An efficient approximation-scheme for Schrödinger-type equations including turning points

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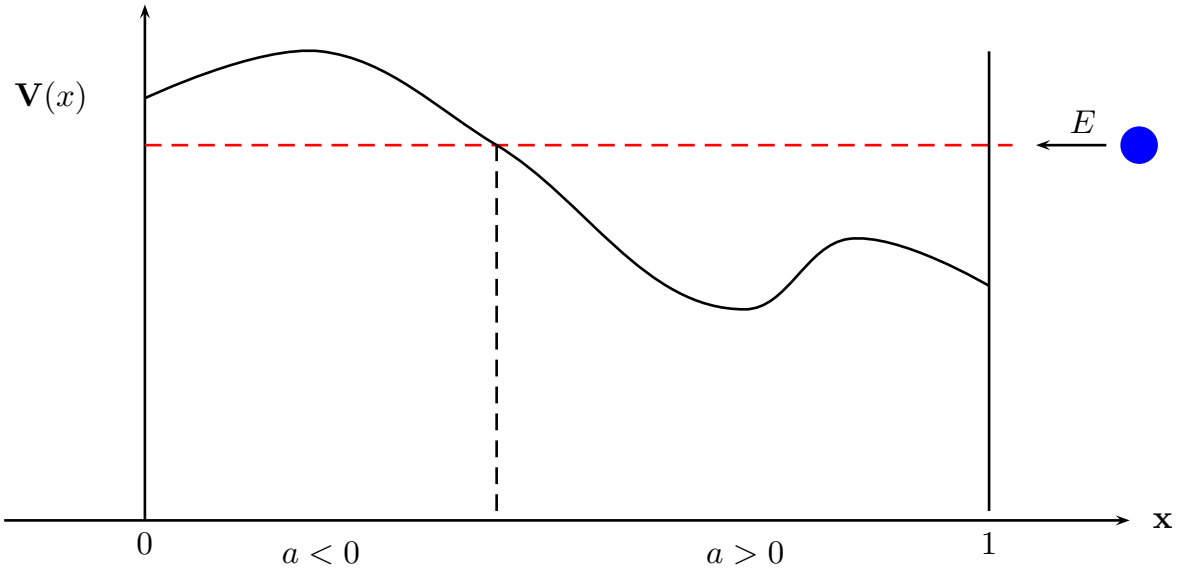
Application: electron injection in semiconductor (diode)



- $\rightsquigarrow$ device scale: nanometers
- $\rightsquigarrow$ electron injection at high energies E
- $\rightsquigarrow$ semiclassical limit $\rightsquigarrow$ quantum effects (e.g. tunneling)

The time-dependent Schrödinger equation

Quantum mechanical model for a single particle in an electric field:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(t,x) = \left(-\frac{\hbar^2}{2m}\Delta_x + V(x)\right)\Psi(t,x)$$

[time-independent potential $V(x)$]

- $\rightsquigarrow$ $\Psi(t,x)$ . . . state/wave function.
- $\rightsquigarrow$ $|\Psi(t,x)|^2$ . . . probability density of the particle.

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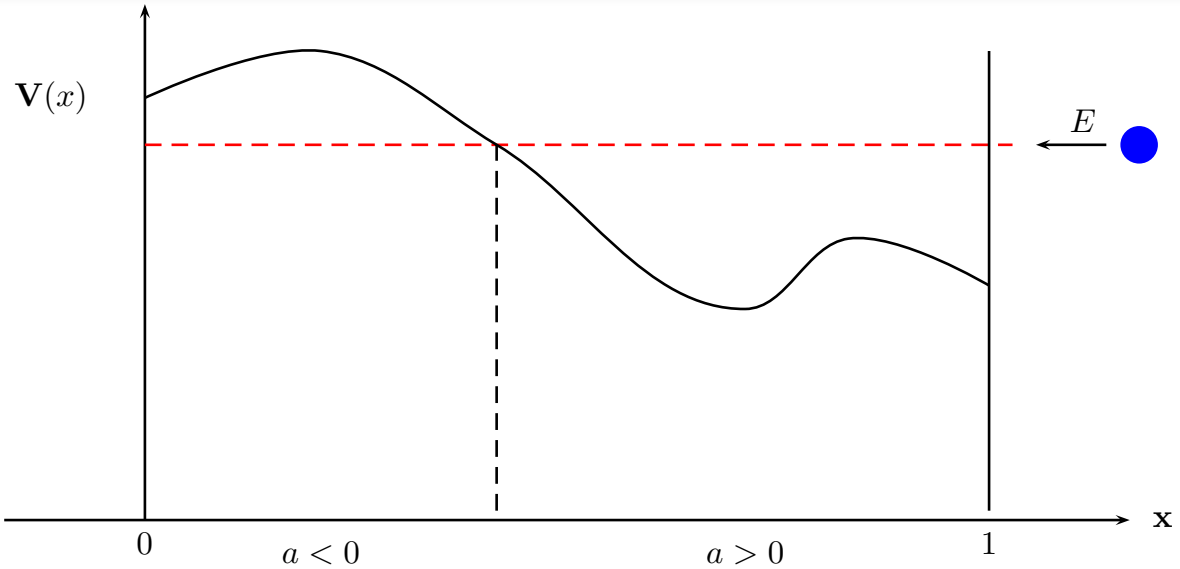
[time-independent potential $V(x)$]

Separation of variables:

$$\Psi(t,x) = \psi(x)f(t)$$

$\rightsquigarrow$ $f(t) = e^{\frac{-\mathrm{i}Et}{\hbar}}$ ... where E represents the total energy of the particle.

Stationary Schrödinger equation (diode $\rightsquigarrow$ 1D model)



$\rightsquigarrow$ stationary Schrödinger equation with open boundary conditions:

$$\begin{cases} \frac{\hbar^2}{2m}\,\psi_{xx}(x) + \big(E - V(x)\big)\psi(x) = 0\,, \quad x \in [0,1] \\ \\ \frac{\hbar}{\sqrt{2m}}\psi_x(0) + \mathrm{i}\sqrt{E - V(0)}\psi(0) = 0 \\ \frac{\hbar}{\sqrt{2m}}\psi_x(1) - \mathrm{i}\sqrt{E - V(1)}\psi(1) = -2\mathrm{i}\sqrt{E - V(1)} \end{cases}$$

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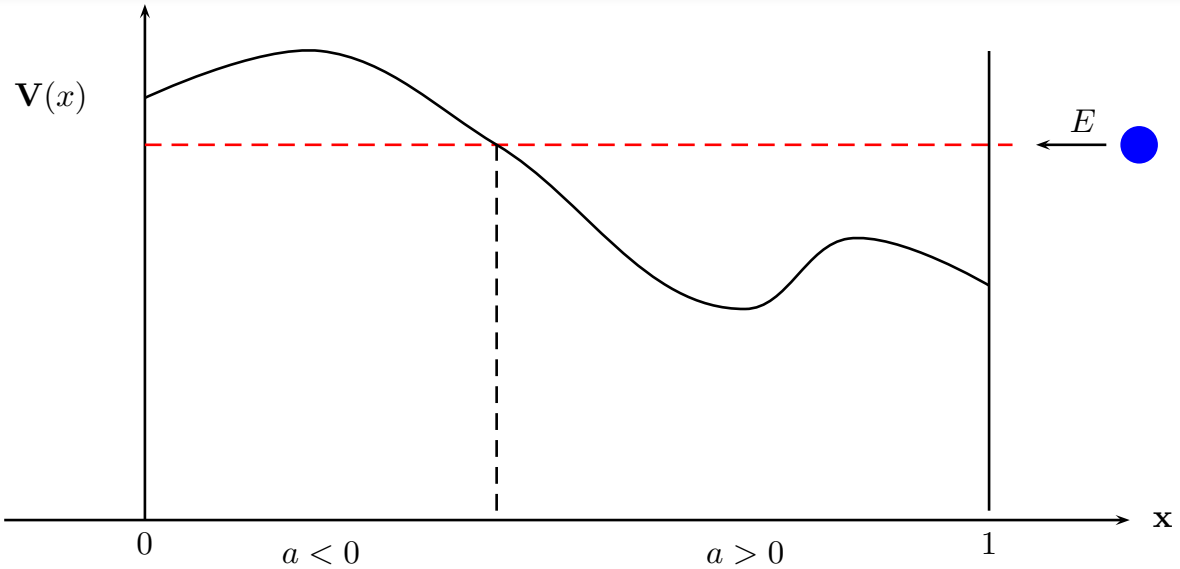
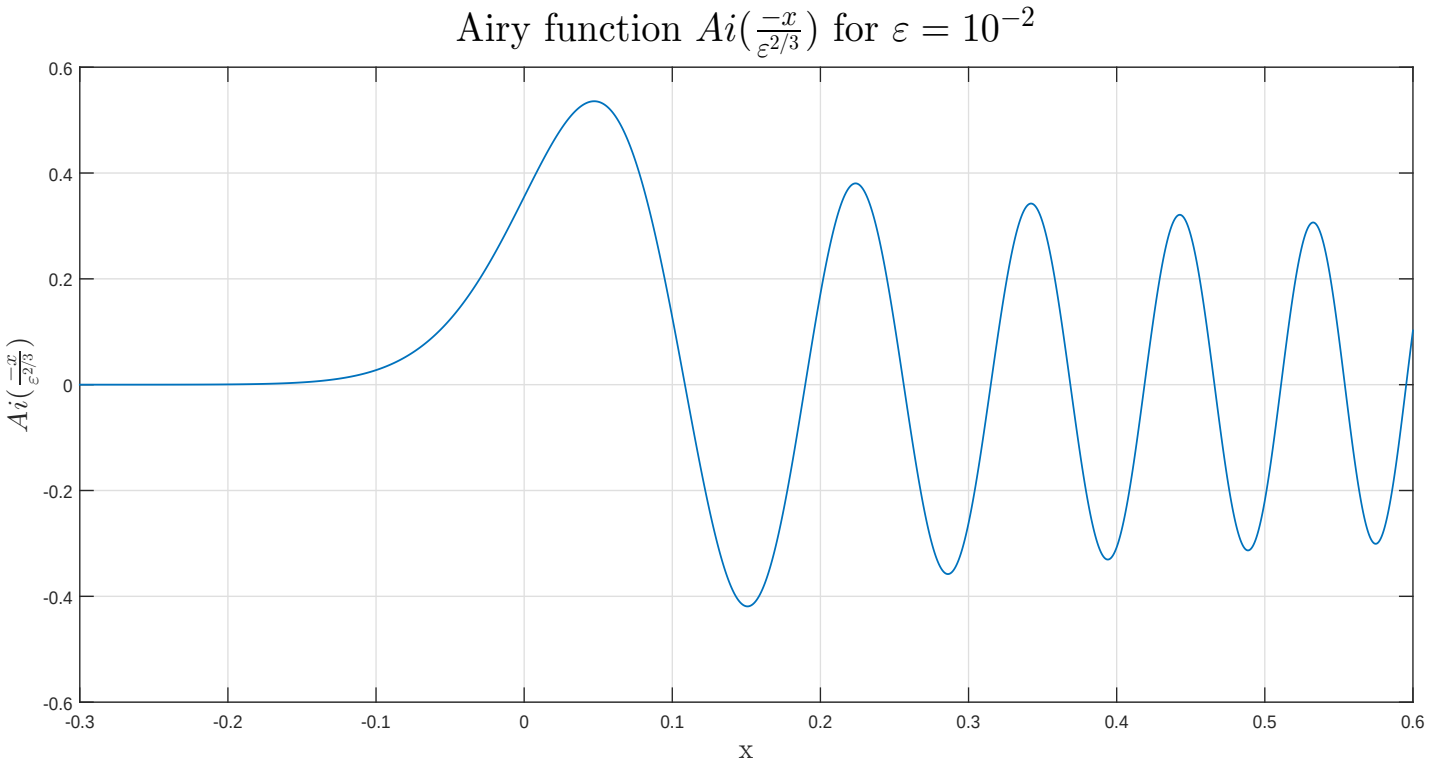


$\rightsquigarrow$ stationary Schrödinger equation with open boundary conditions:

$$\begin{cases} \varepsilon^2 \psi_{xx}(x) + a(x)\psi(x) = 0\,, \quad x \in [0,1] \\ \\ \varepsilon\psi_x(0) + \mathrm{i}\sqrt{a(0)}\psi(0) = 0 \\ \varepsilon\psi_x(1) - \mathrm{i}\sqrt{a(1)}\psi(1) = -2\mathrm{i}\sqrt{a(1)} \end{cases}$$

Airy function

Airy equation: $\varepsilon^2 \psi_{xx}(x) + x\psi(x) = 0$



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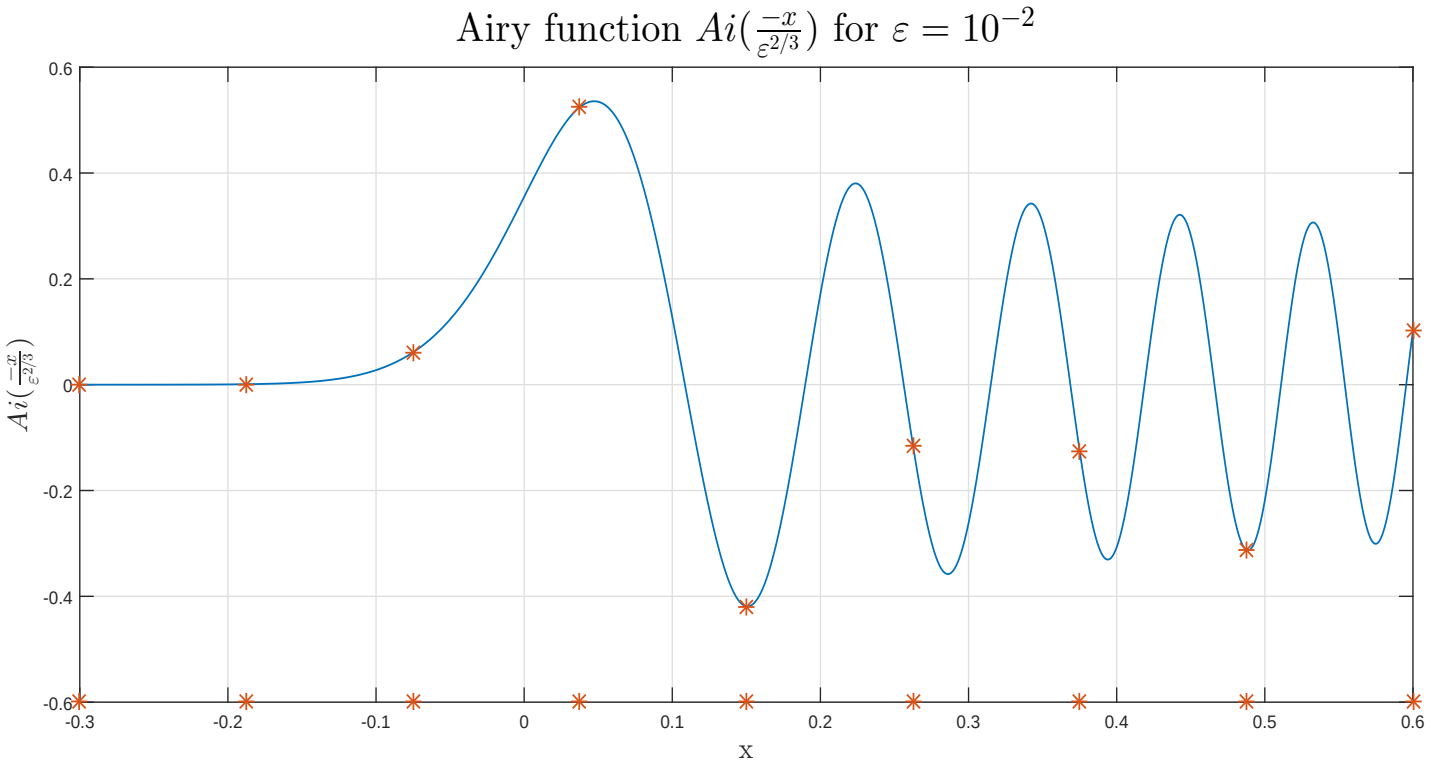
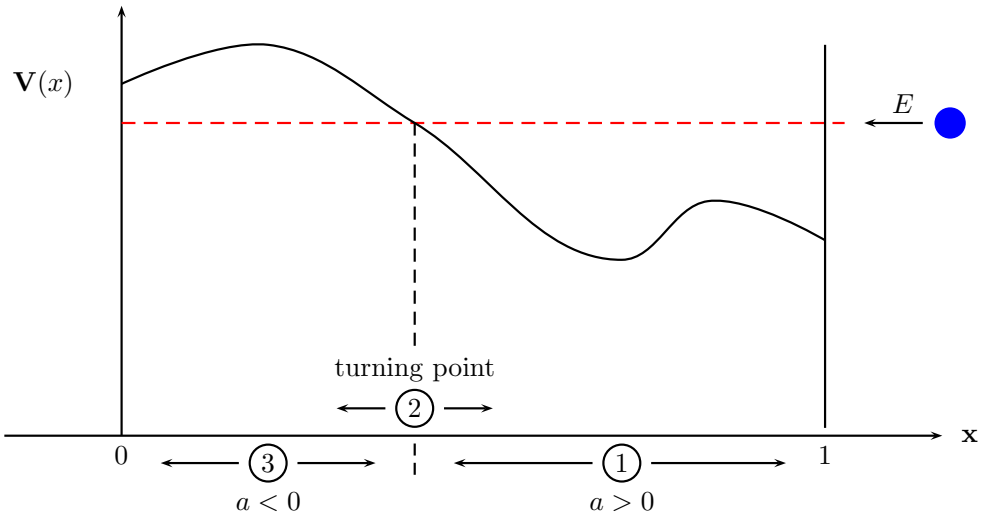


$\rightsquigarrow$ wavelength $\sim \frac{\varepsilon}{\sqrt{a(x)}}$ (restricted stepsize $h < \varepsilon$ to resolve oscillations)

$\rightsquigarrow$ want (coarse) stepsize h independent of the wavelength

Known results



- ⇝ standard WKB methods: ① + ③
- ⇝ [Lorenz - Jahnke - Lubich (2005)]: ①
  ε-uniform; error $\mathcal{O}(h^2)$, for $h \leq \mathcal{O}(\sqrt{\varepsilon})$;
- ⇝ [Negulescu (2005)]: ③
  FEM-based
- ⇝ [Arnold - B. Abdallah - Negulescu (2011)]: ①
  ε-asymptotically correct scheme; error $\mathcal{O}(\varepsilon^3 h^2)$

Hybrid method for an ε-uniform scheme

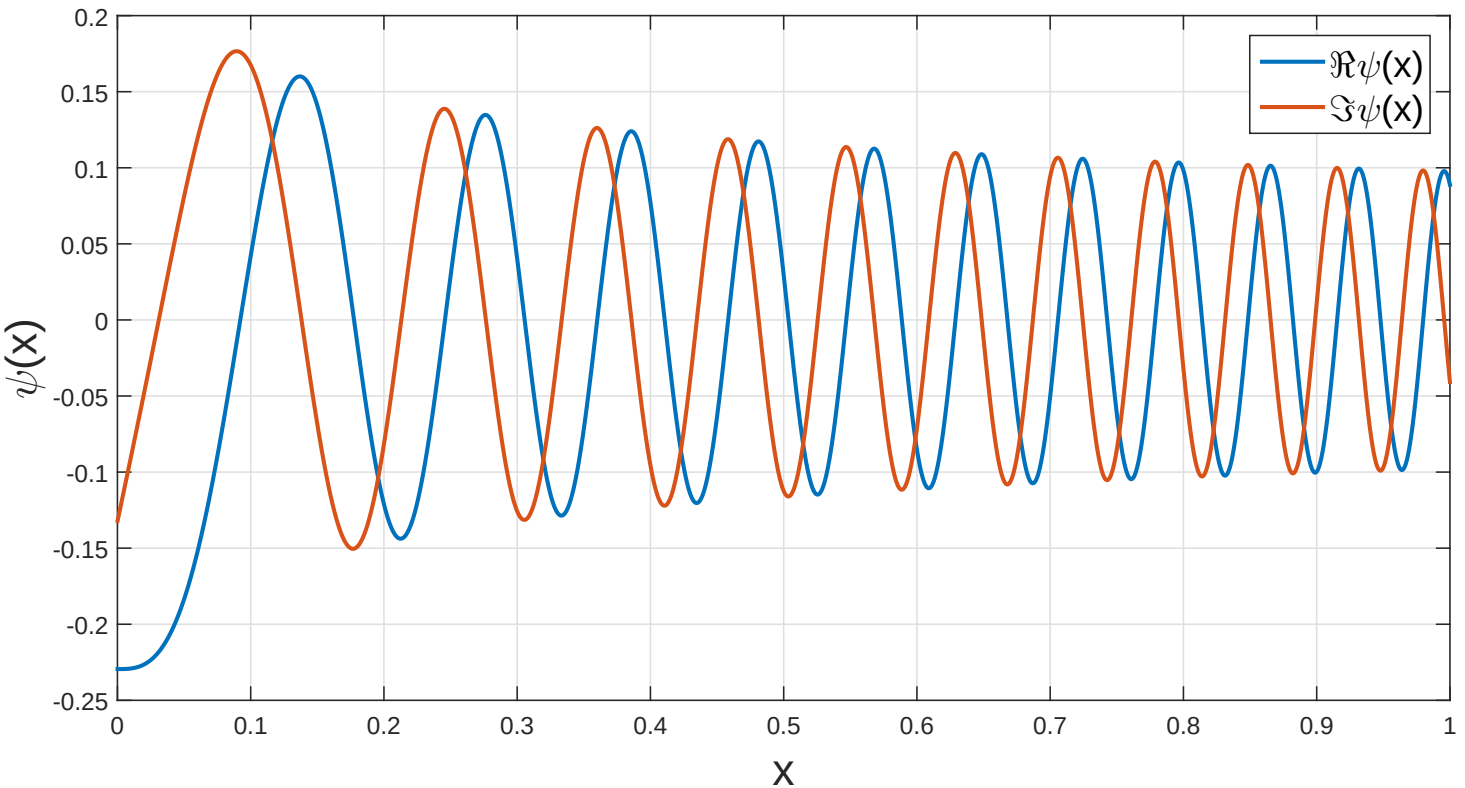
The approach for the oscillatory regime incl. a turning point consists of two main steps:

- (1) analytic preprocessing of ODE to eliminate the dominant oscillations
- (2) numerical (ε-asymptotically correct) scheme for approximating oscillatory integrals

Hankel function

$$\varepsilon^2\psi_{xx}(x) + x^\alpha\psi(x) = 0 \quad \rightsquigarrow \quad \psi(x) = \sqrt{x}H_\nu^{(j)}\left(-\frac{2\nu x^{\frac{1}{2\nu}}}{\varepsilon}\right)$$

$H_\nu^{(j)}(x)$ ... Hankel functions (Bessel functions of the third kind) ... $\nu = \frac{1}{\alpha+2}$.



Choice of the ansatz functions ω_j for general $a(x)$

Motivated by the case $a(x) = x^\alpha$ we make a product ansatz with Hankel functions [Langer, 1931] where $a(x)$ has a root of order $\alpha > 0$ and $\nu = \frac{1}{\alpha+2}$:

$$\boxed{\psi(x) \quad \overset{\varepsilon \to 0}{\sim} \quad \omega_j(x) := \rho(x) \cdot H_\nu^{(j)}\left(\frac{1}{\varepsilon}\phi(x)\right)}, \qquad j = 1, 2$$

$$\phi(x) := \int_{x_0}^{x} \sqrt{a(s)}ds, \qquad \rho(x) := \sqrt{\frac{\phi(x)}{|\phi'(x)|}}$$

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Phase and Modulus of the Hankel functions for $\nu \geq 0$ and $z > 0$:

$$H_\nu^{(j)}(z) = M_\nu(z)e^{\pm i\theta_\nu(z)}$$

Transformation to a 1^{st} order system

We transform into the system

$$U(x) := \begin{pmatrix} \psi(x) \\ \varepsilon\psi'(x) \end{pmatrix}$$

$$\rightsquigarrow U' = \frac{1}{\varepsilon} \begin{pmatrix} 0 & 1 \\ -a(x) & 0 \end{pmatrix} U\,, \qquad x \in (0,1)\,, \qquad U(0) = U_l.$$

The transformed system

Further transformation via our ansatz functions ω_j and a diagonalizing term

$$Z(x) =: \begin{pmatrix} e^{-\mathrm{i}\int_{x_0}^{x}\beta_\varepsilon(\hat{x})d\hat{x}} & 0 \\ 0 & e^{\mathrm{i}\int_{x_0}^{x}\beta_\varepsilon(\hat{x})d\hat{x}} \end{pmatrix} \begin{pmatrix} \omega_1(x) & \omega_2(x) \\ \varepsilon\omega_1'(x) & \varepsilon\omega_2'(x) \end{pmatrix}^{-1} U(x).$$

is done to obtain the following system:

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$$\rightsquigarrow \qquad \boxed{Z'(x) = \mathrm{i}\beta_\varepsilon(x)\,\mathbf{B}_\varepsilon(x)\,Z(x)}\,, \quad x \in (0,1)\,, \quad Z(0) = Z_I\,,$$

where $$\beta_\varepsilon(x) := \frac{\pi}{4}\left(\rho\rho'' + \frac{\nu^2}{\rho^2}\right) M_\nu(\frac{\phi(x)}{\varepsilon})^2$$

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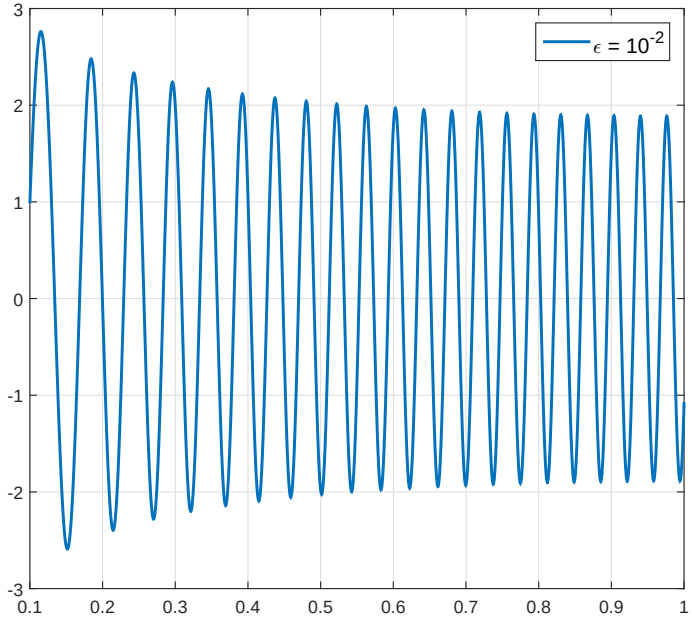
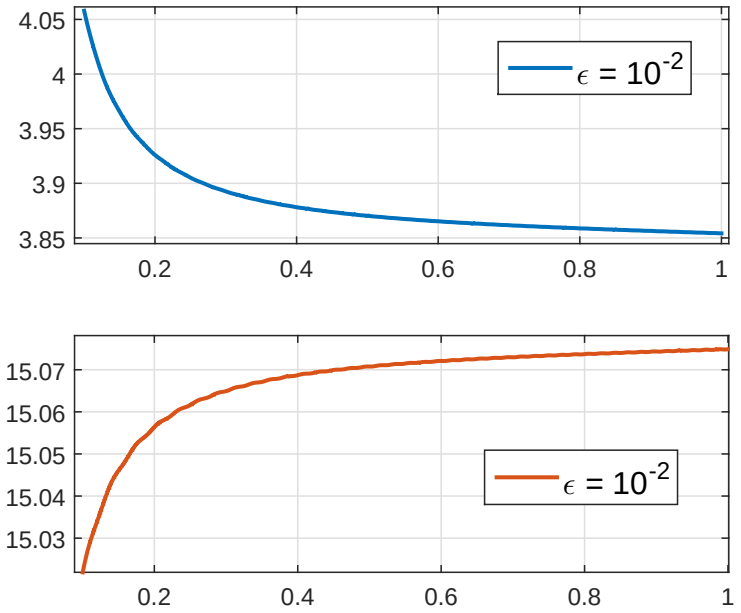
strong asymptotic limit $Z(x) = const = Z_I$ for $\varepsilon \to 0$.

Illustration: dominant oscillations eliminated:



solution $\Re\psi(x)$ for $\varepsilon = 10^{-2}$
$\rightsquigarrow$ amplitude ~ 2



$\Re Z_1(x)$ and $\Im Z_1(x)$:
$\rightsquigarrow$ twice the frequency
$\rightsquigarrow$ amplitude $= \mathcal{O}(10^{-3})$

An ε-asymptotically correct numerical scheme

Design a method with error that vanishes as $\varepsilon \to 0$.

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Applying Picard iteration to the system in Z and and truncating yields a truncation error γ_1

$$Z(x_{n+1}) = Z(x_n) + \int_{x_n}^{x_{n+1}} \underbrace{\mathrm{i}\beta(y)}_{\in\mathbb{R}} \underbrace{\mathbf{B}_\varepsilon(y)}_{\in\mathbb{R}^{2\times 2}} dy \cdot \underbrace{Z(x_n)}_{\in\mathbb{R}^2} + \gamma_1$$

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$$= Z(x_n) + \quad \tilde{\mathbf{B}}(x_{n+1}; x_n)\, Z(x_n) + \gamma_2 \quad + \gamma_1$$

For a method $\tilde{\mathbf{B}}(x; a)$ approximating the remaining *oscillatory* integral an approximation error γ_2 occurs.

Asymptotic method

To control the approximation error of the oscillatory integrals γ_2 in terms of ε, we make use of the *asymptotic method* for oscillatory integrals [Olver, 2006]

$$\underbrace{\int_{x_n}^{x_{n+1}} f(x) e^{\frac{i}{\varepsilon}\phi(x)} dx}_{\mathcal{O}(h)} = -(i\varepsilon) \left[\frac{f(x)}{\phi'(x)} e^{\frac{i}{\varepsilon}\phi(x)} \right]_{x_n}^{x_{n+1}} + \mathcal{O}(\varepsilon h)$$

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[Arnold-B.Abdallah-Negulescu, 2011]

$\rightsquigarrow$ *shifted asymptotic method*: error control in terms of the stepsize h.

Result

The resulting one-step scheme

$$Z_{n+1} := \left(\mathbb{I} + \tilde{\mathbf{B}}(x_{n+1}; x_n)\right) Z_n \tag{1}$$

is 1^{st} order consistent and exhibits the following approximation error.

Theorem (K.D., A. Arnold)

Let $a(x)$ have a zero of order α. For the scheme (1) introduced above it holds

$$||Z(x_n) - Z_n|| \quad \leq \quad C\varepsilon^{4\nu} \min(\varepsilon^{2\nu}, h) \,,$$

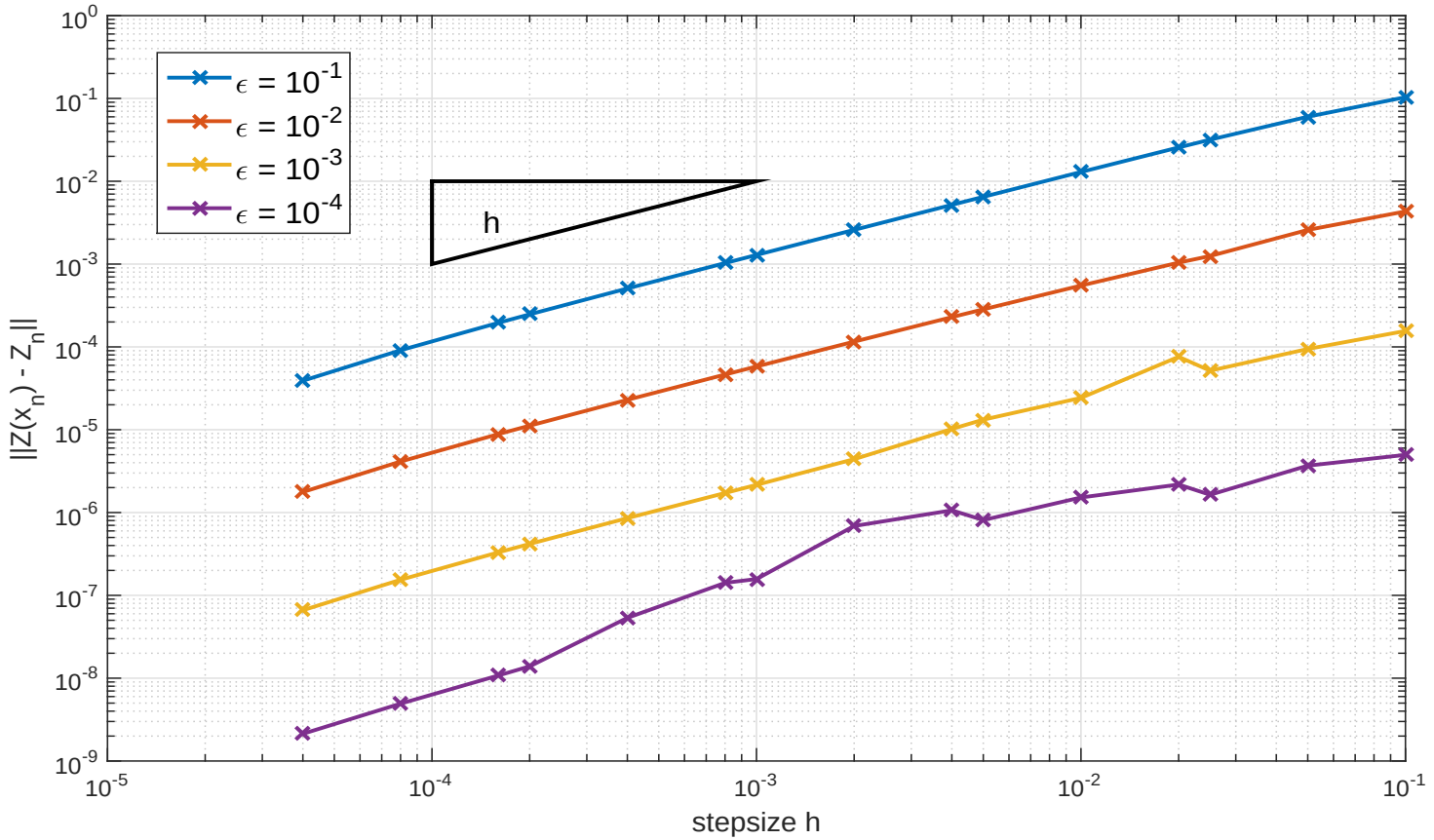
for $1 \leq n \leq N$, $0 < \varepsilon, h \leq 1$ and $\nu = \frac{1}{\alpha+2}$.

i.e. the error vanishes as $\varepsilon \to 0$ even for fixed step size h.

Error

ex: $a(x) = 2x - x^2 \rightsquigarrow$ turning point at $x = 0$

$\rightsquigarrow$ error $\mathcal{O}(\varepsilon^{\frac{4}{3}} h)$



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