Ensemble control of n-level systems via combined adiabatic and rotating wave approximations

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System

Let us consider a continuum of n-level systems described by the Schrödinger equation

$$i\dot{\psi}(t) = (H(\alpha) + \omega(t)H_c(\delta))\psi(t), \tag{1}$$

where $\omega(\cdot)$ is a real-valued control. Here we assume $H(\alpha)$ is determined by an unknown parameter α in a closed and connected domain $\mathcal{D}$ of $\mathbb{R}^m$ and has the following structure

$$H(\alpha) = \begin{pmatrix} \lambda_1(\alpha) & 0 & \dots & 0 \\ 0 & \lambda_2(\alpha) & 0 & \vdots \\ \vdots & 0 & \ddots & 0 \\ 0 & \dots & 0 & \lambda_n(\alpha) \end{pmatrix},$$

where $\lambda_j : \mathcal{D} \to \mathbb{R}$ is a continuous function for each $j \in \{1, \dots, n\}$.

System

$H_c(\delta)$ is a self-adjoint matrix that describes the control coupling between the eigenstates of the system and has the form

$$H_c(\delta) = \begin{pmatrix} 0 & \delta_{12} & \cdots & \delta_{1n} \\ \delta_{12} & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \delta_{n-1,n} \\ \delta_{1n} & \cdots & \delta_{n-1,n} & 0 \end{pmatrix},$$

We assume that each δ_{jk} is unknown but that it belongs to some closed interval $\mathcal{I}_{jk} = \left[\delta_{jk}^0, \delta_{jk}^1\right]$ in $\mathbb{R}$ such that $0 \notin \mathcal{I}_{jk}$.

Objective

For $p, q \in \{1, \dots, n\}$ s.t. $p \neq q$, one would like to find a uniform control $\omega(\cdot)$ for the family of quantum systems s.t. if at $t = 0$, all systems are at the same initial state $\psi(0) = \mathbf{e}_p$, then at time T the systems are close to final states of form $e^{i\theta}\mathbf{e}_q$ for some $\theta \in \mathbb{R}$.

Two-level system with complex control

Consider a two-level system with a complex control

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = \begin{pmatrix} E+\alpha & \omega(t) \\ \omega^*(t) & -E-\alpha \end{pmatrix}\psi(t), \tag{2}$$

where α is in an unknown parameter in an interval $[\alpha_0, \alpha_1]$. For $\epsilon > 0$, choose the control

$$\omega_\epsilon(t) = u(\epsilon t)e^{-i\left(2Et+\frac{\Delta(\epsilon t)}{\epsilon}\right)}, \tag{3}$$

where u and Δ are real-valued functions on $[0, T]$. Let us apply the change of variables

$$\psi(t) = \begin{pmatrix} e^{-i\left(Et+\frac{\Delta(\epsilon t)}{2\epsilon}\right)} & 0 \\ 0 & e^{i\left(Et+\frac{\Delta(\epsilon t)}{2\epsilon}\right)} \end{pmatrix}\Psi(t). \tag{4}$$

Two-level system with complex control

Then we can obtain that

$$i\frac{\mathrm{d}}{\mathrm{d}t}\Psi = \begin{pmatrix} \alpha - v(\epsilon t) & u(\epsilon t) \\ u(\epsilon t) & -\alpha + v(\epsilon t) \end{pmatrix} \Psi, \tag{5}$$

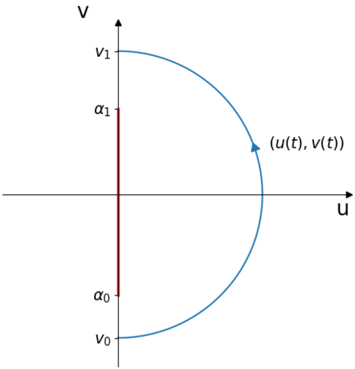
where $v(s) = \Delta'(s)/2$. Assume that

$$\sqrt{(\alpha - v(s))^2 + u(s)^2} > 0, \quad \forall s \in [0, T]. \tag{6}$$

Then by adiabatic theorem (e.g. [Teufel, 2003]), when $\epsilon \to 0$, if $\Psi(0)$ is in the eigenspace associated with $\lambda_+(0)$ (respectively, $\lambda_-(0)$), then the state will remain close to the eigenspace associated with $\lambda_+(t)$ (respectively, $\lambda_-(t)$).

Two-level system with complex control

Fix $T = 1$. Define $u(\cdot)$ and $v(\cdot)$ as follow



Therefore, the solution ψ of (2) with initial state $(0, 1)$ and corresponding to ω_ϵ satisfies $\left|\psi(T/\epsilon) - (e^{i\theta}, 0)\right| \leq C\epsilon$ for some $\theta \in \mathbb{R}$.

Two-level system with real control

Consider a two-level system with a real-valued control

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = \begin{pmatrix} E+\alpha & \omega(t) \\ \omega(t) & -E-\alpha \end{pmatrix}\psi(t), \tag{7}$$

and the real chirped pulse

$$\omega_\epsilon(t) = 2u(\epsilon t)\cos\left(2Et + \Delta(\epsilon t)/\epsilon\right), \tag{8}$$

and apply the change of variables from (4). We obtain

$$i\frac{\mathrm{d}}{\mathrm{d}t}\Psi = \left[\begin{pmatrix} \alpha - v(\epsilon t) & u(\epsilon t) \\ u(\epsilon t) & -\alpha + v(\epsilon t) \end{pmatrix} + R(t,\epsilon)\right]\Psi, \tag{9}$$

$$R(t,\epsilon) = \begin{pmatrix} 0 & u(\epsilon t)e^{i(4Et+2\Delta(\epsilon t)/\epsilon)} \\ u(\epsilon t)e^{-i(4Et+2\Delta(\epsilon t)/\epsilon)} & 0 \end{pmatrix}.$$

The adiabatic theorem discussed above is no longer valid.

RWA(Rotating wave approximations)

If $\alpha = 0$, the dynamics of a system with complex-valued control can be simulated with a real-valued control. For $\epsilon > 0$, consider the control

$$\omega_\epsilon(t) = 2\epsilon u(\epsilon t)\cos(2Et + \Delta(\epsilon t)). \tag{10}$$

Applying the change of variable

$$\psi(t) = \begin{pmatrix} e^{-i(Et+\Delta(\epsilon t)/2)} & 0 \\ 0 & e^{i(Et+\Delta(\epsilon t)/2)} \end{pmatrix} \hat{\psi}(t), \tag{11}$$

and the change of variable $\tilde{\psi}(s) = \hat{\psi}(\epsilon t)$, we obtain

$$i\frac{\mathrm{d}}{\mathrm{d}s}\tilde{\psi} = \left[\begin{pmatrix} -v(s) & u(s) \\ u(s) & v(s) \end{pmatrix} + \begin{pmatrix} 0 & e^{i(4Es/\epsilon+2\Delta(s))}u(s) \\ e^{-i(4Es/\epsilon+2\Delta(s))}u(s) & 0 \end{pmatrix}\right]\tilde{\psi}.$$

By classical averaging result, the second term induces a perturbation of order ϵ to the solution.

RWA(Rotating wave approximations)

However, when the resonance is not precisely known $\alpha \in [\alpha_0, \alpha_1]$,

$$i\frac{\mathrm{d}}{\mathrm{d}s}\tilde{\psi}_\alpha = \left[\begin{pmatrix} \alpha/\epsilon - v(s) & u(s) \\ u(s) & -\alpha/\epsilon + v(s) \end{pmatrix} + B(s,\epsilon)\right]\tilde{\psi}_\alpha,$$

where $B(s,\epsilon)$ denotes the second term in the previous equation. The adiabatic following is no longer valid since $\lim_{\epsilon\to 0}\alpha_1/\epsilon = +\infty$ and $\lim_{\epsilon\to 0}\alpha_0/\epsilon = -\infty$.

Combination of RWA and AA (Robin, Augier, Boscain, Sigalotti, 2022)

Consider two time scales $\epsilon_1, \epsilon_2 > 0$ and a control law of the type

$$\omega_{\epsilon_1,\epsilon_2}(t) = 2\epsilon_1\delta u(\epsilon_1\epsilon_2 t)\cos\left(2Et + \frac{\Delta(\epsilon_1\epsilon_2 t)}{\epsilon_1\epsilon_2}\right). \qquad (12)$$

Here u, Δ are real-valued smooth functions on [0,T] and $\delta \in \mathbb{R}^*$ is an unknown parameter.

Combination of RWA and AA in population inversion

Theorem (Robin, Augier, Boscain, Sigalotti, 2022)

Assume that $v_0 < 0 < v_1$ are such that $3(E + v_0) \geq E + v_1$. Fix $T > 0$ and $u, \Delta : [0, T] \to \mathbb{R}$ smooth (e.g., $u \in \mathcal{C}^2$ and $\Delta \in \mathcal{C}^3$) 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 $\psi^{\alpha}_{\epsilon_1,\epsilon_2}$ the solution of (7) with initial condition $\psi^{\alpha}_{\epsilon_1,\epsilon_2}(0) = (0, 1)$ and control $\omega_{\epsilon_1,\epsilon_2}$ as in (12). 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 $\eta > 0$ such that for every $\alpha \in I$ and every $(\epsilon_1, \epsilon_2) \in (0, \eta)^2$,

$$\left|\psi_{\epsilon_1,\epsilon_2}(T/(\epsilon_1\epsilon_2)) - (e^{i\theta}, 0)\right| < C_{N_0} \max(\epsilon_2/\epsilon_1, \epsilon_1^{N_0-1}/\epsilon_2) \tag{13}$$

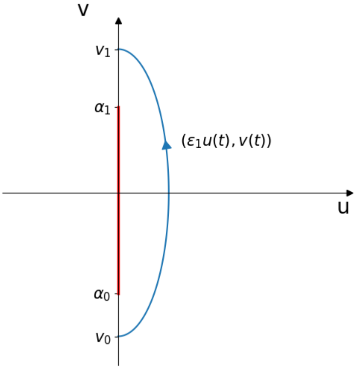
for some $\theta \in \mathbb{R}$. Moreover, the constant C_{N_0} can be taken locally uniform with respect to the parameter $\delta > 0$ appearing in (12).

Combination of RWA and AA in population inversion

The conditions in the theorem ensures that we can simulate the dynamics

$$\frac{\mathrm{d}}{\mathrm{d}t}\psi_{\text{slow}} = \begin{pmatrix} v(\epsilon_1\epsilon_2 t) - \alpha & \epsilon_1 u(\epsilon_1\epsilon_2 t) \\ \epsilon_1 u(\epsilon_1\epsilon_2 t) & -v(\epsilon_1\epsilon_2 t) + \alpha \end{pmatrix} \psi_{\text{slow}}. \tag{14}$$

A non-classical adiabatic theorem can be applied with an error $\mathcal{O}(\epsilon_2/\epsilon_1)$.



N-level system

Recall the n-level system

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi(t) = \begin{pmatrix} \lambda_1(\alpha) & \delta_{1,2}\omega(t) & \dots & \delta_{1,n}\omega(t) \\ \delta_{1,2}\omega(t) & \lambda_2(\alpha) & \ddots & \vdots \\ \vdots & \ddots & \ddots & \delta_{n-1,n}\omega(t) \\ \delta_{1,n}\omega(t) & \dots & \delta_{n-1,n}\omega(t) & \lambda_n(\alpha) \end{pmatrix}\psi(t),$$

and the control law

$$\omega_{\epsilon_1\epsilon_2}(t) = 2\epsilon_1 u(\epsilon_1\epsilon_2 t)\cos\left(\int_0^t f(\epsilon_1\epsilon_2\tau)\mathrm{d}\tau\right), \qquad (15)$$

where $u, f : [0, T] \to \mathbb{R}$ are functions to be chosen.

Theorem

Let us assume that for all $1 \leq j < k \leq n$, and for all $\alpha \in \mathcal{D}$, $\lambda_k(\alpha) - \lambda_j(\alpha) > 0$. Fix $1 \leq p < q \leq n$ and assume that there exist $0 < v_0 < v_1$ such that

1. For $\alpha \in \mathcal{D}$, $\lambda_p(\alpha) - \lambda_q(\alpha) \in (v_0, v_1)$ and, for all $1 \leq j < k \leq n$ such that $(j, k) \neq (p, q)$, we have that $\forall \alpha \in \mathcal{D}$, $\lambda_k(\alpha) - \lambda_j(\alpha) \notin [v_0, v_1]$.
2. For all $1 \leq j < k \leq n$ and all $\alpha \in \mathcal{D}$, $\lambda_k(\alpha) - \lambda_j(\alpha) \notin [2v_0, 2v_1]$.

Theorem

Then we can fix $T > 0$ and take $u, f \in \mathcal{C}^2([0, T], \mathbb{R})$ such that

i) $(u(0), f(0)) = (0, v_0)$ and $(u(T), f(T)) = (0, v_1)$;

ii) $\forall s \in (0, T), u(s) > 0, f'(s) > 0$.

Denote by $\psi_{\epsilon_1,\epsilon_2}$ the solution of (1) with initial condition $\psi_{\epsilon_i,\epsilon_2}(0) = \mathbf{e}_p$ and the control law $\omega_{\epsilon_1,\epsilon_2}$ as in (15). Then there exist $C > 0$ and $\eta > 0$ such that for every $\alpha \in \mathcal{D}$ and every $(\epsilon_1, \epsilon_2) \in (0, \eta)^2$,

$$\left\| \psi_{\epsilon_1,\epsilon_2}\left(\frac{T}{\epsilon_1\epsilon_2}\right) - \exp(i\theta)\mathbf{e}_q \right\| < C \max\left(\frac{\epsilon_1^2}{\epsilon_2}, \frac{\epsilon_2}{\epsilon_1}\right) \tag{16}$$

for some $\theta \in \mathbb{R}$.

Proof

For $E \in \mathbb{R}$ and $1 \leq j \leq k \leq n$, let us define

$$A_{jk}(E) = \begin{cases} \exp(iE)\mathbf{e}_{jk} + \exp(-iE)\mathbf{e}_{kj} & \text{if } j < k, \\ \cos(E)\mathbf{e}_{jj} & \text{if } j = k, \end{cases}$$

$$B_{jk}(E) = \begin{cases} i\exp(iE)\mathbf{e}_{jk} - i\exp(-iE)\mathbf{e}_{kj} & \text{if } j < k, \\ -\sin(E)\mathbf{e}_{jj} & \text{if } j = k. \end{cases}$$

For $1 \leq j < k \leq n$ and $\sigma \in \mathbb{Z}$, $\phi_{jk}^{\sigma}(t)$ is defined by

$$\phi_{jk}^{\sigma}(t) = (\lambda_j - \lambda_k)t + \sigma \int_0^t f(\epsilon_1\epsilon_2\tau)\mathrm{d}\tau.$$

Let us recast (1) in the interaction frame $\psi(t) = \exp(-itH(\alpha))\psi_I(t)$. The dynamics of ψ_I is characterized by the Hamiltonian

$$H_I(t) = \sum_{j=1}^{n-1} \sum_{k=j+1}^{n} \delta_{j,k} u(\epsilon_1\epsilon_2 t) \left[A_{jk}(\phi_{jk}^{1}(t)) + A_{jk}(\phi_{jk}^{-1}(t)) \right].$$

Proof

Assume that hypothesis 1 of Theorem is satisfied. Then there exist a function $X_1(t)$ on $[0, 1/(\epsilon_1\epsilon_2)]$ and a change of variables

$$\psi_I(t) = \exp(i\epsilon_1 X_1(t))\hat{\psi}_1(t), \tag{17}$$

such that the dynamics of $\hat{\psi}_1$ is characterized by the Hamiltonian

$$\hat{H}_1(t) = \epsilon_1\delta_{pq}u(\epsilon_1\epsilon_2 t)A_{pq}\left(\phi^1_{pq}(t)\right) + \sum_{(j,k,\sigma)\in\mathcal{J}} \epsilon_1^2 h^\sigma_{jk}(\epsilon_1\epsilon_2 t)A_{jk}\left(\phi^\sigma_{jk}(t)\right) + \mathcal{O}(\epsilon_1^3 + \epsilon_1^2\epsilon_2),$$

where $\mathcal{J} = \{(j,k,\sigma) \mid 1 \le j \le k \le n, \sigma \in \{-2,0,2\}\}$ and $h^\sigma_{jk}(\cdot)$ are functions on $[0,1]$.

Proof

Similar to the reasoning above, with Hypothesis 2, there exist a function $X_2(t)$ on $[0, 1/(\epsilon_1\epsilon_2)]$ and a change of variables

$$\hat{\psi}_1(t) = \exp(i\epsilon_1^2 X_2(t))\hat{\psi}_2(t),$$

such that the dynamics of $\hat{\psi}_2(t)$ is characterized by the Hamiltonian

$$\begin{aligned}\hat{H}_2(t) &= \hat{H}_1(t) + \epsilon_1^2 \frac{\mathrm{d}}{\mathrm{d}t} X_2(t) + \mathcal{O}(\epsilon_1^3) \\ &= \epsilon_1 \delta_{pq} u(\epsilon_1\epsilon_2 t) A_{pq}(\phi_{pq}^1(t)) + \sum_{j=1}^{n} \epsilon_1^2 h_{jj}^0(\epsilon_1\epsilon_2 t)\mathbf{e}_{jj} + \mathcal{O}(\epsilon_1^3 + \epsilon_1^2\epsilon_2).\end{aligned}$$

Since $u(0) = u(1) = 0$, we deduce that $h_{jk}^{\sigma}(0) = h_{jk}^{\sigma}(1) = 0$ for every $(j, k, \sigma) \in \mathcal{J}$. Then $X_1(0) = X_1\left(\frac{1}{\epsilon_1\epsilon_2}\right) = 0$ and $X_2(0) = X_2\left(\frac{1}{\epsilon_1\epsilon_2}\right) = 0$. Hence, $\psi_I(0) = \hat{\psi}_1(0) = \hat{\psi}_2(0)$ and $\psi_I\left(\frac{1}{\epsilon_1\epsilon_2}\right) = \hat{\psi}_1\left(\frac{1}{\epsilon_2\epsilon_2}\right) = \hat{\psi}_2\left(\frac{1}{\epsilon_2\epsilon_2}\right)$.

Proof

Assume that $\psi_I(0) \in V = \mathbf{span}\,(\mathbf{e}_p, \mathbf{e}_q)$, let us first project $\hat{H}_2(t)$ on V and introduce the following truncation

$$H_{rwa}(t) = \epsilon_1 \delta_{pq} u(\epsilon_1\epsilon_2 t) A_{pq}\left(\phi^1_{pq}(t)\right) + \sum_{j\in\{p,q\}} \epsilon_1^2 h^0_{jj}(\epsilon_1\epsilon_2 t)\mathbf{e}_{jj},$$

and the system

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi_{\text{rwa}}(t) = H_{\text{rwa}}(t)\psi_{\text{rwa}}(t), \quad \psi_{\text{rwa}}(0) = \psi_I(0).$$

We can prove that

$$\left\|\psi_I\left(1/(\epsilon_1\epsilon_2)\right) - \psi_{\text{rwa}}\left(1/(\epsilon_1\epsilon_2)\right)\right\| = \mathcal{O}(\epsilon_1^2/\epsilon_2 + \epsilon_1).$$

Proof

Introduce the unitary change of variables with $\psi_{\text{rwa}}(t) = U(t)\psi_{\text{slow}}(t)$ with

$$U(t) = e_{pp} + \exp\left(-i\phi^1_{pq}(t)\right)\mathbf{e}_{qq}. \tag{18}$$

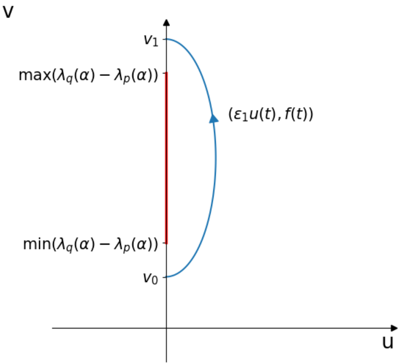
The dynamics of ψ_{slow} is characterized by the Hamiltonian

$$\begin{aligned} H_{\text{slow}}(t) = \epsilon_1^2 h^0_{pp}(\epsilon_1\epsilon_2 t)\mathbf{e}_{pp} + \epsilon_1\delta_{pq}u(\epsilon_1\epsilon_2 t)(\mathbf{e}_{pq} + \mathbf{e}_{qp}) \\ + \left((\lambda_2 - \lambda_1 - f(\epsilon_1\epsilon_2 t) + \epsilon_1^2 h^0_{qq}(\epsilon_1\epsilon_2 t)\right)\mathbf{e}_{qq}. \end{aligned}$$

Remark

It has been shown in [Robin, Augier, Boscain, Sigalotti, 2022] that the diagonal terms $\epsilon_1^2 h^0_{qq}(\epsilon_1\epsilon_2 t)\mathbf{e}_{qq}$ and $\epsilon_1^2 h^0_{pp}(\epsilon_1\epsilon_2 t)\mathbf{e}_{pp}$ can be neglected when applying the adiabatic theorem.

Proof



We can then apply Lemma 30 in [Robin, Augier, Boscain, Sigalotti, 2022] and obtain that, for the control $\omega_{\epsilon_1,\epsilon_2}(\cdot)$ given in (15), there exists $C' > 0$ such that for $\psi_{\text{rwa}}(0) = \mathbf{e}_p$

$$\min_{\theta \in [0,2\pi]} \left\| \psi_{\text{rwa}}\left(1/(\epsilon_1 \epsilon_2)\right) - \exp(i\theta)\mathbf{e}_q \right\| \leq C' \epsilon_2 / \epsilon_1.$$

Proof

We deduce that, in the interaction frame, there exists $C > 0$ such that

$$\min_{\theta \in [0,2\pi]} \left\| \psi_I \left(\frac{1}{\epsilon_1 \epsilon_2} \right) - \exp(i\theta) \mathbf{e}_q \right\| \leq C \max \left(\frac{\epsilon_1^2}{\epsilon_2}, \frac{\epsilon_2}{\epsilon_1} \right).$$

It follows that

$$\min_{\theta \in [0,2\pi]} \left\| \psi_{\epsilon_1, \epsilon_2} \left(\frac{1}{\epsilon_1 \epsilon_2} \right) - \exp(i\theta) \mathbf{e}_q \right\| < C \max \left(\frac{\epsilon_1^2}{\epsilon_2}, \frac{\epsilon_2}{\epsilon_1} \right).$$

We can thus conclude the proof.

Example

Consider a system as in (1) with drift and control Hamiltonians

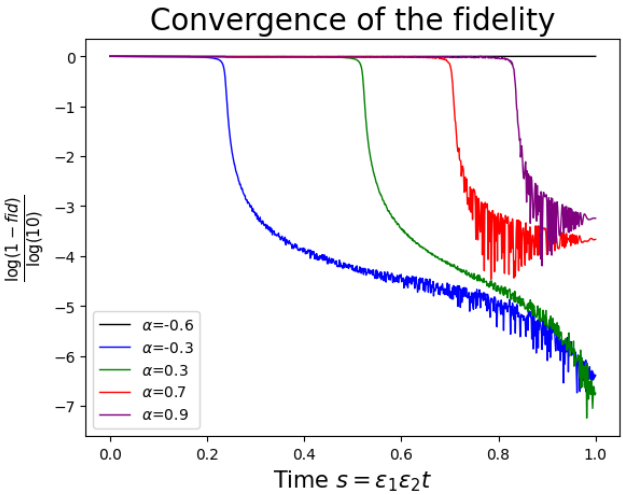
$$H(\alpha) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1.5+\alpha & 0 \\ 0 & 0 & 8 \end{pmatrix}, \quad H_c = \begin{pmatrix} 0 & 1 & 5 \\ 1 & 0 & 5 \\ 5 & 5 & 0 \end{pmatrix}.$$

In order to realize a population inversion between the first and the second eigenstates, we fix $T = 1$, $(\epsilon_1, \epsilon_2) = (10^{-2}, 10^{-7/2})$, $\psi_{\epsilon_1,\epsilon_2}(0) = (1,0,0)^\top$ and use the control law given in (15) with $v_0 = 1$, $v_1 = 2.5$. The fidelity at $s \in [0,1]$ is defined as

$$\mathrm{fid}(s) = 1 - \min_{\theta \in [0,2\pi]} \left\| \psi_{\epsilon_1,\epsilon_2}\left(\frac{s}{\epsilon_1\epsilon_2}\right) - e^{i\theta}\mathbf{e}_q \right\|. \qquad (19)$$

Here, the target state $\mathbf{e}_q = (0,1,0)^\top$.

Example



Convergence of the fidelity
0
−1
−2
−3
−4
−5
−6
−7
$\frac{\log(1-fid)}{\log(10)}$
α=-0.6
α=-0.3
α=0.3
α=0.7
α=0.9
0.0
0.2
0.4
0.6
0.8
1.0
Time $s = \varepsilon_1 \varepsilon_2 t$