jump}}\rangle}{\sqrt{p_k}}$.

In a simulation one selects the state $|\psi^{k_{jump}}_{t_{jump}}\rangle$ by drawing a random number $s \in [0,1]$ and selects the state for which

$$\max_{k_{jump}} \sum_{m=1}^{k_{jump}} p_m < s .$$

example: (4 jumps possible)





The state $|\psi^{k_{jump}}_{t_{jump}}\rangle$ is selected as new initial state and the procedure starts over.

In order to calculate expectation values of observables, one calculates the corresponding expectation value for each trajectory and then averages over many trajectories.

- Example: two-level atom with decay