Quadrature methods for highly oscillatory singular integrals

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Abstract

We address the evaluation of highly oscillatory integrals, with power-law and logarithmic singularities. Such problems arise in numerical methods in engineering. Notably, the evaluation of oscillatory integrals dominates the run-time for wave-enriched boundary integral formulations for wave scattering, and many of these exhibit singularities. We show that the asymptotic behaviour of the integral depends on the integrand and its derivatives at the singular point of the integrand, the stationary points and the endpoints of the integral. A truncated asymptotic expansion achieves an error that decays faster for increasing frequency. Based on the asymptotic analysis, a Filon-type method is constructed to approximate the integral. Unlike an asymptotic expansion, the Filon method achieves high accuracy for both small and large frequency. Complex-valued quadrature involves interpolation at the zeros of polynomials orthogonal to a complex weight function. Numerical results indicate that the complex-valued Gaussian quadrature achieves the highest accuracy when the three methods are compared. However, while it achieves higher accuracy for the same number of function evaluations, it requires significant additional cost of computation of orthogonal polynomials and their zeros.

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1 Introduction

In this paper, we shall consider four kinds of highly oscillatory singular integrals: with singular non-oscillatory component,

$$I[f] = \int_0^b x^{-\alpha} f(x) \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x, \tag{1.1}$$

$$I[f] = \int_0^b \log x f(x) \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x, \tag{1.2}$$

and where the singularity appears in the phase function [22]

$$I[f] = p\int_0^b x^{-\alpha} f(x) \mathrm{e}^{\mathrm{i}\omega x^{-p}} \mathrm{d}x, \quad \alpha \in (0,1), \quad p > 0, \tag{1.3}$$

$$I[f] = \int_0^b \log x f(x) \mathrm{e}^{\mathrm{i}\omega \log x} \mathrm{d}x, \tag{1.4}$$

where f and g are sufficiently smooth functions, independent of $|\omega| \gg 1$.

Oscillatory integrals are encountered in a wide range of applications in science and engineering. In cases where the integrand exhibits a singularity of one of the above types, this further complicates the evaluation of the integral. Such integrals arise in applications in electromagnetics [17, 18] and electromagnetic shielding problems [10]. In the present work we focus on the frequency-domain, wave-enriched boundary integral formulations as a particular example to motivate this work.

Acoustic wave propagation problems in 2-D unbounded regions are governed by the Helmholtz differential equation

$$\Delta u(\mathrm{p}) + \omega^2 u(\mathrm{p}) = 0, \quad \mathrm{p} \in \mathbb{R}^2 \backslash \overline{\Omega},$$

where $u \in \mathbb{C}$ is the acoustic potential sought as the solution, p is the position, λ is the wave length, $\omega = 2\pi/\lambda$, Ω is a bounded obstacle with a boundary Γ and $\overline{\Omega} = \Omega \cup \Gamma$. Three classical numerical methods that are widely used in industry for the analysis of wave propagation problems are the Finite Difference Method (FDM), Finite Element Method (FEM) and Boundary Element Method (BEM). However, complications arise for wave scattering problems in infinite domains. In particular, FDM and FEM discretisations require truncation of the domain and the application of some non-reflecting boundary conditions on the artificial exterior boundary. BEM formulations are therefore often preferable to volumetric discretisations for these problems since the meshing is restricted to the boundary of the scatterer(s), leading to the efficient solution of problems in unbounded geometries.

The first step of the BEM is to transform the Helmholtz equation into a boundary integral equation. The Robin boundary condition

$$\nabla u(\mathrm{q}) \cdot n(\mathrm{q}) = \gamma u(\mathrm{q}) + \beta, \quad \mathrm{q} \in \Gamma$$

is imposed, where γ and β may be derived from the impedance characteristics of the material(s) forming the scatterer boundaries, and $n(\mathrm{q})$ is the unit normal at q pointing outward from the solution domain. Applying Green' second theorem and Sommerfeld radiation conditions yields the boundary integral equation

$$\frac{u(\mathrm{p})}{2} + \int_\Gamma \left[\frac{\partial G(\mathrm{p},\mathrm{q})}{\partial \mathrm{n}(\mathrm{q})} - \gamma G(\mathrm{p},\mathrm{q})\right] u(\mathrm{q}) \mathrm{d}\Gamma_\mathrm{q} = \int_\Gamma \beta G(\mathrm{p},\mathrm{q}) \mathrm{d}\Gamma(q) + u^i(\mathrm{p}),$$

where G is the Green's function for the Helmholtz equation and u^i is the incident wave. The source point is $\mathrm{p} \in \Gamma$ and the observation point is q. To discretise the boundary integral equation, the boundary (line) Γ is partitioned into N_e elements and each element e is mapped onto the parametric space, $\Gamma = \sum_{e=1}^{N_e} \Gamma_e$, $\Gamma_e = \{q(\xi) : \xi \in [-1, 1]\}$. The traditional boundary element expansion for the potential at a point q on an element e is

$$\sum_{j=1}^{J} N_j(\xi)\hat{u}_j,$$

where J is the number of nodes of the element and N_j is the usual Lagrangian polynomial shape function for node j. Applying the collocation method results in the linear algebraic system

$$(\mathcal{C} + \mathcal{S} + \mathcal{D})\, \hat{\mathrm{u}} = \hat{\mathrm{f}},$$

where $\mathcal{C}$ is the identity matrix. Each entry of matrices $\mathcal{S} = \{\mathcal{S}_{ej}\}$ and $\mathcal{D} = \{\mathcal{D}_{ej}\}$ can be represented by the integrals

$$\begin{aligned}
\mathcal{S}_{ej} &= \int_{-1}^{1} H_1^{(1)}(\omega \mathrm{r}(\xi)) N_j(\xi) \frac{\partial \mathrm{r}(\xi)}{\partial n(\xi)} |J| \mathrm{d}\xi, \\
\mathcal{D}_{ej} &= \int_{-1}^{1} H_0^{(1)}(\omega \mathrm{r}(\xi)) \alpha(q(\xi)) N_j(\xi) |J| \mathrm{d}\xi,
\end{aligned}$$

where $H_0^{(1)}(\cdot)$ and $H_1^{(1)}(\cdot)$ are the Hankel functions of the first kind and order 0 and 1, respectively. The distance is denoted by $\mathrm{r} = |\mathrm{q} - \mathrm{p}|$, while J is a Jacobian defined by $\mathrm{d}\Gamma = J(\xi)\mathrm{d}\xi$. Once the coefficient matrices are determined, application of an iterative method yields the numerical solution.

However, if the parameter ω is very large, the wavelength under consideration is much less than the dimension of the scatterer. A consequence of this is that a greater degree of discretisation is required to accurately determine the oscillatory solution u using traditional quadrature methods. The dimension of the collocation matrices therefore increases with the parameter ω as $\mathcal{O}\left(\omega^d\right)$, where d is the dimension of the problem.

To reduce the dependence on ω, high-frequency BEMs have been presented. These methods select the product of a polynomial and oscillatory functions as the basis, replacing N_j. The new basis can approximate the oscillatory solution more accurately. One effective method is the Hybrid Numerical Asymptotic BEM (HNA-BEM) [4, 8]. However, this requires some properties of the solution to be known in advance. An alternative is the Partition of Unity Boundary Element Method (PUBEM) [21], whereby the plane wave enrichment

$$\begin{gathered}
\sum_{j=1}^{J} N_j(\xi) \sum_{m=1}^{M} A_{jm} \mathrm{e}^{\mathrm{i}\omega \mathrm{d}_{jm} \cdot \mathrm{q}(\xi)}, \\
\mathrm{d}_{jm} = (\cos\theta_{jm}, \sin\theta_{jm}), \quad \theta_{jm} = \frac{2\pi(m-1)}{M} + \theta^I
\end{gathered}$$

is proposed, where A_{jm} is the unknown amplitude of the basis function $N_j(\xi_e)\mathrm{e}^{\mathrm{i}\omega \mathrm{d}_{jm} \cdot \mathrm{q}}$ and θ^I is the incident angle. This has been shown to bring about a large reduction in the requirement size for short-wave scattering problems, from 10 degrees of freedom to 2–3 per wavelength. However, this reduction comes at the cost of a requirement to evaluate a large number of highly oscillatory integrals of the form

$$-\frac{\mathrm{i}\gamma}{4} \int_{-1}^{1} H_0^{(1)}(\omega \mathrm{r}) N_j(\xi) \mathrm{e}^{\mathrm{i}\omega \mathrm{d}_m \cdot \mathrm{q}(\xi)} J(\xi) \mathrm{d}\xi.$$

A numerical steepest descent method was successfully applied for this integral in [11] to reduce the computational effort. Yet, this approach needs careful implementation in order to be robust in the presence of singularities in the integrand in the complex plane formed on a real axis aligned with ξ. To design a robust and effective quadrature method, we are interested in the asymptotic analysis of this kind of integral. Note that as the distance r goes to zero, the Hankel function behaves as

$$H_0^{(1)}(\omega\mathrm{r}) \sim \frac{2\mathrm{i}}{\pi}\log(\omega\mathrm{r}),$$

referenced from the website `http://dlmf.nist.gov/10.7`. This calls for asymptotic analysis of a highly oscillatory integral with a logarithmic singularity.

The computation of the highly oscillatory integrals, even without singularity, by conventional quadrature methods is exceedingly expensive and inefficient: essentially, the number of quadrature points [5] must be $\mathcal{O}(\omega)$ and this becomes prohibitive for large $|\omega|$. Unlike traditional quadrature methods, based upon local Taylor expansions, a new type of highly oscillatory quadrature algorithms – asymptotic expansions and Filon-type methods introduced by Iserles and Nørsett [13, 14], Levin methods [7, 16, 20] and the numerical steepest descent methods of Huybrechs and Vandewalle [12] – excel in the presence of high oscillation. All such methods are based upon asymptotic expansions and their accuracy scales like $\mathcal{O}\left(\omega^{-p-1}\right)$ for some $p \geq 1$. In other words, their precision *increases* with growing frequency, while cost remains constant. Furthermore, complex-valued Gaussian quadrature studied in [2, 6] attains an optimal asymptotic order and exceedingly small error. All such methods build upon an asymptotic expansion [7] of the solution in inverse (but not necessarily integer) powers of ω. The existing theory of highly oscillatory quadrature, however, does not extend to the presence of singular integrands. The extension is nontrivial because the weak singularity at the origin interacts with other aspects of the asymptotic expansion.

We note in passing that the computation of singular highly oscillatory integrals has been already considered in literature [1, 9, 15, 19]. For the weak singularities mentioned in this paper, although there are some estimates provided, such as [24], asymptotic analysis is incomplete, as is the design of effective quadrature methods. The theme of this paper is the development of efficient quadrature schemes for integrals of the form of (1.1–1.4). This is not a straightforward generalisation of standard theory and it compels us to commence from asymptotic analysis of highly oscillatory singular integrals to provide insight into the subsequent development of quadrature schemes.

We explore three typical quadrature schemes for highly oscillatory integration with singularities. Their asymptotic properties and related expansions are formulated in Section 2. Based on this analysis, Filon methods are constructed in Section 3. Both sections are accompanied by relevant numerical examples. Section 4 displays the numerical results for complex-valued Gaussian quadrature.

The main ideas that have inspired modern analysis of highly oscillatory integrals – in particular asymptotic expansions and Filon-type methods – form the cornerstone of this paper. While these ideas are not new and the analysis of this paper follows along similar signposts as [7], the analysis is considerably more demanding and presence of singularities calls for much extra care.

Before we commence asymptotic analysis, we first define generalised moments of $I[f]$

in (1.1) and (1.2)

$$\begin{aligned}\mu_j(\alpha,\omega) &= \int_0^b x^{j-\alpha}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x,\\ \nu_j(\omega) &= \int_0^b x^j \log x \mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x.\end{aligned}$$

2 Asymptotic analysis of highly oscillatory integrals with power-law and logarithmic singularities

In this section we are concerned with the asymptotic analysis of highly oscillatory power-law integrals (1.1, 1.3) and logarithmic integrals (1.2, 1.4). Given that the presence of a stationary point is a game changer in asymptotic analysis, we will present the theory first without and subsequently with stationary points.

2.1 Asymptotic analysis of power-law singularity

We commence with the case $g'(x) \neq 0$ for the integral (1.1). In contrast to the non-singular oscillatory integral [14], our first step is to examine the behaviour of the moment function $\mu(\alpha,\omega)$, an essential ingredient in asymptotic analysis. Firstly, the moment function is bounded,

$$|\mu_0(\alpha,\omega)| = \left|\int_0^b x^{-\alpha}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x\right| \leq \int_0^b x^{-\alpha}\mathrm{d}x = \frac{b^{1-\alpha}}{1-\alpha}.$$

To get a sharper upper bound, we separate the interval of integration into

$$\int_0^b x^{-\alpha}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x = \int_0^\varepsilon x^{-\alpha}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x + \int_\varepsilon^b x^{-\alpha}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x,$$

where a small number $\varepsilon > 0$ will be set momentarily. Different choices of ε determine different upper bounds and in the next lemma we choose an optimal value of ε to get the lowest upper bound.

Lemma 1. *Given $\omega \gg 1$ and $g'(x) \neq 0$, $x \in [0,b]$, the zeroth moment function $\mu_0(\alpha,\omega)$ satisfies*

$$|\mu_0(\alpha,\omega)| = \left|\int_0^b x^{-\alpha}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x\right| \sim \mathcal{O}\Big(\omega^{-(1-\alpha)}\Big).$$

Proof. Assume a small number $\varepsilon > 0$. We write the moment in the form

$$\int_0^b x^{-\alpha}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x = \int_0^\varepsilon x^{-\alpha}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x + \int_\varepsilon^b x^{-\alpha}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x.$$

The first integral on the right side is $\mathcal{O}\left(\varepsilon^{1-\alpha}\right)$. The remaining integral is non-singular and can be calculated using integration by parts,

$$\begin{aligned}\int_\varepsilon^b x^{-\alpha}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x &= \frac{1}{\mathrm{i}\omega}\left[\frac{b^{-\alpha}}{g'(b)}\mathrm{e}^{\mathrm{i}\omega g(b)} - \frac{\varepsilon^{-\alpha}}{g'(\varepsilon)}\mathrm{e}^{\mathrm{i}\omega g(\varepsilon)}\right]\\ &\quad - \frac{1}{\mathrm{i}\omega}\int_\varepsilon^b \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{x^{-\alpha}}{g'(x)}\right)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x \sim \mathcal{O}\left(\omega^{-1}\varepsilon^{-\alpha}\right).\end{aligned}$$

Together then, the integral is bounded by $\mathcal{O}\left(\varepsilon^{1-\alpha}\right) + \mathcal{O}\left(\omega^{-1}\varepsilon^{-\alpha}\right)$. We take $\varepsilon = \omega^{-1}$ to get the desired result. □

It directly follows from Lemma 1 that

$$\left|\int_0^b x^{-\alpha} f(x) \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x\right| \leq C_1 \omega^{-(1-\alpha)}, \tag{2.1}$$

where f is a sufficiently smooth function and the constant C_1 is related to the upper bound of f.

Based on (2.1), we deduce the following theorem.

Theorem 2. *Assume that f is a smooth function and $g'(x) \neq 0$. Then for $s \in \mathbb{N}$ and $\omega \gg 1$, the first $2s$ terms of the asymptotic expansion of $I[f]$ are*

$$Q^{A,s}[f] \sim \mu_0(\alpha,\omega) \sum_{k=0}^{s-1} \frac{1}{(-i\omega)^k} \sigma_k[f](0) - \sum_{k=1}^{s} \frac{1}{(-i\omega)^k} \frac{\sigma_{k-1}[f](b) - \sigma_{k-1}[f](0)}{b^\alpha g'(b)} \mathrm{e}^{\mathrm{i}\omega g(b)},$$

where

$$\begin{aligned} \sigma_0[f](x) &= f(x), \\ \sigma_{k+1}[f](x) &= x^\alpha \frac{\mathrm{d}}{\mathrm{d}x} \frac{\sigma_k[f](x) - \sigma_k[f](0)}{x^\alpha g'(x)}, \qquad k \geq 0. \end{aligned}$$

The corresponding asymptotic error is

$$I[f] - Q^{A,s}[f] \sim \mathcal{O}\Big(\omega^{-s-(1-\alpha)}\Big), \qquad |\omega| \gg 1. \tag{2.2}$$

The proof is given in Appendix A.1.

In particular, in the important case of the Fourier oscillator $g(x) = x$ with $\omega \gg 1$, we have

$$\int_0^b x^{-\alpha} f(x) \mathrm{e}^{\mathrm{i}\omega x} \mathrm{d}x \sim \mu_0(\alpha,\omega) \sum_{k=0}^{s-1} \frac{1}{(-\mathrm{i}\omega)^k} \sigma_k[f](0) - \sum_{k=1}^{s} \frac{1}{(-\mathrm{i}\omega)^k} \frac{\sigma_{k-1}(b) - \sigma_{k-1}(0)}{b^\alpha} \mathrm{e}^{\mathrm{i}\omega b},$$

where

$$\sigma_k(x) = \sum_{j=0}^{\infty} \frac{(j+k-\alpha)\cdots(j+2-\alpha)(j+1-\alpha)}{(j+k)!} f^{(j+k)}(0) x^j, \qquad k \geq 0.$$

Also in the case of a stationary point the key to asymptotic analysis is repeated integration by parts. Once $g'(x) = 0$ at one or more points in $[0, b]$, the form of the asymptotic expansion depends on the stationary points, the endpoints and the order of the singularity. Assume for simplicity that the integral (1.1) possesses just a single stationary point at $\xi \in [0, b]$. (The extension to the case of more stationary points is straightforward.) In addition, we only explore the asymptotic analysis for $\xi = 0$ since the case $\xi > 0$ is very similar but somewhat easier. To start with, we analyse the asymptotic order of the moment $\mu_j(\alpha,\omega)$ based on the method of stationary phase [3, p. 279], generalising the familiar *van der Corput lemma* [23] to the setting of integrands with singularities.

Lemma 3. *Suppose that $\omega \gg 1$ and $g(x)$ has a stationary point of order r at $x = 0$, that is $g'(0) = \cdots = g^{(r)}(0) = 0$, $g^{(r+1)}(0) \neq 0$, then*

$$|\mu_j(\alpha,\omega)| = \left|\int_0^b x^{j-\alpha} \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x\right| \sim \mathcal{O}\Big(\omega^{-\min\left(\frac{j+1-\alpha}{r+1},1\right)}\Big). \tag{2.3}$$

Proof. We separate μ_j into two terms:

$$\int_0^b x^{j-\alpha} \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x = \int_0^\infty - \int_b^\infty .$$

Using integration by parts, the second integral on the right behaves as

$$\int_b^\infty x^{j-\alpha} \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x \sim \mathcal{O}\big(\omega^{-1}\big) ,$$

since it is a proper integral without a stationary point in the interval $[b, \infty]$.

Here, without loss of generality, we assume $g(0) = 0$. To obtain the essential behaviour of the first integral on the right, we expand the function $g(x)$ in a Taylor series

$$g(x) \sim \sum_{m=0}^{r} \frac{g^{(m)}(0)}{m!} x^m + \frac{g^{(r+1)}(x)}{(r+1)!} x^{r+1} + \cdots = \frac{g^{(r+1)}(\xi)}{(r+1)!} x^{r+1}$$

for some $\xi \in [0, x]$, since $g^{(m)}(0) = 0$, $m = 0, 1, \cdots, r$, and $g^{(r+1)}(0) \neq 0$. This gives

$$\int_0^\infty x^{j-\alpha} \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x \sim \int_0^\infty x^{j-\alpha} \mathrm{e}^{\mathrm{i}\omega \frac{g^{(r+1)}(\xi)}{(r+1)!} x^{r+1}} \mathrm{d}x.$$

Then we rotate the contour of integration from the real-x axis by an angle $\frac{\pi}{2(r+1)}$ if $g^{(r+1)}(\xi) > 0$ and make the substitution

$$x = \mathrm{e}^{\frac{\mathrm{i}\pi}{2(r+1)}} \left[\frac{(r+1)!u}{\omega g^{(r+1)}(\xi)} \right]^{1/(r+1)} ,$$

where u is real (we rotate by an angle $\frac{-\pi}{2(r+1)}$ if $g^{(r+1)}(\xi) < 0$ with $x = \mathrm{e}^{\frac{-\mathrm{i}\pi}{2(r+1)}} \left[\frac{(r+1)!u}{\omega |g^{(r+1)}(\xi)|} \right]^{1/(r+1)}$). This yields

$$\begin{aligned} \int_0^\infty x^{j-\alpha} \mathrm{e}^{\mathrm{i}\omega \frac{g^{(r+1)}(\xi)}{(r+1)!} x^{r+1}} \mathrm{d}x \quad &\sim \quad C\omega^{-\frac{j+1-\alpha}{r+1}} \int_0^\infty e^{-u} u^{\frac{j+1-\alpha}{r+1}-1} \mathrm{d}u \\ &\sim \quad C\omega^{-\frac{j+1-\alpha}{r+1}} \Gamma\left(\frac{j+1-\alpha}{r+1}\right) \sim \mathcal{O}\left(\omega^{-\frac{j+1-\alpha}{r+1}}\right) . \end{aligned}$$

Comparing the two orders, it follows that

$$|\mu_j(\alpha, \omega)| \sim \mathcal{O}\left(\max\left(\omega^{-\frac{j+1-\alpha}{r+1}}, \omega^{-1}\right)\right) .$$

Thus, we arrive at the exponent $\min\left(\frac{j+1-\alpha}{r+1}, 1\right)$. This completes the proof of (2.3). $\square$

Based on Lemma 3, it follows that

$$\left| \int_0^b x^{-\alpha} f(x) \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x \right| \leq C_2 \omega^{-\frac{1-\alpha}{r+1}}, \tag{2.4}$$

where the constant C_2 is related to the bound of the smooth function f as $\omega \to \infty$.

We commence from the basic case $g'(0) = 0$, $g''(0) \neq 0$: progression to the general setting will be easy.

Theorem 4. *Assume that $g'(0)=0$, $g''(0)\neq 0$ and $g'(x)\neq 0$, $x\in(0,b]$. For every smooth function f and $\omega \gg 0$, it is true that*

$$\begin{aligned} I[f] \;\sim\; & \mu_0(\alpha,\omega)\sum_{k=0}^{s-1}\frac{\rho_k[f](0)}{(-\mathrm{i}\omega)^k}+\mu_1(\alpha,\omega)\sum_{k=0}^{s-1}\frac{\rho_k'[f](0)}{(-\mathrm{i}\omega)^k} \\ & -\sum_{k=1}^{s}\frac{1}{(-\mathrm{i}\omega)^k}\frac{\rho_{k-1}[f](b)-\rho_{k-1}[f](0)-\rho_{k-1}'[f](0)b}{b^\alpha g'(b)}\mathrm{e}^{\mathrm{i}\omega g(b)} \end{aligned} \tag{2.5}$$

with an error of $\mathcal{O}\left(\omega^{-s-(1-\alpha)/2}\right)$, where

$$\begin{aligned} &\rho_0[f](x)=f(x), \\ &\rho_k[f](x)=x^\alpha\frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\rho_{k-1}[f](x)-\rho_{k-1}[f](0)-\rho_{k-1}'[f](0)x}{x^\alpha g'(x)}\right], \qquad k\geq 1. \end{aligned}$$

Letting $s\to\infty$ we obtain the asymptotic expansion of $I[f]$.

Proof. Following along the same lines as Theorem 2 and Lemma 3. We omit the details for the sake of brevity. □

Integrals with higher-order stationary points are important and common in applications [23]. The asymptotic expansion in Theorem 2 can be readily extended to the case of $g(x)$ having a single stationary point of order $r\geq 1$ at 0, in other words

$$0=g(0)=g'(0)=\cdots=g^{(r)}(0)=0, \qquad g^{(r+1)}(0)\neq 0$$

and $g'(x)\neq 0$ for $x\in(0,b]$. If $g(0)\neq 0$, we can simply transform the integral into the form

$$I[f]=\int_0^b x^{-\alpha}f(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x=\mathrm{e}^{\mathrm{i}\omega g(\xi)}\int_0^b x^{-\alpha}f(x)\mathrm{e}^{\mathrm{i}\omega[g(x)-g(\xi)]}\mathrm{d}x.$$

Consequently, setting

$$\begin{aligned} \rho_0[f](x) &= f(x), \\ \rho_{k+1}[f](x) &= x^\alpha\frac{\mathrm{d}}{\mathrm{d}x}\frac{\rho_k[f](x)-\sum_{j=0}^{r}\frac{\rho_k^{(j)}[f](0)}{j!}x^j}{x^\alpha g'(x)}, \qquad k\geq 0, \end{aligned}$$

we obtain the general form of the asymptotic expansion,

$$I[f]\sim\sum_{j=0}^{r}\frac{\mu_j(\alpha,\omega)}{j!}\sum_{k=0}^{s-1}\frac{\rho_k^{(j)}[f](0)}{(-i\omega)^k}-\sum_{k=1}^{s}\frac{\mathrm{e}^{\mathrm{i}\omega g(b)}}{(-i\omega)^k}\frac{\rho_{k-1}[f](b)-\sum_{j=0}^{r}\frac{\rho_{k-1}^{(j)}[f](0)}{j!}b^j}{b^\alpha g'(b)}, \tag{2.6}$$

the remainder term being $O\Big(\omega^{-(s+\frac{1-\alpha}{r+1})}\Big)$.

As we have shown in our analysis, evaluating the integral by computing a truncation of (2.6) can reduce the asymptotic error very effectively indeed for $|\omega|\gg 1$. However, it does not work for a small $|\omega|$. We consider the integral without stationary points

$$\int_0^1 x^{-\alpha}f(x)\mathrm{e}^{\mathrm{i}\omega x}\mathrm{d}x \tag{2.7}$$

where $f(x) = (1+x)^{-1}$ and $\alpha = \frac{1}{2}$, which also will be considered as a test example for the Filon method and complex-valued Gaussian quadrature, which will be considered in the sequel. This is a form of singularity in the PUBEM integrals. The terms in the truncated expansion for $s = 1, 2, 3$ are

$$\begin{aligned} Q^{A,1}[f](\omega) &= \mu_0(\alpha,\omega) + \frac{\mathrm{i}}{2\omega}\mathrm{e}^{\mathrm{i}\omega}, \\ &\quad \text{originating in } f(0), f(1); \\ Q^{A,2}[f](\omega) &= Q^{A,1}[f](\omega) - \frac{\mathrm{i}}{2\omega}\mu_0(\alpha,\omega) + \frac{\mathrm{e}^{\mathrm{i}\omega}}{2\omega^2}, \\ &\quad \text{originating in } f(0), f'(0), f(1), f'(1); \\ Q^{A,3}[f](\omega) &= Q^{A,2}[f](\omega) - \frac{3}{4\omega^2}\mu_0(\alpha,\omega) - \frac{7\mathrm{i}}{8\omega^3}\mathrm{e}^{\mathrm{i}\omega}, \\ &\quad \text{originating in } f(0), f'(0), f''(0), f(1), f'(1), f''(0), \end{aligned}$$

and their asymptotic error is $\mathcal{O}\left(\omega^{-s-\frac{1}{2}}\right)$. In Fig. 2.1 we depict the magnitude of the error, $\log_{10}\left|Q^{A,s}[f] - I[f]\right|$, $s = 1, 2, 3$. As we mentioned, the error blows up near $\omega = 0$ and decreases rapidly when $\omega > 10$. Needless to say, an inclusion of more terms in the expansion produces a better error for $|\omega| \gg 1$.

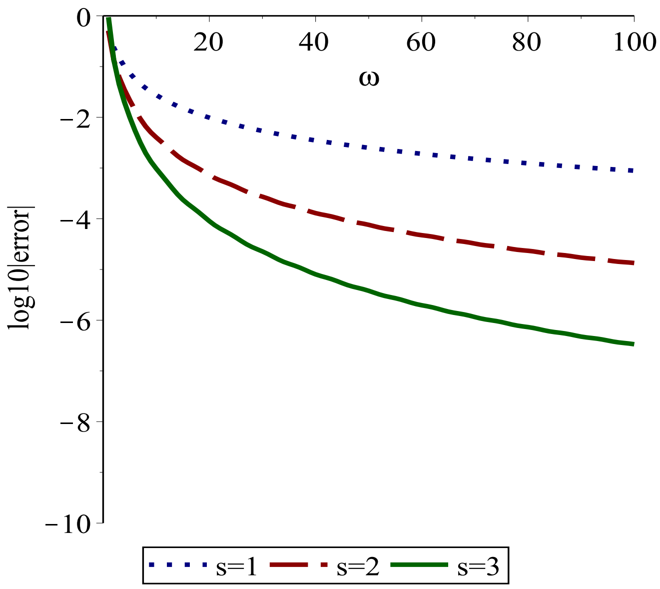

Figure 2.1: The error $\log_{10}\left|Q^{A,s}[f] - I[f]\right|$ with $x^{-\frac{1}{2}}$ and $g(x) = x$. The colours are navy blue (the top, dotted), dark red (the middle, dashed) and dark green (the bottom, solid) for $s = 1, 2, 3$.

We now consider the same example but with an order-1 stationary point, i.e. calculate the integral

$$\int_0^1 x^{-\alpha} f(x) \mathrm{e}^{\mathrm{i}\omega x^2} \mathrm{d}x \tag{2.8}$$

where $f(x) = (1+x)^{-1}$, $\alpha = \frac{1}{2}$. Throughout this paper, this integral will be calculated as an example with a stationary point to illustrate the performance of different numerical quadratures. We truncate the expansion in Theorem 2 as $Q^{A,s}[f]$, $s = 1, 2, 3$ with the asymptotic error $\mathcal{O}\left(\omega^{-s-\frac{1}{4}}\right)$,

$$\begin{aligned}
Q^{A,1}[f](\omega) &= \mu_0(\alpha,\omega) - \mu_1(\alpha,\omega) - \frac{\mathrm{i}}{4\omega}\mathrm{e}^{\mathrm{i}\omega}, \\
&\quad \text{originating in } f(1), f^{(j)}(0), \quad j=0,1; \\
Q^{A,2}[f](\omega) &= Q^{A,1}[f](\omega) + \frac{\mathrm{i}}{4\omega}\mu_0(\alpha,\omega) - \frac{3\mathrm{i}}{4\omega}\mu_1(\alpha,\omega) + \frac{\mathrm{e}^{\mathrm{i}\omega}}{4\omega^2}, \\
&\quad \text{originating in } f(1), f'(1), f^{(j)}(0), \quad j=0,\cdots,3; \\
Q^{A,3}[f](\omega) &= Q^{A,2}[f](\omega) + \frac{-5}{16\omega^2}\mu_0(\alpha,\omega) + \frac{21}{16\omega^2}\mu_1(\alpha,\omega) + \frac{31\mathrm{i}}{64\omega^3}\mathrm{e}^{\mathrm{i}\omega}, \\
&\quad \text{originating in } f(1), f'(1), f''(1), f^{(j)}(0), \quad j=0,\cdots,5.
\end{aligned}$$

Fig. 2.2 demonstrates the error order of the asymptotic expansion for different terms. Similar error behaviour has been observed in Figs. 2.1 and 2.2 and it is evident that the stationary point is not detrimental to the performance of the asymptotic method, provided that we subtract the singularity originating in both the stationary point and singular points.

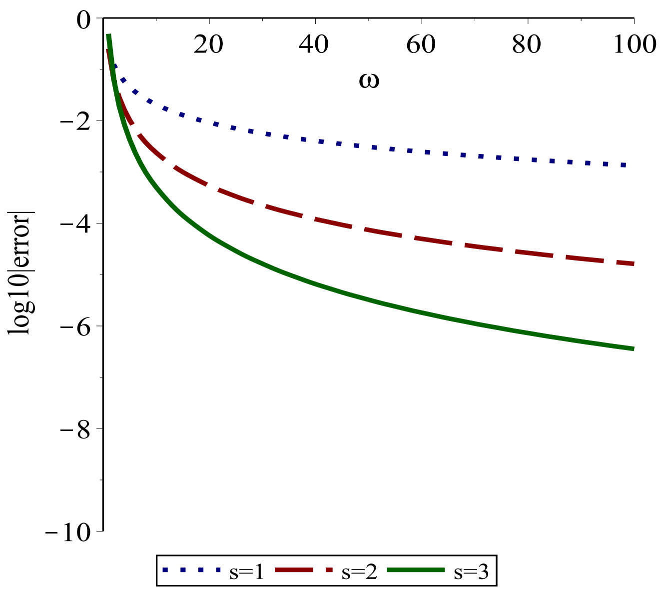

Figure 2.2: The error $\log_{10}\left|Q^{A,s}[f] - I[f]\right|$ with $x^{-\frac{1}{2}}$ and $g(x) = x^2$, for $s = 1$ (navy blue, the top, dotted), $s = 2$ (dark red, the middle, dashed), $s = 3$ (dark green, the bottom, solid).

2.2 Asymptotic analysis for logarithmic singularity

Our second instance of a singular oscillatory integral originates in the logarithmic singularity (1.2). Our analysis is similar to the case of a power-law singularity, hence we present it with greater brevity. As before, we commence with the case without a stationary point, i.e $g' \neq 0$, $x \in [0, b]$. In that case

$$\begin{aligned}
I[f] &= \int_0^b \log x f(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x \\
&= \int_0^b \log x \left[f(x) - f(0)\right]\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x + f(0)\int_0^b \log x \mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x
\end{aligned}$$

$$= \int_0^b \log x \, [f(x) - f(0)] \, \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x + f(0)\nu_0,$$

where

$$\nu_k = \int_0^b x^k \log x \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x, \qquad k \geq 0.$$

The function $\log x \, [f(x) - f(0)]$ is non-singular and analytic in the interval $[0, b]$. We define

$$\begin{aligned}
\sigma_0[f](x) &= f(x), \\
\sigma_j[f](x) &= \frac{\mathrm{d}}{\mathrm{d}x} \left[\frac{\sigma_{j-1}[f](x) - \sigma_{j-1}[f](0)}{g'(x)} \right], \qquad j = 1, \ldots, k+1.
\end{aligned}$$

Integrating by parts,

$$\begin{aligned}
I[f] &= \int_0^b \log x \, [f(x) - f(0)] \, \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x + f(0) \, \nu_0 \\
&= f(0)\nu_0 + \frac{1}{\mathrm{i}\omega} \int_0^b \log x \frac{(f(x) - f(0))}{g'(x)} \mathrm{d}\mathrm{e}^{\mathrm{i}\omega g(x)} \\
&= f(0)\nu_0 + \frac{1}{\mathrm{i}\omega} \left[\log x \frac{f(x) - f(0)}{g'(x)} \right] \mathrm{e}^{\mathrm{i}\omega g(x)} \Big|_0^b - \frac{1}{\mathrm{i}\omega} \int_0^b \frac{f(x) - f(0)}{x g'(x)} \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x \\
&\quad - \frac{1}{\mathrm{i}\omega} \int_0^b \log x \sigma_1[f](x) \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x.
\end{aligned}$$

Iterating the procedure results in the asymptotic expansion

$$\begin{aligned}
I[f] &= \nu_0(\omega) \sum_{k=0}^{s-1} \frac{\sigma_k[f](0)}{(-\mathrm{i}\omega)^k} - \sum_{k=1}^{s} \frac{\mathrm{e}^{\mathrm{i}\omega g(b)}}{(-\mathrm{i}\omega)^k} \frac{\log b \, (\sigma_{k-1}[f](b) - \sigma_{k-1}[f](0))}{g'(b)} \\
&\quad + \sum_{k=1}^{s} \frac{1}{(-\mathrm{i}\omega)^k} \int_0^b \frac{\sigma_{k-1}[f](x) - \sigma_{k-1}[f](0)}{x g'(x)} \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x \\
&\quad + \frac{1}{(-\mathrm{i}\omega)^s} \int_0^b \log x \sigma_s[f](x) \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x, \qquad (2.9)
\end{aligned}$$

provided that

$$\lim_{x \to 0} \left[\log x \frac{(\sigma_{k-1}[f](x) - \sigma_{k-1}[f](0))}{g'(x)} \right] = 0.$$

Note the presence of non-singular highly oscillatory integrals in the expansion.

Before determining the asymptotic order of (2.9), we need to estimate the behaviour of the zeroth moment. The following lemma clarifies this issue.

Lemma 5. *Given $\omega \gg 1$ and $g'(x) \neq 0$, $x \in [0, b]$, the function $\nu_0(\omega)$ satisfies*

$$|\nu_0(\omega)| = \left| \int_0^b \log x \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x \right| \sim \mathcal{O}\big(\omega^{-1} \log \omega\big) .$$

Proof. Similar to that of Lemma 3. Consider a small positive number $\varepsilon \to 0$ and separate the integral into two parts

$$\int_0^b \log x \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x = \int_0^\varepsilon + \int_\varepsilon^b ,$$

where

$$\int_\varepsilon^b \log x \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x \sim \mathcal{O}\left(\omega^{-1} \log \varepsilon\right)$$

and

$$\left|\int_0^\varepsilon \log x \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x\right| \le -\int_0^\varepsilon \log x \mathrm{d}x \sim \mathcal{O}\left(\varepsilon \log \varepsilon\right).$$

Comparing both error bounds, an optimal upper bound is $\mathcal{O}\left(\omega^{-1}\log\omega\right)$, once $\varepsilon = \omega^{-1}$. □

It follows at once that

$$\int_0^b \log x f(x) \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x \sim \mathcal{O}\left(\omega^{-1}\log\omega\right).$$

Likewise, in the expansion (2.9), truncating after the first s terms the asymptotic error is $\mathcal{O}\big(\omega^{-(s+1)}\log\omega\big)$. Note however that nonsingular oscillatory integrals in the asymptotic expansion (2.9) must be calculated with an error which is consistent with the above asymptotic decay. We denote the number of truncation terms in the nonsingular oscillatory integral by L_k noting its dependence on the index k. These oscillatory integrals without logarithmic integrands are expanded by the asymptotic expansion from [14],

$$\begin{aligned}&\int_0^b \frac{\sigma_{k-1}[f](x)-\sigma_{k-1}[f](0)}{xg'(x)}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x\\ \sim\quad & -\sum_{\ell=0}^{L_k-1}\frac{1}{(-\mathrm{i}\omega)^{\ell+1}}\left[\frac{\gamma_{k-1,\ell}[f](b)}{g'(b)}\mathrm{e}^{\mathrm{i}\omega g(b)}-\frac{\gamma_{k-1,\ell}[f](0)}{g'(0)}\mathrm{e}^{\mathrm{i}\omega g(0)}\right]\end{aligned} \tag{2.10}$$

with a truncation error of $\mathcal{O}\big(\omega^{-L_k-1}\big)$, where

$$\begin{aligned}\gamma_{k-1,0}[f](x) &= \frac{\sigma_{k-1}[f](x)-\sigma_{k-1}[f](0)}{xg'(x)},\\ \gamma_{k-1,j}[f](x) &= \frac{\mathrm{d}}{\mathrm{d}x}\frac{\gamma_{k-1,j-1}[f](x)}{g'(x)}, \qquad j=1,\ldots,\ell.\end{aligned}$$

Inserting (2.10) into the expansion (2.9) gets rid of the highly oscillatory integrals there and yields a complete asymptotic expansion,

$$\begin{aligned}I[f] \;\sim\; & \nu_0(\omega)\sum_{k=0}^{s-1}\frac{\sigma_k[f](0)}{(-\mathrm{i}\omega)^k}-\sum_{k=1}^{s}\frac{\mathrm{e}^{\mathrm{i}\omega g(b)}}{(-\mathrm{i}\omega)^k}\frac{\log b\left(\sigma_{k-1}[f](b)-\sigma_{k-1}[f](0)\right)}{g'(b)}\\ & -\sum_{k=1}^{s}\frac{1}{(-\mathrm{i}\omega)^k}\sum_{\ell=0}^{L_k-1}\frac{1}{(-\mathrm{i}\omega)^{\ell+1}}\left[\frac{\gamma_{k-1,\ell}[f](b)}{g'(b)}\mathrm{e}^{\mathrm{i}\omega g(b)}-\frac{\gamma_{k-1,\ell}[f](0)}{g'(0)}\mathrm{e}^{\mathrm{i}\omega g(0)}\right]\\ & -\sum_{k=1}^{s}\frac{1}{(-\mathrm{i}\omega)^k}\mathcal{O}\Big(\omega^{-(L_k+1)}\Big)+\mathcal{O}\Big(\omega^{-(s+1)}\log\omega\Big).\end{aligned} \tag{2.11}$$

To ensure an error of $\mathcal{O}\left(\omega^{-s-1}\log\omega\right)$, the index L_k must satisfy the inequality $L_k \ge s-k$.

We summarize the above analysis into one theorem as follows:

Theorem 6. *Assume that $g'(x)\neq 0$. Then for $s\in\mathbb{N}$, $\omega\gg 1$, the integral (1.2) can be expanded into the asymptotic expansion*

$$\begin{aligned}Q^{A,s}[f] \;\sim\; & \nu_0(\omega)\sum_{k=0}^{s-1}\frac{\sigma_k[f](0)}{(-\mathrm{i}\omega)^k}-\sum_{k=1}^{s}\frac{\mathrm{e}^{\mathrm{i}\omega g(b)}}{(-\mathrm{i}\omega)^k}\frac{\log b\left(\sigma_{k-1}[f](b)-\sigma_{k-1}[f](0)\right)}{g'(b)}\\ & -\sum_{k=1}^{s}\frac{1}{(-\mathrm{i}\omega)^k}\sum_{\ell=0}^{L_k-1}\frac{1}{(-\mathrm{i}\omega)^{\ell+1}}\left[\frac{\gamma_{k-1,\ell}[f](b)}{g'(b)}\mathrm{e}^{\mathrm{i}\omega g(b)}-\frac{\gamma_{k-1,\ell}[f](0)}{g'(0)}\mathrm{e}^{\mathrm{i}\omega g(0)}\right],\end{aligned}$$

where

$$\begin{aligned}
\sigma_0[f](x) &= f(x), \\
\sigma_1[f](x) &= \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\sigma_1[f](x)-\sigma_0[f](0)}{g'(x)}\right], \\
&\vdots \\
\sigma_{k+1}[f](x) &= \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\sigma_k[f](x)-\sigma_k[f](0)}{g'(x)}\right], \\
\gamma_{k-1,0}[f](x) &= \frac{\sigma_{k-1}[f](x)-\sigma_{k-1}[f](0)}{xg'(x)}, \\
\gamma_{k-1,1}[f](x) &= \frac{\mathrm{d}}{\mathrm{d}x}\frac{\gamma_{k-1,0}[f](x)}{g'(x)}, \\
&\vdots \\
\gamma_{k-1,\ell}[f](x) &= \frac{\mathrm{d}}{\mathrm{d}x}\frac{\gamma_{k-1,\ell-1}[f](x)}{g'(x)}.
\end{aligned}$$

For each k, $k=1,2,\cdots,s$, if $L_k \geq s-k$, then the corresponding truncation error is

$$I[f]-Q^{A,s}[f] \sim \mathcal{O}\Big(\omega^{-(s+1)}\log\omega\Big).$$

Next, we intend to derive the asymptotic expansion for the more complicated oscillatory case with stationary points. If the stationary point is located at $\xi \neq 0$, we can separate the integral into two parts

$$\int_0^b \log x\, f(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x = \int_0^{\xi/2} + \int_{\xi/2}^b,$$

whereby the first integral has no stationary points and can be expanded with (2.9) and the second has no singularity and is amenable to a standard expansion from [14]. Therefore in the following subsection we assume that $\xi = 0$, thus

$$g(0)=g'(0)=g^{(2)}(0)=\cdots=g^{(r)}(0)=0, \qquad g^{(r+1)}(0)\neq 0.$$

Let us assume that the moments ν_j can be calculated explicitly. The function f being analytic, we use the subtraction technique again to remove the logarithmic singularity,

$$\begin{aligned}
I[f] &= \int_0^b \log x f(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x \\
&= \sum_{j=0}^{r}\frac{f^j(0)}{j!}\nu_j(\omega) + \int_0^b \log x\left[f(x)-\sum_{j=0}^{r}\frac{f^j(0)}{j!}x^j\right]\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x.
\end{aligned}$$

Therefore, integrating by parts,

$$\begin{aligned}
\frac{1}{\mathrm{i}\omega}\int_0^b \log x\frac{f(x)-\sum\limits_{j=0}^{r}\frac{f^j(0)}{j!}x^j}{g'(x)}\mathrm{d}\mathrm{e}^{\mathrm{i}\omega g(x)} &= \frac{1}{\mathrm{i}\omega}\left[\log x\frac{f(x)-\sum\limits_{j=0}^{r}\frac{f^j(0)}{j!}x^j}{g'(x)}\mathrm{e}^{\mathrm{i}\omega g(x)}\right]\Bigg|_0^b \\
&- \frac{1}{\mathrm{i}\omega}\int_0^b\frac{\mathrm{d}}{\mathrm{d}x}\left[\log x\frac{f(x)-\sum\limits_{j=0}^{r}\frac{f^j(0)}{j!}x^j}{g'(x)}\right]\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x.
\end{aligned}$$

Iterating this process results in an asymptotic expansion,

$$I[f] \sim \sum_{k=0}^{s-1}\sum_{j=0}^{r} \frac{\nu_j}{j!}\frac{\rho_k^{(j)}[f](0)}{(-\mathrm{i}\omega)^k} - \sum_{k=1}^{s} \frac{\mathrm{e}^{\mathrm{i}\omega g(b)}}{(-\mathrm{i}\omega)^k}\frac{\log b}{g'(b)}\left[\rho_{k-1}[f](b) - \sum_{j=0}^{r}\frac{\rho_{k-1}^{(j)}[f](0)}{j!}b^j\right]$$

$$+\sum_{k=1}^{s}\frac{1}{(-\mathrm{i}\omega)^k}\int_0^b \frac{\rho_{k-1}[f](x) - \sum_{j=0}^{r}\frac{\rho_{k-1}^{(j)}[f](0)}{j!}x^j}{xg'(x)}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x + \frac{1}{(-\mathrm{i}\omega)^s}I[\rho_s[f](x)], \quad (2.12)$$

where

$$\rho_0[f](x) = f(x), \qquad \rho_k[f](x) = \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\rho_{k-1}[f](x) - \sum_{j=0}^{r}\frac{\rho_{k-1}^{(j)}[f](0)}{j!}x^j}{g'(x)}\right], \quad k \geq 1,$$

and

$$\lim_{x\to 0}\frac{\rho_k[f](x) - \sum_{j=0}^{r}\frac{\rho_k^j[f](0)}{j!}x^j}{g'(x)} = 0.$$

Prior to determining the error involved in truncating the expansion, we need to examine the behaviour of the generalized moments ν_j.

Lemma 7. *Assuming $g(0) = g'(0) = \cdots = g^{(r)}(0) = 0$, $g^{(r+1)}(0) \neq 0$, we have*

$$|\nu_j(\omega)| = \left|\int_0^b x^j \log x \mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x\right| \sim \mathcal{O}\Big(\omega^{-(j+1)/(r+1)}\log\omega\Big), \qquad j \leq r, \quad (2.13)$$

$$|\nu_j(\omega)| \sim \mathcal{O}\big(\omega^{-1}\big), \qquad j \geq r+1, \quad (2.14)$$

Proof. Since g is an analytic function, it may be written as a Taylor series about $x = 0$,

$$g(x) = \sum_{m=0}^{r}\frac{g^{(m)}(0)}{m!}x^m + \frac{g^{(r+1)}(\tau)}{(r+1)!}x^{r+1} = \frac{g^{(r+1)}(\tau)}{(r+1)!}x^{r+1},$$

where $\tau \in [0, x]$ is an intermediate point. We may thus assume that $g(x) = cx^{r+1}$ for some $c \neq 0$.

To prove (2.13) we proced similarly to the proof of Lemma 5, setting a small positive number $\varepsilon > 0$ and decomposing the integral of ν_j,

$$\nu_j(\omega) = \int_0^\varepsilon + \int_\varepsilon^b,$$

where

$$\int_\varepsilon^b x^j \log x \mathrm{e}^{\mathrm{i}\omega c x^{r+1}}\mathrm{d}x \sim \mathcal{O}\left(\omega^{-1}\varepsilon^{j-r}\log\varepsilon\right),$$

since x^{r+1} is a non-singular function in $[\varepsilon, b]$. For the first integral on the right, we deduce that

$$\left|\int_0^\varepsilon x^j \log x \mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x\right| \leq \int_0^\varepsilon x^j \log x \mathrm{d}x = \int_0^\varepsilon x^j \mathrm{d}(x\log x - x) \sim \mathcal{O}\big(\varepsilon^{j+1}\log\varepsilon\big).$$

Comparing the two error bounds, we determine the error bound to be $\mathcal{O}\big(\omega^{-(j+1)/(r+1)}\log\omega\big)$ by equating $\omega^{-1}\varepsilon^{j-r} = \varepsilon^{j+1}$.

When $j \geq r+1$ the formula (2.14) can be derived by integration by parts,

$$\begin{aligned}
\nu_j(\omega) &= \int_0^b x^j \log x \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x = \frac{1}{\mathrm{i}\omega} \int_0^b \frac{x^j \log x}{g'(x)} \mathrm{d}\left(\mathrm{e}^{\mathrm{i}\omega g(x)}\right) \\
&= \frac{1}{\mathrm{i}\omega} \left[\frac{x^j \log x}{g'(x)} \mathrm{e}^{\mathrm{i}\omega g(x)} \right]\Bigg|_0^b - \mathcal{O}\left(\omega^{-\frac{3}{2}}\right) \sim \mathcal{O}\left(\omega^{-1}\right).
\end{aligned}$$

□

It follows from Lemma 7 that the asymptotic order of the expansion in (2.12) is $O\left(\omega^{-\left(s+\frac{1}{r+1}\right)} \log \omega\right)$. This indicates the asymptotic order of expansion of the oscillatory integrals in (2.12). Setting

$$\begin{aligned}
\eta_{k-1,0}[f](x) &= \frac{\rho_{k-1}[f](x) - \sum_{j=0}^{r} \frac{\rho_{k-1}^{(j)}[f](0)}{j!} x^j}{x g'(x)}, \\
\eta_{k-1,j}[f](x) &= \frac{\mathrm{d}}{\mathrm{d}x} \left[\frac{\eta_{k-1,j-1}[f](x) - \sum_{n=0}^{r-1} \frac{\eta_{k-1,j-1}^{(n)}[f](0)}{n!} x^n}{g'(x)} \right], \qquad j = 1, \ldots, \ell+1,
\end{aligned}$$

we have

$$\begin{aligned}
\int_0^b \eta_{k-1,0}[f](x) \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x &= \sum_{\ell=0}^{L_k-1} \frac{1}{(-\mathrm{i}\omega)^\ell} \sum_{n=0}^{r-1} \frac{\mu_n(0,\omega)}{n!} \eta_{k-1,\ell}^{(n)}[f](0) \\
&\quad - \sum_{\ell=1}^{L_k} \frac{1}{(-\mathrm{i}\omega)^\ell} \left[\frac{\eta_{k-1,\ell-1}[f](x) - \sum_{n=0}^{r-1} \frac{\eta_{k-1,\ell-1}^{(n)}[f](0)}{n!} x^n}{g'(x)} \mathrm{e}^{\mathrm{i}\omega g(x)} \right]\Bigg|_0^b \\
&\quad + \frac{1}{(-\mathrm{i}\omega)^{L_k}} \int_0^b \eta_{k-1,L_k}[f](x) \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x. \qquad (2.15)
\end{aligned}$$

Recalling that $\mu_0 \sim \mathcal{O}\left(\omega^{-\frac{1}{r+1}}\right)$, we confirm that the error order of the integral on the left side of (2.15) is $\mathcal{O}\left(\omega^{-L_k-\frac{1}{r+1}}\right)$.

Putting together the expansions (2.12) and (2.15), we obtain an asymptotic expansion for the integral (1.2) with an order-r stationary point at $x = 0$, which is formulated into the following theorem:

Theorem 8. *Assume that $g(0) = g'(0) = \cdots = g^{(r)}(0) = 0$, $g^{(r+1)}(0) \neq 0$. Then for $s \in \mathbb{N}$, $\omega \gg 1$, the integral (1.2) can be expanded into the asymptotic expansion*

$$\begin{aligned}
I[f] \sim Q^{A,s}[f] &= \sum_{k=0}^{s-1} \frac{1}{(-\mathrm{i}\omega)^k} \sum_{j=0}^{r} \frac{\nu_j}{j!} \rho_k^{(j)}[f](0) - \sum_{k=1}^{s} \frac{\mathrm{e}^{\mathrm{i}\omega g(b)}}{(-\mathrm{i}\omega)^k} \frac{\log b}{g'(b)} \left[\rho_{k-1}[f](b) - \sum_{j=0}^{r} \frac{\rho_{k-1}^{(j)}[f](0)}{j!} b^j \right] \\
&\quad + \sum_{k=1}^{s} \frac{1}{(-\mathrm{i}\omega)^k} \sum_{\ell=0}^{L_k-1} \frac{1}{(-\mathrm{i}\omega)^\ell} \sum_{n=0}^{r-1} \frac{\mu_n(0,\omega)}{n!} \eta_{k-1,\ell}^{(n)}[f](0) \\
&\quad - \sum_{k=1}^{s} \frac{1}{(-\mathrm{i}\omega)^k} \sum_{\ell=1}^{L_k} \frac{1}{(-\mathrm{i}\omega)^\ell} \left[\frac{\eta_{k-1,\ell-1}[f](x) - \sum_{n=0}^{r-1} \frac{\eta_{k-1,\ell-1}^{(n)}[f](0)}{n!} x^n}{g'(x)} \mathrm{e}^{\mathrm{i}\omega g(x)} \right]\Bigg|_0^b, \qquad (2.16)
\end{aligned}$$

where

$$
\begin{aligned}
\rho_0[f](x) &= f(x),\\
\rho_k[f](x) &= \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\rho_{k-1}[f](x)-\sum\limits_{j=0}^{r}\frac{\rho_{k-1}^{(j)}[f](0)}{j!}x^j}{g'(x)}\right], \quad k\geq 1,\\
\eta_{k-1,0}[f](x) &= \frac{\rho_{k-1}[f](x)-\sum\limits_{j=0}^{r}\frac{\rho_{k-1}^{(j)}[f](0)}{j!}x^j}{xg'(x)},\\
\eta_{k-1,1}[f](x) &= \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\eta_{k-1,0}[f](x)-\sum\limits_{n=0}^{r-1}\frac{\eta_{k-1,0}^{(n)}[f](0)}{n!}x^n}{g'(x)}\right],\\
&\vdots\\
\eta_{k-1,\ell+1}[f](x) &= \frac{\mathrm{d}}{\mathrm{d}x}\left[\frac{\eta_{k-1,\ell}[f](x)-\sum\limits_{n=0}^{r-1}\frac{\eta_{k-1,\ell}^{(n)}[f](0)}{n!}x^n}{g'(x)}\right].
\end{aligned}
$$

Furthermore, for each k, $k = 1, 2, \cdots, s$, when $L_k \geq s-k$, then the corresponding truncation error is

$$I[f]-Q^{A,s}[f]\sim\mathcal{O}\left(\omega^{-s-\frac{1}{r+1}}\log\omega\right).$$

As an example of the asymptotic expansion method for the logarithmic highly oscillatory integral, consider the integral

$$\int_0^1\frac{\log x}{1+x}\mathrm{e}^{\mathrm{i}\omega x}\mathrm{d}x. \tag{2.17}$$

The expansion (2.11) is truncated to $s = 1, 2, 3$ with the associated asymptotic error $\mathcal{O}\big(\omega^{-s-1}\log\omega\big)$. The truncated expansions are

$$
\begin{aligned}
Q^{A,1}[f](\omega) &= \nu_0(\omega),\\
Q^{A,2}[f](\omega) &= Q^{A,1}[f](\omega)-\frac{\mathrm{i}}{\omega}\nu_0(\omega)+\frac{-\frac{\mathrm{e}^{\mathrm{i}\omega}}{2}+1}{\omega^2},\\
Q^{A,3}[f](\omega) &= Q^{A,2}[f](\omega)+\frac{-2}{\omega^2}\nu_0(\omega)+\frac{\mathrm{i}\left(\frac{\mathrm{e}^{\mathrm{i}\omega}}{4}-1\right)}{\omega^3}+\frac{\mathrm{i}\left(\frac{3}{4}\mathrm{e}^{\mathrm{i}\omega}-2\right)}{\omega^3}.
\end{aligned}
$$

Fig. 2.3 displays the error for the asymptotic methods $Q^{A,s}$, $s = 1, 2, 3$ for increasing ω. Again, inclusion of more terms results in a reduced error.

In the stationary-point case we consider the same integral but with $g(x) = x^2$,

$$\int_0^1\frac{\log x}{1+x}\mathrm{e}^{\mathrm{i}\omega x^2}\mathrm{d}x. \tag{2.18}$$

Asymptotic expansion terms are calculated based on formula (2.16) for $s = 1, 2, 3$,

$$Q^{A,1}[f](\omega) = \nu_0(\omega)-\nu_1(\omega),$$

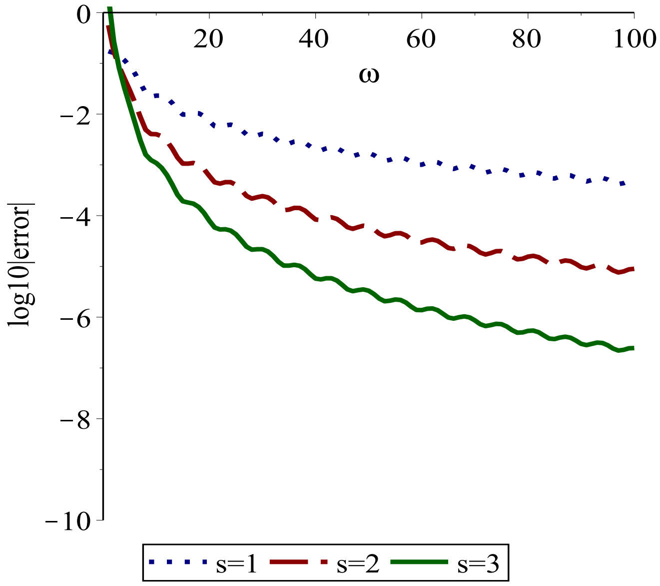

Figure 2.3: The error, $\log_{10}\left|Q^{A,s}[f]-I[f]\right|$, as a function of ω with $g(x)=x$. The colours are navy blue (the top, dotted), dark red (the middle, dashed) and dark green (the bottom, solid) for $s=1,2,3$.

$$\begin{aligned}
Q^{A,2}[f](\omega) &= Q^{A,1}[f](\omega)+\frac{\mathrm{i}}{2\omega}\nu_0(\omega)-\frac{\mathrm{i}}{\omega}\nu_1(\omega)+\frac{\mathrm{i}}{2\omega}\mu_0(0,\omega)+\frac{-\frac{\mathrm{e}^{\mathrm{i}\omega}}{8}+\frac{1}{4}}{\omega^2},\\
Q^{A,3}[f](\omega) &= Q^{A,2}[f](\omega)-\frac{3}{4\omega^2}\nu_0(\omega)+\frac{2}{\omega^2}\nu_1(\omega)-\frac{1}{\omega^2}\mu_0(0,\omega)\\
&\quad+\frac{\mathrm{i}\left(-\frac{3\mathrm{e}^{\mathrm{i}\omega}}{32}+\frac{1}{4}\right)}{\omega^3}+\frac{\mathrm{i}\left(-\frac{7\mathrm{e}^{\mathrm{i}\omega}}{32}+\frac{1}{2}\right)}{\omega^3}.
\end{aligned}$$

The order of the error is $O\left(\omega^{-s-\frac{1}{2}}\log\omega\right)$, $s=1,2,3$. As is evident from Fig. 2.4 (and expected from our analysis), the error of an asymptotic expansion method for the logarithmic oscillatory integral with stationary points decreases with increasing $|\omega|$ but blows up for small $|\omega|$.

2.3 Asymptotic analysis of a power-law singularity in the phase function

Applying the variable transformation $x^{-p}=t$, the integral (1.3) is transformed into

$$\begin{aligned}
I[f] &= p\int_0^1 x^{-\alpha}f(x)\mathrm{e}^{\mathrm{i}\omega x^{-p}}\mathrm{d}x=\int_1^\infty t^{\frac{\alpha-1}{p}-1}f\left(t^{-\frac{1}{p}}\right)\mathrm{e}^{\mathrm{i}\omega t}\mathrm{d}t=\int_1^\infty t^{\frac{\alpha-1}{p}-1}h(t)\mathrm{e}^{\mathrm{i}\omega t}\mathrm{d}t\\
&= \int_1^\infty t^{-\beta}h(t)\mathrm{e}^{\mathrm{i}\omega t}\mathrm{d}t=I[h],
\end{aligned}$$

where $h(t)=f\left(t^{-\frac{1}{p}}\right)$ and $\beta=-\frac{\alpha-1}{p}+1$. Since asymptotic analysis is fundamental to the quadrature methods, we commence from the asymptotic expansion for the integral (1.3). Assuming $\left|f\left(t^{-\frac{1}{p}}\right)\right|\le C_3$, the integral is bounded by

$$|I[f]|\le C_3\left|\int_1^\infty t^{-\beta}\mathrm{d}t\right|=C_3\left|\mathrm{Ei}\left(\beta,-\mathrm{i}\omega\right)\right|,$$

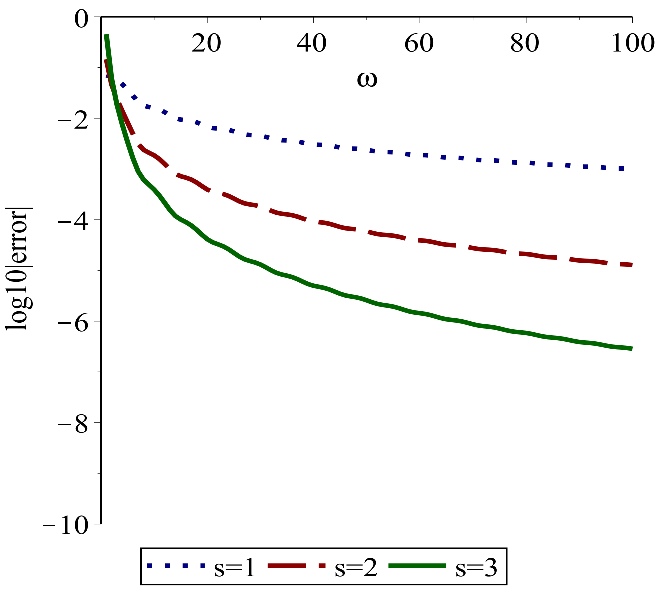

Figure 2.4: The error, $\log_{10}\left|Q^{A,s}[f]-I[f]\right|$, as a function of ω with $g(x)=x^2$. Navy blue (the top, dotted), dark red (the middle, dashed) and dark green (the bottom, solid) plots correspond to $s=1,2,3$, respectively.

where Ei is the *exponential integral,* with the asymptotic expansion

$$\operatorname{Ei}(\beta,-\mathrm{i}\omega)\sim\frac{\mathrm{e}^{\mathrm{i}\omega}}{(-\mathrm{i}\omega)}\sum_{\ell=0}^{\infty}(-1)^{\ell}\frac{(\beta)_\ell}{(-\mathrm{i}\omega)^{\ell}},\qquad \omega\gg 1 \tag{2.19}$$

(cf. http://dlmf.nist.gov/8.20), where $(\beta)_\ell=\beta(\beta+1)\cdots(\beta+\ell-1)$ is the *Pochhammer symbol.* Thus, for fixed β and $\omega\to\infty$, this yields $|I[f]|\sim\mathcal{O}\left(\omega^{-1}\right)$.

We construct the asymptotic expansion by integration by parts,

$$\begin{aligned}
I[h] &= \int_1^\infty t^{-\beta}h(t)\mathrm{e}^{\mathrm{i}\omega t}\mathrm{d}t\\
&= -\frac{h(1)\mathrm{e}^{\mathrm{i}\omega}}{\mathrm{i}\omega}-\frac{1}{\mathrm{i}\omega}\int_1^\infty t^{-\beta}\left(-\beta t^{-1}h(t)+h'(t)\right)\mathrm{e}^{\mathrm{i}\omega t}\mathrm{d}t\\
&= -\frac{h(1)\mathrm{e}^{\mathrm{i}\omega}}{\mathrm{i}\omega}-\frac{1}{\mathrm{i}\omega}\int_1^\infty t^{-\beta}\rho_1(t)\mathrm{e}^{\mathrm{i}\omega t}\mathrm{d}t,
\end{aligned}$$

where

$$\rho_1(t)=-\beta t^{-1}h(t)+h'(t)$$

is analytic functions in $[1,\infty)$. Repeating the process s times, we obtain the following theorem.

Theorem 9. *For two real numbers $0<\alpha<1$, $p>0$, setting $\beta=1-\frac{\alpha-1}{p}$, the asymptotic expansion of $I[f]$ is*

$$Q^{A,s}[h]\sim\sum_{k=1}^{s}\frac{\rho_{k-1}[h](1)\mathrm{e}^{\mathrm{i}\omega}}{(-i\omega)^k}+\frac{(-1)^s}{(\mathrm{i}\omega)^s}\int_1^\infty t^{-\beta}\rho_s[h](t)\mathrm{e}^{\mathrm{i}\omega t}\mathrm{d}t$$

for any smooth function h, where

$$\rho_0[h](t)=h(t),$$

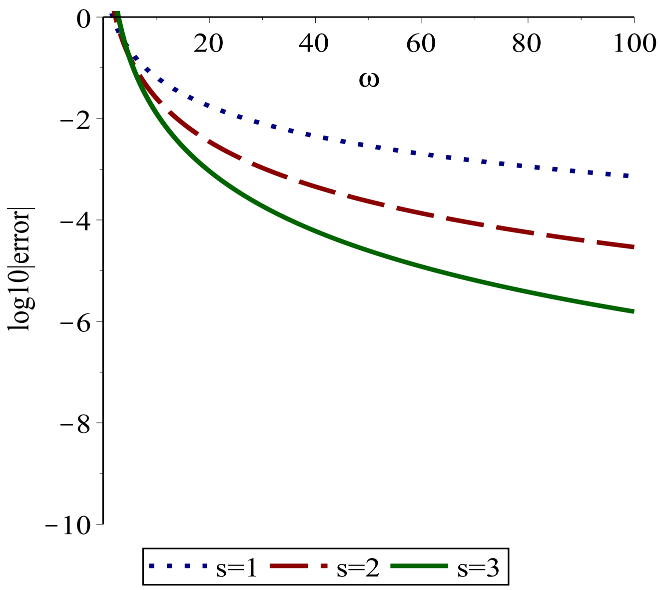

Figure 2.5: The error, $\log_{10}\left|Q^{A,s}[h](\omega) - I[h](\omega)\right|$, with $h(t) = \mathrm{e}^{t^{-1}}$ and $\alpha = \frac{1}{3}$. Navy blue (the top, dotted), dark red (the middle, dashed) and dark green (the bottom, solid) correspond to $s = 1, 2, 3$, respectively.

$$\rho_{k+1}[h](t) = t^{\beta}\frac{\mathrm{d}}{\mathrm{d}t}\left(t^{-\beta}\rho_k[h](t)\right), \qquad k \geq 0.$$

The corresponding truncation error is

$$I[h] - Q^{A,s}[h] \sim \mathcal{O}\left(\omega^{-s-1}\right). \tag{2.20}$$

We deduce that the singularity in the phase function does not affect the asymptotic order.As an example, the integral (1.3) is considered with $f(x) = \mathrm{e}^x$, $\alpha = \frac{1}{3}$, $p = 1$. The corresponding asymptotic expansions for $s = 1, 2, 3$ are

$$\begin{aligned}
Q^{A,1}[h] &= -\frac{h(1)\mathrm{e}^{\mathrm{i}\omega}}{\mathrm{i}\omega}, \\
Q^{A,2}[h] &= Q^{A,1}[h] + \frac{(-\beta h(1) + h'(1))\mathrm{e}^{\mathrm{i}\omega}}{(\mathrm{i}\omega)^2}, \\
Q^{A,3}[h] &= Q^{A,2}[h] - \frac{[-\beta(-\beta h(1) + h'(1)) + \beta h(1) - \beta h'(1) + h''(1)]\mathrm{e}^{\mathrm{i}\omega}}{(\mathrm{i}\omega)^3}.
\end{aligned}$$

We plot the errors $\left|I[h] - Q^{A,1}[h]\right|$(navy blue, the top), $\left|I[h] - Q^{A,2}[h]\right|$ (dark red, the middle), $\left|I[h] - Q^{A,3}[h]\right|$(dark green, the bottom) in Fig. 2.5. It is confirmed that the asymptotic order is $\mathcal{O}\left(\omega^{s-1}\right)$.

2.4 Asymptotic analysis for the logarithmic singularity in the phase function

Integration by parts the expression (1.4),

$$\begin{aligned}
I[f] &= \int_0^1 \log x f(x)\mathrm{e}^{\mathrm{i}\omega\log x}\mathrm{d}x = \int_{-\infty}^0 tf(\mathrm{e}^t)\mathrm{e}^{(\mathrm{i}\omega+1)t}\mathrm{d}t \\
&= -\frac{1}{\mathrm{i}\omega+1}\int_{-\infty}^0 f(\mathrm{e}^t)\mathrm{e}^{(\mathrm{i}\omega+1)t}\mathrm{d}t - \frac{1}{\mathrm{i}\omega+1}\int_{-\infty}^0 tf'(\mathrm{e}^t)\mathrm{e}^{(\mathrm{i}\omega+2)t}\mathrm{d}t.
\end{aligned}$$

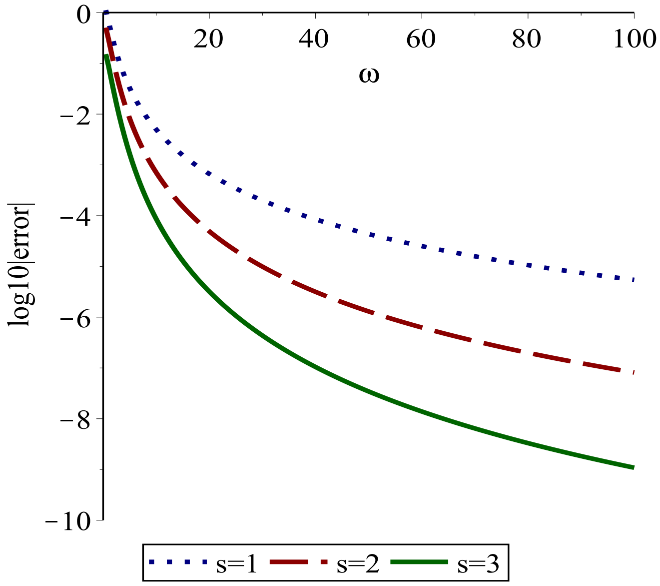

Figure 2.6: The graphs of $\log_{10}\left|Q^{A,s}[f](\omega) - I[f](\omega)\right|$, for $f(x) = \mathrm{e}^x$, $g(x) = \log(x)$. The navy blue (the top, dotted), dark red (the middle, dashed) and dark green (the bottom, solid) are for $s = 1, 2, 3$.

Continuing in this vain, we prove

Theorem 10. *An asymptotic expansion of (1.4) for analytic f is*

$$I[f] = -\sum_{k=1}^{s} \frac{(-1)^{k-1}}{(\mathrm{i}\omega+1)_k} \sum_{\ell=0}^{s-k} \frac{(-1)^{\ell} f^{(k+\ell-1)}(1)}{(\mathrm{i}\omega+k)_{\ell+1}} + \mathcal{O}\left(\frac{1}{\omega^{s+1}}\right), \tag{2.21}$$

where the symbol $(z)_k$ denotes the Pochhammer symbol $z(z+1)\cdots(z+k-1)$.

A detailed proof can be found in Appendix A.2.

We apply the above asymptotic expansion methodto $f(x) = \mathrm{e}^x$. The errors of the first three asymptotic expansions

$$\begin{aligned}
Q^{A,1}[f] &= -\frac{f(1)}{(\mathrm{i}\omega+1)^2}, \\
Q^{A,2}[f] &= Q^{A,1}[f] + \left(\frac{1}{(\mathrm{i}\omega+1)^2(\mathrm{i}\omega+2)} + \frac{1}{(\mathrm{i}\omega+1)(\mathrm{i}\omega+2)^2}\right) f'(1), \\
Q^{A,3}[f] &= Q^{A,2}[f] + \left(\frac{1}{(\mathrm{i}\omega+1)^2(\mathrm{i}\omega+2)(\mathrm{i}\omega+3)} + \frac{1}{(\mathrm{i}\omega+1)(\mathrm{i}\omega+2)^2(\mathrm{i}\omega+3)}\right. \\
&\qquad \left. + \frac{1}{(\mathrm{i}\omega+1)(\mathrm{i}\omega+2)(\mathrm{i}\omega+3)^2}\right) f''(1)
\end{aligned}$$

are plotted in Fig. 2.6: the asymptotic order is consistent with Theorem 10.

3 The Filon method for singular highly oscillatory integrals

3.1 A Filon method for a power-law singularity in (1.1)

Filon-type methods constitute a powerful alternative to asymptotic expansion: they are as good as the latter for $|\omega| \gg 1$ while delivering good accuracy for small $|\omega|$ [7]. The essence of the technique is to replace the non-oscillatory function $f(x)$ by a polynomial subject to interpolation conditions that are determined by the asymptotic expansion. Given interpolation nodes $c_1 = 0 < c_2 < \cdots < c_\nu = b$ with multiplicities $m_1, m_2, \cdots, m_\nu \in \mathbb{N}$, respectively, we interpolate $f(x)$ by $p_n(x) = \sum_{m=0}^{n} d_m x^m$, $n = \sum_{\ell=1}^{\nu} m_\ell - 1$ and determine the coefficients d_m by the Hermite interpolation conditions

$$p_n^{(j)}(c_\ell) = f^{(j)}(c_\ell), \quad \ell = 1, \cdots, \nu; \quad j = 0, 1, \cdots, m_\ell - 1.$$

A Filon method is defined by

$$Q^F[f] = \int_0^b x^{-\alpha} p_n(x) \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x = \sum_{m=0}^{n} d_m I[x^m], \tag{3.1}$$

where $I[x^m]$ is the mth moment.

Theorem 11. *Letting $\nu \geq 2$, $c_0 = 0, c_\nu = b$, $\min\{m_1, m_\nu\} \geq s$, we have*

$$I[f] - Q^F[f] \sim \mathcal{O}\Big(\omega^{-s-(1-\alpha)}\Big).$$

The proof is relegated to Appendix A.3.

Once $x = 0$ is an order-r stationary point for the integral, the interpolation conditions for a Filon method are based on the expansion (2.6).

Theorem 12. *Given $\nu \geq 2$ and $c_0 = 0$, $c_\nu = b$ and letting $m_1 \geq s(r+1)$ and $m_\nu \geq s$, we have*

$$I[f] - Q^F[f] \sim \mathcal{O}\Big(\omega^{-s-(1-\alpha)/(r+1)}\Big).$$

The proof is given in Appendix A.4.

While inheriting the asymptotic behaviour of its counterparts from Section 2, a Filon method reduces to *Hermite–Birkhoff quadrature* as $\omega = 0$ [7], thereby being very effective uniformly for all $\omega \in \mathbb{R}$.

To illustrate our theoretical analysis, we revisit the example (2.7) and construct a Filon-type method as follows

$$\begin{aligned}
Q^{F,1}[f](\omega) &= -\frac{\mu_1(\alpha,\omega)}{2} + \mu_0(\alpha,\omega), \\
&\quad \text{with} \quad f(0) = p_n(0), \quad f(1) = p_n(1), \\
Q^{F,2}[f](\omega) &= -\frac{\mu_3(\alpha,\omega)}{4} + \frac{3\mu_2(\alpha,\omega)}{4} - \mu_1(\alpha,\omega) + \mu_0(\alpha,\omega), \\
&\quad \text{with} \quad f^{(j)}(0) = p_n^{(j)}(0), \quad j = 0,1, \quad f^{(j)}(1) = p_n^{(j)}(1), \quad j = 0,1, \\
Q^{F,3}[f](\omega) &= -\frac{\mu_5(\alpha,\omega)}{8} + \frac{\mu_4(\alpha,\omega)}{2} - \frac{7\mu_3(\alpha,\omega)}{8} + \mu_2(\alpha,\omega) \\
&\quad - \mu_1(\alpha,\omega) + \mu_0(\alpha,\omega), \\
&\quad \text{with} \quad f^{(j)}(0) = p_n^{(j)}(0), \quad j = 0,1,2, \quad f^{(j)}(1) = p_n^{(j)}(1), \quad j = 0,1,2.
\end{aligned}$$

We display the error $\log_{10}\left|Q^{F,s} - I\right|$ in Fig. 3.1 for $s = 1, 2, 3$. Unlike in Fig. 2.1, the error does not blow up when ω is near 0, while when $\omega \to \infty$, the error of the Filon method behaves better than that of the asymptotic method with the same s.

Next we consider the same integral with $g(x) = x^2$. Again, three Filon methods are presented,

$$Q^{F,1}[f](\omega) = \frac{\mu_2(\alpha,\omega)}{2} - \mu_1(\alpha,\omega) + \mu_0(\alpha,\omega),$$

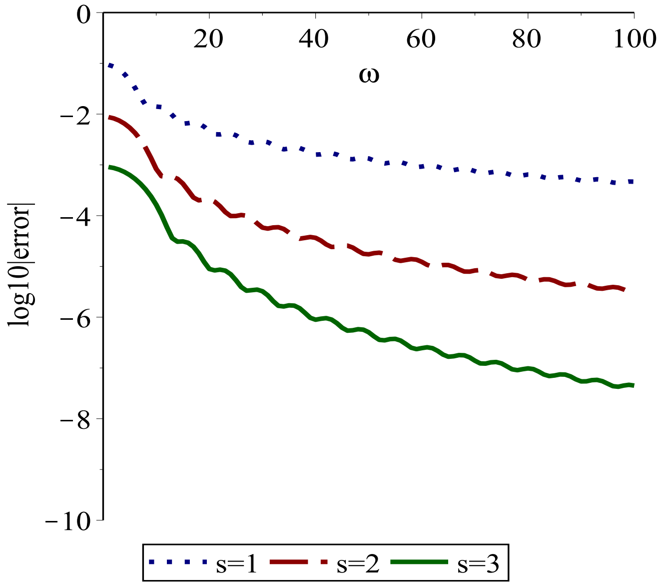

Figure 3.1: The error, $\log_{10}\left|Q^{F,s}[f]-I[f]\right|$, as a function of ω with $g(x)=x$, for $s=1$ (navy blue, the top, dotted), $s=2$ (dark red, the middle, dashed) and $s=3$ (dark green, the bottom, solid).

$$
\begin{aligned}
& \text{with} \quad f^{(j)}(0)=p_n^{(j)}(0), \quad j=0,\cdots,1, \quad f(1)=p_n(1), \\
Q^{F,2}[f](\omega) &= \frac{\mu_5(\alpha,\omega)}{-4}+\frac{3\mu_4(\alpha,\omega)}{4}-\mu_3(\alpha,\omega)+\mu_2(\alpha,\omega)-\mu_1(\alpha,\omega)+\mu_0(\alpha,\omega), \\
& \text{with} \quad f^{(j)}(0)=p_n^{(j)}(0), \quad j=0,\cdots,3, \quad f^{(j)}(1)=p_n^{(j)}(1), \quad j=0,1, \\
Q^{F,3}[f](\omega) &= \frac{\mu_8(\alpha,\omega)}{8}-\frac{\mu_7(\alpha,\omega)}{2}+\frac{7\mu_6(\alpha,\omega)}{8}-\mu_5(\alpha,\omega)+\mu_4(\alpha,\omega)-\mu_3(\alpha,\omega) \\
& +\mu_2(\alpha,\omega)-\mu_1(\alpha,\omega)+\mu_0(\alpha,\omega), \\
& \text{with} \quad f^{(j)}(0)=p_n^{(j)}(0), \quad j=0,\cdots,5, \quad f^{(j)}(1)=p_n^{(j)}(1), \quad j=0,1,2.
\end{aligned}
$$

The error $\log_{10}\left|Q^{F,s}-I\right|$ is plotted in Fig 3.2, for $s=1,2,3$. Note that the error of the Filon method is substantially smaller than the asymptotic method even for large ω.

3.2 A Filon method for the logarithmic singularity in (1.2)

Similarly to (3.1), for a logarithmic integral without a stationary point we let

$$Q^F[f]=\int_0^b \log x\, p_n(x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x=\sum_{m=0}^{n} d_m I[x^m].$$

Theorem 13. *Supposing that $g'(x)\neq 0$, $x\in[0,b]$, then*

$$I[f]-Q^F[f]\sim\mathcal{O}\left(\omega^{-s-1}\log\omega\right),$$

for $q\geq 2$, where $c_1=0$, $c_q=b$, $m_1\geq s$, $m_q\geq s$.

The proof is presented in Appendix A.5.

We consider the same example as in (2.17). The interpolation function p_n is formed in a similar manner to that in Section 3.1 except that $\mu_m(\alpha,\omega)$ is replaced by $\nu_m(\omega)$. In

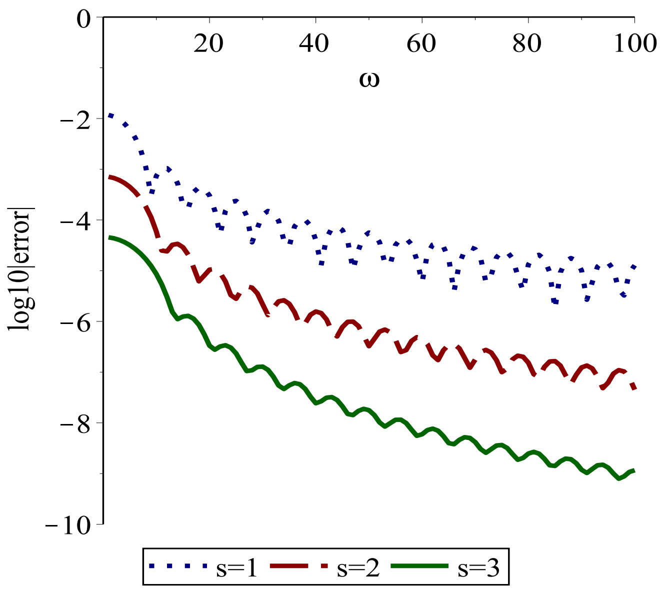

Figure 3.2: The error, $\log_{10} \left|Q^{F,s}[f] - I[f]\right|$, as a function of ω with $g(x) = x^2$. The colours are navy blue (the top, dotted), dark red (the middle, dashed) and dark green (the bottom, solid) for $s = 1, 2, 3$.

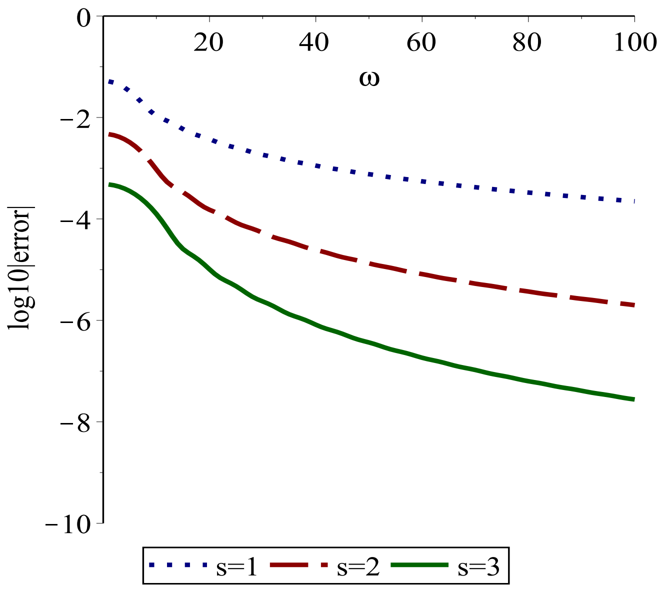

Figure 3.3: The error, $\log_{10} \left|Q^{F,s}[f] - I[f]\right|$, as a function of ω with $g(x) = x$ and $\omega \in [1, 100]$. Navy blue (the top, dotted), dark red (the middle, dashed) and dark green (the bottom, solid) correspond to $s = 1, 2, 3$ respectively.

Fig. 3.3, we depict the error function $\log\left|Q^{F,s} - I\right|$ for $s = 1$ (navy blue, dotted), $s = 2$ (dark red, dashed) and $s = 3$ (dark green, solid). All the plots are consistent with an error of $\mathcal{O}\left(\omega^{-s-1}\log\omega\right)$.

Next we consider the case with stationary points.

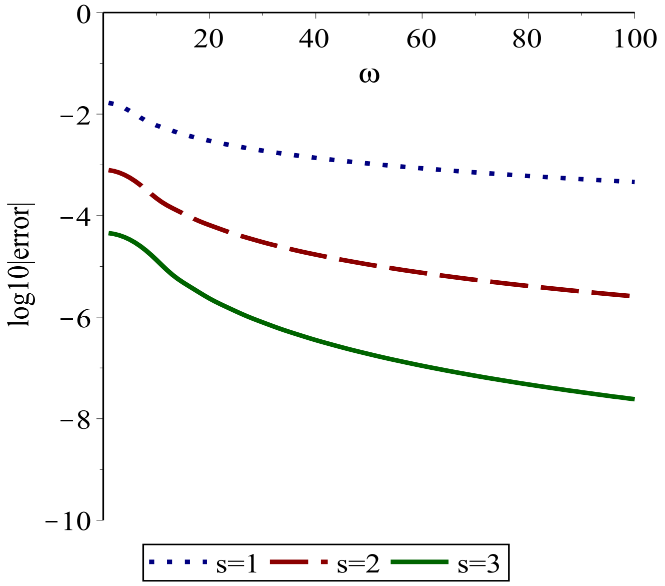

Figure 3.4: The error, $\log_{10}\left|Q^{F,s}[f]-I[f]\right|$, as a function of ω for the highly oscillatory integral with $g(x) = x^2$ and $\omega \in [1, 100]$. The colours navy blue, dark red, dark green correspond to $s = 1$ (the top, dotted), 2 (the middle, dashed), 3 (the bottom, solid) respectively.

Theorem 14. *Given $q \geq 2$, let $c_1 = 0$, $c_q = b$, $m_1 \geq s(r+1)$ and $m_q \geq s$. Then*

$$I[f] - Q^F[f] \sim \mathcal{O}\Big(\omega^{-(s+1/(r+1))}\log\omega\Big), \qquad \textit{where} \qquad Q^F[f] = \sum_{m=0}^{n} d_m I[x^m].$$

The proof is presented in Appendix A.6. Our example is (2.18): we form the interpolation polynomial p_n with $\nu_m(\omega)$ instead of $\mu_m(\alpha,\omega)$. The plot in Fig. 3.2 displays the logarithmic error of Filon methods $Q^{F,1}$, $Q^{F,2}$ and $Q^{F,3}$. The asymptotic order is $\mathcal{O}\Big(\omega^{-(s+\frac{1}{2})}\log\omega\Big)$ and our numerical results are in complete agreement with Theorem 14.

3.3 A Filon method for the singular oscillatory integral (1.3)

There are two issues that need be analysed to construct a Filon method from the asymptotic expansion (2.20). One is the connection between the asymptotic order and the derivatives of $f(t)$. It follows by induction from (2.20) that $\rho_k[f](1)$ is a linear combination of $f^{(j)}(1)$, $j = 0, 1, \cdots, k$. As long as the interpolating polynomial $P_n(t) = \sum_{m=0}^{n} d_m t^{-m/p}$ satisfies

$$P_n^{(j)}(1) = f^{(j)}(1), \quad j = 0, 1, \cdots, s-1, \tag{3.2}$$

the asymptotic expansion gives the asymptotic order $\mathcal{O}\left(\omega^{-s-1}\right)$.

Theorem 15. *If the polynomial $P_n(t)$ is constructed by the Hermite interpolation conditions (3.2) then the quadrature $Q^F[f] = \sum_{m=0}^{s-1} d_m I\left[t^{-m/p}\right]$ results in an error*

$$I[f] - Q^F[f] \sim \mathcal{O}\left(\omega^{-s-1}\right).$$

The second ingredient required for the Filon method is the computation of the moments $I\left[t^{-m/p}\right]$, $m = 0, 1, \cdots, s-1$. They are calculated explicitly in terms of exponential

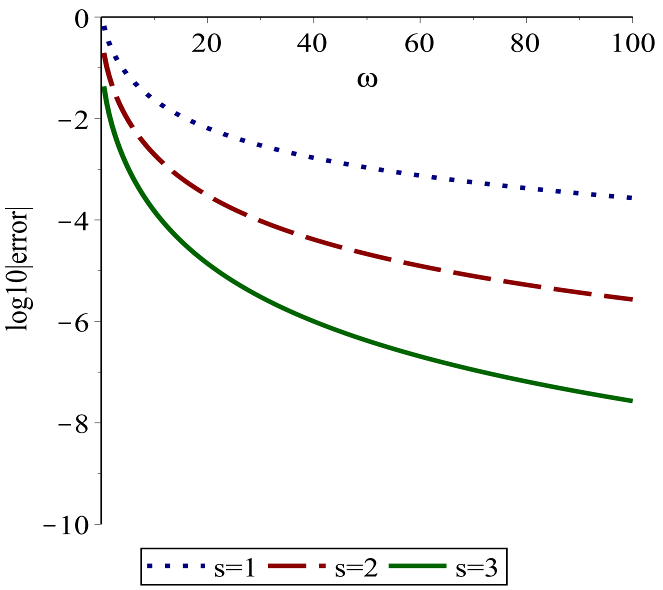

Figure 3.5: The error, $\log_{10}\left|Q^{F,s}[f]-I[f]\right|$, with $g(x)=x^{-1}$ and $\omega\in[1,100]$. The colours navy blue, dark red, dark green correspond to $s=1$ (the top, dotted), $s=2$ (the middle, dashed), $s=3$ (the bottom, solid).

integrals,

$$I\left[t^{-m/p}\right]=\int_1^\infty t^{-m/p-\beta}\mathrm{e}^{\mathrm{i}\omega t}\mathrm{d}t=\mathrm{Ei}\left(\frac{m}{p}+\beta,-\mathrm{i}\omega\right).$$

As an example, consider $f(t)=\mathrm{e}^t$, $\alpha=\frac{1}{3}$ and $p=1$. We have

$$\begin{aligned}Q_1^F[f] &= \mathrm{e}\,\mathrm{Ei}\left(\beta,-\mathrm{i}\omega\right),\\ Q_2^F[f] &= \mathrm{e}\,\mathrm{Ei}\left(\frac{1}{p}+\beta,-\mathrm{i}\omega\right),\\ Q_3^F[f] &= \frac{\mathrm{e}}{2}\,\mathrm{Ei}\left(\beta,-\mathrm{i}\omega\right)+\frac{\mathrm{e}}{2}\,\mathrm{Ei}\left(\frac{2}{p}+\beta,-\mathrm{i}\omega\right).\end{aligned}$$

The errors are depicted in Fig. 3.5 for $s=1$ (the top), $s=2$ (the middle) and $s=3$ (the bottom), respectively. Compared to the Fig. 2.5, it is noted that the error is uniformly smaller, another demonstration of the advantage of Filon method.

3.4 Filon method for the integral (1.4)

The two vital steps in the construction of Filon method are the computation of the moments and the determination of interpolation conditions from an asymptotic expansion. It follows from (2.21) that interpolation at $f^{(j)}(1)$, $j=0,1,\cdots,s-1$ ensured an asymptotic order of $\mathcal{O}\left(\omega^{-s-1}\right)$. The moments are are simple integrals,

$$\mu_m(\omega)=\int_0^1 x^m\log(x)\mathrm{e}^{\mathrm{i}\omega\log(x)}\mathrm{d}x=\int_{-\infty}^0 t\mathrm{e}^{(\mathrm{i}\omega+m+1)t}\mathrm{d}t=-\frac{1}{(\mathrm{i}\omega+m+1)^2}.$$

For the same example as in Section 2.4, the Filon method $Q^{F,s}[f]=\sum_{m=0}^{s-1}d_m\mu_m$ is constructed for $s=1,2,3$, as follows:

$$Q^{F,1}[f]=\mathrm{e}\mu(0,\omega),\qquad Q^{F,2}[f]=\mathrm{e}\mu(1,\omega),\qquad Q^{F,3}[f]=\frac{\mathrm{e}}{2}\mu(2,\omega)+\frac{\mathrm{e}}{2}\mu(0,\omega).$$

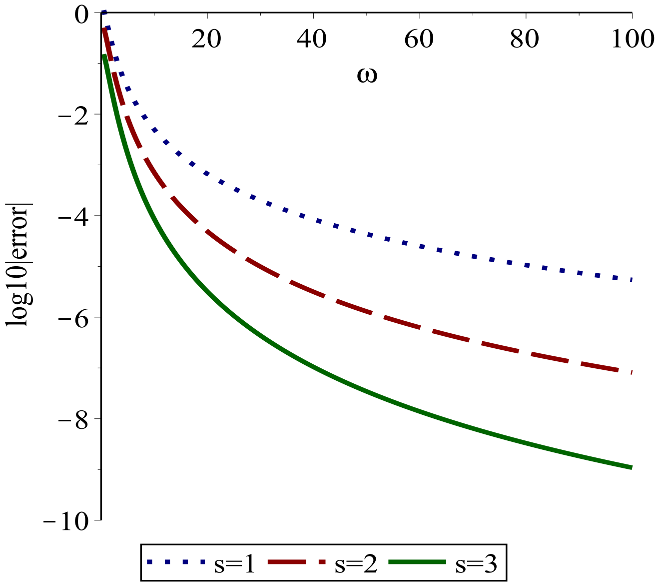

Figure 3.6: The error, $\log_{10}\left|Q^{F,s}[f]-I[f]\right|$, with $g(x) = \log x$ and $\omega \in [1, 100]$. The colours navy blue, dark red, dark green correspond to $s = 1$ (the top), $s = 2$ (the middle), $s = 3$ (the bottom).

In Fig. 3.6 the error graphs $\log_{10}\left|Q^{F,s}[f]-I[f]\right|$ are presented, conforming that the asymptotic order decays with increasing ω and s.

4 Complex-valued Gaussian quadrature

A powerful alternative to standard methods of quadrature for highly oscillatory functions is complex-valued Gaussian quadrature. While an early analysis has been presented in [6] for the integral $\int_{-1}^{1} f(x)e^{i\omega x}dx$, our understanding of this approach is incomplete. Yet, this should not prevent a practical use of this technique. In this section, we are concerned with complex-valued Gaussian quadrature for singular highly oscillatory integrals of the form

$$I[f] = \int_0^b f(x)h(x)e^{i\omega g(x)}dx, \quad \omega \gg 1,$$

where either $h(x) = x^{-\alpha}$ or $h(x) = \log x$ is weakly singular at $x = 0$ and f is an analytic function. We seek an n-point Gaussian quadrature formula

$$I[f] \sim \sum_{j=1}^{n} w_j f(x_j) = Q^{G,n}[f](\omega) \tag{4.1}$$

where x_j, $j = 1, \cdots, n$ are the zeros of an nth-degree monic orthogonal polynomial $p_n^\omega(x)$ in $[0, b]$ with the *complex* weight function $h(x)e^{i\omega g(x)}$,

$$\int_0^b p_n^\omega(x)x^j h(x)e^{i\omega g(x)}dx = 0, \qquad j = 0, \cdots, n-1, \quad n \in \mathbb{Z}_+,$$

and w_j are the corresponding weights. Note that the existence of p_n^ω is not assured for every n and ω and that, once it exists, its zeros are complex.

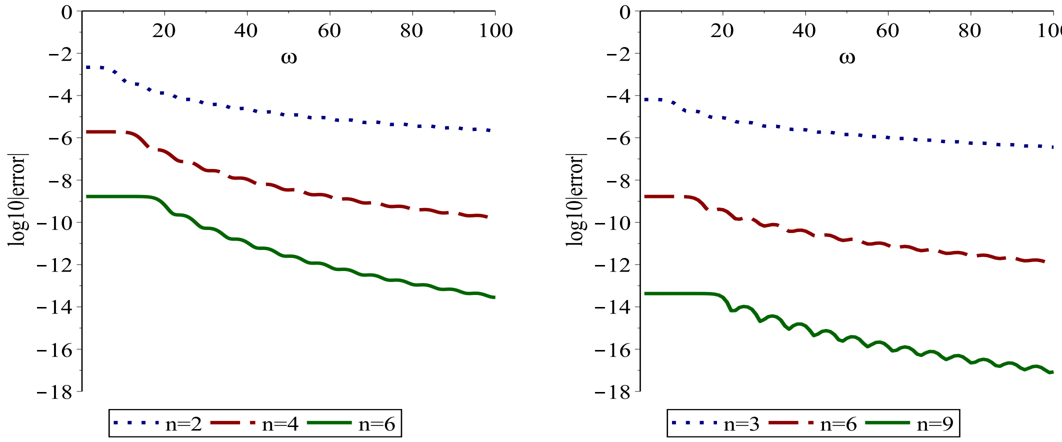

Figure 4.1: $\log_{10}\left|Q^{G,n}[f](\omega) - I[f](\omega)\right|$ as a function of ω for the integral with a power-law singularity. The left: $g(x) = x$. The colours are navy blue (the top, dotted), dark red (the middle, dashed) and dark green (the bottom, solid) for $n = 2, 4, 6$; The right: $g(x) = x^2$ and the same colour scheme for $n = 3, 6, 9$.

We first construct p_n^ω. To do this, consider the *Hankel matrix* formed by the moments μ_j for power singularity (or ν_j for logarithmic singularity).

$$H_n = \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_n \\ \mu_1 & \mu_2 & \cdots & \mu_{n+1} \\ \vdots & \vdots & & \vdots \\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n} \end{bmatrix}, \qquad h_n = \det H_n, \quad n \in \mathbb{N}.$$

Then

$$p_n^\omega(x) = \frac{1}{h_{n-1}} \det \begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_{n-1} & 1 \\ \mu_1 & \mu_2 & \cdots & \mu_n & x \\ \vdots & \vdots & & \vdots & \vdots \\ \mu_n & \mu_{n+1} & \cdots & \mu_{2n-1} & x^n \end{bmatrix}.$$

While the properties of polynomials orthogonal with respect to the complex weight $\mathrm{e}^{\mathrm{i}\omega x}$ are discussed in detail [2, 6] in this paper, we are concerned just with the accuracy of complex Gaussian quadrature. A more comprehensive analysis is bound to await better theoretical understanding of this new construct. We note that, while easy to construct (and difficult to analyse!), complex-valued Gaussian quadrature is significantly more expensive than, say, the Filon approach. Yet, as will be evident in the sequel, it is significantly more accurate.

To compare complex-valued quadrature to Filon methods from Section 3, we set n equal to the number of the interpolation conditions (hence, the number of function evaluations) in a corresponding Filon method.

4.1 Numerical experiments for power-law singularity

We apply the complex-valued Gaussian quadrature to the integrals in (2.7) and (2.8) and display the error $\log_{10}\left|Q^{G,n}[f] - I[f]\right|$ in Fig. 4.1. The case without stationary points is on the left and the case of one stationary point is on the right. We set $n = 2, 4, 6$ on the left and $n = 3, 6, 9$ on the right. When $n = 2$, we obtain the two zeros of $p_2(x) = 0$ and the quadrature in (4.1) involves two function evaluations. Counting function evaluations, this

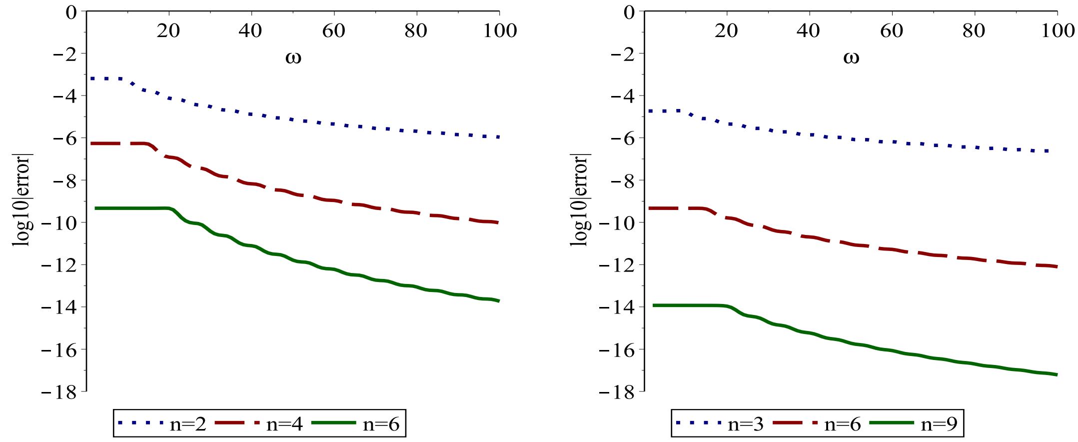

Figure 4.2: $\log_{10}\left|Q^{G,n}[f](\omega)-I[f](\omega)\right|$ as a function of ω for the integral with a logarithmic singularity. The left plot: $g(x)=x$. The colours are navy blue (the top, dotted), dark red (the middle, dashed) and dark green (the bottom, solid) for $n=2,4,6$; The right: $g(x)=x^2$ and the same colour scheme for $n=3,6,9$.

is equivalent to $Q^{F,1}$, which involves function evaluations at $x=0$ and $x=1$. However, when the results in Fig. 4.1 are compared to those in Fig. 3.1, it can be seen that the error of $Q^{G,2}$ is considerably smaller. Similarly, although $Q^{G,4}$ involves the same number of function evaluations as $Q^{F,2}$, its accuracy is greater than even $Q^{F,3}$. Next consider the case with a stationary point. We examine the result for $n=3$. The number of function evaluations for $Q^{G,3}$ is the same as $Q^{F,1}$ as both involve three function evaluations. However, when the result in Fig. 4.1 is compared to that in Fig. 3.2, the size of the error is similar to that of $Q^{F,3}$ clearly indicating its superior accuracy for the same number of function evaluations. Similar conclusions can be drawn for $n=6$.

4.2 Numerical experiments for logarithmic singularity

We calculate the integrals in (2.17) and (2.18). The logarithmic errors $\log_{10}\left|Q^{G,n}-I[f]\right|$ are displayed in Fig. 4.2: $n=2,4,6$ for $g(x)=x$ are on the left and $n=3,6,9$ for $g(x)=x^2$ on the right. The difference between the precision of the complex-valued Gaussian quadrature and Filon method is again striking. Complex-valued Gaussian quadrature delivers substantially higher accuracy for the same number of function evaluations. However, it should be noted that in complex quadrature there is the additional cost of the computation of the orthogonal polynomial and its zeros. In other words, a simple comparison of function evaluations is incomplete, because it disregards the considerably higher price tag of linear algebra for complex-valued Gaussian quadrature.

5 Conclusions

In this paper, motivated by numerical problems in wave inverse scattering, we have extended the modern theory of highly oscillatory integrals and their computation to the realm of singular integrals. Specifically, we have presented three general approaches. The first is a truncated asymptotic expansion. While this method is accurate for high frequencies, it fails for low frequencies, yet it is fundamental in underpinning our second approach, Filon-type methods. They overcome the divergence at low frequencies and numerical results confirm their superiority *vis-à-vis* the asymptotic expansion method. The final method is complex-valued Gaussian quadrature. While it is poorly understood from an analytic standpoint, numerical results indicate that this approach achieves by far the least error throughout the full range of frequencies.

The main thrust of this paper is in demonstrating that existing theory of highly oscillatory quadrature can be extended to the singular case, although this requires great care and attention to detail. Once correct quadrature methods are employed, singular highly oscillatory integrals can be approximated by affordable and precise computations. We expect this to have a significant impact in accelerating computational schemes to simulate wave propagation.

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A Proofs of theorems

In this section, we give the detailed proofs of our theorems.

A.1 Proof of Theorem 2

Proof. Firstly, use subtraction to remove the singularity of $x^{-\alpha}$,

$$\int_0^b x^{-\alpha} f(x) \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x = f(0) \int_0^b x^{-\alpha} \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x + \int_0^b x^{-\alpha} [f(x) - f(0)] \mathrm{e}^{\mathrm{i}\omega g(x)} \mathrm{d}x$$

$$\begin{aligned} &= f(0)\mu_0(\alpha,\omega) + \int_0^b x^{-\alpha}[f(x) - f(0)]\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x \\ &= f(0)\mu_0(\alpha,\omega) + I_2, \end{aligned}$$

where $\mu_0(\alpha,\omega)$ is bounded and

$$I_2 = \int_0^b x^{-\alpha}[f(x) - f(0)]\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x.$$

The first term in the expansion of I_2 is determined from

$$\begin{aligned} I_2 &= \int_0^b x^{-\alpha}[f(x) - f(0)]\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x = \frac{1}{\mathrm{i}\omega}\int_0^b \frac{f(x) - f(0)}{x^\alpha g'(x)}\mathrm{d}\mathrm{e}^{\mathrm{i}\omega g(x)} \\ &= \frac{1}{\mathrm{i}\omega}\frac{f(b) - f(0)}{b^\alpha g'(b)}\mathrm{e}^{\mathrm{i}\omega g(b)} - \frac{1}{\mathrm{i}\omega}\left[\lim_{x\to 0}\frac{f(x) - f(0)}{x^\alpha g'(x)}\right]\mathrm{e}^{\mathrm{i}\omega g(0)} \\ &\quad - \frac{1}{\mathrm{i}\omega}\int_0^b \frac{\mathrm{d}}{\mathrm{d}x}\frac{f(x) - f(0)}{x^\alpha g'(x)}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x \\ &= \frac{1}{\mathrm{i}\omega}\frac{f(b) - f(0)}{b^\alpha g'(b)}\mathrm{e}^{\mathrm{i}\omega g(b)} \\ &\quad - \frac{1}{\mathrm{i}\omega}\int_0^b x^{-\alpha}\frac{f'(x)g'(x) - [f(x) - f(0)][\frac{\alpha g'(x)}{x} + g''(x)]}{g'^2(x)}\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x \end{aligned}$$

provided that the function $\frac{f(x)-f(0)}{x^\alpha g'(x)}$ is continuous and that $\lim\limits_{x\to 0}\frac{f(x)-f(0)}{x^\alpha g'(x)} = 0$. Since

$$\frac{\sigma_{k-1}(x) - \sigma_{k-1}(0)}{x^\alpha g'(x)}|_{x=0} = \lim_{x\to 0}\frac{\sigma_{k-1}(x) - \sigma_{k-1}(0)}{x^\alpha g'(x)} = 0,$$

we deduce the remaining terms using integration by parts,

$$
\begin{aligned}
I[f] \;&\sim\; \mu_0(\alpha,\omega)\sum_{k=0}^{s-1}\frac{1}{(-\mathrm{i}\omega)^k}\sigma_k[f](0)-\sum_{k=1}^{s}\frac{1}{(-\mathrm{i}\omega)^k}\frac{\sigma_{k-1}[f](b)-\sigma_{k-1}[f](0)}{b^\alpha g'(b)}\mathrm{e}^{\mathrm{i}\omega g(b)}\\
&\quad+\frac{1}{(-\mathrm{i}\omega)^s}\int_0^b x^{-\alpha}\sigma_s[f](x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x.
\end{aligned}
$$

The result (2.17) follows. ☐

A.2 Proof of Theorem 10

Proof. Commencing from the formula

$$
\begin{aligned}
\int_{-\infty}^0 f^{(k-1)}\big(\mathrm{e}^t\big)\,\mathrm{e}^{(k+\mathrm{i}\omega)t}\mathrm{d}t \;&=\; \sum_{\ell=0}^{L-1}\frac{(-1)^\ell f^{(k+\ell-1)}(1)}{(\mathrm{i}\omega+k)_{\ell+1}}+\frac{(-1)^{L-1}}{(\mathrm{i}\omega+k)_{L-1}}\\
&\qquad\int_{-\infty}^0 f^{(k+L-1)}\big(\mathrm{e}^t\big)\,\mathrm{e}^{(\mathrm{i}\omega+k+L)t}\mathrm{d}t\\
&\sim\; \sum_{\ell=0}^{L-1}\frac{(-1)^\ell f^{(k+\ell-1)}(1)}{(\mathrm{i}\omega+k)_{\ell+1}}+\mathcal{O}\Big(\frac{1}{\omega^L}\Big),
\end{aligned}
$$

and integrating (1.4) by parts, we get

$$
\begin{aligned}
I[f] \;&=\; -\sum_{k=1}^{s}\frac{(-1)^{k-1}}{(\mathrm{i}\omega+1)_k}\int_{-\infty}^0 f^{(k-1)}\big(\mathrm{e}^t\big)\,\mathrm{e}^{(\mathrm{i}\omega+k)t}\mathrm{d}t\\
&\quad+\frac{(-1)^s}{(\mathrm{i}\omega+1)_s}\int_{-\infty}^0 tf^{(s)}\big(\mathrm{e}^t\big)\,\mathrm{e}^{(s+1+\mathrm{i}\omega)t}\mathrm{d}t\\
&\sim\; -\sum_{k=1}^{s}\frac{(-1)^{k-1}}{(\mathrm{i}\omega+1)_k}\left[\sum_{\ell=0}^{L-1}\frac{(-1)^\ell f^{(k+\ell-1)}(1)}{(\mathrm{i}\omega+k)_{\ell+1}}+\mathcal{O}\Big(\frac{1}{\omega^L}\Big)\right]+\mathcal{O}\Big(\frac{1}{\omega^{s+1}}\Big).
\end{aligned}
$$

To get the asymptotic order $\mathcal{O}(\omega^{-s-1})$, the truncation parameter L should be chosen so that $L \geq s-k+1$. This completes the proof. ☐

A.3 Proof of Theorem 11

Proof. Let $r = f - p_n$, whereby

$$
\begin{aligned}
I[r(x)] \;&\sim\; \mu_0(\alpha,\omega)\sum_{k=0}^{s-1}\frac{\sigma_k[r](0)}{(-\mathrm{i}\omega)^k}-\sum_{k=1}^{s}\frac{1}{(-\mathrm{i}\omega)^k}\frac{\sigma_{k-1}[r](b)-\sigma_{k-1}[r](0)}{b^\alpha g'(b)}\mathrm{e}^{\mathrm{i}\omega g(b)}\\
&\quad+\frac{1}{(-\mathrm{i}\omega)^s}\int_0^b x^{-\alpha}\sigma_s[r](x)\mathrm{e}^{\mathrm{i}\omega g(x)}\mathrm{d}x,
\end{aligned}
$$

where we recall from Theorem 1 that

$$
\begin{aligned}
\sigma_0[f](x) \;&=\; f(x),\\
\sigma_{k+1}[f](x) \;&=\; x^\alpha\frac{\mathrm{d}}{\mathrm{d}x}\frac{\sigma_k[f](x)-\sigma_k[f](0)}{x^\alpha g'(x)},\qquad k\geq 0,
\end{aligned}
$$

is determined from the error function $r(x)$. If

$$
\sigma_k[r](0)=0,\qquad \sigma_k[r](b)=0,\quad k=0,1,\cdots,s-1, \tag{A.1}
$$

then the error is $\mathcal{O}\big(\omega^{-s-(1-\alpha)}\big)$.

Next we determine the requirements for meeting these conditions. Following from its definition, $\sigma_1[f](0)$ depends on $f'(0)$. Let

$$f(x)=\sum_{j=0}^{\infty}\frac{f^{(j)}(0)}{j!}x^j,\qquad g(x)=\sum_{j=0}^{\infty}\frac{g^{(j)}(0)}{j!}x^j,\qquad \sigma_k[f](x)=\sum_{j=0}^{\infty}\frac{\sigma_k^{(j)}[f](0)}{j!}x^j,\quad k\ge 0.$$

Since $\sigma_k[f]$ is analytic,

$$\sigma_2[f](x)=\frac{(1-\alpha)\sigma_1'[f](0)}{g'(0)}+\mathcal{O}(x)$$

indicating that $\sigma_2[f](0)$ is determined by $f'(0)$ and $f''(0)$. Similarly, $\sigma_k[f](0)$ is a linear combination of $f'(0)$, $f''(0)$, $\cdots$, $f^{(k)}(0)$. In addition, for $x\neq 0$, it may be shown easily that each $\sigma_k[f](x)$, is a linear combination of $f(x)$, $f(0)$, $f'(x)$, $f'(0)$, $\cdots$, $f^{(k-1)}(x)$, $f^{(k-1)}(0)$, $f^{(k)}(x)$. Therefore, the conditions in (A.1) are met if

$$\begin{aligned} r(0)&=r'(0)=\cdots=r^{(s-1)}(0)=0,\\ r(b)&=r'(b)=\cdots=r^{(s-1)}(b)=0.\end{aligned}$$

Setting

$$p_n^{(j)}(c_\ell)=f^{(j)}(c_\ell),\quad \ell=1,\cdots,\nu;\quad j=0,1,\cdots,m_\ell-1.$$

the conditions in (A.1) follow and the error is therefore $\mathcal{O}\big(\omega^{-s-(1-\alpha)}\big)$. □

A.4 Proof of Theorem 12

Proof. Substituting $r=f-p_n$ into (2.6),we observe that if $\rho_k^{(j)}[r](0)=0$, $k=0,\cdots,s-1$, $j=0,\cdots,r$ and $\rho_k[r](b)=0$, $k=0,1,\cdots,s-1$, then the error is $\mathcal{O}\big(\omega^{-s-(1-\alpha)/(r+1)}\big)$. We examine in detail the calculation of $\rho_k[f](x)$ in (2.6) and show that it depends on $f(x)$, $f'(x)$, $\cdots$, $f^{(k)}(x)$, $x\neq 0$. Let

$$f(x)=\sum_{j=0}^{\infty}\frac{f^{(j)}(0)}{j!}x^j,\qquad g(x)=\sum_{j=r+1}^{\infty}\frac{g^{(j)}(0)}{j!}x^j,$$

then

$$\begin{aligned}\rho_1[f](x)&=x^\alpha\frac{\mathrm{d}}{\mathrm{d}x}\frac{f(x)-\sum\limits_{j=0}^{r}\frac{f^{(j)}(0)}{j!}x^j}{x^\alpha g'(x)}\\ &=\frac{\sum\limits_{j=r}^{\infty}\frac{f^{(j+1)}(0)}{j!}x^j}{\sum\limits_{j=r}^{\infty}\frac{g^{(j+1)}(0)}{j!}x^j}-\alpha\frac{\sum\limits_{j=r+1}^{\infty}\frac{f^{(j)}(0)}{j!}x^j}{\sum\limits_{j=r+1}^{\infty}\frac{g^{j}(0)}{(j-1)!}x^j}-\frac{\left[\sum\limits_{j=r+1}^{\infty}\frac{f^{(j)}(0)}{j!}x^j\right]\left[\sum\limits_{j=r-1}^{\infty}\frac{g^{(j+2)}(0)}{j!}x^j\right]}{\left[\sum\limits_{j=r}^{\infty}\frac{g^{(j+1)}(0)}{j!}x^j\right]\left[\sum\limits_{j=r}^{\infty}\frac{g^{(j+1)}(0)}{j!}x^j\right]}.\end{aligned}$$

It follows that

$$\rho_1[f](0)=\left(1-\frac{r+\alpha}{r+1}\right)\frac{f^{(r+1)}(0)}{g^{(r+1)}(0)}.$$

Moreover,

$$\rho_1^{(1)}[f](0)=\lim_{x\to 0}\frac{\rho_1[f](x)-\rho_1[f](0)}{x}$$

is a linear combination of $f^{(r+1)}(0)$ and $f^{(r+2)}(0)$. We thus deduce that $\rho_1^{(j)}[f](0)$ depends on $f^{(\ell)}$, $\ell=r+1,r+2,\cdots,r+1+j$. Similarly, assuming $\rho_1[f](x)=\sum\limits_{j=0}^{\infty}\frac{\rho_1^{(j)}[f](0)}{j!}x^j$, $\rho_2[f](0)$

is determined by $\rho_1^{(r+1)}[f](0)$, that is, the derivatives $f^{(\ell)}(0)$, $\ell = r+1, r+2, \cdots, 2(r+1)$ determine the value of $\rho_2[f](0)$. Likewise, the r-th order derivative $\rho_2^{(r)}[f](0)$ is a linear combination of $f^{(\ell)}(0)$, $\ell = r+1, r+2, \cdots, 2(r+1)+r$. Thus, we conclude that $\rho_k[f](0)$ involves $f^{(\ell)}(0)$, $\ell = r+1, r+2, \cdots, k(r+1)$ and $\rho_k^{(j)}[f](0)$ is a linear combination of $f^{(\ell)}(0)$, $\ell = r+1, r+2, \cdots, k(r+1)+j$. Hence the theorem follows by setting

$$\begin{aligned} r^{(\ell)}(0) &= 0, \qquad \ell = 0, 1, \cdots, (s-1)(r+1)+r, \\ r^{(\ell)}(b) &= 0, \qquad \ell = 0, 1, \cdots, s-1, \end{aligned}$$

or, equivalently,

$$\rho_k^{(j)}[r](0) = 0, \quad k = 0, \cdots, s-1, j = 0, \cdots, r, \qquad \rho_k[r](b) = 0, k = 0, 1, \cdots, s-1.$$

□

A.5 Proof of Theorem 13

Proof. In the asymptotic expansion (2.11) we have for every $k \geq 0$ and $p = 0, \cdots, k$

$$\sigma_k[f](x) = \sum_{p=0}^{k} \sigma_{k,p}(x) f^{(p)}(x) + \sigma_{0,p}(x) f(0),$$

where $\sigma_{k,k}(x) \neq 0$ and $\sigma_{k,p}$ is a combination of derivatives of $g(x)$. We compute

$$\begin{aligned} \gamma_{k-1,0}[f](x) &= \sum_{p=0}^{k-1} \frac{\sigma_{k-1,p}(x) f^{(p)}(x) - \sigma_{k-1,p}(0) f^{(p)}(0)}{x g'(x)} + [\sigma_{0,p}(x) - \sigma_{0,p}(0)] f(0), \\ \gamma_{k-1,1}[f](x) &= \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\gamma_{k-1,0}[f](x)}{g'(x)} \right). \end{aligned}$$

Hence, we deduce that $\sigma_{s-1}[f](b)$ and $\gamma_{s-1,\ell}[f](b)$ are a linear combination of $f^{(j)}(b)$, $j = 0, \cdots, s-1$. Also $\sigma_{s-1}[f](0)$ and $\gamma_{s-1,\ell}[f](0)$ can be expressed in terms of the $f^{(j)}(0)$, $j = 0, 1, \cdots, s-1$. Hence, with nodes c_j and multiplicities m_j, $j = 1, 2, \cdots, q$, if we substitute the error function $r(x) = f(x) - p_n(x)$ into the asymptotic expansion, the result is an error of $\mathcal{O}\big(\omega^{-(s+1)} \log \omega\big)$. □

A.6 Proof of Theorem 14

Proof. Consider a first-order stationary point at $x = 0$. We need to analyse the relationships among $\rho_{k-1}[f](x)$, $\eta_{k-1,\ell-1}[f](x)$, f and its derivatives in (2.16). Based on the definitions, it can be deduced that $\rho_{k-1}[f](b)$ is a combination of $f^{(j)}(b)$, $j = 0, 1, \cdots, k-1$. Likewise, $\eta_{k-1,\ell-1}[f](b)$ is also determined by $f^{(j)}(b)$, $j = 0, 1, \cdots, k+\ell-2$ for $k = 1, \cdots, s$ and $\ell = 1, \cdots, L_k$, $L_k = s-k+1$. Thus, the values of $\rho_{k-1}[f](b)$ and $\eta_{k-1,\ell-1}[f](b)$ in the asymptotic expansion depend upon $f^{(j)}(b)$, $j = 0, 1, \cdots, s-1$.

Now consider the endpoint $x = 0$. Let

$$f(x) = \sum_{j=0}^{\infty} \frac{f^{(j)}(0)}{j!} x^j, \qquad g(x) = \sum_{j=r+1}^{\infty} \frac{g^{(j)}(0)}{j!} x^j.$$

Incorporating this into the definition of ρ_k yields

$$\rho_1[f](0) = \frac{\mathrm{d}}{\mathrm{d}x} \left[\frac{\sum\limits_{j=r+1}^{\infty} \frac{f^{(j)}(0)}{j!} x^j}{\sum\limits_{j=r}^{\infty} \frac{g^{(j+1)}(0)}{j!} x^j} \right] \Bigg|_0 = \frac{f^{(r+1)}(0)}{(r+1) g^{(r+1)}(0)},$$

which implies that $\rho_1^{(k)}[f](0)$ depends on $f^{(j)}(0)$, $j = r+1, r+2, \cdots, r+1+k$. Since

$$\rho_2[f](0) = \frac{\rho_1^{(r+1)}[f](0)}{(r+1)g^{(r+1)}(0)},$$

it follows that $\rho_2[f](0)$ is a linear combination of $f^{(j)}(0)$, $j = r+1, r+2, \cdots, 2(r+1)$. An immediate consequence is that $\rho_{k-1}[f](0)$ is a combination of $f^{(j)}(0)$, $j = r+1, r+2, \cdots, (k-1)(r+1)$. In addition,

$$\eta_{k-1,0}[f](0) = \left. \frac{\sum\limits_{j=r+1}^{\infty} \frac{\rho_{k-1}^{(j)}[f](0)}{j!} x^j}{\sum\limits_{j=r+1}^{\infty} \frac{g^{(j)}(0)}{(j-1)!} x^j} \right|_0 = \frac{\rho_{k-1}^{(r+1)}[f](0)}{(r+1)g^{(r+1)}(0)},$$

in which $\rho_{k-1}^{(r+1)}[f](0)$ depends on $f^{(j)}(0)$, $j = r+1, r+2, \cdots, k(r+1)$. Applying the same technique to $\eta_{k-1,1}[f]$, we observe that $\eta_{k-1,1}[f](0)$ depends linearly on $\eta_{k-1,0}^{(r)}[f](0)$ and $\eta_{k-1,0}^{(r+1)}[f](0)$ which involves a linear combination of $f^{(j)}(0)$, $j = r+1, r+2, \cdots, (k+1)(r+1)$. More generally, it is deduced that $\eta_{k-1,\ell}[f](0)$ is a linear combination $f^{(j)}(0)$, $j = r+1, r+2, \cdots, (k+\ell)(r+1)$ and $\eta_{k-1,\ell}^{(n)}[f](0)$ is a linear combination of $f^{(j)}(0)$, $j = r+1, r+2, \cdots, (k+\ell)(r+1)+n$.

Hence the theorem follows once we substitute the error function $r = f - p_n$ into the asymptotic expansion (2.16). $\square$