Quantum systems and control 1

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ABSTRACT. This paper describes several methods used by physicists for manipulations of quantum states. For each method, we explain the model, the various time-scales, the performed approximations and we propose an interpretation in terms of control theory. These various interpretations underlie open questions on controllability, feedback and estimations. For 2-level systems we consider: the Rabi oscillations in connection with averaging; the Bloch-Siegert corrections associated to the second order terms; controllability versus parametric robustness of open-loop control and an interesting controllability problem in infinite dimension with continuous spectra. For 3-level systems we consider: Raman pulses and the second order terms. For spin/spring systems we consider: composite systems made of 2-level sub-systems coupled to quantized harmonic oscillators; multi-frequency averaging in infinite dimension; controllability of 1D partial differential equation of Shrödinger type and affine versus the control; motion planning for quantum gates. For open quantum systems subject to decoherence with continuous measures we consider: quantum trajectories and jump processes for a 2-level system; Lindblad-Kossakovsky equation and their controllability.

RÉSUMÉ. Ce papier décrit plusieurs méthodes utilisées par les physiciens pour la manipulation d'états quantiques. Pour chaque méthode, nous expliquons la modélisation, les diverses échelles de temps, les approximations faites et nous proposons une interprétation en termes de contrôle. Ces diverses interprétations servent de base à la formulation de questions ouvertes sur la commandabilité et aussi sur le feedback et l'estimation, renouvelant un peu certaines questions de base en théorie des systèmes non-linéaires. Pour les systèmes à deux niveaux, dits aussi de spin $\frac{1}{2}$, il s'agit: des oscillations de Rabi et d'une approximation au premier ordre de la théorie des perturbations (transition à un photon); des corrections de Bloch-Siegert et d'approximation au second ordre; de commandabilité et de robustesse paramétrique pour des contrôles en boucle ouverte, robustesse liée à des questions largement ouvertes sur la commandabilité en dimension infinie où le spectre est continu. Pour les systèmes à trois niveaux, il s'agit: de pulses Raman; d'approximations au second ordre. Pour les systèmes spin/ressort, il s'agit: des systèmes composés de sous-systèmes à deux niveaux couplés à des oscillateurs harmoniques quantifiés; de théorie des perturbations à plusieurs fréquences en dimension infinie; de commandabilité d'équations aux dérivées partielles de type Schrödinger sur $\mathbb{R}$ et affine en contrôle; de planification de trajectoires pour la synthèse portes logiques quantiques. Pour les systèmes ouverts soumis à la décohérence avec des mesures en continu, il s'agit: de trajectoires quantiques de Monte-Carlo et de processus à sauts sur un systèmes à deux niveaux; des équations de Lindblad-Kossakovsky avec leur commandabilité.

KEYWORDS : Quantum systems, Schrödinger equations, decoherence and open quantum systems, controllability, averaging and second order approximation.

MOTS-CLÉS : Systèmes quantiques, équation de Schrödinger, dé-cohérence et systèmes quantiques ouverts, contrôlabilité, moyennisation et approximation du second order.

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1. Introduction

Since several years physicists have developed experiments where they manipulate with high precision quantum states (see the recent book [15] for a tutorial and up-to-date exposure). The goal of this paper is to convince the reader that such experiment can be examined with a control theoretical point of view. We focuse on modeling and control of typical quantum systems where the control inputs correspond to pulse sequences in the radio-frequency or optical domain. The control goals are then the generation of intricate states and the design of quantum gates, the key components of a future (and hypothetical) quantum computer [29].

We consider here methods explained in [15] and based on resonance and perturbations theory. These methods are essentially open-loop and solve motion planning problems for systems described by Schrödinger equations of finite and infinite dimension. We do not consider in details feedback and estimations questions that are strongly connected to measurement theory, to the interpretation of the wave function and to de-coherence. Nevertheless, due to the central role played by feedback and filtering in mathematical system theory, we consider also this aspect by presenting, for a simple but representative example, the input/output model structure: the input is a classical deterministic signal; the output is a deterministic or probabilistic signal associated to a photo-detector. For more elaborated models stemming from quantum optics and open quantum systems see [6, 3, 14].

Section 2 is devoted to coherent evolution of 2-level systems also called $\frac{1}{2}$-spin systems. Section 3 presents, for 2-level systems only, decoherence and irreversible effects due to measures and/or environment. In section 4 we consider infinite dimensional systems of spin/spring type and made of 2-level systems coupled to quantized harmonic oscillators. These sections are structured in several subsections ending most of the time with comments on recent contributions and open-problems.

In subsection 2.1 we detail the Schrödinger equation with a scalar control input for a 2-level system described by a wave function $|\psi\rangle$ in $\mathbb{C}^2$. We exploit the Bra and Ket notations recalled in appendix A. Subsection 2.2 explains the passage between the wave function $|\psi\rangle$, the density operator ρ and the Bloch vector for a 2-level system. Subsection 2.3 shows that a control of small amplitude but in resonance with the system provides large changes of the wave function with Rabi oscillations. Such resonant open-loop controls underly motion planning methods widely used in experiments and based on averaging theorem and first order approximations recalled in appendix C. In subsection 2.4, such first order approximations are extended to second order with the Bloch-Siegert shift: the obtained system still obeys a Shrödinger equation but the dependence versus the control becomes nonlinear. This second order approximation is less usual but can be of some interest when the control amplitude is not very small. Subsection 2.5 presents adiabatic strategy: the control input varies slowly but its variations could be large on long time intervals. Subsection 2.6 treats Raman transitions for a 3-level system: it is as if we have a fictitious 2-level system whose Hamiltonian depends non-linearly on the complex amplitudes defining the control. This Hamiltonian results from a second order approximation. The way we conduct the calculations is, as far as we know, not standard. It relies on a short-cut method due to Kapitsa, explained in appendix C et that probably admits a nice interpretation in non-standard analysis.

Both subsections 3.1 and 3.2 describe, for a 2-level system, two models, (stochastic for a single system and deterministic for a population of identical systems) taking into account coupling to the environment and the perturbations due to the measure process. Such models are suitable for feedback et estimation (see, e.g., [14, 25, 28]).

In subsection 4.1 we recall the spectral decomposition of the quantized harmonic oscillator, the operators creating and annihilating quantum of vibration. Next subsection 4.2 presents the Jaynes and Cummings Hamiltonian that described the behavior of a 2-level atom resonantly coupled to the quantized mode of an electro-magnetic cavity. This Hamiltonian is associated to a system of two partial differential equations with one space variable in $\mathbb{R}$ and of Shrödinger type. Subsection 4.3 is devoted to an ion, catched in a Paul trap represented by a quadratic potential, and with two internal electronic levels excited by a resonant laser. As in previous subsection, we detail the various steps leading to the average Hamiltonian and we discuss the controllability of the attached partial differential system. In subsection 4.4, we present directly the average Hamiltonian for two ions in the same trap, each of them being controlled by it own laser. We describe the pulses sequence defining the open-loop control steering the system from the separated state where each ion is in its ground state to an intricate state (Bell state).

In appendix A, we recall the main notations used to describe quantum systems, the Copenhagen interpretation and its measurement theory based on the collapse of the wave packet. Appendix B gathers useful computational formulae with Pauli matrices. Appendix C presents in an elementary way perturbation theory and averaging for finite dimension system with a single frequency. We recall and complete also a short-cut method, due to Kapitsa, for computing the second order correction terms.

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2. Two-level systems

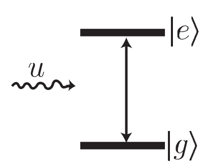

Figure 1. *a 2-level system*

2.1. The controlled Schrödinger equation

Take the system of figure 1. Typically, it corresponds to an electron around an atom. This electron is either in the ground state $|g\rangle$ of energy E_g, or in the excited state $|e\rangle$ of energy E_e ($E_g < E_e$). We discard the other energy levels. We proceed here similarly to flexible mechanical systems where one usually considers only few vibration modes: instead of looking at the partial differential Schrödinger equation describing the time evolution of the electron wave function, we consider only its components along two eigenmodes, one corresponds to the fundamental state and the other to the excited state. We will see below that controls are close to resonance and thus such an approximation is very naturel (at least for physicists).

The quantum state, described by $|\psi\rangle \in \mathbb{C}^2$ of length 1, $\langle\psi|\psi\rangle = 1$, is a linear superposition of $|g\rangle \in \mathbb{C}^2$, the ground state, and $|e\rangle \in \mathbb{C}^2$, the excited state, two orthogonal states, $\langle g|e\rangle = 0$, of length 1, $\langle g|g\rangle = \langle e|e\rangle = 1$:

$$|\psi\rangle = \psi_g |g\rangle + \psi_e |e\rangle$$

with $\psi_g, \psi_e \in \mathbb{C}$ the probability complex amplitude (see appendix A). This state $|\psi\rangle$ depends on time t. For this simple 2-level system, the Schrödinger equation is just an ordinary differential equation

$$\imath\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle = \Big(E_g |g\rangle\langle g| + E_e |e\rangle\langle e|\Big)|\psi\rangle$$

completely characterized by H, the Hamiltonian operator (Hermitian $H^\dagger = H$) corresponding to the energy ($\hbar$ is the Planck constant and $\frac{H}{\hbar}$ is homogenous to a frequency).

Since energies are defined up to a scalar, the Hamiltonians H and $H + \hbar u_0(t) I$ (with $u_0(t) \in \mathbb{R}$ arbitrary) describe the same physical system. If $|\psi\rangle$ obeys $\imath\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle$ then $|\chi\rangle = e^{-\imath\theta_0(t)}|\psi\rangle$ with $\frac{d}{dt}\theta_0 = u_0$ satisfies $\imath\hbar\frac{d}{dt}|\chi\rangle = (H + \hbar u_0 I)|\chi\rangle$. Thus for all θ_0, $|\psi\rangle$ and $e^{-\imath\theta_0}|\psi\rangle$ are attached to the same physical system. The global phase of the quantum state $|\psi\rangle$ can be arbitrarily chosen. It is as if we can add a control u_0 of the global phase, this control input u_0 being arbitrary (gauge degree of freedom relative to the origin of the energy scale). Thus the one parameter family of Hamiltonian

$$\Big((E_g + \hbar u_0)|g\rangle\langle g| + (E_e + \hbar u_0)|e\rangle\langle e|\Big)_{u_0 \in \mathbb{R}}$$

describes the same system. It is then natural to take $\hbar u_0 = -\frac{E_e - E_g}{2}$ and to set $\Omega = \frac{E_e - E_g}{\hbar}$, the pulsation of the photon emitted or absorbed during the transition between the ground and excited states. This frequency is associated to the light emitted by the electron during the jump from $|e\rangle$ to $|g\rangle$. This light is observed experimentally in spectroscopy: its frequency is a signature of the atom.

For the isolated system, the dynamics of $|\psi\rangle$ reads:

$$\imath\frac{d}{dt}|\psi\rangle = \frac{\Omega}{2}(|e\rangle\langle e| - |g\rangle\langle g|)|\psi\rangle .$$

Thus

$$|\psi\rangle_t = \psi_{g0}\, e^{\frac{\imath\Omega t}{2}}\, |g\rangle + \psi_{e0}\, e^{\frac{-\imath\Omega t}{2}}\, |e\rangle$$

where $|\psi\rangle_0 = \psi_{g0}|g\rangle + \psi_{e0}|e\rangle$. Usually, we denote by

$$\sigma_z = |e\rangle\langle e| - |g\rangle\langle g|$$

this Pauli matrix (see appendix B). Since $\sigma_z^2 = 1$, we have $e^{\imath\theta\sigma_z} = \cos\theta + \imath\sin\theta\sigma_z$ ($\theta \in \mathbb{R}$) and another expression of the time evolution of $|\psi\rangle$ is:

$$|\psi\rangle_t = e^{-\frac{\imath\Omega t}{2}\sigma_z}|\psi\rangle_0 = \cos\left(\frac{\Omega t}{2}\right)|\psi\rangle_0 - \imath\sin\left(\frac{\Omega t}{2}\right)\sigma_z|\psi\rangle_0 .$$

Assume now that the system is in interaction with a classical electro-magnetic field described by the control input $u(t) \in \mathbb{R}$. Then the evolution of $|\psi\rangle$ still results from a Schrödinger equation with an Hamiltonian depending on $u(t)$. In many cases, this controlled Hamiltonian admits the following form (dipolar and long wave-length approximations):

$$\frac{H(t)}{\hbar} = \frac{\Omega}{2}(|e\rangle\langle e| - |g\rangle\langle g|) + \frac{u(t)}{2}(|e\rangle\langle g| + |g\rangle\langle e|)$$

where u is homogenous to a frequency. The Schrödinger equation $\imath\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle$ reads also

$$\imath\frac{d}{dt}\begin{pmatrix}\psi_e\\ \psi_g\end{pmatrix} = \frac{\Omega}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}\psi_e\\ \psi_g\end{pmatrix} + \frac{u(t)}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\psi_e\\ \psi_g\end{pmatrix}.$$

At this point, it is very convenient to use the Pauli matrices (see appendix B):

$$\sigma_x = |e\rangle\langle g| + |g\rangle\langle e|\,,\ \sigma_y = -\imath\,|e\rangle\langle g| + \imath\,|g\rangle\langle e|\,,\ \sigma_z = |e\rangle\langle e| - |g\rangle\langle g|\,.$$

The controlled Hamiltonian is then :

$$\frac{H}{\hbar} = \frac{\Omega}{2}\sigma_z + \frac{u(t)}{2}\sigma_x.$$

Since σ_z and σ_x do not commute, there is no simple expression for the solution of the Cauchy problem, $\imath\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle$, when u depends on t.

It is interesting to notice that such systems are very similar to those considered by Claude Lobry in his seminal work on nonlinear controllability [21, 22]. If we add the phase control u_0, we have a two input control system

$$\imath\frac{d}{dt}|\psi\rangle = \left(\frac{\Omega}{2}\sigma_z + \frac{u(t)}{2}\sigma_x + u_0(t)I_d\right)|\psi\rangle$$

those controllability is characterized by the Lie algebra generated by the skew-Hermitian matrices $\imath\sigma_z$, $\imath\sigma_x$ and $\imath I_d$. Since $[\sigma_z, \sigma_x] = 2\imath\sigma_y$, we obtain all $u(2)$, the set of all skew-Hermitian matrices of dimension 2. Thus this system is controllable. We refer to the recent paper [2] for complete results on various notions of controllability for quantum systems and their characterization in terms of Lie algebra.

Notice that, without the phase control u_0, this system is not differentially flat since this single input system is not linearizable by static feedback (σ_x and $[\sigma_z, \sigma_x] = 2\imath\sigma_y$ do no commute, see [16, 7, 12]). It is only orbitally flat [11]. But, with the phase control u_0 this system is differentially flat: a possible flat output reads $(\Im(\psi_g\psi_e^*), \arg(\psi_g))$.

2.2. Density operator and Bloch sphere

We start with $|\psi\rangle$ satisfying $\imath\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle$. We consider the orthogonal projector $\rho = |\psi\rangle\langle\psi|$, called density operator. Then ρ is Hermitian and ≥ 0, satisfies $\text{tr}\,(\rho) = 1$, $\rho^2 = \rho$ and obeys the following equation:

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

where $[,]$ is the commutator: $[H, \rho] = H\rho - \rho H$. During the passage from $|\psi\rangle$ to the projector ρ we loose the global phase: for any angle θ, $|\psi\rangle$ and $e^{\imath\theta}|\psi\rangle$ yield to the same ρ. For a 2-level system $|\psi\rangle = \psi_g|g\rangle + \psi_e|e\rangle$ we have

$$|\psi\rangle\langle\psi| = |\psi_g|^2|g\rangle\langle g| + \psi_g\psi_e^*|g\rangle\langle e| + \psi_g^*\psi_e|e\rangle\langle g| + |\psi_e|^2|e\rangle\langle e|\,.$$

With

$$x = 2\Re(\psi_g \psi_e^*), \quad y = 2\Im(\psi_g \psi_e^*), \quad z = |\psi_e|^2 - |\psi_g|^2$$

we get the following expression

$$\rho = \frac{I + x\sigma_x + y\sigma_y + z\sigma_z}{2}.$$

Thus $(x, y, z) \in \mathbb{R}^3$ can be seen as the coordinates in the orthogonal frame $(\vec{\imath}, \vec{\jmath}, \vec{k})$ of a vector $\vec{M}$ in $\mathbb{R}^3$, called the Bloch vector:

$$\vec{M} = x\vec{\imath} + y\vec{\jmath} + z\vec{k}.$$

Since tr $\left(\rho^2\right) = x^2 + y^2 + z^2 = 1$, $\vec{M}$ is of length one. It evolves on the unit sphere, called the Bloch sphere, according to

$$\frac{d}{dt}\vec{M} = (u\vec{\imath} + \Omega\vec{k}) \times \vec{M},$$

another equivalent writing for $\frac{d}{dt}\rho = -\imath\left[\frac{\Omega}{2}\sigma_z + \frac{u}{2}\sigma_x,\ \rho\right]$. Thus $u\vec{\imath} + \Omega\vec{k}$ is the instantaneous rotation velocity. Such geometric interpretation of the $|\psi\rangle$ dynamics on the Bloch sphere is very popular in magnetic resonance where the 2-level system corresponds to a $\frac{1}{2}$-spin one. The knowledge of $\vec{M}$ is equivalent to the knowledge $|\psi\rangle$, up to a global phase. The $\vec{M}$ dynamics is flat with $y = \vec{M} \cdot \vec{\jmath} =$ tr $(\rho\sigma_y)$ as flat output.

2.3. Resonant control and Rabi oscillations

In the Schrödinger equation, $\imath \frac{d}{dt}|\psi\rangle = \left(\frac{\Omega}{2}\sigma_z + \frac{u}{2}\sigma_x\right)|\psi\rangle$, it is often unrealistic[1]to have u and Ω of the same magnitude order. The control is thus in general very small: $|u| \ll \Omega$. In this case, the simplest and efficient strategy is to take an oscillating u with a pulsation Ω^L close to Ω and to exploit resonance.

Let us begin by a change of variables, $|\psi\rangle = e^{-\frac{\imath\Omega t}{2}\sigma_z}|\phi\rangle$, called by physicists inter-action frame: the goal is to cancel the drift term $\frac{\Omega}{2}\sigma_z$ in the Hamiltonian. The dynamics of $|\phi\rangle$ reads:

$$\imath\frac{d}{dt}|\phi\rangle = \frac{u}{2}e^{\frac{\imath\Omega t}{2}\sigma_z}\sigma_x e^{-\frac{\imath\Omega t}{2}\sigma_z}|\phi\rangle = \frac{H_{\text{int}}}{\hbar}|\phi\rangle$$

with

$$\frac{H_{\text{int}}}{\hbar} = \frac{u}{2}e^{\imath\Omega t}\sigma_+ + \frac{u}{2}e^{-\imath\Omega t}\sigma_-$$

the Hamiltonian in the inter-action frame and where

$$\sigma_+ = |e\rangle\langle g| = \frac{\sigma_x + \imath\sigma_y}{2}, \quad \sigma_- = |g\rangle\langle e| = \frac{\sigma_x - \imath\sigma_y}{2}.$$

The operators (non Hermitian) σ_+ and σ_- are associated to the quantum jump from $|g\rangle$ to $|e\rangle$ and from $|e\rangle$ to $|g\rangle$, respectively. It is then very efficient to take u quasi-resonant with a pulsation $\Omega^L \approx \Omega$

$$u = \mathbf{u}e^{\imath\Omega^L t} + \mathbf{u}^* e^{-\imath\Omega^L t}$$

1. Excepted if we can use very intense electro-magnetic field, but in this case one has to take into account new phenomena and the model is no more valid.

and $\mathbf{u}$ is a small complex amplitude varying slowly:

$$\left|\frac{d}{dt}\mathbf{u}\right| \ll \Omega|\mathbf{u}|, \quad |\mathbf{u}| \ll \Omega, \quad |\Omega^L - \Omega| \ll \Omega.$$

Thus we have

$$\imath\frac{d}{dt}\left|\phi\right\rangle = \left(\left(\frac{\mathbf{u}e^{\imath(\Omega+\Omega^L)t} + \mathbf{u}^* e^{\imath\Delta t}}{2}\right)\sigma_+ + \left(\frac{\mathbf{u}e^{-\imath\Delta t} + \mathbf{u}^* e^{-2\imath(\Omega+\Omega^L)t}}{2}\right)\sigma_-\right)\left|\phi\right\rangle$$

with $\Delta = \Omega - \Omega^L$ the de-tuning between the control frequency and the system frequency. This system is in standard form for averaging (see appendix C) with $\epsilon = \frac{|\mathbf{u}|}{\Omega+\Omega^L}$ as small parameter. The secular approximation, also called rotating wave approximation (RWA), just consists in neglecting terms oscillating at pulsation $\Omega + \Omega^L$ and with zero average. Thus $|\phi\rangle$ obeys, up to second order terms in ϵ, the average dynamics:

$$\imath\frac{d}{dt}\left|\phi\right\rangle = \left(\frac{\mathbf{u}e^{-\imath\Delta t}}{2}\sigma_- + \mathbf{u}^*\frac{e^{\imath\Delta t}}{2}\sigma_+\right)\left|\phi\right\rangle.$$

The change of variables $|\phi\rangle = e^{\frac{-\imath\Delta t}{2}\sigma_z}\left|\chi\right\rangle$ yields an autonomous equation

$$\imath\frac{d}{dt}\left|\chi\right\rangle = \left(\frac{\Delta}{2}\sigma_z + \frac{\mathbf{u}}{2}\sigma_- + \frac{\mathbf{u}^*}{2}\sigma_+\right)\left|\chi\right\rangle.$$

It still remains of Schrödinger kind but with the effective Hamiltonian

$$\frac{H_{eff}}{\hbar} = \frac{\Delta}{2}\sigma_z + \frac{\mathbf{u}}{2}\sigma_- + \frac{\mathbf{u}^*}{2}\sigma_+.$$

Let us assume, until the end of this subsection, $\Delta = 0$ and $\mathbf{u} = \omega_r e^{\imath\theta}$ with $\omega_r > 0$ and θ real and constant. Then

$$\frac{\mathbf{u}^*\sigma_+ + \mathbf{u}\sigma_-}{2} = \frac{\omega_r}{2}\left(\cos\theta\sigma_x + \sin\theta\sigma_y\right)$$

and the solution $|\chi\rangle$ oscillates between $|e\rangle$ and $|g\rangle$ with the Rabi pulsation $\frac{\omega_r}{2}$. Since $(\cos\theta\sigma_x + \sin\theta\sigma_y)^2 = 1$, we have

$$e^{-\frac{\imath\omega_r t}{2}(\cos\theta\sigma_x+\sin\theta\sigma_y)} = \cos\left(\frac{\omega_r t}{2}\right) - \imath\sin\left(\frac{\omega_r t}{2}\right)\left(\cos\theta\sigma_x + \sin\theta\sigma_y\right),$$

and the solution of $\frac{d}{dt}\left|\chi\right\rangle = \frac{-\imath\omega_r}{2}\left(\cos\theta\sigma_x + \sin\theta\sigma_y\right)\left|\chi\right\rangle$ reads

$$\left|\chi\right\rangle_t = \cos\left(\frac{\omega_r t}{2}\right)\left|g\right\rangle - \imath\sin\left(\frac{\omega_r t}{2}\right)e^{-\imath\theta}\left|e\right\rangle, \quad \text{when} \quad \left|\chi\right\rangle_0 = \left|g\right\rangle,$$

$$\left|\chi\right\rangle_t = \cos\left(\frac{\omega_r t}{2}\right)\left|e\right\rangle - \imath\sin\left(\frac{\omega_r t}{2}\right)e^{\imath\theta}\left|g\right\rangle, \quad \text{when} \quad \left|\chi\right\rangle_0 = \left|e\right\rangle,$$

With the ground state as initial condition, $\left|\chi\right\rangle_0 = \left|g\right\rangle$, let us take $\mathbf{u} = -\imath\omega_r$ constant on $[0, T]$ (pulse of length T). Then

$$\left|\chi\right\rangle_T = \cos\left(\frac{\omega_r T}{2}\right)\left|g\right\rangle + \sin\left(\frac{\omega_r T}{2}\right)\left|e\right\rangle,$$

and we see that:

– if $\omega_r T = \pi$ then $|\chi\rangle_T = |e\rangle$ and we have a transition between the ground state to the excited one by stimulated absorption of one photon of energy $\hbar\Omega$. If we measure the energy in the final state we always find E_e. This is a π-pulse.

– if $\omega_r T = \pi/2$ then $|\chi\rangle_T = (|g\rangle + |e\rangle)/\sqrt{2}$ 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 $|\psi\rangle = e^{-\frac{\imath\Omega^L t}{2}\sigma_z}|\chi\rangle$, we see that a π-pulse transfers $|\psi\rangle$ from $|g\rangle$ at $t=0$ to $e^{\imath\alpha}|e\rangle$ at $t = T = \frac{\pi}{\omega_r}$ where the phase $\alpha \approx \frac{\Omega^L}{\omega_r}\pi$ is very large since $\omega_r \ll \Omega^L$. Similarly, a $\frac{\pi}{2}$-pulse, transfers $|\psi\rangle$ from $|g\rangle$ at $t=0$ to $\frac{e^{-\imath\alpha}|g\rangle + e^{\imath\alpha}|e\rangle}{\sqrt{2}}$ at $t = T = \frac{\pi}{2\omega_r}$ with a very large relative half-phase $\alpha \approx \frac{\Omega^L}{2\omega_r}\pi$. Thus, this kind of pulses is well adapted when the initial state, $|\psi\rangle_0$, and final state, $|\psi\rangle_T$, are characterized by $|\langle\psi|g\rangle|^2$ and $|\langle\psi|e\rangle|^2$ where these phases disappear. One speak then of populations since $|\langle\psi|g\rangle|^2$ (resp. $|\langle\psi|e\rangle|^2$) is the probability to find E_g (resp. E_e) when we measure the energy of the isolated system $H_0 = E_g|g\rangle\langle g| + E_e|e\rangle\langle e|$.

The fact to take a resonant open-loop control u is indeed optimal for population transfer as proved by the nice result [5] for systems with two and three states. In [30] motion planing for the propagator $U(t) \in SU(2)$,

$$\imath\frac{d}{dt}U = \left(\frac{\Delta}{2}\sigma_z + \frac{\mathbf{u}}{2}\sigma_- + \frac{\mathbf{u}^*}{2}\sigma_+\right)U, \qquad U(0) = I_d,$$

is solved explicitly et analytically for any goal matrix $U(T) \in SU(2)$: we exploit the fact that this flat system is invariant versus right translation on $SU(2)$; the non-commutative computations are done with quaternions and they generalize those already done for the non-holonomic car where $SU(2)$ replaces $SE(2)$ [31]. The resulting open-loop controls $\mathbf{u}$ are very smooth. Such an approach could be interesting practically if it can be extended to higher dimension. For 4-level systems, such hypothetical extensions could be an alternative, for the design of a quantum gate (such as the Cnot-gate), to complicated sequences of several pulses (see, e.g., [15, page 493]).

Let us finish by an interesting robustness notion encountered in magnetic resonance: ensemble controllability as stated in [20] when we face a continuum of parameter values. For the system

$$\imath\frac{d}{dt}|\psi\rangle = \left(\frac{\Delta}{2}\sigma_z + \frac{\mathbf{u}}{2}\sigma_- + \frac{\mathbf{u}^*}{2}\sigma_+\right)|\psi\rangle$$

depending on the parameter Δ, the problem reads as follows: find a unique open-loop control $[0,T] \ni t \mapsto \mathbf{u}(t) \in \mathbb{C}$ ensuring the (approximated) transfer of $|\psi\rangle_0^\Delta = |g\rangle$ towards $|\psi\rangle_T^\Delta = |e\rangle$ where $|\psi\rangle_t^\Delta$ is the solution corresponding to the parameter Δ:

$$\imath\frac{d}{dt}|\psi\rangle^\Delta = \left(\frac{\Delta}{2}\sigma_z + \frac{\mathbf{u}}{2}\sigma_- + \frac{\mathbf{u}^*}{2}\sigma_+\right)|\psi\rangle^\Delta .$$

The difficulty stems from the fact that Δ takes any value in the interval $[\Delta_0, \Delta_1]$ ($\Delta_0 < \Delta_1$ are given) whereas $\mathbf{u}(t)$ is independent of Δ. The goal is to control via the same input an infinite number (a continuum) of similar systems differing only by the value of Δ. This is a special controllability problem of infinite dimension with continuous spectra: for $\mathbf{u} = 0$, the spectrum is on the imaginary axis, $\left[\frac{-\imath\Delta_1}{2}, \frac{-\imath\Delta_0}{2}\right] \cup \left[\frac{\imath\Delta_0}{2}, \frac{\imath\Delta_1}{2}\right]$. This infinite dimensional system is particularly interesting if we want to understand controllability with a continuous part in the spectrum, a situation that has never been considered except in [24].

2.4. Resonant control and Bloch-Siegert shift

When the assumption $|\mathbf{u}| \ll \Omega$ is not very well satisfied, it could be interesting to compute second order correction terms. In fact, the rotation wave approximation is a first order approximation in the sense of perturbations theory. Second order terms can be easily obtained by following the short-cut method recalled in appendix C. Set $|\phi\rangle = |\bar{\phi}\rangle + |\delta\phi\rangle$ where $|\bar{\phi}\rangle$ evolves slowly and where $|\delta\phi\rangle$ is small, oscillates and admits a zero average:

$$\imath \frac{d}{dt}\left(|\bar{\phi}\rangle + |\delta\phi\rangle\right) = \left(\frac{\mathbf{u}e^{\imath(\Omega+\Omega^L)t} + \mathbf{u}^* e^{\imath\Delta t}}{2}\right)\sigma_+ \left(|\bar{\phi}\rangle + |\delta\phi\rangle\right) + \left(\frac{\mathbf{u}e^{-\imath\Delta t} + \mathbf{u}^* e^{-\imath(\Omega+\Omega^L)t}}{2}\right)\sigma_- \left(|\bar{\phi}\rangle + |\delta\phi\rangle\right).$$

Then identify the terms of same order and oscillating ($|\mathbf{u}| \sim \epsilon\Omega$, $|\delta\phi\rangle \sim \epsilon$ and $\frac{d}{dt}|\delta\phi\rangle \sim \epsilon$ oscillate, $|\bar{\phi}\rangle \sim 1$ and $\frac{d}{dt}|\bar{\phi}\rangle \sim \epsilon$ does not oscillate):

$$\imath \frac{d}{dt}|\delta\phi\rangle \approx \frac{\mathbf{u}e^{\imath(\Omega+\Omega^L)t}}{2}\sigma_+ |\bar{\phi}\rangle + \mathbf{u}^* \frac{e^{-\imath(\Omega+\Omega^L)t}}{2}\sigma_- |\bar{\phi}\rangle$$

Thus $|\delta\phi\rangle \approx -\frac{\mathbf{u}e^{\imath(\Omega+\Omega^L)t}}{2(\Omega+\Omega^L)}\sigma_+ |\bar{\phi}\rangle + \mathbf{u}^* \frac{e^{-\imath(\Omega+\Omega^L)t}}{2(\Omega+\Omega^L)}\sigma_- |\bar{\phi}\rangle$. The average of

$$\imath \frac{d}{dt}|\bar{\phi}\rangle = \frac{\mathbf{u}e^{\imath(\Omega+\Omega^L)t} + \mathbf{u}^* e^{\imath\Delta t}}{2}\sigma_+ |\delta\phi\rangle + \frac{\mathbf{u}^* e^{\imath\Delta t}}{2}\sigma_+ |\bar{\phi}\rangle + \frac{\mathbf{u}^* e^{-\imath(\Omega+\Omega^L)t} + \mathbf{u}e^{-\imath\Delta t}}{2}\sigma_- |\delta\phi\rangle + \frac{\mathbf{u}e^{-\imath\Delta t}}{2}\sigma_- |\bar{\phi}\rangle$$

gives, after the substitution of the value of $|\delta\phi\rangle$ versus $|\bar{\phi}\rangle$,

$$\imath \frac{d}{dt}|\bar{\phi}\rangle = \frac{|\mathbf{u}|^2}{4(\Omega+\Omega^L)}\sigma_z |\bar{\phi}\rangle + \frac{\mathbf{u}e^{-\imath\Delta t}}{2}\sigma_- |\bar{\phi}\rangle + \frac{\mathbf{u}^* e^{\imath\Delta t}}{2}\sigma_+ |\bar{\phi}\rangle$$

With $|\bar{\phi}\rangle = e^{\frac{-\imath\Delta t}{2}\sigma_z}|\chi\rangle$ we get

$$\imath \frac{d}{dt}|\chi\rangle = \left(\frac{|\mathbf{u}|^2}{4(\Omega+\Omega^L)} + \frac{\Delta}{2}\right)\sigma_z |\chi\rangle + \frac{\mathbf{u}}{2}\sigma_- |\chi\rangle + \frac{\mathbf{u}^*}{2}\sigma_+ |\chi\rangle$$

The effective Hamiltonian becomes now

$$\frac{H_{eff}}{\hbar} = \left(\frac{|\mathbf{u}|^2}{4(\Omega+\Omega^L)} + \frac{\Delta}{2}\right)\sigma_z + \frac{\mathbf{u}}{2}\sigma_- + \frac{\mathbf{u}^*}{2}\sigma_+.$$

The second order correction corresponds to $\frac{|\mathbf{u}|^2}{4(\Omega+\Omega^L)}\sigma_z$ and is called the Bloch-Siegert shift. At order 2, the effective Hamiltonian depends nonlinearly on the complex amplitude $\mathbf{u}$. We will see a similar dependence for the Raman Hamiltonian.

2.5. Slowly varying Control

We first recall the quantum version of adiabatic invariance. All the details can be found in the recent book of Teufel [35] with extension to infinite dimensional systems. We restrict here the exposure to the simplest version, i.e. in finite dimension and without the exponentially precise estimations. Take $m+1$ Hermitian matrices $n\times n$: $H_0,\dots,H_m$. For $u\in\mathbb{R}^m$ set $H(u):=H_0+\sum_{k=1}^m u_k\, H_k$. Then we have to following two results:

1) for any u exists an ortho-normal frame $(|\phi_k^u\rangle)_{k\in\{1,\dots,n\}}$ of $\mathbb{C}^n$ made of eigenvectors of $H(u)$ those dependence in u is analytic (locally).

2) For $0<\epsilon\ll 1$, we consider the solution $\left[0,\frac{1}{\epsilon}\right]\ni t\mapsto |\psi\rangle_t^\epsilon$ of

$$\imath\hbar\frac{d}{dt}\,|\psi\rangle_t^\epsilon = H(u(\epsilon t))\,|\psi\rangle_t^\epsilon$$

where $u(s)$ is a continuously differentiable function of $s\in[0,1]$. If for any $u(s)$, $s\in[0,1]$, the eigenvalues of $H(u(s))$ are all distinct, then, for all $\eta>0$, exists $\nu>0$ such that, $\forall\epsilon\in]0,\nu]$, $\forall t\in\left[0,\frac{1}{\epsilon}\right]$ and $\forall k\in\{1,...,n\}$,

$$\left|\,\left|\left\langle \psi_t^\epsilon|\phi_k^{u(\epsilon t)}\right\rangle\right|^2 - \left|\left\langle \psi_0^\epsilon|\phi_k^{u(0)}\right\rangle\right|^2\,\right| \le \eta$$

This means that the solution of $\imath\hbar\frac{d}{dt}\,|\psi\rangle = H\left(\frac{t}{T}\right)\psi$ follows the spectral decomposition of $H\left(\frac{t}{T}\right)$ as soon as T is large enough and when $H\left(\frac{t}{T}\right)$ does not admit multiple eigenvalues (non degenerate spectrum). 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 [34]), to the same ground state. The non-degeneracy of the spectrum is important as we will see at the end of this subsection.

Let us take a 2-level system. Since we do not care for global phase, we will use the Bloch vector of subsection 2.2:

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

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 unitary 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: $\vec{M}(t)\approx\vec{\beta}\left(\frac{t}{T}\right)$: $\vec{M}$ 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 $\imath\frac{d}{dt}\,|\psi\rangle = \left(\frac{u}{2}\sigma_x+\frac{v}{2}\sigma_y+\frac{w}{2}\sigma_z\right)|\psi\rangle$ and to apply the adiabatic theorem recalled here above. The absence of spectrum degeneracy results from the fact that ϖ never vanishes

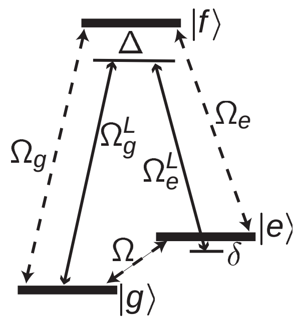

Figure 2. *Raman transition for a* 3*-level system*

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, $|\psi\rangle_t$ 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 $H(t)$, 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 [37, 1] for related control theoretic results.

2.6. Raman transition

This transition strategy is commonly used[2] for 3-level systems (cf figure 2) where the additional sate $|f\rangle$ admits an energy E_f much greater than E_g and E_e. However, we will see that the effective Hamiltonian 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 $\Omega = \frac{E_e - E_g}{\hbar}$, but with a control based on two frequencies Ω_g^L and Ω_e^L, in the vicinity of $\Omega_g = \frac{E_f - E_g}{\hbar}$ and $\Omega_e = \frac{E_f - E_e}{\hbar}$ and those difference is very close to Ω. Such transitions result from a nonlinear phenomena and second order perturbations. The main practical advantage comes from the fact that Ω_e^L and Ω_g^L are optical frequencies (around 10^{15} rad/s) whereas Ω is a radio frequency (around 10^{10} rad/s). The wave length of the laser generating u is around 1 μm and thus spacial resolution is much better with optical waves than with radio-frequency ones.

2. See, e.g., [8] where π and $\pi/2$ Raman pulses are applied on a cloud of cold atoms in order to measure with very high precision the gravity g.

Take the 3-level system ($|g\rangle$, $|e\rangle$ and $|f\rangle$ of energy E_g, E_e and E_f) of figure 2. The atomic pulsations are denoted as follows:

$$\Omega_g = \frac{E_f - E_g}{\hbar},\ \Omega_e = \frac{E_f - E_e}{\hbar},\ \Omega = \frac{E_e - E_g}{\hbar}.$$

We assume an Hamiltonian of the form

$$\frac{H}{\hbar} = \frac{E_g}{\hbar}\left|g\right\rangle\left\langle g\right| + \frac{E_e}{\hbar}\left|e\right\rangle\left\langle e\right| + \frac{E_f}{\hbar}\left|f\right\rangle\left\langle f\right| \\ + \mu_g u(\left|g\right\rangle\left\langle f\right| + \left|f\right\rangle\left\langle g\right|) + \mu_e u(\left|e\right\rangle\left\langle f\right| + \left|f\right\rangle\left\langle e\right|)$$

where μ_g and μ_e are coupling coefficients with the electro-magnetic field described by $u(t)$. We assume also that $\Omega \ll \Omega_g, \Omega_e$. Notice the absence of direct coupling between $|g\rangle$ and $|e\rangle$ via u, i.e., of terms like $u(\left|g\right\rangle\left\langle e\right| + \left|e\right\rangle\left\langle g\right|)$. To go from $|g\rangle$ to $|e\rangle$ with u, we need the coupling of $|g\rangle$ and $|e\rangle$ with the supplementary state $|f\rangle$[3].

We take a quasi-resonant control defined by the complex amplitudes $\mathbf{u}_g$ and $\mathbf{u}_e$ slowly varying,

$$u = \mathbf{u}_g e^{\imath\Omega_g^L t} + \mathbf{u}_g^* e^{-\imath\Omega_g^L t} + \mathbf{u}_e e^{\imath\Omega_e^L t} + \mathbf{u}_e^* e^{-\imath\Omega_e^L t}$$

where the pulsation Ω_g^L and Ω_e^L are close to but different of Ω_g and Ω_e, and their difference is very close to Ω. With

$$\Delta = \Omega_g - \Omega_g^L, \qquad \delta = \Omega - (\Omega_g^L - \Omega_e^L)$$

this means that, on one side

$$|\Omega_g^L - \Omega_g| \ll \Omega_g, \quad |\Omega_e^L - \Omega_e| \ll \Omega_e$$

but on the other side

$$|\Delta| \ll \Omega_g, \quad |\Delta| \ll \Omega_e$$

and

$$|\delta| \ll |\Delta|, \quad |\delta| \ll |\Delta + \Omega|, \quad |\delta| \ll |\Delta - \Omega|.$$

To summarize, we have three time-scales:

1) the fast scale associated to Ω_g, Ω_e, Ω_g^L and Ω_e^L.

2) the intermediate scale associated to Δ and $\Delta \pm \Omega$

3) the slow scale associated to δ, $\mu_g|\mathbf{u}_g|$, $\mu_g|\mathbf{u}_e|$, $\mu_e|\mathbf{u}_g|$ and $\mu_e|\mathbf{u}_e|$.

We assume thus that $\mathbf{u}_g$ and $\mathbf{u}_e$ satisfy

$$|\mu_g \mathbf{u}_g|, |\mu_e \mathbf{u}_g|, |\mu_g \mathbf{u}_e|, |\mu_e \mathbf{u}_e| \ll |\Delta|, |\Delta \pm \Omega|$$

and

$$\left|\frac{d}{dt}\mathbf{u}_g\right| \ll |\Delta||\mathbf{u}_g|, \quad \left|\frac{d}{dt}\mathbf{u}_e\right| \ll |\Delta||\mathbf{u}_e|.$$

3. Let us remark that, even if a term like $\mu u(\left|g\right\rangle\left\langle e\right| + \left|e\right\rangle\left\langle g\right|)$ is present in the Hamiltonian, the fact to take a small u oscillating at frequencies much higher that Ω, does not change the result of this subsection and the obtained second order approximation will remain unchanged.

Notice that Ω could be relevant of the slow or of the intermediate scale, or Ω could be in between.

In the interaction frame (passage from $|\psi\rangle$ to $|\phi\rangle$),

$$|\psi\rangle = \left(e^{-\frac{\imath E_g t}{\hbar}} |g\rangle \langle g| + e^{-\frac{\imath E_e t}{\hbar}} |e\rangle \langle e| + e^{-\frac{\imath E_f t}{\hbar}} |f\rangle \langle f|\right) |\phi\rangle$$

the Hamiltonian becomes $\frac{H_{\text{int}}}{\hbar}$:

$$\mu_g \left(\mathbf{u}_g e^{\imath\Omega_g^L t} + \mathbf{u}_e e^{\imath\Omega_e^L t} + \mathbf{u}_g^* e^{-\imath\Omega_g^L t} + \mathbf{u}_e^* e^{-\imath\Omega_e^L t}\right) \left(e^{\imath\Omega_g t} |g\rangle \langle f| + e^{-\imath\Omega_g t} |f\rangle \langle g|\right)$$
$$+ \mu_e \left(\mathbf{u}_g e^{\imath\Omega_g^L t} + \mathbf{u}_e e^{\imath\Omega_e^L t} + \mathbf{u}_g^* e^{-\imath\Omega_g^L t} + \mathbf{u}_e^* e^{-\imath\Omega_e^L t}\right) \left(e^{\imath\Omega_e t} |e\rangle \langle f| + e^{-\imath\Omega_e t} |f\rangle \langle e|\right)$$

We average terms oscillating at pulsation $\Omega_\xi^L + \Omega_\zeta$ ($\xi, \zeta = g, e$) to get the effective Hamiltonian $\frac{H_{eff}}{\hbar}$:

$$\mu_g \left(\mathbf{u}_g e^{\imath(\Omega_g^L - \Omega_g)t} + \mathbf{u}_e e^{\imath(\Omega_e^L - \Omega_g)t}\right) |f\rangle \langle g| + \mu_g \left(\mathbf{u}_g^* e^{-\imath(\Omega_g^L - \Omega_g)t} + \mathbf{u}_e^* e^{-\imath(\Omega_e^L - \Omega_g)t}\right) |g\rangle \langle f|$$
$$+ \mu_e \left(\mathbf{u}_g e^{\imath(\Omega_g^L - \Omega_e)t} + \mathbf{u}_e e^{\imath(\Omega_e^L - \Omega_e)t}\right) |f\rangle \langle e| + \mu_e \left(\mathbf{u}_g^* e^{-\imath(\Omega_g^L - \Omega_e)t} + \mathbf{u}_e^* e^{-\imath(\Omega_e^L - \Omega_e)t}\right) |e\rangle \langle f|$$

By assumptions concerning the different time-scales,

$$\Omega_g - \Omega_g^L = \Delta, \quad \Omega_g - \Omega_e^L = \Delta + \Omega - \delta, \quad \Omega_e - \Omega_g^L = \Delta - \Omega, \quad \Omega_e - \Omega_e^L = \Delta - \delta$$

are all much larger than δ and $\mu_\xi |\mathbf{u}_\zeta|$ ($\xi, \zeta = g, e$). Since we are interested by the slow time-scale, we have to remove the oscillating terms associated to the intermediate scale. Since all terms in H_{eff} have a zero average, the first order approximation yields 0. We have to compute the second order one in order to obtain a nonzero Hamiltonian. We use the method already employed for the Bloch-Siegert shift by setting

$$|\phi\rangle = |\bar{\phi}\rangle + |\delta\phi\rangle$$

in the Schrödinger equation $\imath\hbar \frac{d}{dt} |\phi\rangle = H_{eff} |\phi\rangle$ and by identifying the oscillating term of same order. We have here multiple frequencies and the short-cut method of appendix C has to be extended to this case. We assume that this can be done. A clear mathematical justification will be welcome.

Thus $\imath \frac{d}{dt} |\delta\phi\rangle = \frac{H_{eff}}{\hbar} |\bar{\phi}\rangle$ where $|\bar{\phi}\rangle$ is assumed constant and H_{eff} is oscillatory. A simple time integration gives $|\delta\phi\rangle$ as

$$\mu_g \left(\frac{\mathbf{u}_g^* e^{-\imath(\Omega_g^L - \Omega_g)t}}{\Omega_g^L - \Omega_g} + \frac{\mathbf{u}_e^* e^{-\imath(\Omega_e^L - \Omega_g)t}}{\Omega_e^L - \Omega_g}\right) |g\rangle \langle f|\bar{\phi}\rangle$$
$$- \mu_g \left(\frac{\mathbf{u}_g e^{\imath(\Omega_g^L - \Omega_g)t}}{\Omega_g^L - \Omega_g} + \frac{\mathbf{u}_e e^{\imath(\Omega_e^L - \Omega_g)t}}{\Omega_e^L - \Omega_g}\right) |f\rangle \langle g|\bar{\phi}\rangle$$
$$+ \mu_e \left(\frac{\mathbf{u}_g^* e^{-\imath(\Omega_g^L - \Omega_e)t}}{\Omega_g^L - \Omega_e} + \frac{\mathbf{u}_e^* e^{-\imath(\Omega_e^L - \Omega_e)t}}{\Omega_e^L - \Omega_e}\right) |e\rangle \langle f|\bar{\phi}\rangle$$
$$- \mu_e \left(\frac{\mathbf{u}_g e^{\imath(\Omega_g^L - \Omega_e)t}}{\Omega_g^L - \Omega_e} + \frac{\mathbf{u}_e e^{\imath(\Omega_e^L - \Omega_e)t}}{\Omega_e^L - \Omega_e}\right) |f\rangle \langle e|\bar{\phi}\rangle .$$

We have neglected second order terms in $\frac{\mu_\xi |\mathbf{u}_\zeta|}{\Omega^L_{\xi'} - \Omega_{\zeta'}}$ ($\xi, \zeta, \xi', \zeta' = g, e$). We have

$$\imath \frac{d}{dt} \left|\bar{\phi}\right\rangle = \frac{H_{eff}}{\hbar} \left|\delta\phi\right\rangle$$

where $|\delta\phi\rangle$ must be replaced by it value versus $\left|\bar{\phi}\right\rangle$ given here above and where we consider only secular terms. This consists in keeping only the secular terms in the product of $\frac{H_{eff}}{\hbar}$ by the operator A defined by $|\delta\phi\rangle = A\left|\bar{\phi}\right\rangle$ and recalled here below:

$$\begin{aligned}
\mu_g \Bigg(\left(\frac{\mathbf{u}_g^* e^{-\imath(\Omega_g^L - \Omega_g)t}}{\Omega_g^L - \Omega_g} + \frac{\mathbf{u}_e^* e^{-\imath(\Omega_e^L - \Omega_g)t}}{\Omega_e^L - \Omega_g} \right) |g\rangle \langle f| \\
- \left(\frac{\mathbf{u}_g e^{\imath(\Omega_g^L - \Omega_g)t}}{\Omega_g^L - \Omega_g} + \frac{\mathbf{u}_e e^{\imath(\Omega_e^L - \Omega_g)t}}{\Omega_e^L - \Omega_g} \right) |f\rangle \langle g| \Bigg) \\
+ \mu_e \Bigg(\left(\frac{\mathbf{u}_g^* e^{-\imath(\Omega_g^L - \Omega_e)t}}{\Omega_g^L - \Omega_e} + \frac{\mathbf{u}_e^* e^{-\imath(\Omega_e^L - \Omega_e)t}}{\Omega_e^L - \Omega_e} \right) |e\rangle \langle f| \\
- \left(\frac{\mathbf{u}_g e^{\imath(\Omega_g^L - \Omega_e)t}}{\Omega_g^L - \Omega_e} + \frac{\mathbf{u}_e e^{\imath(\Omega_e^L - \Omega_e)t}}{\Omega_e^L - \Omega_e} \right) |f\rangle \langle e| \Bigg)
\end{aligned}$$

But $\frac{H_{eff}}{\hbar} A$ is a linear combination of the diagonal operators

$$|g\rangle \langle g|\,,\ |e\rangle \langle e|\,,\ |f\rangle \langle f|$$

and non diagonal ones

$$|e\rangle \langle g|\,, \quad |g\rangle \langle e|\,.$$

Thus the average slow dynamics of $\left|\bar{\phi}\right\rangle$ along $|f\rangle$ is decoupled from the ones along $|g\rangle$ and $|e\rangle$: if $\left\langle f|\bar{\phi}\right\rangle_{t=0} = 0$ then $\left\langle f|\bar{\phi}\right\rangle_t \approx 0$ for $t > 0$. Once we have eliminate the oscillating terms of pulsation Δ and $\Delta \pm \Omega$, we get the following Raman Hamiltonian H_{Raman}:

$$\begin{aligned}
\frac{H_{\text{Raman}}}{\hbar} = \mu_g^2 \left(\frac{|\mathbf{u}_g|^2}{\Delta} + \frac{|\mathbf{u}_e|^2}{\Delta + \Omega} \right) |g\rangle \langle g| + \mu_e^2 \left(\frac{|\mathbf{u}_g|^2}{\Delta - \Omega} + \frac{|\mathbf{u}_e|^2}{\Delta} \right) |e\rangle \langle e| \\
+ \frac{\mu_g \mu_e}{\Delta} \left(\mathbf{u}_g^* \mathbf{u}_e e^{\imath\delta t}\ |g\rangle \langle e| + \mathbf{u}_g \mathbf{u}_e^* e^{-\imath\delta t}\ |e\rangle \langle g| \right) \\
- \left(\frac{|\mu_g \mathbf{u}_g|^2 + |\mu_e \mathbf{u}_e|^2}{\Delta} + \frac{|\mu_g \mathbf{u}_e|^2}{\Delta + \Omega} + \frac{|\mu_e \mathbf{u}_g|^2}{\Delta - \Omega} \right) |f\rangle \langle f|
\end{aligned}$$

We have neglected δ versus Δ and $\Delta \pm \Omega$. This approximation is justify since it impacts only higher order correction terms. This ensures that H_{Raman} is rigorously Hermitian and not up to higher orders term.

The restriction of the dynamics to the sub-space spanned by $|g\rangle$ and $|e\rangle$ is possible as soon as $\langle\psi|f\rangle_0 = 0$, and we have an effective 2-level system obeying

$$\imath \frac{d}{dt} |\phi\rangle = \left(v_g\, |g\rangle \langle g| + v_e\, |e\rangle \langle e| + \frac{U_{eff} e^{-\imath\delta t}}{2}\ |e\rangle \langle g| + \frac{U_{eff}^* e^{\imath\delta t}}{2}\ |g\rangle \langle e| \right) |\phi\rangle$$

where $v_g, v_e \in \mathbb{R}$ and $U_{eff} \in \mathbb{C}$ are the control input:

$$v_g = \mu_g^2 \left(\frac{|\mathbf{u}_g|^2}{\Delta} + \frac{|\mathbf{u}_e|^2}{\Delta + \Omega} \right), \; v_e = \mu_e^2 \left(\frac{|\mathbf{u}_g|^2}{\Delta - \Omega} + \frac{|\mathbf{u}_e|^2}{\Delta} \right), \; U_{eff} = \frac{\mu_g \mu_e}{2\Delta} \mathbf{u}_g \mathbf{u}_e^*$$

The frame change $|\chi\rangle = e^{\frac{\imath \int_0^t (v_g + v_d)}{2}} e^{\frac{-\imath \delta t}{2} \sigma_z} |\phi\rangle$ yields

$$\imath \frac{d}{dt} |\chi\rangle = \left(\frac{U}{2} (|e\rangle \langle e| - |g\rangle \langle g|) + \frac{U_{eff}}{2} \; |e\rangle \langle g| + \frac{U_{eff}^*}{2} \; |g\rangle \langle e| \right) |\chi\rangle$$

with the scalar control $v_e - v_g - \delta = U \in \mathbb{R}$.

To summarize: up to a diagonal change on $|\psi\rangle$ and under the above three time-scales assumptions, the average slow dynamics of $|\psi\rangle$ follows the ones of a 2-level system as soon as $\langle \psi | f \rangle_{t=0} = 0$:

$$\imath \frac{d}{dt} |\psi\rangle = \left(\frac{U}{2} (|e\rangle \langle e| - |g\rangle \langle g|) + \frac{U_{eff}}{2} \; |e\rangle \langle g| + \frac{U_{eff}^*}{2} \; |g\rangle \langle e| \right) |\psi\rangle$$

with controls, $U \in \mathbb{R}$ and $U_{eff} \in \mathbb{C}$ related to complex laser amplitudes, $\mathbf{u}_g$ and $\mathbf{u}_e$, by

$$U + \delta = |\mathbf{u}_g|^2 \left(\frac{\mu_e^2}{\Delta - \Omega} - \frac{\mu_g^2}{\Delta} \right) + |\mathbf{u}_e|^2 \left(\frac{\mu_e^2}{\Delta} - \frac{\mu_g^2}{\Delta + \Omega} \right), \; U_{eff} = \frac{\mu_g \mu_e}{2\Delta} \mathbf{u}_g \mathbf{u}_e^*,$$

the physical control being $u = \mathbf{u}_g e^{\imath \Omega_g^L t} + \mathbf{u}_g^* e^{-\imath \Omega_g^L t} + \mathbf{u}_e e^{\imath \Omega_e^L t} + \mathbf{u}_e^* e^{-\imath \Omega_e^L t}$.

It suffices to take $U = 0$ and $U_{eff} = \omega_r \ll |\Delta|$ where $\omega_r > 0$ is constant to recover the Rabi oscillation:

$$|\psi\rangle_t = e^{-\frac{\imath \omega_r t}{2}} \sigma_x |\psi\rangle_0 .$$

As for a 2-level system, we have π-pulse (resp. $\frac{\pi}{2}$-pulse) when the time length T verifies $\omega_r T = \pi$ (resp. $\omega_r T = \frac{\pi}{2}$).

During such Raman pulses, the intermediate state $|f\rangle$ remains almost empty (i.e. $\langle \psi | f \rangle \approx 0$) and thus, as physicists say, the life time of $|f\rangle$ does not require to be long. This point should be studied in more details: in parallel to the three existing time-scales, we have to consider Γ, the inverse of the life time of $|f\rangle$; it seems, but we do not find any precise justification, that, if Γ and Δ are of same magnitude order, the approximations remain valid and there is no need to consider the instability of $|f\rangle$. This could also be true even if $|\Delta| \ll \Gamma \ll \Omega_g, \Omega_e$.

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 life-time. The incorporation into the $|\psi\rangle$-dynamics of such irreversible effects, is analogue to the incorporation of friction and viscous effects in classical Hamiltonian dynamics. Since more than 20 years, physicists have developed and also simplified the first models including environment and decoherence. In next section, we present two such models, one is stochastic and the other is deterministic: both are typical models used to described open quantum systems (see chapter 4 of [15] for a tutorial exposure and [6, 3] for more detailed presentations).

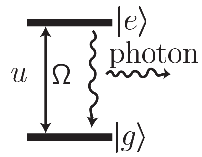

Figure 3. *2-level system, similar to figure 1, with spontaneous emission of one photon from the excited $|e\rangle$ of finite life-time Γ^{-1}.*

3. Decoherence for a 2-level system

3.1. Monte Carlo quantum trajectories

We consider, as illustrated on figure 3, a two level system with an unstable excited state $|e\rangle$ that could emit a spontaneous photon of pulsation $\Omega = \frac{E_e - E_g}{\hbar}$ followed by a quasi-instantaneous jump to the ground state $|g\rangle$. Such spontaneous emission is a stochastic process with jump. Between jumps occurring at random times and where the quantum state $|\psi\rangle$ is projected onto $|g\rangle$, $|\psi\rangle$ evolves according to a deterministic dynamics.

Spontaneous emission is characterized by the following non-Hermitian operator:

$$L = \sqrt{\Gamma}\,|g\rangle\,\langle e|$$

where Γ is homogenous to a frequency and its inverse coincides with the life-time of $|e\rangle$. The deterministic evolution between jumps depends on the usual controlled Hamiltonian

$$\frac{H}{\hbar} = \frac{\Omega}{2}(|e\rangle\,\langle e| - |g\rangle\,\langle g|) + \frac{u}{2}(|e\rangle\,\langle g| + |g\rangle\,\langle e|)$$

where $u(t) \in \mathbb{R}$. The system is still described by the quantum state $|\psi\rangle \in \mathbb{C}^2$ of length one but it obeys now to the Monte Carlo dynamics described here below.

Take a small time-step $\delta t > 0$ such that

$$\Gamma\delta t \ll 1, \quad \Omega\delta t \ll \quad \text{and} \quad |u|\delta t \ll 1.$$

The transition between $|\psi(t)\rangle$ and $|\psi(t+\delta t)\rangle$ follows the following rules:

1) Compute the probability p

$$p = \langle\psi(t)|\,L^\dagger L\,|\psi(t)\rangle\,\delta t = \Gamma|\psi_e|^2\delta t$$

for a jump to occur between t and $t+\delta t$. Since $\Gamma\delta t \ll 1$, we have $0 \leq p \ll 1$.

2) Take randomly a variable σ in $[0,1]$ according to the uniform distribution on $[0,1]$.

3) If $0 \leq \sigma \leq 1-p$, there is no jump, no photon emission and thus no click at the photo-detector. In this case:

$$|\psi(t+\delta t)\rangle = \frac{1 - \imath\delta t\frac{H}{\hbar} - \delta t\frac{L^\dagger L}{2}}{\sqrt{1-p}}\;|\psi(t)\rangle$$

Since $p \ll 1$ and $\Omega\delta t, |u|\delta t, \Gamma\delta t \ll 1$ we see that $|\psi(t+\delta t)\rangle$ is very close to $|\psi(t)\rangle$. This corresponds to a continuous evolution. Moreover the division by $\sqrt{1-p}$ ensures that $|\psi(t+\delta t)\rangle$ remains, up to order 2 in δt, of length 1.

4) If $1-p<\sigma\leq 1$, then a jump occurs with emission of a photon and thus with a click at the photo-detector. In this case we have

$$|\psi(t+\delta t)\rangle = \frac{L\,|\psi(t)\rangle}{\sqrt{p/\delta t}}$$

and up to a global phase $|\psi(t+\delta t)\rangle$ coincides with $|g\rangle$. It is a true jump and $|\psi(t+\delta t)\rangle$ is not close to $|\psi(t)\rangle$.

When $\Gamma = 0$, i.e. when the life time of $|e\rangle$ is infinite, $L=0$, there is no jump, no spontaneous emitted photon and $|\psi\rangle$ obeys the usual Schrödinger dynamics $\imath\hbar\,\frac{d}{dt}\,|\psi\rangle = H\,|\psi\rangle$.

Such jump processes describe the input/output relationship for a single 2-level system, such as two electronic level of an ion in a Paul trap. The input is the control u representing a classical electro-magnetic wave generated by a laser, for example. The output is then the signal of a photo-detector that captures the emitted photon and for each captured photon, the photo-detector generates a simple click and increment a counter. In practice the photo-detector captures in average one photon on a set of n emitted photon, n being around 10 and $\eta = 1/n\ \in]0,1[$ being then the efficiency of the detection process. We could imagine an output feedback loop for such input/ouput system: how to change the control u in real-time and according the past click sequences of the photo-detector to ensure a certain control goal. For instance, if u is quasi-resonant, $u = \mathbf{u}e^{\imath\Omega^L t} + \mathbf{u}^* e^{-\imath\Omega^L t}$ with $\Omega^L \approx \Omega$, how to adjust Ω^L in order to lock the laser frequency Ω^L exactly to the atomic one Ω. The goal will be to find a real-time synchronization feedback loop that could be an alternative to the synchronization scheme invented by physicist for atomic clocks (see, e.g., the thesis [33]). A first response to this problem is proposed in [28].

3.2. Lindblad-Kossakowski master equation

For a large number of identical 2-level systems without interaction and submitted to the same control u, the previous input/output relationship can be described by a deterministic dynamics of internal state ρ, the density operator that satisfies the Lindblad-Kossakowski master differential equation. The link with the above quantum trajectories is as follows. Consider the average, at the same time t, of a large number N of quantum trajectories $\left|\psi^k(t)\right\rangle$, $k=1,\ldots,N$, each of them follows the same stochastic process with the same control u (N realizations of the same stochastic process). The average is performed via the density matrix:

$$\rho(t) = \frac{\sum_{k=1}^{N}\left|\psi^k(t)\right\rangle\left\langle\psi^k(t)\right|}{N}.$$

For N large ρ satisfies the following differential matrix equation (Lindblad-Kossakowski master equation)

$$\frac{d}{dt}\rho = -\frac{\imath}{\hbar}[H,\rho] + L\rho L^\dagger - \frac{1}{2}\left(L^\dagger L\rho + \rho L^\dagger L\right)$$

where $y(t) = \eta\mathrm{tr}\left(\rho L^\dagger L\right)$ is the number of clicks per time-unit and $\eta\in]0,1[$ is the detection efficiency.

Contrarily to the Schrödinger equation (see, e.g., [36, 2]), the controllability of such master equation is not well understood, up-to now. Concerning the input/output relation between u and y, control techniques have to be adapted to the design of output feedback in order to exploit fully the very specific structure of this input/output relationship.

4. Spin/spring systems

4.1. Harmonic oscillator

A complete and much more tutorial exposure is available in [9]. We just recall here the basic facts needed in the next subsections. The Hamiltonian formulation of a classical harmonic oscillator of pulsation ω, $\frac{d^2}{dt^2}x = -\omega^2 x$, reads:

$$\frac{d}{dt}x = \omega p = \frac{\partial \mathcal{H}}{\partial p}, \quad \frac{d}{dt}p = -\omega x = -\frac{\partial \mathcal{H}}{\partial x}$$

where the classical Hamiltonian $\mathcal{H} = \frac{\omega}{2}(p^2+x^2)$. The correspondence principle gives directly, from the classical Hamiltonian formulation, its quantization. The classical Hamiltonian becomes then a operator, H, operating on complex-value functions of one real variable $x \in \mathbb{R}$. The quantum state $|\psi\rangle$ is thus a function of x and t. It is also denoted here by $\psi(x,t)$. This function admits complex value and, for each time t, its square module is integrable over $x \in \mathbb{R}$ with $\int |\psi(x,t)|^2 dx = 1$: at each time t, $|\psi\rangle_t \in L^2(\mathbb{R}, \mathbb{C})$.

The Hamiltonian operator H is obtained by replacing, in the classical Hamiltonian $\mathcal{H}$, x by the operator X, the multiplication by x, p by the derivation $P = -\imath \frac{\partial}{\partial x}$. Thus we have

$$\frac{H}{\hbar} = \frac{\omega}{2}(P^2 + X^2) = -\frac{\omega}{2}\frac{\partial^2}{\partial x^2} + \frac{\omega}{2}x^2.$$

The Schrödinger equation

$$\imath\hbar\frac{d}{dt}|\psi\rangle = H|\psi\rangle$$

is then a partial differential equation that determines the evolution of the probability amplitude wave function $\psi(x,t)$:

$$\imath\frac{\partial \psi}{\partial t}(x,t) = -\frac{\omega}{2}\frac{\partial^2 \psi}{\partial x^2}(x,t) + \frac{\omega}{2}x^2\psi(x,t), \quad x \in \mathbb{R}.$$

The averaged position is

$$\bar{X}(t) = \langle \psi | X | \psi \rangle = \int_{-\infty}^{+\infty} x|\psi|^2 dx,$$

and averaged impulsion reads

$$\bar{P}(t) = \langle \psi | P | \psi \rangle = -\imath \int_{-\infty}^{+\infty} \psi^* \frac{\partial \psi}{\partial x} dx.$$

One can verify via integration by part that $P(t)$ is real. With the annihilation and creation operators, a and $a^\dagger$,

$$a = \frac{X + \imath P}{\sqrt{2}} = \frac{1}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right), \quad a^\dagger = \frac{X - \imath P}{\sqrt{2}} = \frac{1}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right)$$

we have

$$[a, a^\dagger] = 1, \quad \frac{H}{\hbar} = \omega\left(a^\dagger a + \tfrac{1}{2}\right).$$

With $[a, a^\dagger] = 1$, the spectral decomposition of $a^\dagger a$ is very simple and justifies the denomination of annihilation and creation operators for a and $a^\dagger$. The Hermitian operator $a^\dagger a$ admits $\mathbb{N}$ as non degenerate spectrum. The unitary eigen-state associated to the eigenvalue $n \in \mathbb{N}$ is denoted by $|n\rangle$: it is also called a Fock state and n is the number of quanta of vibration (phonon or photon). Moreover for any $n > 0$,

$$a|n\rangle = \sqrt{n}\,|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle.$$

The ground state $|0\rangle$ satisfies $a|0\rangle = 0$ and corresponds to the Gaussian function:

$$\psi_0(x) = \frac{1}{\pi^{1/4}}\exp(-x^2/2).$$

The operator a (resp. $a^\dagger$) is the annihilation (resp. creation) operator since it transfers $|n\rangle$ to $|n-1\rangle$ (resp. $|n+1\rangle$) and thus decreases (resp. increases) the quantum number by one unit.

Add a control u and consider the controlled harmonic oscillator $\frac{d^2}{dt^2}x = -\omega^2 x - \frac{1}{\sqrt{2}}u$. Its quantization yields the following controlled Hamiltonian [4]

$$\frac{H}{\hbar} = \omega\left(a^\dagger a + \tfrac{1}{2}\right) + u(a + a^\dagger).$$

One can prove that this system is not controllable (Lie algebra of dimension 4). This result is known since more than 40 years in the physics community but under another formulation. The control theoretic version was given recently in [26] and [27].

4.2. A two-level atom in a cavity

This composite system is made of a 2-level system of states $|g\rangle$ and $|e\rangle$ and a quantized harmonic oscillator with a control u. Physically, an atom with two electronic levels is resonantly in interaction with a quantized mode of an electro-magnetic cavity (cavity quantum electro-dynamic with a Rydberg atom [15]). The quantum state $|\psi\rangle$ lives thus in the tensor product of $\mathbb{C}^2$ and $L^2(\mathbb{R}, \mathbb{C})$[5]. Thus $|\psi\rangle$ admits two components $(\psi_g(x,t), \psi_e(x,t))$ where, for each t, the complex value functions ψ_g and ψ_e belong to $L^2(\mathbb{R}, \mathbb{C})$. The Hamiltonian of this composite system is the sum of three Hamiltonians: the Hamiltonian H_a of the 2-level system alone (a for atom), the Hamiltonian of the controlled harmonic oscillator alone H_c (c for cavity) and finally the interaction Hamiltonian H_{int} (int for interaction). We have

$$\frac{H_a}{\hbar} = \frac{\Omega}{2}(|e\rangle\langle e| - |g\rangle\langle g|) = \frac{\Omega}{2}\sigma_z, \quad \frac{H_c}{\hbar} = \omega\left(a^\dagger a + \tfrac{1}{2}\right) + u(a + a^\dagger)$$

with $\Omega \approx \omega$. Since $|\psi\rangle \in \mathbb{C}^2 \otimes L^2(\mathbb{R}, \mathbb{C})$, we should write (to be rigorous):

$$\frac{H_a}{\hbar} = \frac{\Omega}{2}\,\sigma_z \otimes I_{L^2(\mathbb{R},\mathbb{C})}, \quad \frac{H_c}{\hbar} = \omega\, I_{\mathbb{C}^2} \otimes \left(a^\dagger a + \tfrac{1}{2}\right) + u\, I_{\mathbb{C}^2} \otimes (a + a^\dagger).$$

4. Notice the similarity with the controlled Hamiltonian of a 2-level system where the annihilation operator a is replaced by $\sigma^- = |g\rangle\langle e|$, the jump operator from the excited state $|e\rangle$ to the ground state $|g\rangle$.

5. See appendix A for some basic fact on composite systems and tensor product.

Since these rigorous notations are quite inefficient and here unnecessary, we abandon the tensor products sign and identity operators, as done previously. Thus H_a and H_c commute since they act on different spaces. However, the interaction Hamiltonian H_{int} is based on a true tensor product of two non trivial operators. It admits the following form (dipolar and long wave-length approximations):

$$\frac{H_{\text{int}}}{\hbar} = \frac{\omega_0}{2}(|e\rangle\langle g| + |g\rangle\langle e|)(a+a^\dagger) = \frac{\omega_0}{2}\sigma_x(a+a^\dagger)$$

where the tensor product is noted as a simple product [6]. The pulsation ω_0 is called the vacuum Rabi pulsation. Thus the complete Hamiltonian, called Jaynes and Cummings Hamiltonian [17], reads with these compact notations:

$$\frac{H_{JC}}{\hbar} = \frac{\Omega}{2}\sigma_z + \omega\left(a^\dagger a + \tfrac{1}{2}\right) + u(a+a^\dagger) + \frac{\omega_0}{2}\sigma_x(a+a^\dagger).$$

The different scale assumptions are:

$$\omega_0 \ll \Omega, \omega, \qquad |\Omega - \omega| \ll \Omega, \omega \qquad \text{and} \qquad |u| \ll \Omega, \omega.$$

The wave function $|\psi\rangle$ obeys to the Schrödinger equation: $\imath\hbar\frac{d}{dt}|\psi\rangle = H_{JC}|\psi\rangle$. With the new wave function $|\phi\rangle$ defined by

$$|\psi\rangle = e^{-\imath\omega t\left(a^\dagger a + \frac{1}{2}\right)} e^{\frac{-\imath\Omega t}{2}\sigma_z}|\phi\rangle$$

the passage to the interaction frame reads,

$$\imath\frac{d}{dt}|\phi\rangle = \left(u(e^{-\imath\omega t}a + e^{\imath\omega t}a^\dagger) + \frac{\omega_0}{2}(e^{-\imath\omega t}a + e^{\imath\omega t}a^\dagger)(e^{-\imath\Omega t}|g\rangle\langle e| + e^{\imath\Omega t}|e\rangle\langle g|)\right)|\phi\rangle.$$

This comes from the following relationships:

$$e^{\frac{\imath\Omega t}{2}\sigma_z}\,\sigma_x e^{-\frac{\imath\Omega t}{2}\sigma_z} = e^{-\imath\Omega t}|g\rangle\langle e| + e^{\imath\Omega t}|e\rangle\langle g|$$

and, since $[a, a^\dagger] = 1$, we have also

$$e^{\imath\omega t\left(a^\dagger a + \frac{1}{2}\right)}\, a\, e^{-\imath\omega t\left(a^\dagger a + \frac{1}{2}\right)} = e^{-\imath\omega t}a \quad \text{and} \quad e^{\imath\omega t\left(a^\dagger a + \frac{1}{2}\right)}\, a^\dagger\, e^{-\imath\omega t\left(a^\dagger a + \frac{1}{2}\right)} = e^{\imath\omega t}a^\dagger.$$

The control magnitude being small, u is chosen in quasi-resonance with the cavity frequency:

$$u = \mathbf{u}e^{\imath\omega^L t} + \mathbf{u}^* e^{-\imath\omega^L t}$$

with $\mathbf{u}$ complex amplitude and

$$|\omega^L - \omega| \ll \omega, \quad |\mathbf{u}| \ll \omega, \quad \left|\frac{d}{dt}\mathbf{u}\right| \ll \omega|\mathbf{u}|.$$

We face an oscillating system with two large pulsations $\omega + \Omega$ and $\omega + \omega^L$. Denote by $\delta = \omega - \omega^L$ the control/cavity de-tuning and by $\Delta = \Omega - \omega$ the cavity/atom de-tuning. By assumptions $|\delta|, |\Delta| \ll \omega$ and thus we use the secular approximation and neglect the highly oscillating terms with zero time-averages. The justification of this

6. The rigorous expression is $\frac{H_{\text{int}}}{\hbar} = \frac{\omega_0}{2}\sigma_x \otimes (a+a^\dagger)$.

approximation is standard for finite dimensional systems. Here, the dimension is infinite and some theoretical cautions could be useful. We do not find precise mathematical results covering directly such situations: some adaptations of the infinite dimensional results in [35] are needed. These mathematical questions are interesting but we abandon them in this paper and we assume that the average Hamiltonian

$$ue^{-\imath\delta t}a + u^* e^{\imath\delta t}a^\dagger + \frac{\omega_0}{2}e^{\imath\Delta t}a\,|e\rangle\,\langle g| + \frac{\omega_0}{2}e^{-\imath\Delta t}a^\dagger\,|g\rangle\,\langle e|$$

describes correctly the dynamics. The change of $|\phi\rangle$ to $|\chi\rangle$ defined by

$$|\phi\rangle = e^{\imath\delta t\left(a^\dagger a+\frac{1}{2}\right)}e^{\frac{\imath\Delta t}{2}\sigma_z}\,|\chi\rangle$$

yields the effective Jaynes-Cummings Hamiltonian:

$$\frac{\bar{H}_{JC}}{\hbar} = \delta\,\left(a^\dagger a + \tfrac{1}{2}\right) + \mathbf{u}a + \mathbf{u}^* a^\dagger + \frac{\Delta}{2}\sigma_z + \frac{\omega_0}{2}a|e\rangle\,\langle g| + \frac{\omega_0}{2}a^\dagger|g\rangle\,\langle e|.$$

Decompose $\bar{H}_{JC}$ according to $H_0 + u_1 H_1 + u_2 H_2$ where $\sqrt{2}\mathbf{u} = u_1 + \imath u_2$ with $u_1, u_2 \in \mathbb{R}$. Then, we have

$$\frac{H_0}{\hbar} = \frac{\delta}{2}(X^2+P^2) + \frac{\Delta}{2}\sigma_z + \frac{\omega_0}{\sqrt{2}}(X\sigma_x - P\sigma_y), \quad \frac{H_1}{\hbar} = X, \quad \frac{H_2}{\hbar} = P.$$

With the commutation rules for the Pauli matrices $\sigma_{x,y,z}$ (see appendix B) and the Heisenberg commutation relation $[X,P] = \imath$, the Lie algebra spanned by $\imath H_0$, $\imath H_1$ and $\imath H_2$ is of infinite dimension. Thus, it is natural to conjecture that this system is controllable. To fix the problem, it is useful to translate it into the partial differential language where powerful tools exist for studying linear and nonlinear controllability (see, e.g., the recent book [10]). Since $a = \frac{1}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right)$ and $a^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right)$, $\imath\hbar\frac{d}{dt}\,|\chi\rangle = \bar{H}_{JC}\,|\chi\rangle$ reads as a system of two partial differential equations affine in the two scalar controls $u_1 = \sqrt{2}\Re(\mathbf{u})$ and $u_2 = \sqrt{2}\Im(\mathbf{u})$. The quantum state $|\chi\rangle$ is described by two elements of $L^2(\mathbb{R},\mathbb{C})$, χ_g and χ_e, those time evolution is given by

$$\begin{aligned}
\imath\frac{\partial\chi_g}{\partial t} &= -\frac{\delta}{2}\frac{\partial^2\chi_g}{\partial x^2} + \frac{\delta x^2 - \Delta}{2}\chi_g + \left(u_1 x + \imath u_2\frac{\partial}{\partial x}\right)\chi_g + \frac{\omega_0}{2\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right)\chi_e \\
\imath\frac{\partial\chi_e}{\partial t} &= -\frac{\delta}{2}\frac{\partial^2\chi_e}{\partial x^2} + \frac{\delta x^2 + \Delta}{2}\chi_e + \left(u_1 x + \imath u_2\frac{\partial}{\partial x}\right)\chi_e + \frac{\omega_0}{2\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right)\chi_g.
\end{aligned}$$

An open question is the controllability on the set of functions (χ_g, χ_e) defined up to a global phase and such that $\|\chi_g\|_{L^2} + \|\chi_e\|_{L^2} = 1$. In a first step, one can take $\delta = 0$ (which is not a limitation in fact) and $\Delta = 0$ (which is a strict sub-case).

4.3. A single trapped ion

It is a composite system with a quantum state similar to the above subsection: $|\psi\rangle$ belongs to $\mathbb{C}^2 \otimes L^2(\mathbb{R},\mathbb{C})$ and the Hamiltonian reads

$$\frac{H}{\hbar} = \omega\left(a^\dagger a + \tfrac{1}{2}\right) + \frac{\Omega}{2}\sigma_z + \left[\mathbf{u}e^{\imath(\Omega^L t - kX)} + \mathbf{u}^* e^{-\imath(\Omega^L t - kX)}\right]\sigma_x$$

where the control is an electro-magnetic wave of complex amplitude $\mathbf{u}$ and with a phase $\Omega^L t - kx$ depending on the spatial coordinate x. It is thus an operator $\Omega t - kX$ with

$kX = \eta(a + a^\dagger)$ where η is the Lamb-Dicke parameter, of small magnitude in general. Such x-dependence ensures the impulsion conservation: when the ion absorbs a photon, its energy changes (increase of $\hbar\Omega^L$) but also its impulsion captures the photon impulsion $\hbar k$. Such impulsion changes excite the vibration mode inside the trap described here as a simple harmonic oscillator. The ion vibration are quantized, each quantum being called a phonon. The scales are as follows:

$$|\Omega_L - \Omega| \ll \Omega, \quad \omega \ll \Omega, \quad |\mathbf{u}| \ll \Omega, \quad \left|\frac{d}{dt}\mathbf{u}\right| \ll \Omega|\mathbf{u}|.$$

In the "laser frame", $|\psi\rangle = e^{-\frac{\imath\Omega^L t}{2}\sigma_z} |\phi\rangle$, the Hamiltonian becomes:

$$\omega\left(a^\dagger a + \tfrac{1}{2}\right) + \frac{\Omega - \Omega^L}{2}\sigma_z + \left(\mathbf{u}e^{2\imath\Omega^L t}e^{-\imath\eta(a+a^\dagger)} + \mathbf{u}^* e^{\imath\eta(a+a^\dagger)}\right)|e\rangle\langle g| \\ + \left(\mathbf{u}e^{-\imath\eta(a+a^\dagger)} + \mathbf{u}^* e^{\imath\eta(a+a^\dagger)}e^{-2\imath\Omega^L t}\right)|g\rangle\langle e|$$

As for the Jaynes-Cummings system, the secular approximation yields the following effective Hamiltonian

$$\frac{\bar{H}}{\hbar} = \left(a^\dagger a + \tfrac{1}{2}\right) + \frac{\Omega - \Omega^L}{2}\sigma_z + \mathbf{u}e^{-\imath\eta(a+a^\dagger)}|g\rangle\langle e| + \mathbf{u}^* e^{\imath\eta(a+a^\dagger)}|e\rangle\langle g|$$

with $\Delta = \Omega - \Omega_L$ the laser de-tuning. The Schrödinger equation $\imath\hbar\frac{d}{dt}|\phi\rangle = \bar{H}|\phi\rangle$ is a partial differential system on the two components (ϕ_g, ϕ_e):

$$\imath\frac{\partial\phi_g}{\partial t} = \frac{\omega}{2}\left(x^2 - \frac{\partial^2}{\partial x^2}\right)\phi_g - \frac{\Delta}{2}\phi_g + \mathbf{u}e^{-\imath\sqrt{2}\eta x}\phi_e$$
$$\imath\frac{\partial\phi_e}{\partial t} = \mathbf{u}^* e^{\imath\sqrt{2}\eta x}\phi_g + \frac{\omega}{2}\left(x^2 - \frac{\partial^2}{\partial x^2}\right)\phi_e + \frac{\Delta}{2}\phi_e.$$

Here $\mathbf{u} \in \mathbb{C}$ is the control input. As for the Jaynes-Cummings system, the controllability of this system is an open question.

Assume that u is a superposition of three mono-chromatic plane waves of pulsation Ω (ion electronic transition) and amplitude $\mathbf{u}$, of pulsation $\Omega - \omega$ (red shift by a vibration quantum) and amplitude $\mathbf{u}_r$, of pulsation $\Omega + \omega$ (blue shift by a vibration quantum) and amplitude $\mathbf{u}_b$. With this control, the Hamiltonian reads

$$\begin{aligned} H =& \omega\left(a^\dagger a + \tfrac{1}{2}\right) + \frac{\Omega}{2}\sigma_z + \left(\mathbf{u}e^{\imath(\Omega t - \eta(a+a^\dagger))} + \mathbf{u}^* e^{-\imath(\Omega t - \eta(a+a^\dagger))}\right)\sigma_x \\ &+ \left(\mathbf{u}_b e^{\imath((\Omega+\omega)t - \eta_b(a+a^\dagger))} + \mathbf{u}_b^* e^{-\imath((\Omega+\omega)t - \eta_b(a+a^\dagger))}\right)\sigma_x \\ &+ \left(\mathbf{u}_r e^{\imath((\Omega-\omega)t - \eta_r(a+a^\dagger))} + \mathbf{u}_r^* e^{-\imath((\Omega-\omega)t - \eta_r(a+a^\dagger))}\right)\sigma_x. \end{aligned}$$

We still have $\omega \ll \Omega$. The Lamb-Dicke parameters $|\eta|, |\eta_b|, |\eta_r| \ll 1$ are almost identical. The amplitudes vary very slowly:

$$\left|\frac{d}{dt}\mathbf{u}\right| \ll \omega|\mathbf{u}|, \quad \left|\frac{d}{dt}\mathbf{u}_r\right| \ll \omega|\mathbf{u}_r|, \quad \left|\frac{d}{dt}\mathbf{u}_b\right| \ll \omega|\mathbf{u}_b|.$$

In the interaction frame, $|\psi\rangle$ is replaced by $|\phi\rangle$ according to

$$|\psi\rangle = e^{-\imath\omega t\left(a^\dagger a+\frac{1}{2}\right)} e^{\frac{-\imath\Omega t}{2}\sigma_z} |\phi\rangle .$$

The Hamiltonian becomes

$$\begin{aligned} e^{\imath\omega t\left(a^\dagger a\right)} &\left(\mathbf{u} e^{\imath\Omega t} e^{-\imath\eta(a+a^\dagger)} + \mathbf{u}^* e^{-\imath\Omega t} e^{\imath\eta(a+a^\dagger)}\right) \\ & \qquad e^{-\imath\omega t\left(a^\dagger a\right)} \left(e^{\imath\Omega t} |e\rangle\langle g| + e^{-\imath\Omega t} |g\rangle\langle e|\right) \\ & + e^{\imath\omega t\left(a^\dagger a\right)} \left(\mathbf{u}_b e^{\imath(\Omega+\omega)t} e^{-\imath\eta_b(a+a^\dagger)} + \mathbf{u}_b^* e^{-\imath(\Omega+\omega)t} e^{\imath\eta_b(a+a^\dagger)}\right) \\ & \qquad e^{-\imath\omega t\left(a^\dagger a\right)} \left(e^{\imath\Omega t} |e\rangle\langle g| + e^{-\imath\Omega t} |g\rangle\langle e|\right) \\ & + e^{\imath\omega t\left(a^\dagger a\right)} \left(\mathbf{u}_r e^{\imath(\Omega-\omega)t} e^{-\imath\eta_r(a+a^\dagger)} + \mathbf{u}_r^* e^{-\imath(\Omega-\omega)t} e^{\imath\eta_r(a+a^\dagger)}\right) \\ & \qquad e^{-\imath\omega t\left(a^\dagger a\right)} \left(e^{\imath\Omega t} |e\rangle\langle g| + e^{-\imath\Omega t} |g\rangle\langle e|\right) \end{aligned}$$

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

$$\begin{aligned} &\left(\mathbf{u} e^{\imath\Omega t}(1 - \imath\eta(e^{-\imath\omega t}a + e^{\imath\omega t}a^\dagger)) + \mathbf{u}^* e^{-\imath\Omega t}(1 + \imath\eta(e^{-\imath\omega t}a + e^{\imath\omega t}a^\dagger))\right) \\ & \qquad \left(e^{\imath\Omega t} |e\rangle\langle g| + e^{-\imath\Omega t} |g\rangle\langle e|\right) \\ & + \left(\mathbf{u}_b e^{\imath(\Omega+\omega)t}(1 - \imath\eta_b(e^{-\imath\omega t}a + e^{\imath\omega t}a^\dagger)) + \mathbf{u}_b^* e^{-\imath(\Omega+\omega)t}(1 + \imath\eta_b(e^{-\imath\omega t}a + e^{\imath\omega t}a^\dagger))\right) \\ & \qquad \left(e^{\imath\Omega t} |e\rangle\langle g| + e^{-\imath\Omega t} |g\rangle\langle e|\right) \\ & + \left(\mathbf{u}_r e^{\imath(\Omega-\omega)t}(1 - \imath\eta_r(e^{-\imath\omega t}a + e^{\imath\omega t}a^\dagger)) + \mathbf{u}_r^* e^{-\imath(\Omega-\omega)t}(1 + \imath\eta_r(e^{-\imath\omega t}a + e^{\imath\omega t}a^\dagger))\right) \\ & \qquad \left(e^{\imath\Omega t} |e\rangle\langle g| + e^{-\imath\Omega t} |g\rangle\langle e|\right) \end{aligned}$$

The oscillating terms (with pulsations 2Ω, $2\Omega\pm\omega$, $2(\Omega\pm\omega)$ and $\pm\omega$) have a zero average. The mean Hamiltonian, illustrated on figure 4, reads

$$\frac{\bar{H}}{\hbar} = \mathbf{u} |g\rangle\langle e| + \mathbf{u}^* |e\rangle\langle g| + \overline{\mathbf{u}}_b a |g\rangle\langle e| + \overline{\mathbf{u}}_b^* a^\dagger |e\rangle\langle g| + \overline{\mathbf{u}}_r a^\dagger |g\rangle\langle e| + \overline{\mathbf{u}}_r^* a |e\rangle\langle g|$$

where we have set $\overline{\mathbf{u}}_b = -\imath\eta_b\mathbf{u}_b$ and $\overline{\mathbf{u}}_r = -\imath\eta_r\mathbf{u}_r$. The above Hamiltonian is "valid" as soon as $|\eta|, |\eta_b|, |\eta_r| \ll 1$ and

$$|\mathbf{u}|, |\mathbf{u}_b|, |\mathbf{u}_r| \ll \omega, \quad \left|\frac{d}{dt}\mathbf{u}\right| \ll \omega|\mathbf{u}|, \left|\frac{d}{dt}\mathbf{u}_b\right| \ll \omega|\mathbf{u}_b|, \left|\frac{d}{dt}\mathbf{u}_r\right| \ll \omega|\mathbf{u}_r|.$$

To interpret the structure of the different operators building this average Hamiltonian, physicists have a nice mnemonics tick based on energy conservation. Take for example $a|g\rangle\langle e|$ attached to the control $\overline{\mathbf{u}}_b$, i.e. to the blue shifted photon of pulsation $\Omega+\omega$. The operator $|g\rangle\langle e|$ corresponds to the quantum jump from $|e\rangle$ to $|g\rangle$ whereas the operator a is the destruction of one phonon. Thus $a|g\rangle\langle e|$ is the simultaneous jump from $|e\rangle$ to

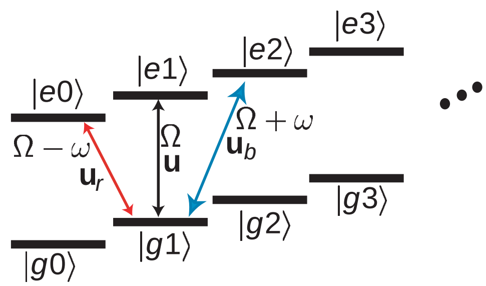

Figure 4. *a trapped ion submitted to three mono-chromatic plane waves of pulsations Ω, $\Omega-\omega$ and $\Omega+\omega$.*

$|g\rangle$ (energy change of $\hbar\Omega$) with destruction of one phonon (energy change of $\hbar\omega$). The emitted photon has to take away the total energy lost by the system, i.e. $\hbar\Omega + \hbar\omega$. Its pulsation is then $\Omega+\omega$ and corresponds thus to $\overline{\mathbf{u}}_b$. We understand why $a^\dagger |g\rangle \langle e|$ is associated to $\mathbf{u}_r$: the system looses $\hbar\Omega$ during the jump from $|e\rangle$ to $|g\rangle$; at the same time, it wins $\hbar\omega$, the phonon energy; the emitted photon takes away $\hbar\Omega - \hbar\omega$ and thus corresponds to $\overline{\mathbf{u}}_r$. This point is illustrated on figure 4 describing the different first order transitions between the different states of definite energy.

The dynamics $\imath\hbar\frac{d}{dt}|\phi\rangle = \bar{H}|\phi\rangle$ depends linearly on 6 scalar controls: it is a driftless system of infinite dimension (non-holonomic system of infinite dimension). The two underlying partial differential equations are

$$\imath\frac{\partial \phi_g}{\partial t} = \left(\mathbf{u} + \frac{\overline{\mathbf{u}}_b}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right) + \frac{\overline{\mathbf{u}}_r}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right)\right)\phi_e$$
$$\imath\frac{\partial \phi_e}{\partial t} = \left(\mathbf{u}^* + \frac{\overline{\mathbf{u}}_b^*}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right) + \frac{\overline{\mathbf{u}}_r^*}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right)\right)\phi_g$$

In the eigen-basis of the operator $\omega\left(a^\dagger a + \frac{1}{2}\right) + \frac{\Omega}{2}\sigma_z$, tensor product of the eigen-basic of the harmonic oscillator, $(|n\rangle)_{n\in\mathbb{N}}$, and of the 2-level system, $(|g\rangle, |e\rangle)$, $\{|gn\rangle, |en\rangle\}_{n\in\mathbb{N}}$, the above partial differential system reads

$$\imath\frac{d}{dt}\psi_{gn} = \mathbf{u}\psi_{en} + \overline{\mathbf{u}}_r\sqrt{n}\psi_{en-1} + \overline{\mathbf{u}}_b\sqrt{n+1}\psi_{en+1}$$
$$\imath\frac{d}{dt}\psi_{en} = \mathbf{u}^*\psi_{gn} + \overline{\mathbf{u}}_r^*\sqrt{n+1}\psi_{gn+1} + \overline{\mathbf{u}}_b^*\sqrt{n}\psi_{gn-1}$$

with $|\psi\rangle = \sum_{n=0}^{+\infty}\psi_{gn}|gn\rangle + \psi_{en}|en\rangle$ and $\sum_{n=0}^{+\infty}|\psi_{gn}|^2 + |\psi_{en}|^2 = 1$.

Law and Eberly [19] have proved that it is always possible (and in any arbitrary time $T>0$) to steer $|\psi\rangle$ from any finite linear superposition of $\{|gn\rangle, |en\rangle\}_{n\in\mathbb{N}}$ at $t=0$, to any other finite linear superposition at time $t=T$. They need only two controls $\mathbf{u}$ and $\overline{\mathbf{u}}_b$ (resp. $\mathbf{u}$ and $\overline{\mathbf{u}}_r$): $\overline{\mathbf{u}}_r$ (resp. $\overline{\mathbf{u}}_b$) remains zero and the supports of $\mathbf{u}$ and $\overline{\mathbf{u}}_b$ (resp. $\mathbf{u}$ and $\overline{\mathbf{u}}_r$) do not overlap. This spectral controllability implies approximate controllability. Is it possible to have a stronger result? Exact controllability? In what kind of functional spaces? Up to now these questions are open.

Notice that the adiabatic approach of [1] directly applies to this system and proves its approximate controllability.

4.4. Two trapped ions

Let us consider two ions catched in the same trap and coupled to one of the two vibration modes, the center of mass mode of frequency ω (see [15, chapitre 8] for detailed explanations and modeling assumptions). Considerations similar to the ones developed in the previous subsection yield to the following average Hamiltonian

$$\begin{aligned}(\mathbf{u}_1 + \mathbf{u}_{1b}a + \mathbf{u}_{1r}a^\dagger)\left(\left|g\right\rangle\left\langle e\right|\right)_1 + (\mathbf{u}_1^* + \mathbf{u}_{1b}^* a^\dagger + \mathbf{u}_{1r}^* a)\left(\left|e\right\rangle\left\langle g\right|\right)_1 \\ + (\mathbf{u}_2 + \mathbf{u}_{2b}a + \mathbf{u}_{2r}a^\dagger)\left(\left|g\right\rangle\left\langle e\right|\right)_2 + (\mathbf{u}_2^* + \mathbf{u}_{2b}^* a^\dagger + \mathbf{u}_{2r}^* a)\left(\left|e\right\rangle\left\langle g\right|\right)_2\end{aligned}$$

where the indices 1 and 2 are relative to ion number 1 and ion number 2, each of them having its own control, u_1 and u_2 that are superpositions of three mono-chromatic plane waves: pulsation Ω with amplitudes $\mathbf{u}_1$ and $\mathbf{u}_2$; pulsation $\Omega + \omega$ with amplitudes proportional to $\mathbf{u}_{1b}$ and $\mathbf{u}_{2b}$; pulsation $\Omega - \omega$ with amplitudes proportional to$\mathbf{u}_{1r}$ and $\mathbf{u}_{2r}$.

The quantum state $|\phi\rangle$ is described by 4 elements of $L^2[\mathbb{R}, \mathbb{C})$, $(\psi_{gg}, \psi_{ge}, \psi_{eg}, \psi_{ee})$. They satisfy the following partial differential system:

$$\begin{aligned}
\imath\frac{\partial}{\partial t}\phi_{gg} &= \left(\mathbf{u}_1 + \frac{\mathbf{u}_{1r}}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right) + \frac{\mathbf{u}_{1b}}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right)\right)\phi_{eg} \\
&\quad + \left(\mathbf{u}_2 + \frac{\mathbf{u}_{2r}}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right) + \frac{\mathbf{u}_{2b}}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right)\right)\phi_{ge} \\
\imath\frac{\partial}{\partial t}\phi_{eg} &= \left(\mathbf{u}_1^* + \frac{\mathbf{u}_{1r}^*}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right) + \frac{\mathbf{u}_{1b}^*}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right)\right)\phi_{gg} \\
&\quad + \left(\mathbf{u}_2 + \frac{\mathbf{u}_{2r}}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right) + \frac{\mathbf{u}_{2b}}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right)\right)\phi_{ee} \\
\imath\frac{\partial}{\partial t}\phi_{ge} &= \left(\mathbf{u}_1 + \frac{\mathbf{u}_{1r}}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right) + \frac{\mathbf{u}_{1b}}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right)\right)\phi_{ee} \\
&\quad + \left(\mathbf{u}_2^* + \frac{\mathbf{u}_{2r}^*}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right) + \frac{\mathbf{u}_{2b}^*}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right)\right)\phi_{gg} \\
\imath\frac{\partial}{\partial t}\phi_{ee} &= \left(\mathbf{u}_1^* + \frac{\mathbf{u}_{1r}^*}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right) + \frac{\mathbf{u}_{1b}^*}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right)\right)\phi_{ge} \\
&\quad + \left(\mathbf{u}_2^* + \frac{\mathbf{u}_{2r}^*}{\sqrt{2}}\left(x + \frac{\partial}{\partial x}\right) + \frac{\mathbf{u}_{2b}^*}{\sqrt{2}}\left(x - \frac{\partial}{\partial x}\right)\right)\phi_{eg}
\end{aligned}$$

We conjecture that this system is controllable (at least approximatively).

We recall here a 4-pulse sequence (see also [15]) that steers in finite time $|\psi\rangle$ from $|gg0\rangle$ at $t = 0$, ions in ground states and 0 phonon, to the intricate state (Bell state) at $t = 4T$,

$$\frac{|gg0\rangle + |ee0\rangle}{\sqrt{2}},$$

a coherent superposition of $|gg0\rangle$ and $|ee0\rangle$ (ions in excited states with 0 phonon). One proceeds in 4 successive pulses of duration $T > 0$ and where only one of the 6 controls is different form zero:

1) $\pi/2$-pulse on $\mathbf{u}_{b1}$: only $\mathbf{u}_{b1}$ differs from 0 and is equal to $-\imath\frac{\pi}{T}$; the Hamiltonian (with this particular control) leaves invariant the sub-space spanned by $|gg0\rangle$ and $|eg1\rangle$; since the initial state is $|gg0\rangle$, we have thus a simple $\pi/2$-pulse of Rabi type; it ends with $|\psi\rangle = \frac{|gg0\rangle+|eg1\rangle}{\sqrt{2}}$, exactly.

2) π-pulse on $\mathbf{u}_2$: we apply $\mathbf{u}_2 = -\imath\frac{2\pi}{T}$ and start with $|\psi\rangle = \frac{|gg0\rangle+|eg1\rangle}{\sqrt{2}}$; we finish the pulse with $|\psi\rangle = \frac{|ge0\rangle+|ee1\rangle}{\sqrt{2}}$

3) π-pulse on $\mathbf{u}_{b2}$: set $\mathbf{u}_{b2} = -\imath\frac{2\pi}{T}$; $|\psi\rangle$ is steered from $\frac{|ge0\rangle+|ee1\rangle}{\sqrt{2}}$ to $\frac{|ge0\rangle-|eg0\rangle}{\sqrt{2}}$ since the state $|ge0\rangle$ is not touched by the control $\mathbf{u}_{b2}$.

4) π-pulse on $\mathbf{u}_1$: we apply $\mathbf{u}_1 = -\imath\frac{2\pi}{T}$; $|\psi\rangle$ is steered from $\frac{|ge0\rangle-|eg0\rangle}{\sqrt{2}}$ to $\frac{|ee0\rangle+|gg0\rangle}{\sqrt{2}}$ a Bell state.

These kinds of open-loop controls have been tested experimentally to generate intricate quantum states and also quantum gates. They are made in a succession of pulses where only a single control is non zero. The situation is similar to what happens in robotics for car-like robot. It is possible to go from one initial position/orientation to any other position/orientation by a succession of two primitive motions: a primitive motion along circle of arbitrary radius and where the speed and the steering angle are both constant; a primitive "motion" where the speed is zero but where the steering angle is changed. It is clear that a usual car driver does not use such control strategy: he changes simultaneously and continuously the speed and the steering angle in a coordinated manner (as flatness-based motion planing algorithms do [31, 23]). We wonder if one cannot control similarly such quantum systems and replace pulses sequences by smooth open-loop controls varying simultaneously.

5. Conclusion

This paper is far from being exhaustive on control of quantum systems. We have just focused here on the most popular methods used by physicists and experimentally tested. Many other contributions are available, in particular in the applied mathematics community, on controllability, motion planing and optimal control of systems governed by Shrödinger equations. For finite dimensional systems, we have the works of Agrachev, Gauthier, Jurdjevic, Coron, Mirrahimi, Altafini, Boscain, Chambrion, ... ; for infinite dimensional systems, there are the contributions of Beauchard, Maday, Turinici, Coron, Mirrahimi, Salomon, Machtyngier, Zuazua, Lasieka, Triggiani, Zhang, Lebeau , Burq, Baudouin, Puel, ...

The current technological evolutions (laser, photo-detectors, optoelectronics, ...) tend to increase the bandwidth of actuators and sensors relevant of quantum systems. Thus questions around quantum feedback and estimation (filtering) to control decoherence will become more and more realistic and will constitute one of the basic subject of an emerging domain called "Quantum Engineering" (see the seminal works of Mabuchi, Belavkin and Rabitz on feedback, filtering and identification).

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A. Bra, Ket, quantum states, measures and composite systems

We just recall here some basic notions of quantum mechanics. We refer to the excellent course [9] where these notions are explained in details. Bra $\langle\bullet|$ and Ket $|\bullet\rangle$ are co-vector and vector. The quantum state is described by the ket $|\psi\rangle$ (belonging to an Hilbert space of finite or infinite dimension) also called (probability amplitude) wave function. For a 2-level system, $|\psi\rangle \in \mathbb{C}^2$ reads $|\psi\rangle = \psi_g |g\rangle + \psi_e |e\rangle$ with $\psi_g, \psi_e \in \mathbb{C}$ and

$$|g\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |e\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

The components of $|\psi\rangle$ are complex probability amplitudes and thus $|\psi_g|^2 + |\psi_e|^2 = 1$. It is usual to denote by $|g\rangle$ the quantum state of smallest energy (ground state) and by $|e\rangle$ the quantum state with the highest energy (excited state). A $\frac{1}{2}$-spin system is a 2-level system. In quantum information, one speaks also of qubit (single qubit) to design a 2-level system and notations are changed according to the correspondence: $|1\rangle = |g\rangle$ and $|0\rangle = |e\rangle$.

The Hermitian conjugate of a Ket is a Bra : $\langle\psi| = |\psi\rangle^\dagger = \psi_g^* \langle g| + \psi_e^* \langle e|$. The Hermitian product is defined as follows: for $|\psi\rangle = \psi_g |g\rangle + \psi_e |e\rangle$ and $|\phi\rangle = \phi_g |g\rangle + \phi_e |e\rangle$, their Hermitian product reads

$$\langle\psi|\phi\rangle = \psi_g^*\phi_g + \psi_e^*\phi_e.$$

An Hermitian operator M is a self-adjoint operator for the Hermitian product. In the ortho-normal frame $(|g\rangle, |e\rangle)$, M writes

$$M = m_g|g\rangle\langle g| + m_e|e\rangle\langle e| + m|e\rangle\langle g| + m^*|g\rangle\langle e|$$

with $m_g, m_e \in \mathbb{R}$ and $m \in \mathbb{C}$.

To each measurement process is attached an Hermitian operator, called also observable. Assume that we measure the energy $H = E_g |g\rangle\langle g| + E_e |e\rangle\langle e|$ with $E_g < E_e$ and that we have, at our disposal, a large number n of identical systems with the same quantum state $|\psi\rangle = \psi_g |g\rangle + \psi_e |e\rangle$. For each system, we measure H. We obtain

1) either E_g and then, just after the measure, $|\psi\rangle = |g\rangle$;

2) or E_e and then, just after the measure, $|\psi\rangle = |e\rangle$.

Denote by n_g (resp. n_e) the number of time we have obtained E_g (resp. E_e). For n large, we have

$$\frac{n_g}{n} \approx |\psi_g|^2, \quad \frac{n_e}{n} \approx |\psi_e|^2$$

(coherent with $n = n_g + n_e$ and $|\psi_g|^2 + |\psi_e|^2 = 1$). The average value of these n measures is thus $|\psi_g|^2 E_g + |\psi_e|^2 E_e$. This is the fundamental reason why one interprets the component of $|\psi\rangle$ as probability amplitudes. More generally, the measure of any observable M of a quantum state $|\psi\rangle$ gives, in average, the value $\langle\psi|M|\psi\rangle$.

A composite system is made of several sub-systems. It is very important to realize that the state space (Hilbert space) of a composite system is not the Cartesian product of the state space of its sub-systems, as it is the case for classical systems. It is the tensor product. This difference is essential. An n-qubit is a composite system made of n single qubits. Its state belongs to $\overbrace{\mathbb{C}^2 \otimes \mathbb{C}^2 \ldots \otimes \mathbb{C}^2}^{n \text{ times}}$ that is isomorphic to $\mathbb{C}^{2^n}$. This is very different from a Cartesian product that will produce $\mathbb{C}^{2n}$. The canonical basis of a 2-qubit is

$$|g\rangle \otimes |g\rangle = |gg\rangle, \quad |g\rangle \otimes |e\rangle = |ge\rangle, \quad |e\rangle \otimes |g\rangle = |eg\rangle, \quad |e\rangle \otimes |e\rangle = |ee\rangle.$$

The canonical basis of 3-qubit reads

$$|ggg\rangle, \quad |gge\rangle, \quad |geg\rangle, \quad |gee\rangle, \quad |egg\rangle, \quad |ege\rangle, \quad |eeg\rangle, \quad |eee\rangle.$$

The measure $\sigma_z = -|g\rangle\langle g| + |e\rangle\langle e|$ of the first qubit of a 2-qubit corresponds to the operator (observable) $M = \sigma_z \otimes I_d$. On the 2-qubit

$$|\psi\rangle = \psi_{gg} |gg\rangle + \psi_{ge} |ge\rangle + \psi_{eg} |eg\rangle + \psi_{ee} |ee\rangle$$

the measure of σ_z of the first qubit, gives, in average,

$$\langle\psi|M|\psi\rangle = -(|\psi_{gg}|^2 + |\psi_{ge}|^2) + (|\psi_{eg}|^2 + |\psi_{ee}|^2)$$

i.e., gives either -1 with a probability $|\psi_{gg}|^2 + |\psi_{ge}|^2$, or $+1$ with a probability $|\psi_{eg}|^2 + |\psi_{ee}|^2$. If, just before the measure of σ_z on the first qubit, the quantum state is $|\psi\rangle = \psi_{gg}\,|gg\rangle + \psi_{ge}\,|ge\rangle + \psi_{eg}\,|eg\rangle + \psi_{ee}\,|ee\rangle$, then, just after the measure, the quantum state is

– either $\frac{\psi_{gg}|gg\rangle+\psi_{ge}|ge\rangle}{\sqrt{|\psi_{gg}|^2+|\psi_{ge}|^2}} = |g\rangle \otimes \left(\frac{\psi_{gg}|g\rangle+\psi_{ge}|e\rangle}{\sqrt{|\psi_{gg}|^2+|\psi_{ge}|^2}}\right)$ if the measure is -1,

– or $\frac{\psi_{eg}|eg\rangle+\psi_{ee}|ee\rangle}{\sqrt{|\psi_{eg}|^2+|\psi_{ee}|^2}} = |e\rangle \otimes \left(\frac{\psi_{eg}|g\rangle+\psi_{ee}|e\rangle}{\sqrt{|\psi_{eg}|^2+|\psi_{ee}|^2}}\right)$ if the measure is $+1$

This is the famous "collapse of the wave packet" associated to any measurement process and on which is based the Copenhagen interpretation of the wave function $|\psi\rangle$.

B. Pauli Matrices

The Pauli matrices are 2×2 Hermitian matrices defined here below:

$$\sigma_x = |e\rangle\langle g| + |g\rangle\langle e|\,,\ \sigma_y = -\imath\,|e\rangle\langle g| + \imath\,|g\rangle\langle e|\,,\ \sigma_z = |e\rangle\langle e| - |g\rangle\langle g|\,.$$

They satisfy the following relations:

$$\sigma_x^2 \;=\; 1, \quad \sigma_y^2 \;=\; 1, \quad \sigma_z^2 \;=\; 1, \quad \sigma_x\sigma_y \;=\; \imath\sigma_z, \quad \sigma_y\sigma_z \;=\; \imath\sigma_x, \quad \sigma_z\sigma_x \;=\; \imath\sigma_y.$$

For any angle $\theta \in \mathbb{R}$ we have

$$e^{\imath\theta\sigma_\alpha} = \cos\theta + \imath\sin\theta\sigma_\alpha, \quad \text{for} \quad \alpha = x, y, z.$$

Thus the solution of the Schrödinger equation ($\Omega \in \mathbb{R}$)

$$\imath\frac{d}{dt}|\psi\rangle = \frac{\Omega}{2}\sigma_z\,|\psi\rangle$$

reads

$$|\psi\rangle_t = e^{\frac{-\imath\Omega t}{2}\sigma_z}\,|\psi\rangle_0 = \left(\cos\left(\frac{\Omega t}{2}\right) - \imath\sin\left(\frac{\Omega t}{2}\right)\sigma_z\right)\,|\psi\rangle_0$$

where $\cos\left(\frac{\Omega t}{2}\right)$ is a short-cut notation for $\cos\left(\frac{\Omega t}{2}\right) I_d$ with I_d the 2×2 identity matrix. For $\alpha, \beta = x, y, z$, $\alpha \neq \beta$ we have the useful formulae:

$$\sigma_\alpha e^{\imath\theta\sigma_\beta} = e^{-\imath\theta\sigma_\beta}\sigma_\alpha, \qquad \left(e^{\imath\theta\sigma_\alpha}\right)^{-1} = \left(e^{\imath\theta\sigma_\alpha}\right)^\dagger = e^{-\imath\theta\sigma_\alpha}$$

and also

$$e^{-\frac{\imath\theta}{2}\sigma_\alpha}\sigma_\beta e^{\frac{\imath\theta}{2}\sigma_\alpha} = e^{-\imath\theta\sigma_\alpha}\sigma_\beta = \sigma_\beta e^{\imath\theta\sigma_\alpha}$$

C. Averaging and oscillating systems

We summarize here the basic result and approximations used in this paper for single-frequency systems. One can consult [32, 13, 4] for much more elaborated results. We emphasize a particular computational trick that simplifies notably second order calculations. This trick is a direct extension of a computation explained in [18] and done by the soviet physicist Kapitsa for deriving the average motion of particle in a highly oscillating force field. We suspect that such nice computational trick has a direct interpretation in the non-standard analysis frame-work.

Consider the oscillating system of dimension n;

$$\frac{dx}{dt} = \varepsilon f(x,t,\varepsilon), \quad x \in \mathbb{R}^n$$

with f smooth and of period T versus t, where ε is a small parameter. For x bounded and $|\varepsilon|$ small enough exists a time-periodic change of variables, close to identity, of the form

$$x = z + \varepsilon w(z,t,\varepsilon)$$

with w smooth function and T-periodic versus t, such that, the differential equation in the z frame reads:

$$\frac{dz}{dt} = \varepsilon \overline{f}(z,\varepsilon) + \varepsilon^2 f_1(z,t,\varepsilon)$$

with

$$\overline{f}(z,\varepsilon) = \frac{1}{T}\int_0^T f(z,t,\varepsilon)\,dt$$

and f_1 smooth and T-periodic versus t.

Thus we can approximate on interval $[0, \frac{T}{\epsilon}]$ the trajectories of the oscillating system $\frac{dx}{dt} = \varepsilon f(x,t,\varepsilon)$ by those of the average one $\frac{dz}{dt} = \varepsilon \overline{f}(z,\varepsilon)$. More precisely, if $x(0) = z(0)$ then $x(t) = z(t) + O(|\varepsilon|)$ for all $t \in [0, \frac{T}{\epsilon}]$. Since this approximation is valid on intervals of length T/ε, we say that this approximation is of order one. One speaks also of secular approximation.

The function $w(z,t,\varepsilon)$ appearing in this change of variables is given by a t-primitive of $f - \bar{f}$. If we replace x by $z + \varepsilon w$ in $\frac{d}{dt}x = \varepsilon f$ we get

$$\left(I_d + \varepsilon \frac{\partial w}{\partial z}\right)\frac{d}{dt}z = \varepsilon f - \varepsilon \frac{\partial w}{\partial t} = \varepsilon \bar{f} + \varepsilon\left(f - \bar{f} - \frac{\partial w}{\partial t}\right).$$

Since for each z, the function $\int_0^t \left(f(z,\tau,\varepsilon) - \bar{f}(z,\varepsilon)\right) d\tau$ is T-periodic, we set

$$w(z,t,\varepsilon) = \int_0^t \left(f(z,\tau,\varepsilon) - \bar{f}(z,\varepsilon)\right)\, d\tau + c(z,\varepsilon)$$

where the integration "constant" $c(z,\varepsilon)$ can be set arbitrarily. We will see that a clever choice for c corresponds to w with a null time-average. We have

$$\left(I_d + \varepsilon \frac{\partial w}{\partial z}(z,t,\varepsilon)\right)\frac{d}{dt}z = \varepsilon \bar{f}(z,\varepsilon) + \varepsilon\left(f(z + \epsilon w(z,t,\varepsilon),t,\varepsilon) - f(z,t,\varepsilon)\right)$$

and thus

$$\frac{d}{dt}z = \varepsilon\left(I_d + \varepsilon\frac{\partial w}{\partial z}(z,t,\varepsilon)\right)^{-1}\left(\,\bar{f}(z,\varepsilon) + f(z+\epsilon w(z,t,\varepsilon),t,\varepsilon) - f(z,t,\varepsilon)\,\right).$$

We obtain the goal form , $\frac{d}{dt}z = \varepsilon\bar{f} + \varepsilon^2 f_1$, with

$$f_1(z,t,\varepsilon) = \frac{1}{\epsilon}\left(\left(\left(I_d + \varepsilon\frac{\partial w}{\partial z}(z,t,\varepsilon)\right)^{-1} - I_d\right)\bar{f}(z,\varepsilon)\right.$$
$$\left. + \left(I_d + \varepsilon\frac{\partial w}{\partial z}(z,t,\varepsilon)\right)^{-1}\frac{f(z+\epsilon w(z,t,\varepsilon),t,\varepsilon) - f(z,t,\varepsilon)}{\varepsilon}\right.$$

Notice that

$$f_1(z,t,\varepsilon) = \frac{\partial f}{\partial z}(z,t,\varepsilon)w(z,t,\varepsilon) - \frac{\partial w}{\partial z}(z,t,\varepsilon)\bar{f}(z,\varepsilon) + O(\varepsilon).$$

The second order approximation is then obtained by taking the time-average of f_1. Its justification is still based on a time-periodic change of variables of type $z = \zeta + \varepsilon^2\varpi(\zeta,t,\varepsilon)$, i.e., close to identity but up-to second order in ε.

If we adjust $c(z,\epsilon)$ in order to have w of null time-average, then the time-average of $\frac{\partial w}{\partial z}$ is also null. Thus, up to order one terms in ε, the time-average of f_1 is then identical to the time average of $\frac{\partial f}{\partial z}w$. For this particular choice of w, the second order approximation reads

$$\frac{d}{dt}x = \varepsilon\bar{f} + \varepsilon^2\overline{\frac{\partial f}{\partial x}w}$$

where the symbol "$\overline{}$" stands for time-average. The solutions of the oscillating system $\frac{d}{dt}x = \varepsilon f$ et those of the second order approximation here above remain close on time intervals of length $\frac{T}{\varepsilon^2}$.

A suggestive manner to compute this second order approximation and very efficient on physical examples is due to Kapitsa [18, page 147]. One decomposes $x = \bar{x} + \delta x$ in a non-oscillating part $\bar{x}$ of order 0 in ε and an oscillating part δx of order 1 in ε and of null time-average. One has

$$\frac{d}{dt}\bar{x} + \frac{d}{dt}\delta x = \varepsilon f(\bar{x} + \delta x, t, \varepsilon).$$

Since $\delta x = 0(\varepsilon)$, we have

$$f(\bar{x} + \delta x, t, \varepsilon) = f(\bar{x},t,\varepsilon) + \frac{\partial f}{\partial x}(\bar{x},t,\varepsilon)\delta x + O(\varepsilon^2).$$

Thus

$$\frac{d}{dt}\bar{x} + \frac{d}{dt}\delta x = \varepsilon f(\bar{x},t,\varepsilon) + \varepsilon\frac{\partial f}{\partial x}(\bar{x},t,\varepsilon)\delta x + O(\varepsilon^3).$$

Since $\frac{d}{dt}\bar{x} = \varepsilon\bar{f}(\bar{x},\varepsilon) + O(\varepsilon^2)$, identification of oscillating terms of null time-average and of first order in ϵ provides

$$\frac{d}{dt}(\delta x) = \varepsilon(f(\bar{x},t,\varepsilon) - \bar{f}(\bar{x},\varepsilon)).$$

This equation can be integrated in time since $\bar{x}$ is almost constant. The integration constant is fixed by the constraint on the time-average of δx. Finally,

$$\delta x = \varepsilon \int_0^t \left(f(\bar{x}, \tau, \varepsilon) - \bar{f}(\bar{x}, \varepsilon) \right) \, d\tau + \varepsilon c(\bar{x}, \varepsilon)$$

is a function of $(\bar{x}, t, \varepsilon)$, $\delta x = \delta x(\bar{x}, t, \varepsilon)$, T-periodic versus t and of null time-average (good choice of $c(\bar{x}, \varepsilon)$). Let us plug this function $\delta x(\bar{x}, t, \varepsilon)$ into the differential equation for $\bar{x}$,

$$\frac{d}{dt}\bar{x} = \varepsilon \bar{f}(\bar{x}, \varepsilon) + \varepsilon \frac{\partial f}{\partial x}(\bar{x}, t, \varepsilon) \delta x(\bar{x}, t, \varepsilon) + O(\varepsilon^3),$$

And let us take its time-average. We get

$$\frac{d}{dt}\bar{x} = \varepsilon \bar{f}(\bar{x}, \varepsilon) + \varepsilon^2 \bar{f}_1(\bar{x}, \varepsilon)$$

with

$$\varepsilon \bar{f}_1(\bar{x}, \varepsilon) = \frac{1}{T} \int_0^T \frac{\partial f}{\partial x}(\bar{x}, t, \varepsilon) \delta x(\bar{x}, t, \varepsilon) \, dt$$

We recover then exactly the previous second order approximation. In subsections 2.4 and 2.6, the calculations of the Bloch-Siegert shift and of the Raman Hamiltonian are conducted exactly along this method that is particularly efficient there.