VIENNA
UNIVERSITY OF
TECHNOLOGY

# A hybrid WKB-based method for the stationary Schrödinger equation in the semi-classical limit

Anton ARNOLD

with C. Negulescu (Toulouse); K. Döpfner; C. Klein (Dijon), B. Ujvari

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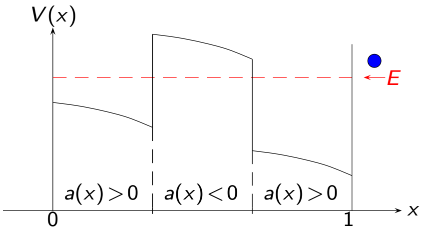
# Application: electron injection in semiconductor (diode)




- stationary Schrödinger equation (1d) - scattering problem:

$$\underbrace{\frac{\hbar^2}{2m}}_{=:\,\varepsilon^2}\,\psi''(x) + \underbrace{\big(E - V(x)\big)}_{=:\,a(x)\neq 0}\,\psi(x) \;=\; 0\,, \quad x \in (0,1)$$

- inhomogeneous open BCs:

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

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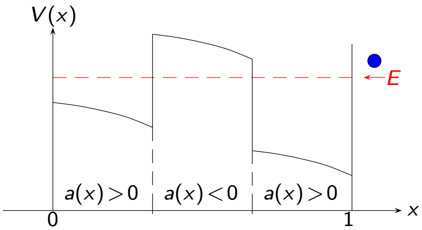


often: coupled problem for all energies $E > 0$;
sharp transmission peaks w.r.t. $E$

$\Rightarrow$ efficient solvers important

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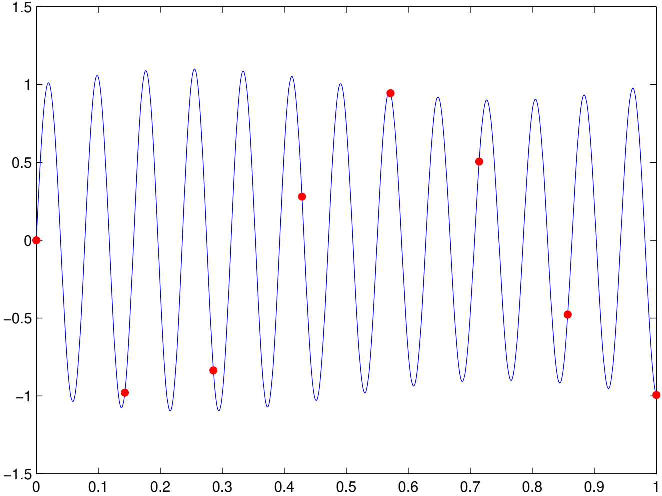



- wavelength $= \mathcal{O}(\varepsilon/\sqrt{a(x)})$; GOAL: use stepsize $h > \lambda$
- $\rightarrow$ accurate scheme that does NOT NEED to resolve the oscillations

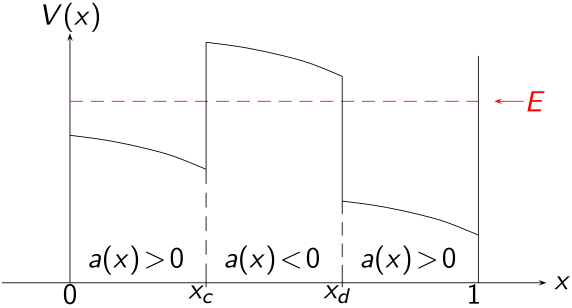
GOAL: hybrid analytic–numerical scheme for $\varepsilon^2\psi'' + a(x)\psi = 0$

## Outline:

1. Domain decomposition method: couple oscillatory ($a > 0$) & evanescent regions ($a < 0$)
2. Oscillatory WKB-method: marching scheme
3. Evanescent WKB-method: FEM with exponential ansatz functions
4. extension to turning points ($a = 0$)

# Difficulties with $\varepsilon^2\psi'' + a(x)\psi = 0 \quad (1)$

- Assume: potential has jump discontinuities (no *turning points*)



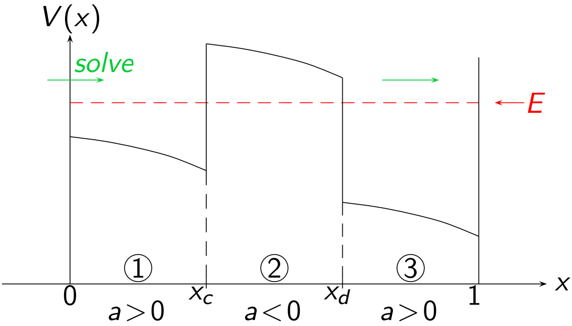

2 challenges:

1) solution of $\varepsilon^2\psi_{xx} + a(x)\psi = 0$ is

- oscillatory for $a(x) > 0$: $\exp\left(\pm i\frac{\sqrt{a}}{\varepsilon}x\right)$ for $a = const$
- evanescent (exponential) for $a(x) < 0$: $\exp\left(\pm\frac{\sqrt{|a|}}{\varepsilon}x\right)$ for $a = const$

$\Rightarrow$ 2 different methods with coarse meshes

# Difficulties with $\varepsilon^2\psi'' + a(x)\psi = 0$ (2)




$2^{nd}$ challenge:

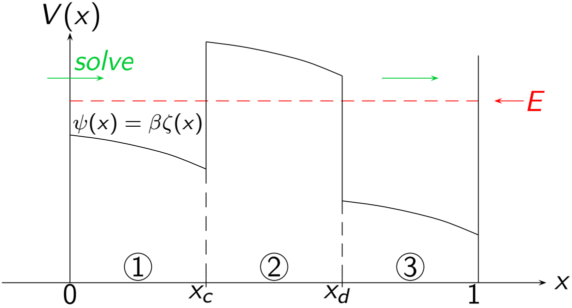
- regions (1)+(3): IVP (marching scheme) more practical than BVP
- region (2) is elliptic: Only BVP is stable! $\rightarrow$ use FEM

$\Rightarrow$ non-overlapping domain decomposition method:
1 sweep (against the incoming wave direction) yields the exact solution.

# Domain decomposition method

- BVP with homogeneous left BC: $\varepsilon\psi'(0) + i\sqrt{a(0)}\psi(0) = 0$ .

$\Rightarrow$ Solve against the incoming wave direction.




Step 1 – IVP for $\zeta$ in oscillatory region (1); $\beta \in \mathbb{C}$:

$$\begin{cases} \varepsilon^2\zeta''(x) + a(x)\zeta(x) = 0\,, & x \in (0, x_c)\,, \\ \zeta(0) = 1\,, & \text{(auxiliary Dirichlet BC)} \\ \varepsilon\zeta'(0) = -i\sqrt{a(0)}\,. & \text{(true left BC)} \end{cases}$$

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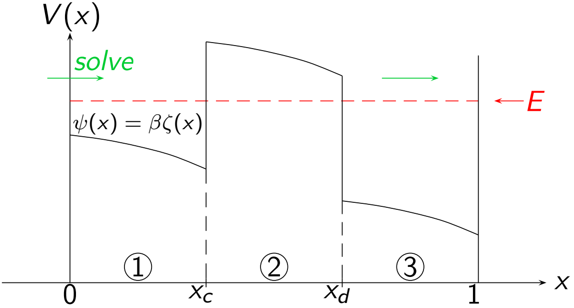


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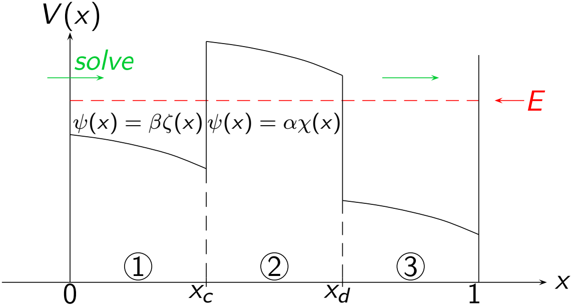
$\Rightarrow \zeta(x) \neq 0 \quad \forall x.$

# Domain decomposition method




Step 2 – BVP for $\chi$ in elliptic region (2); $\alpha \in \mathbb{C}$:

$$\begin{cases} \varepsilon^2 \chi''(x) + a(x)\chi(x) = 0\,, \quad x \in (x_c, x_d)\,, & \\ \dfrac{\chi'(x_c)}{\chi(x_c)} = \dfrac{\zeta'(x_c)}{\zeta(x_c)}\,, & \text{(continuity of } \frac{\psi'}{\psi} \text{ is scaling invariant)} \\ \varepsilon\chi'(x_d) = 1\,. & \text{(auxiliary Neumann BC)} \end{cases}$$

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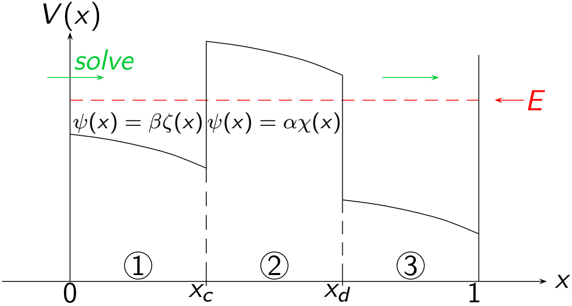


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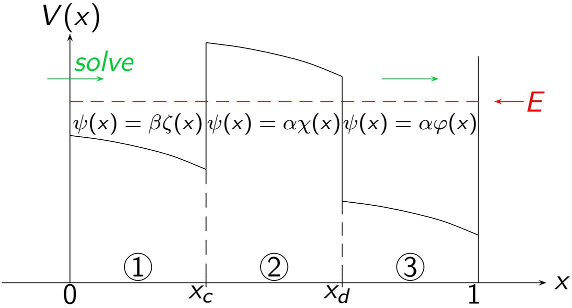
- $\exists!$ solution of BVP (since $\zeta'/\zeta \notin \mathbb{R}$).

# Domain decomposition method

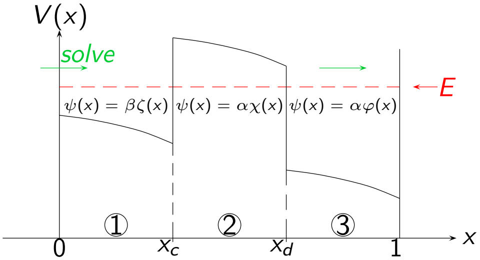



Step 3 – IVP for $\varphi$ in oscillatory region (3):

$$\begin{cases} \varepsilon^2\varphi''(x) + a(x)\varphi(x) = 0\,, \quad x \in (x_d, 1)\,, \\ \varphi(x_d) = \chi(x_d)\,, \qquad \text{(implies continuity of } \psi \text{ at } x_d) \\ \varphi'(x_d) = \chi'(x_d)\,. \qquad \text{(implies continuity of } \psi' \text{ at } x_d) \end{cases}$$

# Domain decomposition method: scaling for $C^1$-continuity

- BVP with right inhomogeneous BC: $\varepsilon\psi'(1) - i\sqrt{a(1)}\psi(1) = -2i\sqrt{a(1)}$




Step 4 – scaling of the auxiliary wave functions; $\alpha,\ \beta \in \mathbb{C}$:

exact solution: $$\psi(x) := \begin{cases} \beta\,\zeta(x)\,, & x \in (0, x_c)\,, \\ \alpha\,\chi(x)\,, & x \in (x_c, x_d)\,, \\ \alpha\,\varphi(x)\,, & x \in (x_d, 1)\,, \end{cases}$$

$$\alpha\,[\varepsilon\varphi'(1) - i\sqrt{a(1)}\,\varphi(1)] = -2i\sqrt{a(1)}\,,$$ (due to true right BC)

$$\beta\,\zeta(x_c) = \alpha\,\chi(x_c)\,.$$ (implies continuity of $\psi$ at $x_c$)

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## Oscillatory WKB-method → analytic preprocessing of ODE

WKB-ansatz for $\varepsilon^2\varphi'' + a(x)\varphi = 0$ (if $a(x) > 0$, oscillatory case):

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

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

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

- second order:

$$\varphi(x) \approx C\,\frac{\exp\left(\pm\frac{i}{\varepsilon}\int_0^x \sqrt{a(y)} - \varepsilon^2\beta(y)\,dy\right)}{\sqrt[4]{a(x)}}, \quad \beta := -\frac{1}{2a^{1/4}}\left(a^{-1/4}\right)''$$

- For each fixed order: asymptotically correct ODE-solution as $\varepsilon \to 0$

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

1. vector system from $\varepsilon^2\varphi'' + a(x)\varphi = 0$:

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

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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:

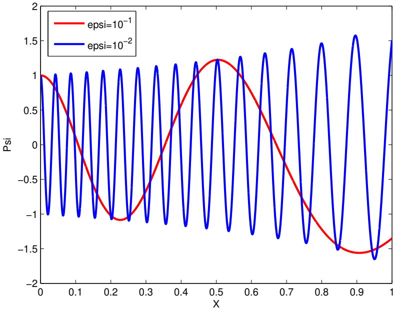
$$Z(x) := \begin{pmatrix} e^{-\frac{i}{\varepsilon}\phi(x)} & 0 \\ 0 & e^{\frac{i}{\varepsilon}\phi(x)} \end{pmatrix} Y(x) \to Z' = \underbrace{\varepsilon \begin{pmatrix} 0 & \beta e^{-\frac{2i}{\varepsilon}\phi(x)} \\ \beta e^{\frac{2i}{\varepsilon}\phi(x)} & 0 \end{pmatrix}}_{\mathcal{O}(\varepsilon)}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

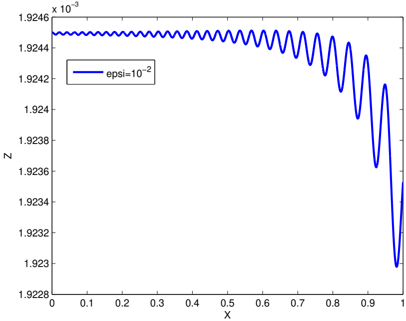
$$\phi(x) := \int_0^x \sqrt{a} - \varepsilon^2\beta \, dy$$ ... phase of $2^{nd}$ order WKB-approximation

# dominant oscillations eliminated:

Ex: $\varepsilon^2\varphi'' + a(x)\varphi = 0\,; \quad a(x) = (x+\frac{1}{2})^2\,, \quad x \in (0,1)$

- $Z$ much smoother than $\varphi \to$ numerics easier




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

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

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

# GOAL: $\varepsilon$–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 $p \geq 2$
- $\varepsilon$–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 [Lorenz-Jahnke-Lubich '05]
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- Remark: lower order WKB-transformations [Lorenz-Jahnke-Lubich '05]
  $\Rightarrow$ only $\varepsilon$–uniformly accurate scheme; i.e. error $= \mathcal{O}_\varepsilon(1)$
- tricky: approximation of oscillatory integral with error $\mathcal{O}(h \min(\varepsilon, h))$

# Resulting method + convergence of WKB–IVP

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

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

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**Theorem ([AA-Ben Abdallah-Negulescu; SIAM NumAnal 2011])**

*Let $a \in C^5$ (piecewise), $a(x) \geq \tau_{os} > 0$.*

$$\Rightarrow \quad ||\varphi(x_n) - \varphi_n|| + \varepsilon||\varphi'(x_n) - \varphi_n'|| \;\leq\; C\frac{h^\gamma}{\varepsilon} + C\varepsilon^3 h^2\,, \quad 1 \leq n \leq N$$

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

- Simpson ($\gamma = 4$) $\Rightarrow$ constraint $h = \mathcal{O}(\sqrt{\varepsilon})$ for $2^{nd}$ order scheme
- $\phi$ exact for potential $a(x)$ piecewise linear (e.g. in RT-diode)
  $\Rightarrow$ $\varepsilon$–asymptotically correct scheme

# Phase integration by spectral method [AA-Klein-Ujvari '18]

problem: constraint $h = \mathcal{O}(\sqrt{\varepsilon})$ due to quadrature error in the phase $\phi(x) = \int_0^x \sqrt{a} - \varepsilon^2 \beta \, dy$ (for $1^{st}$ order scheme; Simpson):

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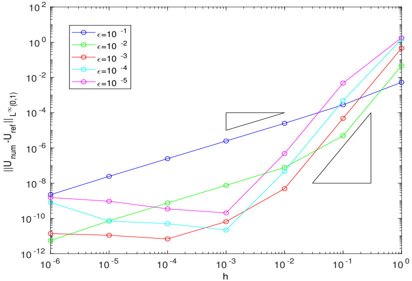
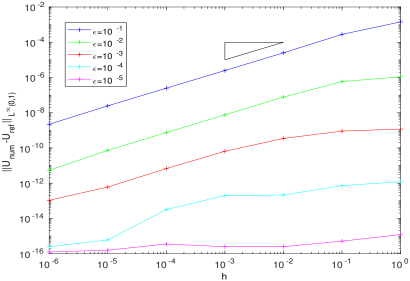
cure: spectral method with barycentric interpolation of phase

Error of $1^{st}$ order WKB-method for $a(x) = e^{-x^2}$ :



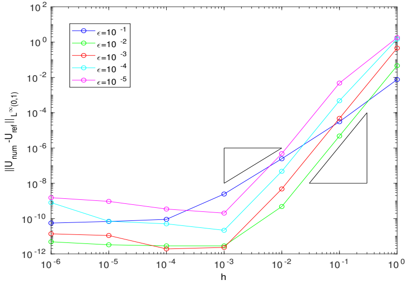

left: phase computation via Simpson rule on each cell $[x_n, x_{n+1}]$

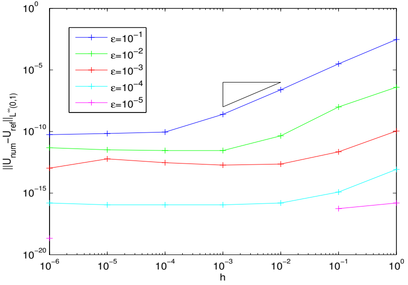
right: Clenshaw-Curtis algorithm (20 pts) on $[0, 1]$ + barycentric interpol.

# Phase integration by spectral method [AA-Klein-Ujvari '18]

Error of $2^{nd}$ order WKB-method for $a(x) = e^{-x^2}$ :

$$||U(x_n) - U_n|| \le C\frac{h^4}{\varepsilon} + C\varepsilon^3 h^2$$

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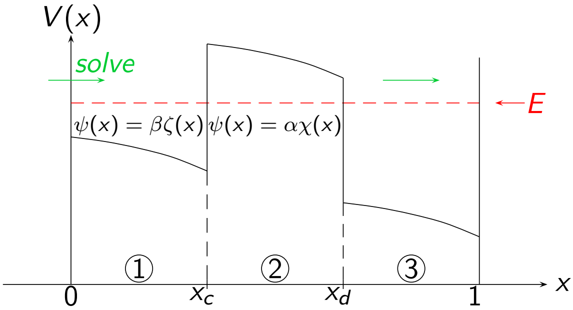
# Domain decomposition method

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# Evanescent WKB-method $\to$ FEM on $[x_c, x_d]$

WKB-ansatz for $\varepsilon^2\varphi'' + a(x)\varphi = 0$ (if $a(x) < 0$, evanescent case):

- first order WKB-functions:

$$\varphi(x) \approx C\,\frac{\exp\left(\pm\frac{1}{\varepsilon}\int_0^x \sqrt{|a|}\,dy\right)}{\sqrt[4]{|a(x)|}}$$

- exponential "hat function" on cell $[x_{n-1}, x_{n+1}]$:

$$\zeta_n(x) := \frac{1}{\sqrt[4]{|a(x)|}} \begin{cases} c\,\sinh\left(\frac{1}{\varepsilon}\int_{x_{n-1}}^x \sqrt{|a|}\,dy\right), & x \in [x_{n-1}, x_n]\,, \\ \tilde{c}\,\sinh\left(\frac{1}{\varepsilon}\int_x^{x_{n+1}} \sqrt{|a|}\,dy\right), & x \in [x_n, x_{n+1}], \\ 0\,, & \text{else}\,. \end{cases}$$

# Convergence of hybrid WKB–method (after scaling step)

- The hybrid scheme is w.r.t. $h$: $2^{nd}$ order for $\psi$, $1^{st}$ order for $\psi'$:

**Theorem ([AA-Negulescu; Numer. Math. 2018])**

*Let $a_{os}(x)$, $a_{ev}(x)$ be bounded away from 0. Asumme $\zeta_n$ has no phase error.*

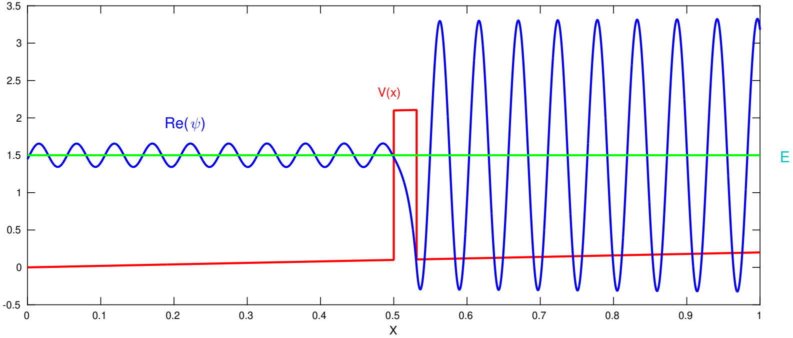
$$\begin{aligned} \Rightarrow \quad \|\tilde{e}_h\|_\infty &\leq C\sqrt{h}\,\min(\varepsilon^{3/2}, h^{3/2})\,, \\ \varepsilon\|\tilde{e}_h'\|_\infty &\leq C\varepsilon\sqrt{h}\,\min(\sqrt{\varepsilon}, \sqrt{h}) \end{aligned}$$

hybrid error:
$\tilde{e}_h(x) := \psi(x) - \psi_h(x)$; $x$ continuous in evanescent region/ discrete in oscillatory region.

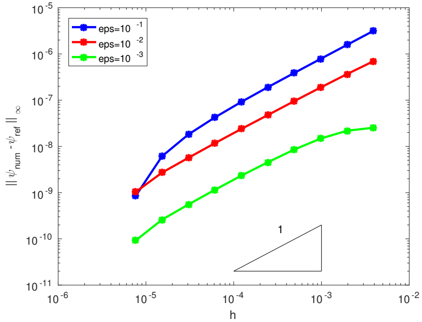
$$\|\tilde{e}_h\|_\infty := \max(\|\tilde{e}_h\|_{L^\infty(x_c,x_d)}\,;\ \max_{n=0,\dots,N} |\tilde{e}_{h,n}|)$$

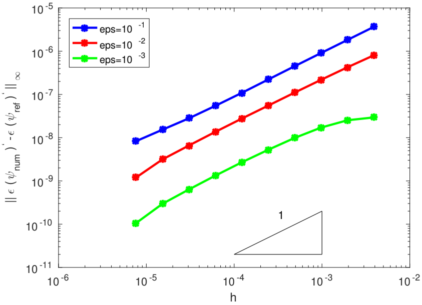
# Numerical results – solution

- tunneling structure: injection of plane wave with energy $E$ at right BC



# Numerical results – hybrid error as function of $h$, $\varepsilon$




$\|\tilde{e}_h\|_\infty$ for 3 values of $\varepsilon$; $\quad\quad \varepsilon\|\tilde{e}_h'\|_\infty$

theoretical estimates:

$$\|\tilde{e}_h\|_\infty = \mathcal{O}\big(\sqrt{h}\,\min(\varepsilon^{3/2}, h^{3/2})\big); \qquad \varepsilon\|\tilde{e}_h'\|_\infty = \mathcal{O}\big(\varepsilon\sqrt{h}\,\min(\sqrt{\varepsilon}, \sqrt{h})\big)$$

# Outline:

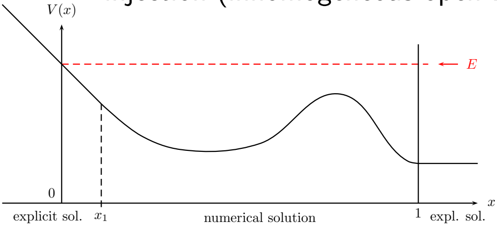
1. Domain decomposition method: couple oscillatory ($a > 0$) & evanescent regions ($a < 0$)
2. Oscillatory WKB-method: marching scheme
3. Evanescent WKB-method: FEM with exponential ansatz functions
4. extension to turning points ($a = 0$)

# Scattering problem with turning point

toy problem: $\varepsilon^2\psi''(x) + a(x)\psi(x) = 0\,, \quad x \in \mathbb{R}$

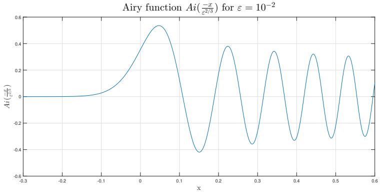
$a(x) = E - V(x) = x\,, \quad x \le x_1$

injection (inhomogeneous open BC) at $x = 1$




- WKB-approximation wrong close to turning point!

$\Rightarrow$ explicit solution for $x \le x_1$:
$\psi_-(x) = c_0 \,\mathrm{Ai}\left(-\frac{x}{\varepsilon^{2/3}}\right)$

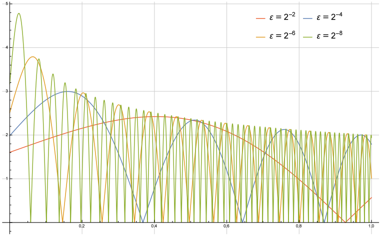


# Scattering problem: blow up at turning point

**Theorem ([AA-Döpfner 2018])**

$$\begin{aligned} \|\psi_\varepsilon\|_{L^\infty(0,1)} &= \mathcal{O}\big(\varepsilon^{-\frac{1}{6}}\big) \\ \varepsilon\|\psi_\varepsilon'\|_{L^\infty(0,1)} &\leq C\,, \qquad \textit{for } \varepsilon \to 0 \end{aligned}$$

Ex: scattering solution $|\psi_\varepsilon|$ for $a(x) = x$ on $(-\infty, 1]$:




$\rightarrow$ Asymptotic unboundedness could polute numerical solution on $[x_1, 1]$.

# Domain decomposition method

Step 1 - WKB-IVP for $\varphi$ in oscillatory region:

$$\begin{cases} \varepsilon^2\varphi''(x) + a(x)\varphi(x) = 0\,, \quad x \in (x_1, 1)\,, \\ \varphi(x_1) = \varepsilon^{-\frac{1}{6}}\mathrm{Ai}\,\big(-\frac{x_1}{\varepsilon^{2/3}}\big)\,, \\ \varepsilon\varphi'(x_1) = -\varepsilon^{\frac{1}{6}}\mathrm{Ai}\,'\big(-\frac{x_1}{\varepsilon^{2/3}}\big)\,. \end{cases}$$

Step 2 - scaling to satisfy true right BC:

$$\psi(x) := \alpha \begin{cases} \mathrm{Ai}\,\big(-\frac{x}{\varepsilon^{2/3}}\big)\,, \quad x \le x_1\,, \\ \varphi(x)\,, \quad x_1 < x \le 1\,. \end{cases}$$

$$\alpha := \frac{-2i\sqrt{a(1)}}{\varepsilon\varphi'(1) - i\sqrt{a(1)}\varphi(1)}$$ includes a numerical error - from WKB

# Convergence of $2^{nd}$ order WKB–Airy method

**Theorem ([AA-Döpfner 2018])**

$$\textit{In } [0,x_1]: \quad \|e_h\|_{C[0,x_1]} \le C\frac{h^\gamma}{\varepsilon^{7/6}} + C\varepsilon^{\frac{17}{6}} h^2\,, \quad \varepsilon\|e_h'\|_{C[0,x_1]} \le C\frac{h^\gamma}{\varepsilon} + C\varepsilon^3 h^2,$$

$$\textit{In } [x_1,1]: \quad |e_{h,n}| + \varepsilon|e_{h,n}'| \le C\frac{h^\gamma}{\varepsilon} + C\varepsilon^3 h^2\,, \quad n = 1,\dots,N$$

- Asymptotic correctness of the scheme (as $\varepsilon \to 0$) over-compensates blow-up at $x = 0$: but $\varepsilon^{-1/6}$ is lost.

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- For Simpson quadrature of the phase ($\gamma = 4$):
  Second order scheme (w.r.t. $h$), if:
  $h = \mathcal{O}(\varepsilon^{1/2})$ ... without turning point
  $h = \mathcal{O}(\varepsilon^{7/12})$ ... with (first order) turning point

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  $h = \mathcal{O}(\varepsilon^{7/12})$ ... with (first order) turning point
- Extension to quadratic potential for $x \le x_1$:
  Airy function $\to$ parabolic cylinder functions

# Conclusion

- (analytic) domain decomposition: oscillatory & evanescent region
- oscillatory WKB-method (marching)
- phase computation: spectral method
- evanescent WKB-method (FEM)
- coupling to turning point

# References


- A. Arnold, C. Negulescu: Stationary Schrödinger equation in the semi-classical limit: numerical coupling of oscillatory and evanescent regions, Numer. Math., 2018.
- A. Arnold, C. Klein, B. Ujvari: WKB-method for the 1D-Schrödinger equation in the semi-classical limit: enhanced phase treatment, submitted 2018.
- A. Arnold, K. Döpfner: Stationary Schrödinger equation in the semi-classical limit: WKB-based scheme coupled to a turning point, submitted 2018.