# From high oscillation to rapid approximation II: Expansions in polyharmonic eigenfunctions 

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September 1, 2006


#### Abstract

We consider the use of eigenfunctions of polyharmonic operators, accompanied by Neumann boundary conditions, to expand analytic functions in compact intervals. Such expansions feature a number of advantages in comparison with classical Fourier series, in particular they exhibit more rapid decay of expansion coefficients for nonperiodic functions.

Having derived an asymptotic formula for expansion coefficients, we examine in detail an explicit form of eigenfunctions and the location of eigenvalues. This is followed by an introduction and analysis of Filon-type quadrature techniques for rapid approximation of expansion coefficients. Finally, we consider special quadrature methods for eigenfunctions corresponding to a multiple zero eigenvalue.


## 1 Introduction

We continue in this paper a theme that we have commenced in (Iserles \& Nørsett 2006), namely the expansion and approximation of nonperiodic analytic functions on bounded real intervals in eigenfunctions of certain differential operators. Such techniques entertain a number of advantages, of both theoretical and numerical nature, once compared to classical Fourier expansions. It thus makes sense to explain briefly the main idea of (Iserles \& Nørsett 2006), an idea that we propose to explore further and generalise in this paper.

Standard Fourier expansions in the interval $[-1,1]$ use the basis

$$
\{\cos \pi n x: n \geq 0\} \cup\{\sin \pi n x: n \geq 1\}
$$

and they exhibit two remarkable properties once we expand a function which is both analytic and periodic of period 2. Firstly, expansion coefficients decay exponentially fast and, secondly, once integral expressions for expansion coefficients are discretized by means of the Discrete Fourier Transform (DFT), we incur an error which decays exponentially in the number of expansion coefficients. These two features, in tandem with the availability of the Fast Fourier Transform to compute the DFT, underlie the astonishing success of Fourier expansions in an exceedingly wide range of applications in science and engineering. Yet, both features are no longer valid once the function in question is nonperiodic. In that case the $n$th Fourier coefficient decays like $\mathcal{O}\left(n^{-1}\right)$ and the error incurred by DFT is $\mathcal{O}\left(n^{-2}\right)$. In that instance we have proposed in (Iserles \& Nørsett 2006) the alternative of employing the basis $\mathcal{G}_{1}=\mathbb{P}_{0} \oplus \mathcal{H}_{1}$, where $\mathbb{P}_{m}$ is the set of $m$ th-degree algebraic polynomials and

$$
\begin{equation*}
\mathcal{H}_{1}=\{\cos \pi n x: n \geq 1\} \cup\left\{\sin \pi\left(n-\frac{1}{2}\right) x: n \geq 1\right\} \tag{1.1}
\end{equation*}
$$

We have proved that $\mathcal{G}_{1}$ is an orthogonal (indeed, orthonormal) basis, which is dense in $\mathrm{L}_{2}[-1,1]$. Moreover, statements equivalent to the classical Fejér and de la Vallée Poussin theorems are valid in this setting and the modified Fourier expansion

$$
f(x) \sim \frac{1}{2} \hat{f}_{0}^{C}+\sum_{n=1}^{\infty}\left[\hat{f}_{n}^{C} \cos \pi n x+\hat{f}_{n}^{S} \sin \pi\left(n-\frac{1}{2}\right) x\right]
$$

where

$$
\hat{f}_{n}^{C}=\int_{-1}^{1} f(x) \cos \pi n x \mathrm{~d} x, \quad \hat{f}_{n}^{S}=\int_{-1}^{1} f(x) \sin \pi\left(n-\frac{1}{2}\right) x \mathrm{~d} x
$$

converges for a Riemann-integrable function $f$ at any $x \in(-1,1)$ where $f$ is Lipschitz. Convergence at the endpoints is also assured (unlike for the classical Fourier expansion) for an analytic $f$.

Once the coefficients $\hat{f}_{n}^{C}$ and $\hat{f}_{n}^{S}$ are expanded asymptotically in powers of $n^{-1}$, we observe that $\hat{f}_{n}^{C}, \hat{f}_{n}^{S}=\mathcal{O}\left(n^{-2}\right)$, a considerably faster decay than that of classical Fourier expansions for analytic, nonperiodic functions. This asymptotic expansion also provides powerful means to compute the first $m$ modified Fourier coefficients $\hat{f}_{n}^{C}$ and $\hat{f}_{n}^{S}$ to high accuracy in just $\mathcal{O}(m)$ operations. This can be further improved by employing Filon-type techniques for the computation of highly oscillatory integrals, that have been introduced by the current authors in (Iserles \& Nørsett 2005). Finally, the few coefficients corresponding to small values of $n$, before asymptotic behaviour sets, can be approximated by nonstandard quadrature formulæ that require just a single extra function evaluation.

To recap, standard Fourier coefficients for analytic functions decay like $\mathcal{O}\left(n^{-1}\right)$, while modified Fourier coefficients display faster decay of $\mathcal{O}\left(n^{-2}\right)$. In this paper we demonstrate that even faster decay of the coefficients can be attained once basis functions are chosen judiciously. The underlying idea is very simple once we understand why using $\mathcal{G}_{1}$ leads to more rapid decay of the coefficients than employing standard Fourier basis. The reason is that both $\cos \pi n x$ and $\sin \pi\left(n-\frac{1}{2}\right) x$ are eigenfunctions of the second-derivative operator $\mathrm{d}^{2} / \mathrm{d} x^{2}$ with Neumann boundary conditions. Supposing that $u$ is such an eigenfunction, $u^{\prime \prime}+\alpha^{2} u=0$, $u^{\prime}( \pm 1)=0$, integrate twice by parts and substitute Neumann boundary conditions,

$$
\int_{-1}^{1} f(x) u(x) \mathrm{d} x=-\frac{1}{\alpha^{2}} \int_{-1}^{1} f(x) u^{\prime \prime}(x) \mathrm{d} x=-\frac{1}{\alpha^{2}}\left[\left.f(x) u^{\prime}(x)\right|_{-1} ^{1}-\int_{-1}^{1} f^{\prime}(x) u^{\prime}(x) \mathrm{d} x\right]
$$

$$
\begin{equation*}
=\frac{1}{\alpha^{2}}\left[\left.f^{\prime}(x) u(x)\right|_{-1} ^{1}-\int_{-1}^{1} f^{\prime \prime}(x) u(x) \mathrm{d} x\right] . \tag{1.2}
\end{equation*}
$$

Since it follows from the standard spectral theory that all eigenvalues are real, positive and $\alpha_{n}^{2}=\mathcal{O}\left(n^{2}\right)$ for the $n$th eigenvalue (Pöschel \& Trubowitz 1987), we deduce that

$$
\int_{-1}^{1} f(x) u(x) \mathrm{d} x=\mathcal{O}\left(n^{-2}\right)
$$

Hence the aforementioned $\mathcal{O}\left(n^{-2}\right)$ decay of the $n$th modified Fourier coefficient.
We note in passing another important feature of (1.2), a key to rapid computation of the coefficients: the expression on the right can be iterated further, a procedure that leads to an asymptotic expansion of the coefficients in inverse powers of $n$. Similar idea will be used in the sequel. Here we just emphasize the crucial importance of Neumann boundary conditions in making expansion terms vanish and accelerating convergence. Note in this context that $\sin \pi n x$ is also an eigenfunction of $\mathrm{d}^{2} / \mathrm{d} x^{2}$, except that with Dirichlet boundary conditions this is precisely why 'its' coefficients decay like $\mathcal{O}\left(n^{-1}\right)$.

Had the eigenfunction $u$ obeyed higher-order Neumann boundary conditions, more terms would have dropped out in (1.2), resulting in more rapid decay. To be in position to impose more zero derivatives, we consider the eigenfunctions of the polyharmonic operator $\mathrm{d}^{2 q} / \mathrm{d} x^{2 q}$, where $q \geq 1$ is an integer. In other words, we seek functions $u$ and numbers $\alpha$ such that

$$
\begin{equation*}
u^{(2 q)}+(-1)^{q+1} \alpha^{2 q} u=0, \quad-1 \leq x \leq 1 \tag{1.3}
\end{equation*}
$$

in tandem with the Neumann boundary conditions

$$
\begin{equation*}
u^{(i)}(-1)=u^{(i)}(+1)=0, \quad i=q, q+1, \ldots, 2 q-1 . \tag{1.4}
\end{equation*}
$$

We will prove in Section 2 a number of important features of eigenfunctions $u$ :

1. There exists a countable number of positive, simple eigenvalues and real eigenfunctions, except that (1.3-4) also has a zero eigenvalue of multiplicity $q$.
2. Denote the $n$th positive eigenvalue by $\kappa_{n}=(-1)^{q} \alpha_{n}^{2 q}$ and the corresponding eigenfunction by $u_{n}$. Then $\mathcal{G}_{q}=\mathbb{P}_{q-1} \oplus \mathcal{H}_{q}$, where

$$
\mathcal{H}_{q}=\left\{u_{n}: n \geq 1\right\}
$$

is dense in $L_{2}[-1,1]$ and $u_{n}$ is orthogonal to $u_{m}$ for $n \neq m$ with respect to the standard Euclidean inner product.
3. It is true that $\kappa_{n} \sim \mathcal{O}\left(n^{2 q}\right)$.
4. Once an analytic function is expanded in the functions $u_{n}$, the $n$th expansion coefficient decays like $\mathcal{O}\left(n^{-q-1}\right)$ for $n \gg 1$.
5. For large $n$ the functions $u_{n}$ oscillate rapidly. Thus, the task of computing the $n$th expansion coefficient $\hat{f}_{n}$ can be tackled by techniques of highly oscillatory quadrature.

In Section 3 we examine in detail the case $q=2$, the first setting ranging beyond the work of (Iserles \& Nørsett 2006). We show that there exist two families of eigenfunctions $u_{n}$, corresponding to two transcendental equations for the computation of $\alpha_{n}$. This work is generalised in Section 4 to general $q \geq 1$.

Rapid decay of expansion coefficients is not just a theoretical curiosity, since (like in the case $q=1$ ) they can be approximated very rapidly by using techniques originally designed in the numerical treatment of highly oscillatory integrals. This is the theme of Section 5.

This paper represents an introductory foray into the entire matter of polyharmonic eigenfunctions as a means to approximate analytic functions. An entire raft of questions have not been addressed here, and in particular we mention the issue of pointwise convergence. In section 6 we list a considerably longer list of open problems and issues for further investigation.

An interesting generalisation of our setting occurs when the $(2 q)$ th derivative in (1.3) is replaced by a more general $(2 q)$-degree linear differential operator, i.e. when we consider

$$
\sum_{l=0}^{2 q} p_{l}(x) u^{(l)}(x)+(-1)^{q+1} \alpha^{2 q} u=0, \quad-1 \leq x \leq 1,
$$

where $p_{2 q}>0$, in tandem with the Neumann boundary conditions (1.4). It is not difficult to prove that the five aforementioned features of (1.3-4) hold in this, considerably more general setting. Having said this, it is unclear at this juncture of time whether this "poly-SturmLiouville setting" has any specific advantages. Therefore, we restrict our attention here to the polyharmonic case (1.3), which exhibits the virtues of simplicity.

Polyharmonic eigenfunctions subjected to Neumann boundary conditions have been considered by Mark Krein, who analysed their properties and proved Lemma 1 (Krein 1935). They have been introduced to approximation theory by Andrei Kolmogorov in his theory of $n$-widths (Kolmogorov 1936). This distinguished pedigree notwithstanding, to the best of our knowledge they have never been used as a means for practical approximation of functions and their highly oscillatory nature has never been exploited for rapid computation of expansion coefficients.

## 2 Expansions in polyharmonic Neumann eigenfunctions

Since $(-1)^{q} \mathrm{~d}^{2 q} / \mathrm{d} x^{2 q}$ (with Neumann boundary conditions) is a semipositive-definite differential operator, we deduce that $\alpha \geq 0$ in (1.3).

We commence by noting that both (1.3) and the boundary conditions (1.4) are satisfied with $\alpha=0$ when $u \in \mathbb{P}_{q-1}$. We thus deduce that 0 is a $q$-fold eigenvalue and that the relevant linear subspace of eigenfunctions is spanned by the Legendre polynomials $\mathrm{P}_{k}, k=$ $0,1, \ldots, q-1$, an orthogonal basis of $\mathbb{P}_{q-1}$.

The remaining $\alpha$ s are positive, whence we can let

$$
u(x)=\frac{(-1)^{q}}{\alpha^{2 q}} u^{(2 q)}(x)
$$

Therefore, integrating by parts and substituting the Neumann boundary conditions,

$$
\int_{-1}^{1} f(x) u(x) \mathrm{d} x=\frac{(-1)^{q}}{\alpha^{2 q}} \int_{-1}^{1} f(x) u^{(2 q)}(x) \mathrm{d} x=\frac{(-1)^{q+1}}{\alpha^{2 q}} \int_{-1}^{1} f^{\prime}(x) u^{(2 q-1)}(x) \mathrm{d} x .
$$

We can next apply similar reasoning to the integral on the right and, indeed, prove by induction that

$$
\int_{-1}^{1} f(x) u(x) \mathrm{d} x=\frac{(-1)^{q+k}}{\alpha^{2 q}} \int_{-1}^{1} f^{(k)}(x) u^{(2 q-k)}(x) \mathrm{d} x, \quad k=0,1, \ldots, q
$$

In particular, letting $k=q$ we obtain the important identity

$$
\begin{equation*}
\int_{-1}^{1} f(x) u(x) \mathrm{d} x=\frac{1}{\alpha^{2 q}} \int_{-1}^{1} f^{(q)}(x) u^{(q)}(x) \mathrm{d} x \tag{2.1}
\end{equation*}
$$

Lemma 1 The eigenfunctions of (1.3-4) are orthogonal with respect to the usual Euclidean inner product and they are dense in $\mathrm{L}_{2}[-1,1]$.

Proof Although the lemma follows at once from standard spectral theory (Krein 1935, Levitan \& Sargsjan 1975), it is instructive to prove orthogonality from first principles, using (2.1). According to spectral theory, positive eigenvalues are simple. We denote them by $\kappa_{n}=(-1)^{q} \alpha_{n}^{2 q}$ and the corresponding nonzero eigenfunctions by $u_{n}$.

It follows at once from (2.1) that $\int_{-1}^{1} f(x) u_{n}(x) \mathrm{d} x=0$ for $f \in \mathbb{P}_{q-1}$, hence $u_{n}$ is orthogonal to all eigenfunctions corresponding to the zero eigenvalue. Moreover, letting $f=$ $u_{m}$ for $m \neq n$ in (2.1) we have

$$
\alpha_{n}^{2 q} \int_{-1}^{1} u_{m}(x) u_{n}(x) \mathrm{d} x=\int_{-1}^{1} u_{m}^{(q)}(x) u_{n}^{(q)}(x) \mathrm{d} x
$$

However, by symmetry,

$$
\alpha_{m}^{2 q} \int_{-1}^{1} u_{m}(x) u_{n}(x) \mathrm{d} x=\int_{-1}^{1} u_{m}^{(q)}(x) u_{n}^{(q)}(x) \mathrm{d} x
$$

and $\alpha_{m} \neq \alpha_{n}, \alpha_{m}, \alpha_{n}>0$, imply that necessarily

$$
\int_{-1}^{1} u_{m}(x) u_{n}(x) \mathrm{d} x=0, \quad m \neq n .
$$

Hence orthogonality.
We note in passing that it follows from the proof that

$$
\int_{-1}^{1} u_{m}^{(q)}(x) u_{n}^{(q)}(x) \mathrm{d} x=0, \quad m \neq n
$$

Before we are carried away, however, we observe that $u_{n}^{(q)}$ is nothing else but the eigenfunction corresponding to the $n$th eigenvalue of (1.3) with the Dirichlet boundary conditions $u^{(i)}( \pm 1)=0, i=0,1, \ldots, q-1$. (The eigenvalues are the same as in the Neumann case, except that the Dirichlet problem has no zero eigenvalues.) Therefore, orthogonality of $q$ th derivatives is another immediate consequence of standard spectral theory.

Lemma 1 justifies the expansion in $\mathcal{G}_{q}=\mathbb{P}_{q-1} \oplus \mathcal{H}_{q}$, where $\mathcal{H}_{q}=\left\{u_{n}: n \geq 1\right\}$, of $\mathrm{L}_{2}[-1,1]$ functions. We thus let

$$
\begin{aligned}
& \hat{f}_{n}^{o}=\int_{-1}^{1} f(x) \mathrm{P}_{n}(x) \mathrm{d} x, \quad n=0, \ldots, q-1, \\
& \hat{f}_{n}=\int_{-1}^{1} f(x) u_{n}(x) \mathrm{d} x, \quad n=1,2, \ldots,
\end{aligned}
$$

where $\mathrm{P}_{m}$ is the $m$ th degree Legendre polynomial. The underlying orthogonal expansion takes the form

$$
\begin{equation*}
\sum_{n=0}^{q-1}\left(n+\frac{1}{2}\right) \hat{f}_{n}^{o} \mathrm{P}_{n}(x)+\sum_{n=1}^{\infty} \frac{\hat{f}_{n}}{\sigma_{n}} u_{n}(x) \tag{2.2}
\end{equation*}
$$

where

$$
\sigma_{n}=\left[\int_{-1}^{1} u_{n}^{2}(x) \mathrm{d} x\right]^{\frac{1}{2}}
$$

and we recall that $\int_{-1}^{1} \mathrm{P}_{n}^{2}(x) \mathrm{d} x=\left(n+\frac{1}{2}\right)^{-1}$.
The identity (2.1) can be iterated further and this provides a convenient route toward an asymptotic expansion of the coefficients $\hat{f}_{n}$ and ultimately, in Section 5, their effective computation. We are no longer allowed to eliminate terms using boundary conditions and repeated integration by parts yields

$$
\begin{aligned}
\hat{f}_{n}= & \frac{1}{\alpha_{n}^{2 q}} \int_{-1}^{1} f^{(q)}(x) u_{n}^{(q)}(x) \mathrm{d} x \\
= & \frac{1}{\alpha_{n}^{2 q}}\left[\left.f^{(q)}(x) u_{n}^{(q-1)}(x)\right|_{-1} ^{1}-\int_{-1}^{1} f^{(q+1)}(x) u_{n}^{(q-1)}(x) \mathrm{d} x\right] \\
= & \frac{1}{\alpha_{n}^{2 q}}\left[\left.f^{(q)}(x) u_{n}^{(q-1)}(x)\right|_{-1} ^{1}-\left.f^{(q+1)}(x) u_{n}^{(q-2)}(x)\right|_{-1} ^{1}+\int_{-1}^{1} f^{(q+2)}(x) u_{n}^{(q-2)}(x) \mathrm{d} x\right] \\
= & \cdots=\frac{1}{\alpha_{n}^{2 q}}\left[\left.\sum_{l=0}^{k-1}(-1)^{l} f^{(q+l)}(x) u_{n}^{(q-1-l)}(x)\right|_{-1} ^{1}\right. \\
& \left.\quad+(-1)^{k} \int_{-1}^{1} f^{(q+k)}(x)(x) u_{n}^{(q-k)}(x) \mathrm{d} x\right]
\end{aligned}
$$

for $k=0,1, \ldots, q$. In particular, letting $k=q$ we have

$$
\begin{align*}
\hat{f}_{n}= & \frac{(-1)^{q}}{\alpha_{n}^{2 q}}\left\{\sum_{k=q}^{2 q-1}(-1)^{k}\left[f^{(k)}(1) u_{n}^{(2 q-k-1)}(1)-f^{(k)}(-1) u_{n}^{(2 q-k-1)}(-1)\right]\right.  \tag{2.3}\\
& \left.+\int_{-1}^{1} f^{(2 q)}(x) u_{n}(x) \mathrm{d} x\right\}
\end{align*}
$$

Note, however, that the integral on the right is the generalized Fourier coefficient of $f^{(2 q)}$. Therefore, (2.3) can be iterated,

$$
\hat{f}_{n}=\frac{(-1)^{q}}{\alpha_{n}^{2 q}} \sum_{k=q}^{2 q-1}(-1)^{k}\left[f^{(k)}(1) u_{n}^{(2 q-k-1)}(1)-f^{(k)}(-1) u_{n}^{(2 q-k-1)}(-1)\right]
$$

$$
\begin{aligned}
& +\frac{(-1)^{2 q}}{\alpha_{n}^{4 q}} \sum_{k=q}^{2 q-1}(-1)^{k}\left[f^{(2 q+k)}(1) u_{n}^{(2 q-k-1)}(1)-f^{(2 q+k)}(-1) u_{n}^{(2 q-k-1)}(-1)\right] \\
& +\frac{(-1)^{2 q}}{\alpha_{n}^{4 q}} \int_{-1}^{1} f^{(4 q)}(x) u_{n}(x) \mathrm{d} x
\end{aligned}
$$

and so on.
Theorem 2 Given $f \in \mathrm{C}^{\infty}[-1,1]$, it is true that
$\hat{f}_{n} \sim \sum_{r=0}^{\infty} \frac{(-1)^{(r+1) q}}{\alpha_{n}^{2(r+1) q}} \sum_{k=q}^{2 q-1}(-1)^{k}\left[f^{(2 q r+k)}(1) u_{n}^{(2 q-k-1)}(1)-f^{(2 q r+k)}(-1) u_{n}^{(2 q-k-1)}(-1)\right]$.

Proof Follows at once from (2.3) by repeated iteration.
To connect (2.4) with the narrative of (Iserles \& Nørsett 2006), we observe that for $q=1$ we have $\alpha_{n}=\frac{1}{2} \pi n$,

$$
u_{2 n-1}(x)=\sin \pi\left(n-\frac{1}{2}\right) x, \quad u_{2 n}(x)=\cos \pi n x
$$

and

$$
\begin{aligned}
\hat{f}_{2 n-1} & \sim(-1)^{n-1} \sum_{r=0}^{\infty} \frac{(-1)^{r}}{\left[\left(n-\frac{1}{2}\right) \pi\right]^{2 r+2}}\left[f^{(2 r+1)}(1)+f^{(2 r+1)}(-1)\right] \\
\hat{f}_{2 n} & \sim(-1)^{n} \sum_{r=0}^{\infty} \frac{(-1)^{r}}{(n \pi)^{2 r+2}}\left[f^{(2 r+1)}(1)-f^{(2 r+1)}(-1)\right]
\end{aligned}
$$

consistently with Theorem 2.
How fast does $\hat{f}_{n}$ decay for $n \gg 1$ ? It "feels" intuitively right that $u_{n}^{(k)}(x) \sim \mathcal{O}\left(\alpha_{n}^{k}\right)$ for large $n$ and, indeed, this will be proved in Section 4. Taking this for granted for the time being, we deduce from (2.4) that

$$
\hat{f}_{n} \sim \mathcal{O}\left(\alpha_{n}^{-q-1}\right), \quad n \gg 1
$$

It is, however, easy to prove that $\alpha_{n} \sim \mathcal{O}(n)$. To this end we note that

$$
\frac{\mathrm{d}^{2 q}}{\mathrm{~d} x^{2 q}}-(-1)^{q} \alpha_{n}^{2 q}=\left(\frac{\mathrm{d}^{2}}{\mathrm{~d} x^{2}}+\alpha_{n}^{2}\right) \sum_{j=0}^{q-1}(-1)^{q-1-j} \alpha_{n}^{2 q-2-2 j} \frac{\mathrm{~d}^{2 j}}{\mathrm{~d} x^{2 j}}
$$

Therefore, $v_{n}^{\prime \prime}+\alpha_{n}^{2} v_{n}=0$, where

$$
v_{n}(x)=\sum_{j=0}^{q-1}(-1)^{q-1-j} \alpha_{n}^{2 q-2-2 j} u_{n}^{(2 j)}(x)
$$

Note that $v_{n} \not \equiv 0$. For suppose that $v_{n} \equiv 0$. In particular, this would have implied $v_{n}( \pm 1)=$ 0 . This, together with the Neumann boundary conditions (1.4), yields an overdetermined
homogeneous linear system for $u_{n}$, hence $u_{n} \equiv 0$, a contradiction. Consequently $v_{n}$ is the $n$th eigenfunction (and $\alpha_{n}^{2}$ the $n$th eigenvalue) of $-\mathrm{d}^{2} / \mathrm{d} x^{2}$ with some mixed boundary conditions at $\pm 1$. Therefore indeed $\alpha_{n}=\mathcal{O}(n)$ (Pöschel \& Trubowitz 1987). We thus deduce that

$$
\begin{equation*}
\hat{f}_{n} \sim \mathcal{O}\left(n^{-q-1}\right), \quad n \gg 1 \tag{2.5}
\end{equation*}
$$

This has important consequences to the subject matter of this paper: the larger $q \geq 1$, the more rapid the decay of expansion coefficients, hence fewer of them are required once we wish to approximate $f$ to given precision.

## 3 The case $q=2$

The general solution of (1.3) for $q=2$ is

$$
u(x)=c_{1} \cos \alpha x+c_{2} \sin \alpha x+c_{3} \cosh \alpha x+c_{4} \sinh \alpha x .
$$

Imposition of $u^{\prime \prime}(-1)=u^{\prime \prime}(1)=0$ results in

$$
c_{3}=c_{1} \frac{\cos \alpha}{\cosh \alpha}, \quad c_{4}=c_{2} \frac{\sin \alpha}{\sinh \alpha}
$$

We substitute these values of $c_{3}$ and $c_{4}$ into $u(x)$ and impose the remaining boundary condition, $u^{\prime \prime \prime}(-1)=u^{\prime \prime \prime}(1)=0$. Since, after straightforward algebra,

$$
\begin{aligned}
\frac{1}{\alpha^{3}}\left[u^{\prime \prime \prime}(1)+u^{\prime \prime \prime}(-1)\right] & =2 c_{2} \frac{\sin \alpha \cosh \alpha-\cos \alpha \sinh \alpha}{\sinh \alpha} \\
\frac{1}{\alpha^{3}}\left[u^{\prime \prime \prime}(1)-u^{\prime \prime \prime}(-1)\right] & =2 c_{1} \frac{\sin \alpha \cosh \alpha+\cos \alpha \sinh \alpha}{\cosh \alpha}
\end{aligned}
$$

we deduce that for $\alpha>0$ we have two possibilities.
Case 1 Letting $c_{2}=0$ and normalising $c_{1}=1 /(\sqrt{2} \cos \alpha)$, we have

$$
\begin{equation*}
u(x)=\frac{\sqrt{2}}{2}\left(\frac{\cos \alpha x}{\cos \alpha}+\frac{\cosh \alpha x}{\cosh \alpha}\right) \tag{3.1}
\end{equation*}
$$

an even function, where $\alpha$ is a positive zero of the transcendental equation

$$
\begin{equation*}
g_{e}(\alpha)=\tan \alpha+\tanh \alpha=0 \tag{3.2}
\end{equation*}
$$

Case 2 Alternatively we let, $c_{1}=0$ and normalise $c_{2}=1 /(\sqrt{2} \sin \alpha)$, whence

$$
\begin{equation*}
u(x)=\frac{\sqrt{2}}{2}\left(\frac{\sin \alpha x}{\sin \alpha}+\frac{\sinh \alpha x}{\sinh \alpha}\right) \tag{3.3}
\end{equation*}
$$

an odd function, where $\alpha$ is a positive zero of

$$
\begin{equation*}
g_{o}(\alpha)=\tan \alpha-\tanh \alpha=0 \tag{3.4}
\end{equation*}
$$

To locate zeros of (3.2) and (3.4), we commence with $g_{e}$ and observe that

$$
g_{e}^{\prime}(\alpha)=2+\tan ^{2} \alpha-\tanh ^{2} \alpha>0, \quad \alpha>0
$$

since $0<\tanh \alpha<1$ for $\alpha>0$. Therefore $g_{e}$ increases monotonically. Moreover, for every $n=1,2, \ldots$.

$$
g_{e}\left(\left(n-\frac{1}{4}\right) \pi\right)=-1+\tanh \left(n-\frac{1}{4}\right) \pi<0, \quad g_{e}(n \pi)=\tanh n \pi>0
$$

and $g_{e}$ has a simple pole at $\left(n-\frac{1}{2}\right) \pi$. We thus deduce that (3.2) has a unique simple zero in each interval of the form $I_{2 n-1}=\left(\left(n-\frac{1}{4}\right) \pi, n \pi\right)$ for all $n=1,2, \ldots$. As a matter of fact we can say considerably more: for small $\varepsilon>0$ we have

$$
\begin{aligned}
g_{e}\left(\left(n-\frac{1}{4}\right) \pi+\varepsilon\right) & =-\frac{\cos \varepsilon-\sin \varepsilon}{\cos \varepsilon+\sin \varepsilon}+\tanh \left(\left(n-\frac{1}{4}\right) \pi+\varepsilon\right) \\
& \geq-\frac{\cos \varepsilon-\sin \varepsilon}{\cos \varepsilon+\sin \varepsilon}+\tanh \left(\left(n-\frac{1}{4}\right) \pi\right) \\
& =2 \varepsilon-2 \mathrm{e}^{-2\left(n-\frac{1}{4}\right) \pi}+\mathcal{O}\left(\varepsilon^{2}, \mathrm{e}^{-4\left(n-\frac{1}{4}\right) \pi}\right)
\end{aligned}
$$

Therefore, letting $\varepsilon=\mathrm{e}^{-2\left(n-\frac{1}{4}\right) \pi}$, we deduce that for sufficiently large $n$ it is true that the unique zero of (3.2) in $I_{n}$ can be confined to

$$
\tilde{I}_{2 n-1}=\left(\left(n-\frac{1}{4}\right) \pi,\left(n-\frac{1}{4}\right) \pi+\mathrm{e}^{-2\left(n-\frac{1}{4}\right) \pi}\right)
$$

an interval of exponentially-small length. Computer search confirms that there is a zero in $\tilde{I}_{2 n-1}$ for all $n \geq 1$, not just for $n \gg 1$.

Similarly, it is easy to verify that $g_{o}$ is strictly monotonically increasing, with a simple pole at $\left(n-\frac{1}{2}\right) \pi$ and that

$$
g_{o}(n \pi)<0<g_{o}\left(\left(n+\frac{1}{4}\right) \pi\right)
$$

for every $n \geq 1$. We thus deduce that $g_{o}$ has a single zero in each interval $I_{2 n}=(n \pi,(n+$ $\left.\frac{1}{4}\right) \pi$ ) and is nonzero elsewhere. Proceeding as before, this zero can be restricted to

$$
\tilde{I}_{2 n}=\left(\left(n+\frac{1}{4}\right) \pi-\mathrm{e}^{-2\left(n+\frac{1}{4}\right) \pi},\left(n+\frac{1}{4}\right) \pi\right) .
$$

To sum up, all parameters $\alpha$ can be confined to intervals which become exceedingly small for $n \gg 1$ : we let $\alpha_{n} \in \tilde{I}_{n}, n=1,2, \ldots$, and denote the corresponding eigenfunction by $u_{n}$. Note that solutions of (3.2) and (3.4) alternate and that, consistently with the analysis of Section 2, $\alpha_{n}=\mathcal{O}(n)$.

The functions $u_{n}$ are already normalized and the proof involves straightforward algebra. For example, given

$$
v(x)=\frac{\cos \alpha x}{\cos \alpha}+\frac{\cosh \alpha x}{\cosh \alpha}
$$

we have, after long calculation,

$$
\int_{-1}^{1} v^{2}(x) \mathrm{d} x=\frac{1}{\cos ^{2} \alpha}+\frac{1}{\cosh ^{2} \alpha}+\frac{3}{\alpha}(\tan \alpha+\tanh \alpha) .
$$



Figure 3.1: The orthogonal functions $u_{n}, n=1,2,3,4$, for $q=2$.

Assuming that $\alpha=\alpha_{2 n-1}$ obeys (3.2), the term in brackets on the right vanishes and, after another easy calculation,

$$
\frac{1}{\cos ^{2} \alpha}+\frac{1}{\cosh ^{2} \alpha}=2
$$

Therefore $u_{2 n-1}(x)=v(x) / \sqrt{2}$ is indeed of unit norm. The calculation for $u_{2 n}$ is identical. Therefore, we may let $\sigma_{n}=1$ in (2.2). Moreover,

$$
u_{n}(-1)=(-1)^{n-1} \sqrt{2}, \quad u_{n}(1)=\sqrt{2}, \quad n=1,2, \ldots
$$

In Figure 3.1 we display the first four functions $u_{n}$. In conformity with our former observations, note that $u_{2 n-1} \mathrm{~s}$ are even, while $u_{2 n} \mathrm{~s}$ are odd. It is evident from the figure that each $u_{n}$ has precisely $n$ simple zeros in $(-1,1)$ and that the zeros interlace. This behaviour is characteristic of Sturm-Liouville eigenfunctions (Levitan \& Sargsjan 1975) and is evidently valid also for biharmonic eigenfunctions. We also note in passing that each $u_{n}$ appears to have $n+1$ zeros. Recall, however, that the functions $u_{n}$ need be complemented by 1 and $x$, the first two Legendre polynomials, with no zeros and a single zero, respectively.

In Figure 3.2 we display the absolute values of the first hundred coefficients $\hat{f}_{n}$. It follows


Figure 3.2: The magnitude of the coefficients $\hat{f}_{n}$ for $q=2$ and $f(x)=\mathrm{e}^{x}$. On the left we display $\left|\hat{f}_{n}\right|$ and on the right scaled values $n^{3}\left|\hat{f}_{n}\right|$.
from Section 2 that $\hat{f}_{n}=\mathcal{O}\left(n^{-3}\right)$, and this is confirmed by the figure on the right, which depicts $n^{3}\left|\hat{f}_{n}\right|$. Note there the very rapid onset of asymptotic behaviour.

Figure 3.3 depicts the pointwise error in the approximation of $f(x)=\mathrm{e}^{x}$ by the truncated expansion

$$
F_{m}(x)=\frac{1}{2} \hat{f}_{0}^{o}+\frac{3}{2} \hat{f}_{1}^{o} x+\sum_{n=1}^{m} \hat{f}_{n} u_{n}(x)
$$

for $m=10,20,40,80$ in the interval $\left(-\frac{9}{10}, \frac{9}{10}\right)$. Note that the error decreases roughly by a factor of eight once the size of $m$ is doubled, indicative of $\mathcal{O}\left(m^{-3}\right)$ decay. It is instructive to compare this figure with Figure 2.1 in (Iserles \& Nørsett 2006), which displays pointwise error for modified Fourier expansions (i.e., polyharmonic eigenfunctions with $q=1$ ), as well as for classical Fourier expansions. Thus, for $q=1$ the pointwise error decay is $\mathcal{O}\left(m^{-1}\right)$ for classical Fourier expansions, $\mathcal{O}\left(m^{-2}\right)$ for $q=1$ and $\mathcal{O}\left(m^{-3}\right)$ in the present case, $q=2$. Of course, all this refers to numerical results: we have proved in (Iserles \& Nørsett 2006) that modified Fourier expansions converge pointwise for any Riemann integrable $f$ at a point where it is Lipschitz, but we have not determined there the rate of convergence. For $q \geq 2$ we lack at present any hard proofs about pointwise convergence or even summability, not to mention the rate of convergence.

An important distinction between classical and modified Fourier expansions is that, for analytic $f$, the latter converge pointwise in all of $[-1,1]$, inclusive of endpoints. However, the convergence at $\pm 1$ is just $\mathcal{O}\left(m^{-1}\right)$, slower than the conjectured convergence at interior points (Iserles \& Nørsett 2006). It is thus interesting to examine pointwise convergence of $F_{m}$ at the endpoints. In Figure 3.4 we have done so for $\mathrm{e}^{x}$ (compare with Figure 2.2 from (Iserles \& Nørsett 2006)), displaying the quantities $m^{2}\left|F_{m}( \pm 1)-\mathrm{e}^{ \pm 1}\right|$ for $m=1, \ldots, 100$. Evidently, it seems that the error at the endpoints decays like $\mathcal{O}\left(m^{-2}\right)$, an order of magnitude


Figure 3.3: The pointwise error in approximating $f(x)=\mathrm{e}^{x}$ by $F_{m}$ for $m=10,20,40$ and 80, respectively.
faster than in the case $q=1$. Although it is reasonable to guess that Figure 3.4 is indicative of general behaviour, we have to date no hard analysis to underpin this conjecture.

## 4 Eigenfunction bases for general $q \geq 1$

The case $q=1$ has been considered in (Iserles \& Nørsett 2006) and $q=2$ in the previous section. Presently we turn our attention to general $q \geq 1$. In other words, we consider functions $u$ such that

$$
\begin{equation*}
u^{(2 q)}+(-1)^{q+1} \alpha^{2 q} u=0, \quad-1 \leq x \leq 1 \tag{4.1}
\end{equation*}
$$



Figure 3.4: Pointwise error, scaled by $m^{2}$, at -1 (left) and +1 in approximating $f(x)=\mathrm{e}^{x}$ by $F_{m}$ for $m=1,2, \ldots, 100$.
subject to

$$
\begin{equation*}
u^{(i)}(-1)=u^{(i)}(+1)=0, \quad i=q, q+1, \ldots, 2 q-1 \tag{4.2}
\end{equation*}
$$

We restrict our attention to $\alpha \neq 0$, since the case of the $q$-fold zero eigenvalue has been dealt with in Section 2.

An immediate observation is that, regardless of our choice of $\alpha$, the $i$ th derivative of $u$ scales like $\alpha^{i}$ for $i \geq 0$. This feature of eigenfunctions has been already employed in Section 2, to prove (2.5), the asymptotic rate of decay of expansion coefficients.

We commence by considering general solutions of the linear equation (4.1). They are necessarily of the form

$$
\begin{equation*}
u(x)=\sum_{k=0}^{2 q-1} c_{k} \mathrm{e}^{\alpha \lambda_{k} x} \tag{4.3}
\end{equation*}
$$

where $\lambda_{0}, \ldots, \lambda_{2 q-1} \in \mathbb{C}$ are solutions of $\lambda^{2 q}=(-1)^{q}$, while $c_{0}, \ldots, c_{2 q-1} \in \mathbb{C}$ are arbitrary constants. The boundary conditions (4.2) will be incorporated once we have brought (4.1) into a more convenient form.

### 4.1 $\quad$ Even $q \geq 2$

It is advantageous to separate the discussion of even and odd values of $q$ and we commence with even $q$. In that case the $\lambda_{k} \mathrm{~s}$ are roots of unity, $\lambda_{k}=\exp \left(\frac{\pi \mathrm{i} k}{q}\right), k=0,1, \ldots, 2 q-1$, and we note that $\lambda_{q+k}=-\lambda_{k}$. Therefore (4.1) simplifies to

$$
u(x)=\sum_{k=0}^{q-1}\left\{c_{k} \mathrm{e}^{\alpha x \cos \frac{\pi k}{q}}\left[\cos \left(\alpha x \sin \frac{\pi k}{q}\right)+\mathrm{i} \sin \left(\alpha x \sin \frac{\pi k}{q}\right)\right]\right\}
$$

$$
\left.+c_{q+k} \mathrm{e}^{-\alpha x \cos \frac{\pi k}{q}}\left[\cos \left(\alpha x \sin \frac{\pi k}{q}\right)-\mathrm{i} \sin \left(\alpha x \sin \frac{\pi k}{q}\right)\right]\right\}
$$

Since we are interested in expressing $u$ in terms of real parameters, we consider two cases:
Case A We let $c_{k}=\frac{1}{2}\left(\beta_{k}+\mathrm{i} \gamma_{k}\right), c_{q+k}=\bar{c}_{k}=\frac{1}{2}\left(\beta_{k}-\mathrm{i} \gamma_{k}\right)$ for $k=0, \ldots, q-1$. Then, following elementary algebra,

$$
\begin{aligned}
u(x)= & \sum_{k=0}^{q-1}\left[\beta_{k} \cos \left(\alpha x \sin \frac{\pi k}{q}\right) \cosh \left(\alpha x \cos \frac{\pi k}{q}\right)\right. \\
& \left.+\gamma_{k} \sin \left(\alpha x \sin \frac{\pi k}{q}\right) \sinh \left(\alpha x \cos \frac{\pi k}{q}\right)\right\}
\end{aligned}
$$

Note that $u$ is an even function.
Since $\beta_{k}$ and $\beta_{q-k}$ multiply identical terms for $k=1,2, \ldots, q / 2-1$, we may assume without loss of generality that $\beta_{q / 2+k}=0$ for $k=1, \ldots, q / 2-1$. Likewise, $\gamma_{k}$ and $\gamma_{q-k}$ for $k=1, \ldots, q / 2-1$ multiply terms that differ just by sign and again they can be aggregated and we may assume that $\gamma_{q / 2+k}=0$ for $k=1, \ldots, q / 2-1$. Finally, $\gamma_{0}$ and $\gamma_{q / 2}$ multiply zero terms, hence we might set them to zero. All that survives is

$$
\begin{align*}
u(x)= & \sum_{k=0}^{q / 2} \beta_{k} \cos \left(\alpha x \sin \frac{\pi k}{q}\right) \cosh \left(\alpha x \cos \frac{\pi k}{q}\right)  \tag{4.4}\\
& +\sum_{k=1}^{q / 2-1} \gamma_{k} \sin \left(\alpha x \sin \frac{\pi k}{q}\right) \sinh \left(\alpha x \cos \frac{\pi k}{q}\right)
\end{align*}
$$

Note that we have in (4.4) exactly $q$ coefficients, $\beta_{k}, k=0, \ldots, q / 2$ and $\gamma_{k}, k=1, \ldots, q / 2-$ 1 , matching the $q$ boundary conditions (4.2).

It is easy to confirm by induction that the derivatives of (4.4) have the explicit form

$$
\begin{aligned}
& \alpha^{-2 s} u^{(2 s)}(x) \\
= & \sum_{k=0}^{q / 2}\left[\left(\beta_{k} \cos \frac{2 \pi k s}{q}+\gamma_{k} \sin \frac{2 \pi k s}{q}\right) \cos \left(\alpha x \sin \frac{\pi k}{q}\right) \cosh \left(\alpha x \cos \frac{\pi k}{q}\right)\right. \\
& \left.+\left(-\beta_{k} \sin \frac{2 \pi k s}{q}+\gamma_{k} \cos \frac{2 \pi k s}{q}\right) \sin \left(\alpha x \sin \frac{\pi k}{q}\right) \sinh \left(\alpha x \cos \frac{\pi k}{q}\right)\right] \\
& \alpha^{-2 s-1} u^{(2 s+1)}(x) \\
= & \sum_{k=0}^{q / 2}\left[\left(\beta_{k} \cos \frac{\pi k(2 s+1)}{q}+\gamma_{k} \sin \frac{\pi k(2 s+1)}{q}\right) \cos \left(\alpha x \sin \frac{\pi k}{q}\right) \sinh \left(\alpha x \cos \frac{\pi k}{q}\right)\right. \\
& \left.+\left(-\beta_{k} \sin \frac{\pi k(2 s+1)}{q}+\gamma_{k} \cos \frac{\pi k(2 s+1)}{q}\right) \sin \left(\alpha x \sin \frac{\pi k}{q}\right) \cosh \left(\alpha x \cos \frac{\pi k}{q}\right)\right] .
\end{aligned}
$$

Letting $x= \pm 1$ for the $i$ th derivative, $i=q, q+1, \ldots, 2 q-1$, and equating to zero is
equivalent to the identity

$$
\Phi_{q}\left[\begin{array}{c}
\boldsymbol{\beta} \\
\boldsymbol{\gamma}
\end{array}\right]=\mathbf{0}, \quad \text { where } \quad \boldsymbol{\beta}=\left[\begin{array}{c}
\beta_{0} \\
\beta_{1} \\
\vdots \\
\beta_{q / 2}
\end{array}\right], \gamma=\left[\begin{array}{c}
\gamma_{1} \\
\gamma_{2} \\
\vdots \\
\gamma_{q / 2-1}
\end{array}\right]
$$

where the $q \times q$ matrix $\Phi_{q}$ is formed consistently with the identities above. Thus, given that we seek a nonzero eigenfunction, we obtain the transcendental algebraic equation

$$
\begin{equation*}
\operatorname{det} \Phi_{q}=0 \tag{4.5}
\end{equation*}
$$

for the coefficient $\alpha$, whence $\left[\begin{array}{l}\boldsymbol{\beta} \\ \gamma\end{array}\right]$ is the eigenvector corresponding to the zero eigenvalue of $\Phi_{q}$.

The first two cases are $q=2$, resulting in

$$
\Phi_{2}=\left[\begin{array}{cc}
\cosh \alpha & -\cos \alpha \\
\sinh \alpha & \sin \alpha
\end{array}\right] \quad \Rightarrow \quad \operatorname{det} \Phi_{2}=\sin \alpha \cosh \alpha+\cos \alpha \cosh \alpha
$$

(the latter is identical to (3.2)) and $q=4$, when
$\Phi_{4}=\left[\begin{array}{ccrc}\cosh \alpha & -\cos \frac{\alpha}{\sqrt{2}} \cosh \frac{\alpha}{\sqrt{2}} & \cos \alpha & \sin \frac{\alpha}{\sqrt{2}} \sinh \frac{\alpha}{\sqrt{2}} \\ \sinh \alpha & -\frac{\sqrt{2}}{2}\left(\cos \frac{\alpha}{\sqrt{2}} \sinh \frac{\alpha}{\sqrt{2}}-\sin \frac{\alpha}{\sqrt{2}} \cosh \frac{\alpha}{\sqrt{2}}\right) & -\sin \alpha & -\left(\frac{\sqrt{2}}{2} \cos \frac{\alpha}{\sqrt{2}} \sinh \frac{\alpha}{\sqrt{2}}+\sin \frac{\alpha}{\sqrt{2}} \cosh \frac{\alpha}{\sqrt{2}}\right) \\ \cosh \alpha & \sin \frac{\alpha}{\sqrt{2}} \sinh \frac{\alpha}{\sqrt{2}} & -\cos \alpha & -\cos \frac{\alpha}{\sqrt{2}} \cosh \frac{\alpha}{\sqrt{2}} \\ \sinh \alpha & \frac{\sqrt{2}}{2}\left(\cos \frac{\alpha}{\sqrt{2}} \sinh \frac{\alpha}{\sqrt{2}}+\sin \frac{\alpha}{\sqrt{2}} \cosh \frac{\alpha}{\sqrt{2}}\right) & \sin \alpha & \frac{\sqrt{2}}{2}\left(\sin \frac{\alpha}{\sqrt{2}} \cosh \frac{\alpha}{\sqrt{2}}-\cos \frac{\alpha}{\sqrt{2}} \sinh \frac{\alpha}{\sqrt{2}}\right)\end{array}\right]$
yields the equation

$$
\begin{aligned}
& \sinh \alpha\left[\sin \alpha(\cosh \sqrt{2} \alpha+\cos \sqrt{2} \alpha)+\frac{\sqrt{2}}{2} \cos \alpha(\sinh \sqrt{2} \alpha-\sin \sqrt{2} \alpha)\right] \\
& -\cosh \alpha\left[\cos \alpha(\cosh \sqrt{2} \alpha-\cos \sqrt{2} \alpha)+\frac{\sqrt{2}}{2} \sin \alpha(\sinh \sqrt{2} \alpha-\sin \sqrt{2} \alpha)\right] .
\end{aligned}
$$

Case B We now let $c_{k}=\frac{1}{2}\left(\beta_{k}+\mathrm{i} \gamma_{k}\right)$ and $c_{q+k}=-\bar{c}_{k}=\frac{1}{2}\left(-\beta_{k}+\mathrm{i} \gamma_{k}\right), k=0, \ldots, q-1$. We now obtain the odd function

$$
\begin{aligned}
u(x)= & \sum_{k=0}^{q-1}\left[\beta_{k} \cos \left(\alpha x \sin \frac{\pi k}{q}\right) \sinh \left(\alpha x \cos \frac{\pi k}{q}\right)\right. \\
& \left.+\gamma_{k} \sin \left(\alpha x \sin \frac{\pi k}{q}\right) \cosh \left(\alpha x \cos \frac{\pi k}{q}\right)\right] .
\end{aligned}
$$

We continue along the same lines as for Case A. Thus, aggregating identical terms, we have

$$
\begin{align*}
u(x)= & \sum_{k=0}^{q / 2-1} \beta_{k} \cos \left(\alpha x \sin \frac{\pi k}{q}\right) \sinh \left(\alpha x \cos \frac{\pi k}{q}\right)  \tag{4.6}\\
& +\sum_{k=1}^{q / 2} \gamma_{k} \sin \left(\alpha x \sin \frac{\pi k}{q}\right) \cosh \left(\alpha x \cos \frac{\pi k}{q}\right)
\end{align*}
$$

- in this case the surviving coefficients are $\beta_{0}, \ldots, \beta_{q / 2-1}$ and $\gamma_{1}, \ldots, \gamma_{q / 2}$. We again form derivatives,

$$
\begin{aligned}
& \alpha^{-2 s} u^{(2 s)}(x) \\
= & \sum_{k=0}^{q / 2}\left[\left(\beta_{k} \cos \frac{2 \pi s k}{q}+\gamma_{k} \sin \frac{2 \pi s k}{q}\right) \cos \left(\alpha x \sin \frac{\pi k}{q}\right) \sinh \left(\alpha x \cos \frac{\pi k}{q}\right)\right. \\
& \left.+\left(-\beta_{k} \sin \frac{2 \pi s k}{q}+\gamma_{k} \cos \frac{2 \pi s k}{q}\right) \sin \left(\alpha x \sin \frac{\pi k}{q}\right) \cosh \left(\alpha x \cos \frac{\pi k}{q}\right)\right] \\
& \alpha^{-2 s-1} u^{(2 s+1)}(x) \\
= & \sum_{k=0}^{q / 2}\left[\left(\beta_{k} \cos \frac{\pi(2 s+1) k}{q}+\gamma_{k} \sin \frac{\pi(2 s+1) k}{q}\right) \cos \left(\alpha x \sin \frac{\pi k}{q}\right) \cosh \left(\alpha x \cos \frac{\pi k}{q}\right)\right. \\
& \left.+\left(-\beta_{k} \sin \frac{\pi(2 s+1) k}{q}+\gamma_{k} \cos \frac{\pi(2 s+1) k}{q}\right) \sin \left(\alpha x \sin \frac{\pi k}{q}\right) \sinh \left(\alpha x \cos \frac{\pi k}{q}\right)\right] .
\end{aligned}
$$

Imposing the boundary conditions (4.2) leads to

$$
\Psi_{q}\left[\begin{array}{c}
\boldsymbol{\beta} \\
\boldsymbol{\gamma}
\end{array}\right]=\mathbf{0}, \quad \text { where } \quad \boldsymbol{\beta}=\left[\begin{array}{c}
\beta_{0} \\
\beta_{1} \\
\vdots \\
\beta_{q / 2-1}
\end{array}\right], \gamma=\left[\begin{array}{c}
\gamma_{1} \\
\gamma_{2} \\
\vdots \\
\gamma_{q / 2}
\end{array}\right]
$$

hence to the transcendental equation

$$
\begin{equation*}
\operatorname{det} \Psi_{q}=0 \tag{4.7}
\end{equation*}
$$

In particular,

$$
\begin{aligned}
\operatorname{det} \Psi_{2}= & \cosh \alpha \sin \alpha-\sinh \alpha \cos \alpha \\
\operatorname{det} \Psi_{4}= & \sinh \alpha\left[\sin \alpha(\cos \sqrt{2} \alpha+\cosh \sqrt{2} \alpha)-\frac{\sqrt{2}}{2} \cos \alpha(\sin \sqrt{2} \alpha+\sinh \sqrt{2} \alpha)\right] \\
& -\cosh \alpha\left[\cos \alpha(\cos \sqrt{2} \alpha-\cosh \sqrt{2} \alpha)+\frac{\sqrt{2}}{2} \sin \alpha(\sin \sqrt{2} \alpha+\sinh \sqrt{2} \alpha)\right]
\end{aligned}
$$

Note that $\operatorname{det} \Psi_{2}=0$ is identical to (3.4).

### 4.2 Odd $q \geq 1$

The treatment of an odd $q$ is identical: we form $u$ in terms of real coefficients $\beta_{k}$ and $\gamma_{k}$, whereby there are two cases, even and odd functions. In each case we aggregate coefficients, form derivatives explicitly and impose the Neumann boundary conditions (4.2). This results in each case in a transcendental equation, setting a determinant of a matrix to zero, whereby the coefficients $\boldsymbol{\beta}$ and $\gamma$ are components of the eigenvector of the matrix in question corresponding to a zero eigenvalue.

The starting point is

$$
u(x)=\sum_{k=0}^{q-1}\left\{c_{k} \mathrm{e}^{\alpha x \cos \frac{\pi\left(k+\frac{1}{2}\right)}{q}}\left[\cos \left(\alpha x \sin \frac{\pi\left(k+\frac{1}{2}\right)}{q}\right)+\mathrm{i} \sin \left(\alpha x \sin \frac{\pi\left(k+\frac{1}{2}\right)}{q}\right)\right]\right.
$$

$$
\left.+c_{q+k} \mathrm{e}^{-\alpha x \cos \frac{\pi\left(k+\frac{1}{2}\right)}{q}}\left[\cos \left(\alpha x \sin \frac{\pi\left(k+\frac{1}{2}\right)}{q}\right)-\mathrm{i} \sin \left(\alpha x \sin \frac{\pi\left(k+\frac{1}{2}\right)}{q}\right)\right]\right\}
$$

Case A Using the same substitution as before and aggregating identical terms, the only surviving coefficients are

$$
\boldsymbol{\beta}=\left[\begin{array}{c}
\beta_{0} \\
\beta_{1} \\
\vdots \\
\beta_{(q-1) / 2}
\end{array}\right] \quad \text { and } \quad \gamma=\left[\begin{array}{c}
\gamma_{0} \\
\gamma_{1} \\
\vdots \\
\gamma_{(q-3) / 2}
\end{array}\right]
$$

All the formulæ are the same as in the case of even $q$, except that we need to adjust the limits of summation and replace $k$ with $k+\frac{1}{2}$ in numerators. This applies both to (4.4) and to the expressions for $\alpha^{-s} u^{(s)}(x)$.

For $q=1$ we obtain $\operatorname{det} \Phi_{1}=\Phi_{1}=-\sin \alpha$ : no surprise here. For $q=3$ we have

$$
\Phi_{3}=\left[\begin{array}{crc}
-\sin \frac{\alpha}{2} \cosh \frac{\sqrt{3} \alpha}{2} & \sin \alpha & \cos \frac{\alpha}{2} \sinh \frac{\sqrt{3} \alpha}{2} \\
-\frac{1}{2} \cos \frac{\alpha}{2} \cosh \frac{\sqrt{3} \alpha}{2}-\frac{\sqrt{3}}{2} \sin \frac{\alpha}{2} \sinh \frac{\sqrt{3} \alpha}{2} & \cos \alpha & \frac{\sqrt{3}}{2} \cos \frac{\alpha}{2} \cosh \frac{\sqrt{3} \alpha}{2}-\frac{1}{2} \sin \frac{\alpha}{2} \sinh \frac{\sqrt{3} \alpha}{2} \\
-\frac{\sqrt{3}}{2} \cos \frac{\alpha}{2} \sinh \frac{\sqrt{3} \alpha}{2}-\frac{1}{2} \sin \frac{\alpha}{2} \cosh \frac{\sqrt{3} \alpha}{2} & -\sin \alpha & \frac{1}{2} \cos \frac{\alpha}{2} \sinh \frac{\sqrt{3} \alpha}{2}-\frac{\sqrt{3}}{2} \sin \frac{\alpha}{2} \cosh \frac{\sqrt{3} \alpha}{2}
\end{array}\right]
$$

and

$$
\operatorname{det} \Phi_{3}=\frac{\sqrt{3}}{4}\left(\cos \alpha \cosh \sqrt{3} \alpha-2+\cos ^{2} \alpha\right)
$$

Case B Again, we proceed like for even $q$. After aggregation we obtain

$$
\boldsymbol{\beta}=\left[\begin{array}{c}
\beta_{0} \\
\beta_{1} \\
\vdots \\
\beta_{(q-3) / 2}
\end{array}\right] \quad \text { and } \quad \gamma=\left[\begin{array}{c}
\gamma_{0} \\
\gamma_{1} \\
\vdots \\
\gamma_{(q-1) / 2}
\end{array}\right]
$$

while (4.6) and the formulæ for derivatives are, again, identical, except for changes in limits of summation and replacement of $k$ by $k+\frac{1}{2}$ in numerators.

For $q=1$ we recover $\operatorname{det} \Psi_{1}=\Psi_{1}=\cos \alpha$, while for $q=3$

$$
\begin{aligned}
\Psi_{3}= & {\left[\begin{array}{ccc}
-\sin \frac{\alpha}{2} \sinh \frac{\sqrt{3} \alpha}{2} & \cos \frac{\alpha}{2} \cosh \frac{\sqrt{3} \alpha}{2} & -\cos \alpha \\
-\frac{1}{2} \cos \frac{\alpha}{2} \sinh \frac{\sqrt{3} \alpha}{2}-\frac{\sqrt{3}}{2} \sin \frac{\alpha}{2} \cosh \frac{\sqrt{3} \alpha}{2} & \frac{\sqrt{3}}{2} \cos \frac{\alpha}{2} \sinh \frac{\sqrt{3} \alpha}{2}-\frac{1}{2} \sin \frac{\alpha}{2} \cosh \frac{\sqrt{3} \alpha}{2} & \sin \alpha \\
-\frac{\sqrt{3}}{2} \cos \frac{\alpha}{2} \cosh \frac{\sqrt{3} \alpha}{2}-\frac{1}{2} \sin \frac{\alpha}{2} \sinh \frac{\sqrt{3} \alpha}{2} \frac{1}{2} \cos \frac{\alpha}{2} \cosh \frac{\sqrt{3} \alpha}{2}-\frac{\sqrt{3}}{2} \sin \frac{\alpha}{2} \sinh \frac{\sqrt{3} \alpha}{2} & \cos \alpha
\end{array}\right], } \\
& \operatorname{det} \Psi_{3}=-\frac{\sqrt{3}}{4} \sin \alpha(\cosh \sqrt{3} \alpha-\cos \alpha) .
\end{aligned}
$$

Note that $\cosh \sqrt{3} \alpha>\cos \alpha$ for $\alpha>0$, therefore we need to consider only the trivial equation $\sin \alpha=0$.

### 4.3 Location of the $\alpha_{n} s$

Let us take stock. We have proved in this section that $u^{(i)}(x)=\mathcal{O}\left(\alpha^{i}\right)$, a result justifying the statement in Section 2 that $\hat{f}_{n}=\mathcal{O}\left(n^{-q-1}\right)$, and derived the functions $u$ in an explicit
form as a linear combination of products of trigonometric and hyperbolic functions. The functions depend on a parameter $\alpha$, which is a solution of a transcendental equation: once $\alpha$ is known, the coefficients in the linear combination can be easily computed by solving an algebraic eigenproblem. Regardless of the value of $q \geq 1$, such functions and corresponding transcendental equations always occur in two cases: even and odd.

All that remains is to look closer into the solutions of the transcendental equations (4.5) and (4.7).

For $q=1$ the situation is clear: the solutions of (4.5) and (4.7) are $n \pi$ and $\left(n-\frac{1}{2}\right) \pi$ respectively. Therefore, the solutions interlace, the "odd" solution comes first, and we let $\alpha_{2 n-1}=\left(n-\frac{1}{2}\right) \pi, \alpha_{2 n}=n \pi$ and label $u_{n}$ accordingly.

We have already considered $q=2$ in Section 3 and proved that the solutions of (4.5) and (4.7) reside in the exponentially small intervals $\tilde{I}_{n}$. Specifically, $\alpha$ s corresponding to even functions are $\approx\left(n-\frac{1}{4}\right) \pi$, while for odd $u$ s we have $\alpha \approx\left(n+\frac{1}{4}\right) \pi$. Again, zeros interlace, except that the order is reversed: we start on the left from a zero corresponding to an even function. We allocate subscripts accordingly: $\alpha_{2 n-1}$ corresponds to an even $u_{2 n-1}$ and $\alpha_{2 n}$ to an odd $u_{2 n}$.

For $q \geq 3$ we have already seen that (4.7) reduces to $\sin \alpha=0$, with the zeros $n \pi$. Insofar as (4.5) is concerned, let

$$
g(x)=\cos x \cosh \sqrt{3} x-2+\cos ^{2} x, \quad \tilde{g}(x)=\frac{g(x)}{\cos x}
$$

Since

$$
\tilde{g}^{\prime}(x)=\sqrt{3} \sinh \sqrt{3} x-\frac{\sin x\left(2+\cos ^{2} x\right)}{\cos ^{2} x}
$$

it follows at once that $\tilde{g}$ monotonically increases for sufficiently large $x$ : as a matter of fact, by numerical calculation, for $x \geq 1.874858$. Moreover, computation shows that (4.5) has no zeros in $(0,2)$, hence we may assume that $\tilde{g}$ increases monotonically. Since it has a simple polar singularity at $\left(n+\frac{1}{2}\right) \pi$ and $\tilde{g}(n \pi)=\cosh \sqrt{3} n \pi-(-1)^{n}>0$ for every $n \geq 1$, we deduce that it must have a single zero in every interval of the form $(n \pi,(n+1) \pi)$. Therefore, zeros of (4.5) and of (4.7) interlace.

Applying a single step of Newton-Raphson iteration to $g(x)=0$, with starting guess $\left(n+\frac{1}{2}\right) \pi$, produces

$$
\alpha \approx\left(n+\frac{1}{2}\right) \pi-4(-1)^{n} \mathrm{e}^{-\sqrt{3}\left(n+\frac{1}{2}\right) \pi}
$$

an extraordinarily good approximation: for $n=10$ and $n=11$ we incur an error of $6.55 \times$ $10^{-49}$ and of $1.23 \times 10^{-53}$, respectively.

In the case $q=4$ we have just numerical results, but they fit the general pattern. Thus, solutions of (4.5) and of (4.7) tend exponentially fast with $n \geq 1$ to $\left(n+\frac{1}{4}\right) \pi$ and to $\left(n+\frac{3}{4}\right) \pi$ respectively.

To sum up our results for $q=1,2,3,4$, we have

| $q$ | $\alpha_{2 n-1}$ | $\alpha_{2 n}$ | the least zero |
| :---: | :---: | :---: | :---: |
| 1 | $\left(n-\frac{1}{2}\right) \pi$ | $n \pi$ | $(4.7)$ |
| 2 | $\rightarrow\left(n-\frac{1}{4}\right) \pi$ | $\rightarrow\left(n+\frac{1}{4}\right) \pi$ | $(4.5)$ |
| 3 | $n \pi$ | $\rightarrow\left(n+\frac{1}{2}\right) \pi$ | (4.7) |
| 4 | $\rightarrow\left(n+\frac{1}{4}\right) \pi$ | $\rightarrow\left(n+\frac{3}{4}\right) \pi$ | (4.5) |

The pattern emerges and we conjecture that for general $q \geq 1$ zeros of (4.5) and of (4.7) interlace, with the leftmost zero being of (4.5) for even $q$, of (4.7) otherwise, and moreover

$$
\begin{equation*}
\alpha_{n} \rightarrow \frac{1}{4}(2 n+q-1) \pi, \quad q, n \geq 1 \tag{4.8}
\end{equation*}
$$

exponentially fast for $n \gg 1$.
Note that this behaviour is consistent with our remark in Section 2 that $\alpha_{n}=\mathcal{O}(n)$ : actually, there is compelling numerical evidence that $\alpha_{n}=\frac{1}{2} \pi n+\mu_{q}+\mathcal{O}\left(n^{-1}\right)$ for some $\mu_{q} \in \mathbb{R}$.

Another valuable observation is that, given exponential tendency to limit in (4.8), the computation of $\alpha_{n}$ by Newton-Raphson iteration is exceedingly easy: just a single iteration is required in IEEE arithmetic for even small values of $n$. Thus, for $q=2$ a single iteration produces an error of $1.49 \times 10^{-20}$ already for $n=4(n=3$ misses the IEEE machine epsilon by a whisker, giving an error of $7.95 \times 10^{-16}$ ).

## 5 Rapid computation of expansion coefficients

A major reason for the extraordinary success of classical Fourier expansions can be attributed to the very fast and accurate means for the evaluation of their coefficients using Fast Fourier Transform. As we have already explained in (Iserles \& Nørsett 2006), modified Fourier expansions provide an alternative means to approximate expansions coefficients to high precision, using asymptotic expansions and other techniques originating in highly oscillatory quadrature. The outcome is a numerical approach that requires very modest data - a relatively small number of function and derivative evaluations of $f$ - and just $\mathcal{O}(m)$ flops to evaluate the first $m$ expansion coefficients. In this section we demonstrate that all this can be generalised to polyharmonic eigenfunctions, regardless of $q \geq 1$. Our point of departure is the asymptotic expansion (2.4) from Theorem 2.

### 5.1 The asymptotic method

Before we commence our discussion of effective numerical approximation of expansion coefficients, we need convenient formalism to express derivative information. We thus let

$$
\boldsymbol{N}_{m}=\{j \in \mathbb{N}: j=2 q r+k \leq m \text { where } r \geq 0, q \leq k \leq 2 q-1\}
$$

and

$$
\boldsymbol{D}_{m}(x)=\left\{f^{(j)}(x): j \in \boldsymbol{N}_{m}\right\}
$$

The first step in our design of an effective algorithm for the calculation of

$$
\hat{f}_{n}=\int_{-1}^{1} f(x) u_{n}(x) \mathrm{d} x, \quad n \geq 1
$$

consists of truncating (2.4). This results in the asymptotic method

$$
\begin{align*}
& \hat{\mathcal{Q}}_{n}^{\left[\rho_{s, p}, \rho_{s, p}\right]}[f]  \tag{5.1}\\
= & \sum_{r=0}^{s-1} \frac{(-1)^{(r+1) q}}{\alpha_{n}^{2(r+1) q}} \sum_{k=q}^{2 q-1}(-1)^{k}\left[f^{(2 q r+k)}(1) u_{n}^{(2 q-k-1)}(1)-f^{(2 q r+k)}(-1) u_{n}^{(2 q-k-1)}(-1)\right]
\end{align*}
$$

$$
+\frac{(-1)^{(s+1) q}}{\alpha_{n}^{2(s+1) q}} \sum_{k=q}^{q+p-1}(-1)^{k}\left[f^{(2 q s+k)}(1) u_{n}^{(2 q-k-1)}(1)-f^{(2 q s+k)}(-1) u_{n}^{(2 q-k-1)}(-1)\right],
$$

where $s \geq 0, p \in\{0, \ldots, q-1\}$ and

$$
\rho_{s, p}= \begin{cases}2 q s-1, & p=0, \\ (2 s+1) q+p-1, & p=1, \ldots, q-1\end{cases}
$$

is the number of derivatives at $\pm 1$.
Theorem 3 It is true for every $s \geq 0$ and $p=0, \ldots, q-1$ that

$$
\begin{equation*}
\hat{\mathcal{Q}}_{n}^{\left[\rho_{s, p}, \rho_{s, p}\right]} \sim \hat{f}_{n}+\mathcal{O}\left(n^{-(2 s+1) q-p-1}\right), \quad n \gg 1 . \tag{5.2}
\end{equation*}
$$

Proof Follows at once by direct comparison of (5.1) with the asymptotic expansion (2.4), distinguishing between the cases $p=0$ and $p \geq 1$, bearing in mind that $\alpha_{n} \sim \mathcal{O}(n)$ and $u_{n}^{(i)} \sim \mathcal{O}\left(n^{i}\right)$.

Once an approximation to $\hat{f}_{n}$ is $\mathcal{O}\left(n^{-N}\right)$ for $n \gg 1$, we say that it is of an asymptotic order $N$. Thus, the asymptotic method (5.1) is of asymptotic order $(2 s+1) q+p+1$. Note that asymptotic order refers to absolute error. Since $\hat{f}_{n}=\mathcal{O}\left(n^{-q-1}\right)$, the relative asymptotic order of (5.1) is $2 s q+p$.

We say that (5.1) employs the data set

$$
\boldsymbol{D}^{\left[\rho_{s, p}, \rho_{s, p}\right]}=\tilde{\boldsymbol{D}}_{q} \cup \boldsymbol{D}_{\rho_{s, p}}(-1) \cup \boldsymbol{D}_{\rho_{s, p}}(1),
$$

where

$$
\tilde{\boldsymbol{D}}_{q}=\left\{f^{(i)}(0): i=0, \ldots, q\right\} .
$$

It will be clear to the observant reader that $\tilde{\boldsymbol{D}}_{q}$ is not, actually, used at all in (5.1). The reason for its inclusion will be apparent in the sequel, in Subsection 5.4.

To illustrate (5.1), we consider $q=2$. We have already noted in Section 3 that

$$
u_{2 n-1}(-1)=\sqrt{2}, \quad u_{2 n-1}(1)=\sqrt{2}, \quad u_{2 n}(-1)=-\sqrt{2}, \quad u_{2 n}(1)=\sqrt{2} .
$$

Moreover, differentiating $u_{n}$ and using (3.2) and (3.4), it is easy to verify that

$$
u_{2 n-1}^{\prime}(-1)=\sqrt{2} \alpha_{2 n-1} \tan \alpha_{2 n-1}, \quad u_{2 n-1}^{\prime}(1)=-\sqrt{2} \alpha_{2 n-1} \tan \alpha_{2 n-1}
$$

and

$$
u_{2 n}^{\prime}(-1)=u_{2 n}^{\prime}(1)=\frac{\sqrt{2} \alpha_{2 n}}{\tan \alpha_{2 n}}
$$

(note that $\left|\tan \alpha_{n}\right| \approx 1$ ). Therefore, the first few asymptotic methods for $q=2$ are

$$
\begin{aligned}
\hat{Q}_{2 n-1}^{[2,2]}[f] & =-\frac{\sqrt{2} \tan \alpha_{2 n-1}}{\alpha_{2 n-1}^{3}}\left[f^{\prime \prime}(1)+f^{\prime \prime}(-1)\right] \\
\hat{Q}_{2 n}^{[2,2]}[f] & =\frac{\sqrt{2} \cot \alpha_{2 n}}{\alpha_{2 n}^{3}}\left[f^{\prime \prime}(1)-f^{\prime \prime}(-1)\right],
\end{aligned}
$$



Figure 5.1: Scaled errors $n^{4}\left(\hat{Q}_{n}^{[2,2]}-\hat{f}_{n}\right), n^{7}\left(\hat{Q}_{n}^{[3,3]}-\hat{f}_{n}\right)$ and $n^{8}\left(\hat{Q}_{n}^{[6,6]}-\hat{f}_{n}\right)$ for $f(x)=\mathrm{e}^{x}$ and $q=2$.

$$
\begin{aligned}
\hat{Q}_{2 n-1}^{[3,3]}[f]= & -\frac{\sqrt{2} \tan \alpha_{2 n-1}}{\alpha_{2 n-1}^{3}}\left[f^{\prime \prime}(1)+f^{\prime \prime}(-1)\right]-\frac{\sqrt{2}}{\alpha_{2 n-1}^{4}}\left[f^{\prime \prime \prime}(1)-f^{\prime \prime \prime}(-1)\right], \\
\hat{Q}_{2 n}^{[3,3]}[f]= & \frac{\sqrt{2} \cot \alpha_{2 n}}{\alpha_{2 n}^{3}}\left[f^{\prime \prime}(1)-f^{\prime \prime}(-1)\right]-\frac{\sqrt{2}}{\alpha_{2 n}^{4}}\left[f^{\prime \prime \prime}(1)+f^{\prime \prime \prime}(-1)\right], \\
\hat{Q}_{2 n-1}^{[6,6]}[f]= & -\frac{\sqrt{2} \tan \alpha_{2 n-1}}{\alpha_{2 n-1}^{3}}\left[f^{\prime \prime}(1)+f^{\prime \prime}(-1)\right]-\frac{\sqrt{2}}{\alpha_{2 n-1}^{4}}\left[f^{\prime \prime \prime}(1)-f^{\prime \prime \prime}(-1)\right] \\
& -\frac{\sqrt{2} \tan \alpha_{2 n-1}}{\alpha_{2 n-1}^{7}}\left[f^{(6)}(1)+f^{(6)}(-1)\right], \\
\hat{Q}_{2 n}^{[6,6]}[f]= & \frac{\sqrt{2} \cot \alpha_{2 n}}{\alpha_{2 n}^{3}}\left[f^{\prime \prime}(1)-f^{\prime \prime}(-1)\right]-\frac{\sqrt{2}}{\alpha_{2 n}^{4}}\left[f^{\prime \prime \prime}(1)+f^{\prime \prime \prime}(-1)\right] \\
& +\frac{\sqrt{2} \cot \alpha_{2 n}}{\alpha_{2 n}^{7}}\left[f^{(6)}(1)-f^{(6)}(-1)\right]
\end{aligned}
$$

and so on. An important observation is that for any $i \geq 3$ the first $m$ coefficients $\hat{\mathcal{Q}}_{n}^{[i, i]}[f]$, $n=1, \ldots, m$, can be computed in $\mathcal{O}(m)$ operations.

In Figure 5.1 we display scaled errors $n^{N}\left(\hat{\mathcal{Q}}_{n}^{[i, i]}[f]-\hat{f}_{n}\right)$, where $N$ is the asymptotic order, for the three choices $i=2,3,6, q=2$ and $f(x)=\mathrm{e}^{x}$ : numerous other computer experiments with other analytic functions $f$ replicate these results. It is clear that computations conform with theory. Absolute and relative (non-scaled) errors for selected values of $n$ are presented in Table 1. Evidently, the error for small $n$ is unacceptably large, but this is hardly surprising since the asymptotic method (5.1) is, as its name implies, effective only for large $n \mathrm{~s}$, when $u_{n} \mathrm{~s}$ become highly oscillatory and asymptotic behaviour sets. Moreover, $\hat{\mathcal{Q}}_{n}^{[2,2]}$ clearly delivers poor relative error even for large $n$. This is not surprising either, since its relative asymptotic order is just one.

|  | $\hat{\mathcal{Q}}_{n}^{[2,2]}[f]$ |  | $\hat{\mathcal{Q}}_{n}^{[3,3]}[f]$ |  | $\hat{\mathcal{Q}}_{n}^{[6,6]}[f]$ |  |
| ---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $n$ | absolute | relative | absolute | relative | absolute | relative |
| 1 | $9.90_{-02}$ | $4.40_{-01}$ | $-7.20_{-03}$ | $-3.20_{-02}$ | $3.17_{-03}$ | $1.41_{-02}$ |
| 2 | $1.82_{-02}$ | $4.50_{-01}$ | $-1.54_{-04}$ | $-4.21_{-03}$ | $7.66_{-05}$ | $2.08_{-03}$ |
| 3 | $3.61_{-03}$ | $1.60_{-01}$ | $-2.48_{-05}$ | $-1.09_{-03}$ | $3.96_{-06}$ | $1.75_{-04}$ |
| 4 | $1.75_{-03}$ | $2.28_{-01}$ | $-3.07_{-06}$ | $-4.01_{-04}$ | $6.99_{-07}$ | $9.15_{-05}$ |
| 10 | $5.90_{-05}$ | $8.65_{-02}$ | $-9.21_{-09}$ | $-1.35_{-05}$ | $7.97_{-10}$ | $1.69_{-06}$ |
| 20 | $4.06_{-06}$ | $4.25_{-02}$ | $-8.88_{-11}$ | $-9.30_{-07}$ | $3.78_{-12}$ | $3.95_{-08}$ |
| 50 | $1.10_{-07}$ | $1.68_{-02}$ | $-1.65_{-13}$ | $-2.53_{-08}$ | $2.78_{-15}$ | $4.25_{-10}$ |
| 100 | $7.02_{-09}$ | $8.39_{-03}$ | $-1.35_{-15}$ | $-1.60_{-09}$ | $1.13_{-17}$ | $1.35_{-11}$ |

Table 1: Absolute and relative errors $\hat{\mathcal{Q}}_{n}^{[i, i]}[f]-\hat{f}_{n}$ for $f(x)=\mathrm{e}^{x}, q=2$ and $i=2,3,6$.

### 5.2 Filon-type methods

The main idea of Filon-type methods is to replace $f$ by an interpolating polynomial $\psi$ inside the integral. Thus, let $-1=c_{1}<c_{2}<\cdots<c_{\nu}=1$ be given nodes and $m_{1}, m_{2}, \ldots, m_{\nu} \in$ $\mathbb{N}$ their multiplicities. We interpolate (in a Hermite sense) $\psi^{(i)}\left(c_{k}\right)=f^{(i)}\left(c_{k}\right)$ for $i=$ $0, \ldots, m_{k}-1, k=1, \ldots, \nu$ and let

$$
\begin{equation*}
\hat{\mathcal{Q}}_{n}[f]=\int_{-1}^{1} \psi(x) u_{n}(x) \mathrm{d} x, \quad n=1,2, \ldots \tag{5.3}
\end{equation*}
$$

(Iserles \& Nørsett 2005). Note that (5.3) can be always integrated exactly, because of the form (4.3) of $u_{n}$. The asymptotic order of (5.3) is $\min \left\{m_{1}, m_{\nu}\right\}$ : in other words, it is influenced solely by function values and derivatives at the endpoints, consistently with the asymptotic expansion. However, further information at the intermediate points $c_{2}, \ldots, c_{\nu-1}$ typically decreases significantly the size of the error (Iserles \& Nørsett 2005).

The Filon method has been reinterpreted in (Iserles \& Nørsett 2006) in the case of modified Fourier expansions, our case $q=1$, and similar reinterpretation applies in the current, more general setting, except that it requires some further work.

Once we contemplate the information (in terms of function and derivative evaluations) required for the formation of $\psi$, we are struck by an important observation. The asymptotic expansion (2.4) requires only some derivatives at the endpoints: specifically, we require only $f^{(2 q r+k)}( \pm 1)$ for $r=0,1, \ldots$ and $k=q, \ldots, 2 q-1$. In particular, $f^{(i)}( \pm 1)$ is not required for $i=0, \ldots, q-1$. It is clearly wasteful to evaluate and interpolate unnecessary values, not just in evaluating derivatives that have no direct bearing on the solution but also in increasing unduly the degree of $\psi$. Following the practice of (Iserles \& Nørsett 2006), we use 'significant' derivatives $f^{(2 q r+k)}\left(c_{k}\right)$ also at the intermediate points $k=2, \ldots, \nu-1$.

This practice leads to savings but is potentially dangerous. The Birkhoff-Hermite interpolation problem, whereby a function is interpolated on a basis of lacunary derivative information (i.e., with some derivatives 'missing') need not have a solution or the solution need not be unique (Lorenz, Jetter \& Riemenschneider 1983). We cannot take it for granted that $\psi$ exists for any configuration of $c_{k} \mathrm{~s}$ and derivative information therein. Although this will not be a problem in particular examples explicitly worked out in the current paper, it is only fair to warn the reader.

Not every multiplicity makes sense in the present context, since not every derivative features in asymptotic expansion. We say that a natural number $J$ is good if there exist $s \geq 0$ and $p \in\{0, \ldots, q-1\}$ such that $J=\rho_{s, p}$ and assume in the sequel that all multiplicities are good numbers.

We seek a polynomial $\psi$ of degree $\sum_{k=1}^{\nu} \iota_{m_{k}}-1$, where $\iota_{m}$ is the number of terms in the set $\boldsymbol{N}_{m}$, such that

$$
\begin{equation*}
\psi^{(j)}\left(c_{k}\right)=f^{(j)}\left(c_{k}\right) \quad j \in N_{m_{k}}, \quad k=1, \ldots, \nu \tag{5.4}
\end{equation*}
$$

and set

$$
\begin{equation*}
\hat{\mathcal{Q}}_{n}^{m}[f]=\int_{-1}^{1} \psi(x) u_{n}(x) \mathrm{d} x, \quad n=1,2, \ldots \tag{5.5}
\end{equation*}
$$

Therefore, the data set of the Filon-type method (5.5) is

$$
\boldsymbol{D}^{\boldsymbol{m}}=\tilde{\boldsymbol{D}}_{q} \cup \bigcup_{k=1}^{\nu} \boldsymbol{D}_{m_{k}}\left(c_{k}\right)
$$

Recalling that the least index in $\boldsymbol{N}_{m}$ is the $q$ th one, it is convenient to replace (5.4) by the interpolation conditions

$$
\varphi^{(j-q)}\left(c_{k}\right)=f^{(i)}\left(c_{k}\right) \quad j \in N_{m_{k}}, \quad k=1, \ldots, \nu
$$

In other words, $\varphi=\psi^{(q)}$ and trivial calculation yields

$$
\begin{equation*}
\psi(x)=\sum_{l=0}^{q-1} \frac{1}{l!} f^{(l)}(0) x^{l}+\frac{1}{(q-1)!} \int_{0}^{x}(x-t)^{q-1} \varphi(t) \mathrm{d} t \tag{5.6}
\end{equation*}
$$

We substitute (5.6) into (5.5) and note that, by Lemma 1, the $u_{n} \mathrm{~s}$ are orthogonal to all polynomials of degree $\leq q-1$. Therefore

$$
\hat{\mathcal{Q}}_{n}^{m}[f]=\frac{1}{(q-1)!} \int_{-1}^{1} \int_{0}^{x}(x-t)^{q-1} \varphi(t) \mathrm{d} t u_{n}(x) \mathrm{d} x, \quad n=1,2, \ldots
$$

Theorem 4 Let $m_{1}=m_{\nu}=\rho_{s, p}$ (recall that all multiplicities are good numbers). The asymptotic order of $\hat{\mathcal{Q}}_{n}^{m}$ is $(2 s+1) q+p+1$.

Proof Identical to the proof of the order of a Filon-type method from (Iserles \& Nørsett 2005), substituting $\psi-f$ into the asymptotic expansion and using Theorem 3 for the order of the asymptotic method.

Proposition 5 It is true that

$$
\begin{equation*}
\hat{\mathcal{Q}}_{n}^{m}[f]=\frac{1}{\alpha_{n}^{2 q}} \int_{-1}^{1} \varphi(x) u_{n}^{(q)}(x) \mathrm{d} x, \quad n=1,2, \ldots . \tag{5.7}
\end{equation*}
$$

Proof We observe that

$$
\frac{\mathrm{d}}{\mathrm{~d} x} \int_{0}^{x}(x-t)^{j} \varphi(t) \mathrm{d} t=j \int_{0}^{x}(x-t)^{j-1} \varphi(t) \mathrm{d} t, \quad j \geq 1
$$

We replace $u_{n}$ with $(-1)^{q} \alpha_{n}^{-2 q} u_{n}^{(2 q)}$, using (1.3), and integrate by parts,

$$
\begin{aligned}
\hat{\mathcal{Q}}_{n}^{m}[f]= & \frac{(-1)^{q}}{(q-1)!\alpha_{n}^{2 q}} \int_{-1}^{1} \int_{0}^{x}(x-t)^{q-1} \varphi(t) \mathrm{d} t u_{n}^{(2 q)}(x) \mathrm{d} x \\
= & \frac{(-1)^{q}}{(q-1)!\alpha_{n}^{2 q}}\left[u_{n}^{(2 q-1)}(1) \int_{0}^{1}(1-t)^{q-1} \varphi(t) \mathrm{d} t\right. \\
& \left.\quad-(-1)^{q} u_{n}^{(2 q-1)}(-1) \int_{-1}^{0}(1+t)^{q-1} \varphi(t) \mathrm{d} t\right] \\
& +\frac{(-1)^{q-1}}{(q-2)!\alpha_{n}^{2 q}} \int_{-1}^{1} \int_{0}^{x}(x-t)^{q-2} \varphi(t) \mathrm{d} t u_{n}^{(2 q-1)}(x) \mathrm{d} x .
\end{aligned}
$$

Because of (1.4), however, $u_{n}^{(2 q-1)}( \pm 1)$, therefore

$$
\hat{\mathcal{Q}}_{n}^{m}[f]=\frac{(-1)^{q-1}}{(q-2)!\alpha_{n}^{2 q}} \int_{-1}^{1} \int_{0}^{x}(x-t)^{q-2} \varphi(t) \mathrm{d} t u_{n}^{(2 q-1)}(x) \mathrm{d} x
$$

We continue by induction, repeatedly integrating by parts and using Neumann boundary conditions (1.4). It thus follows that

$$
\hat{\mathcal{Q}}_{n}^{m}[f]=\frac{(-1)^{q-k}}{(q-k)!\alpha_{n}^{2 q}} \int_{-1}^{1} \int_{0}^{x}(x-t)^{q-k-1} \varphi(t) \mathrm{d} t u_{n}^{(2 q-k)}(x) \mathrm{d} x
$$

for $k=0,1, \ldots, q-1$. Letting $k=q-1$, integrating again by parts and substituting zero Neumann boundary conditions, we obtain

$$
\hat{\mathcal{Q}}_{n}^{m}[f]=-\frac{1}{\alpha_{n}^{2 q}} \int_{-1}^{1} \int_{0}^{x} \varphi(t) \mathrm{d} t u_{n}^{(q+1)}(x) \mathrm{d} x=\frac{1}{\alpha_{n}^{2 q}} \int_{-1}^{1} \varphi(x) u_{n}^{(q)}(x) \mathrm{d} x
$$

This completes the proof.
Note that $u_{n}^{(q)} \sim \mathcal{O}\left(\alpha_{n}^{q}\right)$, therefore $\hat{\mathcal{Q}}_{n}^{m}[f] \sim \mathcal{O}\left(\alpha_{n}^{-q-1}\right)$, as expected. Note further that $v_{n}=u_{n}^{(q)}$ is an eigenfunction of (1.3) corresponding to the Dirichlet boundary conditions

$$
v_{n}^{(i)}( \pm 1)=0, \quad i=0,1, \ldots, q-1
$$

(the eigenvalues for Dirichlet and Neumann conditions are the same for (1.3)).
Each $\varphi$ is a linear combination of derivative values,

$$
\varphi(x)=\sum_{k=1}^{\nu} \sum_{j \in \mathrm{~N}_{m_{k}}\left(c_{k}\right)} \varphi_{k, j}(x) f^{(j)}\left(c_{k}\right)
$$

where the $\varphi_{k, j}$ s are cardinal polynomials of Birkhoff-Hermite interpolation. Therefore, letting

$$
b_{k, j}(n)=\frac{1}{\alpha_{n}^{2 q}} \int_{-1}^{1} \varphi_{k, j}(x) u_{n}^{(q)}(x) \mathrm{d} x, \quad j \in \boldsymbol{N}_{m_{k}}, k=1, \ldots, \nu
$$

we have

$$
\begin{equation*}
\hat{\mathcal{Q}}_{n}^{m}[f]=\sum_{k=1}^{\nu} \sum_{j \in \boldsymbol{N}_{m_{k}}} b_{k, j}(n) f^{(j)}\left(c_{k}\right) \tag{5.8}
\end{equation*}
$$

As an example, we let $q=2, \nu=4, \boldsymbol{c}=[-1,-c, c, 1]$ and $\boldsymbol{m}=[2,2,2,2]$, where $c \in(0,1)$. Since for $q=2$ we have $\boldsymbol{N}_{2}=\{ \}$, our data set is

$$
\begin{equation*}
\left\{f(0), f^{\prime}(0), f^{\prime \prime}(0), f^{\prime \prime}(-1), f^{\prime \prime}(-c), f^{\prime \prime}(c), f^{\prime \prime}(1)\right\} \tag{5.9}
\end{equation*}
$$

Simple calculation confirms that the cardinal polynomials are

$$
\begin{aligned}
& \varphi_{1,2}(x)=-\frac{1}{2} \frac{(1-x)\left(c^{2}-x^{2}\right)}{1-c^{2}} \\
& \varphi_{2,2}(x)=\frac{1}{2} \frac{\left(1-x^{2}\right)(c-x)}{c\left(1-c^{2}\right)} \\
& \varphi_{3,2}(x)=\frac{1}{2} \frac{\left(1-x^{2}\right)(c+x)}{c\left(1-c^{2}\right)} \\
& \varphi_{4,2}(x)=-\frac{1}{2} \frac{(1+x)\left(c^{2}-x^{2}\right)}{1-c^{2}}
\end{aligned}
$$

The fastest way of calculating the weights $b_{k, j}$ is probably by treating $\alpha_{n}$ as a parameter, calculating the integral and finally using (3.2) and (3.4) to simplify he expressions. The outcome is appealing in its simplicity,

$$
\begin{aligned}
b_{1,2}(2 n-1) & =b_{4,2}(2 n-1)=-\frac{\sqrt{2} \tan \alpha_{2 n-1}}{\alpha_{2 n-1}^{3}}-\frac{2 \sqrt{2}}{1-c^{2}} \frac{1}{\alpha_{2 n-1}^{4}} \\
b_{2,2}(2 n-1) & =b_{3,2}(2 n-1)=\frac{2 \sqrt{2}}{1-c^{2}} \frac{1}{\alpha_{2 n-1}^{4}} \\
b_{1,2}(2 n) & =-\frac{\sqrt{2} \cot \alpha_{2 n}}{\alpha_{2 n}^{3}}+\frac{\sqrt{2}\left(3-c^{2}\right)}{1-c^{2}} \frac{1}{\alpha_{2 n}^{4}}, \quad b_{4,2}(2 n)=-b_{1,2}(2 n), \\
b_{2,2}(2 n) & =-\frac{2 \sqrt{2}}{c\left(1-c^{2}\right)} \frac{1}{\alpha_{2 n}^{4}}, \quad b_{3,2}(2 n)=-b_{2,2}(2 n) .
\end{aligned}
$$

Comparing with $\hat{\mathcal{Q}}_{n}^{[2,2]}$, we thus deduce that

$$
\begin{gather*}
\hat{\mathcal{Q}}_{2 n-1}^{[2,2,2,2]}[f]=\hat{\mathcal{Q}}_{2 n-1}^{[2,2]}[f]-\frac{1}{\alpha_{2 n-1}^{4}} \frac{2 \sqrt{2}}{1-c^{2}}\left[f^{\prime \prime}(1)-f^{\prime \prime}(c)-f^{\prime \prime}(-c)+f^{\prime \prime}(-1)\right],  \tag{5.10}\\
\begin{array}{c}
\hat{\mathcal{Q}}_{2 n}^{[2,2,2,2]}[f]=\hat{\mathcal{Q}}_{2 n}^{[2,2]}[f]-\frac{1}{\alpha_{2 n}^{4}} \frac{\sqrt{2}}{c\left(1-c^{2}\right)}\left\{c\left(3-c^{2}\right)\left[f^{\prime \prime}(1)-f^{\prime \prime}(-1)\right]-2\left[f^{\prime \prime}(c)\right.\right. \\
\\
\left.\left.-f^{\prime \prime}(-c)\right]\right\} .
\end{array}
\end{gather*}
$$

We deduce that, like in the case of asymptotic methods, $\hat{\mathcal{Q}}_{n}^{[2,2,2,2]}[f]$ for $n=1,2, \ldots, m$ can be computed in $\mathcal{O}(m)$ operations. Indeed, it is evident from (5.8) that this is the case for all $\hat{\mathcal{Q}}_{n}^{m}[f]$.

### 5.3 Another take on Filon-type methods

The method (5.10), as well as several examples of such methods for $q=1$ in (Iserles \& Nørsett 2006), can be written in the form

$$
\begin{align*}
\hat{\mathcal{Q}}_{2 n-1}^{m}[f] & =\hat{\mathcal{Q}}_{2 n-1}^{\left[\rho_{p, s}, \rho_{p, s}\right]}[f]+\frac{G_{1}(n)}{\alpha_{2 n-1}^{N}} \sum_{k=1}^{\nu} \sum_{j \in \boldsymbol{N}_{m_{k}}} a_{k, j} f^{(j)}\left(c_{k}\right),  \tag{5.11}\\
\hat{\mathcal{Q}}_{2 n}^{m}[f] & =\hat{\mathcal{Q}}_{2 n}^{\left[\rho_{p, s}, \rho_{p, s}\right]}[f]+\frac{G_{2}(n)}{\alpha_{2 n}^{N}} \sum_{k=1}^{\nu} \sum_{j \in \boldsymbol{N}_{m_{k}}} d_{k, j} f^{(j)}\left(c_{k}\right),
\end{align*}
$$

where $m_{1}=m_{\nu}=\rho_{p, m}$ and $N=(2 s+1) q+p+1$, while $G_{1}$ and $G_{2}$ are given functions ( $G_{1}, G_{2} \equiv 1$ in (5.10)). This can be reinterpreted in the following manner: we are using derivative information to approximate the $N$ th term in the asymptotic expansion. This procedure minimises the magnitude of the error by replacing the leading truncated term in the asymptotic expansion, a linear combination of derivatives, with an error incurred while approximating these derivatives.

Thus, letting $h=f^{\prime \prime}$, we can easily verify that

$$
\begin{aligned}
\frac{2}{1-c^{2}}[h(1)-h(c)-h(-c)+h(-1)] & \approx h^{\prime}(1)-h^{\prime}(-1), \\
\frac{1}{c\left(1-c^{2}\right)}\left\{c\left(3-c^{2}\right)[h(1)-h(-1)]-2[h(c)-h(-c)]\right\} & \approx h^{\prime}(1)+h^{\prime}(-1)
\end{aligned}
$$

is correct for every $h \in \mathbb{P}_{3}$ and $h \in \mathbb{P}_{4}$, respectively. (It is impossible to make it correct for higher order polynomials, since this would have required $c=1$.)

The form (5.11) has two crucial advantages. Firstly, it provides a transparent means to compute first $m$ approximated expansion coefficients in $\mathcal{O}(m)$ operations. Secondly, it is considerably easier to derive than through an interpolation polynomial and its integration.

Note that we do not claim that every Filon-type method $\hat{Q}_{n}^{m}$ can be expressed in the form (5.11). All the cases we have considered fit this pattern and we believe that this is true in general, but as things stand we cannot confirm this by a proof.

To illustrate how to form methods (5.11) directly and with ease, without constructing and integrating interpolating polynomials, we consider $\boldsymbol{m}=[3,3,3,3]$, hence asymptotic order $N=7, \rho_{s, p}=3$ and

$$
G_{1}(n)=-\sqrt{2} \tan \alpha_{2 n-1}, \quad G_{2}(n)=\sqrt{2} \cot \alpha_{2 n} .
$$

Letting $h=f^{\prime \prime}$, the task in hand is to approximate $h^{(i v)}(1)+h^{(i v)}(-1)$ (for odd $n$ ) and $h^{(i v)}(1)-h^{(i v)}(-1)$ (for even $n$ ) by a linear combination of

$$
h(-1), h^{\prime}(-1), h(-c), h^{\prime}(-c), h(c), h^{\prime}(c), h(1), h^{\prime}(1) .
$$

It is easy to find optimal linear combinations of this kind: specifically

$$
\begin{aligned}
h^{(i v)}(1)+h^{(i v)}(-1)= & -\frac{1440}{\left(1-c^{2}\right)^{3}}[h(1)-h(c)-h(-c)+h(-1)] \\
& +\frac{360}{c\left(1-c^{2}\right)^{2}}\left[c h^{\prime}(1)+h^{\prime}(c)-h^{\prime}(-c)-c h^{\prime}(-1)\right]
\end{aligned}
$$

is correct for every $h \in \mathbb{P}_{7}$, while

$$
\begin{aligned}
h^{(i v)}(1)-h^{(i v)}(-1)= & -\frac{120\left(14-7 c^{2}+c^{4}\right)}{\left(1-c^{2}\right)^{3}}[h(1)-h(-1)] \\
& -\frac{60\left(5-28 c^{2}+7 c^{4}\right)}{c^{3}\left(1-c^{2}\right)^{3}}[h(c)-h(-c)] \\
& +\frac{120\left(3-c^{2}\right)}{\left(1-c^{2}\right)^{2}}\left[h^{\prime}(1)+h^{\prime}(-1)\right]+\frac{60\left(5-c^{2}\right)}{c^{2}\left(1-c^{2}\right)^{2}}\left[h^{\prime}(c)+h^{\prime}(-c)\right]
\end{aligned}
$$

for all $h \in \mathbb{P}_{8}$. Therefore

$$
\begin{aligned}
\hat{\mathcal{Q}}_{2 n-1}^{[3,3,3,3]}[f]= & \hat{\mathcal{Q}}_{2 n-1}^{[3,3]}[f]-\frac{\sqrt{2} \tan \alpha_{2 n-1}}{\alpha_{2 n-1}^{7}}\left\{-\frac{1440}{\left(1-c^{2}\right)^{3}}\left[f^{\prime \prime}(1)-f^{\prime \prime}(c)-f^{\prime \prime}(-c)\right.\right. \\
& \left.\left.+f^{\prime \prime}(-1)\right]+\frac{360}{c\left(1-c^{2}\right)^{2}}\left[c f^{\prime \prime \prime}(1)+f^{\prime \prime \prime}(c)-f^{\prime \prime \prime}(-c)-c f^{\prime \prime \prime}(-1)\right]\right\} \\
\hat{\mathcal{Q}}_{2 n}^{[3,3,3,3]}[f]= & \hat{\mathcal{Q}}_{2 n}^{[3,3]}[f]-\frac{\sqrt{2} \cot \alpha_{2 n}}{\alpha_{2 n}^{7}}\left\{-\frac{120\left(14-7 c^{2}+c^{4}\right)}{\left(1-c^{2}\right)^{3}}\left[f^{\prime \prime}(1)-f^{\prime \prime}(-1)\right]\right. \\
& -\frac{60\left(5-28 c^{2}+7 c^{4}\right)}{c^{3}\left(1-c^{2}\right)^{3}}\left[f^{\prime \prime}(c)-f^{\prime \prime}(-c)\right]+\frac{120\left(3-c^{2}\right)}{\left(1-c^{2}\right)^{2}}\left[f^{\prime \prime \prime}(1)+f^{\prime \prime \prime}(-1)\right] \\
& \left.+\frac{60\left(5-c^{2}\right)}{c^{2}\left(1-c^{2}\right)^{2}}\left[f^{\prime \prime \prime}(c)+f^{\prime \prime \prime}(-c)\right]\right\} .
\end{aligned}
$$

### 5.4 Exotic quadrature

Our formulæ for $\hat{\mathcal{Q}}_{n}^{[2,2,2,2]}$ and $\hat{\mathcal{Q}}_{n}^{[3,3,3,3]}$ feature a free parameter $c \in(0,1)$. The reason is twofold. Firstly, this leads to less cluttered and more transparent notation. Secondly, we have not yet formulated a good criterion for the choice of the node $c$.

Once we attempt to construct the expansion (2.2), we need to compute not just $\hat{f}_{n}$ for $n \geq$ 1 but also the nonoscillatory integrals $\hat{f}_{0}^{0}, \ldots, \hat{f}_{q-1}^{o}$. In principle, we could have computed them with, say, Gaussian quadrature: given that only $q$ coefficients need be computed, the $\mathcal{O}(m)$ operation count remains valid. We can do better, however, by reusing derivatives that have been already used in forming our approximations to the $\hat{f}_{n} \mathrm{~s}$, complemented by a small number of lower derivatives. Specifically, we let each $\hat{f}_{n}^{o}, n=0, \ldots, q-1$, be a linear combination of values from the data set $D^{m}$ :

$$
\begin{equation*}
\int_{-1}^{1} f(x) \mathrm{P}_{n}(x) \mathrm{d} x \approx \hat{\mathcal{P}}_{n}^{m}[f]=\sum_{k=1}^{\nu} \sum_{j \in \boldsymbol{N}_{m_{k}}} \delta_{k, j}(n) f^{(j)}\left(c_{k}\right), \quad n=0, \ldots, q-1 \tag{5.12}
\end{equation*}
$$

We call (5.12) an exotic quadrature, to underly its difference from more standard computational methods for nonoscillatory integrals. Note that a precursor of this idea has been named in (Iserles \& Nørsett 2006) an "underlying classical quadrature", surely more of a mouthful than "exotic".

The data set for $\hat{\mathcal{Q}}_{n}^{[2,2,2,2]}$ is

$$
\boldsymbol{D}^{[2,2,2,2]}=\left\{f(0), f^{\prime}(0), f^{\prime \prime}(-1), f^{\prime \prime}(-c), f^{\prime \prime}(0), f^{\prime \prime}(c), f^{\prime \prime}(1)\right\}
$$

and simple algebra confirms that the exotic quadrature

$$
\begin{aligned}
\hat{\mathcal{P}}_{0}^{[2,2,2,2]}[f]= & 2 f(0)+\frac{1}{420} \frac{2-7 c^{2}}{1-c^{2}}\left[f^{\prime \prime}(1)+f^{\prime \prime}(-1)\right]+\frac{1}{84} \frac{1}{c^{2}\left(1-c^{2}\right)}\left[f^{\prime \prime}(c)+f^{\prime \prime}(-c)\right] \\
& -\frac{1}{210} \frac{5-63 c^{2}}{c^{2}} f^{\prime \prime}(0)
\end{aligned}
$$

is of order 7 (i.e., correct for all $f \in \mathbb{P}_{7}$ ) for generic $c$ and of order 9 for $c=\sqrt{210} / 30$. Likewise,

$$
\hat{\mathcal{P}}_{1}^{[2,2,2,2]}[f]=\frac{2}{3} f^{\prime}(0)+\frac{1}{420} \frac{3-14 c^{2}}{1-c^{2}}\left[f^{\prime \prime}(1)-f^{\prime \prime}(-1)\right]+\frac{11}{420} \frac{1}{c\left(1-c^{2}\right)}\left[f^{\prime \prime}(c)-f^{\prime \prime}(-c)\right]
$$

is in general of order 6 , except that $c=\sqrt{187} / 33$ results in order 8 . Since we wish to maximise the least order of $\hat{\mathcal{P}}_{k}^{[2,2,2,2]}[f], k=0,1$, we thus choose $c=\sqrt{187} / 33$ in both Filon-type and exotic quadrature for $\boldsymbol{m}=[2,2,2,2]$.

Longer algebra produces exotic quadrature coefficients for $\hat{\mathcal{Q}}_{n}^{[3,3,3,3]}$,

$$
\begin{aligned}
\hat{\mathcal{P}}_{0}^{[3,3,3,3]}[f]= & 2 f(0)+\frac{1}{13860} \frac{68-404 c^{2}+935 c^{4}-396 c^{6}}{\left(1-c^{2}\right)^{3}}\left[f^{\prime \prime}(1)+f^{\prime \prime}(-1)\right] \\
& -\frac{1}{13860} \frac{25-328 c^{2}+506 c^{4}}{c^{4}\left(1-c^{2}\right)^{3}}\left[f^{\prime \prime}(c)+f^{\prime \prime}(-c)\right] \\
& +\frac{1}{6930} \frac{25-253 c^{2}+1914 c^{4}}{c^{4}} f^{\prime \prime}(0) \\
& -\frac{1}{55440} \frac{27-154 c^{2}+330 c^{4}}{\left(1-c^{2}\right)^{2}}\left[f^{\prime \prime \prime}(1)-f^{\prime \prime \prime}(-1)\right] \\
& +\frac{1}{55440} \frac{50-253 c^{2}}{c^{3}\left(1-c^{2}\right)^{2}}\left[f^{\prime \prime \prime}(c)-f^{\prime \prime \prime}(-c)\right], \\
\hat{\mathcal{P}}_{1}^{[3,3,3,3]}[f]= & \frac{2}{3} f^{\prime}(0)+\frac{1}{166320} \frac{1015-6671 c^{2}+19558 c^{4}-7722 c^{6}}{\left(1-c^{2}\right)^{3}}\left[f^{\prime \prime}(1)-f^{\prime \prime}(-1)\right] \\
& -\frac{1}{166320} \frac{259-6707 c^{2}+12628 c^{4}}{c^{3}\left(1-c^{2}\right)^{3}}\left[f^{\prime \prime}(c)-f^{\prime \prime}(-c)\right] \\
& -\frac{1}{166320} \frac{115-748 c^{2}+2178 c^{4}}{\left(1-c^{2}\right)^{2}}\left[f^{\prime \prime \prime}(1)+f^{\prime \prime \prime}(-1)\right] \\
& +\frac{1}{166320} \frac{259-1804 c^{2}}{c^{2}\left(1-c^{2}\right)^{2}}\left[f^{\prime \prime \prime}(c)-f^{\prime \prime \prime}(-c)\right]
\end{aligned}
$$

of orders 11 and 10 , respectively. No real value of $c$ results in a higher-order exotic quadrature.


Figure 5.2: Scaled errors $n^{4}\left|\hat{\mathcal{Q}}_{n}^{[2,2,2,2]}[f]-\hat{f}_{n}\right|$ and $n^{7}\left|\hat{\mathcal{Q}}_{n}^{[3,3,3,3]}[f]-\hat{f}_{n}\right|$ for $f(x)=\mathrm{e}^{x}$ and $q=2$.

|  | $\hat{\mathcal{P}}_{n}^{[2,2,2,2]}[f]$ |  | $\hat{\mathcal{P}}_{n}^{[3,3,3,3]}[f]$ |  |
| ---: | :---: | :---: | ---: | ---: |
| $n$ | absolute | relative | absolute | relative |
| 0 | $2.11_{-06}$ | $8.96_{-07}$ | $-1.21_{-10}$ | $-5.15_{-11}$ |
| 1 | $2.48_{-07}$ | $3.37_{-07}$ | $-3.49_{-09}$ | $-4.74_{-09}$ |
|  | $\hat{\mathcal{Q}}_{n}^{[2,2,2,2]}[f]$ |  | $\hat{\mathcal{Q}}_{n}^{[3,3,3,3]}[f]$ |  |
| $n$ | absolute | relative | absolute | relative |
| 1 | $-4.91_{-04}$ | $-2.18_{-03}$ | $-1.75_{-04}$ | $-7.78_{-04}$ |
| 2 | $1.84_{-05}$ | $5.00_{-04}$ | $7.59_{-05}$ | $2.07_{-03}$ |
| 3 | $2.05_{-04}$ | $9.04_{-03}$ | $-5.31_{-06}$ | $-2.35_{-04}$ |
| 4 | $1.34_{-05}$ | $1.75_{-03}$ | $6.88_{-07}$ | $8.98_{-05}$ |
| 10 | $5.46_{-07}$ | $8.01_{-04}$ | $7.68_{-10}$ | $1.27_{-06}$ |
| 20 | $3.81_{-08}$ | $3.99_{-04}$ | $3.51_{-12}$ | $3.68_{-08}$ |
| 50 | $1.04_{-09}$ | $1.59_{-04}$ | $2.30_{-15}$ | $3.52_{-10}$ |
| 100 | $6.62_{-11}$ | $7.90_{-05}$ | $7.43_{-18}$ | $8.87_{-12}$ |

Table 2: Absolute and relative errors $\hat{\mathcal{P}}_{n}^{[i, i, i, i]}[f]-\hat{f}_{n}^{o}$ and $\hat{\mathcal{Q}}_{n}^{[i, i, i, i]}[f]-\hat{f}_{n}$ for $f(x)=\mathrm{e}^{x}$, $q=2$ and $i=2,3$.

Other things being equal, we opt for algebraically simple coefficients and let $c=\frac{1}{2}$ in $\hat{\mathcal{Q}}_{n}^{[3,3,3,3]}$ and $\hat{\mathcal{P}}_{n}^{[3,3,3,3]}$.

Fig. 5.2 depicts scaled errors produced by the two Filon-type methods that we have described earlier and it should be compared with Fig. 5.1. It is evident that, although the asymptotic order is the same, the use of additional data inside $(-1,1)$ decreases the error by a significant factor. The same conclusion emerges from Table 2. In particular, the improvement
for small $n s$ is tangible, although the errors there are still excessive for many uses. Of course, they can be decreased further by using larger $\nu$.

Table 2 also presents the error committed by exotic quadrature when approximating the expansion coefficients $\hat{f}_{0}^{o}$ and $\hat{f}_{1}^{o}$. Clearly, the error is very small indeed! It is, as a matter of fact, significantly smaller than the error of Filon-type methods for small $n$, when the integrand is nonoscillatory. Indeed, one possible remedy for small $n s$ is to use there appropriate exotic quadrature (on the same data set) in preference to Filon.

## 6 Conclusions and challenges

This is the moment to take stock and briefly review what have we done in this paper and what remains to be done.

Our point of departure being modified Fourier expansions, whose coefficients decay like $\mathcal{O}\left(n^{-2}\right)$ for analytic functions (Iserles \& Nørsett 2006), we have generalized the framework to approximation bases originating in eigenfunctions of polyharmonic operators with Neumann boundary conditions. These bases exhibit faster rate of decay of expansion coefficients. In particular, we have analysed in greater detail bases with $\mathcal{O}\left(n^{-3}\right)$ decay. We have expanded the $n$th coefficient $\hat{f}_{n}$ asymptotically in powers of $n^{-1}$ and presented the underlying orthogonal functions in an explicit manner. Such functions always separate into two sets: they are either even or odd. They depend on a parameter which can be obtained by solving a scalar nonlinear algebraic equation.

Theoretical analysis has been followed by the introduction of three numerical techniques for rapid approximation of expansion coefficients.

- Firstly, we have used a truncated asymptotic expansion. Requiring a small number of derivative evaluations and linear cost, it results in impressively small error once asymptotic behaviour sets, but the error might be unacceptably large for small ns .
- Secondly, we have considered Filon-type methods which, in addition to derivatives at the endpoints, require additional derivatives elsewhere in the interval. The outcome is a family of methods that produce significantly smaller error, also for lower $n \mathrm{~s}$. We have reinterpreted Filon-type methods of (Iserles \& Nørsett 2005) as a combination of an asymptotic method with a scaled approximation to derivatives. This interpretation allows for a relatively painless practical derivation of such methods in a manner which is of the right form to allow their implementation in linear time.
- Thirdly, we have reused derivative information for "exotic quadrature" algorithms. The latter can be used very effectively indeed for the computation of coefficients corresponding to the zero eigenvalue of the polyharmonic operator.

Although our examples focused on the case $q=2$, corresponding to $\mathcal{O}\left(n^{-3}\right)$ decay, the underlying techniques apply to all $q \geq 1$. It is fair to comment, however, that underlying functions are becoming increasingly complicated with $q$.

This paper introduces a new mathematical approach and new numerical techniques. The treatment of neither mathematical nor computational aspects is comprehensive and many substantive problems remain. Indeed, bearing in mind the monumental intellectual effort that went into the last two centuries of harmonic analysis, it would have been surprising had we
been able to answer similar questions in a considerably more demanding and complicated framework in a single paper! We wish to single out the following problems and challenges for future work:

1. Pointwise convergence. It is known that classical Fourier expansions, truncated after $m$ terms, converge pointwise at the rate of $\mathcal{O}\left(\mathrm{m}^{-1}\right)$ away from the boundary for analytic, nonperiodic functions (Körner 1988). The standard proof consists of two major steps: proof of summability (the Fejér Theorem) is used as a stepping stone in the proof of pointwise convergence (the de la Vallée Poussin Theorem). Both the Fejér Theorem and the de la Vallée Poussin Theorem have been generalized in (Iserles \& Nørsett 2006) for modified Fourier expansions, the simplest instance of approximation bases considered in this paper.

However, numerical experiments indicate that modified Fourier expansions of analytic functions converge like $\mathcal{O}\left(m^{-2}\right)$, yet this has never been proved. Insofar as the more general approximation bases of this paper are concerned, we believe that they converge pointwise inside the interval and uniformly in any closed subset at the rate of $\mathcal{O}\left(n^{-q-1}\right)$. Needless to say, this is just a conjecture and we have at present neither proof nor even a tentative idea how to seek a proof.
An important difference between classical and modified Fourier expansions is that the latter converge at the boundary (for nonperiodic analytic functions) at the decreased rate of $\mathcal{O}\left(n^{-1}\right)$ (Iserles \& Nørsett 2006). Based on numerical experimentation, we believe that bases of polyharmonic eigenfunctions converge at the endpoints at the rate of $\mathcal{O}\left(n^{-q}\right)$, but cannot prove it yet. Note that the method of proof in (Iserles \& Nørsett 2006) relies specifically on the (very simple) form of modified Fourier expansions and cannot be extended to general $q \geq 1$.
2. Properties of the $\alpha_{n} s$. The parameters $\alpha_{n}$ are zeros of the nonlinear algebraic equations (4.5) and (4.7). The cases $q=1,2,3$, as well as numerical investigation for $q=4$, indicate that all such zeros are simple, they interlace and the least zero is that of (4.5) for even $q$ and of (4.7) otherwise. Moreover, the $\alpha_{n}$ s appear to tend to $\frac{1}{4}(2 n+q-1) \pi$ exponentially fast with $n$. All this, for general $q \geq 1$, is purely a matter of conjecture.
3. Properties of the functions $u_{n}$. It is enough to examine Fig. 3.1 to persuade ourselves of the many features of the eigenfunctions $u_{n}$. In particular, each $u_{n}$ appears to have $n+q$ simple zeros in $(-1,1)$ and these zeros interlace. Of course, interlace of zeros of eigenfunctions is well known in the case of Sturm-Liouville operators, but we are not aware of similar results for polyharmonic operators.
4. Filon-type quadrature. The design of Filon-type quadrature in the form (5.11), exploiting its interpretation as "asymptotic method plus scaled approximation to derivatives" is fairly straightforward and can be performed, at least in principle, for any reasonable number of nodes $c_{1}, c_{2}, \ldots, c_{\nu}$. This can deal with lower accuracy at low frequencies, apparent in Tables 1 and 2. It is of interest, however, to obtain good, reliable and affordable error bounds and error estimates. In (Iserles \& Nørsett 2004) we have considered practical means of estimating the error in Filon-type quadrature. However, the techniques therein are effective mainly for large frequencies, while our interest is also in low frequencies, before the onset of asymptotic behaviour. We thus need an alternative approach. An intriguing idea is to use the Peano Kernel Theorem (Powell 1981):
this is fairly standard for derivative approximations but might be more of a challenge for the asymptotic-expansion part.
A pertinent issue is the stability of Filon-type methods (5.11) for large $\nu$. Approximation to derivatives is known as an ill-conditioned numerical problem - does this impact on the conditioning of Filon-type methods? Does it lead to large coefficients and to loss of accuracy? Clearly, we need to understand such issues these better and obtain a wealth of practical numerical experience with many $\nu$ s and many functions $f$.
5. Avoiding the use of derivatives. We have already described in (Iserles \& Nørsett 2006) how to replace derivatives by finite differences in Filon-type methods for modified Fourier expansions. As long as the spacing is sufficiently fine, results are practically indistinguishable from using derivatives. We see absolutely no reason why this approach cannot be extended to arbitrary $q \geq 1$.
6. Alternative highly oscillatory quadrature. Four main approaches to highly oscillatory quadrature came off age in the last few years: asymptotic and Filon-type methods (Iserles \& Nørsett 2005), but also Levin-type methods (Olver 2006) and the method of numerical stationary phase (Huybrechs \& Vandewalle 2006). Can such methods provide a competing, perhaps superior means to evaluate expansion coefficients $\hat{f}_{n}$ ?
7. Exotic quadrature. Classical interpolatory quadrature is exceedingly well understood (Davis \& Rabinowitz 1984). In particular, optimal choice of quadrature nodes is easily explained in terms of orthogonal polynomials. No such theory exists for exotic quadrature and we do not even know what is its attainable order. In one case, $\boldsymbol{m}=[2,2,2,2]$, we were able to optimize order by an appropriate choice of internal nodes, but for $\boldsymbol{m}=[3,3,3,3]$ no choice of nodes in the interior of the interval leads to better order. We believe that such a theory is within reach and are already assembling preliminary results.
Another challenge is to produce reliable and tight bounds on the error. This, we believe, can be accomplished with the Peano Kernel Theorem in a standard manner.
Yet another challenge in this context is to use exotic quadrature also for the first few coefficients $\hat{f}_{n}$, before the onset of asymptotic behaviour, where it might produce better outcome than the underlying Filon method. This does not seem to be unduly complicated, at least not for $q=1,2$, but the underlying ground work needs to be done.
Fourier analysis and fast Fourier transform techniques have proved themselves extraordinarily successful in modern mathematics and its applications. It is neither the intention nor the message of this paper to challenge this. Expansions in polyharmonic functions address themselves to just a single application area of Fourier techniques: the expansion of analytic, nonperiodic functions and its potential uses, e.g. in the numerical solution of differential equations. It is a tribute to the breadth and success of Fourier analysis that even this single application area is so important and has so many ramifications.

## Acknowledgments

We wish to thank Brian Davies (King's College, London), Andy Hausrath (University of Arizona), Daan Huybrechs (Katholieke Universiteit Leuven), Michael Levitin (HeriotWatt

University, Edinburgh), Alexei Shadrin (DAMTP, University of Cambridge), Jared Tanner (University of Utah) and Enrique Zuazua (Universidad Autonoma de Madrid) for helpful discussions and comments.

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