

Modeling and Control of the LKB Photon-Box: ¹ Spin Systems

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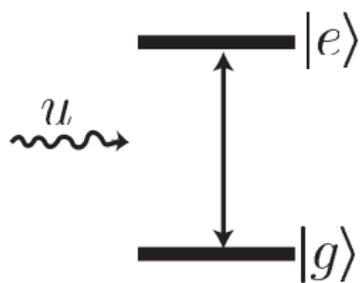
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¹LKB: Laboratoire Kastler Brossel, ENS, Paris.

Several slides have been used during the IHP course (fall 2010) given with Mazyar Mirrahimi (INRIA) see:

<http://cas.ensmp.fr/~rouchon/QuantumSyst/index.html> 

- 1 The 2-level system
- 2 RWA and averaging
- 3 Adiabatic control
- 4 Complements
 - Multi-frequency averaging: second order
 - STIRAP
 - Controllability of finite dimensional Schrödinger systems



The simplest quantum system: a ground state $|g\rangle$ of energy ω_g ; an excited state $|e\rangle$ of energy ω_e . The quantum state $|\psi\rangle \in \mathbb{C}^2$ is a linear superposition $|\psi\rangle = \psi_g |g\rangle + \psi_e |e\rangle$ and obeys to the Schrödinger equation (ψ_g and ψ_e depend on t).

Schrödinger equation for the uncontrolled 2-level system ($\hbar = 1$):

$$i \frac{d}{dt} |\psi\rangle = H_0 |\psi\rangle = (\omega_e |e\rangle \langle e| + \omega_g |g\rangle \langle g|) |\psi\rangle$$

where H_0 is the Hamiltonian, a Hermitian operator $H_0^\dagger = H_0$. Energy is defined up to a constant: H_0 and $H_0 + \varpi(t)\mathbf{1}$ ($\varpi(t) \in \mathbb{R}$ arbitrary) are attached to the same physical system. If $|\psi\rangle$ satisfies $i \frac{d}{dt} |\psi\rangle = H_0 |\psi\rangle$ then $|\chi\rangle = e^{-i\vartheta(t)} |\psi\rangle$ with $\frac{d}{dt} \vartheta = \varpi$ obeys to $i \frac{d}{dt} |\chi\rangle = (H_0 + \varpi I) |\chi\rangle$. Thus for any ϑ , $|\psi\rangle$ and $e^{-i\vartheta} |\psi\rangle$ represent the same physical system: The **global phase** of a quantum system $|\psi\rangle$ can be chosen **arbitrarily at any time**.

Take origin of energy such that ω_g (resp. ω_e) becomes $-\frac{\omega_e - \omega_g}{2}$ (resp. $\frac{\omega_e - \omega_g}{2}$) and set $\omega_{eg} = \omega_e - \omega_g$

The solution of $i\frac{d}{dt}|\psi\rangle = H_0|\psi\rangle = \frac{\omega_{eg}}{2}(|e\rangle\langle e| - |g\rangle\langle g|)|\psi\rangle$ is

$$|\psi\rangle_t = \psi_{g0} e^{\frac{i\omega_{eg}t}{2}} |g\rangle + \psi_{e0} e^{-\frac{i\omega_{eg}t}{2}} |e\rangle.$$

With a classical electromagnetic field described by $u(t) \in \mathbb{R}$, **the coherent evolution** the controlled Hamiltonian

$$H(t) = \frac{\omega_{eg}}{2} \sigma_z + \frac{u(t)}{2} \sigma_x = \frac{\omega_{eg}}{2} (|e\rangle\langle e| - |g\rangle\langle g|) + \frac{u(t)}{2} (|e\rangle\langle g| + |g\rangle\langle e|)$$

The controlled Schrödinger equation $i\frac{d}{dt}|\psi\rangle = (H_0 + uH_1)|\psi\rangle$ reads:

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

The 3 Pauli Matrices²

$$\sigma_x = |e\rangle\langle g| + |g\rangle\langle e|, \quad \sigma_y = -i|e\rangle\langle g| + i|g\rangle\langle e|, \quad \sigma_z = |e\rangle\langle e| - |g\rangle\langle g|$$

²They correspond, up to multiplication by i , to the 3 imaginary quaternions. 

$$\sigma_x = |e\rangle\langle g| + |g\rangle\langle e|, \quad \sigma_y = -i|e\rangle\langle g| + i|g\rangle\langle e|, \quad \sigma_z = |e\rangle\langle e| - |g\rangle\langle g|$$

$$\sigma_x^2 = \mathbf{1}, \quad \sigma_x\sigma_y = i\sigma_z, \quad [\sigma_x, \sigma_y] = 2i\sigma_z, \quad \text{circular permutation} \dots$$

- Since for any $\theta \in \mathbb{R}$, $e^{i\theta\sigma_x} = \cos\theta + i\sin\theta\sigma_x$ (idem for σ_y and σ_z), the solution of $i\frac{d}{dt}|\psi\rangle = \frac{\omega_{eg}}{2}\sigma_z|\psi\rangle$ is

$$|\psi\rangle_t = e^{\frac{-i\omega_{eg}t}{2}\sigma_z} |\psi\rangle_0 = \left(\cos\left(\frac{\omega_{eg}t}{2}\right) \mathbf{1} - i\sin\left(\frac{\omega_{eg}t}{2}\right) \sigma_z \right) |\psi\rangle_0$$

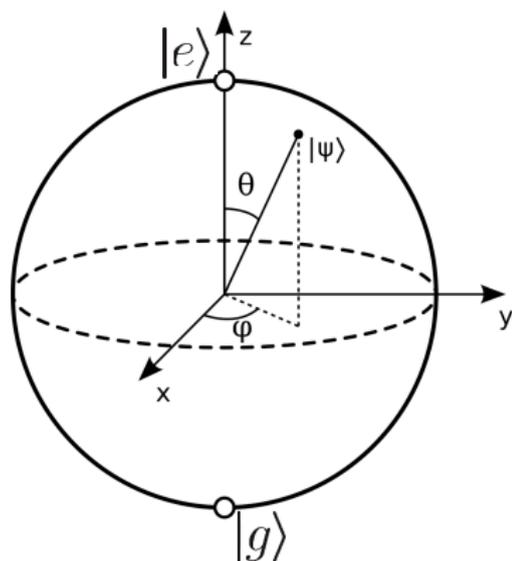
- For $\alpha, \beta = x, y, z$, $\alpha \neq \beta$ we have

$$\sigma_\alpha e^{i\theta\sigma_\beta} = e^{-i\theta\sigma_\beta} \sigma_\alpha, \quad \left(e^{i\theta\sigma_\alpha}\right)^{-1} = \left(e^{i\theta\sigma_\alpha}\right)^\dagger = e^{-i\theta\sigma_\alpha}.$$

and also

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

Bloch sphere representation of a 2-level system



if $|\psi\rangle$ obeys $\frac{d}{dt}|\psi\rangle = -iH|\psi\rangle$, then projector $\rho = |\psi\rangle\langle\psi|$ obeys:

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

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

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

Set $x = 2\Re(\psi_g\psi_e^*)$, $y = 2\Im(\psi_g\psi_e^*)$ and $z = |\psi_e|^2 - |\psi_g|^2$ we get

$$\rho = \frac{\mathbf{1} + x\sigma_x + y\sigma_y + z\sigma_z}{2}.$$

The Bloch vector $\vec{M} = x\vec{i} + y\vec{j} + z\vec{k}$ evolves on the unit sphere of \mathbb{R}^3 :

$$i\frac{d}{dt}|\psi\rangle = \left(\frac{\omega_x}{2}\sigma_x + \frac{\omega_y}{2}\sigma_y + \frac{\omega_z}{2}\sigma_z\right)|\psi\rangle \quad \sim \quad \frac{d}{dt}\vec{M} = (\omega_x\vec{i} + \omega_y\vec{j} + \omega_z\vec{k}) \times \vec{M}$$

Bloch vector \vec{M} with Euler angles (θ, ϕ) corresponds to

$$|\psi\rangle = e^{i\phi} \sin\left(\frac{\theta}{2}\right)|g\rangle + \cos\left(\frac{\theta}{2}\right)|e\rangle.$$

Un-measured quantum system \rightarrow **Bilinear Schrödinger equation**

$$i \frac{d}{dt} |\psi\rangle = (H_0 + u(t)H_1) |\psi\rangle,$$

- $|\psi\rangle \in \mathcal{H}$ the system's wavefunction with $\| |\psi\rangle \|_{\mathcal{H}} = 1$;
- the free Hamiltonian, H_0 , is a Hermitian operator defined on \mathcal{H} ;
- the control Hamiltonian, H_1 , is a Hermitian operator defined on \mathcal{H} ;
- the control $u(t) : \mathbb{R}^+ \mapsto \mathbb{R}$ is a scalar control.

Here we consider the case of finite dimensional \mathcal{H} for mathematical proof.

Almost periodic control

We consider the controls of the form

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

- $\epsilon > 0$ is a small parameter;
- $\epsilon \mathbf{u}_j$ is the constant complex amplitude associated to the pulsation $\omega_j \geq 0$;
- r stands for the number of independent pulsations ($\omega_j \neq \omega_k$ for $j \neq k$).

We are interested in approximations, for ϵ tending to 0^+ , of trajectories $t \mapsto |\psi_\epsilon\rangle_t$ on $t \in [0, 1/\epsilon]$ of

$$\frac{d}{dt} |\psi_\epsilon\rangle = \left(A_0 + \epsilon \left(\sum_{j=1}^r \mathbf{u}_j e^{i\omega_j t} + \mathbf{u}_j^* e^{-i\omega_j t} \right) A_1 \right) |\psi_\epsilon\rangle$$

where $A_0 = -iH_0$ and $A_1 = -iH_1$ are skew-Hermitian.

Rotating frame

Consider the following change of variables

$$|\psi_\epsilon\rangle_t = e^{A_0 t} |\phi_\epsilon\rangle_t.$$

The resulting system is said to be in the “interaction frame”

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

where $B(t)$ is a skew-Hermitian operator whose time-dependence is almost periodic:

$$B(t) = \sum_{j=1}^r \mathbf{u}_j e^{i\omega_j t} e^{-A_0 t} A_1 e^{A_0 t} + \mathbf{u}_j^* e^{-i\omega_j t} e^{-A_0 t} A_1 e^{A_0 t}.$$

Main idea

We can write

$$B(t) = \bar{B} + \frac{d}{dt} \tilde{B}(t),$$

where \bar{B} is a constant skew-Hermitian matrix and $\tilde{B}(t)$ is a bounded almost periodic skew-Hermitian matrix.

Multi-frequency averaging: first order

Consider the two systems

$$\frac{d}{dt} |\phi_\epsilon\rangle = \epsilon \left(\bar{B} + \frac{d}{dt} \tilde{B}(t) \right) |\phi_\epsilon\rangle,$$

and

$$\frac{d}{dt} \left| \phi_\epsilon^{1st} \right\rangle = \epsilon \bar{B} \left| \phi_\epsilon^{1st} \right\rangle,$$

initialized at the same state $\left| \phi_\epsilon^{1st} \right\rangle_0 = |\phi_\epsilon\rangle_0$.

Theorem: first order approximation (Rotating Wave Approximation)

Consider the functions $|\phi_\epsilon\rangle$ and $\left| \phi_\epsilon^{1st} \right\rangle$ initialized at the same state and following the above dynamics. Then, there exist $M > 0$ and $\eta > 0$ such that for all $\epsilon \in]0, \eta[$ we have

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

Proof's idea

Almost periodic change of variables:

$$|\chi_\epsilon\rangle = (1 - \epsilon\tilde{B}(t))|\phi_\epsilon\rangle$$

well-defined for $\epsilon > 0$ sufficiently small.

The dynamics can be written as

$$\frac{d}{dt}|\chi_\epsilon\rangle = (\epsilon\bar{B} + \epsilon^2 F(\epsilon, t))|\chi_\epsilon\rangle$$

where $F(\epsilon, t)$ is uniformly bounded in time.

Approximation recipes

We consider the Hamiltonian

$$H = H_0 + \sum_{k=1}^m u_k H_k, \quad u_k(t) = \sum_{j=1}^r \mathbf{u}_{k,j} e^{\omega_j t} + \mathbf{u}_{k,j}^* e^{-\omega_j t}.$$

The Hamiltonian in interaction frame

$$H_{\text{int}}(t) = \sum_{k,j} \left(\mathbf{u}_{k,j} e^{\omega_j t} + \mathbf{u}_{k,j}^* e^{-\omega_j t} \right) e^{iH_0 t} H_k e^{-iH_0 t}$$

We define the **first order Hamiltonian**

$$H_{\text{rwa}}^{1\text{st}} = \overline{H_{\text{int}}} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T H_{\text{int}}(t) dt,$$

Remark

In the above analysis we have assumed the complex amplitudes $\mathbf{u}_{k,j}$ to be constant. However, the whole analysis holds for the case where each one $\mathbf{u}_{k,j}$'s is of a small magnitude, admits a finite number of discontinuities and, between two successive discontinuities, is a slowly time varying function that is continuously differentiable.

In $i\frac{d}{dt}|\psi\rangle = \left(\frac{\omega_{eg}}{2}\sigma_z + \frac{u}{2}\sigma_x\right)|\psi\rangle$, take a resonant control $u = \mathbf{u}e^{i\omega_{eg}t} + \mathbf{u}^*e^{-i\omega_{eg}t}$ with \mathbf{u} slowly varying complex amplitude $|\frac{d}{dt}\mathbf{u}| \ll \omega_{eg}|\mathbf{u}|$. Set $H_0 = \frac{\omega_{eg}}{2}\sigma_z$ and $\epsilon H_1 = \frac{u}{2}\sigma_x$ and consider $|\psi\rangle = e^{-\frac{i\omega_{eg}t}{2}\sigma_z}|\phi\rangle$ to eliminate the **drift** H_0 and to get the **Hamiltonian in the interaction frame**:

$$i\frac{d}{dt}|\phi\rangle = \frac{u}{2}e^{\frac{i\omega_{eg}t}{2}\sigma_z}\sigma_x e^{-\frac{i\omega_{eg}t}{2}\sigma_z}|\phi\rangle = H_{\text{int}}|\phi\rangle$$

$$\text{with } H_{\text{int}} = \frac{u}{2}e^{i\omega_{eg}t} \overbrace{\frac{\sigma_x + i\sigma_y}{2}}^{\sigma^+ = |e\rangle\langle g|} + \frac{u}{2}e^{-i\omega_{eg}t} \overbrace{\frac{\sigma_x - i\sigma_y}{2}}^{\sigma^- = |g\rangle\langle e|}$$

The RWA consists in neglecting the oscillating terms at frequency $2\omega_{eg}$ when $|\mathbf{u}| \ll \Omega$:

$$H_{\text{int}} = \left(\frac{\mathbf{u}e^{2i\omega_{eg}t} + \mathbf{u}^*}{2}\right)\sigma^+ + \left(\frac{\mathbf{u} + \mathbf{u}^*e^{-2i\omega_{eg}t}}{2}\right)\sigma^-.$$

Thus

$$\overline{H_{\text{int}}} = \frac{\mathbf{u}^*\sigma^+ + \mathbf{u}\sigma^-}{2}.$$

$$i \frac{d}{dt} |\phi\rangle = \frac{(\mathbf{u}^* \sigma^+ + \mathbf{u} \sigma^-)}{2} |\phi\rangle = \frac{(\mathbf{u}^* |e\rangle \langle g| + \mathbf{u} |g\rangle \langle e|)}{2} |\phi\rangle$$

We set $\mathbf{u} = \Omega_r e^{i\theta}$ with $\Omega_r > 0$ and θ real.

$$\frac{\mathbf{u}^* \sigma^+ + \mathbf{u} \sigma^-}{2} = \frac{\Omega_r}{2} (\cos \theta \sigma_x + \sin \theta \sigma_y)$$

The system oscillates between $|e\rangle$ and $|g\rangle$ with the **Rabi pulsation** $\frac{\Omega_r}{2}$. Since $(\cos \theta \sigma_x + \sin \theta \sigma_y)^2 = \mathbf{1}$ and

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

the solution of $\frac{d}{dt} |\phi\rangle = \frac{-i\Omega_r}{2} (\cos \theta \sigma_x + \sin \theta \sigma_y) |\phi\rangle$ reads

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

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

We start always from $|\phi\rangle_0 = |g\rangle$ we light on the resonant control with the constant amplitude $\mathbf{u} = -i\Omega_r$ during $[0, T]$ (pulse length T). Since

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

we see that

- if $\Omega_r T = \pi$ (π -pulse) then $|\phi\rangle_T = |e\rangle$: stimulate absorption of one photon. If we measure the system energy (measurement operator $\frac{\omega_{eg}}{2} |e\rangle\langle e| - \frac{\omega_{eg}}{2} |g\rangle\langle g|$), then we will find deterministically $\frac{\omega_{eg}}{2}$.
- if $\Omega_r T = \pi/2$ ($\pi/2$ -pulse) when $|\phi\rangle_T = (|g\rangle + |e\rangle)/\sqrt{2}$, a **coherent superposition** of $|g\rangle$ and $|e\rangle$. If we measure the energy, the result is stochastic and the probability to get $\frac{\omega_{eg}}{2}$ is $\frac{1}{2}$ and to get $-\frac{\omega_{eg}}{2}$ is also $\frac{1}{2}$.

Take the first order approximation

$$(\Sigma) \quad i \frac{d}{dt} |\phi\rangle = \frac{(\mathbf{u}^* \sigma^+ + \mathbf{u} \sigma^-)}{2} |\phi\rangle = \frac{(\mathbf{u}^* |e\rangle \langle g| + \mathbf{u} |g\rangle \langle e|)}{2} |\phi\rangle$$

with control $\mathbf{u} \in \mathbb{C}$.

- 1 Take constant control $\mathbf{u}(t) = \Omega_r e^{i\theta}$ for $t \in [0, T]$, $T > 0$. Show that $i \frac{d}{dt} |\phi\rangle = \frac{\Omega_r (\cos \theta \sigma_x + \sin \theta \sigma_y)}{2} |\phi\rangle$.
- 2 Set $\Theta_r = \frac{\Omega_r}{2} T$. Show that the solution at T of the propagator $U_t \in SU(2)$, $i \frac{d}{dt} U = \frac{\Omega_r (\cos \theta \sigma_x + \sin \theta \sigma_y)}{2} U$, $U_0 = \mathbf{1}$ is given by

$$U_T = \cos \Theta_r \mathbf{1} - i \sin \Theta_r (\cos \theta \sigma_x + \sin \theta \sigma_y),$$

- 3 Take a wave function $|\bar{\phi}\rangle$. Show that exist Ω_r and θ such that $U_T |g\rangle = e^{i\alpha} |\bar{\phi}\rangle$, where α is some global phase.
- 4 Prove that for any given two wave functions $|\phi_a\rangle$ and $|\phi_b\rangle$ exists a piece-wise constant control $[0, 2T] \ni t \mapsto \mathbf{u}(t) \in \mathbb{C}$ such that the solution of (Σ) with $|\phi\rangle_0 = |\phi_a\rangle$ satisfies $|\phi\rangle_T = e^{i\beta} |\phi_b\rangle$ for some global phase β .

Take $[0, 1] \ni s \mapsto H(s)$ a C^2 family of Hermitian matrices $n \times n$: set $s = \epsilon t \in [0, 1]$ and ϵ a small positive parameter. Consider a solution $[0, \frac{1}{\epsilon}] \ni t \mapsto |\psi\rangle_t^\epsilon$ of

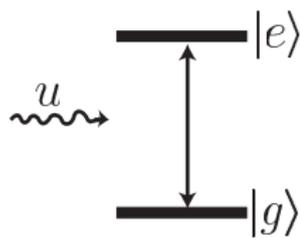
$$i \frac{d}{dt} |\psi\rangle_t^\epsilon = H(\epsilon t) |\psi\rangle_t^\epsilon.$$

Take $[0, s] \ni s \mapsto P(s)$ a **family of orthogonal projectors** such that for each $s \in [0, 1]$, $H(s)P(s) = \omega(s)P(s)$ where $\omega(s)$ is an eigenvalue of $H(s)$. Assume that $[0, s] \ni s \mapsto P(s)$ is C^2 and that, **for almost all** $s \in [0, 1]$, $P(s)$ is the **orthogonal projector on the eigen-space** associated to the eigen-value $\omega(s)$. Then

$$\lim_{\epsilon \rightarrow 0^+} \left(\sup_{t \in [0, \frac{1}{\epsilon}]} \left| \|P(\epsilon t) |\psi\rangle_t^\epsilon\|^2 - \|P(0) |\psi\rangle_0^\epsilon\|^2 \right| \right) = 0.$$

³Theorem 6.2, page 175 of *Adiabatic Perturbation Theory in Quantum Dynamics*, by S. Teufel, Lecture notes in Mathematics, Springer, 2003. 

Chirped control of a 2-level system (1)



$i\frac{d}{dt}|\psi\rangle = \left(\frac{\omega_{eg}}{2}\sigma_z + \frac{u}{2}\sigma_x\right)|\psi\rangle$ with quasi-resonant control ($|\omega_r - \omega_{eg}| \ll \omega_{eg}$)
 $u(t) = v(t) \left(e^{i(\omega_r t + \theta(t))} + e^{-i(\omega_r t + \theta(t))} \right)$

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

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

Passage to the interaction frame $|\psi\rangle = e^{-i\frac{\omega_r t + \theta(t)}{2}\sigma_z}|\phi\rangle$:

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

Set $\Delta_r = \omega_{eg} - \omega_r$ and $w(t) = -\frac{d\theta}{dt}$, RWA yields following averaged Hamiltonian

$$H_{\text{chirp}} = \frac{\Delta_r + w(t)}{2}\sigma_z + \frac{v(t)}{2}\sigma_x$$

where (v, w) are two real control inputs.

Chirped control of a 2-level system (2)

In $H_{\text{chirp}} = \frac{\Delta_r + w}{2} \sigma_z + \frac{v}{2} \sigma_x$ set, for $s = \epsilon t$ varying in $[0, \pi]$, $w = a \cos(\epsilon t)$ and $v = b \sin^2(\epsilon t)$. **Spectral decomposition** of H_{chirp} for $s \in]0, \pi[$:

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

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

where $\alpha \in]-\frac{\pi}{2}, \frac{\pi}{2}[$ is defined by $\tan \alpha = \frac{\Delta_r + w}{v}$. With $a > |\Delta_r|$ and $b > 0$

$$\lim_{s \rightarrow 0^+} \alpha = \frac{\pi}{2} \quad \text{implies} \quad \lim_{s \rightarrow 0^+} |-\rangle_s = |g\rangle, \quad \lim_{s \rightarrow 0^+} |+\rangle_s = |e\rangle$$

$$\lim_{s \rightarrow \pi^-} \alpha = -\frac{\pi}{2} \quad \text{implies} \quad \lim_{s \rightarrow \pi^-} |-\rangle_s = -|e\rangle, \quad \lim_{s \rightarrow \pi^-} |+\rangle_s = |g\rangle.$$

Adiabatic approximation: the solution of $i \frac{d}{dt} |\phi\rangle = H_{\text{chirp}}(\epsilon t) |\phi\rangle$ starting from $|\phi\rangle_0 = |g\rangle$ reads

$$|\phi\rangle_t \approx e^{i\vartheta_t} |-\rangle_{s=\epsilon t}, \quad t \in [0, \frac{\pi}{\epsilon}], \quad \text{with } \vartheta_t \text{ time-varying global phase.}$$

At $t = \frac{\pi}{\epsilon}$, $|\psi\rangle$ coincides with $|e\rangle$ up to a global phase: **robustness** versus Δ_r , a and b (**ensemble controllability**).

- The chirped dynamics $i\frac{d}{dt}\phi = \left(\frac{\Delta_r+w}{2}\sigma_z + \frac{v}{2}\sigma_x\right) |\phi\rangle$ with $w = a\cos(\epsilon t)$ and $v = b\sin^2(\epsilon t)$ reads

$$\frac{d}{dt}\vec{M} = \underbrace{(b\sin^2(\epsilon t)\vec{v} + (\Delta_r + a\cos(\epsilon t))\vec{k})}_{=\vec{\Omega}_t} \times \vec{M}$$

- The initial condition $|\phi\rangle_0 = |g\rangle$ means that $\vec{M}_0 = -\vec{k}$ and $\vec{\Omega}_0 = (\Delta_r + a)\vec{k}$ with $\Delta_r + a > 0$.
- Since $\vec{\Omega}$ never vanishes for $t \in [0, \frac{\pi}{\epsilon}]$, adiabatic theorem implies that \vec{M} follows the direction of $-\vec{\Omega}$, i.e. that $\vec{M} \approx -\frac{\vec{\Omega}}{\|\vec{\Omega}\|}$ (see matlab simulations `AdiabaticBloch.m`).
- At $t = \frac{\pi}{\epsilon}$, $\vec{\Omega} = (\Delta_r - a)\vec{k}$ with $\Delta_r - a < 0$: $\vec{M}_{\frac{\pi}{\epsilon}} = \vec{k}$ and thus $|\phi\rangle_{\frac{\pi}{\epsilon}} = e^{i\vartheta} |e\rangle$.

Consider the propagator $U \in SU(2)$, solution of

$$\frac{d}{dt}U(t) = -iH(\epsilon t)U(t) = -i\left(\frac{\Delta_r}{2}\sigma_z + \frac{v(\epsilon t)}{2}\sigma_y\right)U(t), \quad U(0) = I$$

assuming $0 < \epsilon \ll 1$, $\Delta_r > 0$ and $v = f(s)$ ($s = \epsilon t$) where $[0, 1] \ni s \mapsto f(s)$ is smooth and $f(0) = f(1) = 0$.

We have

$$U(1/\epsilon) = e^{-i\bar{\vartheta}\sigma_z} + O(\epsilon)$$

where $\bar{\vartheta}$ is given by the integral:

$$\bar{\vartheta} = \frac{1}{2} \int_0^{1/\epsilon} \sqrt{\Delta_r^2 + f^2(\epsilon t)} dt.$$

The phase $\bar{\vartheta}$ is only due to the time integral of the $H(\epsilon t)$ eigenvalues (dynamic phase only, no Berry phase for such adiabatic evolution).

Adiabatic propagator $U(t)$ for $H(\epsilon t) = \frac{\Delta_r}{2}\sigma_z + \frac{v(\epsilon t)}{2}\sigma_y$ (2)

The frame $(|-\rangle_s, |+\rangle_s)$ that diagonalize $H(s)$ ($s = \epsilon t$)

$H(s)|\pm\rangle_s = \pm \frac{\sqrt{\Delta_r^2 + f^2(s)}}{2} |\pm\rangle_s$, reads

$$|-\rangle_s = \cos \xi_s |g\rangle + i \sin \xi_s |e\rangle, \quad |+\rangle_s = i \sin \xi_s |g\rangle + \cos \xi_s |e\rangle$$

where $\mu_s = \sqrt{1 + (f(s)/\Delta_r)^2}$ gives

$$\cos \xi_s = \sqrt{(\mu_s + 1)/(2\mu_s)}, \quad \sin \xi_s = \sqrt{(\mu_s - 1)/(2\mu_s)}$$

The passage from the $(|g\rangle, |e\rangle)$ to $(|-\rangle_s, |+\rangle_s)$ corresponds, in the Bloch sphere representation, to a rotation around the X -axis of angle $-2\xi_s$:

$$|-\rangle_s = e^{i\xi_s\sigma_x} |g\rangle, \quad |+\rangle_s = e^{i\xi_s\sigma_x} |e\rangle$$

Thus we have

$$\frac{\Delta_r}{2}\sigma_z + \frac{f(s)}{2}\sigma_y = \frac{\sqrt{\Delta_r^2 + f^2(s)}}{2} e^{-i\xi_s\sigma_x} \sigma_z e^{i\xi_s\sigma_x}.$$

Adiabatic propagator $U(t)$ for $H(\epsilon t) = \frac{\Delta_r}{2}\sigma_z + \frac{v(\epsilon t)}{2}\sigma_y$ (3)

Consider $\frac{d}{dt}|\psi\rangle = -iH(\epsilon t)|\psi\rangle$, set

$$\vartheta(t) = \frac{1}{2} \int_0^t \sqrt{\Delta_r^2 + f^2(\epsilon\tau)} d\tau$$

set $|\psi\rangle = e^{i\xi_{\epsilon t}\sigma_x} e^{-i\vartheta(t)\sigma_z} |\phi\rangle$. Then, with $\xi'_s = \frac{d}{ds}\xi_s$,

$$\frac{d}{dt}|\phi\rangle = -i\epsilon\xi'_{\epsilon t} e^{i\vartheta(t)\sigma_z} \sigma_x e^{-i\vartheta(t)\sigma_z} |\phi\rangle = -i\epsilon\xi'_{\epsilon t} \sigma_x e^{-2i\vartheta(t)\sigma_z} |\phi\rangle.$$

In average $\xi'_{\epsilon t} \sigma_x e^{-2i\vartheta(t)\sigma_z}$ gives zero up to first order terms in ϵ (use $\int_0^t e^{-2i\vartheta(\tau)\sigma_z} d\tau = A(t)$ with $A(t)$ bounded on $[0, 1/\epsilon]$). Then $|\phi\rangle_t \approx |\phi\rangle_0 = e^{-i\xi_0\sigma_x} |\psi\rangle_0$ is almost constant and thus

$$|\psi\rangle_t = e^{i\xi_{\epsilon t}\sigma_x} e^{-i\vartheta(t)\sigma_z} e^{-i\xi_0\sigma_x} |\psi\rangle_0 + O(\epsilon).$$

The propagator reads then for $t \in [0, 1/\epsilon]$,

$$U(t) = e^{i\xi_{\epsilon t}\sigma_x} e^{-i\vartheta(t)\sigma_z} + O(\epsilon)$$

since $\xi_0 = 0$ results from $f(0) = 0$.

Multi-frequency averaging: second order

Consider the two systems

$$\frac{d}{dt} |\phi_\epsilon\rangle = \epsilon \left(\bar{B} + \frac{d}{dt} \tilde{B}(t) \right) |\phi_\epsilon\rangle,$$

and

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

initialized at the same state $\left| \phi_\epsilon^{2\text{nd}} \right\rangle_0 = |\phi_\epsilon\rangle_0$.

Theorem: second order approximation

Consider the functions $|\phi_\epsilon\rangle$ and $\left| \phi_\epsilon^{2\text{nd}} \right\rangle$ initialized at the same state and following the above dynamics. Then, there exist $M > 0$ and $\eta > 0$ such that for all $\epsilon \in]0, \eta[$ we have

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

Proof's idea

Another almost periodic change of variables

$$|\xi_\epsilon\rangle = \left(\mathbf{1} - \epsilon^2 \left([\bar{B}, \tilde{C}(t)] - \tilde{D}(t) \right) \right) |\chi_\epsilon\rangle.$$

The dynamics can be written as

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

where G is almost periodic and therefore uniformly bounded in time.

Approximation recipes

We consider the Hamiltonian

$$H = H_0 + \sum_{k=1}^m u_k H_k, \quad u_k(t) = \sum_{j=1}^r \mathbf{u}_{k,j} e^{\omega_j t} + \mathbf{u}_{k,j}^* e^{-\omega_j t}.$$

The Hamiltonian in interaction frame

$$H_{\text{int}}(t) = \sum_{k,j} \left(\mathbf{u}_{k,j} e^{\omega_j t} + \mathbf{u}_{k,j}^* e^{-\omega_j t} \right) e^{iH_0 t} H_k e^{-iH_0 t}$$

We define the **first order Hamiltonian**

$$H_{\text{rwa}}^{1\text{st}} = \overline{H_{\text{int}}} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T H_{\text{int}}(t) dt,$$

and the **second order Hamiltonian**

$$H_{\text{rwa}}^{2\text{nd}} = H_{\text{rwa}}^{1\text{st}} - i \overline{(H_{\text{int}} - \overline{H_{\text{int}}}) \left(\int_t (H_{\text{int}} - \overline{H_{\text{int}}}) \right)}$$

In $i\frac{d}{dt}|\psi\rangle = \left(\frac{\omega_{eg}}{2}\sigma_z + \frac{u}{2}\sigma_x\right)|\psi\rangle$, take a resonant control $u = \mathbf{u}e^{i\omega_{eg}t} + \mathbf{u}^*e^{-i\omega_{eg}t}$ with \mathbf{u} slowly varying complex amplitude $|\frac{d}{dt}\mathbf{u}| \ll \omega_{eg}|\mathbf{u}|$. Set $H_0 = \frac{\omega_{eg}}{2}\sigma_z$ and $\epsilon H_1 = \frac{u}{2}\sigma_x$ and consider $|\psi\rangle = e^{-\frac{i\omega_{eg}t}{2}\sigma_z}|\phi\rangle$ to eliminate the drift H_0 and to get the **Hamiltonian in the interaction frame**:

$$i\frac{d}{dt}|\phi\rangle = \frac{u}{2}e^{\frac{i\omega_{eg}t}{2}\sigma_z}\sigma_x e^{-\frac{i\omega_{eg}t}{2}\sigma_z}|\phi\rangle = H_{\text{int}}|\phi\rangle$$

$$\text{with } H_{\text{int}} = \frac{u}{2}e^{i\omega_{eg}t} \overbrace{\frac{\sigma_x + i\sigma_y}{2}}^{\sigma^+ = |e\rangle\langle g|} + \frac{u}{2}e^{-i\omega_{eg}t} \overbrace{\frac{\sigma_x - i\sigma_y}{2}}^{\sigma^- = |g\rangle\langle e|}$$

The RWA consists in neglecting the oscillating terms at frequency $2\omega_{eg}$ when $|\mathbf{u}| \ll \Omega$:

$$H_{\text{int}} = \left(\frac{\mathbf{u}e^{2i\omega_{eg}t} + \mathbf{u}^*}{2}\right)\sigma^+ + \left(\frac{\mathbf{u} + \mathbf{u}^*e^{-2i\omega_{eg}t}}{2}\right)\sigma^-.$$

Thus

$$\overline{H_{\text{int}}} = \frac{\mathbf{u}^*\sigma^+ + \mathbf{u}\sigma^-}{2}.$$

The decomposition of H_{int} ,

$$H_{\text{int}} = \underbrace{\frac{\mathbf{u}^*}{2}\sigma_+ + \frac{\mathbf{u}}{2}\sigma_-}_{\overline{H_{\text{int}}}} + \underbrace{\frac{\mathbf{u}e^{2i\omega_{eg}t}}{2}\sigma_+ + \frac{\mathbf{u}^*e^{-2i\omega_{eg}t}}{2}\sigma_-}_{H_{\text{int}} - \overline{H_{\text{int}}}},$$

provides the **first order approximation** (RWA)

$H_{\text{rwa}}^{1\text{st}} = \overline{H_{\text{int}}} = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T H_{\text{int}}(t) dt$, and also the second order approximation $H_{\text{rwa}}^{2\text{nd}} = H_{\text{rwa}}^{1\text{st}} - i \overline{(H_{\text{int}} - \overline{H_{\text{int}}}) \left(\int_t (H_{\text{int}} - \overline{H_{\text{int}}}) \right)}$. Since $\int_t H_{\text{int}} - \overline{H_{\text{int}}} = \frac{\mathbf{u}e^{2i\omega_{eg}t}}{4i\omega_{eg}}\sigma_+ - \frac{\mathbf{u}^*e^{-2i\omega_{eg}t}}{4i\omega_{eg}}\sigma_-$, we have

$$\overline{(H_{\text{int}} - \overline{H_{\text{int}}}) \left(\int_t (H_{\text{int}} - \overline{H_{\text{int}}}) \right)} = -\frac{|\mathbf{u}|^2}{8i\omega_{eg}}\sigma_z$$

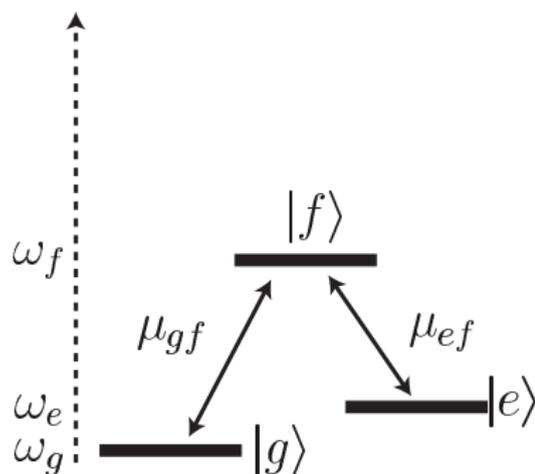
(use $\sigma_+^2 = \sigma_-^2 = 0$ and $\sigma_z = \sigma_+\sigma_- - \sigma_-\sigma_+$).

The **second order approximation** reads:

$$H_{\text{rwa}}^{2\text{nd}} = H_{\text{rwa}}^{1\text{st}} + \left(\frac{|\mathbf{u}|^2}{8\omega_{eg}} \right) \sigma_z = \frac{\mathbf{u}^*}{2}\sigma_+ + \frac{\mathbf{u}}{2}\sigma_- + \left(\frac{|\mathbf{u}|^2}{8\omega_{eg}} \right) \sigma_z.$$

The 2nd order correction $\frac{|\mathbf{u}|^2}{4\omega_r}\sigma_z$ is called the **Bloch-Siegert shift**.

Stimulated Raman Adiabatic Passage (STIRAP) (1)



$$H = \omega_g |g\rangle \langle g| + \omega_e |e\rangle \langle e| + \omega_f |f\rangle \langle f| \\ + u\mu_{gf} (|g\rangle \langle f| + |f\rangle \langle g|) \\ + u\mu_{ef} (|e\rangle \langle f| + |f\rangle \langle e|).$$

Set $\omega_{gf} = \omega_f - \omega_g$, $\omega_{ef} = \omega_f - \omega_e$ and $u = u_{gf} \cos(\omega_{gf}t) + u_{ef} \cos(\omega_{ef}t)$ with slowly varying small real amplitudes u_{gf} and u_{ef} .

Put $i\frac{d}{dt}|\psi\rangle = H|\psi\rangle$ in the interaction frame:

$$|\psi\rangle = e^{-it(\omega_g|g\rangle\langle g| + \omega_e|e\rangle\langle e| + \omega_f|f\rangle\langle f|)}|\phi\rangle.$$

Rotation Wave Approximation yields $i\frac{d}{dt}|\phi\rangle = H_{\text{rwa}}|\phi\rangle$ with

$$H_{\text{rwa}} = \frac{\Omega_{gf}}{2}(|g\rangle\langle f| + |f\rangle\langle g|) + \frac{\Omega_{ef}}{2}(|e\rangle\langle f| + |f\rangle\langle e|)$$

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

Stimulated Raman Adiabatic Passage (STIRAP) (2)

Spectral decomposition: as soon as $\Omega_{gf}^2 + \Omega_{ef}^2 > 0$,

$\frac{\Omega_{gf}(|g\rangle\langle f| + |f\rangle\langle g|)}{2} + \frac{\Omega_{ef}(|e\rangle\langle f| + |f\rangle\langle e|)}{2}$ admits 3 distinct eigen-values,

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

They correspond to the following 3 eigen-vectors,

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

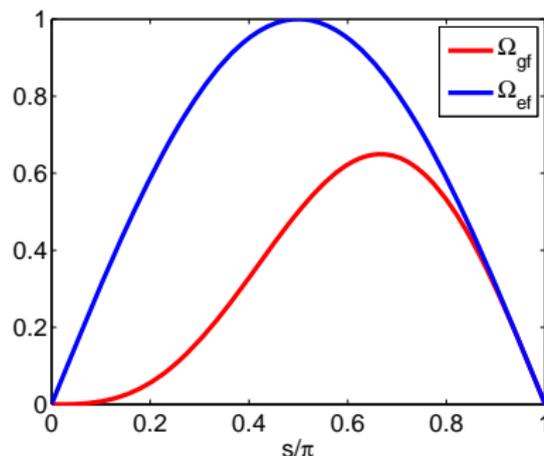
For $\epsilon t = s \in [0, \frac{3\pi}{2}]$ and $\bar{\Omega}_g, \bar{\Omega}_e > 0$, the adiabatic control

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

provides the passage from $|g\rangle$ at $t = 0$ to $|e\rangle$ at $\epsilon t = \frac{3\pi}{2}$.
(see matlab simulations `stirap.m`).

Exercise

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



Take, e.g., $s = \epsilon t \in [0, \pi]$
and $\bar{\Omega} > 0$, and set

$$\Omega_{gf}(s) = \frac{\bar{\Omega}}{2} \sin s - \frac{\bar{\Omega}}{4} \sin 2s$$

$$\Omega_{ef}(s) = \bar{\Omega} \sin s$$

Results from $|0\rangle = \frac{-\Omega_{ef}}{\sqrt{\Omega_{gf}^2 + \Omega_{ef}^2}} |g\rangle + \frac{\Omega_{gf}}{\sqrt{\Omega_{gf}^2 + \Omega_{ef}^2}} |e\rangle$

Schrödinger equation

$$i \frac{d}{dt} |\psi\rangle = \left(H_0 + \sum_{k=1}^m u_k H_k \right) |\psi\rangle$$

State controllability

For any $|\psi_a\rangle$ and $|\psi_b\rangle$ on the unit sphere of \mathcal{H} , there exist a time $T > 0$, a global phase $\theta \in [0, 2\pi[$ and a piecewise continuous control $[0, T] \ni t \mapsto u(t)$ such that the solution with initial condition $|\psi\rangle_0 = |\psi_a\rangle$ satisfies $|\psi\rangle_T = e^{i\theta} |\psi_b\rangle$.

⁴See, e.g., *Introduction to Quantum Control and Dynamics* by D. D'Alessandro. Chapman & Hall/CRC, 2008.

Controllability of bilinear Schrödinger equations

Propagator equation:

$$i \frac{d}{dt} U = \left(H_0 + \sum_{k=1}^m u_k H_k \right) U, \quad U(0) = \mathbf{1}$$

We have $|\psi\rangle_t = U(t) |\psi\rangle_0$.

Operator controllability

For any unitary operator V on \mathcal{H} , there exist a time $T > 0$, a global phase θ and a piecewise continuous control $[0, T] \ni t \mapsto u(t)$ such that the solution of propagator equation satisfies $U_T = e^{i\theta} V$.

Operator controllability implies state controllability

Lie-algebra rank condition

$$\frac{d}{dt} U = \left(A_0 + \sum_{k=1}^m u_k A_k \right) U$$

with $A_k = H_k/i$ are skew-Hermitian. We define

$$\mathcal{L}_0 = \text{span}\{A_0, A_1, \dots, A_m\}$$

$$\mathcal{L}_1 = \text{span}(\mathcal{L}_0, [\mathcal{L}_0, \mathcal{L}_0])$$

$$\mathcal{L}_2 = \text{span}(\mathcal{L}_1, [\mathcal{L}_1, \mathcal{L}_1])$$

\vdots

$$\mathcal{L} = \mathcal{L}_\nu = \text{span}(\mathcal{L}_{\nu-1}, [\mathcal{L}_{\nu-1}, \mathcal{L}_{\nu-1}])$$

Lie Algebra Rank Condition

Operator controllable if, and only if, the Lie algebra generated by the $m + 1$ skew-Hermitian matrices $\{-iH_0, -iH_1, \dots, -iH_m\}$ is either $su(n)$ or $u(n)$.

Exercise

Show that $i \frac{d}{dt} |\psi\rangle = \left(\frac{\omega_{eg}}{2} \sigma_z + \frac{u}{2} \sigma_x \right) |\psi\rangle$, $|\psi\rangle \in \mathbb{C}^2$ is controllable.

A simple sufficient condition

We consider $H = H_0 + uH_1$, $(|j\rangle)_{j=1,\dots,n}$ the eigenbasis of H_0 .

We assume $H_0 |j\rangle = \omega_j |j\rangle$ where $\omega_j \in \mathbb{R}$, we consider a graph G :

$$V = \{|1\rangle, \dots, |n\rangle\}, \quad E = \{(|j_1\rangle, |j_2\rangle) \mid 1 \leq j_1 < j_2 \leq n, \langle j_1 | H_1 | j_2 \rangle \neq 0\}.$$

G admits a degenerate transition if there exist $(|j_1\rangle, |j_2\rangle) \in E$ and $(|l_1\rangle, |l_2\rangle) \in E$, admitting the same transition frequencies,

$$|\omega_{j_1} - \omega_{j_2}| = |\omega_{l_1} - \omega_{l_2}|.$$

A sufficient controllability condition

Remove from E , all the edges with identical transition frequencies.

Denote by $\bar{E} \subset E$ the reduced set of edges without degenerate transitions and by $\bar{G} = (V, \bar{E})$. If \bar{G} is connected, then the system is operator controllable.