

Asymptotically correct finite difference schemes for highly oscillatory ODEs

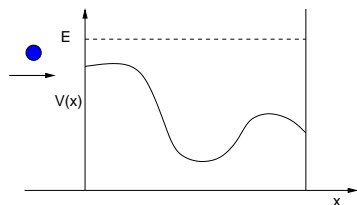
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UCLA, March 2009

Application: electron injection in semiconductor



often: coupled problem for all energies $E > 0$;
sharp transmission peaks w.r.t. E

future: couple oscillatory to evanescent regime: $E < V(x)$

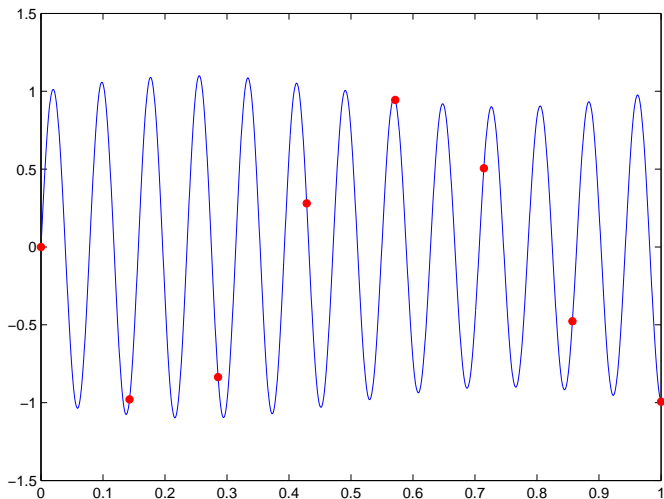
- stationary Schrödinger equation (1d):

$$\underbrace{\frac{\hbar^2}{2m}}_{=\varepsilon^2} \varphi_{xx}(x) + \underbrace{(E - V(x))}_{=a(x) \geq \alpha > 0} \varphi(x) = 0, \quad x \in (0, 1)$$

- inhomogeneous open BCs:

$$\varepsilon \varphi_x(0) + i\sqrt{a(0)}\varphi(0) = 2i\sqrt{a(0)}, \quad \varepsilon \varphi_x(1) - i\sqrt{a(1)}\varphi(1) = 0$$

- reformulate as (backward) IVP for ψ : $\varphi(x) = \frac{2i\sqrt{a(0)}}{\varepsilon\psi_x(0) + i\sqrt{a(0)}\psi(0)} \psi(x)$



- wavelength = $\mathcal{O}(\varepsilon/\sqrt{a(x)})$; **GOAL:** use stepsize $h > \varepsilon$
- \rightarrow accurate scheme that does NOT NEED to resolve the oscillations

GOAL: numerical scheme for $\varepsilon^2 \varphi_{xx} + a(x)\varphi = 0$

Outline:

- 1 analytic WKB-transformation of scalar ODE \rightarrow separate highly oscillatory term & smooth perturbation
- 2 scheme: correct uniformly in ε
- 3 approximation of oscillatory integrals
- 4 error estimates
- 5 numerical example
- 6 extension to vector systems

(1) WKB-method \rightarrow for analytic preprocessing of ODE

WKB-ansatz for $\varepsilon^2 \varphi_{xx} + a(x)\varphi = 0$:

$$\varphi(x) \sim \exp\left(\frac{1}{\varepsilon} \sum_{p=0}^{\infty} \varepsilon^p \phi_p(x)\right)$$

- zeroth order: $\varphi(x) \approx C \exp\left(\pm \frac{i}{\varepsilon} \int_0^x \sqrt{a} d\tau\right)$

- first order:

$$\varphi(x) \approx C \frac{\exp\left(\pm \frac{i}{\varepsilon} \int_0^x \sqrt{a} d\tau\right)}{\sqrt[4]{a(x)}}$$

- second order:

$$\varphi(x) \approx C \frac{\exp\left(\pm \frac{i}{\varepsilon} \int_0^x \sqrt{a(\tau)} - \varepsilon^2 \beta(\tau) d\tau\right)}{\sqrt[4]{a(x)}}, \quad \beta := \frac{a''}{8a^{3/2}} - \frac{5(a')^2}{32a^{5/2}}$$

- all: asymptotically correct for $\varepsilon \rightarrow 0$

WKB-FEM

[Ben Abdallah-Pinaud, 2006], [Negulescu, 2008]:

- 1st order WKB-approximation on (x_n, x_{n+1}) :

$$\psi(x) = \frac{1}{\sqrt[4]{a(x)}} \left(A_n e^{i\frac{\phi_n(x)}{\varepsilon}} + B_n e^{-i\frac{\phi_n(x)}{\varepsilon}} \right)$$

$$\text{phase: } \phi_n(x) = \int_{x_n}^x \sqrt{a(\tau)} d\tau,$$

- real WKB-basis functions on cell (x_n, x_{n+1}) :

$$\alpha_n(x) = -\frac{\sin \frac{\phi_{n+1}(x)}{\varepsilon}}{\sin \frac{\phi_n(x_{n+1})}{\varepsilon}} \sqrt[4]{\frac{a(x_n)}{a(x)}}, \quad \beta_n(x) = \frac{\sin \frac{\phi_n(x)}{\varepsilon}}{\sin \frac{\phi_n(x_{n+1})}{\varepsilon}} \sqrt[4]{\frac{a(x_{n+1})}{a(x)}}$$

- need “no-resonance condition” for linear independence:

$$\left| \frac{\phi_n(x_{n+1})}{\varepsilon} - k\pi \right| \geq \gamma > 0, \quad \forall k \in \mathbb{Z}$$

⇒ use finite differences instead

2nd order WKB transformation [AA-B.Abdallah-Negulescu]

① vector system:

$$U(x) := \begin{pmatrix} \sqrt[4]{a}\varphi(x) \\ \frac{\varepsilon(\sqrt[4]{a}\varphi)'(x)}{\sqrt{a}(x)} \end{pmatrix} \rightarrow U' = \left[\frac{1}{\varepsilon} \begin{pmatrix} 0 & \sqrt{a} \\ -\sqrt{a} & 0 \end{pmatrix} + \varepsilon \begin{pmatrix} 0 & 0 \\ 2\beta(x) & 0 \end{pmatrix} \right] U$$

2nd order WKB transformation [AA-B.Abdallah-Negulescu]

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② diagonalize dominant part:

$$Y(x) := \frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} U \rightarrow Y' = \left[\frac{i}{\varepsilon} \begin{pmatrix} \sqrt{a} - \varepsilon^2\beta & 0 \\ 0 & -\sqrt{a} + \varepsilon^2\beta \end{pmatrix} + \varepsilon \begin{pmatrix} 0 & \beta \\ \beta & 0 \end{pmatrix} \right] Y$$

2nd order WKB transformation [AA-B.Abdallah-Negulescu]

1 vector system:

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2 diagonalize dominant part:

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3 eliminate leading oscillation:

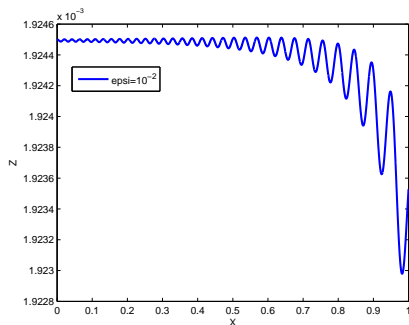
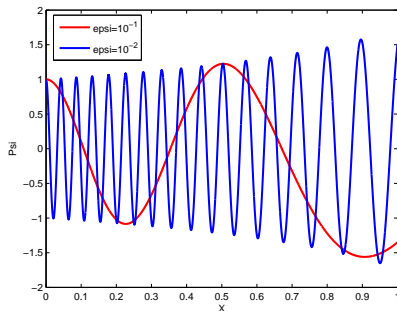
$$Z(x) := \begin{pmatrix} e^{-\frac{i}{\varepsilon}\phi(x)} & 0 \\ 0 & e^{\frac{i}{\varepsilon}\phi(x)} \end{pmatrix} Y(x) \rightarrow Z' = \underbrace{\varepsilon \begin{pmatrix} 0 & \beta e^{-\frac{2i}{\varepsilon}\phi(x)} \\ \beta e^{\frac{2i}{\varepsilon}\phi(x)} & 0 \end{pmatrix}}_{\mathcal{O}(\varepsilon)} Z$$

$$\phi(x) := \int_0^x \sqrt{a} - \varepsilon^2\beta \, d\tau \quad \dots \text{ phase of 2}^{nd} \text{ order WKB-approximation}$$

dominant oscillations eliminated:

ex: $\varepsilon^2 \varphi_{xx} + a(x)\varphi = 0$; $a(x) = (x + \frac{1}{2})^2$, $x \in (0, 1)$

- Z much smoother than φ or $U \rightarrow$ numerics easier



solution $\Re \varphi(x)$ for 2 values of ε ;

solution $\Re z_1(x)$: same frequency,
amplitude = $\mathcal{O}(10^{-5})$

$$\|U\|_{L^\infty(0,1)} \leq C, \quad \|U'\|_{L^\infty(0,1)} \leq \frac{C}{\varepsilon}; \quad \|Z - Z_I\|_\infty \leq C\varepsilon^2, \quad \|Z'\|_\infty \leq C\varepsilon$$

(2) GOAL: ε -uniform scheme

$$Z' = \varepsilon \underbrace{\begin{pmatrix} 0 & \beta(x)e^{-\frac{2i}{\varepsilon}\phi(x)} \\ \beta(x)e^{\frac{2i}{\varepsilon}\phi(x)} & 0 \end{pmatrix}}_{=:N(x)=\mathcal{O}(1)} Z, \quad x \in (0, 1); Z(0) = Z_I$$

- **strong asymptotic limit** $Z^{\varepsilon=0}(x) = Z_I$... trivial to capture numerically
 \Rightarrow **asymptotically correct scheme**; i.e. error = $\mathcal{O}(\varepsilon^p)$ for some $p \geq 2$
- **ε -uniform approximation** (truncated Picard iteration):

$$Z(x) = Z_I + \varepsilon \int_0^x N(y_1) dy_1 Z_I + \varepsilon^2 \int_0^x N(y_1) \int_0^{y_1} N(y_2) dy_2 dy_1 Z_I + \mathcal{O}(\varepsilon^3 x^2 \min(\varepsilon, x))$$

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- Remark: lower order WKB-transformations \rightarrow **non-const. limit** $Z^{\varepsilon=0}$
 \Rightarrow only **ε -uniform scheme**; i.e. error = $\mathcal{O}(1)$
[Lorenz-Jahnke-Lubich, 2005]

(3) Approximation of oscillatory integrals

GOAL: ε -uniform approximation of $J = \int_{x_n}^{x_{n+1}} \underbrace{\beta(y)}_{\text{smooth}} \underbrace{e^{\frac{2i}{\varepsilon}\phi(y)}}_{\text{oscillatory}} dy$

(+ iterated \int 's)

+ to arbitrary h -order !

- **asymptotic method** [Iserles-Nørsett, 2005]:

$$J = -i\varepsilon \left[\frac{\beta}{2\phi'} e^{\frac{2i}{\varepsilon}\phi} \right]_{x_n}^{x_{n+1}} + \mathcal{O}(\min(\varepsilon^2, \varepsilon h))$$

integration by parts yields higher ε -orders but *no* h -consistency for ODE

- **Filon method** [Iserles-Nørsett, 2005]:

would need exact moments $J \approx \int_{x_n}^{x_{n+1}} \underbrace{\pi(y)}_{\text{polynomial}} e^{\frac{2i}{\varepsilon}\phi(y)} dy$

modified asympt. method [AA-B.Abdallah-Negulescu '09]

$$\begin{aligned} J &= e^{\frac{2i}{\varepsilon}\phi(x_n)} \int_{x_n}^{x_{n+1}} \beta(y) e^{\frac{2i}{\varepsilon}[\phi(y)-\phi(x_n)]} dy \\ &= -i\varepsilon e^{\frac{2i}{\varepsilon}\phi(x_n)} \int_{x_n}^{x_{n+1}} \frac{\beta}{2\phi'} \frac{d}{dy} \left(e^{\frac{2i}{\varepsilon}[\phi(y)-\phi(x_n)]} - 1 \right) dy \\ &= -i\varepsilon e^{\frac{2i}{\varepsilon}\phi(x_n)} \frac{\beta}{2\phi'}(x_{n+1}) \left(e^{\frac{2i}{\varepsilon}[\phi(x_{n+1})-\phi(x_n)]} - 1 \right) + \mathcal{O}(\min(\varepsilon h, h^2)) \end{aligned}$$

- idea: include a **zero of oscillatory factor** by shift
⇒ **change ε -power to h -power**
- 1^{st} order consistent, ε -asymptotically correct ODE-method

Resulting methods

- first h -order: $Z_{n+1} = (I + A_n^1) Z_n$
- second h -order: $Z_{n+1} = (I + A_n^1 + A_n^2) Z_n$

$$A_n^1 := -i\varepsilon^2 \frac{\beta}{2\phi'}(x_{n+1}) \begin{pmatrix} 0 & e^{-\frac{2i}{\varepsilon}\phi(x_n)} - e^{-\frac{2i}{\varepsilon}\phi(x_{n+1})} \\ e^{\frac{2i}{\varepsilon}\phi(x_{n+1})} - e^{\frac{2i}{\varepsilon}\phi(x_n)} & 0 \end{pmatrix}$$

$$A_n^2 := \dots$$

(4) Error estimates

Theorem ([ABN '09])

$$\|Z(x_n) - Z_n\| \leq C \varepsilon^p h^{\alpha-1} \min(\varepsilon, h), \quad 1 \leq n \leq N,$$

$$\|U(x_n) - U_n\| \leq C \frac{h^\gamma}{\varepsilon} + C \varepsilon^p h^{\alpha-1} \min(\varepsilon, h), \quad 1 \leq n \leq N$$

$p = 1$

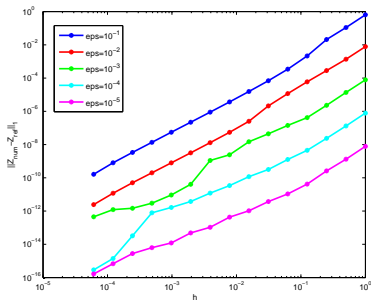
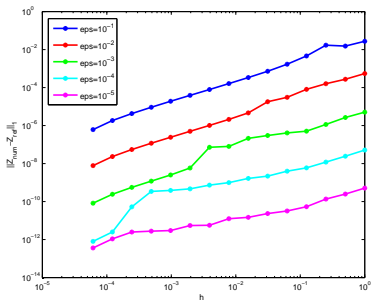
$\alpha = 1, 2 \dots$ h -order of method

$\gamma \dots$ order of quadrature rule for phase $\phi(x) = \int_0^x \sqrt{a} - \varepsilon^2 \beta \, d\tau$

- Simpson ($\gamma = 4$) \Rightarrow constraint $h = \mathcal{O}(\sqrt{\varepsilon})$ for 2nd order scheme
- ϕ exact for potential $a(x)$ piecewise linear (e.g. in RTD)
 $\Rightarrow \varepsilon$ -asymptotically correct scheme also for U
- simple improvement: $p = 2$ (note: $\|Z(x) - Z_I\| \leq C\varepsilon^2$)

(5) Numerical example

- $\varepsilon^2 \varphi_{xx} + a(x)\varphi = 0$ with $a(x) = (x + \frac{1}{2})^2$
→ phase $\phi = \int_0^x \sqrt{a(\tau)} - \varepsilon^2 \beta(\tau) d\tau$ explicitly integrable



- $L^1(0, 1)$ -error of Z (as function of h) for first & second order schemes
- schemes are asymptotically correct (error = $\mathcal{O}(\varepsilon^2)$, for h fixed !)

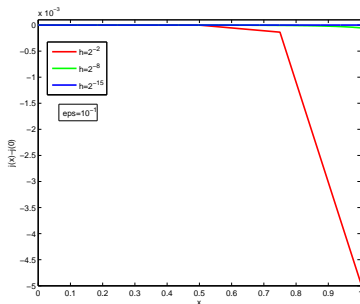
Current conservation

- continuous current:

$$j(x) := \varepsilon \Im(\bar{\varphi}(x)\varphi'(x)) = \frac{1}{2} Z(x)^\top \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \bar{Z}(x) = \text{const in } x$$

- discrete current: $j_n := \frac{1}{2} Z_n^\top \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \bar{Z}_n$

- slightly drifts: $j_{n+1} - j_n =: -\varepsilon^4 \lambda^2 j_n$



- simple fix by scaling possible: $\tilde{Z}_{n+1} = (1 - \varepsilon^4 \lambda^2)^{-1/2} (I + A_n^1) \tilde{Z}_n$

(6) Vector valued ODEs

- initial value problem: $\varphi(x) \in \mathbb{C}^d$

$$\begin{aligned}\varphi''(x) + \frac{1}{\varepsilon^2} A(x) \varphi(x) &= 0, \\ \varphi(0) &= \varphi_0, \\ \varphi'(0) &= \varphi'_0.\end{aligned}$$

- assumptions: $\mathbb{R}^{d \times d} \ni A(x) = Q(x)a(x)Q^*(x) > 0$

- ▶ $Q(x)$... orthogonal, smooth
- ▶ eigenvalues a_j remain separated:

$$|a_k(x) - a_l(x)| \geq \delta > 0, \quad a_k(x) \geq \frac{1}{2}\delta, \quad k \neq l$$

- ▶ $\Rightarrow a(x)$... diagonal matrix, smooth

analytic transformation I: 0^{th} order WKB [LJL]

1 vector system:

$$U(x) := \begin{pmatrix} \varphi \\ \varepsilon A^{-\frac{1}{2}} \varphi' \end{pmatrix} \in \mathbb{C}^{2d} \rightarrow U' = \left[\begin{array}{c} \frac{1}{\varepsilon} \begin{pmatrix} 0 & A^{\frac{1}{2}} \\ -A^{\frac{1}{2}} & 0 \end{pmatrix} - \underbrace{\begin{pmatrix} 0 & 0 \\ 0 & A^{-\frac{1}{2}} (A^{\frac{1}{2}})' \end{pmatrix}}_{\text{only } \mathcal{O}(1)} \end{array} \right] U$$

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2 diagonalize dominant part:

$$Y(x) := \frac{1}{\sqrt{2}} \begin{pmatrix} Q^*(x) & -iQ^*(x) \\ -iQ^*(x) & Q^*(x) \end{pmatrix} U$$

$$\rightarrow Y' = \left[\begin{array}{c} \frac{i}{\varepsilon} \begin{pmatrix} a^{\frac{1}{2}} & 0 \\ 0 & -a^{\frac{1}{2}} \end{pmatrix} - \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \otimes \mu + I \otimes (Q^* Q') \end{array} \right] Y,$$

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

(\otimes ... Kronecker product)

analytic transformation II: 0th order WKB [LJL]

- 3 eliminate leading oscillation:

$$Z(x) := \begin{pmatrix} e^{-\frac{i}{\varepsilon}\phi(x)} & 0 \\ 0 & e^{\frac{i}{\varepsilon}\phi(x)} \end{pmatrix} Y(x) \rightarrow Z' = \left[-\frac{1}{4} \begin{pmatrix} a^{-1}a' & 0 \\ 0 & a^{-1}a' \end{pmatrix} + \underbrace{N^\varepsilon(x)}_{=\mathcal{O}(1)} \right] Z$$

$$\phi(x) := \int_0^x a^{\frac{1}{2}}(\tau) d\tau \dots \text{phase of } 0^{\text{th}}/1^{\text{st}} \text{ order WKB-approx., diag. matrix}$$

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$\phi(x) := \int_0^x a^{\frac{1}{2}}(\tau) d\tau$... phase of 0^{th} / 1^{st} order WKB-approx., diag. matrix

- 4 optional improvement – 1^{st} order WKB:

$$\tilde{Z}(x) := \begin{pmatrix} a^{\frac{1}{4}}(x)e^{-\frac{i}{\varepsilon}\phi(x)} & 0 \\ 0 & a^{\frac{1}{4}}(x)e^{\frac{i}{\varepsilon}\phi(x)} \end{pmatrix} Y(x) \rightarrow \tilde{Z}' = \underbrace{\tilde{N}^\varepsilon(x)}_{\text{off diag., } \mathcal{O}(1)} \tilde{Z}$$

$$\Rightarrow \tilde{Z} = Z_I + \mathcal{O}(\varepsilon)$$

2 approaches for vector systems

- [LJL '05]: 0th order WKB; standard treatment of oscillatory integrals
- [Geier-AA '09]: 1st order WKB;
for oscillatory integrals: shifted asymptotic method or moment-free Filon-type [Olver '06]
- both second h -order

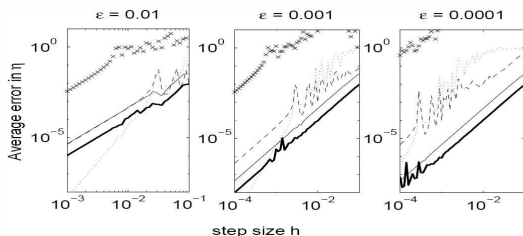
Numerical example

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

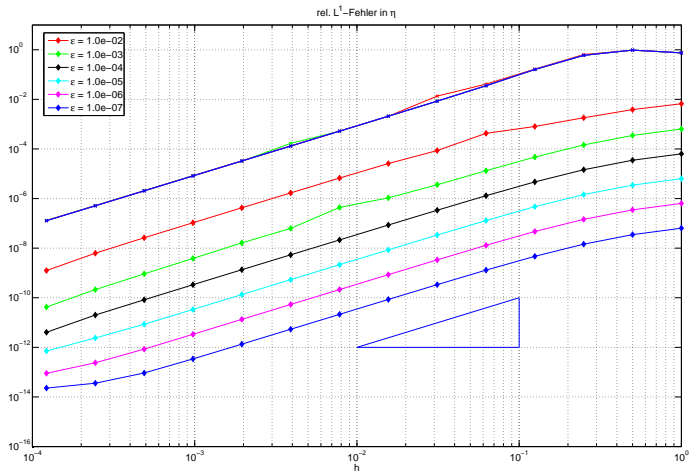
$$a^{\frac{1}{2}}(x) = \left(\frac{3}{2}x + 3\right) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{\sqrt{x^2+4}}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$Q(x) = \begin{pmatrix} \cos \xi(x) & -\sin \xi(x) \\ \sin \xi(x) & \cos \xi(x) \end{pmatrix}, \text{ with}$$

$$\xi(x) = \frac{\pi}{4} + \frac{1}{2} \arctan\left(\frac{x}{2}\right), \quad \phi(x) \text{ exactly computable}$$



- [LJL '05]: error $= \mathcal{O}(h^2)$ (uniformly in ε), but NO ε -convergence of Z



← [LJL'05]

[Geier-AA]

● error in $Z = \mathcal{O}(\epsilon h^2)$