Highly-oscillatory evolution equations : averaging and numerics

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A class of Highly-oscillatory problems

Highly-oscillatory ODEs

$$\frac{dy^\varepsilon}{dt} = \frac{\gamma(t)}{\varepsilon} A y^\varepsilon + R_\varepsilon(y^\varepsilon), \quad t \in [0, T], \qquad y^\varepsilon(0) = y_0,$$

where A is supposed a skew-adjoint operator with all its eigenvalues in $i\mathbb{Z}$. Assume $\gamma(t) \geq 0$ for simplicity. $\varepsilon \in (0, 1]$.

Two important cases:

Case I :

$$\gamma(t) \geq \gamma_0 > 0$$

Case II :

$$\gamma(t_0) = 0 \quad \text{for some} \quad t_0 \in [0, T].$$

Numerical difficulties

- Standard schemes of order p lead to

$$\|u^\varepsilon - u^{\varepsilon,\Delta t}\| \leq C\frac{(\Delta t)^p}{\varepsilon^q}, \quad q > 0,$$

forcing $\Delta t \sim \varepsilon$ and thus formidable costs for small values of ε.

- More sophisticated schemes of order p can be constructed in some situations but suffer from the "order reduction" phenomena :

$$\|u^\varepsilon - u^{\varepsilon,\Delta t}\| \leq C(\Delta t)^q, \qquad q << p.$$

- Partial remedy: Averaging methods lead to

$$\|u^\varepsilon - \tilde{u}^{\varepsilon,\Delta t}\| \leq C((\Delta t)^p + \varepsilon^q).$$

- Aim: Provide with systematic methods allowing the conventional numerical schemes of order p to be uniformly accurate, i.e. such that

$$\sup_{\varepsilon\in(0,1]} \|u^\varepsilon - u^{\varepsilon,\Delta t}\| \leq C(\Delta t)^p.$$

A first example : Vlasov equation with a given strong magnetic field

$$\partial_t f^\varepsilon + v \cdot \nabla_x f^\varepsilon + E \cdot \nabla_v f^\varepsilon + \frac{v \times B}{\varepsilon} \cdot \nabla_v f^\varepsilon = 0$$

Caracteritics :

$$\dot{x}(t) = v(t)$$
$$\dot{v}(t) = \frac{1}{\varepsilon} v(t) \times B(x(t)) + E(x(t))$$

Numerics : widely developed in collaboration with Chartier, Crouseilles, Méhats, X. Zhao.
Asymptotics : widely developed by Bostan *et al.*.

- Monofrequency case : constant modulus $|B(x)| = 1.$ The oscillatory part generates a 2π- periodic trajectory.
- General case : B with varying intensity and direction. In this case, we introduce a new time s and consider t as a function of s.

$$\frac{d}{ds} t(s) = \frac{1}{|B(\widetilde{x}(s))|}, \qquad \frac{d}{ds} \widetilde{x}(s) = \frac{\widetilde{v}(s)}{|B(\widetilde{x}(s))|},$$

$$\frac{d}{ds} \widetilde{v}(s) = \frac{1}{\varepsilon} \widetilde{v}(t) \times \frac{B}{|B(\widetilde{x}(s))|} + \frac{E}{|B(\widetilde{x}(s))|}.$$

Main Assumption : $|B(x)| \geq Constant > 0.$

A second example : transition between quantum states

- Landau-Zener 2×2 system

$$\frac{du^\varepsilon}{dt} = -\frac{i}{\varepsilon} \begin{pmatrix} -t & \delta \\ \delta & t \end{pmatrix} u^\varepsilon + \text{corrective terms.}$$

- Transport in graphene in semiclassical regime (*Morandi-Schürrer, 2012*). Joint work with *Crouseilles , Jin and Méhats.*

Unknowns are the Wigner disitributions $f_+(t,x,p)$, $f_-(t,x,p)$, $f(t,x,p)$:

$$\partial_t f^+ + \frac{p}{|p|} \cdot \nabla_x f^+ - \nabla_x V \cdot \nabla_p f^+ = -\frac{p^\perp \cdot \nabla_x V}{|p|^3} \Im\left((p_1 + ip_2) f\right),$$

$$\partial_t f^- - \frac{p}{|p|} \cdot \nabla_x f^- - \nabla_x V \cdot \nabla_p f^- - = \frac{p^\perp \cdot \nabla_x V}{|p|^3} \Im\left((p_1 + ip_2) f\right),$$

$$\partial_t f - \nabla_x V \cdot \nabla_p f = -\frac{2i|p|}{\varepsilon} f + i\frac{p^\perp \cdot \nabla_x V}{|p|^2} f + \frac{i}{2}\frac{p^\perp \cdot \nabla_x V}{|p|^3}(p_1 - ip_2)(f^+ - f^-).$$

where $p = (p_1, p_2)$ and $p^\perp = (-p_2, p_1)$.
This semi-classical model is derived from the Von-Neumann equation for two mixed states, by taking the Wigner transform and keeping only terms of the order of $1/\varepsilon$ and 1. The quantities f_+ and f_- are the diagonal terms in the Wigner matrix and f is the off-diagonal coefficient.
Main Assumption : 1D problem in x and p, with $p_2 > 0$ as a fixed parameter.

Generic problem

$$\frac{dy^\varepsilon}{dt} = \frac{\gamma(t)}{\varepsilon} A y^\varepsilon + R(y^\varepsilon), \quad t \in [0, T], \qquad y^\varepsilon(0) = y_0,$$

- Setting

$$u^\varepsilon(t) = \exp\left(\frac{S(t)}{\varepsilon} A\right) y^\varepsilon(t), \qquad \text{with} \qquad S(t) = \int_0^t \gamma(s) ds$$

$$\frac{d}{dt} u^\varepsilon(t) = F\left(\frac{S(t)}{\varepsilon}, u^\varepsilon\right), \qquad F(\theta, u) = e^{-\theta A} R\left(e^{\theta A} u\right).$$
$$u^\varepsilon(0) = y_0,$$

- F is periodic in θ.
- In all cases (vanishing or not), the limit model is

$$\frac{d}{dt}\underline{u} = \langle F(\cdot, \underline{u}) \rangle, \qquad \underline{u}(0) = y_0, \qquad \text{where}$$

$$\langle F(\cdot, u) \rangle = \frac{1}{2\pi} \int_0^{2\pi} F(\theta, u)\, d\theta.$$

Asymptotic models: constant frequency $\gamma = 1$

$$\frac{d}{dt}u^\varepsilon(t) = F\left(\frac{t}{\varepsilon}, u^\varepsilon\right), \quad u^\varepsilon(0) = y_0, \qquad F(\theta, u) = e^{-\theta A} R\left(e^{\theta A} u\right).$$

- Averaging techniques or two-scale expansions : Bogoliubov-Mitropolsky 1930', Perko 1968, ...

$$u^\varepsilon(t) = \Phi^\varepsilon_{t/\varepsilon}(\underline{u}^\varepsilon(t)) = \underline{u}^\varepsilon(t) + \varepsilon U_1(t/\varepsilon, \underline{u}^\varepsilon(t)) + \varepsilon^2 U_2(t/\varepsilon, \underline{u}^\varepsilon(t)) + ...$$

$$\begin{aligned} &\frac{d}{dt}\underline{u}^\varepsilon(t) = K_0(\underline{u}^\varepsilon(t)) + \varepsilon K_1(\underline{u}^\varepsilon(t)) + ... = K^\varepsilon(\underline{u}^\varepsilon(t)) \\ &\underline{u}^\varepsilon(0) = (\Phi^\varepsilon_0)^{-1}(y_0), \end{aligned}$$

Φ_θ is periodic in θ. No constructive method for Φ^ε and K^ε.

- Equivalently,

$$u^\varepsilon(t) = \Phi^\varepsilon_{t/\varepsilon} \circ \Psi_t \circ (\Phi^\varepsilon_0)^{-1}(y_0),$$

with

$$\frac{d\Psi_t}{dt} = K^\varepsilon(\Psi_t), \quad \Psi_0 = Id.$$

Constructive methods and structure (Lie structure, Hamiltonian and divergence free properties) : Chartier, Murua and Sanz-Serna, Castella, Méhats (2011-2012-2015) ...

- Equation on Φ_θ^ε

$$\partial_\theta \Phi_\theta(u) = -\varepsilon \partial_u \Phi_\theta(u) K^\varepsilon(u) + \varepsilon f_\theta \circ \Phi_\theta(u),$$
$$K^\varepsilon = \langle \partial_u \Phi_\theta(u)\rangle^{-1} \langle f_\theta \circ \Phi_\theta(u)\rangle.$$

- Integrating this equation with $\langle \Phi_\theta \rangle = \mathrm{id}$,

$$\Phi_\theta^{[0]} = \mathrm{id}, \quad \Phi_\theta^{[n+1]} = \mathrm{id} + \varepsilon \int_0^\theta \Big(f_\tau \circ \Phi_\tau^{[n]} - \partial_u \Phi_\tau^{[n]} K^{[n]} \Big)\, d\tau$$
$$- \varepsilon \left\langle \int_0^\theta \Big(f_\tau \circ \Phi_\tau^{[n]} - \partial_u \Phi_\tau^{[n]} K^{[n]} \Big)\, d\tau \right\rangle$$
$$K^{[0]} = \langle f \rangle, \quad K^{[n+1]} = \langle f \circ \Phi^{[n+1]} \rangle.$$

- Averaged model

$$\frac{d\underline{u}}{dt} = K_0(\underline{u}) = \langle F(\cdot, \underline{u})\rangle = \frac{1}{2\pi} \int_0^{2\pi} F(\theta, \underline{u}) d\theta.$$

- Error estimate. Let u_N^ε be the truncated averaging expansion up to ε^N, then

$$u^\varepsilon - u_N^\varepsilon = O\left(\varepsilon^{N+1}\right),$$

provided we have enough regularity on F.

- The first asymptotic models may be obtained by hand (Chapman-Enskog like expansion), starting from an equation on $U(t, \theta = t/\varepsilon) = u^\varepsilon(t)$

$$\partial_t U - F(\theta, U) = -\frac{1}{\varepsilon} \partial_\theta U.$$

Asymptotic models: varying frequency $\gamma(t) \geq \gamma_0 > 0$

$$\frac{d}{dt}u^\varepsilon(t) = F\left(\frac{S(t)}{\varepsilon}, u^\varepsilon\right), \quad F(\theta, u) = e^{-\theta A}K\left(e^{\theta A}u\right), \quad S(t) = \int_0^t \gamma(t')dt'$$

- Perform a change of time

$$s = S(t), \quad v^\varepsilon(s) = u^\varepsilon(t).$$

- We can see this as an equation on $(v^\varepsilon(s), t(s))$:

$$\frac{dv^\varepsilon}{ds} = \frac{1}{\gamma(t)}F\left(\frac{s}{\varepsilon}, v^\varepsilon\right), \qquad \frac{dt}{ds} = \frac{1}{\gamma(t)}$$

- Averaging techniques can be applied since the quantity $\frac{1}{\gamma(t)}$ is smooth. u^ε strongly converges to $\underline{u}$ solution to

$$\frac{d}{dt}\underline{u}(t) = \langle F\left(\cdot, \underline{u}(t)\right)\rangle, \quad \underline{v}(0) = u_0.$$

- We still have the error estimate

$$u^\varepsilon - \underline{u} = O(\varepsilon).$$

First numerical method when $\gamma(t) \geq \gamma_0 > 0$: a two-scale approach

$$\frac{d}{dt}u^\varepsilon(t) = F\left(\frac{t}{\varepsilon}, u^\varepsilon\right), \qquad u^\varepsilon(0) = u_0.$$

(Crouseilles, Méhats, L. JCP, 2013, and then with Chartier, Zhao, 2015-2019) with applications to Schrödinger equations, and Vlasov equations with strong magnetic field.

- Imbed the problem into an augmented one allowing to separate the fast variable from the slow one: Set $U(t, \theta = t/\varepsilon) = u^\varepsilon(t)$

$$\partial_t U - F(\theta, U) = -\frac{1}{\varepsilon}\partial_\theta U.$$

- The only condition we have at time $t = 0$ is $U(0,0) = u_0$. An additional degree a freedom is available on the initial condition $U(0, \theta)$.
- For any $N \in \mathbb{N}$, there exists a suitable initial condition $U(0, \theta)$ such that
  - $U(0,0) = u_0$, and
  - the resulting solution $U(t, \theta)$ has uniformly bounded derivatives in time and θ up to the order $N + 1$.

Two-scale approach

- for $N = 1$, a good choice of initial condition is

$$U(0, \theta) = u_0 + \varepsilon \int_0^\theta \left(F(\sigma, u_0) - \langle F(\cdot, u_0)\rangle\right) d\sigma.$$

  More generally for arbitrary N:

$$U(0, \theta) = \Phi_\theta^{[N]} \circ \left(\Phi_0^{[N]}\right)^{-1} (u_0),$$

  where $\Phi_\theta^{[N]}$ is the truncation up to the order ε^N of the expansion of Φ_θ^ε.
- This ensures the uniform boundeness of the time derivatives of U up to order $N + 1$.
- Uniformly accurate numerical schemes of order N (or even $N + 1$) can be constructed on this two-scale formulation, with applications to Schrodinger and kinetic equations.

Second appraoch for $\gamma(t) \geq \gamma_0 > 0$: a micro-macro approach

The two-scale equation uses an additional variable θ. To avoid this, we have introduced Micro-macro decomposition (with Chartier, Méhats, and Vilmart, Found. Comput. Math. 2020).

$$\frac{d}{dt}u^\varepsilon(t) = F\left(\frac{t}{\varepsilon}, u^\varepsilon\right), \qquad u(0) = u_0.$$

- The idea is to write the solution u^ε as

$$u^\varepsilon(t) = \Phi^{[N]}_{t/\varepsilon}\left(\underline{u}^\varepsilon(t)\right) + v^\varepsilon(t),$$

where $\Phi^{[N]}_\theta \circ \underline{u}(t)$ is the asymptotic expansion up to some order N. The change of variable Φ^ε_θ is periodic in θ, and $\underline{u}^\varepsilon(t)$ is the solution to a smooth averaged equation:

$$\frac{d}{dt}\underline{u}^\varepsilon(t) = K^{[N]}_\varepsilon \underline{u}^\varepsilon(t), \qquad \underline{u}^\varepsilon(0) = \left(\Phi^{[N]}_0\right)^{-1}(u_0).$$

$$\begin{aligned}\frac{d}{dt}v^\varepsilon(t) &= F\left(t/\varepsilon, \Phi^{[N]}_{t/\varepsilon}(\underline{u}^\varepsilon(t)) + v^\varepsilon\right) - \left(\frac{1}{\varepsilon}\partial_\theta \Phi^{[N]}_{t/\varepsilon}(\underline{u}^\varepsilon) + \partial_u \Phi^{[N]}_{t/\varepsilon}(\underline{u}^\varepsilon) K^\varepsilon \underline{u}^\varepsilon\right).\\ &= F\left(t/\varepsilon, \Phi^{[N]}_{t/\varepsilon}(\underline{u}^\varepsilon(t)) + v^\varepsilon\right) - F\left(t/\varepsilon, \Phi^{[N]}_{t/\varepsilon}(\underline{u}^\varepsilon(t))\right) + O(\varepsilon^N).\end{aligned}$$

- Solve the equations on v^ε and $\underline{u}^\varepsilon$, instead of the original equation on u^ε

Micro-macro approach

$$u^\varepsilon(t) = \Phi^{[N]}_{t/\varepsilon}\left(\underline{u}^\varepsilon(t)\right) + v^\varepsilon(t)$$

- Case $N = 0$: $u^\varepsilon(t) = \underline{u}(t) + v^\varepsilon(t)$, with

$$\frac{d}{dt}\underline{u} = \langle F(\cdot, \underline{u})\rangle, \qquad \underline{u}(0) = u_0;$$

$$\frac{d}{dt}v^\varepsilon = F\left(t/\varepsilon, \underline{u} + v^\varepsilon\right) - \langle F(\cdot, \underline{u})\rangle, \quad v^\varepsilon(0) = 0.$$

- Case $N = 1$: $u^\varepsilon(t) = \Phi^{[1]}_{t/\varepsilon}\left(\underline{u}^\varepsilon(t)\right) + v^\varepsilon(t)$ where

$$\Phi^{[1]}_\theta(u) = u + \varepsilon(Id - \langle . \rangle)\int_0^\theta \left(F(\sigma, u) - \langle F(\cdot, u)\rangle\right) d\sigma.$$

$$\frac{d}{dt}\underline{u}^\varepsilon = \langle F(\cdot, \Phi^{[1]}_\theta(\underline{u}^\varepsilon(t)))\rangle, \qquad \underline{u}^\varepsilon(0) = \left(\Phi^{[1]}_0\right)^{-1}(u_0)$$

- The construction is done in a such way that, if we truncate to N the expansions of Φ^ε and of the averaged vector field K^ε, then
  - $v^\varepsilon(t) = O(\varepsilon^{N+1})$ and has uniformly bounded time derivatives up to $N + 1$,
  - the equation satisfied by $v^\varepsilon(t)$ does not contain singularities in ε.

Asymptotic models: vanishing frequency $\gamma(t_0) = 0,\ t_0 \geq 0.$

(with Chartier, Méhats, and Vilmart, SIAM, 2020)

$$\gamma(t) = (p+1)|t - t_0|^p, \quad S(t) = \text{sign}(t - t_0)|t - t_0|^{p+1} + t_0^{p+1}.$$

$$\frac{d}{dt} u^\varepsilon(t) = F\left(\frac{S(t)}{\varepsilon}, u^\varepsilon\right), \quad F(\theta, u) = e^{-\theta A} f\left(e^{\theta A} u\right).$$

- Perform the change of time $s = S(t), \quad v^\varepsilon(s) = u^\varepsilon(t) = u^\varepsilon\left(S^{-1}(s)\right).$

$$\gamma(t) = |s - s_0|^{\frac{p}{p+1}}, \qquad s_0 = S(t_0).$$

$$\frac{d}{ds} v^\varepsilon = \frac{1}{\gamma(t)} F\left(\frac{s}{\varepsilon}, v^\varepsilon\right), \qquad \frac{dt}{ds} = \frac{1}{\gamma(t)}.$$

- Averaging techniques can no longer be applied since the quantity $\frac{1}{\gamma(t)}$ is not smooth at $t = t_0$.
- We no longer have the estimate $u^\varepsilon - \underline{u} = O(\varepsilon)$ but rather

$$u^\varepsilon - \underline{u} = O\left(\varepsilon^{\frac{1}{p+1}}\right)$$

Vanishing frequency: stationary phase effect.

$$\frac{d}{ds}v^\varepsilon = |s-s_0|^{-\frac{p}{p+1}} F\left(\frac{s}{\varepsilon}, v^\varepsilon\right).$$

- We rather write (taking $t_0 = s_0 = 0$ for simplicity)

$$v^\varepsilon(s) = v^\varepsilon(0) + \int_0^s \sigma^{-\frac{p}{p+1}} F\left(\frac{\sigma}{\varepsilon}, v^\varepsilon(\sigma)\right) d\sigma.$$

$$v^\varepsilon(s) = v^\varepsilon(0) + \int_0^s \sigma^{-\frac{p}{p+1}} \langle F(\cdot, v^\varepsilon(\sigma))\rangle d\sigma + R_\varepsilon,$$

where

$$R_\varepsilon = \int_0^s \sigma^{-\frac{p}{p+1}} \left(F\left(\frac{\sigma}{\varepsilon}, v^\varepsilon(\sigma)\right) - \langle F(\cdot, v^\varepsilon(\sigma))\rangle\right) d\sigma$$

- Typically, if $F(\sigma, u) = (1 + e^{i\sigma})u$, we have

$$R_\varepsilon = \int_0^s \sigma^{-\frac{p}{p+1}} \exp\left(i\sigma/\varepsilon\right) v^\varepsilon(\sigma) d\sigma.$$

- A change of variable $\sigma/\varepsilon \to \sigma$ gives

$$R_\varepsilon = \varepsilon^{\frac{1}{p+1}} \int_0^{s/\varepsilon} \sigma^{-\frac{p}{p+1}} e^{i\sigma} v^\varepsilon(\varepsilon\sigma) d\sigma$$

Vanishing frequency: stationary phase effect.

- Let

$$\Omega(s) = \int_s^{+\infty} \sigma^{-\frac{p}{p+1}} e^{i\sigma} d\sigma$$

and perform integration by parts

$$R_\varepsilon = \varepsilon^{\frac{1}{p+1}} \left(\Omega(0)v^\varepsilon(0) - \Omega(s/\varepsilon)v^\varepsilon(s)\right) + \varepsilon^{\frac{2}{p+1}} \int_0^{s/\varepsilon} \sigma^{-\frac{p}{p+1}} \Omega(\sigma) v^\varepsilon(\varepsilon\sigma)(1+e^{i\sigma}) d\sigma.$$

- Next term: Observing that $|\Omega(s)| \leq C(1+s)^{-\frac{p}{p+1}}$, we get

$$\varepsilon^{\frac{2}{p+1}} \left| \int_0^{s/\varepsilon} \sigma^{-\frac{p}{p+1}} \Omega(\sigma) v^\varepsilon(\varepsilon\sigma)(1+e^{i\sigma}) d\sigma \right| \leq C\varepsilon^{\frac{2}{p+1}} \int_0^{s/\varepsilon} \sigma^{-\frac{p}{p+1}} (1+\sigma)^{-\frac{p}{p+1}} d\sigma.$$

We then get a $O(\varepsilon^{\frac{2}{p+1}})$ for $p > 1$ and $O(\varepsilon \log(\varepsilon))$ for $p = 1$.

Rigorous estimate up to $\varepsilon^{2/(p+1)}$

Let

$$G(\theta,u)=\int_0^\theta (F(\sigma,u)-\langle F(\cdot,u)\rangle)d\sigma-\langle\int_0^s (F(\sigma,u)-\langle F(\cdot,u)\rangle)d\sigma\rangle,$$

$$\Omega(s,u)=\int_s^{+\infty}\sigma^{-p/(p+1)}(F(\sigma,u)-\langle F(\cdot,u)\rangle)d\sigma.$$

Let $\underline{u}$ the solution to

$$\frac{d\underline{u}}{dt}=\langle F(\cdot,\underline{u}(t))\rangle,\qquad \underline{u}(0)=u_0+\frac{\varepsilon^{1/(p+1)}}{p+1}\Omega(0,u_0).$$

Truncation error estimate

We have

$$u^\varepsilon=\widetilde{u}+w^\varepsilon,\quad \text{with}\quad |w^\varepsilon(t)|\le C\varepsilon^{\frac{2}{p+1}},\quad \forall t\in[0,T],$$

and $\tilde{u}(t)=\Phi_{\frac{S(t)}{\varepsilon}}(\underline{u}(t))$ and

$$\Phi_\theta(\underline{u})=\underline{u}-\frac{\varepsilon^{1/(p+1)}}{p+1}\Omega\left(\theta,\underline{u}(t)\right)+\frac{\delta_p}{4}\varepsilon\log\left(1+\theta\right)\langle(\partial_2 G)F\rangle(u_0),$$

$\delta_p=1$ if $p=1$ and 0 otherwise.

Micro-Macro decomposition

Set

$$u^\varepsilon(t) = \widetilde{u}(t) + w^\varepsilon(t).$$

Uniform estimate on the time derivatives of w^ε, for $p = 1$.

We have

$$\forall t \in [0, T], \qquad |w^\varepsilon(t) \le C\varepsilon$$

$$\left|\frac{dw^\varepsilon}{dt}\right| \le C\sqrt{\varepsilon}, \qquad \left|\frac{d^2 w^\varepsilon}{dt^2}\right| \le C.$$

- Instead of solving numerically the stiff equation on u, our strategy consists in solving the system of the two smooth equations on $\underline{u}$ and w^ε. Then compute $\tilde{u}$ and finally $u^\varepsilon(t) = \tilde{u}(t) + w^\varepsilon(t)$.
- The computation of $\tilde{u}$ requires the computation of the function $\Omega(\theta, u)$. Using Fourier expansions for F, we are left with functions of "Erf" type.

The vanishing-frequency case

We test our method on the Hénon-Heiles system $y^\varepsilon = (q_1, q_2, p_1, p_2)$ with a time-varying parameter $\gamma(t) = 2(t - t_0)$

$$\dot{y}^\varepsilon(t) = \left(\frac{\gamma(t)}{\varepsilon} p_1, p_2, -\frac{\gamma(t)}{\varepsilon} q_1 - 2q_1 q_2, -q_2 - q_1^2 + q_2^2 \right), \ t \in [0, 1],$$
$$y^\varepsilon(0) = (0.9, 0.6, 0.8, 0.5).$$

The filtered unknown $u^\varepsilon(t) \in \mathbb{R}^4$ is defined by

$$u^\varepsilon(t) = (\cos(\theta) q_1(t) - \sin(\theta)\, p_1(t), q_2(t), \sin(\theta) q_1(t) + \cos(\theta) p_1(t), p_2(t)),$$

with $\theta = \frac{(t - t_0)|t - t_0| + t_0^2}{\varepsilon}$, and satisfies

$$\dot{u}^\varepsilon(t) = (F_1, F_2, F_3, F_4)(\theta, u^\varepsilon(t)),$$

with

$$F_1(\theta, u) = 2 \sin\theta \,(u_1 \cos\theta + u_3 \sin\theta)\, u_2, \qquad F_2(\theta, u) = u_4,$$
$$F_3(\theta, u) = -2 \cos\theta \,(u_1 \cos\theta + u_3 \sin\theta)\, u_2, \quad F_4(\theta, u) = -\left(u_1 \cos\theta + u_3 \sin\theta\right)^2 + u_2^2 - u_2).$$

In our tests, several values for t_0 has been taken in $[0, 1]$, $h = 1/N$ for some $N \in \mathbb{N}^*$ and $t^{[k]} = kh$, $k = 0, \ldots, N$.

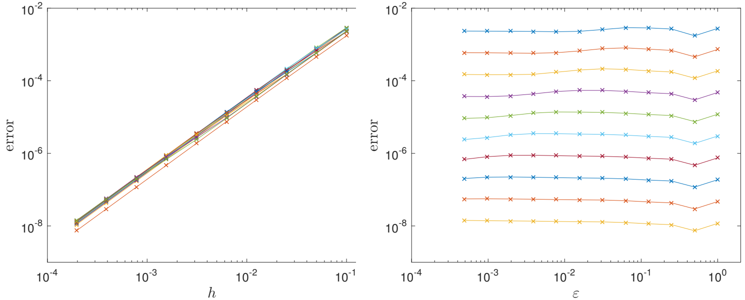


Figure: Error as a function of h for $\varepsilon \in \{2^{-k},\ k = 0, \cdots, 11\}$ (left) and error as a function of ε for $h \in \{0.1/2^{-k},\ k = 0, \cdots, 9\}$ (right). $p = 1$.

Time-space oscillations and transport model for graphene

$$\partial_t f - \nabla_x V \cdot \nabla_p f = -\frac{2i|p|}{\varepsilon} f + \cdots .$$

(with N. Crouseilles, S. Jin and F. Méhats, 2020).

Combine ideas from nonlinear geometric optics (with Crouseilles and Jin, M3AS, 2017), with the above micro-macro decomposition.

Transport of electrons in graphene : Wigner distributions $f_+(t,x,p)$, $f_-(t,x,p)$, $f(t,x,p)$, and ε is the semiclassical parameter:

$$\partial_t f^+ + \frac{p}{|p|} \cdot \nabla_x f^+ - \nabla_x V \cdot \nabla_p f^+ = -\frac{p^\perp \cdot \nabla_x V}{|p|^3} \Im\left((p_x + ip_y) f\right),$$

$$\partial_t f^- - \frac{p}{|p|} \cdot \nabla_x f^- - \nabla_x V \cdot \nabla_p f^- = \frac{p^\perp \cdot \nabla_x V}{|p|^3} \Im\left((p_x + ip_y) f\right),$$

$$\partial_t f - \nabla_x V \cdot \nabla_p f = -\frac{2i|p|}{\varepsilon} f + i\frac{p^\perp \cdot \nabla_x V}{|p|^2} f + \frac{i}{2}\frac{p^\perp \cdot \nabla_x V}{|p|^3}(p_x - ip_y)(f^+ - f^-).$$

where $|p| = (p_x^2 + p_y^2)^{1/2}$ and $p^\perp = (-p_y, p_x)$.
We construct a uniformly accurate second order method.
Important assumption: We consider a $1D$ problem in x so that p_y becomes a parameter. We suppose that $p_y \geq \nu_0 > 0$, so that $|p|$ does not vanish.

It is not a time oscillatory model!

$$\partial_t f - \nabla_x V \cdot \nabla_p f = -\frac{2i|p|}{\varepsilon} f + \cdots .$$

- Because of its dependence in p, the stiff term does not generate a periodic solution and cannot be filtered out as before.
- The main oscillation should involve all the variables (t, x, p). We introduce the phase of oscillations:

$$s = S(t,x,p), \qquad \partial_t S - \nabla_x V \cdot \nabla_p S = 2|p|, \qquad S(0,x,p) = 0.$$

  in order to bring down the problem to a time-oscillatory problem and apply the micro/macro strategy.
- The function $g(s = S(t,x,p), x, p) = f(t,x,p)$

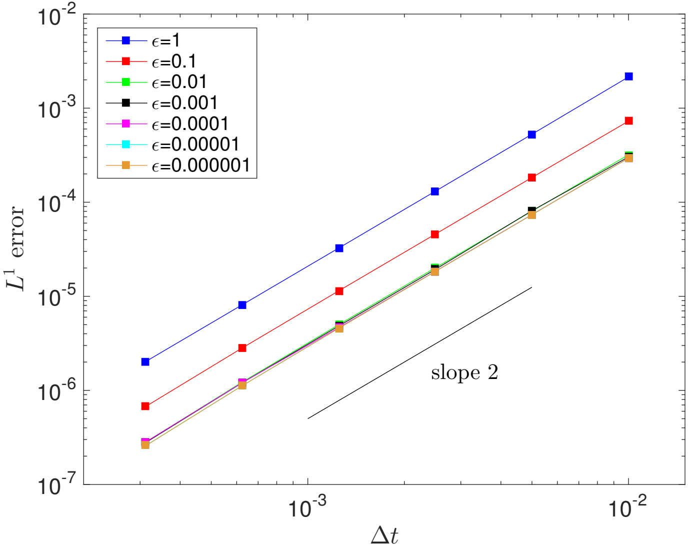
$$\partial_s g - \frac{\nabla_x V}{2|p|} \cdot \nabla_p g = -\frac{i}{\varepsilon} g + \frac{1}{2|p|} \times \text{the other terms.}$$

- This phase equation can be solved explicitly here:

$$S(t,x,p_x,p_y) = \frac{p_y^2}{E}\left[\xi\left(\frac{p_x + Et}{p_y}\right) - \xi\left(\frac{p_x}{p_y}\right)\right].$$

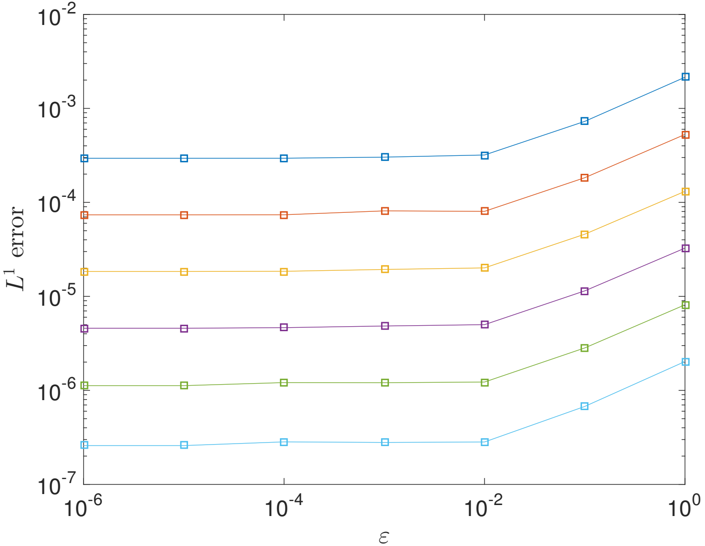
$$\xi(u) = u\sqrt{1+u^2} + \log(u + \sqrt{1+u^2})$$

Error curves as a function of Δt



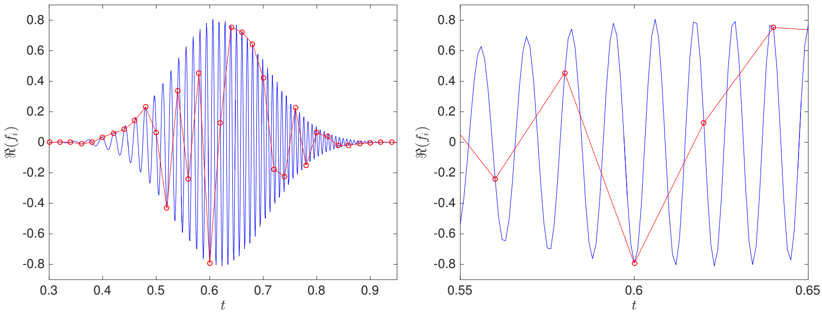
Error with respect to Δt for $\varepsilon \in \{1, 0.1, 0.01, 0.001, 0.0001, 0.00001, 0.000001\}$.
$N_x = 128, N_{p_x} = 128$.

Error curves as a function of ε



Error with respect to ε for various values of Δt: $\Delta t = 2^{-k} \times 10^{-2}, k = 0, ..., 5.$

Oscillations



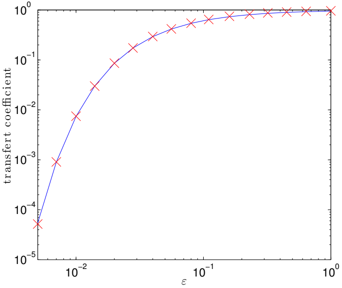
For $\varepsilon = 0.005$: $\Re(f)(t, -2.16, -1.18)$ as a function of t.
Blue: reference solution, Red: solution computed with our scheme. The right figure is a zoom of the left figure. $N_x = 64, N_{p_x} = 128, \Delta t = 0.02$.

Landau-Zener transition rate

We plot the transition rate as a function of ε, and compare with the theoretical Landau-Zener transition rate:

$$f_+(0,x,p_x) = \frac{4}{\pi} e^{-4(x+2)^2 - 4(p_x-1.3)^2}, \quad f_-(0,x,p_x) = 0, \quad f_i(0,x,p_x) = 0.$$

$$T = \frac{\int f_-(t_f,x,p_x)dxdp_x}{\int f_+(0,x,p_x)dxdp_x}, \qquad T_{Landau-Zener} = \exp\left(-\frac{\pi p_y^2}{\varepsilon E}\right).$$



Landau-Zener probability. Red crosses=numerically computed transfert coefficient. Blue curve=theoretical coefficient. $N_x = 64, N_{p_x} = 64, \Delta t = 0.005$.

Computing Φ_θ by a derivative-free algorithm

$$\frac{du}{dt} = f_{t/\varepsilon}(u), \qquad u(t) = \Phi_{t/\varepsilon} \circ \Psi_t \circ (\Phi_0)^{-1}(u_0).$$

- Equation on Φ_θ^ε

$$\partial_\theta \Phi_\theta(u) = -\varepsilon \partial_u \Phi_\theta(u) K^\varepsilon(u) + \varepsilon f_\theta \circ \Phi_\theta(u),$$
$$K^\varepsilon = \langle \partial_u \Phi_\theta(u) \rangle^{-1} \langle f_\theta \circ \Phi_\theta(u) \rangle.$$

- Integrating this equation with $\langle \Phi_\theta \rangle = \mathrm{id}$,

$$\Phi_\theta^{[0]} = \mathrm{id}, \quad \Phi_\theta^{[n+1]} = \mathrm{id} + \varepsilon \int_0^\theta \left(f_\tau \circ \Phi_\tau^{[n]} - \partial_u \Phi_\tau^{[n]} K^{[n]} \right) d\tau$$
$$- \varepsilon \left\langle \int_0^\theta \left(f_\tau \circ \Phi_\tau^{[n]} - \partial_u \Phi_\tau^{[n]} K^{[n]} \right) d\tau \right\rangle$$
$$K^{[0]} = \langle f \rangle, \quad K^{[n+1]} = \langle f \circ \Phi^{[n+1]} \rangle.$$

A free derivative recursive formula

- Computing the explicit form of $\partial_u \Phi_\theta^{[n]}$ becomes very complicated for large k as it involves high-order derivatives of $f_\theta(u)$. Necessity to have at our disposal the derivatives of f_θ
- To overcome this, we replace the derivatives $\partial_u g$ by the following

$$D_\eta g(u) = \frac{1}{\eta}\left(g\left(u+\eta v\right) - g(u)\right), \qquad \eta = \varepsilon^n,$$

and get the following iterative scheme ,

$$\widetilde{\Phi}_\theta^{[0]} = \mathrm{id}, \qquad \widetilde{\Phi}_\theta^{[n+1]} = \mathrm{id} + \varepsilon \int_0^\theta \Big(f_\tau \circ \widetilde{\Phi}_\tau^{[n]} - D_{\varepsilon^n} \widetilde{\Phi}_\tau^{[n]}\, \widetilde{K}^{[n]}\Big) d\tau$$

$$- \varepsilon \left\langle \int_0^\theta \Big(f_\tau \circ \widetilde{\Phi}_\tau^{[n]} - D_{\varepsilon^n} \widetilde{\Phi}_\tau^{[n]} \widetilde{K}^{[n]}\Big) d\tau \right\rangle$$

$$\widetilde{K}^{[0]} = \langle f \rangle \qquad \widetilde{K}^{[n+1]} = \langle f \circ \widetilde{\Phi}^{[n+1]} \rangle.$$

- Note that $\widetilde{\Phi}_\theta^{[0]} = \Phi_\theta^{[0]}$ and $\widetilde{\Phi}_\theta^{[1]} = \Phi_\theta^{[1]}$.
- Online code in a Julia package : Yves Mocquard, Pierre Navaro et N. Crouseilles : https://github.com/ymocquar/HOODESolver.jl

Conlusion

- Several strategies based on averaging techniques have been briefly presented : they provide uniformly accurate (UA) schemes for highly oscillatory models.
- Usual averaging techniques do not work in the case of vanishing frequency : the fast and the slow variable strongly interact in the asymptotics. Stationary-phase like computations are needed.
- Systematic derivation and structure of asymptotic models in this case is an open question.
- This a first step towards the development of efficient methods for more "realistic" quantum-kinetic models: quantum transition rates in 2D graphene for example.
- Other applications in Fluid Mechanics : rotating fluids, vibrating traps or bubbles ...

Thank you for your attention