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WKB-based schemes for the Schrödinger equation in the semi-classical limit

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Abstract

An efficient and accurate numerical method is presented for the solution of highly oscillatory differential equations. While standard methods would require a very fine grid to resolve the oscillations, the presented approach uses first an analytic (second order) WKB-type transformation, which filters out the dominant oscillations. The resulting ODE is much smoother and can hence be discretized on a much coarser grid, with significantly reduced numerical costs.

In many practically relevant examples, the method is even asymptotically correct w.r.t. the small parameter ε that identifies the oscillation wave length. Indeed, in these cases, the error then vanishes for $\varepsilon \to 0$, even on a fixed spatial mesh. Applications to the stationary Schrödinger equation are presented.

Keywords : Schrödinger equation; highly oscillating wave functions; epsilon–independent second order numerical scheme; higher order WKB-approximation; asymptotically correct finite difference scheme; asymptotic analysis.

1 Introduction

This paper deals with an asymptotic scheme for the numerical solution of highly oscillating differential equations of the type

$$\varepsilon^2 \varphi''(x) + a(x)\varphi(x) = 0\,, \tag{1.1}$$

where $0 < \varepsilon \ll 1$ is a very small parameter and $a(x) \geq a_0 > 0$ a sufficiently smooth function. For very small $\varepsilon > 0$, the wave length $\lambda = \frac{\varepsilon}{\sqrt{a(x)}}$ is very small, such that the solution φ becomes highly oscillating. But a highly oscillatory solution requires a very fine mesh in order to accurately resolve the oscillations, typically at least 10 grid points per oscillation (see Figure 1). And a fine mesh means high numerical costs, implying thus the inefficiency of standard methods.

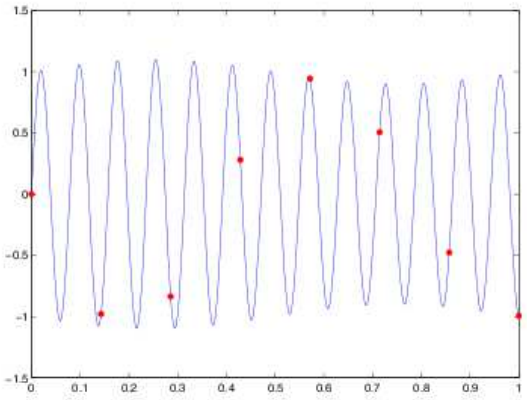

Figure 1: In standard numerical methods highly oscillating solutions require a very fine mesh to capture the oscillations. However, with the analytic pre-processing of our method an accurate solution can be obtained on a coarse grid.

Such problems that require the numerical integration of highly oscillatory equations play an essential role in a wide range of physical phenomena: electromagnetic and acoustic scattering (Maxwell and Helmholtz equations in the high frequency regime), wave evolution problems in quantum and plasma physics (Schrödinger equation in the semiclassical regime), stiff mechanical systems, and so on. Due to the high oscillations, these problems render the mathematical analysis and computation very challenging.

The application we are interested in here is the numerical solution of the stationary 1D Schrödinger equation

$$\begin{cases} -\varepsilon^2 \psi_E''(x) + V(x)\psi_E(x) = E\psi_E(x)\,, \quad x \in (0,1)\,, \\ \psi_E'(0) + ik(0)\psi_E(0) = 0\,, \\ \psi_E'(1) - ik(1)\psi_E(1) = -2ik(1)\,. \end{cases} \tag{1.2}$$

It describes the state of an electron that is injected with the prescribed energy E from the right boundary (or lead) into an electronic device (diode, e.g.), modeled on the interval $[0,1]$. The corresponding (complex valued) wave function is denoted by $\psi_E(x)$, where $|\psi_E(x)|^2$ is related to the spatial probability density of the electron. Due to the continuous injection of a plane wave function at $x = 1$, we cannot expect $|\psi_E|^2$ to be

normalized here. The small parameter ε is the rescaled Planck constant and V is the given electrostatic potential. We suppose that $E > V(x)$ all along the device which characterizes the problematic oscillatory regime. In contrast, the evanescent regime, i.e. $E < V(x)$, is rather harmless since the solution is then smooth, and consequently we are not considering this case in the present work. The boundary conditions in (1.2) are the so called open or transparent boundary conditions, permitting an electron wave to enter or leave the device without reflections [13]. And finally, the wave vector k and the corresponding de Broglie wave-length λ are given by

$$k(x) := \frac{\sqrt{E - V(x)}}{\varepsilon}\,, \quad \lambda(x) := \frac{1}{k(x)} = \frac{\varepsilon}{\sqrt{E - V(x)}}\,.$$

Solving one single ODE like (1.2) is, of course, no numerical challenge today. However, a rapid resolution of the Schrödinger equation (1.2) is a crucial element in the simulation of the electron transport in nanoscale semiconductor devices, like quantum wave-guides [1], resonant tunneling diodes (RTDs) [3], MOSFETs [17], etc. In such applications, macroscopic quantities like the electron density n and the current density j are given by the formulae

$$n(x) = \int_0^\infty f(k)|\psi_{E(k)}(x)|^2\,dk\,, \quad j(x) = \varepsilon \int_0^\infty f(k)\Im(\overline{\psi_{E(k)}(x)}\psi'_{E(k)}(x))\,dk\,,$$

where f represents the injection statistics of the electrons, described by the Fermi-Dirac or the Boltzmann distribution function. Thus, the Schrödinger equation (1.2) has to be solved many times (once per injection energy E) in order to compute the macroscopic quantities n and j. In fact, one needs here a very fine grid in E, since the transition probability for the electrons through the device is very peaked w.r.t. E (cf. [3]). Hence, efficient methods for the solution of (1.2) will lead to a considerable gain in the simulation time.

In order to put into perspective the numerical method proposed in §2, we first review the well-known WKB-approximation (cf. [12]) for the singularly perturbed ODE (1.1). The WKB-ansatz

$$\varphi(x) = \exp\left(\frac{1}{\varepsilon}\sum_{p=0}^{\infty}\varepsilon^p\phi_p(x)\right)\,, \tag{1.3}$$

inserted in (1.1), leads after comparison of the ε^p-terms to

$$\begin{aligned}
\phi_0(x) &= \pm i\int_0^x \sqrt{a(\tau)}\,d\tau + const.\,,\\
\phi_1(x) &= \ln a(x)^{-1/4} + const.\,,\\
\phi_2(x) &= \mp i\int_0^x \beta(\tau)\,d\tau + const.\,, \quad \beta := \frac{a''}{8a^{3/2}} - \frac{5(a')^2}{32a^{5/2}}\,.
\end{aligned}$$

In [14] the zeroth order WKB-approximation $\varphi(x) \approx C\exp\left(\pm\frac{i}{\varepsilon}\int_0^x\sqrt{a}\,d\tau\right)$ was used to eliminate the dominant oscillations. After transformation, the resulting smoother

variables were approximated numerically. A localized variant of this transformation is also the background for the *modified Magnus method* for (1.1), developed in §5 of [8].

Truncating the Ansatz (1.3) after $p = 1$ yields the asymptotic approximation

$$\varphi(x) \approx C \, \frac{\exp\left(\pm \frac{i}{\varepsilon} \int_0^x \sqrt{a}\, d\tau\right)}{\sqrt[4]{a(x)}}\,, \tag{1.4}$$

which is the basis to construct a WKB-finite element scheme for (1.1) in [16, 17]. While that FEM required a non-resonance condition on h, our new method is valid without any such restriction. Using the first order WKB-approximation (1.4) to transform (1.1) into a smoother problem was also mentioned in §2.6 of [14], but it was not pursued there numerically.

Our method below is related to a second order WKB-approximation (i.e. truncation of the Ansatz (1.3) after $p = 2$), which uses the refined asymptotics

$$\varphi(x) \approx C \, \frac{\exp\left(\pm \frac{i}{\varepsilon} \int_0^x \phi(\tau)\, d\tau\right)}{\sqrt[4]{a(x)}}\,, \quad \phi(x) := \sqrt{a(x)} - \varepsilon^2 \beta(x)\,. \tag{1.5}$$

Let us briefly sketch our strategy. It is closely related to the procedure in [14], but yields a refinement to higher ε–order:

1. *Analytic pre-processing* of (1.1) by a second order WKB-transformation of the form (1.5). The equation (1.1) is transformed into a smoother problem that can be solved accurately and efficiently on a coarse grid (see Fig. 1).

2. ε–uniform *discretization of the oscillatory integral* $\int \beta(y) \exp\left(\frac{2i}{\varepsilon}\phi(y)\right)\, dy$ (and multiple iterates of it) appearing in the numerical scheme for the transformed, smoother problem (cf. (2.6) below).

3. *Numerical integration of the phase* $\phi(x)$ in (1.5). Here, numerical errors of order $\mathcal{O}(h^\gamma)$ in the phase-computation will typically induce $\mathcal{O}(h^\gamma/\varepsilon)$ errors in the oscillatory integral. However, this phase integral can be computed explicitly in several relevant examples (e.g. RTDs).

In [14] the oscillatory integral is dealt with by first using a Taylor expansion of β and ϕ, followed by an integration by parts. But recently, quite refined techniques for the quadrature of oscillatory integrals were developed. The goal of the methods in [9, 15, 18] is to provide approximations for $\int_x^{x+h} \beta(y) \exp\left(\frac{2i}{\varepsilon}\phi(y)\right)\, dy$ of arbitrarily high ε–order. But for solving oscillatory ODEs there are of course additional requirements: The local discretization error must also be of sufficiently high h–order. Therefore let us first discuss, under this perspective, the existing techniques. The *asymptotic method* [9, 18] provides approximations of arbitrarily high ε–order. But since it does not yield high h–orders (cf. §2.2 for details), it is not usable for constructing ODE schemes. In *Filon-type quadrature* [9, 15], the oscillatory integral is approximated by integrals $\int_x^{x+h} \pi(y) \exp\left(\frac{2i}{\varepsilon}\phi(y)\right)\, dy$, where π is a polynomial interpolation of β, assuming that

the resulting moment integrals can be evaluated exactly. Since this is not the case here, Filon-type quadrature would not apply to our situation. In the *moment free Levin-type methods* [18, 19], the function β in the oscillatory integral is approximated (Hermite interpolation) by a function $L[v](y) := v' + \frac{2i}{\varepsilon}\phi' v$. Then the resulting integral can be evaluated exactly. With growing interpolation order, the error has increasing orders of εh. Hence, this method would appear suitable for oscillatory ODEs. But –to the authors' knowledge– it has not been used yet.

In §2.2 we shall present a new variant of the asymptotic method that trades ε–powers into h–powers. The idea is to subtract from the oscillatory term $\exp\left(\frac{2i}{\varepsilon}\phi(y)\right)$ of the integrand a trigonometric polynomial of the phase ϕ (which is appropriately compensated in the integration by parts). This procedure creates zeros in the integrand and increases the h–order of the error.

Standard methods for (1.1) (like in [6, 7]) used to require a step size $h = \mathcal{O}(\varepsilon)$ for accurate resolution. With a zeroth order WKB-transformation, the second order 2-step scheme of [14] reduces that limitation to $h = \mathcal{O}(\sqrt{\varepsilon})$. With the choice $\gamma = 4$ (Simpson rule) our second order 1-step scheme has, in general, the same h-limitation (see Theorems 3.1, 3.5). But for explicitly integrable phases, h can be chosen independently of ε in our scheme.

This *asymptotic correctness* w.r.t. ε is an additional novel feature of our scheme: RTD-models typically have piecewise linear potentials. Hence, the phase function ϕ in (1.5) can be integrated exactly. As a consequence, the numerical error decreases to zero as $\varepsilon \to 0$, even when using a fixed step size $h > 0$. Hence, the scheme with e.g. just 2 grid points on $[0, 1]$ becomes asymptotically correct in the highly oscillatory limit, which was a-priori the most difficult scenario.

We remark that the basic "philosophy" of this asymptotic correctness is closely related to *relaxation schemes* or *asymptotic preserving schemes*. These numerical schemes are developed for PDE-families that involve a small parameter ε, and they stay uniformly accurate also in the scaling limit $\varepsilon \to 0$. Examples include the diffusive limits of kinetic equations [10], kinetic to fluid dynamical limits [11], and the semiclassical limit of the time dependent Schrödinger equation [4].

This paper is organized as follows. In Section 2 we present the numerical method for solving the highly oscillating equation (1.1). In Section 3 the convergence of the numerical scheme is analyzed and the main result of this paper is stated in Theorem 3.1. The modified first and second order schemes of §3.2 present in addition a second order behaviour in ε. The advantages of the introduced methods and their (ε, h)–dependent error behavior are illustrated on a numerical example in §3.3.

2 Description of the method

The objective of this paper is to solve efficiently the following highly oscillating initial value problem (IVP):

$$\begin{cases} \varepsilon^2\varphi''(x) + a(x)\varphi(x) = 0\,, \quad x \in (0,1)\,, \\ \varphi(0) = \varphi_0\,, \\ \varepsilon\varphi'(0) = \varphi_1\,. \end{cases} \tag{2.1}$$

Here we are concerned with the scalar problem, with possibly complex valued initial conditions. The more technical vector valued situation will be addressed in a subsequent work.

To make the connection with our application presented in the introduction, we can put

$$a(x) = E - V(x)\,, \quad \varphi_0 = 1\,,\ \varphi_1 = -i\sqrt{a(0)}\,,$$

where E can be considered as fixed and $0 < \varepsilon < 1$ as arbitrarily small. The solution φ of the IVP (2.1) and that one of the BVP (1.2) are then related by

$$\psi_E(x) = -\frac{2ik(1)}{\varphi'(1) - ik(1)\varphi(1)}\varphi(x)\,.$$

The existence of a solution to problem (2.1) is stated in the following proposition.

Proposition 2.1 *[2, 16] Let $a \in W^{1,\infty}(0,1)$ be a given real function, satisfying $a(x) \geq a_0 > 0$ in $[0,1]$ and let $0 < \varepsilon < 1$ be fixed. Then the Schrödinger equation (2.1) admits a unique solution $\varphi \in W^{2,\infty}(0,1)$ verifying*

$$||\varphi||_{L^\infty(0,1)} \leq C\,, \quad ||\varepsilon\varphi'||_{L^\infty(0,1)} \leq C\,, \quad ||\varepsilon^2\varphi''||_{L^\infty(0,1)} \leq C\,,$$

with a constant $C > 0$ independent of ε.

This predicted oscillating behaviour of φ can be observed in Figure 2 (left) for two different ε-values.

We shall now introduce an efficient numerical method for solving (2.1). The idea is to first reformulate the oscillatory problem in order to get a new equation with "smoother" unknowns. This is the objective of Section 2.1. Then, this new problem can be solved numerically on a coarse grid (in §2.2). The originality of this procedure is that one fixed grid, independent of the wave-length $\varepsilon/\sqrt{a(x)}$, can be used to solve the "smooth" equation accurately, permitting thus a considerable gain in computational costs.
For simplicity only, we shall suppose all along this paper that a is smooth enough. Note, however, that piecewise smoothness of a would be enough. At discontinuities of a, the IVP could just be "restarted".

Hypothesis A *Let $a \in C^\infty[0,1]$ be a fixed smooth (real valued) function, satisfying $a(x) \geq a_0 > 0$ in $[0,1]$, which means that we are in the oscillatory regime. Besides, let $0 < \varepsilon < 1$ be an arbitrary real number.*

2.1 Reformulation of the continuous problem

The first step in our reformulation is to pass from the second order differential equation (2.1) to a system of first order differential equations. Setting

$$U(x) = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} := \begin{pmatrix} a^{1/4}\varphi(x) \\ \dfrac{\varepsilon(a^{1/4}\varphi)'(x)}{\sqrt{a(x)}} \end{pmatrix},$$

we have

$$\begin{cases} U'(x) = [A_0(x) + \varepsilon A_1(x)]\, U(x)\,, \quad 0 < x < 1 \\ U(0) = U_I\,, \end{cases} \tag{2.2}$$

with the two matrices

$$A_0(x) = \frac{\sqrt{a(x)}}{\varepsilon} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}; \quad A_1(x) = \begin{pmatrix} 0 & 0 \\ 2\beta(x) & 0 \end{pmatrix},$$

where

$$\beta = \frac{a''}{8a^{3/2}} - \frac{5(a')^2}{32a^{5/2}}\,.$$

Note that in (2.2) the matrix $A_0 = \mathcal{O}(\varepsilon^{-1})$ is dominant and gives rise to the highly oscillatory part in the solution. On the other hand, εA_1 is a small $\mathcal{O}(\varepsilon)$–perturbation. In contrast, [14] uses $\tilde{U}(x) := (\varphi(x),\, \varepsilon\varphi'(x)/\sqrt{a(x)})^\top$ to transform (2.1) to a first order system. And this results in an $\mathcal{O}(1)$–perturbation of the dominant matrix $A_0(x)$.

Proposition 2.1 implies the existence of a unique solution $U \in (W^{1,\infty}(0,1))^2$ of (2.2), satisfying

$$||U||_{L^\infty(0,1)} \le C \quad ; \quad ||U'||_{L^\infty(0,1)} \le \frac{C}{\varepsilon}\,, \tag{2.3}$$

with a constant $C > 0$ independent of ε.

As a second step we diagonalize now the dominant part of the system (2.2) by performing the change of variable

$$Y(x) := PU(x)\,,$$

where

$$P := \frac{1}{\sqrt{2}} \begin{pmatrix} i & 1 \\ 1 & i \end{pmatrix} \quad ; \quad P^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} -i & 1 \\ 1 & -i \end{pmatrix}.$$

The equation for Y reads

$$\begin{cases} \dfrac{dY}{dx} = \dfrac{i}{\varepsilon} D^\varepsilon Y + \varepsilon N Y\,, \quad 0 < x < 1\,, \\ Y(0) = Y_I\,, \end{cases} \tag{2.4}$$

with

$$D^\varepsilon(x) = \begin{pmatrix} D_1^\varepsilon(x) & 0 \\ 0 & D_2^\varepsilon(x) \end{pmatrix} = \begin{pmatrix} \sqrt{a} - \varepsilon^2\beta & 0 \\ 0 & -\sqrt{a} + \varepsilon^2\beta \end{pmatrix} \quad ; \quad N(x) = \beta(x) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

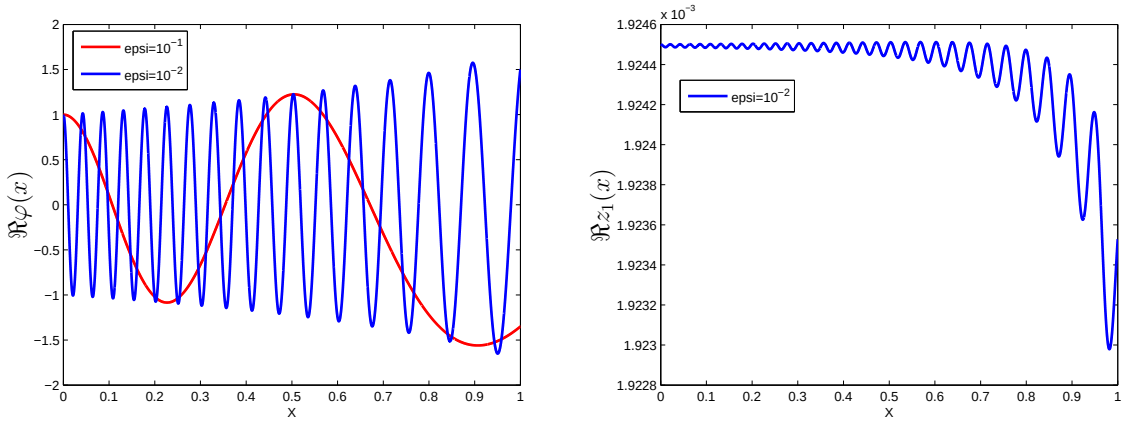

Figure 2: Left: solution $\Re\varphi(x)$ of (2.1) for 2 values of ε. Right: solution $\Re z_1(x)$ of (2.6). The simulation is performed for the same potential $a = (x + 1/2)^2$ as in §3.3.

Again, the matrix $\frac{i}{\varepsilon}D^\varepsilon$ gives rise to highly oscillatory solutions, while εN is a small perturbation.
In our final transformation step we eliminate the leading oscillations by defining the diagonal matrix

$$\Phi^\varepsilon(x) := \int_0^x D^\varepsilon(y)\,dy = \begin{pmatrix} \phi^\varepsilon & 0 \\ 0 & -\phi^\varepsilon \end{pmatrix},$$

with the (real valued) phase function

$$\phi^\varepsilon(x) := \int_0^x \left(\sqrt{a(\tau)} - \varepsilon^2\beta(\tau)\right) d\tau\,. \tag{2.5}$$

Note that this is precisely the phase in the second order WKB-approximation (1.5). Making the change of unknown

$$Z(x) = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} := \exp\left(-\frac{i}{\varepsilon}\Phi^\varepsilon(x)\right) Y(x)\,,$$

leads to the system

$$\begin{cases} \dfrac{dZ}{dx} = \varepsilon N^\varepsilon Z\,, \quad 0 < x < 1\,, \\ Z(0) = Z_I = Y_I\,. \end{cases} \tag{2.6}$$

Here, the matrix

$$N^\varepsilon = \exp(-\frac{i}{\varepsilon}\Phi^\varepsilon)\, N\, \exp(\frac{i}{\varepsilon}\Phi^\varepsilon)\,,$$

is bounded independently of ε. It is off-diagonal, with the entries

$$N^\varepsilon_{1,2}(x) = \beta(x)e^{-\frac{2i}{\varepsilon}\phi^\varepsilon(x)}\,, \quad N^\varepsilon_{2,1}(x) = \beta(x)e^{\frac{2i}{\varepsilon}\phi^\varepsilon(x)}\,.$$

Note that, due to our higher order WKB-transformation, the ODE (2.6) has a trivial limit (for $\varepsilon \to 0$), while the r.h.s. of the corresponding equation in §2.5 of [14] was only

$\mathcal{O}(1)$. Hence, the solution to our equation (2.6) converges as $\varepsilon \to 0$ to $Z^0(x) := Z_I$ (uniformly in x). This limit is trivial to capture numerically and the core of the above mentioned asymptotic correctness (w.r.t. ε) of the presented scheme. The importance of recovering numerically such *adiabatic invariants* of (2.1) was already mentioned in §3 of [8].

The principal idea of this paper is that, instead of solving (2.2), we shall solve numerically (2.6) and recover then the original solution by

$$U(x) = P^{-1} e^{\frac{i}{\varepsilon}\Phi^\varepsilon(x)} Z(x)\,. \tag{2.7}$$

In particular this inverse transform of the asymptotic limit $Z_I = (z_1, z_2)^\top$ is given by

$$\varphi(x) = \frac{1}{\sqrt{2}\sqrt[4]{a(x)}} \left(-i\, e^{\frac{i}{\varepsilon}\phi^\varepsilon(x)} z_1 + e^{-\frac{i}{\varepsilon}\phi^\varepsilon(x)} z_2 \right) ,$$

which is a combination of the second order WKB-functions (1.5).
Let us explain in some words the essential advantage of doing so. For small ε, the function U is highly oscillating, with amplitude of order $\mathcal{O}(1)$ (see (2.3) and Figure 2). Thus, a very fine grid (e.g. 10 discretization points per wave length) has to be chosen in order to solve accurately enough the system (2.2). The function Z is also highly oscillating – approximately with the same frequency as U. But, as a great advantage, Z oscillates around a smooth function, with an amplitude only of the order $\mathcal{O}(\varepsilon^2)$ (see (2.9) and Figure 2). Hence, if we take a coarse grid with a step size $h \gg \varepsilon$ (step size superior to the wave-length), then we shall incur at maximum an error of the order $\mathcal{O}(\varepsilon^2)$ when solving (2.6), whereas for (2.2) the error would be of the order $\mathcal{O}(1)$. This is summarized in the following proposition.

Proposition 2.2 *Under Hypothesis A, the problem (2.6) admits a unique solution $Z \in C^\infty[0,1]$ with the explicit form*

$$Z(x) = Z_I + \sum_{p=1}^{\infty} \varepsilon^p M_p^\varepsilon(x;0) Z_I\,, \tag{2.8}$$

where the matrices M_p^ε are defined in (2.11). Moreover we have

$$||Z - Z_I||_{L^\infty(0,1)} \le C\varepsilon^2\,, \quad ||Z'||_{L^\infty(0,1)} \le C\varepsilon\,, \quad ||Z''||_{L^\infty(0,1)} \le C\,, \tag{2.9}$$

with a constant $C > 0$ independent of ε.

Proof Integrating the equation for Z (2.6) over the interval (s,t), we find

$$\begin{aligned} Z(t) &= Z(s) + \varepsilon \int_s^t N^\varepsilon(y_1) Z(y_1)\, dy_1 \\ &= Z(s) + \varepsilon \left(\int_s^t N^\varepsilon(y_1)\, dy_1 \right) Z(s) + \varepsilon^2 \int_s^t N^\varepsilon(y_1) \int_s^{y_1} N^\varepsilon(y_2) Z(y_2)\, dy_2\, dy_1 \\ &= Z(s) + \sum_{p=1}^{\infty} \varepsilon^p M_p^\varepsilon(t;s) Z(s), \end{aligned} \tag{2.10}$$

where $M_0^\varepsilon = Id$ and for $p \geq 1$

$$\begin{aligned} M_p^\varepsilon(t;s) &= \int_s^t \int_s^{y_1} \cdots \int_s^{y_{p-1}} N^\varepsilon(y_1) \cdots N^\varepsilon(y_p)\, dy_p \cdots dy_1\,, \\ M_p^\varepsilon(t;s) &= \int_s^t N^\varepsilon(y) M_{p-1}^\varepsilon(y;s)\, dy\,. \end{aligned} \tag{2.11}$$

Since N^ε is oscillating at the frequency $\frac{1}{\varepsilon}$, it is clear that $M_1^\varepsilon(t;s) = \mathcal{O}(\min(\varepsilon, |t-s|))$. This implies immediately that

$$M_p^\varepsilon(t;s) = \mathcal{O}\left(\frac{|t-s|^{p-1}}{p!}\min(p\varepsilon, |t-s|)\right)\,, \tag{2.12}$$

so that the terms involved in the expansion of $Z(t)$ are of the order $\varepsilon \min(p\varepsilon, |t-s|)(\varepsilon|t-s|)^{p-1}/p!$. This gives immediately rise to the estimates (2.9) and it shows the convergence of (2.8). □

To summarize, the solution U of the initial problem (2.2) is highly oscillating for $\varepsilon \ll 1$ and demands thus the use of very fine meshes in standard methods. To compute U, we will solve instead the reformulated problem (2.6) and transform back via (2.7). As will be seen in Section 3, this procedure allows to use coarser grids ($h > \varepsilon$), leading to a considerably gain in simulation time.

2.2 Numerical discretization of the transformed problem

The aim of this section is to introduce a first order and a second order scheme to solve the IVP

$$\begin{cases} \dfrac{dZ}{dx} = \varepsilon N^\varepsilon Z\,, \quad 0 < x < 1\,, \\ Z(0) = Z_I = Y_I\,. \end{cases} \tag{2.13}$$

Since N^ε is highly oscillatory, we shall pay attention to the ε–uniform discretization of the oscillatory integrals. Let $0 = x_1 < \cdots < x_n < \cdots < x_N = 1$ be a discretization of the interval $(0,1)$ and $h := \max_{n=1,\cdots,N-1} |x_{n+1} - x_n|$. In the following, for simplicity, we shall often denote the cell $I_n := (x_n, x_{n+1})$ simply by (s,t), i.e. $s = x_n$ and $t = x_{n+1}$.

In order to design a scheme of order k, we shall use the formula (2.8) (limit of Picard iteration)

$$Z(t) = Z(s) + \sum_{p=1}^{\infty} \varepsilon^p M_p^\varepsilon(t;s) Z(s)\,, \tag{2.14}$$

and truncate the series at order k, the remainder being of the order $\varepsilon^{k+1} h^k \min(\varepsilon, h)$. This will lead to a scheme of order k for $h < \varepsilon$. Now the additional difficulty comes from the fact that the highly oscillating integrals M_p^ε cannot be computed exactly, such that further errors will be introduced. Good approximations are thus needed, with errors controlled independently of ε. The idea is to use integration by parts to filter out the oscillations. We present now this procedure for the expansions of M_1^ε and M_2^ε.

Expansion of M_1^ε. Since N^ε is off-diagonal and its entries are complex conjugate of one another, we only have to compute $m_1^\varepsilon = (M_1^\varepsilon)_{2,1}$ for instance. This gives

$$\begin{aligned}
m_1^\varepsilon(t;s) =& \int_s^t \beta(y) e^{\frac{2i}{\varepsilon}\phi(y)}\, dy = e^{\frac{2i}{\varepsilon}\phi(s)} \int_s^t \beta(y) e^{\frac{2i}{\varepsilon}(\phi(y)-\phi(s))} dy \\
=& -(i\varepsilon)\, e^{\frac{2i}{\varepsilon}\phi(s)} \int_s^t \frac{\beta}{2\phi'}(y) \frac{d}{dy}\left(e^{\frac{2i}{\varepsilon}(\phi(y)-\phi(s))} - 1 \right) dy \\
=& -(i\varepsilon) e^{\frac{2i}{\varepsilon}\phi(s)} \left\{ \left[\beta_0(y) H_1\!\left(\frac{2}{\varepsilon}(\phi(y)-\phi(s)) \right) \right]_s^t - \int_s^t \beta_0'(y) H_1\!\left(\frac{2}{\varepsilon}(\phi(y)-\phi(s)) \right) dy \right\} \\
=& -(i\varepsilon) e^{\frac{2i}{\varepsilon}\phi(s)} \left\{ \beta_0(t) H_1\!\left(\frac{2}{\varepsilon}(\phi(t)-\phi(s)) \right) + i\varepsilon \int_s^t \beta_1(y) H_2\!\left(\frac{2}{\varepsilon}(\phi(y)-\phi(s)) \right)' dy \right\} \\
=& -(i\varepsilon) e^{\frac{2i}{\varepsilon}\phi(s)} \left\{ \beta_0(t) H_1\!\left(\frac{2}{\varepsilon}(\phi(t)-\phi(s)) \right) + i\varepsilon \beta_1(t) H_2\!\left(\frac{2}{\varepsilon}(\phi(t)-\phi(s)) \right) \right\} \\
& \qquad + \mathcal{O}(h^2 \min(\varepsilon, h))\,,
\end{aligned} \tag{2.15}$$

where

$$H_k(t) := e^{it} - \sum_{p=0}^{k-1} \frac{(it)^p}{p!},$$

$$\beta_0(y) := \frac{\beta}{2\phi'}(y) = \frac{\beta}{2(\sqrt{a} - \varepsilon^2 \beta)}(y); \qquad \beta_{k+1} := \frac{1}{2\phi'(y)} \frac{d}{dy}\left(\beta_k\right)(y).$$

Continuing iteratively we obtain the asymptotic expansion

$$m_1^\varepsilon(t;s) \sim -\sum_{k=1}^{\infty} (i\varepsilon)^k e^{\frac{2i}{\varepsilon}\phi(s)} \beta_{k-1}(t) H_k\left(\frac{2}{\varepsilon}(\phi(t) - \phi(s)) \right). \tag{2.16}$$

But just as in §3.1 of [9], the series (2.16) might not converge.

Note that (2.5) and Hypothesis A imply $\phi'(x) \geq \phi_0 > 0$ for ε sufficiently small. Hence, the phase ϕ has no stationary point and $\|\beta_k\|_{L^\infty(0,1)}$ is uniformly bounded w.r.t. small ε. Since

$$H_k(t) = \mathcal{O}(\min(t^k, t^{k-1}))\,, \tag{2.17}$$

the k^{th} term of the expansion of m_1^ε is of the order $h^{k-1}\min(\varepsilon, h)$, for $k \geq 1$. Keeping only the first term yields a consistency error of order $h\min(\varepsilon, h)$ thus producing an order 1 scheme in the region $h < \varepsilon$. Keeping the first two terms yields an error of order $h^2 \min(\varepsilon, h)$, thus producing an order 2 scheme for $h < \varepsilon$.
This expansion is reminiscent of the *asymptotic method* for oscillatory integrals (cf. §2 of [9], §2 of [18]). Indeed

$$\begin{aligned}
m_1^\varepsilon(t;s) =& -(i\varepsilon)\left[\beta_0(y) e^{\frac{2i}{\varepsilon}\phi(y)} \right]_s^t - (i\varepsilon)^2 \left[\beta_1(y) e^{\frac{2i}{\varepsilon}\phi(y)} \right]_s^t + (i\varepsilon)^2 \int_s^t \beta_1'(y) e^{\frac{2i}{\varepsilon}\phi(y)}\, dy \\
\sim& -\sum_{k=1}^{\infty} (i\varepsilon)^k \left[\beta_{k-1}(t) e^{\frac{2i}{\varepsilon}\phi(t)} - \beta_{k-1}(s) e^{\frac{2i}{\varepsilon}\phi(s)} \right],
\end{aligned} \tag{2.18}$$

where the remainder integral after two partial integrations is of the order $\mathcal{O}(\varepsilon^2 \min(\varepsilon, h))$. Note that our expansion in (2.15) yields higher h–orders with each integration by parts (due to the k–th order zero of H_k at $t = 0$), while the asymptotic method (2.18) yields higher ε–orders. In §3.2 we shall derive a modified expansion with the "intermediate" truncation error of order $\varepsilon h \min(\varepsilon, h)$.

We remark that finite truncations of the asymptotic expansion (2.16) do not preserve the original skew-symmetry of $m_1^\varepsilon(t;s)$ w.r.t. interchanging t and s. If this property of the approximation is desirable, it is easily recovered by rather extracting the factor $\exp\left(\frac{2i}{\varepsilon}\phi(\frac{s+t}{2})\right)$ in the first step of (2.15) instead of $\exp\left(\frac{2i}{\varepsilon}\phi(s)\right)$. This will however only intricate the formulae without improving them, such that we shall not pursue this direction in the following.

Expansion of M_2^ε. The expansion of M_2^ε is only needed for the construction of the second order scheme. We have

$$M_2^\varepsilon(t;s) = \int_s^t N^\varepsilon(y) M_1^\varepsilon(y;s)\, dy,$$

such that we shall use the expansion of M_1^ε to approximate M_2^ε. Since N^ε and M_1^ε are off-diagonal, the M_2^ε-matrix is diagonal and the entries are conjugate of one another. Thus we will only study the term $m_2^\varepsilon = (M_2^\varepsilon)_{1,1}$. Since we are looking at the corrections needed for the second order scheme, we only need the first term of the expansion of M_1^ε, which gives

$$\begin{aligned}
m_2^\varepsilon(t;s) &= \int_s^t N_{1,2}^\varepsilon(y)(M_1^\varepsilon)_{2,1}(y;s)\, dy \\
&= i\varepsilon \int_s^t N_{1,2}^\varepsilon(y) \left[\beta_0(y)(e^{\frac{2i}{\varepsilon}\phi(s)} - e^{\frac{2i}{\varepsilon}\phi(y)}) + \mathcal{O}(\frac{h}{\varepsilon}\min(\varepsilon, h))\right] dy \\
&= i\varepsilon \int_s^t \beta(y)\beta_0(y) \left(e^{-\frac{2i}{\varepsilon}[\phi(y)-\phi(s)]} - 1\right) dy + \mathcal{O}(h^2 \min(\varepsilon, h)) \qquad (2.19) \\
&= (i\varepsilon)^2 \int_s^t (\beta_0(y))^2 \left(H_2(-\frac{2}{\varepsilon}[\phi(y) - \phi(s)])\right)' dy + \mathcal{O}(h^2 \min(\varepsilon, h)) \\
&= (i\varepsilon)^2 (\beta_0(t))^2 \left(H_2(-\frac{2}{\varepsilon}[\phi(t) - \phi(s)])\right) + \mathcal{O}(h^2 \min(\varepsilon, h))\,.
\end{aligned}$$

We have now all the necessary elements to introduce the first and the second order schemes for solving the reformulated equation (2.6) in the unknown Z.
Let $Z_1 := Z_I$ be the initial condition and let $n = 1, \cdots, N$.

First order scheme.

$$Z_{n+1} = Z_n + A_n^1 Z_n, \qquad (2.20)$$

with the 2×2 matrix

$$\begin{aligned} A_n^1 &:= -i\varepsilon^2\beta_0(x_{n+1}) \begin{pmatrix} 0 & e^{-\frac{2i}{\varepsilon}\phi(x_n)} - e^{-\frac{2i}{\varepsilon}\phi(x_{n+1})} \\ e^{\frac{2i}{\varepsilon}\phi(x_{n+1})} - e^{\frac{2i}{\varepsilon}\phi(x_n)} & 0 \end{pmatrix} \\ &= -i\varepsilon^2\beta_0(x_{n+1}) \begin{pmatrix} 0 & -e^{-\frac{2i}{\varepsilon}\phi(x_n)} H_1(-\frac{2}{\varepsilon}S_n) \\ e^{\frac{2i}{\varepsilon}\phi(x_n)} H_1(\frac{2}{\varepsilon}S_n) & 0 \end{pmatrix}, \end{aligned} \tag{2.21}$$

and the phase

$$S_n := \phi(x_{n+1}) - \phi(x_n) = \int_{x_n}^{x_{n+1}} \Big(\sqrt{a(\tau)} - \varepsilon^2\beta(\tau) \Big)\, d\tau.$$

In this scheme we assume that the function β (involving the derivatives a', a'') is explicitly "available". Alternatively, a' and a'' could be approximated numerically.

Second order scheme.

$$Z_{n+1} = Z_n + (A_n^1 + A_n^2) Z_n, \tag{2.22}$$

where A_n^1 is given by (2.21) and

$$\begin{aligned} A_n^2 &:= \varepsilon^3\beta_1(x_{n+1}) \begin{pmatrix} 0 & e^{-\frac{2i}{\varepsilon}\phi(x_n)} H_2(-\dfrac{2S_n}{\varepsilon}) \\ e^{\frac{2i}{\varepsilon}\phi(x_n)} H_2(\dfrac{2S_n}{\varepsilon}) & 0 \end{pmatrix} \\ &\quad -\varepsilon^4(\beta_0(x_{n+1}))^2 \begin{pmatrix} H_2(-\dfrac{2S_n}{\varepsilon}) & 0 \\ 0 & H_2(\dfrac{2S_n}{\varepsilon}) \end{pmatrix}. \end{aligned} \tag{2.23}$$

In order to compute the solution of (2.2) and thus get the wave function φ as well as its derivative φ', we have to transform back via

$$Y_n = e^{\frac{i}{\varepsilon}\Phi^\varepsilon(x_n)} Z_n\,, \quad U_n = P^{-1} Y_n\,, \quad n = 1, ..., N\,. \tag{2.24}$$

We shall now discuss if these two schemes preserve the current conservation property of problem (2.1). In the continuous case the current density satisfies

$$\begin{aligned} j(x) &:= \varepsilon\Im(\overline{\varphi}(x)\varphi'(x)) = -\frac{1}{2i} U(x)^\top \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \overline{U}(x) \\ &= -\frac{1}{2i} Z(x)^\top e^{\frac{i}{\varepsilon}\Phi^\varepsilon(x)} P^{-1} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} P e^{-\frac{i}{\varepsilon}\Phi^\varepsilon(x)} \overline{Z}(x) \\ &= \frac{1}{2} Z(x)^\top \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \overline{Z}(x)\,, \end{aligned} \tag{2.25}$$

which is constant along the domain $(0,1)$ due to (2.6). Analogously we have on the discrete level

$$j_n := \frac{1}{2} Z_n^\top \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \overline{Z}_n \,, \quad 1 \le n \le N \,. \tag{2.26}$$

As we shall see in Prop. 3.3, the above schemes do not keep the discrete current perfectly constant, but up to a small error of the order $\mathcal{O}(\varepsilon^2 \min(\varepsilon, h))$. However, this can be easily adjusted.

In Section 3 we first analyze the convergence of the first order scheme (2.20), (2.21), (2.24) and of the second order scheme (2.22), (2.23), (2.24). Then we shall present numerical results obtained with the above schemes, including a check on the (almost) preservation of the current by (2.26).

3 Error analysis and numerical results

3.1 Convergence of the method

The next theorem is the essential result of this paper. Let us denote in the following by $Z(x)$ (resp. $U(x)$) the exact solution of the continuous problem (2.6) (resp. (2.2)). And $(Z_n)_{n=1}^N$ (resp.$(U_n)_{n=1}^N$) denotes the numerical approximation of $Z(x_n)$ (resp. $U(x_n)$), computed via the first order scheme (2.20), (2.21), (2.24) or the second order scheme (2.22), (2.23), (2.24) presented in Section 2.2. Then we have the following error estimates.

Theorem 3.1 *Let Hypothesis A be satisfied. Then the global errors of the numerical schemes introduced in §2.2 satisfy*

$$||Z(x_n) - Z_n||_2 \le C\varepsilon h^\alpha \min(\varepsilon, h) \,, \quad 1 \le n \le N \,, \tag{3.1}$$

$$||U(x_n) - U_n||_2 \le C\frac{h^\gamma}{\varepsilon} + C\varepsilon h^\alpha \min(\varepsilon, h) \,, \quad 1 \le n \le N \,, \tag{3.2}$$

with C independent of h and ε. Here, $\gamma > 0$ is the order of the chosen numerical integration method for the computation of the phase integral

$$\Phi^\varepsilon(x) = \int_0^x \left(\sqrt{a(\tau)} - \varepsilon^2 \beta(\tau) \right) d\tau \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{3.3}$$

The discretization step size is $h > 0$, and we have $\alpha = 0$ for the first order scheme and $\alpha = 1$ for the second order scheme.

Proof Both schemes can be written under the form

$$Z_{n+1} = (I + B_n^k) Z_n \,, \quad k = 1, 2 \,, \tag{3.4}$$

where $B_n^1 = A_n^1$ (first order scheme) and $B_n^2 = A_n^1 + A_n^2$ (second order scheme). With (2.17) we have

$$A_n^k = \mathcal{O}(\varepsilon h^{k-1} \min(\varepsilon, h)) \,, \quad k = 1,\, 2 \,.$$

Hence, both schemes are stable, with an ε–independent stability constant.

The consistency error for the first order scheme is given by

$$e_n := \left[\varepsilon M_1^\varepsilon(x_{n+1};x_n) - A_n^1\right] Z(x_n) + \gamma_n\,, \quad \gamma_n := \sum_{p=2}^{\infty} \varepsilon^p M_p^\varepsilon(x_{n+1};x_n) Z(x_n)\,, \tag{3.5}$$

with the order of magnitude of these terms given by (2.12), i.e.

$$M_1^\varepsilon(x_{n+1};x_n) = \mathcal{O}(\min(\varepsilon,h))\,, \quad \gamma_n = \mathcal{O}(\varepsilon^2 h \min(\varepsilon,h))\,.$$

The construction of A_n^1 (see (2.16)) yields moreover

$$\varepsilon M_1^\varepsilon(x_{n+1};x_n) - A_n^1 = \mathcal{O}(\varepsilon h \min(\varepsilon,h))\,. \tag{3.6}$$

And this proves the assertion (3.1) for $\alpha = 0$.

For the second order scheme we have

$$\begin{aligned} e_n &:= \left[\varepsilon M_1^\varepsilon(x_{n+1};x_n) + \varepsilon^2 M_2^\varepsilon(x_{n+1};x_n) - B_n^2\right] Z(x_n) + \gamma_n\,, \\ \gamma_n &:= \sum_{p=3}^{\infty} \varepsilon^p M_p^\varepsilon(x_{n+1};x_n) Z(x_n)\,, \end{aligned}$$

where $\gamma_n = \mathcal{O}(\varepsilon^3 h^2 \min(\varepsilon,h))$. By the construction of A_n^1 and A_n^2 we deduce

$$\begin{aligned} \varepsilon M_1^\varepsilon(x_{n+1};x_n) + \varepsilon^2 M_2^\varepsilon(x_{n+1};x_n) - B_n^2 &= \mathcal{O}(\varepsilon h^2 \min(\varepsilon,h)) + \mathcal{O}(\varepsilon^2 h^2 \min(\varepsilon,h)) \\ &= \mathcal{O}(\varepsilon h^2 \min(\varepsilon,h))\,, \end{aligned}$$

implying for the second order scheme

$$||Z(x_{n+1}) - Z_{n+1}||_2 \le C\varepsilon h \min(\varepsilon,h)\,. \tag{3.7}$$

To obtain now the initially "desired" solution U of (2.2), we have to transform back Z. This often introduces some additional errors, in particular due to the numerical computation of the phase-matrix (3.3). Indeed,

$$\begin{aligned} U(x_{n+1}) - U_{n+1} &= P^{-1} e^{\frac{i}{\varepsilon}\Phi^\varepsilon(x_{n+1})} Z(x_{n+1}) - P^{-1} e^{\frac{i}{\varepsilon}\Phi^\varepsilon_{n+1}} Z_{n+1} \\ &= P^{-1}\left\{\left[e^{\frac{i}{\varepsilon}\Phi^\varepsilon(x_{n+1})} - e^{\frac{i}{\varepsilon}\Phi^\varepsilon_{n+1}}\right] Z(x_{n+1}) + e^{\frac{i}{\varepsilon}\Phi^\varepsilon_{n+1}}\left[Z(x_{n+1}) - Z_{n+1}\right]\right\}. \end{aligned} \tag{3.8}$$

Thus we have

$$||U(x_{n+1}) - U_{n+1}||_2 \le C||e^{\frac{i}{\varepsilon}\Phi^\varepsilon(x_{n+1})} - e^{\frac{i}{\varepsilon}\Phi^\varepsilon_{n+1}}||_2 + C||Z(x_{n+1}) - Z_{n+1}||_2\,. \tag{3.9}$$

The first term on the right hand side of (3.9) is rather unfavourable as it depends on $\frac{1}{\varepsilon}$. Indeed, if we choose an integration method of order γ to compute the phase Φ^ε (for example $\gamma = 4$ for the Simpson rule), we will have an error with

$$||e^{\frac{i}{\varepsilon}\Phi^\varepsilon(x_n)} - e^{\frac{i}{\varepsilon}\Phi^\varepsilon_n}||_2 \le C\frac{h^\gamma}{\varepsilon}\,.$$

And this yields the error estimate (3.2) for U. □

Remark 3.2 *Theorem 3.1 shows that the back-transformation (2.24) from Z to U introduces an unsatisfactory error behaving like $1/\varepsilon$, due to the numerical approximation of the phase Φ^ε. However, this error term can be avoided in some interesting applications. For example, RTD-models typically involve a piecewise linear potential $a(x)$, for which the phase can be integrated exactly.*

Let us now study the discrete current conservation of (2.26).

Proposition 3.3 *Under Hypothesis A the numerical schemes introduced in §2.2 conserve the discrete current defined in (2.25), up to an error of*

$$|j_{n+1} - j_n| \le C\varepsilon^2(\min(\varepsilon, h))^2\,, \quad n = 1, ..., N-1\,,$$

which yields $j_n = j_I + \mathcal{O}(\varepsilon^2 \min(\varepsilon, h))$ for each $n = 2, \cdots, N$, where $j_I := \varepsilon\Im(\overline{\varphi}(0)\varphi'(0))$ is the initial current.

Proof For the first order scheme (2.20) we have with (2.26)

$$\begin{aligned} j_{n+1} - j_n &= \frac{1}{2} Z_n^\top \left\{ (I + A_n^1)^\top \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} (I + \overline{A}_n^1) - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \overline{Z}_n \\ &= \frac{1}{2} Z_n^\top (A_n^1)^\top \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \overline{A}_n^1 \overline{Z}_n = -\frac{1}{2} (A_n^1)_{12} (A_n^1)_{21} Z_n^\top \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \overline{Z}_n \\ &= -\varepsilon^4 \beta_0^2(x_{n+1}) |H_1(\tfrac{2}{\varepsilon} S_n)|^2 j_n\,. \end{aligned} \tag{3.10}$$

□

Remark 3.4 *Note from (3.10) that the error of the current has a (negative) sign. Hence, the error does not oscillate around the correct value j_I, but rather drifts away slowly (see Fig. 3). If perfect conservation of the discrete current is required, one could easily modify the first order scheme (2.20) as follows:*

$$\tilde{Z}_{n+1} = \left(1 - \varepsilon^4 \beta_0^2(x_{n+1}) |H_1(\frac{2}{\varepsilon} S_n)|^2 \right)^{-1/2} (I + A_n^1) \tilde{Z}_n\,.$$

And the resulting first order scheme still satisfies the convergence estimate of Theorem 3.1. A similar modification would also be possible for the modified first order scheme of §3.2 below.

3.2 A modified first and second order scheme

In this section we shall derive a slightly modified first order method which is an improvement (w.r.t. its ε–order) of the first order scheme presented in §2.2. In the quantum mechanical applications presented in the introduction we are particularly interested in the regime $h \gg \varepsilon$. There, Theorem 3.1 gives an error estimate of $\mathcal{O}(\varepsilon^2)$ for the first order Z-scheme in this regime. But, as shown in Proposition 2.2, it is sufficient to take

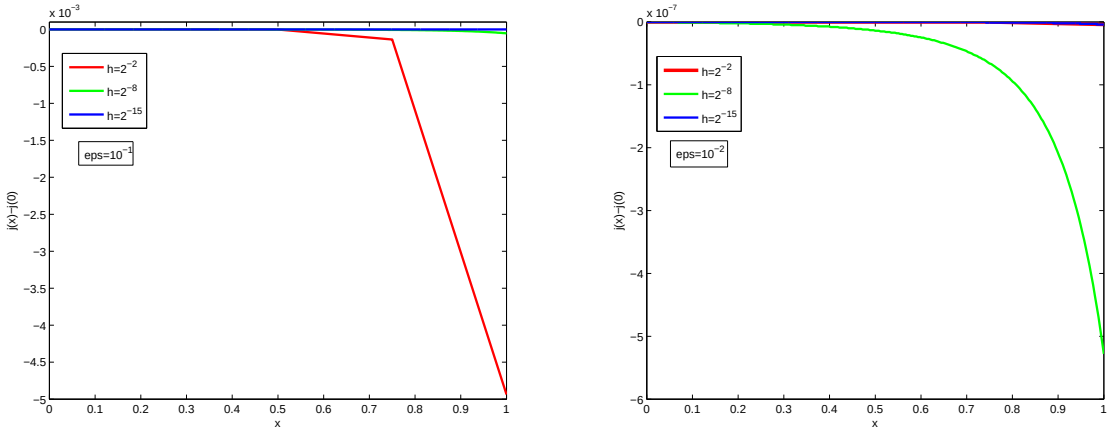

Figure 3: Quasi current conservation: current drift $j(x) - j_I$ for different step sizes h and different ε-values.

(without any computation!) $Z_n = Z_I$ for $n = 1, \cdots, N$ in order to get an error of $\mathcal{O}(\varepsilon^2)$. Thus an improvement of the presented first order scheme would be desirable.

We have seen that

$$Z(x_{n+1}) = Z(x_n) + \varepsilon M_1^\varepsilon(x_{n+1}; x_n) Z(x_n) + \gamma_n\,, \quad \text{with} \quad \gamma_n = \mathcal{O}(\varepsilon^2 h \min(\varepsilon, h))\,.$$

The idea is now to expand $M_1^\varepsilon(x_{n+1}; x_n)$ differently from (2.16) in order to reduce the consistency error to the same magnitude as γ_n. This will improve the error estimate (3.1) by one ε-order. To this end two different partial integrations will be performed. First we make one step of the standard asymptotic method (2.18). This increases the ε–power of the error to $\mathcal{O}(\varepsilon \min(\varepsilon, h))$:

$$\begin{aligned} m_1^\varepsilon(t;s) = & \int_s^t \beta(y) e^{\frac{2i}{\varepsilon}\phi(y)}\, dy = -i\varepsilon \int_s^t \beta_0(y) \left[e^{\frac{2i}{\varepsilon}\phi(y)}\right]' dy \\ = & -i\varepsilon \left[\beta_0(y) e^{\frac{2i}{\varepsilon}\phi(y)}\right]_s^t + i\varepsilon \int_s^t \beta_0'(y) e^{\frac{2i}{\varepsilon}\phi(y)} dy = -i\varepsilon \left[\beta_0(y) e^{\frac{2i}{\varepsilon}\phi(y)}\right]_s^t + T_\varepsilon(t,s)\,. \end{aligned} \tag{3.11}$$

Next we make one step of the "shifted asymptotic method" (2.15). This increases the order of the method w.r.t. h. Indeed,

$$\begin{aligned} T_\varepsilon(t,s) = & \; i\varepsilon \int_s^t \beta_0'(y) e^{\frac{2i}{\varepsilon}\phi(y)} dy = -(i\varepsilon)^2 e^{\frac{2i}{\varepsilon}\phi(s)} \int_s^t \beta_1(y) \left[e^{\frac{2i}{\varepsilon}(\phi(y)-\phi(s))} - 1\right]' dy \\ = & \; -(i\varepsilon)^2 e^{\frac{2i}{\varepsilon}\phi(s)} \left[\beta_1(y) H_1(\tfrac{2}{\varepsilon}(\phi(y) - \phi(s)))\right]_s^t + \mathcal{O}(\varepsilon h \min(\varepsilon, h))\,. \end{aligned} \tag{3.12}$$

This will lead to a consistency error of the order $\mathcal{O}(\varepsilon^2 h \min(\varepsilon, h))$.

Thus the **modified first order scheme** reads now

$$Z_{n+1} = (I + A^1_{n,mod})Z_n\,, \tag{3.13}$$

with the 2×2 matrix

$$\begin{aligned} A^1_{n,mod} &:= \varepsilon^3\beta_1(x_{n+1}) \begin{pmatrix} 0 & e^{-\frac{2i}{\varepsilon}\phi(x_n)}H_1(-\frac{2}{\varepsilon}S_n) \\ e^{\frac{2i}{\varepsilon}\phi(x_n)}H_1(\frac{2}{\varepsilon}S_n) & 0 \end{pmatrix} \\ &-i\varepsilon^2 \begin{pmatrix} 0 & \beta_0(x_n)e^{-\frac{2i}{\varepsilon}\phi(x_n)} - \beta_0(x_{n+1})e^{-\frac{2i}{\varepsilon}\phi(x_{n+1})} \\ \beta_0(x_{n+1})e^{\frac{2i}{\varepsilon}\phi(x_{n+1})} - \beta_0(x_n)e^{\frac{2i}{\varepsilon}\phi(x_n)} & 0 \end{pmatrix}, \end{aligned} \tag{3.14}$$

and the phase increments

$$S_n := \phi(x_{n+1}) - \phi(x_n) = \int_{x_n}^{x_{n+1}} \Big(\sqrt{a(\tau)} - \varepsilon^2\beta(\tau)\Big)\,d\tau.$$

Now we turn to the second order scheme (2.22), (2.23), (2.24). According to Theorem 3.1 it has an error of $\mathcal{O}(\varepsilon^2 h)$ for $h \gg \varepsilon$. With a modification of the scheme we shall now improve on this ε–power. Truncating (2.14) at $p = 2$ yields

$$\begin{aligned} Z(x_{n+1}) &= Z(x_n) + \left[\varepsilon M^\varepsilon_1(x_{n+1}; x_n) + \varepsilon^2 M^\varepsilon_2(x_{n+1}; x_n)\right] Z(x_n) + \theta_n\,, \quad \text{with} \\ \theta_n &= \mathcal{O}(\varepsilon^3 h^2 \min(\varepsilon, h))\,. \end{aligned} \tag{3.15}$$

Proceeding similarly to (3.11) we shall now improve the consistency error of the second order scheme to $\mathcal{O}(\varepsilon^2 h^2 \min(\varepsilon, h))$. Note that, due to (3.15), a further improvement to $\mathcal{O}(\varepsilon^3 h^2 \min(\varepsilon, h))$ would be possible, by adding one more term for the M^ε_1– and M^ε_2–approximations.

We proceed as in (3.11), but add a second step of the "shifted asymptotic method". This yields

$$\begin{aligned} m^\varepsilon_1(t; s) &= -i\varepsilon \left[\beta_0(y)e^{\frac{2i}{\varepsilon}\phi(y)}\right]_s^t - (i\varepsilon)^2 e^{\frac{2i}{\varepsilon}\phi(s)} \left[\beta_1(y)H_1\left(\tfrac{2}{\varepsilon}(\phi(y) - \phi(s))\right)\right]_s^t \\ &\quad -(i\varepsilon)^3 e^{\frac{2i}{\varepsilon}\phi(s)} \left[\beta_2(y)H_2\left(\tfrac{2}{\varepsilon}(\phi(y) - \phi(s))\right)\right]_s^t \\ &\quad +(i\varepsilon)^3 e^{\frac{2i}{\varepsilon}\phi(s)} \int_s^t \beta_2'(y)H_2\left(\frac{2}{\varepsilon}(\phi(y) - \phi(s))\right) dy\,, \end{aligned} \tag{3.16}$$

and the last integral is of the order $\mathcal{O}(\varepsilon h^2 \min(\varepsilon, h))$. This will lead to a consistency error of the order $\mathcal{O}(\varepsilon^2 h \min(\varepsilon, h))$, since the expansion of m^ε_2 from (2.19) needs no modification.

Thus the **modified second order scheme** reads now

$$Z_{n+1} = (I + A^1_{n,mod} + A^2_{n,mod})Z_n\,. \tag{3.17}$$

$A^1_{n,mod}$ is given in (3.14), $A^2_{n,mod}$ is the 2×2 matrix

$$\begin{aligned} A^2_{n,mod} \;:=\; & i\varepsilon^4 \beta_2(x_{n+1}) \begin{pmatrix} 0 & -e^{-\frac{2i}{\varepsilon}\phi(x_n)} H_2(-\frac{2S_n}{\varepsilon}) \\ e^{\frac{2i}{\varepsilon}\phi(x_n)} H_2(\frac{2S_n}{\varepsilon}) & 0 \end{pmatrix} \\ & -\varepsilon^4 [\beta_0(x_{n+1})]^2 \begin{pmatrix} H_2(-\frac{2S_n}{\varepsilon}) & 0 \\ 0 & H_2(\frac{2S_n}{\varepsilon}) \end{pmatrix}, \end{aligned} \tag{3.18}$$

with the phase increments

$$S_n := \phi(x_{n+1}) - \phi(x_n) = \int_{x_n}^{x_{n+1}} \Big(\sqrt{a(\tau)} - \varepsilon^2 \beta(\tau) \Big)\, d\tau.$$

The convergence result for the two modified schemes (3.13)–(3.14) and (3.17)–(3.18) is summarized in the following theorem.

Theorem 3.5 *Let Hypothesis A be satisfied. Then, the global error for solving (2.6) via the modified first or second order scheme reads*

$$||Z(x_n) - Z_n||_2 \le C\varepsilon^2 h^\alpha \min(\varepsilon, h)\,, \quad 1 \le n \le N\,, \tag{3.19}$$

$$||U(x_n) - U_n||_2 \le C\frac{h^\gamma}{\varepsilon} + C\varepsilon^2 h^\alpha \min(\varepsilon, h)\,, \quad 1 \le n \le N\,, \tag{3.20}$$

where $\gamma > 0$ is the order of the chosen numerical integration method for the computation of the phase integral $\Phi^\varepsilon(x)$, and $h > 0$ is the discretization step size. Moreover, $\alpha = 0$ for the first order scheme and $\alpha = 1$ for the second order scheme.

3.3 Numerical results

We shall present now the numerical results obtained with the two schemes introduced in Section 2.2 as well as with the modified first order scheme presented in Section 3.2. For our numerical tests we chose $a(x) = (x + 1/2)^2$, such that the phase

$$\Phi^\varepsilon(x) = \int_0^x \Big(\sqrt{a(\tau)} - \varepsilon^2 \beta(\tau) \Big)\, d\tau \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

is explicitly computable. Hence, the h^γ/ε–term in (3.2) drops and the scheme is asymptotically correct w.r.t. ε in this example. Thus, even for $h = 1$ fixed, the error decays like $\mathcal{O}(\varepsilon^2)$ (cf. Fig. 4). This remarkable behavior is not shared by other schemes from the literature.

Figure 4 shows the numerical error of the first order scheme (2.20), (2.21) as a function of the discretization step h, and for various ε-values. Plotted are the errors

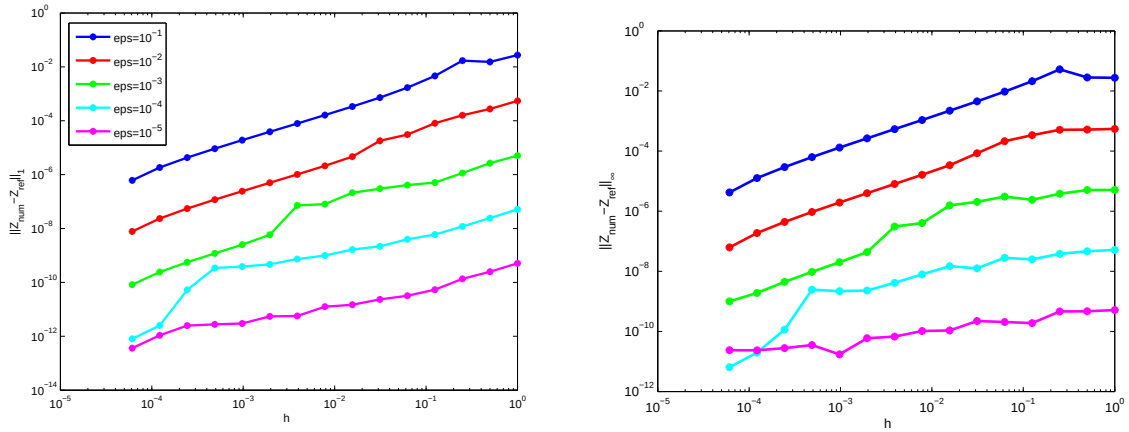

Figure 4: Absolute error between the computed solution Z_{num} and a reference solution Z_{ref} as a function of h, for the first order scheme: in the $L^1(0,1)$–norm (left) and the $L^\infty(0,1)$–norm (right).

between the numerical solution and a reference solution, which is computed with the same method on a very fine grid. Note that the ε–asymptotics of the errors is actually much better (i.e. smaller) than estimated in Theorem 3.1. Indeed, one can read from the plots an error of the order $\mathcal{O}(\varepsilon^2 h)$ rather than the expected $\mathcal{O}(\varepsilon \min(\varepsilon, h))$. To understand this phenomenon we shall analyze in the next section in much more detail the error estimate obtained in Theorem 3.1.
For the second order scheme we observe the same tendency. The error estimate of Theorem 3.1 (i.e. $\mathcal{O}(\varepsilon h \min(\varepsilon, h))$) seems to be worse than the actual numerical errors (presumably $\mathcal{O}(\varepsilon^2 h^2)$), as plotted in Figure 5. The explanation for this difference is again a cancellation as for the first order scheme.

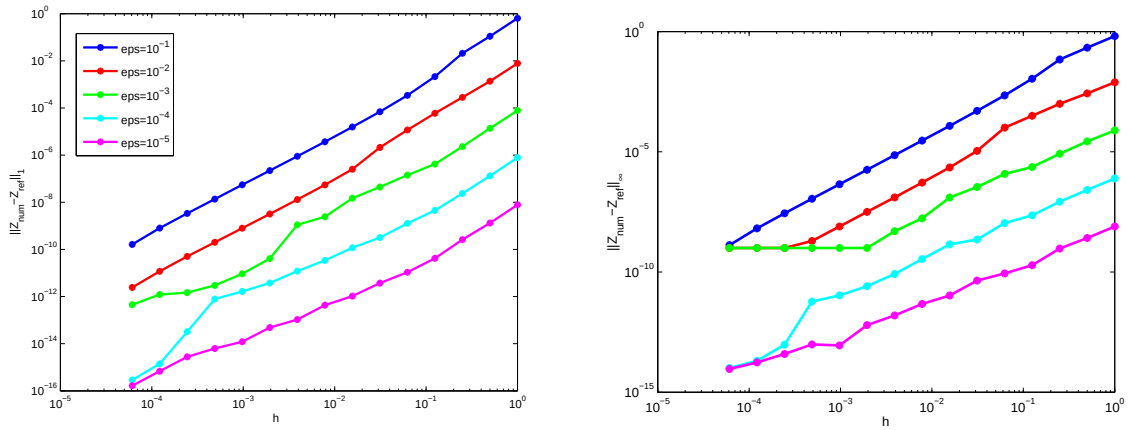

Figure 5: Absolute error between the computed solution Z_{num} and a reference solution Z_{ref} as a function of h, for the second order scheme: in the $L^1(0,1)$–norm (left) and the $L^\infty(0,1)$–norm (right).

And finally, the error plots for the modified first order scheme are presented in Figure

6. No more cancellation can be observed, the mathematical error estimate of Theorem 3.5 (i.e. $\mathcal{O}(\varepsilon^2 \min(\varepsilon, h))$) is very close to the numerical results.

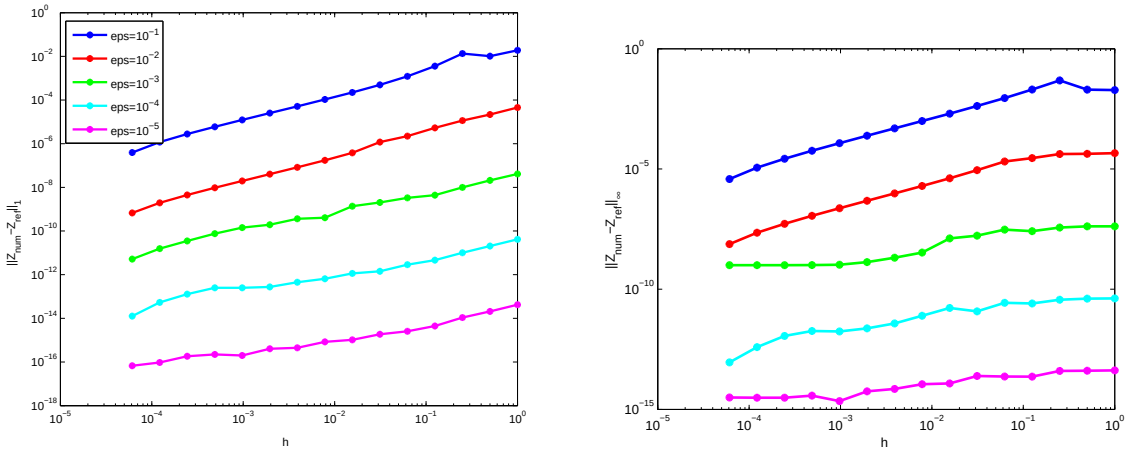

Figure 6: Absolute error between the computed solution Z_{num} and a reference solution Z_{ref} as a function of h, for the modified first order scheme: in the $L^1(0,1)$–norm (left) and the $L^\infty(0,1)$–norm (right).

3.4 Cancelation in the error estimate

The aim of this section is to present an improved error analysis for the first order scheme (2.20), (2.21) in order to explain the phenomenon detected in the Figures 4 and 5: The error behavior of the numerical simulations is apparently better than predicted by Theorem 3.1. For example, for the first order scheme, Figure 4 suggests an error of the order $\mathcal{O}(\varepsilon^2 h)$, while Theorem 3.1 only predicts $\mathcal{O}(\varepsilon h \min(\varepsilon, h))$. And Figure 5 gives a similar indication for the second order scheme.

With the usual error propagation in the one–step ODE–schemes we obtain

$$||Z(x_{n+1}) - Z_{n+1}||_2 \leq ||\sum_{j=1}^{n} \left[\Pi_{l=j+1}^{n}(I + A_l^1)\right] e_j||_2\,, \quad 1 \leq n \leq N\,,$$

with $e_j := \left[\varepsilon M_1^\varepsilon(x_{j+1}; x_j) - A_j^1\right] Z(x_j) + \gamma_j$. In particular we are interested in a better estimation of the term

$$T_n := ||\sum_{j=1}^{n} \left[\Pi_{l=j+1}^{n}(I + A_l^1)\right] (\varepsilon M_1^\varepsilon(x_{j+1}; x_j) - A_j^1) Z(x_j)||_2\,, \quad 1 \leq n < N\,,$$

since $\sum_{j=1}^{n} \left[\Pi_{l=j+1}^{n}(I + A_l^1)\right] \gamma_j$ is already of the order $\mathcal{O}(\varepsilon^2 \min(\varepsilon, h))$. Due to the fact that $A_l^1 = \mathcal{O}(\varepsilon \min(\varepsilon, h))$, we can show that $\Pi_{l=j+1}^{n}(I + A_l^1) = I + \mathcal{O}(N\varepsilon \min(\varepsilon, h)) = I + \mathcal{O}(\varepsilon)$, with $N = 1 + 1/h$ the number of grid points. This means, with (3.6)

$$T_n \leq ||\sum_{j=1}^{n} (\varepsilon M_1^\varepsilon(x_{j+1}; x_j) - A_j^1) Z(x_j)||_2 + \mathcal{O}(\varepsilon^2 \min(\varepsilon, h))\,. \tag{3.21}$$

As $Z(x) = Z_I + \mathcal{O}(\varepsilon^2)$ we have

$$||\sum_{j=1}^{n}(\varepsilon M_1^\varepsilon(x_{j+1};x_j) - A_j^1)Z(x_j)||_2 \le C||\sum_{j=1}^{n}(\varepsilon M_1^\varepsilon(x_{j+1};x_j) - A_j^1)||_2 + \mathcal{O}(\varepsilon^3 \min(\varepsilon,h))\,.$$

Thus, the improvement visible in Figure 4 can only come from some cancellation in the term $E_n := \sum_{j=1}^{n}(\varepsilon M_1^\varepsilon(x_{j+1};x_j) - A_j^1)$. Let us analyze this term in more detail:

$$(E_n)_{21} = \sum_{j=1}^{n}\left(\varepsilon M_1^\varepsilon(x_{j+1};x_j) - A_j^1\right)_{21} = i\varepsilon^2 \sum_{j=1}^{n} e^{\frac{2i}{\varepsilon}\phi(x_j)} \int_{x_j}^{x_{j+1}} \beta_0'(y) H_1\left(\frac{2}{\varepsilon}(\phi(y)-\phi(x_j))\right) dy\,.$$

A rough estimate will lead at this step to $E_n = \mathcal{O}(\varepsilon \min(\varepsilon,h))$, which is exactly what we got in Theorem 3.1. But continuing by partial integration leads to

$$\begin{aligned}
(E_n)_{21} &= -\varepsilon^3 \sum_{j=1}^{n} e^{\frac{2i}{\varepsilon}\phi(x_j)} \int_{x_j}^{x_{j+1}} \beta_1(y) H_2\left(\frac{2}{\varepsilon}(\phi(y)-\phi(x_j))\right)' dy \\
&= \varepsilon^3 \sum_{j=1}^{n} e^{\frac{2i}{\varepsilon}\phi(x_j)} \left\{ \int_{x_j}^{x_{j+1}} \beta_1'(y) H_2\left(\frac{2}{\varepsilon}(\phi(y)-\phi(x_j))\right) dy - \beta_1(x_{j+1}) H_2(\frac{2}{\varepsilon}S_j) \right\} \\
&= \mathcal{O}(\varepsilon h \min(\varepsilon,h)) - \varepsilon^3 \sum_{j=1}^{n} e^{\frac{2i}{\varepsilon}\phi(x_j)} \beta_1(x_{j+1}) H_2(\frac{2}{\varepsilon}S_j) \\
&= \mathcal{O}(\varepsilon h \min(\varepsilon,h)) - \varepsilon h \min(\varepsilon,h) \sum_{j=1}^{n} c_j e^{\frac{2i}{\varepsilon}\phi(x_j)}\,,
\end{aligned} \tag{3.22}$$

with some constants $c_j > 0$ bounded independently of N and ε. Thus, all depends on the term

$$\tau := \sum_{j=1}^{n} c_j e^{\frac{2i}{\varepsilon}\phi(x_j)}\,, \quad 1 \le n < N\,.$$

A cancellation in this term would explain the "good" numerical error as plotted in Figure 4. In the worst case, for example for $c_j = C$ and $\phi(x_j) = k_j \pi\varepsilon$ with some $k_j \in \mathbb{Z}$, we would have $\tau = \mathcal{O}(1/h)$. Then, (3.21), (3.22) would lead to an error of

$$||Z(x_{n+1}) - Z_{n+1}||_2 = \mathcal{O}(\varepsilon^2 \min(\varepsilon,h)) + \mathcal{O}(\varepsilon h \min(\varepsilon,h)) + \mathcal{O}(\varepsilon \min(\varepsilon,h)) = \mathcal{O}(\varepsilon \min(\varepsilon,h))\,,$$

which was asserted in Theorem 3.1. More generally, if we take for example $c_j = C$ and the linear phase function $\phi(x_j) := x_j = (j-1)h$ for $j = 1, \cdots, N$, we have

$$\tau = C \sum_{j=1}^{n} \left(e^{\frac{2i}{\varepsilon}h}\right)^{j-1} = C \frac{1 - e^{\frac{2i}{\varepsilon}hn}}{1 - e^{\frac{2i}{\varepsilon}h}}\,.$$

Thus, far from $h/\varepsilon = k\pi$ ($k \in \mathbb{N}$), e.g. in the case $h \ll \varepsilon$, the term τ remains bounded w.r.t. N, i.e. $\tau = \mathcal{O}(1)$. And this yields an over all error of the order $\mathcal{O}(\varepsilon^2 \min(\varepsilon,h)) + \mathcal{O}(\varepsilon h \min(\varepsilon,h)) = \mathcal{O}(\varepsilon^2 h)$, which is exactly what we see in Figure 4. For $h \gg \varepsilon$, we may

have $\tau = \mathcal{O}(1/h)$, leading to a total error of $\mathcal{O}(\varepsilon^2)$.
Next we consider $c_j = C$ and the quadratic phase function $\phi(x_j) := x_j^2 = (j-1)^2 h^2$; $j = 1, \cdots, N$, which is related to our test example. This yields

$$\tau = C \sum_{j=1}^{n} e^{\frac{2i}{\varepsilon} h^2 (j-1)^2} = C \sum_{j=1}^{n} e^{i\pi\sigma(j-1)^2},$$

where $\sigma = \frac{2}{\pi\varepsilon} h^2$. Hardy and Littlewood [5] studied this type of series, with the result that for irrational σ, we have

$$\sum_{j=1}^{n} e^{i\pi\sigma(j-1)^2} = o(n) = o(1/h),$$

where $ho(1/h) \to 0$ for $h \to 0$. This implies the following error estimate for the Z-scheme:

$$||Z(x_{n+1}) - Z_{n+1}||_2 = \mathcal{O}(\varepsilon^2 \min(\varepsilon, h)) + \mathcal{O}(\varepsilon h \min(\varepsilon, h)) + \mathcal{O}(\varepsilon h \min(\varepsilon, h) o(1/h)).$$

Hence, we have for $\varepsilon \ll h$ an error of $\mathcal{O}(\varepsilon^2 \max(h, h\, o(1/h))) = \mathcal{O}(\varepsilon^2)$ and for $\varepsilon \gg h$ an error of $\mathcal{O}(\varepsilon^2 h)$, which is again what we can see in Figure 4. For rational $\sigma = \frac{2}{\pi\varepsilon} h^2$, we have unfortunately only $\tau = \mathcal{O}(1/h)$, leading to the results of Theorem 3.1. To sum up, the results of the main Theorem 3.1 are correct and sharp (in general), but "most of the time" we will get better estimates as seen in Figure 4.

4 Conclusion

We have introduced in this paper a new method for solving highly oscillating differential equations. This method differs from standard numerical methods by using first an analytic reformulation of the problem in order to extract the troublesome oscillations of the solution. The transformed "smooth" equation was then numerically discretized. Error estimates underlined the advantages of the new method.

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