Filon-Clenshaw-Curtis rules for highly-oscillatory integrals with algebraic singularities and stationary points

V. Domínguez*        I.G. Graham†        T. Kim ‡

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Abstract

In this paper we propose and analyse composite Filon-Clenshaw-Curtis quadrature rules for integrals of the form

\[ I^{[a,b]}_k(f,g) := \int_a^b f(x) \exp(ikg(x)) \, dx, \]

where \( k \geq 0, \) \( f \) may have integrable singularities and \( g \) may have stationary points. Our composite rule is defined on a mesh with \( M \) subintervals and requires \( MN + 1 \) evaluations of \( f \). It satisfies an error estimate of the form

\[ C_N k^{-r} M^{-N-1+r}, \]

where \( r \) is determined by the strength of any singularity in \( f \) and the order of any stationary points in \( g \) and \( C_N \) is a constant which is independent of \( k \) and \( M \), but depends on \( N \). The regularity requirements on \( f \) and \( g \) are explicit in the error estimates. For fixed \( k \), the rate of convergence of the rule as \( M \to \infty \) is the same as would be obtained if \( f \) was smooth. Moreover, the quadrature error decays at least as fast as \( k \to \infty \) as does the original integral \( I^{[a,b]}_k(f,g) \). For the case of nonlinear oscillators \( g \), the algorithm requires the evaluation of \( g^{-1} \) at non-stationary points. Numerical results demonstrate the sharpness of the theory. An application to the implementation of boundary integral methods for the high-frequency Helmholtz equation is given.

Keywords Oscillatory integrals, Clenshaw-Curtis quadrature, Integrable singularities, Stationary points, Graded meshes.

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1 Introduction

Oscillatory integrals of the form

\[ I^{[a,b]}_k(f,g) := \int_a^b f(x) \exp(ikg(x)) \, dx \]  \hspace{1cm} (1.1)

where \( f \in L^1[a,b] \) and \( k > 0 \) regularly appear in applications. If \( f \) and \( g \) are smooth and \( g' \) does not vanish then \( I^{[a,b]}_k(f,g) \) decays with at least \( O(k^{-1}) \) as \( k \to \infty \). The decay is faster than \( O(k^{-1}) \) if \( f \) and some of its derivatives vanish at both end-points \( a, b \), but is generally slower if \( f \) has a singularity or if \( g \) has a stationary point in \( [a,b] \). In practice one may be interested in computing (1.1) efficiently and to controllable accuracy for a range of values of \( k \) and for quite general \( f \) and \( g \). The purpose of this paper is to provide stable quadrature rules for this task and

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*Dep. Ingeniería Matemática e Informática, E.T.S.I.I.T. Universidad Pública de Navarra. Campus de Tudela 31500 - Tudela (SPAIN), email:victor.dominguez@unavarra.es
†Department of Mathematical Sciences, University of Bath, Bath, BA2 7AY, United Kingdom. E-mail: I.G.Graham@bath.ac.uk
‡Department of Mathematical Sciences, University of Bath, Bath, BA2 7AY, United Kingdom. E-mail: T.Kim@bath.ac.uk
to prove error estimates demonstrating the quality of the methods. We also demonstrate the
efficiency of our rules by applying them to an example coming from boundary integral methods
for high-frequency wave scattering.

Restricting first to the case $g(x) = x$, a recent paper [5] studied the convergence of Filon-
Clenshaw-Curtis (FCC) rules for computing the special case of (1.1):

$$I_k(f) := \int_{-1}^{1} f(x) \exp(ikx) \, dx .$$  \hfill (1.2)

These rules (denoted by $I_{k,N}(f)$), approximate (1.2) (when $k \geq 1/2$) by replacing $f$ by its poly-
nomial interpolant of degree $N$ at the Clenshaw-Curtis (or Chebyshev) points $t_{j,N} = \cos(jN/\pi)$,
$j = 0, \ldots, N$. (When $k < 1/2$, standard Clenshaw Curtis rules are used instead.) A stability
theory is given in [5] and a slight extension of the error estimates given in [5] (see Theorem 2.1
below) shows that, for $r \in [0,2]$ and $m > \max\{1/2, \rho(r)\}$,

$$|I_k(f) - I_{k,N}(f)| \leq C \left( \frac{1}{k} \right)^r \left( \frac{1}{N} \right)^{m-\rho(r)} \|f_c\|_{H^m} , \quad N \geq 1 ,$$ \hfill (1.3)

where $f_c(\theta) = f(\cos \theta)$, $\rho(r) = r$, $r \in [0,1]$, $\rho(r) = 5r/2 - 3/2$, $r \in [1,2]$ and $\| \cdot \|_{H^m}$ denotes the
norm of the Sobolev space of order $m$ on $[-\pi, \pi]$. Thus fast convergence of the rule with respect
to $N$ and decay of the error with order up to $O(k^{-2})$ is obtained if $f$ is sufficiently regular.

However the convergence rate of the FCC rule is significantly impaired when $f$ has one or
more (integrable) singularities. Thus in this paper we consider composite rules for (1.1) (first for
$g(x) = x$), obtained by subdividing $[a,b]$ into a mesh with $M$ subintervals, chosen so that any
singular points of $f$ coincide with mesh points. We then construct a composite rule which uses
the FCC rule on each mesh subinterval not containing the singularities, and, on subintervals
containing the singularities, either zero or a very simple two-point rule is used, depending on
the strength of the singularity. (See Section 3.4 for precise description of the algorithm.) To
give a flavour of our results, we show, for example, that if $f$ has a singularity of form $|x - x_0|^\beta$
for $x_0 \in [a,b]$ and $\beta \in (-1,1) \setminus \{0\}$, then with suitable mesh refinement near $x_0$, our rules have
error $E(f)$ which satisfies the estimate (see Theorem 3.6):

$$E(f) \leq C_N \left( \frac{1}{k} \right)^r \left( \frac{1}{M} \right)^{N+1-r} \|f\| ,$$ \hfill (1.4)

where $r \in [0,1+\beta]$ and the norm on $f$ is an appropriate weighted norm which takes into account
the singularity at $x_0$. The estimate (1.4) decays at least as fast with $k$ as does the corresponding
integral (1.1), since the latter decays in general with $O(k^{-r})$ where $r = \min\{1+\beta, 1\}$ – see
Lemmas 3.1 - 3.3.

In order to prove (1.4) (and its generalisations), in this paper a non-trivial extension of the esti-
mate (1.3) (quoted from [5]) is first obtained in [2]. Since the error estimate (1.3) depends on
the regularity of $f$ through the norm of $f_c$, this estimate does not provide the correct scaling with
respect to $h$ when it is transported to an interval of size $h$. Therefore in Theorem 2.5 we prove a vari-
ant of (1.3), where $\|f_c\|_{H^m}$ is replaced by the Chebyshev weighted norm of $f^{(m)}$. This new
estimate has the correct scaling behaviour, as is shown in Theorem 2.6. In [3] we obtain the
error analysis for the composite FCC rule applied to (1.1) with $g(x) = x$ when $f$ has integrable
singularities at a finite set of points, in particular obtaining error estimates of the form (1.4). In
[4] we further extend to the case where $g$ may have a finite number of stationary points in $[a,b]$.
The latter case can be reduced to that studied in [3] provided we assume that the inverse of $g$
is known (or is evaluated numerically) on subintervals between stationary points, and indeed
the action of \( g^{-1} \) is required for the implementation of the algorithm. In §5 we give numerical experiments, utilising the public domain code [3] which indicate that as \( M \) increases, the error decays with \( O(M^{-N-1}) \), provided the parameters of the mesh are appropriately chosen, relative to the regularity of \( f \) and stationary points in \( g \). Moreover, when \( k \) increases the error decays roughly with \( O(k^{-r}) \), where \( r \in [0, 1 + \beta] \) indicating the sharpness of our theory. The numerical experiments also indicate that applying the composite FCC on a graded mesh to integrals with singularities yields much more accurate results than applying FCC globally, and using the same number of integrand evaluations.

In this paper we restrict our error estimates to the case of \( k > 0 \) for convenience only; the rules also work well for all \( k \in \mathbb{R} \) and the error estimates can be easily extended to that case (see, e.g., [5] Corollary 2.3). As is also shown in [5], the FCC rules for (1.2) have a stable implementation for all \( k \) and \( N \) which, via FFT, costs \( O(N \log N) \) operations. The composite rules presented here require the evaluation of \( f \) at \( MN + 1 \) points.

Although oscillatory integration is well-studied in the classical literature, some problems of interest to numerical analysts (even in 1D) still remain unsolved today. Thus this field has enjoyed a recent upsurge of interest, partly because of its importance in wave scattering applications. (See [2] and [5] for some more detailed historical remarks.) In particular, the construction and analysis of Filon-type methods has been examined in Iserles [10 11], Iserles and Nørset [12], Olver [16], Xiang [21] and Huybrechs and Olver [9]. (Other related methods include those of Levin-type [14, 17, 18] and those using numerical steepest descent [8].) In all these references, however, the analysis concentrates on accelerating the convergence as \( k \to \infty \), generally assuming either that \( f \) is sufficiently regular or \( f \) has a particular type of singularity so that the moments (i.e. integrals (1.1) where \( f \) is replaced by polynomials) can be computed using special functions. By contrast, we propose Filon-type method for computing (1.1) where \( f \) has algebraic singularities and \( g \) may have stationary points and where the moments can be obtained readily. Our method converges superalgebraically with respect to the number of quadrature points for any strength of singularity, provided the parameters of the mesh are chosen appropriately, and also converges with respect to \( k \) at least as fast the integral itself converges to zero as \( k \to \infty \). Our error estimates explicitly indicate the regularity requirements on \( f \) and \( g \). Other papers [15] and [5] provide analogous estimates for pure (non-composite) Filon rules, where \( f \) and \( g \) are sufficiently regular (and \( g' \neq 0 \) ). But apart from these we know of no other contributions in this direction.

Finally we mention that our methods add something to traditional asymptotic methods. The method of stationary phase produces an accurate approximation to an integral if \( k \) is sufficiently large, whereas our methods work for all \( k \) and are superalgebraically convergent with respect to the number of function evaluations. Our methods also yield a relative error which is superalgebraically convergent uniformly in \( k \) and may indeed even decay with \( k \).

2 The Basic Filon Clenshaw-Curtis Rule

In this and the next section we will consider only the linear oscillator \( g(x) = x \) in (1.1). (See §4 for the case of nonlinear \( g \).) Also, we introduce the notation

\[
I_k^{[a,b]}(f) := \int_a^b f(x) \exp(ikx) \, dx .
\]  

(2.1)

When \([a,b] = [-1, 1]\) we will denote (2.1) simply as \( I_k(f) \).
2.1 Integrals over the fundamental interval $[-1,1]$

The FCC rule in its simplest form approximates $I_k(f)$, by replacing $f$ by its algebraic polynomial interpolant $Q_N f$ at the Clenshaw-Curtis points $t_{j,N} := \cos(j\pi/N)$, $j = 0, \ldots, N$ where $N \geq 1$. Then for $k \geq 1/2$, the rule is

$$I_{k,N}(f) := \int_{-1}^{1} Q_N f(x) \exp(ikx) \, dx = \sum_{n=0}^{N} \alpha_{n,N}(f) \omega_n(k),$$

(2.2)

where, for $n \geq 0$, $\omega_n(k) := \int_{-1}^{1} T_n(x) \exp(ikx) \, dx$, $T_n(x) = \cos(n \arccos(x))$ is the $n$th Chebyshev polynomial, and

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

(2.3)

The notation $\sum''$ means that the first and last terms in the sum are multiplied by $1/2$.

When $0 < k < 1/2$ the integrand in (2.1) is non-oscillatory and we then apply the standard Clenshaw-Curtis rule:

$$I_{k,N}(f) := \int_{-1}^{1} Q_N f_k(x) \, dx = \sum_{n=0}^{N} \alpha_{n,N}(f_k) \omega_n(0), \quad f_k(x) := f(x) \exp(ikx).$$

(2.4)

We point out that $\omega_n(0) = 2/(1 - n^2)$ if $n$ is even, 0 otherwise. For $k \geq 1/2$, the computation of $\omega_n(k)$ turns out to be more delicate. However in [5] a stable and efficient scheme for computing these weights is presented. After an initial application of the discrete cosine transform (via FFT, costing $O(N \log N)$ operations), the rule (2.2)-(2.4) can then be applied to any $f$ in an additional $O(N)$ operations - see [5] for more detail. In the error analysis in this section, we shall make use of the Sobolev space $H^m$ of $2\pi$–periodic functions with the norm

$$\|\varphi\|_{H^m}^2 := |\hat{\varphi}(0)|^2 + \sum_{\mu \neq 0} |\mu|^2 |\hat{\varphi}(\mu)|^2, \quad \hat{\varphi}(\mu) := \frac{1}{2\pi} \int_{-\pi}^{\pi} \varphi(\theta) \exp(-i\mu \theta) \, d\theta.$$  

(2.5)

For $\phi \in H^0 = L^2[-\pi, \pi]$ and any $J \geq 0$, we introduce the truncated Fourier series:

$$(S_J \phi)(\theta) = \sum_{\mu = -J}^{J} \hat{\phi}(\mu) \exp(i\mu \theta)$$

which converges to $\phi \in H^0$ as $J \to \infty$. In fact when $\phi$ is even, we have

$$(S_J \phi)(\theta) := \hat{\phi}(0) + 2 \sum_{\mu = 1}^{J} \hat{\phi}(\mu) \cos(\mu \theta), \quad \text{where} \quad \hat{\phi}(\mu) = \frac{1}{\pi} \int_{0}^{\pi} \phi(\theta) \cos(\mu \theta) d\theta,$$

(2.6)

where the second sum is void if $J = 0$.

Introducing the notation $f_c(\theta) = f(\cos \theta)$, and $\rho(r) = r$, $r \in [0, 1]$, and $\rho(r) = 5r/2 - 3/2$, $r \in [1, 2]$, the following theorem is then a minor extension of [5] Theorem 2.2.

**Theorem 2.1** There exists a constant $C > 0$ such that, for all $r \in [0,2]$ and all integers $m > \max\{1/2, \rho(r)\}$, the estimate

$$|I_k(f) - I_{k,N}(f)| \leq C \left(\frac{1}{k}\right)^r \left(\frac{1}{N}\right)^{m-\rho(r)} \|f_c\|_{H^m}, \quad k \geq 1, \quad N \geq 1$$

(2.7)

holds when $f_c \in H^m$. 


Proof. In [5] the estimate (2.7) was obtained for \( k \geq 1/2 \), for \( r = 0, 1, 2 \). Hence for any \( \theta \in [0, 1] \) we can write
\[
|I_k(f) - I_{k,N}(f)| = |I_k(f) - I_{k,N}(f)|^\theta |I_k(f) - I_{k,N}(f)|^{1-\theta}.
\] (2.8)
Then using estimate (2.7) with \( r = 1 \) (respectively \( r = 2 \)) to bound the first (respectively second) factor on the right hand side of (2.8) we obtain
\[
|I_k(f) - I_{k,N}(f)| \leq C \left( \frac{1}{k} \right)^{2-\theta} \left( \frac{1}{N} \right)^{m-7/2+5\theta/2} \|f_c\|_{H^m}.
\]
Then setting \( \theta = 2-r \) we obtain (2.7) for \( r \in [1, 2] \) and for \( k \geq 1 \). An even simpler interpolation argument obtains the estimate for \( r \in [0, 1] \). For \( k < 1/2 \), i.e., for the classical Clenshaw-Curtis rule, the case \( r = 0 \) follows by the same arguments used in [5, Theorem 2.2] to prove (2.7). For \( r \in (0, 2) \) the result is obvious since \( k \) is bounded.

Theorem 2.2 ensures arbitrarily high convergence for the FCC rule as \( N \to \infty \), provided \( f \) is sufficiently smooth. When \( f \) is not smooth it is better to apply the FCC rule in a composite fashion on meshes graded suitably towards the singular point(s). These composite rules then typically have fixed \( N \) and converge as the subinterval size shrinks to zero. In order to obtain good error estimates for the composite rules we need to modify the error estimate in Theorem 2.1 so that derivatives of \( f \) rather than derivatives of \( f_c \) appear in the bound. This will be done in Theorem 2.5 which in turn is used to obtain Theorem 2.6 showing how the error of the FCC rule, when applied on an arbitrary interval, depends on the length of the interval. In order to prove Theorem 2.6 we first need two lemmas.

**Lemma 2.2** Let \( f \) be such that \((f')_c \in L^1[-\pi, \pi]\). Then
\[
\hat{f}_c(\mu) = \frac{1}{2\mu} \left[ (f')_c(\mu) - (f')_c(\mu + 1) \right], \quad \text{for} \quad \mu \neq 0.
\] (2.9)

**Proof.** Since \( f_c \) is even we use (2.6) and integrate by parts to obtain
\[
\hat{f}_c(\mu) = \frac{1}{\pi} \int_0^\pi f_c(\theta) \cos(\mu \theta) d\theta = -\frac{1}{\pi \mu} \int_0^\pi (f_c)'(\theta) \sin(\mu \theta) d\theta
= \frac{1}{\mu \pi} \int_0^\pi f'(\cos \theta) \sin \theta \sin(\mu \theta) d\theta
= \frac{1}{2\mu \pi} \int_0^\pi (f')_c(\theta) [\cos((\mu - 1) \theta) - \cos((\mu + 1) \theta)] d\theta,
\]
and the result follows. \(\Box\)

Using Lemma 2.2 we now estimate the error in the truncated Fourier cosine series of \( f_c \).

**Lemma 2.3** For all \( 0 \leq m \leq N + 1 \) there exist constants \( \sigma_{m,N} > 0 \) such that
\[
\|(I - S_N)f_c\|_{H^m} \leq \sigma_{m,N} \|(f^{(m)})_c\|_{H^0}.
\] (2.10)

**Proof.** Since \( S_N \) is the orthogonal projection of \( H^0 \) onto span\{exp(\pi j \theta) : 0 \leq |j| \leq N\}, the result is trivial for \( m = 0 \). So let us assume now that \( m \geq 1 \). Since \( f_c \) is even, from (2.6) we have, for all \( J \geq 0 \),
\[
(I - S_J)f_c = 2 \sum_{\mu \geq J+1} \hat{f}_c(\mu) \cos(\mu \theta), \quad \text{and} \quad \|(I - S_J)f_c\|_{H^m}^2 = 2 \sum_{\mu \geq J+1} \mu^{2m} |\hat{f}_c(\mu)|^2.
\]

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**Proof.** Since \( S_N \) is the orthogonal projection of \( H^0 \) onto \( \text{span}\{\exp(\pi j \theta) : 0 \leq |j| \leq N\} \), the result is trivial for \( m = 0 \). So let us assume now that \( m \geq 1 \). Since \( f_c \) is even, from (2.6) we have, for all \( J \geq 0 \),
\[
(I - S_J)f_c = 2 \sum_{\mu \geq J+1} \hat{f}_c(\mu) \cos(\mu \theta), \quad \text{and} \quad \|(I - S_J)f_c\|_{H^m}^2 = 2 \sum_{\mu \geq J+1} \mu^{2m} |\hat{f}_c(\mu)|^2.
\]
Then, using Lemma 2.2 we obtain
\[
\| (I - S_J) f_c \|_{H^m}^2 \leq \frac{1}{2} \sum_{\mu \geq J+1} \mu^{2m-2} \left| (f')^c(\mu - 1) - (f')^c(\mu + 1) \right|^2 \\
\leq \sum_{\mu \geq J+1} \mu^{2m-2} \left| (f')^c(\mu - 1) \right|^2 + \sum_{\mu \geq J+1} \mu^{2m-2} \left| (f')^c(\mu + 1) \right|^2 \\
= \sum_{\mu \geq J} (\mu + 1)^{2m-2} \left| (f')^c(\mu) \right|^2 + \sum_{\mu \geq J+2} (\mu - 1)^{2m-2} \left| (f')^c(\mu) \right|^2 \\
\leq 2 \sum_{\mu \geq J} (\mu + 1)^{2m-2} \left| (f')^c(\mu) \right|^2.
\]
(2.11)

Hence, in the case \( J \geq 1 \), we have,
\[
\| (I - S_J) f_c \|_{H^m} \leq 2 \left( \frac{J+1}{J} \right)^{2m-2} \sum_{\mu \geq J} \mu^{2m-2} \left| (f')^c(\mu) \right|^2 \\
= \left( \frac{J+1}{J} \right)^{2m-2} \| (I - S_{J-1}) (f')^c \|_{H^{m-1}}.
\]
(2.12)

Using this identity \( m - 1 \) times (recalling that \( m \leq N + 1 \)), we obtain
\[
\| (I - S_N) f_c \|_{H^m} \leq \left( \frac{N+1}{N} \right)^{m-1} \left( \frac{N}{N-1} \right)^{m-2} \ldots \left( \frac{N-m+3}{N-m+2} \right) \| (I - S_{N-m+1}) (f^{(m-1)})^c \|_{H^1},
\]
which we write as
\[
\| (I - S_N) f_c \|_{H^m} \leq \sigma_{m,N} \| (I - S_{N-m+1}) (f^{(m-1)})^c \|_{H^1}.
\]
(2.13)

Now, if \( m < N + 1 \), we can use (2.12) one more time and use the fact that \( S_{N-m} \) is an orthogonal projection on \( H^0 \) to obtain the required result. On the other hand if \( m = N + 1 \) we can use the fact that
\[
\| (I - S_0) (f^{(m-1)})^c \|_{H^1} \leq \| (f^{(m)})^c \|_{H^0},
\]
which is easily obtained from (2.11), to deduce (2.10). \( \square \)

**Remark 2.4.** To estimate the constants \( \sigma_{m,N} \), note that in each pair of terms in the product, we can cancel the denominator in the left-hand term with the numerator in the right-hand term to obtain, for \( m \geq 1 \),
\[
\sigma_{m,N} = \frac{(N+1)^{m-1}}{N(N-1) \ldots (N-m+2)} = m \prod_{j=1}^{m-1} \left( \frac{N+1}{N+1-j} \right),
\]
(with the product being interpreted as 1 when \( m = 1 \)). Thus for fixed \( m \geq 1 \), \( \sigma_{m,N} \to 1 \) as \( N \to \infty \). Moreover letting \( m \) grown with \( N \) (for example \( m = N + 1 \)), we have
\[
\sigma_{N+1,N} = \frac{(N+1)^N}{N!} = \frac{N^N}{N!} \left( 1 + \frac{1}{N} \right)^N \sim \frac{e^{N+1}}{\sqrt{2\pi N}},
\]
where the last relation is obtained using Stirling’s formula. Since in this paper we will use fixed order methods (i.e. \( N \) fixed) and obtain convergence for composite methods as the mesh size
shrinks, the growth of $\sigma_{N+1,N}$ is not of essential importance to us here. However if we wanted to use $hp$ quadrature then this growth would be important and would need to be cancelled by suitable decay of the derivatives of $f$ in order to obtain convergence. Estimates of this type are in [15].

Now in Theorem 2.5 below we will obtain the analogue of Theorem 2.1, but with (appropriate weighted norms of) derivatives of $f$, rather than $f_c$ on the right-hand side. For any integer $m \geq 0$, and a function $f$ defined on $[a,b]$, we introduce the weighted seminorm

$$|f|_{H^m[a,b]} := \left\{ \int_a^b \frac{|f^{(m)}(x)|^2}{\sqrt{(b-x)(x-a)}} \, dx \right\}^{1/2}. \quad (2.14)$$

When $[a,b] = [-1,1]$ we just write $| \cdot |_{H^m}$ and we note that

$$|f|_{H^m} = \left\{ \int_{-\pi}^{\pi} |(f^{(m)})_c(\theta)|^2 \, d\theta \right\}^{1/2} = \sqrt{\pi} \| (f^{(m)})_c \|_{H^0}. \quad (2.15)$$

**Theorem 2.5** Let $r \in [0,2]$ and $0 \leq m \leq N + 1$. There exist constants $\sigma'_{m,N}$ such that

$$|I_k(f) - I_{k,N}(f)| \leq \sigma'_{m,N} \left( \frac{1}{k} \right)^r \left( \frac{1}{N} \right)^{m-\rho(r)} |f|_{H^m}, \quad (2.16)$$

when $|f|_{H^m} < \infty$. Moreover $\sigma'_{m,N} = C\sigma_{m,N}$ with $C$ independent of $m, N$.

**Proof.** Note that if $|f|_{H^m} < \infty$ then $f \in L^2[-1,1]$ and so we can define an algebraic polynomial $p$ of degree $N$ by

$$p(x) = \hat{f}_c(0) + 2 \sum_{n=1}^N \hat{f}_c(n) T_n(x). \quad (2.17)$$

Clearly (recalling (2.6)), $p_c(\theta) = (S_N f_c)(\theta)$, for all $\theta \in [-\pi, \pi]$. Since $I_{k,N}$ is exact for all polynomials of degree up to $N$, we have, using Theorem 2.1

$$|I_k(f) - I_{k,N}(f)| = |I_k(f - p) - I_{k,N}(f - p)| \leq C \left( \frac{1}{k} \right)^r \left( \frac{1}{N} \right)^{m-\rho(r)} \| (f - p)_c \|_{H^m} = C \left( \frac{1}{k} \right)^r \left( \frac{1}{N} \right)^{m-\rho(r)} \| (I - S_N)f_c \|_{H^m}. \quad (2.18)$$

Then, using Lemma 2.3

$$|I_k(f) - I_{k,N}(f)| \leq C\sigma_{m,N} \left( \frac{1}{k} \right)^r \left( \frac{1}{N} \right)^{m-\rho(r)} \| (f^{(m)})_c \|_{H^0} \quad (2.18)$$

and the result follows from (2.15). □
2.2 Integrals over \([a, b]\)

Now we consider the integral (2.1) for general \([a, b]\). To apply the FCC quadrature, we first transform the integral using the following linear change of variables:

\[
x = c + h t, \quad t \in [-1, 1], \quad \text{where} \quad c := \frac{b + a}{2}, \quad \text{and} \quad h := \frac{b - a}{2}.
\]  

(2.19)

Then we may write

\[
I_{k}^{[a, b]}(f) = h \exp(i k c) I_{k}^{[\tilde{f}]}(f),
\]

(2.20)

where \(\tilde{k} = h k\) and \(\tilde{f}\) is the function on \([-1, 1]\):

\[
\tilde{f}(t) = f(c + h t), \quad t \in [-1, 1].
\]

(2.21)

Then we apply the quadrature rule (2.2)-(2.4) to the integral on the right-hand side of (2.20) to obtain the approximation

\[
I_{k,N}^{[a, b]}(f) := h \exp(i k c) I_{k,N}^{[\tilde{f}]}(f) \approx I_{k}^{[a, b]}(f).
\]

(2.22)

The following theorem is the corresponding extension of Theorem 2.5.

**Theorem 2.6** Let \(r \in [0, 2]\) and \(0 \leq m \leq N + 1\). Then, when \(|f|_{H_{w}^{m}}^{[a, b]} < \infty\), we have

\[
\left|I_{k}^{[a, b]}(f) - I_{k,N}^{[a, b]}(f)\right| \leq \sigma'_{m,N} \left(\frac{1}{k}\right)^{r} h^{m+1-r} \left(\frac{1}{N}\right)^{m-\rho(r)} |f|_{H_{w}^{m}}^{[a, b]}.
\]

(2.23)

**Proof.** From (2.20), (2.22) and then Theorem 2.5 we obtain

\[
\left|I_{k}^{[a, b]}(f) - I_{k,N}^{[a, b]}(f)\right| = h \left|I_{k}^{[\tilde{f}]}(f) - I_{k,N}^{[\tilde{f}]}(f)\right|
\leq \sigma'_{m,N} h \left(\frac{1}{k}\right)^{r} \left(\frac{1}{N}\right)^{m-\rho(r)} |\tilde{f}|_{H_{w}^{m}}^{[a, b]}
\approx \sigma'_{m,N} \left(\frac{1}{k}\right)^{r} h^{1-r} \left(\frac{1}{N}\right)^{m-\rho(r)} |\tilde{f}|_{H_{w}^{m}}^{[a, b]}. \tag{2.24}
\]

Now \(\tilde{f}^{(m)}(t) = h^{m} f^{(m)}(c + h t)\), and so

\[
|\tilde{f}|_{H_{w}^{m}}^{2} = h^{2m} \int_{-1}^{1} \frac{|f^{(m)}(c + h t)|^2}{\sqrt{1 - t^2}} \, dt = h^{2m} |f|_{H_{w}^{m}}^{2} \tag{2.25}
\]

and the result follows. \(\square\)

The most important use of this theorem will be for the case when \(N\) is fixed and convergence is obtained by letting \(h \to 0\) (as arises when composite versions of the FCC rule are used). For this case we have the following corollary, which is obtained using Theorem 2.6 with \(m = N + 1\).

**Corollary 2.7** Let \(r \in [0, 2]\). For each \(N \geq 1\), there exists a constant \(c_{N} = C \sigma'_{N+1,N}(1/N)^{N+1-\rho(r)}\), such that

\[
\left|I_{k}^{[a, b]}(f) - I_{k,N}^{[a, b]}(f)\right| \leq c_{N} \left(\frac{1}{k}\right)^{r} h^{N+2-r} \max_{x \in [a, b]} |f^{(N+1)}(x)| \tag{2.26}
\]

when \(f \in C^{N+1}[a, b]\).
3 Composite Clenshaw-Curtis Rules

In this section, we will consider the computation of \( I_k^{[a,b]}(f) \), where \( f \) is allowed to have an algebraic or logarithmic singularity in \([a,b]\). To control the length of the paper, we restrict to functions \( f \) which are not continuously differentiable. Singularities in higher derivatives can be treated in an analogous way.

Without loss of generality we set \([a,b] = [0,1]\) and assume that the only singularity occurs at the origin. The case of a finite number of singularities on \([a,b]\) can be treated by splitting \([a,b]\) up into subintervals, each with only one singularity at an end point, and then mapping each interval onto \([0,1]\) in an obvious affine way. Hence, for \( \beta \in (0,1) \) and \( m \geq 1 \), we introduce

\[
\| v \|_{m,\beta} := \max \left\{ \sup_{x \in [0,1]} |v(x)|, \sup_{x \in [0,1]} \left| x^{(j-\beta)} v^{(j)}(x) \right|, \quad j = 1, \ldots, m \right\}.
\]

We denote by \( C^{m}_{\beta}[0,1] \) the space of all functions \( v \in C[0,1] \) such that \( \| v \|_{m,\beta} < \infty \). Similarly, for \( \beta \in (-1,0) \) we define

\[
\| v \|_{m,\beta} := \max \left\{ \sup_{x \in [0,1]} \left| x^{(j-\beta)} v^{(j)}(x) \right|, \quad j = 0, \ldots, m \right\},
\]

and choose \( C^{m}_{\beta}[0,1] \) to be the space of all \( v \in C(0,1) \) such that \( \| v \|_{m,\beta} < \infty \). Finally, we cover the case of logarithmic singularities via the norm

\[
\| v \|_{m,0} := \max \left\{ \sup_{x \in [0,1]} |(\log x) + 1|^{-1} v(x)|, \sup_{x \in [0,1]} \left| x^j v^{(j)}(x) \right|, \quad j = 1, \ldots, m \right\}
\]

and introduce the associated space \( C^{m}_{0}[0,1] \). Note that \( C^{m}_{\beta}[0,1] \subset L^1[0,1] \) for all \( \beta \in (-1,1) \).

3.1 The composite algorithm

When \( f \in C^{m}_{\beta}[0,1] \), for \( \beta \in (-1,1) \), our strategy for computing \( I_k^{[0,1]}(f) \) is to apply the FCC rule in a composite fashion on a mesh graded towards the singularity. With the right choice of mesh the error of the quadrature can then be made to satisfy a uniform error estimate on subintervals and be small overall. Let us recall the classical graded mesh

\[
\Pi_{M,q} := \left\{ x_j := \left( \frac{j}{M} \right)^q : j = 0, 1, \ldots, M \right\},
\]

where \( q \geq 1 \) is the grading parameter to be chosen. This mesh - originally proposed in [19] - is well-known to give optimal approximation of functions with singularities by fixed order piecewise polynomials. An application to quadrature was given in [7]. This paper contains an extension of these results to the computation of oscillatory integrals with singularities. Writing

\[
I_k^{[0,1]}(f) = I_k^{[x_0,x_1]}(f) + \sum_{j=2}^{M} I_k^{[x_{j-1},x_j]}(f),
\]

we approximate each term in the sum on the right-hand side by applying the FCC rule as defined in [22]. The strategy for approximating the first term on the right-hand side depends on whether \( \beta \leq 0 \) or \( \beta > 0 \). Precisely we define the approximation

\[
\tilde{I}_k^{[x_0,x_1]}(f) := \begin{cases} 
I_k^{[x_0,x_1]}(f), & \text{if } \beta \in (0,1), \\
0, & \text{if } \beta \in (-1,0).
\end{cases}
\]

(3.5)
Note that for $\beta \in (0,1)$,

$$I_{k,1}^{[x_0,x_1]}(f) = \begin{cases} \int_{x_0}^{x_1} \left( Q_1^{[x_0,x_1]} f \right)(x) \exp(ikx) \, dx, & \text{if } x_1k \geq 1 \\ \int_{x_0}^{x_1} \left( Q_1^{[x_0,x_1]} (f \exp(ik\cdot)) \right)(x) \, dx, & \text{if } x_1k < 1 \end{cases}$$

where $Q_1^{[x_0,x_1]} f$ is the linear function interpolating $(x_0, f(x_0))$ and $(x_1, f(x_1))$. (To obtain this formula, recall that from (2.20), $I_{k,1}^{[x_0,x_1]}(f) = h \exp(ikc) I_{k,1}^1(\tilde{f})$ where $k = kx_1/2$, and recall (2.2) and (2.4)). The composite quadrature rule is

$$I_{k,N,M,q}^{0,1}(f) := \tilde{I}_k^{[x_0,x_1]}(f) + \sum_{j=2}^M I_{k,N}^{[x_{j-1},x_j]}(f). \quad (3.6)$$

The corresponding error may then be bounded by

$$E_{k,N,M,q}(f) := |I_k^{0,1}(f) - I_{k,N,M,q}^{0,1}(f)| \leq |\tilde{e}_1| + \sum_{j=2}^M |e_j|, \quad (3.7)$$

where

$$\tilde{e}_1 = I_k^{[x_0,x_1]}(f) - \tilde{I}_k^{[x_0,x_1]}(f), \quad \text{and}$$

$$e_j = I_k^{[x_{j-1},x_j]}(f) - I_{k,N}^{[x_{j-1},x_j]}(f), \quad \text{for } j = 2, \ldots, M. \quad (3.8)$$

In the following two sections, we derive results which will help us estimate $|\tilde{e}_1|$. These are subsequently used to estimate the total error $E_{k,N,M,q}(f)$ in Theorem 3.6.

### 3.2 Estimates on the size of the integrals

In the following two lemmas, we analyse the integrals $I_k^{0,\varepsilon}(f)$, where $f \in C_\beta^1[0,1]$, making explicit the rate of decay as both $\varepsilon \to 0$ and $k \to \infty$.

**Lemma 3.1** For any $\beta \in (-1,0)$ and any $f \in C_\beta^1[0,1]$ there exists $C_\beta > 0$ such that for $\varepsilon \in (0,1]$ we have

$$|I_k^{0,\varepsilon}(f)| \leq C_\beta \varepsilon^{1+\beta-s} \left( \frac{1}{k} \right)^s \|f\|_{1,\beta} \quad (3.10)$$

where $s \in [0,1+\beta]$. Furthermore, for any $f \in C_\beta^1[0,1]$ there exists $C_0 > 0$ such that for $\varepsilon \in (0,1]$, we have

$$|I_k^{0,\varepsilon}(f)| \leq C_0 (\varepsilon + \varepsilon |\log \varepsilon|)^{1-s} \left( \frac{1 + \log k}{k} \right)^s \|f\|_{1,0} \quad (3.11)$$

where $s \in [0,1]$.

**Proof.** We will prove the lemma for the case when $\beta \in (-1,0)$. The case when $\beta = 0$ follows similarly. First note that for all $\varepsilon \in (0,1]$, we have

$$|I_k^{0,\varepsilon}(f)| \leq \int_0^\varepsilon x^\beta \, dx \|f\|_{0,\beta} = \frac{1}{1+\beta} \varepsilon^{1+\beta} \|f\|_{0,\beta} \leq \frac{1}{1-|\beta|} \varepsilon^{1+\beta} \|f\|_{1,\beta}. \quad (3.12)$$

We show now

$$|I_k^{0,\varepsilon}(f)| \leq \frac{1}{1-|\beta|} \left[ \frac{2}{|\beta|} \right] \left( \frac{1}{k} \right)^{1+\beta} \|f\|_{1,\beta}. \quad (3.13)$$
and the result follows by interpolation of (3.12) and (3.13).

To obtain (3.13), note first that it follows trivially from (3.12) if \( \varepsilon k \leq 1 \). Therefore, let us assume that \( \varepsilon > 1/k \), and write

\[
I_k^{[0,\varepsilon]}(f) = I_k^{[0,1/k]}(f) + I_k^{[1/k,\varepsilon]}(f). 
\]  
(3.14)

Now again from (3.12)

\[
|I_k^{[0,1/k]}(f)| \leq \frac{1}{1 - |\beta|} \left( \frac{1}{k} \right)^{1+\beta} \|f\|_{0,\beta}. 
\]  
(3.15)

On the other hand, integration by parts yields

\[
I_k^{[1/k,\varepsilon]}(f) = \frac{1}{ik} \left[ f(x) \exp(ikx) \right]_{x=1/k}^{x=\varepsilon} - \frac{1}{ik} \int_{1/k}^{\varepsilon} f'(x) \exp(ikx) \, dx. 
\]

Thus

\[
|I_k^{[1/k,\varepsilon]}(f)| \leq \frac{1}{k} \left[ |f(\varepsilon)| + |f(1/k)| + \int_{1/k}^{\varepsilon} |f'(x)| \, dx \right]. 
\]

Now for any \( x > 0 \), \( |f(x)| \leq x^\beta \|f\|_{1,\beta} \) and also

\[
\int_{1/k}^{\varepsilon} |f'(x)| \, dx \leq \int_{1/k}^{\varepsilon} x^{\beta-1} \|f\|_{1,\beta} \leq \frac{1}{|\beta|} \left[ \varepsilon^\beta + \left( \frac{1}{k} \right)^\beta \right] \|f\|_{1,\beta}.
\]

Thus

\[
|I_k^{[1/k,\varepsilon]}(f)| \leq \frac{1}{k} \left[ 1 + \frac{1}{|\beta|} \right] \left[ \varepsilon^\beta + \left( \frac{1}{k} \right)^\beta \right] \|f\|_{1,\beta},
\]

and, since \( \varepsilon^\beta < (1/k)^\beta \) we obtain

\[
|I_k^{[1/k,\varepsilon]}(f)| \leq 2 \left[ \frac{1 + |\beta|}{|\beta|} \right] \left( \frac{1}{k} \right)^{1+\beta} \|f\|_{1,\beta}. 
\]  
(3.16)

Substituting (3.16) and (3.15) into (3.14) we obtain

\[
I_k^{[0,\varepsilon]}(f) \leq \left[ |\beta| + 2(1 - |\beta|^2) \right] \left( \frac{1}{k} \right)^{1+\beta} \|f\|_{1,\beta}
\]

thus proving (3.13).

\[ \square \]

**Lemma 3.2** For any \( \beta \in (0,1) \) and for any \( f \in C_{\beta}^2[0,1] \) there exists \( C_{\beta} > 0 \) such that for \( \varepsilon \in (0,1] \) and \( s \in [0,1] \) we have

\[
|I_k^{[0,\varepsilon]}(f)| \leq C_{\beta} \varepsilon^{1-s} \left( \frac{1}{k} \right)^s \|f\|_{1,\beta}.
\]  
(3.17)

Moreover, if \( s \in [1,1+\beta] \),

\[
|I_k^{[0,\varepsilon]}(f)| \leq \frac{1}{k} \left[ |f(0)| + |f(\varepsilon)| \right] + C_{\beta} \varepsilon^{1+\beta-s} \left( \frac{1}{k} \right)^s \|f'\|_{1,\beta-1}
\]

\[
\leq \frac{2}{k} \|f\|_{0,\beta} + C_{\beta} \varepsilon^{1+\beta-s} \left( \frac{1}{k} \right)^s \|f\|_{2,\beta}.
\]  
(3.18)
Lemma 3.3

For all $\varepsilon \in (0, 1)$,

$$|I_k^{[0,\varepsilon]}(f)| \leq \varepsilon \|f\|_{0,\beta}. \quad (3.19)$$

On the other hand, integration by parts yields

$$|I_k^{[0,\varepsilon]}(f)| \leq 1 \left| f(0) + |f'(\varepsilon)| \right| + \frac{1}{k} \left| \int_{0}^{\varepsilon} f''(x) \exp(ikx) \, dx \right| \quad (3.20)$$

and substitution of (3.22) into (3.21) yields

$$|I_k^{[0,\varepsilon]}(f)| \leq 2 \|f\|_{0,\beta} + \frac{1}{k} \left| \int_{0}^{\varepsilon} f'(x) \exp(ikx) \, dx \right|. \quad (3.21)$$

Also, we have

$$\left| \int_{0}^{\varepsilon} f'(x) \exp(ikx) \, dx \right| \leq \left[ \int_{0}^{\varepsilon} x^{\beta-1} \, dx \right] \|f\|_{1,\beta} = \frac{1}{\beta} \varepsilon^\beta \|f\|_{1,\beta} \quad (3.22)$$

and substitution of (3.22) into (3.21) yields

$$|I_k^{[0,\varepsilon]}(f)| \leq \left( 2 + \frac{1}{\beta} \right) \frac{1}{k} \|f\|_{1,\beta}. \quad \text{Interpolation of this with (3.19) yields (3.17).}
$$

To obtain (3.18), we also note $f' \in C_{\beta-1}^{[0,1]}$ so by Lemma 3.1 we also have

$$\left| \int_{0}^{\varepsilon} f'(x) \exp(ikx) \, dx \right| \leq C_{\beta-1} \varepsilon^{\beta-s'} \left( \frac{1}{k} \right)^{s'} \|f'\|_{1,\beta-1} \leq C_{\beta-1} \varepsilon^{\beta-s'} \left( \frac{1}{k} \right)^{s'} \|f\|_{2,\beta}$$

for all $s' \in [0, \beta]$. Substituting this into (3.20) and putting $s = 1 + s'$, we obtain the result. \(\square\)

In the next lemma we shall verify the sharpness of the estimates in Lemmas 3.1-3.2 as $k \to \infty$.

This result concerns the family of functions

$$f_\beta(x) = \begin{cases} x^\beta, & \beta \in (-1, 0) \cup (0, 1), \\ \log x, & \beta = 0. \end{cases} \quad (3.23)$$

Lemma 3.3 For all $\beta \in (-1, 1)$, there exists a constant $A_\beta > 0$ such that, for all $k$ sufficiently large,

$$k^{\min\{1+\beta,1\}} |I_k^{[0,1]}(f_\beta)| \geq A_\beta, \quad \text{when } \beta \neq 0 \quad (3.24)$$

$$\frac{k}{\log k} |I_k^{[0,1]}(f_0)| \geq A_0. \quad (3.25)$$

Proof. Let us consider first $\beta \in (-1, 0) \cup (0, 1)$. Using [3] (3.761.1),(3.761.6), we obtain

$$I_k^{[0,1]}(f_\beta) = \frac{1}{1+\beta} 1 F_1 (1 + \beta, 2 + \beta; ik), \quad (3.26)$$

where $1 F_1(a,b,z)$ denotes the confluent hypergeometric function (also called Kummer’s function and denoted $M(a,b,z)$ in [1] Section 13). At large values of $|z|$, with $-\pi/2 < \arg z < 3\pi/2$, for fixed $a$ and $b$, the function $1 F_1(a,b,z)$ has the following asymptotics, see [1] (13.5.1):

$$1 F_1(a,b,z) = \Gamma(b) \left( \frac{e^{\pi a} z^{-a}}{\Gamma(b-a)} + \frac{e^{\pi a} z^{-b}}{\Gamma(a)} \right) (1 + O(|z|^{-1})).$$
Then, from (3.26) and since \( \Gamma(1 + z) = z\Gamma(z) \), we obtain,
\[
I_{k}^{[0,1]}(f_{\beta}) = \left( \Gamma(1 + \beta)e^{i\pi(1+\beta)}(ik)^{-1-\beta} + e^{i(k)k^{-1}} \right)(1 + O(k^{-1})).
\]

Therefore, for \( k \) sufficiently large, we have, for \( \beta \in (-1,0) \),
\[
|I_{k}^{[0,1]}(f_{\beta})| \geq \frac{1}{2} \left( \Gamma(1 + \beta)k^{-1-\beta} - k^{-1} \right) \geq \frac{1}{4} \Gamma(1 + \beta)k^{-1-\beta},
\]
and for \( \beta \in (0,1) \),
\[
|I_{k}^{[0,1]}(f_{\beta})| \geq \frac{1}{2} \left( k^{-1} - \Gamma(1 + \beta)k^{-1-\beta} \right) \geq \frac{1}{4} k^{-1}.
\]

These prove the estimate (3.24).

To verify (3.25), we use the formulae [6, (4.381.1), (4.381.2)] to obtain
\[
I_{k}^{[0,1]}(f_{0}) = -\frac{1}{k} \left( \frac{\pi}{2} + i\gamma + i\log k \right) + \frac{i}{k} \left( ci(k) + isi(k) \right)
\]
where \( si \) and \( ci \) are the sine and cosine integral functions:
\[
si(x) := -\frac{\pi}{2} + \int_{0}^{x} \frac{\sin t}{t} \, dt, \quad ci(x) := \gamma + \log x + \int_{0}^{x} \frac{\cos t - 1}{t} \, dt,
\]
and \( \gamma \approx 0.5772 \) is the Euler-Macheroti constant. (Note that, in the notation of \([1]\), \( si(x) = -\pi/2 + \text{Si}(x) \) and \( ci(x) = \text{Ci}(x) \).) Then using the asymptotics for large arguments of \( \text{Si} \) and \( \text{Ci} \) in \([1\ 5.2.34\), (5.2.35)\] and \([1\ 5.2.8,\ 5.2.9]\), we deduce that
\[
\lim_{k \to \infty} \text{si}(k) = O(1/k), \quad \lim_{k \to \infty} \text{ci}(k) = O(1/k).
\]

Thus
\[
I_{k}^{[0,1]}(f_{0}) = -\frac{1}{k} \left( \frac{\pi}{2} + i\gamma + i\log k \right) + O \left( \frac{1}{k^{2}} \right).
\]

Thus, for all \( k \) sufficiently large
\[
|I_{k}^{[0,1]}(f_{0})| \geq \frac{\log k}{2k},
\]
proving the estimate (3.25). \( \square \)

### 3.3 The total error for the composite Filon-Clenshaw-Curtis method

In Theorem 3.6 below we use (3.7) to estimate the total error of the composite FCC rule. The first contribution \( |\tilde{e}_{1}| \) is estimated either by a direct application of Lemma 3.1 (when \( \beta \in (-1,0) \)), or via an integration by parts argument (when \( \beta \in (0,1) \)). This is done in Lemma 3.5 below, but first the remaining sum on the right-hand side is estimated in the following lemma. Since the proof uses fairly classical graded mesh arguments we shall be brief.

**Lemma 3.4** Let \( f \in C_{\beta}^{N+1}[0,1], \ \beta \in (-1,1), \ \text{let} \ \ r \geq 0 \ \text{and choose}
\[
q > (N + 1 - r)/(\beta + 1 - r), \quad \text{for} \ \ r < 1 + \beta.
\]

Then there exists a constant \( C \) which depends on \( N, \ \beta \ \text{and} \ q \) such that
\[
\sum_{j=2}^{M} |e_{j}| \leq C \left( \frac{1}{k} \right)^{r} \left( \frac{1}{M} \right)^{N+1-r} \|f\|_{N+1,\beta},
\]

\[3.28\]
Lemma 3.5 Under the same hypothesis as Lemma 3.4, there exists a constant \( C \) which depends on \( \beta \) and \( q \) such that, for \( N \geq 1 \)

\[
|\tilde{c}_1| \leq C \left( \frac{1}{k} \right)^r \left( \frac{1}{M} \right)^{N+1-r} \begin{cases} 
\|f\|_{2,\beta}, & \text{when } \beta \in (-1, 0) \cup (0, 1), \\
(1 + \log k)^r (\log M)^{1-r} \|f\|_{2,0}, & \text{when } \beta = 0.
\end{cases}
\]

Proof. Throughout we use the fact that \( x_0 = 0 \). Consider first \( \beta \in (0, 1) \) and note that

\[
|(Q_1^{[0,x_1]} f)'| = \left| \frac{f(x_1) - f(0)}{x_1} \right| = \left| \frac{1}{x_1} \int_0^{x_1} f'(x) \, dx \right| \leq \frac{1}{x_1} \int_0^{x_1} |f'(x)| \, dx \leq \frac{1}{x_1} \int_0^{x_1} |f'(x)| \, dx \leq \frac{1}{\beta} x_1^{\beta-1} \|f\|_{1,\beta}.
\]

Moreover, for any \( t \in [0, x_1] \) and any \( f \in C_{\beta}^1[0, 1] \), we have

\[
|f(t) - Q_1^{[0,x_1]} f(t)| = \left| \int_0^t (f - Q_1^{[0,x_1]} f)'(x) \, dx \right| \leq \int_0^{x_1} |f'(x)| \, dx + x_1 |(Q_1^{[0,x_1]} f)'| \leq \frac{2}{\beta} x_1^{\beta} \|f\|_{1,\beta}.
\]

Then, from (3.5), we have from (3.32), when \( f \in C_{\beta}^1[0, 1] \),

\[
|\tilde{c}_1| = \left| \int_0^{x_1} (f(x) - Q_1^{[0,x_1]} f(x)) \exp(ikx) \, dx \right| \leq \frac{2}{\beta} x_1^{1+\beta} \|f\|_{1,\beta}.
\]
On the other hand, integrating the formula for $\tilde{e}_1$ by parts, we obtain

$$\tilde{e}_1 = -\frac{1}{ik} \int_0^{x_1} \left( f(x) - (Q_1^{[0,x_1]} f)(x) \right)' \exp(ikx)dx .$$

(3.34)

Since $f' \in C^N_{\beta-1}$, to treat the first term on the right-hand side of (3.34) we can use Lemma 3.1 with $\epsilon$ replaced by $\beta - 1$ and $s$ chosen to be $\beta$, thus obtaining

$$\left| \int_0^{x_1} f'(x) \exp(ikx)dx \right| \leq C_\beta \left( \frac{1}{k} \right)^\beta \| f' \|_{1,\beta-1} \leq C_\beta \left( \frac{1}{k} \right)^\beta \| f \|_{2,\beta} .$$

(3.35)

Moreover, to treat the second term in (3.34), since $(Q_1^{[0,x_1]} f)'$ is constant, we have by (3.34),

$$\left| \int_0^{x_1} (Q_1^{[0,x_1]} f)' \exp(ikx)dx \right| = \left| (Q_1^{[0,x_1]} f)' \right| \left| \int_0^{x_1} \exp(ikx)dx \right| \leq \frac{x_1^{\beta-1}}{\beta k} \| f \|_{1,\beta} .$$

(3.36)

Hence combining (3.35) and (3.36) with (3.34), we obtain

$$|\tilde{e}_1| \leq C'_\beta \left( \frac{1}{k} \right)^{1+\beta} + \frac{x_1^{\beta-1}}{k^2} \| f \|_{2,\beta} \leq C'_\beta \left( \frac{1}{k} \right)^{1+\beta} \left[ 1 + (x_1k)^{\beta-1} \right] \| f \|_{2,\beta} .$$

(3.37)

Hence if $x_1k \geq 1$ we can interpolate (3.37) and (3.33), to deduce that

$$|\tilde{e}_1| \leq C''_\beta \left( \frac{1}{k} \right)^r x_1^{1+\beta-r} \| f \|_{N+1,\beta} \leq C''_\beta \left( \frac{1}{k} \right)^r \left( \frac{1}{M} \right)^{N+1-r} \| f \|_{2,\beta} ,$$

(3.38)

for any $r \in [0, 1+\beta]$.

On the other hand, if $kx_1 < 1$, and defining $f_k(x) := f(x) \exp(ikx)$, (3.32) yields

$$|\tilde{e}_1| = \left| \int_0^{x_1} (f_k(x) - Q_1^{[0,x_1]} f_k(x)) dx \right| \leq \frac{2}{\beta} x_1^{1+\beta} \| f_k \|_{1,\beta} \leq \frac{2}{\beta} \left( \frac{1}{k} \right)^r x_1^{1+\beta-r} \| f \|_{1,\beta} \leq \frac{2}{\beta} \left( \frac{1}{k} \right)^r \left( \frac{1}{M} \right)^{N+1-r} \| f \|_{1,\beta} .$$

(3.39)

and (3.38), (3.39) prove the result for $\beta \in (0, 1)$.

For $\beta \in (-1, 0]$ note that the integral over the first subinterval is approximated by zero, and so the result follows readily from Lemma 3.1 (with $\epsilon = x_1$ and $s = r$).

The proof of the following result now follows directly from Lemmas 3.4 and 3.5.

**Theorem 3.6** Under the same hypothesis as Lemma 3.4, there exists a constant $C$ which depends on $N$, $\beta$ and $q$ such that

$$E_{k,N,M,q}(f) \leq C \left( \frac{1}{k} \right)^r \left( \frac{1}{M} \right)^{N+1-r} \begin{cases} \| f \|_{N+1,\beta} , & \text{when } \beta \in (-1, 0) \cup (0, 1), \\ (1 + \log k)^r (\log M)^{1-r} \| f \|_{N+1,0} , & \text{when } \beta = 0. \end{cases}$$
4 Nonlinear oscillators

In this section we return to the integral \( I_k^{[a,b]}(f,g) \) defined in (4.1), and consider a general nonlinear \( g \). We will assume for simplicity that \( g \in C^\infty[a,b] \). For less smooth \( g \) the arguments will be analogous but the exposition would be more technical. Our methods will be based on the change of variable

\[
\tau = g(x). \tag{4.1}
\]

If \( g \) has no stationary points (i.e. \( g' \) does not vanish), then \( g^{-1} \in C^\infty[a,b] \), \( (g^{-1})' = 1/(g' \circ g^{-1}) \) and

\[
I_k^{[a,b]}(f,g) = I_k^{[g(a),g(b)]}(F), \quad \text{with} \quad F = (f \circ g^{-1})|(g^{-1})'| = (f \circ g^{-1})(g' \circ g^{-1})^{-1}. \tag{4.2}
\]

Now, assuming also that \( f \in C^\infty[a,b] \), then (4.2) can be computed using the FCC rules described in [2] with the additional cost being the evaluation of the inverse function \( g^{-1} \) at the quadrature points. Moreover if \( f \) has singularities then these induce singularities in \( F \) and the composite FCC rules in [3] could be used instead. (Here we assume implicitly that \( g(a) > g(b) \). If \( g(b) > g(a) \) then the integral can be transferred to one over the interval \([g(b),g(a)]\) by a simple affine change of variables. We make similar implicit assumptions below.)

If now \( g \) has a stationary point at one or more \( \xi \in [a,b] \), the transformation (4.1) may still be applied, but singularities appear in \( F \) at the points \( g(\xi) \). To describe these, we may, without loss of generality, consider a single stationary point \( \xi \in [a,b] \) of order \( n \geq 1 \) with property

\[
g'(\xi) = g''(\xi) = \ldots = g^{(n)}(\xi) = 0, \quad g^{(n+1)}(\xi) > 0 \quad \text{and} \quad g'(x) \neq 0, \quad \text{for} \quad x \in [a,b] \setminus \{\xi\}. \tag{4.3}
\]

Then \( g \) is monotone on each of the intervals \([a,\xi] \) and \((\xi,b] \). The change of variables (4.1) can be applied on each interval separately to obtain

\[
I_k^{[a,b]}(f,g) = \left( \int_{g(a)}^{g(\xi)} + \int_{g(\xi)}^{g(b)} \right) F(\tau) \exp(ik\tau)d\tau \tag{4.4}
\]

with \( F \) as in (4.2). (One of the integrals in (4.4) is interpreted as void if \( \xi = a \) or \( b \).) The regularity of the resulting function \( F \) is summarised in the following theorem. Here and throughout the rest of this section we use the convenient notation \( \alpha = 1/(n+1) \).

**Theorem 4.1** Assume that \( f \) and \( g \) are in \( C^\infty[a,b] \) and that \( g \) has a single stationary point \( \xi \) of order \( n \) as in (4.3). Then for each \( p \in \mathbb{N}_0 := \mathbb{N} \cup \{0\} \), there exists \( C_p > 0 \) such that

\[
|F^{(p)}(\tau)| \leq C_p |\tau - g(\xi)|^{n-p-1}, \quad \tau \in [g(a),g(\xi)] \cup (g(\xi),g(b)]. \tag{4.5}
\]

The proof of Theorem 4.1 requires Lemma 4.2 (below) and both these results require the Faà di Bruno formula for the derivatives of the composition of two univariate functions. For \( p \in \mathbb{N}_0 \), let \( f^{(p)} \) denote the \( p \)th derivative of any sufficiently differentiable function \( f \). Then, if \( \phi, \psi \) are suitably smooth functions and the composition \( \phi \circ \psi \) is well-defined, we have the formula

\[
(\phi \circ \psi)^{(p)} = \sum_{m} \frac{p!}{m!} \left( \phi^{(|m|)} \circ \psi \right) \left( \prod_{j=1}^{p} (\psi^{(j)})^{m_j} \right), \tag{4.6}
\]

where the sum in (4.6) is over all multiindices \( m \in (\mathbb{N}_0)^p \) which satisfy \( m_1 + 2m_2 + \ldots + pm_p = p \). Moreover \( |m| = m_1 + m_2 + \ldots + m_p \) and \( m! = m_1!m_2! \ldots m_p! \). A suitable reference is ([20], Theorem 2)].
Lemma 4.2 Assume \( g \in C^\infty[a, b] \) and that \( g \) has a single stationary point \( \xi \) of order \( n \) as in (4.3). Then, for all \( p \in \mathbb{N} \), there exists a constant \( C_p > 0 \) such that
\[
\left| (g^{-1})^{(p)}(\tau) \right| \leq C_p |\tau - g(\xi)|^{n-p}.
\]

Proof. Without loss of generality we assume \( \xi < b \), that \( g \) is increasing in \([\xi, b]\) and we consider the case \( \tau \in (\xi, b) \) only. (The case \( \tau \in [a, \xi) \) is completely analogous.) By Taylor’s theorem with integral remainder and (4.3),
\[
g(x) = g(\xi) + (x - \xi)g'(\xi) + \ldots + \frac{(x - \xi)^n}{n!}g^{(n)}(\xi) + R_\xi(x) = g(\xi) + R_\xi(x),
\]
for all \( x \in (\xi, b) \), where
\[
R_\xi(x) = \frac{1}{n!} \int_\xi^x (x - t)^n g^{(n+1)}(t) \, dt.
\]
With the change of variables \( t \mapsto y = (t - \xi)/(x - \xi) \) in (4.9), we obtain
\[
R_\xi(x) = (x - \xi)^{n+1} T_\xi(x), \quad \text{where} \quad T_\xi(x) = \frac{1}{n!} \int_0^1 (1 - y)^n g^{(n+1)}(\xi + y(x - \xi)) \, dy.
\]
Then, for all \( x \in (\xi, b) \), \( R_\xi(x) > 0 \) and \( T_\xi(x) > 0 \). Also, since \( g \in C^\infty[a, b] \), we have \( T_\xi \in C^\infty[\xi, b] \) and \( T_\xi(\xi) = \frac{1}{(n+1)!} g^{(n+1)}(\xi) > 0 \).

Now, recall \( \alpha = 1/(n + 1) \) and define
\[
h_\xi(x) = (g(x) - g(\xi))^\alpha = (R_\xi(x))^\alpha = (T_\xi(x))^\alpha(x - \xi).
\]
Then \( h_\xi \in C^\infty(\xi, b) \) and, for all \( x \in (\xi, b) \), \( h_\xi'(x) = \alpha(g(x) - g(\xi))^\alpha - 1 g'(x) > 0 \). Moreover since also \( h_\xi(\xi) = (T_\xi(\xi))^\alpha > 0 \) it follows that \( h_\xi \) is positive valued on \([\xi, b]\) and so \( h_\xi : [\xi, b] \to \mathbb{R} \) is invertible and \( (h_\xi)^{-1} \in C^\infty[h_\xi(\xi), h_\xi(b)] \). Thus, inserting (4.11) (and \( x = g^{-1}(\tau) \)) into (4.11), we have
\[
g^{-1}(\tau) = x = h_\xi^{-1}((\tau - g(\xi))^\alpha).
\]
To prove the estimates (4.7) we now apply the Faà di Bruno formula (4.6) with \( \phi = h_\xi^{-1} \) and \( \psi(\tau) = (\tau - g(\xi))^\alpha \) to obtain derivatives of (4.12). Consider any term in the resulting sum (4.6).

Since \( h_\xi^{-1} \) is smooth, the first factor in round brackets is bounded, while the second factor in round brackets can be estimated by
\[
|\tau - g(\xi)|^{(\alpha-1)m_1 + (\alpha-2)m_2 + \ldots + (\alpha-p)m_p},
\]
times a constant. Recalling the remarks following (4.6), the index in (4.13) is \( \alpha/m - p \geq \alpha - p \), so (4.7) follows.

\[
\text{Proof of Theorem 4.1.} \quad \text{Again, without loss of generality, we work with } \tau \in (g(\xi), g(b)]. \quad \text{We first observe that since } g' \text{ is one-signed, so is } (g^{-1})'. \quad \text{Thus we can write } F = \pm(f \circ g^{-1})(g^{-1})' \text{ and hence, by the Leibnitz rule, } F^{(p)} \text{ is a linear combination of terms of the form}
\]
\[
(f \circ g^{-1})^{(l)}(g^{-1})^{(p-l+1)}, \quad l = 0, \ldots, p.
\]
Referring again to formula (4.6), and recalling that \( f \) is smooth, the first term in (4.14) may be estimated by a constant times
\[
\left| \prod_{j=1}^l ((g^{-1})^{(j)})^{m_j} \right|,
\]
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where \( m_1 + 2m_2 + \ldots + lm_l = l \). Using the same argument as in the proof of Lemma 4.2 this product has the estimate \(|τ - g(ξ)|^{α-l}\) (modulo a constant factor).

Now, returning to the products (4.14), we see that for \( l \neq 0 \) each of these can be estimated (modulo a constant factor) by

\[
|τ - g(ξ)|^{α-l}|τ - g(ξ)|^{α-p+1-l} = |τ - g(ξ)|^{2α-p-1}.
\]

However, when \( l = 0 \) the bound is \(|τ - g(ξ)|^{α-p}\) and since \( α > 0 \), the result (4.5) follows. □

### 4.1 Accurate implementation

Now let us return to the computation of (4.2). Under the assumption of Theorem 4.1, we write

\[
I_{k}^{[a,b]}(f,g) = \left( \int_{g(a)}^{g(b)} + \int_{g(ξ)}^{g(ξ)} \right) F(τ) \exp(ikτ)dτ .
\]  

(4.15)

Each of these two integrals can be transformed in an affine way to an integral over \([0, 1]\) so that the singularity is placed at the origin. The composite FCC algorithm given in (3.3) can then be applied, with error estimates given by Theorem 4.4. For example, consider the second integral in (4.15). Under the change of variable \( τ = g(ξ) + c\tilde{ξ} \) where \( c = g(b) - g(ξ) \) and \( \tilde{ξ} \in [0, 1] \) this becomes

\[
I_{k}^{[0,1]}(\tilde{F}) \text{ where } \tilde{F}(\tilde{ξ}) = c\exp(ikg(ξ))F(g(ξ) + c\tilde{ξ}) ,
\]  

(4.16)

and, by Theorem 4.1, \( \tilde{F} \in C_β[0, 1] \), with \( β = α - 1 = -n/(n + 1) \in (-1, 0) \).

In the implementation of the composite FCC rules for (4.16) some care must be taken to accurately evaluate the integrand \( F(g(ξ) + c\tilde{ξ}) \) at very small arguments \( \tilde{ξ} \) (as arise in the case of finely graded meshes). This is a delicate matter since if \( g(ξ) \gg c\tilde{ξ} \), rounding error may pollute the direct calculation of \( g(ξ) + c\tilde{ξ} \), in turn making \( \tilde{F}(\tilde{ξ}) \) inaccurate. To solve this problem, recall that \( F \) is defined in (4.2) in terms of the composition of smooth functions \( f \) and \( g' \) with \( g^{-1} \). Our task is therefore reduced to devising an accurate evaluation of the quantity \( x := g^{-1}(g(ξ) + ε) \) for small \( ε \).

The required \( x \) is then a solution to the equation \( g(x) - g(ξ) = ε \) and, recalling the proof of Lemma 4.2, we see that this is in turn equivalent to \((T_ξ(x))^{α}(x - ξ) = ε^α\). Thus \( x \) solves the nonlinear parameter dependent problem

\[
G(x, ε) := (T_ξ(x))^{α}(x - ξ) - ε^α = 0 .
\]

Since \( T_ξ(ξ) > 0 \) (see also the proof of Lemma 4.2), we have \( G(ξ, 0) = 0 \neq G_x(ξ, 0) \) and so the Implicit Function Theorem implies that, near \( ε = 0 \), \( x \) is a smooth function of \( ε^α \) and there exists a constant \( C_1 \) so that \(|x - ξ| \leq C_1ε^α\), for small enough \( ε \). Moreover \( x \) is also a solution to the fixed point problem

\[
x = ξ + \left( \frac{ε}{T_ξ(x)} \right)^α =: H(x) .
\]

Since \( T_ξ(ξ) > 0 \) and \( T_ξ \) is smooth in a neighbourhood of \( ξ \), it is easy to see that \( H \) is Lipschitz in a ball centred on \( ξ \) and its Lipschitz constant is \( C_2ε^α \) for some constant \( C_2 \). So for small enough \( ε \), \( x \) is the unique fixed point of \( H \) and fixed point iteration converges. This suggests that for \( ε \) small, a suitable approximation to \( x \) can be chosen as \( \tilde{x} := H(ξ) \), with error

\[
|\tilde{x} - x| = |H(ξ) - H(x)| \leq C_2ε^α|ξ - x| = O(ε^2α) .
\]

The approximation \( \tilde{x} \) to \( g^{-1}(g(ξ) + ε) \) when \( ε \) is small is used in the computations in §5.2.
5 Numerical Experiments

In this section, we first carry out some numerical experiments which illustrate the convergence estimates of Theorem 3.6 using computations of the model integral with linear oscillator:

\[ I_{k}^{[0,1]}(f_{\beta}) = \int_{0}^{1} f_{\beta}(x) \exp(ikx) \, dx, \]  

(5.1)

for various \( \beta \in (-1, 1) \), with \( f_{\beta} \) defined in (3.23). Then we compute a model problem with a nonlinear oscillator motivated by the implementation of hybrid numerical-asymptotic boundary integral methods in high-frequency scattering.

5.1 Linear oscillator

Experiment 1

Our first set of experiments studies the case \( M \to \infty \), for fixed \( k \). From Theorem 3.6 with \( r = 0 \), we see that in this case the composite FCC rule for (5.1) should converge with order \( O(M^{-(N+1)}) \) as \( M \to \infty \) provided \( q > (N+1)/(\beta+1) \) for \( \beta \neq 0 \). When \( \beta = 0 \) an additional factor of \( \log M \) appears in the estimate. To illustrate this result we compute the errors \( E_{k,N,M,q}(f_{\beta}) \) for \( k = 1000 \) with various \( N \) and \( q = (N+1)/(\beta+1) + 0.1 \) as \( M \) increases. The exact value of (5.1) can be computed analytically and so the errors can be found exactly. The results for the three values \( \beta = 1/2, 0, -1/4 \) are given in the three sub-tables in Table 1. The columns headed “error” contain the values of \( E_{k,N,M,q}(f_{\beta}) \) while the columns headed “ratio” contain the empirical convergence rates with respect to \( M \) computed by extrapolation. The expected convergence rate is \( N+1 \) (modulo a log factor when \( \beta = 0 \)) and this is given in the row marked “expected ratio”. In all cases the empirical convergence rate is close to the predicted rate, except when the error has almost reached machine precision in which case, naturally, rather unsteady empirical convergence rates are obtained. It is worth noting that in this computation some of the subintervals in the composite rule are very small, in fact with \( N = 8 \) and \( M = 64 \) the smallest subinterval of the mesh is of size about \( 10^{-34} \). Nevertheless the algorithm appears to show no instability and converges to machine precision as \( M \) increases.

Experiment 2

Here we fix \( M = 10, N = 3 \) and \( q = 12 \) and we study convergence as \( k \) increases, for various \( \beta \). In Table 2, the columns headed “ratio” contain the empirical convergence rates with respect to \( M \) computed by extrapolation. From Theorem 3.6 we see that the composite FCC rule for (5.1) should converge with order \( O(k^{-r}) \) as \( k \to \infty \) where \( r < (q(\beta + 1) - (N - 1))/(q - 1) \). In the row marked “best expected ratio” this upper bound on \( r \) is given for each \( \beta \), using our choice of \( N, q \). We see from Table 2 that the empirical convergence rate as \( k \) increases for \( \beta > 0 \) is close to the theoretically predicted best rate of convergence. When \( \beta < 0 \), the empirical rates are a bit slower than the theoretical best rate.

Experiment 3

In Table 3 we study the computation of (5.1) with \( f_{\beta}(x) = \log x \), for \( M = 12 \) and \( N = 3 \) as \( k \) increases for various \( q \). For each value of \( q \) and \( N \), the error of the composite FCC rule should converge with order \( O(k^{-r}) \), with \( r < (q - N - 1)/(q - 1) \). The row marked “best expected ratio” contains the upper bound on \( r \) while the columns marked “ratio” contain the empirical convergence rates. The table shows that when when \( q = 12 \) the empirical convergence rate is
\[ \beta = 1/2 \]

| \( M \) | \( N = 4 \) | \( N = 6 \) | \( N = 8 \) |
|-------|-------|-------|-------|
|       | error | ratio | error | ratio | error | ratio |
| 8     | 4.3e-006 | 5.2e-008 | 1.7e-009 |
| 16    | 5.7e-010 | 6.50e-008 | 8.06e-008 |
| 32    | 7.3e-011 | 2.0e-012 | 9.30e-012 |
| 64    | 8.1e-011 | 6.50e-008 | 6.37e-008 |

| \( \beta = 0 \) | \( N = 4 \) | \( N = 6 \) | \( N = 8 \) |
|-------|-------|-------|-------|
|       | error | ratio | error | ratio | error | ratio |
| 8     | 2.7e-004 | 7.9e-006 | 1.0e-006 |
| 16    | 7.3e-008 | 6.77e-008 | 8.82e-008 |
| 32    | 3.0e-012 | 7.4e-010 | 9.53e-012 |
| 64    | 1.9e-015 | 4.87e-012 | 10.59e-012 |

| \( \beta = -1/4 \) | \( N = 4 \) | \( N = 6 \) | \( N = 8 \) |
|-------|-------|-------|-------|
|       | error | ratio | error | ratio | error | ratio |
| 8     | 4.5e-005 | 1.6e-005 | 6.0e-006 |
| 16    | 8.0e-008 | 7.62e-008 | 8.22e-008 |
| 32    | 9.1e-010 | 6.43e-010 | 10.91e-010 |
| 64    | 3.9e-012 | 7.88e-012 | 8.51e-012 |

Table 1: Numerical Results for Experiment 1

close the the theoretical best rate. When \( q = 4 \), the empirical convergence rate is even better than the best expected rate which in this case indicates that no convergence should be observed at all. On the other hand, when \( q = 8 \) and \( q = 16 \) rather unsteady convergence rates are obtained. However, when \( q = 8 \) as \( k \) increases the empirical rates become bounded by the best expected rate, while for \( q = 16 \) the empirical rates are either bounded by or are slightly better than the the best expected rate.

**Experiment 4**

Here we illustrate the power of the composite FCC rule compared to the non-composite version for computing (5.1) when \( \beta = 1/2 \). The parameter \( N \) for the non-composite FCC rule takes values \( N_i = \{ 24 \times 2^i, i = 0, 1, 2, 3 \} \), while for the composite rule, we fix parameters \( q = 12 \) and \( M = 6 \) and take \( N_i = \{ 4 \times 2^i, i = 0, 1, 2, 3 \} \). The total number of function evaluations in both cases is therefore the same. The superiority of the composite version is clearly seen.

**5.2 An example from boundary integral methods in high-frequency scattering**

Finally, we describe an application to the computation of acoustic scattering at high frequency by numerical-asymptotic methods. When an incident plane wave \( \exp(ikx \cdot d) \) is scattered by a smooth convex sound-soft obstacle with boundary \( \Gamma \), the scattered field can be computed by solving the integral equation

\[
\int_{\Gamma} \mathbf{i} \frac{1}{4} H_0^{(1)}(k|x - y|)v(y) \, ds(y) = \exp(ikx \cdot \hat{d}) , \quad x \in \Gamma.
\]

where \( H_0^{(1)} \) is the Hankel function of the first kind of order 0. (In fact this problem is not well-posed for all values of \( k \) and in practice a related “combined potential” formulation is used. However this formulation illustrates the essential quadrature challenge which arises in all
\[
\beta = \frac{1}{8}, \quad \beta = \frac{1}{4}, \quad \beta = \frac{1}{2}, \quad \beta = \frac{3}{4}
\]

| \(k_i\)   | \(\beta = 1/8\) | \(\beta = 1/4\) | \(\beta = 1/2\) | \(\beta = 3/4\) |
|-----------|-----------------|-----------------|-----------------|-----------------|
|           | error ratio     | error ratio     | error ratio     | error ratio     |
| 10^3      | 4.9e-006        | 4.0e-006        | 1.2e-006        | 2.2e-007        |
| 10^4      | 4.7e-007        | 2.7e-007        | 1.1e-006        | 1.4e-008        |
| 10^5      | 5.7e-008        | 2.6e-008        | 1.0e-007        | 1.3e-009        |
| 10^6      | 1.2e-008        | 3.8e-009        | 8.9e-010        | 1.8e-012        |
| 10^7      | 1.3e-009        | 2.5e-010        | 1.1e-012        | 7.1e-014        |

Table 2: Numerical Results for Experiment 2

| \(k_i\)   | \(\beta = -1/16\) | \(\beta = -1/8\) | \(\beta = -1/4\) | \(\beta = -1/2\) |
|-----------|-------------------|-------------------|-------------------|-------------------|
|           | error ratio       | error ratio       | error ratio       | error ratio       |
| 10^3      | 9.3e-006          | 2.9e-005          | 1.4e-004          | 1.6e-003          |
| 10^4      | 1.5e-006          | 5.4e-006          | 3.7e-005          | 1.2e-003          |
| 10^5      | 2.5e-007          | 1.0e-006          | 8.6e-006          | 4.8e-004          |
| 10^6      | 9.0e-008          | 4.4e-007          | 5.1e-006          | 3.4e-004          |
| 10^7      | 2.3e-008          | 1.5e-007          | 3.1e-006          | 8.0e-004          |

Table 3: Numerical results for Experiment 3

| \(k_i\)   | \(q = 4\) | \(q = 8\) | \(q = 12\) | \(q = 16\) |
|-----------|-----------|-----------|-----------|-----------|
|           | error ratio | error ratio | error ratio | error ratio |
| 10^1      | 5.5e-004  | 1.5e-004  | 1.1e-003  | 3.6e-003  |
| 10^2      | 5.2e-004  | 5.6e-005  | 3.7e-005  | 3.5e-004  |
| 10^3      | 5.2e-004  | 3.3e-005  | 3.8e-005  | 1.0e-004  |
| 10^4      | 5.0e-004  | 6.7e-006  | 7.0e-006  | 8.4e-006  |
| 10^5      | 1.4e-004  | 9.1e-007  | 1.1e-006  | 1.9e-006  |
| 10^6      | 2.0e-005  | 3.9e-007  | 2.0e-007  | 2.4e-007  |
| 10^7      | 1.9e-006  | 1.3e-007  | 5.1e-008  | 8.5e-008  |

Table 4: Numerical results for Experiment 4
formulations. Even for moderate values of $k$ is useful to apply the “physical optics approximation” which amounts to writing $v(y) = V(y) \exp(iky \cdot \hat{d})$, and computing the less oscillatory component $V$ rather than the highly oscillatory $v$ - see [4], [2].

Using the fact that $H_1^0(kr) \exp(-ikr)$ is a non-oscillatory function, smooth for $r > 0$ but with a logarithmic singularity at $r = 0$ and introducing a smooth parameterization $x : [0, 2\pi] \to \Gamma$, the problem above can be reformulated, for $s \in [0, 2\pi]$ as

$$
\int_0^{2\pi} M_k(s, t) \exp(ik \Psi_s(t)) V(t) \, dt = 1, \quad \Psi_s(t) := |x(s) - x(t)| - (x(s) - x(t)) \cdot \hat{d}.
$$

(5.2)

The function $M_k(s, t)$ is non-oscillating and smooth except as $t = s$ where a logarithmic singularity occurs. (More details are in [12].) It can be proved that when $s$ is chosen so that $x(s)$ is in the “illuminated” part of $\Gamma$ (where the incident waves hits the obstacle), there is only one stationary point, i.e., there exists a unique $t$ so that $(\Psi_s)'(t) = 0$. Moreover, $x(t)$ is a point in the shadow part. Conversely, if $x(s)$ lies in the shadow, we have three stationary points, with two of them in the shadow and one in the illuminated part. Thus (5.2) is a good example for application of the methods of [4].

As an illustration we compute the integral in (5.2) when $\Gamma$ is the unit circle, $x(s) = (\cos s, \sin s)$ and set $\hat{d} = (1, 0)$ so that

$$
\Psi_s(t) = 2 \left| \sin \left( \frac{s - t}{2} \right) \right| - \cos s + \cos t.
$$

The integral is computed using the following strategy. First, $[0, 2\pi]$ is divided into subintervals so that each of them contains at most one point which is either the singular point $s$ or a stationary point. Next, any subinterval of length greater than one is split into two subintervals of equal length and this process is continued until we obtain a subdivision of $[0, 2\pi]$ in say $J$ subintervals of length smaller than 1. This is done to avoid working with graded meshes on relatively long intervals. Then, with the change of variable $\tau = \Psi_s(t)$, we have to approximate the integral

$$
\int_{\Psi_s(a_j)}^{\Psi_s(b_j)} F_s(\tau) \exp(ik \tau) \, d\tau, \quad F_s(\tau) := M_k(s, \Psi_s^{-1}(\tau)) V(\Psi_s^{-1}(\tau)) \frac{1}{(\Psi_s)'(\Psi_s^{-1}(\tau))}, \quad j = 1, \ldots, J.
$$

Given $L$ a positive integer, we compute the approximation of these integrals as follows: If $[a_j, b_j]$ does not contain $s$ or a stationary point, the function $F_s$ is smooth, and therefore we can apply the simple Filon Clenshaw-Curtis rule with $\min\{L + 1, 129\}$ points. If $s \in [a_j, b_j]$, after an affine change of variables, $F_s$ belongs to $C_0^\infty[0, 1]$. On the other hand, if either $a_j$ or $b_j$ is a stationary point of order $n \geq 1$, $F \in C_{-n/(n+1)}^\infty[0, 1]$ cf. Theorem 3.6. In both cases, we introduce meshes appropriately graded towards the singularity, according Theorem 3.6 with $L$ subintervals and apply the composite FCC rule with $N + 1$ points. In our experiment we have taken $V \equiv 1$ and $s = 3\pi/4$, which corresponds to a point in the illuminated part. The only stationary point $t = 23\pi/24$ is of order 1.

In Table 5 we display the results obtained with $N = 6$, $q = (N + 1)/(1 + \beta) + 1/10$, which corresponds to $r = 0$ in Theorem 3.6. Here $\beta = 0$ or $-1/2$ depending on the singularity of the integrand. From Theorem 3.6 we can expect that the error decreases with as $O(L^{-7})$ (but there is no predicted decay with respect to $k$ in this case). In Table 6 we give results for $N = 4$ and $q = (N + 1)/(1 + \beta - 1/4) + 1/10$, leading to the error estimate $O(k^{-1/4}L^{-4.75})$. Although the convergence in Table 5 is irregular, in contrast to Table 5 the error decreases with $k$ as predicted by the theory.

In this experiment over 90% of the CPU time is spent in computing the change of variable, since any evaluation in $\tau$ requires the solution of a non-linear equation. This is carried out in our
implementation using the fzero of Matlab. In the case that \((5.2)\) has to be computed for many different functions \(V\), for instance in assembling the matrix of a Boundary Element Method, these calculations have to be done only once, resulting in a speed up of the the method. We run our programs in a modest laptop, a Core 2 Duo with 4Gb of Ram memory, and show in Table 7 the CPU time required to construct some columns of Table 5. We clearly see that the cost is linear in \(L\).

| \(k\)     | \(10\) | \(100\) | \(1,000\) | \(10,000\) | \(100,000\) |
|-----------|--------|--------|----------|------------|------------|
| \(L\)     | error  | ratio  | error    | ratio      | error      | ratio      |
| 12        | 4.5e-07| 2.4e-07| 1.2e-07  | 1.6e-08    | 7.9e-08    |            |
| 24        | 5.0e-09| 6.5    | 1.0e-09  | 6.0        | 3.6        | 6.2        |
| 48        | 4.6e-11| 6.8    | 5.1e-12  | 7.6        | 8.1e-12    | 7.4        |
| 96        | 2.3e-13| 7.6    | 1.1e-13  | 6.8        | 1.0e-13    | 6.3        |
| 192       | 8.3e-15| 4.8    | 6.4e-15  | 4.1        | 1.1e-15    | 6.6        |

Table 5: Results for \(N = 6\), \(M = L\) and \(q = (N + 1)\) for intervals with log singularities and \(q = (N + 1)/(1 - 1/2)\) for integrals having a stationary point (so \(r = 0\)).

| \(k\)     | \(10\) | \(100\) | \(1,000\) | \(10,000\) | \(100,000\) |
|-----------|--------|--------|----------|------------|------------|
| \(L\)     | error  | ratio  | error    | ratio      | error      | ratio      |
| 12        | 4.7e-05| 1.9e-05| 2.4e-06  | 8.2e-07    | 1.8e-07    |            |
| 24        | 6.0e-07| 6.3    | 1.7e-07  | 4.3        | 3.9e-07    | 4.1        |
| 48        | 1.2e-08| 5.7    | 1.4e-08  | 5.0        | 2.4e-08    | 5.9        |
| 96        | 3.1e-10| 5.2    | 3.9e-10  | 5.1        | 7.0e-12    | 5.1        |
| 192       | 1.4e-11| 4.5    | 3.3e-11  | 3.6        | 3.7e-12    | 9.0e-13    |

Table 6: Results for \(N = 4\), \(M = L\) and \(q = (N + 1)/(1 - 1/4)\) for intervals with log singularities and \(q = (N + 1)/(1 - 1/2 - 1/4)\) for intervals having a stationary point (so \(r = 1/4\)).

| \(L\)     | \(k = 10\) | \(k = 1000\) | \(k = 10,000\) |
|-----------|------------|---------------|---------------|
| 12        | 0.77""     | 0.83""        | 0.78""        |
| 24        | 1.41""     | 1.34""        | 1.45""        |
| 48        | 2.44""     | 2.49""        | 2.42""        |
| 96        | 4.50""     | 4.64""        | 4.48""        |
| 192       | 8.48""     | 8.46""        | 8.37""        |

Table 7: CPU time consumed for computing Table 5

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