# Numerical solution of Sturm–Liouville problems via Fer streamers: Absolutely integrable potentials and self-adjoint boundary conditions

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**Abstract**

In (Ramos and Iserles, "Numerical solution of Sturm–Liouville problems via Fer streamers", 2013), the present author and Arieh Iserles put forth a new numerical method to compute eigenvalues and eigenfunctions of regular Sturm–Liouville problems in Liouville's normal form, with continuous and piecewise analytic potentials and self-adjoint separated boundary conditions. In this paper we revisit and extend the results of (Ramos and Iserles, 2013) to the general case with absolutely integrable potentials and self-adjoint separated, real coupled or complex coupled boundary conditions. We prove that the numerical method in (Ramos and Iserles, 2013), which is based on a non-standard truncation of Fer expansions, called 'Fer streamers', retains the same four properties either in the original setting or in this general case: *i*) it does not impose any restriction on the step size for eigenvalues which are greater or equal than a certain constant, *ii*) it requires only a mild restriction on the step size for the remaining finite number of eigenvalues, *iii*) it can attain any convergence rate, which grows exponentially with the number of terms, and is uniform for every eigenvalue, and *iv*) it lends itself to a clear understanding of the manner in which the potential affects local and global errors.

## 1 Introduction

Regular Sturm–Liouville problems in Liouville's normal form with absolutely integrable potentials and self-adjoint separated, real coupled or complex coupled boundary conditions are ubiquitous in applications and it is of great interest to develop numerical methods to compute their eigenvalues and eigenfunctions.

In (Ramos and Iserles, 2013), the present author and Arieh Iserles put forth a new numerical method to compute eigenvalues and eigenfunctions of regular Sturm–Liouville problems in Liouville's normal form, with continuous and piecewise analytic potentials and self-adjoint separated boundary conditions.

The point of departure in (Ramos and Iserles, 2013) is to interpret the problem setting in a Lie-group/Lie-algebra formalism and to capitalize on the low-dimensionality of the Lie algebra to rewrite any analytic function of any commutator matrix in a very useful form. This basic idea was then melded with Fer expansions to produce a new concept called 'Fer streamers', setting the stage for a non-standard truncation of Fer expansions.

This new concept was nurtured throughout (Ramos and Iserles, 2013) and resulted in a numerical method, which *i*) does not impose any restriction on the step size for eigenvalues which are greater or equal than a certain constant, *ii*) requires only a mild restriction on the step size for the remaining finite number of eigenvalues, *iii*) can attain any convergence rate, which grows exponentially with the number of terms, and is uniform for every eigenvalue, and *iv*) lends itself to a clear understanding of the manner in which the potential affects the local and global errors.

It is of note that there exist numerical methods that possess one or two of these four properties, e.g., (Moan, 1998), (Iserles et al., 2000), (Ixaru, 2000) and (Ledoux et al., 2010), but the numerical method based on Fer streamers is the only one that enjoys all four (Ramos and Iserles, 2013)!

In this paper, we revisit and extend the results of (Ramos and Iserles, 2013) to the general case with absolutely integrable potentials and self-adjoint separated, real coupled or complex coupled boundary conditions.

In particular, we prove that the numerical method in (Ramos and Iserles, 2013) retains the aforementioned four properties either in the original setting or in this general case.

Continuity and piecewise analyticity are often used as a means to develop and increase the local and global order of a numerical method, either by bounding the approximation error of function by a polynomial around a point, by bounding the interpolation error of a function by a polynomial in a interval, or perhaps by using integration by parts to derive an asymptotic expansion. For example, (Moan, 1998), (Iserles et al., 2000), (Ixaru, 2000) and (Ledoux et al., 2010) use continuity and piecewise analyticity as basic tools to develop their numerical methods. In addition, (Moan, 1998) and (Iserles et al., 2000) invoke boundedness and piecewise analyticity to increase the order of their commutators, while (Ixaru, 2000) and (Ledoux et al., 2010) call upon boundedness to compute constant approximations of their potentials and exploit piecewise analyticity to increase the order of their approximations.

Our first contribution in the extension of Fer streamers is to observe that (Ramos and Iserles, 2013) does not call upon continuity and piecewise analyticity as basic tools to develop the numerical method: they are used to increase the local and global order, but nothing else! Taking this into account, we prove that it is possible to leave the comfort and security of continuity and piecewise analyticity, and consider absolutely integrable potentials. Although the basic idea is the concept of Fer streamers introduced in (Ramos and Iserles, 2013), this general case presents several subtleties which need to be identified and addressed. In particular, we identify four different classes of potentials which require different treatment, e.g., different inequalities, different restrictions on the step size, different selection criteria on the numerical mesh, different flows or different non-linear characterizations of the eigenvalues. For example, the last three points are especially important whenever the potential is absolutely integrable but not in $\mathrm{L}^p([a,b],\mathbb{R})$, $p \in (1,\infty]$, since *i*) the mesh points, which are not boundary points, have to be Lebesgue points of the potential (this is always possible according to Lebesgue's differentiation theorem), and *ii*) if the left boundary point is not a Lebesgue point of the potential then the flow needs to be separated into 'positive' and 'negative' parts and the non-linear characterization of the eigenvalues needs to be changed. These endeavours account for the main part of the paper.

Self-adjoint separated boundary conditions are sometimes used as a constituent part of a numerical method. For example, this is the case with Prüfer's method which relies on self-adjoint separated boundary conditions to characterize the eigenvalues as the solutions of a certain non-linear equation, which is written in terms of the solution of a non-linear first-order differential equation called the Prüfer angle (Pryce, 1993).

Our second contribution in the extension of Fer streamers is to observe that self-adjoint separated boundary conditions are not essential to develop the numerical method in (Ramos and Iserles, 2013), and that it is also possible to consider self-adjoint real coupled or complex coupled boundary conditions.

### 1.1 Problem statement

In this paper we consider the solution of regular Sturm–Liouville problems in Liouville's normal form with absolutely integrable potentials,

$$\begin{aligned} &-y_\lambda''(t) + q(t)y_\lambda(t) = \lambda y_\lambda(t) \text{ a.e. } t \in [a,b], \quad a,b \in \mathbb{R}, \\ &q \in \mathrm{L}^1([a,b],\mathbb{R}), \quad \lambda \in \mathbb{R}, \quad y_\lambda, y_\lambda' \in \mathrm{AC}([a,b],\mathbb{C}), \end{aligned} \tag{1.1}$$

and self-adjoint separated, real coupled or complex coupled boundary conditions

$$\boldsymbol{C}_a \begin{bmatrix} y_\lambda(a) \\ y_\lambda'(a) \end{bmatrix} + \boldsymbol{C}_b \begin{bmatrix} y_\lambda(b) \\ y_\lambda'(b) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{1.2}$$

where

$$\boldsymbol{C}_a, \boldsymbol{C}_b \in \mathbb{C}^{2\times 2}, \quad \boldsymbol{C}_a \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \boldsymbol{C}_a^\dagger = \boldsymbol{C}_b \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \boldsymbol{C}_b^\dagger, \quad \operatorname{rank}(\boldsymbol{C}_a : \boldsymbol{C}_b) = 2$$

and where $a$, $b$, $q$, $\boldsymbol{C}_a$ and $\boldsymbol{C}_b$ are known, while the eigenvalue and eigenfunction pairs $(\lambda, y_\lambda)$ are unknown.

It is instructive to note (c.f., (Zettl, 2005, Chapter 4)) that regular Sturm–Liouville problems in Liouville's normal form with absolutely integrable potentials and self-adjoint boundary conditions (1.1)–(1.2), possess an infinite but countable number of eigenvalues which are real, isolated with no finite accumulation point, bounded below, not bounded above and such that the multiset

$$\{\lambda_j\}_{j\in\mathbb{Z}_0^+}$$

has multiplicity one or two, i.e., that each eigenvalue is either simple or double. Moreover, the multiset can be ordered to satisfy

$$-\infty < \lambda_0 \le \lambda_1 \le \lambda_2 \ldots, \quad \lim_{j\to+\infty} \lambda_j = +\infty. \tag{1.3}$$

## 1.2 Four classes of potentials

It is insightful to cluster the set of $\mathrm{L}^1([a,b],\mathbb{R})$ potentials in four different classes according to their regularity. In particular, it is of the utmost importance to identify the largest

$$p \in [1,\infty]$$

such that

$$q \in \mathrm{L}^p([a,b],\mathbb{R}).$$

**Class I** (Essentially Piecewise Absolutely Continuous Potentials)**.** A potential $q$ is said to belong to this class if

$$p = \infty$$

and there exist

$$m \in \mathbb{Z}^+, \tag{1.4}$$

$$c_0 = a < c_1 < \cdots < c_{m-1} < c_m = b, \tag{1.5}$$

$$h_{\min} := \min_{k\in\{0,1,\ldots,m-1\}} \{c_{k+1} - c_k\}, \tag{1.6}$$

$$h_{\max} := \max_{k\in\{0,1,\ldots,m-1\}} \{c_{k+1} - c_k\}, \tag{1.7}$$

$$p' \in [1,\infty], \tag{1.8}$$

$$q_0 \in \mathrm{AC}([c_0,c_1],\mathbb{R}), \ldots, q_{m-1} \in \mathrm{AC}([c_{m-1},c_m],\mathbb{R}), \tag{1.9}$$

such that, for all $k \in \{0,1,\ldots,m-1\}$,

$$q_k' \in \mathrm{L}^{p'}([c_k,c_{k+1}],\mathbb{R}), \tag{1.10}$$

$$q(t) = q_k(t) \text{ a.e. } t \in [c_k,c_{k+1}]. \tag{1.11}$$

In this case, it is assumed that the numerical mesh (1.4)–(1.7) has been refined in such a way that

$$\lambda \ge \operatorname{ess\,inf}\{q\} \implies h_{\max} \le (\operatorname{ess\,sup}\{q\} - \operatorname{ess\,inf}\{q\})^{-\frac{1}{2}}, \tag{1.12}$$

$$\lambda \le \operatorname{ess\,inf}\{q\} \implies h_{\max}^2 (\operatorname{ess\,sup}\{q\} - \lambda) \le 1, \tag{1.13}$$

$$\frac{h_{\max}}{h_{\min}} \le 2, \tag{1.14}$$

and that the big $\mathcal{O}$ notation and the small $o$ notation refers to one of the three asymptotic regimes

$$h_{\max} \to 0^+ \text{ uniformly with respect to } \begin{cases} k \in \{0,1,\dots,m-1\}, \\ t \in [c_k, c_{k+1}], \\ |\lambda - \operatorname{ess\,sup}\{q\}| \leq h_{\max}^{-2}, \end{cases} \tag{1.15}$$

$$h_{\max} \to 0^+ \text{ uniformly with respect to } \begin{cases} k \in \{0,1,\dots,m-1\}, \\ t \in [c_k, c_{k+1}], \\ \lambda - \operatorname{ess\,sup}\{q\} \geq h_{\max}^{-2}, \end{cases} \tag{1.16}$$

$$h_{\max} \to 0^+ \text{ uniformly with respect to } \begin{cases} k \in \{0,1,\dots,m-1\}, \\ t \in [c_k, c_{k+1}], \\ \lambda - \operatorname{ess\,sup}\{q\} \geq -h_{\max}^{-2}. \end{cases} \tag{1.17}$$

**Class II** (Essentially Bounded Potentials)**.** A potential $q$ is said to belong to this class if

$$p = \infty.$$

In this case, it is assumed that the numerical mesh (1.4)–(1.7) is such that (1.12), (1.13) and (1.14) hold true and that the big $\mathcal{O}$ notation and the small $o$ notation refers to one of the three asymptotic regimes (1.15), (1.16) and (1.17).

**Class III.** A potential $q$ is said to lie in this class if

$$p \in (1, \infty).$$

In this case, it is assumed that the numerical mesh (1.4)–(1.7) is such that

$$\lambda \geq 0 \quad \Longrightarrow \quad h_{\max} \leq \left(4\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right)^{-\frac{p}{2p-1}}, \tag{1.18}$$

$$\lambda \leq 0 \quad \Longrightarrow \quad h_{\max}^{\frac{2p-1}{p}} \|q\|_{\mathrm{L}^p([a,b],\mathbb{R})} + h_{\max}^2 |\lambda| \leq 1, \tag{1.19}$$

$$\frac{h_{\max}}{h_{\min}} \leq 2, \tag{1.20}$$

and that the big $\mathcal{O}$ notation and the small $o$ notation refers to one of the three asymptotic regimes

$$h_{\max} \to 0^+ \text{ uniformly w.r.t. } \begin{cases} k \in \{0,1,\dots,m-1\}, \\ t \in [c_k, c_{k+1}], \\ |\lambda| \leq h_{\max}^{-2} \left(1 - h_{\max}^{\frac{2p-1}{p}} \|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right), \end{cases} \tag{1.21}$$

$$h_{\max} \to 0^+ \text{ uniformly w.r.t. } \begin{cases} k \in \{0,1,\dots,m-1\}, \\ t \in [c_k, c_{k+1}], \\ \lambda \geq h_{\max}^{-2} \left(1 - h_{\max}^{\frac{2p-1}{p}} \|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right), \end{cases} \tag{1.22}$$

$$
h_{\max} \to 0^+ \text{ uniformly w.r.t. } \begin{cases} k \in \{0, 1, \dots, m-1\}, \\ t \in [c_k, c_{k+1}], \\ \lambda \geq -h_{\max}^{-2} \left(1 - h_{\max}^{\frac{2p-1}{p}} \|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right). \end{cases} \tag{1.23}
$$

**Class IV** (Absolutely Integrable Potentials)**.** A potential $q$ is said to lie in this class if

$$
p = 1.
$$

In this case, it is assumed that the numerical mesh (1.4)–(1.7) is such that

$$
c_1, \dots, c_{m-1} \text{ are Lebesgue points of } q,
$$

that (1.18), (1.19) and (1.20) hold true with $p = 1$, and that the big $\mathcal{O}$ notation and the small $o$ notation refers to one of the three asymptotic regimes (1.21), (1.22) and (1.23) with $p = 1$.

## 1.3 Three types of self-adjoint boundary conditions

Classically, it has been extremely fruitful in the theory of Sturm–Liouville problems to note that the self-adjoint boundary conditions (1.2) are invariant under multiplication by a non-singular matrix, and to divide them into three mutually exclusive types, deemed canonical in view of the aforementioned invariance (Zettl, 2005, Chapter 4). We do not require this division, but we present it here for completeness and the reader's convenience.

**Type I** (Self-Adjoint Canonical Separated Boundary Conditions)**.** All instances where

$$
\begin{bmatrix}\alpha_1 & \alpha_2\end{bmatrix} \in \mathbb{R}^{1\times 2}, \quad \begin{bmatrix}\alpha_1 & \alpha_2\end{bmatrix} \neq \begin{bmatrix}0 & 0\end{bmatrix}, \quad \boldsymbol{C}_a = \begin{bmatrix}\alpha_1 & \alpha_2 \\ 0 & 0\end{bmatrix},
$$
$$
\begin{bmatrix}\beta_1 & \beta_2\end{bmatrix} \in \mathbb{R}^{1\times 2}, \quad \begin{bmatrix}\beta_1 & \beta_2\end{bmatrix} \neq \begin{bmatrix}0 & 0\end{bmatrix}, \quad \boldsymbol{C}_b = \begin{bmatrix}0 & 0 \\ \beta_1 & \beta_2\end{bmatrix}.
$$

These boundary conditions lead to simple eigenvalues, i.e., to strict inequalities everywhere in (1.3) (Zettl, 2005, Theorem 4.3.1). Special cases include zero Dirichlet boundary conditions ($\alpha_2 = \beta_2 = 0$) and zero Neumann boundary conditions ($\alpha_1 = \beta_1 = 0$).

**Type II** (Self-Adjoint Canonical Real Coupled Boundary Conditions)**.** All cases where

$$
\boldsymbol{K} \in \mathrm{SL}(2,\mathbb{R}), \quad \boldsymbol{C}_a = \boldsymbol{K}, \quad \boldsymbol{C}_b = -\begin{bmatrix}1 & 0 \\ 0 & 1\end{bmatrix}.
$$

These boundary conditions lead to simple or double eigenvalues (Zettl, 2005, Theorem 4.3.1). In particular, $\boldsymbol{K} = \begin{bmatrix}1 & 0 \\ 0 & 1\end{bmatrix}$ encodes periodic boundary conditions.

**Type III** (Self-Adjoint Canonical Complex Coupled Boundary Conditions)**.** All cases where

$$\boldsymbol{K} \in \mathrm{SL}(2,\mathbb{R}), \quad \gamma \in (-\pi,0)\cup(0,\pi), \quad \boldsymbol{C}_a = e^{i\gamma}\boldsymbol{K}, \quad \boldsymbol{C}_b = -\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

These boundary conditions lead to simple eigenvalues, i.e., to strict inequalities everywhere in (1.3) (Zettl, 2005, Theorem 4.3.1).

## 1.4 Methodology

Our approach consists of a three-step procedure: Firstly, when dealing with potentials in Classes I or II, we divide (1.12) and (1.13) into the two pieces

$$\lambda \in \left[\operatorname{ess\,sup}\{q\} - h_{\max}^{-2}, \operatorname{ess\,sup}\{q\} + h_{\max}^{-2}\right] \cup \left[\operatorname{ess\,sup}\{q\} + h_{\max}^{-2}, +\infty\right),$$

and when dealing with potentials in Classes III or IV, we divide (1.18) and (1.19) into the two pieces

$$\lambda \in \left[-h_{\max}^{-2}\left(1 - h_{\max}^{\frac{2p-1}{p}} \|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right), h_{\max}^{-2}\left(1 - h_{\max}^{\frac{2p-1}{p}} \|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right)\right] \cup$$
$$\cup \left[h_{\max}^{-2}\left(1 - h_{\max}^{\frac{2p-1}{p}} \|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right), +\infty\right).$$

Then, we let

$$d \text{ be any point in } [a,b]$$

when dealing with potentials in Classes I, II or III and

$$d \text{ be any Lebesgue point of } q \text{ in } [a,b]$$

when dealing with potentials in Class IV, and approximate the solution of

$$\boldsymbol{\Phi}_\lambda'(t) = \begin{bmatrix} 0 & 1 \\ q(t)-\lambda & 0 \end{bmatrix} \boldsymbol{\Phi}_\lambda(t) \text{ a.e. } t \in [a,b], \quad a \le d \le b,$$
$$q \in \mathrm{L}^1([a,b],\mathbb{R}), \quad \lambda \in \mathbb{R}, \quad \boldsymbol{\Phi}_\lambda(\cdot) \in \mathrm{AC}([a,b],\mathrm{SL}(2,\mathbb{C})), \tag{1.24}$$

with initial condition

$$\boldsymbol{\Phi}_\lambda(d) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{1.25}$$

in the two asymptotic regimes (1.15) and (1.16) when dealing with potentials in Classes I or II, and in the two asymptotic regimes (1.21) and (1.22) when dealing with potentials in Classes III or IV. To this end, we consider the auxiliary initial value problems

$$\boldsymbol{\Phi}_\lambda^{+\prime}(d,t) = \begin{bmatrix} 0 & 1 \\ q(t)-\lambda & 0 \end{bmatrix} \boldsymbol{\Phi}_\lambda^{+}(d,t) \text{ a.e. } t \in [d,b], \quad a \le d \le b,$$
$$q \in \mathrm{L}^1([a,b],\mathbb{R}), \quad \lambda \in \mathbb{R}, \quad \boldsymbol{\Phi}_\lambda^{+}(d,\cdot) \in \mathrm{AC}([d,b],\mathrm{SL}(2,\mathbb{C})) \tag{1.26}$$

with initial condition

$$\mathbf{\Phi}_\lambda^+(d,d) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{1.27}$$

and

$$\mathbf{\Phi}_\lambda^-{}'(-d,t) = -\begin{bmatrix} 0 & 1 \\ q(-t)-\lambda & 0 \end{bmatrix} \mathbf{\Phi}_\lambda^-(-d,t) \text{ a.e. } t \in [-d,-a], \quad -b \le -d \le -a,$$

$$q \in \mathrm{L}^1\left([a,b],\mathbb{R}\right), \quad \lambda \in \mathbb{R}, \quad \mathbf{\Phi}_\lambda^-(-d,\cdot) \in \mathrm{AC}\left([-d,-a],\mathrm{SL}(2,\mathbb{C})\right) \tag{1.28}$$

with initial condition

$$\mathbf{\Phi}_\lambda^-(-d,-d) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}. \tag{1.29}$$

We note that

$$\begin{bmatrix} y_\lambda(b) \\ y'_\lambda(b) \end{bmatrix} = \mathbf{\Phi}_\lambda(b)\left(\mathbf{\Phi}_\lambda(d)\right)^{-1}\begin{bmatrix} y_\lambda(d) \\ y'_\lambda(d) \end{bmatrix} = \mathbf{\Phi}_\lambda^+(d,b)\begin{bmatrix} y_\lambda(d) \\ y'_\lambda(d) \end{bmatrix},$$

$$\begin{bmatrix} y_\lambda(a) \\ y'_\lambda(a) \end{bmatrix} = \mathbf{\Phi}_\lambda(a)\left(\mathbf{\Phi}_\lambda(d)\right)^{-1}\begin{bmatrix} y_\lambda(d) \\ y'_\lambda(d) \end{bmatrix} = \mathbf{\Phi}_\lambda^-(-d,-a)\begin{bmatrix} y_\lambda(d) \\ y'_\lambda(d) \end{bmatrix}.$$

Secondly, we approximate the unknown eigenvalues $\lambda$ via

$$\{\lambda_j\}_{j\in\mathbb{Z}_0^+} = \left\{\lambda \in \mathbb{R} : \det\left(\boldsymbol{C}_a\mathbf{\Phi}_\lambda^-(-d,-a) + \boldsymbol{C}_b\mathbf{\Phi}_\lambda^+(d,b)\right) = 0\right\},$$

which relates (1.1)–(1.2) and (1.24)–(1.25), by approximating $\mathbf{\Phi}_\lambda^-(-d,-a)$ and $\mathbf{\Phi}_\lambda^+(d,b)$ with Fer streamers, and solving the resulting equation with the use of a root-finding algorithm.

If the task at hand is to compute every eigenvalue within a given compact interval or, given a positive integer $k$ and a real number $c$, compute the smallest $k$ eigenvalues which are larger than $c$, then our aim is to convert it to a computation of the zeros of a continuous function in a compact interval or, to an iteration of this procedure, with a well-defined stopping criteria in view of (1.3). This is a well-posed numerical problem.

If the task at hand is, given two non-negative integers $k$ and $l$, to compute $\lambda_k, \lambda_{k+1}, \ldots \lambda_{k+l}$, then this is not a well-posed numerical problem, but it can be made well-posed by pre-computing a certain $\mu_0$ which is such that "there is one and only one eigenvalue in the interval $(-\infty,\mu_0]$ and it is $\lambda_0$" (c.f., (Zettl, 2005, Remark 4.6.1) and (Zettl, 2005, Remark 4.8.1)) and proceeding as above.

Thirdly, having approximated the eigenvalues, we continue by estimating the corresponding eigenfunctions $y_\lambda$.

# 2 Fer expansions and streamers

We begin by recalling Fer expansions and revisiting the basic idea in (Ramos and Iserles, 2013), which is to rewrite the problem statement in a Lie-group/Lie-algebra formalism and to call upon Fer expansions and the low-dimensionality of the underlying Lie algebra to introduce a new concept called Fer streamers, which played a pivotal role in that paper. We continue by extending the numerical method based on Fer streamers in (Ramos and Iserles, 2013) from the original setting with continuous and piecewise analytic potentials to the general case with absolutely integrable potentials.

## 2.1 Fer expansions

**Definition 2.1.** Let $\boldsymbol{X}, \boldsymbol{Y} \in \mathfrak{sl}(2,\mathbb{C})$, and define the exponential, the adjoint representation, and the derivative of the adjoint representation as

$$\begin{aligned}\exp(\boldsymbol{X}) &:= \sum_{j=0}^{\infty} \frac{\boldsymbol{X}^j}{j!},\\ \mathrm{Ad}_{\exp(\boldsymbol{X})}\boldsymbol{Y} &:= \exp(\boldsymbol{X})\,\boldsymbol{Y}\exp(-\boldsymbol{X}),\\ \mathrm{ad}_{\boldsymbol{X}}\boldsymbol{Y} &:= \boldsymbol{X}\boldsymbol{Y} - \boldsymbol{Y}\boldsymbol{X}.\end{aligned}$$

**Definition 2.2.** Let $l \in \mathbb{Z}^+$ and $t \in [\pm c_k, \pm c_{k\pm 1}]$, and set

$$\begin{aligned}\boldsymbol{B}^{\pm}_{\lambda,0}(\pm c_k, t) &:= \pm\begin{bmatrix} 0 & 1\\ q(\pm t) - \lambda & 0\end{bmatrix},\\ \boldsymbol{D}^{\pm}_{\lambda,0}(\pm c_k, t) &:= \int_{[\pm c_k, t]} \boldsymbol{B}^{\pm}_{\lambda,0}(\pm c_k, \xi)d\xi,\\ \boldsymbol{B}^{\pm}_{\lambda,l}(\pm c_k, t) &:= \sum_{j=1}^{\infty}(-1)^j \frac{j}{(j+1)!}\mathrm{ad}^j_{\boldsymbol{D}^{\pm}_{\lambda,l-1}(\pm c_k,t)}\boldsymbol{B}^{\pm}_{\lambda,l-1}(\pm c_k, t),\\ \boldsymbol{D}^{\pm}_{\lambda,l}(\pm c_k, t) &:= \int_{[c_k, t]} \boldsymbol{B}^{\pm}_{\lambda,l}(\pm c_k, \xi)d\xi.\end{aligned}$$

**Theorem 2.1** ((Fer, 1958), (Iserles, 1984, Theorem 3), (Iserles et al., 2000, p. 267–270))**.** If $q$ is absolutely integrable, then, the solution of (1.26)–(1.27), $\boldsymbol{\Phi}^+_\lambda(d,t)$, and the solution of (1.28)–(1.29), $\boldsymbol{\Phi}^-_\lambda(-d,t)$, are given by the Fer expansions

$$t \geq \pm c_k \geq \pm d \Rightarrow \boldsymbol{\Phi}^{\pm}_\lambda(\pm d, t) = e^{\boldsymbol{D}^{\pm}_{\lambda,0}(\pm c_k,t)} e^{\boldsymbol{D}^{\pm}_{\lambda,1}(\pm c_k,t)} e^{\boldsymbol{D}^{\pm}_{\lambda,2}(\pm c_k,t)} \cdots \boldsymbol{\Phi}^{\pm}_\lambda(\pm d, \pm c_k).$$

## 2.2 Fer streamers

### 2.2.1 Closed-form expressions

**Definition 2.3.** For every $\boldsymbol{E} \in \mathfrak{sl}(2, \mathbb{C})$, let

$$\begin{aligned}\boldsymbol{\pi}\left(\boldsymbol{E}\right) &:= \begin{bmatrix}[\boldsymbol{E}]_{1,1}\\ [\boldsymbol{E}]_{1,2}\\ [\boldsymbol{E}]_{2,1}\end{bmatrix},\\ \mathscr{C}_{\boldsymbol{E}} &:= \begin{bmatrix}0 & -[\boldsymbol{E}]_{2,1} & [\boldsymbol{E}]_{1,2}\\ -2[\boldsymbol{E}]_{1,2} & 2[\boldsymbol{E}]_{1,1} & 0\\ 2[\boldsymbol{E}]_{2,1} & 0 & -2[\boldsymbol{E}]_{1,1}\end{bmatrix},\\ \rho(\boldsymbol{E}) &:= 2\sqrt{-\det\left(\boldsymbol{E}\right)}.\end{aligned}$$

**Theorem 2.2.** If $l \in \mathbb{Z}^{+}$ and $\boldsymbol{E}, \boldsymbol{F} \in \mathfrak{sl}(2, \mathbb{C})$, then

$$\boldsymbol{\pi}\left(\mathrm{ad}_{\boldsymbol{E}}\boldsymbol{F}\right) = \mathscr{C}_{\boldsymbol{E}}\boldsymbol{\pi}\left(\boldsymbol{F}\right), \quad \mathscr{C}_{\boldsymbol{E}}^{2l-1} = \rho^{2l-2}(\boldsymbol{E})\mathscr{C}_{\boldsymbol{E}}, \quad \mathscr{C}_{\boldsymbol{E}}^{2l} = \rho^{2l-2}(\boldsymbol{E})\mathscr{C}_{\boldsymbol{E}}^{2}.$$

*Proof.* The first assertion follows by straightforward computation, and the last two follow by induction from

$$\mathscr{C}_{\boldsymbol{E}}^{3} = \rho^{2}(\boldsymbol{E})\mathscr{C}_{\boldsymbol{E}}.$$

□

**Definition 2.4.** Let

$$\psi(z) := \sum_{j=1}^{\infty}(-1)^{j}\frac{j}{(j+1)!}z^{j} = -\frac{e^{-z}(e^{z}-1-z)}{z}$$

and

$$\begin{aligned}\varphi(z) &:= \frac{\psi(z)-\psi(-z)}{2z} = -\sum_{j=0}^{\infty}\frac{2j+1}{(2j+2)!}z^{2j} = \frac{\cosh(z)-1-z\sinh(z)}{z^{2}},\\ \phi(z) &:= \frac{\psi(z)+\psi(-z)}{2z^{2}} = \sum_{j=0}^{\infty}\frac{2j+2}{(2j+3)!}z^{2j} = \frac{z\cosh(z)-\sinh(z)}{z^{3}}.\end{aligned}$$

**Remark 2.1.** In the sequel, it will be crucial to observe that both $\varphi$ and $\phi$ are bounded along the imaginary axis:

$$\begin{aligned}\varphi(ix) &= \sum_{j=0}^{\infty}(-1)^{j+1}\frac{2j+1}{(2j+2)!}x^{2j} = \left(\frac{1-\cos(x)}{x} - \sin(x)\right)\frac{1}{x},\\ \phi(ix) &= \sum_{j=0}^{\infty}(-1)^{j}\frac{2j+2}{(2j+3)!}x^{2j} = \left(\frac{\sin\left(x\right)}{x} - \cos\left(x\right)\right)\frac{1}{x^{2}}.\end{aligned}$$

The exact closed-form expressions which appear in the following theorem are named *Fer streamers*.

**Theorem 2.3.** If $l \in \mathbb{Z}^+$ and $t \in [\pm c_k, \pm c_{k\pm 1}]$, then, it follows that

$$\boldsymbol{\pi}\left(\boldsymbol{B}^{\pm}_{\lambda,l}(\pm c_k, t)\right) = \varphi\left(\rho\left(\boldsymbol{D}^{\pm}_{\lambda,l-1}(\pm c_k, t)\right)\right)\mathscr{C}_{\boldsymbol{D}^{\pm}_{\lambda,l-1}(\pm c_k,t)}\boldsymbol{\pi}\left(\boldsymbol{B}^{\pm}_{\lambda,l-1}(\pm c_k, t)\right) + \\ + \phi\left(\rho\left(\boldsymbol{D}^{\pm}_{\lambda,l-1}(\pm c_k, t)\right)\right)\mathscr{C}^2_{\boldsymbol{D}^{\pm}_{\lambda,l-1}(\pm c_k,t)}\boldsymbol{\pi}\left(\boldsymbol{B}^{\pm}_{\lambda,l-1}(\pm c_k, t)\right).$$

*Proof.* The proof follows as in (Ramos and Iserles, 2013, Appendix A) by calling upon Definition 2.2 and Theorem 2.2. ☐

**Remark 2.2.** As an example, let $t \in [\pm c_k, \pm c_{k\pm 1}]$ and note that since

$$\boldsymbol{\pi}\left(\boldsymbol{B}^{\pm}_{\lambda,0}(\pm c_k, t)\right) = \pm\begin{bmatrix} 0 \\ 1 \\ q(\pm t) - \lambda \end{bmatrix}$$

we have that

$$\rho\left(\boldsymbol{D}^{\pm}_{\lambda,0}(\pm c_k, t)\right) = 2|t \mp c_k|\sqrt{\frac{\int_{[\pm c_k,t]} q(\pm\xi)d\xi}{|t \mp c_k|} - \lambda}$$

and that Theorem 2.3 yields (see Appendix A)

$$\boldsymbol{\pi}\left(\boldsymbol{B}^{\pm}_{\lambda,1}(\pm c_k, t)\right) = \\ = \begin{bmatrix} \varphi\left(\rho\left(\boldsymbol{D}^{\pm}_{\lambda,0}(\pm c_k, t)\right)\right)|t \mp c_k|\left(q(\pm t) - \frac{\int_{[\pm c_k,t]} q(\pm\xi)d\xi}{|t\mp c_k|}\right) \\ \mp 2\phi\left(\rho\left(\boldsymbol{D}^{\pm}_{\lambda,0}(\pm c_k, t)\right)\right)|t \mp c_k|^2\left(q(\pm t) - \frac{\int_{[\pm c_k,t]} q(\pm\xi)d\xi}{|t\mp c_k|}\right) \\ \pm\frac{1}{2}\phi\left(\rho\left(\boldsymbol{D}^{\pm}_{\lambda,0}(\pm c_k, t)\right)\right)\rho^2\left(\boldsymbol{D}^{\pm}_{\lambda,0}(\pm c_k, t)\right)\left(q(\pm t) - \frac{\int_{[\pm c_k,t]} q(\pm\xi)d\xi}{|t\mp c_k|}\right) \end{bmatrix}.$$

### 2.2.2 Estimates

It is important to observe that the $\pm$ and $\mp$ signs in Remark 2.2 do not change its overall features. This is one of the reasons to consider the 'positive' flow $\boldsymbol{\Phi}^{+}_{\lambda}(d, t)$ and the 'negative' flow $\boldsymbol{\Phi}^{-}_{\lambda}(-d, t)$, instead of the normal flow $\boldsymbol{\Phi}_{\lambda}(t)$ and the inverse flow $(\boldsymbol{\Phi}_{\lambda}(t))^{-1}$. Another reason to consider positive and negative flows instead of normal and inverse flows is due to the fact that the normal Fer expansion is given by an infinite product of exponentials from left to right, whereas the inverse of the Fer expansion is given by an infinite product of exponentials from right to left, and this leads to asymmetric formulas and less tidy analysis.

It is also important to emphasize that with positive and negative flows it is possible to assume without loss of generality that $d = a$. The reason is that it is always possible to partition $[a, b] = [a, d] \cup [d, b]$, to identify $[a, d]$ with $[-d, -a]$ and to consider the positive flow in $[d, b]$ and the negative flow in $[-d, -a]$. This is assumed throughout this subsubsection.

**Definition 2.5.** Let

$$\epsilon_1 := \begin{cases} 2h_{\max} & \Leftarrow \text{Classes I or II, and asymptotic regime (1.15),} \\ (\lambda - \operatorname{ess\,sup}\{q\})^{-\frac{1}{2}} & \Leftarrow \text{Classes I or II, and asymptotic regime (1.16),} \\ 2h_{\max} & \Leftarrow \text{Classes III or IV, and asymptotic regime (1.21),} \\ 2\lambda^{-\frac{1}{2}} & \Leftarrow \text{Classes III or IV, and asymptotic regime (1.22),} \end{cases}$$

and

$$\epsilon_2 := \begin{cases} \frac{3}{4}\|q'\|_{\mathrm{L}^\infty([a,b],\mathbb{R})} h_{\max}^2 & \Leftarrow \text{Class I and } p' = \infty, \\ \frac{(3p'-1)p'}{(2p'-1)^2}\|q'\|_{\mathrm{L}^{p'}([a,b],\mathbb{R})} o\left(h_{\max}^{\frac{2p'-1}{p'}}\right) & \Leftarrow \text{Class I and } p' \in (1, \infty), \\ 2\|q'\|_{\mathrm{L}^1([a,b],\mathbb{R})} o\left(h_{\max}\right) & \Leftarrow \text{Class I and } p' = 1, \\ 2\|q\|_{\mathrm{L}^\infty([a,b],\mathbb{R})} h_{\max} & \Leftarrow \text{Class II,} \\ \frac{2p-1}{p-1}\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})} o\left(h_{\max}^{\frac{p-1}{p}}\right) & \Leftarrow \text{Class III,} \\ \|q\|_{\mathrm{L}^1([a,b],\mathbb{R})} o\left(1\right) & \Leftarrow \text{Class IV.} \end{cases}$$

**Theorem 2.4.** If $q$ is in Class I, II, III or IV, and $l \in \mathbb{Z}^+$, then,

$$e^{\boldsymbol{D}^+_{\lambda,0}(c_k,c_{k+1})} \cdots e^{\boldsymbol{D}^+_{\lambda,0}(a,c_1)} = \begin{bmatrix} \mathcal{O}(1) & \mathcal{O}(\epsilon_1) \\ \mathcal{O}\left(\epsilon_1^{-1}\right) & \mathcal{O}(1) \end{bmatrix},$$

$$\boldsymbol{\pi}\left(\boldsymbol{D}^+_{\lambda,l}(c_k, t)\right) = \epsilon_2^{2^{l-1}} \epsilon_1^{2^{l-1}-1} \begin{bmatrix} \mathcal{O}(\epsilon_1) \\ \mathcal{O}\left(\epsilon_1^2\right) \\ \mathcal{O}(1) \end{bmatrix}.$$

*Proof.* See Appendix A. □

**Definition 2.6.** Let $n \in \mathbb{Z}^+$, and define the

$$\begin{aligned}
\text{exact flow:} \quad & \boldsymbol{\Psi}_{\lambda}^{+}(c_k, c_{k+1}) := \prod_{l=0}^{\infty} e^{\boldsymbol{D}_{\lambda,l}^{+}(c_k,c_{k+1})}, \\
\text{exact solution:} \quad & \boldsymbol{\Phi}_{\lambda}^{+}(a, c_{k+1}) \ = \boldsymbol{\Psi}_{\lambda}^{+}(c_k, c_{k+1}) \cdots \boldsymbol{\Psi}_{\lambda}^{+}(c_1, c_2) \boldsymbol{\Psi}_{\lambda}^{+}(a, c_1), \\
\text{approximate flow:} \quad & \tilde{\boldsymbol{\Psi}}_{\lambda,n}^{+}(c_k, c_{k+1}) := \prod_{l=0}^{n} e^{\boldsymbol{D}_{\lambda,l}^{+}(c_k,c_{k+1})}, \\
\text{approximate solution:} \quad & \tilde{\boldsymbol{\Phi}}_{\lambda,n}^{+}(a, c_{k+1}) := \tilde{\boldsymbol{\Psi}}_{\lambda,n}^{+}(c_k, c_{k+1}) \cdots \tilde{\boldsymbol{\Psi}}_{\lambda,n}^{+}(c_1, c_2) \tilde{\boldsymbol{\Psi}}_{\lambda,n}^{+}(a, c_1), \\
\text{local error:} \quad & \boldsymbol{L}_{\lambda,n}^{+}(c_k, c_{k+1}) := \log\left( \boldsymbol{\Psi}_{\lambda}^{+}(c_k, c_{k+1}) \left( \tilde{\boldsymbol{\Psi}}_{\lambda,n}^{+}(c_k, c_{k+1}) \right)^{-1} \right), \\
\text{global error:} \quad & \boldsymbol{G}_{\lambda,n}^{+}(a, c_{k+1}) := \log\left( \boldsymbol{\Phi}_{\lambda}^{+}(a, c_{k+1}) \left( \tilde{\boldsymbol{\Phi}}_{\lambda,n}^{+}(a, c_{k+1}) \right)^{-1} \right).
\end{aligned}$$

**Theorem 2.5.** If $q$ is in Class I, II, III or IV, and $n \in \mathbb{Z}^+$, then

$$\boldsymbol{\pi}\left( \boldsymbol{L}_{\lambda,n}^{+}(c_k, c_{k+1}) \right) = \epsilon_2^{2^n} \epsilon_1^{2^n - 1} \begin{bmatrix} \mathcal{O}(\epsilon_1) \\ \mathcal{O}(\epsilon_1^2) \\ \mathcal{O}(1) \end{bmatrix},$$

$$\boldsymbol{\pi}\left( \boldsymbol{G}_{\lambda,n}^{+}(a, c_{k+1}) \right) = h_{\max}^{-1} \epsilon_2^{2^n} \epsilon_1^{2^n - 1} \begin{bmatrix} \mathcal{O}(\epsilon_1) \\ \mathcal{O}(\epsilon_1^2) \\ \mathcal{O}(1) \end{bmatrix}.$$

*Proof.* The proof follows as in (Ramos and Iserles, 2013, Appendix C). The main obstacle in estimating the local and global errors is the fact that the lower-left entry of $\exp\left(\boldsymbol{D}_{\lambda,0}^{+}\right)$ is very large. This is circumvented by calling upon three Baker–Campbell–Hausdorff (BCH) type formulas. Firstly, the local error is estimated by calling upon Definition 2.6, the aforementioned BCH type formulas and Theorem 2.4. Secondly, the global error is estimated by invoking Definition 2.6, the aforementioned BCH type formulas, Theorem 2.4 as well as assumption (1.14) (when dealing with Classes I or II) or assumption (1.20) (when dealing with Classes III or IV). This is done by observing that the global error obeys a certain recurrence relation. □

Theorem 2.5 can now be specialized to the following notable cases. These are important to write down, since they make clear what is what.

**Corollary 2.1.** If $q$ is in Class I, $p' = \infty$ and $n \in \mathbb{Z}^+$, then, in the asymptotic regime (1.17),

$$\boldsymbol{\pi}\left(\boldsymbol{L}_{\lambda,n}^{+}(c_k,c_{k+1})\right)=\left(\frac{3}{4}\|q'\|_{\mathrm{L}^\infty([a,b],\mathbb{R})}\right)^{2^n} h_{\max}^{3\times 2^n-1}\begin{bmatrix}\mathcal{O}\left(h_{\max}\right)\\ \mathcal{O}\left(h_{\max}^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix},$$

$$\boldsymbol{\pi}\left(\boldsymbol{G}_{\lambda,n}^{+}(a,c_{k+1})\right)=\left(\frac{3}{4}\|q'\|_{\mathrm{L}^\infty([a,b],\mathbb{R})}\right)^{2^n} h_{\max}^{3\times 2^n-2}\begin{bmatrix}\mathcal{O}\left(h_{\max}\right)\\ \mathcal{O}\left(h_{\max}^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix}.$$

**Corollary 2.2.** If $q$ is in Class I, $p'\in(1,\infty)$ and $n\in\mathbb{Z}^+$, then, in the asymptotic regime (1.17),

$$\boldsymbol{\pi}\left(\boldsymbol{L}_{\lambda,n}^{+}(c_k,c_{k+1})\right)=\left(\frac{(3p'-1)p'}{(2p'-1)^2}\|q'\|_{\mathrm{L}^{p'}([a,b],\mathbb{R})}\right)^{2^n} h_{\max}^{\frac{3p'-1}{p'}\times 2^n-1}\begin{bmatrix}o\left(h_{\max}\right)\\ o\left(h_{\max}^2\right)\\ o\left(1\right)\end{bmatrix},$$

$$\boldsymbol{\pi}\left(\boldsymbol{G}_{\lambda,n}^{+}(a,c_{k+1})\right)=\left(\frac{(3p'-1)p'}{(2p'-1)^2}\|q'\|_{\mathrm{L}^{p'}([a,b],\mathbb{R})}\right)^{2^n} h_{\max}^{\frac{3p'-1}{p'}\times 2^n-2}\begin{bmatrix}o\left(h_{\max}\right)\\ o\left(h_{\max}^2\right)\\ o\left(1\right)\end{bmatrix}.$$

**Corollary 2.3.** If $q$ is in Class I, $p'=1$ and $n\in\mathbb{Z}^+$, then, in the asymptotic regime (1.17),

$$\boldsymbol{\pi}\left(\boldsymbol{L}_{\lambda,n}^{+}(c_k,c_{k+1})\right)=\left(2\|q'\|_{\mathrm{L}^1([a,b],\mathbb{R})}\right)^{2^n} h_{\max}^{2\times 2^n-1}\begin{bmatrix}o\left(h_{\max}\right)\\ o\left(h_{\max}^2\right)\\ o\left(1\right)\end{bmatrix},$$

$$\boldsymbol{\pi}\left(\boldsymbol{G}_{\lambda,n}^{+}(a,c_{k+1})\right)=\left(2\|q'\|_{\mathrm{L}^1([a,b],\mathbb{R})}\right)^{2^n} h_{\max}^{2\times 2^n-2}\begin{bmatrix}o\left(h_{\max}\right)\\ o\left(h_{\max}^2\right)\\ o\left(1\right)\end{bmatrix}.$$

**Corollary 2.4.** If $q$ is in Class II and $n\in\mathbb{Z}^+$, then, in the asymptotic regime (1.17),

$$\boldsymbol{\pi}\left(\boldsymbol{L}_{\lambda,n}^{+}(c_k,c_{k+1})\right)=\left(2\|q\|_{\mathrm{L}^\infty([a,b],\mathbb{R})}\right)^{2^n} h_{\max}^{2\times 2^n-1}\begin{bmatrix}\mathcal{O}\left(h_{\max}\right)\\ \mathcal{O}\left(h_{\max}^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix},$$

$$\boldsymbol{\pi}\left(\boldsymbol{G}_{\lambda,n}^{+}(a,c_{k+1})\right)=\left(2\|q\|_{\mathrm{L}^\infty([a,b],\mathbb{R})}\right)^{2^n} h_{\max}^{2\times 2^n-2}\begin{bmatrix}\mathcal{O}\left(h_{\max}\right)\\ \mathcal{O}\left(h_{\max}^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix}.$$

**Corollary 2.5.** If $q$ belongs to Class III and $n \in \mathbb{Z}^+$, then, in the asymptotic regime (1.23),

$$\boldsymbol{\pi}\left(\boldsymbol{L}^+_{\lambda,n}(c_k, c_{k+1})\right) = \left(\frac{2p-1}{p-1}\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right)^{2^n} h_{\max}^{\frac{2p-1}{p}\times 2^n - 1} \begin{bmatrix} o\left(h_{\max}\right) \\ o\left(h_{\max}^2\right) \\ o\left(1\right) \end{bmatrix},$$

$$\boldsymbol{\pi}\left(\boldsymbol{G}^+_{\lambda,n}(a, c_{k+1})\right) = \left(\frac{2p-1}{p-1}\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right)^{2^n} h_{\max}^{\frac{2p-1}{p}\times 2^n - 2} \begin{bmatrix} o\left(h_{\max}\right) \\ o\left(h_{\max}^2\right) \\ o\left(1\right) \end{bmatrix}.$$

**Corollary 2.6.** If $q$ belongs to Class IV and $n \in \mathbb{Z}^+$, then, in the asymptotic regime (1.23),

$$\boldsymbol{\pi}\left(\boldsymbol{L}^+_{\lambda,n}(c_k, c_{k+1})\right) = \left(\|q\|_{\mathrm{L}^1([a,b],\mathbb{R})}\right)^{2^n} h_{\max}^{1\times 2^n - 1} \begin{bmatrix} o\left(h_{\max}\right) \\ o\left(h_{\max}^2\right) \\ o\left(1\right) \end{bmatrix},$$

$$\boldsymbol{\pi}\left(\boldsymbol{G}^+_{\lambda,n}(a, c_{k+1})\right) = \left(\|q\|_{\mathrm{L}^1([a,b],\mathbb{R})}\right)^{2^n} h_{\max}^{1\times 2^n - 2} \begin{bmatrix} o\left(h_{\max}\right) \\ o\left(h_{\max}^2\right) \\ o\left(1\right) \end{bmatrix}.$$

# 3 Conclusions

We have seen that the numerical method based on Fer streamers put forth in (Ramos and Iserles, 2013) can be extended to cover not only regular Sturm–Liouville problems in Liouville's normal form, with continuous and piecewise analytic potentials and self-adjoint separated boundary conditions, but also regular Sturm–Liouville problems in Liouville's normal form, with absolutely integrable potentials and self-adjoint separated, real coupled or complex coupled boundary conditions. Much remains to be done and future work include:

- Efficient discretization schemes,
- Singular Sturm–Liouville problems.

## 3.1 Efficient discretization schemes

These are particularly challenging because of their highly oscillatory nature which was already present when dealing with continuous and piecewise analytic potentials (Ramos and Iserles, 2013, Subsection 4.1), but also because of their lack of regularity which was not present in the original setting (Ramos and Iserles, 2013). For example, in this case, it is not clear whether it is possible to call upon integration by parts or similar techniques which rely on derivatives, in order to resolve the high oscillations.

## 3.2 Singular Sturm–Liouville problems

Extending the numerical method based on Fer streamers to this setting involves at least two new and exciting problems: infinite intervals and boundary conditions. Infinite intervals have to be transformed into compact intervals or approximated by compact intervals. Boundary conditions depend on the nature of the singularity: limit-circle (boundary conditions are required, but are different and lead to a different non-linear characterization of the eigenvalues) or limit-point (boundary conditions are not required or allowed) (Zettl, 2005, Parts 3 and 4).

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# A Proof of Theorem 2.4

## A.1 Estimating $\exp\left(\boldsymbol{D}^+_{\lambda,0}(c_k, c_{k+1})\right) \cdots \exp\left(\boldsymbol{D}^+_{\lambda,0}(a, c_1)\right)$

### A.1.1 Classes I and II

In this subsubsection it is assumed that $q$ belongs to Class I or to Class II. Recall Definitions 2.2 and 2.3 and note that

$$\rho\left(\boldsymbol{D}^+_{\lambda,0}(c_k, t)\right) = 2|t - c_k|\sqrt{\frac{\int_{[c_k,t]} q(\xi)d\xi}{|t - c_k|} - \lambda}. \tag{A.1}$$

Note further that (A.1) and assumptions (1.12) and (1.13) ensure that

$$\begin{aligned}
&\lambda \in \left[\operatorname{ess\,sup}\{q\} - h_{\max}^{-2}, \operatorname{ess\,inf}\{q\}\right] \Rightarrow \\
&\Rightarrow \rho\left(\boldsymbol{D}^+_{\lambda,0}(c_k, t)\right) \in [0, 2h_{\max}\sqrt{\operatorname{ess\,sup}\{q\} - \lambda}] \subseteq [0, 2], && \text{(A.2)}\\
&\lambda \in [\operatorname{ess\,inf}\{q\}, \operatorname{ess\,sup}\{q\}] \Rightarrow \\
&\Rightarrow \left|\rho\left(\boldsymbol{D}^+_{\lambda,0}(c_k, t)\right)\right| \leq 2h_{\max}\sqrt{\operatorname{ess\,sup}\{q\} - \operatorname{ess\,inf}\{q\}} \leq 2, && \text{(A.3)}\\
&\lambda \in \left[\operatorname{ess\,sup}\{q\}, \operatorname{ess\,sup}\{q\} + h_{\max}^{-2}\right] \Rightarrow \\
&\Rightarrow \rho\left(\boldsymbol{D}^+_{\lambda,0}(c_k, t)\right) \in i[0, 2], && \text{(A.4)}\\
&\lambda \geq \operatorname{ess\,sup}\{q\} + h_{\max}^{-2} \Rightarrow \\
&\Rightarrow \rho\left(\boldsymbol{D}^+_{\lambda,0}(c_k, t)\right) \in i\Big[2\,|t - c_k|\,(\lambda - \operatorname{ess\,sup}\{q\})^{\frac{1}{2}}, +\infty\Big), && \text{(A.5)}
\end{aligned}$$

which, together with Definition 2.4 and Remark 2.1, lead to the following estimates in the asymptotic regime (1.15)

$$\left|\varphi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)|t-c_k|\right| \leq 2h_{\max}, \tag{A.6}$$

$$\left|\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)|t-c_k|^2\right| \leq (2h_{\max})^2, \tag{A.7}$$

$$\left|\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)\rho^2\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right| \leq 2, \tag{A.8}$$

and to the following estimates in the asymptotic regime (1.16)

$$\left|\varphi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)|t-c_k|\right| \leq (\lambda-\operatorname{ess\,sup}\{q\})^{-\frac{1}{2}}, \tag{A.9}$$

$$\left|\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)|t-c_k|^2\right| \leq (\lambda-\operatorname{ess\,sup}\{q\})^{-1}, \tag{A.10}$$

$$\left|\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)\rho^2\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right| \leq 2. \tag{A.11}$$

If $q$ belongs to Class I, observe that assumptions (1.8), (1.9), (1.10) and (1.11) and Hölder's inequality imply that

$$\begin{aligned}
&\left|q(t)-\frac{\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|}\right| = \\
&= \left|q_k(t)-\frac{\int_{[c_k,t]}q_k(\xi)d\xi}{|t-c_k|}\right| \quad \text{a.e. } t\in[c_k,c_{k+1}] \\
&= \left|\left(q_k(c_k)+\int_{[c_k,t]}q_k'(\xi_2)d\xi_2\right)-\frac{\int_{[c_k,t]}\left(q_k(c_k)+\int_{[c_k,\xi]}q_k'(\xi_2)d\xi_2\right)d\xi}{|t-c_k|}\right| \\
&\leq \int_{[c_k,t]}|q_k'(\xi_2)|d\xi_2+\frac{\int_{[c_k,t]}\int_{[c_k,\xi]}|q_k'(\xi_2)|d\xi_2 d\xi}{|t-c_k|} \\
&\leq |t-c_k|^{\frac{p'-1}{p'}}\|q_k'\|_{\mathrm{L}^{p'}([c_k,c_{k+1}],\mathbb{R})}+\frac{\int_{[c_k,t]}|\xi-c_k|^{\frac{p'-1}{p'}}\|q_k'\|_{\mathrm{L}^{p'}([c_k,c_{k+1}],\mathbb{R})}d\xi}{|t-c_k|} \\
&= \frac{3p'-1}{2p'-1}\|q_k'\|_{\mathrm{L}^{p'}([c_k,c_{k+1}],\mathbb{R})}|t-c_k|^{\frac{p'-1}{p'}} \\
&= \frac{3p'-1}{2p'-1}\|q'\|_{\mathrm{L}^{p'}([c_k,c_{k+1}],\mathbb{R})}|t-c_k|^{\frac{p'-1}{p'}}
\end{aligned}$$

and result in

$$\int_{[c_k,t]} \left| q(\xi) - \frac{\int_{[c_k,\xi]} q(\xi_2) d\xi_2}{|\xi - c_k|} \right| d\xi \leq$$
$$\leq \frac{(3p'-1)p'}{(2p'-1)^2} \|q'\|_{\mathrm{L}^{p'}([c_k,c_{k+1}],\mathbb{R})} h_{\max}^{\frac{2p'-1}{p'}}$$
$$\leq \begin{cases} \frac{3}{4}\|q'\|_{\mathrm{L}^{\infty}([a,b],\mathbb{R})} h_{\max}^2 & \Leftarrow p' = \infty, \\ \frac{(3p'-1)p'}{(2p'-1)^2} \|q'\|_{\mathrm{L}^{p'}([a,b],\mathbb{R})} o\left(h_{\max}^{\frac{2p'-1}{p'}}\right) & \Leftarrow p' \in (1,+\infty), \\ 2\|q'\|_{\mathrm{L}^{1}([a,b],\mathbb{R})} o\left(h_{\max}\right) & \Leftarrow p' = 1. \end{cases} \tag{A.12}$$

If $q$ belongs to Class II, observe that Hölder's inequality yields

$$\begin{aligned} \int_{[c_k,t]} \left| q(\xi) - \frac{\int_{[c_k,\xi]} q(\xi_2) d\xi_2}{|\xi - c_k|} \right| d\xi &\leq 2\|q\|_{\mathrm{L}^{\infty}([c_k,c_{k+1}],\mathbb{R})} h_{\max} \\ &\leq 2\|q\|_{\mathrm{L}^{\infty}([a,b],\mathbb{R})} h_{\max}. \end{aligned} \tag{A.13}$$

Finally, we are in a position to estimate

$$\exp\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right) \cdots \exp\left(\boldsymbol{D}^{+}_{\lambda,0}(a,c_1)\right).$$

To this end, we require a different approach for each of the two asymptotic regimes (1.15) and (1.16). Firstly, in the asymptotic regime (1.15), we have

$$e^{\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})} =$$
$$= \cosh \frac{\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} +$$
$$+ \frac{\sinh \frac{\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}{2}}{\frac{\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}{2}} \begin{bmatrix} 0 & c_{k+1}-c_k \\ (c_{k+1}-c_k)^{-1}\left(\frac{\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}{2}\right)^2 & 0 \end{bmatrix}$$
$$= \mathcal{O}(1) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \mathcal{O}(1) \begin{bmatrix} 0 & \mathcal{O}(1)(2h_{\max}) \\ \mathcal{O}(1)(2h_{\max})^{-1} & 0 \end{bmatrix}$$

where we have called upon assumptions (1.13) and (1.14) as well as (A.2), (A.3) and (A.4). Secondly, in the asymptotic regime (1.16), we have

$$
\begin{aligned}
&e^{\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})} = \\
&= \cos\frac{\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}{2i}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} + \\
&\quad + \sin\frac{\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}{2i}\begin{bmatrix}0 & \frac{c_{k+1}-c_k}{(2i)^{-1}\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}\\ -\frac{(2i)^{-1}\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}{c_{k+1}-c_k} & 0\end{bmatrix} \\
&= \mathcal{O}(1)\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} + \mathcal{O}(1)\begin{bmatrix}0 & \mathcal{O}(1)\left(\lambda-\operatorname{ess\,sup}\{q\}\right)^{-\frac{1}{2}}\\ \mathcal{O}(1)\left(\left(\lambda-\operatorname{ess\,sup}\{q\}\right)^{-\frac{1}{2}}\right)^{-1} & 0\end{bmatrix}
\end{aligned}
$$

where we have taken advantage of (A.5) and of the fact that assumption (1.12) ensures that

$$
\begin{aligned}
\left|\frac{c_{k+1}-c_k}{(2i)^{-1}\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}\right| &= \frac{1}{\sqrt{\lambda-\frac{\int_{[c_k,c_{k+1}]}q(\xi)d\xi}{c_{k+1}-c_k}}} \\
&\leq 1\cdot\frac{1}{\sqrt{\lambda-\operatorname{ess\,sup}\{q\}}}, \\
\left|\frac{(2i)^{-1}\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}{c_{k+1}-c_k}\right| &= \sqrt{\lambda-\frac{\int_{[c_k,c_{k+1}]}q(\xi)d\xi}{c_{k+1}-c_k}} \\
&\leq \sqrt{\frac{\lambda-\operatorname{ess\,inf}\{q\}}{\lambda-\operatorname{ess\,sup}\{q\}}}\cdot\sqrt{\lambda-\operatorname{ess\,sup}\{q\}} \\
&\leq \sqrt{1+h^2_{\max}(\operatorname{ess\,sup}\{q\}-\operatorname{ess\,inf}\{q\})}\cdot\sqrt{\lambda-\operatorname{ess\,sup}\{q\}} \\
&\leq \sqrt{2}\cdot\sqrt{\lambda-\operatorname{ess\,sup}\{q\}}.
\end{aligned}
$$

The result now follows from Definition 2.5.

### A.1.2 Classes III and IV

In this subsubsection it is assumed that $q$ belongs to either Class III or IV. The treatment follows that of the previous subsection, but presents new subtleties which require additional care. Rewrite (A.1) as

$$
\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right) = 2|t-c_k|^{\frac{2p-1}{2p}}\sqrt{|t-c_k|^{\frac{1-p}{p}}\int_{[c_k,t]}q(\xi)d\xi-|t-c_k|^{\frac{1}{p}}\lambda}
$$

and observe that assumptions (1.18)–(1.19) and Hölder's inequality yield

$$
\left||t-c_k|^{\frac{1-p}{p}}\int_{[c_k,t]}q(\xi)d\xi\right| \leq \|q\|_{\mathrm{L}^p([a,b],\mathbb{R})} \tag{A.14}
$$

and

$$|\lambda| \leq h_{\max}^{-2}\left(1 - h_{\max}^{\frac{2p-1}{p}}\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right) \Rightarrow |\rho\left(\boldsymbol{D}_{\lambda,0}^{+}(c_k,t)\right)| \leq 2, \tag{A.15}$$

$$\lambda \geq h_{\max}^{-2}\left(1 - h_{\max}^{\frac{2p-1}{p}}\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right) \Rightarrow \rho\left(\boldsymbol{D}_{\lambda,0}^{+}(c_k,t)\right) \in [0,2] \cup i\mathbb{R}_0^{+}. \tag{A.16}$$

Like before, (A.15), Definition 2.4 and Remark 2.1, lead to the following estimates in the asymptotic regime (1.21)

$$\left|\varphi\left(\rho\left(\boldsymbol{D}_{\lambda,0}^{+}(c_k,t)\right)\right)|t-c_k|\right| \leq 2h_{\max}, \tag{A.17}$$

$$\left|\phi\left(\rho\left(\boldsymbol{D}_{\lambda,0}^{+}(c_k,t)\right)\right)|t-c_k|^2\right| \leq (2h_{\max})^2, \tag{A.18}$$

$$\left|\phi\left(\rho\left(\boldsymbol{D}_{\lambda,0}^{+}(c_k,t)\right)\right)\rho^2\left(\boldsymbol{D}_{\lambda,0}^{+}(c_k,t)\right)\right| \leq 2. \tag{A.19}$$

The new subtlety appears in the asymptotic regime (1.22). Unlike before, (A.16) does not lead to 'good' estimates. A possible workaround is to partition

$$[c_k, c_{k+1}] = \left[c_k, c_k + \lambda^{-\frac{1}{2}}\right] \cup \left[c_k + \lambda^{-\frac{1}{2}}, c_{k+1}\right].$$

If $t \in \left[c_k, c_k + \lambda^{-\frac{1}{2}}\right]$, then it is clear that (A.16) results in

$$\left|\varphi\left(\rho\left(\boldsymbol{D}_{\lambda,0}^{+}(c_k,t)\right)\right)|t-c_k|\right| \leq 2\lambda^{-\frac{1}{2}}, \tag{A.20}$$

$$\left|\phi\left(\rho\left(\boldsymbol{D}_{\lambda,0}^{+}(c_k,t)\right)\right)|t-c_k|^2\right| \leq \left(2\lambda^{-\frac{1}{2}}\right)^2, \tag{A.21}$$

$$\left|\phi\left(\rho\left(\boldsymbol{D}_{\lambda,0}^{+}(c_k,t)\right)\right)\rho^2\left(\boldsymbol{D}_{\lambda,0}^{+}(c_k,t)\right)\right| \leq 2. \tag{A.22}$$

If $t \in \left[c_k + \lambda^{-\frac{1}{2}}, c_{k+1}\right]$, then it follows from assumption (1.18), (A.14), (A.16) and the inequalities

$$\begin{aligned}
&|t-c_k|^{\frac{1-p}{p}}\int_{[c_k,t]} q(\xi)d\xi - |t-c_k|^{\frac{1}{p}}\lambda \leq \\
&\leq \|q\|_{\mathrm{L}^p([a,b],\mathbb{R})} - \lambda^{\frac{2p-1}{2p}} \\
&\leq -h_{\max}^{-\frac{2p-1}{p}}\left(\left(1 - h_{\max}^{\frac{2p-1}{p}}\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right)^{\frac{2p-1}{2p}} - h_{\max}^{\frac{2p-1}{p}}\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right) \\
&\leq -\frac{h_{\max}^{-\frac{2p-1}{p}}}{2} \\
&< 0
\end{aligned}$$

and

$$\left|\frac{|t-c_k|^{\frac{1-p}{p}}\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|^{\frac{1}{p}}\lambda}\right| \le \|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\lambda^{-\frac{2p-1}{2p}}$$

$$\le \frac{h_{\max}^{\frac{2p-1}{p}}\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}}{\left(1-h_{\max}^{\frac{2p-1}{p}}\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right)^{\frac{2p-1}{2p}}}$$

$$\le \frac{1}{3}$$

that

$$\begin{aligned}
&\left|\varphi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)|t-c_k|\right| = \\
&= \left|\frac{\varphi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)}{2}\frac{2|t-c_k|}{\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)}\right| \\
&\le \lambda^{-\frac{1}{2}}\left(\frac{|t-c_k|^{\frac{1}{p}}\lambda}{|t-c_k|^{\frac{1}{p}}\lambda-|t-c_k|^{\frac{1-p}{p}}\int_{[c_k,t]}q(\xi)d\xi}\right)^{\frac{1}{2}} \\
&= \lambda^{-\frac{1}{2}}\left(1-\frac{|t-c_k|^{\frac{1-p}{p}}\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|^{\frac{1}{p}}\lambda}\right)^{-\frac{1}{2}} \\
&\le 2\lambda^{-\frac{1}{2}},
\end{aligned}$$

$$\begin{aligned}
&\left|\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)|t-c_k|^2\right| = \\
&= \left|\frac{\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)\rho^2\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)}{4}\frac{4|t-c_k|^2}{\rho^2\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)}\right| \\
&\le \lambda^{-1}\frac{|t-c_k|^{\frac{1}{p}}\lambda}{|t-c_k|^{\frac{1}{p}}\lambda-|t-c_k|^{\frac{1-p}{p}}\int_{[c_k,t]}q(\xi)d\xi} \\
&= \lambda^{-1}\left(1-\frac{|t-c_k|^{\frac{1-p}{p}}\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|^{\frac{1}{p}}\lambda}\right)^{-1} \\
&\le \left(2\lambda^{-\frac{1}{2}}\right)^2
\end{aligned}$$

and

$$\left|\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)\rho^2\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right| \le 2.$$

If $q$ belongs to Class III, then Hölder's inequality yields

$$\int_{[c_k,t]} \left| q(\xi) - \frac{\int_{[c_k,\xi]} q(\xi_2) d\xi_2}{|\xi - c_k|} \right| d\xi \leq \frac{2p-1}{p-1} \|q\|_{\mathrm{L}^p([c_k,c_{k+1}],\mathbb{R})} h_{\max}^{\frac{p-1}{p}}$$
$$\leq \frac{2p-1}{p-1} \|q\|_{\mathrm{L}^p([a,b],\mathbb{R})} o\left(h_{\max}^{\frac{p-1}{p}}\right). \tag{A.23}$$

If $q$ belongs to Class IV and $c_k$ is a Lebesgue point of $q$, then Lebesgue's fundamental theorem of calculus ensures that the mapping

$$\xi \in [c_k,t] \to \int_{[c_k,\xi]} |q(\xi_2)| d\xi_2 \in \mathbb{R}_0^+$$

is continuous and Lebesgue's differentiation theorem ensures that

$$\exists \lim_{\xi \to c_k^+} \frac{\int_{[c_k,\xi]} |q(\xi_2)| d\xi_2}{|\xi - c_k|} < +\infty.$$

Hence,

$$\xi \in [c_k,t] \to \frac{\int_{[c_k,\xi]} |q(\xi_2)| d\xi_2}{|\xi - c_k|} \in \mathbb{R}_0^+$$

is continuous (with removable singularity) and

$$\int_{[c_k,t]} \left| q(\xi) - \frac{\int_{[c_k,\xi]} q(\xi_2) d\xi_2}{|\xi - c_k|} \right| d\xi \leq$$
$$\leq \|q\|_{\mathrm{L}^1([a,b],\mathbb{R})} \left( \frac{\int_{[c_k,c_{k+1}]} |q(\xi)| d\xi}{\|q\|_{\mathrm{L}^1([a,b],\mathbb{R})}} + \frac{\int_{[c_k,t]} \frac{\int_{[c_k,\xi]} |q(\xi_2)| d\xi_2}{|\xi - c_k|} d\xi}{\|q\|_{\mathrm{L}^1([a,b],\mathbb{R})}} \right)$$
$$\leq \|q\|_{\mathrm{L}^1([a,b],\mathbb{R})} \left( o\left(1\right) + \mathcal{O}\left(h_{\max}\right) \right). \tag{A.24}$$

Finally, we have the capacity to estimate

$$\exp\left( \boldsymbol{D}_{\lambda,0}^+(c_k,c_{k+1}) \right) \cdots \exp\left( \boldsymbol{D}_{\lambda,0}^+(a,c_1) \right).$$

To this end we require a different way of dealing with each of the two asymptotic regimes (1.21) and (1.22). Firstly, in the asymptotic regime (1.21), we have, like before,

$$e^{\boldsymbol{D}_{\lambda,0}^+(c_k,c_{k+1})} =$$
$$= \cosh \frac{\rho\left(\boldsymbol{D}_{\lambda,0}^+(c_k,c_{k+1})\right)}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} +$$
$$+ \frac{\sinh \frac{\rho\left(\boldsymbol{D}_{\lambda,0}^+(c_k,c_{k+1})\right)}{2}}{\frac{\rho\left(\boldsymbol{D}_{\lambda,0}^+(c_k,c_{k+1})\right)}{2}} \begin{bmatrix} 0 & c_{k+1} - c_k \\ (c_{k+1} - c_k)^{-1} \left( \frac{\rho\left(\boldsymbol{D}_{\lambda,0}^+(c_k,c_{k+1})\right)}{2} \right)^2 & 0 \end{bmatrix}$$
$$= \mathcal{O}\left(1\right) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \mathcal{O}\left(1\right) \begin{bmatrix} 0 & \mathcal{O}\left(1\right)\left(2h_{\max}\right) \\ \mathcal{O}\left(1\right)\left(2h_{\max}\right)^{-1} & 0 \end{bmatrix}$$

where we have called upon assumptions (1.19)–(1.20) and (A.15). Secondly, in the asymptotic regime (1.22), we have, unlike before,

$$
\begin{aligned}
&e^{\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})} = \\
&= \cos\frac{\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}{2i}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} + \\
&\quad + \sin\frac{\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}{2i}\begin{bmatrix}0 & \frac{c_{k+1}-c_k}{(2i)^{-1}\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}\\ -\frac{(2i)^{-1}\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,c_{k+1})\right)}{c_{k+1}-c_k} & 0\end{bmatrix}\\
&= \mathcal{O}(1)\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} + \mathcal{O}(1)\begin{bmatrix}0 & \mathcal{O}(1)\left(2\lambda^{-\frac{1}{2}}\right)\\ \mathcal{O}(1)\left(2\lambda^{-\frac{1}{2}}\right)^{-1} & 0\end{bmatrix}
\end{aligned}
$$

where we have capitalized upon (A.16) as well as the fact that assumption (1.18), assumption (1.20) and (A.14) ensure that

$$
\begin{aligned}
&(c_{k+1}-c_k)^{\frac{1-p}{p}}\int_{[c_k,c_{k+1}]} q(\xi)d\xi - (c_{k+1}-c_k)^{\frac{1}{p}}\lambda \leq\\
&\leq \|q\|_{\mathrm{L}^p([a,b],\mathbb{R})} - \left(\frac{h_{\min}}{h_{\max}}\right)^{\frac{1}{p}} h_{\max}^{\frac{1}{p}}\lambda\\
&\leq -h_{\max}^{-\frac{2p-1}{p}}\left(\frac{1}{2} - \frac{3}{2}h_{\max}^{\frac{2p-1}{p}}\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}\right)\\
&\leq -\frac{h_{\max}^{-\frac{2p-1}{p}}}{8}\\
&< 0,
\end{aligned}
$$

$$
\begin{aligned}
\left|\frac{(c_{k+1}-c_k)^{\frac{1-p}{p}}\int_{[c_k,c_{k+1}]} q(\xi)d\xi}{(c_{k+1}-c_k)^{\frac{1}{p}}\lambda}\right| &\leq \left(\frac{h_{\max}}{h_{\min}}\right)^{\frac{1}{p}}\frac{\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}}{h_{\max}^{\frac{1}{p}}\lambda}\\
&\leq 2\frac{h_{\max}^{\frac{2p-1}{p}}\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}}{1-h_{\max}^{\frac{2p-1}{p}}\|q\|_{\mathrm{L}^p([a,b],\mathbb{R})}}\\
&\leq \frac{2}{3}
\end{aligned}
$$

and

$$\left|\frac{c_{k+1}-c_k}{(2i)^{-1}\rho\left(\boldsymbol{D}^+_{\lambda,0}(c_k,c_{k+1})\right)}\right| = \lambda^{-\frac{1}{2}}\left(1-\frac{(c_{k+1}-c_k)^{\frac{1-p}{p}}\int_{[c_k,c_{k+1}]}q(\xi)d\xi}{\lambda\left(c_{k+1}-c_k\right)^{\frac{1}{p}}}\right)^{-\frac{1}{2}}$$
$$\leq \frac{\sqrt{3}}{2}\cdot\left(2\lambda^{-\frac{1}{2}}\right),$$
$$\left|\frac{(2i)^{-1}\rho\left(\boldsymbol{D}^+_{\lambda,0}(c_k,c_{k+1})\right)}{c_{k+1}-c_k}\right| = \lambda^{\frac{1}{2}}\left(1-\frac{(c_{k+1}-c_k)^{\frac{1-p}{p}}\int_{[c_k,c_{k+1}]}q(\xi)d\xi}{\lambda\left(c_{k+1}-c_k\right)^{\frac{1}{p}}}\right)^{\frac{1}{2}}$$
$$\leq \frac{2\sqrt{5}}{\sqrt{3}}\cdot\left(2\lambda^{-\frac{1}{2}}\right)^{-1}.$$

The result now follows from Definition 2.5.

## A.2 Estimating $\boldsymbol{\pi}\left(\boldsymbol{B}^+_{\lambda,1}(c_k,t)\right)$ and $\boldsymbol{\pi}\left(\boldsymbol{D}^+_{\lambda,1}(c_k,t)\right)$

Contrary to the previous subsection, it is now possible and convenient to cover every class and asymptotic regime simultaneously. To this end, recall Definition 2.5 and rewrite (A.6)–(A.8), (A.9)–(A.11), (A.17)–(A.19) and (A.20)–(A.22) as

$$\left|\varphi\left(\rho\left(\boldsymbol{D}^+_{\lambda,0}(c_k,t)\right)\right)|t-c_k|\right| \leq \epsilon_1, \tag{A.25}$$
$$\left|\phi\left(\rho\left(\boldsymbol{D}^+_{\lambda,0}(c_k,t)\right)\right)|t-c_k|^2\right| \leq \epsilon_1^2, \tag{A.26}$$
$$\left|\phi\left(\rho\left(\boldsymbol{D}^+_{\lambda,0}(c_k,t)\right)\right)\rho^2\left(\boldsymbol{D}^+_{\lambda,0}(c_k,t)\right)\right| \leq 2, \tag{A.27}$$

and (A.12), (A.13), (A.23) and (A.24) as

$$\int_{[c_k,t]}\left|q(\xi)-\frac{\int_{[c_k,\xi]}q(\xi_2)d\xi_2}{|\xi-c_k|}\right|d\xi \leq \epsilon_2. \tag{A.28}$$

Note that (A.25)–(A.27), in turn, imply that

$$\varphi\left(\rho\left(\boldsymbol{D}^+_{\lambda,0}(c_k,t)\right)\right)\mathscr{C}_{\boldsymbol{D}^+_{\lambda,0}(c_k,t)}\boldsymbol{\pi}\left(\boldsymbol{B}^+_{\lambda,0}(c_k,t)\right) =$$
$$= \begin{bmatrix}\varphi\left(\rho\left(\boldsymbol{D}^+_{\lambda,0}(c_k,t)\right)\right)|t-c_k|\left(q(t)-\frac{\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|}\right)\\ 0\\ 0\end{bmatrix}$$
$$= \left(q(t)-\frac{\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|}\right)\begin{bmatrix}\mathcal{O}\left(\epsilon_1\right)\\ 0\\ 0\end{bmatrix}$$

and

$$\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)\mathscr{C}^{2}_{\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)}\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,0}(c_k,t)\right)=$$
$$=\begin{bmatrix} 0 \\ -2\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)|t-c_k|^2\left(q(t)-\frac{\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|}\right) \\ \frac{1}{2}\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)\rho^2\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\left(q(t)-\frac{\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|}\right)\end{bmatrix}$$
$$=\left(q(t)-\frac{\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|}\right)\begin{bmatrix}0\\ \mathcal{O}\left(\epsilon_1^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix}$$

which, according to Theorem 2.3, lead to

$$\begin{aligned}\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,1}(c_k,t)\right)&=\varphi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)\mathscr{C}_{\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)}\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,0}(c_k,t)\right)+\\ &\quad+\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)\right)\right)\mathscr{C}^{2}_{\boldsymbol{D}^{+}_{\lambda,0}(c_k,t)}\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,0}(c_k,t)\right)\\ &=\left(q(t)-\frac{\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|}\right)\begin{bmatrix}\mathcal{O}\left(\epsilon_1\right)\\ \mathcal{O}\left(\epsilon_1^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix}\end{aligned}$$

and (c.f., (A.28))

$$\boldsymbol{\pi}\left(\boldsymbol{D}^{+}_{\lambda,1}(c_k,t)\right)=\int_{[c_k,t]}\boldsymbol{B}^{+}_{\lambda,1}(c_k,\xi)d\xi=\epsilon_2\begin{bmatrix}\mathcal{O}\left(\epsilon_1\right)\\ \mathcal{O}\left(\epsilon_1^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix}.$$

## A.3 Estimating $\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,l}(c_k,t)\right)$ and $\boldsymbol{\pi}\left(\boldsymbol{D}^{+}_{\lambda,l}(c_k,t)\right)$ for $l\geq 2$

Our estimate follows by induction. The induction claim is that

$$\begin{aligned}\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,l}(c_k,t)\right)&=\left(q(t)-\frac{\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|}\right)\epsilon_2^{2^{l-1}-1}\epsilon_1^{2^{l-1}-1}\begin{bmatrix}\mathcal{O}\left(\epsilon_1\right)\\ \mathcal{O}\left(\epsilon_1^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix},\\ \boldsymbol{\pi}\left(\boldsymbol{D}^{+}_{\lambda,l}(c_k,t)\right)&=\epsilon_2^{2^{l-1}}\epsilon_1^{2^{l-1}-1}\begin{bmatrix}\mathcal{O}\left(\epsilon_1\right)\\ \mathcal{O}\left(\epsilon_1^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix}.\end{aligned}$$

### A.3.1 First step: $l=2$

Given Definition 2.4 and the uniform estimates for $\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,1}(c_k,t)\right)$ in the previous subsection, it is now clear that

$$\begin{aligned}\varphi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,1}(c_k,t)\right)\right)&=-\frac{1}{2}+\epsilon_2^2\mathcal{O}\left(\epsilon_1^2\right),\\ \phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,1}(c_k,t)\right)\right)&=\frac{1}{3}+\epsilon_2^2\mathcal{O}\left(\epsilon_1^2\right),\end{aligned}$$

and, according to Theorem 2.3, that

$$\begin{aligned}\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,2}(c_k,t)\right) &= \varphi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,1}(c_k,t)\right)\right)\mathscr{C}_{\boldsymbol{D}^{+}_{\lambda,1}(c_k,t)}\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,1}(c_k,t)\right)+\\ &\quad+\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,1}(c_k,t)\right)\right)\mathscr{C}^{2}_{\boldsymbol{D}^{+}_{\lambda,1}(c_k,t)}\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,1}(c_k,t)\right)\\ &= \left(q(t)-\frac{\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|}\right)\epsilon_2\epsilon_1\begin{bmatrix}\mathcal{O}\left(\epsilon_1\right)\\ \mathcal{O}\left(\epsilon_1^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix}\end{aligned}$$

and (c.f., (A.28))

$$\boldsymbol{\pi}\left(\boldsymbol{D}^{+}_{\lambda,2}(c_k,t)\right)=\int_{[c_k,t]}\boldsymbol{B}^{+}_{\lambda,2}(c_k,\xi)d\xi=\epsilon_2^2\epsilon_1\begin{bmatrix}\mathcal{O}\left(\epsilon_1\right)\\ \mathcal{O}\left(\epsilon_1^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix}.$$

### A.3.2 Induction step: $l \Rightarrow l+1$

Given the induction claim, it is now clear that

$$\begin{aligned}\varphi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,l}(c_k,t)\right)\right) &= -\frac{1}{2}+\epsilon_2^{2^l}\mathcal{O}\left(\epsilon_1^{2^l}\right),\\ \phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,l}(c_k,t)\right)\right) &= \frac{1}{3}+\epsilon_2^{2^l}\mathcal{O}\left(\epsilon_1^{2^l}\right),\end{aligned}$$

and, according to Theorem 2.3, that

$$\begin{aligned}\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,l+1}(c_k,t)\right) &= \varphi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,l}(c_k,t)\right)\right)\mathscr{C}_{\boldsymbol{D}^{+}_{\lambda,l}(c_k,t)}\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,l}(c_k,t)\right)+\\ &\quad+\phi\left(\rho\left(\boldsymbol{D}^{+}_{\lambda,l}(c_k,t)\right)\right)\mathscr{C}^{2}_{\boldsymbol{D}^{+}_{\lambda,l}(c_k,t)}\boldsymbol{\pi}\left(\boldsymbol{B}^{+}_{\lambda,l}(c_k,t)\right)\\ &= \left(q(t)-\frac{\int_{[c_k,t]}q(\xi)d\xi}{|t-c_k|}\right)\epsilon_2^{2^l-1}\epsilon_1^{2^l-1}\begin{bmatrix}\mathcal{O}\left(\epsilon_1\right)\\ \mathcal{O}\left(\epsilon_1^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix}\end{aligned}$$

and (c.f., (A.28))

$$\boldsymbol{\pi}\left(\boldsymbol{D}^{+}_{\lambda,l+1}(c_k,t)\right)=\int_{[c_k,t]}\boldsymbol{B}^{+}_{\lambda,l+1}(c_k,\xi)d\xi=\epsilon_2^{2^l}\epsilon_1^{2^l-1}\begin{bmatrix}\mathcal{O}\left(\epsilon_1\right)\\ \mathcal{O}\left(\epsilon_1^2\right)\\ \mathcal{O}\left(1\right)\end{bmatrix}.$$

## References


Fer, F. (1958), ‘Résolution del l‘equation matricielle $\dot{U}=pU$ par produit infini d‘exponentielles matricielles’, *Bulletin de la Classe des Sciences Académie Royale de Belgique* **44**, 818–829.

Iserles, A. (1984), 'Solving linear ordinary differential equations by exponentials of iterated commutators', *Numerische Mathematik* **45**(2), 183–199.

Iserles, A., Munthe-Kaas, H. Z., Nørsett, S. and Zanna, A. (2000), 'Lie-group methods', *Acta Numerica* **9**, 215–365.

Ixaru, L. (2000), 'CP methods for the Schrödinger equation', *Journal of Computational and Applied Mathematics* **125**(1-2), 347–357.

Ledoux, V., Daele, M. and van den Berghe, G. (2010), 'Efficient numerical solution of the 1D Schrödinger eigenvalue problem using Magnus integrators', *IMA Journal of Numerical Analysis* **30**, 751–776.

Moan, P. C. (1998), Efficient approximation of Sturm–Liouville problems using Lie-group methods, Technical report, Department of Applied Mathematics and Theoretical Physics, University of Cambridge, United Kingdom.

Pryce, J. (1993), *Numerical Solution of Sturm–Liouville Problems*, Oxford University Press.

Ramos, A. and Iserles, A. (2013), Numerical solution of Sturm–Liouville problems via Fer streamers, Technical report, Department of Applied Mathematics and Theoretical Physics, University of Cambridge, United Kingdom. Available online at:
(http://www.damtp.cam.ac.uk/user/na/NA_papers/NA2013_09.pdf).

Zettl, A. (2005), *Sturm–Liouville Theory*, American Mathematical Society.