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Asymptotically correct finite difference schemes for highly oscillatory ODEs

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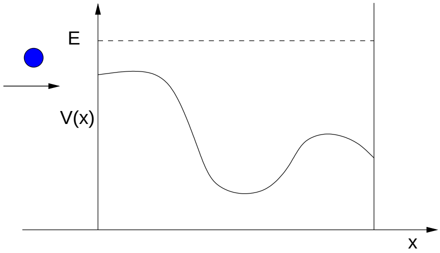
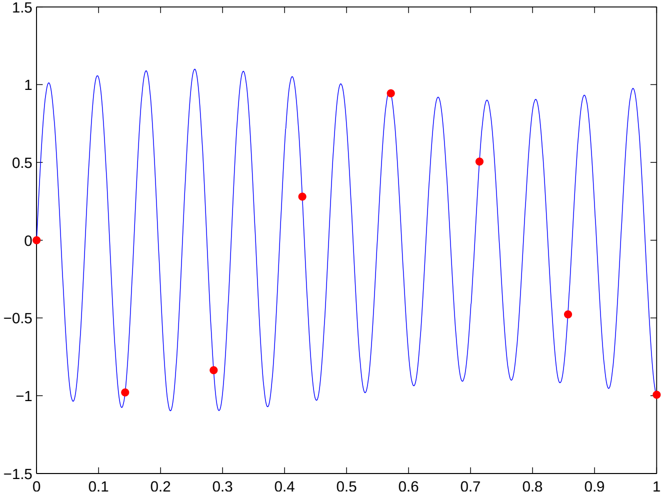
Goal

- stationary Schrödinger equation (1d):

$$\frac{\hbar^2}{2m}\psi_{xx}(x) + \underbrace{\big(E - V(x)\big)}_{\geq \alpha > 0}\psi(x) \quad = \quad 0$$

with inhomogeneous open BCs $\rightarrow$ reformulate as IVP





GOAL: accurate numerical scheme that does NOT NEED to resolve the oscillations

Outline:

1. transformation of ODE $\longrightarrow$ separate highly oscillatory term & smooth perturbation
2. approximation of oscillatory integrals
3. error orders
4. numerical example

vector valued ODEs

- revisit problem of Lorenz, Jahnke, Lubich [LJL 2005]
- inital value problem: $\psi(x) \in \mathbb{C}^d$

$$\begin{aligned} \psi''(x) + \frac{1}{\varepsilon^2} A(x)\,\psi(x) &= 0\,, \quad x \in (x_0, x_{end}) \\ \psi(x_0) &= \psi_0\,, \\ \psi'(x_0) &= \psi_0'\,. \end{aligned}$$

- assumptions: $\mathbb{R}^{d\times d} \ni A(x) = Q(x)a(x)Q^*(x) > 0$
  - $Q(x)$ orthogonal, smooth
  - a diagonal smooth
  - eigenvalues a_j remain separated:

$$|a_k(x) - a_l(x)| \geq \delta\,, \qquad a_k(x) \geq \tfrac{1}{2}\delta, \quad k \neq l$$

Separation of highly oscillatory term + slow perturbation

- the ansatz $u_1 := \psi$, $u_2 := \varepsilon A^{-\frac{1}{2}}\psi'$ yields

$$u' = \frac{1}{\varepsilon}\begin{pmatrix} 0 & A^{\frac{1}{2}} \\ -A^{\frac{1}{2}} & 0 \end{pmatrix} u - \begin{pmatrix} 0 & 0 \\ 0 & A^{-\frac{1}{2}}(A^{\frac{1}{2}})' \end{pmatrix} u\,.$$

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- diagonalisation of the first matrix via $v := Pu$:

$$v' = \frac{i}{\varepsilon}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes a^{\frac{1}{2}}\, v - \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \otimes \mu\, v + I \otimes \left(Q^{*\prime} Q\right) v \,,$$

$$\mu := \tfrac{1}{2} Q^* A^{-\frac{1}{2}}(A^{\frac{1}{2}})' Q \,.$$

($\otimes$ denotes the *Kronecker* product)

Explicit transformation of high oscillations

- to simplify notation let $d = 1$ (Schrödinger equ., $a(x) = V(x) - E$):

$$v' = \frac{i}{\varepsilon} a^{\frac{1}{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} v - \frac{a'}{4a} \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} v$$

- def. phase (exactly integrable for $V(x)$ piecewise linear, e.g.):

$$\phi(x) := \int_{x_0}^{x} a^{\frac{1}{2}}(s)\, ds \qquad (\omega = e^{-\frac{i\phi}{\varepsilon}})$$

$$F(x) := \exp\left(-\frac{i}{\varepsilon} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \phi(x) \right) =: \begin{pmatrix} \omega & 0 \\ 0 & \overline{\omega} \end{pmatrix}$$

- let $\eta := F\, v$

$$\eta' = -\frac{a'}{4a} \begin{pmatrix} 1 & -i\omega^2 \\ i\overline{\omega}^2 & 1 \end{pmatrix} \eta =: \Omega\, \eta$$

$\Rightarrow$ new system matrix is ε–uniformly bounded $\Rightarrow$ η "smoother"

numerical integration

- let $x_0 < x_1 < \cdots < x_N = x_{end}$ be an equidistant grid with stepsize $h = |x_n - x_{n+1}|$
- goal: second order scheme
- integration from x_n to x_{n+1} yields

$$\begin{aligned}
\eta_{n+1} &= \eta_n + \int_{x_n}^{x_{n+1}} \Omega(s)\, ds\, \eta_n \\
&\quad + \int_{x_n}^{x_{n+1}} \Omega(s) \int_{x_n}^{s} \Omega(r)\eta(r)\, dr\, ds \\
&= \eta_n + \int_{x_n}^{x_{n+1}} \Omega(s)\, ds\, \eta_n \\
&\quad + \int_{x_n}^{x_{n+1}} \Omega(s) \int_{x_n}^{s} \Omega(r)\, dr\, ds\, \eta_n + \mathcal{O}(h^3)
\end{aligned}$$

Approximation of the Integral

- use standard quadrature rules for the diagonal of the first integral (non-oscillating entries)
- the off-diagonal elements have the same structure, i.e.

$$\mathcal{I} \;:=\; \int_{x_n}^{x_{n+1}} \Omega_{21}(s)\, ds \;=\; -\int_{x_n}^{x_{n+1}} e^{\frac{2i}{\varepsilon}\phi(s)} \cdot \frac{a'(s)}{4a(s)}\, ds$$

- two strategies
  1. replacing ϕ by $\phi_n + s\phi_n' + \frac{s^2}{2}\phi_n''$ leads to the *adiabatic midpoint rule* proposed by [LJL] (integration interval: $[x_{n-1}, x_{n+1}]$!)
  2. manipulate $\frac{a'}{4a}$ in order to exactly integrate the remaining integral (*AA, Ben Abdallah, Negulescu*)

Details for integral strategy (2)

- factorize the integrand ($\phi' = a$) in:

$$\mathcal{I} = -\int_{x_n}^{x_{n+1}} \underbrace{e^{\frac{2i}{\varepsilon}\phi(s)} \frac{2i\phi'(s)}{\varepsilon}}_{=\left(e^{\frac{2i}{\varepsilon}\phi}\right)' \text{ ... oscill.}} \cdot \underbrace{\frac{\varepsilon}{2i\phi'(s)} \frac{a'(s)}{4a(s)}}_{=:f \text{ ... “smooth”}} ds$$

IDEA: approximate only the smooth factor, integrate oscill. factor exactly

- approximate f:
  $f \approx \alpha + \beta\phi$ ($\rightarrow$ second order)
  α, β are determined by interpolation
- the double integral is treated analogously

Properties of the scheme

- both strategies yield a scheme of $\mathcal{O}(h^2)$
- error estimates independent of ε,
  even for $h > \varepsilon$ (if phase $\Phi = \int \sqrt{a(s)}\, ds$ is exact)
- both methods are exact for constant A
- the oscillatory integrals are of order ε:

$$\int_a^b e^{\frac{\phi(x)}{\varepsilon}} f(x)\, dx = \int_a^b e^{\frac{\phi}{\varepsilon}} \frac{\phi'}{\varepsilon} \cdot \frac{\varepsilon}{\phi'} f\, dx$$

$$= e^{\frac{\phi}{\varepsilon}} \frac{\varepsilon}{\phi'} f \Big|_{x=a}^{b} - \varepsilon \int_a^b e^{\frac{\phi}{\varepsilon}} \left(\frac{f}{\phi'}\right)' dx$$

Is it possible to benefit from these property?

Improved scheme

- previous equation:

$$\eta' = -\frac{a'}{4a}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\eta + i\frac{a'}{4a}\begin{pmatrix} 0 & \omega^2 \\ -\overline{\omega}^2 & 0 \end{pmatrix}\eta$$

- "remove" the diagonal part by transformation: $w := a^{\frac{1}{4}}(x)\,\eta$

$$w' = i\frac{a'}{4a}\begin{pmatrix} 0 & \omega^2 \\ -\overline{\omega}^2 & 0 \end{pmatrix} w = \tilde{\Omega}\, w, \quad \omega = e^{-i\frac{\Phi}{\varepsilon}}$$

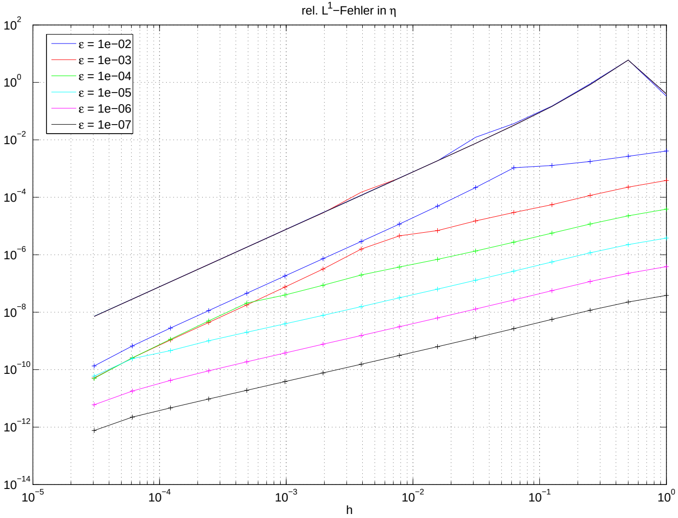
- same structure as η–equation
  $\Rightarrow$ replace Ω by $\tilde{\Omega}$ in the previous numerical scheme
- strong ε–limit: $w(x) = w(x_0)$ (for $a(x)$ smooth)
- improved error estimate: $\mathcal{O}(\min(h,\varepsilon)\cdot h)$!
- scheme asymptotically correct as $\varepsilon \to 0$ (for $h = const$!)

Numerical Example

- example from [LJL 2005]: $d = 2$, $x \in [-1, 1]$

$$
\begin{aligned}
a^{\frac{1}{2}}(x) &= \left(\tfrac{3}{2}x + 3\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \tfrac{\sqrt{x^2+4}}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
Q(x) &= \begin{pmatrix} \cos\xi(x) & -\sin\xi(x) \\ \sin\xi(x) & \cos\xi(x) \end{pmatrix}, \text{ with} \\
\xi(x) &= \tfrac{\pi}{4} + \tfrac{1}{2}\arctan\left(\tfrac{x}{2}\right)
\end{aligned}
$$

- error in [LJL 2005]: $\mathcal{O}(h^2)$ (uniformly in ε)



- error of improved scheme: $\mathcal{O}(\min(h, \varepsilon) \cdot h)$
- work in progress: error $= \mathcal{O}(\varepsilon h^2)$ (with "better" transformations)