Dynamics and Control of Open Quantum Systems
Lecture 10 (December 2023):
Open-loop control: state preparation and logical gates

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This lecture investigates two types of questions:

1. State preparation: for $|\psi\rangle$ obeying a controlled Schrödinger equation $i\frac{d}{dt}|\psi\rangle = (\boldsymbol{H}_0 + \sum_{k=1}^m u_k \boldsymbol{H}_k)|\psi\rangle$ with a given initial condition $|\psi_i\rangle$, find an open-loop control $[0,T] \ni t \mapsto u(t) = (u_1(t), u_2(t), \cdots, u_m(t))$ such that at a final time T, $|\psi\rangle$ has reached a pre-specified target state $|\psi_f\rangle$.

2. Logical gates: for the unitary propagator $\boldsymbol{U}$ obeying the controlled Schrödinger equation $i\frac{d}{dt}\boldsymbol{U} = (\boldsymbol{H}_0 + \sum_{k=1}^m u_k \boldsymbol{H}_k)\boldsymbol{U}$ with initial condition $\boldsymbol{U}(0) = \boldsymbol{I}$, find an open-loop control $[0,T] \ni t \mapsto u(t) = (u_1(t), u_2(t), \cdots, u_m(t))$ such that at a final time T, $\boldsymbol{U}$ has reached a pre-specified target unitary operation $\boldsymbol{U}_f$. This target unitary operation is the so-called logical gate we seek to implement.

In different sections, emphasis is put on different methods to construct efficient open-loop steering controls: resonant control and the rotation wave approximation are treated in section 1; quasi-static controls exploiting adiabatic invariance are presented in section 2; optimal control techniques are investigated in section 3. All these control techniques are routinely used in experiments that could be modeled as spins, springs or composite spin-spring systems. Therefore, while we provide a general framework for these techniques, we will emphasize on their application to spin-spring systems.

Note once again that $|\psi\rangle$ and $e^{i\theta}|\psi\rangle$ for any phase $\theta \in [0, 2\pi[$ represent the same physical state. Therefore, the relevant state preparation control problem consists of, finding for a given initial and final state, $|\psi_i\rangle$ and $|\psi_f\rangle$, a set of piecewise continuous controls $[0,T] \ni t \mapsto u_k(t)$ such that the solution for $|\psi\rangle_0 = |\psi_i\rangle$ satisfies $|\psi\rangle_T = e^{i\theta}|\psi_f\rangle$. In a similar manner, in case of generating a unitary propagator $\boldsymbol{U}_f$ associated to a logical gate, the unitary can be prepared up to a an arbitrary phase $\boldsymbol{U}(T) = e^{i\theta}\boldsymbol{U}_f$.

1 Resonant control, rotating wave approximation

1.1 Multi-frequency averaging

Let us consider the system

$$i\frac{d}{dt}|\psi\rangle = \frac{1}{\hbar}\left(\boldsymbol{H}_0 + \sum_{k=1}^m u_k \boldsymbol{H}_k\right)|\psi\rangle, \qquad |\psi(0)\rangle = |\psi_i\rangle \tag{1}$$

defined on a finite-dimensional Hilbert space $\mathcal{H}$ (while we will consider infinite dimensional examples later through this chapter, we will present the general framework only for the finite-dimensional case). Note furthermore that the analysis below directly applies to the propagator

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version of this equation

$$i\frac{d}{dt}\boldsymbol{U} = \frac{1}{\hbar}\left(\boldsymbol{H}_0 + \sum_{k=1}^{m} u_k \boldsymbol{H}_k\right)\boldsymbol{U}, \qquad \boldsymbol{U}(0) = \boldsymbol{I}. \tag{2}$$

For simplicity sakes, we also consider a single control, $m = 1$. We define the skew-Hermitian matrices $\boldsymbol{A}_k = -i\boldsymbol{H}_k/\hbar$, $k = 0, 1$. Assume that the single scalar control is of small amplitude and admits an almost periodic time-dependence

$$u(t) = \epsilon\left(\sum_{j=1}^{r} u_j e^{i\omega_j t} + u_j^* e^{-i\omega_j t}\right) \tag{3}$$

where $\epsilon > 0$ is a small parameter, ϵu_j is the constant complex amplitude associated to the frequency $\omega_j \geq 0$ and r stands for the number of independent frequencies ($\omega_j \neq \omega_k$ for $j \neq k$). We are interested in approximations, for ϵ tending to 0^+, of trajectories $t \mapsto |\psi_\epsilon(t)\rangle$ of (1) (resp. $t \mapsto \boldsymbol{U}_\epsilon(t)$ of (2)). Such approximations should be explicit and valid on time intervals of length $O(\frac{1}{\epsilon})$ (first order approximation) or $O(\frac{1}{\epsilon^2})$ (second order approximation). The wave function $|\psi_\epsilon\rangle$ obeys the following linear time-varying differential equation

$$\frac{d}{dt}|\psi_\epsilon\rangle = \left(\boldsymbol{A}_0 + \epsilon\left(\sum_{j=1}^{r} u_j e^{i\omega_j t} + u_j^* e^{-i\omega_j t}\right)\boldsymbol{A}_1\right)|\psi_\epsilon\rangle. \tag{4}$$

Consider the following change of variables

$$|\psi_\epsilon(t)\rangle = e^{\boldsymbol{A}_0 t}|\phi_\epsilon(t)\rangle \tag{5}$$

where $|\psi_\epsilon\rangle$ is replaced by $|\phi_\epsilon\rangle$. Through this change of variables, we put the system in the so-called "interaction frame":

$$\frac{d}{dt}|\phi_\epsilon\rangle = \epsilon\boldsymbol{B}(t)|\phi_\epsilon\rangle \tag{6}$$

where $\boldsymbol{B}(t)$ is a skew-Hermitian operator whose time-dependence is almost periodic[2]:

$$\boldsymbol{B}(t) = \sum_{j=1}^{r} u_j e^{i\omega_j t} e^{-\boldsymbol{A}_0 t}\boldsymbol{A}_1 e^{\boldsymbol{A}_0 t} + u_j^* e^{-i\omega_j t} e^{-\boldsymbol{A}_0 t}\boldsymbol{A}_1 e^{\boldsymbol{A}_0 t}.$$

More precisely each entry of $\boldsymbol{B}$ is a linear combination of oscillating terms of the form $e^{i\omega' t}$ with $\omega' \neq 0$. This results from the spectral decomposition of $\boldsymbol{A}_0$ to compute $e^{\boldsymbol{A}_0 t}$. Thus one can always decompose $\boldsymbol{B}(t)$ into a constant skew-Hermitian operator $\bar{\boldsymbol{B}}$ and the time derivative of a bounded and almost periodic skew-Hermitian operator $\widetilde{\boldsymbol{B}}(t)$ whose entries are linear combinations of $e^{i\omega' t}$ with $\omega' \neq 0$:

$$\boldsymbol{B}(t) = \bar{\boldsymbol{B}} + \frac{d}{dt}\widetilde{\boldsymbol{B}}(t). \tag{7}$$

[2]An almost periodic time function f is equal by definition to $F(\varpi_1 t, \ldots, \varpi_p t)$ where the function F is a 2π-periodic function of each of its p arguments and the ϖ_j's form a set of p different frequencies.

Notice that we can always set $\widetilde{\boldsymbol{B}}(t) = \frac{d}{dt}\widetilde{\boldsymbol{C}}(t)$ where $\widetilde{\boldsymbol{C}}$ is also an almost periodic skew-Hermitian operator. Then (6) reads $\frac{d}{dt}\left|\phi_\epsilon\right\rangle = \left(\epsilon\bar{\boldsymbol{B}} + \epsilon\frac{d}{dt}\widetilde{\boldsymbol{B}}\right)\left|\phi_\epsilon\right\rangle$ and suggests the following almost periodic change of variables

$$\left|\chi_\epsilon\right\rangle = (\boldsymbol{I} - \epsilon\widetilde{\boldsymbol{B}}(t))\left|\phi_\epsilon\right\rangle \tag{8}$$

well defined for ϵ small enough and then close to identity. In the $\left|\chi_\epsilon\right\rangle$ frame, the dynamics reads

$$\frac{d}{dt}\left|\chi_\epsilon\right\rangle = \epsilon\left(\bar{\boldsymbol{B}} - \epsilon\widetilde{\boldsymbol{B}}\bar{\boldsymbol{B}} - \epsilon\widetilde{\boldsymbol{B}}\frac{d}{dt}\widetilde{\boldsymbol{B}}\right)\left(\boldsymbol{I} - \epsilon\widetilde{\boldsymbol{B}}\right)^{-1}\left|\chi_\epsilon\right\rangle.$$

Since $\widetilde{\boldsymbol{B}}(t)$ is almost periodic and $\left(\boldsymbol{I} - \epsilon\widetilde{\boldsymbol{B}}\right)^{-1} = \boldsymbol{I} + \epsilon\widetilde{\boldsymbol{B}} + O(\epsilon^2)$, the dynamics of $\left|\chi_\epsilon\right\rangle$ reads

$$\frac{d}{dt}\left|\chi_\epsilon\right\rangle = \left(\epsilon\bar{\boldsymbol{B}} + \epsilon^2[\bar{\boldsymbol{B}}, \widetilde{\boldsymbol{B}}(t)] - \epsilon^2\widetilde{\boldsymbol{B}}(t)\frac{d}{dt}\widetilde{\boldsymbol{B}}(t) + \epsilon^3\boldsymbol{E}(\epsilon, t)\right)\left|\chi_\epsilon\right\rangle$$

where the operator $\boldsymbol{E}(\epsilon, t)$ is still almost periodic versus t but now its entries are no more linear combinations of time exponentials. The operator $\widetilde{\boldsymbol{B}}(t)\frac{d}{dt}\widetilde{\boldsymbol{B}}(t)$ is an almost periodic operator whose entries are linear combinations of oscillating time exponentials. Thus we have

$$\widetilde{\boldsymbol{B}}(t)\frac{d}{dt}\widetilde{\boldsymbol{B}}(t) = \bar{\boldsymbol{D}} + \frac{d}{dt}\widetilde{\boldsymbol{D}}(t)$$

where $\widetilde{\boldsymbol{D}}(t)$ is almost periodic. With these notations we have

$$\frac{d}{dt}\left|\chi_\epsilon\right\rangle = \left(\epsilon\bar{\boldsymbol{B}} - \epsilon^2\bar{\boldsymbol{D}} + \epsilon^2\frac{d}{dt}\left([\bar{\boldsymbol{B}}, \widetilde{\boldsymbol{C}}(t)] - \widetilde{\boldsymbol{D}}(t)\right) + \epsilon^3\boldsymbol{E}(\epsilon, t)\right)\left|\chi_\epsilon\right\rangle \tag{9}$$

where the skew-Hermitian operators $\bar{\boldsymbol{B}}$ and $\bar{\boldsymbol{D}}$ are constants and the other ones $\widetilde{\boldsymbol{C}}$, $\widetilde{\boldsymbol{D}}$, and $\boldsymbol{E}$ are almost periodic.

The first order approximation of $\left|\phi_\epsilon\right\rangle$ is given by the solution $\left|\phi_\epsilon^{1^{\text{st}}}\right\rangle$ of

$$\frac{d}{dt}\left|\phi_\epsilon^{1^{\text{st}}}\right\rangle = \epsilon\bar{\boldsymbol{B}}\left|\phi_\epsilon^{1^{\text{st}}}\right\rangle \tag{10}$$

where $\bar{\boldsymbol{B}}$ can be interpreted as the averaged value of $\boldsymbol{B}(t)$:

$$\bar{\boldsymbol{B}} = \lim_{T\mapsto\infty}\frac{1}{T}\int_0^T \boldsymbol{B}(t)\,dt = \lim_{T\mapsto\infty}\frac{1}{T}\int_0^T\left(\sum_{j=1}^r u_j e^{i\omega_j t}e^{-\boldsymbol{A}_0 t}\boldsymbol{A}_1 e^{\boldsymbol{A}_0 t} + u_j^* e^{-i\omega_j t}e^{-\boldsymbol{A}_0 t}\boldsymbol{A}_1 e^{\boldsymbol{A}_0 t}\right)dt.$$

Approximating $\boldsymbol{B}(t)$ by $\bar{\boldsymbol{B}}$ in (6) is called the Rotating Wave Approximation (RWA). The second order approximation reads then

$$\frac{d}{dt}\left|\phi_\epsilon^{2^{\text{nd}}}\right\rangle = (\epsilon\bar{\boldsymbol{B}} - \epsilon^2\bar{\boldsymbol{D}})\left|\phi_\epsilon^{2^{\text{nd}}}\right\rangle. \tag{11}$$

In (10) and (11), the operators $\epsilon\bar{\boldsymbol{B}}$ and $\epsilon\bar{\boldsymbol{B}} - \epsilon^2\bar{\boldsymbol{D}}$ are skew-Hermitian: these approximate dynamics remain of Schrödinger type and are thus characterized by the approximate Hamiltonians

$$\bar{H}^{1^{\text{st}}} = i\epsilon\bar{\boldsymbol{B}} \quad\text{and}\quad \bar{H}^{2^{\text{nd}}} = i(\epsilon\bar{\boldsymbol{B}} - \epsilon^2\bar{\boldsymbol{D}}).$$

A very similar analysis yields a second order approximation of the propagator dynamics

$$\frac{d}{dt}\boldsymbol{U}_\epsilon^{2^{\text{nd}}} = (\epsilon\bar{\boldsymbol{B}} - \epsilon^2\bar{\boldsymbol{D}})\boldsymbol{U}_\epsilon^{2^{\text{nd}}}. \tag{12}$$

1.2 Approximation recipes

Such first order and second order approximations extend without any difficulties to the case of m scalar oscillating controls in (1). They can be summarized as follows (without introducing the small parameter ϵ and the skew-Hermitian operators $\boldsymbol{A}_k$). Consider the controlled Hamiltonian associated to $|\psi\rangle$

$$\boldsymbol{H} = \boldsymbol{H}_0 + \sum_{k=1}^{m} u_k \boldsymbol{H}_k \tag{13}$$

with m oscillating real controls

$$u_k(t) = \sum_{j=1}^{r} u_{k,j} e^{\omega_j t} + u_{k,j}^* e^{-\omega_j t}$$

where $u_{k,j}$ is the slowly varying complex amplitude associated to control number k and frequency ω_j. In the sequel, all the computations are done assuming $u_{k,j}$ constant. Nevertheless, the obtained approximate Hamiltonians given in (15) are also valid for slowly time-varying amplitudes.[3]

The interaction Hamiltonian

$$\boldsymbol{H}_{\text{int}}(t) = \sum_{k,j} \left(u_{k,j} e^{\omega_j t} + u_{k,j}^* e^{-\omega_j t}\right) e^{i\boldsymbol{H}_0 t} \boldsymbol{H}_k e^{-i\boldsymbol{H}_0 t} \tag{14}$$

is associated to the interaction frame via the unitary transformation $|\phi\rangle = e^{i\boldsymbol{H}_0 t} |\psi\rangle$. It admits the decomposition

$$\boldsymbol{H}_{\text{int}}(t) = \boldsymbol{H}_{\text{rwa}}^{1^{\text{st}}} + \frac{d}{dt}\boldsymbol{I}_{\text{osc}}(t)$$

where $\boldsymbol{H}_{\text{rwa}}^{1^{\text{st}}}$ is the averaged Hamiltonian corresponding to the non-oscillating part of $\boldsymbol{H}_{\text{int}}$ (secular part) and $\boldsymbol{I}_{\text{osc}}$ is the time integral of the oscillating part. $\boldsymbol{I}_{\text{osc}}$ is an almost periodic Hermitian operator whose entries are linear combinations of oscillating time-exponentials. The Rotating Wave Approximation consists in approximating the time-varying Hamiltonian $\boldsymbol{H}_{\text{int}}(t)$ by $\boldsymbol{H}_{\text{rwa}}^{1^{\text{st}}}$. This approximation is valid when the amplitudes $u_{k,j}$ are small. It is of first order. The second order approximation is then obtained by adding to $\boldsymbol{H}_{\text{rwa}}^{1^{\text{st}}}$ a second order correction made by the averaged part $\boldsymbol{J}_{\text{rwa}}$ of the almost periodic Hamiltonian

$$i\left(\frac{d}{dt}\boldsymbol{I}_{\text{osc}}(t)\right)\boldsymbol{I}_{\text{osc}}(t) = \boldsymbol{J}_{\text{rwa}} + \frac{d}{dt}\boldsymbol{J}_{\text{osc}}(t)$$

with $\boldsymbol{J}_{\text{osc}}$ almost periodic. Notice $\boldsymbol{J}_{\text{rwa}}$ is also Hermitian since $\frac{d}{dt}\boldsymbol{I}_{\text{osc}}^2 = \frac{d}{dt}\boldsymbol{I}_{\text{osc}}\boldsymbol{I}_{\text{osc}} + \boldsymbol{I}_{\text{osc}}\frac{d}{dt}\boldsymbol{I}_{\text{osc}}$. We can summarize these approximations as the following recipes:

$$\boldsymbol{H}_{\text{rwa}}^{1^{\text{st}}} = \overline{\boldsymbol{H}_{\text{int}}}, \quad \boldsymbol{H}_{\text{rwa}}^{2^{\text{nd}}} = \boldsymbol{H}_{\text{rwa}}^{1^{\text{st}}} - i\overline{\left(\boldsymbol{H}_{\text{int}} - \overline{\boldsymbol{H}_{\text{int}}}\right)\left(\int_t (\boldsymbol{H}_{\text{int}} - \overline{\boldsymbol{H}_{\text{int}}})\right)} \tag{15}$$

where the over-line means taking the average.

[3] More precisely and according to exercise 1, we can assume that each $u_{k,j}$ is of small magnitude, admits a finite number of discontinuities and, between two successive discontinuities, is a slowly time varying function that is continuously differentiable.

1.3 Two approximation lemmas

A precise justification of the rotating wave approximation is given by the following lemma.

Lemma 1 (First order approximation)**.** *Consider the solution of* (6) *with initial condition* $|\phi_\epsilon(0)\rangle = |\phi_a\rangle$ *and denote by* $\left|\phi_\epsilon^{1^{st}}\right\rangle$ *the solution of* (10) *with the same initial condition,* $\left|\phi_\epsilon^{1^{st}}(0)\right\rangle = |\phi_a\rangle$*. Then, there exist* $M > 0$ *and* $\eta > 0$ *such that for all* $\epsilon \in]0, \eta[$ *we have*

$$\max_{t\in\left[0,\frac{1}{\epsilon}\right]} \left\| |\phi_\epsilon(t)\rangle - \left|\phi_\epsilon^{1^{st}}(t)\right\rangle \right\| \leq M\epsilon$$

Proof. Denote by $|\chi_\epsilon\rangle$ the solution of (9) with $|\chi_\epsilon(0)\rangle = (\boldsymbol{I} - \epsilon\widetilde{\boldsymbol{B}}(0))\,|\phi_a\rangle$. According to (8), there exist $M_1 > 0$ and $\eta_1 > 0$, such that for all $\epsilon \in]0, \eta_1]$ and $t > 0$ we have $\| |\chi_\epsilon(t)\rangle - |\phi_\epsilon(t)\rangle \| \leq M_1\epsilon$. But (9) admits the following form $\frac{d}{dt}|\chi_\epsilon\rangle = \left(\epsilon\bar{\boldsymbol{B}} + \epsilon^2\boldsymbol{F}(t)\right)|\chi_\epsilon\rangle$ where the operator $\boldsymbol{F}(t)$ is uniformly bounded versus t. Thus, there exist $M_2 > 0$ and $\eta_2 > 0$ such that the solution $\left|\varphi_\epsilon^{1^{\text{st}}}\right\rangle$ of (11) with initial condition $(\boldsymbol{I} - \epsilon\widetilde{\boldsymbol{B}}(0))\,|\phi_a\rangle$ satisfies, for all $\epsilon \in]0, \eta_2]$,

$$\max_{t\in\left[0,\frac{1}{\epsilon}\right]} \left\| \left|\varphi_\epsilon^{1^{\text{st}}}(t)\right\rangle - |\chi_\epsilon(t)\rangle \right\| \leq M_2\epsilon.$$

The propagator of (10) is unitary and thus

$$\left\| \left|\varphi_\epsilon^{1^{\text{st}}}(t)\right\rangle - \left|\phi_\epsilon^{1^{\text{st}}}(t)\right\rangle \right\| = \left\| \left|\varphi_\epsilon^{1^{\text{st}}}(0)\right\rangle - \left|\phi_\epsilon^{1^{\text{st}}}(0)\right\rangle \right\| = \epsilon \left\| \widetilde{\boldsymbol{B}}(0)\,|\phi_a\rangle \right\|.$$

We conclude with the triangular inequality

$$\left\| |\phi_\epsilon\rangle_t - \left|\phi_\epsilon^{1^{\text{st}}}\right\rangle_t \right\| \leq \| |\phi_\epsilon\rangle_t - |\chi_\epsilon\rangle_t \| + \left\| |\chi_\epsilon\rangle_t - \left|\varphi_\epsilon^{1^{\text{st}}}\right\rangle_t \right\| + \left\| \left|\varphi_\epsilon^{1^{\text{st}}}\right\rangle_t - \left|\phi_\epsilon^{1^{\text{st}}}\right\rangle_t \right\|.$$

□

The following lemma underlies the second order approximation:

Lemma 2 (Second order approximation)**.** *Consider the solution of* (6) *with initial condition* $|\phi_\epsilon(0)\rangle = |\phi_a\rangle$ *and denote by* $\left|\phi_\epsilon^{2^{nd}}\right\rangle$ *the solution of* (11) *with the same initial condition,* $\left|\phi_\epsilon^{2^{nd}}(0)\right\rangle = |\phi_a\rangle$*. Then, there exist* $M > 0$ *and* $\eta > 0$ *such that for all* $\epsilon \in]0, \eta[$ *we have*

$$\max_{t\in\left[0,\frac{1}{\epsilon^2}\right]} \left\| |\phi_\epsilon(t)\rangle - \left|\phi_\epsilon^{2^{nd}}(t)\right\rangle \right\| \leq M\epsilon$$

Proof. As for the proof of Lemma 1, we introduce $|\chi_\epsilon\rangle$, $\left|\varphi_\epsilon^{2^{\text{nd}}}\right\rangle$ solution of (11) starting from $\left|\varphi_\epsilon^{2^{\text{nd}}}(0)\right\rangle = (\boldsymbol{I} - \epsilon\widetilde{\boldsymbol{B}}(0))\,|\phi_a\rangle$. Using similar arguments, it is then enough to prove the existence of $M_3, \eta_3 > 0$ such that, for all $\epsilon \in]0, \eta_3[$, $\max_{t\in\left[0,\frac{1}{\epsilon}\right]} \left\| \left|\varphi_\epsilon^{2^{\text{nd}}}(t)\right\rangle - |\chi_\epsilon(t)\rangle \right\| \leq M_3\epsilon$. This estimate is a direct consequence of the almost periodic change of variables

$$|\xi_\epsilon\rangle = \left(\boldsymbol{I} - \epsilon^2\left([\bar{\boldsymbol{B}}, \widetilde{\boldsymbol{C}}(t)] - \widetilde{\boldsymbol{D}}(t)\right)\right)|\chi_\epsilon\rangle$$

that transforms (9) into

$$\frac{d}{dt}|\xi_\epsilon\rangle = \left(\epsilon\bar{\boldsymbol{B}} - \epsilon^2\bar{\boldsymbol{D}} + \epsilon^3\boldsymbol{F}(\epsilon,t)\right)|\xi_\epsilon\rangle$$

where $\boldsymbol{F}$ is almost periodic. This cancels the oscillating operator $\epsilon^2\frac{d}{dt}\left([\bar{\boldsymbol{B}},\widetilde{\boldsymbol{C}}(t)] - \widetilde{\boldsymbol{D}}(t)\right)$ appearing in (9): the equation satisfied by $|\xi_\epsilon\rangle$ and the second order approximation (11) differ only by third order almost periodic operator $\epsilon^3\boldsymbol{F}(\epsilon,t)$. □

Exercice 1. *The goal is to prove that, even if the amplitudes u_j are slowly varying, i.e., $u_j = u_j(\epsilon t)$ where $\tau \mapsto u_j(\tau)$ is continuously differentiable, the first and second order approximations remain valid. We have then two time-dependancies for*

$$\boldsymbol{B}(t,\tau) = \sum_{j=1}^{r} u_j(\tau)e^{i\omega_j t}e^{-\boldsymbol{A}_0 t}\boldsymbol{A}_1 e^{\boldsymbol{A}_0 t} + u_j^*(\tau)e^{-i\omega_j t}e^{-\boldsymbol{A}_0 t}\boldsymbol{A}_1 e^{\boldsymbol{A}_0 t}$$

with $\tau = \epsilon t$. Then $\frac{d}{dt}\boldsymbol{B} = \frac{\partial \boldsymbol{B}}{\partial t} + \epsilon\frac{\partial \boldsymbol{B}}{\partial \tau}$.

1. *Extend the decomposition (7) to*

$$\boldsymbol{B}(t,\tau) = \bar{\boldsymbol{B}}(\tau) + \frac{\partial \widetilde{\boldsymbol{B}}}{\partial t}(t,\tau)$$

   where $\widetilde{\boldsymbol{B}}(t,\tau)$ is t-almost periodic with zero mean in t (τ is fixed here).

2. *Show that the approximation Lemma 1 is still valid where (10) is replaced by*

$$\frac{d}{dt}\left|\phi_\epsilon^{1^{st}}\right\rangle = \epsilon\bar{\boldsymbol{B}}(\epsilon t)\left|\phi_\epsilon^{1^{st}}\right\rangle$$

3. *Show that the approximation Lemma 2 is still valid where (11) is replaced by*

$$\frac{d}{dt}\left|\phi_\epsilon^{2^{nd}}\right\rangle = (\epsilon\bar{\boldsymbol{B}}(\epsilon t) - \epsilon^2\bar{\boldsymbol{D}}(\epsilon t))\left|\phi_\epsilon^{2^{nd}}\right\rangle$$

   and where $\widetilde{\boldsymbol{B}}(t,\tau)\frac{\partial \widetilde{\boldsymbol{B}}}{\partial t}(t,\tau) = \bar{\boldsymbol{D}}(\tau) + \frac{\partial \widetilde{\boldsymbol{D}}}{\partial t}(t,\tau)$ with $\widetilde{\boldsymbol{D}}(t,\tau)$ almost periodic versus t and with zero t-mean.

4. *Extend the above approximation lemma when $\tau \mapsto u_j(\tau)$ is piecewise continuous and, on each interval where it remains continuous, it is also continuously differentiable ($\tau \mapsto u_j(\tau)$ is made by the concatenation of continuously differentiable functions).*

1.4 Rabi oscillations and single qubit logical gates

Let us consider the spin-half system described below and fix the phase of the drive, so that the controlled dynamics is given by:

$$i\frac{d}{dt}|\psi\rangle = \left(\tfrac{\omega_{\text{eg}}}{2}\boldsymbol{\sigma_z} + \tfrac{u(t)}{2}\boldsymbol{\sigma_x}\right)|\psi\rangle\,.$$

Furthermore, we assume that $u(t) = ve^{i\omega_r t} + v^* e^{-i\omega_r t}$ where the complex amplitude v is chosen such that $|v| \ll \omega_{\text{eg}}$ and the frequency ω_r is close to ω_{eg}, i.e., $|\omega_{\text{eg}} - \omega_r| \ll \omega_{\text{eg}}$. Denote by

$\Delta_r = \omega_{\text{eg}} - \omega_r$ the detuning between the control and the system then we get the standard form (13) with $m = 2$, $\boldsymbol{H}_0 = \frac{\omega_r}{2}\boldsymbol{\sigma_z}$, $u_1\boldsymbol{H}_1 = \frac{\Delta_r}{2}\boldsymbol{\sigma_z}$ and $u_2\boldsymbol{H}_2 = \frac{ve^{i\omega_r t}+v^*e^{-i\omega_r t}}{2}\boldsymbol{\sigma_x}$ with $\|\boldsymbol{H}_0\|$ much larger than $\|u_1\boldsymbol{H}_1 + u_2\boldsymbol{H}_2\|$. A direct computation yields to the following interaction Hamiltonian defined by (14):

$$\boldsymbol{H}_{\text{int}} = \frac{\Delta_r}{2}\boldsymbol{\sigma_z} + \tfrac{ve^{i\omega_r t}+v^*e^{-i\omega_r t}}{2} e^{\frac{i\omega_r t}{2}\boldsymbol{\sigma_z}}\boldsymbol{\sigma_x} e^{-\frac{i\omega_r t}{2}\boldsymbol{\sigma_z}}.$$

With the identities $e^{i\theta\boldsymbol{\sigma_z}} = \cos\theta \boldsymbol{I} + i\sin\theta\boldsymbol{\sigma_z}$ and $\boldsymbol{\sigma_z}\boldsymbol{\sigma_x} = i\boldsymbol{\sigma_y}$ we get the formula

$$e^{i\theta\boldsymbol{\sigma_z}}\boldsymbol{\sigma_x}e^{-i\theta\boldsymbol{\sigma_z}} = e^{2i\theta}\boldsymbol{\sigma}_+ + e^{-2i\theta}\boldsymbol{\sigma}_-.$$

Thus we have

$$\boldsymbol{H}_{\text{int}} = \tfrac{\Delta_r}{2}\boldsymbol{\sigma_z} + \tfrac{ve^{2i\omega_r t}+v^*}{2}\boldsymbol{\sigma}_+ + \tfrac{v^*e^{-2i\omega_r t}+v}{2}\boldsymbol{\sigma}_-.$$

The decomposition of $\boldsymbol{H}_{\text{int}} = \boldsymbol{H}_{\text{rwa}}^{1^{\text{st}}} + \frac{d}{dt}\boldsymbol{I}_{\text{osc}}$ reads:

$$\boldsymbol{H}_{\text{int}} = \underbrace{\tfrac{\Delta_r}{2}\boldsymbol{\sigma_z} + \tfrac{v^*}{2}\boldsymbol{\sigma}_+ + \tfrac{v}{2}\boldsymbol{\sigma}_-}_{\boldsymbol{H}_{\text{rwa}}^{1^{\text{st}}}} + \underbrace{\tfrac{ve^{2i\omega_r t}}{2}\boldsymbol{\sigma}_+ + \tfrac{v^*e^{-2i\omega_r t}}{2}\boldsymbol{\sigma}_-}_{\frac{d}{dt}\boldsymbol{I}_{\text{osc}}}.$$

Thus the first order approximation of any solution $|\psi\rangle$ of

$$i\frac{d}{dt}|\psi\rangle = \left(\tfrac{\omega_r+\Delta_r}{2}\boldsymbol{\sigma_z} + \tfrac{ve^{i\omega_r t}+v^*e^{-i\omega_r t}}{2}\boldsymbol{\sigma_x}\right)|\psi\rangle$$

is given by $e^{-i\frac{\omega_r t}{2}\boldsymbol{\sigma_z}}|\phi\rangle$ where $|\phi\rangle$ is solution of the linear time-invariant equation

$$i\frac{d}{dt}|\phi\rangle = \left(\tfrac{\Delta_r}{2}\boldsymbol{\sigma_z} + \tfrac{v^*}{2}\boldsymbol{\sigma}_+ + \tfrac{v}{2}\boldsymbol{\sigma}_-\right)|\phi\rangle, \quad |\phi(0)\rangle = |\psi(0)\rangle. \tag{16}$$

According to (15), the second order approximation requires the computation of the secular term in $\boldsymbol{I}_{\text{osc}}\frac{d}{dt}\boldsymbol{I}_{\text{osc}}$. Since $\boldsymbol{I}_{\text{osc}} = \frac{ve^{2i\omega_r t}}{4i\omega_r}\boldsymbol{\sigma}_+ - \frac{v^*e^{-2i\omega_r t}}{4i\omega_r}\boldsymbol{\sigma}_-$, we have

$$\boldsymbol{I}_{\text{osc}}\frac{d}{dt}\boldsymbol{I}_{\text{osc}} = \tfrac{|v|^2}{8i\omega_r}\boldsymbol{\sigma_z}$$

where we have also applied $\boldsymbol{\sigma}_+{}^2 = \boldsymbol{\sigma}_-{}^2 = 0$ and $\boldsymbol{\sigma_z} = \boldsymbol{\sigma}_+\boldsymbol{\sigma}_- - \boldsymbol{\sigma}_-\boldsymbol{\sigma}_+$. The second order approximation resulting from (15) reads:

$$i\frac{d}{dt}|\phi\rangle = \left(\left(\tfrac{\Delta_r}{2} + \tfrac{|v|^2}{8\omega_r}\right)\boldsymbol{\sigma_z} + \tfrac{v^*}{2}\boldsymbol{\sigma}_+ + \tfrac{v}{2}\boldsymbol{\sigma}_-\right)|\phi\rangle, \quad |\phi(0)\rangle = |\psi(0)\rangle. \tag{17}$$

We observe that (16) and (17) differ only by a correction of $\frac{|v|^2}{4\omega_r}$ added to the detuning Δ_r. This correction is called the Bloch-Siegert shift.

Set $v = \Omega_r e^{i\theta}$ and $\Delta_r' = \Delta_r + \frac{\Omega_r^2}{4\omega_r}$ with $\Omega_r > 0$ and θ real and constant. Then

$$\left(\left(\tfrac{\Delta_r}{2} + \tfrac{|v|^2}{8\omega_r}\right)\boldsymbol{\sigma_z} + \tfrac{v^*}{2}\boldsymbol{\sigma}_+ + \tfrac{v}{2}\boldsymbol{\sigma}_-\right) = \frac{\Omega_r}{2}\left(\cos\theta\boldsymbol{\sigma_x} + \sin\theta\boldsymbol{\sigma_y}\right) + \frac{\Delta_r'}{2}\boldsymbol{\sigma_z}. \tag{18}$$

Set

$$\Omega_r' = \sqrt{\left(\Delta_r + \tfrac{\Omega_r^2}{4\omega_r}\right)^2 + \Omega_r^2}, \quad \boldsymbol{\sigma_r} = \frac{\Omega_r\left(\cos\theta\boldsymbol{\sigma_x} + \sin\theta\boldsymbol{\sigma_y}\right) + \Delta_r'\boldsymbol{\sigma_z}}{\Omega_r'}.$$

Then ${\boldsymbol{\sigma_r}}^2 = \boldsymbol{I}$ and thus the solution of (17),

$$|\phi(t)\rangle = e^{-i\frac{\Omega'_r t}{2}\boldsymbol{\sigma_r}} |\phi(0)\rangle = \cos\left(\tfrac{\Omega'_r t}{2}\right)|\phi(0)\rangle - i\sin\left(\tfrac{\Omega'_r t}{2}\right)\boldsymbol{\sigma_r}|\phi(0)\rangle ,$$

oscillates between $|\phi(0)\rangle$ and $-i\boldsymbol{\sigma_r}|\phi(0)\rangle$ with the Rabi frequency $\frac{\Omega'_r}{2}$.

For $\Delta_r = 0$ and neglecting second order terms in Ω_r, we have $\Omega'_r \approx \Omega_r$, $\Delta'_r \approx 0$ and $\boldsymbol{\sigma_r} \approx \cos\theta\boldsymbol{\sigma_x} + \sin\theta\boldsymbol{\sigma_y}$. When $|\phi(0)\rangle = |g\rangle$ we see that, up-to second order terms, $|\phi(t)\rangle$ oscillates between $|g\rangle$ and $e^{-i(\theta+\frac{\pi}{2})}|e\rangle$. With $\theta = -\frac{\pi}{2}$, we have

$$|\chi(t)\rangle = \cos\left(\tfrac{\Omega_r t}{2}\right)|g\rangle + \sin\left(\tfrac{\Omega_r t}{2}\right)|e\rangle ,$$

and we see that, with a constant amplitude $v = \Omega_r e^{i\eta}$ for $t \in [0, T]$, we have the following transition, depending on the pulse-length $T > 0$:

- if $\Omega_r T = \pi$ then $|\phi(T)\rangle = |e\rangle$ and we have a transition between the ground state to the excited one, together with stimulated absorption of a photon of energy ω_{eg}. If we measure the energy in the final state we always find E_e. This is a π-pulse in reference to the Bloch sphere interpretation of (17).
- if $\Omega_r T = \frac{\pi}{2}$ then $|\phi(T)\rangle = (|g\rangle + |e\rangle)/\sqrt{2}$ and the final state is a coherent superposition of $|g\rangle$ and $|e\rangle$. A measure of the energy of the final state yields either E_g or E_e with a probability of 1/2 for both E_g and E_e. This is a $\frac{\pi}{2}$-pulse.

Since $|\psi\rangle = e^{-\frac{i\omega_r t}{2}\boldsymbol{\sigma_z}}|\phi\rangle$, we see that a π-pulse transfers $|\psi\rangle$ from $|g\rangle$ at $t = 0$ to $e^{i\alpha}|e\rangle$ at $t = T = \frac{\pi}{\Omega_r}$ where the phase $\alpha \approx \frac{\omega_r}{\Omega_r}\pi$ is very large since $\Omega_r \ll \omega_r$. Similarly, a $\frac{\pi}{2}$-pulse, transfers $|\psi\rangle$ from $|g\rangle$ at $t = 0$ to $\frac{e^{-i\alpha}|g\rangle + e^{i\alpha}|e\rangle}{\sqrt{2}}$ at $t = T = \frac{\pi}{2\Omega_r}$ with a very large relative half-phase $\alpha \approx \frac{\omega_r}{2\Omega_r}\pi$.

Exercice 2. *Take the first order approximation (16) with $\Delta_r = 0$ and $v \in \mathbb{C}$ as control.*

1. *Set $\Theta_r = \frac{\Omega_r}{2}T$. Show that the solution at T of the propagator $\boldsymbol{U}(t) \in SU(2)$, $i\frac{d}{dt}\boldsymbol{U} = \frac{\Omega_r(\cos\theta\boldsymbol{\sigma_x} + \sin\theta\boldsymbol{\sigma_y})}{2}\boldsymbol{U}$, $U_0 = \boldsymbol{I}$ is given by*

$$\boldsymbol{U}(T) = \cos\Theta_r \boldsymbol{I} - i\sin\Theta_r\left(\cos\theta\boldsymbol{\sigma_x} + \sin\theta\boldsymbol{\sigma_y}\right),$$

2. *Take a wave function $|\bar{\phi}\rangle$. Show that there exist Ω_r and θ such that $\boldsymbol{U}(T)|g\rangle = e^{i\alpha}|\bar{\phi}\rangle$, where α is some global phase.*
3. *Prove that for any given two wave functions $|\phi_a\rangle$ and $|\phi_b\rangle$ exists a piece-wise constant control $[0, 2T] \ni t \mapsto v(t) \in \mathbb{C}$ such that the solution of (16) with $|\phi(0)\rangle = |\phi_a\rangle$ and $\Delta_r = 0$ satisfies $|\phi(T)\rangle = e^{i\beta}|\phi_b\rangle$ for some global phase β.*
4. *Generalize the above question when $|\phi\rangle$ obeys the second order approximation (17) with Δ_r as additional control.*

Following the above analysis, the second order approximation of the solution $\boldsymbol{U}$ of the propagator equation

$$i\frac{d}{dt}\boldsymbol{U} = \left(\tfrac{\omega_r + \Delta_r}{2}\boldsymbol{\sigma_z} + \tfrac{v e^{i\omega_r t} + v^* e^{-i\omega_r t}}{2}\boldsymbol{\sigma_x}\right)\boldsymbol{U}, \qquad \boldsymbol{U}(0) = \boldsymbol{I},$$

is given by

$$\boldsymbol{U}^{2^{\rm nd}}(t) = e^{-i\frac{\omega_r t}{2}\boldsymbol{\sigma_z}} e^{-it\boldsymbol{H}^{2^{\rm nd}}}, \qquad \boldsymbol{H}^{2^{\rm nd}} = \frac{\Delta_r'}{2}\boldsymbol{\sigma_z} + \frac{\Omega_r\cos(\theta)}{2}\boldsymbol{\sigma_x} + \frac{\Omega_r\sin(\theta)}{2}\boldsymbol{\sigma_y}. \tag{19}$$

Note that by varying the parameters Δ_r, Ω_r and θ, corresponding respectively to the frequency, amplitude and phase of the driving control $u(t)$, the Hamiltonian $\boldsymbol{H}^{2^{\rm nd}}$ varies over the ensemble of Hermitian operators over $\mathbb{C}^2$ up to the addition of a constant multiple of identity. In consequence, it is easy to see (by further varying T) that the unitary operator $\boldsymbol{U}^{2^{\rm nd}}(T)$ varies over the ensemble of unitary operators on $\mathbb{C}^2$ up to a global phase. Therefore, by varying the parameters of the driving control, we can generate all possible unitary operations (logical gates) on a single qubit.

1.5 Λ-systems and Raman transition

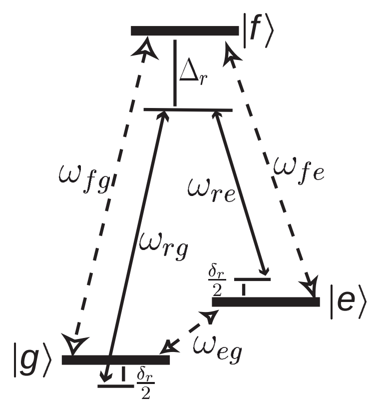

Figure 1: Raman transition for a Λ-level system ($\delta_r < 0$ and $\Delta_r > 0$ on the figure).

This transition strategy is used for a three-levem Λ-system. In such a 3-level system defined on the Hilbert space $\mathcal{H} = \{c_g|g\rangle + c_e|e\rangle + c_f|f\rangle, (c_g, c_e, c_f) \in \mathbb{C}^3\}$, we assume the three energy levels $|g\rangle$, $|e\rangle$ and $|f\rangle$ to admit the energies E_g, E_e and E_f (see Figure 1). The atomic frequencies are denoted as follows:

$$\omega_{\rm fg} = \frac{(E_f - E_g)}{\hbar},\ \omega_{fe} = \frac{(E_f - E_e)}{\hbar},\ \omega_{eg} = \frac{(E_e - E_g)}{\hbar}.$$

We assume a Hamiltonian of the form

$$\frac{\boldsymbol{H}(t)}{\hbar} = \frac{E_g}{\hbar}|g\rangle\langle g| + \frac{E_e}{\hbar}|e\rangle\langle e| + \frac{E_f}{\hbar}|f\rangle\langle f| + \tfrac{u(t)}{2}\Big(\mu_g(|g\rangle\langle f| + |f\rangle\langle g|) + \mu_e(|e\rangle\langle f| + |f\rangle\langle e|)\Big) \tag{20}$$

where μ_g and μ_e are coupling coefficients with the electromagnetic field described by $u(t)$. Assuming the third level $|f\rangle$ to admit an energy E_f much greater than E_e and E_g, we will see that the averaged Hamiltonian (after the rotating wave approximation) is very similar to the one describing Rabi oscillations and the state $|f\rangle$ can be ignored. The transition from $|g\rangle$ to $|e\rangle$ is no more performed via a quasi-resonant control with a single frequency close to $\omega_{eg} = (E_e - E_g)/\hbar$, but with a control based on two frequencies ω_{rg} and ω_{re}, in a neighborhood of $\omega_{\rm fg} = (E_f - E_g)/\hbar$ and $\omega_{fe} = (E_f - E_e)/\hbar$, with $\omega_{rg} - \omega_{re}$ close to ω_{eg}. Such transitions result from a nonlinear phenomena and second order perturbations. The main practical advantage comes from the fact that ω_{re} and ω_{rg} are in many examples optical frequencies (around 10^{15} rad/s) whereas ω_{eg} is a radio frequency (around 10^{10} rad/s). The wave length of the laser generating u is around 1 μm and thus spatial resolution is much better with optical waves than with radio-frequency ones.

Indeed, in the Hamiltonian (20), we take a quasi-resonant control defined by the constant complex amplitudes u_g and u_e,

$$u(t) = u_g e^{i\omega_{rg}t} + u_g^* e^{-i\omega_{rg}t} + u_e e^{i\omega_{re}t} + u_e^* e^{-i\omega_{re}t}$$

where the frequencies ω_{rg} and ω_{re} are close to $\omega_{\rm fg}$ and ω_{fe}. According to Figure 1 set

$$\omega_{\rm fg} = \omega_{rg} + \Delta_r - \tfrac{\delta_r}{2}, \quad \omega_{fe} = \omega_{re} + \Delta_r + \tfrac{\delta_r}{2},$$

and assume that

$$\begin{aligned}\big(\max(|\mu_g|,|\mu_e|)\max(|u_g|,|u_e|)\big) \text{ and } |\delta_r| \\ \ll \min\left(\omega_{rg},\omega_{re},\omega_{\rm fg},\omega_{fe},|\Delta_r|,|\omega_{re}-\omega_{rg}+\Delta_r|,|\omega_{re}-\omega_{rg}-\Delta_r|\right).\end{aligned}$$

In the interaction frame (passage from $|\psi\rangle$ where $i\frac{d}{dt}|\psi\rangle = \frac{\boldsymbol{H}(t)}{\hbar}|\psi\rangle$ to $|\phi\rangle$),

$$|\psi\rangle = \Big(e^{-i\left(E_g+\frac{\delta_r}{2}\right)t}|g\rangle\langle g| + e^{-i\left(E_e-\frac{\delta_r}{2}\right)t}|e\rangle\langle e| + e^{-iE_f t}|f\rangle\langle f|\Big)|\phi\rangle$$

the Hamiltonian becomes ($i\frac{d}{dt}|\phi\rangle = \frac{\boldsymbol{H}_{\rm int}(t)}{\hbar}|\phi\rangle$):

$$\begin{aligned}\frac{\boldsymbol{H}_{\rm int}(t)}{\hbar} &= \tfrac{\delta_r}{2}(|e\rangle\langle e| - |g\rangle\langle g|) \\ &+ \mu_g\left(u_g e^{i\omega_{rg}t} + u_e e^{i\omega_{re}t} + u_g^* e^{-i\omega_{rg}t} + u_e^* e^{-i\omega_{re}t}\right)\Big(e^{i(\omega_{rg}+\Delta_r)t}|g\rangle\langle f| + e^{-i(\omega_{rg}+\Delta_r)t}|f\rangle\langle g|\Big) \\ &+ \mu_e\left(u_g e^{i\omega_{rg}t} + u_e e^{i\omega_{re}t} + u_g^* e^{-i\omega_{rg}t} + u_e^* e^{-i\omega_{re}t}\right)\Big(e^{i(\omega_{re}+\Delta_r)t}|e\rangle\langle f| + e^{-i(\omega_{re}+\Delta_r)t}|f\rangle\langle e|\Big).\end{aligned}$$

It is clear from (15), that $\frac{\boldsymbol{H}_{\rm rwa}^{\rm 1st}}{\hbar} = \frac{\delta_r}{2}(|e\rangle\langle e| - |g\rangle\langle g|)$ and thus second order terms should be considered and $\boldsymbol{H}_{\rm rwa}^{\rm 2nd}$ has to be computed for a meaningfull approximation. Simple but tedious computations show that $\int(\boldsymbol{H}_{\rm int} - \boldsymbol{H}_{\rm rwa}^{\rm 1st})/\hbar$ (the time primitive of zero mean) is given by

$$\begin{aligned}&\tfrac{\mu_g}{2}\left(\tfrac{u_g e^{i(2\omega_{rg}+\Delta_r)t}}{i(2\omega_{rg}+\Delta_r)} + \tfrac{u_e e^{i(\omega_{rg}+\omega_{re}+\Delta_r)t}}{i(\omega_{rg}+\omega_{re}+\Delta_r)} + \tfrac{u_g^* e^{i\Delta_r t}}{i\Delta_r} + \tfrac{u_e^* e^{i(\omega_{rg}-\omega_{re}+\Delta_r)t}}{i(\omega_{rg}-\omega_{re}+\Delta_r)}\right)|g\rangle\langle f| \\ &\quad + \tfrac{\mu_e}{2}\left(\tfrac{u_g e^{i(\omega_{rg}+\omega_{re}+\Delta_r)t}}{i(\omega_{rg}+\omega_{re}+\Delta_r)} + \tfrac{u_e e^{i(2\omega_{re}+\Delta_r)t}}{i(2\omega_{re}+\Delta_r)} + \tfrac{u_g^* e^{i(\omega_{re}-\omega_{rg}+\Delta_r)t}}{i(\omega_{re}-\omega_{rg}+\Delta_r)} + \tfrac{u_e^* e^{i\Delta_r t}}{i\Delta_r}\right)|e\rangle\langle f| \\ &\quad - \tfrac{\mu_g}{2}\left(\tfrac{u_g^* e^{-i(2\omega_{rg}+\Delta_r)t}}{i(2\omega_{rg}+\Delta_r)} + \tfrac{u_e^* e^{-i(\omega_{rg}+\omega_{re}+\Delta_r)t}}{i(\omega_{rg}+\omega_{re}+\Delta_r)} + \tfrac{u_g e^{-i\Delta_r t}}{i\Delta_r} + \tfrac{u_e e^{-i(\omega_{rg}-\omega_{re}+\Delta_r)t}}{i(\omega_{rg}-\omega_{re}+\Delta_r)}\right)|f\rangle\langle g| \\ &\quad - \tfrac{\mu_e}{2}\left(\tfrac{u_g^* e^{-i(\omega_{rg}+\omega_{re}+\Delta_r)t}}{i(\omega_{rg}+\omega_{re}+\Delta_r)} + \tfrac{u_e^* e^{-i(2\omega_{re}+\Delta_r)t}}{i(2\omega_{re}+\Delta_r)} + \tfrac{u_g e^{-i(\omega_{re}-\omega_{rg}+\Delta_r)t}}{i(\omega_{re}-\omega_{rg}+\Delta_r)} + \tfrac{u_e e^{-i\Delta_r t}}{i\Delta_r}\right)|f\rangle\langle e|.\end{aligned}$$

The non-oscillating terms of $i\left(\int_t \left(\boldsymbol{H}_{\text{int}} - \boldsymbol{H}^{1^{\text{st}}}_{\text{rwa}}\right)/\hbar\right)\left(\boldsymbol{H}_{\text{int}} - \boldsymbol{H}^{1^{\text{st}}}_{\text{rwa}}\right)/\hbar$ are then given by simple but tedious computations:

$$
\begin{aligned}
\frac{\boldsymbol{H}^{2^{\text{nd}}}_{\text{rwa}}}{\hbar} &= \tfrac{\mu_g\mu_e}{4}\left(\tfrac{1}{\omega_{rg}+\omega_{re}+\Delta_r} + \tfrac{1}{\Delta_r}\right)\left(u_g^* u_e \left|g\right\rangle\left\langle e\right| + u_g u_e^* \left|e\right\rangle\left\langle g\right|\right) + \tfrac{\delta_r}{2}\left(\left|e\right\rangle\left\langle e\right| - \left|g\right\rangle\left\langle g\right|\right) \\
&+ \tfrac{\mu_g^2}{4}\left(\tfrac{|u_g|^2}{2\omega_{rg}+\Delta_r} + \tfrac{|u_g|^2}{\Delta_r} + \tfrac{|u_e|^2}{\omega_{rg}-\omega_{re}+\Delta_r}\right)\left|g\right\rangle\left\langle g\right| + \tfrac{\mu_e^2}{4}\left(\tfrac{|u_e|^2}{2\omega_{re}+\Delta_r} + \tfrac{|u_e|^2}{\Delta_r} + \tfrac{|u_g|^2}{\omega_{re}-\omega_{rg}+\Delta_r}\right)\left|e\right\rangle\left\langle e\right| \\
&- \tfrac{1}{4}\left(\tfrac{\mu_g^2|u_g|^2}{2\omega_{rg}+\Delta_r} + \tfrac{\mu_e^2|u_e|^2}{2\omega_{re}+\Delta_r} + \tfrac{\mu_g^2|u_g|^2+\mu_e^2|u_e|^2}{\omega_{rg}+\omega_{re}+\Delta_r} + \tfrac{\mu_g^2|u_g|^2+\mu_e^2|u_e|^2}{\Delta_r} + \tfrac{\mu_g^2|u_g|^2}{\omega_{re}-\omega_{rg}+\Delta_r} + \tfrac{\mu_e^2|u_e|^2}{\omega_{rg}-\omega_{re}+\Delta_r}\right)\left|f\right\rangle\left\langle f\right|.
\end{aligned}
\tag{21}
$$

This expression simplfies if we assume additionnally that

$$
|\Delta_r|,\ |\omega_{re} - \omega_{rg} + \Delta_r|,\ |\omega_{re} - \omega_{rg} - \Delta_r| \ll \omega_{rg},\ \omega_{re},\ \omega_{\text{fg}},\ \omega_{fe}.
$$

With these additional assumptions we have 3 time-scales:

1. The slow one associated to δ_r, $\mu_g|u_g|$, $\mu_g|u_e|$, $\mu_e|u_g|$ and $\mu_e|u_e|$
2. The intermediate one attached to Δ_r, $|\omega_{re} - \omega_{rg} + \Delta_r|$ and $|\omega_{re} - \omega_{rg} - \Delta_r|$
3. The fast one related to ω_{rg}, ω_{re}, ω_{fg} and ω_{fe}.

We have then the following approximation of the average Hamiltonian

$$
\begin{aligned}
\frac{\boldsymbol{H}^{2^{\text{nd}}}_{\text{rwa}}}{\hbar} \approx\ & \tfrac{\mu_g\mu_e u_g^* u_e}{4\Delta_r}\left|g\right\rangle\left\langle e\right| + \tfrac{\mu_g\mu_e u_g u_e^*}{4\Delta_r}\left|e\right\rangle\left\langle g\right| + \tfrac{\delta_r}{2}\left(\left|e\right\rangle\left\langle e\right| - \left|g\right\rangle\left\langle g\right|\right) \\
&+ \tfrac{\mu_g^2}{4}\left(\tfrac{|u_g|^2}{\Delta_r} + \tfrac{|u_e|^2}{\omega_{rg}-\omega_{re}+\Delta_r}\right)\left|g\right\rangle\left\langle g\right| + \tfrac{\mu_e^2}{4}\left(\tfrac{|u_e|^2}{\Delta_r} + \tfrac{|u_g|^2}{\omega_{re}-\omega_{rg}+\Delta_r}\right)\left|e\right\rangle\left\langle e\right| \\
&- \tfrac{1}{4}\left(\tfrac{\mu_g^2|u_g|^2+\mu_e^2|u_e|^2}{\Delta_r} + \tfrac{\mu_g^2|u_g|^2}{\omega_{re}-\omega_{rg}+\Delta_r} + \tfrac{\mu_e^2|u_e|^2}{\omega_{rg}-\omega_{re}+\Delta_r}\right)\left|f\right\rangle\left\langle f\right|.
\end{aligned}
$$

If $\left\langle\phi(0)|f\right\rangle = 0$ then $\left\langle\phi(t)|f\right\rangle = 0$ up to third order terms: the space $\text{span}\{\left|g\right\rangle, \left|e\right\rangle\}$ and $\text{span}\{\left|f\right\rangle\}$ are invariant space of $\boldsymbol{H}^{2^{\text{nd}}}_{\text{rwa}}$. Thus, if the initial state belongs to $\text{span}\{\left|g\right\rangle, \left|e\right\rangle\}$, we can forget the $\left|f\right\rangle\left\langle f\right|$ term in $\boldsymbol{H}^{2^{\text{nd}}}_{\text{rwa}}$ (restriction of the dynamics to this invariant subspace) and we get a 2-level Hamiltonian, called Raman Hamiltonian, that lives on $\text{span}\{\left|g\right\rangle, \left|e\right\rangle\}$:

$$
\begin{aligned}
\frac{\boldsymbol{H}_{\text{Raman}}}{\hbar} =\ & \tfrac{\mu_g\mu_e u_g^* u_e}{4\Delta_r}\left|g\right\rangle\left\langle e\right| + \tfrac{\mu_g\mu_e u_g u_e^*}{4\Delta_r}\left|e\right\rangle\left\langle g\right| + \tfrac{\delta_r}{2}\left(\left|e\right\rangle\left\langle e\right| - \left|g\right\rangle\left\langle g\right|\right) \\
&+ \tfrac{\mu_g^2}{4}\left(\tfrac{|u_g|^2}{\Delta_r} + \tfrac{|u_e|^2}{\omega_{rg}-\omega_{re}+\Delta_r}\right)\left|g\right\rangle\left\langle g\right| + \tfrac{\mu_e^2}{4}\left(\tfrac{|u_e|^2}{\Delta_r} + \tfrac{|u_g|^2}{\omega_{re}-\omega_{rg}+\Delta_r}\right)\left|e\right\rangle\left\langle e\right|.
\end{aligned}
\tag{22}
$$

that is similar (up to a global phase shift) to the average Hamiltonian underlying Rabi oscillations (18) with

$$
\begin{aligned}
\Delta_r' &= \delta_r + \tfrac{\mu_e^2}{4}\left(\tfrac{|u_e|^2}{\Delta_r} + \tfrac{|u_g|^2}{\omega_{re}-\omega_{rg}+\Delta_r}\right) - \tfrac{\mu_g^2}{4}\left(\tfrac{|u_g|^2}{\Delta_r} + \tfrac{|u_e|^2}{\omega_{rg}-\omega_{re}+\Delta_r}\right), \\
\Omega_r e^{i\theta} &= \tfrac{\mu_g\mu_e u_g^* u_e}{2\Delta_r}.
\end{aligned}
$$

During such Raman pulses, the intermediate state $\left|f\right\rangle$ remains almost empty (i.e. $\left\langle\psi|f\right\rangle \approx 0$) and thus, this protocol remains rather robust with respect to an eventual instability of the state $|f\rangle$, not modeled through such Schrödinger dynamics. To tackle such questions, one has to consider non-conservative dynamics for $|\psi\rangle$ and to take into account decoherence effects due to the coupling of $|f\rangle$ with the environment, coupling leading to a finite lifetime. The incorporation into the $|\psi\rangle$-dynamics of such irreversible effects, is analogous to the incorporation of friction and viscous effects in classical Hamiltonian dynamics. Later on through these lecture notes, we will present such models to describe open quantum systems (see also chapter 4 of [12] for a tutorial exposure and [7, 3] for more mathematical presentations).

1.6 Jaynes-Cummings model

Consider the following spin-spring interaction Hamiltonian $\boldsymbol{H}_{tot}$ that governs the dynamics of $|\psi\rangle$,

$$i\frac{d}{dt}|\psi\rangle = \left(\tfrac{\omega_{\rm eg}}{2}\boldsymbol{\sigma_z} + \omega_c\left(\boldsymbol{a}^\dagger\boldsymbol{a} + \frac{\mathbf{I}}{2}\right) + u(t)(\boldsymbol{a}+\boldsymbol{a}^\dagger) + i\tfrac{\Omega}{2}\boldsymbol{\sigma_x}(\boldsymbol{a}^\dagger - \boldsymbol{a})\right)|\psi\rangle\,,$$

where we have additionally considered a drive of real amplitude $u(t)$ applied on the harmonic oscillator. Assume that $u(t) = ve^{i\omega_r t} + v^* e^{-i\omega_r t}$ where the complex amplitude v is constant. Define the following detunings

$$\Delta_c = \omega_c - \omega_r, \quad \Delta_{eg} = \omega_{\rm eg} - \omega_r$$

and assume that

$$|\Delta_c|,\ |\Delta_{eg}|,\ |\Omega|, |v| \ll \omega_{\rm eg},\ \omega_c,\ \omega_r.$$

Then $\boldsymbol{H}_{tot} = \boldsymbol{H}_0 + \epsilon\boldsymbol{H}_1$ where ϵ is a small parameter and

$$\begin{aligned}\frac{\boldsymbol{H}_0}{\hbar} &= \tfrac{\omega_r}{2}\boldsymbol{\sigma_z} + \omega_r\left(\boldsymbol{a}^\dagger\boldsymbol{a}+\frac{\mathbf{I}}{2}\right)\\ \epsilon\frac{\boldsymbol{H}_1}{\hbar} &= \left(\tfrac{\Delta_{eg}}{2}\boldsymbol{\sigma_z} + \Delta_c\left(\boldsymbol{a}^\dagger\boldsymbol{a}+\frac{\mathbf{I}}{2}\right) + (ve^{i\omega_r t} + v^*e^{-i\omega_r t})(\boldsymbol{a}+\boldsymbol{a}^\dagger) + i\tfrac{\Omega}{2}\boldsymbol{\sigma_x}(\boldsymbol{a}^\dagger - \boldsymbol{a})\right).\end{aligned}$$

Even if the system is infinite dimensional, we apply here heuristically the rotating wave approximation summarized in Subsection 1.2. First we have to compute the Hamiltonian in the interaction frame via the following change of variables $|\psi\rangle \mapsto |\phi\rangle$:

$$|\psi\rangle = e^{-i\omega_r t\left(\boldsymbol{a}^\dagger\boldsymbol{a}+\frac{\mathbf{I}}{2}\right)} e^{\frac{-i\omega_r t}{2}\boldsymbol{\sigma_z}}\,|\phi\rangle$$

We get the following interaction Hamiltonian

$$\begin{aligned}\frac{\boldsymbol{H}_{\rm int}}{\hbar} = \tfrac{\Delta_{eg}}{2}\boldsymbol{\sigma_z} + \Delta_c\left(\boldsymbol{a}^\dagger\boldsymbol{a}+\frac{\mathbf{I}}{2}\right) + \left(ve^{i\omega_r t} + v^*e^{-i\omega_r t}\right)\left(e^{-i\omega_r t}\boldsymbol{a} + e^{i\omega_r t}\boldsymbol{a}^\dagger\right)\\ + i\tfrac{\Omega}{2}(e^{-i\omega_r t}\boldsymbol{\sigma_-} + e^{i\omega_r t}\boldsymbol{\sigma_+})(e^{i\omega_r t}\boldsymbol{a}^\dagger - e^{-i\omega_r t}\boldsymbol{a})\end{aligned}$$

where we have applied the following identities:

$$e^{\frac{i\theta}{2}\boldsymbol{\sigma_z}}\ \boldsymbol{\sigma_x} e^{-\frac{i\theta}{2}\boldsymbol{\sigma_z}} = e^{-i\theta}\boldsymbol{\sigma_-} + e^{i\theta}\boldsymbol{\sigma_+}, \quad e^{i\theta\left(\boldsymbol{a}^\dagger\boldsymbol{a}+\frac{\mathbf{I}}{2}\right)}\ \boldsymbol{a}\ e^{-i\theta\left(\boldsymbol{a}^\dagger\boldsymbol{a}+\frac{\mathbf{I}}{2}\right)} = e^{-i\theta}\boldsymbol{a}$$

The secular part of $\boldsymbol{H}_{\rm int}$ is given by

$$\frac{\boldsymbol{H}^{1^{\rm st}}_{\rm rwa}}{\hbar} = \tfrac{\Delta_{eg}}{2}\boldsymbol{\sigma_z} + \Delta_c\left(\boldsymbol{a}^\dagger\boldsymbol{a}+\frac{\mathbf{I}}{2}\right) + v\boldsymbol{a} + v^*\boldsymbol{a}^\dagger + i\tfrac{\Omega}{2}(\boldsymbol{\sigma_-}\boldsymbol{a}^\dagger - \boldsymbol{\sigma_+}\boldsymbol{a}). \tag{23}$$

This precisely corresponds to the Jaynes-Cummings approximation. The oscillating part of $\boldsymbol{H}_{\text{int}}$ is given by

$$\frac{(\boldsymbol{H}_{\text{int}} - \boldsymbol{H}^{1^{\text{st}}}_{\text{rwa}})}{\hbar} = ve^{2i\omega_r t}\boldsymbol{a}^\dagger + v^* e^{-2i\omega_r t}\boldsymbol{a} + i\tfrac{\Omega}{2}(e^{2i\omega_r t}\boldsymbol{\sigma_+}\boldsymbol{a}^\dagger - e^{-2i\omega_r t}\boldsymbol{\sigma_-}\boldsymbol{a}).$$

Then we have

$$\int_t \frac{(\boldsymbol{H}_{\text{int}} - \boldsymbol{H}^{1^{\text{st}}}_{\text{rwa}})}{\hbar} = \tfrac{1}{2i\omega_r}\left(ve^{2i\omega_r t}\boldsymbol{a}^\dagger - v^* e^{-2i\omega_r t}\boldsymbol{a} + i\tfrac{\Omega}{2}(e^{2i\omega_r t}\boldsymbol{\sigma_+}\boldsymbol{a}^\dagger + e^{-2i\omega_r t}\boldsymbol{\sigma_-}\boldsymbol{a})\right)$$

and, following (15), the second order approximation reads

$$\frac{\boldsymbol{H}^{2^{\text{nd}}}_{\text{rwa}}}{\hbar} = \tfrac{\Delta_{eg} + \frac{\Omega^2}{8\omega_r}}{2}\boldsymbol{\sigma_z} + \Delta_c\left(\boldsymbol{a}^\dagger\boldsymbol{a} + \frac{\mathbf{I}}{2}\right) + v\boldsymbol{a} + v^*\boldsymbol{a}^\dagger + i\tfrac{\Omega}{2}(\boldsymbol{\sigma_-}\boldsymbol{a}^\dagger - \boldsymbol{\sigma_+}\boldsymbol{a})$$
$$+ i\tfrac{\Omega}{4\omega_r}(v\boldsymbol{\sigma_-} - v^*\boldsymbol{\sigma_+}) + \tfrac{\Omega^2}{8\omega_r}\boldsymbol{\sigma_z}\boldsymbol{a}^\dagger\boldsymbol{a} - \left(\tfrac{\Omega^2}{16\omega_r} + \tfrac{|v|^2}{2\omega_r}\right)\boldsymbol{I} \quad (24)$$

(use $[\boldsymbol{a}, \boldsymbol{a}^\dagger] = 1$, $\boldsymbol{\sigma_+}\boldsymbol{\sigma_-} = |e\rangle\langle e|$ and $\boldsymbol{\sigma_-}\boldsymbol{\sigma_+} = |g\rangle\langle g|$).

Consider now that the average Hamiltonian $\boldsymbol{H}^{1^{\text{st}}}_{\text{rwa}}$ defined by (23) with $v \in \mathbb{C}$ as control. It splits into $\boldsymbol{H}_0 + v_1\boldsymbol{H}_1 + v_2\boldsymbol{H}_2$ where $v = \frac{1}{2}(v_1 + iv_2)$ with $v_1, v_2 \in \mathbb{R}$ and

$$\frac{\boldsymbol{H}_0}{\hbar} = \tfrac{\Delta_{eq}}{2}\boldsymbol{\sigma_z} + \Delta_c(\boldsymbol{X}^2 + \boldsymbol{P}^2) - \frac{\Omega}{2}(\boldsymbol{X}\boldsymbol{\sigma_y} + \boldsymbol{P}\boldsymbol{\sigma_x}), \qquad \frac{\boldsymbol{H}_1}{\hbar} = \tfrac{\boldsymbol{a}+\boldsymbol{a}^\dagger}{2} = \boldsymbol{X}, \quad \frac{\boldsymbol{H}_2}{\hbar} = \tfrac{\boldsymbol{a}-\boldsymbol{a}^\dagger}{2i} = \boldsymbol{P}. \quad (25)$$

The controlled system $i\frac{d}{dt}|\phi\rangle = (\boldsymbol{H}_0 + v_1\boldsymbol{H}_1 + v_2\boldsymbol{H}_2)|\phi\rangle$ reads as a system of two partial differential equations, affine in the two scalar controls $u_1 = v_1/\sqrt{2}$ and $u_2 = v_2/\sqrt{2}$. The quantum state $|\phi\rangle$ is described by two elements of $L^2(\mathbb{R}, \mathbb{C})$, ϕ_g and ϕ_e, whose time evolution is given by

$$\begin{aligned} i\frac{\partial\phi_g}{\partial t} &= -\tfrac{\Delta_c}{2}\frac{\partial^2\phi_g}{\partial x^2} + \left(\frac{\Delta_c x^2 - \Delta_{eg}}{2}\right)\phi_g + \left(u_1 x + iu_2\frac{\partial}{\partial x}\right)\phi_g + i\tfrac{\Omega}{2\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right)\phi_e \\ i\frac{\partial\phi_e}{\partial t} &= -\tfrac{\Delta_c}{2}\frac{\partial^2\phi_e}{\partial x^2} + \left(\frac{\Delta_c x^2 + \Delta_{eg}}{2}\right)\phi_e + \left(u_1 x + iu_2\frac{\partial}{\partial x}\right)\phi_e - i\tfrac{\Omega}{2\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right)\phi_g \end{aligned} \quad (26)$$

since $\boldsymbol{X}$ stands for $\frac{x}{\sqrt{2}}$ and $\boldsymbol{P}$ for $-\frac{i}{\sqrt{2}}\frac{\partial}{\partial x}$. An open question is the controllability (see Appendix A) on the set of functions (ϕ_g, ϕ_e) defined up to a global phase and such that $\|\phi_g\|_{L^2} + \|\phi_e\|_{L^2} = 1$. In a first step, one can take $\Delta_c = 0$ (which is not a limitation in fact) and $\Delta_{eg} = 0$ (which is a strict sub-case).

Exercice 3. *Consider* $i\frac{d}{dt}|\psi\rangle = \frac{(\boldsymbol{H}_0 + v_1\boldsymbol{H}_1 + v_2\boldsymbol{H}_1)}{\hbar}|\psi\rangle$ *with* $\boldsymbol{H}_0$, $\boldsymbol{H}_1$ *and* $\boldsymbol{H}_2$ *given by* (25) *with* $\Delta_{eg} = \Delta_c = 0$, $\Omega > 0$ *and* (v_1, v_2) *as control. The system is therefore given by*

$$i\frac{d}{dt}|\psi\rangle = \left(i\tfrac{\Omega}{2}(\boldsymbol{\sigma_-}\boldsymbol{a}^\dagger - \boldsymbol{\sigma_+}\boldsymbol{a}) + v\boldsymbol{a}^\dagger + v^*\boldsymbol{a}\right)|\psi\rangle$$

with $v = \frac{v_1 + iv_2}{2}$.

1. *Set* $\nu \in \mathbb{C}$ *solution of* $\frac{d}{dt}\nu = -iv$ *and consider the following change of frame* $|\phi\rangle = \boldsymbol{D}_{-\nu}|\psi\rangle$ *with the displacement operator* $\boldsymbol{D}_{-\nu} = e^{-\nu \boldsymbol{a}^\dagger + \nu^* \boldsymbol{a}}$. *Show that, up to a global phase change, we have*

$$i\frac{d}{dt}|\phi\rangle = \left(\tfrac{i\Omega}{2}(\boldsymbol{\sigma_-}\boldsymbol{a}^\dagger - \boldsymbol{\sigma_+}\boldsymbol{a}) + (\tilde{v}\boldsymbol{\sigma_+} + \tilde{v}^*\boldsymbol{\sigma_-})\right)|\phi\rangle$$

with $\tilde{v} = i\frac{\Omega}{2}\nu$.

2. *Take the orthonormal basis* $\{|g,n\rangle, |e,n\rangle\}$ *with* $n \in \mathbb{N}$ *being the photon number and where for instance* $|g,n\rangle$ *stands for the tensor product* $|g\rangle \otimes |n\rangle$. *Set* $|\phi\rangle = \sum_n \phi_{g,n}|g,n\rangle + \phi_{e,n}|e,n\rangle$ *with* $\phi_{g,n}, \phi_{e,n} \in \mathbb{C}$ *depending on* t *and* $\sum_n |\phi_{g,n}|^2 + |\phi_{e,n}|^2 = 1$. *Show that, for* $n \geq 0$

$$i\frac{d}{dt}\phi_{g,n+1} = i\frac{\Omega}{2}\sqrt{n+1}\phi_{e,n} + \tilde{v}^*\phi_{e,n+1}, \quad i\frac{d}{dt}\phi_{e,n} = -i\tfrac{\Omega}{2}\sqrt{n+1}\phi_{g,n+1} + \tilde{v}\phi_{g,n}$$

and $i\frac{d}{dt}\phi_{g,0} = \tilde{v}^*\phi_{e,0}$.

3. *Assume that* $|\phi(0)\rangle = |g,0\rangle$. *Construct an open-loop control* $[0,T] \ni t \mapsto \tilde{v}(t)$ *such that* $|\phi(T)\rangle = |g,1\rangle$ *(hint: take* $\tilde{v} = \bar{v}\delta(t)$ *and adjust the constants* $\bar{v}$ *and* $T > 0$, $\delta(t)$ *Dirac distribution at* 0*).*

4. *Generalize the above open-loop control when the goal state* $|\phi(T)\rangle$ *is* $|g,n\rangle$ *with any arbitrary photon number* n.

1.7 Single trapped ion and Law-Eberly method

Through this subsection, we study the laser control of a single trapped ion. The Hamiltonian is given by

$$\frac{\boldsymbol{H}}{\hbar} = \frac{\omega_{\text{eg}}}{2}\boldsymbol{\sigma_z} + \omega_m(\boldsymbol{a}^\dagger\boldsymbol{a} + \frac{\mathbf{I}}{2}) + (u^*(t)\boldsymbol{\sigma_+}\ e^{i\eta(\boldsymbol{a}+\boldsymbol{a}^\dagger)} + u(t)\boldsymbol{\sigma_-}\ e^{-i\eta(\boldsymbol{a}+\boldsymbol{a}^\dagger)}). \tag{27}$$

The Schrödinger equation $i\frac{d}{dt}|\psi\rangle = \frac{\tilde{\boldsymbol{H}}}{\hbar}|\psi\rangle$ is equivalent to a system of partial differential equations on the two components (ψ_g, ψ_e):

$$\begin{aligned} i\frac{\partial\psi_g}{\partial t} &= \tfrac{\omega_m}{2}\left(x^2 - \frac{\partial^2}{\partial x^2}\right)\psi_g - \tfrac{\omega_{\text{eg}}}{2}\psi_g + u(t)e^{-i\sqrt{2}\eta x}\psi_e \\ i\frac{\partial\psi_e}{\partial t} &= \tfrac{\omega_m}{2}\left(x^2 - \frac{\partial^2}{\partial x^2}\right)\psi_e + \tfrac{\omega_{\text{eg}}}{2}\psi_e + u^*(t)e^{i\sqrt{2}\eta x}\psi_g, \end{aligned} \tag{28}$$

where $u \in \mathbb{C}$ is the control input. In [11] this system is proven to be approximately controllable for (ψ_g, ψ_e) on the unit sphere of $(L^2(\mathbb{R},\mathbb{C}))^2$. The proof proposed in [11] relies on the Law-Eberly proof of spectral controllability for a secular approximation when $u(t)$ is a superposition of three mono-chromatic plane waves: first one of frequency ω_{eg} (ion electronic transition) and amplitude v; second one of frequency $\omega_{\text{eg}} - \omega_m$ (red shift by a vibration quantum) and amplitude v_r; third one of frequency $\omega_{\text{eg}} + \omega_m$ (blue shift by a vibration quantum) and amplitude v_b. With this control, the Hamiltonian reads

$$\begin{aligned}\frac{\boldsymbol{H}}{\hbar} =&\omega_m\left(\boldsymbol{a}^\dagger\boldsymbol{a}+\frac{\mathbf{I}}{2}\right)+\frac{\omega_{\text{eg}}}{2}\boldsymbol{\sigma_z}+\left(v\boldsymbol{\sigma_-}e^{i(\omega_{\text{eg}}t-\eta(\boldsymbol{a}+\boldsymbol{a}^\dagger))}+v^*\boldsymbol{\sigma_+}e^{-i(\omega_{\text{eg}}t-\eta(\boldsymbol{a}+\boldsymbol{a}^\dagger))}\right)\\ &+\left(v_b\boldsymbol{\sigma_-}e^{i((\omega_{\text{eg}}+\omega_m)t-\eta_b(\boldsymbol{a}+\boldsymbol{a}^\dagger))}+v_b^*\boldsymbol{\sigma_+}e^{-i((\omega_{\text{eg}}+\omega_m)t-\eta_b(\boldsymbol{a}+\boldsymbol{a}^\dagger))}\right)\\ &+\left(v_r\boldsymbol{\sigma_-}e^{i((\omega_{\text{eg}}-\omega_m)t-\eta_r(\boldsymbol{a}+\boldsymbol{a}^\dagger))}+v_r^*\boldsymbol{\sigma_+}e^{-i((\omega_{\text{eg}}-\omega_m)t-\eta_r(\boldsymbol{a}+\boldsymbol{a}^\dagger))}\right).\end{aligned}$$

We have the following separation of scales (vibration frequency much smaller than the qubit frequency and slowly varying laser amplitudes v, v_r, v_b):

$$\omega_m \ll \omega_{\text{eg}}, \quad \left|\frac{d}{dt}\right| \ll \omega_m|v|, \quad \left|\frac{d}{dt}v_r\right| \ll \omega_m|v_r|, \quad \left|\frac{d}{dt}v_b\right| \ll \omega_m|v_b|.$$

Furthermore the Lamb-Dicke parameters $|\eta|, |\eta_b|, |\eta_r| \ll 1$ are almost identical. In the interaction frame, $|\psi\rangle$ is replaced by $|\phi\rangle$ according to

$$|\psi\rangle = e^{-i\omega t\left(\boldsymbol{a}^\dagger\boldsymbol{a}+\frac{\mathbf{I}}{2}\right)}e^{\frac{-i\omega_{\text{eg}}t}{2}\boldsymbol{\sigma_z}}|\phi\rangle\,.$$

The Hamiltonian becomes

$$\begin{aligned}\frac{\boldsymbol{H}_{\text{int}}}{\hbar} &= e^{i\omega_m t\left(\boldsymbol{a}^\dagger\boldsymbol{a}\right)}\left(v\boldsymbol{\sigma_-}e^{-i\eta(\boldsymbol{a}+\boldsymbol{a}^\dagger)}+v^*\boldsymbol{\sigma_+}e^{i\eta(\boldsymbol{a}+\boldsymbol{a}^\dagger)}\right)e^{-i\omega_m t\left(\boldsymbol{a}^\dagger\boldsymbol{a}\right)}\\ &\quad+e^{i\omega t\left(\boldsymbol{a}^\dagger\boldsymbol{a}\right)}\left(v_b\boldsymbol{\sigma_-}e^{i\omega_m t}e^{-i\eta_b(\boldsymbol{a}+\boldsymbol{a}^\dagger)}+v_b^*\boldsymbol{\sigma_+}e^{-i\omega_m t}e^{i\eta_b(\boldsymbol{a}+\boldsymbol{a}^\dagger)}\right)e^{-i\omega_m t\left(\boldsymbol{a}^\dagger\boldsymbol{a}\right)}\\ &\qquad+e^{i\omega_m t\left(\boldsymbol{a}^\dagger\boldsymbol{a}\right)}\left(v_r\boldsymbol{\sigma_-}e^{-i\omega_m t}e^{-i\eta_r(\boldsymbol{a}+\boldsymbol{a}^\dagger)}+v_r^*\boldsymbol{\sigma_+}e^{i\omega_m t}e^{i\eta_r(\boldsymbol{a}+\boldsymbol{a}^\dagger)}\right)e^{-i\omega_m t\left(\boldsymbol{a}^\dagger\boldsymbol{a}\right)}.\end{aligned}$$

With the approximation $e^{i\epsilon(a+a^\dagger)} \approx 1+i\epsilon(a+a^\dagger)$ for $\epsilon = \pm\eta, \eta_b, \eta_r$, the Hamiltonian becomes (up to second order terms in ϵ),

$$\begin{aligned}\frac{\boldsymbol{H}_{\text{int}}}{\hbar} &= v\boldsymbol{\sigma_-}(1-i\eta(e^{-i\omega_m t}\boldsymbol{a}+e^{i\omega_m t}\boldsymbol{a}^\dagger))+v^*\boldsymbol{\sigma_+}(1+i\eta(e^{-i\omega_m t}\boldsymbol{a}+e^{i\omega_m t}\boldsymbol{a}^\dagger))\\ &+v_b e^{i\omega_m t}\boldsymbol{\sigma_-}(1-i\eta_b(e^{-i\omega_m t}\boldsymbol{a}+e^{i\omega_m t}\boldsymbol{a}^\dagger))+v_b^* e^{-i\omega t}\boldsymbol{\sigma_+}(1+i\eta_b(e^{-i\omega_m t}\boldsymbol{a}+e^{i\omega_m t}\boldsymbol{a}^\dagger))\\ &+v_r e^{-i\omega_m t}\boldsymbol{\sigma_-}(1-i\eta_r(e^{-i\omega_m t}\boldsymbol{a}+e^{i\omega_m t}\boldsymbol{a}^\dagger))+v_r^* e^{i\omega_m t}\boldsymbol{\sigma_+}(1+i\eta_r(e^{-i\omega_m t}\boldsymbol{a}+e^{i\omega_m t}\boldsymbol{a}^\dagger))\end{aligned}$$

The oscillating terms (with frequencies $\pm\omega_m$ and $\pm 2\omega_m$) have zero average. The mean Hamiltonian, illustrated on Figure 2, reads

$$\frac{\boldsymbol{H}^{1^{\text{st}}}_{\text{rwa}}}{\hbar} = v\boldsymbol{\sigma_-}+v^*\boldsymbol{\sigma_+}+\bar{v}_b\boldsymbol{a}\boldsymbol{\sigma_-}+\bar{v}_b^*\boldsymbol{a}^\dagger\boldsymbol{\sigma_+}+\bar{v}_r\boldsymbol{a}^\dagger\boldsymbol{\sigma_-}+\bar{v}_r^*\boldsymbol{a}\boldsymbol{\sigma_+}$$

where we have set $\bar{v}_b = -i\eta_b v_b$ and $\bar{v}_r = -i\eta_r v_r$. The above Hamiltonian is "valid" as soon as $|\eta|, |\eta_b|, |\eta_r| \ll 1$ and

$$|v|, |v_b|, |v_r| \ll \omega_m, \quad \left|\frac{d}{dt}v\right| \ll \omega_m|v|, \quad \left|\frac{d}{dt}v_b\right| \ll \omega_m|v_b|, \quad \left|\frac{d}{dt}v_r\right| \ll \omega_m|v_r|.$$

To interpret the structure of the different operators building this average Hamiltonian, physicists have a nice mnemonic trick based on energy conservation. Take for example $\boldsymbol{a}\boldsymbol{\sigma_-}$ attached to the control $\bar{v}_b$, i.e. to the blue shifted photon of frequency $\omega_{\text{eg}}+\omega_m$. The operator

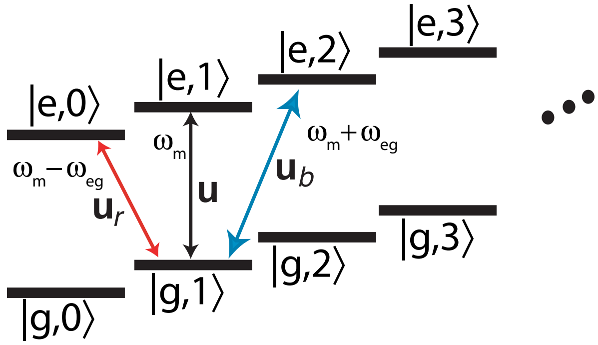

Figure 2: a trapped ion submitted to three mono-chromatic plane waves of frequencies $\omega_{\rm eg}$, $\omega_{\rm eg} - \omega_m$ and $\omega_{\rm eg} + \omega_m$.

$\boldsymbol{\sigma_-}$ corresponds to the quantum jump from $|e\rangle$ to $|g\rangle$ whereas the operator $\boldsymbol{a}$ is the destruction of one phonon. Thus $\boldsymbol{a\sigma_-}$ is the simultaneous jump from $|e\rangle$ to $|g\rangle$ (energy change of $\omega_{\rm eg}$) with destruction of one phonon (energy change of ω_m). The emitted photon has to take away the total energy lost by the system, i.e. $\omega_{\rm eg} + \omega_m$. Its frequency is then $\omega_{\rm eg} + \omega_m$ and corresponds thus to $\bar{v}_b$. We understand why $\boldsymbol{a}^\dagger\boldsymbol{\sigma_-}$ is associated to $\bar{v}_r$: the system loses $\omega_{\rm eg}$ during the jump from $|e\rangle$ to $|g\rangle$; at the same time, it wins ω_m, the phonon energy; the emitted photon takes away $\omega_{\rm eg} - \omega_m$ and thus corresponds to $\bar{v}_r$. This point is illustrated on Figure 2 describing the first order transitions between the different states of definite energy.

The dynamics $i\frac{d}{dt}|\phi\rangle = \frac{\boldsymbol{H}^{1^{\rm st}}_{\rm rwa}}{\hbar}|\phi\rangle$ depends linearly on 6 scalar controls: it is a drift-less system of infinite dimension (non-holonomic system of infinite dimension). The two underlying partial differential equations are

$$i\frac{\partial \phi_g}{\partial t} = \left(v + \frac{\bar{v}_b}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right) + \frac{\bar{v}_r}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right)\right)\phi_e$$
$$i\frac{\partial \phi_e}{\partial t} = \left(v^* + \frac{\bar{v}_b^*}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right) + \frac{\bar{v}_r^*}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right)\right)\phi_g$$

We write the above dynamics in the eigenbasis, $\{|g,n\rangle, |e,n\rangle\}_{n\in\mathbb{N}}$, of the operator $\omega_m\left(\boldsymbol{a}^\dagger\boldsymbol{a} + \frac{\mathbf{I}}{2}\right) + \frac{\omega_{\rm eg}}{2}\boldsymbol{\sigma_z}$:

$$i\frac{d}{dt}\phi_{g,n} = v\phi_{e,n} + \bar{v}_r\sqrt{n}\phi_{e,n-1} + \bar{v}_b\sqrt{n+1}\phi_{e,n+1}$$
$$i\frac{d}{dt}\phi_{e,n} = v^*\phi_{g,n} + \bar{v}_r^*\sqrt{n+1}\phi_{g,n+1} + \bar{v}_b^*\sqrt{n}\phi_{g,n-1}$$

with $|\phi\rangle = \sum_{n=0}^{+\infty}\phi_{g,n}|g,n\rangle + \phi_{e,n}|e,n\rangle$ and $\sum_{n=0}^{+\infty}|\phi_{g,n}|^2 + |\phi_{e,n}|^2 = 1$.

Law and Eberly [15] illustrated that it is always possible (and in any arbitrary time $T > 0$) to steer $|\phi\rangle$ from any finite linear superposition of $\{|g,n\rangle, |e,n\rangle\}_{n\in\mathbb{N}}$ at $t = 0$, to any other finite linear superposition at time $t = T$ (spectral controllability). One only needs two controls v and $\bar{v}_b$ (resp. v and $\bar{v}_r$): $\bar{v}_r$ (resp. $\bar{v}_b$) remains zero and the supports of v and $\bar{v}_b$ (resp. v and $\bar{v}_r$) do not overlap. This spectral controllability implies approximate controllability.

Let us detail now the main idea behind the Law-Eberly method to prove spectral controllability. Take $n > 0$ and denote by $\mathcal{H}_n$ the truncation to n-phonon space:

$$\mathcal{H}_n = \text{span}\{|g,0\rangle, |e,0\rangle, \ldots, |g,n\rangle, |e,n\rangle\}$$

We consider an initial condition $|\phi(0)\rangle \in \mathcal{H}_n$ and $T > 0$. Then for $t \in [0, \frac{T}{2}]$ the control

$$\bar{v}_r(t) = \bar{v}_b(t) = 0, \quad v(t) = \tfrac{2i}{T} \arctan \left| \tfrac{\phi_{e,n}(0)}{\phi_{g,n}(0)} \right| e^{i \arg(\phi_{g,n}(0)\phi^*_{e,n}(0))}$$

ensures that $\phi_{e,n}(T/2) = 0$. For $t \in [\frac{T}{2}, T]$, the control

$$\bar{v}_b(t) = v(t) = 0, \quad \bar{v}_r(t) = \tfrac{2i}{T\sqrt{n}} \arctan \left| \frac{\phi_{g,n}(\frac{T}{2})}{\phi_{e,n-1}(\frac{T}{2})} \right| e^{i \arg\left(\phi_{g,n}(\frac{T}{2})\phi^*_{e,n-1}(\frac{T}{2})\right)}$$

ensures that $\phi_{e,n}(t) \equiv 0$ and that $\phi_{g,n}(T) = 0$. Thus with this two-pulse control, the first one on v and the second one on $\bar{v}_r$, we have $|\phi(T)\rangle \in \mathcal{H}_{n-1}$.

After n iterations of this two-pulse process $|\phi(nT)\rangle$ belongs to $\mathcal{H}_0$. Then for $t \in [nT, (n+\frac{1}{2})T]$, the control

$$\bar{v}_r(t) = \bar{v}_b(t) = 0, \quad v(t) = \tfrac{2i}{T} \arctan \left| \tfrac{\phi_{e,0}(nT)}{\phi_{g,0}(nT)} \right| e^{i \arg\left(\phi_{g,0}(nT)\phi^*_{e,0}(nT)\right)}$$

guaranties that $\left|\phi\left((n+\frac{1}{2})T\right)\right\rangle = e^{i\theta}|g,0\rangle$.

Up to a global phase, we can steer, in any arbitrary time and with a piecewise constant control, any element of $\mathcal{H}_n$ to $|g,0\rangle$. Since the system is driftless ($t \mapsto -t$ and $(v, \bar{v}_b, \bar{v}_r) \mapsto -(v, \bar{v}_b, \bar{v}_r)$ leave the system unchanged) we can easily reverse the time and thus can also steer $|g,0\rangle$ to any element of $\mathcal{H}_n$. To steer $|\phi\rangle$ form any initial state in $\mathcal{H}_n$ to any final state also in $\mathcal{H}_n$, it is enough to steer the initial state to $|g,0\rangle$ and then to steer $|g,0\rangle$ to the final state. To summarize: on can always steer, with piecewise constant controls and in an arbitrary short time, any finite linear superposition of $(|g,\nu\rangle, |e,\nu\rangle)_{\nu\geq 0}$ to any other one.

1.8 Cirac-Zoller two-qubit gate

In this subsection, we apply the tools of the previous subsections to introduce a two-qubit entangling gate implementation proposed by Cirac and Zoller [10]. This implementation proposed for trapped ions is a central ingredient of a quantum computer based on trapped ions. Indeed such a C-phase gate (controlled-phase gate), in combination with the single-qubit gates discussed in Subsection 1.4, provides a universal set of logical gates. This means that by combining such single-qubit and two-qubit gates, one can perform any arbitrary unitary operation on a multi-qubit quantum computer (see [16] for a detailed discussion of universal quantum gates). Such a C-phase gate corresponds to the following two-qubit unitary operation:

$$\boldsymbol{U}_{\text{C-phase}} = |g^c\rangle\langle g^c| \otimes \boldsymbol{I}^t + |e^c\rangle\langle e^c| \otimes \boldsymbol{\sigma_z}^t. \tag{29}$$

Here the superscripts c and t stand for control and target qubits (t not to be confused with the time). This unitary operation can be understood as follows: we apply the identity operation on the target qubit if the control qubit is in the ground state $|g\rangle$, and we apply the Pauli $\boldsymbol{\sigma_z}$ operation on the target qubit, if the control qubit is in its excited state $|e\rangle$. This is an entangling gate, as starting from the separable state $(|g^c\rangle + |e^c\rangle) \otimes (|g^t\rangle + |e^t\rangle)/2$ and applying the C-phase unitary, we reach the state

$$\frac{1}{2}|g^c\rangle \otimes (|e^t\rangle + |g^t\rangle) + \frac{1}{2}|e^c\rangle \otimes (|e^t\rangle - |g^t\rangle)$$

which cannot be written as the tensor product of two local states on the control and target qubits.

In Cirac and Zoller's proposal for realizing such a gate with trapped ions, one considers two ions out of a string of trapped ions. The vibrational degree of freedom of the center of mass of the string is used as a quantum bus to transfer information from one qubit to the other and to perform such a two-qubit unitary operation without any direct interaction between the ions. This vibrational degree of freedom being modelled as a quantum harmonic oscillator, we are again in presence of a spin-spring system with a single harmonic oscillator (frequency ω_m) coupled to two qubits (frequencies ω^c_{eg} and ω^t_{eg}). Another ingredient of this gate is a third auxiliary energy level of the ion that gets populated throughout the gate operation, even though at the final time it remains unpopulated. More precisely, we consider a third energy level f with a transition frequency ω_{fg} between the levels $|g\rangle$ and $|f\rangle$. Therefore the free Hamiltonian in absence of driving lasers is given by

$$\frac{\boldsymbol{H}_0}{\hbar} = \omega_m(\boldsymbol{a}^\dagger\boldsymbol{a} + \frac{\boldsymbol{I}}{2}) + \omega^c_{\text{eg}}\,|e^c\rangle\langle e^c| + \omega^c_{\text{fg}}\,|f^c\rangle\langle f^c| + \omega^t_{\text{eg}}\,|e^t\rangle\langle e^t| + \omega^t_{\text{fg}}\,|f^t\rangle\langle f^t|\,.$$

Note that, compared to the previous subsection, here we have redefined the origin of energy such that the energy value of $|0_m\rangle \otimes |g^c\rangle \otimes |g^t\rangle$ is 0. This is why the Hamiltonian $\omega_{\text{eg}}/2\boldsymbol{\sigma_z}$ is replaced by $\omega_{\text{eg}}\,|e\rangle\langle e|$.

Now, in order to perform a C-phase gate between the two qubits, we apply individual laser fields on the two ions. On the control ion, we apply a laser field at frequency $\omega^c_{\text{eg}} - m$ with a real amplitude v^c, and on the target ion, we apply a laser field at frequcny $\omega^t_{\text{fg}} - m$ with a real amplitude v^t. The total Hamiltonian is given by$\boldsymbol{H}_{tot}(\tau) = \boldsymbol{H}_0 + \boldsymbol{H}^c(\tau) + \boldsymbol{H}^t(\tau)$ (note that in this subsection, we denote time by τ to avoid confusion with the superscript t standing for the target qubit). Here, the interaction Hamiltonians are defined as follows

$$\frac{\boldsymbol{H}^c(\tau)}{\hbar} = v^c(|g^c\rangle\langle e^c|\, e^{i((\omega^c_{\text{eg}}-\omega_m)\tau - \eta^c(\boldsymbol{a}+\boldsymbol{a}^\dagger))} + |e^c\rangle\langle g^c|\, e^{-i((\omega^c_{\text{eg}}-\omega_m)\tau - \eta^c(\boldsymbol{a}+\boldsymbol{a}^\dagger))})$$
$$\frac{\boldsymbol{H}^t(\tau)}{\hbar} = v^t(|g^c\rangle\langle f^c|\, e^{i((\omega^t_{\text{fg}}-\omega_m)\tau - \eta^t(\boldsymbol{a}+\boldsymbol{a}^\dagger))} + |f^t\rangle\langle g^t|\, e^{-i((\omega^t_{\text{eg}}-\omega_m)\tau - \eta^t(\boldsymbol{a}+\boldsymbol{a}^\dagger))})$$

Following a similar analysis to the previous subsection, after going to the rotating frame of the Hamiltonian $\boldsymbol{H}_0$ and performing a first-order rotating-wave approximation, we obtain the Hamiltonian

$$\frac{\boldsymbol{H}^{1^{\text{st}}}_{\text{rwa}}}{\hbar} = \bar{v}^c(|g^c\rangle\langle e^c|\,\boldsymbol{a}^\dagger + |e^c\rangle\langle g^c|\,\boldsymbol{a}) + \bar{v}^t(|g^t\rangle\langle f^t|\,\boldsymbol{a}^\dagger + |f^t\rangle\langle g^t|\,\boldsymbol{a}).$$

The control sequence to perform a C-phase gate is as follows:

1. We let the laser amplitude v^t to be zero and turn on a constant non-zero v^c . By applying this laser field on the control qubit over a time duration $T = \pi/2v^c$, we apply a unitary operation

$$\boldsymbol{U}^c = \exp(-i\pi/2(|g^c\rangle\langle e^c|\,\boldsymbol{a}^\dagger + |e^c\rangle\langle g^c|\,\boldsymbol{a})).$$

2. Next, we turn off the laser field on the control qubit and turn on the one on the target. We apply a constant non-zero amplitude v^t over a time duration $T = \pi/v^t$, which gives the unitary operation

$$\boldsymbol{U}^t = \exp(-i\pi(|g^t\rangle\langle f^t|\,\boldsymbol{a}^\dagger + |f^t\rangle\langle g^c|\,\boldsymbol{a})).$$

3. Finally, we turn on the laser on the control qubit and turn off the one target, performing the same exact unitary operation as in step 1.

Exercice 4. *For* $\boldsymbol{H}_{JC} = \omega\left(\boldsymbol{\sigma_z} \otimes \boldsymbol{I}_c/2 + \boldsymbol{I}_q \otimes \boldsymbol{N} + \boldsymbol{I}_q \otimes \boldsymbol{I}_c/2\right) + i\frac{\Omega}{2}(\boldsymbol{\sigma}_- \otimes \boldsymbol{a}^\dagger - \boldsymbol{\sigma}_+ \otimes \boldsymbol{a})$ *show that the propagator, the t-dependant unitary operator* $\boldsymbol{U}$ *solution of* $i\frac{d}{dt}\boldsymbol{U} = \boldsymbol{H}_{JC}\boldsymbol{U}$ *with* $\boldsymbol{U}(0) = \boldsymbol{I}$*, reads* $\boldsymbol{U}(t) = e^{-i\omega t\left(\frac{\boldsymbol{\sigma_z}\otimes\boldsymbol{I}_c}{2} + \boldsymbol{I}_q\otimes\boldsymbol{N} + \frac{\boldsymbol{I}_q\otimes\boldsymbol{I}_c}{2}\right)} e^{\frac{\Omega t}{2}(\boldsymbol{\sigma}_-\otimes\boldsymbol{a}^\dagger - \boldsymbol{\sigma}_+\otimes\boldsymbol{a})}$ *where for any angle* θ*,*

$$e^{\theta(\boldsymbol{\sigma}_-\otimes\boldsymbol{a}^\dagger - \boldsymbol{\sigma}_+\otimes\boldsymbol{a})} = |g\rangle\langle g| \otimes \cos(\theta\sqrt{\boldsymbol{N}}) + |e\rangle\langle e| \otimes \cos(\theta\sqrt{\boldsymbol{N}+\boldsymbol{I}}) - \boldsymbol{\sigma}_+ \otimes \boldsymbol{a}\,\frac{\sin(\theta\sqrt{\boldsymbol{N}})}{\sqrt{\boldsymbol{N}}} + \boldsymbol{\sigma}_- \otimes \frac{\sin(\theta\sqrt{\boldsymbol{N}})}{\sqrt{\boldsymbol{N}}}\,\boldsymbol{a}^\dagger$$

where

$$\exp\left(i\theta\left(\frac{\boldsymbol{\sigma_z}\otimes\boldsymbol{I}_c}{2} + \boldsymbol{I}_q\otimes\boldsymbol{N} + \frac{\boldsymbol{I}_q\otimes\boldsymbol{I}_c}{2}\right)\right) = e^{i\theta/2}\left(e^{i\theta/2}|e\rangle\langle e| + e^{-i\theta/2}|g\rangle\langle g|\right) \otimes \sum_{n=0}^{\infty} e^{i\theta n}|n\rangle\langle n|,$$

$$\cos(\theta\sqrt{\boldsymbol{N}}) = \sum_{n=0}^{\infty}\cos(\theta\sqrt{n})|n\rangle\langle n|$$

$$\cos(\theta\sqrt{\boldsymbol{N}+\boldsymbol{I}}) = \sum_{n=0}^{\infty}\cos(\theta\sqrt{n+1})|n\rangle\langle n|$$

$$\frac{\sin(\theta\sqrt{\boldsymbol{N}})}{\sqrt{\boldsymbol{N}}} = \sum_{n=0}^{\infty}\frac{\sin(\sqrt{n}\theta)}{\sqrt{n}}|n\rangle\langle n|.$$

Show then that

$$\boldsymbol{U}^c = |g^c\rangle\langle g^c| \otimes \cos(\pi\sqrt{\boldsymbol{N}}/2) + |e^c\rangle\langle e^c| \otimes \cos(\pi\sqrt{\boldsymbol{N}+\boldsymbol{I}}/2) + |f^c\rangle\langle f^c| \otimes \boldsymbol{I} - i\,|e^c\rangle\langle g^c| \otimes \boldsymbol{a}\,\frac{\sin(\pi\sqrt{\boldsymbol{N}}/2)}{\sqrt{\boldsymbol{N}}} - i\,|g^c\rangle\langle e^c| \otimes \frac{\sin(\pi\sqrt{\boldsymbol{N}}/2)}{\sqrt{\boldsymbol{N}}}\,\boldsymbol{a}^\dagger$$

$$\boldsymbol{U}^t = |g^t\rangle\langle g^t| \otimes \cos(\pi\sqrt{\boldsymbol{N}}) + |e^t\rangle\langle e^t| \otimes \boldsymbol{I} + |f^t\rangle\langle f^t| \otimes \cos(\pi\sqrt{\boldsymbol{N}+\boldsymbol{I}}) - i\,|f^t\rangle\langle g^t| \otimes \boldsymbol{a}\,\frac{\sin(\pi\sqrt{\boldsymbol{N}})}{\sqrt{\boldsymbol{N}}} - i\,|g^t\rangle\langle f^t| \otimes \frac{\sin(\pi\sqrt{\boldsymbol{N}})}{\sqrt{\boldsymbol{N}}}\,\boldsymbol{a}^\dagger$$

Whenever the harmonic oscillator is initialized in its vacuum state $|0\rangle$, the above combination of unitary operations $\boldsymbol{U}^c\boldsymbol{U}^t\boldsymbol{U}^c$ performs effectively a C-phase unitary on the two qubits. This can be seen by following the action of the above unitary operations on the four basis states of the two-qubit system. Indeed, we have

$$\begin{array}{ccccccc}
|g^c\rangle|g^t\rangle|0\rangle & \xrightarrow{\boldsymbol{U}^c} & |g^c\rangle|g^t\rangle|0\rangle & \xrightarrow{\boldsymbol{U}^t} & |g^c\rangle|g^t\rangle|0\rangle & \xrightarrow{\boldsymbol{U}^c} & |g^c\rangle|g^t\rangle|0\rangle \\
|g^c\rangle|e^t\rangle|0\rangle & \xrightarrow{\boldsymbol{U}^c} & |g^c\rangle|e^t\rangle|0\rangle & \xrightarrow{\boldsymbol{U}^t} & |g^c\rangle|e^t\rangle|0\rangle & \xrightarrow{\boldsymbol{U}^c} & |g^c\rangle|e^t\rangle|0\rangle \\
|e^c\rangle|g^t\rangle|0\rangle & \xrightarrow{\boldsymbol{U}^c} & -i|g^c\rangle|g^t\rangle|1\rangle & \xrightarrow{\boldsymbol{U}^t} & i|g^c\rangle|g^t\rangle|1\rangle & \xrightarrow{\boldsymbol{U}^c} & |e^c\rangle|g^t\rangle|0\rangle \\
|e^c\rangle|e^t\rangle|0\rangle & \xrightarrow{\boldsymbol{U}^c} & -i|g^c\rangle|e^t\rangle|1\rangle & \xrightarrow{\boldsymbol{U}^t} & -i|g^c\rangle|e^t\rangle|1\rangle & \xrightarrow{\boldsymbol{U}^c} & -|e^c\rangle|e^t\rangle|0\rangle.
\end{array}$$

Thus whenever the harmonic oscillator is initialized in $|0\rangle$, and the state of the two ions are spanned by the computational basis elements $|g\rangle$ and $|e\rangle$, by linearity, the unitary operation $\boldsymbol{U}^c\boldsymbol{U}^t\boldsymbol{U}^c$ effectively acts as a C-phase unitary operation on the two-qubit state.

2 Adiabatic control

2.1 Time-adiabatic approximation without gap conditions

We first recall the quantum version of adiabatic invariance. We restrict here the exposure to finite dimensions and without the exponentially precise estimations. However we give the simplest version of a time-adiabatic approximation result without any gap conditions. All the details can be found in a book by Teufel [20] with extension to infinite dimensional case.

Theorem 1. *Take $m+1$ Hermitian matrices of size $n \times n$: $\boldsymbol{H}_0, \ldots, \boldsymbol{H}_m$. For $u \in \mathbb{R}^m$ set $H(u) := \boldsymbol{H}_0 + \sum_{k=1}^m u_k \, \boldsymbol{H}_k$. Assume that u is a slowly varying time-function: $u = u(s)$ with $s = \epsilon t \in [0,1]$ and ϵ a small positive parameter. Consider a solution $\left[0, \frac{1}{\epsilon}\right] \ni t \mapsto |\psi^\epsilon(t)\rangle$ of*

$$i \frac{d}{dt} |\psi^\epsilon(t)\rangle = \frac{\boldsymbol{H}(u(\epsilon t))}{\hbar} |\psi^\epsilon(t)\rangle .$$

Take $[0,s] \ni s \mapsto \boldsymbol{P}(s)$ a family of orthogonal projectors such that for each $s \in [0,1]$, $\boldsymbol{H}(u(s))\boldsymbol{P}(s) = E(s)\boldsymbol{P}(s)$ where $E(s)$ is an eigenvalue of $\boldsymbol{H}(u(s))$. Assume that $[0,s] \ni s \mapsto \boldsymbol{H}(u(s))$ is C^2, $[0,s] \ni s \mapsto \boldsymbol{P}(s)$ is C^2 and that, for almost all $s \in [0,1]$, $\boldsymbol{P}(s)$ is the orthogonal projector on the eigenspace associated to the eigenvalue $E(s)$. Then

$$\lim_{\epsilon \mapsto 0^+} \left(\sup_{t \in [0, \frac{1}{\epsilon}]} \Big| \| \boldsymbol{P}(\epsilon t) |\psi^\epsilon(t)\rangle \|^2 - \| \boldsymbol{P}(0) |\psi^\epsilon(0)\rangle \|^2 \Big| \right) = 0.$$

This theorem is a finite dimensional version of Theorem 6.2, page 175, in [20] where, for simplicity sake, we have removed the so-called adiabatic Hamiltonian and adiabatic propagator that intertwines the spectral subspace of the slowly time-dependent Hamiltonian $\boldsymbol{H}(u(\epsilon t))$.

This theorem implies that the solution of $i\frac{d}{dt}|\psi\rangle = \frac{\boldsymbol{H}\left(u(\frac{t}{T})\right)}{\hbar}|\psi\rangle$ follows the spectral decomposition of $\boldsymbol{H}\left(u(\frac{t}{T})\right)$ as soon as T is large enough and when $\boldsymbol{H}\left(u(\frac{t}{T})\right)$ does not admit multiple eigenvalues (non-degenerate spectrum): apply the above theorem with $\boldsymbol{P} = \boldsymbol{P}_k$ where $\boldsymbol{P}_k$ is the orthogonal projection on the k'th eigenstate of $\boldsymbol{H}$ to conclude that the population on state $|k\rangle$ is approximatively constant. If, for instance, $|\psi\rangle$ starts at $t=0$ in the ground state and if $u(0) = u(1)$ then $|\psi\rangle$ returns at $t = T$, up to a global phase (related to the Berry phase [18]), to the same ground state.

Whenever, for some value of s, the spectrum of $\boldsymbol{H}(u(s))$ becomes degenerate the above theorem says that the populations follow the smooth decomposition versus s of $\boldsymbol{H}(u(s))$. For example, assume that the spectrum of $\boldsymbol{H}$ is not degenerate except at $\bar{s}$ where only two eigenvalues become identical: for all s we assume that the n eigenvalues of $\boldsymbol{H}(u(s))$ are labeled according to their order

$$E_1(s) < E_2(s) < \ldots < E_{\bar{k}}(s) \leq E_{\bar{k}+1}(s) < E_{k+2}(s) < \ldots < E_n(s)$$

and $E_{\bar{k}}(s) = E_{\bar{k}+1}(s)$ only when $s = \bar{s}$ for some $\bar{k} \in \{1, \ldots, n\}$. Since $s \mapsto \boldsymbol{H}(u(s))$ is smooth, there always exists a spectral decomposition of $\boldsymbol{H}(u(s))$ that is smooth versus s (this comes from the fact that the spectral decomposition of a Hermitian matrix depends smoothly on its entries). Thus we have only two cases:

1. the non-crossing case where $s \mapsto E_{\bar{k}}(s)$ and $s \mapsto E_{\bar{k}+1}(s)$ are smooth functions

2. the crossing case where

$$s \mapsto \begin{cases} E_{\bar{k}}(s), & \text{for } s \leq \bar{s}; \\ E_{\bar{k}+1}(s), & \text{for } s \geq \bar{s}. \end{cases} \quad \text{and} \quad s \mapsto \begin{cases} E_{\bar{k}+1}(s), & \text{for } s \leq \bar{s}; \\ E_{\bar{k}}(s), & \text{for } s \geq \bar{s}. \end{cases}$$

are smooth functions.

In the non-crossing case the projectors that satisfy the theorem's assumption are the orthogonal projectors $\boldsymbol{P}_k(s)$ on the k'th eigen-direction associated to $E_k(s)$. In the crossing case, the projectors on the eigenspaces associated to $E_{\bar{k}}$ and $E_{\bar{k}+1}$ have to be exchanged when s passes through $\bar{s}$ to guaranty at least the continuity of $\boldsymbol{P}_{\bar{k}}(s)$ and $\boldsymbol{P}_{\bar{k}+1}(s)$: for $s < \bar{s}$, $\boldsymbol{P}_{\bar{k}}$ (resp. $\boldsymbol{P}_{\bar{k}+1}$ is the projector of the eigenspace associated to $E_{\bar{k}}$ (resp. $E_{\bar{k}+1}$); for $s > \bar{s}$, $\boldsymbol{P}_{\bar{k}}$ (resp. $\boldsymbol{P}_{\bar{k}+1}$) is the projector of the eigenspace associated to $E_{\bar{k}+1}$ (resp. $E_{\bar{k}}$); for $s = \bar{s}$, $\boldsymbol{P}_{\bar{k}}$ and $\boldsymbol{P}_{\bar{k}+1}$ are extended by continuity and correspond to orthogonal projectors on two orthogonal eigen-directions that span the eigenspace of dimension two associated to $E_{\bar{k}}(\bar{s}) = E_{\bar{k}+1}(\bar{s})$. This corresponds to so-called conic intersection that can be exploited to construct explicit open-loop control laws (see e.g. [4]).

2.2 Adiabatic motion on the Bloch sphere

Let us take a qubit system. Since we do not care for global phase, we will use the Bloch vector formulation:

$$\frac{d}{dt}\vec{M} = (u\vec{\imath} + v\vec{\jmath} + w\vec{k}) \times \vec{M}$$

where we assume that $\vec{B} = (u\vec{\imath}+v\vec{\jmath}+w\vec{k})$, a vector in $\mathbb{R}^3$, is the control (in magnetic resonance, $\vec{B}$ is the magnetic field). We set $\omega \in \mathbb{R}$ and $\vec{B} = \omega\vec{b}$ where $\vec{b}$ is a unit vector in $\mathbb{R}^3$. Thus we have

$$\frac{d}{dt}\vec{M} = \omega\vec{b} \times \vec{M}, \quad \text{with, as control input, } \omega \in \mathbb{R}, \vec{b} \in \mathbb{S}^2.$$

Assume now that $\vec{B}$ varies slowly: we take $T > 0$ large (i.e., $\omega T \gg 1$), and set $\omega(t) = \varpi\left(\frac{t}{T}\right)$, $\vec{b}(t) = \vec{\beta}\left(\frac{t}{T}\right)$ where ϖ and $\vec{\beta}$ depend regularly on $s = \frac{t}{T} \in [0, 1]$. Assume that, at $t = 0$, $\vec{M}_0 = \vec{\beta}(0)$. If, for any $s \in [0, 1]$, $\varpi(s) > 0$, then the trajectory of $\vec{M}$ with the above control $\vec{B}$ verifies: $\vec{M}(t) \approx \vec{\beta}\left(\frac{t}{T}\right)$, i.e. $\vec{M}$ follows adiabatically the direction of $\vec{B}$. If $\vec{b}(T) = \vec{b}(0)$, i.e., if the control $\vec{B}$ makes a loop between 0 and T ($\beta(0) = \beta(1)$) then $\vec{M}$ follows the same loop (in direction).

To justify this point, it suffices to consider $|\psi\rangle$ that obeys the Schrödinger equation $i\frac{d}{dt}|\psi\rangle = \left(\frac{u}{2}\sigma_x + \frac{v}{2}\sigma_y + \frac{w}{2}\sigma_z\right)|\psi\rangle$ and to apply the adiabatic theorem of the previous subsection. The absence of spectrum degeneracy results from the fact that ϖ never vanishes and remains always strictly positive. The initial condition $\vec{M}_0 = \vec{\beta}(0)$ corresponds to $|\psi\rangle_0$ in the ground state of $\frac{u(0)}{2}\sigma_x + \frac{v(0)}{2}\sigma_y + \frac{w(0)}{2}\sigma_z$. Thus $|\psi\rangle_t$ follows the ground state of $\frac{u(t)}{2}\sigma_x + \frac{v(t)}{2}\sigma_y + \frac{w(t)}{2}\sigma_z$, i.e., $\vec{M}(t)$ follows $\vec{\beta}\left(\frac{t}{T}\right)$.

The assumption concerning the non degeneracy of the spectrum is important. If it is not satisfied, $|\psi(t)\rangle$ can jump smoothly from one branch to another branch when some eigenvalues cross. In order to understand this phenomenon (analogue to monodromy), assume that $\varpi(s)$ vanishes only once at $\bar{s} \in]0, 1[$ with $\varpi(s) > 0$ (resp. < 0) for $s \in [0, \bar{s}[$ (resp. $s \in]\bar{s}, 1]$). Then, around $t = \bar{s}T$, $|\psi\rangle_t$ changes smoothly from the ground state to the excited state of $\boldsymbol{H}(t)$, since their energies coincide for $t = \bar{s}T$. With such a choice for ϖ, $\vec{B}$ performs a loop if, additionally

$\vec{b}(0) = -\vec{b}(1)$ and $\varpi(0) = -\varpi(1)$, whereas $|\psi\rangle_t$ does not. It starts from the ground state at $t = 0$ and ends on the excited state at $t = T$. In fact, $\vec{M}(t)$ follows adiabatically the direction of $\vec{B}(t)$ for $t \in [0, \bar{s}T]$ and then the direction of $-\vec{B}(t)$ for $t \in [\bar{s}T, T]$. Such quasi-static motion planing method is particularly robust and widely used in practice. We refer to [21, 1, 17] for related control theoretical results. In the following subsections we detail some important examples.

2.3 Stimulated Raman Adiabatic Passage (STIRAP)

Consider the Λ-system of Figure 1. The controlled Hamiltonian reads

$$\frac{\boldsymbol{H}(t)}{\hbar} = \omega_g |g\rangle\langle g| + \omega_e |e\rangle\langle e| + \omega_f |f\rangle\langle f| + u(t)\left(\mu_{gf}(|g\rangle\langle f| + |f\rangle\langle g|) + \mu_{ef}(|e\rangle\langle f| + |f\rangle\langle e|)\right).$$

Assume $\omega_{gf} = \omega_f - \omega_g > \omega_{ef} = \omega_f - \omega_e > 0$. We take a quasi-periodic and small control involving perfect resonances with transitions $g \leftrightarrow f$ and $e \leftrightarrow f$:

$$u = u_{gf}\cos(\omega_{gf}t) + u_{ef}\cos(\omega_{ef}t)$$

with slowly varying small real amplitudes u_{gf} and u_{ef}. Put the system in the interaction frame via the unitary transformation $e^{-it(\omega_g|g\rangle\langle g| + \omega_e|e\rangle\langle e| + \omega_f|f\rangle\langle f|)}$. We apply the rotating wave approximation (order 1 in (15)) to get the average Hamiltonian

$$\boldsymbol{H}^{1^{\text{st}}}_{\text{rwa}}/\hbar = \tfrac{\Omega_{gf}}{2}(|g\rangle\langle f| + |f\rangle\langle g|) + \tfrac{\Omega_{ef}}{2}(|e\rangle\langle f| + |f\rangle\langle e|)$$

with slowly varying Rabi pulsations $\Omega_{gf} = \mu_{gf}u_{gf}$ and $\Omega_{ef} = \mu_{ef}u_{ef}$.

Let us now analyze the dependence of the spectral decomposition of $\boldsymbol{H}^{1^{\text{st}}}_{\text{rwa}}$ on the two parameters Ω_{gf} and Ω_{ef}. When $\Omega_{gf}^2 + \Omega_{ef}^2 \neq 0$, spectrum of $\boldsymbol{H}^{1^{\text{st}}}_{\text{rwa}}/\hbar$ admits three distinct eigenvalues:

$$\Omega_- = -\tfrac{\sqrt{\Omega_{gf}^2 + \Omega_{ef}^2}}{2}, \quad \Omega_0 = 0, \quad \Omega_+ = \tfrac{\sqrt{\Omega_{gf}^2 + \Omega_{ef}^2}}{2}$$

associated to the following eigenvectors :

$$\begin{aligned}
|-\rangle &= \tfrac{\Omega_{gf}}{\sqrt{2(\Omega_{gf}^2 + \Omega_{ef}^2)}}|g\rangle + \tfrac{\Omega_{ef}}{\sqrt{2(\Omega_{gf}^2 + \Omega_{ef}^2)}}|e\rangle - \tfrac{1}{\sqrt{2}}|f\rangle \\
|0\rangle &= \tfrac{-\Omega_{ef}}{\sqrt{\Omega_{gf}^2 + \Omega_{ef}^2}}|g\rangle + \tfrac{\Omega_{gf}}{\sqrt{\Omega_{gf}^2 + \Omega_{ef}^2}}|e\rangle \\
|+\rangle &= \tfrac{\Omega_{gf}}{\sqrt{2(\Omega_{gf}^2 + \Omega_{ef}^2)}}|g\rangle + \tfrac{\Omega_{ef}}{\sqrt{2(\Omega_{gf}^2 + \Omega_{ef}^2)}}|e\rangle + \tfrac{1}{\sqrt{2}}|f\rangle.
\end{aligned}$$

Assume now that the Rabi frequencies depend on $s \in [0, \frac{3\pi}{2}]$ according to the following formula

$$\Omega_{gf}(s) = \begin{cases} \bar{\Omega}_g \cos^2 s, & \text{for } s \in [\frac{\pi}{2}, \frac{3\pi}{2}]; \\ 0, & \text{elsewhere.} \end{cases}, \qquad \Omega_{ef}(s) = \begin{cases} \bar{\Omega}_e \sin^2 s, & \text{for } s \in [0, \pi]; \\ 0, & \text{elsewhere.} \end{cases}$$

with $\bar{\Omega}_g > 0$ and $\bar{\Omega}_e > 0$ constant parameter. With such s dependence, we have three analytic branches of the spectral decomposition:

- for $s \in]0, \frac{\pi}{2}[$ we have

$$\begin{aligned} \Omega_-(s) = -\bar{\Omega}_e \sin s \text{ with } \left|-\right\rangle_s = \tfrac{|e\rangle - |f\rangle}{\sqrt{2}}. \\ \Omega_0 = 0 \text{ with } \left|0\right\rangle_s = -\left|g\right\rangle \\ \Omega_+(s) = \bar{\Omega}_e \sin s \text{ with } \left|+\right\rangle_s = \tfrac{|e\rangle + |f\rangle}{\sqrt{2}}. \end{aligned}$$

- for $s \in]\frac{\pi}{2}, \pi[$ we have

$$\begin{aligned} \Omega_-(s) = -\sqrt{\bar{\Omega}_g^2 \cos^4 s + \bar{\Omega}_e^2 \sin^4 s} \text{ with } \left|-\right\rangle_s = \tfrac{\bar{\Omega}_g \cos^2 s |g\rangle + \bar{\Omega}_e \sin^2 s |e\rangle}{\sqrt{2(\bar{\Omega}_g^2 \cos^4 s + \bar{\Omega}_e^2 \sin^4 s)}} - \tfrac{1}{\sqrt{2}} \left|f\right\rangle \\ \Omega_0 = 0 \text{ with } \left|0\right\rangle_s = \tfrac{-\bar{\Omega}_e \sin^2 s |g\rangle + \bar{\Omega}_g \cos^2 s |e\rangle}{\sqrt{\bar{\Omega}_g^2 \cos^4 s + \bar{\Omega}_e^2 \sin^4 s}} \\ \Omega_+(s) = \sqrt{\bar{\Omega}_g^2 \cos^4 s + \bar{\Omega}_e^2 \sin^4 s} \text{ with } \left|+\right\rangle_s = \tfrac{\bar{\Omega}_g \cos^2 s |g\rangle + \bar{\Omega}_e \sin^2 s |e\rangle}{\sqrt{2(\bar{\Omega}_g^2 \cos^4 s + \bar{\Omega}_e^2 \sin^4 s)}} + \tfrac{1}{\sqrt{2}} \left|f\right\rangle. \end{aligned}$$

- for $s \in]\pi, \frac{3\pi}{2}[$ we have

$$\begin{aligned} \Omega_-(s) = -\bar{\Omega}_g |\cos s| \text{ with } \left|-\right\rangle_s = \tfrac{|g\rangle - |f\rangle}{\sqrt{2}}. \\ \Omega_0 = 0 \text{ with } \left|0\right\rangle_s = \left|e\right\rangle \\ \Omega_+(s) = \bar{\Omega}_g |\cos s| \text{ with } \left|+\right\rangle_s = \tfrac{|g\rangle + |f\rangle}{\sqrt{2}}. \end{aligned}$$

Let us consider the eigenvalue Ω_0: it is associated to the projector $\boldsymbol{P}_0(s)$ on $\left|0\right\rangle_s$ that depends smoothly on $s \in [0, \frac{3\pi}{2}]$ as shown by the concatenation of the above formula on the three intervals $]0, \frac{\pi}{2}[$, $]\frac{\pi}{2}, \pi[$ and $]\pi, \frac{3\pi}{2}[$. Thus assume that $\left|\psi\right\rangle_0 = \left|g\right\rangle$ then adiabatic Theorem 1 shows that, for $\epsilon > 0$ small enough, the solution of $i\frac{d}{dt}\left|\psi\right\rangle = \frac{\boldsymbol{H}_{\text{rwa}}^{1^{\text{st}}}}{\hbar}\left|\psi\right\rangle$ with the time-varying control amplitudes

$$[0, \tfrac{3\pi}{2\epsilon}] \ni t \mapsto (u_{fg}, u_{ef}) = \left(\tfrac{\Omega_{gf}(\epsilon t)}{\mu_{gf}}, \tfrac{\Omega_{ef}(\epsilon t)}{\mu_{ef}}\right)$$

is approximatively given by

$$\left|\psi\right\rangle_t \approx e^{i\theta_t}\left|0\right\rangle_{\epsilon t} = e^{i\theta_t} \begin{cases} -\left|g\right\rangle, & \text{for } t \in [0, \frac{\pi}{2\epsilon}]; \\ \frac{-\bar{\Omega}_e \sin^2(\epsilon t)|g\rangle + \bar{\Omega}_g \cos^2(\epsilon t)|e\rangle}{\sqrt{\bar{\Omega}_g^2 \cos^4(\epsilon t) + \bar{\Omega}_e^2 \sin^4(\epsilon t)}}, & \text{for } t \in [\frac{\pi}{2\epsilon}, \frac{\pi}{\epsilon}]; \\ \left|e\right\rangle, & \text{for } t \in [\frac{\pi}{\epsilon}, \frac{3\pi}{2\epsilon}]; \end{cases}$$

where θ_t is a time-varying global phase. Thus at the final time $t = \frac{3\pi}{2\epsilon}$, $\left|\psi\right\rangle$ coincides, up to a global phase to $\left|e\right\rangle$. It is surprising that during this adiabatic passage from $\left|g\right\rangle$ to $\left|e\right\rangle$ the control u_{ef} driving the transition $e \leftrightarrow f$ is turned on first whereas the control u_{gf} driving transition $g \leftrightarrow f$ is turned on later. It is also very interesting that the precise knowledge of the coupling parameter μ_{gf} and μ_{ef} is not necessary (robustness with respect to uncertainty in these parameters). However the precise knowledge of the transition frequencies ω_{gf} and ω_{ef} is required. Such adiabatic control strategies are widely used (see, e.g., the recent review article [14]).

Exercice 5. *Design an adiabatic passage $s \mapsto (\Omega_{gf}(s), \Omega_{ef}(s))$ from $\left|g\right\rangle$ to $\frac{-|g\rangle + |e\rangle}{\sqrt{2}}$, up to a global phase.*

2.4 Chirped pulse for a 2-level system

Let us start with $\frac{\boldsymbol{H}}{\hbar} = \frac{\omega_{\text{eg}}}{2}\boldsymbol{\sigma_z} + \frac{u}{2}\boldsymbol{\sigma_x}$ considered in Subsection 1.4 and take the quasi-resonant control ($|\omega_r - \omega_{\text{eg}}| \ll \omega_{\text{eg}}$)

$$u(t) = v\left(e^{i(\omega_r t+\theta)} + e^{-i(\omega_r t+\theta)}\right)$$

where $v, \theta \in \mathbb{R}$, $|v|$ and $|\frac{d\theta}{dt}|$ are small and slowly varying

$$|v|, \left|\frac{d\theta}{dt}\right| \ll \omega_{\text{eg}}, \quad \left|\frac{dv}{dt}\right| \ll \omega_{\text{eg}}|v|, \quad \left|\frac{d^2\theta}{dt^2}\right| \ll \omega_{\text{eg}}\left|\frac{d\theta}{dt}\right|.$$

Following similar computations to those of Subsection 1.4, consider the following change of frame $|\psi\rangle = e^{-i\frac{\omega_r t+\theta}{2}\boldsymbol{\sigma_z}}|\phi\rangle$. Then $i\frac{d}{dt}|\psi\rangle = \frac{\boldsymbol{H}}{\hbar}|\psi\rangle$ becomes

$$i\frac{d}{dt}|\phi\rangle = \left(\frac{\omega_{\text{eg}}-\omega_r-\frac{d}{dt}\theta}{2}\boldsymbol{\sigma_z} + \frac{ve^{2i(\omega_r t+\theta)}+v}{2}\boldsymbol{\sigma_+} + \frac{ve^{-2i(\omega_r t-\theta)}+v}{2}\boldsymbol{\sigma_-}\right)|\phi\rangle.$$

With $\Delta_r = \omega_{\text{eg}} - \omega_r$ and $w = -\frac{d}{dt}\theta$ and using the first order rotating wave approximation (see (15) with $\boldsymbol{H}^{1^{\text{st}}}_{\text{rwa}}$) we get the following averaged control Hamiltonian

$$\frac{\boldsymbol{H}_{\text{chirp}}}{\hbar} = \frac{\Delta_r+w}{2}\boldsymbol{\sigma_z} + \frac{v}{2}\boldsymbol{\sigma_x}$$

where (v, w) are two real control inputs. Take three constant parameters $a > |\Delta_r|$, $b > 0$, $0 < \epsilon \ll a, b$. Set

$$w = a\cos(\epsilon t), \quad v = b\sin^2(\epsilon t).$$

Set $s = \epsilon t$ varying in $[0, \pi]$. These explicit expressions are not essential. Only the shape of $s \mapsto w(s)$ and of $s \mapsto v(s)$ are important here: w decreases regularly from a to $-a$; v is a bump function that remains strictly positive for $s \in]0, \pi[$ and that vanishes with its derivatives at $s = 0$ and $s = \pi$.

The spectral decomposition of $\boldsymbol{H}_{\text{chirp}}/\hbar$ for $s \in]0, \pi[$ is standard with two distinct and opposite eigenvalues.

$$\Omega_- = -\frac{\sqrt{(\Delta_r+w)^2+v^2}}{2} \text{ associated to eigenstate } |-\rangle = \frac{\cos\alpha\,|g\rangle - (1-\sin\alpha)\,|e\rangle}{\sqrt{2(1-\sin\alpha)}}$$

$$\Omega_+ = \frac{\sqrt{(\Delta_r+w)^2+v^2}}{2} \text{ associated to eigenstate } |+\rangle = \frac{(1-\sin\alpha)\,|g\rangle + \cos\alpha\,|e\rangle}{\sqrt{2(1-\sin\alpha)}}$$

where $\alpha \in]\frac{-\pi}{2}, \frac{\pi}{2}[$ is defined by $\tan\alpha = \frac{\Delta_r+w}{v}$. Since $\lim_{s\mapsto 0^+}\alpha = \frac{\pi}{2}$ and $\lim_{s\mapsto\pi^-}\alpha = -\frac{\pi}{2}$

$$\lim_{s\mapsto 0^+}|-\rangle_s = |g\rangle, \quad \lim_{s\mapsto 0^+}|+\rangle_s = |e\rangle, \quad \lim_{s\mapsto\pi^-}|-\rangle_s = -|e\rangle, \quad \lim_{s\mapsto\pi^-}|+\rangle_s = |g\rangle.$$

Consequently the adiabatic approximation of Theorem 1 implies that the solution $|\phi\rangle$ of

$$i\frac{d}{dt}|\phi\rangle = \left(\frac{\Delta_r+a\cos(\epsilon t)}{2}\boldsymbol{\sigma_z} + \frac{b\sin^2(\epsilon t)}{2}\boldsymbol{\sigma_x}\right)|\phi\rangle, \quad |\phi\rangle_{t=0} = |g\rangle$$

is given approximatively, for ϵ small and $t \in [0, \frac{\pi}{\epsilon}]$, by

$$|\phi\rangle_t = e^{i\vartheta_t}|-\rangle_{s=\epsilon t}$$

with ϑ_t a time-varying global phase. Thus for $t = \frac{\pi}{\epsilon}$, $|\phi\rangle$ coincides with $|e\rangle$ up to a global phase. Notice the remarkable robustness of such adiabatic control strategy. We do not need to know precisely neither the detuning Δ_r nor the chirp and control amplitudes a and b. This means in particular that such adiabatic chirp control from g to e is insensitive to all parameters appearing in a 2-level system.

This adiabatic chirp passage can be extended to any ladder configuration that is slightly an-harmonic.

2.5 Principle of adiabatic quantum computation

An alternative approach towards quantum computing is based on the adiabatic control detailed in this section. This is for instance the case of annealing machines developed by one of the D-Wave Systems Inc. a Canadian company. The main idea in this approach is that many combinatorial optimization problems can be encoded as the problem of finding the ground state of a multi-qubit Hamiltonian. Let us assume that we are interested in a classically hard combinatorial optimization problem that is encoded as the problem of finding the ground state of the Hamiltonian $\boldsymbol{H}_f$. Starting from a different Hamiltonian $\boldsymbol{H}_0$ for which the ground state is well-known, we try to find an implementable time-dependent $\boldsymbol{H}(t)$, such that $\boldsymbol{H}(0) = 0$ and $\boldsymbol{H}(T) = \boldsymbol{H}_f$. Initializing the system in the well-known ground state of $\boldsymbol{H}_0$, and assuming a slow variation of the Hamiltonian, and non-degeneracy of the ground state during the evolution, the state of the system at time T should be close to the ground state of $\boldsymbol{H}_f$. Below, we present a typical example.

Consider the following classical omptimization problem: for a large $n > 0$ and a collection $(\lambda_{i,j})_{1\leq i,j\leq n}$ of real numbers, find the argument $\bar{x}$ of the minimization problem

$$\min_{x\in\{-1,+1\}^n} \Lambda(x), \qquad \Lambda(x) := \sum_{i,j} \lambda_{i,j} x_i x_j.$$

In order to solve this hard classical optimization problem, we consider an n-qubit system (with the wave-function $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n} \equiv \mathbb{C}^{2^n}$). We consider the Hamiltonian

$$\boldsymbol{H}_u = \sum_{i,j} \lambda_{i,j} \boldsymbol{\sigma_z}^{(i)} \boldsymbol{\sigma_z}^{(j)} + u \sum_i \boldsymbol{\sigma_x}^{(i)}.$$

Now, considering a smooth decreasing function f on $[0,1]$ with $f(0) \gg \max_{1\leq i,j\leq n} |\lambda_{i,j}|$ and $f(1) = 0$, we assume that the smallest eigenvalue of $\boldsymbol{H}_u$ is not degenerate for any $u \in [0, f(0)]$. The ground state of $\boldsymbol{H}_{f(0)}$ is close to the ground state of $u \sum_i \boldsymbol{\sigma_x}^{(i)}$, which is given by the well-known separable state

$$|\psi_0\rangle = \left(\frac{|g\rangle - |e\rangle}{\sqrt{2}}\right)^{\otimes n}.$$

Also, note that the ground state of $\boldsymbol{H}_0$ is given by the separable state $|q_1\rangle \otimes |q_2\rangle \otimes \cdots \otimes |q_n\rangle$ where $|q_i\rangle = |g\rangle$ (resp. $|e\rangle$) when $\bar{x}_i = -1$ (resp. $\bar{x}_i = +1$). Therefore, considering the slowly varying Hamiltonian $\boldsymbol{H}(t) = \boldsymbol{H}_{f(\epsilon t)}$, and initializing all the n qubits in the state $(|g\rangle - |e\rangle)/\sqrt{2}$, the solution of the Schrödinger equation at time $t = 1/\epsilon$ is close to the state $|q_1\rangle \otimes |q_2\rangle \otimes \cdots \otimes |q_n\rangle$ (solution of the optimization problem). By measuring the Pauli $\boldsymbol{\sigma_z}$ operator on each qubit, we can therefore identify this solution $\bar{x}$.

3 Optimal control

In this section, we introduce a widely used optimization technique for finding a control field $u(t) = (u_1(t), \cdots, u_m(t))$ that steers the state $|\psi_u(t)\rangle$ of the system

$$i\frac{d}{dt}|\psi_u\rangle = (\boldsymbol{H}_0 + \sum_{k=1}^{m} u_k(t)\boldsymbol{H}_k)|\psi_u\rangle, \qquad |\psi_u(0)\rangle = |\psi_i\rangle \tag{30}$$

from its initial state $|\psi_i\rangle$ to a desired target state $|\psi_f\rangle$. As we will see, the same technique can also be used to generate arbitrary unitary operations $\boldsymbol{U}_f$.

3.1 Gradient ascent pulse engineering for state transfer

This approach, also known under the acronym GRAPE [13], has for goal to maximize the functional

$$u \mapsto F(u) := |\langle \psi_f \mid \psi_u(T)\rangle|^2,$$

where ψ_u satisfies the equation (30). The space of control functions u over which we want to solve the above optimization problem could for instance be $L^\infty([0,T];\mathbb{R}^m)$. However the GRAPE algorithm assumes a descretization of the time domain to N identical time intervals of duration $\Delta t = T/N$. We therefore look into maximizing the above functional over the space of piecewise constant functions

$$u(t) = (u_1(t), \cdots, u_m(t)) = (u_1^j, \cdots, u_m^j), \qquad \text{for } t \in [(j-1)\Delta t, j\Delta t[,\ j = 1, 2, \cdots, N.$$

Therefore the functional $F(u)$ can be written as follows

$$F(u) = |\langle\psi_f|\boldsymbol{U}_N\boldsymbol{U}_{N-1}\cdots\boldsymbol{U}_1|\psi_i\rangle|^2, \qquad \boldsymbol{U}_j = \exp\left(-i\Delta t(\boldsymbol{H}_0 + \sum_{k=1}^{m} u_k^j\boldsymbol{H}_k)\right).$$

The optimization is simply done by a gradient ascent method, where at each iteration, we calculate the gradient of the functional with respect to u_k^j, k'th control amplitude over the j'th time step and we update the associated control value by going in the direction of this gradient. More precisely, we update the control value u_k^j as follows

$$u_k^j \longrightarrow u_k^j + \epsilon\frac{\partial F}{\partial u_k^j}, \tag{31}$$

where ϵ is a small step size. We further note that this gradient is analytically given by the following simple computation. First, we note that the functional F can be written as follows

$$F(u) = |\langle\psi_f|\boldsymbol{U}_N\boldsymbol{U}_{N-1}\cdots\boldsymbol{U}_1|\psi_i\rangle|^2 = |\langle\psi_{j,f} \mid \psi_{j,i}\rangle|^2,$$

where

$$|\psi_{j,i}\rangle = \boldsymbol{U}_j\boldsymbol{U}_{j-1}\cdots\boldsymbol{U}_1|\psi\rangle \quad \text{and} \quad |\psi_{j,f}\rangle = \boldsymbol{U}_{j+1}^\dagger\boldsymbol{U}_{j+2}^\dagger\cdots\boldsymbol{U}_N^\dagger|\psi_f\rangle.$$

Furthermore, noting that none of $\boldsymbol{U}_r$'s, except for $\boldsymbol{U}_j$, does depend on u_k^j, we can calculate

$$\frac{\partial\boldsymbol{U}_j}{\partial u_k^j} = -i\Delta t\widetilde{\boldsymbol{H}}_k\boldsymbol{U}_j, \qquad \widetilde{\boldsymbol{H}}_k = \frac{1}{\Delta t}\int_0^{\Delta t} e^{-i\tau(\boldsymbol{H}_0+\sum_{r=1}^m u_r^j\boldsymbol{H}_r)}\boldsymbol{H}_k e^{i\tau(\boldsymbol{H}_0+\sum_{r=1}^m u_r^j\boldsymbol{H}_r)}d\tau. \tag{32}$$

To prove the above equation, we have used the identity

$$\frac{d}{dx}e^{\boldsymbol{A}+x\boldsymbol{B}}\Big|_{x=0} = \left(\int_0^1 e^{\boldsymbol{A}\tau}\boldsymbol{B}e^{-\boldsymbol{A}\tau}d\tau\right)e^{\boldsymbol{A}}.$$

Exercice 6. *Prove the above identity, by showing the more general identity for an x-dependent matrix $\boldsymbol{A}(x)$,*

$$\frac{d}{dx}e^{\boldsymbol{A}(x)} = \int_0^1 dy e^{(1-y)\boldsymbol{A}(x)}\frac{d\boldsymbol{A}}{dx}e^{y\boldsymbol{A}(x)}.$$

Hint: proceed by expanding the exponentials.

In the equation (32), for small Δt ($\Delta t \ll \|\boldsymbol{H}_0 + \sum_k u_k^j \boldsymbol{H}_k\|^{-1}$), we can take the approximation $\widetilde{\boldsymbol{H}}_k \approx \boldsymbol{H}_k$. Thus

$$\frac{\partial F}{\partial u_k^j} \approx -i\Delta t \left(\langle \psi_{j,f} | \boldsymbol{H}_k | \psi_{j,i} \rangle \langle \psi_{j,i} \mid \psi_{j,f} \rangle - \langle \psi_{j,i} | \boldsymbol{H}_k | \psi_{j,f} \rangle \langle \psi_{j,f} \mid \psi_{j,i} \rangle \right). \tag{33}$$

We can therefore summarize the basic GRAPE algorithm as follows:

1. Start with an initial control guess u_k^j, for $k = 1, \cdots, m$ and $j = 1, \cdots, N$.
2. Starting from $|\psi_i\rangle$, calculate for all $j = 1, \cdots, N$, $|\psi_{j,i}\rangle = \boldsymbol{U}_j \cdots \boldsymbol{U}_1 |\psi_i\rangle$.
3. Starting from $|\psi_f\rangle$, calculate for all $j = 1, \cdots N$, $|\psi_{j,f}\rangle = \boldsymbol{U}_{j+1}^\dagger \cdots \boldsymbol{U}_N^\dagger |\psi_f\rangle$.
4. Evaluate $\partial F/\partial u_k^j$ according to (33) and update the $m \times N$ control amplitudes u_k^j according to (31).
5. Go to step 2.

The algorithm terminates if the change in the functional F from an iteration to the next one is smaller than a threshold. Here are a few remarks on the algorithm.

Remark 1. *In case we want to ensure limited control amplitudes (L^2-norm for instance), we can add a penalty F_{pen} to the above functional, with*

$$F_{pen} = -\alpha\Delta t \sum_{j=1}^{N}\sum_{k=1}^{m} |u_k^j|^2.$$

This leads to the update rule

$$u_k^j \longrightarrow u_k^j + \epsilon\frac{\partial F}{\partial u_k^j} - 2\alpha\epsilon\Delta t u_k^j.$$

Remark 2. *The gradient ascent algorithms ensure a monotonic convergence towards a local maximum of the functional. Therefore, the initial control guess is rather important to avoid getting trapped in such local maxima instead of converging towards the global one.*

Remark 3. *The step size ϵ needs to be small to ensure the convergence, but at the same time choosing a too small step size leads to a slow convergence. One other possibility is to vary the step size ϵ at each iteration by choosing an optimal value. This would lead to more computations at each iteration but perhaps a faster convergence.*

3.2 Gradient ascent pulse engineering for unitary generation

The same tool can be used to address the synthesis of unitary transformations, for instance multi-qubit gates. The equation of motion for the propagator of the quantum system is given by

$$\frac{d}{dt}\boldsymbol{U} = -i(\boldsymbol{H}_0 + \sum_{k=1}^{m} u_k(t)\boldsymbol{H}_k)\boldsymbol{U}, \qquad \boldsymbol{U}(0) = \boldsymbol{I}.$$

We consider the problem of generating a desired unitary $\boldsymbol{U}_f$, by maximizing the functional

$$F(u) = |\operatorname{Tr}\left(\boldsymbol{U}_f^* \boldsymbol{U}(T)\right)|^2.$$

Note that as soon as $\boldsymbol{U}(T) = e^{i\theta}\boldsymbol{U}_f$, we have $F(u) = 1$.

Exercice 7. *Prove that for any two unitary operators* $\boldsymbol{U}$ *and* $\boldsymbol{V}$

$$|\operatorname{Tr}(\boldsymbol{U}^*\boldsymbol{V})| \leq 1.$$

Once again descretizing the time to N steps of length Δt, we have

$$\boldsymbol{U}(T) = \boldsymbol{U}_N \boldsymbol{U}_{N-1} \cdots \boldsymbol{U}_1, \qquad \boldsymbol{U}_j = exp\left(-i\Delta t(\boldsymbol{H}_0 + \sum_{k=1}^{m} u_k^j \boldsymbol{H}_k)\right).$$

We define for $j = 1, \cdots, N$,

$$\boldsymbol{V}_j := \boldsymbol{U}_j \boldsymbol{U}_{j-1} \cdots \boldsymbol{U}_1, \qquad \boldsymbol{W}_j := \boldsymbol{U}_{j+1}^\dagger \boldsymbol{U}_{j+2}^\dagger \cdots \boldsymbol{U}_N^\dagger \boldsymbol{U}_F.$$

Therefore, we have

$$F(u) = |\operatorname{Tr}\left(\boldsymbol{U}_f^* \boldsymbol{U}(T)\right)|^2 = |\operatorname{Tr}\left(\boldsymbol{W}_j^\dagger \boldsymbol{V}_j\right)|^2.$$

Simple calculations, similar to the previous subsection, lead to

$$\frac{\partial \boldsymbol{U}}{\partial u_k^j} = 2\Delta t \operatorname{Im}\left(\operatorname{Tr}\left(\boldsymbol{W}_j^\dagger \boldsymbol{H}_k \boldsymbol{V}_j\right)\operatorname{Tr}\left(\boldsymbol{V}_j^\dagger \boldsymbol{W}\right)\right).$$

With this formulation of the gradient, the implementation of the GRAPE algorithm is precisely the same as in the previous subsection.

3.3 Other optimal control strategies

Take the n-level system $i\frac{d}{dt}|\psi\rangle = \frac{1}{\hbar}(\boldsymbol{H}_0 + \sum_{k=1}^m u_k \boldsymbol{H}_k)|\psi\rangle$, initial and final states $|\psi_a\rangle$ and $|\psi_b\rangle$ and a transition time $T > 0$ ($\langle\psi_a|\psi_a\rangle = \langle\psi_b|\psi_b\rangle = 1$). We are looking for optimal controls $[0,T] \ni t \mapsto u(t)$ minimizing $\int_0^T(\sum_{k=1}^m u_k^2)$ and steering $|\psi\rangle$ from $|\psi_a\rangle$ at $t = 0$ to $|\psi_b\rangle$ at $t = T$ (assuming the system to be controllable, we consider only the cases where such a control exists). Thus we are considering the following problem

$$\min_{\substack{u_k \in L^2([0,T],\mathbb{R}),\ k=1,\ldots,m \\ i\frac{d}{dt}|\psi\rangle = \frac{1}{\hbar}(\boldsymbol{H}_0 + \sum_{k=1}^m u_k \boldsymbol{H}_k)|\psi\rangle,\ t\in(0,T) \\ |\psi(0)\rangle = |\psi_a\rangle,\ |\langle\psi_b|\psi\rangle|_{t=T}^2 = 1}} \frac{1}{2}\int_0^T \left(\sum_{k=1}^m u_k^2(t)\right) dt \tag{34}$$

for given T, $|\psi_a\rangle$ and $|\psi_b\rangle$ ($\langle\psi_a|\psi_a\rangle = \langle\psi_b|\psi_b\rangle = 1$). Notice that $|\langle\psi_b|\psi\rangle|^2 = 1$ means that $|\psi(T)\rangle = e^{i\theta}|\psi_b\rangle$ where $\theta \in \mathbb{R}$ is an arbitrary global phase.

Since the initial and final constraints are difficult to satisfy simultaneously from a numerical point of view, we will consider also the second problem where the final constraint is relaxed

$$\min_{\substack{u_k \in L^2([0,T],\mathbb{R}),\ k=1,\dots,m \\ i\frac{d}{dt}|\psi\rangle = \frac{1}{\hbar}(\boldsymbol{H}_0 + \sum_{k=1}^m u_k \boldsymbol{H}_k)|\psi\rangle,\ t\in(0,T) \\ |\psi(0)\rangle = |\psi_a\rangle}} \frac{1}{2}\int_0^T \left(\sum_{k=1}^m u_k^2(t)\right) dt + \frac{\alpha}{2}(1 - |\langle\psi_b|\psi(T)\rangle|^2) \tag{35}$$

with the positive penalization coefficient $\alpha > 0$. Notice that for α large this problem tends to the original one (34).

3.3.1 First order stationary condition

Pontryaguin's Maximum Principle (PMP) introduced in Appendix B provides necessary optimality conditions. In our case, these necessary conditions are given as follows. Notice that the adjoint state can be seen as a Ket, denoted by $|p\rangle \in \mathbb{C}^n$ (of constant norm but not necessarily 1 in general) since it satisfies the same Schrödinger equation as $|\psi\rangle$.

For problem (34), the first order stationary conditions read:

$$\begin{cases} i\frac{d}{dt}|\psi\rangle = \frac{1}{\hbar}(\boldsymbol{H}_0 + \sum_{k=1}^m u_k \boldsymbol{H}_k)|\psi\rangle,\ t\in(0,T) \\ i\frac{d}{dt}|p\rangle = \frac{1}{\hbar}(\boldsymbol{H}_0 + \sum_{k=1}^m u_k \boldsymbol{H}_k)|p\rangle,\ t\in(0,T) \\ u_k = -\frac{1}{\hbar}\Im\Big(\langle p|\boldsymbol{H}_k|\psi\rangle\Big), k=1,\dots,m,\quad t\in(0,T) \\ |\psi(0)\rangle = |\psi_a\rangle,\ |\langle\psi_b|\psi(T)\rangle|^2 = 1 \end{cases} \tag{36}$$

For the relaxed problem (35), the first order stationary conditions read:

$$\begin{cases} i\frac{d}{dt}|\psi\rangle = \frac{1}{\hbar}(\boldsymbol{H}_0 + \sum_{k=1}^m u_k \boldsymbol{H}_k)|\psi\rangle,\ t\in(0,T) \\ i\frac{d}{dt}|p\rangle = \frac{1}{\hbar}(\boldsymbol{H}_0 + \sum_{k=1}^m u_k \boldsymbol{H}_k)|p\rangle,\ t\in(0,T) \\ u_k = -\frac{1}{\hbar}\Im\Big(\langle p|\boldsymbol{H}_k|\psi\rangle\Big), k=1,\dots,m,\quad t\in(0,T) \\ |\psi(0)\rangle = |\psi_a\rangle,\ |p(T)\rangle = -\alpha\langle\psi_b|\psi(T)\rangle\ |\psi_b\rangle. \end{cases} \tag{37}$$

These optimality conditions differ only by the boundary conditions at $t = 0$ and $t = T$: the common part

$$\begin{aligned} i\frac{d}{dt}|\psi\rangle &= \frac{1}{\hbar}(\boldsymbol{H}_0 + \textstyle\sum_{k=1}^m u_k \boldsymbol{H}_k)|\psi\rangle,\ t\in(0,T) \\ i\frac{d}{dt}|p\rangle &= \frac{1}{\hbar}(\boldsymbol{H}_0 + \textstyle\sum_{k=1}^m u_k \boldsymbol{H}_k)|p\rangle,\ t\in(0,T) \\ u_k &= -\frac{1}{\hbar}\Im\left(\langle p|\boldsymbol{H}_k|\psi\rangle\right), k=1,\dots,m,\quad t\in(0,T) \end{aligned}$$

is a Hamiltonian system with $|\psi\rangle$ and $|p\rangle$ being the conjugate variables. The underlying Hamiltonian function is given by : $\overline{\mathbb{H}}(|\psi\rangle, |p\rangle) = \min_{u\in\mathbb{R}^m} \mathbb{H}(|\psi\rangle, |p\rangle, u)$ where

$$\mathbb{H}(|\psi\rangle, |p\rangle, u) = \frac{1}{2}\left(\sum_{k=1}^m u_k^2\right) + \frac{1}{\hbar}\Im\left(\left\langle p\left|\boldsymbol{H}_0 + \sum_{k=1}^m u_k \boldsymbol{H}_k\right|\psi\right\rangle\right). \tag{38}$$

Thus for any solutions $(|\psi\rangle, |p\rangle, u)$ of (36) or (37), $\mathbb{H}(|\psi\rangle, |p\rangle, u)$ is independent of t. Notice that

$$\overline{\mathbb{H}}(|\psi\rangle, |p\rangle) = \Im\left(\left\langle p \left| \frac{\boldsymbol{H}_0}{\hbar} \right| \psi \right\rangle\right) - \tfrac{1}{2}\left(\sum_{k=1}^m \Im\Big(\left\langle p|\frac{\boldsymbol{H}_k}{\hbar}|\psi\right\rangle\Big)^2\right).$$

3.3.2 Monotonic numerical scheme

For the relaxed problem (35), there exists a general monotonic iterative scheme to find the solution. Defining the cost function

$$J(u) = \tfrac{1}{2}\int_0^T \left(\sum_{k=1}^m u_k^2(t)\right) dt + \tfrac{\alpha}{2}(1 - |\langle\psi_b|\psi_u(T)\rangle|^2)$$

where $|\psi_u\rangle$ denotes the solution of $i\frac{d}{dt}|\psi\rangle = \frac{1}{\hbar}(\boldsymbol{H}_0 + \sum_{k=1}^m u_k \boldsymbol{H}_k)|\psi\rangle$ starting from $|\psi_a\rangle$, and starting from an initial guess $u^0 \in L^2([0,T], \mathbb{R}^m)$, this scheme generates a sequence of controls $u^\nu \in L^2([0,T], \mathbb{R}^m)$, $\nu = 1, 2, \ldots$, such that the cost $J(u^\nu)$ is decreasing, $J(u^{\nu+1}) \le J(u^\nu)$.

This scheme does not guaranty in general the convergence to an optimal solution. But applied on several examples, with a correct tuning of the penalization coefficient α, it produces interesting controls with $|\psi(T)\rangle$ close to $|\psi_b\rangle$. Such monotonic schemes have been proposed for quantum systems in [19] (see also [22] for a slightly different version). We follow here the presentation of [5] which also provides an extension to infinite dimensional case. See also [9] for much earlier results on optimal control in infinite dimensional cases.

Take $u, v \in L^2([0,T], \mathbb{R}^m)$, denote by $\boldsymbol{P} = |\psi_b\rangle\langle\psi_b|$ the orthogonal projector on $|\psi_b\rangle$, then

$$J(u) - J(v) = -\frac{\alpha\Big(\langle\psi_u - \psi_v|\boldsymbol{P}|\psi_u - \psi_v\rangle_T + \langle\psi_u - \psi_v|\boldsymbol{P}|\psi_v\rangle_T + \langle\psi_v|\boldsymbol{P}|\psi_u - \psi_v\rangle_T\Big)}{2} + \int_0^T \frac{\sum_{k=1}^m (u_k - v_k)(u_k + v_k)}{2}.$$

Denote by $|p_v\rangle$ the adjoint associated to v, i.e. the solution of the backward systems

$$i\frac{d}{dt}|p_v\rangle = \frac{1}{\hbar}\left(\boldsymbol{H}_0 + \sum_{k=1}^m v_k \boldsymbol{H}_k\right)|p_v\rangle, \; |p_v(T)\rangle = -\alpha\boldsymbol{P}|\psi_v(T)\rangle.$$

We have

$$i\frac{d}{dt}(|\psi_u\rangle - |\psi_v\rangle) = \frac{1}{\hbar}\left(\boldsymbol{H}_0 + \sum_{k=1}^m v_k \boldsymbol{H}_k\right)(|\psi_u\rangle - |\psi_v\rangle) + \frac{1}{\hbar}\left(\sum_{k=1}^m (u_k - v_k)\boldsymbol{H}_k\right)|\psi_u\rangle.$$

We consider the Hermitian product of this equation with the adjoint state $|p_v\rangle$:

$$\left\langle p_v \left| \tfrac{d(\psi_u - \psi_v)}{dt} \right.\right\rangle = \frac{1}{\hbar}\left\langle p_v \left| \tfrac{\boldsymbol{H}_0 + \sum_{k=1}^m v_k \boldsymbol{H}_k}{i} \right| \psi_u - \psi_v \right\rangle + \frac{1}{\hbar}\left\langle p_v \left| \tfrac{\sum_{k=1}^m (u_k - v_k)\boldsymbol{H}_k}{i} \right| \psi_u \right\rangle.$$

An integration by parts yields

$$\begin{aligned}\int_0^T \left\langle p_v \left| \tfrac{d(\psi_u - \psi_v)}{dt} \right.\right\rangle &= \langle p_v|\psi_u - \psi_v\rangle_T - \langle p_v|\psi_u - \psi_v\rangle_0 - \int_0^T \left\langle \tfrac{dp_v}{dt} \right| \psi_u - \psi_v \Big\rangle \\ &= -\alpha\langle\psi_v|\boldsymbol{P}|\psi_u - \psi_v\rangle_T + \frac{1}{\hbar}\int_0^T \left\langle p_v \left| \tfrac{\boldsymbol{H}_0 + \sum_{k=1}^m v_k \boldsymbol{H}_k}{i} \right| \psi_u - \psi_v \right\rangle\end{aligned}$$

since $|\psi_v(0)\rangle = |\psi_u(0)\rangle$, $|p_v(T)\rangle = -\alpha \boldsymbol{P} |\psi_v(T)\rangle$ and $\frac{d}{dt}\langle p_v| = -\frac{1}{\hbar}\langle p_v| \left(\frac{\boldsymbol{H}_0 + \sum_{k=1}^m v_k \boldsymbol{H}_k}{i}\right)$. We get:

$$-\alpha \langle \psi_v | \boldsymbol{P} | \psi_u - \psi_v \rangle_T = \frac{1}{\hbar}\int_0^T \left\langle p_v \left| \frac{\sum_{k=1}^m (u_k - v_k)\boldsymbol{H}_k}{i} \right| \psi_u \right\rangle.$$

Thus $\alpha \Re\left(\langle \psi_v | \boldsymbol{P} | \psi_u - \psi_v \rangle_T\right) = -\frac{1}{\hbar}\int_0^T \Im\left(\langle p_v | \sum_{k=1}^m (u_k - v_k)\boldsymbol{H}_k | \psi_u \rangle\right)$. Finally we have

$$J(u) - J(v) = -\tfrac{\alpha}{2}\left(\langle \psi_u - \psi_v | \boldsymbol{P} | \psi_u - \psi_v \rangle\right)_T \\ + \tfrac{1}{2}\sum_{k=1}^m \left(\int_0^T (u_k - v_k)\left(u_k + v_k + \frac{2}{\hbar}\Im\left(\langle p_v | \boldsymbol{H}_k | \psi_u \rangle\right)\right) dt\right).$$

If each u_k satisfies $u_k = -\frac{1}{\hbar}\Im\left(\langle p_v | \boldsymbol{H}_k | \psi_u \rangle\right)$ for all $t \in [0, T)$ we have

$$J(u) - J(v) = -\tfrac{\alpha}{2}\left(\langle \psi_u - \psi_v | \boldsymbol{P} | \psi_u - \psi_v \rangle\right)_T - \tfrac{1}{2}\sum_{k=1}^m \left(\int_0^T (u_k - v_k)^2\right)$$

and thus $J(u) \le J(v)$.

These computations suggest the following iterative scheme. Assume that, at step ν, we have computed the control u^ν, the associated quantum state $|\psi^\nu\rangle = |\psi_{u^\nu}\rangle$ and its adjoint $|p^\nu\rangle = |p_{u^\nu}\rangle$. We get their new time values $u^{\nu+1}$, $|\psi^{\nu+1}\rangle$ and $|p^{\nu+1}\rangle$ in two steps:

1. Imposing $u_k^{\nu+1} = -\frac{1}{\hbar}\Im\left(\langle p^\nu | \boldsymbol{H}_k | \psi^{\nu+1}\rangle\right)$ as a feedback, one get $u^{\nu+1}$ just by a forward integration of the nonlinear Schrödinger equation,

$$i\frac{d}{dt}|\psi\rangle = \frac{1}{\hbar}\left(\boldsymbol{H}_0 - \sum_{k=1}^m \Im\left(\left\langle p^\nu \left| \frac{\boldsymbol{H}_k}{\hbar} \right| \psi \right\rangle\right)\boldsymbol{H}_k\right)|\psi\rangle, \quad |\psi(0)\rangle = |\psi_a\rangle,$$

   that provides $[0, T] \ni t \mapsto |\psi^{\nu+1}\rangle$ and the m new controls $u_k^{\nu+1}$.

2. Backward integration from $t = T$ to $t = 0$ of

$$i\frac{d}{dt}|p\rangle = \frac{1}{\hbar}\left(\boldsymbol{H}_0 + \sum_{k=1}^m u_k^{\nu+1}(t)\boldsymbol{H}_k\right)|p\rangle, \quad |p\rangle_T = -\alpha \langle \psi_b | \psi^{\nu+1}(T)\rangle |\psi_b\rangle$$

   yields to the new adjoint trajectory $[0, T] \ni t \mapsto |p^{\nu+1}\rangle$.

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A Concepts of control theory

A large part of control theory is based on differential equations: this is the so-called state space representation of deterministic systems in continuous time (versus stochastic systems using stochastic differential equations). It goes as follows: consider a physical system (e.g. a satellite, a car,...), described by its state $x(t)$ at time t (e.g. position and speed), on which one can act a every time by means of a *control* u (e.g. engine push for a satellite). We represent the state by a vector of $\mathbb{R}^n$, the control by a vector of $\mathbb{R}^m$, and we model evolution of the vector $x(t)$ by a *control system* (or controlled differential equation)

$$(\Sigma) \ : \qquad \frac{d}{dt}x(t) = f(t, x(t), u(t)), \qquad t \in [0, \tau],$$

where $\tau > 0$.

What is the meaning of the latter expression? The function $u(t)$, $t \in [0, \tau]$, called *control law* is the mean of action on the system (Σ): it will be chosen in terms of the goals to be achieved. To a control law $u(\cdot)$, is associated an ordinary differential equation

$$(\Sigma_u) \ : \qquad \frac{d}{dt}x(t) = f_u(t, x(t)), \qquad t \in [0, \tau],$$

where $f_u(t, x) := f(t, x, u(t))$. Hence, a function $x(\cdot)$ is solution of System (Σ) if there exists a control law $u(\cdot)$ such that $x(\cdot)$ is solution of (Σ_u).

The main concepts to address are the following.

Controllability given an initial state $x_0 \in \mathbb{R}^n$, a final state $v \in \mathbb{R}^n$ and a time $t = \tau > 0$, is it possible to find a control law $u(\cdot)$ steering System (Σ) initially in $x(0)$ at $t = 0$ to the state v at time $t = \tau$? Equivalently, is it possible to *control* System (Σ) from x_0 to v in time τ?

Motion planning To the above structural question, corresponds the more practical problem of determining an effective procedure which associates, to a pair of states $x_0, v \in \mathbb{R}^n$ and a time τ, a control law $u(\cdot)$ steering the system from $x(0)$ to v in time $t = \tau$.

Stabilization Is it possible to build a control law $u(\cdot)$ which *asymptotically stabilizes* System (Σ) at an equilibrium point x_0, i.e., such that, for every initial condition $x(0)$, one has

$$\lim_{t \to +\infty} x(t) = x_0?$$

Observability In order to achieve a control goal (motion planning, stabilization, etc...) and therefore to choose the appropriate control law, a certain amount of information on the state x of the system is available at every time t. It is usually obtained by measurement. However, it is not possible to measure in general (one says *to observe* in control theory) directly the full state $x(t)$ but only a function $y(t)$ of the state and the control

$$y(t) = g(x(t), u(t), t).$$

One must then "reconstruct" the state $x(\cdot)$ from the *output* $y(\cdot)$. The observability issue resumes therefore to the following: does the knowledge of $y(t)$ and $u(t)$ for every $t \in [0, \tau]$ allow one to determine the state $x(\cdot)$ for every $t \in [0, \tau]$ (or, let say the initial state $x(0)$)?

B Pontryaguin Maximum Principe

This appendix is a summary of the necessary optimality conditions called Pontryaguin Maximum Principle (PMP) for finite dimensional systems (for tutorial exposures see [8] or [2]).

Take a control system of the form $\frac{d}{dt}x = f(x, u)$, $x \in \mathbb{R}^n$, $u \in U \subset \mathbb{R}^m$ with a cost to maximize of the form $J = \int_0^T c(x, u)dt$ $(T > 0)$, initial condition $x(0) = x^a$ and final condition $x(T) = x^b$. The functions $f \in \mathbb{R}^n$ and $c \in \mathbb{R}$ are assumed to be C^1 functions of their arguments. If the couple $[0, T] \ni t \mapsto (x(t), u(t)) \in \mathbb{R}^n \times U$ is optimal, then there exists a never vanishing and absolutely continuous function[4] $[0, T] \ni t \mapsto p \in \mathbb{R}^n$ and a constant $p_0 \in]-\infty, 0]$ such that:

(i) with $\mathbb{H}(x, p, u) = p_0 c(x, u) + \sum_{i=1}^n p_i f_i(x, u)$, x and p are solutions of

$$\frac{d}{dt}x = \frac{\partial \mathbb{H}}{\partial p}(x, p, u), \quad \frac{d}{dt}p = -\frac{\partial \mathbb{H}}{\partial x}(x, p, u),$$

(ii) for almost all $t \in [0, T]$

$$\mathbb{H}(x(t), p(t), u(t)) = \overline{\mathbb{H}}(x(t), p(t)) \quad \text{where} \quad \overline{\mathbb{H}}(x, p) = \max_{v \in U} \mathbb{H}(x, p, v).$$

(iii) $\overline{\mathbb{H}}(x(t), p(t))$ is independent of t and its value $\bar{h}$, depends on T if the final time is fixed to T or $\bar{h} = 0$ if T is free (as for minimum time problem with U bounded and $c = -1$).

Conditions (i), (ii) and (iii) form the Pontryaguin Maximum Principle (PMP). Couples $[0, T] \ni t \mapsto (x(t), u(t))$ satisfying these conditions are called extremals: if $p_0 = 0$ the extremal is called abnormal; if $p_0 < 0$ the extremal is called normal. Strictly abnormal extremals are abnormal ((x, p) satisfies (i), (ii) and (iii) with $p_0 = 0$) and not normal ((x, p) never satisfies (i), (ii) and (iii) for $p_0 < 0$). Abnormal extremals do not depend on the cost $c(x, u)$ but only on the system itself $\frac{d}{dt}x = f(x, u)$: they are strongly related to system controllability (for driftless systems where $f(x, u)$ is linear versus x, see [6]).

[4] An absolutely continuous function $[0, T] \ni t \mapsto z \in \mathbb{R}^m$ satisfies, by definition, the following condition: for all $\epsilon > 0$, there exits $\eta > 0$ such that, for any ordered sequence $0 \le t_1 \le \ldots \le t_k \le T$ of arbitrary length k fulfilling $\sum_{i=1}^{k-1} |t_{i+1} - t_i| \le \eta$, we have $\sum_{i=1}^{k-1} |z(t_{i+1}) - z(t_i)| \le \epsilon$. Such functions are differentiable versus t, for almost all $t \in [0, T]$ and, moreover we have $z(t) = z(0) + \int_0^t z(s)ds$.

Assume that we have a normal extremal (x,u), i.e. satisfying conditions (i), (ii) and (iii) with $p_0 < 0$. Assume also that $u \mapsto \mathbb{H}(x,p,u)$ is differentiable, α concave, bounded from above, infinite at infinity and that $U = \mathbb{R}^m$. Then condition (ii) is then equivalent to $\frac{\partial \mathbb{H}}{\partial u} = 0$. Replacing p by p/p_0, PMP conditions (i), (ii) and (iii) coincide with the usual *first order stationary conditions* († means transpose here):

$$\frac{d}{dt}x = f, \quad \frac{d}{dt}p = -\left(\frac{\partial f}{\partial x}\right)^\dagger p - \left(\frac{\partial c}{\partial x}\right)^\dagger, \quad \left(\frac{\partial f}{\partial u}\right)^\dagger p + \left(\frac{\partial c}{\partial u}\right)^\dagger = 0 \tag{39}$$

with the boundary condtions $x(0) = x^a$, $x(T) = x^b$. From static equations in (39) we can express generally u as a function of (x,p), denoted here by $u = k(x,p)$. Then $\overline{\mathbb{H}}(x,p) = \mathbb{H}(x,p,k(x,p))$ and the first order stationary conditions form an Hamiltonian system

$$\frac{d}{dt}x = \frac{\partial \overline{\mathbb{H}}}{\partial p}(x,p), \quad \frac{d}{dt}p = -\frac{\partial \overline{\mathbb{H}}}{\partial x}(x,p)$$

since $\frac{\partial \overline{\mathbb{H}}}{\partial p} = \frac{\partial \mathbb{H}}{\partial p} + \frac{\partial \mathbb{H}}{\partial u}\frac{\partial k}{\partial p} = \frac{\partial \mathbb{H}}{\partial p}$ because $\frac{\partial \mathbb{H}}{\partial u} \equiv 0$ (idem for $\frac{\partial \overline{\mathbb{H}}}{\partial x}$). In general, this Hamiltonian system is not integrable in the Arnol'd-Liouville sense and numerical methods are then used.

These first order stationary conditions can be obtained directly using standard variation calculus based on the Lagrange method. The adjoint state p is the Lagrange multipliers associated to the constraint $\frac{d}{dt}x = f(x,u)$. Assume T given and consider the Lagrangian $L(x,\dot{x},p,u) = c(x,u) + \sum_{i=1}^n p_i(f_i(x,u) - \dot{x}_i)$ associated to

$$\max_{\substack{u,x \\ f(x,u) - \frac{d}{dt}x = 0 \\ x(0) = x^a,\ x(T) = x^b}} \int_0^T c(x,u)dt.$$

The first variation $\delta\mathcal{L}$ of $\mathcal{L} = \int_0^T L(x,\dot{x},p,u)dt$ should vanish for any variation δx, δp and δu such that $\delta x(0) = \delta x(T) = 0$:

- $\delta\mathcal{L} = 0$ for any δp yields to $\frac{d}{dt}x = f(x,u)$;
- $\delta\mathcal{L} = 0$ for any δx with $\delta x(0) = \delta x(T) = 0$ yields to $\frac{d}{dt}p = -\left(\frac{\partial f}{\partial x}\right)^\dagger p - \left(\frac{\partial c}{\partial x}\right)^\dagger$
- $\delta\mathcal{L} = 0$ for any δu yields to $\frac{\partial c}{\partial u} + \sum_i p_i \frac{\partial f_i}{\partial u} = 0$

We recover the stationary conditions (39).

It is then simple to show that the stationary conditions for

$$\max_{\substack{u,x \\ f(x,u) - \frac{d}{dt}x = 0 \\ x(0) = x^a}} \int_0^T c(x,u)dt + l(x(T)),$$

where the final condition $x(T) = x^b$ is replaced by a final cost $l(x(T)$ (l a C^1 function), remain unchanged except for the boundary conditions that become

$$x(0) = x^a, \quad p(T) = \left(\frac{\partial l}{\partial x}\right)^\dagger (x(T)).$$