Journal of Computational and Applied Mathematics 457 (2025) 116240

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Optimally truncated WKB approximation for the 1D stationary Schrödinger equation in the highly oscillatory regime

Anton Arnold [a,*], Christian Klein [b,c], Jannis Körner [a], Jens Markus Melenk [a]

[a] *Institute of Analysis and Scientific Computing, Technische Universität Wien, Wiedner Hauptstr. 8-10, A–1040 Wien, Austria*
[b] *Institut de Mathématiques de Bourgogne, Université de Bourgogne-Franche-Comté, 9 avenue Alain Savary, 21078 Dijon Cedex, France*
[c] *Institut Universitaire de France, France*

ARTICLE INFO

MSC:
34E20
81Q20
65L11
65M70

Keywords:
Schrödinger equation
Highly oscillatory wave functions
Higher order WKB approximation
Optimal truncation
Asymptotic analysis
Airy function
Spectral methods

ABSTRACT

This paper is dedicated to the efficient numerical computation of solutions to the 1D stationary Schrödinger equation in the highly oscillatory regime. We compute an approximate solution based on the well-known WKB-ansatz, which relies on an asymptotic expansion w.r.t. the small parameter ε. Assuming that the coefficient in the equation is analytic, we derive an explicit error estimate for the truncated WKB series, in terms of ε and the truncation order N. For any fixed ε, this allows to determine the optimal truncation order N_{opt} which turns out to be proportional to ε^{-1}. When chosen this way, the resulting error of the *optimally truncated WKB series* behaves like $\mathcal{O}(\exp(-r/\varepsilon))$, with some parameter $r > 0$. The theoretical results established in this paper are confirmed by several numerical examples.

1. Introduction

In this paper we are concerned with the numerical solution of the stationary 1D Schrödinger equation

$$\begin{cases} \varepsilon^2\varphi''(x) + a(x)\varphi(x) = 0\,, \quad x \in I := [\xi,\eta]\,, \\ \varphi(\xi) = \varphi_0\,, \\ \varepsilon\varphi'(\xi) = \varphi_1\,, \end{cases} \tag{1}$$

which yields highly oscillatory solutions. Here, $0 < \varepsilon \ll 1$ is a very small parameter and a is a real-valued function satisfying $a(x) \geq a_0 > 0$ and, for a quantum mechanical problem, it is related to the potential. The constants $\varphi_0, \varphi_1 \in \mathbb{C}$ may depend on ε but are assumed to be ε-uniformly bounded. It is known that the (local) wavelength λ of the solution φ to (1) is proportional to ε. More precisely, it can be expressed as $\lambda(x) = (2\pi\varepsilon)/\sqrt{a(x)}$. Consequently, for a small parameter ε the solution becomes highly oscillatory, particularly in the semi-classical limit $\varepsilon \to 0$.

Highly oscillatory problems such as (1) occur across a broad range of applications, e.g., plasma physics [1,2], inflationary cosmology [3,4] and electron transport in semiconductor devices such as resonant tunneling diodes [5–7]. More specifically, the state of an electron of mass m that is injected with the prescribed energy E from the right boundary into an electronic device

* Corresponding author.
E-mail addresses: anton.arnold@tuwien.ac.at (A. Arnold), Christian.Klein@u-bourgogne.fr (C. Klein), jannis.koerner@tuwien.ac.at (J. Körner), melenk@tuwien.ac.at (J.M. Melenk).

https://doi.org/10.1016/j.cam.2024.116240
Received 18 January 2024; Received in revised form 30 July 2024
Available online 29 August 2024

(e.g., diode), modeled on the interval $[\xi,\eta]$, can be described by the following boundary value problem (BVP) (e.g., see [8] or [7, Chap. 2]):

$$\begin{cases} -\varepsilon^2\psi_E''(x) + V(x)\psi_E(x) = E\psi_E(x)\,, & x\in(\xi,\eta)\,, \\ \psi_E'(\xi) + \mathrm{i}\,k(\xi)\psi_E(\xi) = 0\,, \\ \psi_E'(\eta) - \mathrm{i}\,k(\eta)\psi_E(\eta) = -2\,\mathrm{i}\,k(\eta)\,. \end{cases} \tag{2}$$

Here, $\varepsilon := \hbar/\sqrt{2m}$ is proportional to the (reduced) Planck constant $\hbar$, $k(x) := \varepsilon^{-1}\sqrt{E-V(x)}$ is the wavevector and the real-valued function V denotes the electrostatic potential. In the context of (2), our assumption $a(x) \geq a_0 > 0$ simply reads $E > V(x)$, which means that we are in the oscillatory regime. One is then often interested in macroscopic quantities such as the charge density n and the current density j, which are given by

$$n(x) = \int_0^\infty |\psi_E(x)|^2 f(E)\,\mathrm{d}E\,, \quad j(x) = \varepsilon\int_0^\infty \mathrm{Im}(\overline{\psi_E(x)}\psi_E'(x))f(E)\,\mathrm{d}E\,. \tag{3}$$

Here, f is the distribution function which represents the injection statistics of the electron and $\mathrm{Im}(\cdot)$ denotes the imaginary part. Thus, in order to compute the quantities (3), one has to use a very fine grid in E which means that the BVP (2) has to be solved many times. Consequently, there exists a substantial demand for efficient numerical methods that are suitable for solving problems like (2). Further, we note that the BVP (2) is strongly connected to IVP (1). Indeed, for suitable initial values, namely, $\varphi_0 = 1$ and $\varphi_1 = -\mathrm{i}\sqrt{a(\xi)}$, the solution φ of IVP (1) and the solution ψ_E of BVP (2) are related by

$$\psi_E(x) = -\frac{2\,\mathrm{i}\,k(\eta)}{\varphi'(\eta) - \mathrm{i}\,k(\eta)\varphi(\eta)}\varphi(x)\,. \tag{4}$$

Thus, any numerical method for solving IVP (1) is also suitable for the numerical treatment of BVP (2).

1.1. Background and approach

Since the solution φ to (1) exhibits rapid oscillations when ε is small, standard numerical methods for ODEs become inefficient as they are typically constrained by grid limitations $h = \mathcal{O}(\varepsilon)$ (h denoting the step size), in order to resolve the oscillations accurately. By contrast, the *phase function method* of [9] is based on the observation that solutions to (1) can be represented accurately by means of a nonoscillatory phase function. Our approach presented below is closer to the *uniformly accurate* (w.r.t. ε) marching methods of [10,11] which yield global errors of order $\mathcal{O}(h^2)$ and allow for reducing the grid limitation to at least $h = \mathcal{O}(\sqrt{\varepsilon})$. The WKB-based (named after the physicists Wentzel, Kramers, Brillouin; cf. [12]) one-step method from [8] is even *asymptotically correct*, i.e. the numerical error goes to zero with $\varepsilon \to 0$, provided that the integrals $\int^x \sqrt{a(\tau)}\,\mathrm{d}\tau$ and $\int^x a(\tau)^{-1/4}(a(\tau)^{-1/4})''\,\mathrm{d}\tau$ for the phase of the solution can be computed exactly. More precisely, the method then yields an error which is of order $\mathcal{O}(\varepsilon^3)$ as $\varepsilon \to 0$ and $\mathcal{O}(h^2)$ as $h \to 0$. If these integrals cannot be evaluated exactly, the asymptotically correct error behavior can be (almost) recovered by employing spectral methods for the integrals, as shown in [13]. Further, in [14] the authors propose a numerical algorithm that switches adaptively between a defect correction iteration (which builds on an asymptotic expansion) for oscillatory regions of the solution, and a conventional Chebyshev collocation solver for smoother regions. Although the method is demonstrated to be highly accurate and efficient, a full error analysis was left for future work.

Our approach here is to implement directly a WKB approximation for the solution of (1), which is asymptotically correct and of arbitrary order w.r.t. ε. The essence of the method is rather an analytic approximation via an asymptotic WKB series with optimal truncation. As such, the main goal is to understand the asymptotic ε-dependence of this truncation strategy and of the resulting error. Thus our strategy is not a classical numerical method with some chosen grid size h and convergence as $h \to 0$. Instead, the resulting approximation error will be of order $\mathcal{O}(\varepsilon^N)$ as $\varepsilon \to 0$, where N refers to the used truncation order in the underlying asymptotic WKB series, see (5)–(6) below. As N can be chosen freely, this approach may prove very practical for applications, especially when the model parameter ε is very small. Since the computation of the terms of the asymptotic series involves several integrals, we will employ highly accurate spectral methods, as already proven useful in [13].

The key question when implementing this WKB approximation is which choice of N is adequate or even optimal, in the sense of minimizing the resulting approximation error. Indeed, since the asymptotic WKB series is typically divergent, the error cannot simply be reduced further by increasing the value of N. This question about the best attainable accuracy of the WKB approximation was already addressed in [4], where the author compared the WKB series with the exact solution represented by a convergent Bremmer series [15,16], or more precisely, by an asymptotic expansion of that Bremmer series. The author finds that in cases where the coefficient function a is analytic, the optimal truncation order is proportional to ε^{-1}, yielding a corresponding optimal accuracy which is exponentially small w.r.t. ε. However, to derive these results, the author makes several additional asymptotic approximations. In the present paper, on the other hand, we shall follow a more rigorous strategy by providing error estimates for the WKB approximation which are explicit w.r.t. ε *and* N. We note, however, that the key assumption from [4], i.e., a being analytic, will also be crucial for the strategy of the present work.

In practical finite precision computations, optimal truncation is not generally needed since it is not useful to add additional terms after reaching machine precision. In this paper we present concrete a-priori estimates for this truncation.

1.2. Main results

Our first main result is Theorem 3.7, which provides an explicit (w.r.t. ε and N) error estimate for the WKB approximation, and implies that the approximation error is of order $\mathcal{O}(\varepsilon^N)$. The explicitness of this estimate then allows for an investigation of the error w.r.t. the truncation order N. Indeed, the optimal truncation order N_{opt} can be predicted by minimizing the established upper error bound w.r.t. N or by determining the smallest term of the asymptotic series, and is found to be proportional to ε^{-1}. This leads to our second main result, namely, Corollary 4.1. It states that, for an adequate choice of $N = N(\varepsilon) \sim \varepsilon^{-1}$, the error of the WKB approximation is of order $\mathcal{O}(\exp(-r/\varepsilon))$, $r > 0$ being some constant. As a consequence, also the error of the optimally truncated WKB approximation is of order $\mathcal{O}(\exp(-r/\varepsilon))$, see also Remark 4.2.

This paper is organized as follows: In Section 2 we introduce the Nth order (w.r.t. ε) WKB approximation as an approximate solution of IVP (1). Section 3 then contains a detailed error analysis for the WKB approximation and includes explicit (w.r.t. ε and the truncation order N) error estimates. In Section 4 we specify the computation of the WKB approximation. This includes the description of the chosen methods for the computation of the terms of the underlying asymptotic series as well as a reasonable truncation strategy. In Section 5 we illustrate the theoretical results established in this paper by several numerical examples. We conclude in Section 6.

2. WKB approximation

In this section we introduce the *WKB approximation* as an approximate solution of IVP (1). The basis for its construction is the well-known WKB-ansatz (cf. [12,17]), which for the ODE (1) reads[1]

$$\varphi(x) \sim \exp\left(\frac{1}{\varepsilon} S(x)\right) , \quad \varepsilon \to 0 , \tag{5}$$

where S is a complex-valued function containing information of the phase as well as the amplitude of the solution φ. To derive WKB approximations it is then convenient to express S as an asymptotic expansion[2] w.r.t. the small parameter ε:

$$S(x) \sim \sum_{n=0}^{\infty} \varepsilon^n S_n(x) , \quad \varepsilon \to 0 ; \quad S_n(x) \in \mathbb{C} . \tag{6}$$

It should be noted that this asymptotic series is typically divergent (as usual for asymptotic series) and must therefore be truncated in order to obtain an approximate solution.

By substituting the ansatz (5)–(6) into (1), one obtains (formally)

$$\left(\sum_{n=0}^{\infty} \varepsilon^n S_n'(x)\right)^2 + \sum_{n=0}^{\infty} \varepsilon^{n+1} S_n''(x) + a(x) = 0. \tag{7}$$

A comparison of ε-powers then yields the following well-known recurrence relation for the functions S_n':

$$S_0' = \pm \mathrm{i} \sqrt{a} , \tag{8}$$

$$S_1' = -\frac{S_0''}{2S_0'} = -\frac{a'}{4a} = -\frac{1}{4}(\ln(a))' , \tag{9}$$

$$S_n' = -\frac{1}{2S_0'} \left(\sum_{j=1}^{n-1} S_j' S_{n-j}' + S_{n-1}'' \right) , \quad n \geq 2 . \tag{10}$$

The computation of each S_n, $n \geq 0$, thus involves one integration constant. Further, the repeated differentiation in (10) indicates that a WKB approximation relying on $N+1$ terms in the truncated series (6) requires $a \in C^N(I)$. Moreover, the fact that the r.h.s. of (8) has two different signs implies that there are two sequences of functions, which solve (8)–(10). This corresponds to the fact that there are two fundamental solutions of the ODE in (1). Let us denote by $(S_n^-)_{n\in\mathbb{N}_0}$ the sequence induced by the choice $S_0' = -\mathrm{i}\sqrt{a}$. The one following from $S_0' = \mathrm{i}\sqrt{a}$ will be denoted by $(S_n^+)_{n\in\mathbb{N}_0}$. Then, a simple observation is the following proposition.

Proposition 2.1.

$$(S_{2n}^-)'(x) = -(S_{2n}^+)'(x) \in \mathrm{i}\,\mathbb{R} , \tag{11}$$

$$(S_{2n+1}^-)'(x) = (S_{2n+1}^+)'(x) \in \mathbb{R} , \tag{12}$$

for all $x \in I$ *and* $n \geq 0$.

[1] We say that two functions $f, g : I \times (0, \varepsilon_0) \to \mathbb{C}$ are *asymptotically equivalent* as $\varepsilon \to 0$, if and only if for any $x \in I$ it holds $f(x,\varepsilon) - g(x,\varepsilon) = o(g(x,\varepsilon))$ as $\varepsilon \to 0$. In this case we write $f(x,\varepsilon) \sim g(x,\varepsilon)$, $\varepsilon \to 0$.

[2] We say that a function $f : I \times (0, \varepsilon_0) \to \mathbb{C}$ has an *asymptotic expansion* as $\varepsilon \to 0$, if and only if there exist sequences of functions $\left(f_n : I \to \mathbb{C}\right)_{n\in\mathbb{N}_0}$ and $(\phi_n : (0,\varepsilon_0) \to \mathbb{C}_{n\in\mathbb{N}_0}$ satisfying for all $n \in \mathbb{N}_0$ and $x \in I$ that $\phi_{n+1}(\varepsilon) f_{n+1}(x) = o(\phi_n(\varepsilon) f_n(x))$ as $\varepsilon \to 0$, such that for all $N \geq 0$ it holds $f(x,\varepsilon) - \sum_{n=0}^{N} \phi_n(\varepsilon) f_n(x) = o(\phi_N(\varepsilon) f_N(x))$ as $\varepsilon \to 0$. In this case we write $f(x,\varepsilon) \sim \sum_{n=0}^{\infty} \phi_n(\varepsilon) f_n(x)$, $\varepsilon \to 0$. We call an asymptotic expansion *uniform* w.r.t. $x \in I$, if all the order symbols hold uniformly in $x \in I$.

Proof. The statement can easily be verified by induction on $n \in \mathbb{N}_0$. $\square$

Since both sequences $(S_n^\pm)_{n\in\mathbb{N}_0}$ lead to an approximate solution of the ODE in (1), the general approximate solution can be written as the linear combination

$$\varphi \approx \varphi_N^{WKB} := \alpha_{N,\varepsilon} \exp\left(\sum_{n=0}^{N} \varepsilon^{n-1} S_n^-\right) + \beta_{N,\varepsilon} \exp\left(\sum_{n=0}^{N} \varepsilon^{n-1} S_n^+\right), \tag{13}$$

with arbitrary $\alpha_{N,\varepsilon}, \beta_{N,\varepsilon} \in \mathbb{C}$. Note that all integration constants in the computation of S_n^- and S_n^+ can be "absorbed" into $\alpha_{N,\varepsilon}$ and $\beta_{N,\varepsilon}$, respectively. Hence, these integration constants can be set to zero without loss of generality. More precisely, we define

$$S_n^\pm(x) := \int_\xi^x \left(S_n^\pm\right)'(\tau)\,\mathrm{d}\tau\,. \tag{14}$$

With this, Proposition 2.1 implies

$$S_{2n}^-(x) = -S_{2n}^+(x) \in \mathrm{i}\,\mathbb{R}\,, \tag{15}$$

$$S_{2n+1}^-(x) = S_{2n+1}^+(x) \in \mathbb{R}\,, \tag{16}$$

for all $x \in I$ and $n \geq 0$. Hence, functions with even indices only contribute to the phase of the WKB approximation φ_N^{WKB}, whereas functions with odd indices only provide corrections to the amplitude.

Note that in general the constants $\alpha_{N,\varepsilon}$ and $\beta_{N,\varepsilon}$ can be uniquely determined by initial or boundary conditions. Here, for the WKB approximation (13) to satisfy the initial conditions in (1), we set

$$\alpha_{N,\varepsilon} = \frac{\varphi_0\left(\sum_{n=0}^N \varepsilon^n (S_n^+)'(\xi)\right) - \varphi_1}{\sum_{n=0}^N \varepsilon^n \left((S_n^+)'(\xi) - (S_n^-)'(\xi)\right)}\,, \tag{17}$$

$$\beta_{N,\varepsilon} = \frac{\varphi_1 - \varphi_0\left(\sum_{n=0}^N \varepsilon^n (S_n^-)'(\xi)\right)}{\sum_{n=0}^N \varepsilon^n \left((S_n^+)'(\xi) - (S_n^-)'(\xi)\right)}\,. \tag{18}$$

In the following we will often simply write S_n whenever one could insert either S_n^- or S_n^+.

According to [17, Sec. 10.2], for the WKB-ansatz (5)–(6) to be valid on the whole interval I, it is necessary that the series $\sum_{n=0}^\infty \varepsilon^{n-1} S_n(x)$ is a uniform asymptotic expansion of $\varepsilon^{-1} S(x)$ as $\varepsilon \to 0$. This implies that for any $n \in \mathbb{N}_0$ the relation

$$\varepsilon^n S_{n+1}(x) = o(\varepsilon^{n-1} S_n(x))\,, \quad \varepsilon \to 0\,, \tag{19}$$

must hold uniformly in $x \in I$. Note that this condition is violated if the interval I includes so-called *turning points*, i.e., points $x_0 \in I$ with $a(x_0) = 0$. Indeed, this is already evident from (9), which implies that S_1 blows up at such turning points.

3. Error analysis

In this section we aim to find an explicit (w.r.t. ε and the truncation order N) error estimate for the WKB approximation (13). One key ingredient will be the following a priori estimate for the solution φ of the inhomogeneous analog of the Schrödinger equation-IVP (1).

Proposition 3.1. *Let $a \in W^{1,\infty}(I)$ with $a(x) \geq a_0 > 0$ and $f \in C(I)$. Further, let $\varphi \in C^2(I)$ be the solution of the inhomogeneous IVP*

$$\begin{cases} \varepsilon^2 \varphi'' + a(x)\varphi = f(x)\,, & x \in I\,, \\ \varphi(\xi) = \hat{\varphi}_0\,, \\ \varepsilon\varphi'(\xi) = \hat{\varphi}_1\,, \end{cases}$$

with constants $\hat{\varphi}_0, \hat{\varphi}_1 \in \mathbb{C}$. Then there exists $C > 0$ independent of ε, f, $\hat{\varphi}_0$, $\hat{\varphi}_1$ such that

$$\|\varphi\|_{L^\infty(I)} \leq \frac{C}{\varepsilon}\|f\|_{L^2(I)} + C\left(|\hat{\varphi}_1| + |\hat{\varphi}_0|\right)\,, \tag{20}$$

$$\|\varepsilon\varphi'\|_{L^\infty(I)} \leq \frac{C}{\varepsilon}\|f\|_{L^2(I)} + C\left(|\hat{\varphi}_1| + |\hat{\varphi}_0|\right)\,. \tag{21}$$

Proof. Estimates (20)–(21) can be derived by finding an upper bound for the real-valued function $E(x) := \varepsilon^2|\varphi'|^2 + a|\varphi|^2$. At first, it holds that

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}x}E(x) &= \varepsilon^2 \frac{\mathrm{d}}{\mathrm{d}x}|\varphi'|^2 + a\frac{\mathrm{d}}{\mathrm{d}x}|\varphi|^2 + a'|\varphi|^2 \\ &= 2\,\mathrm{Re}((\varepsilon^2\varphi'' + a\varphi)\overline{\varphi'}) + a'|\varphi|^2 \\ &= 2\,\mathrm{Re}(f\overline{\varphi'}) + a'|\varphi|^2 \\ &\leq 2|f||\varphi'| + \|a'\|_{L^\infty(I)}|\varphi|^2\,. \end{aligned} \tag{22}$$

Using Young's inequality, we obtain

$$2|f||\varphi'| \le \frac{1}{\varepsilon^2}|f|^2 + \varepsilon^2|\varphi'|^2 . \tag{23}$$

Moreover, $a(x) \ge a_0 > 0$ implies that

$$\|a'\|_{L^\infty(I)}|\varphi|^2 \le \frac{\|a'\|_{L^\infty(I)}}{a_0} a|\varphi|^2 . \tag{24}$$

Thus, from (22)–(24) we obtain with $c := \max(1, \frac{\|a'\|_{L^\infty(I)}}{a_0}) \ge 1$

$$\frac{\mathrm{d}}{\mathrm{d}x} E(x) \le \frac{1}{\varepsilon^2}|f(x)|^2 + cE(x) . \tag{25}$$

Applying Gronwall's inequality (i.e., multiply (25) by $\exp(-cx)$ and integrate), we therefore get

$$\begin{aligned} E(x) &\le \frac{1}{\varepsilon^2}\int_\xi^x |f(s)|^2\, \mathrm{e}^{c(x-s)}\,\mathrm{d}s + E(\xi)\,\mathrm{e}^{c(x-\xi)} \\ &\le \left(\frac{1}{\varepsilon^2}\|f\|^2_{L^2(I)} + E(\xi)\right)\mathrm{e}^{c(x-\xi)} \\ &\le \mathrm{e}^{c(\eta-\xi)}\left(\frac{1}{\varepsilon^2}\|f\|^2_{L^2(I)} + |\hat\varphi_1|^2 + a(\xi)|\hat\varphi_0|^2\right) , \end{aligned} \tag{26}$$

which implies the estimates (20)–(21). □

In order to derive an error estimate for the WKB approximation (13) that is explicit not only w.r.t. ε but also w.r.t. the truncation order N, it is essential to control the growth of the functions S_n w.r.t. $n \in \mathbb{N}_0$. As a first step, we aim to establish upper bounds for the derivatives S_n', which are given by recurrence relation (8)–(10). To this end, we employ a strategy similar to [18, Lemma 2], which relies heavily on Cauchy's integral formula. To enable us to apply this tool, we shall assume that S_0' is not only defined on the real interval I, but also on a complex neighborhood $G \subset \mathbb{C}$ of I and holomorphic there. This leads us to introduce the following assumption.

Hypothesis A. Let S_0' be holomorphic (complex analytic) on a complex, bounded, simply connected neighborhood $G \subset \mathbb{C}$ of I, satisfying $S_0'(z) \ne 0$ for any $z \in G$.

As a consequence of Hypothesis A, the function a and all S_n, $n \in \mathbb{N}$, are holomorphic on G. In particular, each S_n is bounded on I. For the next lemma, we introduce, for $\delta > 0$, the open sets

$$G_\delta := \{z \in G \mid \mathrm{dist}(z, \partial G) > \delta\}. \tag{27}$$

Lemma 3.2. *Let Hypothesis A be satisfied and let $0 < \delta \le 1$ be such that $G_\delta \ne \emptyset$. Then there exists a constant $K > 0$ depending only on G and S_0' such that*

$$\|S_n'\|_{L^\infty(G_\delta)} \le \|S_0'\|_{L^\infty(G)} K^n n^n \delta^{-n} , \quad n \in \mathbb{N}_0 . \tag{28}$$

Here, we define 0^0 as 1.

Proof. Define the auxiliary functions $\hat S_n' := -(2S_0')^{-1}S_n'$. By using (8)–(10) we then find that the functions $\hat S_n'$ satisfy the following recurrence relation

$$\hat S_0' = -\frac{1}{2} , \tag{29}$$

$$\hat S_n' = \left(\sum_{j=1}^{n-1} \hat S_j' \hat S_{n-j}'\right) + \left(2S_0'\right)^{-2}(-2S_0'\hat S_{n-1}')' , \quad n \ge 1 . \tag{30}$$

Note that since S_0' is holomorphic on G, it follows from recurrence relation (8)–(10) that S_n', and hence also $\hat S_n'$, is holomorphic on G, for every $n \in \mathbb{N}_0$. We will now prove by induction on n that

$$\|\hat S_n'\|_{L^\infty(G_\delta)} \le \frac{1}{2}K^n n^n \delta^{-n} , \quad n \in \mathbb{N}_0 . \tag{31}$$

Obviously, this estimate does hold for $n = 0$, according to (29). Assume that the estimate in (31) holds for $0 \le j \le n-1$ with some fixed $n \ge 1$. We will now prove it for n. Let $0 < \kappa < 1$ and $z \in G_\delta$. We denote with $\partial B_{\kappa\delta}(z)$ a circle of radius $\kappa\delta$ around z, see the left panel of Fig. 1. Then Cauchy's integral formula implies

$$|(-2S_0'\hat S_{n-1}')'(z)| = \frac{1}{2\pi}\left|\int_{\partial B_{\kappa\delta}(z)} \frac{-2S_0'(\zeta)\hat S_{n-1}'(\zeta)}{(\zeta - z)^2}\,\mathrm{d}\zeta\right| \le \frac{2\pi\kappa\delta}{2\pi} 2\|S_0'\|_{L^\infty(G)}\|\hat S_{n-1}'\|_{L^\infty(\partial B_{\kappa\delta}(z))}(\kappa\delta)^{-2} . \tag{32}$$

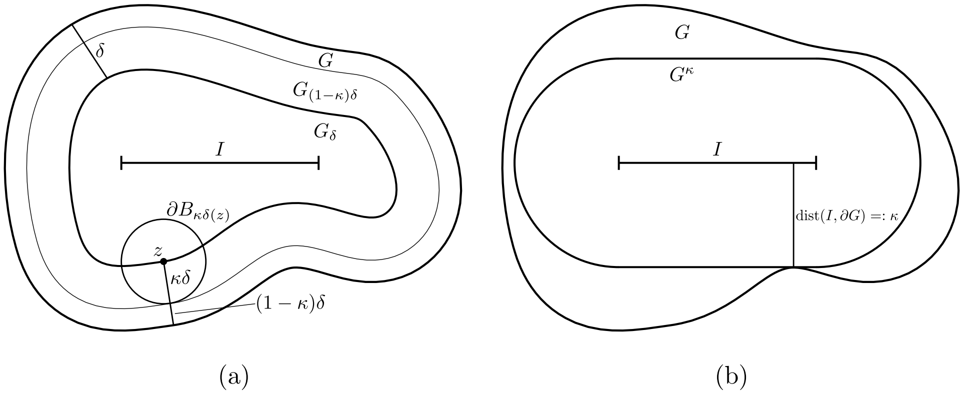

Fig. 1. (a) Exemplary sketch of the situation from the proof of Lemma 3.2: $G_\delta \subset G_{(1-\kappa)\delta} \subset G$, where G is a complex neighborhood of the interval I. Here, the point $z \in G_\delta$ is very close to the boundary ∂G_δ, which makes it clear why one has to consider $G_{(1-\kappa)\delta}$ in the r.h.s. of (33). (b) Every possible candidate G for the minimum on the l.h.s. of (41) can be reduced to a set $G^\kappa := \{z \in \mathbb{C} \mid \operatorname{dist}(z, I) < \kappa\}$, where $\kappa := \operatorname{dist}(I, \partial G) > 0$.

This, together with the fact that $\partial B_{\kappa\delta}(z) \subseteq \overline{G_{(1-\kappa)\delta}}$ yields

$$\|(-2S_0'\hat{S}_{n-1}')'\|_{L^\infty(G_\delta)} \leq 2\|S_0'\|_{L^\infty(G)}(\kappa\delta)^{-1}\|\hat{S}_{n-1}'\|_{L^\infty(G_{(1-\kappa)\delta})}\,. \tag{33}$$

By applying estimate (33) and the induction hypothesis to (30), we find

$$\begin{aligned}\|\hat{S}_n'\|_{L^\infty(G_\delta)} &\leq \sum_{j=1}^{n-1}\|\hat{S}_j'\|_{L^\infty(G_\delta)}\|\hat{S}_{n-j}'\|_{L^\infty(G_\delta)} \quad + \frac{1}{4}\|(S_0')^{-2}\|_{L^\infty(G_\delta)}2\|S_0'\|_{L^\infty(G)}(\kappa\delta)^{-1}\|\hat{S}_{n-1}'\|_{L^\infty(G_{(1-\kappa)\delta})} \\ &\leq \frac{1}{4}K^n\delta^{-n}\sum_{j=1}^{n-1}j^j(n-j)^{n-j} \quad + \frac{1}{4}\|(S_0')^{-2}\|_{L^\infty(G_\delta)}\|S_0'\|_{L^\infty(G)}\delta^{-n}K^{n-1}\frac{(n-1)^{n-1}}{\kappa(1-\kappa)^{n-1}}\,.\end{aligned} \tag{34}$$

Since $j^j(n-j)^{n-j} \leq (n-1)^{n-1}$ for all $1 \leq j \leq n-1$, we can bound the sum in the first term of (34) by $(n-1)^n$. Thus, we obtain

$$\|\hat{S}_n'\|_{L^\infty(G_\delta)} \leq \frac{1}{2}K^n n^n\delta^{-n}\left[\frac{1}{2}\left(\frac{n-1}{n}\right)^n + \frac{\|(S_0')^{-2}\|_{L^\infty(G_\delta)}\|S_0'\|_{L^\infty(G)}}{2K\kappa(1-\kappa)^{n-1}n}\left(\frac{n-1}{n}\right)^{n-1}\right]\,. \tag{35}$$

It now suffices to show that the expression in the square brackets is less than or equal to 1. By further estimating $\left(\frac{n-1}{n}\right)^n \leq \frac{1}{\mathrm{e}}$, and choosing $\kappa = \frac{1}{n}$, we get

$$\|\hat{S}_n'\|_{L^\infty(G_\delta)} \leq \frac{1}{2}K^n n^n\delta^{-n}\left[\frac{1}{2\,\mathrm{e}} + \frac{\|(S_0')^{-2}\|_{L^\infty(G_\delta)}\|S_0'\|_{L^\infty(G)}}{2K}\right] \tag{36}$$

Thus it is sufficient to choose

$$K := \frac{\mathrm{e}}{2\,\mathrm{e}-1}\|(S_0')^{-2}\|_{L^\infty(G)}\|S_0'\|_{L^\infty(G)}\,. \tag{37}$$

The estimate $\|(S_0')^{-2}\|_{L^\infty(G_\delta)} \leq \|(S_0')^{-2}\|_{L^\infty(G)}$ concludes the proof. □

A simple but important implication of Lemma 3.2 is the fact that we are now able to provide estimates not only for all the derivatives of S_n but also for S_n itself:

Corollary 3.3. *Let Hypothesis A be satisfied. Then there exist constants $K_1, K_2 > 0$ depending only on G and S_0' such that*

$$\|S_n\|_{L^\infty(I)} \leq (\eta-\xi)\|S_0'\|_{L^\infty(G)}K_2^n n^n\,, \quad n \in \mathbb{N}_0\,, \tag{38}$$

$$\|S_n^{(k)}\|_{L^\infty(I)} \leq \|S_0'\|_{L^\infty(G)}(k-1)!\,K_1^{k-1}K_2^n n^n\,, \quad n \in \mathbb{N}_0\,, \quad k \in \mathbb{N}\,. \tag{39}$$

Here we define 0^0 as 1.

Proof. Since G is a complex neighborhood of I, there is some $0 < \delta \leq 1$ such that $I \subset G_{2\delta}$. To prove estimate (39), we start with the trivial estimate $\|S_n^{(k)}\|_{L^\infty(I)} \leq \|S_n^{(k)}\|_{L^\infty(G_{2\delta})}$. Then, for any $k \in \mathbb{N}$ and $z \in G_{2\delta}$, Cauchy's integral formula implies

$$|S_n^{(k)}(z)| = \frac{(k-1)!}{2\pi}\left|\int_{\partial B_\delta(z)}\frac{S_n'(z)}{(\zeta-z)^k}\,\mathrm{d}\zeta\right| \leq (k-1)!\,\delta^{-k+1}\|S_n'\|_{L^\infty(G_\delta)}\,. \tag{40}$$

By applying Lemma 3.2 on the r.h.s. of (40) we conclude that (39) holds with $K_1 := 1/\delta$ and $K_2 := K/\delta$. Estimate (38) then follows from (39) for $k = 1$ and by the definition of S_n, see (14). □

Remark 3.4. Of course, it is of great interest to find a constant K_2 from Corollary 3.3 that is as small as possible. To this end one would have to minimize the constant K/δ in estimate (28). In particular, one has to fix some complex neighborhood G of I as well as a constant $0 < \delta \le 1$ such that it holds $I \subset G_\delta$. Further, the proof of Lemma 3.2 indicates that K can be reduced by choosing G small, see (37). However, this means that one is forced to reduce also the value of δ. Hence, this procedure usually results in a trade-off between the magnitudes of K and δ. More precisely, one is led to solve the following minimization problem:

$$\inf_{\substack{0<\delta\le 1\\ G\subset\mathbb{C}\\ I\subset G_\delta}} \frac{\|(S_0')^{-2}\|_{L^\infty(G)}\|S_0'\|_{L^\infty(G)}}{\delta} = \min_{0<\delta\le 1} \frac{\|(S_0')^{-2}\|_{L^\infty(G^\delta)}\|S_0'\|_{L^\infty(G^\delta)}}{\delta}, \tag{41}$$

where $G^\delta := \{z \in \mathbb{C} \mid \operatorname{dist}(z, I) < \delta\}$. Equality in (41) holds for the following reasons: First, on the l.h.s. of (41) one only needs to consider sets $G \subset \mathbb{C}$ of the form $G = G^\kappa := \{z \in \mathbb{C} \mid \operatorname{dist}(z, I) < \kappa\}$, with $\kappa > 0$. For any $0 < \delta \le 1$ such that $I \subset G_\delta$, this follows since the numerator on the l.h.s. of (41) is not increased when replacing G by $G^{\operatorname{dist}(I,\partial G)}$, see the right panel of Fig. 1. The condition $I \subset G_\delta$ then simply reads $\kappa > \delta$. Second, since for a fixed $0 < \delta \le 1$ and $\delta < \kappa_1 < \kappa_2$ it holds that $G^{\kappa_1} \subset G^{\kappa_2}$, it is sufficient to consider simply the sets $G^{\delta+\epsilon}$, with $\epsilon > 0$ being an arbitrarily small number. The equality in (41) then follows from the fact that $\bigcap_{\epsilon>0} G^{\delta+\epsilon} = \overline{G^\delta}$.

We will later make use of the residual of the WKB approximation (13) w.r.t. the ODE in (1). For this, the following lemma will be helpful.

Lemma 3.5. *Denote with* $L_\varepsilon := \varepsilon^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} + a(x)$ *the linear operator appearing in the Schrödinger Eq. (1) and let* $\widetilde{\varphi}_N := \exp\left(\sum_{n=0}^N \varepsilon^{n-1} S_n\right)$, $N \in \mathbb{N}_0$. *Then it holds*

$$L_\varepsilon \widetilde{\varphi}_N = \widetilde{\varphi}_N f_{N,\varepsilon}, \tag{42}$$

where

$$f_{N,\varepsilon} = \varepsilon^{N+1}(-2S_0' S_{N+1}') + \sum_{n=2}^N \sum_{k=2+N-n}^N \varepsilon^{n+k} S_n' S_k'; \tag{43}$$

for $N < 2$ *the double sum is dropped.*

Proof. First we observe that

$$L_\varepsilon \widetilde{\varphi}_N = \varepsilon^2 \widetilde{\varphi}_N'' + a(x)\widetilde{\varphi}_N = \varepsilon^2 \widetilde{\varphi}_N \left(\left(\frac{1}{\varepsilon} \sum_{n=0}^N \varepsilon^n S_n' \right)^2 + \frac{1}{\varepsilon} \sum_{n=0}^N \varepsilon^n S_n'' \right) + a(x)\widetilde{\varphi}_N = \widetilde{\varphi}_N \left(\sum_{n=0}^N \sum_{k=0}^N \varepsilon^{n+k} S_n' S_k' + \sum_{n=0}^N \varepsilon^{n+1} S_n'' + a(x) \right). \tag{44}$$

Let us denote the second factor in (44) by $f_{N,\varepsilon}$. We will now show that $f_{N,\varepsilon}$ reduces to (43). To this end, let us first rewrite $f_{N,\varepsilon}$ as

$$f_{N,\varepsilon} = \left(S_0'^2 + a\right) + \left(\sum_{n=0}^N \sum_{k=\max(0,1-n)}^{N-n} \varepsilon^{n+k} S_n' S_k' + \sum_{n=0}^{N-1} \varepsilon^{n+1} S_n'' \right) + \left(\sum_{n=1}^N \varepsilon^{N+1} S_{N+1-n}' S_n' + \varepsilon^{N+1} S_N'' \right) + \sum_{n=2}^N \sum_{k=N+2-n}^N \varepsilon^{n+k} S_n' S_k'. \tag{45}$$

Now, the first term in (45) vanishes due to (8). The second term also vanishes since

$$\sum_{n=0}^N \sum_{k=\max(0,1-n)}^{N-n} \varepsilon^{n+k} S_n' S_k' = \sum_{n=0}^{N-1} \varepsilon^{n+1} \sum_{j=0}^{n+1} S_j' S_{n+1-j}' = \sum_{n=0}^{N-1} \varepsilon^{n+1} \left(2S_0' S_{n+1}' + \sum_{j=1}^n S_j' S_{n+1-j}' \right) = -\sum_{n=0}^{N-1} \varepsilon^{n+1} S_n'', \tag{46}$$

where we used in the last equation recurrence relation (10) for the function S_{n+1}'. Finally, by using (10) for the function S_{N+1}', the third term in (45) simplifies to $\varepsilon^{N+1}(-2S_0' S_{N+1}')$. The claim follows. □

Recalling that $S_0(x) \in \mathrm{i}\mathbb{R}$ we note that $\widetilde{\varphi}_N(x)$ is, for fixed $x \in I$, uniformly bounded w.r.t. $\varepsilon \in (0, 1]$. Thus the r.h.s. of (42) is of the order $\mathcal{O}(\varepsilon^{N+1})$, and we conclude from Lemma 3.5 that the function $\widetilde{\varphi}_N$ satisfies the ODE $L_\varepsilon \varphi = 0$ asymptotically, as $\varepsilon \to 0$. This is one of the main properties we can utilize to show that also the numerical error of the WKB approximation (13) will approach 0 as $\varepsilon \to 0$, at least for $N \ge 1$. To this end we need the following lemma.

Lemma 3.6. *Let Hypothesis A be satisfied and define* $\varphi_N^\pm := \exp\left(\sum_{n=0}^N \varepsilon^{n-1} S_n^\pm\right)$, $N \in \mathbb{N}_0$. *Then there exist constants* $\varepsilon_0 \in (0, 1)$ *and* $C > 0$ *such that it holds for* $\varepsilon \in (0, \varepsilon_0]$:

$$\|\alpha_{N,\varepsilon} \varphi_N^-\|_{L^\infty(I)} \le C \left(|\varphi_0| \, \|S_0'\|_{L^\infty(G)} \sum_{n=0}^N \varepsilon^n K_2^n n^n + |\varphi_1| \right) \exp\left((\eta - \xi) \|S_0'\|_{L^\infty(G)} \sum_{n=0}^{\lfloor \frac{N-1}{2} \rfloor} \varepsilon^{2n} K_2^{2n+1} (2n+1)^{2n+1} \right), \tag{47}$$

with $\alpha_{N,\varepsilon}$ *from (17). For* $N = 0$ *the last sum is dropped. The same estimate holds for* $\|\beta_{N,\varepsilon}\varphi_N^+\|_{L^\infty(I)}$. *In particular, since the initial values* φ_0 *and* φ_1 *are assumed to be uniformly bounded w.r.t.* ε, *so is* φ_N^{WKB} *in* $L^\infty(I)$.

Proof. We will prove only the estimate for $\alpha_{N,\varepsilon}\varphi_N^-$. For $\beta_{N,\varepsilon}\varphi_N^+$ it is fully analogous. First notice that Proposition 2.1 implies that

$$|\alpha_{N,\varepsilon}| = \frac{\left|\varphi_0 \sum_{n=0}^{N} \varepsilon^n (S_n^+)'(\xi) - \varphi_1\right|}{2\left|\sum_{n=0}^{\lfloor \frac{N}{2} \rfloor} \varepsilon^{2n} (S_{2n}^+)'(\xi)\right|} . \tag{48}$$

Due to $a(x) \geq a_0 > 0$, we have $|(S_0^+)'(\xi)| \geq \sqrt{a_0} > 0$. Thus, there exists $\varepsilon_0 \in (0,1)$ sufficiently small such that

$$\left|\sum_{n=0}^{\lfloor \frac{N}{2} \rfloor} \varepsilon^{2n} (S_{2n}^+)'(\xi)\right| \geq \left|(S_0^+)'(\xi)\right| - \sum_{n=1}^{\lfloor \frac{N}{2} \rfloor} \varepsilon^{2n} \left|(S_{2n}^+)'(\xi)\right| \geq \sqrt{a_0} - \sum_{n=1}^{\lfloor \frac{N}{2} \rfloor} \varepsilon^{2n} \left|(S_{2n}^+)'(\xi)\right| \geq \frac{1}{2C} \tag{49}$$

for all $\varepsilon \in (0, \varepsilon_0]$ and some $C > 0$ (since $(S_{2n}^+)'$ is bounded on I). Hence, we obtain

$$|\alpha_{N,\varepsilon}| \leq C \left|\varphi_0 \sum_{n=0}^{N} \varepsilon^n (S_n^+)'(\xi) - \varphi_1\right| . \tag{50}$$

Next, (15)–(16) imply $|\varphi_N^-(x)| \leq \exp\left(\sum_{n=0}^{\lfloor \frac{N-1}{2} \rfloor} \varepsilon^{2n} \left|S_{2n+1}^-(x)\right|\right)$ for all $x \in I$. Together with (50) this yields

$$|\alpha_{N,\varepsilon}\varphi_N^-(x)| \leq C \left(|\varphi_0| \sum_{n=0}^{N} \varepsilon^n \left|(S_n^+)'(\xi)\right| + |\varphi_1| \right) \exp\left(\sum_{n=0}^{\lfloor \frac{N-1}{2} \rfloor} \varepsilon^{2n} \left|S_{2n+1}^-(x)\right| \right) \tag{51}$$

for all $x \in I$. Applying Corollary 3.3 then yields the claim. □

Finally, we provide an error estimate for the WKB approximation (13).

Theorem 3.7. *Let Hypothesis A be satisfied and let $\varphi \in C^2(I)$ be the solution of IVP (1). There exist constants $\varepsilon_0 \in (0,1)$ and $C > 0$ independent of N and ε such that it holds for $\varepsilon \in (0, \varepsilon_0]$:*

$$\begin{aligned} \|\varphi - \varphi_N^{WKB}\|_{L^\infty(I)} \leq{}& C\|S_0'\|_{L^\infty(G)}^2 \left(|\varphi_0|\, \|S_0'\|_{L^\infty(G)} \sum_{n=0}^{N} \varepsilon^n K_2^n n^n + |\varphi_1| \right) \\ &\times \exp\left((\eta - \xi)\|S_0'\|_{L^\infty(G)} \sum_{n=0}^{\lfloor \frac{N-1}{2} \rfloor} \varepsilon^{2n} K_2^{2n+1} (2n+1)^{2n+1} \right) \\ &\times \left(\varepsilon^N K_2^{N+1} (N+1)^{N+1} + \sum_{n=2}^{N} \sum_{k=2+N-n}^{N} \varepsilon^{n+k-1} K_2^{n+k} n^n k^k \right) . \end{aligned} \tag{52}$$

For $N = 0$ the sum in the exponential function is dropped, and for $N < 2$ the double sum is dropped.

Proof. To compute the residual of the WKB approximation (13), we notice that $\varphi_N^{WKB} = \alpha_{N,\varepsilon}\varphi_N^- + \beta_{N,\varepsilon}\varphi_N^+$, where $\varphi_N^\pm = \exp\left(\sum_{n=0}^{N} \varepsilon^{n-1} S_n^\pm\right)$. By applying Lemma 3.5, we obtain

$$L_\varepsilon(\varphi - \varphi_N^{WKB}) = -\alpha_{N,\varepsilon} L_\varepsilon \varphi_N^- - \beta_{N,\varepsilon} L_\varepsilon \varphi_N^+ = -\alpha_{N,\varepsilon}\varphi_N^- f_{N,\varepsilon}^- - \beta_{N,\varepsilon}\varphi_N^+ f_{N,\varepsilon}^+ , \tag{53}$$

where the functions $f_{N,\varepsilon}^\pm$ are given by (43) when inserting $S_n^\pm$ for S_n. Further, since φ_N^{WKB} satisfies the initial conditions in (1), we have $(\varphi - \varphi_N^{WKB})(\xi) = 0$ and $\varepsilon(\varphi - \varphi_N^{WKB})'(\xi) = 0$. Thus, Proposition 3.1 for $\hat{\varphi}_0, \hat{\varphi}_1 = 0$ implies (note that $f_{N,\varepsilon}^\pm \in C(I)$ and $a \in W^{1,\infty}(I)$) the existence of some $C > 0$ independent of N and ε such that

$$\begin{aligned} \|\varphi - \varphi_N^{WKB}\|_{L^\infty(I)} &\leq \frac{C}{\varepsilon} \|\alpha_{N,\varepsilon}\varphi_N^- f_{N,\varepsilon}^- + \beta_{N,\varepsilon}\varphi_N^+ f_{N,\varepsilon}^+\|_{L^2(I)} \\ &\leq \frac{\widetilde{C}}{\varepsilon} \left(\|\alpha_{N,\varepsilon}\varphi_N^-\|_{L^\infty(I)} \|f_{N,\varepsilon}^-\|_{L^\infty(I)} + \|\beta_{N,\varepsilon}\varphi_N^+\|_{L^\infty(I)} \|f_{N,\varepsilon}^+\|_{L^\infty(I)} \right) , \end{aligned} \tag{54}$$

where $\widetilde{C} := \sqrt{\eta - \xi}\, C$. Further, according to Corollary 3.3,

$$\begin{aligned} \|f_{N,\varepsilon}^\pm\|_{L^\infty(I)} &\leq 2\varepsilon^{N+1} \|S_0'\|_{L^\infty(I)} \|S_{N+1}'\|_{L^\infty(I)} + \sum_{n=2}^{N} \sum_{k=2+N-n}^{N} \varepsilon^{n+k} \|S_n'\|_{L^\infty(I)} \|S_k'\|_{L^\infty(I)} \\ &\leq \|S_0'\|_{L^\infty(G)}^2 \left(2\varepsilon^{N+1} K_2^{N+1} (N+1)^{N+1} + \sum_{n=2}^{N} \sum_{k=2+N-n}^{N} \varepsilon^{n+k} K_2^{n+k} n^n k^k \right) . \end{aligned} \tag{55}$$

Estimate (52) now follows from (54)–(55) by applying Lemma 3.6. This concludes the proof. □

Remark 3.8. As a consequence of Theorem 3.7, we have that

$$\|\varphi - \varphi_N^{WKB}\|_{L^\infty(I)} = \mathcal{O}(\varepsilon^N), \quad \varepsilon \to 0. \tag{56}$$

3.1. Refined error estimate incorporating quadrature errors

Theorem 3.7 yields an explicit (w.r.t. ε and N) error estimate for the WKB approximation (13). However, in practice one cannot expect to be able to compute (13) exactly. Indeed, even though for a given function a one can compute the derivatives $(S_n^\pm)'$ exactly through (8)–(10), one still has to deal with the integrals $\int_\xi^x (S_n^\pm)'\,\mathrm{d}\tau$ in (14) in order to compute the functions $S_n^\pm$. For a detailed description of the method we use to approximate these integrals, we refer to Section 4.1.

For now, let us assume we are given numerical approximations $\widetilde{S}_n^\pm$, $n \in \mathbb{N}_0$, of the functions $S_n^\pm$ that satisfy $\|\widetilde{S}_n^\pm - S_n^\pm\|_{L^\infty(I)} \le e_n$ with positive constants e_n. We then define the corresponding "perturbed" WKB approximation as

$$\widetilde{\varphi}_N^{WKB} := \alpha_{N,\varepsilon} \exp\left(\sum_{n=0}^N \varepsilon^{n-1} \widetilde{S}_n^-\right) + \beta_{N,\varepsilon} \exp\left(\sum_{n=0}^N \varepsilon^{n-1} \widetilde{S}_n^+\right). \tag{57}$$

Notice that we use here the exact constants $\alpha_{N,\varepsilon}$ and $\beta_{N,\varepsilon}$ as given by formulas (17)–(18) (since the values $(S_n^\pm)'(\xi)$ are exactly known from (8)–(10)).

We are now interested in an error estimate for the perturbed WKB approximation (57). Such an estimate is provided by the following theorem:

Theorem 3.9. *Let Hypothesis A be satisfied and let $\varphi \in C^2(I)$ be the solution of IVP (1). Further assume $\widetilde{S}_{2n}^\pm(x) \in \mathrm{i}\mathbb{R}$, $n \in \mathbb{N}_0$, for any $x \in I$. Then, there exist constants $\varepsilon_0 \in (0,1)$ and $C > 0$ independent of N and ε such that it holds for $\varepsilon \in (0, \varepsilon_0]$:*

$$\begin{aligned}\|\varphi - \widetilde{\varphi}_N^{WKB}\|_{L^\infty(I)} \le{}& \exp\left((\eta-\xi)\|S_0'\|_{L^\infty(G)} \sum_{n=0}^{\lfloor \frac{N-1}{2} \rfloor} \varepsilon^{2n} K_2^{2n+1}(2n+1)^{2n+1}\right) \\ &\times \Bigg[C\|S_0'\|^2_{L^\infty(G)} \left(|\varphi_0|\,\|S_0'\|_{L^\infty(G)} \sum_{n=0}^N \varepsilon^n K_2^n n^n + |\varphi_1|\right) \\ &\quad \times \left(\varepsilon^N K_2^{N+1}(N+1)^{N+1} + \sum_{n=2}^N \sum_{k=2+N-n}^N \varepsilon^{n+k-1} K_2^{n+k} n^n k^k\right) \\ &\quad + \left(|\alpha_{N,\varepsilon}| + |\beta_{N,\varepsilon}|\right)\left(\sum_{n=0}^N \varepsilon^{n-1} e_n\right) \exp\left(\sum_{n=0}^{\lfloor \frac{N-1}{2} \rfloor} \varepsilon^{2n} e_{2n+1}\right)\Bigg]. \end{aligned} \tag{58}$$

For $N = 0$ the sums in the exponential functions drop, and for $N < 2$ the double sum is dropped.

Proof. We have that

$$\|\varphi - \widetilde{\varphi}_N^{WKB}\|_{L^\infty(I)} \le \|\varphi - \varphi_N^{WKB}\|_{L^\infty(I)} + \|\varphi_N^{WKB} - \widetilde{\varphi}_N^{WKB}\|_{L^\infty(I)}. \tag{59}$$

Now, the first term in (59) can be estimated using Theorem 3.7 and enforces the restriction $\varepsilon \in (0, \varepsilon_0]$. For the second term we estimate

$$\begin{aligned}\|\varphi_N^{WKB} - \widetilde{\varphi}_N^{WKB}\|_{L^\infty(I)} \le{}& |\alpha_{N,\varepsilon}| \left\| \exp\left(\sum_{n=0}^N \varepsilon^{n-1} S_n^-\right) - \exp\left(\sum_{n=0}^N \varepsilon^{n-1} \widetilde{S}_n^-\right)\right\|_{L^\infty(I)} \\ &+ |\beta_{N,\varepsilon}| \left\| \exp\left(\sum_{n=0}^N \varepsilon^{n-1} S_n^+\right) - \exp\left(\sum_{n=0}^N \varepsilon^{n-1} \widetilde{S}_n^+\right)\right\|_{L^\infty(I)}. \end{aligned} \tag{60}$$

Let us introduce the abbreviation $\Delta S_n^\pm := \widetilde{S}_n^\pm - S_n^\pm$ and estimate

$$\begin{aligned}&\left\| \exp\left(\sum_{n=0}^N \varepsilon^{n-1} S_n^\pm\right) - \exp\left(\sum_{n=0}^N \varepsilon^{n-1} \widetilde{S}_n^\pm\right)\right\|_{L^\infty(I)} \\ &= \left\| \int_0^1 \frac{\mathrm{d}}{\mathrm{d}t} \exp\left(\sum_{n=0}^N \varepsilon^{n-1}\left(S_n^\pm + t\Delta S_n^\pm\right)\right) \mathrm{d}t \right\|_{L^\infty(I)} \\ &\le \left(\int_0^1 \left\| \exp\left(\sum_{n=0}^N \varepsilon^{n-1}\left(S_n^\pm + t\Delta S_n^\pm\right)\right)\right\|_{L^\infty(I)} \mathrm{d}t\right)\left(\sum_{n=0}^N \varepsilon^{n-1}\|\Delta S_n^\pm\|_{L^\infty(I)}\right)\end{aligned}$$

$$\leq \left(\int_0^1 \exp\left(\sum_{n=0}^{\lfloor \frac{N-1}{2} \rfloor} \varepsilon^{2n}\left(\|S_{2n+1}^{\pm}\|_{L^\infty(I)} + t\|\Delta S_{2n+1}^{\pm}\|_{L^\infty(I)}\right)\right) \mathrm{d}t\right)\left(\sum_{n=0}^{N} \varepsilon^{n-1}\|\Delta S_n^{\pm}\|_{L^\infty(I)}\right)$$

$$\leq \exp\left(\sum_{n=0}^{\lfloor \frac{N-1}{2} \rfloor} \varepsilon^{2n}\left(\|S_{2n+1}^{\pm}\|_{L^\infty(I)} + \|\Delta S_{2n+1}^{\pm}\|_{L^\infty(I)}\right)\right)\left(\sum_{n=0}^{N} \varepsilon^{n-1}\|\Delta S_n^{\pm}\|_{L^\infty(I)}\right)$$

$$\leq \exp\left((\eta-\xi)\|S_0'\|_{L^\infty(G)} \sum_{n=0}^{\lfloor \frac{N-1}{2} \rfloor} \varepsilon^{2n} K_2^{2n+1}(2n+1)^{2n+1}\right) \exp\left(\sum_{n=0}^{\lfloor \frac{N-1}{2} \rfloor} \varepsilon^{2n} e_{2n+1}\right)\left(\sum_{n=0}^{N} \varepsilon^{n-1} e_n\right), \quad (61)$$

where we used in the third step that $S_{2n}^{\pm}(x) + t\Delta S_{2n}^{\pm}(x) \in \mathrm{i}\,\mathbb{R}$ for every $t \in [0,1]$ and $x \in I$, which is a direct consequence of (15) and the assumption $\widetilde{S}_{2n}^{\pm}(x) \in \mathrm{i}\,\mathbb{R}$. Moreover, in the last step we used Corollary 3.3. The claim now follows by combining (59)–(61). □

Let us compare the extended error estimate (58) with (52). The new (additional) second term inside the square brackets in (58) is due to the perturbed functions $\widetilde{S}_n^{\pm}$ and includes the approximation error bounds e_n. In particular, the factor $\sum_{n=0}^{N} \varepsilon^{n-1} e_n$ is rather unfavorable, as it is of order $\mathcal{O}(\varepsilon^{-1})$, as $\varepsilon \to 0$. We note that the appearance of this $\mathcal{O}(\varepsilon^{-1})$-term in estimate (58) is strongly related to the appearance of the $\mathcal{O}(\varepsilon^{-1})$-terms in [8, Theorem 3.1], [13, Theorem 3.2] and [11, Eq. (35)]. There it implied an upper step size limit $h \leq \bar{h}(\varepsilon) = \varepsilon^{\gamma}$ with some $\gamma \in (0,1)$. Similarly, it would require here some ε-dependent upper bound on the quadrature error e_0 of $\widetilde{S}_0^{\pm}$ in order to compensate at least the $\mathcal{O}(\varepsilon^{-1})$-error term. In practice this will necessitate to use some finer grid for computing $\widetilde{S}_0^{\pm}$, as ε decreases. We specify this observation in the following remark.

Remark 3.10. It is evident from (50) that $\alpha_{N,\varepsilon} = \mathcal{O}(1)$, $\varepsilon \to 0$. The same holds for $\beta_{N,\varepsilon}$. Hence, we see from (58) that

$$\|\varphi - \widetilde{\varphi}_N^{WKB}\|_{L^\infty(I)} = \mathcal{O}(\varepsilon^N) + \sum_{n=0}^{N} \mathcal{O}(\varepsilon^{n-1}) e_n, \quad \varepsilon \to 0. \quad (62)$$

Thus, asymptotically, as $\varepsilon \to 0$, the approximation error of $\widetilde{S}_0^{\pm}$ has the biggest impact on the overall error since it is multiplied by a factor $\mathcal{O}(\varepsilon^{-1})$. In order to recover an overall $\mathcal{O}(\varepsilon^N)$ error behavior, as in Theorem 3.7, one should hence aim for highly accurate approximations of the functions $S_n^{\pm}$, with an ε-dependent error order of at most $e_n = \mathcal{O}(\varepsilon^{N-n+1})$.

4. Computation of the WKB approximation

In this section we present the methods we use to compute the (perturbed) WKB approximation (13), (57). This process can be divided into two steps. First, the computation of the functions S_n. Second, an adequate truncation of the asymptotic series (6).

4.1. Computation of the functions S_n

The computation of the functions S_n relies on recurrence relation (8)–(10) as well as on definition (14). Since the latter involves the evaluation of an integral, one cannot expect to be able to compute S_n exactly, in general. Consequently, we will instead compute approximations $\widetilde{S}_n \approx S_n = \int_{\xi}^{x} S_n' \,\mathrm{d}\tau$ which satisfy the assumption $\widetilde{S}_{2n}(x) \in \mathrm{i}\,\mathbb{R}$, $n \in \mathbb{N}_0$, such that the resulting error for the corresponding perturbed WKB approximation can be controlled by Theorem 3.9.

As the first step, we compute the derivatives S_n' through (8)–(10) exactly, employing symbolic computations[3]. Secondly, we employ a highly accurate quadrature for approximating the integral in (14). For this, we use the well-known Clenshaw–Curtis algorithm [20], which we shall briefly explain in the following.

The basic idea of Clenshaw–Curtis quadrature is to expand the integrand f in terms of Chebyshev polynomials, the integrals of which are known. More precisely, one considers a truncated Chebyshev series for the integrand, i.e., $f(l) \approx \sum_{r=0}^{M} a_r T_r(l)$, $l \in [-1,1]$, where $T_r(l) = \cos(r \arccos(l))$, $r \in \mathbb{N}_0$, are the Chebyshev polynomials. Here, the spectral coefficients a_r are determined with a collocation method at the Chebyshev collocation points $l_k = \cos(k\pi/M)$, $k = 0,\dots,M$, by solving the $M+1$ equations $f(l_k) = \sum_{r=0}^{M} a_r \cos\left(\frac{rk\pi}{M}\right)$ for the a_r, $r = 0,\dots,M$. Therefore, the spectral coefficients can be computed by the discrete cosine transformation (DCT) of the function f sampled at the collocations points. We note that the DCT is related to the discrete Fourier transform and can be computed efficiently using the fast Fourier transform algorithm after some preprocessing (e.g., see [21, Chap. 8]).

Then, the antiderivative of f can be approximated again by a Chebyshev sum,

$$\int_{-1}^{l} f(\tau)\,\mathrm{d}\tau \approx \sum_{r=0}^{M} b_r T_r(l), \quad (63)$$

[3] As an alternative to (8)–(10), in [19] the authors established an almost explicit formula for the derivatives S_n', depending on a and its derivatives $a', \dots, a^{(n)}$. Although not used here, this approach may prove advantageous with regard to the computational time.

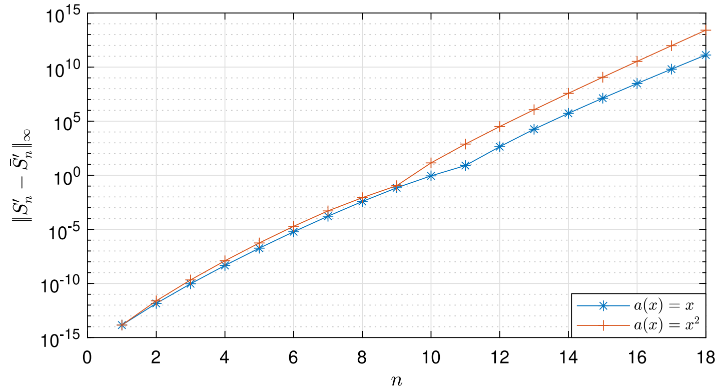

Fig. 2. $L^\infty(I)$-norm of the error of the approximation $\bar{S}_n'$ for the examples $a(x) = x$ and $a(x) = x^2$ on the interval $I = [1,2]$. Here, we set $M = 20$.

where the coefficients b_r are related to the a_r, see [20] for the detailed formulas. In [22] it was shown that the Clenshaw–Curtis method approximates integrals of analytic functions with spectral accuracy, i.e., the numerical error decreases exponentially with the number of modes M.

An integration over the interval $x \in [\xi, \eta]$ is realized by mapping $x = \eta(1+l)/2 + \xi(1-l)/2$, $l \in [-1,1]$ to the interval $[-1,1]$. Thus, by sampling the derivatives S_n' at the transformed Chebyshev points x_k, $k = 0,\dots,M$ in the interval $I = [\xi,\eta]$, we obtain the approximations $\widetilde{S}_n(x_k) \approx S_n(x_k)$. Notably, the coefficients b_r are such that the r.h.s. of (63) vanishes at $l = -1$, implying $\widetilde{S}_n(\xi) = 0$. Hence, the perturbed WKB approximation (57) satisfies the first initial condition in (1), namely, $\widetilde{\varphi}_N^{WKB}(\xi) = \alpha_{N,\varepsilon} + \beta_{N,\varepsilon} = \varphi_0$. Finally, it is worth mentioning that when employing the Clenshaw–Curtis algorithm for the integrals in (14), it follows that $\widetilde{S}_{2n}(x_k) \in \mathrm{i}\,\mathbb{R}$. As a consequence, the error of the corresponding perturbed WKB approximation (57) can be controlled with the aid of Theorem 3.9.

We note that an alternative and efficient way of approximating the functions S_n can be realized without the need for symbolic computation of the derivatives S_n'. Indeed, one can instead employ a spectral method to perform the differentiation of the predecessor S_{n-1}' in the recursion (10). For instance, by using the $(M+1)\times(M+1)$ Chebyshev differentiation matrices $\mathbf{D}_M$ as described in [21, Chap. 6], one can efficiently approximate the derivative of a function at Chebyshev grid points $l_k \in [-1,1]$, $k = 0,1,\dots,M$. Thus, to approximate the derivative of a function sampled at transformed Chebyshev points $x_k \in [\xi,\eta]$, it is necessary to use the scaled matrix $\widetilde{\mathbf{D}}_M := \frac{2}{\eta-\xi}\mathbf{D}_M$. Following recurrence relation (8)–(10), we can therefore approximate the derivatives S_n' sampled at Chebyshev points x_k through the following pointwise definition on the grid:

$$\bar{S}_1'(x_k) := -\frac{\sum_{l=0}^{M} (\widetilde{\mathbf{D}}_M)_{k+1,l+1} S_0'(x_l)}{2S_0'(x_k)}\,, \tag{64}$$

$$\bar{S}_n'(x_k) := -\frac{\sum_{j=1}^{n-1} \bar{S}_j'(x_k)\bar{S}_{n-j}'(x_k) + \sum_{l=0}^{M} (\widetilde{\mathbf{D}}_M)_{k+1,l+1} \bar{S}_{n-1}'(x_l)}{2S_0'(x_k)}\,, \quad n \ge 2\,, \tag{65}$$

for $k = 0,\dots,M$. One then obtains approximations $\widetilde{S}_n(x_k) \approx S_n(x_k)$ by employing the Clenshaw–Curtis algorithm using the approximations $\bar{S}_n'(x_k) \approx S_n'(x_k)$, $k = 0,\dots,M$.

However, note that approximating S_n' using (64)–(65) can lead to a rapid accumulation of errors, as repeated numerical differentiation is intrinsically unstable. The reason for this behavior lies in the ill-conditioned Chebyshev differentiation matrices $\mathbf{D}_M$. It is known that the condition number of these matrices is of order $\mathcal{O}(M^2)$ (e.g., see [23,24]). In a finite precision approach this leads to a big loss, which means that in each application of the recurrence relation we lose a finite amount of accuracy in the computation of the S_n' (see Fig. 2 for two examples). Consequently, it can be recommended to employ this approach only for small values of N.

4.2. Truncation of the WKB series

When truncating the asymptotic series

$$f \sim \sum_{n=0}^{\infty} \varepsilon^n f_n\,, \quad \varepsilon \to 0 \tag{66}$$

after some finite order N, one would like to analyze the difference $f - \sum_{n=0}^{N} \varepsilon^n f_n$. But since the function S in (5)–(6) remains unknown, we shall investigate the numerical error of the WKB approximation, as started in Section 3.

Recall that for a fixed $N \ge 0$, Theorem 3.7 guarantees that $\|\varphi - \varphi_N^{WKB}\|_{L^\infty(I)} = \mathcal{O}(\varepsilon^N)$ as $\varepsilon \to 0$, see also Remark 3.8. In practical applications, however, the situation is exactly the opposite, namely, the small parameter ε is fixed and N can be chosen freely. Note also that just including more terms into the series (6) does not necessarily reduce the error of the WKB approximation, simply since the asymptotic series is typically divergent. Hence the question arises which choice of N will minimize $\|\varphi-\varphi_N^{WKB}\|_{L^\infty(I)}$, often referred to as *optimal truncation*. In this context, we denote by $N_{opt}=N_{opt}(\varepsilon):=\operatorname{argmin}_{N\in\mathbb{N}_0}\|\varphi-\varphi_N^{WKB}\|_{L^\infty(I)}$ the *optimal truncation order*. In general, an *optimally truncated* asymptotic series is sometimes referred to as *superasymptotics* (e.g., see [25]). The corresponding error of an optimally truncated series is then typically of the form $\sim\exp(-c/\varepsilon)$, as $\varepsilon\to0$, with some constant $c>0$.

In practice, a useful heuristic for finding the optimal truncation order for a fixed ε is given in [25]. It suggests that it can be obtained by truncating the asymptotic series before its smallest term. In our case, we would hence have to find the minimizer $N_{heu}=N_{heu}(\varepsilon)$ of $n\mapsto\varepsilon^n\|S_{n+1}\|_{L^\infty(I)}$. This can either be found by "brute force", comparing the size of each term up to some prescribed maximal order N_{max}, or by utilizing Corollary 3.3 to (roughly) predict N_{heu}. Indeed, for any $N\in\mathbb{N}_0$, estimate (38) implies

$$\varepsilon^N\|S_{N+1}\|_{L^\infty(I)}\le(\eta-\xi)\|S_0'\|_{L^\infty(G)}\varepsilon^N K_2^{N+1}(N+1)^{N+1}\,. \tag{67}$$

Treating N as a continuous variable for the moment, we find the minimum of

$$g(N):=\ln\left(\varepsilon^N K_2^{N+1}(N+1)^{N+1}\right) \tag{68}$$

at

$$\hat N_{heu}=\hat N_{heu}(\varepsilon)=\frac{1}{\mathrm{e}K_2\varepsilon}-1\,. \tag{69}$$

Hence, the minimum of the right-hand side of (67) is

$$(\eta-\xi)\|S_0'\|_{L^\infty(G)}\exp\left(g(\hat N_{heu})\right)=\frac{(\eta-\xi)\|S_0'\|_{L^\infty(G)}}{\varepsilon}\exp\left(-\frac{1}{\mathrm{e}K_2\varepsilon}\right)\,. \tag{70}$$

So, the first term of the remainder of the asymptotic series appearing in the WKB-ansatz (5)–(6), truncated at the nearest integer value to $\hat N_{heu}$, is exponentially small w.r.t. ε. Recalling that the term $\exp(g(N))=\varepsilon^N K_2^{N+1}(N+1)^{N+1}$ also appears in estimate (52), we therefore might also expect the error $\|\varphi-\varphi_N^{WKB}\|_{L^\infty(I)}$ to be exponentially small w.r.t. ε, if N is chosen adequately. Indeed, this is guaranteed by the following corollary of Theorem 3.7.

Corollary 4.1. *Let Hypothesis A be satisfied and let $\varphi\in C^2(I)$ be the solution of IVP (1). Then there exist $\tilde\varepsilon_0\in(0,1)$ and $N=N(\varepsilon)\in\mathbb{N}$ such that it holds for $\varepsilon\in(0,\tilde\varepsilon_0]$:*

$$\|\varphi-\varphi_N^{WKB}\|_{L^\infty(I)}\le C\exp\left(-\frac{r}{\varepsilon}\right)\,, \tag{71}$$

with constants $C,r>0$ independent of ε.

Proof. We prove estimate (71) by applying Theorem 3.7 for a specific choice of $N=N(\varepsilon)$. First, choose $0<\tilde\varepsilon_0<\min(\varepsilon_0,\frac{1}{K_2})$ with $\varepsilon_0\in(0,1)$ being the constant from Theorem 3.7 and K_2 from Corollary 3.3. Then there exists some constant $c\in[\mathrm{e}K_2\tilde\varepsilon_0,\mathrm{e})$ implying that $N:=\lfloor\frac{c}{\mathrm{e}K_2\varepsilon}\rfloor-1\ge0$ for any $\varepsilon\in(0,\tilde\varepsilon_0]$. The idea is now to majorize, for this choice of N, several sums in (52) by convergent geometric series. First, we have

$$\sum_{n=0}^N(\varepsilon K_2 n)^n\le\sum_{n=0}^N(\varepsilon K_2(N+1))^n\le\sum_{n=0}^\infty\left(\frac{c}{\mathrm{e}}\right)^n=\frac{1}{1-\frac{c}{\mathrm{e}}}\,, \tag{72}$$

where we used $\varepsilon K_2(N+1)\le\frac{c}{\mathrm{e}}$. Similarly, we get

$$\begin{aligned}\sum_{n=0}^{\lfloor\frac{N-1}{2}\rfloor}\varepsilon^{2n}(K_2(2n+1))^{2n+1}&\le K_2\sum_{n=0}^{\lfloor\frac{N-1}{2}\rfloor}(\varepsilon K_2(N+1))^{2n}(2n+1)\le K_2\sum_{n=0}^N\left(\frac{c}{\mathrm{e}}\right)^n(n+1)\le K_2\left(\sum_{n=0}^\infty\left(\frac{c}{\mathrm{e}}\right)^n n+\sum_{n=0}^\infty\left(\frac{c}{\mathrm{e}}\right)^n\right)\\&=K_2\frac{\mathrm{e}^2}{(\mathrm{e}-c)^2}\,,\end{aligned} \tag{73}$$

where we used the geometric series variant $\sum_{n=0}^\infty q^n n=\frac{q}{(1-q)^2}$ for any $q\in\mathbb{R}$ with $|q|<1$. At this point, Theorem 3.7 and (72)–(73) imply for $\varepsilon\in(0,\tilde\varepsilon_0]$

$$\|\varphi-\varphi_N^{WKB}\|_{L^\infty(I)}\le C\varepsilon^N K_2^{N+1}(N+1)^{N+1}+C\sum_{n=2}^N\sum_{k=2+N-n}^N\varepsilon^{n+k-1}K_2^{n+k}n^n k^k\,, \tag{74}$$

where $C>0$ is some constant independent of ε. Now, for the first term in (74) we have that

$$\varepsilon^N K_2^{N+1}(N+1)^{N+1}\le\frac{1}{\varepsilon}\left(\frac{c}{\mathrm{e}}\right)^{\lfloor\frac{c}{\mathrm{e}K_2\varepsilon}\rfloor}\le\frac{\mathrm{e}}{c\varepsilon}\left(\frac{c}{\mathrm{e}}\right)^{\frac{c}{\mathrm{e}K_2\varepsilon}}=\frac{\mathrm{e}}{c\varepsilon}\exp\left(-\frac{\tilde r}{\varepsilon}\right)\,, \tag{75}$$

with $\tilde r:=\frac{c\ln(\mathrm{e}/c)}{\mathrm{e}K_2}>0$. Finally, the second term in (74) can be estimated as follows:

$$\sum_{n=2}^N\sum_{k=2+N-n}^N\varepsilon^{n+k-1}K_2^{n+k}n^n k^k\le\frac{1}{\varepsilon}\sum_{n=2}^N\sum_{k=2+N-n}^N(\varepsilon K_2 N)^n(\varepsilon K_2 N)^k=\frac{1}{\varepsilon}(\varepsilon K_2 N)^{N+2}\sum_{n=0}^{N-2}\sum_{k=0}^n(\varepsilon K_2 N)^k$$

$$\leq \frac{1}{\varepsilon}(\varepsilon K_2 N)^{N+2} \sum_{n=0}^{N-2} \sum_{k=0}^{\infty} \left(\frac{c}{\mathrm{e}}\right)^k = \frac{1}{\varepsilon}(\varepsilon K_2 N)^{N+2} \frac{N-1}{1-\frac{c}{\mathrm{e}}} \leq \frac{K_2}{1-\frac{c}{\mathrm{e}}} \left(\frac{c}{\mathrm{e}\, K_2 \varepsilon}\right)^2 \left(\frac{c}{\mathrm{e}}\right)^{\left\lfloor \frac{c}{\mathrm{e} K_2 \varepsilon} \right\rfloor}$$
$$\leq \frac{c}{(\mathrm{e}-c)K_2\varepsilon^2} \left(\frac{c}{\mathrm{e}}\right)^{\frac{c}{\mathrm{e} K_2 \varepsilon}} = \frac{c}{(\mathrm{e}-c)K_2\varepsilon^2} \exp\left(-\frac{\tilde{r}}{\varepsilon}\right). \tag{76}$$

We observe that the r.h.s. of (75) can be bounded by the r.h.s. of (76) (up to a multiplicative constant) for $\varepsilon \in (0, \tilde{\varepsilon}_0]$. Thus, the claim follows with $r := \tilde{r}/2$ and adapting C. □

Remark 4.2. We note that the specific value N from the proof of Corollary 4.1 is not necessarily equal to the optimal truncation order N_{opt}. However, as a consequence of Corollary 4.1, and by the definition of N_{opt}, we conclude that for some $r > 0$

$$\|\varphi - \varphi^{WKB}_{N_{opt}}\|_{L^\infty(I)} = \mathcal{O}(\exp(-r/\varepsilon)), \quad \varepsilon \to 0. \tag{77}$$

Finally, we note that, apart from N_{heu} and $\hat{N}_{heu}$, another option for predicting the optimal truncation order N_{opt} is to find the minimizer of error estimate (52) (for ε fixed), say $\hat{N}_{opt} = \hat{N}_{opt}(\varepsilon)$, although this rather complicated expression can only be minimized numerically by brute force.

At this point, it seems convenient to summarize the notations and meanings of the different mentioned truncation orders which aim to estimate N_{opt} – see Table 1. In the next section we will compare results for each truncation order from Table 1, since it is not clear a priori which of these orders provides the most accurate prediction of N_{opt}. Nonetheless, let us note that in our experiments N_{opt}, $\hat{N}_{opt}$, and N_{heu} can only be determined by brute force, while $\hat{N}_{heu}$ is given explicitly by formula (69).

5. Numerical simulations

In this section we present several numerical simulations to illustrate some of the theoretical results we derived in Section 3. To this end, we will compute the (perturbed) WKB approximation as described in Section 4.1. That is, the functions S_n' are pre-computed symbolically and are then integrated numerically using the Clenshaw–Curtis algorithm based on a Chebyshev grid with $M+1$ grid points, where M will be specified later. All computations are carried out using Matlab version 9.13.0.2049777 (R2022b). Further, since we are dealing with very small errors for the WKB approximation, especially when investigating the optimal truncation order, we use the Advanpix Multiprecision Computing Toolbox for Matlab [26] with quadruple-precision to avoid roundoff errors.

5.1. Example 1: Airy equation

Consider the initial value problem

$$\begin{cases} \varepsilon^2\varphi''(x) + x\varphi(x) = 0, \quad x \in [1,2], \\ \varphi(1) = \mathrm{Ai}(-\frac{1}{\varepsilon^{2/3}}) + \mathrm{i}\,\mathrm{Bi}(-\frac{1}{\varepsilon^{2/3}}), \\ \varepsilon\varphi'(1) = -\varepsilon^{1/3}\left(\mathrm{Ai}'(-\frac{1}{\varepsilon^{2/3}}) + \mathrm{i}\,\mathrm{Bi}'(-\frac{1}{\varepsilon^{2/3}})\right), \end{cases} \tag{78}$$

where the exact solution is given by

$$\varphi_{exact}(x) = \mathrm{Ai}(-\frac{x}{\varepsilon^{2/3}}) + \mathrm{i}\,\mathrm{Bi}(-\frac{x}{\varepsilon^{2/3}}). \tag{79}$$

Here, Ai and Bi denote the Airy functions of first and second kind, respectively (e.g., see [27, Chap. 9]). Note that for this example, where $a(x) = x$, the derivatives S_n' are given by powers of x (up to a constant factor). Hence, the functions $S_n^\pm$ can be computed exactly from (14); however, we shall use them here only as reference solutions for the approximations $\tilde{S}_n^\pm$. Indeed, for a fixed number $M+1$ of Chebyshev grid points, we are then able to compute explicitly the approximation error $\|S_n^\pm - \tilde{S}_n^\pm\|_{L^\infty(I)} =: e_n$. Since $\tilde{S}_n^\pm$ is only available at the grid points, we actually compute the discrete analog of this norm.

The left panel of Fig. 3 shows the real part of φ_{exact} for the choice $\varepsilon = 2^{-8}$, which illustrates well the highly oscillatory behavior of the solution. Let us first investigate numerically the result from Corollary 3.3. For this, let us compute a constant K_2, as indicated

Table 1
Terminology for the different truncation orders mentioned in Section 4. The numbers $\hat{N}_{opt}$ and $\hat{N}_{heu}$ are predictions for N_{opt} and N_{heu} by means of (52) and (67), respectively. (For numerical values in two concrete examples see Figs. 6 and 9.)

N_{opt}	minimizer of $\|\varphi - \varphi_N^{WKB}\|_{L^\infty(I)}$ (optimal truncation order)
$\hat{N}_{opt}$	minimizer of error estimate (52) (prediction of N_{opt})
N_{heu}	minimizer of $\varepsilon^N \|S_{N+1}\|_{L^\infty(I)}$ (heuristic prediction of N_{opt})
$\hat{N}_{heu}$	minimizer of the r.h.s. of (67) (prediction of N_{heu})

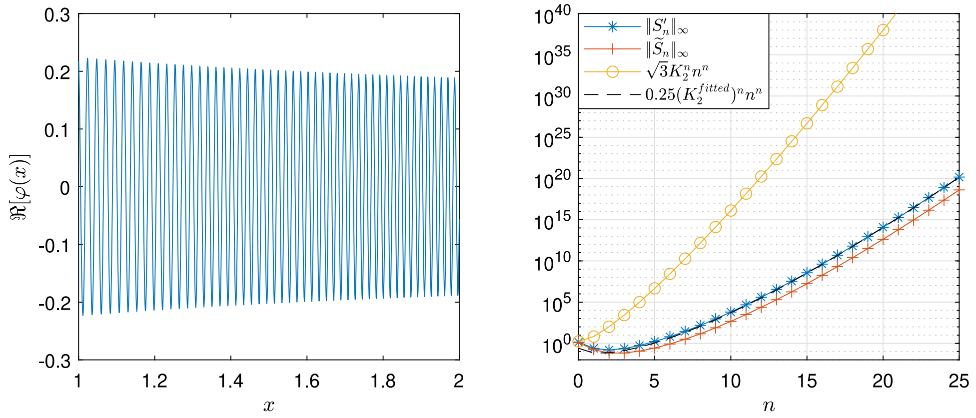

Fig. 3. Left: Real part of the exact solution (79) of IVP (78) for the choice $\varepsilon = 2^{-8}$. Right: $L^\infty(I)$-norm of S_n' and $\widetilde{S}_n$ as functions of n for the example $a(x) = x$ on the interval $I = [1, 2]$.

by the proof of Corollary 3.3 and Remark 3.4. Indeed, by using the minimization strategy from (41), we find that (note that here $S_0'(z) = \pm \mathrm{i}\sqrt{z}$; $\delta_{opt} = \frac{\sqrt{97}-7}{6} \approx 0.4748$)

$$K_2 = \frac{\mathrm{e}}{2\,\mathrm{e}-1} \min_{0<\delta\le 1} \frac{\sqrt{2+\delta}}{\delta(1-\delta)} = \frac{\mathrm{e}}{2\,\mathrm{e}-1} \frac{\sqrt{2+\delta_{opt}}}{\delta_{opt}(1-\delta_{opt})} \approx 3.8653 \tag{80}$$

is a suitable constant within the context of Corollary 3.3. In the right panel of Fig. 3, we present the $L^\infty(I)$-norms of the functions S_n' and the approximations $\widetilde{S}_n$ when using $M = 25$, along with the theoretical bound (39) on $\|S_n'\|_{L^\infty(I)}$. We observe that the true norms consistently remain below the theoretical bound. Additionally, we include as a dashed line the theoretical bound (39) when replacing K_2 and $\|S_0'\|_{L^\infty(G)}$ by the experimentally fitted values $K_2^{fitted} = 10/37 \approx 0.27$ and 0.25, respectively.[4] We observe very good agreement between the norms $\|S_n'\|_{L^\infty(I)}$ and the dashed line. This demonstrates well that, in the present example, the norms $\|S_n'\|_{L^\infty(I)}$ grow as Corollary 3.3 suggests, i.e., $\|S_n'\|_{L^\infty(I)} \sim C K_2^n n^n$ as $n \to \infty$, for some appropriate constants $C, K_2 > 0$. In general, however, this may not be the case. We refer to Appendix A and Section 5.3 for an example, where the functions S_n' and S_n even decay as $n \to \infty$.

Next, we investigate numerically the behavior of the WKB approximation error $\|\varphi - \widetilde{\varphi}_N^{WKB}\|_{L^\infty(I)}$ as a function of ε. We may compare the results with the error "estimate" (62). As a first test, we set $M = 8$ to compute $\widetilde{\varphi}_N^{WKB}$. This results in an approximation error for S_n of $e_n \approx 10^{-8}$, $n = 0, \dots, 4$. On the left of Fig. 4 we plot for $N = 0, \dots, 4$ the error as a function of ε: For $N = 2, 3, 4$ and small values of ε, the $\mathcal{O}(\varepsilon^{-1})e_0$-term is dominant. In contrast, for $N = 0$ and $N = 1$ this error term is not visible for the given range of ε-values so that the $\mathcal{O}(\varepsilon^N)$-term is dominant. As a second test, we set again $M = 8$, but now use in $\widetilde{\varphi}_N^{WKB}$ the exactly computed function S_0. The $\mathcal{O}(\varepsilon^{-1})e_0$-term from (62) is thus eliminated. On the right of Fig. 4 we show again the error $\|\varphi - \widetilde{\varphi}_N^{WKB}\|_{L^\infty(I)}$ as a function of ε: For $N = 2, 3, 4$ and small ε-values, the $\mathcal{O}(\varepsilon^0)e_1$-term, which is the next term in the sum in (62), now dominates. Indeed, the error curves show an almost constant value of approximately $2 \cdot 10^{-9}$ for small values of ε. For larger ε, the error curves behave like $\mathcal{O}(\varepsilon^N)$. As a third test, we set $M = 25$ and approximate again all functions S_n, $n = 0, \dots, 4$ (as in the first test). The corresponding approximation errors of S_n are $e_n \approx 10^{-23}$, $n = 0, \dots, 4$. On the left of Fig. 5 we present the resulting WKB approximation errors. We observe that, on this scale, all $\mathcal{O}(\varepsilon^{n-1})e_n$-terms in the sum of (62) are essentially eliminated, since all the shown error curves behave like $\mathcal{O}(\varepsilon^N)$. Overall, we observe very good agreement between the numerical results of each of the three tests and the statements from Theorem 3.9 and Remark 3.10.

Next we investigate the error of the (perturbed) WKB approximation as a function of the truncation order N. For this, we set again $M = 25$, yielding approximation errors of S_n as $e_n \approx 10^{-23}$ for $n = 0, 1, \dots$. We may therefore neglect the errors caused by approximating the functions S_n. On the right of Fig. 5 we plot the actual error $\|\varphi - \widetilde{\varphi}_N^{WKB}\|_{L^\infty(I)}$ and its error estimate (52) while again using $K_2^{fitted} = 10/37$, both as functions of N, for several ε-values. We observe that, even when using the fitted constant K_2^{fitted}, the "optimal" truncation order $\widehat{N}_{opt}$, as predicted by the estimate (52), is smaller than N_{opt} (determined as the argmin of the actual error curve). For instance, we have $\widehat{N}_{opt}(2^{-4}) \approx 14 < 22 \approx N_{opt}(2^{-4})$ and $\widehat{N}_{opt}(2^{-5}) \approx 29 < 44 \approx N_{opt}(2^{-5})$, respectively. This is not a paradox, but it is implied in this example by the strong over-estimation (52) of the error for large N.

In Fig. 6 we plot on the left the optimal truncation order $N_{opt}(\varepsilon)$ as a function of ε as well as its predictions $\widehat{N}_{opt}(\varepsilon)$, $N_{heu}(\varepsilon)$, and $\widehat{N}_{heu}(\varepsilon)$. The plot suggests that N_{opt}, $\widehat{N}_{opt}$, and N_{heu} are all proportional to ε^{-1}, as $\varepsilon \to 0$ (for $\widehat{N}_{heu}$ this is already evident from (69)). Further, for $\varepsilon = 2^{-1}, 2^{-3}, 2^{-4}, 2^{-5}$ we observe that $N_{opt} = N_{heu}$. On the right of Fig. 6 we plot the corresponding optimal error which is achieved by using N_{opt} as well as error estimate (52) when using $N = \widehat{N}_{opt}$, both as a function of $1/\varepsilon$. As indicated by the dashed line, the optimal error decays like $\mathcal{O}(\exp(-r/\varepsilon))$, with $r \approx 1.36$ being a fitted value, in good agreement with Remark 4.2.

[4] Dividing (39) by n^n and taking the logarithm we used a linear approximation to obtain K_2^{fitted}.

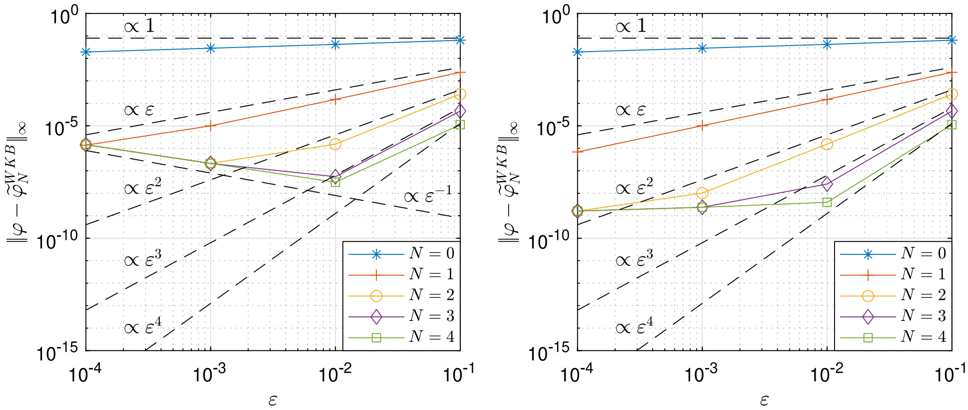

Fig. 4. $L^\infty(I)$-norm of the error of the WKB approximation as a function of ε, for the IVP (78) and several choices of N. Left: $M = 8$. Right: $M = 8$; using the exact function S_0.

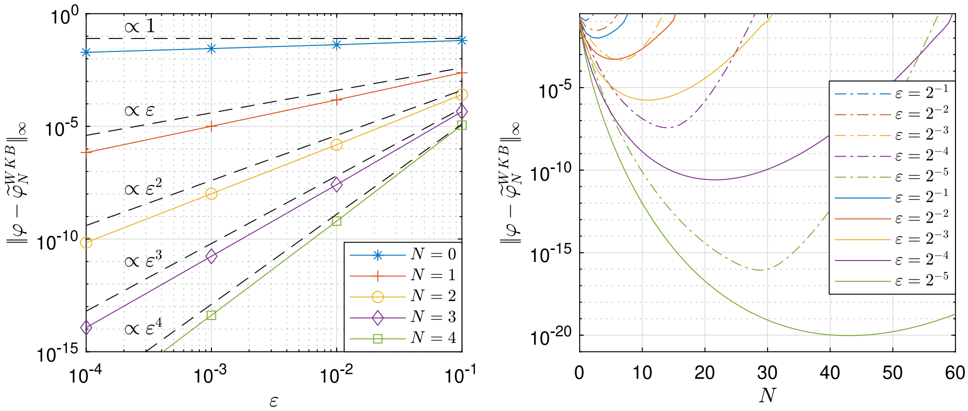

Fig. 5. Left: $L^\infty(I)$-norm of the error of the WKB approximation as a function of ε for the IVP (78) and several choices of N. Here, we set $M = 25$. Right: $L^\infty(I)$-norm of the error of the WKB approximation as a function of N for the IVP (78) and several choices of ε. The dash-dotted lines correspond to the error estimate according to Theorem 3.7 and the solid lines correspond to the actual error of the WKB approximation. (In both plots the curves have the same top-down ordering as the legend.).

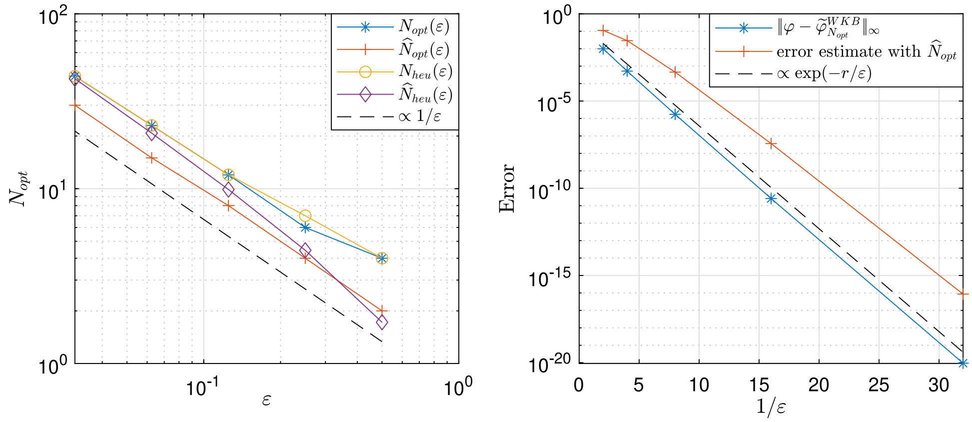

Fig. 6. Left: The optimal truncation order N_{opt} as well as the predicted "optimal" orders $\widehat{N}_{opt}$, N_{heu}, and $\widehat{N}_{heu}$ as functions of ε. The dashed line is proportional to $1/\varepsilon$. Right: The optimal error achieved by using N_{opt} as well as error estimate (52) when using $N = \widehat{N}_{opt}$, both as functions of $1/\varepsilon$. The dashed line is proportional to $\exp(-\frac{r}{\varepsilon})$ with $r \approx 1.36$.

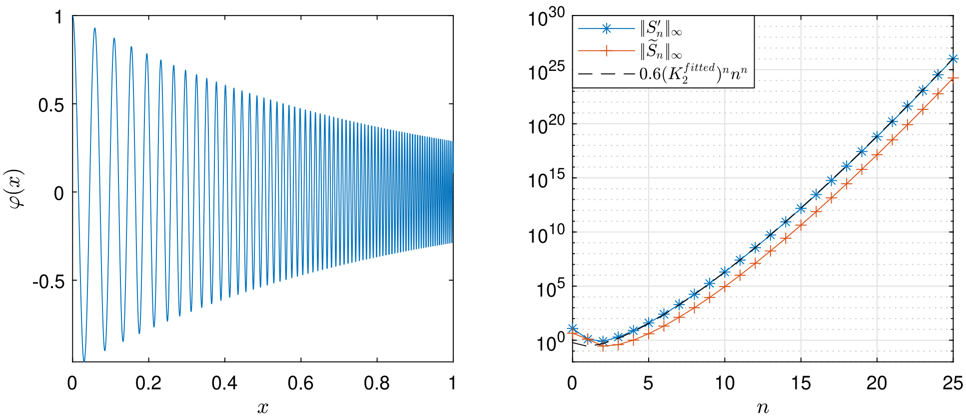

Fig. 7. Left: Exact solution (82) of IVP (81) for the choice $\varepsilon = 10^{-2}$. Right: $L^\infty(I)$-norm of S_n' and $\widetilde{S}_n$ as functions of n for the example $a(x) = \exp(5x)$ on the interval $I = [0,1]$.

5.2. Example 2

As our second example let us consider the initial value problem

$$\begin{cases} \varepsilon^2\varphi''(x) + \mathrm{e}^{5x}\,\varphi(x) = 0\,, \quad x \in [0,1]\,, \\ \varphi(0) = 1\,, \\ \varepsilon\varphi'(0) = 0\,, \end{cases} \tag{81}$$

where the exact solution is given by[5]

$$\varphi_{exact}(x) = \frac{J_0\left(\frac{2}{5\varepsilon}\,\mathrm{e}^{5x/2}\right)Y_1\left(\frac{2}{5\varepsilon}\right) - Y_0\left(\frac{2}{5\varepsilon}\,\mathrm{e}^{5x/2}\right)J_1\left(\frac{2}{5\varepsilon}\right)}{J_0\left(\frac{2}{5\varepsilon}\right)Y_1\left(\frac{2}{5\varepsilon}\right) - J_1\left(\frac{2}{5\varepsilon}\right)Y_0\left(\frac{2}{5\varepsilon}\right)}\,. \tag{82}$$

Here, J_ν and Y_ν denote the Bessel functions of first and second kind of order ν, respectively (e.g., see [27, Chap. 10]).

On the left of Fig. 7 the exact solution φ_{exact} is plotted for the choice $\varepsilon = 10^{-2}$. Throughout the whole interval, due to the fast growth of the function $a(x) = \exp(5x)$, the solution exhibits a rapid increase of its oscillatory behavior. Further, we plot on the right of Fig. 7 the $L^\infty(I)$-norms of the derivatives S_n' and the approximations $\widetilde{S}_n$ when using $M = 30$. As indicated by the dashed line, the smallest (fitted) constant K_2 such that estimate (39) holds is $K_2^{fitted} \approx 9/20$ (here we also replaced $\|S_0'\|_{L^\infty(G)}$ in (39) by the fitted value 0.6). In Fig. 8 we present the WKB approximation error $\|\varphi - \widetilde{\varphi}_N^{WKB}\|_{L^\infty(I)}$ as a function of ε and may again compare the results with the error "estimate" (62). We observe that, on this scale, all $\mathcal{O}(\varepsilon^{n-1})e_n$-terms are essentially eliminated, since all the shown error curves behave like $\mathcal{O}(\varepsilon^N)$. Overall, we observe very good agreement with the statements from Theorem 3.9 and Remark 3.10. Finally, we plot in Fig. 9 on the left the optimal truncation order N_{opt} as well as its predictions $\widehat{N}_{opt}$, N_{heu}, and $\widehat{N}_{heu}$, as functions of ε. We find that N_{opt} is proportional to ε^{-1}, as $\varepsilon \to 0$. On the right of Fig. 9 we present the corresponding optimal error as well as error estimate (52) when using $N = \widehat{N}_{opt}$, both as a function of $1/\varepsilon$. As the dashed line indicates, the error decays like $\mathcal{O}(\exp(-r/\varepsilon))$, with $r \approx 0.81$ being a fitted value. This is in good agreement with Remark 4.2.

5.3. Example 3: Convergent WKB approximation

As a final example, let us consider $a(x) = (1 + x + x^2)^{-2}$. We are interested in investigating the initial value problem

$$\begin{cases} \varepsilon^2\varphi''(x) + (1 + x + x^2)^{-2}\varphi(x) = 0\,, \quad x \in [0,1]\,, \\ \varphi(0) = 1\,, \\ \varepsilon\varphi'(0) = 1\,, \end{cases} \tag{83}$$

where the exact solution φ_{exact} is given by[6]

$$\varphi_{exact}(x) = \frac{a(x)^{-1/4}}{\sqrt{3}\gamma(\varepsilon)}\sin\left(\gamma(\varepsilon)\left(\arctan\left(\frac{2x+1}{\sqrt{3}}\right) - \frac{\pi}{6}\right)\right) - a(x)^{-1/4}\cos\left(\gamma(\varepsilon)\left(\arctan\left(\frac{2x+1}{\sqrt{3}}\right) - \frac{\pi}{6}\right)\right)\,, \tag{84}$$

[5] We found the exact solution by using the Symbolic Math Toolbox of MATLAB.

[6] We found the exact solution by using the Symbolic Math Toolbox of MATLAB.

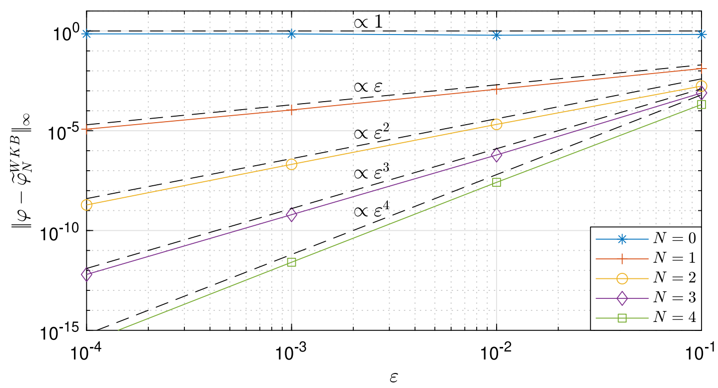

Fig. 8. $L^\infty(I)$-norm of the error of the WKB approximation as a function of ε for the IVP (81) and several choices of N. Here, we set $M = 30$.

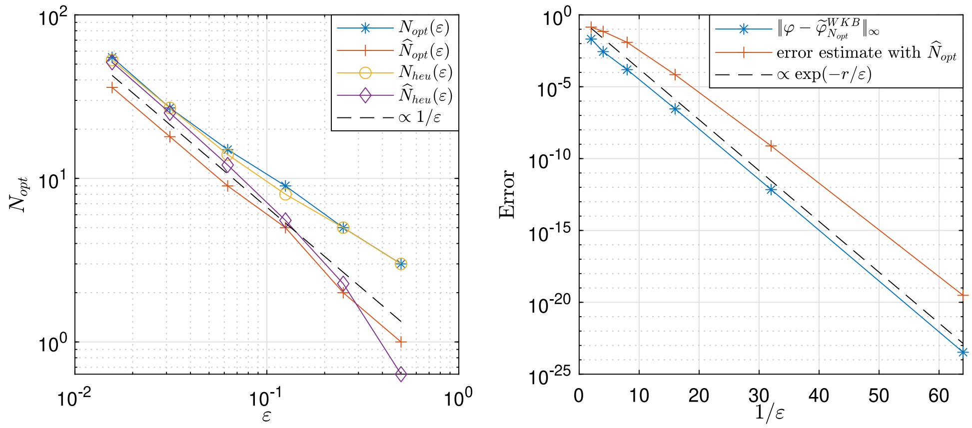

Fig. 9. Left: The optimal truncation order N_{opt} as well as the predicted "optimal" orders $\widehat{N}_{opt}$, N_{heu}, and $\widehat{N}_{heu}$ as functions of ε. The dashed line is proportional to $1/\varepsilon$. Right: The optimal error achieved by using N_{opt} as well as error estimate (52) when using $N = \widehat{N}_{opt}$, both as functions of $1/\varepsilon$. The dashed line is proportional to $\exp(-\frac{r}{\varepsilon})$ with $r \approx 0.81$.

where $\gamma(\varepsilon) := \sqrt{3\varepsilon^2 + 4}/(\sqrt{3}\varepsilon)$.

This example is special in the sense that $a(x) = (1 + x + x^2)^{-2}$ belongs to the class of functions represented as $(C_1 + C_2 x + C_3 x^2)^{-2}$, with constants C_i, $i = 1, 2, 3$, satisfying $|C_2| + |C_3| > 0$ and $C_2^2 \neq 4C_1C_3$. Further details regarding this class of functions are discussed in Appendix A, particularly with regard to the corresponding WKB series. Notably, for such functions it holds that $S_1' \not\equiv 0$, $S_2' \not\equiv 0$ and $S_3' \equiv 0$, see Remark A.2. Moreover, according to Proposition A.1 and Remark A.3, it follows that

$$S_{2n}' = \mathcal{O}\left((n-1)^{-3/2} |C_1C_3 - C_2^2/4|^{n-1}\right) , \quad n \to \infty , \tag{85}$$

$$S_{2n+1}' \equiv 0 , \quad n \geq 1 . \tag{86}$$

Consequently, this implies that the underlying asymptotic series (6) is (geometrically) convergent for any $\varepsilon \leq |C_1C_3 - C_2^2/4|^{-1/2}$, see again Remark A.3. In this case, given that $|C_1C_3 - C_2^2/4| = 3/4$, the functions S_{2n}' (and hence S_{2n}) exhibit exponential decay as $n \to \infty$, uniformly in $x \in I$. The corresponding WKB series is convergent for any $\varepsilon \in (0, 2/\sqrt{3}]$.

In Fig. 10 on the left we plot φ_{exact} for the choice $\varepsilon = 2^{-9}$. Moreover, on the right of Fig. 10 we plot the $L^\infty(I)$-norm of S_n' and $\widetilde{S}_n$, both as a function of n. Here, we set $M = 30$ for the numerical integration of the functions S_n'. We observe that the norms indeed decay exponentially, in agreement with Remark A.3. Here, the dashed line is precisely given by the r.h.s. of (92) with $C_1 = C_2 = C_3 = 1$. In Fig. 11 on the left we plot for $N = 0, \dots, 4$ the error of the WKB approximation $\|\varphi - \widetilde{\varphi}_N^{WKB}\|_{L^\infty(I)}$ as a function of ε. By comparing the results with (62), we observe that all $\mathcal{O}(\varepsilon^{n-1})e_n$-terms are essentially eliminated. Further, the error curves for $N = 0, 1, 3$ behave like $\mathcal{O}(\varepsilon^N)$ whereas the curves corresponding to the choices $N = 2, 4$ behave like $\mathcal{O}(\varepsilon^{N+1})$. This is because the given function a implies $S_{2n+1}' \equiv 0$, for any $n \geq 1$, which means $\varphi_N^{WKB} = \varphi_{N+1}^{WKB}$ for any even $N \geq 2$.

Finally, on the right of Fig. 11 we plot the error $\|\varphi - \widetilde{\varphi}_N^{WKB}\|_{L^\infty(I)}$ as a function of the truncation order N, for several ε-values. We observe that all shown error curves are decreasing functions in N, up to the point where they reach values of approximately 10^{-22}. This is due to the approximation of the functions S_n. More precisely, the first term of the sum in (62), namely, the $\mathcal{O}(\varepsilon^{-1})e_0$-term corresponding to the approximation of S_0, becomes dominant at this point. For this reason, the minimum achievable error level

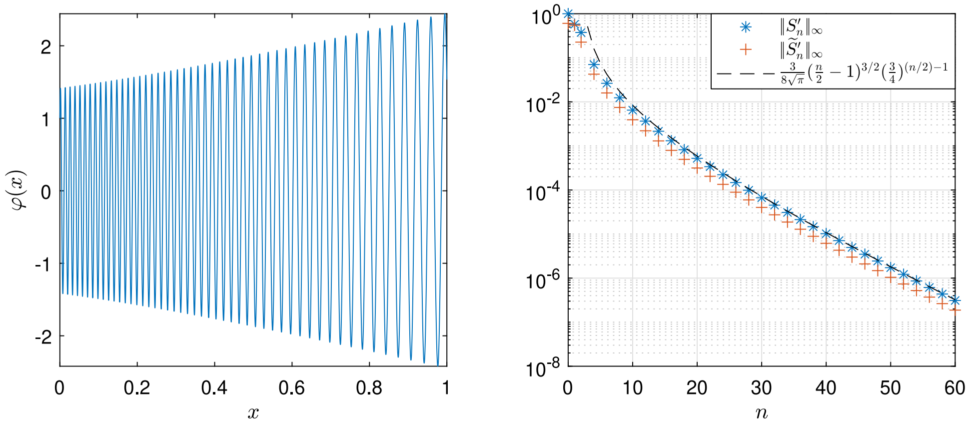

Fig. 10. Left: Exact solution (84) of IVP (83) for the choice $\varepsilon = 2^{-9}$. Right: $L^\infty(I)$-norm of S_n' and $\widetilde{S}_n$ as functions of even n, for the example $a(x) = (1 + x + x^2)^{-2}$ on the interval $I = [0, 1]$. The dashed line is proportional to the r.h.s. of (92) with $C_1 = C_2 = C_3 = 1$.

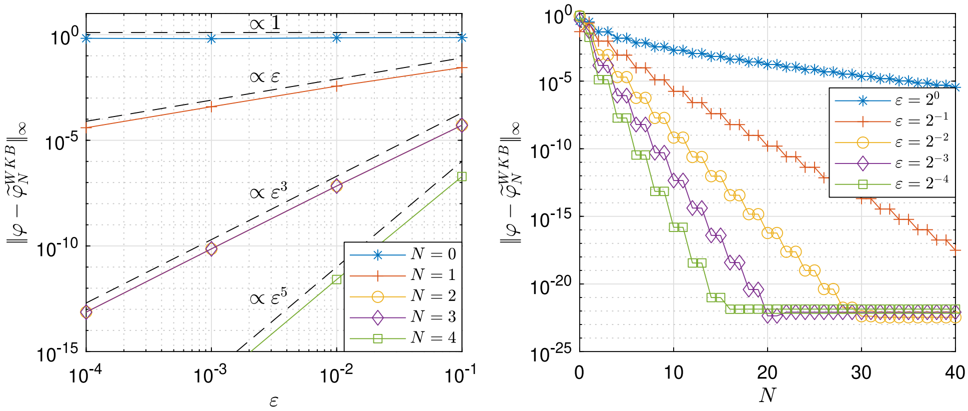

Fig. 11. Left: $L^\infty(I)$-norm of the error of the WKB approximation as a function of ε, for the IVP (83) and several choices of N. Here, we set $M = 30$. The yellow curve for $N = 2$ is the same as for $N = 3$ and hence not visible in the shown plot. Right: $L^\infty(I)$-norm of the error of the WKB approximation as a function of N, for the IVP (83) and several choices of ε. Here, we set $M = 30$.

is growing with decreasing ε. Besides from this saturation effect, the plot aligns well with Remark A.3, suggesting that the WKB approximation converges to the exact solution of IVP (83) as $N \to \infty$, for all displayed ε-values. Furthermore, one can observe again the fact that $\varphi_N^{WKB} = \varphi_{N+1}^{WKB}$ for even $N \geq 2$, as indicated by the step-like behavior of all shown error curves.

6. Conclusion

In the present paper we analyzed the WKB approximation of the solution to a highly oscillatory initial value problem. Assuming that the potential in the equation is analytic, we found explicit upper bounds for the terms occurring in the asymptotic WKB series of the approximate solution. Building on that, we proved error estimates which are explicit not only w.r.t. the small parameter ε but also w.r.t. N, the chosen number of terms in the truncated asymptotic series. We showed that the optimal truncation order N_{opt} is proportional to ε^{-1}, and this results in an approximation error that is exponentially small w.r.t. ε. We confirmed our theoretical results by several numerical experiments.

Data availability

Data will be made available on request.

Acknowledgments

The authors J. Körner, A. Arnold, and J. M. Melenk acknowledge support by the Austrian Science Fund (FWF) project 10.55776/F65, and the authors A. Arnold and C. Klein also by the bi-national FWF-project I3538-N32. C. Klein thanks for support by the ANR-17-EURE-0002 EIPHI and by the European Union Horizon 2020 research and innovation program under the Marie Sklodowska-Curie RISE 2017 grant agreement no. 778010 IPaDEGAN.

Appendix A. Convergent WKB series

In this appendix we provide examples where the asymptotic series (6) is convergent in $L^\infty(I)$. In practice, the norms $\|S_n'\|_{L^\infty(I)}$ (and $\|S_n\|_{L^\infty(I)}$) often decrease up to a certain number of n before they start to increase rapidly, e.g., see the right plot of Fig. 3. However, there are examples where one can easily verify that this is not the case. For instance, consider the simplest case in which $a \equiv a_0$ is constant. By (9) this is equivalent to $S_1' \equiv 0$, which by (10) then implies $S_n' \equiv 0$ for every $n \geq 1$. Similarly, one easily verifies that $S_2' \equiv 0$ is equivalent to a having the form $a(x) = (C_1 + C_2 x)^{-4}$ for some constants C_1 and C_2, see also [17, Problem 10.2]. It then holds $S_n' \equiv 0$ for every $n \geq 2$. Thus, in both of the just mentioned cases, the asymptotic series (6) terminates automatically and is therefore convergent. The corresponding WKB approximation (13) with $N \geq 0$ (respectively $N \geq 1$) is then the exact solution to IVP (1). Indeed, revisiting (43), it is clear that the r.h.s. in (54) then vanishes, i.e. $\|\varphi - \varphi_N^{WKB}\|_{L^\infty(I)} = 0$.

In the subsequent discussion, we will give examples of convergent WKB series which do not terminate automatically.

Proposition A.1. *Let $S_3' \equiv 0$. Then it holds*

$$S_{2n}' = S_2' \left(-\frac{S_2'}{2S_0'} \right)^{n-1} a_n \,, \tag{87}$$

$$S_{2n+1}' \equiv 0 \,, \tag{88}$$

for $n \geq 2$. Here, the sequence a_n is recursively defined by $a_1 := 1$ and

$$a_{n+1} := \sum_{j=1}^{n} a_j a_{n+1-j} \,, \quad n \geq 1 \,. \tag{89}$$

Proof. It is easy to check, that (87) and (88) hold for $n = 2$. We proceed now by induction on n. To this end, assume that formulas (87) and (88) hold for all $2 \leq k \leq n$ for some fixed $n \geq 2$. We shall now prove them for $n+1$. The induction hypothesis implies that $S_{2n+1}'' \equiv 0$ as well as $S_j' \equiv 0$ for all odd indices j such that $1 \leq j \leq 2n+1$. Hence,

$$S_{2n+2}' = -\frac{1}{2S_0'} \left(\sum_{j=1}^{2n+1} S_j' S_{2n+2-j}' + S_{2n+1}'' \right) = -\frac{1}{2S_0'} \sum_{j=1}^{n} S_{2j}' S_{2(n+1-j)}' = S_2' \left(-\frac{S_2'}{2S_0'} \right)^n \sum_{j=1}^{n} a_j a_{n+1-j} = S_2' \left(-\frac{S_2'}{2S_0'} \right)^n a_{n+1} \,, \tag{90}$$

where we have again used the induction hypothesis in the third equation. Differentiating (90) and using $\frac{S_0''}{S_0'} = -2S_1'$ we further obtain

$$S_{2n+2}'' = \left(-\frac{S_2'}{2S_0'} \right)^n \left(2n S_1' S_2' + (n+1) S_2'' \right) a_{n+1} \,. \tag{91}$$

Moreover, the induction hypothesis implies $S_j' S_{2n+3-j}' \equiv 0$ for $2 \leq j \leq 2n+1$ since either j or $2n+3-j$ is odd. Therefore, we get

$$\begin{aligned} S_{2n+3}' &= -\frac{1}{2S_0'} \left(\sum_{j=1}^{2n+2} S_j' S_{2n+3-j}' + S_{2n+2}'' \right) = -\frac{1}{2S_0'} \left(2S_1' S_{2n+2}' + S_{2n+2}'' \right) \\ &= \left(-\frac{S_2'}{2S_0'} \right)^n \left(-\frac{1}{2S_0'} \right) \left(2(n+1) S_1' S_2' + (n+1) S_2'' \right) a_{n+1} = \left(-\frac{S_2'}{2S_0'} \right)^n (n+1) S_3' a_{n+1} \equiv 0 \,, \end{aligned}$$

by assumption on S_3'. This concludes the proof. □

Remark A.2. Proposition A.1 assumes $S_3' \equiv 0$, which is equivalent to $a(x)$ satisfying the third order nonlinear ODE $15a'^3 + 4a^2 a''' - 18 a a' a'' = 0$. With the aid of MATLAB's Symbolic Math Toolbox we find that the general solution to this ODE is given by $a(x) = (C_1 + C_2 x + C_3 x^2)^{-2}$, where C_1, C_2 and C_3 are constants. A simple computation then shows that if $|C_2| + |C_3| > 0$ and $C_2^2 \neq 4C_1 C_3$, the coefficient function a does not have one of the two forms mentioned before Proposition A.1, i.e., $S_1' \not\equiv 0$ and $S_2' \not\equiv 0$. Thus, due to Proposition A.1, the corresponding WKB series does not terminate in this case.

Remark A.3. The numbers $a_n =: c_{n-1}$ in Proposition A.1 are the so-called Catalan numbers (e.g., see [28]), which are known to grow asymptotically as $c_n \sim \frac{4^n}{n^{3/2}\sqrt{\pi}}$, for $n \to \infty$. Let us assume that $a(x) = (C_1 + C_2 x + C_3 x^2)^{-2}$ such that $S_3' \equiv 0$, see Remark A.2. We then have $S_2'(x)/S_0'(x) = C_1 C_3/2 - C_2^2/8$. According to (87), we thus have for $n \geq 2$

$$\begin{aligned} \|S_{2n}'\|_{L^\infty(I)} \leq \|S_2'\|_{L^\infty(I)} \left\| \frac{S_2'}{2S_0'} \right\|_{L^\infty(I)}^{n-1} c_{n-1} &\sim \frac{\|S_2'\|_{L^\infty(I)}}{(n-1)^{3/2}\sqrt{\pi}} \left\| \frac{2S_2'}{S_0'} \right\|_{L^\infty(I)}^{n-1} , \quad n \to \infty \\ &= \frac{\|S_2'\|_{L^\infty(I)}}{(n-1)^{3/2}\sqrt{\pi}} \left| C_1 C_3 - \frac{C_2^2}{4} \right|^{n-1} . \end{aligned} \tag{92}$$

By definition (14), we conclude that

$$\|S_{2n}\|_{L^\infty(I)} = \mathcal{O}\left((n-1)^{-3/2}|C_1C_3 - C_2^2/4|^{n-1}\right), \quad n \to \infty\,. \tag{93}$$

Thus, the constants C_i, $i = 1, 2, 3$, determine whether the function $\|S_{2n}\|_{L^\infty(I)}$ is exponentially growing or decaying as $n \to \infty$. Note that Proposition A.1 also implies that $S_{2n+1} \equiv 0$ for $n \geq 1$. A short calculation then shows that (93) implies that the corresponding WKB series $\exp(\sum_{n=0}^{\infty} \varepsilon^{n-1} S_n(x))$ is (geometrically) convergent for any $x \in I$, if $\varepsilon \leq |C_1C_3 - C_2^2/4|^{-1/2}$.

References

[1] E.D. Courant, H.S. Snyder, Theory of the alternating-gradient synchrotron, Ann. Physics 281 (1958) 360–408.
[2] H.R. Lewis, Motion of a Time-Dependent Harmonic Oscillator, and of a Charged Particle in a Class of Time-Dependent, Axially Symmetric Electromagnetic Fields, Phys. Rev. 172 (1968) 1313–1315.
[3] J. Martin, D.J. Schwarz, WKB approximation for inflationary cosmological perturbations, Phys. Rev. D 67 (2003) 083512.
[4] S. Winitzki, Cosmological particle production and the precision of the WKB approximation, Phys. Rev. D 72 (2005) 104011.
[5] J.-F. Mennemann, A. Jüngel, H. Kosina, Transient Schrödinger-Poisson simulations of a high-frequency resonant tunneling diode oscillator, J. Comput. Phys. 239 (2013) 187–205.
[6] J. Sun, G.I. Haddad, P. Mazumder, J.N. Schulman, Resonant tunneling diodes: models and properties, Proc. IEEE 86 (1998) 641–660.
[7] C. Negulescu, Asymptotical models and numerical schemes for quantum systems (Ph.D. thesis), Université Paul Sabatier, Toulouse, 2005.
[8] A. Arnold, N.B. Abdallah, C. Negulescu, WKB-based schemes for the oscillatory 1D Schrödinger equation in the semiclassical limit, SIAM J. Numer. Anal. 49 (2011) 1436–1460.
[9] J. Bremer, On the numerical solution of second order ordinary differential equations in the high-frequency regime, Appl. Comput. Harmon. Anal. 44 (2018) 312–349.
[10] K. Lorenz, T. Jahnke, C. Lubich, Adiabatic integrators for highly oscillatory second-order linear differential equations with time-varying eigendecomposition, BIT Numer. Math. 45 (2005) 91–115.
[11] T. Jahnke, C. Lubich, Numerical integrators for quantum dynamics close to the adiabatic limit, Numer. Math. 94 (2003) 289–314.
[12] L.D. Landau, E.M. Lifschitz, Quantenmechanik, Akademie-Verlag, 1985.
[13] A. Arnold, C. Klein, B. Ujvari, WKB-method for the 1D Schrödinger equation in the semi-classical limit: enhanced phase treatment, BIT Numer. Math. 62 (2022) 1–22.
[14] F.J. Agocs, A.H. Barnett, An adaptive spectral method for oscillatory second-order linear ODEs with frequency-independent cost, SIAM J. Numer. Anal. 62 (2024) 295–321.
[15] H. Bremmer, The WKB approximation as the first term of a geometric-optical series, Comm. Pure Appl. Math. 4 (1951) 105–115.
[16] F. Atkinson, Wave propagation and the Bremmer series, J. Math. Anal. Appl. 1 (1960) 255–276.
[17] C.M. Bender, S.A. Orszag, Advanced mathematical methods for scientists and engineers I: asymptotic methods and perturbation theory., first ed., Springer New York, NY, 1999.
[18] J.M. Melenk, On the robust exponential convergence of *hp* finite element methods for problems with boundary layers, IMA J. Numer. Anal. 17 (1997) 577–601.
[19] M. Robnik, V.G. Romanovski, Some properties of WKB series, J. Phys. A 33 (2000) 5093–5104.
[20] C.W. Clenshaw, A.R. Curtis, A method for numerical integration on an automatic computer, Numer. Math. 2 (1960) 197–205.
[21] L.N. Trefethen, Spectral Methods in Matlab, in: vol. 10 of Software, Environments, and Tools, Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2000.
[22] M.M. Chawla, Error estimates for the Clenshaw-Curtis quadrature, Math. Comp. 22 (1968) 651–656.
[23] K.S. Breuer, R.M. Everson, On the errors incurred calculating derivatives using Chebyshev polynomials, J. Comput. Phys. 99 (1992) 56–67.
[24] D. Funaro, A Preconditioning Matrix for the Chebyshev Differencing Operator, SIAM J. Numer. Anal. 24 (1987) 1024–1031.
[25] J.P. Boyd, The Devil's invention: Asymptotic, superasymptotic and hyperasymptotic series, Acta Appl. Math. 56 (1999) 1–98.
[26] Advanpix LLC, Multiprecision computing toolbox for Matlab version 5.1.0.15432, Advanpix LLC, 2023.
[27] F.W.J. Olver, D.W. Lozier, R.F. Boisvert, C.W. Clark, NIST Handbook of Mathematical Functions, Cambridge University Press, 2010.
[28] R.L. Graham, D.E. Knuth, O. Patashnik, Concrete mathematics - a foundation for computer science, Addison-Wesley Publishing Company, 1991.