A stroboscopic averaging technique for highly-oscillatory Schrödinger equation

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Saint-Malo Workshop, January 26-28, 2011

Goal of the present study

Numerical schemes and **asymptotic study** for nonlinear Schrödinger equations of the form

$$i\partial_t \psi^\varepsilon(t,x) = \frac{H_x}{\varepsilon}\psi^\varepsilon(t,x) + F\left(|\psi^\varepsilon(t,x)|^2\right)\,\psi^\varepsilon(t,x),$$

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

$$H_x = -\frac{1}{2}\Delta_x + \frac{1}{2}|x|^2.$$

and F is a given nonlinear function.

Context: Bose-Einstein condensates

$\longrightarrow$ H_x/ε represents **strong confinement** in x.

$\longrightarrow$ nonlinear term describes bosons' **interactions.**

Goal of the present study (2)

References (in that context):
Bao, Markowich, Schmeiser, Weishäupl (M3AS, 2005),
Ben Abdallah, Méhats (JMPA, 2005),
Ben Abdallah, Méhats, Schmeiser, Weishäupl (SIAM, 2005).

See also, in the context of fluid mechanics:
Grenier (JMPA, 1997),
Schochet (JDE, 1994),
Métivier, Schochet (JDE 2003),

and, for other Schrödinger-like or Vlasov-like equations:
Bidégaray, Castella, Degond (DCDS 2004),
Castella, Degond, Goudon (JSP 2006).

Rough analysis (and wrong approach)

⟶ **Linear part**: Eigenvalues of H_x :

$$\{E_n = n_1 + \cdots + n_d + \frac{d}{2}\,;\, n = (n_1, \ldots, n_d) \in \mathbb{N}^d\},$$

Eigenfunctions: explicitely known $\chi_n(x)$'s ($n \in \mathbb{N}^d$),

Hermite polynomial $\times$ Gaussian.

⟶ **Project**

$$\psi^\varepsilon(t,x) = \sum_n \psi_n^\varepsilon(t)\,\chi_n(x),$$

and write, say if $F(|\psi|^2)\psi = |\psi|^2\psi$,

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

$$\left(\text{with } A_{n,p,q,r} = \int_{\mathbb{R}^d} \psi_p^\varepsilon(t)^*\,\psi_q^\varepsilon(t)\,\psi_r^\varepsilon(t)\right).$$

Rough analysis (and wrong approach) (2)

$\longrightarrow$ **Filter out** the oscillatory term and introduce

$$\phi_n^\varepsilon(t,x) = \exp\left(+it\frac{E_n}{\varepsilon}\right)\psi^\varepsilon(t,x).$$

It satisfies

$$i\partial_t\phi_n^\varepsilon(t) = \sum_{p,q,r} A_{n,p,q,r}\ \exp\left(it\frac{E_n+E_p-E_q-E_r}{\varepsilon}\right)\phi_p^\varepsilon(t)^*\,\phi_q^\varepsilon(t)\,\phi_r^\varepsilon(t).$$

$\longrightarrow$ System of the form

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

with G **periodic** (E_n's are half-integers)

and $u^\varepsilon = (\phi_0^\varepsilon, \phi_1^\varepsilon, \dots)$ (**infinite**, **nonlinearly coupled** system).

Rough analysis (and wrong approach) (3)

$\longrightarrow$ **Questions**

• How to **numerically average out** the ODE

$$\partial_t u^\varepsilon = G\left(\frac{t}{\varepsilon}, u^\varepsilon\right) \ ?$$

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

• How to control the **norms** of u^ε, and that of the **nonlinear term** G (*i.e.*, typically ϕ^ε and the sums $\sum_{p,q,r} \cdots$: it is not clear that the Sobolev smoothness $\sum_n n^\alpha |\phi_n|^2 < +\infty$ implies $\sum_n n^\alpha \left|\sum_{p,q,r} \cdots\right|^2 < +\infty$, because of the $A_{n,p,q,r}$'s) ?

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

Right approach and analytic framework

$\longrightarrow$ **Avoid projecting** on the χ_n's and write directly (Ben Abdallah, Castella, Méhats)

$$\phi^\varepsilon(t,x) = \exp\left(+it\frac{H_x}{\varepsilon}\right)\,\psi^\varepsilon(t,x).$$

$\longrightarrow$ It satisfies $i\partial_t\phi^\varepsilon(t,x) = G\left(\frac{t}{\varepsilon},\phi^\varepsilon(t,x)\right)$,

where, for $u = u(x)$ given, we have $\left(\widetilde{F}(z) = F(|z|^2)z\right)$

$$G\left(\frac{t}{\varepsilon},u\right) = \exp\left(+it\frac{H_x}{\varepsilon}\right)\widetilde{F}\left(\exp\left(-it\frac{H_x}{\varepsilon}\right)\,u(x)\right)$$

Right approach and analytic framework (2)

Bounds on the **nonlinear terms** $G(t/\varepsilon, \phi^\varepsilon)$ or $\widetilde{F}(\psi^\varepsilon)$?

When $F \equiv 0$, we have (take a large $N \in \mathbb{N}$)

$$i\partial_t \psi^\varepsilon = \frac{H_x}{\varepsilon}\psi^\varepsilon$$

$$\Longrightarrow \partial_t \left\| H_x^N \psi^\varepsilon \right\|_{L^2}^2 = 2\mathrm{Re} \left\langle H_x^N \left(-i\frac{H_x}{\varepsilon}\psi^\varepsilon \right), H_x^N \psi^\varepsilon \right\rangle_{L^2} = 0,$$

(H_x commutes with H_x^N **and** H_x is self-adjoint)

$$\Longrightarrow \left\| H_x^N \psi^\varepsilon \right\|_{L^2}^2 \leq \mathrm{const.}$$

while

$$\partial_t \left\| \partial_x^N \psi^\varepsilon \right\|_{L^2}^2 = \mathcal{O}\left(\frac{1}{\varepsilon}\right) \Longrightarrow \text{ no uniform in } \varepsilon \text{ bound on } \left\| \partial_x^N \psi^\varepsilon \right\|_{L^2}^2 .$$

Right approach and analytic framework (3)

This is due to

$$\partial_t \left\| \partial_x^N \psi^\varepsilon \right\|_{L^2}^2 = 2\mathrm{Re} \left\langle \partial_x^N \left(-i \frac{H_x}{\varepsilon} \psi^\varepsilon \right) , \partial_x^N \psi^\varepsilon \right\rangle_{L^2}$$
$$= 2\mathrm{Re} \left\langle \partial_x^N \left(-i \frac{|x|^2}{\varepsilon} \psi^\varepsilon \right) , \partial_x^N \psi^\varepsilon \right\rangle_{L^2}$$
$$= \mathcal{O}\left(\frac{1}{\varepsilon} \right).$$

$\longrightarrow$ Only a uniform bound on $\|H_x^N \psi^\varepsilon\|_{L^2}$ (and not on $\|\partial_x^N \psi^\varepsilon\|_{L^2}$) can be obtained in the general case.

$\longrightarrow$ The "good norm" is $\|u\|_{B^N} = \|u\|_{L^2} + \|H_x^N u\|_{L^2}$,

instead of the Sobolev scale $\|u\|_{H^N} = \|u\|_{L^2} + \|\partial_x^N u\|_{L^2}$.

Right approach and analytic framework (4)

Note that : $$\left\| H_x^N \phi^\varepsilon \right\|_{L^2} = \left\| H_x^N \exp\left(+it \frac{H_x}{\varepsilon} \right) \psi^\varepsilon \right\|_{L^2}$$
$$= \left\| \exp\left(+it \frac{H_x}{\varepsilon} H_x^N \right) \psi^\varepsilon \right\|_{L^2} \quad \text{(commutation)}$$
$$= \left\| H_x^N \psi^\varepsilon \right\|_{L^2} \quad \text{(self-adjointness)}$$

Remaining question: we know ($\|u\|_{H^N} := \|u\|_{L^2} + \|\partial_x^N u\|_{L^2}$)

$$\left\| \widetilde{F}(\psi^\varepsilon) \right\|_{H^N} \leq \text{const.}\left(\|\psi^\varepsilon\|_{H^N} \right),$$

yet **is it true that** ($\|u\|_{B^N} := \|u\|_{L^2} + \|H_x^N u\|_{L^2}$)

$$\left\| \widetilde{F}(\psi^\varepsilon) \right\|_{B^N} \leq \text{const.}\left(\|\psi^\varepsilon\|_{B^N} \right) \ ?$$

Right approach and analytic framework (5)

Answer (Ben Abdallah, Castella, Méhats, see also Helffer, Nier, and Bony, Chemin — requires Weyl-Hörmander calculus for general Hamiltonians):
Yes because of the following

Theorem ($H_x = -\Delta_x + |x|^2$)

For any N, we have the equivalence of norms

$$\|u\|_{L^2} + \|\partial_x^{2N} u\|_{L^2} + \||x|^{2N} u\|_{L^2} \sim \|u\|_{L^2} + \|(-\partial_x^2 + |x|^2)^N u\|_{L^2}$$

or, in other words

$$\|u\|_{L^2} + \|\partial_x^{2N} u\|_{L^2} + \||x|^{2N} u\|_{L^2} \sim \|u\|_{B^N}.$$

Right approach and analytic framework (6)

By standard nonlinear analysis (Gronwall $+$ the above nonlinear estimates on $\|\widetilde{F}(u)\|_{B^N}$ $+$ standard fixed point in the original PDE),

this immediately implies the existence of $T_0 > 0$ such that

$$\|\psi^\varepsilon(t,x)\|_{B^N}, \quad \|\phi^\varepsilon(t,x)\|_{B^N} \leq \text{const.} \qquad (0 \leq t \leq T_0),$$

and all nonlinear terms are well defined and uniformly bounded in the space B_N

$\longrightarrow$ there remains to average out, in the space B^N, the equation

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

Highly oscillatory ODE's

Problems of the form

$$\dot{y} = \frac{dy}{dt} = f(y, t/\varepsilon), \quad y(0) = y_0,$$

where :

- ε is a small parameter (the inverse of the frequency).
- f is a **smooth** vector-field, 2π-periodic in t/ε.

Assumptions:

- a clear and explicit separation of the time-scales
- a periodic (and not only quasi-periodic at this stage) dependence in the fast time

Highly oscillatory ODE's (2)

Appears in various forms:

- "Standard" form in KAM theory
- Two-scale expansions in quantum mechanics (Wentzel-Kramers-Brillouin, 1926)
- Magnus expansions (A. Iserles, 2002)
- Modulated Fourier expansions (D. Cohen, E. Hairer and Chr. Lubich, 2003)

Theory has been gradually improved:

- Krylov and Bogoliubov (1934) : basic idea
- Bogoliubov and Mitropolski (1958) : rigorous statement for second order approximation and general scheme
- Perko (1969) : almost complete theory with error estimates for the periodic and quasi-periodic cases (see also the book Sanders, Verhulst and Murdock, 2007)

Highly oscillatory ODE's (3)

Theorem (Perko, SIAM 1969 : Averaging of high-order)

Under a smoothness assumption on f and a non-resonance condition on ω , given the system

$$\begin{cases} y' = \varepsilon f(y,\theta) \in \mathbb{R}^n, & y(0) = y_0, \\ \theta' = \omega \in \mathbb{T}^d, & \theta(0) = \theta_0, \end{cases}$$

there exists a transformation from $\mathbb{R}^n \times \mathbb{T}^d$ to $\mathbb{R}^n$

$$y = U(Y,\theta) = Y + \varepsilon u_1(Y,\theta) + \ldots + \varepsilon^k u_k(Y,\theta)$$

such that

$$Y' = \varepsilon F_1(Y) + \ldots + \varepsilon^k F_k(Y), Y(0) = \xi.$$

and

$$\|y(\tau) - U(Y(\tau), \theta_0 + \tau\omega)\| \leq C\varepsilon^k \text{ for } \tau \leq C/\varepsilon.$$

Highly oscillatory ODE's (4)

The functions u_i (and thus F_i) are not unique except F_1

$$\tilde{F}_1(Y) = f(y,\theta),$$

$$\tilde{F}_j(Y,\theta) = \sum_{k=1}^{j-1} \left[\frac{1}{k!} \sum_{i_1+\ldots+i_k=j-1} \frac{\partial^k f}{\partial y^k}\left(u_{i_1},\ldots,u_{i_k}\right) - \frac{\partial u_k}{\partial Y} F_{j-k} \right],$$

$$F_j(Y) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \tilde{F}_j(Y,\theta) d\theta,$$

$$\omega \cdot \frac{\partial u_j}{\partial \theta}(Y,\theta) = \tilde{F}_j(Y,\theta) - F_j(Y).$$

For $d = 1$, one can impose $u_j(Y,0) = 0$: this is **stroboscopic** averaging, in the sense that $U(Y, 2k\pi) = Y$.

An example

For $f(y,\tau) = 1 + \cos(\tau)y$, we have

$$\Phi_{\tau_0}^{\tau}(y_0) = \varepsilon e^{\varepsilon \sin(\tau)} \int_{\tau_0}^{\tau} e^{-\varepsilon \sin(s)} ds + e^{\varepsilon(\sin(\tau) - \sin(\tau_0))} y_0,$$

so that

$$\Phi_{\tau_0}^{\tau_0 + 2\pi}(y_0) = 2\pi\varepsilon\nu e^{\varepsilon \sin(\tau_0)} + y_0, \quad \nu = \frac{1}{2\pi} \int_0^{2\pi} e^{-\varepsilon \sin(\tau)} d\tau.$$

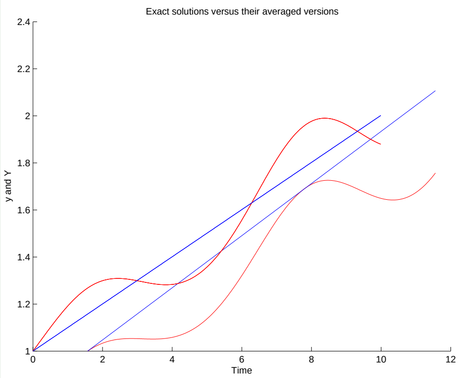
We see that $\left(\Phi_{\tau_0}^{\tau_0+2\pi}\right)^k (y_0)$ coincides with the solution at points $\tau = 2k\pi$ of the differential equation

$$\begin{cases} Y'(\tau) = \varepsilon\nu e^{\varepsilon \sin(\tau_0)} \\ Y(0) = y_0 \end{cases},$$

which happens to be the modified equation we are looking for.

An example (2)

Example



We search for a differential equation whose flow coincides at times that are multiple of 2π with the flow of the highly-oscillatory equation.

B-series expansions

Mode-coloured B-series with time-dependent coefficients

Consider the rescaled system expanded in Fourier coefficients

$$\begin{cases} y'(\tau) = \varepsilon \sum_{k\in\mathbb{Z}} e^{ik\tau} f_k(y), & y(0) = y_0 \\ \theta'(\tau) = 1, & \theta(0) = \theta_0 \end{cases}$$

where the f_k's are the Fourier coefficients of f. Chartier, Murua and Sanz-Serna [FOCM 2010] consider B-series of the form

$$y_0 + \sum_{u\in\mathcal{T}} \varepsilon^{|u|} \frac{\alpha_u(\tau)}{\sigma_u} \mathcal{F}_u(y_0)$$

where

- $\mathcal{T}$ is a set of mode-decorated trees.
- $\mathcal{F}_u(y_0)$ are associated derivatives of the f_k's .
- σ_u is a normalisation coefficient.
- $\alpha_u(\tau)$ are coefficients defining the series.

B-series expansions (2)

Tree	Order	σ_u	$\mathcal{F}_u$
$\bullet_k$	1	1	f_k
$= [\bullet_k]_l$	2	1	$f_l' f_k$
$= [\bullet_k, \bullet_l]_m$	3	$1 + \delta_{k,l}$	$f_m''(f_k, f_l)$
$[[\bullet_k]_l]_m =$	3	1	$f_m' f_l' f_k$

Table: Mode-decorated trees and their associated coefficients

B-series expansions (3)

Nota : The general procedure is described as in Chartier, Murua, Sanz-Serna, FOCM 2010

Construction of averaged vector field F from $\varepsilon f(y,\tau)$:

1. Compute the B-series expansion of the **exact** solution

$$y(\tau) = y_0 + \sum_{u\in\mathcal{T}} \varepsilon^{|u|} \frac{\alpha_u(\tau)}{\sigma_u} \mathcal{F}_u(y_0)$$

2. Notice that $\alpha_u(\tau) = P^u(\tau,\theta)|_{\theta=\tau}$ with $P^u(\tau,\theta) = \sum a^u_{kl}\tau^l e^{ik\theta}$
3. Define **averaged** (or frozen) solution by $\bar{\alpha}_u(\tau) = P^u(\tau,0)$

$$Y(\tau) = y_0 + \sum_{u\in\mathcal{T}} \varepsilon^{|u|} \frac{\bar{\alpha}_u(\tau)}{\sigma_u} \mathcal{F}_u(y_0)$$

4. Define averaged vector field $\varepsilon F(Y,\tau)$ such that

$$\begin{cases} Y'(\tau) & = & \varepsilon F(Y(\tau),\tau) \\ Y(0) & = & y_0 \end{cases}$$

5. Notice that F is **autonomous** and **Hamiltonian** as soon as f is Hamiltonian.

The averaged vector field is autonomous

The vector field corresponding to $Y(\tau) = \bar{\Phi}_{\tau_0}^{\tau}(y_0)$ writes

$$F(Y,\tau) = \left(\frac{\partial \bar{\Phi}_{\tau_0}^{\tau}}{\partial \tau} \circ \left(\bar{\Phi}_{\tau_0}^{\tau}\right)^{-1}\right)(Y) = \sum_{u \in \mathcal{T}} \varepsilon^{|u|} \frac{\bar{\beta}_u(\tau)}{\sigma_u} \mathcal{F}_u(Y)$$

where $\bar{\beta}(\tau) = \bar{\alpha}^{-1}(\tau) * \bar{\alpha}'(\tau)$. Since $Y(\tau_{j+k}) = \left(\Phi_{\tau_0}^{\tau_0+2\pi}\right)^{j+k}(y_0)$:

$$\bar{\alpha}_u(\tau_j + \tau_k) = \bar{\alpha}_u(\tau_k) * \bar{\alpha}_u(\tau_j) = \bar{\alpha}_u(\tau_j) * \bar{\alpha}_u(\tau_k), \quad j,k = 0, \pm 1, \pm 2, \ldots$$

and by an interpolation argument

$$\forall k, \quad \forall \tau, \quad \bar{\alpha}_u(\tau + \tau_k) = \bar{\alpha}_u(\tau_k) * \bar{\alpha}_u(\tau).$$

Differentiating and taking the value at $\tau = 0$ gives

$$\forall k, \quad \bar{\alpha}'(\tau_k) = \bar{\alpha}(\tau_k) * \bar{\alpha}'(0),$$

so that by interpolation once again,

$$\forall \tau, \quad \bar{\alpha}'(\tau) = \bar{\alpha}(\tau) * \bar{\alpha}'(0) \text{ i.e. } \forall \tau, \quad \bar{\alpha}^{-1}(\tau) * \bar{\alpha}'(\tau) = \bar{\alpha}'(0).$$

The averaged vector field is Hamiltonian

If α is symplectic, the B-series $\bar{\alpha}$ remains symplectic

Since $\alpha_u(\tau) = P^u(\tau, \tau)$ with $P^u(\tau, \theta) := \sum a^u_{lk} \tau^l e^{ik\theta}$ we see that the symplecticity relation

$$\forall \tau, \quad \alpha_{u \circ v}(\tau) + \alpha_{v \circ u}(\tau) = \alpha_u(\tau) \alpha_v(\tau)$$

implies

$$\forall \tau, \forall \theta, \quad P_{u \circ v}(\tau, \theta) + P_{v \circ u}(\tau, \theta) = P_u(\tau, \theta) P_v(\tau, \theta)$$

and hence

$$\forall \tau, \quad \bar{\alpha}_{u \circ v}(\tau) + \bar{\alpha}_{v \circ u}(\tau) = \bar{\alpha}_u(\tau) \bar{\alpha}_v(\tau)$$

The numerical scheme

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

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

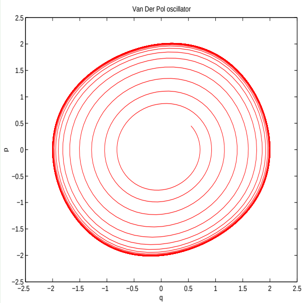
$$F(Y) \approx \frac{1}{4\pi}(\Phi_0^{2\pi}(Y) - \Phi_0^{-2\pi}(Y))$$

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

Nota : in the formulation $\dot{y} = f(t/\varepsilon, y)$, this gives rise to micro-steps $\delta t \ll \varepsilon$ alternating with macro-steps $\varepsilon \ll \Delta t \ll 1$.

The numerical scheme (2)

Example (Van Der Pol oscillator)



$$\begin{cases} \dot{q} &= p \\ \dot{p} &= -q + \varepsilon(1 - q^2)p \end{cases}$$

which, after the change of variables

$$\begin{aligned} q &= \cos(t)x + \sin(t)y \\ p &= -\sin(t)x + \cos(t)y \end{aligned}$$

writes

$$\begin{cases} \dot{x} &= -\sin(t)\,\varepsilon\,\left(1 - (\cos(t)\,x + \sin(t)\,y)^2\right)(-\sin(t)\,x + \cos(t)\,y) \\ \dot{y} &= \cos(t)\,\varepsilon\,\left(1 - (\cos(t)\,x + \sin(t)\,y)^2\right)(-\sin(t)\,x + \cos(t)\,y) \end{cases}$$

The numerical scheme (3)

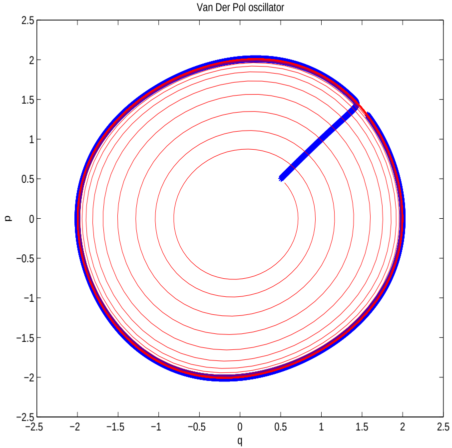


Figure: Exact solution (red) and numerical solution obtained by SAM (blue)

The numerical scheme : references

- P. Chartier, J.M. Sanz-Serna and A. Murua, Higher-order averaging, formal series and numerical integration I: B-series, FOCM, 2010.
- M.P. Calvo, P. Chartier, J.M. Sanz-Serna and A. Murua, A stroboscopic numerical method for highly oscillatory problems, submitted.
- P. Chartier, J.M. Sanz-Serna and A. Murua, Higher-order averaging, formal series and numerical integration II: the multi-frequency case, in preparation.

Application to the considered nonlinear Schrödinger equations

Theorem
The Perko formulae apply in our context, when conveniently rephrased in the B^N spaces:

one can define functions u_j, Y_j as in Perko, and averaging can be performed at any order, to provided $\phi_K^\varepsilon(t,x)$'s such that $\phi_K^\varepsilon(t,x) = \phi^\varepsilon(t,x) + \mathcal{O}(\varepsilon^K)$ in B^N, whenever $0 \leq t \leq T_0$.

Numerical counterpart
The above described numerical scheme, when conveniently adapted, provides the following results.

Application to the considered nonlinear Schrödinger equations (2)

In the case of

$$i\partial_t \psi^\varepsilon = \frac{1}{\varepsilon}\Delta_x + |\psi^\varepsilon|^2 \psi^\varepsilon$$

$x \in [0,1]$ with periodic boundary conditions, $t \in [0, \sqrt{2}/2\pi]$.

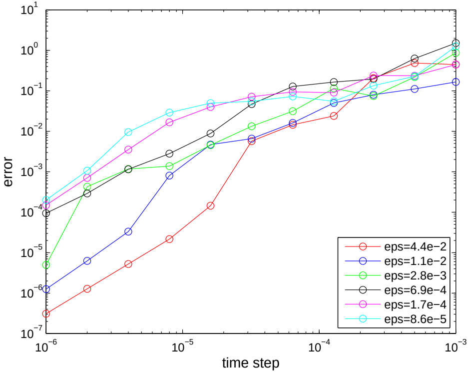


Figure: direct Strang splitting (order 2 if $\varepsilon \sim 1$)

Application to the considered nonlinear Schrödinger equations (3)

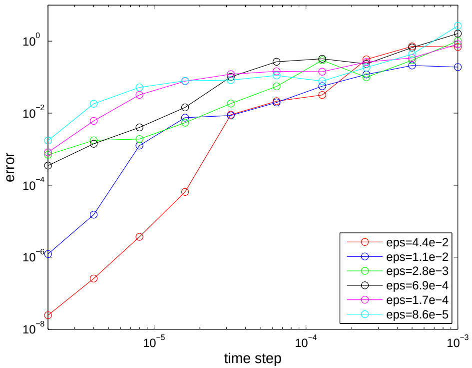


Figure: direct order 4 splitting

Application to the considered nonlinear Schrödinger equations (4)

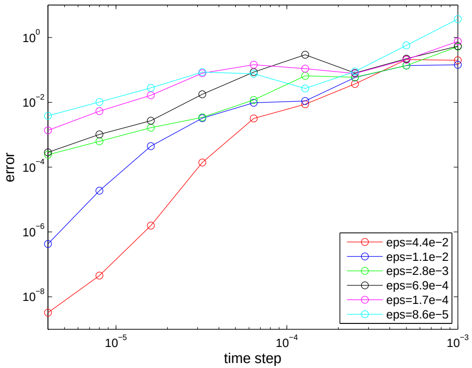


Figure: direct order 6 splitting

Application to the considered nonlinear Schrödinger equations (5)

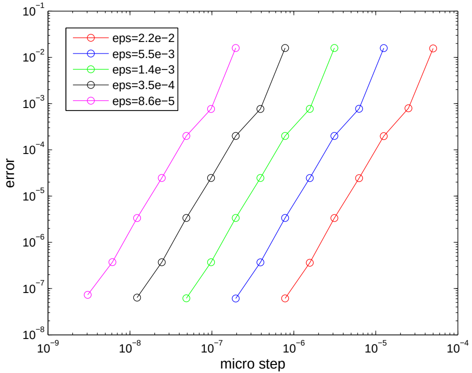


Figure: Stroboscopic averaging – constant numerical cost, various values of ε

Application to the considered nonlinear Schrödinger equations (6)

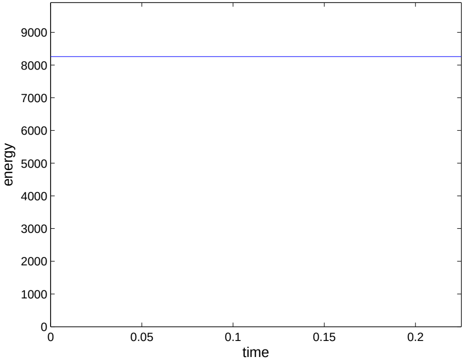


Figure: Energy conservation.

Application to the considered nonlinear Schrödinger equations (7)

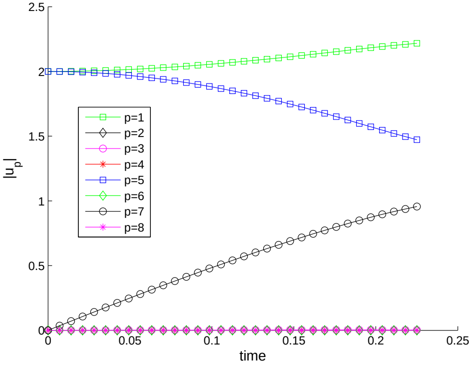


Figure: Evolution of modes 1 to 8 in the cubic NLS: modes 1 and 5 feed mode 7 (and only this mode).