Appendix A

Technical Lemmas

Here we present the proofs of two technical lemmas, Lemmas 2.1 and 2.6, that play an important role in the convergence rate results of Chapter 2. Neither of these results is very difficult to obtain, but since the technical nature of the proofs obscures the essence of the convergence rate results, we place them here in the appendix.

A.1 Bound on Fourier Coefficient of Green's Function

To prove that solutions to the approximate integral equation (2.3) exist and to prove the convergence rates, we need a bound on the decay rate of the Fourier coefficients of the Green's function, $\mathcal{J}_\ell(a, r)$ as defined in (2.1). This decay rate is given in Lemma 2.1. However, although the proof of this lemma is not difficult, it is somewhat technical. Hence, we first derive two simple bounds that aid in the proof.

Lemma A.1. *Given $\alpha > 0$ and a positive integer k, there exists a constant $C > 0$ such that*

$$\frac{\alpha^\ell}{\ell!} \leq \frac{C}{\max\{1, \ell^k\}},$$

for all integers $\ell \geq 0$.

Proof. If we let $\ell = 0$, then we require that $C \geq 1$ for the lemma to hold. Now consider $\ell \geq 1$. Equivalently we require that

$$\ell \log \alpha - \sum_{p=2}^{\ell} \log \ell + k \log \ell \leq \log C.$$

We bound the sum by the following integral

$$\sum_{p=2}^{\ell} \log \ell \geq \int_{1}^{\ell} \log x dx = \ell \log \ell - \ell + 1.$$

Thus, we require that

$$\ell \left[\log \alpha + 1 + k \frac{\log \ell}{\ell} \right] - \ell \log \ell \leq \log C + 1.$$

It is not difficult to see that the left-hand side of this equation is bounded from above for $\ell \geq 1$ since $\ell \log \ell$ eventually dominates. Hence, we can choose a constant $C \geq 1$ such that the result holds. □

According to [2, p. 362], for all integers $\ell \geq 0$ and for any real, non-negative z,

$$|J_\ell(z)| \leq \frac{1}{\ell!} \left(\frac{z}{2} \right)^{\ell}. \tag{A.1}$$

The following lemma provides a similar bound for $|Y_\ell(z)|$.

Lemma A.2. *For all integers $\ell \geq 1$ and for any real, non-negative z,*

$$|Y_\ell(z)| \leq \frac{(\ell-1)!}{\pi} \left(\frac{z}{2} \right)^{-\ell} e^{\left(\frac{z}{2}\right)^2} + \frac{2}{\pi \ell!} \left| \log \left(\frac{z}{2} \right) \right| \left(\frac{z}{2} \right)^{\ell} + \frac{2}{\pi} \left(\frac{z}{2} \right)^{\ell} e^{\left(\frac{z}{2}\right)^2}. \tag{A.2}$$

For $\ell = 0$,

$$|Y_\ell(z)| \leq \frac{2}{\pi} \left| \log \left(\frac{z}{2} \right) \right| + \frac{2}{\pi} e^{\left(\frac{z}{2}\right)^2}.$$

Proof. By [10, p. 51], $Y_\ell(z)$ for any non-negative integer ℓ is given by

$$Y_\ell(z) = \frac{2}{\pi} J_\ell(z) \log \left(\frac{z}{2} \right) - \frac{1}{\pi} \sum_{k=0}^{\ell-1} \frac{(\ell-k-1)!}{k!} \left(\frac{z}{2} \right)^{2k-\ell} - \frac{1}{\pi} \sum_{k=0}^{\infty} \frac{\psi(\ell+k) + \psi(k)}{(-1)^k k! (k+\ell)!} \left(\frac{z}{2} \right)^{2k+\ell},$$

where $\psi(0) = -\gamma \approx -0.5772$ and $\psi(k) = -\gamma + \sum_{j=1}^{k} \frac{1}{j}$ for $k \geq 1$.

For $\ell \geq 1$,

$$\begin{aligned}\sum_{k=0}^{\ell-1} \frac{(\ell-k-1)!}{k!}\left(\frac{z}{2}\right)^{2k} &\leq (\ell-1)!\sum_{k=0}^{\infty}\frac{1}{k!}\left[\left(\frac{z}{2}\right)^2\right]^k \\ &\leq (\ell-1)!e^{\left(\frac{z}{2}\right)^2}.\end{aligned}$$

Also note that for $k \geq 1$, $|\psi(0)| \leq 1$ and

$$\begin{aligned}0 \leq \psi(k) &\leq -\gamma + \sum_{j=1}^{k} 1 \\ &= -\gamma + k \\ &\leq k.\end{aligned}$$

Hence, $|\psi(k)| \leq \max\{1, k\}$.

Now observe that $|\psi(\ell+k)+\psi(k)| \leq 2\max\{1, \ell+k\}$ and

$$\frac{|\psi(k)|}{k!} \leq 1,$$

for $k \geq 0$. Therefore, for $\ell \geq 0$

$$\begin{aligned}\sum_{k=0}^{\infty}\frac{|\psi(\ell+k)+\psi(k)|}{k!(k+\ell)!}\left(\frac{z}{2}\right)^{2k} &\leq 2\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{z}{2}\right)^{2k} \\ &\leq 2e^{\left(\frac{z}{2}\right)^2}.\end{aligned}$$

Hence, by these individual bounds and (A.1) we obtain the desired result. □

With these two results in hand, we turn to the proof of the main lemma.

Proof of Lemma 2.1. First note that

$$\begin{aligned}\int_{R_0}^{R_1} |\mathcal{J}_\ell(a,r)|\, r dr &= |H_\ell^1(\kappa a)| \int_{R_0}^{a} |J_\ell(\kappa r)| r dr + |J_\ell(\kappa a)| \int_{a}^{R_1} |H_\ell^1(\kappa r)| r dr \\ &\leq |J_\ell(\kappa a)| \int_{R_0}^{R_1} |J_\ell(\kappa r)| r dr + |J_\ell(\kappa a)| \int_{a}^{R_1} |Y_\ell(\kappa r)| r dr \\ &\quad + |Y_\ell(\kappa a)| \int_{R_0}^{a} |J_\ell(\kappa r)| r dr \\ &\leq I_{J,J} + I_{J,Y} + I_{Y,J},\end{aligned}$$

where

$$\begin{aligned} I_{J,J} &= |J_\ell(\kappa a)| \int_0^{R_1} |J_\ell(\kappa r)| r dr, \\ I_{J,Y} &= |J_\ell(\kappa a)| \int_a^{R_1} |Y_\ell(\kappa r)| r dr, \\ I_{Y,J} &= |Y_\ell(\kappa a)| \int_0^{a} |J_\ell(\kappa r)| r dr. \end{aligned}$$

Note that $|J_{-\ell}(z)| = |(-1)^\ell J_\ell(z)| = |J_\ell(z)|$ and similarly $|Y_{-\ell}(z)| = |Y_\ell(z)|$. Hence, it suffices to bound these integrals for $\ell \geq 0$.

We use (A.1) as well as Lemmas A.1 and A.2 to bound each of these integrals. For $\ell \geq 0$

$$\begin{aligned} I_{J,J} &\leq \frac{1}{(\ell!)^2} R_1^2 \left(\frac{\kappa R_1}{2}\right)^{2l} \\ &\leq \frac{C_{J,J}}{\max\{1, \ell^2\}}, \end{aligned}$$

where the last inequality follows from Lemma A.1 and $C_{J,J}$ depends only on κ and R_1.

The bound for $I_{J,Y}$ consists of three parts from each of the three terms in (A.2). For $\ell > 2$,

$$\begin{aligned} \frac{\kappa^\ell}{2^\ell \ell!} a^\ell \int_a^{R_1} \frac{2^\ell (\ell-1)!}{\pi \kappa^\ell} r^{-\ell+1} e^{(\frac{\kappa r}{2})^2} dr &\leq \frac{{R_1}^2}{\pi \ell (\ell-2)} e^{(\frac{\kappa R_1}{2})^2} \left(\left(\frac{a}{R_1}\right)^2 - \left(\frac{a}{R_1}\right)^\ell \right) \\ &\leq \frac{C_{J,Y}^{(1)}}{\max\{1, \ell^2\}}. \end{aligned}$$

For $\ell = 0$ this term does not appear in (A.2) and for $\ell = 1, 2$, a similar argument yields the same bound. Continuing with the next term in (A.2)

$$\begin{aligned} \frac{(\kappa a)^\ell}{2^\ell \ell!} \int_a^{R_1} \frac{2\kappa^\ell}{\pi 2^\ell \ell!} \left|\log\left(\frac{\kappa r}{2}\right)\right| r^{\ell+1} dr &\leq \left(\frac{\kappa R_1}{2}\right)^{2\ell} \frac{2R_1}{\pi (\ell!)^2} \int_0^{R_1} \left|\log\left(\frac{\kappa r}{2}\right)\right| dr \\ &\leq \frac{C_{J,Y}^{(2)}}{\max\{1, \ell^2\}}, \end{aligned}$$

by Lemma A.1 and since $\int_0^{R_1} \left|\log\left(\frac{\kappa r}{2}\right)\right| dr$ is bounded. Finally, by similar arguments one can show that the third term is similarly bounded.

We also bound $I_{Y,J}$ by considering the three terms in (A.2). For $\ell \geq 1$,

$$\begin{aligned} \frac{2^\ell(\ell-1)!}{\pi\kappa^\ell} a^{-\ell} e^{\left(\frac{\kappa a}{2}\right)^2} \int_0^a \frac{\kappa^\ell}{2^\ell \ell!} r^{\ell+1} dr &\leq \frac{1}{\pi\ell(\ell+2)} e^{\left(\frac{\kappa a}{2}\right)^2} {R_1}^2 \\ &\leq \frac{C^{(1)}_{Y,J}}{\max\{1,\ell^2\}} \,. \end{aligned}$$

Continuing with the second term,

$$\begin{aligned} \frac{2}{\pi\ell!}\left|\log\left(\frac{\kappa a}{2}\right)\right|\left(\frac{\kappa a}{2}\right)^\ell \int_0^a \frac{1}{\ell!}\left(\frac{\kappa r}{2}\right)^\ell r dr &\leq \frac{1}{\pi(\ell!)^2}\left(\frac{\kappa R_1}{2}\right)^{2\ell} a^2 \left|\log\left(\frac{\kappa a}{2}\right)\right| \\ &\leq \frac{C^{(2)}_{Y,J}}{\max\{1,\ell^2\}} \,, \end{aligned}$$

since $a^2 \left|\log\left(\frac{\kappa a}{2}\right)\right|$ is bounded for $0 \leq a \leq R_1$. The bound for the last term also takes this form and can be obtained similarly. Hence,

$$I_{J,J} + I_{J,Y} + I_{Y,J} \leq \frac{C}{\max\{1,\ell^2\}},$$

for some constant $C > 0$ that depends only on κ and R_1. □

A.2 Bound on Integral Operator

In this section, we prove the bound on $K_\ell u^T$ as given in Lemma 2.6, which plays a primary role in our derivation of the convergence rates. As mentioned previously, some care is required to obtain tight bounds on the convergence rates. Hence, the proof of the lemma is somewhat technical.

Proof of Lemma 2.6. Define the annular region $A = \{(a,\phi) : R_0 \leq a \leq R_1\}$. Then (2.7), Lemma 2.4 and Theorem 2.5 imply that if $m \in C^{k,\alpha}(A) \cap C^{k+2,\alpha}_{pw}(A)$, then $u \in C^{k+2,\alpha}(A) \cap C^{k+4,\alpha}_{pw}(A)$ and there exists a constant $C > 0$ such that

$$\begin{aligned} \left\|K_\ell u^T\right\|_\infty &\leq \frac{C}{\max\{1,\ell^2\}} \sum_{|j|>M} \frac{1}{\max\{1,|\ell-j|^{k+2}\}} \frac{1}{\max\{1,|j|^{k+4}\}} \\ &= \frac{C}{\max\{1,\ell^2\}} \sum_{j>M} \frac{1}{j^{k+4}} \left(\frac{1}{(j-\ell)^{k+2}} + \frac{1}{(j+\ell)^{k+2}}\right) \\ &\leq \frac{2C}{\max\{1,\ell^2\}} \sum_{j>M} \frac{1}{j^{k+4}} \frac{1}{(j-|\ell|)^{k+2}}, \end{aligned} \tag{A.3}$$

for $\ell = -M, \ldots, M$. This expression also holds for $m \in L^\infty(A) \cap C^{1,\alpha}_{pw}(A)$ with $k = -1$.

Clearly, we need only consider $\ell = 0, \ldots, M$.

$$\begin{aligned}
\sum_{j>M} \frac{1}{j^{k+4}} \frac{1}{(j-\ell)^{k+2}} &\leq \frac{1}{(M+1)^{k+4}} \frac{1}{(M+1-\ell)^{k+2}} + \int_{M+1}^{\infty} \frac{1}{x^{k+4}} \frac{1}{(x-\ell)^{k+2}} \\
&= \frac{1}{(M+1)^{k+4}} \frac{1}{(M+1-\ell)^{k+2}} \\
&\quad + \frac{1}{2k+5} \frac{1}{(M+1)^{2k+5}} F\left(k+2, 2k+5; 2k+6; \frac{\ell}{M+1}\right),
\end{aligned}$$

where F is the hypergeometric function [2, p. 556]

$$\begin{aligned}
F(a,b;c;z) \equiv {}_2F_1(a,b;c;z) &= \frac{\Gamma(c)}{\Gamma(b)\Gamma(c-b)} \int_0^1 t^{b-1}(1-t)^{c-b-1}(1-tz)^{-a} dt \\
&= \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)\Gamma(b+n)}{\Gamma(c+n)} \frac{z^n}{n!},
\end{aligned}$$

for $|z| < 1$.

We need a few simple bounds on F in order to obtain the final result. It is easily verified that for positive integers a, b,

$$F(a,b;b;z) = \sum_{n=0}^{\infty} \frac{(a+n-1)!}{(a-1)!n!} z^n = (1-z)^{-a}.$$

Using this result, if $a > 1$ and $b > 0$ are integers and $a \leq b+1$, then

$$\begin{aligned}
F(a,b;b+1;z) &= \frac{b}{a-1} \sum_{n=0}^{\infty} \frac{a+n-1}{b+n} \frac{(a+n-2)!}{(a-2)!n!} z^n \\
&\leq \frac{b}{a-1}(1-z)^{-(a-1)}.
\end{aligned}$$

Finally, for integers $a = 1$ and $b > 0$, we have

$$\begin{aligned}
F(1,b;b+1;z) &= b \sum_{n=0}^{\infty} \frac{1}{b+n} z^n \\
&\leq 1 - b\log(1-z).
\end{aligned}$$

Hence, for $k \geq 0$ and $\ell = 0, \ldots, M$, we obtain

$$\begin{aligned} \sum_{j>M} \frac{1}{j^{k+4}} \frac{1}{(j-\ell)^{k+2}} &\leq \frac{1}{(M+1)^{k+4}} \frac{1}{(M+1-\ell)^{k+2}} + \frac{1}{k+1} \frac{1}{(M+1)^{k+4}} \frac{1}{(M+1-\ell)^{k+1}} \\ &\leq \frac{2}{M^{k+4}} \frac{1}{(M+1-\ell)^{k+1}}. \end{aligned} \tag{A.4}$$

For $k = -1$ and $\ell = 0, \ldots, M$,

$$\begin{aligned} \sum_{j>M} \frac{1}{j^3} \frac{1}{j-\ell} &\leq \frac{1}{(M+1)^3} \frac{1}{M+1-\ell} + \frac{1}{3(M+1)^3} + \frac{1}{(M+1)^3} \log\left(\frac{M+1}{M+1-\ell}\right) \\ &\leq \frac{1}{3M^3} + \frac{1}{M^2} \frac{1}{M+1-\ell}, \end{aligned} \tag{A.5}$$

where we have used the fact that $\log x \leq x$. Combining (A.3) with (A.4) and (A.5) give the desired results for $m \in L^\infty(A) \cap C^{1,\alpha}_{pw}(A)$ and $m \in C^{k,\alpha}(A) \cap C^{k+2,\alpha}_{pw}(A)$, respectively. □

Remark A.3. Finally, we note that the bounds for $m \in L^\infty(A) \cap C^{1,\alpha}_{pw}(A)$ and $m \in C^{0,\alpha}(A) \cap C^{2,\alpha}_{pw}(A)$ can be obtained more simply as follows.

$$\begin{aligned} \|K_\ell u^T\| &\leq \frac{2C}{\max\{1, \ell^2\}} \sum_{j>M} \frac{1}{j^{k+4}} \frac{1}{(j-|\ell|)^{k+2}} \\ &\leq \frac{2C}{\max\{1, \ell^2\}} \frac{1}{(M+1-|\ell|)^{k+2}} \sum_{j>M} \frac{1}{j^{k+4}} \\ &\leq \frac{\hat{C}}{\max\{1, \ell^2\}} \frac{1}{(M+1-|\ell|)^{k+2}} \frac{1}{M^{k+3}}, \end{aligned}$$

for some constant $\hat{C} > 0$. However, this simple bound does not capture the interesting convergence rate jumps in the results of Theorem 2.7 for $m \in C^{k,\alpha}(A) \cap C^{k+2,\alpha}_{pw}(A)$, $k \geq 1$.

Appendix B

Accurate and Efficient Computation of Scaled Bessel Functions

As explained in Section 3.1.2, the rapid decay of the $J_\ell(z)$ and the rapid growth of the $Y_\ell(z)$ as ℓ increases produces factors that underflow and overflow, respectively, but whose product is machine-representable. We overcome these and other related issues by computing scaled versions of the Bessel functions. The leading order asymptotic behavior of $J_\ell(z)$ and $Y_\ell(z)$ near the origin are given respectively by

$$J_\ell(z) \sim \frac{1}{\ell!}\left(\frac{z}{2}\right)^\ell$$

and

$$Y_\ell(z) \sim -\frac{(\ell-1)!}{\pi}\left(\frac{z}{2}\right)^{-\ell}$$

for $\ell > 0$. Thus, we scale the Bessel functions by their asymptotic representations, i.e., for $\ell > 0$

$$\tilde{J}_\ell(z) = \ell!\left(\frac{z}{2}\right)^{-\ell} J_\ell(z), \tag{B.1}$$

$$\tilde{Y}_\ell(z) = -\frac{\pi}{(\ell-1)!}\left(\frac{z}{2}\right)^{\ell} Y_\ell(z). \tag{B.2}$$

We use these scaled Bessel functions to compute products and quotients of J_ℓ, Y_ℓ and H^1_ℓ in many combinations. For example, we can compute the product $J_\ell(z_1)Y_\ell(z_2)$ for $\ell > 0$ as

$$J_\ell(z_1)Y_\ell(z_2) = -\frac{1}{\pi\ell}\tilde{J}_\ell(z_1)\tilde{Y}_\ell(z_2). \tag{B.3}$$

Typically, the unscaled Bessel functions are computed by means of their recurrence relations

$$J_{\ell+1}(z) = \frac{2\ell}{z} J_\ell(z) - J_{\ell-1}(z), \tag{B.4}$$

$$Y_{\ell+1}(z) = \frac{2\ell}{z} Y_\ell(z) - Y_{\ell-1}(z). \tag{B.5}$$

Note that these recurrence relations are identical, signifying the fact that the underlying difference equation has linearly independent solutions $J_\ell(z)$ and $Y_\ell(z)$ for each z. Hence, in theory, given either $J_0(z)$ and $J_1(z)$ or $Y_0(z)$ and $Y_1(z)$, these recurrence relations allow us to obtain $J_\ell(z)$ or respectively $Y_\ell(z)$ for all ℓ. In practice, this works well for $Y_\ell(z)$. However, this procedure works for $J_\ell(z)$ only if $z > \ell$. Unfortunately, when computing $J_\ell(z)$ for $z < \ell$ (in which we are primarily interested), since $Y_\ell(z)$ is an exponentially growing solution, the recurrence relation is numerically unstable for increasing ℓ, i.e., the round-off error in $J_0(z)$ and $J_1(z)$ is rapidly amplified by the recurrence. On the other hand, this instability for increasing ℓ also implies that the recurrence relation is stable when computing $J_\ell(z)$ for *decreasing* ℓ, i.e., the round-off error in the starting values is quickly damped by the recurrence. Thus, we can begin the downward recurrence with two arbitrary values and the recurrence will rapidly converge to $\alpha J_\ell(z)$ where α is an unknown normalization constant. Finally, to obtain the correct values of $J_\ell(z)$, we compute α by means of the relationship

$$1 = J_0(z) + 2\sum_{n=1}^{\infty} J_{2n}(z). \tag{B.6}$$

This sum is not difficult to approximate accurately since $J_\ell(z)$ decays exponentially for $z < \ell$ (for more details, see [45, pp. 173–175]).

Hence, when computing $Y_\ell(z)$ for arbitrary z and ℓ or when computing $J_\ell(z)$ for $z > \ell$, we first compute $Y_0(z)$ and $Y_1(z)$ or, respectively, $J_0(z)$ and $J_1(z)$ (perhaps by means of an asymptotic expansion). We then use the recurrence relation with increasing ℓ to compute $Y_\ell(z)$ or $J_\ell(z)$. For $z < \ell$, on the other hand, we iterate several times through the downward recurrence with two arbitrary starting values to converge onto the correct sequence of $\alpha J_\ell(z)$. Then, in the process of the downward recurrence, we collect the sum (B.6) and normalize the sequence by the result.

To compute the scaled Bessel functions, we derive a new set of recurrence relations related to the recurrence relations (B.4) and (B.5). From the definitions (B.1) and (B.2), and using (B.4) and (B.5), we obtain

$$\tilde{J}_{\ell+1}(z) = \ell(\ell+1)\left(\frac{2}{z}\right)^2\left[\tilde{J}_{\ell}(z) - \tilde{J}_{\ell-1}(z)\right], \tag{B.7}$$

$$\tilde{Y}_{\ell+1}(z) = \tilde{Y}_{\ell}(z) - \frac{1}{\ell(\ell+1)}\left(\frac{z}{2}\right)^2\tilde{Y}_{\ell-1}. \tag{B.8}$$

In this case, as a result of the scaling, neither $\tilde{J}_\ell(z)$ or $\tilde{Y}_\ell(z)$ grows (or decays) exponentially. It is not difficult to show by means of a few numerical experiments that the recurrence for $\tilde{J}_\ell$ is unstable and the recurrence for $\tilde{Y}_\ell$ is stable for increasing ℓ. Hence, after computing $Y_0(z)$ and $Y_1(z)$ as done previously, we then scale these values and use the recurrence relation (B.8) to compute $\tilde{Y}_\ell(z)$. To compute $\tilde{J}_\ell(z)$, we use a downward recurrence and the normalization sum (B.6) as before.

The implementation of this algorithm involves only relatively simple modifications to any existing algorithm for computing Bessel functions $J_\ell(z)$ or $Y_\ell(z)$. In our application, we modified the Fortran77 routines *rjbesl* and *rybesl*, which one can easily obtain from the Netlib repository [1].

Appendix C

High-Order Evaluation of Fourier Integrals

Given a smooth, compactly supported, real-valued function $g(t)$ for $t \in \mathbb{R}$, we seek to compute the integral

$$I(\omega) = \int_a^b g(t)e^{i\omega t}dt$$

for various values of $\omega \in [\omega_{min}, \omega_{max}]$. Clearly, since $g(t)$ is real-valued, $I(-\omega) = \overline{I(\omega)}$ and, therefore, we may restrict our attention to $\omega_{min} \geq 0$.

We present a modified version of the method suggested in [45, pp. 577–584]. Through appropriate combinations of Lagrange interpolating polynomials of order q, we obtain a high-order approximation of $g(t)$. In particular, there exist piecewise smooth interpolating polynomials $\psi(s)$ of order q where $-q \leq s \leq q$ such that $\psi(0) = 1$ and $\psi(s) = 0$ for integer values $s = -q, \ldots, q$. To further simplify the approach, we consider only even functions $\psi(s)$. (We describe specific choices of $\psi(s)$ for $q = 2, 4$ in the following sections.) Thus, we can construct a high-order approximation of $g(t)$ as

$$g(t) \approx \sum_{k=-(q-1)}^{N+(q-1)} g_k \psi\left(\frac{t - t_k}{\delta}\right),$$

where $\delta = (b - a)/N$, $t_k = a + k\delta$ and $g_k = g(t_k)$. Note that this approximation requires knowledge of g outside of the interval $[a, b]$. This presents no difficulties in our application since the integrands $p(\rho)$ and $\rho\, p(\rho)$ are given by analytic expressions.

After some simplification, the integral becomes

$$I(\omega) \approx \delta e^{i\omega a}\left[W(\theta)S(\theta) + \nu(\theta) + e^{i\omega(b-a)}\overline{\mu(\theta)}\right],$$

where $\theta = \omega\delta$,

$$S(\theta) = \sum_{k=0}^{N} g_k e^{i\theta k},$$

$$W(\theta) = \int_{-p}^{p} \psi(s)\cos(\theta s)ds,$$

$$\nu(\theta) = g_0\gamma_0(\theta) + \sum_{k=1}^{q-1}\left[g_k\gamma_k(\theta) - g_{-k}\overline{\gamma_k(\theta)}\right],$$

$$\mu(\theta) = g_N\gamma_0(\theta) + \sum_{k=1}^{q-1}\left[g_{N-k}\gamma_k(\theta) - g_{N+k}\overline{\gamma_k(\theta)}\right],$$

and

$$\gamma_k(\theta) = e^{i\theta k}\int_k^q \psi(s)e^{i\theta s}ds.$$

Thus, the computation involves a simple sum of $N+1$ terms, $S(\theta)$, the quantity $W(\theta)$ and a relatively small number of endpoint corrections, $\nu(\theta)$ and $\mu(\theta)$. Furthermore, since $\psi(s)$ is known analytically, $W(\theta)$ and $\gamma_k(\theta)$ can be computed exactly for each choice of ψ.

The only approximation in the method to this point is the high-order interpolation of $g(t)$. Thus, we require only enough points to accurately approximate $g(t)$ instead of the highly oscillatory function $g(t)e^{i\omega t}$. Furthermore, since we only approximate $g(t)$, the accuracy of the approximation is *independent of* ω. Hence, given any $\epsilon > 0$, we can choose N sufficiently large so that the error in $I(\omega)$ is less than ϵ, *uniformly in* ω.

Note that to decrease the error one may either increase the number of interpolation points N or increase q (thereby increasing the order of the interpolation). As can be easily demonstrated, the order of the method depends on q in much the same way as with Newton-Cotes integration methods. More precisely, for q odd, the error decays like $\mathcal{O}(N^{-(q+1)})$ and for q even, the error decays like $\mathcal{O}(N^{-(q+2)})$. Hence, we most generally choose $q = 2$ (fourth-order convergence) or $q = 4$ (sixth-order convergence). The values of $W(\theta)$ and $\gamma_k(\theta)$ for $q = 2$ and $q = 4$ are found in Sections C.1 and C.2, respectively.

In general, we may need to evaluate $I(\omega)$ for many different values of ω. (In our application, $\omega = \kappa \pm 2\pi|c_\ell|$ with $(c_\ell)_q = \ell_q/(B_q - A_q)$ and where $|\ell_q| \leq \widetilde{N}_q/2$.) This is not difficult to obtain for $W(\theta)$, $\nu(\theta)$ and $\mu(\theta)$ since they involve only a few of the g_k. However, straightforward evaluation of the sum $S(\theta)$ has quadratic complexity. To reduce the complexity, we use an FFT to compute $S(\theta)$ at $\theta_n = 2\pi n/N_F$ for $n = 0, \ldots, N_F - 1$, where

$N_F > N$. More precisely,

$$S(\theta) = \sum_{k=0}^{N} g_k e^{i\theta_n k} = \sum_{k=0}^{N_F-1} g_k e^{2\pi i k n/N_F},$$

where we set $g_k = 0$ for $k > N$. Since $S(\theta)$ is periodic in θ with period 2π, we thereby obtain the value of the $S(\theta)$ at $\theta = \theta_n + 2\pi r$, $r \in \mathbb{Z}$.

Thus, given an arbitrary $\theta = \omega\delta$, we interpolate to find $S(\theta)$, which together with $W(\theta)$, $\nu(\theta)$ and $\mu(\theta)$ give us $I(\omega)$. The number of interpolation points N_p determines the order of the interpolation. While a large value of N_p yields high-order accuracy, it is well known that choosing N_p too large can lead to numerical instabilities. Hence, we generally choose $N_p \leq 10$. Furthermore, although increasing the value of N_F also increases the accuracy of the interpolated value $S(\theta)$, the actual value of N_F is less important than the ratio N_F/N, called the oversampling rate β. This is the number of points per wavelength with which the most oscillatory mode in $S(\theta)$ is sampled. We have found that for a partition of unity $p(\rho)$ with $t_0 = 1/2$ and $t_1 = 1$ (see (4.5)) the values $q = 4$, $N = 1024$, $\beta = 128$, $N_p = 10$ as well as $q = 2$, $N = 8192$, $\beta = 128$, $N_p = 10$ give us nearly full double precision accuracy. The choice between these two possibilities depends on the problem size. When $q = 4$, the FFT is faster since $N_F = \beta N$ is smaller. When $q = 2$, the interpolation is faster since the endpoint corrections, ν and μ, are simpler. Hence, in smaller problems, we prefer the $q = 4$ values, and in larger problems, we prefer the $q = 2$ values.

C.1 Second-Order Interpolating Polynomials

For the case of $q = 2$, $\psi(s)$ is given by a sum of second-order Lagrange interpolating polynomials. More precisely, define

$$\begin{aligned}
\psi_1(s) &= \begin{cases} \frac{(s+2)}{2}\frac{(s+1)}{1}, & \text{if } -2 \leq s \leq 0 \\ 0, & \text{otherwise,} \end{cases} \\
\psi_2(s) &= \begin{cases} \frac{(s+1)}{1}\frac{(s-1)}{-1}, & \text{if } -1 \leq s \leq 1 \\ 0, & \text{otherwise,} \end{cases} \\
\psi_3(s) &= \begin{cases} \frac{(s-1)}{-1}\frac{(s-2)}{-2}, & \text{if } 0 \leq s \leq 2 \\ 0, & \text{otherwise.} \end{cases}
\end{aligned}$$

Notice that ψ_1 and ψ_3 form the usual piecewise second-order Lagrange interpolation scheme when the point $s = 0$ lies on the boundary of two subintervals. On the other hand, ψ_2 is the usual Lagrange interpolating polynomial when the point $s = 0$ lies at the center of the subinterval. Addition and normalization leads to

$$\psi(s) = \frac{1}{2}\left[\psi_1(s) + \psi_2(s) + \psi_3(s)\right].$$

The functions $W(\theta)$ and $\gamma_k(\theta)$ can now be obtained:

$$\begin{aligned}
W(\theta) &= \frac{4\sin^3(\theta/2)\left[2\cos(\theta/2) + \theta\sin(\theta/2)\right]}{\theta^3}, \\
\gamma_0(\theta) &= -\frac{2i + (3 + 4i\theta)\theta - 4(\theta + i)e^{i\theta} + (\theta + 2i)e^{2i\theta}}{4\theta^3}, \\
\gamma_1(\theta) &= -\frac{e^{i\theta}\left[-2i + \theta + (2 + it)e^{i\theta}\right]}{4\theta^3}.
\end{aligned}$$

It is important to note that for $\theta \ll 1$ the numerical evaluation of these functions can produce a significant amount of cancellation error. To avoid this problem, for sufficiently small θ, we approximate $W(\theta)$ and $\gamma_k(\theta)$ with a power series. Through experiment, we determine the value of θ at which to switch (for approximately double precision accuracy) from one method to the other. For example, for the function $W(\theta)$ above, we switch to the power series method for $\theta < 10^{-4}$; and for $\gamma_1(\theta)$, we switch for $\theta < 8/10$.

C.2 Fourth-Order Interpolating Polynomials

For $q = 4$, we similarly construct $\psi(s)$ as a sum of fourth-order Lagrange interpolating polynomials. Define

$$\psi_1(s) = \begin{cases} \frac{(s+4)}{4}\frac{(s+3)}{3}\frac{(s+2)}{2}\frac{(s+1)}{1}, & \text{if } -4 \leq s \leq 0 \\ 0, & \text{otherwise,} \end{cases}$$

$$\psi_2(s) = \begin{cases} \frac{(s+3)}{3}\frac{(s+2)}{2}\frac{(s+1)}{1}\frac{(s-1)}{-1}, & \text{if } -3 \leq s \leq 1 \\ 0, & \text{otherwise,} \end{cases}$$

$$\psi_3(s) = \begin{cases} \frac{(s+2)}{2}\frac{(s+1)}{1}\frac{(s-1)}{-1}\frac{(s-2)}{-2}, & \text{if } -2 \leq s \leq 2 \\ 0, & \text{otherwise,} \end{cases}$$

$$\psi_4(s) = \begin{cases} \frac{(s+1)}{1}\frac{(s-1)}{-1}\frac{(s-2)}{-2}\frac{(s-3)}{-3}, & \text{if } -1 \leq s \leq 3 \\ 0, & \text{otherwise,} \end{cases}$$

$$\psi_5(s) = \begin{cases} \frac{(s-1)}{-1}\frac{(s-2)}{-2}\frac{(s-3)}{-3}\frac{(s-4)}{-4}, & \text{if } 0 \leq s \leq 4 \\ 0, & \text{otherwise.} \end{cases}$$

Then, as with $q = 2$, $\psi(s)$ is given by the normalized sum of these piecewise smooth polynomials

$$\psi(s) = \frac{1}{4}\sum_{j=0}^{5}\psi_j(s).$$

In this case for $W(\theta)$ and $\gamma_k(\theta)$, we obtain

$$\begin{aligned} W(\theta) &= \frac{4\sin^5\left(\frac{\theta}{2}\right)}{3\theta^5} \quad \left\{2\theta\left[12 - \theta^2 + 3(6-\theta^2)\cos\theta\right]\sin\left(\frac{\theta}{2}\right)\right. \\ &\qquad \left. + (12+\theta^2)\cos\left(\frac{\theta}{2}\right) + (12 - 11\theta^2)\cos\left(\frac{3\theta}{2}\right)\right\}, \end{aligned}$$

$$
\begin{aligned}
\gamma_0 &= \frac{1}{48\theta^5} \Big[\left(12i + 30\theta - 35i\theta^2 + 25\theta^3 - 48i\theta^4\right) + \left(-48i - 108\theta + 104i\theta^2 + 48\theta^3\right) e^{i\theta} \\
&\quad + \left(72i + 144\theta - 114i\theta^2 - 36\theta^3\right) e^{2i\theta} + \left(-48i - 84\theta + 56i\theta^2 + 16\theta^3\right) e^{3i\theta} \\
&\quad + \left(12i + 18\theta - 11i\theta^2 - 3\theta^3\right) e^{4i\theta} \Big], \\
\gamma_1 &= \frac{1}{48\theta^5} \Big[\left(-36i - 66\theta + 33i\theta^2 - 29\theta^3\right) e^{i\theta} + \left(72i + 144\theta - 114i\theta^2 - 36\theta^3\right) e^{2i\theta} \\
&\quad + \left(-48i - 84\theta + 56i\theta^2 + 16\theta^3\right) e^{3i\theta} + \left(12i + 18\theta - 11i\theta^2 - 3\theta^3\right) e^{4i\theta} \Big], \\
\gamma_2 &= \frac{1}{48\theta^5} \Big[\left(36i + 42\theta + 3i\theta^2 + 7\theta^3\right) e^{2i\theta} + \left(-48i - 84\theta + 56i\theta^2 + 16\theta^3\right) e^{3i\theta} \\
&\quad + \left(12i + 18\theta - 11i\theta^2 - 3\theta^3\right) e^{4i\theta} \Big], \\
\gamma_3 &= \frac{1}{48\theta^5} \Big[\left(-12i - 6\theta - i\theta^2 - \theta^3\right) e^{3i\theta} + \left(12i + 18\theta - 11i\theta^2 - 3\theta^3\right) e^{4i\theta} \Big].
\end{aligned}
$$