From high oscillation to rapid approximation II: Expansions in Birkhoff series

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Abstract

We consider the use of eigenfunctions of polyharmonic operators, equipped with homogeneous Neumann boundary conditions, to approximate nonperiodic functions in compact intervals. Such expansions feature a number of advantages in comparison with classical Fourier series, including uniform convergence and more rapid decay of expansion coefficients.

Having derived an asymptotic formula for expansion coefficients, we describe a systematic means to find eigenfunctions and eigenvalues. Next we demonstrate uniform convergence of the expansion and give estimates for the rate of convergence. This is followed by the 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

The practical expansion of smooth, nonperiodic functions on bounded domains in eigenfunctions of the Laplace operator equipped with homogeneous Neumann boundary conditions has been the subject of a number of recent papers. This theme, commenced in (Iserles & Nørsett 2008) for functions defined on compact intervals, has been generalised to tensor product domains (Iserles & Nørsett 2009) as well as the equilateral triangle (Huybrechs, Iserles & Nørsett 2010*b*). Such an approach entertains a number of advantages, of both theoretical and practical nature, over classical Fourier expansions and polynomial-based approximations. To date, so-called *modified Fourier expansions* have found applications in a number of areas, including the spectral discretization of boundary value problems (Adcock 2009, Adcock 2010*b*) and the computation of spectra of highly oscillatory integral operators (Brunner, Iserles & Nørsett 2009).

In this paper we pursue a different generalisation of this approach: namely, the expansion of functions defined on compact intervals in eigenfunctions of certain higher order differential operators. The purpose of this generalisation is to attain higher degrees of convergence whilst retaining the benefits of modified Fourier expansions. In particular, as we demonstrate, expansion coefficients can be calculated to high accuracy using straightforward generalisations of the quadratures developed in (Iserles & Nørsett 2008). In doing this, we exhibit a sharp contrast with the Fast Fourier Transform (FFT). Rather than being specific to the approximation scheme (i.e. Fourier series or expansions in Chebyshev polynomials), the quadratures utilised are applicable to a broad family of expansions.

It is not our intention to suggest that modified Fourier expansions, and their generalisation that we develop in this paper, will outperform well established algorithms in all scenarios. Clearly, an analytic, periodic function defined in a d-variate cube is best approximated by its Fourier series. Moreover, in many circumstances it may be advantageous to use orthogonal polynomials instead. Regardless, in light of the applications mentioned above, where modified Fourier expansions have been found to convey a number of important advantages, we feel that a study of this particular generalisation is warranted.

This paper thus marks an introductory foray towards the development of numerical methods based on polyharmonic expansions. A great deal of future effort, beyond the scope of one paper, is required to design efficient, stable algorithms based on this approach. In Section 7 we discuss a number of such challenges in greater detail.

Before developing the ideas of polyharmonic–Neumann expansions further, it makes sense to first explain briefly the main concepts of (Iserles & Nørsett 2008), including those that we intend to generalise in this paper.

1.1 Modified Fourier expansions

Classical Fourier expansions on $[-1, 1]$ use the basis

$$\{\cos \pi n x \,:\, n \in \mathbb{Z}_+\} \cup \{\sin \pi n x \,:\, n \in \mathbb{N}\}$$

and provide an incredibly powerful tool for the approximation of functions which are both analytic and periodic of period 2. By using the FFT to evaluate the first m coefficients, the truncated expansion can be constructed in $\mathcal{O}\left(m \log m\right)$ operations. Moreover, the coefficients decay exponentially fast and the error committed by the truncated expansion is exponentially small in m. These features underlie the astonishing success of Fourier expansions in an exceedingly wide range of applications in science and engineering.

However, once periodicity is no longer present, Fourier expansions are far less attractive. In contrast to the periodic case, the nth expansion coefficient decays like $\mathcal{O}\left(n^{-1}\right)$ and the expansion, truncated after m terms, commits an $\mathcal{O}\left(m^{-1}\right)$ error in $(-1,1)$. Moreover, uniform convergence is lacking and $\mathcal{O}\left(1\right)$ oscillations occur near the endpoints (the Gibbs phenomenon).

To approximate such functions it was proposed in (Iserles & Nørsett 2008) to employ the alternative basis $\mathcal{G}_1 = \mathbb{P}_0 \oplus \mathcal{H}_1$, where $\mathbb{P}_m$ is the set of mth-degree algebraic polynomials and

$$\mathcal{H}_1 = \{\cos \pi n x \,:\, n \in \mathbb{N}\} \cup \{\sin \pi (n - \tfrac{1}{2})x \,:\, n \in \mathbb{N}\}. \tag{1.1}$$

It has been shown that $\mathcal{G}_1$ is an orthonormal basis of $\mathrm{L}_2[-1,1]$ (Iserles & Nørsett 2008). However, in contrast to the Fourier basis, $\mathcal{G}_1$ is also orthogonal and dense in the Sobolev space $\mathrm{H}_1[-1,1]$, meaning that the *modified Fourier expansion*

$$f(x) \sim \tfrac{1}{2}\hat{f}^C_0 + \sum_{n=1}^{\infty} [\hat{f}^C_n \cos \pi n x + \hat{f}^S_n \sin \pi (n - \tfrac{1}{2})x],$$

where

$$\hat{f}^C_n = \int_{-1}^{1} f(x) \cos \pi n x \mathrm{d}x, \qquad \hat{f}^S_n = \int_{-1}^{1} f(x) \sin \pi (n - \tfrac{1}{2}) x \mathrm{d}x, \tag{1.2}$$

converges uniformly on $[-1,1]$ for $f \in \mathrm{H}_1[-1,1]$ (Adcock 2009). If this expansion is truncated after m terms, an error of $\mathcal{O}\left(m^{-1}\right)$ is committed uniformly throughout $[-1,1]$, provided f is sufficiently smooth. Away from the endpoints, this figure is $\mathcal{O}\left(m^{-2}\right)$ (Olver 2009).

The improvement offered by (1.1) over the Fourier basis is also seen in the decay of the coefficients. Once $\hat{f}^C_n$ and $\hat{f}^S_n$ are expanded asymptotically in powers of n^{-1}, we observe that $\hat{f}^C_n, \hat{f}^S_n = \mathcal{O}\left(n^{-2}\right)$ as opposed to $\mathcal{O}\left(n^{-1}\right)$ for the corresponding Fourier coefficients (Iserles & Nørsett 2008). This asymptotic expansion also provides the starting point for the design of numerical quadrature schemes to calculate the coefficients $\hat{f}^C_n$ and $\hat{f}^S_n$. As n increases, the functions $\cos \pi n x$ and $\sin \pi (n - \frac{1}{2})x$ become highly oscillatory. Hence, Filon-type techniques (Iserles & Nørsett 2005) can be employed for the computation of the highly oscillatory integrals (1.2). The few coefficients corresponding to small values of n, before asymptotic behaviour sets in, can be approximated by particular nonstandard classical quadrature formulæ (i.e. based on maximising polynomial order), involving both function values and certain derivatives. This method allows for computation of the first m coefficients to high accuracy in just $\mathcal{O}(m)$ operations—a full factor of $\log m$ faster than the FFT and without the requirement that m be highly composite. Unlike the FFT, this approach is also completely adaptive: increasing m does not require recalculation of existing values.

The purpose of this paper is to demonstrate that these ideas can be successfully generalised to a larger family of expansions. By a judicious choice of approximation basis, we introduce expansions with coefficients that can be computed using the aforementioned techniques and that decay at the increased rate of $\mathcal{O}\left(n^{-q-1}\right)$ for *any* fixed $q \in \mathbb{N}$. Correspondingly, the convergence rate of the truncated expansion is $\mathcal{O}\left(m^{-q-1}\right)$ away from the endpoints and $\mathcal{O}\left(m^{-q}\right)$ uniformly.

To achieve this objective, however, we first need to understand why $\mathcal{G}_1$ leads to an improvement over the standard Fourier basis.

1.2 Birkhoff expansions

Central to the understanding of $\mathcal{G}_1$ is the observation that $\cos \pi n x$ and $\sin \pi(n-\frac{1}{2})x$ are *eigenfunctions of the Laplace operator* $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ *equipped with homogeneous Neumann boundary conditions*. Supposing that u is such an eigenfunction, $-u'' = \alpha^2 u$, $u'(\pm 1) = 0$ with nonzero eigenvalue $\kappa = \alpha^2$, two integrations by parts and a substitution of the Neumann boundary conditions gives

$$\int_{-1}^{1} f(x)u(x)\mathrm{d}x = -\frac{1}{\alpha^2}\int_{-1}^{1} f(x)u''(x)\mathrm{d}x = -\frac{1}{\alpha^2}\left[f(x)u'(x)\Big|_{-1}^{1} - \int_{-1}^{1} f'(x)u'(x)\mathrm{d}x\right]$$
$$= \frac{1}{\alpha^2}\left[f'(x)u(x)\Big|_{-1}^{1} - \int_{-1}^{1} f''(x)u(x)\mathrm{d}x\right]. \tag{1.3}$$

It follows from the standard spectral theory that all eigenvalues are real, non-negative and $\alpha_n^2 = \mathcal{O}\left(n^2\right)$ for the nth eigenvalue (Pöschel & Trubowitz 1987). We deduce that $\hat{f}_n^C, \hat{f}_n^S = \mathcal{O}\left(n^{-2}\right)$, hence the aforementioned $\mathcal{O}\left(n^{-2}\right)$ decay of the nth modified Fourier coefficient. As evidenced by (1.3), Neumann boundary conditions are key to this observation: had we employed Dirichlet boundary conditions, for example, only $\mathcal{O}\left(n^{-1}\right)$ decay would occur. The interpretation of the function $\sin \pi n x$ as a Laplace–Dirichlet eigenfunction precisely explains the slow decay of the standard Fourier sine coefficient.

The expansion of a function in Laplace eigenfunctions is just one example of the much larger field of *Birkhoff expansions* (Naimark 1968). The route to extending modified Fourier expansions lies with first understanding this more general scenario. To this end, suppose that $\mathcal{L} = (-1)^q \frac{\mathrm{d}^{2q}}{\mathrm{d}x^{2q}} + \cdots$ is a self-adjoint linear differential operator of order $2q$ with smooth coefficients. (We could, in theory, drop the assumption of self-adjointness. However, since our eventual goal is practical computations, for which, for example, real eigenvalues are desirable, it makes sense to enforce this condition. Nothing is gained in terms of convergence or rate of decay of expansion coefficients by considering the non self-adjoint case.) Suppose further that $U_1(u), \ldots, U_{2q}(u)$, $u \in C^{2q-1}[-1,1]$, are $2q$ linearly independent, linear functions of the values $u(\pm 1), u'(\pm 1), \ldots, u^{(2q-1)}(\pm 1)$ giving rise to homogeneous boundary conditions $U_i(u) = 0$, $i = 1, \ldots, 2q$. Such forms can be augmented to form a dual basis $U_1, \ldots, U_{4q}$ of the $4q$-dimensional vector space

$$\left\{\left(u(-1), u'(-1), \ldots, u^{(2q-1)}(-1), u(1), u'(1), \ldots, u^{(2q-1)}(1)\right) : u \in C^{2q-1}[-1,1]\right\}$$

for which the condition

$$\int_{-1}^{1} \mathcal{L}u(x)v(x)\mathrm{d}x = \sum_{i=1}^{4q} U_i(u)U_{4q+1-i}(v) + \int_{-1}^{1} u(x)\mathcal{L}v(x)\mathrm{d}x \tag{1.4}$$

holds for all $u, v \in C^{2q}[-1,1]$.

Under mild assumptions, the spectrum of $\mathcal{L}$ equipped with boundary conditions $U_1, \ldots U_{2q}$ is countable, with real eigenvalues $0 \le \kappa_1 \le \kappa_2 \le \ldots$, and normalised eigenfunctions $u_1, u_2, \ldots$ (Naimark 1968). Hence we may expand a function $f \in \mathrm{L}_2[-1,1]$ as

$$f(x) \sim \sum_{n=1}^{\infty} \hat{f}_n u_n(x), \quad \text{where} \quad \hat{f}_n = \int_{-1}^{1} f(x)u_n(x)\mathrm{d}x.$$

Since we wish to develop practical approximation schemes based on such eigenfunctions, we select the operator $\mathcal{L}$ and corresponding boundary conditions according to the following two criteria: rapid decay of expansions coefficients and simplicity of eigenfunctions and eigenvalues. Considering the first criterion, we let u be an eigenfunction of $\mathcal{L}$ with eigenvalue $\kappa = \alpha^{2q}$. Using (1.4) and applying the boundary conditions $U_i(u) = 0$, $i = 1, \ldots, 2q$, gives

$$\begin{aligned}\int_{-1}^{1} f(x)u(x)\mathrm{d}x &= \frac{1}{\kappa}\int_{-1}^{1} f(x)\mathcal{L}u(x)\mathrm{d}x \\ &= \frac{1}{\kappa}\sum_{i=1}^{4q} U_i(u)U_{4q+1-i}(f) + \frac{1}{\kappa}\int_{-1}^{1}\mathcal{L}f(x)u(x)\mathrm{d}x \\ &= \frac{1}{\kappa}\sum_{i=2q+1}^{4q} U_i(u)U_{4q+1-i}(f) + \frac{1}{\kappa}\int_{-1}^{1}\mathcal{L}f(x)u(x)\mathrm{d}x.\end{aligned}$$

It is known that $u^{(i)}(\pm 1) = \mathcal{O}\left(\alpha^i\right)$ and that the nth value $\alpha_n = \mathcal{O}\left(n\right)$ (Naimark 1968). Hence

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

where r is the maximal order of derivative appearing in the forms $U_{2q+1}, \ldots, U_{4q}$. We now seek to minimise r over all possible boundary conditions. Since the forms $U_1, \ldots, U_{4q}$ are linearly independent, simple arguments demonstrate that $r = q - 1$ is the minimal value. In this case, the highest derivative in both U_i and U_{q+i} is of order $q + i - 1$ for $i = 1, \ldots q$ (after a possible reordering). Though numerous different boundary conditions have this property, it makes sense to choose the simplest. These are the *Neumann boundary conditions*

$$U_i(u) = u^{(q+i-1)}(-1), \quad U_{q+i}(u) = u^{(q+i-1)}(1), \quad i = 1, \ldots, q.$$

It follows that $\hat{f}_n = \mathcal{O}\left(n^{-q-1}\right)$.

Having prescribed 'optimal' boundary conditions, we now turn our attention to the operator $\mathcal{L}$. Throughout this derivation, aside from the order q and imposition of self-adjointness, $\mathcal{L}$ was arbitrary. Once again, given freedom to choose, we make the most simple choice. This leads naturally to the polyharmonic operator $(-1)^q \frac{\mathrm{d}^{2q}}{\mathrm{d}x^{2q}}$. For these reasons, the remainder of this paper is devoted to the practical construction of expansions based on polyharmonic–Neumann eigenfunctions:

$$(-1)^q u^{(2q)} = \alpha^{2q} u, \qquad u^{(i)}(\pm 1) = 0, \quad i = q, q+1, \ldots, 2q-1. \tag{1.5}$$

We remark in passing that, though considerations of simplicity naturally lead us to (1.5), there is also sound theoretical justification. As described in (Naimark 1968), both the eigenvalues and eigenfunctions of a general operator $\mathcal{L}$ are well understood in the asymptotic regime $|\alpha| \to \infty$. In fact, under some mild assumptions, both the eigenfunctions and eigenvalues of a general $2q$th order operator $\mathcal{L}$ are asymptotic to those of the polyharmonic operator with the same boundary conditions. In other words, *no advantage is gained* from expansions based on eigenfunctions of a more general operator.

Birkhoff expansions have a well developed theory. Much is known about their convergence in various norms and the asymptotic behaviour of both the eigenvalues and eigenfunctions (Benzinger 1972, Naimark 1968). However, a number of omissions exist. The apparently obvious statement that Neumann boundary conditions yield uniformly convergent expansions and the fastest possible rate of convergence seems to be lacking. Indeed, many studies consider only the worst case scenario, including, for example, the *Dirichlet boundary conditions*

$$u^{(i)}(\pm 1) = 0, \quad i = 0, \ldots, q-1, \tag{1.6}$$

which lack uniform convergence and give the slowest possible convergence rate. Moreover, as we discuss later, polyharmonic–Neumann eigenvalues, eigenfunctions and corresponding expansions exhibit asymptotic behaviour insufficiently described by such general theory.

The particular example of polyharmonic–Neumann eigenfunctions has been considered by Mark Krein (Krein 1935), who analysed their properties and proved density in the $\mathrm{L}_2[-1,1]$ norm. They have been introduced to approximation theory by Andrei Kolmogorov in his theory of n-widths (Kolmogorov 1936). Their distinguished pedigree notwithstanding, to the best of our knowledge no attempts have been made to devise practical approximation schemes based on such eigenfunctions. There are two principal reasons for this omission: namely, construction and computation of the eigenvalues and eigenfunctions, and numerical evaluation of the coefficients $\hat{f}_n$. In this paper we demonstrate how both these issues can be addressed in a systematic manner.

1.3 Plan of the paper

The key results and observations of this paper are as follows:

1. There exist countably many eigenvalues and eigenfunctions of (1.5). Aside from the q-fold zero eigenvalue, all eigenvalues are positive and simple. If we denote the nth positive eigenvalue by $\kappa_n = \alpha_n^{2q}$ and the corresponding eigenfunction by u_n, then $\mathcal{G}_q = \mathcal{H}_q \oplus \mathcal{K}_q$, where $\mathcal{H}_q = \{u_n : n \in \mathbb{N}\}$ and $\mathcal{K}_q$ is an orthogonal basis for $\mathbb{P}_{q-1}$, is orthogonal and dense in $\mathrm{L}_2[-1,1]$.

2. The basis $\mathcal{G}_q$ is dense and orthogonal in $\mathrm{H}_q[-1,1]$ with respect to the inner product

$$(f,g)_q = \int_{-1}^{1} \left[f(x)g(x) + f^{(q)}(x)g^{(q)}(x) \right] \mathrm{d}x, \qquad f,g \in \mathrm{H}_q[-1,1]. \tag{1.7}$$

3. Once a function $f \in \mathrm{H}_{q+1}[-1,1]$ is expanded in the functions u_n, the nth expansion coefficient $\hat{f}_n$ decays like $\mathcal{O}\big(n^{-q-1}\big)$ for $n \gg 1$.

4. The truncated expansion f_m of a function $f \in \mathrm{H}_q[-1,1]$ in polyharmonic–Neumann eigenfunctions converges uniformly to f. Provided $f \in \mathrm{H}_{q+2}[-1,1]$, the error $f(x) - f_m(x)$ is $\mathcal{O}\left(m^{-q-1}\right)$ in $(-1,1)$ and $\mathcal{O}\left(m^{-q}\right)$ at the endpoints.

5. For each n, the value α_n lies within an interval of exponentially small width and can be computed extremely easily using Newton–Raphson iterations. The corresponding eigenfunction u_n occurs in two cases, even and odd, and can be written as a sum of products of trigonometric and hyperbolic functions with coefficients that can be easily computed by solving an algebraic eigenproblem.

6. For large n, the functions u_n oscillate rapidly. Thus the task of computing the nth expansion coefficient $\hat{f}_n$ can be tackled by highly oscillatory quadrature formulæ. Using such techniques, any m coefficients can be computed in $\mathcal{O}\left(m\right)$ operations.

The remainder of this paper is arranged as follows. In Section 2 we introduce the fundamentals of polyharmonic–Neumann expansions. Section 3 is devoted to a close examination of the case $q = 2$. In Section 4 we extend this to general $q \geq 1$, and in Section 5 we provide analysis of convergence of such expansions. Finally, in Section 6 we address the numerical computation of the expansion coefficients.

2 Expansions in polyharmonic–Neumann eigenfunctions

Since $(-1)^q \frac{\mathrm{d}^{2q}}{\mathrm{d}x^{2q}}$ (equipped with Neumann boundary conditions) is a semipositive-definite differential operator, we deduce that its eigenvalues are non-negative. As in (1.5) we write $\kappa = \alpha^{2q}$. If $\alpha = 0$ then necessarily $u \in \mathbb{P}_{q-1}$. Hence 0 is a q-fold eigenvalue and the relevant linear subspace of eigenfunctions is spanned by the Legendre polynomials P_k, $k = 0, 1, \ldots, q-1$, an orthogonal basis of $\mathbb{P}_{q-1}$.

The remaining values α are positive. For such α and corresponding u, we have

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

Integrating by parts q times and substituting the boundary conditions yields the identity

$$\int_{-1}^{1} f(x)u(x)\mathrm{d}x = \frac{1}{\alpha^{2q}} \int_{-1}^{1} f^{(q)}(x)u^{(q)}(x)\mathrm{d}x, \quad \forall f \in \mathrm{H}_q[-1,1]. \tag{2.1}$$

Lemma 1 *The eigenfunctions of (1.5) are orthogonal and dense in* $\mathrm{L}_2[-1,1]$ *with respect to the usual Euclidean inner product.*

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 $\kappa_n = \alpha_n^{2q}$ 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

$$\alpha_n^{2q} \int_{-1}^{1} u_m(x)u_n(x)\mathrm{d}x = \int_{-1}^{1} u_m^{(q)}(x)u_n^{(q)}(x)\mathrm{d}x.$$

However, by symmetry,

$$\alpha_m^{2q} \int_{-1}^{1} u_m(x)u_n(x)\mathrm{d}x = \int_{-1}^{1} u_m^{(q)}(x)u_n^{(q)}(x)\mathrm{d}x.$$

Since $\alpha_m \neq \alpha_n$, $\alpha_m, \alpha_n > 0$, orthogonality follows immediately. □

We note in passing that it follows from this proof that

$$\int_{-1}^{1} u_m^{(q)}(x)u_n^{(q)}(x)\mathrm{d}x = 0, \qquad m \neq n.$$

Before we get carried away, however, we observe that $u_n^{(q)}$ is nothing else but the eigenfunction corresponding to the nth eigenvalue of the polyharmonic operator equipped with Dirichlet boundary conditions (1.6). (The eigenvalues are the same as in the Neumann case, except that the Dirichlet problem has no zero eigenvalues.) Therefore, orthogonality of qth derivatives is another immediate consequence of standard spectral theory. We shall return to this observation in Section 5.

Lemma 1 justifies the expansion of a function $f \in \mathrm{L}_2[-1,1]$ in the basis $\mathcal{G}_q = \mathbb{P}_{q-1} \oplus \mathcal{H}_q$. We thus let

$$\begin{aligned} \hat{f}_n^o &= \int_{-1}^{1} f(x)\mathrm{P}_n(x)\mathrm{d}x, \qquad n = 0,\ldots,q-1, \\ \hat{f}_n &= \int_{-1}^{1} f(x)u_n(x)\mathrm{d}x, \qquad n = 1,2,\ldots, \end{aligned} \tag{2.2}$$

where P_n is the nth degree Legendre polynomial. The expansion now takes the form

$$f(x) \sim \sum_{n=0}^{q-1}(n+\tfrac{1}{2})\hat{f}_n^o\mathrm{P}_n(x) + \sum_{n=1}^{\infty}\frac{\hat{f}_n}{\sigma_n}u_n(x), \tag{2.3}$$

where $\sigma_n = \int_{-1}^{1} u_n^2(x)\mathrm{d}x$ and we recall that $\int_{-1}^{1}\mathrm{P}_n^2(x)\mathrm{d}x = (n+\frac{1}{2})^{-1}$. Truncating this infinite sum after m terms leads to the approximation f_m given by

$$f_m(x) = \sum_{n=0}^{q-1}(n+\tfrac{1}{2})\hat{f}_n^o\mathrm{P}_n(x) + \sum_{n=1}^{m}\frac{\hat{f}_n}{\sigma_n}u_n(x). \tag{2.4}$$

Standard arguments establish that f_m is the best approximation to f in the $\mathrm{L}_2[-1,1]$ norm from the set $\mathcal{G}_{q,m} = \mathbb{P}_{q-1} \oplus \mathcal{H}_{q,m}$, where $\mathcal{H}_{q,m} = \{u_1,\ldots,u_m\}$. Convergence of f_m to f in this norm is thus an easy consequence of Lemma 1. A version of Parseval's lemma (Körner 1988) is also readily obtained. If $\|g\|^2 = \int_{-1}^{1} g(x)^2\mathrm{d}x$ is the standard $\mathrm{L}_2[-1,1]$ norm, then

$$\|f\|^2 = \sum_{n=0}^{q-1}(n+\tfrac{1}{2})|\hat{f}_n^o|^2 + \sum_{n=1}^{\infty}\frac{|\hat{f}_n|^2}{\sigma_n}. \tag{2.5}$$

2.1 Asymptotic expansion of the coefficients $\hat{f}_n$

The rate of decay of the coefficients $\hat{f}_n$ has important consequences for this paper: a faster rate of decay means that fewer expansion terms are required to approximate a function f to given precision. To determine this decay we first provide an asymptotic expansion of the coefficients. Such expansion is not only a useful theoretical tool, but it also forms the basis of the quadrature methods employed in Section 6 to evaluate coefficients numerically.

Our starting point is the identity (2.1). Integrating this expression by parts l times (noticing that the boundary terms do not vanish) gives

$$\hat{f}_n = \frac{1}{\alpha_n^{2q}}\sum_{k=0}^{l-1}(-1)^k f^{(q+k)}(x)u_n^{(q-1-k)}(x)\Big|_{-1}^{1} + \frac{(-1)^l}{\alpha_n^{2q}}\int_{-1}^{1} f^{(q+l)}(x)u_n^{(q-l)}(x)\mathrm{d}x \tag{2.6}$$

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

$$\begin{aligned}\hat{f}_n =& \frac{(-1)^q}{\alpha_n^{2q}} \sum_{k=q}^{2q-1} (-1)^k \left[f^{(k)}(1) u_n^{(2q-k-1)}(1) - f^{(k)}(-1) u_n^{(2q-k-1)}(-1) \right] \\ &+ \frac{(-1)^q}{\alpha_n^{2q}} \int_{-1}^{1} f^{(2q)}(x) u_n(x) \mathrm{d}x. \end{aligned} \tag{2.7}$$

The integral on the right is nothing more than the coefficient of $f^{(2q)}$ corresponding to u_n. Therefore (2.7) can be iterated,

$$\begin{aligned}\hat{f}_n =& \frac{(-1)^q}{\alpha_n^{2q}} \sum_{k=q}^{2q-1} (-1)^k [f^{(k)}(1) u_n^{(2q-k-1)}(1) - f^{(k)}(-1) u_n^{(2q-k-1)}(-1)] \\ &+ \frac{(-1)^{2q}}{\alpha_n^{4q}} \sum_{k=q}^{2q-1} (-1)^k [f^{(2q+k)}(1) u_n^{(2q-k-1)}(1) - f^{(2q+k)}(-1) u_n^{(2q-k-1)}(-1)] \\ &+ \frac{(-1)^{2q}}{\alpha_n^{4q}} \int_{-1}^{1} f^{(4q)}(x) u_n(x) \mathrm{d}x \end{aligned}$$

and so on.

Theorem 2 *Given* $f \in \mathrm{C}^\infty[-1,1]$, *it is true that*

$$\hat{f}_n \sim \sum_{r=0}^{\infty} \frac{(-1)^{(r+1)q}}{\alpha_n^{2(r+1)q}} \sum_{k=q}^{2q-1} (-1)^k [f^{(2qr+k)}(1) u_n^{(2q-k-1)}(1) - f^{(2qr+k)}(-1) u_n^{(2q-k-1)}(-1)]. \tag{2.8}$$

Proof Follows at once from (2.7) by repeated iteration. □

We emphasise that (2.8) holds only in an asymptotic sense. It certainly does not converge for fixed n. In fact, it is not even clear *a priori* that (2.8) is an asymptotic expansion in inverse powers of n. To establish this, we require the observations that $\alpha_n = \mathcal{O}(n)$ and $u_n^{(k)}(x) = \mathcal{O}\left(\alpha_n^k\right)$ for $n \gg 1$ and all $k \in \mathbb{N}$. Both results are standard (a proof in the more general setting of Birkhoff expansions is given in (Naimark 1968)). It turns out, however, that far more accurate expressions for α_n and $u_n^{(k)}(x)$ can be derived, as we discuss further in the sequel.

Returning to $\hat{f}_n$, we are now able to deduce that

$$\hat{f}_n = \mathcal{O}\left(n^{-q-1}\right), \qquad n \gg 1. \tag{2.9}$$

We mention in passing that this estimate remains valid under lower regularity assumptions. In fact, using (2.6) with $l = 1$, it follows that $\hat{f}_n$ obeys (2.9) provided $f \in \mathrm{H}_{q+1}[-1,1]$.

To connect (2.8) with the narrative of (Iserles & Nørsett 2008), we observe that for $q = 1$ we have $\alpha_n = \frac{1}{2}\pi n$,

$$u_{2n-1}(x) = \sin \pi(n - \tfrac{1}{2})x, \qquad u_{2n}(x) = \cos \pi n x$$

and

$$\hat{f}_{2n-1} \sim (-1)^{n-1} \sum_{r=0}^{\infty} \frac{(-1)^r}{[(n-\frac{1}{2})\pi]^{2r+2}} [f^{(2r+1)}(1) + f^{(2r+1)}(-1)],$$
$$\hat{f}_{2n} \sim (-1)^n \sum_{r=0}^{\infty} \frac{(-1)^r}{(n\pi)^{2r+2}} [f^{(2r+1)}(1) - f^{(2r+1)}(-1)],$$

consistently with Theorem 2.

3 The case $q = 2$

The biharmonic–Neumann eigenvalue problem warrants further attention. It presents the first setting ranging beyond the work of (Iserles & Nørsett 2008), and exhibits a number of distinct features that remain in place for general $q \geq 2$.

The general solution of $u^{(4)} = \alpha^4 u$ 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 $u''(-1) = u''(1) = 0$ results in

$$c_3 = c_1 \frac{\cos \alpha}{\cosh \alpha}, \qquad c_4 = c_2 \frac{\sin \alpha}{\sinh \alpha}.$$

We substitute these values of c_3 and c_4 into $u(x)$ and impose the remaining boundary condition, $u'''(-1) = u'''(1) = 0$. Since, after straightforward algebra,

$$\frac{1}{\alpha^3}[u'''(1) + u'''(-1)] = 2c_2 \frac{\sin \alpha \cosh \alpha - \cos \alpha \sinh \alpha}{\sinh \alpha},$$
$$\frac{1}{\alpha^3}[u'''(1) - u'''(-1)] = 2c_1 \frac{\sin \alpha \cosh \alpha + \cos \alpha \sinh \alpha}{\cosh \alpha},$$

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

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

an *even* function, where α is a positive zero of the transcendental equation

$$g_e(\alpha) = \tan \alpha + \tanh \alpha = 0. \tag{3.2}$$

Case 2 Alternatively we let, $c_1 = 0$ and normalise $c_2 = 1/(\sqrt{2} \sin \alpha)$, whence

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

an *odd* function, where α is a positive zero of

$$g_o(\alpha) = \tan \alpha - \tanh \alpha = 0. \tag{3.4}$$

As in the case $q = 1$, the eigenfunctions split into even and odd cases respectively. However, unlike Laplace–Neumann eigenvalues, their biharmonic–Neumann counterparts are not given explicitly. Rather, they are solutions of the equations (3.2) and (3.4). Despite this, such values can be computed to high accuracy with ease, as we now describe.

To locate zeros of (3.2) and (3.4), we commence with g_e and observe that

$$g_e'(\alpha) = 2 + \tan^2\alpha - \tanh^2\alpha > 0, \qquad \alpha > 0,$$

since $|\tanh\alpha| < 1$. Therefore g_e increases monotonically. Moreover, for every $n = 1, 2, \ldots$

$$g_e((n - \tfrac{1}{4})\pi) = -1 + \tanh(n - \tfrac{1}{4})\pi < 0, \qquad g_e(n\pi) = \tanh n\pi > 0$$

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

$$\begin{aligned} g_e((n - \tfrac{1}{4})\pi + \varepsilon) &= \frac{\sin\varepsilon - \cos\varepsilon}{\sin\varepsilon + \cos\varepsilon} + \tanh((n - \tfrac{1}{4})\pi + \varepsilon) \\ &> \frac{\sin\varepsilon - \cos\varepsilon}{\sin\varepsilon + \cos\varepsilon} + \tanh((n - \tfrac{1}{4})\pi). \end{aligned}$$

The function $h(x) = \frac{\sin x - \cos x}{\sin x + \cos x}$ satisfies

$$h(x) \geq h(0) + (h(1) - h(0))\, x = -1 + 2\frac{\sin 1}{\sin 1 + \cos 1} x, \qquad 0 \leq x \leq 1.$$

Since $\tanh x \geq 1 - 2\mathrm{e}^{-2x}$ for all $x \geq 0$, we obtain

$$g_e((n - \tfrac{1}{4})\pi + \varepsilon) > 2\frac{\sin 1}{\sin 1 + \cos 1}\varepsilon - 2\mathrm{e}^{-2(n - \frac{1}{4})\pi}.$$

Therefore, letting $\epsilon = ce^{-2(n - \frac{1}{4})\pi}$, where $c = \frac{\cos 1 + \sin 1}{\sin 1}$, we deduce that, for all n, the unique zero of (3.2) in I_{2n-1} can be confined to

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

an interval of exponentially small width. Similarly, it is easy to verify that g_o is strictly monotonically increasing, with a simple pole at $(n - \frac{1}{2})\pi$ and that

$$g_o(n\pi) < 0 < g_o((n + \tfrac{1}{4})\pi)$$

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

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

with c as defined above.

To sum up, all parameters α 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

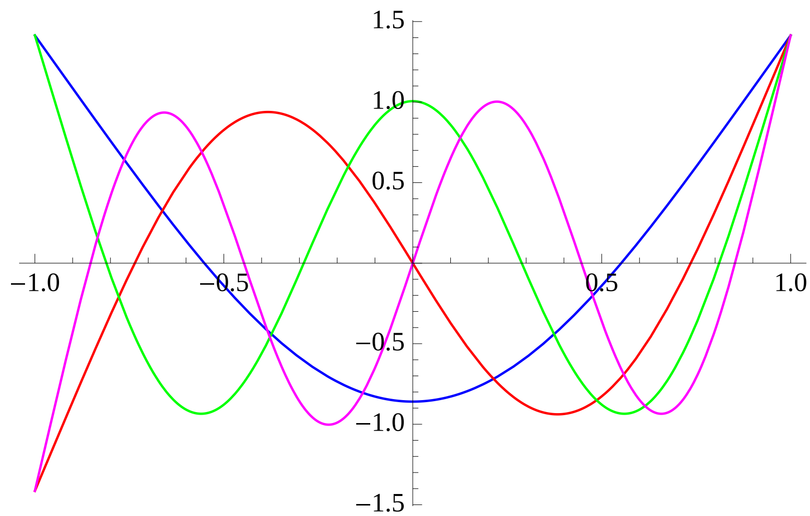

Figure 3.1: The orthogonal functions u_n, $n = 1, 2, 3, 4$, for $q = 2$.

u_n. Note that solutions of (3.2) and (3.4) alternate and that, consistently with general theory, $\alpha_n = \mathcal{O}(n)$.

Numerical computation of the values $\alpha_n \in \tilde{I}_n$ is extremely easy. The exponential tendency to the limiting values $(n \pm \frac{1}{4})\pi$ means that the Newton–Raphson algorithm converges exceedingly quickly in IEEE arithmetic even for small values of n: just a single iteration produces an error of 1.49×10^{-20} already for $n = 4$ ($n = 3$ misses the IEEE machine epsilon by a whisker, giving an error of 7.95×10^{-16}).

We now turn our attention to the corresponding eigenfunctions u_n. Straightforward, but lengthy, algebra verifies that the functions u_n, as given by (3.1) and (3.3), are already normalised. Therefore, we may let $\sigma_n = 1$ in (2.3). Moreover,

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

In Figure 3.1 we display the first four functions u_n. In conformity with our former observations, note that u_{2n-1}s are even, while u_{2n}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. (In fact, each u_n appears to have $n + 1$ zeros. Recall, however, that the functions u_n need to be complemented by 1 and x, the first two Legendre polynomials, with no zeros and a single zero, respectively.) Simple arguments, along similar lines to those already given, demonstrate that these observations are valid for all n when $q = 2$. Such behaviour is characteristic of Sturm–Liouville eigenfunctions (Levitan & Sargsjan 1975). Moreover, it is known to hold also for eigenfunctions corresponding to a wide variety of higher order differential operators, including the polyharmonic operator under current consideration. This result is a by-product of the theory of n-widths (Pinkus 1968, chpt. 3).

Several other features of polyharmonic eigenfunctions are highlighted by the case $q = 2$. First, much like a classical plane wave, the zeros of the nth eigenfunction converge to a

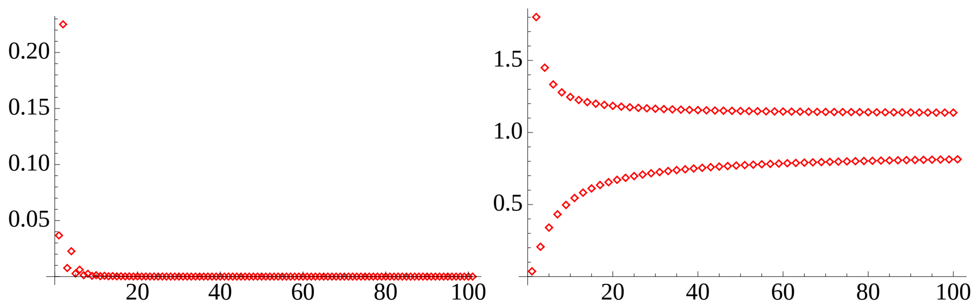

Figure 3.2: The magnitude of the coefficients $\hat{f}_n$ for $q = 2$ and $f(x) = \mathrm{e}^x$. On the left we display $|\hat{f}_n|$ and on the right scaled values $n^3|\hat{f}_n|$.

uniform distribution as $n \to \infty$. Second, away from the endpoints $x = \pm 1$, the eigenfunction u_n behaves like a regular oscillator. In fact,

$$\begin{aligned} u_{2n-1}(x) &= (-1)^n \cos(n - \tfrac{1}{4})\pi x + \mathcal{O}\left(\mathrm{e}^{(1-|x|)(n-\frac{1}{4})\pi}\right) \\ u_{2n}(x) &= (-1)^n \sin(n + \tfrac{1}{4})\pi x + \mathcal{O}\left(\mathrm{e}^{(1-|x|)(n+\frac{1}{4})\pi}\right). \end{aligned}$$

We return to this observation in Section 5.

Having described the biharmonic–Neumann eigenvalues and eigenfunctions, we now scrutinize the approximation of a smooth function f by the truncated expansion f_m, as given by (2.4). In Figure 3.2 we display the absolute values of the first hundred coefficients $\hat{f}_n$. It follows from Section 2.1 that $\hat{f}_n = \mathcal{O}\left(n^{-3}\right)$, and this is confirmed by the figure on the right, which depicts $n^3|\hat{f}_n|$. Note the very rapid onset of asymptotic behaviour.

Figure 3.3 depicts the pointwise error committed by the approximation f_m to the function $f(x) = \mathrm{e}^x$ in the interval $(-\frac{9}{10}, \frac{9}{10})$ for $m = 10, 20, 40, 80$. 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. This is verified in Figure 3.4, which plots the scaled error $m^3|f(x_0) - f_m(x_0)|$ for $x_0 = \frac{1}{8}, \frac{1}{4}$.

It is instructive to compare this to known results. Classical Fourier expansions exhibit $\mathcal{O}\left(m^{-1}\right)$ pointwise error, and, as proved in (Olver 2009), this figure is $\mathcal{O}\left(m^{-2}\right)$ in the $q = 1$ case. As we consider further in Section 5, approximation by polyharmonic eigenfunctions increases this value to $\mathcal{O}\left(m^{-q-1}\right)$.

An important distinction between classical and modified Fourier expansions is that, for $f \in \mathrm{H}_1[-1, 1]$, the latter converge pointwise in *all* of $[-1, 1]$, inclusive of the endpoints (Adcock 2009). However, the convergence at ± 1 is just $\mathcal{O}\big(m^{-1}\big)$, one power of m slower than at interior points. Figure 3.4 demonstrates that polyharmonic expansions exhibit similar behaviour. Uniform convergence occurs, but at a rate of $\mathcal{O}\left(m^{-q}\right)$ as opposed to $\mathcal{O}\left(m^{-q-1}\right)$. This conjecture is proved in Section 5.

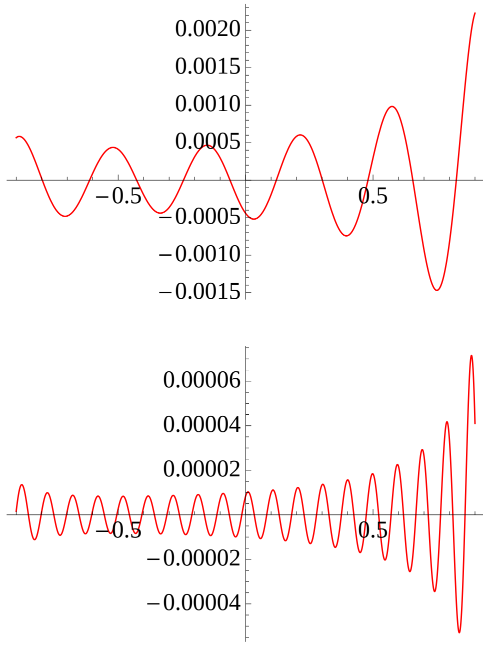

Figure 3.3: The pointwise error in approximating $f(x) = \mathrm{e}^x$ by f_m for $m = 10, 20, 40$ and 80, respectively.

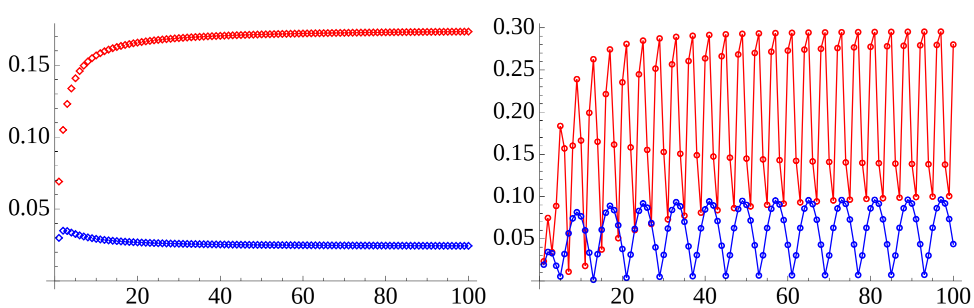

Figure 3.4: Scaled pointwise error in approximating $f(x) = \mathrm{e}^x$ by f_m for $m = 1, 2, \ldots, 100$. Left: $m^2|f(x_0) - f_m(x_0)|$ for $x_0 = +1$ (top) and $x_0 = -1$ (bottom). Right: $m^3|f(x_0) - f_m(x_0)|$ for $x_0 = \frac{1}{4}$ and $x_0 = \frac{1}{8}$.

4 Eigenfunction bases for general $q \geq 1$

Though the spectral properties of linear differential operators in the unit interval have been extensively studied, few attempts have been made to perform practical computations. Vital to such endeavour is a systematic approach for the construction and evaluation of eigenfunctions and eigenvalues. In this section we address this issue in the polyharmonic–Neumann setting.

The case $q = 1$ has been considered in (Iserles & Nørsett 2008) 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

$$(-1)^q u^{(2q)} = \alpha^{2q} u, \quad -1 \leq x \leq 1, \quad u^{(i)}(\pm 1) = 0, \qquad i = q, q+1, \ldots, 2q-1. \tag{4.1}$$

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

We commence by noting that the general solution of $(-1)^q u^{(2q)} = \alpha^{2q} u$ is

$$u(x) = \sum_{k=0}^{2q-1} c_k \mathrm{e}^{\alpha \lambda_k x}, \tag{4.2}$$

where $\lambda_0, \ldots, \lambda_{2q-1} \in \mathbb{C}$ are the solutions of $\lambda^{2q} = (-1)^q$, while $c_0, \ldots, c_{2q-1} \in \mathbb{C}$ are arbitrary constants. The boundary conditions $u^{(q+i)}(\pm 1) = 0$, $i = 0, \ldots, q-1$, will be incorporated once we have brought (4.2) into a more convenient form. To do so, we consider two cases: even $q \geq 2$ and odd $q \geq 1$.

4.1 Even $q \geq 2$

For even q the values λ_k are roots of unity, $\lambda_k = \exp\left(\frac{\pi \mathrm{i} k}{q}\right)$, $k = 0, 1, \ldots, 2q-1$, and we note that $\lambda_{q+k} = -\lambda_k$. Our goal is to write u in terms of real parameters. To do so, we first observe that

$$\begin{aligned}\frac{1}{2}\left(\mathrm{e}^{\alpha\lambda_k x} + \mathrm{e}^{-\alpha\lambda_k x}\right) &= \cos\left(\alpha x \sin\frac{\pi k}{q}\right)\cosh\left(\alpha x \cos\frac{\pi k}{q}\right) \\ &\quad + \mathrm{i}\sin\left(\alpha x \sin\frac{\pi k}{q}\right)\sinh\left(\alpha x \cos\frac{\pi k}{q}\right) \\ &= \phi_k^e(x) + \mathrm{i}\psi_k^e(x),\end{aligned}$$

for $k = 0, \ldots, q-1$ and that

$$\begin{aligned}\frac{1}{2}\left(\mathrm{e}^{\alpha\lambda_k x} - \mathrm{e}^{-\alpha\lambda_k x}\right) &= \cos\left(\alpha x \sin\frac{\pi k}{q}\right)\sinh\left(\alpha x \cos\frac{\pi k}{q}\right) \\ &\quad + \mathrm{i}\sin\left(\alpha x \sin\frac{\pi k}{q}\right)\cosh\left(\alpha x \cos\frac{\pi k}{q}\right) \\ &= \phi_k^o(x) + \mathrm{i}\psi_k^o(x).\end{aligned}$$

Note that $\phi_{q-k}^e = \phi_k^e$ and $\psi_{q-k}^e = -\psi_k^e$ for $k = 1, 2, \ldots, \frac{q}{2}-1$ and that $\psi_0^e = \psi_{\frac{q}{2}}^e = 0$. Similar relations hold for ϕ_k^o and ψ_k^o, so we deduce that u can be written as $u(x) = u_e(x) + u_o(x)$ where

$$\begin{aligned}u_e(x) = &\sum_{k=0}^{\frac{q}{2}} \beta_k^e \cos\left(\alpha x \sin\frac{\pi k}{q}\right)\cosh\left(\alpha x \cos\frac{\pi k}{q}\right) \\ &+ \sum_{k=1}^{\frac{q}{2}-1} \gamma_k^e \sin\left(\alpha x \sin\frac{\pi k}{q}\right)\sinh\left(\alpha x \cos\frac{\pi k}{q}\right),\end{aligned} \tag{4.3}$$

and

$$
\begin{aligned}
u_o(x) = &\sum_{k=0}^{\frac{q}{2}-1} \beta_k^o \cos\left(\alpha x \sin\frac{\pi k}{q}\right) \sinh\left(\alpha x \cos\frac{\pi k}{q}\right) \\
&+ \sum_{k=1}^{\frac{q}{2}} \gamma_k^o \sin\left(\alpha x \sin\frac{\pi k}{q}\right) \cosh\left(\alpha x \cos\frac{\pi k}{q}\right),
\end{aligned}
\tag{4.4}
$$

and $\beta_k^e, \gamma_k^e, \beta_k^o, \gamma_k^o \in \mathbb{R}$ are arbitrary constants. Note that we have exactly $2q$ coefficients, matching the number of boundary conditions.

We observe that u_e is an even function, whilst u_o is odd. Note that the boundary conditions $u^{(q+i)}(\pm 1) = 0$, $i = 0, \ldots, q-1$, can be rewritten as

$$
u^{(q+i)}(1)+(-1)^{q+i}u^{(q+i)}(-1) = u^{(q+i)}(1)+(-1)^{q+i+1}u^{(q+i)}(-1) = 0, \quad i = 0, \ldots, q-1,
$$

with the former being automatically satisfied by an odd function and the latter satisfied by an even function. Therefore, polyharmonic–Neumann eigenfunctions are necessarily even or odd functions given by (4.3) or (4.4) respectively, and we may consider each case separately.

Even u: In this case u is of the form (4.3) with coefficients β_k, γ_k (dropping the e sub- and superscripts). It is easy to confirm by induction that the derivatives of (4.3) have the explicit form

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

Letting $x = 1$ for the ith derivative, $i = q, q+1, \ldots, 2q-1$, and equating to zero yields the identity

$$
\Phi_q \begin{bmatrix} \boldsymbol{\beta} \\ \boldsymbol{\gamma} \end{bmatrix} = \mathbf{0}, \qquad \text{where} \qquad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{\frac{q}{2}} \end{bmatrix}, \ \boldsymbol{\gamma} = \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_{\frac{q}{2}-1} \end{bmatrix},
$$

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

$$
\det \Phi_q = 0 \tag{4.5}
$$

for the coefficient α, whence $\begin{bmatrix} \boldsymbol{\beta} \\ \boldsymbol{\gamma} \end{bmatrix}$ is the eigenvector corresponding to the zero eigenvalue of Φ_q. The first two cases are $q = 2$, resulting in

$$\Phi_2 = \begin{bmatrix} \cosh\alpha & -\cos\alpha \\ \sinh\alpha & \sin\alpha \end{bmatrix} \qquad \Rightarrow \qquad \sin\alpha\cosh\alpha + \cos\alpha\sinh\alpha = 0$$

(the latter is identical to (3.2)) and $q = 4$, where

$$\Phi_4 = \begin{bmatrix} \cosh\alpha & -\cos\frac{\alpha}{\sqrt{2}}\cosh\frac{\alpha}{\sqrt{2}} & \cos\alpha & \sin\frac{\alpha}{\sqrt{2}}\sinh\frac{\alpha}{\sqrt{2}} \\ \sinh\alpha & -\frac{\sqrt{2}}{2}\left(\cos\frac{\alpha}{\sqrt{2}}\sinh\frac{\alpha}{\sqrt{2}} - \sin\frac{\alpha}{\sqrt{2}}\cosh\frac{\alpha}{\sqrt{2}}\right) & -\sin\alpha & -\left(\frac{\sqrt{2}}{2}\cos\frac{\alpha}{\sqrt{2}}\sinh\frac{\alpha}{\sqrt{2}} + \sin\frac{\alpha}{\sqrt{2}}\cosh\frac{\alpha}{\sqrt{2}}\right) \\ \cosh\alpha & \sin\frac{\alpha}{\sqrt{2}}\sinh\frac{\alpha}{\sqrt{2}} & -\cos\alpha & -\cos\frac{\alpha}{\sqrt{2}}\cosh\frac{\alpha}{\sqrt{2}} \\ \sinh\alpha & \frac{\sqrt{2}}{2}\left(\cos\frac{\alpha}{\sqrt{2}}\sinh\frac{\alpha}{\sqrt{2}} + \sin\frac{\alpha}{\sqrt{2}}\cosh\frac{\alpha}{\sqrt{2}}\right) & \sin\alpha & \frac{\sqrt{2}}{2}\left(\sin\frac{\alpha}{\sqrt{2}}\cosh\frac{\alpha}{\sqrt{2}} - \cos\frac{\alpha}{\sqrt{2}}\sinh\frac{\alpha}{\sqrt{2}}\right) \end{bmatrix}$$

which yields the equation

$$\begin{aligned} &\sinh\alpha[\sin\alpha(\cosh\sqrt{2}\alpha + \cos\sqrt{2}\alpha) + \tfrac{\sqrt{2}}{2}\cos\alpha(\sinh\sqrt{2}\alpha - \sin\sqrt{2}\alpha)] \\ &- \cosh\alpha[\cos\alpha(\cosh\sqrt{2}\alpha - \cos\sqrt{2}\alpha) + \tfrac{\sqrt{2}}{2}\sin\alpha(\sinh\sqrt{2}\alpha - \sin\sqrt{2}\alpha)] = 0. \end{aligned}$$

Odd u: The function u, given by (4.4), has derivatives satisfying

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

Imposing the boundary conditions leads to

$$\Psi_q \begin{bmatrix} \boldsymbol{\beta} \\ \boldsymbol{\gamma} \end{bmatrix} = \mathbf{0}, \qquad \text{where} \qquad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_{q/2-1} \end{bmatrix}, \ \boldsymbol{\gamma} = \begin{bmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_{q/2} \end{bmatrix},$$

and hence to the transcendental equation

$$\det \Psi_q = 0. \tag{4.6}$$

In particular,

$$\begin{aligned} \det\Psi_2 &= \cosh\alpha\sin\alpha - \sinh\alpha\cos\alpha, \\ \det\Psi_4 &= \sinh\alpha[\sin\alpha(\cos\sqrt{2}\alpha + \cosh\sqrt{2}\alpha) - \tfrac{\sqrt{2}}{2}\cos\alpha(\sin\sqrt{2}\alpha + \sinh\sqrt{2}\alpha)] \\ &\quad - \cosh\alpha[\cos\alpha(\cos\sqrt{2}\alpha - \cosh\sqrt{2}\alpha) + \tfrac{\sqrt{2}}{2}\sin\alpha(\sin\sqrt{2}\alpha + \sinh\sqrt{2}\alpha)]. \end{aligned}$$

Note that $\det \Psi_2 = 0$ is identical to (3.4).

4.2 Odd $q \geq 1$

The treatment of an odd q is identical. We express u in terms of real coefficients β_k and γ_k, whereby there are two cases, even and odd functions:

$$\begin{aligned} u(x) = & \sum_{k=0}^{\frac{q-1}{2}} \beta_k \cos\left(\alpha x \sin \frac{\pi(k+\frac{1}{2})}{q}\right) \cosh\left(\alpha x \cos \frac{\pi(k+\frac{1}{2})}{q}\right) \\ & + \sum_{k=0}^{\frac{q-3}{2}} \gamma_k \sin\left(\alpha x \sin \frac{\pi(k+\frac{1}{2})}{q}\right) \sinh\left(\alpha x \cos \frac{\pi(k+\frac{1}{2})}{q}\right), \end{aligned}$$

and

$$\begin{aligned} u(x) = & \sum_{k=0}^{\frac{q-3}{2}} \beta_k \cos\left(\alpha x \sin \frac{\pi(k+\frac{1}{2})}{q}\right) \sinh\left(\alpha x \cos \frac{\pi(k+\frac{1}{2})}{q}\right) \\ & + \sum_{k=0}^{\frac{q-1}{2}} \gamma_k \sin\left(\alpha x \sin \frac{\pi(k+\frac{1}{2})}{q}\right) \cosh\left(\alpha x \cos \frac{\pi(k+\frac{1}{2})}{q}\right), \end{aligned}$$

respectively. Proceeding as before, we form derivatives and impose Neumann boundary conditions. In each case this results in a transcendental equation, setting a determinant of a matrix to zero, whereby the coefficients $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ are components of the eigenvector of the matrix in question corresponding to a zero eigenvalue.

For $q = 1$ we obtain $\det \Phi_1 = \Phi_1 = -\sin\alpha$ and $\det \Psi_1 = \Psi_1 = \cos\alpha$: no surprise here. For $q = 3$ we have

$$\Phi_3 = \begin{bmatrix} -\sin\frac{\alpha}{2}\cosh\frac{\sqrt{3}\alpha}{2} & \sin\alpha & \cos\frac{\alpha}{2}\sinh\frac{\sqrt{3}\alpha}{2} \\ -\frac{1}{2}\cos\frac{\alpha}{2}\cosh\frac{\sqrt{3}\alpha}{2} - \frac{\sqrt{3}}{2}\sin\frac{\alpha}{2}\sinh\frac{\sqrt{3}\alpha}{2} & \cos\alpha & \frac{\sqrt{3}}{2}\cos\frac{\alpha}{2}\cosh\frac{\sqrt{3}\alpha}{2} - \frac{1}{2}\sin\frac{\alpha}{2}\sinh\frac{\sqrt{3}\alpha}{2} \\ -\frac{\sqrt{3}}{2}\cos\frac{\alpha}{2}\sinh\frac{\sqrt{3}\alpha}{2} - \frac{1}{2}\sin\frac{\alpha}{2}\cosh\frac{\sqrt{3}\alpha}{2} & -\sin\alpha & \frac{1}{2}\cos\frac{\alpha}{2}\sinh\frac{\sqrt{3}\alpha}{2} - \frac{\sqrt{3}}{2}\sin\frac{\alpha}{2}\cosh\frac{\sqrt{3}\alpha}{2} \end{bmatrix}$$

$$\det \Phi_3 = \frac{\sqrt{3}}{4}(\cos\alpha\cosh\sqrt{3}\alpha - 2 + \cos^2\alpha),$$

and

$$\Psi_3 = \begin{bmatrix} -\sin\frac{\alpha}{2}\sinh\frac{\sqrt{3}\alpha}{2} & \cos\frac{\alpha}{2}\cosh\frac{\sqrt{3}\alpha}{2} & -\cos\alpha \\ -\frac{1}{2}\cos\frac{\alpha}{2}\sinh\frac{\sqrt{3}\alpha}{2} - \frac{\sqrt{3}}{2}\sin\frac{\alpha}{2}\cosh\frac{\sqrt{3}\alpha}{2} & \frac{\sqrt{3}}{2}\cos\frac{\alpha}{2}\sinh\frac{\sqrt{3}\alpha}{2} - \frac{1}{2}\sin\frac{\alpha}{2}\cosh\frac{\sqrt{3}\alpha}{2} & \sin\alpha \\ -\frac{\sqrt{3}}{2}\cos\frac{\alpha}{2}\cosh\frac{\sqrt{3}\alpha}{2} - \frac{1}{2}\sin\frac{\alpha}{2}\sinh\frac{\sqrt{3}\alpha}{2} & \frac{1}{2}\cos\frac{\alpha}{2}\cosh\frac{\sqrt{3}\alpha}{2} - \frac{\sqrt{3}}{2}\sin\frac{\alpha}{2}\sinh\frac{\sqrt{3}\alpha}{2} & \cos\alpha \end{bmatrix},$$

$$\det \Psi_3 = -\frac{\sqrt{3}}{4}\sin\alpha(\cosh\sqrt{3}\alpha - \cos\alpha).$$

Note that $\cosh\sqrt{3}\alpha > \cos\alpha$ for $\alpha > 0$. Therefore, the values α corresponding to odd eigenfunctions satisfy the trivial equation $\sin\alpha = 0$.

4.3 Construction of polyharmonic–Neumann eigenfunctions

In this section, we have proffered a systematic approach for constructing polyharmonic eigenfunctions as linear combinations of products of trigonometric and hyperbolic functions. The functions depend on a parameter α, which is a solution of a transcendental equation. Once α 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. We remark in passing that the estimate $u^{(i)}(x) = \mathcal{O}\left(\alpha^i\right)$ is a direct consequence of this analysis, a result justifying the statement of Section 2 that $\hat{f}_n = \mathcal{O}\left(n^{-q-1}\right)$.

All that remains is to scrutinise the roots of the transcendental equations (4.5) and (4.6) and their computation. The asymptotic nature of these roots is well-known. A classical theory, valid for a large class of linear differential operators and boundary conditions, gives

$$\alpha_n = \frac{1}{4}(2n + q - 1)\pi + \mathcal{O}\left(n^{-1}\right), \qquad n \gg 1 \tag{4.7}$$

(Naimark 1968). However, there is compelling evidence from the cases $q = 1, 2$ that this remainder term is *exponentially small* for polyharmonic–Neumann eigenvalues. In other words, that

$$\alpha_n = \frac{1}{4}(2n + q - 1)\pi + \mathcal{O}\left(\mathrm{e}^{-c_q n}\right), \qquad n \gg 1, \tag{4.8}$$

for some constant c_q independent of n—a greatly improved estimate. To the best of our knowledge (4.8) does not currently exist in literature. The overbearing reason for this appears to be that such an estimate is not valid under even minor perturbations of the operator or boundary conditions. As far as we can ascertain, only a polyharmonic operator with particularly simple boundary conditions exhibits (4.8). We shall present a proof of this conjecture in a future paper. We mention in passing that (4.8) is not just of interest in and of itself. As we discuss briefly in Section 5, it is key to establishing accurate estimates for the error committed by truncated polyharmonic–Neumann expansions.

Aside from theoretical significance, this exponentially small remainder term means that computation of the values α_n can be carried out with extreme ease using Newton–Raphson iterations. Furthermore, for even moderate n we may use the approximation $\alpha_n \approx \frac{1}{4}(2n + q - 1)\pi$ instead. This fact was observed for $q = 2$ in Section 3 and is presently demonstrated in Table 1 for $q = 4$. In both cases, no more than 4 Newton–Raphson iterations are required to calculate α_n to machine epsilon, and for $n \geq 20$ the approximation $\frac{1}{4}(2n + q - 1)\pi$ suffices.

To connect this discussion to the narrative of Section 1.2, we remark that by choosing both the most simple operator and boundary conditions, we have greatly aided the task of computing the values α_n. If we were to choose an operator and boundary conditions for which only (4.7) holds, then computation would be less simple.

Two further remarks regarding practical issues are worthy of mention. First, as q increases, so does the computational cost of constructing and evaluating the eigenfunctions u_n. Moreover, it becomes extremely cumbersome to derive analytic expressions for the coefficients β_k, γ_k of such eigenfunctions. For $q = 4$ we resorted to a symbolic algebra package for this task. Second, since the eigenfunctions involve increasing numbers of hyperbolic functions for large q, there is increasing susceptibility to round-off error in calculations. As a result, it appears inadvisable to use values of q much beyond $q = 4$. However, as we discuss in Section 7, the true impact of the aforementioned issues is a topic for future investigation.

n	1	2	3	4	5	10	15	20	25	30
e_n	2.35	4.63	4.42	5.44	6.97	11.6	16.8	21.5	26.5	31.4
a_n	4	3	3	2	2	1	1	0	0	0

Table 1: Numerical computation of the values α_n for $q = 4$. The values $e_n = -\log_{10}\left(|\alpha_n - \frac{1}{4}(2n+q-1)\pi|/\alpha_n\right)$ measure the number of significant digits and a_n is the number of Newton–Raphson iterations required to obtain machine epsilon.

5 Convergence of polyharmonic–Neumann expansions

Suppose that f_m, as given by (2.4), is the truncated expansion of a function $f \in \mathrm{L}_2[-1,1]$ in polyharmonic–Neumann eigenfunctions. In this section we address the convergence and rate of convergence of f_m to f.

We recall that convergence in the $\mathrm{L}_2[-1,1]$ norm is guaranteed by standard spectral theory (see Lemma 1). The first result of this section is that much stronger convergence is also automatically guaranteed. To establish this, we require the following lemma:

Lemma 3 *The bilinear form (1.7) is an inner product on* $\mathrm{H}_q[-1,1]$ *with associated norm* $\|f\|_q = \sqrt{(f,f)_q}$ *equivalent to the standard norm on* $\mathrm{H}_q[-1,1]$.

Proof This result follows immediately from the additive inequality

$$\|f^{(i)}\| \leq c\left(\|f\| + \|f^{(q)}\|\right) \qquad i = 0,\ldots,q,$$

which holds for all $f \in \mathrm{H}_q[-1,1]$ with constant $c > 0$ independent of f (Adams 1975). □

Theorem 4 *The set of polyharmonic–Neumann eigenfunctions is orthogonal and dense in* $\mathrm{H}_q[-1,1]$ *with respect to the inner product* $(\cdot,\cdot)_q$. *In particular, for* $f \in \mathrm{H}_q[-1,1]$, $f_m \to f$ *in the* $\mathrm{H}_q[-1,1]$ *norm.*

Proof As noted in Section 2, the function $u_n^{(q)}$ is nothing more than the nth polyharmonic–Dirichlet eigenfunction. Orthogonality now follows immediately. To demonstrate density it suffices to show that $f_m^{(q)} \to f^{(q)}$ in the $\mathrm{L}_2[-1,1]$ norm. Assuming that u_n is normalised, let $u_n^{(q)} = c_n v_n$ where $\|v_n\| = 1$. We first show that $c_n^2 = \alpha_n^{2q}$. Indeed, using (2.1), we have

$$\alpha_n^{2q} = \alpha_n^{2q}\int_{-1}^{1} u_n(x)u_n(x)\mathrm{d}x = \int_{-1}^{1} u_n^{(q)}(x)u_n^{(q)}(x)\mathrm{d}x = c_n^2\int_{-1}^{1} v_n^2(x)\mathrm{d}x = c_n^2.$$

Now suppose that $f \in \mathrm{H}_q[-1,1]$. Applying (2.1) to $\hat{f}_n$ gives

$$\hat{f}_n = \frac{1}{\alpha_n^{2q}}\int_{-1}^{1} f^{(q)}(x)u_n^{(q)}(x)\mathrm{d}x = \frac{c_n}{\alpha_n^{2q}}\int_{-1}^{1} f^{(q)}(x)v_n^{(q)}(x)\mathrm{d}x.$$

Combining this with the previous result, we obtain

$$f_m^{(q)}(x) = \sum_{n=1}^{m} \hat{f}_n u_n^{(q)}(x) = \sum_{n=1}^{m}\left[\int_{-1}^{1} f^{(q)}(x)v_n(x)\mathrm{d}x\right] v_n(x).$$

In other words, the function $f_m^{(q)}$ is precisely the mth truncated expansion of $f^{(q)} \in \mathrm{L}_2[-1,1]$ in polyharmonic–Dirichlet eigenfunctions. As in Lemma 1, the result now follows immediately from standard spectral theory. $\square$

We mention in passing that the following version of Parseval's lemma for $\|\cdot\|_q$ is a straightforward consequence of this result:

$$\|f\|_q^2 = \sum_{n=0}^{q-1} (n+\tfrac{1}{2})|\hat{f}_n^o|^2 + \sum_{n=1}^{\infty} (1+\alpha_n^{2q}) \frac{|\hat{f}_n|^2}{\sigma_n}, \quad \forall f \in \mathrm{H}_q[-1,1]. \tag{5.1}$$

Another immediate outcome of Theorem 4 is uniform convergence of the expansion f_m and its first $q-1$ derivatives:

Corollary 1 *Suppose that $f \in \mathrm{H}_q[-1,1]$. Then $f_m \to f$ uniformly in $[-1,1]$. Moreover $f_m^{(i)} \to f^{(i)}$ uniformly for $i = 0, \ldots, q-1$.*

Proof In view of the continuous imbedding $\mathrm{H}_q[-1,1] \hookrightarrow \mathrm{C}_{q-1}[-1,1]$, we have $f - f_m \in C_{q-1}[-1,1]$. Furthermore, there is a constant c independent of f and m such that $\|f^{(i)} - f_m^{(i)}\|_\infty \le c\|f - f_m\|_q$, $i = 0, \ldots, q-1$. The result now follows from Theorem 4. $\square$

Standard means of establishing convergence of Birkhoff expansions involve writing the expansion as the convolution of the function f and a meromorphic kernel (Naimark 1968). Similar ideas were pursued for the case $q = 1$ in (Iserles & Nørsett 2008). The (arguably simpler) technique presented above was used in (Adcock 2010*b*) for $q = 1$.

With convergence in hand, we now turn our attention to the rate of convergence:

Corollary 2 *Suppose that $f \in \mathrm{H}_{q+1}[-1,1]$. Then $f(x) - f_m(x) = \mathcal{O}(m^{-q})$ uniformly in $x \in [-1,1]$. Moreover $f^{(i)}(x) - f_m^{(i)}(x) = \mathcal{O}\left(m^{i-q}\right)$ for $i = 0, \ldots, q-1$.*

Proof For such a function, applications of (2.6) with $l = 1$ and the estimates $\alpha_n = \mathcal{O}(n)$, $\|u_n^{(i)}\|_\infty = \mathcal{O}\left(\alpha_n^i\right)$ yield the bound

$$|\hat{f}_n| \le c n^{-q-1} \|f\|_{q+1}. \tag{5.2}$$

Since uniform convergence is guaranteed by Corollary 1, we may write

$$\left| f^{(i)}(x) - f_m^{(i)}(x) \right| \le \sum_{n>m} |\hat{f}_m| \|u_n^{(i)}\|_\infty \le c\|f\|_{q+1} \sum_{n>m} n^{i-q-1} \le c\|f\|_{q+1} m^{i-q},$$

as required. $\square$

As mentioned in previous sections, the pointwise convergence rate away from the endpoints $x = \pm 1$ is one power of m faster. A full proof of this result is beyond the scope of this paper. The proof is contingent on the three following observations. First, the values α_n satisfy the asymptotic estimate (4.8). Second, the eigenfunctions u_n, appropriately normalised, are described by

$$u_n(x) = \cos\left[\tfrac{1}{4}(2n+q-1)\pi x + \tfrac{1}{2}(n+q-1)\pi\right] + \mathcal{O}\left(\mathrm{e}^{-c_q(1-|x|)n}\right), \tag{5.3}$$

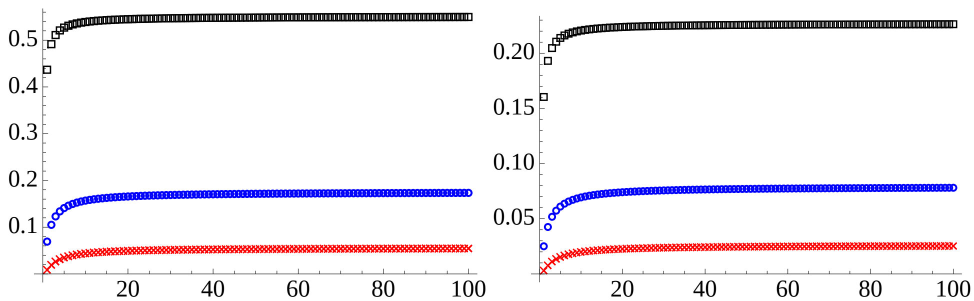

Figure 5.1: Error in approximating $f(x) = \mathrm{e}^x$ by $f_m(x)$ for $q = 1$ (squares), $q = 2$ (circles) and $q = 3$ (crosses). Left: scaled error $m^q \|f - f_m\|_\infty$ for $m = 1, 2, \ldots, 100$. Right: scaled error $m^{q+\frac{1}{2}} \|f - f_m\|$.

and, finally, $u_n(1) = c'_q(-1)^n + \mathcal{O}\left(\mathrm{e}^{-c_q n}\right)$ for constants c_q, c'_q independent of n. With these observations to hand, the result is established along the same lines as the proof given in (Olver 2009) for $q = 1$. Not only can the estimate $f(x) - f_m(x) = \mathcal{O}\left(m^{-q-1}\right)$ be demonstrated, but a full asymptotic expansion of the error at any point $x \in (-1, 1)$ can also be derived. A future paper will give proofs of these conjectures and establish such estimates. Note that (5.3) indicates that polyharmonic eigenfunctions are well approximated by trigonometric functions inside the domain. This is a particular example of a general phenomenon for Birkhoff expansions known as *equiconvergence* (Minkin 1999). As with the values α_n, however, (5.3) improves upon known results.

Estimates for the rate of convergence in various other norms can also be provided:

Lemma 5 *Suppose that $f \in \mathrm{H}_{q+1}[-1, 1]$. Then, for $i = 0, \ldots, q$, $\|f - f_m\|_i = \mathcal{O}(m^{i-q-\frac{1}{2}})$, where $\|\cdot\|_i$ is the standard $\mathrm{H}_i[-1, 1]$ norm.*

Proof Consider first the case $i = 0$. Due to the bound (5.2) and the identity (2.5), we have

$$\|f - f_m\|^2 = \sum_{n>m} |\hat{f}_n|^2 \leq c\|f\|_q^2 \sum_{n>m} n^{-2(q+1)} \leq c\|f\|_q^2 m^{-2q-1},$$

as required. Identical arguments, using (5.1) as opposed to (2.5), also demonstrate the corresponding result for $i = q$. When $i = 1, \ldots, q - 1$ we use the interpolation inequality

$$\|g\|_i \leq c_{i,q} \|g\|^{1-\frac{i}{q}} \|g\|_q^{\frac{i}{q}}, \quad \forall g \in \mathrm{H}_q[-1, 1],$$

(Adams 1975). Setting $g = f - f_m$ gives the full result. □

In Figure 5.1 we verify the results of Corollary 2 and Lemma 5. Figure 5.2 demonstrates the accuracy gained by increasing q. When $q = 3$ and $m = 40$, for example, the uniform error is approximately 10^{-4}, whereas when $q = 1$ this value is only 10^{-1}.

6 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 the Fast

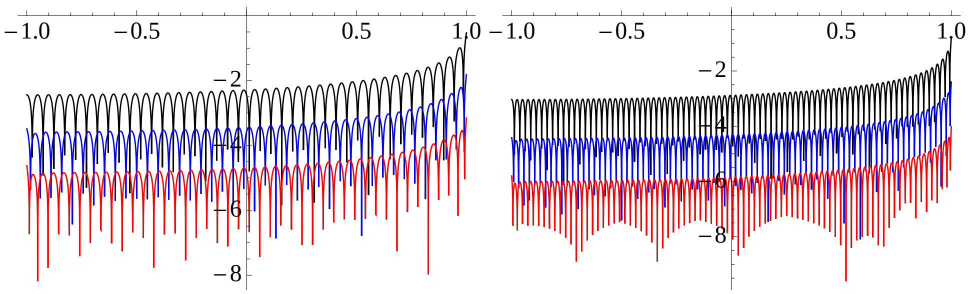

Figure 5.2: Log error $\log_{10}|f(x)-f_m(x)|$ against x for $q=1,2,3$ (in descending order) and $f(x)=x^2\mathrm{e}^{2x}$ with $m=20$ (left) and $m=40$ (right).

Fourier Transform. However, as has been described in (Iserles & Nørsett 2008), compelling alternative means exist for the calculation of modified Fourier expansion coefficients to high precision. Such methods are based on asymptotic expansions and related numerical quadrature schemes for highly oscillatory integrals.

In the context of modified Fourier ($q=1$) expansions, so-called *Filon-type* methods have been introduced in (Iserles & Nørsett 2008), with generalisations to d-variate cubes and the equilateral triangle pursued in (Iserles & Nørsett 2009) and (Huybrechs et al. 2010*b*) respectively. 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 any m expansion coefficients. Unlike the FFT, such methods are adaptive: increasing m does not require recalculation of any existing values. 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 (2.8).

6.1 The asymptotic method

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

$$\hat{f}_n=\int_{-1}^{1} f(x)u_n(x)\mathrm{d}x, \qquad n\in\mathbb{N},$$

consists of truncating (2.8). This results in the *asymptotic method*

$$\begin{aligned}&\hat{\mathcal{Q}}_n^{[\rho_{s,p},\rho_{s,p}]}[f] \qquad\qquad (6.1)\\ &=\sum_{r=0}^{s-1}\frac{(-1)^{(r+1)q}}{\alpha_n^{2(r+1)q}}\sum_{k=q}^{2q-1}(-1)^k[f^{(2qr+k)}(1)u_n^{(2q-k-1)}(1)-f^{(2qr+k)}(-1)u_n^{(2q-k-1)}(-1)]\\ &+\frac{(-1)^{(s+1)q}}{\alpha_n^{2(s+1)q}}\sum_{k=q}^{q+p-1}(-1)^k[f^{(2qs+k)}(1)u_n^{(2q-k-1)}(1)-f^{(2qs+k)}(-1)u_n^{(2q-k-1)}(-1)],\end{aligned}$$

where $s\geq 0$, $p\in\{0,\ldots,q-1\}$ ($p\neq 0$ when $s=0$) and

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

is the maximal order of derivative appearing in $\hat{\mathcal{Q}}_n^{[\rho_{s,p},\rho_{s,p}]}[f]$.

Theorem 6 *It is true for every $s \ge 0$ and $p = 0, \dots, q-1$ that*

$$\hat{\mathcal{Q}}_n^{[\rho_{s,p},\rho_{s,p}]} \sim \hat{f}_n + \mathcal{O}\Big(n^{-(2s+1)q-p-1}\Big), \qquad n \gg 1. \tag{6.2}$$

Proof This result follows at once by direct comparison of (6.1) with the asymptotic expansion (2.8), bearing in mind that $\alpha_n = \mathcal{O}(n)$ and $\|u_n^{(i)}\|_\infty = \mathcal{O}(\alpha_n^i)$. □

Once an approximation to $\hat{f}_n$ is $\mathcal{O}(n^{-N})$ for $n \gg 1$, we say that it is of an *asymptotic order* N. Thus, the asymptotic method (6.1) is of asymptotic order $(2s+1)q+p+1$. Note that asymptotic order refers to absolute error. Since $\hat{f}_n = \mathcal{O}(n^{-q-1})$, the *relative asymptotic order* of (6.1) is $2sq+p$.

It is convenient to introduce the following formalism to express derivative information. We thus let

$$\boldsymbol{N}_m = \{j \in \mathbb{N} \,:\, j = 2qr + k \le m \text{ where } r \ge 0,\ q \le k \le 2q-1\}$$

and $\boldsymbol{D}_m(x) = \{f^{(j)}(x) \,:\, j \in \boldsymbol{N}_m\}$. In view of this, we say that (6.1) employs the *data set*

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

where $\tilde{\boldsymbol{D}}_q = \{f^{(i)}(0) \,:\, i = 0, \dots, q\}$. It will be clear to the observant reader that $\tilde{\boldsymbol{D}}_q$ is not, actually, used at all in (6.1). The reason for its inclusion will be apparent in the sequel.

To illustrate (6.1), we consider $q = 2$. We have already noted in Section 3 that

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

Moreover, differentiating u_n and using (3.2) and (3.4), it is easy to verify that

$$u'_{2n-1}(\pm 1) = \mp\sqrt{2}\alpha_{2n-1}\tan\alpha_{2n-1}, \qquad u'_{2n}(\pm 1) = \frac{\sqrt{2}\alpha_{2n}}{\tan\alpha_{2n}}$$

(note that $|\tan\alpha_n| \approx 1$). Therefore, the first few asymptotic methods for $q = 2$ are

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

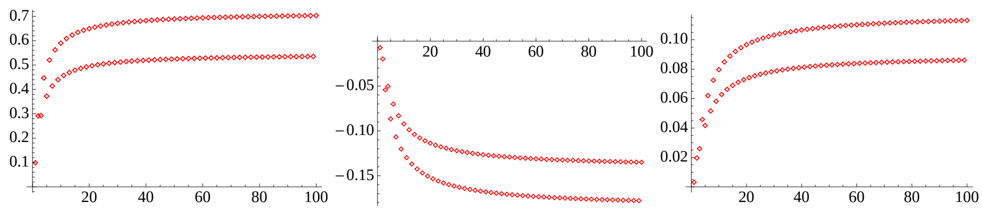

Figure 6.1: Scaled errors $n^4(\hat{Q}_n^{[2,2]} - \hat{f}_n)$, $n^7(\hat{Q}_n^{[3,3]} - \hat{f}_n)$ and $n^8(\hat{Q}_n^{[6,6]} - \hat{f}_n)$ (left to right) for $f(x) = \mathrm{e}^x$ and $q = 2$.

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

and so on. An important observation is that, once $D^{[i,i]}$ has been determined, any m coefficients $\hat{\mathcal{Q}}_n^{[i,i]}[f]$, $n = 1, \ldots, m$, can be computed in $\mathcal{O}(m)$ operations.

In Figure 6.1 we display the scaled errors $n^N(\hat{\mathcal{Q}}_n^{[i,i]}[f] - \hat{f}_n)$, where N is the asymptotic order, for the three choices $i = 2, 3, 6$, $q = 2$ and $f(x) = \mathrm{e}^x$. It is clear that computations conform with theory. Absolute and relative (non-scaled) errors for selected values of n are presented in Table 2. Evidently, the error for small n is unacceptably large, but this is hardly surprising since the asymptotic method (6.1) is, as its name implies, effective only for large ns, when u_ns become highly oscillatory and asymptotic behaviour sets in. 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.

6.2 Filon-type methods

The main idea of Filon-type methods is to replace f by an interpolating polynomial ψ 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) $\psi^{(i)}(c_k) = f^{(i)}(c_k)$ for $i = 0, \ldots, m_k - 1$, $k = 1, \ldots, \nu$ and let

$$\hat{\mathcal{Q}}_n[f] = \int_{-1}^{1} \psi(x) u_n(x) \mathrm{d}x, \qquad n = 1, 2, \ldots \tag{6.3}$$

(Iserles & Nørsett 2005). Note that (6.3) can be always integrated exactly, because of the form (4.2) of u_n. The asymptotic order of (6.3) is determined by $\min\{m_1, m_\nu\}$: 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 magnitude of the error (Iserles & Nørsett 2005).

Once we contemplate the information (in terms of function and derivative evaluations) required for the formation of ψ, we are struck by an important observation. The asymptotic expansion (2.8) requires only *some* derivatives at the endpoints: specifically, we require only $f^{(2qr+k)}(\pm 1)$ for $r = 0, 1, \ldots$ and $k = q, \ldots, 2q-1$. 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 ψ. Following the practice of (Iserles & Nørsett 2008), we use only 'significant' derivatives $f^{(2qr+k)}(c_k)$ also at the intermediate points $k = 2, \ldots, \nu - 1$.

This practice leads to significant 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 ψ exists for any configuration of c_ks 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.

Another potential problem is that this method requires exact derivative values. However, as described in (Iserles & Nørsett 2008) for modified Fourier expansions, these can be replaced by finite differences provided the spacing is sufficiently fine. Since numerical results with or without derivatives are practically indistinguishable, we shall continue to use exact derivatives in this paper.

Returning to the problem at hand, we note that not every multiplicity makes sense in the present context, since not every derivative features in asymptotic expansion. To this end, 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 thus seek a polynomial ψ such that

$$\psi^{(j)}(c_k) = f^{(j)}(c_k) \qquad j \in \boldsymbol{N}_{m_k}, \quad k = 1, \ldots, \nu \tag{6.4}$$

and set

$$\hat{\mathcal{Q}}_n^{\boldsymbol{m}}[f] = \int_{-1}^{1} \psi(x) u_n(x) \mathrm{d}x, \qquad n \in \mathbb{N}. \tag{6.5}$$

Hence, the data set of the Filon-type method (6.5) is

$$\boldsymbol{D}^{\boldsymbol{m}} = \tilde{\boldsymbol{D}}_q \cup \bigcup_{k=1}^{\nu} \boldsymbol{D}_{m_k}(c_k).$$

Recalling that the least index in $\boldsymbol{N}_m$ is the qth one, it is convenient to replace (6.4) by the interpolation conditions

$$\varphi^{(j-q)}(c_k) = f^{(j)}(c_k) \qquad j \in \boldsymbol{N}_{m_k}, \quad k = 1, \ldots, \nu.$$

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

$$\psi(x) = \sum_{l=0}^{q-1} \frac{1}{l!} f^{(l)}(0)x^l + \frac{1}{(q-1)!}\int_0^x (x-t)^{q-1}\varphi(t)\mathrm{d}t. \tag{6.6}$$

We substitute (6.6) into (6.5) and note that, by Lemma 1, the u_ns are orthogonal to all polynomials of degree $\le q-1$. Therefore

$$\hat{\mathcal{Q}}_n^{\boldsymbol{m}}[f] = \frac{1}{(q-1)!}\int_{-1}^1 \int_0^x (x-t)^{q-1}\varphi(t)\mathrm{d}t u_n(x)\mathrm{d}x, \qquad n \in \mathbb{N}.$$

Theorem 7 *Let $m_1 = m_\nu = \rho_{s,p}$ (recall that all multiplicities are good numbers). The asymptotic order of $\hat{\mathcal{Q}}_n^{\boldsymbol{m}}$ is $(2s+1)q+p+1$.*

Proof We substitute $\psi - f$ into the asymptotic expansion and use Theorem 6 for the order of the asymptotic method. □

Proposition 8 *It is true that*

$$\hat{\mathcal{Q}}_n^{\boldsymbol{m}}[f] = \frac{1}{\alpha_n^{2q}}\int_{-1}^1 \varphi(x)u_n^{(q)}(x)\mathrm{d}x, \qquad n \in \mathbb{N}. \tag{6.7}$$

Proof It follows from (2.1) that

$$\hat{\mathcal{Q}}_n^{\boldsymbol{m}}[f] = \frac{1}{\alpha_n^{2q}(q-1)!}\int_{-1}^1 \frac{\mathrm{d}^q}{\mathrm{d}x^q}\left[\int_0^x (x-t)^{q-1}\varphi(t)\mathrm{d}t\right] u_n^{(q)}(x)\mathrm{d}x.$$

Since

$$\frac{\mathrm{d}}{\mathrm{d}x}\int_0^x (x-t)^j\varphi(t)\mathrm{d}t = j\int_0^x (x-t)^{j-1}\varphi(t)\mathrm{d}t, \qquad j \ge 1,$$

we have $\frac{\mathrm{d}^q}{\mathrm{d}x^q}\int_0^x (x-t)^{q-1}\varphi(t)\mathrm{d}t = (q-1)!\varphi(x)$, which gives the result. □

This proposition gives a convenient approach to form the approximation $\hat{\mathcal{Q}}_n^{\boldsymbol{m}}[f]$. Writing φ as a linear combination of derivative values

$$\varphi(x) = \sum_{k=1}^{\nu} \sum_{j \in \mathrm{N}_{m_k}(c_k)} \varphi_{k,j}(x) f^{(j)}(c_k),$$

where the $\varphi_{k,j}$s are cardinal polynomials of Birkhoff–Hermite interpolation, it follows that

$$\hat{\mathcal{Q}}_n^{\boldsymbol{m}}[f] = \sum_{k=1}^{\nu} \sum_{j \in \boldsymbol{N}_{m_k}} b_{k,j}(n) f^{(j)}(c_k), \tag{6.8}$$

where

$$b_{k,j}(n) = \frac{1}{\alpha_n^{2q}}\int_{-1}^1 \varphi_{k,j}(x)u_n^{(q)}(x)\mathrm{d}x, \qquad j \in \boldsymbol{N}_{m_k},\ k = 1,\ldots,\nu.$$

Once the polynomials $\varphi_{k,j}$ have been constructed, determination of $\hat{\mathcal{Q}}_n^{\boldsymbol{m}}[f]$ requires only evaluation of the integrals $b_{k,j}(n)$. This is best achieved by using the asymptotic expansion (2.8): since $\varphi_{k,j}$ is a polynomial, this expansion terminates after a finite number of terms and equals the value $b_{k,j}(n)$.

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 $\boldsymbol{N}_2 = \{2\}$, our data set is

$$\{f(0), f'(0), f''(0), f''(-1), f''(-c), f''(c), f''(1)\}. \tag{6.9}$$

Simple calculation confirms that the cardinal polynomials are

$$\varphi_{1,2}(x) = -\tfrac{1}{2}\frac{(1-x)(c^2-x^2)}{1-c^2}, \qquad \varphi_{2,2}(x) = \tfrac{1}{2}\frac{(1-x^2)(c-x)}{c(1-c^2)},$$
$$\varphi_{3,2}(x) = \tfrac{1}{2}\frac{(1-x^2)(c+x)}{c(1-c^2)}, \qquad \varphi_{4,2}(x) = -\tfrac{1}{2}\frac{(1+x)(c^2-x^2)}{1-c^2},$$

and thus

$$b_{1,2}(2n-1) = b_{4,2}(2n-1) = -\frac{\sqrt{2}\tan\alpha_{2n-1}}{\alpha_{2n-1}^3} - \frac{2\sqrt{2}}{1-c^2}\frac{1}{\alpha_{2n-1}^4},$$
$$b_{2,2}(2n-1) = b_{3,2}(2n-1) = \frac{2\sqrt{2}}{1-c^2}\frac{1}{\alpha_{2n-1}^4};$$

$$b_{1,2}(2n) = -b_{4,2}(2n) = -\frac{\sqrt{2}\cot\alpha_{2n}}{\alpha_{2n}^3} + \frac{\sqrt{2}(3-c^2)}{1-c^2}\frac{1}{\alpha_{2n}^4},$$
$$b_{2,2}(2n) = -b_{3,2}(2n) = -\frac{2\sqrt{2}}{c(1-c^2)}\frac{1}{\alpha_{2n}^4}.$$

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

$$\hat{\mathcal{Q}}_{2n-1}^{[2,2,2,2]}[f] = \hat{\mathcal{Q}}_{2n-1}^{[2,2]}[f] - \frac{1}{\alpha_{2n-1}^4}\frac{2\sqrt{2}}{1-c^2}[f''(1) - f''(c) - f''(-c) + f''(-1)], \tag{6.10}$$
$$\hat{\mathcal{Q}}_{2n}^{[2,2,2,2]}[f] = \hat{\mathcal{Q}}_{2n}^{[2,2]}[f] - \frac{1}{\alpha_{2n}^4}\frac{2\sqrt{2}}{c(1-c^2)}\{\tfrac{c(3-c^2)}{2}[f''(1) - f''(-1)] - [f''(c) - f''(-c)]\}.$$

As in the case of the asymptotic method, any m values $\hat{\mathcal{Q}}_n^{[2,2,2,2]}[f]$ can be computed in $\mathcal{O}(m)$ operations. Indeed, it is evident from (6.8) that this is the case for all $\hat{\mathcal{Q}}_n^{\boldsymbol{m}}[f]$.

6.3 Another take on Filon-type methods

The method (6.10), as well as numerous examples of such methods for $q = 1$ (Iserles & Nørsett 2008, Iserles & Nørsett 2009), can be written in the form

$$\hat{\mathcal{Q}}_{2n-1}^{\boldsymbol{m}}[f] = \hat{\mathcal{Q}}_{2n-1}^{[\rho_{p,s},\rho_{p,s}]}[f] + \frac{G_1(n)}{\alpha_{2n-1}^N}\sum_{k=1}^{\nu}\sum_{j\in\boldsymbol{N}_{m_k}}\alpha_{k,j}f^{(j)}(c_k), \tag{6.11}$$
$$\hat{\mathcal{Q}}_{2n}^{\boldsymbol{m}}[f] = \hat{\mathcal{Q}}_{2n}^{[\rho_{p,s},\rho_{p,s}]}[f] + \frac{G_2(n)}{\alpha_{2n}^N}\sum_{k=1}^{\nu}\sum_{j\in\boldsymbol{N}_{m_k}}\beta_{k,j}f^{(j)}(c_k),$$

where $m_1 = m_\nu = \rho_{p,m}$ and $N = (2s+1)q + p + 1$, while G_1 and G_2 are given functions ($G_1, G_2 \equiv 1$ in (6.10)) and $\alpha_{k,j}$, $\beta_{k,j}$ are constants. This can be reinterpreted in the following manner: we are using derivative information to approximate the Nth term in the asymptotic expansion. This procedure minimises the magnitude of the error by replacing the leading term in the truncated asymptotic expansion, a linear combination of derivatives, with an error incurred while approximating these derivatives. To connect this interpretation with the example (6.10), we can easily verify that

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

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 (6.11) has two crucial advantages. Firstly, it provides a transparent means to compute any 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 $\hat{Q}_n^{\boldsymbol{m}}$ can be expressed in the form (6.11). 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 (6.11) 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

$$G_1(n) = -\sqrt{2}\tan\alpha_{2n-1}, \qquad G_2(n) = \sqrt{2}\cot\alpha_{2n}.$$

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

$$h(-1), h'(-1), h(-c), h'(-c), h(c), h'(c), h(1), h'(1).$$

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

$$\begin{aligned} h^{(iv)}(1) + h^{(iv)}(-1) = &-\frac{72(9-c^2)}{(1-c^2)^3}[h(1) - h(c) - h(-c) + h(-1)] \\ &+ \frac{24(7-c^2)}{(1-c^2)^2}[h'(1) - h'(-1)] + \frac{12(13-c^2)}{c(1-c^2)^2}[h'(c) - h'(-c)] \end{aligned}$$

is correct for every $h \in \mathbb{P}_7$, while

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

for all $h \in \mathbb{P}_8$. Therefore

$$\begin{aligned}\hat{\mathcal{Q}}^{[3,3,3,3]}_{2n-1}[f] =& \hat{\mathcal{Q}}^{[3,3]}_{2n-1}[f] \\ & - \frac{\sqrt{2}\tan\alpha_{2n-1}}{\alpha^7_{2n-1}} \left\{ -\frac{72(9-c^2)}{(1-c^2)^3}\left[f''(1) - f''(c) - f''(-c) + f''(-1)\right] \right. \\ & \left. + \frac{24(7-c^2)}{(1-c^2)^2}\left[f'''(1) - f'''(-1)\right] + \frac{12(13-c^2)}{c(1-c^2)^2}\left[f'''(c) - f'''(-c)\right] \right\}, \\ \hat{\mathcal{Q}}^{[3,3,3,3]}_{2n}[f] =& \hat{\mathcal{Q}}^{[3,3]}_{2n}[f] - \frac{\sqrt{2}\cot\alpha_{2n}}{\alpha^7_{2n}} \left\{ -\frac{120(14-7c^2+c^4)}{(1-c^2)^3}[f''(1) - f''(-1)] \right. \\ & - \frac{60(5-28c^2+7c^4)}{c^3(1-c^2)^3}[f''(c) - f''(-c)] + \frac{120(3-c^2)}{(1-c^2)^2}[f'''(1) + f'''(-1)] \\ & \left. + \frac{60(5-c^2)}{c^2(1-c^2)^2}[f'''(c) + f'''(-c)] \right\}.\end{aligned}$$

6.4 Exotic quadrature

Our formulæ for $\hat{\mathcal{Q}}^{[2,2,2,2]}_n$ and $\hat{\mathcal{Q}}^{[3,3,3,3]}_n$ 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 (2.3), we need to compute not just $\hat{f}_n$ for $n \geq 1$ but also the nonoscillatory integrals $\hat{f}^0_0, \ldots, \hat{f}^o_{q-1}$. 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. However, since we desire optimal strategies with the least computational cost, an integration scheme for these coefficients should reuse derivatives that have been already used in forming our approximations to the $\hat{f}_n$s. Specifically, we let each $\hat{f}^o_n$, $n = 0, \ldots, q-1$, be approximated by a linear combination of values from the data set $\boldsymbol{D}^{\boldsymbol{m}}$:

$$\int_{-1}^{1} f(x)\mathrm{P}_n(x)\mathrm{d}x \approx \hat{\mathcal{P}}^{\boldsymbol{m}}_n[f] = \sum_{k=1}^{\nu} \sum_{j \in \boldsymbol{N}_{m_k}} \delta_{k,j}(n) f^{(j)}(c_k), \qquad n = 0, \ldots, q-1. \quad (6.12)$$

We call (6.12) an *exotic quadrature* to underline its difference from more standard computational methods for nonoscillatory integrals. Note that a precursor of this idea has been named in (Iserles & Nørsett 2008) as “underlying classical quadrature”, surely more of a mouthful than “exotic”. Note further that (6.12) is a special case of *Birkhoff quadrature* (Bojanov & Nikolov 1990).

Returning to the first example of the previous section, $\hat{\mathcal{Q}}^{[2,2,2,2]}_n$, we seek an exotic quadrature using the data set

$$\boldsymbol{D}^{[2,2,2,2]} = \{f(0), f'(0), f''(-1), f''(-c), f''(0), f''(c), f''(1)\}.$$

Simple algebra confirms that the quadrature

$$\begin{aligned}\hat{\mathcal{P}}^{[2,2,2,2]}_0[f] =& 2f(0) + \tfrac{1}{420}\frac{2-7c^2}{1-c^2}[f''(1) + f''(-1)] + \tfrac{1}{84}\frac{1}{c^2(1-c^2)}[f''(c) + f''(-c)] \\ & - \tfrac{1}{210}\frac{5-63c^2}{c^2}f''(0)\end{aligned}$$

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,

$$\hat{\mathcal{P}}_1^{[2,2,2,2]}[f] = \tfrac{2}{3}f'(0) + \tfrac{1}{420}\frac{3-14c^2}{1-c^2}[f''(1) - f''(-1)] + \tfrac{11}{420}\frac{1}{c(1-c^2)}[f''(c) - f''(-c)]$$

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 corresponding to the second example $\hat{\mathcal{Q}}_n^{[3,3,3,3]}$,

$$\begin{aligned}
\hat{\mathcal{P}}_0^{[3,3,3,3]}[f] =& 2f(0) + \tfrac{1}{13860}\frac{68 - 404c^2 + 935c^4 - 396c^6}{(1-c^2)^3}[f''(1) + f''(-1)] \\
&- \tfrac{1}{13860}\frac{25 - 328c^2 + 506c^4}{c^4(1-c^2)^3}[f''(c) + f''(-c)] \\
&+ \tfrac{1}{6930}\frac{25 - 253c^2 + 1914c^4}{c^4}f''(0) \\
&- \tfrac{1}{55440}\frac{27 - 154c^2 + 330c^4}{(1-c^2)^2}[f'''(1) - f'''(-1)] \\
&+ \tfrac{1}{55440}\frac{50 - 253c^2}{c^3(1-c^2)^2}[f'''(c) - f'''(-c)], \\
\hat{\mathcal{P}}_1^{[3,3,3,3]}[f] =& \tfrac{2}{3}f'(0) + \tfrac{1}{166320}\frac{1015 - 6671c^2 + 19558c^4 - 7722c^6}{(1-c^2)^3}[f''(1) - f''(-1)] \\
&- \tfrac{1}{166320}\frac{259 - 6707c^2 + 12628c^4}{c^3(1-c^2)^3}[f''(c) - f''(-c)] \\
&- \tfrac{1}{166320}\frac{115 - 748c^2 + 2178c^4}{(1-c^2)^2}[f'''(1) + f'''(-1)] \\
&+ \tfrac{1}{166320}\frac{259 - 1804c^2}{c^2(1-c^2)^2}[f'''(c) - f'''(-c)],
\end{aligned}$$

of orders 11 and 10, respectively. No real value of c results in a higher order exotic quadrature. 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 $\hat{\mathcal{P}}_n^{[3,3,3,3]}$.

Figure 6.2 depicts scaled errors produced by the Filon-type methods $\hat{\mathcal{Q}}_n^{[i,i,i,i]}[f]$ for $i = 2, 3, 6$ (note that the case $i = 6$ can be obtained in an identical manner to the $i = 2, 3$ cases explicitly derived earlier). Upon comparison with Figure 6.1, it follows immediately that, despite the asymptotic order being the same, the use of additional data inside $(-1, 1)$ decreases the error by a significant factor. The same conclusion emerges from Table 3. In particular, the improvement for small ns is tangible, although the errors in this regime are still excessive for many uses. Of course, they can be decreased further by using larger ν.

Table 3 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! For this reason, and in view of the shortfall of Filon-type methods for small values of n, it makes sense to use

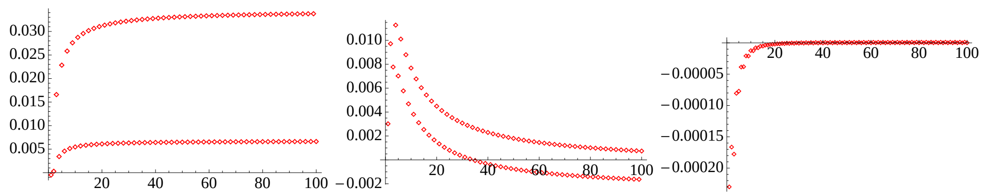

Figure 6.2: Scaled errors $n^4(\hat{Q}_n^{[2,2,2,2]} - \hat{f}_n)$, $n^7(\hat{Q}_n^{[3,3,3,3]} - \hat{f}_n)$ and $n^8(\hat{Q}_n^{[6,6,6,6]} - \hat{f}_n)$ for $f(x) = \mathrm{e}^x$ and $q = 2$.

	$\hat{\mathcal{P}}_n^{[2,2,2,2]}[f]$		$\hat{\mathcal{P}}_n^{[3,3,3,3]}[f]$		$\hat{\mathcal{P}}_n^{[6,6,6,6]}[f]$	
n	absolute	relative	absolute	relative	absolute	relative
0	2.11_{-06}	8.96_{-07}	1.21_{-10}	5.15_{-11}	2.60_{-15}	1.11_{-15}
1	2.48_{-07}	3.37_{-07}	3.49_{-09}	4.74_{-09}	9.60_{-15}	1.31_{-14}

	$\hat{\mathcal{Q}}_n^{[2,2,2,2]}[f]$		$\hat{\mathcal{Q}}_n^{[3,3,3,3]}[f]$		$\hat{\mathcal{Q}}_n^{[6,6,6,6]}[f]$	
n	absolute	relative	absolute	relative	absolute	relative
1	4.90_{-04}	2.18_{-03}	3.02_{-03}	1.34_{-02}	2.30_{-04}	1.02_{-03}
2	1.84_{-05}	5.00_{-04}	7.59_{-05}	2.07_{-03}	6.50_{-07}	1.77_{-05}
3	2.05_{-04}	9.04_{-03}	3.55_{-06}	1.57_{-04}	2.71_{-08}	1.20_{-06}
4	1.34_{-05}	1.75_{-03}	6.88_{-07}	8.98_{-05}	1.23_{-09}	1.60_{-07}
10	5.46_{-07}	8.01_{-04}	7.68_{-10}	1.13_{-06}	1.24_{-13}	1.81_{-10}
20	3.81_{-08}	3.99_{-04}	3.51_{-12}	3.68_{-08}	7.84_{-17}	8.22_{-13}
50	1.04_{-09}	1.59_{-04}	2.30_{-15}	3.52_{-10}	1.12_{-21}	1.70_{-16}
100	6.62_{-11}	7.90_{-05}	7.43_{-18}	8.87_{-12}	1.03_{-23}	1.23_{-17}

Table 3: 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 $i = 2, 3, 6$.

exotic quadrature for not just the nonoscillatory coefficients, but also the first few integrals $\hat{f}_n$. As demonstrated in Table 4, this approach works well for those values of n for which the Filon-type method does not deliver sufficient accuracy.

	$\hat{\mathcal{P}}_n^{[2,2,2,2]}[f]$		$\hat{\mathcal{P}}_n^{[3,3,3,3]}[f]$		$\hat{\mathcal{P}}_n^{[6,6,6,6]}[f]$	
n	absolute	relative	absolute	relative	absolute	relative
1	2.73_{-06}	1.21_{-05}	9.62_{-11}	4.28_{-10}	2.55_{-15}	1.13_{-14}
2	1.83_{-05}	5.00_{-04}	1.16_{-09}	3.15_{-08}	1.45_{-14}	3.95_{-13}
3	1.98_{-06}	8.75_{-05}	3.08_{-11}	1.36_{-09}	1.12_{-15}	4.96_{-14}
4	1.34_{-05}	1.74_{-03}	1.24_{-10}	1.61_{-08}	8.98_{-15}	1.17_{-12}

Table 4: Absolute and relative errors $\hat{\mathcal{P}}_n^{[i,i,i,i]}[f] - \hat{f}_n$for $f(x) = \mathrm{e}^x$, $q = 2$ and $i = 2, 3, 6$.

7 Conclusions and challenges

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

Our point of departure being modified Fourier expansions, with coefficients that decay like $\mathcal{O}(n^{-2})$ (Iserles & Nørsett 2008), we have generalised the framework to certain Birkhoff expansions. Practical considerations, combined with theoretical justification, mean that we have considered expansions in eigenfunctions of polyharmonic operators with Neumann boundary conditions. These bases exhibit faster rate of decay of expansion coefficients and faster convergence of the truncated expansion. In particular, we have analysed in greater detail bases with $\mathcal{O}(n^{-3})$ decay and $\mathcal{O}(m^{-2})$ uniform convergence rate.

Two central practical issues have been successfully addressed. First, we have presented a systematic means to construct eigenfunctions explicitly. Such functions always separate into two sets: they are either even or odd. They also depend on a parameter which can be calculated extremely easily by numerically solving a scalar nonlinear algebraic equation. Second, we have introduced a combination of classical and highly oscillatory quadratures to evaluate expansion coefficients numerically. In doing so, we have demonstrated the broad applicability of such quadratures to a wide variety of expansions, in contrast to the FFT.

The highly oscillatory quadratures employed, Filon-type methods, have been reinterpreted as a combination of a truncated asymptotic expansion 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. However, Filon-type methods cannot be utilised for non-oscillatory coefficients and do not produce sufficient accuracy for small n. In this setting, we have successfully reused derivative information in "exotic quadrature" algorithms to obtain high accuracy.

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! As we now indicate, much further investigation is required to produce efficient methods which are competitive against more mature algorithms. In view of this, we wish to single out the following problems and challenges for future work:

1. *Filon-type quadrature.* The design of Filon-type quadrature in the form (6.11), 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 2 and 3. 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 present more of a challenge for the asymptotic expansion part.

A pertinent issue is the *stability* of Filon-type methods (6.11) for large ν. 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 better and obtain a wealth of practical numerical experience with many νs and many functions f.

2. *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 except for fairly general statements on Birkhoff quadrature, which help little to illuminate the issue at hand. In particular, we do not even know what is the 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 future work shall address this issue in greater detail.

   Another challenge is to produce reliable and tight bounds on the error. This, we believe, can also be accomplished with the Peano Kernel Theorem.

   As demonstrated in this paper, for high accuracy we should use exotic quadrature for the first few coefficients and Filon quadrature for the remainder. However, a criterion for determining which method is appropriate has not yet been established. Additionally, derivative-based quadratures are susceptible to round-off error if, for example, the approximated function is itself oscillatory. In (Brunner et al. 2009), this issue was circumvented when $q = 1$ by using a variant of the FFT to compute those coefficients corresponding to small values of n. Since the zeroes of the nth polyharmonic–Neumann eigenfunction ϕ_n are asymptotically uniformly distributed as $n \to \infty$ (this follows directly from (5.3)), it may be possible to develop a similar approach for general $q \geq 1$. Alternatively, in (Dominguez, Graham & Smyshlyaev 2010) a 'derivative-free' Filon-type scheme has been proposed, for which robust error bounds (explicit in both the coefficient n and the number of quadrature nodes) are known.

3. *Large q.* As discussed in Section 4.3, numerical considerations become an important issue for larger q. Beyond $q = 4$, the increased cost of forming the approximation and the susceptibility to round-off error may present limitations to the scope of this approach. However, much future work is required, incorporating those questions posed above relating to the quadratures employed, to assess the impact of these issues on polyharmonic expansions.

   Insofar as the application of such approximations to the numerical solution of differential equations is concerned, this may not present such an issue. Eighth or higher order problems are of little interest, whereas biharmonic or triharmonic problems are much more frequently studied.

4. *Properties of the eigenvalues and eigenfunctions.* The asymptotic behaviour of eigenvalues and eigenfunctions of linear differential operators subject to regular boundary conditions has been extensively studied (Naimark 1968). In Section 5, we stated several improved results for the polyharmonic–Neumann setting. A future paper shall present proofs of these results and several consequences, including a proof of the $\mathcal{O}\left(m^{-q-1}\right)$ pointwise convergence rate away from the endpoints.

5. *Multivariate expansions.* Multivariate modified Fourier expansions have been successfully developed in the d-variate cube (Iserles & Nørsett 2009). The corresponding generalisation of polyharmonic–Neumann expansions presents a number of challenges, both theoretical and numerical in character. Immediately the analogy with the polyharmonic operator is lost: multivariate polyharmonic eigenfunctions cannot be expressed in terms of simple functions, and are thus unsuitable for practical approximation schemes. Instead, an appropriate multivariate basis consists of Cartesian products of univariate polyharmonic eigenfunctions. These are precisely the eigenfunctions of the *subpolyharmonic* operator $(-1)^q \partial_{x_1}^{2q} + \ldots + (-1)^q \partial_{x_d}^{2q}$. We are currently compiling a theory of such expansions, and will present this in detail in a future paper.

   Modified Fourier expansions have also been introduced in the equilateral triangle (Huybrechs et al. 2010*b*). At this moment, it is unknown whether an appropriate generalisation of univariate polyharmonic expansions can be developed for this domain.

6. *Convergence acceleration.* The development of convergence acceleration strategies for modified Fourier expansions, pursued in (Huybrechs, Iserles & Nørsett 2010*a*) and (Adcock 2010*a*), has proved extremely beneficial in improving the performance of such approximations when compared to more standard methods. We see no reason why such techniques cannot be adapted to the polyharmonic setting, provided the relevant theoretical and numerical details are properly addressed.

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 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.

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