Stability and error estimates for Filon-Clenshaw-Curtis rules for highly-oscillatory integrals

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Abstract

In this paper we obtain new results on Filon-type methods for computing oscillatory integrals of the form $\int_{-1}^{1} f(s)\exp(\mathrm{i}ks)\,\mathrm{d}s$. We use a Filon approach based on interpolating f at the classical Clenshaw-Curtis points $\cos(j\pi/N)$, $j = 0,\ldots,N$. The rule may be implemented in $\mathcal{O}(N\log N)$ operations. We prove error estimates which show explicitly how the error depends both on the parameters k and N and on the Sobolev regularity of f. In particular we identify the regularity of f required to ensure the maximum rate of decay of the error as $k\to\infty$. We also describe a method for implementating the method and prove its stability both when $N\le k$ and $N>k$. Numerical experiments illustrate both the stability of the algorithm and the sharpness of the error estimates.

Keywords Numerical integration. Highly oscillating integrals. Clenshaw-Curtis quadrature.
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1 Introduction

In this note we consider the evaluation of integrals of the form

$$I_k(f) \ := \ \int_{-1}^{1} f(s)\exp(\mathrm{i}ks)\ \mathrm{d}s \tag{1}$$

for k ranging over all positive real values. All the results presented and proven in this paper can be extended for negative values of k in a straighforward way.

We propose rules $I_{k,N}(f)$ which compute $I_k(f)$ using $N+1$ evaluations of the function f and which enjoy an error estimate of the form (see Corollary 2.3):

$$|I_k(f) - I_{k,N}(f)| \ \le \ C_r(f)\ \min\left\{1, \left(\frac{1}{k}\right)^2\right\}\ \left(\frac{1}{N}\right)^r\ , \quad \text{for all } N\ge 1 \ \text{ and } r\ge 0\ , \tag{2}$$

where $C_r(f)$ depends only on r and on a suitable Sobolev norm of f. Our rules are effective both when k is large relative to N and when N is large relative to k. In particular, since in general $I_k(f)\approx\mathcal{O}(k^{-1})$, our method even has a relative error which decays as $\mathcal{O}(k^{-1}N^{-r})$ uniformly in $k\to\infty$, $N\to\infty$, for all r, provided f is sufficiently smooth.

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We shall use a "Filon-like" approach, based on replacing f by its degree N polynomial interpolant $Q_N f$ at the Clenshaw-Curtis points $t_{j,N} := \cos(j\pi/N)$, $j = 0, \dots, N$, yielding the "Filon-Clenshaw-Curtis" quadrature rule:

$$I_{k,N}(f) \ := \ \int_{-1}^{1} (Q_N f)(s) \exp(\mathrm{i}ks) \ \mathrm{d}s. \tag{3}$$

Since $Q_N f$ may be expressed (using FFT) as a linear combination of the Chebyshev polynomials of the first kind $\{T_n : n = 0, \dots, N\}$, the implementation of (3) reduces to the computation of the weights

$$\omega_n(k) := \int_{-1}^{1} T_n(s) \exp(\mathrm{i}ks) \ \mathrm{d}s \ , \quad n = 0, \dots, N \ , \tag{4}$$

and the cost of the implementation is $\mathcal{O}(N \log N)$ (see Remark 5.4).

A standard recursive algorithm for computing $\omega_n(k)$, for $n = 0, 1, \dots$ may be based on three term recurrence relations for orthogonal polynomials. However this algorithm is only stable when $N \ \leq \ k$ and it is inappropriate for evaluating (4) when $N > k$. However in this case the required additional values $\{\omega_n(k) : \ k \ < \ n \ \leq \ N\}$ may be computed by adding a second phase to the algorithm in which a tridiagonal system of size about $N - k$ is solved. The right-hand side of this tridiagonal system is determined by an asymptotic argument and the resulting "composite algorithm" is accurate and stable for all N and k.

Our algorithm may be found in the classical literature on Clenshaw-Curtis rules (where it is referred to as a "modified Clenshaw-Curtis" or "product-integration rule" [31, 18, 7, 6]) However, while the classical literature contains remarks about the stability (or lack of it) of these rules, there seems no proof of stability for the composite algorithm proposed here. Additional novel results in the present paper are (i) the rigorous justification of the asymptotic argument (previously used heuristically) in the second phase of the algorithm and (ii) the proof of the error estimate (2), which also seems to be a new result. We remark that our algorithm for computing (4) may be more generally useful. For example, if one wants to compute the first K Fourier coefficients of the first N Chebyshev polynomials, it could be applied.

A particular attraction of rules based on Clenshaw-Curtis points (and one reason for their historical popularity) is the fact that they are nested: If $I_{k,N}(f)$ has been computed, then computation of $I_{k,2N}(f)$ requires only N additional evaluations of f. Thus an inexpensive adaptive procedure can be based on comparing $I_{k,2N}(f)$ and $I_{k,N}(f)$.

The easy implementation of the rule (3) and its good stability and convergence properties for a wide range of N and k make it particularly well-suited for the implementation of boundary integral equation methods in high-frequency scattering, which is our main target application see, e.g. [9, 17]. In that application, integrals of the form

$$\int_{a}^{b} g(x) \exp(\mathrm{i}kx) \ \mathrm{d}x \tag{5}$$

arise, with complicated (but non-oscillatory) functions g (often themselves defined as integrals involving special functions), and possibly small interval length $b-a$. With the change of variable $x = \alpha + \delta s$, $s \in [-1, 1]$, where $\alpha = (b + a)/2$ and $\delta = (b - a)/2$, (5) becomes

$$I_{\delta k}(f) \ = \ \int_{-1}^{1} f(s) \exp(\mathrm{i}\delta ks) \ \mathrm{d}s \tag{6}$$

where $f(s) = \delta \exp(\mathrm{i}k\alpha) g(\alpha + \delta\, s)$, $\quad s \in [-1, 1]$. If f is complicated, then N may need to be taken fairly large in (3). If in addition δ is small then the case $N > \delta k$ may well arise and so the stability theory of our algorithm for all N becomes relevant.

The Clenshaw-Curtis rule in its original form, for integrating a function f without a weight (i.e. (1) in the case $k = 0$) dates back to [5]. Because of its high rate of convergence for smooth f, the fact that its points are nested and its weights can be computed by FFT, the method quickly gained popularity and many subsequent papers were devoted to its practical implementation, e.g. [10]. Surveys of these results may be found in text books such as [7, 18, 6].

Subsequent attention focussed on adapting the Clenshaw-Curtis method for the computation of integrals of the general form:

$$\int_{-1}^{1} f(s)w(s)\ \mathrm{d}s\ , \tag{7}$$

where f is a possibly complicated (but relatively smooth) function and w is a simple function with some sort of "difficult" behaviour (e.g. containing singularities or oscillations). These "modified Clenshaw-Curtis rules" (or "product integration rules with Clenshaw-Curtis points") were developed for example in [26, 23, 24, 31] (see also [22] for a more recent survey). These papers developed methods for computing the weights $\int_{-1}^{1} T_n(s)w(s)\ \mathrm{d}s$ (analogous to (4)) and were included in the Fortran quadrature toolbox Quadpack [25]. However when we examine how these results apply to (3) (i.e. $w(s) = \exp(\mathrm{i}ks)$) they neither yield error estimates for (3) which are explicit in both k and the regularity of f nor prove stability of the method for computing the weights for all N and k.

More recently, the question of computing highly oscillatory integrals has enjoyed a substantial renaissance and a number of authors have been concerned in particular with identifying quadrature rules for (1) with error which decays with high negative powers of k. The pioneering paper [13] analysed particular types of Filon approach based on replacing $f(x)$ with an interpolating polynomial for a general class of oscillatory integrals, including (1). For (3), the results in [13] imply that the error will decay like $\mathcal{O}(k^{-2})$ as $k \to \infty$ provided the interpolation points include the endpoints ± 1. Our convergence theorem, Theorem 2.2 below, provides more detailed information for the particular rule (3), in that it provides error bounds which are explicit in N (the number of interpolation points) and k (and also in the Sobolev regularity of f), and is valid for all $N \geq 2$ and $k \geq k_0$. Such estimates are useful since they indicate explicitly how the rate of convergence depends on the amount of computational work.

The renewed recent interest in oscillatory integration sparked a number of subsequent papers. For example [14] concerned (among other things) the case when the oscillatory factor in (1) is replaced with $\exp(\mathrm{i}kh(x))$, while [15] obtained methods which converged with higher negative powers of k by using interpolation of derivatives at the end points of the domain of integration. Related methods with the same property and again using higher order derivative information were obtained by [34]. Methods with high order error decay as $k \to \infty$ were also considered in [28, 30], which concerned oscillatory factors of the form $\exp(ik\,h(s))$, where h is allowed to have stationary points inside the interval of integration. Moreover [29] concerned the application of modern Krylov subspace methods for computing an antiderivative of a given function. Such techniques lead to efficient methods for oscillatory integration, as was originally pointed out in Levin's work [19].

In [11], generalisations of the method of steepest descent are employed, which allow the fast evaluation of (1) by converting it to an integral in the complex plane. These methods were applied in the context of boundary integral equation methods in scattering in [12]. Another paper concerned with the solution of boundary integral equations is [4]. This includes a way to compute (4) (which is different from the one proposed in this paper), by expanding in a truncated series of Bessel funtions and then approximating these by a combination of recurrence relations and asymptotic approximation. (The same expansion appears also in [26]).

The plan of this paper is as follows. In §2 we give some more details of the basic properties of $I_{k,N}(f)$ and prove (2). In §3 we present the composite algorithm for computing the weights. In particular the proof of stability for large N requires an asymptotic expansion for (4) for large values of n. This asymptotic expansion is proved in §4. We will prove the stability of the algorithm in §5 and we finish by showing in §6 some numerical experiments to show the stability of the algorithm and the sharpness of the error estimate (2). A public domain Matlab code which implements the algorithm is available at [8].

Remark 1.1 *We end this section by giving a little more detail of boundary integral equation methods for wave scattering problems, and explaining why the Clenshaw-Curtis rules are well-suited to implementing these.*

Let Ω *be a bounded obstacle with boundary* Γ *and let* $\Omega' = \mathbb{R}^2 \backslash \overline{\Omega}$*. Consider the computation of the scattered wave which results when a plane wave* $\exp(ik\mathbf{x}.\widehat{\mathbf{a}})$, $\mathbf{x} \in \Omega'$ *is incident on* Γ*. Here the unit vector* $\widehat{\mathbf{a}} \in \mathbb{R}^2$ *specifies the incidence direction. Under the assumption that the total wave (which is the sum of the incident and scattered waves) vanishes on* Γ *(i.e. the scatterer is "sound-soft"), this problem can be formulated as a boundary integral equation*

$$\int_\Gamma \frac{\mathrm{i}}{4} H_0^{(1)}(k|\mathbf{x}-\mathbf{y}|)v(\mathbf{y})\ \mathrm{d}s(\mathbf{y}) \ = \ \exp(ik\mathbf{x}.\widehat{\mathbf{a}}) \ , \tag{8}$$

where $H_0^{(1)}$ *is the Hankel function of the first kind of order zero, and the unknown* v *is the normal derivative of the total wave wave. (Actually this formulation fails for a countable set of wave-numbers* k *and a modified version of* (8) *is usually used in practice, but* (8) *is sufficient to illustrate the quadrature problems which arise.) In high frequency applications it is often beneficial to write* $v(\mathbf{x}) = V(\mathbf{x})\exp(ik\mathbf{x}.\widehat{\mathbf{a}})$*, since under appropriate geometrical assumptions,* V *is then less oscillatory than* v*. (This is the "geometric optics approximation".) Inserting this ansatz into* (8)*, multiplying by* $\exp(-ik\mathbf{x}.\widehat{\mathbf{a}})$ *and identifying explicitly the large* k *asymptotics of the Hankel function, we obtain*

$$\int_\Gamma \exp\left(\mathrm{i}k[|\mathbf{x}-\mathbf{y}| - (\mathbf{x}-\mathbf{y}).\widehat{\mathbf{a}}]\right) F(\mathbf{x},\mathbf{y})V(\mathbf{y})\ \mathrm{d}s(\mathbf{y}) \ = \ 1 \ , \quad \mathbf{x} \in \Gamma \ , \tag{9}$$

where F *is complicated (and also depends on* k*) but is non-oscillatory. Discretizations of this problem (e.g. via the Galerkin method) commonly require computation of integrals of the form*

$$I := \int_{\Gamma^0} \exp\left(\mathrm{i}k[|\mathbf{x}-\mathbf{y}| - (\mathbf{x}-\mathbf{y}).\widehat{\mathbf{a}}]\right) F(\mathbf{x},\mathbf{y})P(\mathbf{y})\ \mathrm{d}s(\mathbf{y}), \quad \textit{for a range of} \quad \mathbf{x} \in \Gamma \ ,$$

where Γ^0 *is some subinterval of* Γ *and* P *is some polynomial on* Γ^0*. If* $\mathbf{x} = \boldsymbol{\gamma}(s)$ *and* $\mathbf{y} = \boldsymbol{\gamma}(t)$*, where* $\boldsymbol{\gamma}$ *denotes arclength parametrization of* Γ *then* I *has the form*

$$I \ = \ \int_a^b \exp(\mathrm{i}k\Psi_{[s]}(t))\, G(s,t)\, \mathrm{d}t \ , \quad \textit{for some range of values of} \ \ s \ , \tag{10}$$

where $\Psi_{[s]}(t) = |\boldsymbol{\gamma}(s) - \boldsymbol{\gamma}(t)| - (\boldsymbol{\gamma}(s) - \boldsymbol{\gamma}(t)).\widehat{\mathbf{a}}$ *and* G *is non-oscillatory with respect to* k *but may be complicated and contain a relatively high degree polynomial factor in* t*.*

When the phase $\Psi_{[s]}$ *has no stationary points in* $[a,b]$ *the change of variable* $\tau = \Psi_{[s]}(t)$ *reduces* I *to an integral of the form* (5)*. The Filon-Clenshaw-Curtis rule is then particularly appropriate for these integrals since only point values and not derivatives of the complicated function* $G(s,\cdot)$ *are needed and also the error can be controlled explicitly with respect to both* k*,* N*, and some Sobolev norm of* $G(s,\cdot)$*, allowing estimates which are uniform over all polynomials* P *in some suitable basis. This is particularly important when performing an error analysis of the boundary integral methods with quadrature. This is done by analysing the "semi-discrete" method (e.g. the Galerkin method without quadrature) and then incorporating errors due to quadrature as perturbations via the the Strang Lemma [16]. (Additional techniques to handle the occurrence of stationary points in* (10) *and the case when* G *contains the log singularity of the Hankel function are described in [16].) In [12] methods for computing these boundary integrals via the method of steepest descent were used. While these give very good results they do not permit the explicit rigorous error estimates which the Filon-Clenshaw-Curtis rules allow. A rather different approach was taken in the earlier work [3, 2], where quadrature rules for* (8) *were* *directly developed by localisation with respect to each* $\mathbf{x}$ *around singular and stationary points and then suitable extensions of the method of stationary phase and local mesh refinement were applied. Since this Nyström-type method is not based on a Galerkin formulation, the analysis of its k-robustness is a challenging open problem. The methods we have developed here permit a full error analysis.*

2 Basic properties and error estimate

Let $\mathcal{P}_N$ denote the algebraic polynomials of degree N and define the polynomial interpolation operator $Q_N : C[-1,1] \to \mathcal{P}_N$ by requiring

$$Q_N f(t_{j,N}) = f(t_{j,N}), \qquad j = 0,\ldots,N \quad \text{where} \quad t_{j,N} := \cos\left(\frac{j\pi}{N}\right).$$

Using the well-known trigonometric identity

$$\frac{2}{N}\sum_{n=0}^{N}{}'' \cos\left(\frac{j'n\pi}{N}\right)\cos\left(\frac{jn\pi}{N}\right) = \begin{cases} 1, & \text{if } j = j' \in \{1,2,\ldots,N-1\},\\ 2, & \text{if } j = j' \in \{0,N\},\\ 0, & \text{otherwise,}\end{cases}$$

($\sum''$ means that the first and the last terms in the sum are to be halved), it can be seen that $Q_N f$ may be written

$$Q_N f(s) = \sum_{n=0}^{N}{}'' \alpha_{n,N}(f) T_n(s) \ , \tag{11}$$

where $T_n(s) = \cos(n \arccos(s))$ are the Chebyshev polynomials of the first kind, and

$$\alpha_{n,N}(f) = \frac{2}{N}\sum_{j=0}^{N}{}'' \cos\left(\frac{jn\pi}{N}\right) f\left(t_{j,N}\right) , \qquad n = 0,\ldots,N. \tag{12}$$

In view of (3) and (11), we may write the rule (3) as

$$I_{k,N}(f) = \sum_{n=0}^{N}{}'' \alpha_{n,N}(f)\omega_n(k) \tag{13}$$

where the weights

$$\omega_n(k) := \int_{-1}^{1} T_n(s)\exp(\mathrm{i}ks)\, \mathrm{d}s \ , \quad n \geq 0 \ , \tag{14}$$

have to be computed.

Remark 2.1 *Let* C *be the* $(N+1)\times(N+1)$ *matrix with entries*

$$C_{n,j} = (2/N)\cos(jn\pi/N) \ , \qquad n,j = 0,\ldots,N$$

and introduce the column vectors

$$\begin{aligned} \boldsymbol{\alpha}_N(f) &= [\alpha_{0,N}(f), \alpha_{1,N}(f), \ldots, \alpha_{N,N}(f)]^\top \ ,\\ \mathbf{f}_N &= [f(t_{0,N})/2, f(t_{1,N}), \ldots, f(t_{N-1,N}), f(t_{N,N})/2]^\top \ . \end{aligned}$$

Then, we may write (12) in compact form as $\boldsymbol{\alpha}_N(f) = C_N \mathbf{f}_N$*. This is a discrete cosine transform (of "type I"), see for instance [6, §4.7.25], and it can be computed by FFT in* $\mathcal{O}(N\log N)$ *time. Moreover, since* C_N *is symmetric, we may write*

$$I_{k,N}(f) = \boldsymbol{\omega}_N^\top \boldsymbol{\alpha}_N(f) = \boldsymbol{\omega}_N^\top C_N \mathbf{f}_N = (C_N^\top \boldsymbol{\omega}_N)^\top \mathbf{f}_N = (C_N\boldsymbol{\omega}_N)^\top \mathbf{f}_N$$

where $\boldsymbol{\omega}_N = [\omega_0(k)/2, \omega_1(k), \ldots, \omega_{N-1}(k), \omega_N(k)/2]^T$*. Thus if we precompute* $C_N\boldsymbol{\omega}_N$*, we can apply the rule (3) to many different* f *without needing further calls to FFT.*

To obtain an error estimate for (3), for a function f on $[-1,1]$, we introduce its "cosine transform" which is the even 2π-periodic function

$$f_c(\theta) \;=\; f(\cos\theta)\;, \quad \theta \in \mathbb{R}\;.$$

From (11) we see that $(Q_N f)_c \in \mathrm{span}\,\{1, \cos\theta, \cos 2\theta, \ldots, \cos N\theta\}$ is the even trigonometric polynomial of degree N which interpolates f_c at the $N+1$ equally spaced points $j\pi/N$, $j = 0, \ldots, N$. There is a beautiful error analysis for such interpolants (see [27, (8.11)]). In particular, for $0 \le \mu \le \nu$ and $\nu \ge \nu_0 > 1/2$, there is a constant $C_{\nu_0,\mu}$ such that

$$\|f_c - (Q_N f)_c\|_{H^\mu} \;\le\; C_{\nu_0,\mu} N^{\mu-\nu} \|f_c\|_{H^\nu}\;, \quad \text{for all} \quad N \ge 2 \tag{15}$$

where

$$\|\varphi\|^2_{H^\nu} := |\widehat{\varphi}(0)|^2 + \sum_{m\neq 0} |m|^{2\nu} |\widehat{\varphi}(m)|^2, \qquad \widehat{\varphi}(m) := \frac{1}{2\pi}\int_{-\pi}^{\pi} \varphi(\theta)\exp(-\mathrm{i}m\theta)\;\mathrm{d}\theta. \tag{16}$$

(Trivially $\|\cdot\|_{H^0}$ is equivalent to the $L^2(-\pi,\pi)$ norm). The periodic Sobolev space of order r is denoted by H^r and can be defined simply as the completion of the trigonometric polynomials in the norm $\|\cdot\|_{H^r}$. This leads us to our first result.

Theorem 2.2 *For $r = 0, 1, 2$ and for all $\nu \ge \nu_0 > \max\{1/2, \rho(r)\}$ there exists $C_{\nu_0} > 0$ such that for all $k > 0$*

$$|I_k(f) - I_{k,N}(f)| \;\le\; C_{\nu_0}\left(\frac{1}{k^r}\right)\left(\frac{1}{N}\right)^{\nu-\rho(r)} \|f_c\|_{H^\nu} \tag{17}$$

where

$$\rho(r) = \begin{cases} 0, & r = 0, \\ 1, & r = 1, \\ 7/2, & r = 2. \end{cases}$$

Besides, (17) *holds also for $\nu = r = 1$.*

Proof. Given f, introduce the even $2\pi-$periodic error function $e_N := f_c - (Q_N f)_c$. Because the Chebyshev points include the end points ± 1, we have

$$e_N(0) \;=\; e_N(\pi) \;=\; 0\;. \tag{18}$$

Now using the cosine transform, integrating by parts and using (18), we have

$$\begin{aligned} I_k(f) - I_{k,N}(f) \;&=\; \int_{-1}^{1} (f - Q_N f)(s)\;\exp(\mathrm{i}ks)\;\mathrm{d}s \\ &=\; \int_0^\pi e_N(\theta)\;\exp(\mathrm{i}k\cos\theta)\sin\theta\;\mathrm{d}\theta \qquad (19) \\ &=\; \frac{1}{\mathrm{i}k}\int_0^\pi e_N'(\theta)\;\exp(\mathrm{i}k\cos\theta)\;\mathrm{d}\theta\;. \qquad (20) \end{aligned}$$

The estimate (17) for $r = 0$ and $r = 1$ and $\nu \ge \nu_0 > \max\{1/2, \rho(r)\}$ now follows from (15) and (19) and (20) respectively. The estimate when $\nu = r = 1$ also follows similarly.

For $r = 2$ a bit more work is required. First observe that $e_N'(\theta) = -(f - Q_N f)'(\cos\theta)\,\sin\theta$, so $e_N'(\theta)$ also vanishes at 0 and π. Hence we can introduce the function

$$\varphi_N(\theta) \;=\; \frac{e_N'(\theta)}{\sin\theta} = -(f - Q_N f)'(\cos\theta)$$

into (20) and then perform another integration by parts to obtain

$$
\begin{aligned}
I_k(f) - I_{k,N}(f) &= \frac{1}{k^2}\left[\varphi_N(\theta)\exp(\mathrm{i}k\cos\theta)\Big|_0^\pi - \int_0^\pi \varphi_N'(\theta)\exp(\mathrm{i}k\cos\theta)\ \mathrm{d}\theta\right] \\
&=: \frac{1}{k^2}\left[E_1 - E_2\right]. \qquad (21)
\end{aligned}
$$

L'Hopital's rule shows that $\varphi_N(0) = e_N''(0)$ and $\varphi_N(\pi) = -e_N''(\pi)$ and so, using the Sobolev embedding theorem and (15) again,

$$
|E_1| \ \le\ |e_N''(0)| + |e_N''(\pi)| \le\ C\|e_N\|_{H^3}\ \le\ C_{\nu_0}\frac{1}{N^{\nu-3}}\|f_c\|_{H^\nu}\ , \qquad (22)
$$

for all $\nu \ge \nu_0 \ge 3$. To estimate E_2, we write e_N as a cosine series

$$
e_N(\theta) \ =\ \sum_{m=1}^{\infty}\widehat{e}_N(m)\cos m\theta\ ,
$$

where

$$
\widehat{e}_N(m) \ =\ \begin{cases} \dfrac{1}{\pi}\displaystyle\int_0^\pi e_N(\theta)\ \mathrm{d}\theta, & m = 0\ , \\[2ex] \dfrac{2}{\pi}\displaystyle\int_0^\pi e_N(\theta)\cos m\theta\ \mathrm{d}\theta, & m \ge 1\ . \end{cases}
$$

Hence

$$
\varphi_N(\theta) \ =\ -\sum_{m=1}^{\infty}\ m\,\widehat{e}_N(m)\,\frac{\sin m\theta}{\sin\theta}\ . \qquad (23)
$$

Then with σ denoting the bounded $\mathcal{C}^\infty$ function $\sigma(\theta) := (\sin\theta)/\theta$ we have $\sigma(\theta) \ge 2/\pi$ for $\theta \in [-\pi/2, \pi/2]$ and so for $\theta \in [0, \pi/2]$ and $m \ge 1$,

$$
\left|\left(\frac{\sin m\theta}{\sin\theta}\right)'\right| \ =\ \left|m\left(\frac{\sigma(m\theta)}{\sigma(\theta)}\right)'\right| \ =\ \left|\ m^2\frac{\sigma'(m\theta)}{\sigma(\theta)} - m\frac{\sigma(m\theta)\sigma'(\theta)}{\sigma^2(\theta)}\right| \ \le\ Cm^2 \qquad (24)
$$

for some constant C. Moreover, writing

$$
\frac{\sin m\theta}{\sin\theta} \ =\ (-1)^{m-1}\frac{\sin m(\theta-\pi)}{\sin(\theta-\pi)}
$$

allows us to extend (24) to $\theta \in [0, \pi]$. Therefore

$$
|E_2| \ \le\ \pi\|\varphi_N'\|_{L^\infty(0,\pi)}\ \le C\sum_{m=1}^{\infty} m^3|\widehat{e}_N(m)|\ . \qquad (25)
$$

To complete the estimate on E_2, we recall the elementary estimates

$$
\sum_{m=1}^{N} m^6 < \frac{(N+1)^7}{7} \qquad \text{and} \qquad \sum_{m=N+1}^{\infty}\frac{1}{m^{1+\alpha}} < \frac{1}{\alpha\,N^\alpha}\ , \quad (\alpha > 0)\,.
$$

Then, splitting the sum (25) for $m \le N$ and $m \ge N+1$, using the Cauchy-Schwarz inequality, (15) and (16), we deduce for all $\nu \ge \nu_0 > 7/2$

$$
\begin{aligned}
|E_2| \ &\le\ C\left\{\left[\sum_{m=1}^{N} m^6\right]^{1/2}\left[\sum_{m=1}^{N}|\widehat{e}_N(m)|^2\right]^{1/2} + \left[\sum_{m=N+1}^{\infty}\frac{1}{m^{2\nu-6}}\right]^{1/2}\left[\sum_{m=N+1}^{\infty} m^{2\nu}|\widehat{e}_N(m)|^2\right]^{1/2}\right\} \\
&\le\ C\left\{\left(\frac{1}{N}\right)^{-7/2}\|e_N\|_{H^0}\ +\ \left(\frac{1}{N}\right)^{\nu-7/2}\|e_N\|_{H^\nu}\right\} \\
&\le\ C_{\nu_0}\left(\frac{1}{N}\right)^{\nu-7/2}\|f_c\|_{H^\nu}\ .
\end{aligned}
$$

with C denoting a generic constant. Combining the estimates for E_1 and E_2 yields the result. $\square$

Minor adjustments can be introduced in the proof above to prove exponential convergence for analytic functions f. In this case f_c is also analytic which ensures that the trigonometric interpolation converges exponentially cf. [27, §10.1]. As a byproduct, so does the quadrature rule (see also [32]). We refer also to [20] where a general theory of Filon quadrature rules for analytic functions is presented covering as a particular case the Clenshaw-Curtis rule studied in this paper. On the other hand, [31] contains a study of the convergence of the quadrature rule for less smooth functions f. Neither [31] or [32] contains the results given here.

The estimate of Theorem 2.2 is not optimal when k is small. However it can easily be extended as in the following corollary.

Corollary 2.3 *Under the conditions of Theorem 2.2, for* $r = 0, 1, 2$ *and for all* $\nu \geq \nu_0 > \max\{1/2, \rho(r)\}$ *there exists* $C_{\nu_0} > 0$

$$|I_k(f) - I_{k,N}(f)| \;\leq\; C_{\nu_0}\; \min\left\{1, \left(\frac{1}{k^r}\right)\right\} \left(\frac{1}{N}\right)^{\nu-\rho(r)} \|f_c\|_{H^\nu}. \tag{26}$$

Proof. The result is clear from Theorem 2.2 when $k \geq 1$. When $k < 1$, it follows from (19) that

$$|I_k(f) - I_{k,N}(f)| \;\leq\; \sqrt{\pi}\|e_N\|_{L^2(0,\pi)}\ ,$$

which yields the result. $\square$

What it is clear at this point is that an efficient implementation of the rule (13) requires a fast and accurate computation of the weights $\omega_n(k)$ given in (14). This is studied in the next section.

3 Accurate computation of the weights

To briefly review the classical the recurrence relation for $\omega_n(k)$, recall the identity $2T_n = U_n - U_{n-2}$, for all $n \geq 2$ [1, eq. (22.5.8)], where

$$U_n = \frac{1}{n+1} T'_{n+1}$$

is the nth Chebyshev polynomial of the second kind. Thus

$$2\omega_n(k) = \rho_{n+1}(k) - \rho_{n-1}(k). \qquad n \geq 2\ , \tag{27}$$

where

$$\rho_n(k) := \int_{-1}^{1} U_{n-1}(s)\exp(\mathrm{i}ks)\ \mathrm{d}s = \frac{1}{n}\int_{-1}^{1} T'_n(s)\exp(\mathrm{i}ks)\ \mathrm{d}s, \quad n \geq 1. \tag{28}$$

On the other hand, integrating the formula (14) for $\omega_n(k)$ by parts, we obtain,

$$\omega_0(k) = \gamma_0(k) \quad \text{and} \quad \omega_n(k) := \gamma_n(k) - \frac{n}{\mathrm{i}k}\rho_n(k)\ , \quad n \geq 1\ , \tag{29}$$

where (see [1, eq. (22.4.4)])

$$\begin{aligned}\gamma_n(k) \quad &:= \quad \frac{1}{\mathrm{i}k} T_n(s)\exp(\mathrm{i}ks)\Big|_{s=-1}^{s=1} = \frac{1}{\mathrm{i}k}\Big[\exp(\mathrm{i}k) - (-1)^n\exp(-\mathrm{i}k)\Big] \\ &= \begin{cases} \dfrac{2\sin k}{k}, & \text{for even } n, \\[2ex] \dfrac{2\cos k}{\mathrm{i}k}, & \text{for odd } n. \end{cases}\end{aligned}$$

Combining (27) and (29) we obtain the recurrence relation

$$2\gamma_n(k) - \frac{2n}{\mathrm{i}k}\rho_n(k) \;=\; \rho_{n+1}(k) - \rho_{n-1}(k)\;, \quad n \geq 2\;. \tag{30}$$

Moreover, since $U_0(s) = 1$, and $U_1(s) = 2s$, we have

$$\rho_1(k) \;:=\; \gamma_0(k), \tag{31}$$

$$\rho_2(k) \;:=\; 2\gamma_1(k) - \frac{2}{\mathrm{i}k}\gamma_0(k). \tag{32}$$

The algorithm to evaluate $\{\omega_n(k)\}$ for $n \leq k$ uses (30) – (32) as a forward recurrence for $\rho_n(k)$. Then we obtain $\{\omega_n(k)\}$ via (29).

Algorithm: for $n \leq \min\{N, k\}$ (first phase)

- Compute

$$\rho_1(k) \;:=\; \gamma_0(k), \tag{33a}$$

$$\rho_2(k) \;:=\; 2\gamma_1(k) - \frac{2}{\mathrm{i}k}\gamma_0(k), \tag{33b}$$

$$\rho_{n+1}(k) \;:=\; 2\gamma_n(k) - \frac{2n}{\mathrm{i}k}\rho_n(k) + \rho_{n-1}(k), \qquad n = 2, \ldots, \min\{N, k\} - 1\;. \tag{33c}$$

- Set

$$\omega_0(k) = \rho_1(k), \qquad \omega_n(k) := \gamma_n(k) - \frac{n}{\mathrm{i}k}\rho_n(k), \qquad n = 1, 2, ..., \min\{N, k\} \tag{34}$$

$\square$

The restriction $n \leq k$ stated in the algorithm has to be imposed because the forward recurrence becomes unstable when $n \geq k$. We give in Theorem 5.1 and Corollary 5.2 the proof of the stability for $n \leq N \leq k$. If $N > k$, an additional phase of the algorithm must be added.

In this case we introduce the integers $n_0 = \lceil k \rceil$ and $M \geq n_0$, the tridiagonal matrix and the right-hand side vector

$$A_M(k) := \begin{bmatrix} \frac{2n_0}{\mathrm{i}k} & 1 & & & \\ -1 & \frac{2(n_0+1)}{\mathrm{i}k} & 1 & & \\ & -1 & \frac{2(n_0+2)}{\mathrm{i}k} & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & -1 & \frac{2(2M-1)}{\mathrm{i}k} \end{bmatrix}, \quad \mathbf{b}_M(k) := \begin{bmatrix} 2\gamma_{n_0}(k) + \rho_{n_0-1}(k) \\ 2\gamma_{n_0+1}(k) \\ 2\gamma_{n_0+2}(k) \\ \vdots \\ 2\gamma_{2M-1}(k) - \rho_{2M}(k) \end{bmatrix}. \tag{35}$$

Clearly,

$$\boldsymbol{\rho}_M(k) := \begin{bmatrix} \rho_{n_0}(k) & \rho_{n_0+1}(k) & \rho_{n_0+2}(k) & \cdots & \rho_{2M-1}(k) \end{bmatrix}^\top$$

is a solution of

$$A_M(k)\mathbf{x} \;=\; \mathbf{b}_M(k)$$

and therefore the required coefficients can be computed by solving a tridiagonal system once the right-hand side $\mathbf{b}_M$ is known. (This is known as Oliver's algorithm [21].) The coefficients $\gamma_n(k)$ are defined above, and $\rho_{n_0-1}(k)$ can be obtained by the first phase algorithm. The value of $\rho_{2M}(k)$ is a priori unknown, but if we take $2M$ sufficiently large we can approximate it accurately using an asymptotic expansion as shown in the next result. The proof is left for the next section.

Theorem 3.1 *Let M be an integer with $M \geq k$, and define*

$$p_0(\theta) := \frac{1}{(2M - k\sin\theta)}, \qquad p_r(\theta) := p_0(\theta)\frac{\mathrm{d}}{\mathrm{d}\theta}p_{r-1}(\theta), \quad r = 1, 2, \ldots.$$

Then,

$$\rho_{2M}(k) = 2\mathrm{i}\left[\sum_{r=0}^{J}(-1)^r p_{2r}(0)\sin k + \sum_{r=0}^{J}(-1)^r p_{2r+1}(0)\cos k\right] + R_J(M,k) \tag{36}$$

where

$$|R_J(M,k)| \leq C_J k M^{-2J-4}$$

and C_J is independent of M and k.

Algorithm: for $k < n \leq N$ (second phase) Set $n_0 = \lceil k \rceil$.

- Take $M \geq \max\{n_0/2, N/2\}$ sufficiently large and compute $\rho_{2M}(k)$ using (36).
- Construct $A_M(k)$, $\mathbf{b}_M(k)$ as in (35) and solve

$$A_M(k)\boldsymbol{\rho}_M(k) = \mathbf{b}_M(k)$$

  with

$$\boldsymbol{\rho}_M(k) := \begin{bmatrix}\rho_{n_0}(k) & \rho_{n_0+1}(k) & \rho_{n_0+2}(k) & \cdots & \rho_{2M-1}(k)\end{bmatrix}^\top$$

- Set

$$\omega_n(k) := \gamma_n(k) - \frac{n}{\mathrm{i}k}\rho_n(k), \qquad n = n_0, \ldots, N.$$

Remark 3.2 *Note that U_{n-1} is even (respectively odd) when n is odd (respectively even) and so by definition of $\rho_n(k)$ in (28), $\rho_n(k)$ is real for odd n and purely imaginary for even n. Hence, defining*

$$\breve{\rho}_n = \mathrm{Re}\rho_n + \mathrm{Im}\rho_n$$

we can rewrite (30) in real arithmetic,

$$2\breve{\gamma}_n(k) - \frac{2n(-1)^n}{k}\breve{\rho}_n(k) = \breve{\rho}_{n+1}(k) - \breve{\rho}_{n-1}(k). \qquad n \geq 2$$

($\breve{\gamma}_n(k)$ is defined accordingly). The same can be said for the asymptotic expansion stated in Theorem 3.1. Hence, the algorithms can be set up and implemented in real arithmetic such as it has been done in [8]. We prefer however to write the algorithm in complex arithmetic to simplify both the exposition of the method and its analysis.

The first seven coefficients in the asymptotic expansion (36) are given by

$$\begin{aligned}
p_0(0) &= \frac{1}{2M},\\
p_1(0) &= \frac{k}{(2M)^3},\\
p_2(0) &= \frac{3k^2}{(2M)^5},\\
p_3(0) &= \frac{(15k^2 - 4M^2)k}{(2M)^7},\\
p_4(0) &= \frac{(105k^2 - 60M^2)k^2}{(2M)^9},\\
p_5(0) &= \frac{(945k^4 - 840k^2M^2 + 16M^4)k}{(2M)^{11}},\\
p_6(0) &= \frac{(-12600k^2M^2 + 1008M^4 + 10395k^4)k^2}{(2M)^{13}}.
\end{aligned} \tag{37}$$

We point out that a similar asymptotic expansion can be proved for $\rho_{2M+1}(k)$.

Finally, for $N > k$, one question which may naturally arise is why not just apply the second phase of the algorithm for computing all the weights $\rho_n(k)$, instead of combining both parts, as has been proposed in this paper. One of the reasons is that the first phase of the algorithm is faster than the second because the second involves solving a tridiagonal system. Of course this is not a very significant difference in practice. The other reason is that in the proof of the stability of the second phase of the algorithm it is essential for the matrix $A_M(k)$ to be diagonally dominant (see Proposition 5.3). This property holds only if the second phase of the algorithm is restricted to computing the coefficients $\rho_n(k)$ for $n \geq k$.

4 An asymptotic expansion

The aim of this section is to prove Theorem 3.1. First, note that, after applying the change of variables $s = \cos\theta$ in (28)

$$\rho_{2M}(k) = \int_{-1}^{1} U_{2M-1}(s)\exp(\mathrm{i}ks)\ \mathrm{d}s = \int_0^{\pi} \exp(\mathrm{i}k\cos\theta)\sin(2M\theta)\ \mathrm{d}\theta,$$

where we have used the fact that

$$U_n(\cos\theta) = \frac{\sin(n+1)\theta}{\sin\theta}.$$

Clearly

$$\begin{aligned} \rho_{2M}(k) &= -\frac{\mathrm{i}}{2}\Big[\int_0^{\pi} \exp(\mathrm{i}k\cos\theta)(\exp(2\mathrm{i}M\theta) - \exp(-2\mathrm{i}M\theta))\ \mathrm{d}\theta\Big] \\ &=: -\frac{\mathrm{i}}{2}\Big[I_k^{+}(M) - I_k^{-}(M)\Big] \end{aligned} \tag{38}$$

where

$$I_k^{\pm}(M) := \int_0^{\pi} \exp(\mathrm{i}S_{\pm}(\theta))\ \mathrm{d}\theta, \qquad S_{\pm}(\theta) := (\pm 2M\theta + k\cos\theta).$$

(We hide the dependence of $S_\pm$ on M and k to simplify forthcoming expressions).

The two following families of smooth functions will be relevant in the sequel

$$p_0^{\pm}(\theta) := \frac{1}{\mathrm{i}S_{\pm}'(\theta)} = \frac{1}{\mathrm{i}(\pm 2M - k\sin\theta)}, \tag{39a}$$

$$p_r^{\pm}(\theta) := \frac{1}{\mathrm{i}S_{\pm}'(\theta)}\frac{\mathrm{d}p_{r-1}^{\pm}(\theta)}{\mathrm{d}\theta}, \quad r = 1, 2\ldots. \tag{39b}$$

Note that $p_r^{\pm}(\theta)$ is real for odd r and purely imaginary for even r.

Lemma 4.1 *For all $r \geq 0$,*

$$p_r^{\pm}(\theta) = \frac{q_r^{\pm}(\theta)}{\mathrm{i}^{r+1}(S_{\pm}'(\theta))^{2r+1}} \tag{40}$$

where $q_r^{\pm}(\theta)$ is a trigonometric polynomial in θ defined recursively by

$$q_0^{\pm} \equiv 1, \qquad q_{r+1}^{\pm} = (q_r^{\pm})'\, S_{\pm}' - (2r+1)\, q_r^{\pm}\, S_{\pm}'', \quad r = 0, 1, 2, \ldots \tag{41}$$

Besides

$$p_r^{\pm}(0) = (-1)^r p_r^{\pm}(\pi), \tag{42a}$$

$$p_r^{+}(0) = -p_r^{-}(0), \qquad p_r^{+}(\pi) = -p_r^{-}(\pi). \tag{42b}$$

Proof. Equation (40) is clearly true for $r = 0$. Assume that it has been proved up to r. Then,

$$\begin{aligned}
p^{\pm}_{r+1}(\theta) &= \frac{1}{\mathrm{i}S'_{\pm}(\theta)}\frac{\mathrm{d}}{\mathrm{d}\theta}\Big[\frac{q^{\pm}_r(\theta)}{\mathrm{i}^{r+1}(S'_{\pm}(\theta))^{2r+1}}\Big] \\
&= \frac{1}{\mathrm{i}^{r+2}S'_{\pm}(\theta)}\Big[\frac{(q^{\pm}_r)'(\theta)}{(S'_{\pm}(\theta))^{2r+1}} - \frac{(2r+1)q^{\pm}_r(\theta)S''_{\pm}(\theta)}{(S'_{\pm}(\theta))^{2r+2}}\Big] \\
&= \frac{1}{\mathrm{i}^{r+2}(S'_{\pm}(\theta))^{2r+3}}\Big[(q^{\pm}_r)'(\theta)S'_{\pm}(\theta) - (2r+1)q^{\pm}_r(\theta)S''_{\pm}(\theta)\Big]
\end{aligned}$$

and the first assertion of the Lemma is proved.

To obtain relations (42) note that

$$S^{(r)}_{\pm}(\theta) = (-1)^{r+1}S^{(r)}_{\pm}(\pi-\theta) = (-1)^r S^{(r)}_{\mp}(-\theta), \qquad r = 1, 2. \tag{43}$$

Then, (42) follows easily provided we prove that

$$q^{\pm}_r(\theta) = (-1)^r q^{\pm}_r(\pi-\theta), \tag{44a}$$

$$q^{+}_r(\theta) = q^{-}_r(-\theta). \tag{44b}$$

To prove (44a) we proceed by induction on (41). For $r = 0$, (44a) is clear since $q^{\pm}_0 \equiv 1$. If (44a) holds for some r, then by (41) and (43),

$$\begin{aligned}
q^{\pm}_{r+1}(\theta) &= (q^{\pm}_r)'(\theta)S'_{\pm}(\theta) - (2r+1)q^{\pm}_r(\theta)S''_{\pm}(\theta) \\
&= (-1)^{r+1}\left[(q^{\pm}_r)'(\pi-\theta)\right](-1)^2S'_{\pm}(\pi-\theta) - (2r+1)(-1)^r\left[q^{\pm}_r(\pi-\theta)\right](-1)^3S''_{\pm}(\pi-\theta) \\
&= (-1)^{r+3}\Big((q^{\pm}_r)'(\pi-\theta)S'_{\pm}(\pi-\theta) - (2r+1)q^{\pm}_r(\pi-\theta)S''_{\pm}(\pi-\theta)\Big) \\
&= (-1)^{r+1}q^{\pm}_{r+1}(\pi-\theta).
\end{aligned}$$

Similarly, (44b) holds for $r = 0$. Assuming that (44b) holds for r, we observe

$$\begin{aligned}
q^{+}_{r+1}(\theta) &= (q^{+}_r)'(\theta)S'_{+}(\theta) - (2r+1)q^{+}_r(\theta)S''_{+}(\theta) \\
&= \left[-(q^{-}_r)'(-\theta)\right]\left(-S'_{-}(-\theta)\right) - (2r+1)\left[q^{-}_r(-\theta)\right](-1)^2S''_{-}(-\theta) \\
&= (q^{-}_r)'(-\theta)S'_{-}(-\theta) - (2r+1)q^{-}_r(-\theta)S''_{-}(-\theta) \\
&= q^{-}_{r+1}(-\theta)
\end{aligned}$$

and the proof is finished. $\square$

Corollary 4.2 *For all $M \geq k$ and $r \geq 1$ there exists $C_r > 0$ independent of M and k such that*

$$|p^{\pm}_r(\theta)| + |(p^{\pm}_r)'(\theta)| \;\leq\; C_r k M^{-r-2}, \qquad \forall\theta \in [0,\pi].$$

Proof. Note that since $q^{\pm}_1(\theta) = k\cos\theta$, one can check easily from (41) that k is a common factor in $q^{\pm}_r$ for all $r \geq 1$. Moreover, for fixed θ, $q^{\pm}_r(\theta)$ is a polynomial in M and k of (total) degree r and its coefficients are continuous in θ (this can be easily verified from its definition in (41)). Hence there exist constants C'_r such that

$$|q^{\pm}_r(\theta)| \;\leq\; C'_r\, k\sum k^{p-1}M^q \;=\; C'_r\, kM^{r-1}\sum\left(\frac{k}{M}\right)^{p-1}M^{q+p-r}$$

where the sum is over all $p \geq 1, q \geq 0$ such that $p + q \leq r$. Hence, since $M > k$,

$$|q^{\pm}_r(\theta)| \;\leq\; C'_r kM^{r-1}\,, \quad \text{for all} \;\; \theta \in [0,\pi]\,.$$

On the other hand,

$$|S'_\pm(\theta)| \geq 2M - k \geq M.$$

Collecting both bounds, we conclude

$$|p_r^\pm(\theta)| = \left|\frac{q_r^\pm(\theta)}{(S'_\pm(\theta))^{2r+1}}\right| \leq \frac{C'_r k M^{r-1}}{M^{2r+1}} = C'_r k M^{-r-2}\ , \quad \theta \in [0,\pi].$$

The estimate for $|(p_r^\pm)'(\theta)|$ is consequence of (39b), since

$$\left|(p_r^\pm)'(\theta)\right| = \left|\mathrm{i}S'_\pm(\theta)p_{r+1}^\pm(\theta)\right| \leq C'_{r+1}(2M+k)kM^{-r-3} \leq 3C'_{r+1}kM^{-r-2}\ , \quad \theta \in [0,\pi].$$

□

Theorem 4.3 *For all $M \geq k$ we have*

$$\rho_{2M}(k) = -2\left[\sum_{r=0}^{J} p_{2r}^+(0)\sin k + \mathrm{i}\sum_{r=0}^{J} p_{2r+1}^+(0)\cos k\right] + R_J(M,k)$$

with

$$|R_J(M,k)|\ \leq\ C_J k M^{-2J-4}$$

and C_J is independent of M and k.

Proof. Integrating $I_k^\pm(M)$ twice by parts,

$$\begin{aligned}
I_k^\pm(M) &= \int_0^\pi \frac{1}{\mathrm{i}S'_\pm(\theta)}\Big[\mathrm{i}S'_\pm(\theta)\exp(\mathrm{i}S_\pm(\theta))\Big]\ \mathrm{d}\theta = \int_0^\pi p_0^\pm(\theta)\Big[\mathrm{i}S'_\pm(\theta)\exp(\mathrm{i}S_\pm(\theta))\Big]\ \mathrm{d}\theta \\
&= p_0^\pm(\theta)\exp(\mathrm{i}S_\pm(\theta))\Big|_0^\pi - \int_0^\pi \frac{\mathrm{d}p_0^\pm(\theta)}{\mathrm{d}\theta}\exp(\mathrm{i}S_\pm(\theta))\ \mathrm{d}\theta \\
&= p_0^\pm(\theta)\exp(\mathrm{i}S_\pm(\theta))\Big|_0^\pi - \int_0^\pi p_1^\pm(\theta)\Big[\mathrm{i}S'_\pm(\theta)\exp(\mathrm{i}S_\pm(\theta))\Big]\ \mathrm{d}\theta \\
&= \sum_{r=0}^{1}(-1)^r p_r^\pm(\theta)\exp(\mathrm{i}S_\pm(\theta))\Big|_0^\pi + \int_0^\pi \frac{\mathrm{d}p_1^\pm(\theta)}{\mathrm{d}\theta}\exp(\mathrm{i}S_\pm(\theta))\ \mathrm{d}\theta.
\end{aligned}$$

Repeating the same argument and using that $S_\pm(0) = k$, $S_\pm(\pi) = \pm 2M\pi - k$, we finally obtain

$$\begin{aligned}
I_k^\pm(M) &= \sum_{r=0}^{2J+2}(-1)^r p_r^\pm(\theta)\exp(\mathrm{i}S_\pm(\theta))\Big|_0^\pi - \int_0^\pi \frac{\mathrm{d}p_{2J+2}^\pm(\theta)}{\mathrm{d}\theta}\exp(\mathrm{i}S_\pm(\theta))\ \mathrm{d}\theta \\
&= -\sum_{r=0}^{2J+2}(-1)^r p_r^\pm(0)\Big[\exp(\mathrm{i}k) + (-1)^{r+1}\exp(-\mathrm{i}k)\Big] \\
&\quad -\int_0^\pi \frac{\mathrm{d}p_{2J+2}^\pm(\theta)}{\mathrm{d}\theta}\exp(\mathrm{i}S_\pm(\theta))\ \mathrm{d}\theta,
\end{aligned}$$

where we have applied now (42a). Thus, from (38),

$$\begin{aligned}
\rho_{2M}(k) &= -\frac{\mathrm{i}}{2}\Big[I_k^+(M) - I_k^-(M)\Big] \\
&= \frac{\mathrm{i}}{2}\sum_{r=0}^{2J+2}(-1)^r(p_r^+(0) - p_r^-(0))\Big[\exp(\mathrm{i}k) + (-1)^{r+1}\exp(-\mathrm{i}k)\Big] \\
&\quad +\frac{\mathrm{i}}{2}\int_0^\pi \left[\frac{\mathrm{d}p_{2J+2}^+(\theta)}{\mathrm{d}\theta}\exp(\mathrm{i}S_+(\theta)) - \frac{\mathrm{d}p_{2J+2}^-(\theta)}{\mathrm{d}\theta}\exp(\mathrm{i}S_-(\theta))\right]\ \mathrm{d}\theta \\
&= -2\left[\sum_{r=0}^{J} p_{2r}^+(0)\sin k + \mathrm{i}\sum_{r=0}^{J} p_{2r+1}^+(0)\cos k\right] + R_J(M,k),
\end{aligned}$$

where we are applied (42b) in the last step. If we now define

$$R_J(M,k) := -2p^+_{2J+2}(0)\sin k + \frac{\mathrm{i}}{2}\int_0^\pi \left[\frac{\mathrm{d}p^+_{2J+2}(\theta)}{\mathrm{d}\theta}\exp(\mathrm{i}S_+(\theta)) - \frac{\mathrm{d}p^-_{2J+2}(\theta)}{\mathrm{d}\theta}\exp(\mathrm{i}S_-(\theta))\right]\mathrm{d}\theta\ ,$$

and finally use Corollary 4.2 we obtain

$$|R_J(M,k)| \le C_J k M^{-2J-4}$$

with a suitable constant C independent of M and k. The result is now proven. □

Proof of Theorem 3.1. It is now a simple consequence of Theorem 4.3, since by (39)

$$p^+_0 = \frac{1}{\mathrm{i}}p_0, \qquad p^+_r(\theta) = p^+_0(\theta)\frac{\mathrm{d}p^+_{r-1}(\theta)}{\mathrm{d}\theta} = \frac{1}{\mathrm{i}^{r+1}}p_0(\theta)\frac{\mathrm{d}p_{r-1}(\theta)}{\mathrm{d}\theta} = \frac{1}{\mathrm{i}^{r+1}}p_r(\theta),$$

that is

$$p_r = \mathrm{i}^{r+1}p^+_r.$$

□

5 Proofs of the stability of the algorithm

First result of this section deals with the stability of the forward reccurrence used in the first phase of the Algorithm.

Theorem 5.1 *Let $(\varepsilon_m)_m \subset \mathbb{C}$ with $|\varepsilon_m| \le \varepsilon$ and define*

$$\begin{aligned}
\widetilde{\rho}_1(k) &:= \rho_1(k) + \varepsilon_1,\\
\widetilde{\rho}_2(k) &:= \rho_2(k) + \varepsilon_2,\\
\widetilde{\rho}_{n+1}(k) &:= 2\gamma_n(k) - \frac{2n}{\mathrm{i}k}\widetilde{\rho}_n(k) + \widetilde{\rho}_{n-1}(k) + \varepsilon_{n+1}, \qquad n = 2,3,\ldots
\end{aligned} \tag{45}$$

Then for all $2 < n < k$

$$|\widetilde{\rho}_n(k) - \rho_n(k)| \ \le\ \left[1\ +\ \frac{4}{3}\frac{nk^{1/2}}{(k^2-n^2)^{1/4}}\right]\varepsilon.$$

Proof. Setting $\delta_n := \widetilde{\rho}_n(k) - \rho_n(k)$, we see that

$$\begin{aligned}
\delta_1 &= \varepsilon_1, \qquad \delta_2 = \varepsilon_2\ ,\\
\delta_n &= -\frac{2(n-1)}{\mathrm{i}k}\delta_{n-1} + \delta_{n-2} + \varepsilon_n, \qquad n = 3,4,\ldots,
\end{aligned}$$

or in matrix notation

$$\begin{bmatrix}\delta_n\\ \delta_{n-1}\end{bmatrix} = \begin{bmatrix}-\frac{2(n-1)}{\mathrm{i}k} & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\delta_{n-1}\\ \delta_{n-2}\end{bmatrix} + \begin{bmatrix}\varepsilon_n\\ 0\end{bmatrix}\ , \quad n \ge 3\ . \tag{46}$$

Introducing the notation

$$\boldsymbol{\delta}_n := \begin{bmatrix}\delta_n\\ \delta_{n-1}\end{bmatrix}, \qquad \boldsymbol{\varepsilon}_2 := \begin{bmatrix}\varepsilon_2\\ \varepsilon_1\end{bmatrix}, \qquad \boldsymbol{\varepsilon}_n := \begin{bmatrix}\varepsilon_n\\ 0\end{bmatrix}, \quad \text{for } n = 3,4,\ldots$$

and the matrix

$$D_n := \begin{bmatrix}-\dfrac{2(n-1)}{\mathrm{i}k} & 1\\ 1 & 0\end{bmatrix}\ ,$$

we see that $\boldsymbol{\delta}_n$ satisfies

$$\boldsymbol{\delta}_n = D_n \boldsymbol{\delta}_{n-1} + \boldsymbol{\varepsilon}_n \ , \quad \text{for} \quad n \geq 3 \ .$$

It is then easily proved by induction that

$$\boldsymbol{\delta}_n = \sum_{j=2}^{n-1} \left[\prod_{i=j}^{n-1} D_{i+1} \right] \boldsymbol{\varepsilon}_j + \boldsymbol{\varepsilon}_n \ , \quad \text{for} \quad n \geq 2 \ ,$$

where the sum on the right-hand side vanishes for $n = 2$ and

$$\prod_{i=j}^{n-1} D_{i+1} := D_n D_{n-1} \cdots D_j \ .$$

For each $j = 2, 3, \ldots$ consider the sequence $\{\boldsymbol{\delta}_n^{(j)}\}_{n=j}^{\infty}$ defined by

$$\boldsymbol{\delta}_j^{(j)} \ := \ \boldsymbol{\varepsilon}_j, \quad \text{and} \quad \boldsymbol{\delta}_n^{(j)} := \left[\prod_{i=j}^{n-1} D_{i+1} \right] \boldsymbol{\varepsilon}_j, \quad n \geq j+1 \ .$$

Then clearly,

$$\boldsymbol{\delta}_n = \sum_{j=2}^{n-1} \boldsymbol{\delta}_n^{(j)} + \boldsymbol{\varepsilon}_n. \tag{47}$$

Now we define

$$\boldsymbol{\delta}_n^{(j)} = \begin{bmatrix} \delta_n^{(j)} \\ \delta_{n-1}^{(j)} \end{bmatrix} \ .$$

Then, since $\boldsymbol{\delta}_n^{(j)} = D_n \boldsymbol{\delta}_{n-1}^{(j)}$, it follows that for each $j \geq 2$, $\{\delta_n^{(j)}\}_{n=j}^{\infty}$ satisfies the following difference equation with respect to n:

$$\delta_n^{(j)} \ = \ -\frac{2(n-1)}{\mathrm{i}k} \delta_{n-1}^{(j)} + \delta_{n-2}^{(j)}, \qquad n \geq j+1 \ , \tag{48}$$

with starting conditions

$$\left. \begin{array}{ll} \delta_1^{(2)} := \varepsilon_1, & \delta_2^{(2)} = \varepsilon_2, \\ \delta_{j-1}^{(j)} := 0, & \delta_j^{(j)} = \varepsilon_j, \quad \text{for } j = 3, 4, \ldots. \end{array} \right\} \tag{49}$$

Consider now the closely related difference equation

$$a_n - \frac{2(n-1)}{x} a_{n-1} + a_{n-2} = 0, \tag{50}$$

and let J_n, Y_n be the Bessel functions of first and second kind respectively. Then, since $\{J_n(x), Y_n(x)\}_{n \geq 1}$ is a fundamental system of solutions for (50) cf. [1, Ch 9], the functions

$$\widetilde{J}_n(k) := \mathrm{i}^n J_n(k), \qquad \widetilde{Y}_n(k) := \mathrm{i}^n Y_n(k)$$

are independent solutions for (48). Hence, for $j \geq 3$, the solution of (48) may be written

$$\delta_n^{(j)} = \alpha^{(j)} \widetilde{J}_n(k) + \beta^{(j)} \widetilde{Y}_n(k), \quad \text{for} \quad n \geq j+1 \ ,$$

where, via (49), $(\alpha^{(j)}, \beta^{(j)})$ has to satisfy

$$\begin{bmatrix} \widetilde{J}_{j-1}(k) & \widetilde{Y}_{j-1}(k) \\ \widetilde{J}_j(k) & \widetilde{Y}_j(k) \end{bmatrix} \begin{bmatrix} \alpha^{(j)} \\ \beta^{(j)} \end{bmatrix} = \begin{bmatrix} 0 \\ \varepsilon_j \end{bmatrix}.$$

Therefore for $j \geq 3$ and for all $n \geq j+1$,

$$\begin{aligned}
\delta_n^{(j)} &= \begin{bmatrix} \widetilde{J}_n(k) & \widetilde{Y}_n(k) \end{bmatrix} \begin{bmatrix} \widetilde{J}_{j-1}(k) & \widetilde{Y}_{j-1}(k) \\ \widetilde{J}_j(k) & \widetilde{Y}_j(k) \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ \varepsilon_j \end{bmatrix} \\
&= \frac{(-1)^{j+1}\pi k \mathrm{i}}{2} \begin{bmatrix} \widetilde{J}_n(k) & \widetilde{Y}_n(k) \end{bmatrix} \begin{bmatrix} \widetilde{Y}_j(k) & -\widetilde{Y}_{j-1}(k) \\ -\widetilde{J}_j(k) & \widetilde{J}_{j-1}(k) \end{bmatrix} \begin{bmatrix} 0 \\ \varepsilon_j \end{bmatrix},
\end{aligned}$$

where we have used the identity (see [1, (9.1.16)])

$$J_j(k)Y_{j-1}(k) - J_{j-1}(k)Y_j(k) = \frac{2}{\pi k}.$$

Defining $M_n(k) := \sqrt{J_n(k)^2 + Y_n(k)^2}$, using the Cauchy-Schwarz inequality and that $|\varepsilon_j| \leq \varepsilon$, we derive

$$|\delta_n^{(j)}| = \left| \frac{(-1)^{j+1}\pi k \mathrm{i}}{2} \begin{bmatrix} \widetilde{J}_n(k) & \widetilde{Y}_n(k) \end{bmatrix} \begin{bmatrix} -\widetilde{Y}_{j-1}(k) \\ \widetilde{J}_{j-1}(k) \end{bmatrix} \varepsilon_j \right| \leq \frac{\pi k}{2} M_n(k) M_{j-1}(k) \varepsilon \,, \quad \text{for} \quad j \geq 3 \,.$$

Proceeding in a similar way with $j = 2$, we derive

$$|\delta_n^{(2)}| \leq \frac{\pi k}{2} M_n(k) \Big(M_1(k) + M_2(k) \Big) \varepsilon.$$

(Note that $\boldsymbol{\delta}_2^{(2)} = (\varepsilon_2, \varepsilon_1)^\top$ in this case). Now observe that (see [33, §13.74])

$$M_n^2(x) \leq \frac{2}{\pi} \frac{1}{\sqrt{x^2 - n^2}}, \quad \text{for} \quad x > n > 1/2 \,.$$

Since we are assuming $2 < n < k$, it then follows that

$$\begin{aligned}
|\delta_n^{(j)}| &\leq \frac{k\epsilon}{(k^2 - n^2)^{1/4}} \left[\frac{1}{(k^2 - (j-1)^2)^{1/4}} \right], \qquad j = 3, 4, \dots, n \\
|\delta_n^{(2)}| &\leq \frac{k\epsilon}{(k^2 - n^2)^{1/4}} \left[\frac{1}{(k^2 - 1)^{1/4}} + \frac{1}{(k^2 - 4)^{1/4}} \right].
\end{aligned}$$

Gathering all together and using the first entry of vector identity (47), we have

$$\begin{aligned}
|\delta_n| &\leq \varepsilon + \frac{k\,\varepsilon}{(k^2 - n^2)^{1/4}} \left[\frac{1}{(k^2 - 1)^{1/4}} + \frac{1}{(k^2 - 4)^{1/4}} + \sum_{j=2}^{n-2} \frac{1}{(k^2 - j^2)^{1/4}} \right] \\
&\leq \varepsilon + \frac{k\,\varepsilon}{(k^2 - n^2)^{1/4}} \left[\frac{1}{(k^2 - 1)^{1/4}} + \frac{1}{(k^2 - (n-1)^2)^{1/4}} + \sum_{j=2}^{n-2} \frac{1}{(k^2 - j^2)^{1/4}} \right] \qquad (51) \\
&= \varepsilon + \frac{k\,\varepsilon}{(k^2 - n^2)^{1/4}} \left[\sum_{j=1}^{n-1} \frac{1}{(k^2 - j^2)^{1/4}} \right]. \qquad (52)
\end{aligned}$$

(The derivation of (51) uses the assumption that $n \geq 3$.)

Now, since $(k^2 - x^2)^{-1/4}$ is an increasing function for $x \in [0, k)$, the Riemann sum in (52) can be bounded as

$$\begin{aligned}
\sum_{j=1}^{n-1} \frac{1}{(k^2 - j^2)^{1/4}} &\leq \int_0^n \frac{\mathrm{d}x}{(k^2 - x^2)^{1/4}} < \frac{1}{k^{1/4}} \int_0^n \frac{\mathrm{d}x}{(k - x)^{1/4}} \\
&= \frac{1}{k^{1/4}} \left[-\frac{4}{3}(k - x)^{3/4} \right]_0^n = \frac{4}{3k^{1/4}} \left[k^{3/4} - (k - n)^{3/4} \right] \\
&= \frac{4k^{1/2}}{3} \left[1 - \left(\frac{k - n}{k} \right)^{3/4} \right] < \frac{4k^{1/2}}{3} \left[1 - \frac{k - n}{k} \right] \\
&= \frac{4}{3} k^{-1/2} n.
\end{aligned}$$

Using this bound in (52), we finish the proof. $\square$

Notice that for $k >> n$, we derive from this result that $|\widetilde{\rho}_n(k) - \rho_n(k)| \lesssim n\varepsilon$, i.e., the computation of these coefficients is stable. The worst case occurs when n is taken close (or equal) to k. The following result gives a bound on the error in this case.

Corollary 5.2 *Under the same asssumptions as Theorem 5.1, for all $2 < n \leq k$ we have*

$$|\widetilde{\rho}_n(k) - \rho_n(k)| \ \leq \ \left[4 + 2^{7/4}k^{5/4}\right]\varepsilon.$$

Proof. For $n \leq k-1$, Theorem 5.1 implies

$$|\delta_n| \ \leq \ \left[1 + \frac{4}{3}\frac{k^{1/2}(k-1)}{(k^2-(k-1)^2)^{1/4}}\right]\varepsilon = \left[1 \ + \ \frac{2^{7/4}}{3}\frac{k^{1/2}(k-1)}{(k-1/2)^{1/4}}\right]\varepsilon \ \leq \ \left[1 + \frac{2^{7/4}k^{5/4}}{3}\right]\varepsilon.$$

For $k - 1 < n \leq k$ we simply notice that

$$|\delta_n| \ \leq \ \varepsilon + \frac{2n}{k}|\delta_{n-1}| + |\delta_{n-2}| \ \leq \ \varepsilon + 2|\delta_{n-1}| + |\delta_{n-2}| \ ,$$

from where the result follows. $\square$

The proof of the Corollary suggests that the recurrence may become unstable when $n > k$. This has been observed by other authors and we illustrate this phenomenon numerically in the final section. Hence the second phase is introduced to avoid this instability.

Proposition 5.3 *Let $M \geq n_0 = \lceil k \rceil$ and $A_M(k)$ and $\mathbf{b}_M(k)$ be defined as in* (35)*. If*

$$A_M(k)\boldsymbol{\rho}_M(k) = \mathbf{b}_M(k), \qquad A_M(k)\widetilde{\boldsymbol{\rho}}_M(k) = \widetilde{\mathbf{b}}_M(k)$$

with

$$\|\widetilde{\mathbf{b}}_M(k) - \mathbf{b}_M(k)\|_\infty \leq \varepsilon$$

then

$$\|\boldsymbol{\rho}_M(k) - \widetilde{\boldsymbol{\rho}}_M(k)\|_\infty \leq \left(\frac{n_0+2}{2}\right)\varepsilon.$$

Proof. Note that

$$(\boldsymbol{\rho}_M(k) - \widetilde{\boldsymbol{\rho}}_M(k)) = A_M^{-1}(k)(\widetilde{\mathbf{b}}_M(k) - \mathbf{b}_M(k)).$$

Therefore

$$\|\widetilde{\boldsymbol{\rho}}_M(k) - \boldsymbol{\rho}_M(k)\|_\infty \leq \|A_M^{-1}(k)\|_\infty \|\widetilde{\mathbf{b}}_M(k) - \mathbf{b}_M(k)\|_\infty$$

and the proof reduces to bounding $\|A_M^{-1}(k)\|_\infty$. Let

$$D_M(k) := \begin{bmatrix} \frac{2n_0}{\mathrm{i}k} & & & & \\ & \frac{2(n_0+1)}{\mathrm{i}k} & & & \\ & & \frac{2(n_0+2)}{\mathrm{i}k} & & \\ & & & \ddots & \\ & & & & \frac{2(2M-1)}{\mathrm{i}k} \end{bmatrix},$$

then

$$A_M(k) := (I_M + K_M(k))D_M(k),$$

where I_M is the identity matrix of order $2M - n_0$ and

$$K_M(k) := \begin{bmatrix} 0 & \frac{\mathrm{i}k}{2(n_0+1)} & & & & \\ -\frac{\mathrm{i}k}{2n_0} & 0 & \frac{\mathrm{i}k}{2(n_0+2)} & & & \\ & -\frac{\mathrm{i}k}{2(n_0+1)} & 0 & \frac{\mathrm{i}k}{2(n_0+3)} & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \\ & & & & -\frac{\mathrm{i}k}{4(M-1)} & 0 \end{bmatrix}.$$

Note that

$$\|K_M(k)\|_\infty = \frac{(n_0+1)k}{n_0(n_0+2)} \leq \frac{n_0+1}{n_0+2} < 1.$$

Therefore,

$$\|A_M^{-1}(k)\|_\infty \leq \|D_M^{-1}(k)\|_\infty \|(I_M + K_M(k))^{-1}\|_\infty \leq \frac{k}{2n_0} \frac{1}{1 - \|K_M(k)\|_\infty} \leq \frac{n_0+2}{2},$$

and the result is proven. □

Collecting Corollary 5.2 and Proposition 5.3 we deduce that for the second phase algorithm we can expect in the worst case that $|\widetilde{\rho}_n(k) - \rho_n(k)| \lesssim k^{9/4}\varepsilon$ for all $n > k$. Since the second phase algorithm is only used for moderate values of k (the greater is k, the greater has to be N to make the second phase of the algorithm necessary), this bound implies the stability of the algorithm for practical computations.

Remark 5.4 *We finish this section by explaining why the implementation of the quadrature rule* (3) *has complexity* $\mathcal{O}(N \log N)$. *The first step in the implementation is the computation of the coefficients* $\{\omega_n(k) : n = 0, \ldots, N\}$. *Since the first phase of the Algorithm involves a three term recurrence relation this requires* $\mathcal{O}(\min\{N, k\}) = \mathcal{O}(N)$ *operations. If the second phase is required then we have to solve an additional tridiagonal system of size* $2M - \lceil k \rceil$ *where* M *is proportional to* N, *resulting in an additional* $\mathcal{O}(N)$ *operations, via the Thomas algorithm for tridiagonal systems. Finally* $I_{k,N}(f)$ *in* (3) *may then be computed by applying the discrete cosine transform which, by FFT, requires* $\mathcal{O}(N \log N)$ *operations.*

6 Numerical Experiments

In this section we present some numerical experiments to illustrate the theoretical results presented in this paper.

Experiment 1

In this experiment we study the rate of decay of the error in the Filon-Clenshaw-Curtis rule for fixed N, as $k \to \infty$, and in particular we study its dependence on the regularity of f, as characterised by the Sobolev norm appearing on the right hand side of (17). To do this, for $\beta > 0$, define

$$f_\beta(s) := \frac{(1+s)^\beta}{1+s^2}, \quad s \in [-1, 1].$$

We compute the error in (17) with $N = 24$ (a 25-point rule):

$$E_k(f_\beta) := \left| \int_{-1}^{1} f_\beta(s) \exp(\mathrm{i}ks) \, \mathrm{d}s - I_{k,24}(f_\beta) \right|.$$

To check convergence rates we give also the quantities:

$$e_k(\beta) = \log_2(E_{k/2}(f_\beta)/E_k(f_\beta)) \ .$$

In Table 1 we tabulate these results for $k = k_i = 100 \times 2^i, \quad i = 0, \ldots, 9$. It is easy to see that for non integers $\beta > 0$, $(f_\beta)_c \in H^{2\beta+1/2-\varepsilon}$ for all $\varepsilon > 0$. Thus Theorem 2.2 will guarantee convergence of $\mathcal{O}(k^{-1})$ for $E_k(f_\beta)$, provided $\beta > 1/4$ and convergence of order $\mathcal{O}(k^{-2})$ provided $\beta > 3/2$. In our experiments we have chosen $\beta \in \{1/4, 7/8, 3/2, 3\}$. In the case $\beta = 3$, f_c is actually smooth. In Table 1 we observe clear $\mathcal{O}(k^{-2})$ behaviour (but no faster) for $\beta = 3$ (the last two figures in this column are probably polluted by rounding) while for $\beta = 3/2$ the convergence is close to $\mathcal{O}(k^{-2})$ illustrating the sharpness of Theorem 2.2 in this case. For $\beta = 1/4$ the observed rate of close to $\mathcal{O}(k^{-5/4})$, is slightly better than theory predicts whereas for $\beta = 7/8$ the rate is somewhere between $\mathcal{O}(k^{-5/4})$ and $\mathcal{O}(k^{-2})$.

k_i	$E_{k_i}(f_{1/4})$	$e_{k_i}(1/4)$	$E_{k_i}(f_{7/8})$	$e_{k_i}(7/8)$	$E_{k_i}(f_{3/2})$	$e_{k_i}(3/2)$	$E_{k_i}(f_3)$	$e_{k_i}(3)$
100	6.64E−04		3.81E−06		3.41E−07		1.36E−11	
200	4.12E−04	0.69	1.93E−06	0.98	1.46E−07	1.22	2.58E−12	2.34
400	2.03E−04	1.02	8.03E−07	1.26	5.34E−08	1.45	5.80E−13	2.15
800	9.30E−05	1.13	3.04E−07	1.40	1.76E−08	1.60	1.40E−13	2.05
1600	4.12E−05	1.17	1.08E−07	1.49	5.44E−09	1.70	3.46E−14	2.01
3200	1.79E−05	1.20	3.62E−08	1.58	1.57E−09	1.79	8.64E−15	2.00
6400	7.68E−06	1.22	1.17E−08	1.63	4.36E−10	1.85	2.16E−15	2.00
12800	3.27E−06	1.23	3.66E−09	1.67	1.18E−10	1.89	5.40E−16	2.00
25600	1.38E−06	1.24	1.12E−09	1.71	3.10E−11	1.93	1.51E−16	1.84
51200	5.85E−07	1.24	3.37E−10	1.73	8.05E−12	1.94	4.29E−17	1.82

Table 1: Results for the first experiment

Experiment 2

In this experiment we study the behaviour of the Filon-Clenshaw-Curtis rule when f has a singularity in the interior of $(-1, 1)$. We see that the rule may perform rather badly in this case. We consider the function

$$f(s) \;=\; \frac{|s + 0.25|^{3/2}}{1 + s^2}$$

The exact value of the integral (1) was computed using a composite application of the Filon-Clenshaw-Curtis rule on graded meshes toward $s = -0.25$ with a large number of subintervals.

N	$k = 100$	e.c.r.	$k = 400$	e.c.r.	$k = 1600$	e.c.r.	$k = 6400$	e.c.r.
24	2.39E−05		4.33E−07		1.11E−08		5.35E−10	
48	1.39E−05	0.78	5.50E−07	−0.35	1.71E−08	−0.62	3.89E−10	0.46
96	1.13E−05	0.29	5.83E−07	−0.84	1.79E−08	−0.70	5.22E−10	−0.43
192	1.29E−06	3.14	5.50E−07	0.83	1.74E−08	0.03	5.35E−10	−0.04
384	1.58E−07	3.03	2.35E−07	1.23	1.66E−08	0.07	5.68E−10	−0.09
786	5.25E−09	4.91	2.41E−08	3.28	1.77E−08	−0.10	5.31E−10	0.01

Table 2: Error for Experiment 2 when the Filon-Clenshaw-Curtis rule is applied on all of $[-1, 1]$

N	$k = 100$	e.c.r.	$k = 400$	e.c.r.	$k = 1600$	e.c.r.	$k = 6400$	
24	2.35E−06		2.29E−07		3.04E−08		2.43E−09	
48	3.68E−07	2.68	7.21E−08	1.67	7.15E−09	2.09	9.53E−10	1.35
96	2.78E−08	3.73	1.15E−08	2.65	2.24E−09	1.67	2.23E−10	2.09
192	7.65E−12	11.8	6.80E−10	4.08	3.65E−10	2.62	7.02E−11	1.67
384	2.39E−13	5.00	4.96E−11	3.78	2.96E−11	3.63	1.15E−11	2.62
786	6.64E−15	5.17	6.72E−15	12.9	1.78E−12	4.05	4.32E−13	4.73

Table 3: Error for Experiment 2 when the Filon-Clenshaw-Curtis rule is applied on $[-1, -0.25]$ and $[-0.25, 1]$ with $N/2{+}1$ points in each subinterval

(See also Experiment 4.) The results are shown in Table 2 with e.c.r. denoting the estimated convergence rate. Here the error exhibits a more chaotic behaviour due to the singularity of f in the interior of the domain. In fact for large k the method is already extremely accurate even for small N and convergence with respect to N is not noticeable until N is sufficiently large. Even the relative error - i.e. the error scaled by multiplication by k is of the order or 10^{-6} for $k = 6400$ and all N considered. This is not a contradiction to Theorem 2.2 which is an upper bound on the error. We then repeated the experiment, but this time applied the rule in a composite fashion on each of the subintervals $[-1, -0.25]$ and $[-0.25, 1]$ separately with $N/2+1$ points in each subinterval. The results displayed in Table 3 show very clearly that the quadrature rule converges faster than in Table 2 and illustrates the importance of having the singularity at the end points. (This phenomenon is of course well known for non-oscillatory integrals but shows up even more forcefully in the oscillatory case.)

Experiment 3

In this experiment we illustrate the stability of the method of evaluation of the weights $\omega_n(k)$ defined in (14). Exact values for these were first computed using the sofware package Mathematica using analytic formulae and evaluation in high-precision arithmetic.

As an illustration of the importance of the second phase of the algorithm, the forward recurrence (33)–(34) was first used to compute $\omega_n(k)$ without switching to Phase 2 of the algorithm even for $n > k$. We observe clearly in Table 4 that the computed weights for $n \le k$ enjoy a very small error, but the accuracy deteriorates very fast as n increases relative to k. In fact, for $n \ge 2k$ the values returned are useless. Note that there is relatively little deterioration when $n \approx k$ indicating that the estimate in Theorem 5.2 may not be sharp. The results are even worse if the relative errors are considered (see Table 5).

If the second phase algorithm is used for computing $\omega_n(k)$ for $n > k$, we can see (Tables 6 and 7) that the instability has (almost) completely dissapeared.

Recall that one of the key steps of the second phase of the algorithm is computing $\rho_{2M}(k)$ with $M > \max\{\lceil k \rceil, N/2\}$ by using the asymptotic expansion in Theorem 3.1. In our implementation, this expansion is used in an adaptive way: Taking seven terms in the expansion, the approximation returned by the asymptotic expansion is accepted if the last term is less than 10^{-15}. If this requirement is not satisfied, we replace M by $\lceil 3M/2 \rceil$ and repeat this process until a valid M is found. The values of M used in the algorithm (notice that we compute $\omega_n(k)$ until $n = 4k$) were $M = 68$ for $k = 10$ and $n = 20$, $M = 90$, for $k = 20$ and $n = 40$, and $M = 120$ for $k = 80$ and $n = 160$. In other words, the size of the tridiagonal matrix in the second phase of the algorithm, which is roughly of size $(2M - k)$, is in the worst case of size 160×160. Having in mind that the system is tridiagonal, this part of the algorithm is also computationally very cheap.

	$k=10$	$k=20$	$k=40$	$k=80$
$n=k/2$	0	5.5E−17	2.78E−17	1.73E−17
$n=k$	3.33E−16	3.33E−16	3.33E−16	4.44E−16
$n=3k/2$	8.07E−15	2.36E−13	1.20E−10	1.52E−05
$n=2k$	2.70E−12	2.54E−08	1.31E+00	1.71E+15

Table 4: Error for $\omega_n(k)$ when the forward reccurence only is used

	$k=10$	$k=20$	$k=40$	$k=80$
$n=k/2$	0	1.88E−16	1.36E−16	1.18E−15
$n=k$	5.21E−16	6.45E−16	8.09E−16	1.36E−15
$n=3k/2$	5.18E−13	1.75E−10	3.12E−07	1.17E+00
$n=2k$	6.69E−10	5.44E−05	6.16E+03	2.17E+20

Table 5: Relative error for $\omega_n(k)$ when the forward reccurence only is used

	$k=10$	$k=20$	$k=40$	$k=80$
$n=2k$	1.36E−16	8.67E−19	5.20E−18	7.45E−20
$n=4k$	3.04E−18	5.15E−18	3.12E−18	3.95E−18

Table 6: Error for $\omega_n(k)$ when the second phase algorithm is included

	$k=10$	$k=20$	$k=40$	$k=80$
$n=2k$	3.36E−14	1.81E−15	2.44E−14	9.43E−15
$n=4k$	2.93E−15	4.12E−14	5.96E−14	1.87E−12

Table 7: Relative error for $\omega_n(k)$ when the second phase algorithm is included

Experiment 4

We finish by illustrating how a combination of graded meshes and the piecewise application of modified Clenshaw-Curtis rule with a variable number of points, can be used to compute integrals with weakly singular kernels. Consider

$$I(k) := \int_0^1 \frac{\log x}{1+x^2}\exp(\mathrm{i}kx)\,\mathrm{d}x.$$

This can be taken as a model integral of those appearing in boundary integral equations for the high-frequency Helmholtz equation in two dimensions, where the kernel has a logarithmic singularity on the diagonal ([9, 17]). To avoid evaluation of the log function at $x=0$, we introduce then the graded mesh

$$x_{-1}=0; \quad \text{and} \quad x_j=\varepsilon+(j/20)^8(1-\varepsilon), \qquad j=0,\ldots,20.$$

The integral in the first subinterval $[x_{-1},x_0]$ is simply approximated by zero. We have taken $\varepsilon=10^{-20}$ which introduces an error well below of the machine precission. For the rest of the subintervals $[x_j,x_{j+1}]$ we apply the Clenshaw-Curtis rule with up to 65 nodes.

To set the number of points used by the quadrature rule on each interval $[x_j,x_{j+1}]$ we implement a strategy whose aim is to reduce the number of function evaluations by exploiting the fact that Clenshaw-Curtis rules are nested. Let us explain it briefly. The first tentative number of points is $n/2+1$ where n is the number of points used in the preceeding subinterval $[x_{j-1},x_j]$). We next compare this result with that returned by the $(n+1)$−point rule (notice

	`Tol` = 1E−6	`Tol` = 1E−9	`Tol` = 1E−12
$k = 10$	212	280	1216
$k = 100$	212	328	1216
$k = 1000$	228	408	1216
$k = 10000$	236	456	1216

Table 8: Number of evaluations of the function in Experiment 4 for different values of the tolerance `TOL`

	`Tol` = 1E−6	`Tol` = 1E−9	`Tol` = 1E−12	ExactValue
$k = 10$	9.70E−10	6.52E−11	2.92E−13	−1.65E−01 − 2.92E−01i
$k = 100$	9.70E−10	6.52E−11	2.92E−13	−1.57E−02 − 5.19E−02i
$k = 1000$	1.06E−09	6.52E−11	2.92E−13	−1.57E−03 − 7.48E−03i
$k = 10000$	1.17E−09	6.51E−11	2.92E−13	−1.57E−04 − 9.79E−04i

Table 9: True error in Experiment 4 for different values of the tolerance `TOL`

that we need only $n/2$ new evaluations to compute the latter). If the difference between these two approximations is less than the tolerance `TOL`, we accept the value returned by the first rule and move to the next interval. Otherwise, we increase the number of points (to $2n + 1$, etc) and repeat the same argument until the difference between two consecutive approximations is less than `TOL` or the maximum number of points (65) is attained. In any case, no more that 65 evalutions are used in each subinterval.

In Table 8 we can see the results obtained for different tolerances and values of k. We observe that the number of evaluations used in the algorithm remains almost unchanged as $k \to \infty$. Moreover, the true error cf. Table 9 is always well below the prescribed values for tolerances.

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