Classical scattering theory and applications to computing invariant manifolds in chemistry

Daniel Blazevski[1,2]
joint with Rafael de la Llave[2] and Jennifer Franklin [1]

[1]Department of Mathematics
UT-Austin

[2]Department of Mathematics
Georgia Institute of Technology

February 23, 2012

Table of contents

Perturbations localized in time

- We consider a general vector field $\mathcal{U}$ in $\mathbb{R}^n$ subject to a perturbation $\mathcal{P}$ that is localized in time

$$\mathcal{V}(x,t) = \mathcal{U}(x,t) + \mathcal{P}(x,t) \tag{1.1}$$

Perturbations localized in time

- We consider a general vector field $\mathcal{U}$ in $\mathbb{R}^n$ subject to a perturbation $\mathcal{P}$ that is localized in time

$$\mathcal{V}(x,t) = \mathcal{U}(x,t) + \mathcal{P}(x,t) \tag{1.1}$$

- where, for instance, $|\mathcal{P}(x,t)| \leq Ce^{-\lambda|t|}$, $\mathcal{P}$ is compactly supported in time, etc.

Perturbations localized in time

- We consider a general vector field $\mathcal{U}$ in $\mathbb{R}^n$ subject to a perturbation $\mathcal{P}$ that is localized in time

$$\mathcal{V}(x,t) = \mathcal{U}(x,t) + \mathcal{P}(x,t) \tag{1.1}$$

- where, for instance, $|\mathcal{P}(x,t)| \leq Ce^{-\lambda|t|}$, $\mathcal{P}$ is compactly supported in time, etc.
- We expect the flow $U_{t_0}^t$ of $\mathcal{U}$ to behave like the flow $V_{t_0}^t$ of $\mathcal{V}$ for $|t|$ large

Perturbations localized in time

- We consider a general vector field $\mathcal{U}$ in $\mathbb{R}^n$ subject to a perturbation $\mathcal{P}$ that is localized in time

$$\mathcal{V}(x,t) = \mathcal{U}(x,t) + \mathcal{P}(x,t) \tag{1.1}$$

- where, for instance, $|\mathcal{P}(x,t)| \leq Ce^{-\lambda|t|}$, $\mathcal{P}$ is compactly supported in time, etc.
- We expect the flow $U_{t_0}^t$ of $\mathcal{U}$ to behave like the flow $V_{t_0}^t$ of $\mathcal{V}$ for $|t|$ large
- Example: Laser-manipulated chemical reactions

Perturbations localized in time

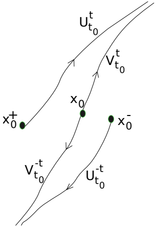
- We consider a general vector field $\mathcal{U}$ in $\mathbb{R}^n$ subject to a perturbation $\mathcal{P}$ that is localized in time

$$\mathcal{V}(x,t) = \mathcal{U}(x,t) + \mathcal{P}(x,t) \tag{1.1}$$

- where, for instance, $|\mathcal{P}(x,t)| \leq Ce^{-\lambda|t|}$, $\mathcal{P}$ is compactly supported in time, etc.
- We expect the flow $U_{t_0}^t$ of $\mathcal{U}$ to behave like the flow $V_{t_0}^t$ of $\mathcal{V}$ for $|t|$ large
- Example: Laser-manipulated chemical reactions
- Example: A satellite being perturbed by the passage of an asteroid or comet

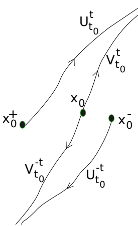
The Wave and scattering maps

- We make precise the notion that the $V_{t_0}^{t}$ behaves like $U_{t_0}^{t}$ for large $|t|$.



The Wave and scattering maps

- We make precise the notion that the $V_{t_0}^t$ behaves like $U_{t_0}^t$ for large $|t|$.

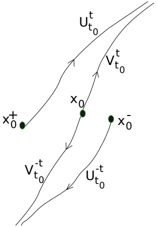


- The wave maps compute x_0^+ and x_0^- knowing x_0

$$\Omega_{\pm}^{t_0} = \lim_{T \to \pm\infty} U_T^{t_0} \circ V_{t_0}^T \tag{1.2}$$

The Wave and scattering maps

- We make precise the notion that the $V_{t_0}^t$ behaves like $U_{t_0}^t$ for large $|t|$.



- The wave maps compute x_0^+ and x_0^- knowing x_0

$$\Omega_\pm^{t_0} = \lim_{T\to\pm\infty} U_T^{t_0} \circ V_{t_0}^T \tag{1.2}$$

- The scattering map takes x_0^- to x_0^+

$$s^{t_0} = \Omega_+^{t_0} \circ \left(\Omega_-^{t_0}\right)^{-1} \tag{1.3}$$

Existence and Intertwining relations

- The Omega maps exist when, roughly speaking, the decay rate of $\mathcal{P}$ is larger than the growth rate $\|DU_{t_0}^t\|$ of $U_{t_0}^t$ (More Later!)

Existence and Intertwining relations

- The Omega maps exist when, roughly speaking, the decay rate of $\mathcal{P}$ is larger than the growth rate $\|DU_{t_0}^t\|$ of $U_{t_0}^t$ (More Later!)
- Implications of the existence of the Omega maps: The intertwining relations

$$\Omega_\pm^s \circ V_{t_0}^s = U_{t_0}^s \circ \Omega_\pm^{t_0} \tag{2.1}$$

Existence and Intertwining relations

- The Omega maps exist when, roughly speaking, the decay rate of $\mathcal{P}$ is larger than the growth rate $\|DU_{t_0}^t\|$ of $U_{t_0}^t$ (More Later!)
- Implications of the existence of the Omega maps: The intertwining relations

$$\Omega_{\pm}^s \circ V_{t_0}^s = U_{t_0}^s \circ \Omega_{\pm}^{t_0} \tag{2.1}$$

- We then obtain the time-dependent conjugacy: $V_{t_0}^s = \left(\Omega_{\pm}^s\right)^{-1} \circ U_{t_0}^s \circ \Omega_{\pm}^{t_0}$

Existence and Intertwining relations

- The Omega maps exist when, roughly speaking, the decay rate of $\mathcal{P}$ is larger than the growth rate $\|DU_{t_0}^t\|$ of $U_{t_0}^t$ (More Later!)
- Implications of the existence of the Omega maps: The intertwining relations

$$\Omega_{\pm}^s \circ V_{t_0}^s = U_{t_0}^s \circ \Omega_{\pm}^{t_0} \tag{2.1}$$

- We then obtain the time-dependent conjugacy: $V_{t_0}^s = \left(\Omega_{\pm}^s\right)^{-1} \circ U_{t_0}^s \circ \Omega_{\pm}^{t_0}$
- If we "automonize" the flows, one can show that the flows $U_{t_0}^t$ and $V_{t_0}^t$ are conjugate in the extended phase space.

Applications to invariant manifolds

- First consider the example: Let U be an autonomous flow and x_0 a fixed point.

Applications to invariant manifolds

- First consider the example: Let U be an autonomous flow and x_0 a fixed point.
- Question: what is the corresponding object in the for the non-autonomous flow $V_{t_0}^t$?

Applications to invariant manifolds

- First consider the example: Let U be an autonomous flow and x_0 a fixed point.
- Question: what is the corresponding object in the for the non-autonomous flow $V_{t_0}^t$?
- For each starting time, we have a point $\bar{x}_0(t_0)$ that satisfies

$$V_{t_0}^t(\bar{x}_0(t_0)) = \bar{x}_0(t) \tag{2.2}$$

Applications to invariant manifolds

- First consider the example: Let U be an autonomous flow and x_0 a fixed point.
- Question: what is the corresponding object in the for the non-autonomous flow $V_{t_0}^t$?
- For each starting time, we have a point $\bar{x}_0(t_0)$ that satisfies

$$V_{t_0}^t(\bar{x}_0(t_0)) = \bar{x}_0(t) \tag{2.2}$$

- This property is called *Time-dependent invariance*

Applications to invariant manifolds

- First consider the example: Let U be an autonomous flow and x_0 a fixed point.
- Question: what is the corresponding object in the for the non-autonomous flow $V_{t_0}^t$?
- For each starting time, we have a point $\bar{x}_0(t_0)$ that satisfies

$$V_{t_0}^t(\bar{x}_0(t_0)) = \bar{x}_0(t) \tag{2.2}$$

- This property is called *Time-dependent invariance*
- If x_0 is *hyperbolic* and has stable and unstable manifolds $W^s(x_0), W^u(x_0)$ then there are corresponding time dependent invariant stable manifolds $W_{t_0}^s(\bar{x}_0(t_0)), W_{t_0}^u(\bar{x}_0(t_0))$

Application to invariant manifolds

- A more general notion: Start with a *time-dependent normally hyperbolic invariant manifold* (TDNHIM) of $U^t_{t_0}$, i.e. a "normally hyperbolic" family M_{t_0} satisfying

$$U^t_{t_0}(M_{t_0}) = M_t \tag{2.3}$$

Proposition

Let M_{t_0} be a TDNHIM for $U^t_{t_0}$ and assume that $\Omega^{t_0}_{\pm}$ exist. Then

$$N^{\pm}_{t_0} := \left(\Omega^{t_0}_{\pm}\right)^{-1}(M_{t_0}) \tag{2.4}$$

is a TDNHIM for $V^t_{t_0}$. Similarly, $\Omega^{\pm}_{t_0}$ takes the stable and unstable manifolds of M_{t_0} to those of N_{t_0}.

Application to invariant manifolds

- A more general notion: Start with a *time-dependent normally hyperbolic invariant manifold* (TDNHIM) of $U_{t_0}^t$, i.e. a "normally hyperbolic" family M_{t_0} satisfying

$$U_{t_0}^t(M_{t_0}) = M_t \tag{2.3}$$

Proposition

Let M_{t_0} be a TDNHIM for $U_{t_0}^t$ and assume that $\Omega_\pm^{t_0}$ exist. Then

$$N_{t_0}^\pm := \left(\Omega_\pm^{t_0}\right)^{-1}(M_{t_0}) \tag{2.4}$$

is a TDNHIM for $V_{t_0}^t$. Similarly, $\Omega_{t_0}^\pm$ takes the stable and unstable manifolds of M_{t_0} to those of N_{t_0}.

- Since $(\Omega_\pm^{t_0})^{-1} \approx V_T^{t_0} \circ U_{t_0}^T$ one can use this to numerically compute invariant objects for $V_{t_0}^t$

Derivation of existence result: Cook's method

- To determine when $\Omega_+^{t_0}$ exist, we consider the truncations of the limiting sequence:

$$\Omega_+^{t_0,T} := U_T^{t_0} \circ V_{t_0}^T \tag{2.5}$$

Derivation of existence result: Cook's method

- To determine when $\Omega_+^{t_0}$ exist, we consider the truncations of the limiting sequence:

$$\Omega_+^{t_0,T} := U_T^{t_0} \circ V_{t_0}^T \tag{2.5}$$

- We show that the sequence $\{\Omega_+^{t_0,N}\}$ is Cauchy in $C^k(B_R)$ for every ball B_R.

Derivation of existence result: Cook's method

- To determine when $\Omega_+^{t_0}$ exist, we consider the truncations of the limiting sequence:

$$\Omega_+^{t_0, T} := U_T^{t_0} \circ V_{t_0}^T \tag{2.5}$$

- We show that the sequence $\{\Omega_+^{t_0,N}\}$ is Cauchy in $C^k(B_R)$ for every ball B_R.
- By the fundamental theorem of calculus we have

$$\Omega_+^{t_0, T+1} - \Omega_+^{t_0, T} = \int_T^{T+1} \frac{d}{d\sigma}\Omega_+^{t_0,\sigma} d\sigma \tag{2.6}$$

Derivation of existence result: Cook's method

- To determine when $\Omega_+^{t_0}$ exist, we consider the truncations of the limiting sequence:

$$\Omega_+^{t_0,T} := U_T^{t_0} \circ V_{t_0}^T \tag{2.5}$$

- We show that the sequence $\{\Omega_+^{t_0,N}\}$ is Cauchy in $C^k(B_R)$ for every ball B_R.
- By the fundamental theorem of calculus we have

$$\Omega_+^{t_0,T+1} - \Omega_+^{t_0,T} = \int_T^{T+1} \frac{d}{d\sigma}\Omega_+^{t_0,\sigma}\, d\sigma \tag{2.6}$$

- We deduce that

$$\sum_{N>t_0} \|\Omega_+^{t_0,N+1} - \Omega_+^{t_0,N}\| \leq \int_{t_0}^{\infty} \left\| \frac{d}{d\sigma}\Omega_+^{t_0,\sigma} \right\| d\sigma \tag{2.7}$$

Computing $\frac{d}{d\sigma}\Omega_+^{t_0,\sigma}$ where $\Omega_+^{t_0,\sigma} = U_\sigma^{t_0} \circ V_{t_0}^{\sigma}$

- We just saw that if

$$\int_{t_0}^{\infty} \left\| \frac{d}{d\sigma} \Omega_+^{t_0,\sigma} \right\| d\sigma < \infty \tag{2.8}$$

Then $\Omega_+^{t_0}$ exists

Computing $\frac{d}{d\sigma}\Omega_+^{t_0,\sigma}$ where $\Omega_+^{t_0,\sigma} = U_\sigma^{t_0} \circ V_{t_0}^\sigma$

- We just saw that if

$$\int_{t_0}^{\infty} \left\| \frac{d}{d\sigma}\Omega_+^{t_0,\sigma} \right\| d\sigma < \infty \tag{2.8}$$

  Then $\Omega_+^{t_0}$ exists
- $\Omega_+^{t_0,\sigma}$ is one-parameter (in σ) family of diffoemorphisms and we can define its *Generator* $\mathcal{O}^+$ by

$$\mathcal{O}_\sigma^+(\Omega_+^{t_0,\sigma}(x)) = \frac{d}{d\sigma}\Omega_+^{t_0,\sigma}(x) \tag{2.9}$$

Computing $\frac{d}{d\sigma}\Omega_+^{t_0,\sigma}$ where $\Omega_+^{t_0,\sigma} = U_\sigma^{t_0} \circ V_{t_0}^\sigma$

- We just saw that if

$$\int_{t_0}^{\infty} \left\| \frac{d}{d\sigma}\Omega_+^{t_0,\sigma} \right\| d\sigma < \infty \tag{2.8}$$

  Then $\Omega_+^{t_0}$ exists
- $\Omega_+^{t_0,\sigma}$ is one-parameter (in σ) family of diffoemorphisms and we can define its *Generator* $\mathcal{O}^+$ by

$$\mathcal{O}_\sigma^+(\Omega_+^{t_0,\sigma}(x)) = \frac{d}{d\sigma}\Omega_+^{t_0,\sigma}(x) \tag{2.9}$$

- Note that the generator of $V_{t_0}^\sigma$ is simply $\mathcal{V}_\sigma$ and we can use *Deformation theory* to compute the generators of compositions (e.g. $U_\sigma^{t_0} \circ V_{t_0}^\sigma$) and inverses (e.g $U_\sigma^{t_0} = \left(U_{t_0}^\sigma\right)^{-1}$)

Existence result

Theorem

[1] *Suppose that*

$$I_\pm(t_0) := \int_{t_0}^{\pm\infty} \| \left(DU_\sigma^{t_0} \left(\mathcal{V}_\sigma - \mathcal{U}_\sigma \right) \right) \circ V_{t_0}^{\sigma} \|_{C^k(B_R)} d\sigma < \infty \tag{2.10}$$

Then the wave maps exist and are in $C^k(B_R)$ for all R.

[1] D. Blazevski and R. de la Llave, *Time-dependent scattering theory for ODEs and applications to reaction dynamics*, Journal of Physics A: Mathematical and Theoretical **44** (2011), no. 19, 195101

Particular cases

- $$I_\pm(t_0) = \int_{t_0}^{\pm\infty} \| \left(DU_\sigma^{t_0} \left(\mathcal{V}_\sigma - \mathcal{U}_\sigma \right) \right) \circ V_{t_0}^\sigma \|_{C^k(B_R)} d\sigma < \infty$$

Particular cases

- $$I_{\pm}(t_0) = \int_{t_0}^{\pm\infty} \| \left(DU_{\sigma}^{t_0} \left(\mathcal{V}_{\sigma} - \mathcal{U}_{\sigma} \right) \right) \circ V_{t_0}^{\sigma} \|_{C^k(B_R)} d\sigma < \infty$$
- This holds if $\mathcal{P}_{\sigma} = \mathcal{V}_{\sigma} - \mathcal{U}_{\sigma}$ is compactly supported in σ

Particular cases

- $$I_{\pm}(t_0) = \int_{t_0}^{\pm\infty} \| \left(DU_\sigma^{t_0} \left(\mathcal{V}_\sigma - \mathcal{U}_\sigma \right) \right) \circ V_{t_0}^{\sigma} \|_{C^k(B_R)} d\sigma < \infty$$
- This holds if $\mathcal{P}_\sigma = \mathcal{V}_\sigma - \mathcal{U}_\sigma$ is compactly supported in σ
- If $\|DU_{t_0}^t\| \leq Ce^{\mu t}$ and $|\mathcal{P}| \leq Ce^{-\lambda t}$ with $\mu < \lambda$

Particular cases

- $$I_{\pm}(t_0) = \int_{t_0}^{\pm\infty} \| \left(DU_{\sigma}^{t_0} \left(\mathcal{V}_{\sigma} - \mathcal{U}_{\sigma} \right) \right) \circ V_{t_0}^{\sigma} \|_{C^k(B_R)} d\sigma < \infty$$
- This holds if $\mathcal{P}_{\sigma} = \mathcal{V}_{\sigma} - \mathcal{U}_{\sigma}$ is compactly supported in σ
- If $\|DU_{t_0}^t\| \leq Ce^{\mu t}$ and $|\mathcal{P}| \leq Ce^{-\lambda t}$ with $\mu < \lambda$
- If $\|DU_{t_0}^t\| \leq Ct$ and $|\mathcal{P}| \leq C/(1 + t^3)$

Invertibility, or *asymptotic completeness*

- When are $\Omega_{\pm}^{t_0}$ invertible?

Invertibility, or *asymptotic completeness*

- When are $\Omega_{\pm}^{t_0}$ invertible?
- The intertwining relations imply: $\Omega_{+}^{s} = U_{t_0}^{s} \circ \Omega_{+}^{t_0} \circ V_{s}^{t_0}$

Invertibility, or *asymptotic completeness*

- When are $\Omega_{\pm}^{t_0}$ invertible?
- The intertwining relations imply: $\Omega_{+}^{s} = U_{t_0}^{s} \circ \Omega_{+}^{t_0} \circ V_{s}^{t_0}$
- Thus, invertibility for one t_0 implies invertbility for all s

Invertibility, or *asymptotic completeness*

- When are $\Omega_{\pm}^{t_0}$ invertible?
- The intertwining relations imply: $\Omega_{+}^{s} = U_{t_0}^{s} \circ \Omega_{+}^{t_0} \circ V_{s}^{t_0}$
- Thus, invertibility for one t_0 implies invertbility for all s
- Recall that we have

$$\Omega_{+}^{t_0,t} - \Omega_{+}^{t_0,s} = \int_s^t \frac{d}{d\sigma}\Omega_{+}^{\sigma} d\sigma \tag{2.11}$$

Invertibility continued

- $$\Omega_+^{t_0,t} - \Omega_+^{t_0,s} = \int_s^{t_0} \frac{d}{d\sigma}\Omega_+^{\sigma}\, d\sigma$$

Invertibility continued

- $$\Omega_+^{t_0,t} - \Omega_+^{t_0,s} = \int_s^{t_0} \frac{d}{d\sigma}\Omega_+^{\sigma} d\sigma$$
- If $s = t_0$ then $\Omega_+^{t_0,t_0}(x) = x$ and we let $t \to \infty$

$$\|\Omega_+^{t_0} - \text{ Id } \| \leq I(t_0) = \int_{t_0}^{\infty} \| \left(DU_\sigma^{t_0} \left(\mathcal{V}_\sigma - \mathcal{U}_\sigma \right) \right) \circ V_{t_0}^{\sigma} \| d\sigma \tag{2.12}$$

Invertibility continued

- $$\Omega_+^{t_0,t} - \Omega_+^{t_0,s} = \int_s^{t_0} \frac{d}{d\sigma}\Omega_+^{\sigma}\, d\sigma$$
- If $s = t_0$ then $\Omega_+^{t_0,t_0}(x) = x$ and we let $t \to \infty$

$$\|\Omega_+^{t_0} - \text{ Id } \| \leq I(t_0) = \int_{t_0}^{\infty} \| \left(DU_\sigma^{t_0} \left(\mathcal{V}_\sigma - \mathcal{U}_\sigma\right)\right) \circ V_{t_0}^{\sigma} \| d\sigma \tag{2.12}$$

- Thus if $I(t_0) \to 0$ as $t_0 \to \infty$ then $\Omega_+^{t_0}$ becomes closer to the identity, and hence invertible

Proposition

If $\lim_{t_0\to\infty} I(t_0) = 0$ *then* $\Omega_+^{t_0}$ *is invertible for all* t_0

Perturbative calculations

- We will now consider the case of

$$\mathcal{V}_t^\epsilon = \mathcal{U}_t + \epsilon \mathcal{P}_t \tag{2.13}$$

and expand $s_\epsilon^{t_0}$ in epsilon.

Perturbative calculations

- We will now consider the case of

$$\mathcal{V}_t^\epsilon = \mathcal{U}_t + \epsilon \mathcal{P}_t \tag{2.13}$$

and expand $s_\epsilon^{t_0}$ in epsilon.

- We write

$$s_\epsilon^{t_0} = \text{ Id } + \epsilon \left(\frac{d}{d\epsilon} s_{t_0}^\epsilon \right) + \mathcal{O}(\epsilon^2) \tag{2.14}$$

Perturbative calculations

- We will now consider the case of

$$\mathcal{V}_t^{\epsilon} = \mathcal{U}_t + \epsilon \mathcal{P}_t \tag{2.13}$$

  and expand $s_{\epsilon}^{t_0}$ in epsilon.
- We write

$$s_{\epsilon}^{t_0} = \text{ Id } + \epsilon \left(\frac{d}{d\epsilon} s_{t_0}^{\epsilon} \right) + \mathcal{O}(\epsilon^2) \tag{2.14}$$

- Again use deformation theory, though this time with respect to ϵ. Generator for V_{ϵ} is given using the variation of parameters formula

Fermi's Golden Rule

Let $U_{t_0}^t$ be the flow for the Hamiltonian H_0 and $V(\epsilon)$ the flow for $H = H_0 + \epsilon h$.

Theorem

Suppose that the wave maps $s_\epsilon^{t_0}$ exists and is smooth. Then $s_\epsilon^{t_0}$ is the time-ϵ map of the Hamiltonian

$$S_\epsilon^{t_0} = \lim_{T \to \infty} \int_{-T}^{T} h \circ V_T^\sigma(\epsilon) \circ U_{t_0}^T d\sigma \tag{2.15}$$

Corollary

Corollary

As a consequence

$$s_\epsilon^{t_0} = \; Id \; + \epsilon J \nabla S_0^{t_0} + \mathcal{O}(\epsilon^2) \tag{2.16}$$

and if F is any observable

$$F \circ s_\epsilon^{t_0} = F + \epsilon \left\{ F, S_0^{t_0} \right\} + \mathcal{O}(\epsilon^2) \tag{2.17}$$

Note that

$$S_0^{t_0} = \lim_{T \to \infty} \int_{-T}^{T} h \circ U_{t_0}^{\sigma} \, d\sigma$$

Perturbative calculations continued

- Application to perturbations of integrable systems: $H(I, \theta) = H_0(I) + \epsilon h(I, \theta)$

Perturbative calculations continued

- Application to perturbations of integrable systems: $H(I, \theta) = H_0(I) + \epsilon h(I, \theta)$
- For H_0 the action I is conserved: $(I(t), \theta(t)) = (I_0, \theta_0 + \nabla H_0(I_0)t)$

Perturbative calculations continued

- Application to perturbations of integrable systems: $H(I, \theta) = H_0(I) + \epsilon h(I, \theta)$
- For H_0 the action I is conserved: $(I(t), \theta(t)) = (I_0, \theta_0 + \nabla H_0(I_0)t)$
- Using averaging or KAM theory one can estimate the slow variable $I_\epsilon(t)$ for the perturbed system for $|t|$ large

Perturbative calculations continued

- Application to perturbations of integrable systems: $H(I,\theta) = H_0(I) + \epsilon h(I,\theta)$
- For H_0 the action I is conserved: $(I(t), \theta(t)) = (I_0, \theta_0 + \nabla H_0(I_0)t)$
- Using averaging or KAM theory one can estimate the slow variable $I_\epsilon(t)$ for the perturbed system for $|t|$ large
- Using scattering theory we can compute the change in any variable, fast or slow, using

$$F \circ s_\epsilon^{t_0} = F + \epsilon \left\{F, S_0^{t_0}\right\} + \mathcal{O}(\epsilon^2) \tag{2.18}$$

which holds for *any* observable, including the coordinate functions, i.e. $F(I,\theta) = \theta$ or $F(I,\theta) = I$.

Comparison to quantum mechanics

- For Schroedinger's equation: $i\partial_t U(t) = H(t)U(t)$ we can still define the wave maps $\Omega_{\pm}^{t_0}$

Comparison to quantum mechanics

- For Schroedinger's equation: $i\partial_t U(t) = H(t)U(t)$ we can still define the wave maps $\Omega_{\pm}^{t_0}$
- Classically, s_0^t computes the asymptotic future knowing the asymptotic past, and quantum mechanically we have

$$\langle u_+ | s^{t_0} | u_- \rangle = \int u_+(x) \overline{s^{t_0} u_-(x)} dx \tag{2.19}$$

does this probabilistically.

Comparison to quantum mechanics

- For Schroedinger's equation: $i\partial_t U(t) = H(t)U(t)$ we can still define the wave maps $\Omega_\pm^{t_0}$
- Classically, s_0^t computes the asymptotic future knowing the asymptotic past, and quantum mechanically we have

$$\langle u_+ | s^{t_0} | u_- \rangle = \int u_+(x) \overline{s^{t_0} u_-(x)} dx \tag{2.19}$$

does this probabilistically.

- For Hamiltonians $H = H_0 + \epsilon H_1$ one can prove that

$$s_\epsilon^{t_0} = s_0^{t_0} + \epsilon \lim_{T\to\infty} U_T^{t_0} \left(\int_{-T}^{T} iH_1 U_{t_0}^T ds \right) U_T^{t_0} + \mathcal{O}(\epsilon^2) \tag{2.20}$$

Application: Numerics for invariant manifolds in chemistry

- We start with the Henon-Heiles Hamiltonian

$$H_0(x, y, p_x, p_y) = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2 y - \frac{1}{3}y^3 \tag{3.1}$$

[2] S. Kawai, A. Bandrauk, C. Jaffe, T. Bartsch, J. Palacian, and T. Uzer, *Transition state theory for laser-driven reactions*, The Journal of Chemical Physics **126** (2007), no. 16, 164306

Application: Numerics for invariant manifolds in chemistry

- We start with the Henon-Heiles Hamiltonian

$$H_0(x, y, p_x, p_y) = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2 y - \frac{1}{3}y^3 \tag{3.1}$$

- And consider the time-dependent perturbation [2]

$$H = H_0 + \mathcal{E}(t)\exp(-\alpha x^2 - \beta y^2) \tag{3.2}$$

and $\mathcal{E}(t)$ is smooth and supported in $[-4.2, 4.2]$.

[2] S. Kawai, A. Bandrauk, C. Jaffe, T. Bartsch, J. Palacian, and T. Uzer, *Transition state theory for laser-driven reactions*, The Journal of Chemical Physics **126** (2007), no. 16, 164306

Application: Numerics for invariant manifolds in chemistry

- We start with the Henon-Heiles Hamiltonian

$$H_0(x, y, p_x, p_y) = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2 y - \frac{1}{3} y^3 \tag{3.1}$$

- And consider the time-dependent perturbation [2]

$$H = H_0 + \mathcal{E}(t) \exp(-\alpha x^2 - \beta y^2) \tag{3.2}$$

  and $\mathcal{E}(t)$ is smooth and supported in $[-4.2, 4.2]$.

- H_0 has 3 unstable fixed points and according to *transition state theory* their stable and unstable manifolds separate regions of phase space leading to an outcome of a reaction

[2] S. Kawai, A. Bandrauk, C. Jaffe, T. Bartsch, J. Palacian, and T. Uzer, *Transition state theory for laser-driven reactions*, The Journal of Chemical Physics **126** (2007), no. 16, 164306

Application continued

- We use scattering theory to compute invariant object for the laser-driven system knowing the invariant object for unperturbed system

Application continued

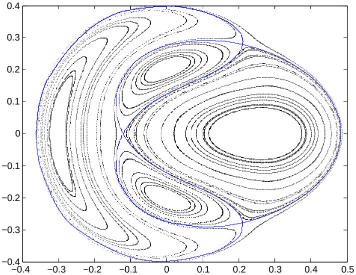
- We use scattering theory to compute invariant object for the laser-driven system knowing the invariant object for unperturbed system
- In this case, we have $\Omega_{\pm}^{t_0} = U_{\pm T}^{t_0} V_{t_0}^{\pm T}$, where $T = 4.2$

Application continued

- We use scattering theory to compute invariant object for the laser-driven system knowing the invariant object for unperturbed system
- In this case, we have $\Omega_{\pm}^{t_0} = U_{\pm T}^{t_0} V_{t_0}^{\pm T}$, where $T = 4.2$
- Recall $N_{t_0} = (\Omega_{\pm}^{t_0})^{-1}(M_{t_0})$, and thus the invariant objects are obtained by integrating trajectories for a finite time

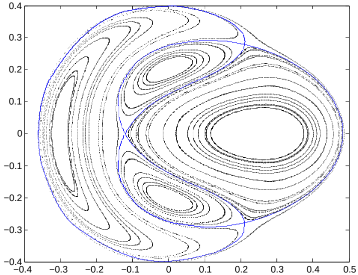
Unperturbed invariant objects

- We fix the energy to be $e = 1/12$ and consider a Poincare section



Unperturbed invariant objects

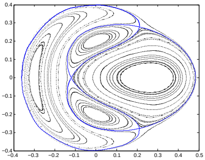
- We fix the energy to be $e = 1/12$ and consider a Poincare section

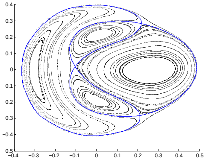


- That is, we take initial condition $(0, y, p_x(y, p_y), p_y)$ and compute "crossings", i.e. when $x = 0$.

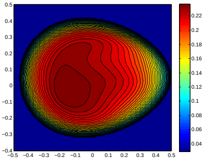
Perturbed invariant objects

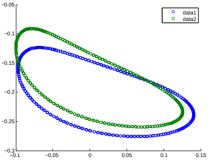
We use the conjugacy $\Omega_+^{t_0}$ with $t_0 = -4.2$ [3]





unperturbed perturbed





$$D(y, p_y) = \| \left(\Omega_+^{t_0}\right)^{-1} - \mathrm{Id} \|$$ Symmetry is broken

[3] D. Blazevski and J. Franklin, *Classical scattering theory and invariant manifolds for the laser-driven henon-heiles system*, In preparation

Concluding remarks

- New areas of applications: In celestial mechanics this could explain the formation of trans-Neptunian binaries [4]

[4] A. G. Suárez, D. Hestroffer, and D. Farrelly, *Formation of the extreme Kuiper-belt binary 2001* QW_{322} *through adiabatic switching of orbital elements*, Celestial Mech. Dynam. Astronom. **106** (2010), no. 3, 245–259. 2600368

Concluding remarks

- New areas of applications: In celestial mechanics this could explain the formation of trans-Neptunian binaries [4]
- Extension to infinite dimensions, e.g. new results for Schroedinger's equation

[4] A. G. Suárez, D. Hestroffer, and D. Farrelly, *Formation of the extreme Kuiper-belt binary 2001* QW_{322} *through adiabatic switching of orbital elements*, Celestial Mech. Dynam. Astronom. **106** (2010), no. 3, 245–259. 2600368

Thank You!

Thank you for your attention!