Quantum Control via Adiabatic Theory and intersection of eigenvalues

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The problem

Want to control the Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(H_0 + u_1(t)H_1 + u_2(t)H_2\right)\psi(x,t)$$

H_0, H_1, H_2 self-adjoint linerar operators on a Hilbert space $\mathcal{H}$
$\mathbf{u} = (u_1, u_2) : \mathbb{R} \to \mathbb{R}^2$ control
$x \in \Omega \subset \mathbb{R}^n$ (possibly the whole $\mathbb{R}^n$)

Assumptions on the Hamiltonians

(H) H_0 is a self-adjoint operator on a Hilbert space $\mathcal{H}$

the discrete spectrum of H_0 is nonempty (and nontrivial).

H_1 and H_2 are bounded and self-adjoint linear operators on $\mathcal{H}$ real with respect to H_0

Typical case:

$H_0 = -\Delta + V(x)$ where Δ is the Laplacian on a domain of $\mathbb{R}^n$, V is a L^1_{loc} real-valued multiplication operator

H_1 and H_2 are measurable bounded real valued multiplication operators.

(Σ) there is an open domain in $\omega \subset \mathbb{R}^2$ where $H(\mathbf{u}) = H_0 + u_1 H_1 + u_2 H_2$, $\mathbf{u} \in \omega$, has a *separated discrete spectrum* .

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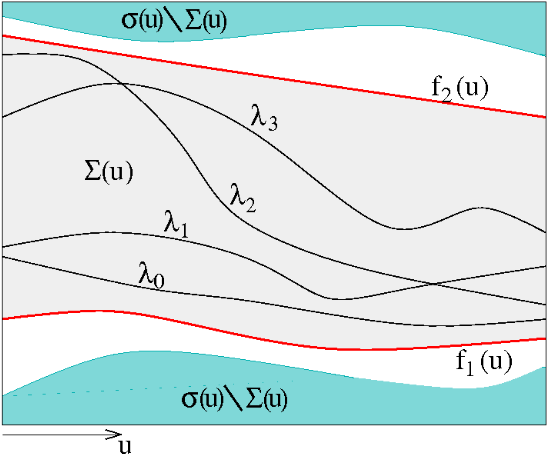
($\boldsymbol{\Sigma}$) there is an open domain in $\omega \subset \mathbb{R}^2$ where
$H(\mathbf{u}) = H_0 + u_1 H_1 + u_2 H_2,\ \mathbf{u} \in \omega$, has a *separated discrete spectrum* .

Example of separated discrete spectrum



Definition of separated discrete spectrum

Definition

Let ω be a domain in $\mathbb{R}^2$. A map Σ defined on ω that associates to each $\mathbf{u} \in \omega$ a subset $\Sigma(\mathbf{u})$ of the discrete spectrum of $H(\mathbf{u})$ is said to be a separated discrete spectrum on ω if there exist two continuous bounded functions $f_1, f_2 : \omega \to \mathbb{R}$ such that:

- $f_1(\mathbf{u}) < f_2(\mathbf{u})$ and $\Sigma(\mathbf{u}) \subset [f_1(\mathbf{u}), f_2(\mathbf{u})] \qquad \forall \mathbf{u} \in \omega$.
- there exists $\Gamma > 0$ such that

$$\inf_{\mathbf{u}\in\omega} dist([f_1(\mathbf{u}), f_2(\mathbf{u})], \sigma(\mathbf{u}) \setminus \Sigma(\mathbf{u})) > \Gamma$$

Notation: $\Sigma = \{\lambda_0 \leq \ldots \leq \lambda_k\}$, where λ_0 is not necessarily the ground state.

$\varphi_i(\mathbf{u}), i = 0, \ldots, k$ real eigenfunction of $H(\mathbf{u})$ relative to $\lambda_i(\mathbf{u})$.

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Definition of Spread Controllability

Definition

Σ be a separated discrete spectrum on ω
$\mathbf{u}^0 \in \omega$ such that $\lambda_i(\mathbf{u}^0) \neq \lambda_j(\mathbf{u}^0)$ $i \neq j$.
We say that the system is approximately spread controllable in $(\omega, \Sigma(\omega))$ if for every
$\Phi_{in} \in \{\varphi_0(\mathbf{u}^0), \ldots, \varphi_k(\mathbf{u}^0)\}$, $\psi(0) = \Phi_{in}$
$p \in [0,1]^{k+1}$ such that $\sum_{i=0}^{k} p_i^2 = 1$
$\varepsilon > 0$
there exists $T > 0$ and a continuous control $\mathbf{u}(\cdot) : [0, T] \to \omega$,
$\mathbf{u}(0) = \mathbf{u}(T) = \mathbf{u}^0$ such that

$$\left[\sum_{i=0}^{k} \left(|\langle \varphi_i(\mathbf{u}^0), \psi(T)\rangle| - p_i \right)^2 \right]^{1/2} \leq \varepsilon$$

where $\psi(T)$ is the solution of the equation $i\dot{\psi}(t) = H(\mathbf{u}(t))\psi(t)$.

Definition of Spread Controllability

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$$\Updownarrow$$

$\exists\, \theta_0,\ldots,\theta_k$ such that $\Phi_f = \sum_{i=0}^{k} e^{i\theta_i} p_i \varphi_i(\mathbf{u}^0)$ and we have

$$\|\Phi_f - \psi(T)\|_{\mathcal{H}} \leq \varepsilon$$

Main result

Theorem

$\Sigma : \omega \to \mathbb{R}^{k+1}$ separated discrete spectrum on $\omega \subset \mathbb{R}^2$
$\exists\ \mathbf{u}_j \in \omega,\ j = 0, \ldots, k-1$, such that

$$\lambda_j(\mathbf{u}_j) = \lambda_{j+1}(\mathbf{u}_j) \text{ conical intersection} \qquad \lambda_i(\mathbf{u}_j) \text{ simple if } i \neq j, j+1.$$

Then the system is approximately spread controllable on Σ, where the final time T in can be chosen of the order $O(1/\varepsilon)$.

Remark

The proof is constructive

Main tools

- Adiabatic Theorem
- Conical intersection

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The Adiabatic Theorem

Consider *slowly varying controls*

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(H_0 + u_1(\varepsilon t)H_1 + u_2(\varepsilon t)H_2\right)\psi(x,t), \quad \varepsilon > 0$$

$$H_a(\tau) = H(\tau) - i\varepsilon P_\Sigma(\tau)\dot{P}_\Sigma(\tau) - i\varepsilon P_\Sigma^\perp(\tau)\dot{P}_\Sigma^\perp(\tau) \qquad \tau = \varepsilon t$$

Theorem (Born-Fock, Kato, Nenciu, Avron, Teufel...)

Assume that $H(t) \in C^2$. Then there is a constant $C > 0$ (depending on the gap) such that for all $\tau, \tau_0 \in \mathbb{R}$

$$\begin{aligned} \|U^\varepsilon(\tau,\tau_0) - U_a^\varepsilon(\tau,\tau_0)\| &\leq C\varepsilon(1 + |\tau - \tau_0|) \qquad (|\tau-\tau_0| = O(1)) \\ &\leq C\varepsilon(1 + \varepsilon|t - t_0|) \qquad (|t-t_0| = O(1/\varepsilon)) \end{aligned}$$

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Conical Intersections

Definition

Let $H(\mathbf{u})$ satisfy hypothesis **(H)**. We say that $\bar{\mathbf{u}} \in \mathbb{R}^2$ is a conical intersection between the eigenvalues λ_1 and λ_2 if

$\lambda_1(\bar{\mathbf{u}}) = \lambda_2(\bar{\mathbf{u}})$

$\exists\, c > 0$ such that for any unit vector $\mathbf{v} \in \mathbb{R}^2$ and $t > 0$ small enough we have that

$$\lambda_2(\bar{\mathbf{u}} + t\mathbf{v}) - \lambda_1(\bar{\mathbf{u}} + t\mathbf{v}) > ct\,.$$

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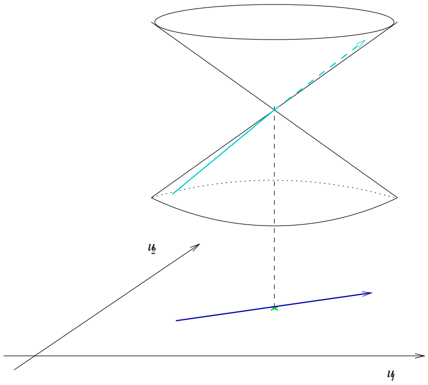
Passage through a conical intersection



$\mathbf{u}^0$ conical intersection between λ_1 and λ_2

$$\mathbf{u}(\tau) = \bar{\mathbf{u}} + \tau(\cos\alpha, \sin\alpha)$$
$$\tau \in [-1, 1]$$

$\psi(\tau)$ solution of
$i\dot{\psi}(t) = H(\mathbf{u}(\tau))\psi(t)$ at time $\tau = 1$
with $\psi(-1) = \varphi_1(\mathbf{u}(-1))$
From adiabatic theory

$$|1 - |\langle \varphi_2(\mathbf{u}(1)), \psi(1)\rangle|| \leq C\sqrt{\varepsilon}$$

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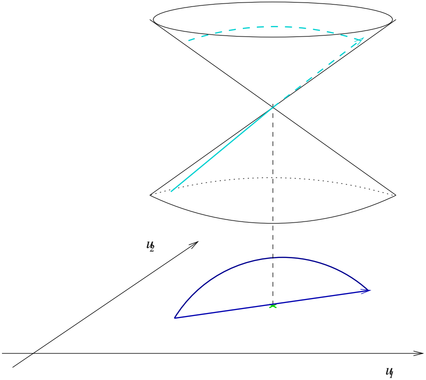

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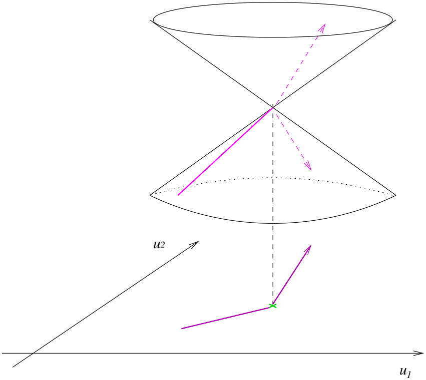

$$\mathbf{u}(\tau) = \begin{cases} \bar{\mathbf{u}} + \tau(\cos\alpha_i, \sin\alpha_i), & \tau \leq 0 \\ \bar{\mathbf{u}} + \tau(\cos\alpha_o, \sin\alpha_o), & \tau \geq 0 \end{cases}$$

Is it possible to spread the probability of occupation of φ_1 and φ_2?

Regularity around a conical intersection

Theorem (Kato-Rellich)

"Along analytic curves the eigenfunctions and the eigenvalues are analytic."

For analytic curves (in particular, straight lines) $\gamma : I \to \omega$ with $\gamma(\bar{t}) = \bar{\mathbf{u}}$ $\exists\ \varphi_1^\gamma, \varphi_2^\gamma$ orthonormal eigenfunctions of $H(\bar{\mathbf{u}})$ relative to $\lambda_1(\bar{\mathbf{u}}) = \lambda_2(\bar{\mathbf{u}})$ such that

$$\lim_{t\to\bar{t}^-} \varphi_j(\gamma(t)) = \varphi_j^\gamma, \qquad j = 1, 2.$$

Proposition

Let γ be a C^1 curve such that $\gamma(\bar{t}) = \bar{\mathbf{u}}$.
Let $r(t)$ be the tangent line to γ at $\bar{\mathbf{u}}$, $r(\bar{t}) = \bar{\mathbf{u}}$. Then

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The Conicity Matrix

Definition

Let $\psi_1, \psi_2 \in \mathcal{H}$. We define the conicity matrix associated to (ψ_1, ψ_2) as

$$\mathcal{M}(\psi_1, \psi_2) = \begin{pmatrix} \langle \psi_1, H_1 \psi_2 \rangle & \frac{1}{2}\big(\langle \psi_2, H_1 \psi_2 \rangle - \langle \psi_1, H_1 \psi_1 \rangle\big) \\ \langle \psi_1, H_2 \psi_2 \rangle & \frac{1}{2}\big(\langle \psi_2, H_2 \psi_2 \rangle - \langle \psi_1, H_2 \psi_1 \rangle\big) \end{pmatrix}.$$

Lemma

$\det \mathcal{M}(\cdot, \cdot)$ *is invariant under rotation of the argument, that is for any* ψ_1, ψ_2 *pair of orthonormal functions of* $\mathcal{H}$ *and for any rotation*

$$\psi_1^\alpha = \cos\alpha\, \psi_1 + \sin\alpha\, \psi_2$$
$$\psi_2^\alpha = -\sin\alpha\, \psi_1 + \cos\alpha\, \psi_2$$

one has $\det \mathcal{M}(\psi_1^\alpha, \psi_2^\alpha) = \det \mathcal{M}(\psi_1, \psi_2)$.

Properties of the conicity matrix

Corollary

$\varphi_1(\mathbf{u}), \varphi_2(\mathbf{u})$ eigenfunctions of $H(\mathbf{u})$ relative to λ_1, λ_2.
The (multi)function $\mathbf{u} \mapsto \det\{-|\mathcal{M}(\varphi_1(\mathbf{u}), \varphi_2(\mathbf{u}))|, |\mathcal{M}(\varphi_1(\mathbf{u}), \varphi_2(\mathbf{u}))|\}$ is well defined as a function of $\mathbf{u} \in \omega$.

Theorem (Characterization of conical intersections)

The intersection is conical if and only if the conicity matrix is non-degenerate at the intersection.

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Proposition

$\bar{\mathbf{u}}$ *conical intersection between* λ_1, λ_2

$\gamma_0(t) = \bar{\mathbf{u}} + (t-1, 0),\ t \geq 0$ *reference curve* $\quad \lim_{t \to 1^-} \varphi_j(\gamma_0(t)) = \varphi_j^0$.

Consider the curve $\gamma_\alpha(t) = \bar{\mathbf{u}} + t(\cos\alpha, \sin\alpha),\ t \geq 0$.

Then there is a monotone C^1 *function* $\boldsymbol{\vartheta} : [0, 2\pi) \to [0, \pi)$ *(or* $(-\pi, 0]$*)* *with* $\boldsymbol{\vartheta}(0) = 0$ *such that*

$$\lim_{t \to 0-} \varphi_j(\gamma_\alpha(t)) = \varphi_j^\alpha \quad j = 1, 2$$

with

$$\begin{aligned} \varphi_1^\alpha &= \cos\boldsymbol{\vartheta}(\alpha)\varphi_1^0 + \sin\boldsymbol{\vartheta}(\alpha)\varphi_2^0 \\ \varphi_2^\alpha &= -\sin\boldsymbol{\vartheta}(\alpha)\varphi_1^0 + \cos\boldsymbol{\vartheta}(\alpha)\varphi_2^0. \end{aligned}$$

Moreover, $\boldsymbol{\vartheta}(\cdot)$ satisfies the following equation:

$$\left(\cos\alpha, \sin\alpha\right) \mathcal{M}(\varphi_1^0, \varphi_2^0) \begin{pmatrix} \cos 2\boldsymbol{\vartheta}(\alpha) \\ \sin 2\boldsymbol{\vartheta}(\alpha) \end{pmatrix} = 0.$$

If $\gamma_\alpha(t) = \bar{\mathbf{u}} + (1 - t, 0),\ \ t \geq 0$, then

$$\theta(\alpha) = (-)\frac{\pi}{2}.$$

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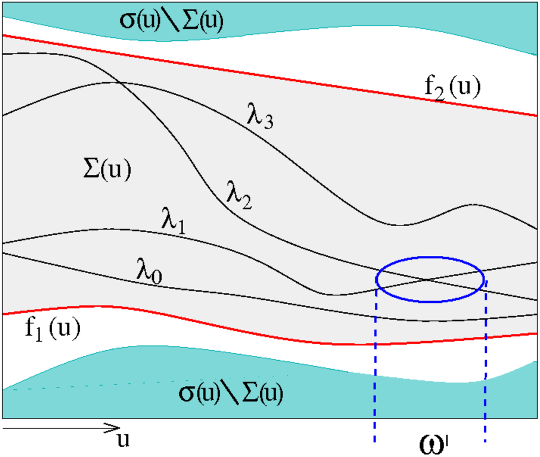
Reduction to 2-d



Representation in $\mathbb{C}^2$

Assumptions:

- $\Sigma(\omega') = \{\lambda_1 \leq \lambda_2\}$ separated discrete spectrum.
- γ C^2 curve in ω' such that φ_1, φ_2 are C^1 along γ.

We can establish an isomorphism $\mathcal{U}(t) : P_{\Sigma(\gamma(t))}(\mathcal{H}) \to \mathbb{C}^2$

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\begin{array}{rcl}
P_{\Sigma(\gamma(t))}(\mathcal{H}) = \mathbb{C}\{\varphi_1(\gamma(t)), \varphi_2(\gamma(t))\} & \simeq & \mathbb{C}^2 \\
\{\varphi_1(\gamma(t)), \varphi_2(\gamma(t))\} & \leftrightarrow & \left\{(1,0)^T, (0,1)^T\right\}
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The effective Hamiltonian

$$H_{\mathrm{eff}}(\tau) = \mathcal{U}(\tau) H_a(\tau) \mathcal{U}^*(\tau) + i\varepsilon \dot{\mathcal{U}}(\tau) \mathcal{U}^*(\tau)$$
$$= \begin{pmatrix} \lambda_\alpha(\tau) & 0 \\ 0 & \lambda_\beta(\tau) \end{pmatrix} + i\varepsilon \begin{pmatrix} 0 & \langle \dot{\varphi}_\alpha(\tau), \varphi_\beta(\tau) \rangle \\ \langle \dot{\varphi}_\alpha(\tau), \varphi_\beta(\tau) \rangle & 0 \end{pmatrix}$$

$U^\varepsilon_{\mathrm{eff}}(\tau, \tau_0)$ evolution operator (on $\mathbb{C}^2$) associated to H_{eff}

$$\left\| \left(U^\varepsilon(\tau, \tau_0) - \mathcal{U}^*(\tau) U^\varepsilon_{\mathrm{eff}}(\tau, \tau_0) \mathcal{U}(\tau_0) \right) P_{\Sigma(\gamma(t))} \right\| \leq C\varepsilon (1 + |\tau - \tau_0|)$$

The non-diagonal terms give a superposition between the two energy levels a priori of order $O(1)$

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The non-mixing Field

$$\langle \dot\varphi_1(\tau), \varphi_2(\tau)\rangle = \frac{\langle \varphi_1, (\dot u_1 H_1 + \dot u_2 H_2)\varphi_2\rangle}{\lambda_2(\tau) - \lambda_1(\tau)}$$

$\langle \dot\varphi_1(\tau), \varphi_2(\tau)\rangle \equiv 0$ along the solutions of the equation

$$\begin{cases} \dot u_1 = -\langle \varphi_1(\mathbf{u}), H_2\varphi_2(\mathbf{u})\rangle \\ \dot u_2 = \langle \varphi_1(\mathbf{u}), H_1\varphi_2(\mathbf{u})\rangle \end{cases} \qquad \left(\begin{cases} \dot u_1 = \langle \varphi_1(\mathbf{u}), H_2\varphi_2(\mathbf{u})\rangle \\ \dot u_2 = -\langle \varphi_1(\mathbf{u}), H_1\varphi_2(\mathbf{u})\rangle \end{cases}\right)$$

Definition

The field $\mathcal{X}_P(\mathbf{u}) = (\pm)(-\langle \varphi_1(\mathbf{u}), H_2\varphi_2(\mathbf{u})\rangle, \langle \varphi_1(\mathbf{u}), H_1\varphi_2(\mathbf{u})\rangle)$ is called the non-mixing field.

- $\mathcal{X}_P$ is well defined and continuous in $\omega' \setminus \{\bar{\mathbf{u}}\}$;
- it is multivalued at $\bar{\mathbf{u}}$.

The non-mixing Field

$$\langle \dot\varphi_1(\tau), \varphi_2(\tau) \rangle = \frac{\langle \varphi_1, (\dot u_1 H_1 + \dot u_2 H_2)\varphi_2 \rangle}{\lambda_2(\tau) - \lambda_1(\tau)}$$

$\langle \dot\varphi_1(\tau), \varphi_2(\tau) \rangle \equiv 0$ along the solutions of the equation

$$\begin{cases} \dot u_1 = -\langle \varphi_1(\mathbf{u}), H_2 \varphi_2(\mathbf{u}) \rangle \\ \dot u_2 = \langle \varphi_1(\mathbf{u}), H_1 \varphi_2(\mathbf{u}) \rangle \end{cases} \qquad \left(\begin{cases} \dot u_1 = \langle \varphi_1(\mathbf{u}), H_2 \varphi_2(\mathbf{u}) \rangle \\ \dot u_2 = -\langle \varphi_1(\mathbf{u}), H_1 \varphi_2(\mathbf{u}) \rangle \end{cases} \right)$$

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The integral curves of $\mathcal{X}_P$

- $$D_{\mathcal{X}_P}(\lambda_2 - \lambda_1)(\mathbf{u}) = |\det \mathcal{M}(\mathbf{u})|$$

  There is a neighbourhood $\bar{\omega}$ of the conical intersection $\bar{\mathbf{u}}$ such that for any $\mathbf{u} \in \bar{\omega}$ the integral curve of $(\pm)\mathcal{X}_P$ starting from $\mathbf{u}$ reaches $\bar{\mathbf{u}}$ in *finite time*
- at the conical intersection $\mathcal{X}_P(\bar{\mathbf{u}})$ covers all possible directions
- the integral curves of $\mathcal{X}_P$ are C^1 ($\bar{\mathbf{u}}$ included) and φ_1, φ_2 are C^1 along them
- the integral curves of $\mathcal{X}_P$ are C^∞ ($\bar{\mathbf{u}}$ included) and φ_1, φ_2 are C^∞ along them

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Climb of one level

Theorem

$\bar{\mathbf{u}}$ conical intersection between λ_1, λ_2
$\gamma : [0,1] \to \omega$ such that

- $\gamma(0) = \mathbf{u}^0 \qquad \gamma(\bar{t}) = \bar{\mathbf{u}} \quad (\bar{t} \in (0,1))$
- $\dot{\gamma}(t) = \mathcal{X}_P(\gamma(t)) \quad t \in [0,\bar{t}) \cup (\bar{t},1]$

Let $\psi(0) = \varphi_1(\mathbf{u}^0)$. Then for any $\varepsilon > 0$ there are $\theta \in [0, 2\pi]$, $T > 0$, $T = O(1/\varepsilon)$, such that

$$\|\psi(T) - e^{i\theta}\varphi_2(\gamma(1))\| \leq \varepsilon,$$

where $\psi(T)$ is the solution of the equation $i\dot{\psi}(t) = H(\gamma(t/T))\psi(t)$.

Distribution of probability between two levels.

Theorem

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- $\gamma(0) = \mathbf{u}^0 \quad \gamma(\bar{t}) = \bar{\mathbf{u}} \ (\ \bar{t} \in (0,1))$
- $\dot{\gamma}(t) = \mathcal{X}_P(\gamma(t)) \quad t \in [0,\bar{t}) \cup (\bar{t},1]$
- *let* α_i, α_o *such that*

$$\lim_{t\to\bar{t}^-} \frac{\dot{\gamma}(t)}{\|\dot{\gamma}(t)\|} = -(\cos\alpha_i, \sin\alpha_i)\,, \quad \lim_{t\to\bar{t}^+} \frac{\dot{\gamma}(t)}{\|\dot{\gamma}(t)\|} = (\cos\alpha_o, \sin\alpha_o).$$

Distribution of probability between two levels.

Fix $\psi(0)=\varphi_1(\mathbf{u}^0)$. *Then for any* $\varepsilon>0$, *there is a* $T>0,\ T=O(1/\varepsilon)$ *such that*

$$\begin{aligned} \big|\,|\langle\varphi_1(\gamma(1)),\psi(T)\rangle| - p_1\big| \le \varepsilon, \\ \big|\,|\langle\varphi_2(\gamma(1)),\psi(T)\rangle| - p_2\big| \le \varepsilon. \end{aligned}$$

where $\psi(T)$ *is the solution of the equation* $i\dot\psi(t)=H(\gamma(t/T))\psi(t)$.

$$p_1 = |\cos(\boldsymbol{\vartheta}(\alpha_o)-\boldsymbol{\vartheta}(\alpha_i))| \quad p_2 = |\sin(\boldsymbol{\vartheta}(\alpha_o)-\boldsymbol{\vartheta}(\alpha_i))|.$$

Inducing a transition $(1,0) \mapsto (p_1^2, p_2^2)$

$\beta \in [0, \pi/2]$ such that $(p_1, p_2) = (\cos\beta, \sin\beta)$

$\gamma_1 : [0, t_1] \to \omega$ such that

- $\gamma_1(0) = \mathbf{u}^0$, $\gamma_1(t_1) = \bar{\mathbf{u}}$
- $\dot\gamma_1(t) = \mathcal{X}_P(\gamma(t)) \quad \forall t \geq t'$, for some $t' \in (0, t_1)$
  $\lim_{t \to t_1^-} \frac{\dot\gamma_1(t)}{\|\dot\gamma_2(t)\|} = -(\cos\alpha_i, \sin\alpha_i)$

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- $\gamma_2(t_1) = \bar{\mathbf{u}}$, $\gamma_2(t_2) = \mathbf{u}^0$
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  $\lim_{t \to t_1^+} \frac{\dot\gamma_2(t)}{\|\dot\gamma_2(t)\|} = (\cos\alpha_o, \sin\alpha_o)$

where

$$\alpha_o = \vartheta^{-1}(\beta + \vartheta(\alpha_i) + k_+\pi) \quad \text{or} \quad \alpha_o = \vartheta^{-1}(-\beta + \vartheta(\alpha_i) + k_-\pi)$$

$k_-, k_+ \in \mathbb{Z}$ in such a way that ϑ^{-1} is well defined.

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$k_-, k_+ \in \mathbb{Z}$ in such a way that $\boldsymbol{\vartheta}^{-1}$ is well defined.

Main results

Theorem

Let $\Sigma = \{\lambda_0(\mathbf{u}) \leq \ldots \leq \lambda_k(\mathbf{u})\}$ be a separated discrete spectrum on ω. Assume that

- $\mathbf{u}^0 \in \omega$ *such that* $\lambda_i(\mathbf{u}^0) \neq \lambda_j(\mathbf{u}^0),\ i \neq j$
- *for every* $i = 0, \ldots, k-1$ *there is* $\bar{\mathbf{u}}_i \in \omega$
  - $\bar{\mathbf{u}}_i$ *conical intersection between* λ_1 *and* λ_2
  - $\lambda_l(\bar{\mathbf{u}}_j) \neq \lambda_{l+1}(\bar{\mathbf{u}}_j)$ *if* $l \neq j$.

Then the system is approximately spread controllable in $(\omega, \Sigma(\omega))$.

Further Perspectives

- study the case $H(\mathbf{u})$ nonlinear w.r.t. $\mathbf{u}$.
- try to obtain a stronger controllability result, that is allowing $|\langle\varphi_i, \psi(0)\rangle| = \pi_i$ with $\sum_{i=1}^{k} \pi_i^2 = 1$.
- looking for a good approximation of the integral curves of $\mathcal{X}_P$ which are more easily computable.