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Lecture 7: Open quantum systems II
The reservoir approach

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In the last lecture, we have started the study of open quantum systems, *i.e.* of situations where a system $\mathcal{S}$ is coupled to another one $\mathcal{R}$, usually assumed to be "large" in a sense that we will make more precise below. This second large system is called a reservoir, a bath, or an environment depending on the context.

The important feature we have found is that due to the coupling between $\mathcal{S}$ and $\mathcal{R}$, the system undergoes a non-unitary evolution: even if $\mathcal{S}$ is initially prepared in a pure state, it will gradually evolve towards a mixed state owing to the entanglement between the system and the reservoir. This non-unitary evolution does not come as a surprise, as already any non isolated *classical* system loses energy in the environment through an energy transfer located on its boundary with the reservoir. This transfer is called heat in thermodynamics. As we are dealing with a subpart $\mathcal{S}$ of the system $\mathcal{S}+\mathcal{R}$, which is isolated, $\mathcal{S}$ must be described by its density matrix $\rho_{\mathcal{S}}$ obtained by tracing the total density matrix $\rho_{\mathcal{SR}}$ over the degrees of freedom of the reservoir $\mathcal{R}$: $\rho_{\mathcal{S}} = \mathrm{Tr}_{\mathcal{R}}[\rho_{\mathcal{SR}}]$.

In the last lecture, we have used the formalism of the Kraus operators to find the equation of evolution of $\rho_{\mathcal{S}}(t)$. Let us recall the method. We assume that at any time t, $\mathcal{S}$ and $\mathcal{R}$ are uncorrelated: $\rho_{\mathcal{SR}}(t) = \rho_{\mathcal{S}}(t) \otimes \rho_{\mathcal{R}}^{\mathrm{eq}}$, with the reservoir $\mathcal{R}$ at equilibrium. At a later time $t+\Delta t$, the density operator $\rho_{\mathcal{S}}(t+\Delta t)$ of the system $\mathcal{S}$ alone is related to its value at t, $\rho_{\mathcal{S}}(t)$, by a transformation called a "quantum map":

$$\rho_{\mathcal{S}}(t+\Delta t) = \sum_{\alpha} \hat{M}_{\alpha}(\Delta t)\rho_{\mathcal{S}}(t)\hat{M}_{\alpha}^{\dagger}(\Delta t)\ , \tag{1}$$

where the $\hat{M}_{\alpha}$'s are the Kraus operators, satisfying $\sum_{\alpha} \hat{M}_{\alpha}^{\dagger}\hat{M}_{\alpha} = \hat{\mathbb{1}}$ and acting in the Hilbert space of $\mathcal{S}$. These Kraus operators $\hat{M}_{\alpha}$, the number of which is $(\mathrm{dim}\mathcal{E}_{\mathcal{S}})^2$ (Kraus' theorem), are the evolution operators of $\mathcal{S}$ conditioned on the state α of the reservoir. The quantum maps is equivalent to the expression we have obtained in Lecture 6, Eq. (23) in the case of an unread measurement of the state of the system, here by the environment. A crucial hypothesis for the quantum map of Eq. (1) to be valid is that $dt \gg \tau_{\mathrm{c}}$, where τ_{c} is the typical time necessary for the reservoir to relax to equilibrium. This assumption, which we will come back to in this lecture, is called the *Markov approximation*: it tells us that the reservoir has no memory. Amazingly enough, the quantum map allowed us to derive the general form of the equation of evolution of $\rho_{\mathcal{S}}(t)$, named the "Master equation", without even knowing the details of the reservoir and its coupling to $\mathcal{S}$.

To obtain the master equation, we expanded the $\hat{M}_\alpha$'s as power series of Δt, distinguishing between the case $\alpha = 0$ where the environment stays at equilibrium in its ground state, thus not evolving, and the case $\alpha \neq 0$ where the reservoir evolves:

$$\begin{aligned} \hat{M}_0(\Delta t) &= \hat{\mathbb{1}} + (\hat{A} - i\hat{H}/\hbar)\Delta t + \mathcal{O}(\Delta t^2) && (2) \\ \hat{M}_{\alpha\neq 0}(\Delta t) &= \hat{L}_\alpha \sqrt{\Delta t} + \mathcal{O}(\Delta t) \ . && (3) \end{aligned}$$

We then obtained the Lindblad form of the master equation, setting $\Delta t \to 0$:

$$\frac{d\rho_{\mathcal{S}}}{dt} = \frac{1}{i\hbar}[H, \rho_{\mathcal{S}}] + \sum_{\alpha\neq 0}(\hat{L}_\alpha \rho_{\mathcal{S}} \hat{L}_\alpha^\dagger - \frac{1}{2}\hat{L}_\alpha^\dagger \hat{L}_\alpha \rho_{\mathcal{S}} - \frac{1}{2}\rho_{\mathcal{S}} \hat{L}_\alpha^\dagger \hat{L}_\alpha) \ . \qquad (4)$$

The operator H is interpreted as the Hamiltonian of the system, as it describes the unitary evolution of $\mathcal{S}$ when no relaxation occurs. The operators $\hat{L}_\alpha$ are called "jump operators". They act in the Hilbert space of the system. Their interpretation is the following: when the system changes its state, it induces a transition (a quantum jump) in the reservoir, as represented in the figure below.

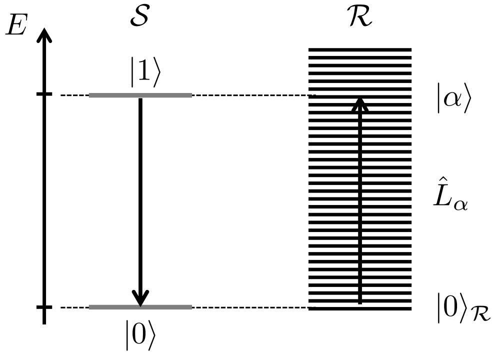

Figure 1: *Quantum jumps: the transition of the qubit, considered as the system $\mathcal{S}$, from state $|1\rangle$ to $|0\rangle$ is associated to an excitation of the reservoir $\mathcal{R}$, supposed here initially in its ground state $|0\rangle_{\mathcal{R}}$, to an excited state $|\alpha\rangle$.*

Two remarks are in order. First Δt was chosen such that $\Delta t \gg \tau_c$. However, it must also fulfill $\Delta t \ll T_{\mathcal{S}}$, where $T_{\mathcal{S}}$ is the typical evolution time of $\rho_{\mathcal{S}}$. We will come back to this in the lecture. As, $\Delta t \gg \tau_c$, we must also remember that the limit $\Delta t \to 0$ is strictly speaking not possible...: the derivative in Eq. (4) thus has to be considered as a "coarse-grain" derivative. Second, the formalism leading to the Lindblad form does not yield any expression for the jump operators $\hat{L}_\alpha$. However, as it gives an intuition of what happens in the reservoir during the jump, one can guess their expression for a particular situation where we have modeled the reservoir. This is what we did in the last lecture for an harmonic oscillator coupled to a thermal bath of oscillators.

The goals of this lecture are twofold. First, we will use the Kraus formalism to derive the Bloch equations that you have encounter in the Light-Matter interaction course, and which are at the heart of the understanding of how electromagnetic waves interact with atoms. Second, we will derive the master equation using a different, more traditional, point of view, sometimes called the “reservoir theory”. As we will see, this approach gives explicit expressions for the Lindblad operators, and allows one to identify the relaxation time τ_c as the correlation time of the reservoir. The approach is however technically more complicated than the Kraus formalism which uses general quantum information theory concepts to obtain in a reasonably straightforward (but arguably more abstract...) way the Lindblad equation.

1 Derivation of the Optical Bloch equations from the Kraus formalism

The Bloch equations are essential tools to describe the coupling between an atom and a *classical* electromagnetic field. We will here consider as a system $\mathcal{S}$ a two-level atom, with states $|g\rangle$ and $|e\rangle$ separated by a transition at frequency ω_0, driven by a field at frequency ω. The reservoir $\mathcal{R}$ is the quantized vacuum electromagnetic field in which the atom is placed: it consists of an infinite number of modes l (frequency ω_l) that the atom can decay in. Do not mix the *classical* EM driving field and the *quantized* field responsible for spontaneous emission in a sense that you have seen in quantum optics.

The Hamiltonian of the atom and classical field is, in the rotating wave approximation ($\omega \approx \omega_0$):

$$H_{\mathcal{S}} = \frac{\hbar\omega_0}{2}\hat{\sigma}_z + \frac{\hbar\Omega}{2}\hat{\sigma}_+ e^{-i\omega t} + \frac{\hbar\Omega^*}{2}\hat{\sigma}_- e^{i\omega t} \ , \tag{5}$$

with $\hat{\sigma}_z = |e\rangle\langle e| - |g\rangle\langle g|$, $\hat{\sigma}_+ = |e\rangle\langle g|$, $\hat{\sigma}_- = |g\rangle\langle e|$. A useful relation: $[\hat{\sigma}_+, \hat{\sigma}_-] = 2\hat{\sigma}_z$.

The reservoir consists here of the modes of the quantized vacuum field with electric part $\mathbf{E}_\mathrm{v}$, considered as harmonic oscillators. The Hamiltonian describing the coupling between the atom and the quantized field has the general form (see Lecture 2):

$$\hat{V}_{\mathcal{SR}} = -\hat{\mathbf{d}} \cdot \hat{\mathbf{E}}_\mathrm{v} = \sum_l (g_l \hat{a}_l + g_l^* \hat{a}_l^+)(\hat{\sigma}_+ + \hat{\sigma}_-) \ . \tag{6}$$

We need to know the state of the vacuum field (reservoir) at equilibrium at a temperature around 300 K for the frequency ω_l around the transition frequency ω_0. The thermal populations of the mode l is

$$n_l(T) = \frac{1}{\exp[\frac{\hbar\omega_l}{k_\mathrm{B}T}] - 1} \tag{7}$$

For an optical transition $\hbar\omega_0 \sim 1\,\mathrm{eV}$, corresponding to a temperature $T \sim 12000\,\mathrm{K}$. Hence $n_l(T = 300\,\mathrm{K}) \sim e^{-40} \ll 1$: one can assume the modes of the vacuum field to be initially empty. One has to be careful when deriving the Bloch equation for microwave transitions: there $\omega_0 \sim 2\pi \times 1 - 10\,\mathrm{GHz}$, corresponding to a temperature $T \sim 1\,\mathrm{K}$. One thus has to account for the initial thermal population of the vacuum modes.

Let us know guess the form of the jump operators. In a spontaneous emission decay, the atom undergoes a transition from $|e\rangle$ to $|g\rangle$, and the reservoir has to be excited according to energy conservation. The corresponding jump operator thus has the form $\hat{L}_- = \sqrt{\Gamma}\,\hat{\sigma}_-$ (remember that the jump operator is associated to a process in the reservoir, but acts on the system). Here, Γ is a constant akin to a rate. The reverse process, by which the reservoir gives energy to the atom, does not occur for an optical transition, as the reservoir is empty at optical frequencies. Hence we need to consider only one jump operator and the Lindblad equation reads:

$$\begin{aligned}\dot{\rho}_{\mathcal{S}} = &\frac{1}{2i\hbar}[\hbar\omega_0\hat{\sigma}_z + \hbar\Omega\hat{\sigma}_+ e^{-i\omega t} + \hbar\Omega^*\hat{\sigma}_- e^{i\omega t}, \rho_{\mathcal{S}}] \\ &+\frac{\Gamma}{2}(2\hat{\sigma}_-\rho_{\mathcal{S}}\hat{\sigma}_+ - \hat{\sigma}_+\hat{\sigma}_-\rho_{\mathcal{S}} - \rho_{\mathcal{S}}\hat{\sigma}_+\hat{\sigma}_-)\ .\end{aligned} \tag{8}$$

When considering the matrix elements, one obtains the Bloch equations for the population $\rho_{ee} = \langle e|\rho_{\mathcal{S}}|e\rangle$ and coherence $\rho_{eg} = \langle e|\rho_{\mathcal{S}}|g\rangle$:

$$\dot{\rho}_{ee} = -\Gamma\rho_{ee} - i\frac{\Omega}{2}e^{-i\omega t}\rho_{ge} + i\frac{\Omega^*}{2}e^{i\omega t}\rho_{eg} \tag{9}$$

$$\dot{\rho}_{eg} = -(i\omega_0 + \frac{\Gamma}{2})\rho_{eg} - i\frac{\Omega}{2}e^{-i\omega t}(\rho_{ee} - \rho_{gg})\ , \tag{10}$$

and $\rho_{gg} = 1 - \rho_{ee}$, $\rho_{eg} = \rho_{ge}^*$.

At this stage we have the general form of the Optical Bloch equations, but we do not know the expression for Γ. To get it, consider the case $\Omega = 0$. Then, for an atom initially in $|e\rangle$, $\rho_{ee}(t) = e^{-\Gamma t}$. For $\Gamma t \ll 1$, $\rho_{ee}(t) \approx 1 - \Gamma t$. We have encountered this expression in quantum optics: Γ is the decay rate of the atom from state $|e\rangle$, obtained by Fermi's rule: $\Gamma = d_{eg}^2\omega_0^3/(3\pi\epsilon_0 c^3\hbar)$.

From equation (10), we also find that when $\Omega = 0$ the coherence $\rho_{eg} \propto e^{-\Gamma t/2}\,e^{-i\omega_0 t}$ decays twice more slowly than the population. It has to be this way: if the population decays at a rate Γ, the power emitted by the atom at the beginning of the decay is $dU/dt = -\Gamma\hbar\omega_0 = -\Gamma U$, with U the energy stored in the atom. Physically, the decay comes from the radiation of the dipole and classical electromagnetism teaches us that the power emitted by a radiating dipole is proportional to $|\langle d(t)\rangle|^2$. As the dipole $\langle d(t)\rangle$ associated to a two-level atom is $\langle d(t)\rangle \propto \rho_{eg}(t)$, this means that for $U(t) \propto e^{-\Gamma t}$, we must get $|\rho_{eg}| \propto e^{-\Gamma t/2}$.

We can recover the same result using another heuristic argument akin to the Wigner-Weisskopf theory (see Quantum Optics course or Basdevant and Dalibard textbook, chapter 17, Sec. 3). Assume that initially the (atom+vacuum field) state is $|\psi(0)\rangle = (\alpha\,|g\rangle + \beta\,|e\rangle) \otimes |n = 0\rangle_{\mathcal{R}}$. Here $|n = 0\rangle_{\mathcal{R}}$ means that the vacuum field contains no photon. Assume that after a time t, the atom has a probability p to still be in its excited state and a probability $1 - p$ to be in $|g\rangle$ having emitted a photon. Then the (atom + vacuum field) state becomes entangled:

$$|\psi(t)\rangle = \alpha\,|g\rangle \otimes |n = 0\rangle_{\mathcal{R}} + \beta\sqrt{p}\,|e\rangle \otimes |n = 0\rangle_{\mathcal{R}} + \beta\sqrt{1-p}\,|g\rangle \otimes |n = 1\rangle_{\mathcal{R}}\ . \tag{11}$$

The density operator of the atom alone is thus

$$\rho_{\mathcal{S}}(t) = \mathrm{Tr}_{\mathcal{R}}[|\psi(t)\rangle\langle\psi(t)|] = \begin{pmatrix} |\alpha|^2 + |\beta|^2(1-p) & \alpha\beta^*\sqrt{p} \\ \alpha^*\beta\sqrt{p} & |\beta|^2 p \end{pmatrix}\ . \tag{12}$$

As $p \propto e^{-\Gamma t}$, the coherences decay as $\sqrt{p} \propto e^{-\Gamma t/2}$.

2 Derivation of the master equation using the reservoir theory

The Kraus formalism led to the Lindblad form of the master equation with almost no other inputs than the fact that information flows from the system to the reservoir, which "reads" the state of the system. We now present a second approach that leads to the Master equation. As a matter of fact, this is the traditional approach described in almost all textbooks on the subject. It starts from an explicit modeling of the $\mathcal{S}+\mathcal{R}$ system. The method is technically heavy. We will therefore only outline it here. However, it will allow us to gain a deeper understanding of the Markov approximation, which appears more explicitly than in the Kraus formalism. Another feature of the method is that it allows calculating explicitly the various decay rates and the jump operators, contrarily to the Kraus approach where they have to be guessed.

2.1 Description of the model

The starting point is again a $\mathcal{S}+\mathcal{R}$ closed (or isolated) system, described by the Hamiltonian: $H = H_\mathcal{S} + H_\mathcal{R} + V_{\mathcal{S}\mathcal{R}}$, where $V_{\mathcal{S}\mathcal{R}}$ is the coupling between the reservoir and the system. Here we model the reservoir as a collection of harmonic oscillators. This is actually quite a general fact that reservoirs can be described in this way: think about spontaneous emission where the vacuum electromagnetic field is an ensemble of modes equivalent to harmonic oscillators; this is also the case of phonons in a solid that are quantized vibrations of the crystal. The Hamiltonian of the reservoir is $H_\mathcal{R} = \sum_l \hbar\omega_l \hat{a}_l^+ \hat{a}_l$. We assume that the frequencies ω_l are closely spaced, so that they form a quasi-continuum: there are therefore many Bohr frequencies $\omega_{nm} = \omega_n - \omega_m$ close to the natural frequencies of the system (for example ω_0 for a two-level atom). To simplify, we will also assume that the reservoir is initially in its ground state $|0\rangle_\mathcal{R}$. You will derive in the HW5 the modification to the formulae below when the reservoir is at thermal equilibrium:

$$\rho_\mathcal{R}^{\rm eq} = \frac{1}{Z} e^{-\beta H_{\rm R}} \ \ \text{with} \ \ \langle \hat{a}_\mu^+ \hat{a}_\nu \rangle = \frac{1}{e^{\beta\hbar\omega_\mu} - 1}\,\delta_{\mu\nu}\ . \tag{13}$$

Finally, let us take a generic form for the (system + reservoir) coupling:

$$V_{\mathcal{S}\mathcal{R}} = \hat{R} \otimes \hat{S} \ \ \text{where} \ \ \hat{R} = \sum_l g_l \hat{a}_l + g_l^* \hat{a}_l^+\ . \tag{14}$$

This expression of $\hat{R}$ would be suitable to describe the quantized electromagnetic field for which the electric field operator has precisely this form, with $g_l = \sqrt{\hbar\omega_l/(2\epsilon_0 V)}$ (see Quantum Optics course or Lecture 2).

2.2 Interaction representation

The dynamics of the density operator $\hat{\rho}_{\mathcal{S}\mathcal{R}}$ of the *isolated* $\mathcal{S}+\mathcal{R}$ system is governed by:

$$\frac{d\rho_{\mathcal{S}\mathcal{R}}}{dt} = \frac{1}{i\hbar}[H, \rho_{SR}]. \tag{15}$$

In order to make the influence of the coupling more transparent and simplify a bit the expressions we will derive, one often uses the *interaction representation*. It consists in eliminating the free evolution due to the Hamiltonians $H_\mathcal{S}$ and $H_\mathcal{R}$. To do so, one defines $\tilde{\rho} = e^{i(H_\mathcal{S}+H_\mathcal{R})t/\hbar}\,\rho_{\mathcal{SR}}\,e^{-i(H_\mathcal{S}+H_\mathcal{R})t/\hbar}$. Then, the density operator in the new representation evolves according to

$$\frac{d\tilde{\rho}}{dt} = \frac{1}{i\hbar}[V(t),\tilde{\rho}]\ , \tag{16}$$

where

$$\begin{aligned} V(t) &= e^{i(H_\mathcal{S}+H_\mathcal{R})t/\hbar}\,V_{\mathcal{SR}}\,e^{-i(H_\mathcal{S}+H_\mathcal{R})t/\hbar} && (17)\\ &= \hat{R}(t)\otimes\hat{S}(t) && (18)\\ &= \sum_l (g_l\hat{a}_l\,e^{-i\omega_l t} + g_l^*\hat{a}_l^+\,e^{i\omega_l t})\otimes e^{iH_\mathcal{S}t/\hbar}\,\hat{S}\,e^{-iH_\mathcal{S}t/\hbar}\ , && (19)\end{aligned}$$

where we have used $\exp(i\omega t\,\hat{a}^+\hat{a})\,\hat{a}\,\exp(-i\omega t\,\hat{a}^+\hat{a}) = \hat{a}\,e^{-i\omega t}$ (check it using the closure relation $\sum_n |n\rangle\langle n| = \hat{\mathrm{Id}}$). We will now solve perturbatively equation (16).

2.3 Perturbative solution

The formal solution to Eq. (16) yields:

$$\tilde{\rho}(t) = \tilde{\rho}(t_0) + \frac{1}{i\hbar}\int_{t_0}^{t}[V(t'),\tilde{\rho}(t')]\,dt'\ . \tag{20}$$

Plugging this expression into Eq. (16) and changing the variable t' to $\tau = t - t'$ leads to:

$$\frac{d\tilde{\rho}}{dt} = \frac{1}{i\hbar}[V(t),\tilde{\rho}(t_0)] - \frac{1}{\hbar^2}\int_0^{t-t0}[V(t),[V(t-\tau),\tilde{\rho}(t-\tau)]]\,d\tau\ . \tag{21}$$

We now want to calculate the density operator of the system $\tilde{\rho}_\mathcal{S}$ (in interaction representation). We therefore trace Eq. (21) over the reservoir:

$$\frac{d\tilde{\rho}_\mathcal{S}}{dt} = \frac{1}{i\hbar}\mathrm{Tr}_\mathcal{R}\{[V(t),\tilde{\rho}(t_0)]\} - \frac{1}{\hbar^2}\int_0^{t-t0}\mathrm{Tr}_\mathcal{R}\{[V(t),[V(t-\tau),\tilde{\rho}(t-\tau)]]\}\,d\tau\ . \tag{22}$$

So far, the result is exact. To calculate the trace, we now assume that at any time the density operator of $\mathcal{S}+\mathcal{R}$ is $\tilde{\rho}(t) = \tilde{\rho}_\mathcal{S}(t)\otimes\tilde{\rho}_\mathcal{R}^{\mathrm{eq}}$, with $\tilde{\rho}_\mathcal{R}^{\mathrm{eq}} = |0\rangle\langle 0|_\mathcal{R}$. This is again the Markov approximation. With this approximation, the first commutator is:

$$\mathrm{Tr}_\mathcal{R}\{[V(t),\tilde{\rho}(t_0)]\} = \mathrm{Tr}_\mathcal{R}\{\hat{R}(t)\tilde{\rho}_\mathcal{R}^{\mathrm{eq}}\}\hat{S}(t)\tilde{\rho}_\mathcal{S}(t_0) - \hat{S}(t)\tilde{\rho}_\mathcal{S}(t_0)\mathrm{Tr}_\mathcal{R}\{\hat{R}(t)\tilde{\rho}_\mathcal{R}^{\mathrm{eq}}\}\ . \tag{23}$$

The trace over the reservoir is the average of $\hat{R}(t)$ given by Eq. (19). As we have assumed $\tilde{\rho}_\mathcal{R}^{\mathrm{eq}} = |0\rangle\langle 0|_\mathcal{R}$ and as $\langle 0|\hat{a}_l|0\rangle = \langle 0|\hat{a}_l^+|0\rangle = 0$, we get $\langle\hat{R}(t)\rangle_{\mathrm{eq}} = 0$ and the commutator (23) is zero.

The trace of the commutator under the integral is more tedious. It involves four terms, such as:

$$\mathrm{Tr}_\mathcal{R}\{\hat{R}(t)\hat{R}(t-\tau)\tilde{\rho}_\mathcal{R}^{\mathrm{eq}}\}\,\hat{S}(t)\hat{S}(t-\tau)\tilde{\rho}_\mathcal{S}(t-\tau)\ . \tag{24}$$

The trace in each of these terms can be calculated explicitly. It corresponds to the *correlation function* of the reservoir $\langle\hat{R}(t)\hat{R}(t-\tau)\rangle$:

$$\begin{aligned}\langle\hat{R}(t)\hat{R}(t-\tau)\rangle_{\text{eq}} &= \text{Tr}_{\mathcal{R}}\{\hat{R}(t)\hat{R}(t-\tau)\tilde{\rho}_{\mathcal{R}}^{\text{eq}}\} \\ &= \langle\sum_l\sum_{l'}(g_l\hat{a}_l\,e^{-i\omega_l t}+g_l^*\hat{a}_l^+\,e^{i\omega_l t})(g_{l'}\hat{a}_{l'}\,e^{-i\omega_{l'}(t-\tau)}+g_{l'}^*\hat{a}_{l'}^+\,e^{i\omega_{l'}(t-\tau)})\rangle \\ &= \sum_l|g_l|^2\,e^{-i\omega_l\tau}=g(\tau)\ . \qquad (25)\end{aligned}$$

This correlation function looks like the Fourier transform of the function $g_l(\omega_l)$, for which we had assumed that the frequencies ω_l of the reservoir form a quasi-continuum. This function is defined over a broad range of frequencies $\Delta\omega$, which characterizes the width of the continuum. Hence $g(\tau)$, Fourier transform of a broad function of ω, is a peaked function of τ with a width $\tau_{\text{c}}\sim 1/\Delta\omega$ called the *correlation time* of the reservoir. It sets the time after which the reservoir has no memory of its initial state. Having introduced the correlation function of the reservoir and calculating the four terms of the commutator, Equation (22) becomes:

$$\frac{d\tilde{\rho}_{\mathcal{S}}}{dt}=\frac{1}{\hbar^2}\int_0^{t-t0}d\tau g(\tau)\{\hat{S}(t)\hat{S}(t-\tau)\tilde{\rho}_{\mathcal{S}}(t-\tau)-\hat{S}(t)\,\tilde{\rho}_{\mathcal{S}}(t-\tau)\hat{S}(t-\tau)\}+\text{h.c.}\ , \qquad (26)$$

where h.c. stands for hermitian conjugate. This integro-differential equation is hard to solve, but considering the fact that $g(\tau)$ is peaked and that $\tilde{\rho}_{\mathcal{S}}$ evolves on a timescale much longer that τ_{c}, we set $\tilde{\rho}_{\mathcal{S}}(t-\tau)\approx\tilde{\rho}_{\mathcal{S}}(t)$. Be careful that such an approximation is *a priori* not possible in $\hat{S}(t-\tau)$ as it may evolve faster than $\tilde{\rho}_{\mathcal{S}}(t)$. Thus

$$\frac{d\tilde{\rho}_{\mathcal{S}}}{dt}=\frac{1}{\hbar^2}\int_0^{t-t0}d\tau g(\tau)\{\hat{S}(t)\hat{S}(t-\tau)\tilde{\rho}_{\mathcal{S}}(t)-\hat{S}(t)\,\tilde{\rho}_{\mathcal{S}}(t)\hat{S}(t-\tau)\}+\text{h.c.} \qquad (27)$$

If $t-t_0\gg\tau_c$, we may replace the upper bound of the integral by $+\infty$. Finally, leaving the interaction representation to put back the free Hamiltonian evolution yields

$$\frac{d\rho_{\mathcal{S}}}{dt}=\frac{1}{i\hbar}[H_{\mathcal{S}},\rho_{\mathcal{S}}]+\frac{1}{\hbar^2}\{U\rho_{\mathcal{S}}(t)\hat{S}+\hat{S}\rho_{\mathcal{S}}(t)U^\dagger-\hat{S}U\rho_{\mathcal{S}}(t)-\rho_{\mathcal{S}}(t)U^\dagger\hat{S}\}\ , \qquad (28)$$

with

$$U=\int_0^{+\infty}g(\tau)\hat{S}(-\tau)\,d\tau\ . \qquad (29)$$

If we compare now equation (28) with Eq. (4), we find that they have the same structure with the dissipator $\hat{L}_\alpha\rho_{\mathcal{S}}\hat{L}_\alpha^\dagger-\frac{1}{2}\hat{L}_\alpha^\dagger\hat{L}_\alpha\rho_{\mathcal{S}}-\frac{1}{2}\rho_{\mathcal{S}}\hat{L}_\alpha^\dagger\hat{L}_\alpha$ that can be calculated from the last term. It has to be done on a case by case basis, for the specific model under consideration.

2.4 Example: spontaneous emission of a qubit

To make things more concrete, let us consider again the case where the system $\mathcal{S}$ is a two-level atom with $H_{\mathcal{S}}=\hbar\omega_0\hat{\sigma}_z/2$, and the reservoir $\mathcal{R}$ is the vacuum field. The coupling between $\mathcal{S}$ and $\mathcal{R}$ is electric dipole so that $\hat{S}=\hat{\sigma}_++\hat{\sigma}_-$. Thus:

$$U=\int_0^{+\infty}g(\tau)\hat{S}(-\tau)\,d\tau=\hbar^2(G_+\hat{\sigma}_++G_-\hat{\sigma}_-) \qquad (30)$$

with

$$G_+ = \frac{1}{\hbar^2}\int_0^{+\infty} g(\tau)\, e^{-i\omega_0\tau}\, d\tau \quad \text{and} \quad G_- = \frac{1}{\hbar^2}\int_0^{+\infty} g(\tau)\, e^{i\omega_0\tau}\, d\tau\ . \tag{31}$$

We have applied here the following formula that you can check directly by looking at the action of the operators on states $|g\rangle$ and $|e\rangle$:

$$\exp[-i\frac{\omega_0\tau}{2}\hat{\sigma}_z]\,\hat{\sigma}_+\,\exp[i\frac{\omega_0\tau}{2}\hat{\sigma}_z] = e^{-i\omega_0\tau}\,\hat{\sigma}_+\ . \tag{32}$$

Using the expression (25), we find

$$\begin{aligned} G_+ &= \sum_l \frac{|g_l|^2}{\hbar^2}\int_0^{+\infty} e^{-i(\omega_0+\omega_l)\tau}\, d\tau = 0\ , & (33)\\ G_- &= \sum_l \frac{|g_l|^2}{\hbar^2}\int_0^{+\infty} e^{i(\omega_0-\omega_l)\tau}\, d\tau = \frac{\pi}{\hbar^2}\sum_l |g_l|^2\,\delta(\omega_l-\omega_0)\ . & (34)\end{aligned}$$

This last expression is nothing but the Fermi's rule! In the case of spontaneous emission, $g_l = d_{eg}\sqrt{\hbar\omega_l/2\epsilon_0 V}$ and we obtain $G_- = \Gamma/2 = d_{eg}^2\omega_0^3/(6\pi\epsilon_0 c^3\hbar)$. Combining the expressions above and inserting them in Eq. (28) leads to:

$$\frac{d\rho_{\mathcal{S}}}{dt} = \frac{1}{i\hbar}[H_{\mathcal{S}}, \rho_{\mathcal{S}}] + \frac{\Gamma}{2}(2\hat{\sigma}_-\rho_{\mathcal{S}}\hat{\sigma}_+ - \hat{\sigma}_+\hat{\sigma}_-\rho_{\mathcal{S}} - \rho_{\mathcal{S}}\hat{\sigma}_+\hat{\sigma}_-)\ . \tag{35}$$

We have used the fact that $\hat{\sigma}_+\hat{\sigma}_+ = \hat{\sigma}_-\hat{\sigma}_- = 0$. This is nothing but the Lindblad form of the optical Bloch equations (8), which we have now derived from first principles!

2.5 Discussion of the perturbative expansion

We finally discuss the validity of the perturbative expansion where we have replaced in Eq. (22) the density operator $\tilde{\rho}(t)$ by $\tilde{\rho}_{\mathcal{S}}(t)\otimes\tilde{\rho}_{\mathcal{R}}^{\rm eq}$. In doing so, we ignore (i) the correlations between the system and the reservoir, and (ii) the modification of the state of the reservoir due to its coupling to the system. The introduction of the correlation function of the reservoir led to the idea that after a typical time $\tau_{\rm c}$, the correlations between $\mathcal{S}$ and $\mathcal{R}$ have disappeared, and that the reservoir has no memory of any correlations, i.e. has relaxed to its equilibrium state.

It turns out (and this is not easy to show, see for example Cohen-Tannoudji, Dupont-Roc and Grynberg, "Atom-photon interactions", Chapter. IV.D) that replacing $\tilde{\rho}(t)$ by $\tilde{\rho}_{\mathcal{S}}(t)\otimes\tilde{\rho}_{\mathcal{R}}^{\rm eq}$ introduces an error of order $v\tau_{\rm c}/\hbar$, with v the order of the magnitude of the matrix elements of the $\mathcal{S}-\mathcal{R}$ coupling $V_{\mathcal{SR}}$. This quantity thus appears as the small parameter in the problem, and for the Markov approximation to be valid we must impose:

$$\frac{v\tau_{\rm c}}{\hbar} \ll 1\ . \tag{36}$$

We therefore obtain a hierarchy in the timescales associated to the relaxation of the reservoir, $\tau_{\rm c}$, the time steps dt used to calculate the evolution of $\tilde{\rho}_{\mathcal{S}}$, and the typical evolution time $T_{\mathcal{S}}$ or $\tilde{\rho}_{\mathcal{S}}$:

$$\tau_{\rm c} \ll dt \ll T_{\mathcal{S}}\ . \tag{37}$$

Let us check that there indeed exists room between τ_{c} and $T_{\mathcal{S}}$ using the following heuristic argument. To calculate the order of magnitude of $T_{\mathcal{S}}$, we consider that during the relaxation time τ_{c} the density operator of the system evolves as $\tilde{\rho}_{\mathcal{S}} \sim e^{-iv\tau_{\mathrm{c}}/\hbar}$. This means that during each relaxation time the phase ϕ accumulated by $\tilde{\rho}_{\mathcal{S}}$ undergoes a random walk with a step $\delta\phi = v\tau_{\mathrm{c}}/\hbar$. In a time t, the number of steps is t/τ_{c}, so that the variance of the accumulated phase is:

$$\Delta\phi^2 \sim \left(\frac{v\tau_{\mathrm{c}}}{\hbar}\right)^2 \frac{t}{\tau_{\mathrm{c}}} \ . \tag{38}$$

The evolution time $T_{\mathcal{S}}$ corresponds to the time for which $\Delta\phi \sim 1$ rad, leading to

$$T_{\mathcal{S}} \sim \frac{\tau_{\mathrm{c}}}{(v\tau_{\mathrm{c}}/\hbar)^2} \gg \tau_c \ . \tag{39}$$

Hence τ_{c} and T_{S} are separated by many orders of magnitude, allowing one to insert the timescale dt between them.

3 The effective Hamiltonian approach

As already said multiple times, coupling a system $\mathcal{S}$ to a reservoir leads to a non-unitary evolution of the system. We can therefore not define the state vector of $\mathcal{S}$, and have to resort to its density operator to describe the evolution. The density operator formalism is usually heavier than the state vector approach, simply by the fact that the number of coefficients required to describe the state vector of, e.g., N qubits is 2^N, while the density matrix has 2^{2N} coefficients. Numerically this is very relevant...

There exists however situations where the description of an open system by a state vector is a good approximation, albeit at the price of giving up the conservation of probability for $\mathcal{S}$ or equivalently by taking a non-hermitian Hamiltonian to calculate the evolution of the state vector. Let us illustrate this approach on the case of a two-level atom driven by a laser and that can spontaneously decay. The Lindblad equation (4) can be written in the following way, using $\hat{\sigma}_+\hat{\sigma}_- = |e\rangle\langle e|$ and $\hat{\sigma}_-\rho_{\mathcal{S}}\hat{\sigma}_+ = \rho_{ee}|g\rangle\langle g|$:

$$\dot{\rho}_{\mathcal{S}} = \frac{1}{i\hbar}[H_{\mathcal{S}} - i\frac{\hbar\Gamma}{2}\,|e\rangle\langle e|, \rho_{\mathcal{S}}] + \Gamma\rho_{ee}|g\rangle\langle g| \ . \tag{40}$$

Note that the commutator for two non-hermitian operators is $[A, B] = AB - B^\dagger A^\dagger$. Introducing the effective, non-hermitian Hamiltonian

$$H_{\mathrm{eff}} = H_{\mathcal{S}} - i\frac{\hbar\Gamma}{2}\,|e\rangle\langle e| = \hbar\begin{pmatrix} 0 & \frac{\Omega}{2}e^{-i\omega t} \\ \frac{\Omega^*}{2}e^{i\omega t} & \omega_0 - i\frac{\Gamma}{2} \end{pmatrix} \ , \tag{41}$$

and assuming that the system is only weakly excited ($\rho_{ee} \ll 1$), the density operator has an evolution that ressembles the one of a closed system. We thus describe the system $\mathcal{S}$ by a state vector $|\psi_{\mathcal{S}}\rangle = \alpha\,|g\rangle + \beta\,|e\rangle$, which fulfills the non-unitary Schrödinger equation:

$$i\hbar\frac{d}{dt}\,|\psi_{\mathcal{S}}(t)\rangle = H_{\mathrm{eff}}\,|\psi_{\mathcal{S}}(t)\rangle \ . \tag{42}$$

The norm of $|\psi_{\mathcal{S}}\rangle$ is not conserved in the evolution... For example, if the system is not driven ($\Omega = 0$) and the atom is initially in $|e\rangle$, one finds $\beta(t) = e^{-\Gamma t/2}\, e^{-i\omega_0 t}$, while $\alpha(t) = 0$ at all time... the system does decay, as it should, but also disappears... One must thus use this formalism with care in order to avoid inconsistent results.

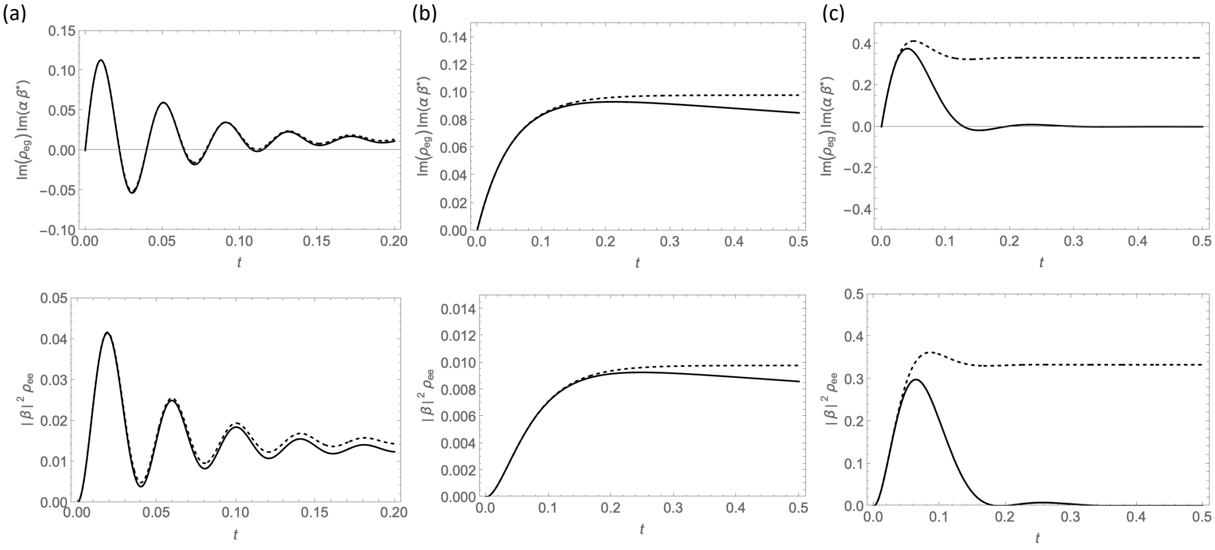

Figure 2: *Examples of evolution of a driven two-level system initially prepared in* $|g\rangle$, *as a function of time* t *in microseconds. The upper row shows the coherences* $\alpha\beta^*$ *for the effective Hamiltonian approach (thick line) and* ρ_{eg} *for the solution of the Bloch equation (dashed line). The bottom row shows the excited state population* $|\beta|^2$ *(effective Hamiltonian) or* ρ_{ee} *(Bloch equations). (a)* $\Omega = 2\pi \times 6$ *MHz,* $\omega - \omega_0 = 2\pi \times 24$ *MHz. (b)* $\Omega = 2\pi \times 0.6$ *MHz,* $\omega = \omega_0$*. (c)* $\Omega = 2\pi \times 0.6$ *MHz,* $\omega = \omega_0$*. The scales vary depending on the parameters.*

Figure 2 shows examples of dynamics under the effective Hamiltonian approach and the solution of the Bloch equation. The agreement is very good, as expected when the system is weakly excited.

A Problem set for Lecture 7

A.1 Reservoir in thermal equilibrium

We have seen in the lecture that the correlation function of an initially empty reservoir is $g(\tau) = \langle R(t)R(t-\tau)\rangle = \sum_l |g_l|^2 e^{-i\omega_l \tau}$ (same notations as in the lecture). Assume now that the reservoir is in thermal equilibrium at a temperature T, described by a density operator

$$\rho_R^{\mathrm{eq}} = \frac{e^{-H_R/k_{\mathrm{B}}T}}{\mathrm{Tr}[e^{-H_R/k_{\mathrm{B}}T}]}\ .$$

1. Show that $\langle a_\lambda\rangle = \langle a_\lambda^+\rangle = 0$ and that $\langle a_\lambda^+ a_\lambda\rangle = n_\lambda = 1/(\exp[\hbar\omega_\lambda/k_{\mathrm{B}}T] - 1)$.

2. What should be the temperature of the reservoir for n_λ to be non negligible for an optical transition and a microwave transition around 10 GHz.

3. Calculate $g(\tau)$ for this thermal reservoir as a function of n_λ. Does it change anything in the argument saying that $g(\tau)$ is a peaked function ?

A.2 Quantum channels

We describe here two processes by which a qubit can lose its coherence. These processes are called quantum channels.

A.2.1 Spin flips

We assume that the qubit (system $\mathcal{S}$) is coupled to a reservoir $\mathcal{R}$. The hamiltonian describing the closed $\mathcal{S}-\mathcal{R}$ system leads to a unitary evolution U_{SR}. Initially, the $\mathcal{S}-\mathcal{R}$ state is $|\psi(0)\rangle = |\psi_S\rangle \otimes |\chi_0\rangle$ with $|\chi_0\rangle$ the state of the reservoir.

1. We assume that the system has a probability $p/3$ to undergo a spin flip around the x, y and z axis, corresponding to the action of $\sigma_{x,y,z}$. Each flip leads to a jump of the state of the reservoir to $|\chi_{x,y,z}\rangle$. What is the state $U_{SR}|\psi(0)\rangle$ after the flips as a function of p.

2. Give the corresponding Kraus operators.

3. Use the quantum map to calculate the density matrix ρ' of the qubit after the flips.

4. Write the matrix representation of ρ'.

A.2.2 Dephasing

We now suppose that the qubit can only undergo a phase flip (action of σ_z) with a probability p. The state of the reservoir following this is $|\chi_z\rangle$.

1. Starting from the same state as before, $|\psi(0)\rangle = |\psi_S\rangle \otimes |\chi_0\rangle$, what is the state of the $\mathcal{S}-\mathcal{R}$ system after the flip as a function of p?

2. Give the corresponding Kraus operators.

3. Write the density matrix corresponding to the quantum map.

4. What is the effect of the dephasing if $p = 1/2$?

5. To understand this, take $|\psi_S\rangle = \alpha|0\rangle + \beta|1\rangle$ and write the state $|\psi_{SR}\rangle$ for $p = 1/2$ in the form $|\psi_{SR}\rangle = \alpha|0\rangle|\phi_0\rangle + \beta|1\rangle|\phi_1\rangle$. Show that $|\phi_0\rangle$ and $|\phi_1\rangle$ are orthogonal, and explain then the loss of coherences.

A.3 Dephasing of a qubit

We take a qubit $|\psi\rangle = \alpha_0 |0\rangle + \beta_0 |1\rangle$, with $|0\rangle$ having an energy $\hbar\omega(t)/2$ and $|1\rangle$ an energy $-\hbar\omega(t)/2$. This frequency varies as a function of time due to fluctuations of the environment.

1. Propose a situation involving a fluctuating magnetic field where the scenario applies.

2. Show that the free evolution of the qubit leads to $\alpha(t) = \alpha_0 e^{-i\Phi/2}$ and $\beta(t) = \beta_0 e^{i\Phi/2}$, with $\Phi = \int_0^t \omega(t')\, dt'$.

3. We now assume that $\omega(t)$ varies randomly every time step j of duration τ by an amount $\delta\omega_j$, around a mean value ω_0. Justify that the population in the density matrix are unchanged.

4. The coherence $\rho_{01} = \langle \alpha\beta^* \rangle$ corresponds to the average over different trajectories. Show that $\rho_{01}(t) = \alpha_0\beta_0^*\, e^{-i\omega_0 t}\langle e^{-i\delta\omega_1\tau} e^{-i\delta\omega_2\tau} e^{-i\delta\omega_3\tau}...\rangle = (\langle e^{-i\delta\omega\tau}\rangle)^n$, where $n = t/\tau$ is the number of time steps from 0 to t.

5. We now assume that the normalized distribution of $\delta\omega$ is gaussian: $p(\delta\omega) = \frac{1}{\sqrt{2\pi}\Delta\omega} \exp[-\frac{\delta\omega^2}{2\Delta\omega^2}]$. Use the integral

   $$\int_{-\infty}^{\infty} e^{-u^2\sigma^2}\, e^{iux}\, du = \frac{\sqrt{\pi}}{\sigma}\, e^{-\frac{x^2}{4\sigma^2}} \ .$$

   to show that $\rho_{01}(t) = \alpha_0\beta_0^*\, e^{-i\omega_0 t} e^{-t/T_2}$. Give the expression of T_2 as a function of $\Delta\omega$ and τ.

6. Write the Bloch equations, i.e. the differential equations satisfied by ρ_{00}, ρ_{11}, ρ_{01} and ρ_{10} when only dephasing is present (the states $|0\rangle, |1\rangle$ have infinite lifetime).

7. We want to recover this equations using the Lindblad formalism. Justify that the jump operator associated to dephasing is $L = \sqrt{\gamma}\sigma_z$.

8. Derive the Bloch equations from the Lindblad form. Take for the hamiltonian of the qubit $H = \frac{\hbar\omega_0}{2}\sigma_z$. What is the link between γ and T_2?

A.4 Parity measurement and fidelity

We analyze here an experiment performed in 2000 [Nature **404**, 256 (2000)] in the group of D.J. Wineland where the researchers prepared and characterized an entangled state between 2 ions. We look here only at the characterization of the entanglement. They used $^9\text{Be}^+$ and two internal state $|0\rangle$ and $|1\rangle$ separated by a transition at a frequency $\omega_0 = 2\pi \times 1.25$ GHz. The two qubit states can be coupled by laser beams and the resulting rotation on the qubit state is described by the unitary matrix

$$\mathcal{R}(\phi) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & ie^{i\phi} \\ ie^{-i\phi} & 1 \end{pmatrix}_{|0\rangle,|1\rangle} , \qquad (43)$$

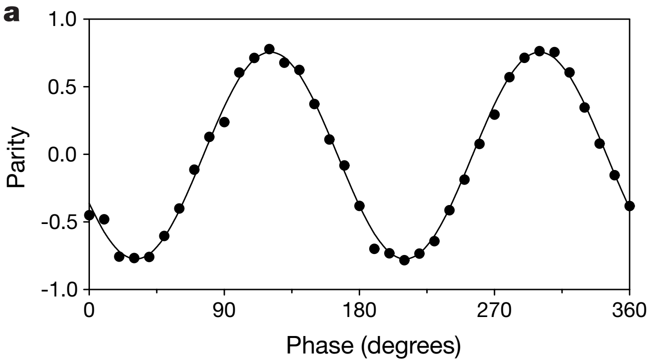

Figure 3: *Parity signal $\Pi(\phi)$ as a function of the phase ϕ following a rotation $\mathcal{R}$ on the two ions at the same time. From [Nature* **404***, 256 (2000)].*

for a $\pi/2$ pulse. The phase ϕ of the lasers can be controlled. The authors wanted to prepare the state $|\psi_+\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$. The experiment actually prepared a density matrix ρ_{exp}.

1. Explain briefly where the matrix $\mathcal{R}(\phi)$ comes from.
2. To assess the quality of the state preparation, they measured the fidelity $\mathcal{F} = \langle\psi_+|\,\rho_{\text{exp}}\,|\psi_+\rangle$. Show that

$$\mathcal{F} = \frac{1}{2}(P_{00} + P_{11}) + \rho_{00,11} \ , \tag{44}$$

   with $P_{00} = \rho_{00,00} = \langle 00|\,\rho\,|00\rangle\,, P_{11} = \rho_{11,11} = \langle 11|\,\rho\,|11\rangle$, and $\rho_{00,11} = \langle 00|\,\rho\,|11\rangle$ (which we assume to be real for simplicity).
3. The experimentalists could decide if the state of the ions was $|0\rangle$ or $|1\rangle$. How could they then measure the probabilities P_{00} and P_{11} by repeating many times the experiment ? They found $P_{00} = 0.43$ and $P_{11} = 0.46$.
4. To measure the coherence $\rho_{00,11}$, they applied the rotation $\mathcal{R}(\phi)$ on the two ions A and B at the same time before measuring their state. After this rotation of angle ϕ, they measured the four probabilities $P_{00}(\phi), P_{01}(\phi), P_{10}(\phi), P_{11}(\phi)$. Explain briefly why the probabilities are

$$\begin{aligned}
P_{00}(\phi) &= \langle 00|\,\mathcal{R}_A^{-1}(\phi)\otimes\mathcal{R}_B^{-1}(\phi)\ \rho\ \mathcal{R}_A(\phi)\otimes\mathcal{R}_B(\phi)\,|00\rangle \ , &(45)\\
P_{01}(\phi) &= \langle 01|\,\mathcal{R}_A^{-1}(\phi)\otimes\mathcal{R}_B^{-1}(\phi)\ \rho\ \mathcal{R}_A(\phi)\otimes\mathcal{R}_B(\phi)\,|01\rangle \ , &(46)\\
P_{10}(\phi) &= \langle 10|\,\mathcal{R}_A^{-1}(\phi)\otimes\mathcal{R}_B^{-1}(\phi)\ \rho\ \mathcal{R}_A(\phi)\otimes\mathcal{R}_B(\phi)\,|10\rangle \ , &(47)\\
P_{11}(\phi) &= \langle 11|\,\mathcal{R}_A^{-1}(\phi)\otimes\mathcal{R}_B^{-1}(\phi)\ \rho\ \mathcal{R}_A(\phi)\otimes\mathcal{R}_B(\phi)\,|11\rangle \ . &(48)
\end{aligned}$$

5. From the probabilities, they calculated the parity signal $\Pi(\phi) = P_{00}(\phi) + P_{11}(\phi) - P_{01}(\phi) - P_{10}(\phi)$. A tedious calculation yields $\Pi(\phi) = A + 2\rho_{00,11}\cos(2\phi)$. Explain briefly how you would do the calculation: calculate for example $P_{01}(\phi) + P_{10}(\phi)$.
6. The measured oscillation is shown in Fig. 3. Extract $\rho_{00,11}$ from it.

7. What is the fidelity of the prepared state then ?

8. We now show that a fidelity $\mathcal{F} > 1/2$ implies that the state prepared in the experiment is entangled. Suppose first that the experiment produces a pure separable state of the two ions $(a\left|0\right\rangle + b\left|1\right\rangle) \otimes (c\left|0\right\rangle + d\left|1\right\rangle)$, with $|a|^2 + |b|^2 = |c|^2 + |d|^2 = 1$. Show that $\mathcal{F} = |ac + bd|^2/2$.

9. Use $|a|^2 + |b|^2 = |c|^2 + |d|^2 = 1$, and write that $|a|^2 + |c|^2 = (|a| - |c|)^2 + 2|ac|$ (similary for $|b|^2 + |d|^2$) to show that $|ac| + |bd| \leq 1$.

10. Conclude that $\mathcal{F} \leq 1/2$ for a separable state and therefore $\mathcal{F} > 1/2$ implies entangled.

11. Suppose now that the two-ion state is described by a mixed separable state $\rho = \sum_k p_k \rho_k$ ($\sum_k p_k = 1$), with ρ_k density matrices of *pure separable* states. Show that the fidelity $\mathcal{F} = \sum_k p_k \left\langle\psi_+\right| \rho_k \left|\psi_+\right\rangle$ and that $\mathcal{F} \leq 1/2$. Hence for if $\mathcal{F} > 1/2$, the mixed state is not separable, i.e. entangled.