Ensemble qubit controllability with a single control via adiabatic and rotating wave approximations.

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Spin dynamics

2-level system (Qubit)

Cauchy problem associated with Schroedinger equation :

$$i\partial_t \psi(t) = H(t)\psi(t), \quad \psi(0) = \psi_0$$

where $\psi_0 \in \mathbb{C}^2$, $|\psi_0| = 1$, $H(t)$ is self-adjoint.

$$H(t) = \begin{pmatrix} a & b+ic \\ b-ic & -a \end{pmatrix} = a\sigma_z + b\sigma_x + c\sigma_y.$$

exemple of physical interpretation

In NMR, a, b, c are respectively the strength of the magnetic field along z, x, y.

Population transfer

Statement of the problem

Let $E > 0$ (strength of the z magnetic field), $-E < \alpha_0 \leq 0 \leq \alpha_1$ the dispersion parameters. For all $\alpha \in [\alpha_0, \alpha_1]$, let
$H^\alpha(v) = \begin{pmatrix} E+\alpha & v \\ v^* & -E-\alpha \end{pmatrix}$.
For any $\epsilon > 0$, can we find $T > 0$ and $w \in \mathcal{C}^2([0,T],\mathbb{K})$ such that the solutions of

$$i\partial_t \psi_w^\alpha = H^\alpha(w(t))\psi_w^\alpha \quad \psi_w^\alpha(0) = e_2$$

satisfies $\forall \alpha \in [\alpha_0, \alpha_1], \exists \theta, |\psi_w^\alpha(T) - e^{i\theta} e_1| \leq \epsilon$?

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Remarks

- This is an ensemble control problem.
- For $\mathbb{K} = \mathbb{C}$ we can use standard adiabatic theory.
- For $\mathbb{K} = \mathbb{R}$, physicists use the Rotating Wave Approximation (RWA) to 'duplicate' a real control into complex one.

Adiabatic Approximation

Interaction frame

Let us choose the pulse w in the form

$$w(t) = u(t)e^{-i(2Et+\Delta(t))},$$

where, $u(\cdot)$ and $\Delta(\cdot)$ are two real-valued smooth functions. Applying the change of variables

$$\psi(t) = \begin{pmatrix} e^{-i(Et+\Delta(t)/2)} & 0 \\ 0 & e^{i(Et+\Delta(t)/2)} \end{pmatrix} \Psi(t),$$

we obtain

$$i\frac{d\Psi}{dt} = \begin{pmatrix} \alpha - v(t) & u(t) \\ u(t) & -\alpha + v(t) \end{pmatrix} \Psi.$$

where $v(t) := \Delta'(t)/2$.

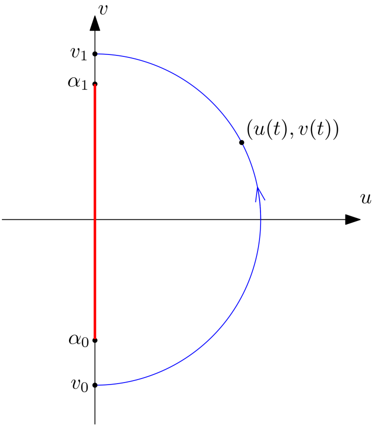
Adiabatic Approximation

Let $H_\alpha(u, v) = (\alpha - v)\sigma_z + u\sigma_x$. The eigenvalues of $H_\alpha(u, v)$ are $\pm\sqrt{(\alpha - v)^2 + u^2}$.

Initial and finite time Hamiltonian

$$H_\alpha(0, v_0) = \begin{pmatrix} \alpha - v_0 & 0 \\ 0 & -\alpha + v_0 \end{pmatrix}$$

$$H_\alpha(0, v_1) = \begin{pmatrix} \alpha - v_1 & 0 \\ 0 & -\alpha + v_1 \end{pmatrix}$$



Adiabatic Approximation

Adiabatic control

Let $v_0, v_1 \in \mathbb{R}$ be such that $v_0 < \alpha_0$ and $\alpha_1 < v_1$ and consider a smooth path $t \mapsto (u(t), v(t))$ lying in the half-plane $u > 0$ except for the initial and final points, where $u = 0$.

Theorem

There exists $C > 0$ such that, for every $\alpha \in [\alpha_0, \alpha_1]$ and every $\varepsilon > 0$, the solution ψ_ε^α of

$$i\frac{d\Psi}{dt} = \begin{pmatrix} \alpha - v_\varepsilon(t) & u_\varepsilon(t) \\ u_\varepsilon(t) & -\alpha + v_\varepsilon(t) \end{pmatrix}\Psi, \quad \psi_\varepsilon^\alpha(0) = e_2$$

with $u_\varepsilon(t) = u(\varepsilon t)$ and $v_\varepsilon(t) = v(\varepsilon t)$ satisfies $|\Psi(T/\varepsilon) - (e^{i\theta}, 0)| \leq C\varepsilon$ for some θ.

Rotating Wave Approximation

Motivation

Consider the controls

$$w_\varepsilon(t) = 2\varepsilon u(\varepsilon t)\cos(2Et + \Delta(\varepsilon t)),$$
$$w_\varepsilon^{\mathrm{R}}(t) = \varepsilon u(\varepsilon t) e^{-i(2Et+\Delta(\varepsilon t))}.$$

In the case where $\alpha = 0$, the evolution associated with the real control in the interaction frame is

$$i\frac{d\hat{\psi}_{w_\varepsilon}}{dt} = \varepsilon\Big[\begin{pmatrix} -\Delta'(\varepsilon t)/2 & u(\varepsilon t) \\ u(\varepsilon t) & \Delta'(\varepsilon t)/2 \end{pmatrix} + \begin{pmatrix} 0 & e^{i(4Et+2\Delta(\varepsilon t))}u(\varepsilon t) \\ e^{-i(4Et+2\Delta(\varepsilon t))}u(\varepsilon t) & 0 \end{pmatrix}\Big]\hat{\psi}_{w_\varepsilon}.$$

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In the case where $\alpha = 0$, the evolution associated with the complex control in the interaction frame is

$$i\frac{d\hat{\psi}^{\mathrm{R}}_{w_\varepsilon}}{dt} = \varepsilon \begin{pmatrix} -\Delta'(\varepsilon t)/2 & u(\varepsilon t) \\ u(\varepsilon t) & \Delta'(\varepsilon t)/2 \end{pmatrix} \hat{\psi}^{\mathrm{R}}_{w_\varepsilon}.$$

Rotating Wave Approximation

Theorem

Let $\alpha = 0$, ψ_{w_ε} and $\psi^{\mathrm{R}}_{w_\varepsilon}$ the evolution of some ψ_0 with the control w_ε and $w^{\mathrm{R}}_\varepsilon$. Then there exist $C > 0$ such that

$$\forall t \in [0, T/\varepsilon], |\psi_{w_\varepsilon}(t) - \psi_{w^R_\varepsilon}(t)| < C\varepsilon.$$

Comparison of the two approximations

RWA

The control

$$w_\varepsilon(t) = 2\varepsilon u(\varepsilon t)\cos(2Et + \Delta(\varepsilon t)),$$
$$w_\varepsilon^{\mathrm{R}}(t) = \varepsilon u(\varepsilon t) e^{-i(2Et+\Delta(\varepsilon t))}.$$

give the same dynamics to an order ε in a Time T/ε. Higher order averaging (add a correction on the Hamiltonian) allow the same order of approximation on T/ε^k.

AA

the control

$$w_\varepsilon(t) = u_\varepsilon(t) e^{-i(2Et+\Delta(\varepsilon t)/\varepsilon)},$$

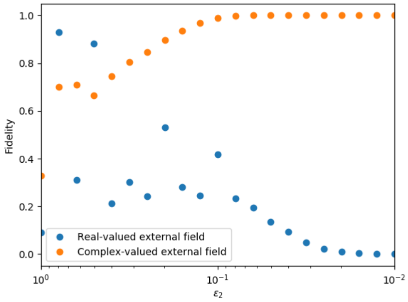
ensure a population transfer for all α up to an order in ε in time T/ε.

First idea

Take u small and use

$$w_\varepsilon(t) = u_\varepsilon(t) 2\cos(2Et + \Delta(\varepsilon t)/\varepsilon) \text{ to simulate } u_\varepsilon(t)e^{-i(2Et+\Delta(\varepsilon t)/\varepsilon)}.$$

Pb: simulations seem to show that it does not work in general.



Comparison of the real-valued and complex-valued chirp scheme of the first point with $E = 0.75$, $\alpha = 0.25$, $\varepsilon_1 = 1$, $v_0 = -0.5$, $v_1 = 0.5$.

The dilemma

RWA

You need small control and not too long final time.

AA

The smaller the control, the longer time you need.

Compatibility

The control

$$w_{\varepsilon_1,\varepsilon_2}(t) = 2\varepsilon_1 u(\varepsilon_1\varepsilon_2 t)\cos\left(2Et + \frac{\Delta(\varepsilon_1\varepsilon_2 t)}{\varepsilon_1\varepsilon_2}\right)$$

Theorem

Assume that $v_0 < 0 < v_1$ are such that $3(E + v_0) \geq E + v_1$. Choose T and $u, \Delta : [0, T] \to \mathbb{R}$ smooth enough (e.g., $u \in C^2$ and $\Delta \in C^3$) such that

1. $(u(0), \Delta'(0)) = (0, 2v_0)$ and $(u(T), \Delta'(T)) = (0, 2v_1)$;
2. $\forall s \in (0, T), u(s) > 0$ and $\Delta''(s) \geq 0$.

Denote by $\psi^{\alpha}_{\varepsilon_1,\varepsilon_2}$ the solution with initial condition $\psi^{\alpha}_{\varepsilon_1,\varepsilon_2}(0) = (0, 1)$ and external field $w_{\varepsilon_1,\varepsilon_2}$. Then, for every $N_0 \in \mathbb{N}$, for every compact interval $I \subseteq (v_0, v_1)$, there exist $C_{N_0} > 0$ and $\delta > 0$ such that for every $\alpha \in I$ and every $(\varepsilon_1, \varepsilon_2) \in (0, \delta)^2$, there exists θ such that
$|\psi^{\alpha}_{\varepsilon_1,\varepsilon_2}(1/\varepsilon_1\varepsilon_2) - (e^{i\theta}, 0)| < C_{N_0} \max(\varepsilon_2/\varepsilon_1, \varepsilon_1^{N_0-1}/\varepsilon_2)$.

Some notations

$$E_1(t) = 2\alpha t - \frac{\Delta(\varepsilon_1\varepsilon_2 t)}{\varepsilon_1\varepsilon_2}, \qquad f_1(t) = \frac{d}{dt}E_1(t),$$
$$E_2(t) = 4Et + 2\alpha t + \frac{\Delta(\varepsilon_1\varepsilon_2 t)}{\varepsilon_1\varepsilon_2}, \qquad f_2(t) = \frac{d}{dt}E_2(t),$$

$$A(E) = \begin{pmatrix} 0 & e^{iE} \\ e^{-iE} & 0 \end{pmatrix}, \qquad B(E) = \begin{pmatrix} 0 & -ie^{iE} \\ ie^{-iE} & 0 \end{pmatrix}.$$

In terms of these new notations, we can rewrite the Hamiltonian in the interaction frame :

$$H_{\mathrm{I}}(t) = \varepsilon_1 u(\varepsilon_1\varepsilon_2 t)A(E_1(t)) + \varepsilon_1 u(\varepsilon_1\varepsilon_2 t)A(E_2(t)), \quad t \in [0, \frac{1}{\varepsilon_1\varepsilon_2}].$$

A technical lemma

Let $\alpha \in (v_0, v_1)$ and assume that $E + \alpha > 0$ and $4E - 3\Delta'(s) > 2\alpha$ for every $s \in [0,1]$. Then, for every $N_0 \in \mathbb{N}$ there exists a Hamiltonian H_{RWA} of the form

$$H_{\mathrm{RWA}}(t) = \varepsilon_1 h_1(\varepsilon_1\varepsilon_2 t) A(E_1(t)) + \varepsilon_1^2 h_2(\varepsilon_1\varepsilon_2 t) B(E_1(t)) + \varepsilon_1^2 h_3(\varepsilon_1\varepsilon_2 t)\sigma_z,$$

with h_1, h_2, h_3 polynomials in $(\varepsilon_1, \varepsilon_2)$ with coefficients in $\mathcal{C}^\infty([0,1], \mathbb{R})$, such that the solution ψ_{RWA} of the Cauchy problem

$$i\frac{d}{dt}\psi_{\mathrm{RWA}} = H_{\mathrm{RWA}}\psi_{\mathrm{RWA}}, \qquad \psi_{\mathrm{RWA}}(0) = \psi_{\mathrm{I}}(0),$$

satisfies $|\psi_{\mathrm{RWA}}(\frac{1}{\varepsilon_1\varepsilon_2}) - \psi_{\mathrm{I}}(\frac{1}{\varepsilon_1\varepsilon_2})| = O(\varepsilon_1^2\varepsilon_2 + \varepsilon_1^{N_0-1}/\varepsilon_2)$. More precisely, there exist $h_{j,p,q} \in \mathcal{C}^\infty([0,1], \mathbb{R})$, for $j = 1,2,3$, $p = 0, \dots, N_0$, and $q = 0, 1$, such that

1. $h_1 = u + \sum_{p=1}^{N_0} \sum_{q=0}^{1} \varepsilon_1^p \varepsilon_2^q h_{1,p,q}$ with $h_{1,p,0}(0) = h_{1,p,0}(1) = 0$,
2. $h_2 = \sum_{p=0}^{N_0} \sum_{q=0}^{1} \varepsilon_1^p \varepsilon_2^q h_{2,p,q}$ with $h_{2,p,0}(0) = h_{2,p,0}(1) = 0$,
3. $h_3 = \sum_{p=0}^{N_0} \sum_{q=0}^{1} \varepsilon_1^p \varepsilon_2^q h_{3,p,q}$ with $h_{3,p,0}(0) = h_{3,p,0}(1) = 0$.

The toward the AA part

Lemma

There exists $\delta > 0$ such that ψ_{RWA} satisfies $|\psi_{\mathrm{RWA}}(\frac{1}{\varepsilon_1\varepsilon_2}) - (e^{i\theta}, 0)| \leq M\varepsilon_2/\varepsilon_1$ for some $\theta \in \mathbb{R}$.

A new change of variable: $\psi_{\mathrm{slow}}(t) = U(t)\psi_{\mathrm{RWA}}(t)$ with

$$U(t) = \begin{pmatrix} e^{i(\alpha t - \frac{\Delta(\epsilon_1\epsilon_2 t)}{2\epsilon_1\epsilon_2})} & 0 \\ 0 & e^{-i(\alpha t - \frac{\Delta(\epsilon_1\epsilon_2 t)}{2\epsilon_1\epsilon_2})} \end{pmatrix}.$$

The new Hamiltonian depends only on $s = \varepsilon_1\varepsilon_2 t$.

$$H_{\mathrm{slow}}(s) = \varepsilon_1 h_1(s)\sigma_x + \varepsilon_1^2 h_2(s)\sigma_y + \Big(\alpha - \frac{\Delta'(s)}{2} + \varepsilon_1^2 h_3(s)\Big)\sigma_z.$$

$$\tilde{H}_{\mathrm{slow}} = \varepsilon_1 u\sigma_x + (\alpha - \Delta'/2)\sigma_z$$

Let $P_{\varepsilon_1,\varepsilon_2}$ be the spectral projector on the negative eigenvalue of H_{slow}. Then :

1. $|P_{\varepsilon_1,\varepsilon_2}(0) - P_{e_1}| = O(\varepsilon_1^2\varepsilon_2)$ and $|P_{\varepsilon_1,\varepsilon_2}(1) - P_{e_2}| = O(\varepsilon_1^2\varepsilon_2)$, where P_{e_i} is the orthogonal projector on $\mathbb{C}e_i$;
2. $\int_0^1 |(\frac{d}{ds}P_{\varepsilon_1,\varepsilon_2})(s)|^2 ds = O(1/\varepsilon_1)$;
3. $\int_0^1 |(\frac{d^2}{ds^2}P_{\varepsilon_1,\varepsilon_2})(s)| ds = O(1/\varepsilon_1)$;
4. $\int_0^1 |\frac{1}{\omega_{\varepsilon_1,\varepsilon_2}(s)^2}\frac{d}{ds}P_{\varepsilon_1,\varepsilon_2}(s)||\frac{d}{ds}H_{\mathrm{slow}}(s)| ds = O(1/\varepsilon_1^2)$.

AA

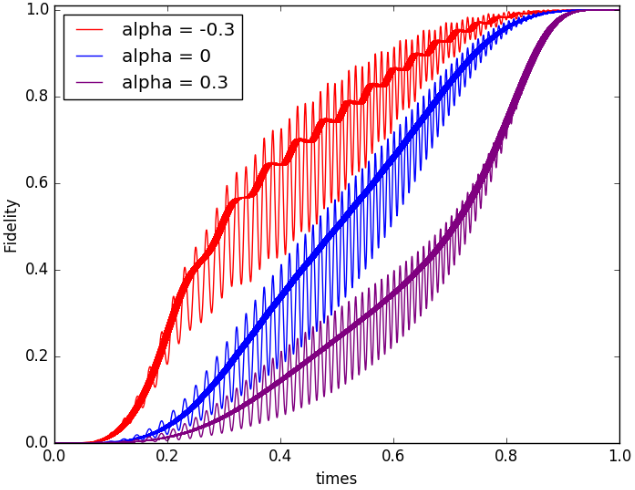
$$\left|\psi_{\mathrm{RWA}}\left(\frac{1}{\varepsilon_1\varepsilon_2}\right) - (e^{i\theta},0)\right| \leq \varepsilon_1\varepsilon_2\Bigg[\frac{|\frac{d}{ds}P_{\varepsilon_1,\varepsilon_2}(1)|}{\omega_{\varepsilon_1,\varepsilon_2}(1)} + \frac{|\frac{d}{ds}P_{\varepsilon_1,\varepsilon_2}(0)|}{\omega_{\varepsilon_1,\varepsilon_2}(0)}$$

$$+\int_0^1 \Big(\frac{2|\frac{d}{ds}P_{\varepsilon_1,\varepsilon_2}(s)|^2}{\omega_{\varepsilon_1,\varepsilon_2}(s)} + \frac{|\frac{d^2}{ds^2}P_{\varepsilon_1,\varepsilon_2}(s)|}{\omega_{\varepsilon_1,\varepsilon_2}(s)} + \frac{|\frac{d}{ds}P_{\varepsilon_1,\varepsilon_2}(s)||\frac{d}{ds}H_{\mathrm{slow}}(s)|}{2\omega_{\varepsilon_1,\varepsilon_2}(s)^2}\Big)ds\Bigg],$$

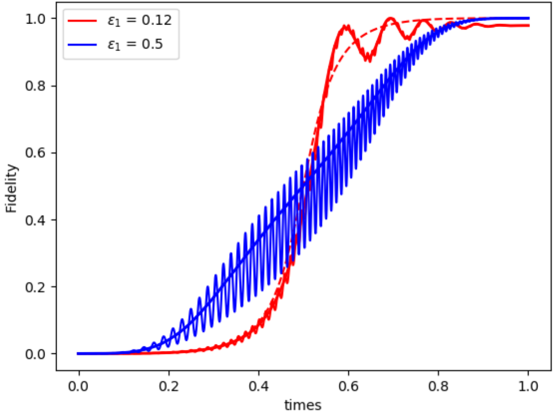
Summary of the proof

Summary of the proof

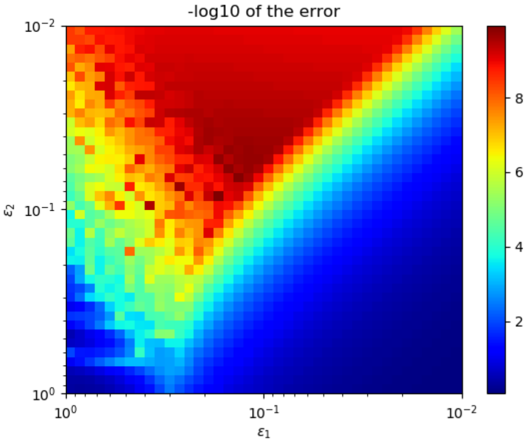
- Thanks to the assumption $3(E + v_0) \geq E + v_1$, it is possible to define a N_0th averaging approximation thanks to an algorithm.
- The complicated Hamiltonian dynamics we obtain stays close to the one of the first order RWA Hamiltonian.
- Convergence of the population transfer for the first order RWA hamiltonian dynamics is ensure when $\varepsilon_2 \ll \varepsilon_1$.



$\varepsilon_1 = 0.5$ and $\varepsilon_2 = 0.1$. In thick line are the trajectories corresponding to the equivalent 1st order RWA system.



$\varepsilon_1\varepsilon_2 = 0.05$, $\alpha = 0$. In thick line are the trajectories corresponding to the equivalent 1st order RWA system and in dotted line the theoretical AA trajectories.



Log of the distance from $\psi^0_{\varepsilon_1,\varepsilon_2}(1/\varepsilon_1\varepsilon_2)$ to the orbit of $(1,0)$.

Li-Khaneja

Let $\mathcal{D} = [E_m, E_M] \times [\delta_m, \delta_M]$ be the compact set of the dispersion parameters and endow $\mathcal{F} := C^0(\mathcal{D}, \mathrm{SU}_2)$ with the usual distance $d_{\mathcal{F}}(f, g) := \max_{d \in \mathcal{D}} \|f(d) - g(d)\|$.

[Li–Khaneja, 2009]

For any control bound $K > 0$, any target distribution $M_F \in \mathcal{F}$, and any $\varepsilon > 0$, there exist some $T > 0$ and controls $u, v \in L^\infty([0, T], [-K, K])$ such that the solution of the equation

$$i \frac{d}{dt} M(E, \delta, t) = (E\sigma_z + \delta u(t)\sigma_x + \delta v(t)\sigma_y) M(E, \delta, t),$$
$$M(E, \delta, 0) = I_2, \quad \forall (E, \delta) \in \mathcal{D}$$

satisfies $d_{\mathcal{F}}(M(\cdot, \cdot, T), M_F(\cdot, \cdot)) < \varepsilon$.

Generalisation of Li-Khaneja

Theorem

Suppose $3E_m > E_M$, let $\mathcal{D} = [E_m, E_M] \times [\delta_m, \delta_M] \subset \mathbb{R}_+^* \times \mathbb{R}_+^*$.
Fix $\epsilon > 0$, $M_F \in \mathcal{F}$ and $K > 0$. Then there exist $T > 0$ and $u \in L^\infty([0,T],[-K,K])$ such that the solution of the ensemble control problem

$$\frac{d}{dt} M(E,\delta,t) = (E\sigma_z + \delta u(t)\sigma_x) M(E,\delta,t), \tag{1}$$

$$M(E,\delta,0) = I_2, \forall (E,\delta) \in \mathcal{D} \tag{2}$$

satisfies $||M(\cdot,\cdot,T) - M_F(\cdot,\cdot)||_{\mathcal{F}} < \varepsilon$.

Main idea

Corollary of AA+RWA part

Suppose that $3E_m > E_M$. Then, for any $K > 0$ and any $\varepsilon > 0$, there exist $T > 0$ and a control $u \in L^\infty([0,T],[-K,K])$ such that the solution of Equation (1) satisfies
$\max_{(E,\delta)\in\mathcal{D}} \min_{\theta\in[0,2\pi]} \|M(E,\delta,T)(0,1)^T - (e^{i\theta},0)^T\| < \varepsilon$.

Reachable propagators

Let $\mathcal{R} = \{M(\cdot,\cdot,T) \mid T > 0$, M is a solution of (1) for some $u \in L^\infty([0,T],[-K,K])\}$

- For all t in $\mathbb{R}$, $(E,\delta) \mapsto e^{-itE\sigma_z}$ is in $\bar{\mathcal{R}}$,
- Let $u \in \mathbb{R}$. Then $(E,\delta) \mapsto e^{u\delta i\sigma_x}$ is in $\bar{\mathcal{R}}$.

A Lie Algebra (of infinite dimension)

Let

$$\mathfrak{g} = \{X \in \mathcal{C}^0(\mathcal{D}, \mathfrak{su}_2) \mid \forall t \in \mathbb{R},\ e^{tX} \in \bar{\mathcal{R}}\}.$$

, Then $\mathfrak{g}$ is stable under brackets and addition.

for any $n, m \in \mathbb{N}$, and any sequence $(b_{k,l})_{k,l}$

$$\sum_{k=0}^{m}\sum_{l=0}^{n} b_{k,l}\delta^{2k+2}E^{2l+1}i\sigma_x \in \mathfrak{g},$$
$$\sum_{k=0}^{m}\sum_{l=0}^{n} c_{k,l}\delta^{2k+1}E^{2l+1}i\sigma_y \in \mathfrak{g},$$
$$\sum_{k=0}^{m}\sum_{l=0}^{n} d_{k,l}\delta^{2k+1}E^{2l+2}i\sigma_z \in \mathfrak{g}.$$

$\implies$ (Stone-Weierstrass) : for any continuous functions $f(d)\sigma_* \in \mathfrak{g}$.
$\implies$ (connectedness of $\mathcal{F}$) : $\bar{\mathcal{R}} = \mathcal{F}$

Conclusion

A few open questions

- Under the assumption $3E_m > E_M$ can we prove convergence for a fixed ε_1?
- What happen in higher dimension? In infinite dimension? We expect the method to work but with conditions depending of N_0.
- Can we extend the controllability result without the assumption $3E_m > E_M$?
- Is there a more efficient way to prove the ensemble controllability (e.g. smaller controllability time).

Thank you for your attention !