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Asymptotically correct finite difference schemes for highly oscillatory ODEs

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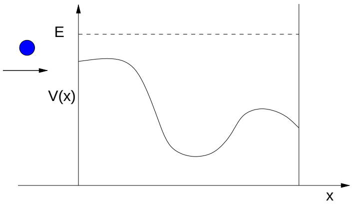
Beijing, April 2009

Application: electron injection in semiconductor (diode)



- stationary Schrödinger equation (1d):

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

- 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: $\varphi(x) = \frac{2i\sqrt{a(0)}}{\varepsilon\psi_x(0)+i\sqrt{a(0)}\psi(0)}\psi(x)$

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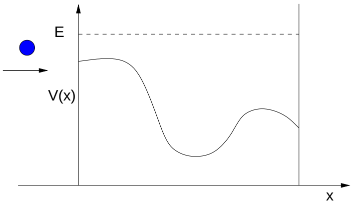

often: coupled problem for all energies $E > 0$;
sharp transmission peaks w.r.t. E

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

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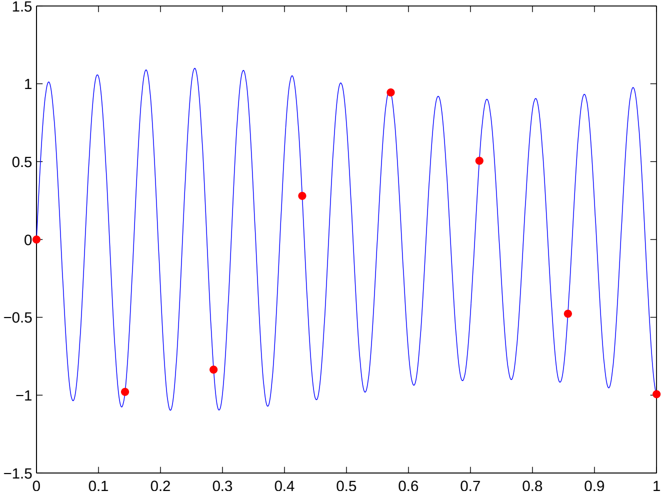

- wavelength $= \mathcal{O}(\varepsilon/\sqrt{a(x)})$; GOAL: use stepsize $h > \lambda$
- $\rightarrow$ accurate scheme that does NOT NEED to resolve the oscillations

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

Outline:

1. analytic WKB-transformation of scalar ODE $\longrightarrow$ 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 → for analytic preprocessing of ODE

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

$$\varphi(x) \sim \exp\left(\frac{i}{\varepsilon}\sum_{p=0}^{\infty}\varepsilon^p \phi_p(x)\right), \quad \phi_p \in \mathbb{C}$$

- 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 $\varepsilon \to 0$

WKB-FEM

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

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

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

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

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

$\Rightarrow$ use finite differences instead

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

1. vector system from $\varepsilon^2\varphi_{xx} + a(x)\varphi = 0$:

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

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2. diagonalize dominant part:

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

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3. eliminate leading oscillation:

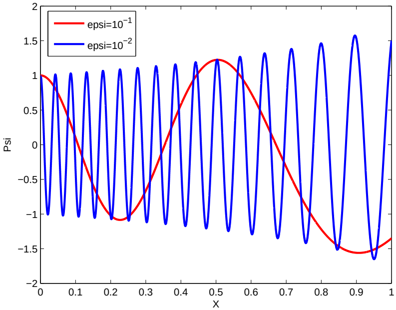
$$Z(x) := \begin{pmatrix} e^{-\frac{i}{\varepsilon}\phi(x)} & 0 \\ 0 & e^{\frac{i}{\varepsilon}\phi(x)} \end{pmatrix} Y(x) \rightarrow Z' = \underbrace{\varepsilon \begin{pmatrix} 0 & \beta e^{-\frac{2i}{\varepsilon}\phi(x)} \\ \beta e^{\frac{2i}{\varepsilon}\phi(x)} & 0 \end{pmatrix}}_{\mathcal{O}(\varepsilon)}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

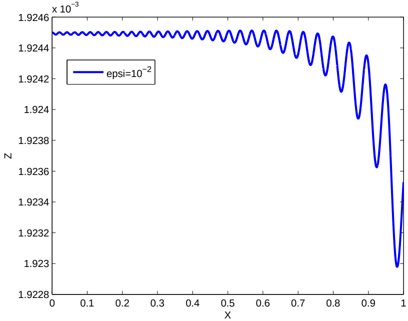
$$\phi(x) := \int_0^x \sqrt{a} - \varepsilon^2\beta \, d\tau$$ ... phase of 2^{nd} order WKB-approximation

dominant oscillations eliminated:

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

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





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

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

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

(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
  $\Rightarrow$ change ε–power to h–power
- 1^{st} order consistent, ε–asymptotically correct ODE-method

Resulting methods

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

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

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

$$A_n^2 := \ \dots$$

(4) Error estimates

Theorem ([ABN '09])

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

$p = 1$

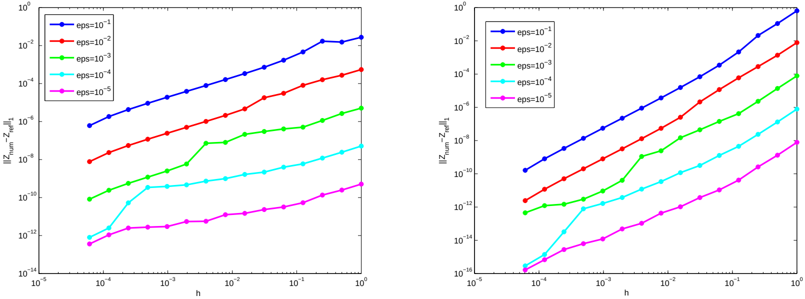
$\alpha = 1, 2$ ... h–order of method

γ ... 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 2^{nd} order scheme
- ϕ exact for potential $a(x)$ piecewise linear (e.g. in RTD) $\Rightarrow$ ε–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 $a(x) = (x + \frac{1}{2})^2$
  $\rightarrow$ phase $\phi = \int_0^x \sqrt{a(\tau)} - \varepsilon^2 \beta(\tau)\, d\tau$ explicitly integrable



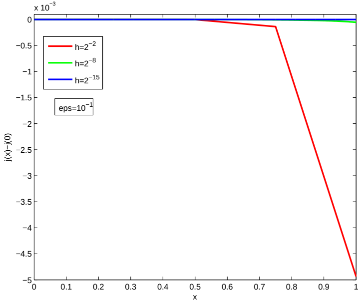
- $L^1(0,1)$–error of Z (as function of h) for first & second order schemes
- schemes are asymptotically correct (error $= \mathcal{O}(\varepsilon^2)$, for h fixed !)

Current conservation

- continuous current:

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

- discrete current: $j_n := \frac{1}{2} Z_n^\top \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \overline{Z}_n$
- slightly drifts: $j_{n+1} - j_n =: -\varepsilon^4 \lambda^2 j_n$



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

(6) Vector valued ODEs

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

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

- 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:

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

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

analytic transformation I: 0^{th} order WKB [L-J-Lubich]

1. vector system:

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

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2. diagonalize dominant part:

$$\begin{aligned} Y(x) &:= \frac{1}{\sqrt{2}} \begin{pmatrix} Q^*(x) & -iQ^*(x) \\ -iQ^*(x) & Q^*(x) \end{pmatrix} U \\ \rightarrow Y' &= \left[\frac{i}{\varepsilon} \begin{pmatrix} a^{\frac{1}{2}} & 0 \\ 0 & -a^{\frac{1}{2}} \end{pmatrix} - \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \otimes \mu + I \otimes (Q^* Q') \right] Y\,, \\ \mu &:= \frac{1}{2} Q^* A^{-\frac{1}{2}} (A^{\frac{1}{2}})' Q \end{aligned}$$

($\otimes$ ... *Kronecker* product)

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

3. eliminate leading oscillation:

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

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

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

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

$\Rightarrow \tilde{Z} = Z_I + \mathcal{O}(\varepsilon) \quad \to$ asymptotically correct scheme possible !

2 approaches for vector systems

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

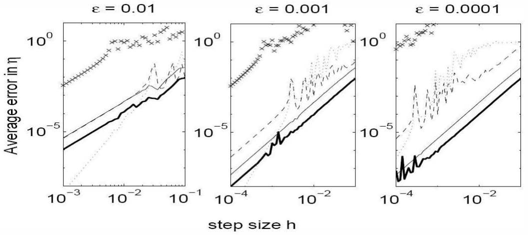
Numerical example

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

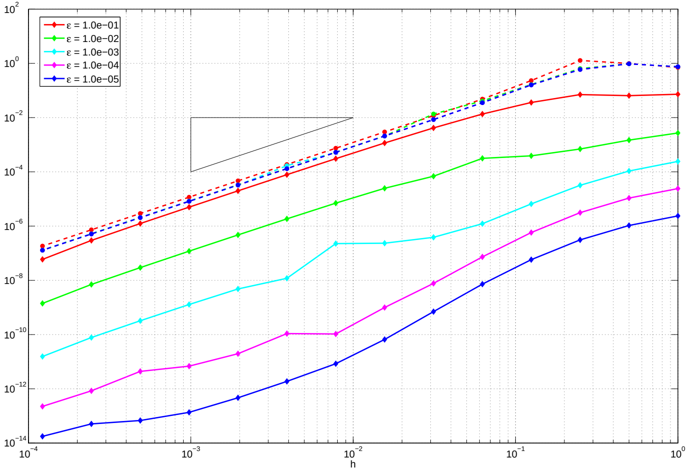
$$a^{\frac{1}{2}}(x) = \left(\tfrac{3}{2}x + 3\right)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{\sqrt{x^2+4}}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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

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



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



← [LJL'05]

[Geier-AA]

- error in $Z = \mathcal{O}(\varepsilon h \min(\varepsilon, h))$