High order averaging for the Gross-Pitaevskii equation

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Goal of this work

Numerical schemes and asymptotic study as $\varepsilon \to 0$ for the Gross-Pitaevskii equation

$$i\partial_t \psi^\varepsilon = \frac{1}{\varepsilon}\mathcal{H}\psi^\varepsilon + f\left(|\psi^\varepsilon|^2\right)\psi^\varepsilon \qquad (\text{NLS}^\varepsilon)$$

where the Hamiltonian $\mathcal{H}$ is the harmonic oscillator ($x \in \mathbb{R}^d$)

$$\mathcal{H} = -\frac{1}{2}\Delta + \frac{1}{2}|x|^2$$

which has a discrete spectrum and f is a smooth function.

The term $\frac{1}{\varepsilon}\mathcal{H}\psi^\varepsilon$ is a forcing term (in infinite dimension). As $\varepsilon \to 0$, we are in a highly oscillatory regime.

Motivation: study the dynamics of Bose-Einstein condensates (BEC) in two asymptotic regimes.

Case 1: strong confinement

$$i\partial_t\psi^\varepsilon = -\frac{1}{2}\Delta\psi^\varepsilon + \frac{|x|^2}{\varepsilon^2}\psi^\varepsilon + f\left(|\psi^\varepsilon|^2\right)\psi^\varepsilon$$

Rescaling the space variable $x = \frac{x'}{\varepsilon}$ leads to (NLS$^\varepsilon$).

Case 2: long-time behavior in the weak interaction regime

$$i\partial_t\psi^\varepsilon = -\frac{1}{2}\Delta\psi^\varepsilon + |x|^2\psi^\varepsilon + \varepsilon f\left(|\psi^\varepsilon|^2\right)\psi^\varepsilon$$

Rescaling the time variable $t = \varepsilon t'$ leads to (NLS$^\varepsilon$).

A variant: highly anisotropic BEC

$$i\partial_t \psi^\varepsilon = -\frac{1}{2}\Delta\psi^\varepsilon + \left(\omega_\| x_1^2 + \omega_\| x_2^2 + \omega_\perp z^2\right)\psi^\varepsilon + f\left(|\psi^\varepsilon|^2\right)\psi^\varepsilon$$

where either $\omega_\perp \gg \omega_\|$ (disk shaped condensate),
or $\omega_\| \gg \omega_\perp$, (cigar shaped condensate).

An adequate anisotropic scaling in (x_1, x_2, z) leads to

$$i\partial_t \psi^\varepsilon = \frac{1}{\varepsilon}(-\partial_z^2 + z^2)\psi^\varepsilon + (-\Delta_x + |x|^2)\psi^\varepsilon + f\left(|\psi^\varepsilon|^2\right)\psi^\varepsilon$$

or

$$i\partial_t \psi^\varepsilon = \frac{1}{\varepsilon}(-\Delta_x + |x|^2)\psi^\varepsilon + (-\partial_z^2 + z^2)\psi^\varepsilon + f\left(|\psi^\varepsilon|^2\right)\psi^\varepsilon$$

Outline

1. First order averaging
   - Rough analysis
   - The good framework
2. High order averaging
   - Equations of stroboscopic averaging
   - A recipe to compute the averaged equations
   - Geometric aspects
3. Application to NLS
   - The main result
   - Numerical experiments

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1. First order averaging
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2. High order averaging
   - Equations of stroboscopic averaging
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   - Geometric aspects
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A few references (in that context):

Bao, Markowich, Schmeiser, Weishäupl (M3AS 2005),
Ben Abdallah, FM, Schmeiser, Weishäupl (SIAM Math. Anal. 2005),
Ben Abdallah, Castella, FM (JDE 2008),
Carles, Markowich, Sparber (Nonlinearity 2008).

See also, in the context of fluid mechanics:

Grenier (JMPA 1997),
Schochet (JDE 1994),
Métivier, Schochet (JDE 2003).

Rough analysis (and wrong approach)

For simplicity, $d = 1$ in what follows. It is known that:

1. The eigenvalues of $\mathcal{H}$ are made of the set

$$\left\{ E_n = n + \frac{1}{2}\,;\, n \in \mathbb{N} \right\}$$

2. The corresponding eigenfunctions $h_n(x)$, $n \in \mathbb{N}$ are (explicitly) known to be products of the form

Hermite polynomial $\times$ Gaussian

It is then rather tempting to

1. Project on the basis $\psi^\varepsilon(t,x) = \sum_n \psi_n^\varepsilon(t)\, h_n(x)$, and write, say if $f(|\psi|^2)\psi = |\psi|^2\psi$,

$$i\partial_t \psi_n^\varepsilon(t) = \frac{E_n}{\varepsilon}\psi_n^\varepsilon(t) + \sum_{p,q,r} A_{n,p,q,r}\, \psi_p^\varepsilon(t)^*\, \psi_q^\varepsilon(t)\, \psi_r^\varepsilon(t)$$

with

$$A_{n,p,q,r} = \int_{\mathbb{R}} h_n(x) h_p(x) h_q(x) h_r(x) dx$$

2. Filter out the oscillatory term by introducing the new unknown $u_n^\varepsilon(t,x) = e^{it\frac{E_n}{\varepsilon}}\psi_n^\varepsilon(t,x)$.

We then obtain an infinite, nonlinearly coupled system

$$i\frac{d}{dt}u_n^\varepsilon(t) = \sum_{p,q,r} A_{n,p,q,r}\, e^{it\frac{E_n+E_p-E_q-E_r}{\varepsilon}}\, u_p^\varepsilon(t)^*\, u_q^\varepsilon(t)\, u_r^\varepsilon(t).$$

of the form

$$\frac{d}{dt}u^\varepsilon = g\left(\frac{t}{\varepsilon}, u^\varepsilon\right), \qquad g(\tau, u) \text{ periodic in } \tau$$

where $u^\varepsilon = (\phi_0^\varepsilon, \phi_1^\varepsilon, \dots)$.

Two questions arise:

1. How to numerically average out the ODE

$$\frac{d}{dt}u^\varepsilon = g\left(\frac{t}{\varepsilon}, u^\varepsilon\right) \ ?$$

   Answer inspired by Chartier, Murua, Sanz-Serna for ODE's.

2. How to control the norms of u^ε and the nonlinear term g ?

   It is not clear that the Sobolev smoothness of u $\sum_n n^\alpha |u_n|^2 < +\infty$ implies the smoothness of the sum $\sum_n n^\alpha \left|\sum_{p,q,r} \cdots\right|^2 < +\infty$, because of the $A_{n,p,q,r}$'s.

   Answer inspired by Ben Abdallah, Castella, FM (functional framework).

The functional framework

The technique we adopt avoids the projection step on the χ_n's and introduces directly the filtered function

$$u^\varepsilon(t,x) = e^{it\frac{\mathcal{H}}{\varepsilon}}\,\psi^\varepsilon(t,x).$$

The filtered function satisfies the equation

$$i\partial_t u^\varepsilon(t,x) = g\left(\frac{t}{\varepsilon}, u^\varepsilon(t,x)\right),$$

where g is now defined, for $u = u(x)$, as follows:

$$g\left(\frac{t}{\varepsilon}, u\right) = e^{it\frac{\mathcal{H}}{\varepsilon}}\left(f\left(|e^{-it\frac{\mathcal{H}}{\varepsilon}}u(x)|^2\right)e^{-it\frac{\mathcal{H}}{\varepsilon}}u(x)\right)$$

The good Sobolev scale

We shall use the following space B^ℓ for $\ell > d/2$:

- $\|u\|_{B^\ell}^2 := \|u\|_{H^\ell}^2 + \||x|^\ell u\|_{L^2}^2$, equivalent to $\|\mathcal{H}^{\ell/2} u\|_{L^2}^2$.
- B^ℓ is continuously embedded in $L^\infty(\mathbb{R}^d)$.
- If $f \in C^\infty(\mathbb{R})$, then $u \in B^\ell \mapsto f(|u|^2)u \in B^\ell$ is C^∞ and satisfies a tame estimate

$$\|f(|u|^2)u\|_{B^\ell} \leq C_f(\|u\|_{L^\infty}) \times \|u\|_{B^\ell}$$

Now, for all $M > 0$ and $u \in B^\ell$ such that $\|u\|_{B^\ell} \leq M$, we have

$$\left\| g\left(\frac{t}{\varepsilon}, u\right) \right\|_{B^\ell} = \left\| \mathcal{H}^{\ell/2} e^{it\frac{\mathcal{H}}{\varepsilon}} f\left(|e^{-it\frac{\mathcal{H}}{\varepsilon}} u|^2\right) e^{-it\frac{\mathcal{H}}{\varepsilon}} u \right\|_{L^2}$$

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$$\left\|g\left(\frac{t}{\varepsilon}, u\right)\right\|_{B^\ell} = \left\|e^{it\frac{\mathcal{H}}{\varepsilon}}\mathcal{H}^{\ell/2} f\left(|e^{-it\frac{\mathcal{H}}{\varepsilon}}u|^2\right)e^{-it\frac{\mathcal{H}}{\varepsilon}}u\right\|_{L^2}$$

(crucial: $e^{-it\frac{\mathcal{H}}{\varepsilon}}$ and $\mathcal{H}^{\ell/2}$ commute together)

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$$\left\| g\left(\frac{t}{\varepsilon}, u\right) \right\|_{B^\ell} = \left\| \mathcal{H}^{\ell/2} f\left(|e^{-it\frac{\mathcal{H}}{\varepsilon}} u|^2 \right) e^{-it\frac{\mathcal{H}}{\varepsilon}} u \right\|_{L^2}$$

($e^{-it\frac{\mathcal{H}}{\varepsilon}}$ is an isometry on L^2)

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- If $f \in C^\infty(\mathbb{R})$, then $u \in B^\ell \mapsto f(|u|^2)u \in B^\ell$ is C^∞ and satisfies a tame estimate

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$$\left\|g\left(\frac{t}{\varepsilon}, u\right)\right\|_{B^\ell} = \left\|f\left(|e^{-it\frac{\mathcal{H}}{\varepsilon}}u|^2\right)e^{-it\frac{\mathcal{H}}{\varepsilon}}u\right\|_{B^\ell}$$

(equivalence of norms)

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- If $f \in C^\infty(\mathbb{R})$, then $u \in B^\ell \mapsto f(|u|^2)u \in B^\ell$ is C^∞ and satisfies a tame estimate

$$\|f(|u|^2)u\|_{B^\ell} \leq C_f(\|u\|_{L^\infty}) \times \|u\|_{B^\ell}$$

Now, for all $M > 0$ and $u \in B^\ell$ such that $\|u\|_{B^\ell} \leq M$, we have

$$\begin{aligned}\left\| g\left(\frac{t}{\varepsilon}, u\right)\right\|_{B^\ell} &= \left\| f\left(|e^{-it\frac{\mathcal{H}}{\varepsilon}} u|^2\right) e^{-it\frac{\mathcal{H}}{\varepsilon}} u \right\|_{B^\ell} \\ &\leq C_{f,M} \left\| \mathcal{H}^{\ell/2} e^{-it\frac{\mathcal{H}}{\varepsilon}} u \right\|_{L^2}\end{aligned}$$

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- If $f \in C^\infty(\mathbb{R})$, then $u \in B^\ell \mapsto f(|u|^2)u \in B^\ell$ is C^∞ and satisfies a tame estimate

$$\|f(|u|^2)u)\|_{B^\ell} \leq C_f(\|u\|_{L^\infty}) \times \|u\|_{B^\ell}$$

Now, for all $M > 0$ and $u \in B^\ell$ such that $\|u\|_{B^\ell} \leq M$, we have

$$\begin{aligned} \left\| g\left(\frac{t}{\varepsilon}, u\right)\right\|_{B^\ell} &= \left\| \mathcal{H}^{\ell/2} f\left(|e^{-it\frac{\mathcal{H}}{\varepsilon}}u|^2\right) e^{-it\frac{\mathcal{H}}{\varepsilon}}u\right\|_{L^2} \\ &\leq C_{f,M}\left\|\mathcal{H}^{\ell/2}e^{-it\frac{\mathcal{H}}{\varepsilon}}u\right\|_{L^2} = C_{f,M}\left\|\mathcal{H}^{\ell/2}u\right\|_{L^2} \end{aligned}$$

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Now, for all $M > 0$ and $u \in B^\ell$ such that $\|u\|_{B^\ell} \leq M$, we have

$$\begin{aligned} \left\| g\left(\frac{t}{\varepsilon}, u\right) \right\|_{B^\ell} &= \left\| \mathcal{H}^{\ell/2} f\left(|e^{-it\frac{\mathcal{H}}{\varepsilon}} u|^2 \right) e^{-it\frac{\mathcal{H}}{\varepsilon}} u \right\|_{L^2} \\ &\leq C_{f,M} \left\| \mathcal{H}^{\ell/2} e^{-it\frac{\mathcal{H}}{\varepsilon}} u \right\|_{L^2} = C_{f,M} \|u\|_{B^\ell} \end{aligned}$$

Consequence: nonlinear analysis

This PDE can be treated by ODE techniques: Gronwall + the above nonlinear estimates + fixed point theorem imply that the Cauchy problem is well-posed on $[0, T_0]$ with $T_0 > 0$ and

$$\|\psi^\varepsilon(t,\cdot)\|_{B^\ell} = \|u^\varepsilon(t,\cdot)\|_{B^\ell} \leq \text{const.} \qquad (0 \leq t \leq T_0),$$

and all nonlinear terms are well defined and uniformly bounded in the space B^ℓ

There remains to average out, in the space B^ℓ, the equation

$$i\partial_t u^\varepsilon(t,x) = g\left(\frac{t}{\varepsilon}, u^\varepsilon(t,x)\right)$$

The (first order) averaging result

Let u^ε solve

$$i\partial_t u^\varepsilon(t,x) = g\left(\frac{t}{\varepsilon}, u^\varepsilon(t,x)\right)$$

and let u solve

$$i\partial_t u(t,x) = g_{av}\left(u(t,x)\right), \qquad g_{av}(u) := \frac{1}{T}\int_0^T g\left(\tau, u\right) d\tau$$

with the same initial data (here T is the period of g).
Then one has

$$\sup_{0\le t\le T_0} \|u^\varepsilon - u\|_{B^\ell} \le C\varepsilon.$$

Proof: write the Duhamel form of the equation satisfied by u^ε and ”integrate by parts” in time.

The projected version of the averaged equation

Recall that if $u(t,x) = \sum_n u_n(t) h_n(x)$, then in the cubic case

$$g(\tau, u) = \sum_{p,q,r} A_{n,p,q,r}\, e^{i\tau(E_n + E_p - E_q - E_r)} u_p^\varepsilon(t)^* \, u_q^\varepsilon(t)\, u_r^\varepsilon(t).$$

Hence the averaged nonlinearity reads

$$g_{av}(u) = \sum_{p,q,r \in \Lambda_n} A_{n,p,q,r}\, u_p^\varepsilon(t)^* \, u_q^\varepsilon(t)\, u_r^\varepsilon(t).$$

where

$$\Lambda_n = \{(p,q,r) : E_n + E_p - E_q - E_r = 0\}$$

A numerical example in dimension 1

$$i\partial_t \psi^\varepsilon = -\frac{1}{\varepsilon}\left(\frac{1}{2}\partial_x^2\psi^\varepsilon + \frac{1}{2}(x^2-1)\right)\psi^\varepsilon + |\psi^\varepsilon|^2\psi^\varepsilon$$

with an initial data on the first two Hermite functions

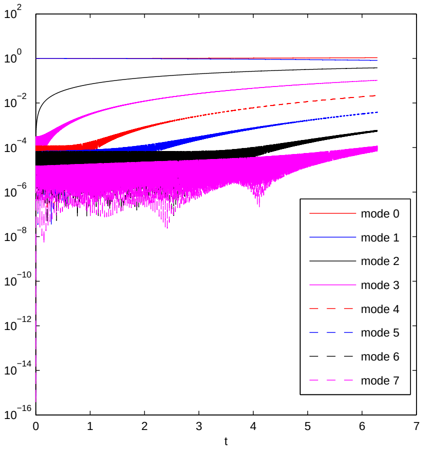
$$\psi(t=0,x) = h_0(x) + h_1(x).$$

Two numerical methods:

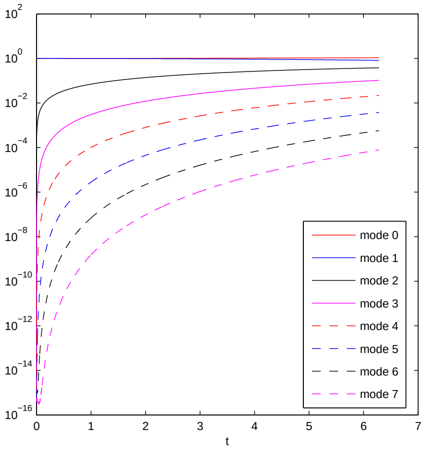
- A direct method on (NLS^ε): Time Splitting Hermite Pseudospectral method (see Bao et al) with $\Delta t = o(\varepsilon)$.
- A numerical integration of the averaged equation with $\Delta t = o(1)$.

$$\begin{aligned} i\partial_t u_n &= \sum_{q+r-p=n} A_{n,p,q,r}\, u_p^\varepsilon(t)^*\, u_q^\varepsilon(t)\, u_r^\varepsilon(t) \\ &= \frac{1}{2\pi}\int_0^{2\pi} e^{i\tau\frac{\mathcal{H}}{\varepsilon}}\left(|e^{-i\tau\frac{\mathcal{H}}{\varepsilon}}u(t,x)|^2 e^{-i\tau\frac{\mathcal{H}}{\varepsilon}}u(t,x)\right)d\tau. \end{aligned}$$

$\varepsilon = 10^{-2}$, representation of the modes $u_n^\varepsilon(t)$



TSHP method



averaged model

- **Observation**

  Simulating only the limit model induces an intrinsic error of order ε and can miss some interesting effects.

- **Goal**

  Search for averaged equations at higher order and associated numerical methods.

Outline

Highly-oscillatory problems with periodic time-dependence

Let X be a Banach space on $\mathbb{R}$. We consider highly oscillatory problems in X of the form

$$\frac{d}{dt}u^\varepsilon = g\left(\frac{t}{\varepsilon}, u^\varepsilon\right), \quad u^\varepsilon(0) = u_0 \in X$$

i.e. after reparametrization of time

$$\frac{d}{d\tau}u^\varepsilon = \varepsilon\, g_\tau(u^\varepsilon), \quad u^\varepsilon(0) = u_0 \in X. \tag{1}$$

- ε is a small parameter (inverse of a frequency).
- $(\theta, u) \mapsto g_\theta(u)$ is given, smooth w.r.t. $u \in X$ and 1-periodic, continuous w.r.t. $\theta \in \mathbb{T} \equiv [0, 1]$.
- There exist $T > 0$, $\varepsilon^* > 0$ and a bounded open subset $K \subset X$ such that, for all $\varepsilon \in]0, \varepsilon^*]$, (1) admits a unique solution $u^\varepsilon \in C^1([0, \frac{T}{\varepsilon}], X)$ with $u^\varepsilon(t) \in K$ for all $t \le \frac{T}{\varepsilon}$.

Averaging for ODEs:

- Krylov and Bogoliubov (1934) : basic idea
- Bogoliubov and Mitropolski (1958) : rigorous statement for second order approximation
- Perko (1969) : polynomial error estimates for the periodic and quasi-periodic cases
- Neihstadt (1984) : exponentially small error estimates for the periodic case
- Chartier, Murua and Sanz-Serna (2010-2012): stroboscopic averaging and quasi-stroboscopic averaging using B-series

Related techniques for ODEs and PDEs:

- Wentzel-Kramers-Brillouin (1926): two-scale expansions in quantum mechanics
- Bambusi, Bourgain, Grébert, Thomann, Villegas-Blas (2003–2012): Birkhoff normal forms (for non-linear PDEs)
- Cohen, Hairer, Gauckler, Lubich (2003–2012): Modulated Fourier expansions for ODEs and some Hamiltonian PDEs (Fermi-Pasta-Ulam, wave equation, Schrödinger equation)

Textbooks:

- Lochak and Meunier (1988) : *Multiphase averaging for classical systems. With applications to adiabatic theorems*
- Sanders, Verhulst and Murdock (2007) : *Averaging methods in nonlinear dynamical systems*

The equations of stroboscopic averaging

The purpose of averaging is to find a 1-periodic smooth change of variable, ε-close to the identity,

$$(\theta, u) \in \mathbb{T} \times K \mapsto \Phi_\theta^\varepsilon(u) \in X$$

such that the solution of $\frac{d}{d\tau} u^\varepsilon = \varepsilon g_\tau(u^\varepsilon)$ takes the form

$$u^\varepsilon(\tau) = \Phi_\tau^\varepsilon \circ \Psi_\tau^\varepsilon(u_0),$$

for u_0 in some open set $U \subset X$, and where Ψ_τ^ε is the flow map of an autonomous differential equation on X:

$$\frac{d}{d\tau} \Psi_\tau^\varepsilon(u_0) = \varepsilon\, G^\varepsilon\left(\Psi_\tau^\varepsilon(u_0)\right).$$

For stroboscopic averaging, one requires in addition $\Phi_0^\varepsilon \equiv id$.

Let us now formally seek the equations satisfied by Φ_θ^ε and Ψ_τ^ε.
By differentiating $u^\varepsilon(\tau) = \Phi_\tau^\varepsilon \circ \Psi_\tau^\varepsilon(u_0)$ w.r.t. τ we get

$$\frac{du^\varepsilon(t)}{d\tau} = \frac{\partial \Phi_\tau^\varepsilon}{\partial \tau}\left(\Psi_\tau^\varepsilon(u_0)\right) + \frac{\partial \Phi_\tau^\varepsilon}{\partial u}\left(\Psi_\tau^\varepsilon(u_0)\right)\frac{d\Psi_\tau^\varepsilon}{d\tau}(u_0).$$

Let us now formally seek the equations satisfied by Φ_θ^ε and Ψ_τ^ε.
By differentiating $u^\varepsilon(\tau) = \Phi_\tau^\varepsilon \circ \Psi_\tau^\varepsilon(u_0)$ w.r.t. τ we get

$$\varepsilon\, g_\tau\left(u^\varepsilon(\tau)\right) = \frac{\partial \Phi_\tau^\varepsilon}{\partial \tau}\left(\Psi_\tau^\varepsilon(u_0)\right) + \varepsilon \frac{\partial \Phi_\tau^\varepsilon}{\partial u}\left(\Psi_\tau^\varepsilon(u_0)\right) G^\varepsilon\left(\Psi_\tau^\varepsilon(u_0)\right).$$

Let us now formally seek the equations satisfied by Φ_θ^ε and Ψ_τ^ε.
By differentiating $u^\varepsilon(\tau) = \Phi_\tau^\varepsilon \circ \Psi_\tau^\varepsilon(u_0)$ w.r.t. τ we get

$$\varepsilon\, g_\tau \left(\Phi_\tau^\varepsilon \circ \Psi_\tau^\varepsilon(u_0)\right) = \frac{\partial \Phi_\tau^\varepsilon}{\partial \tau} \left(\Psi_\tau^\varepsilon(u_0)\right) + \varepsilon \frac{\partial \Phi_\tau^\varepsilon}{\partial u} \left(\Psi_\tau^\varepsilon(u_0)\right) G^\varepsilon \left(\Psi_\tau^\varepsilon(u_0)\right).$$

Let us now formally seek the equations satisfied by Φ_θ^ε and Ψ_τ^ε.
By differentiating $u^\varepsilon(\tau) = \Phi_\tau^\varepsilon \circ \Psi_\tau^\varepsilon(u_0)$ w.r.t. τ we get

$$\varepsilon\, g_\tau\left(\Phi_\tau^\varepsilon \circ \Psi_\tau^\varepsilon(u_0)\right) = \frac{\partial \Phi_\tau^\varepsilon}{\partial \tau}\left(\Psi_\tau^\varepsilon(u_0)\right) + \varepsilon \frac{\partial \Phi_\tau^\varepsilon}{\partial u}\left(\Psi_\tau^\varepsilon(u_0)\right) G^\varepsilon\left(\Psi_\tau^\varepsilon(u_0)\right).$$

Taking $u_0 = \Psi_{-\tau}^\varepsilon(u)$ and replacing τ by $\theta \in \mathbb{T}$ we obtain

Transport equation

$$\frac{\partial \Phi_\theta^\varepsilon}{\partial \theta}(u) + \varepsilon \frac{\partial \Phi_\theta^\varepsilon}{\partial u}(u)\, G^\varepsilon(u) = \varepsilon\, g_\theta\left(\Phi_\theta^\varepsilon(u)\right).$$

Let us now formally seek the equations satisfied by Φ^ε_θ and Ψ^ε_τ.
By differentiating $u^\varepsilon(\tau) = \Phi^\varepsilon_\tau \circ \Psi^\varepsilon_\tau(u_0)$ w.r.t. τ we get

$$\varepsilon\, g_t\left(\Phi^\varepsilon_t \circ \Psi^\varepsilon_t(u_0)\right) = \frac{\partial \Phi^\varepsilon_t}{\partial t}\left(\Psi^\varepsilon_t(u_0)\right) + \varepsilon \frac{\partial \Phi^\varepsilon_t}{\partial u}\left(\Psi^\varepsilon_t(u_0)\right) G^\varepsilon\left(\Psi^\varepsilon_t(u_0)\right).$$

Taking $u_0 = \Psi^\varepsilon_{-t}(u)$ and replacing t by $\theta \in \mathbb{T}$ we obtain

Transport equation

$$\frac{\partial \Phi^\varepsilon_\theta}{\partial \theta}(u) + \varepsilon \frac{\partial \Phi^\varepsilon_\theta}{\partial u}(u)\, G^\varepsilon(u) = \varepsilon\, g_\theta\left(\Phi^\varepsilon_\theta(u)\right).$$

If $f_\theta(u)$ is periodic with respect to θ, then $\langle f \rangle$ will be its average:

$$\langle f \rangle(u) := \int_0^1 f_\theta(u)\, d\theta.$$

Taking averages in θ of both sides of the transport equation:

$$\frac{\partial\langle\Phi^\varepsilon\rangle}{\partial u}(u)\, G^\varepsilon(u) = \langle g\circ\Phi^\varepsilon\rangle\,(u)\,.$$

Assuming that $\frac{\partial\langle\Phi^\varepsilon\rangle}{\partial u}(u)$ is invertible, the outcome are the

Main equations of averaging

$$\text{(i)}\quad \frac{d}{d\tau}\Psi^\varepsilon_\tau(u_0) = \varepsilon\, G^\varepsilon\left(\Psi^\varepsilon_\tau(u_0)\right)$$

$$\text{(ii)}\quad G^\varepsilon(u) := \left(\frac{\partial\langle\Phi^\varepsilon\rangle}{\partial u}(u)\right)^{-1}\langle g\circ\Phi^\varepsilon\rangle\,(u),$$

$$\text{(iii)}\quad \frac{\partial\Phi^\varepsilon_\theta}{\partial\theta}(u) + \varepsilon\frac{\partial\Phi^\varepsilon_\theta}{\partial u}(u)\left(\frac{\partial\langle\Phi^\varepsilon\rangle}{\partial u}(u)\right)^{-1}\langle g\circ\Phi^\varepsilon\rangle\,(u) = \varepsilon\, g_\theta\circ\Phi^\varepsilon_\theta(u)$$

Solving these equations: find a fixed-point of the operator

$$\Gamma_\theta^\varepsilon(\varphi)(u) = u + \varepsilon \int_0^\theta \left(g_\xi \circ \varphi_\xi(u) - \frac{\partial \varphi_\xi}{\partial u}(u) \left(\frac{\partial \langle \varphi \rangle}{\partial u}(u) \right)^{-1} \langle g \circ \varphi \rangle (u) \right) d\xi$$

in an "appropriate subspace" of periodic functions.

However: Γ^ε is non-local, non-linear, and this equation can be solved only up to an exponentially small error term in ε.

Picard iteration is adopted here:

Construct a sequence of analytic functions

$$\Phi_\theta^{[0]} = id, \quad \Phi_\theta^{[k+1]} = \Gamma_\theta^\varepsilon(\Phi_\theta^{[k]}), \quad k = 0, 1, 2, \ldots, n,$$

at the price of a gradual thinning of their domains of definition (due to the loss of derivatives in u).

Contraction property of the mapping

From

$$\Gamma_\theta^\varepsilon(\varphi) - \Gamma_\theta^\varepsilon(\widetilde{\varphi}) = \mathcal{O}(\varepsilon),$$

one deduces the ”convergence” property

$$\Phi_\theta^{[k+1]} - \Phi_\theta^{[k]} = \mathcal{O}(\varepsilon^k).$$

At this point, we have “solved” the equation for Φ^ε and we can consider the associate sequence of vector fields

$$G^{[k]}(u) := \left(\frac{\partial\langle\Phi^{[k]}\rangle}{\partial u}(u)\right)^{-1} \langle g \circ \Phi^{[k]}\rangle(u)$$

From polynomial to exponential errors: optimal truncation

$$(n_\varepsilon + 1) = \lfloor \varepsilon_0/(2\varepsilon) \rfloor, \quad \widetilde{\Phi}_\theta^\varepsilon = \Phi_\theta^{[n_\varepsilon]} \text{ and } \widetilde{G}^\varepsilon = G^{[n_\varepsilon]}.$$

Theorem

For small enough $\varepsilon > 0$*, the following holds. Introduce* $\widetilde{\Psi}_t^\varepsilon$ *the* t*-flow of the* autonomous *diff. equation*

$$\frac{dU}{dt} = \varepsilon \widetilde{G}^\varepsilon(U),$$

then the solution $u^\varepsilon(t)$ *of the IVP satisfies*

$$\forall \tau \in [0, T/\varepsilon], \quad \left\| u^\varepsilon(\tau) - \widetilde{\Phi}_\tau^\varepsilon \circ \widetilde{\Psi}_\tau^\varepsilon(u_0) \right\|_{X_\mathbb{C}} \leq C \exp\left(-\frac{C}{\varepsilon}\right).$$

Note: due to the choice of stroboscopic averaging $\widetilde{\Phi}_0^\varepsilon = id$, one has $\widetilde{\Phi}_{\tau_n}^\varepsilon = id$ at the stroboscopic times $\tau_n = n$ so

$$\left\| u^\varepsilon(\tau_n) - \widetilde{\Psi}_{\tau_n}^\varepsilon(u_0) \right\|_{X_\mathbb{C}} \leq C \exp\left(-\frac{C}{\varepsilon}\right).$$

In the linear case

$$g_\theta(u) \equiv A_\theta u,$$

where A_θ is a bounded linear operator on X, our iterative procedure actually converges and

$$u^\varepsilon(\tau) = \Phi^\varepsilon_\tau \circ \Psi^\varepsilon_\tau(u_0).$$

A recipe to compute the averaged equations

1. Implement the pre-Lie product $h = f \lhd g$ of the fields f_t, g_t

$$h_t(u) = \int_0^t \left(\frac{\partial f_s(u)}{\partial u} g_t(u) - \frac{\partial g_t(u)}{\partial u} f_s(u) \right) ds.$$

2. Compute recursively the terms of the expansion

$$\varepsilon R_t^\varepsilon(u) = \varepsilon R_t^{[1]}(u) + \varepsilon^2 R_t^{[2]}(u) + \varepsilon^3 R_t^{[3]}(u) + \cdots$$

by solving the equation

$$\varepsilon g = \varepsilon R^\varepsilon + \frac{\varepsilon^2}{2} R^\varepsilon \lhd R^\varepsilon + \frac{\varepsilon^3}{3!} R^\varepsilon \lhd (R^\varepsilon \lhd R^\varepsilon) + \frac{\varepsilon^4}{4!} R^\varepsilon \lhd (R^\varepsilon \lhd (R^\varepsilon \lhd R^\varepsilon)) + \cdots$$

3. Compute the averages $G_i(u) = \langle R^{[i]} \rangle (u)$.

First terms read $G_1 = \langle g \rangle$, $\quad G_2 = -\frac{1}{2} \left\langle \int_0^t [g_s(u), g_t(u)]\, ds \right\rangle$, $\cdots$

Geometric aspects

$X \subset Z$ are Hilbert spaces, equipped with $(\cdot,\cdot)_X$ and $(\cdot,\cdot)_Z$ and X is dense in Z (e.g. $X = B^\ell(\mathbb{R}^d)$ and $Z = L^2(\mathbb{R}^d)$).

Definition and assumption

g_θ is assumed to be Hamiltonian: $\exists$ a bounded inv. linear map $J : X \to X$, skew-symmetric w.r.t. $(\cdot,\cdot)_Z$, and an analytic H_θ, s.t.

$$g_\theta = J^{-1}\nabla_u H_\theta.$$

A smooth map Φ_θ is said to be symplectic if

$$\forall (\theta, u, v, w) \in \mathbb{T}\times K \times X^2, \quad \langle J\partial_u \Phi_\theta(u)v \,,\, \partial_u \Phi_\theta(u)w\rangle_Z = \langle Jv, w\rangle_Z.$$

Theorem

$\Phi_\theta^{[n]}$ and $G^{[n]}$ are respectively symplectic and Hamiltonian up to ε^{n+1}-perturbation terms: for all $u \in K$, $v, w \in X$, we have

$$\Big(J\partial_u \Phi_\theta^{[n]}(u)v, \partial_u \Phi_\theta^{[n]}(u)w\Big)_Z = (Jv, w)_Z + \mathcal{O}(\varepsilon^{n+1}\|v\|_X \|w\|_X).$$

$$G^{[n]}(u) = J^{-1}\nabla_u H^{[n]}(u) + \mathcal{O}(\varepsilon^{n+1}),$$

where $H^{[n]}$ is defined by

$$H^{[n]}(u) = \Big\langle H_\theta \circ \Phi_\theta^{[n+1]}(u)\Big\rangle - \frac{1}{2\varepsilon}\Big\langle \Big(J\partial_\theta \Phi_\theta^{[n+1]}(u), \Phi_\theta^{[n+1]}(u)\Big)_Z \Big\rangle.$$

Remark:

This implies that each term in the ε–expansion of $G^{[n]}$ is Hamiltonian.

Assume that the exact solution admits an invariant (possibly depending on ε) $Q_\theta : \mathbb{T} \times X \to \mathbb{R}$:

$$\forall u \in K,\ \forall \theta \in \mathbb{T}, \qquad \frac{\partial Q_\theta}{\partial \theta}(u) + \varepsilon \frac{\partial Q_\theta}{\partial u}(u)\, g_\theta(u) = 0.$$

For instance, $Q(u) = \|u\|_Z^2$ is an invariant if, for all u, one has $(g_\theta(u), u)_Z = 0$: this is the case in our application to NLS.

Theorem

The change of variable $\Phi_\theta^{[n]}$ and the averaged vector field $G^{[n]}$ satisfy the relations

$$\forall u \in K,\ \forall \theta \in \mathbb{T}, \qquad \begin{aligned} & Q_\theta(\Phi_\theta^{[n]}(u)) = Q_0(u) + \mathcal{O}(\varepsilon^{n+1}), \\ & (\partial_u Q_0)(u)\, G^{[n]}(u) = \mathcal{O}(\varepsilon^n). \end{aligned}$$

Outline

The main result

Theorem

For small ε, there exist smooth $G^\varepsilon(u)$ and $\Phi^\varepsilon_\theta(u)$ with $\Phi^\varepsilon_0 = \mathrm{id}$, such that for all $\|\psi_0\|_{B^\ell} \le M$, the NLS solution satisfies

$$\sup_{0\le t\le T} \left\| \psi^\varepsilon(t) - e^{-it\frac{\mathcal{H}}{\varepsilon}} \Phi^\varepsilon_{t/\varepsilon}\left(\widetilde{\psi}^\varepsilon(t)\right) \right\|_{B^\ell} \le C \exp\left(-\frac{C}{\varepsilon}\right),$$

where $\widetilde{\psi} \in C^1([0,T], X)$ solves the autonomous equation

$$\frac{\partial \widetilde{\psi}^\varepsilon}{\partial t} = G^\varepsilon(\widetilde{\psi}^\varepsilon), \qquad \widetilde{\psi}^\varepsilon(0) = \psi_0.$$

Moreover, $G^\varepsilon(u) = J^{-1}\nabla H^\varepsilon(u)$, and if

$$H(\psi) = \frac{1}{2}(\mathcal{H}\psi, \psi)_{L^2} + \frac{\varepsilon}{2}\int F\left(|\psi|^2\right)(t,x)dx,$$

then for $t \le T$,

$$\|\widetilde{\psi}^\varepsilon(t)\|^2_{L^2} = \|\psi_0\|^2_{L^2} \quad \text{and} \quad H(\widetilde{\psi}^\varepsilon(t)) = H(\psi_0) + \mathcal{O}(e^{-C/\varepsilon}).$$

Numerical experiments

To design high order numerical methods, do not write explicitely the averaged equation (its form is in general too complicated !)

Stroboscopic Averaging Method (Chartier, Murua, Sanz-Serna):

Simulation of the autonomous averaged equation, using micro-integrations in order to compute approximatively the vector field.

The idea is to solve the averaged equation at two levels, in the spirit of *Heterogeneous Multiscale Methods*:

- Approximate the averaged vector field G by central differences of the form

$$G(U) \approx \frac{1}{4\pi\varepsilon}\left(S_{2\pi\varepsilon}(U) - S_{-2\pi\varepsilon}(U)\right)$$

  with a numerical method with constant stepsizes (micro-steps δt). Here we have denoted by $S_t(u)$ the solution of the highly-oscillatory equation

$$\frac{d}{dt}u = g\left(\frac{t}{\varepsilon}, u(t)\right), \; u(0) = U.$$

- Solve the averaged equation by a numerical method with possibly variable stepsizes (macro-steps Δt).

More precisely, let us choose for instance

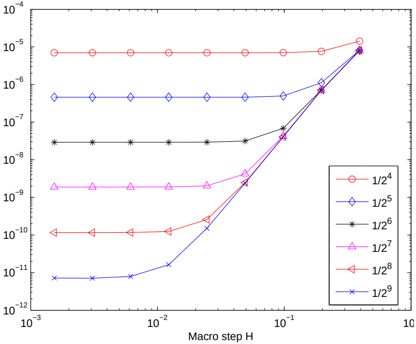
- fourth order (in time) Time Splitting Hermite Pseudospectral method for the micro-steps,
- a fourth-order Runge-Kutta method for the macro-steps,
- a fourth-order interpolation method for the calculation of the averaged field.

Then one can bound the error formally by

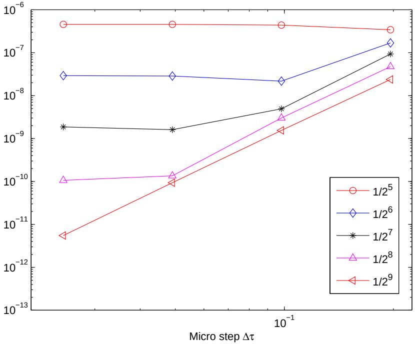
$$\text{error} = \mathcal{O}\left(\varepsilon^4 + (\Delta t)^4 + \varepsilon\left(\frac{\delta t}{\varepsilon}\right)^4\right).$$

Recall that the micro integrations are done on intervals of size $\mathcal{O}(\varepsilon)$. The cost of the method does not increase as $\varepsilon \to 0$.

Accuracy curves for the Stroboscopic Averaging Method

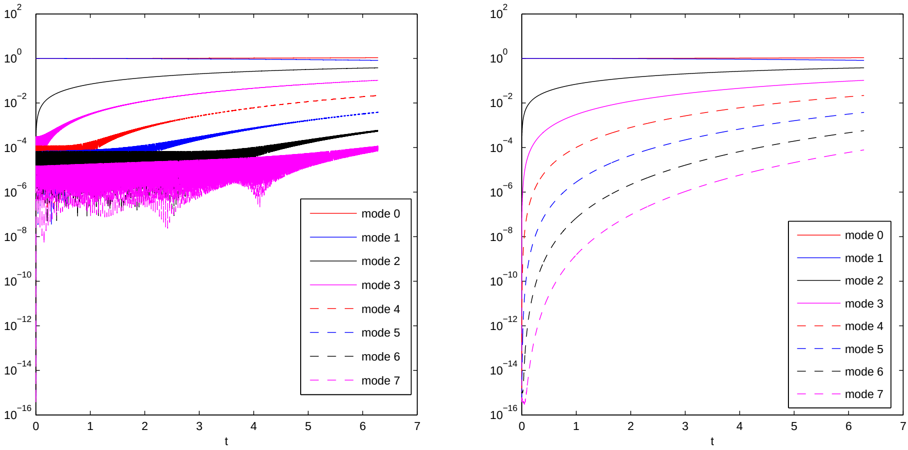


order 4 in the macro step



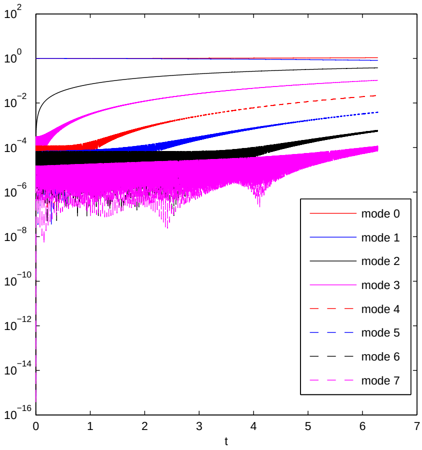
order 4 in the micro step

$\varepsilon = 10^{-2}$, representation of the modes $u_n^\varepsilon(t)$

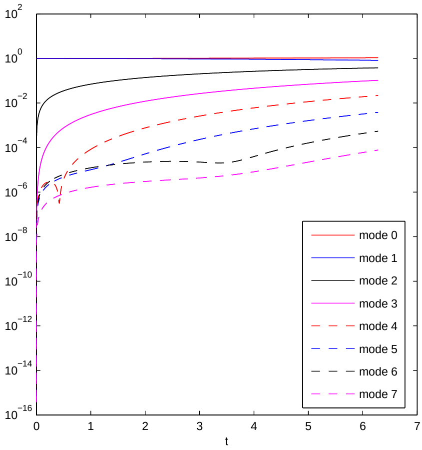


TSHP method — averaged model

$\varepsilon = 10^{-2}$, representation of the modes $u_n^\varepsilon(t)$



TSHP method



Stroboscopic Averaging Method

Thank you for your attention !