

Fourier Analysis of Finite Difference Schemes for the Helmholtz Equation in 1D with Dirichlet Conditions: Sharp Estimates and Relative Errors*

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Abstract

We consider the Dirichlet problem of the indefinite Helmholtz equation in 1D, $u'' + k^2 u = f$ in $(0, 1)$, $u(0) = g_0$, $u(1) = g_1$, with a constant wavenumber $k \in (0, \infty) \setminus \pi\mathbb{N}$ and a source term $f \in H_0^p(0, 1)$, $p \geq 4$. We propose an approach based on Fourier analysis to derive wavenumber explicit sharp estimates of absolute and relative errors of *finite difference* methods. Such results have been well known for *finite element* methods (FEM). We use the approach to analyze the classical centered finite difference scheme. For the Fourier interpolants of the discrete solution with homogeneous (or inhomogeneous) Dirichlet conditions, we show rigorously, under the two assumptions $k > 20$ and $k(kh)^2/\sigma_k \leq 4/(\pi - 2)$ with $\sigma_k := \text{dist}(k, \pi\mathbb{N})$, that the worst case attainable convergence order of the absolute error with $\sum_{p=0}^4 k^{-p} \|f^{(p)}\|_{L^2} = O(1)$ (or $|g_i| \asymp k^{-1}$) is $(kh)^2/\sigma_k^2$ in the L^2 -norm and $k(kh)^2/\sigma_k^2$ in the H^1 -semi-norm, and that of the relative error is $k(kh)^2/\sigma_k$ in both L^2 - and H^1 -semi-norms if $\|u^{(p)}\|_{L^2}/\|u^{(p-2)}\|_{L^2} \asymp k^2$ for $p = 2, 3$. In particular, the lower bounds of these error estimates are established rigorously in the same orders as the upper bounds, which is the main novelty of this work. We show also that the Fourier analysis approach can be used as a convenient visual tool for evaluating finite difference schemes in presence of source terms, which is beyond the scope of dispersion analysis. The results from the theory and visual analysis are corroborated by numerical experiments.

Key words: finite difference, Helmholtz equation, error estimate, wavenumber, Fourier analysis

1 Introduction

The Helmholtz equation $\Delta u + k^2 u = f$ is a common model of time-harmonic waves in acoustics [26], geophysics [39] and electrical engineering [4], etc. Standard discretization of the Helmholtz equation suffers from the so-called “*pollution effect*”, explained by [13] as that “the rule of the thumb taking a certain number of elements per wavelength” is insufficient to “keep the total error under control” albeit “sufficient to keep the interpolation error constant”. It is proved in [28] that the linear finite element method for the 1D scattering problem on $(0, 1)$ with $u(0) = 0$ and $u'(1) - iku(1) = 0$ has the error in the H^1 -norm bounded from above by $C(hk + h^2 k^3)\|f\|_{L^2}$ with $C > 0$ independent of h , k and f , where $Ch^2 k^3\|f\|_{L^2}$ is called the “*pollution term*” which indicates the accuracy deterioration with the “rule of thumb” keeping kh constant. Since then, a lot of progress has been made in wavenumber explicit error estimates of finite element methods [14, 34, 36, 41, 48, 53], including the recent extension to heterogeneous media [6, 8, 9, 23, 32] and multiscale methods [7, 10, 20, 24, 35, 38].

While finite element methods are more advanced and powerful, finite difference methods are still used for their simplicity in some applications [2, 25, 37, 42, 43]. In particular, it was found in [43] for full waveform inversion that “a 27-point stencil on a regular Cartesian grid” is “*more computationally efficient*” than “a P_3 finite element method on h -adaptive tetrahedral mesh”. It is pressing to have a theoretical support for methods in use. But wavenumber explicit error estimates are rarely seen in the

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literature of finite difference methods [18, 40, 45, 47, 50]. Error estimates of some compact fourth order schemes in 2D are given in [21] based on the assumption that the coefficient matrix of the discretized system is positive definite (which is true only for small wavenumber k). In [46], arbitrarily high order and dispersion free schemes in 1D are derived, and an error analysis following the approach of [21] is given. Recently, in [11] it is shown for a dispersion free 3-point scheme in 1D that the maximum-norm error is bounded from above by $(\frac{1}{k}\|f''\|_{L^\infty} + k^2\|f\|_{L^\infty})h^2$ up to a constant factor. An earlier dispersion free scheme in 1D was proposed in the seminal paper [5] and analyzed in the finite element framework giving the H^1 -semi-norm error less than $ch\|f\|_{H^1}$ for the scattering problem with c seemingly $O(k)$.

It has been well noted that the pollution effect is intuitively related to the fact that the numerical solution “has a wavelength that is different from the exact one”, called “dispersion” [13]. Therefore, [13] advocated “a tool in order to measure quantitatively the dispersion for various of the proposed methods as a measure of the pollution”. “This measure allows to compare the different methods that have been proposed to reduce the pollution and compare their efficiency.” The tool called “dispersion analysis” [1] had been used before mainly for time-dependent problems [44].

The idea of dispersion analysis in 1D is to find Fourier modes $e^{i\xi x}$ satisfying the discretized homogeneous Helmholtz equation, e.g. $e^{i\xi(x-h)} + (k^2h^2 - 2)e^{i\xi x} + e^{i\xi(x+h)} = 0$, and from the resulting constraint on ξ , e.g. $2\cos(\xi h) = 2 - k^2h^2$, find the discrete wavenumber $k^h := |\xi|$. If the original Helmholtz equation $(e^{i\xi x})'' + k^2e^{i\xi x} = 0$ is used instead of the discretized one, then we find the constraint $|\xi| = k$. Such Fourier modes $e^{i\xi x}$ are called “plane waves”. The “phase difference” $|k - k^h|$ measures the dispersion error between the original plane wave $e^{\pm ikx}$ and the discretized dispersive ($k^h \neq k$) plane wave $e^{\pm ik^h x}$.

It is shown in [29] for polynomial finite element methods in 1D that the pollution term is of the same order as the phase difference. That partially explains why reducing the phase difference leads to reducing the pollution effect. Sharp dispersion error estimates are obtained in [3]. By providing a practical criterion, dispersion analysis can also guide optimization of the discretization parameters; see [52] for the continuous interior penalty finite element method and [11, 12, 42, 49] for finite difference methods. Recently, dispersion reduction has been generalized in [33] to unstructured meshes by minimizing the residual of the original plane waves in the discretized equation; see also the earlier work [19]. A similar approach based on minimizing “average truncation error of plane waves” is adopted in [18] for some high order finite difference methods.

Albeit intuitive, it is not trivial to translate the “dispersion error” into the “pollution effect”. As remarked in [27]: “dispersion analysis gives valuable information on several physical phenomena inherent to the discrete solution and thus leads to qualitative insight into the sources of numerical error,” but “it does not yield, by its nature, quantitative statements on the numerical error itself”. That is why so many efforts have been made in wavenumber explicit error estimation, as we mentioned above.

Moreover, dispersion analysis is insufficient because it considers only the zero source problem and the Fourier modes constrained by the dispersion relation, while nonzero source terms and the other Fourier modes stimulated by the source term are not taken into account. We shall see in Section 4 that three dispersion free schemes in 1D can behave differently with a source term. Indeed, in [5] a discretization in 1D was proposed with zero truncation error “for as many right hand sides as possible”, not only the zero right hand side. An eigenvalue (Fourier) analysis is carried out in [15] for the Dirichlet boundary value problem with a point source.

Inspired by [15] which calculated the eigenvalue difference of the continuous and discrete Helmholtz operators, we develop here an approach to wavenumber explicit error estimation based on Fourier analysis for general smooth source terms, Dirichlet boundary conditions and non-resonant wavenumbers $k \notin \pi\mathbb{N}$ in 1D. We analyze in detail a classical centered *finite difference* scheme in 1D because it is simple yet not fully understood. Actually, we have not found any other wavenumber explicit estimate for *finite difference* schemes than that in [11], and in particular none for the classical centered *finite difference* scheme, though the folklore says a p th order *finite difference* scheme has the (relative) error $O(k^{p+1}h^p)$ (see e.g. [15]).

It should be well noted that such results have been proved and considered as standard for *finite element* methods. For example, as pointed out by an anonymous reviewer, for arbitrary order finite element methods in a general domain $\Omega \subset \mathbb{R}^d$, combining [9, Theorem 4.11] with the estimate $\gamma_s^* \leq Ck/\delta$ gives a sharp upper bound for the Dirichlet problem.

Regarding our work here for the classical centered finite difference scheme in 1D, all the upper bounds

are attainable and the equality cases are given explicitly. The pollution term is located in Fourier frequencies, and its *exact* order in k and h is found *by two-sided bounds*. In particular, the lower bounds contribute to the main novelty of this work. We also give a sharp estimate for relative errors with source terms. Wavenumber explicit estimates for relative errors have not been studied as much as for absolute errors. Recent progress for finite element methods can be found in [22, 31].

Moreover, by plotting the symbol errors we can see clearly how the error is distributed over Fourier frequencies. In this sense, it becomes a practical tool for comparing different schemes, e.g. those of the same order and those before and after dispersion correction, which complements the dispersion analysis for working with or without a source term. This aspect has been briefly demonstrated in [51] for some compact high order schemes, where sharp orders in k , h are found in Fourier domain and verified numerically.

In the following sections, we first introduce the model problem and Fourier decomposition in Section 2, then carry out the theoretical analysis of the classical scheme in Section 3, and illustrate the practical aspect of the tool in Section 4. Those results are corroborated numerically in Section 5. Some discussions are included at the end.

2 Model problem in 1D and downsampling error

We first introduce the 1D Helmholtz equation in a closed cavity, and the Fourier form of the solution. Then we analyze the component of the discretization error due to sampling of the solution on grids.

2.1 Model problem

Let $k > 0$ be the wavenumber. The Helmholtz equation with Dirichlet boundary conditions in 1D is

$$u'' + k^2 u = f \text{ in } (0, 1), \quad u(0) = g_0, \quad u(1) = g_1. \quad (1)$$

For well-posedness of (1), we assume that k/π is not an integer. By linearity, we separate the two cases:

- (i) homogeneous Dirichlet boundary condition $g_0 = g_1 = 0$, and
- (ii) zero source $f = 0$.

In case (i) $g_0 = g_1 = 0$, we assume $f \in H_0^p(0, 1)$ with $p \geq 1$. For $f \in L^2(0, 1)$, we have $u \in H^2(0, 1) \cap H_0^1(0, 1)$. For the corresponding theory, we refer to [17]. Smoothness of f is a crucial assumption and needed in our analysis of discretization schemes for (1). For example, [5] used the condition $f \in H^1(0, 1)$. Here $f \in H_0^p(0, 1)$ and $u \in H^2(0, 1) \cap H_0^1(0, 1)$ admit odd extension to the domain $(-1, 1)$ and the convergent sine series in the corresponding spaces $H^p(-1, 1)$ and $H^2(-1, 1)$:

$$\begin{aligned} f(x) &= \sum_{(\xi/\pi)=1}^{\infty} \hat{f}(\xi) \sin(\xi x), \quad \hat{f}(\xi) = 2 \int_0^1 f(x) \sin(\xi x) \, dx, \\ u(x) &= \sum_{(\xi/\pi)=1}^{\infty} \hat{u}(\xi) \sin(\xi x), \quad \hat{u}(\xi) = 2 \int_0^1 u(x) \sin(\xi x) \, dx. \end{aligned}$$

From (1) and the sine series, we have $(k^2 - \xi^2)\hat{u}(\xi) = \hat{f}(\xi)$. Well-posedness of (1) amounts to $\lambda(\xi) := k^2 - \xi^2 \neq 0$ for all $\xi \in \pi\mathbb{N}$. In case (ii) $f = 0$, the exact solution is

$$u(x) = \frac{g_1 - g_0 \cos k}{\sin k} \sin(kx) + g_0 \cos(kx). \quad (2)$$

To analyze the discretization error for the homogeneous problem (ii), one just needs to find the closed form solution of the discretized problem. Usually, the discretization incurs a perturbation of the wavenumber k in the solution basis $\{\sin(kx), \cos(kx)\}$, which explains the error, and requires dispersion analysis.

2.2 Downsampling error

We shall discretize (1) on uniform grids with grid points $x_j := jh$, $j = 0, \dots, N$ where $Nh = 1$. Suppose $\mu := \frac{kh}{2} \leq C_\mu$ for a constant $C_\mu \in (0, \frac{\pi}{2})$. In a finite difference scheme, f is simply evaluated at the grid points x_j to give $f^h(x_j) := f(x_j)$. This causes aliasing of the sinusoidal modes in case (i), and gives the discrete sine transform

$$f^h(x_j) = \sum_{(\xi/\pi)=1}^{N-1} \widehat{f^h}(\xi) \sin(\xi x_j), \quad \widehat{f^h}(\xi) := 2 \sum_{j=1}^{N-1} h \sin(\xi x_j) f^h(x_j) = \hat{f}(\xi) + \sum_{s=\pm 1} s \sum_{m=1}^{\infty} \hat{f}(s\xi + 2mN\pi),$$

where the last equality comes from the fact $f^h(x_j) = f(x_j)$ and the rearrangement of

$$f(x_j) = \sum_{(\xi/\pi)=1}^{\infty} \hat{f}(\xi) \sin(\xi x_j) = \sum_{(\xi/\pi)=1}^{N-1} \left(\hat{f}(\xi) + \sum_{s=\pm 1} s \sum_{m=1}^{\infty} \hat{f}(s\xi + 2mN\pi) \right) \sin(\xi x_j)$$

permitted by the absolute convergence

$$\sum_{(\xi/\pi)=1}^{\infty} |\hat{f}(\xi)| \leq \sqrt{\sum_{(\xi/\pi)=1}^{\infty} \frac{1}{\xi^2}} \cdot \sqrt{\sum_{(\xi/\pi)=1}^{\infty} |\xi \hat{f}(\xi)|^2} < \infty.$$

Indeed, it is well known that $\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}$, and by Parseval's identity $\sum_{(\xi/\pi)=1}^{\infty} |\xi \hat{f}(\xi)|^2 = 2 \int_0^1 |f'|^2 dx$.

Let $u^h(x_j)$ be the finite difference solution defined by some scheme, e.g. (9). To calculate the error $e^h := u - u^h$ for case (i), we interpolate $u^h(x_j)$ to the domain $x \in (0, 1)$ by the discrete sine transform¹

$$u^h(x) = \sum_{(\xi/\pi)=1}^{N-1} \widehat{u^h}(\xi) \sin(\xi x), \quad x \in (0, 1), \quad \widehat{u^h}(\xi) := 2 \sum_{j=1}^{N-1} h \sin(\xi x_j) u^h(x_j).$$

So the error for case (i) can be expanded in the sine basis into

$$e^h(x) = \sum_{(\xi/\pi)=1}^{N-1} (\hat{u} - \widehat{u^h})(\xi) \sin(\xi x) + \sum_{(\xi/\pi)=N}^{\infty} \hat{u}(\xi) \sin(\xi x) =: e_1^h(x) + e_2^h(x). \quad (3)$$

We first estimate the H^1 -semi-norm of e_2^h . Note that

$$(e_2^h)'(x) = \sum_{(\xi/\pi)=N}^{\infty} \hat{u}(\xi) \xi \cos(\xi x) = \sum_{(\xi/\pi)=N}^{\infty} \frac{\xi}{k^2 - \xi^2} \hat{f}(\xi) \cos(\xi x). \quad (4)$$

Parseval's identity for the above cosine series reads

$$|e_2^h|_1^2 := \int_0^1 |(e_2^h)'|^2 dx = \frac{1}{2} \sum_{(\xi/\pi)=N}^{\infty} \frac{\xi^2}{(k^2 - \xi^2)^2} |\hat{f}(\xi)|^2. \quad (5)$$

By our assumption that $\frac{kh}{2} \leq C_\mu < \frac{\pi}{2}$, it holds $k < N\pi$, and for $\xi \geq N\pi$,

$$\frac{\xi^2}{(k^2 - \xi^2)^2} \leq \frac{(N\pi)^2}{((N\pi)^2 - k^2)^2} = \frac{\pi^2 h^2}{(\pi^2 - k^2 h^2)^2} \leq \frac{\pi^2 h^2}{(\pi^2 - 4C_\mu^2)^2}.$$

Hence, we obtain

$$|e_2^h|_1^2 \leq \frac{\pi^2 h^2}{(\pi^2 - 4C_\mu^2)^2} \cdot \frac{1}{2} \sum_{(\xi/\pi)=N}^{\infty} |\hat{f}(\xi)|^2.$$

¹The sine interpolation is chosen to facilitate our analysis because the continuous solution u is expanded to sine series. In [5], piecewise linear interpolation is used for analysis of a linear finite element method.

We distinguish the quantities that can and can not be resolved on the mesh,

$$f_{\text{low}} := \sum_{(\xi/\pi)=1}^{N-1} \hat{f}(\xi) \sin(\xi x), \quad f_{\text{high}} := \sum_{(\xi/\pi)=N}^{\infty} \hat{f}(\xi) \sin(\xi x), \quad \|f\| := \int_0^1 |f(x)|^2 dx, \quad (6)$$

where low and high are w.r.t. π/h , but not k (similarly, we also distinguish u_{low} and $u_{\text{high}} = e_2^h$). An ideal mesh is such that the low frequencies cover k i.e. $k < \pi/h$, and f_{high} is small compared to f_{low} . Then, it follows that

$$|e_2^h|_1 \leq \frac{\pi h}{\pi^2 - 4C_\mu^2} \|f_{\text{high}}\|.$$

Using higher regularity $f \in H_0^p(0, 1)$ allows the split $\frac{\xi^2}{(k^2 - \xi^2)^2} \frac{1}{\xi^{2p}} |\xi^p \hat{f}(\xi)|^2$ in (5) and yields

$$|e_2^h|_1 \leq \frac{h(kh)^p}{(\pi^2 - 4C_\mu^2)\pi^{p-1}} k^{-p} |f_{\text{high}}|_p, \quad |f|_p := \|f^{(p)}\| \text{ with } f^{(p)} \text{ the } p\text{th derivative}, \quad (7)$$

and also the L^2 -norm of the downsampling error estimate

$$\|e_2^h\| \leq \frac{h^2(kh)^p}{(\pi^2 - 4C_\mu^2)\pi^p} k^{-p} |f_{\text{high}}|_p. \quad (8)$$

Remark 1. Note that the separation $f = f_{\text{low}} + f_{\text{high}}$ depends on the mesh size $h = 1/N$. We have $f_{\text{low}} \rightarrow f$ and $f_{\text{high}} \rightarrow 0$ in $H^p(0, 1)$ as $N \rightarrow \infty$. By Parseval's identity or orthogonality of the basis, we see that $|f|_l^2 = |f_{\text{low}}|_l^2 + |f_{\text{high}}|_l^2$ for all $l = 0, \dots, p$. If $|f_{\text{high}}|_p = O(k^p)$ and $kh = O(1)$, then (7) and (8) say $|e_2^h|_1 = O(h)$ and $\|e_2^h\| = O(h^2)$, so the higher regularity does not improve the estimates.

The estimation of e_1^h in case (i) and the error in case (ii) both depend on the particular finite difference schemes, which we shall discuss as follows.

3 Analysis of classical 3-point centered scheme

The scheme uses the approximation $u''(x) \approx (u(x+h) - 2u(x) + u(x-h))/h^2$ to find u^h satisfying

$$(k^2 - \frac{2}{h^2})u^h(x_j) + \frac{1}{h^2}u^h(x_{j-1}) + \frac{1}{h^2}u^h(x_{j+1}) = f(x_j), \quad u^h(x_0) = g_0, \quad u^h(x_N) = g_1. \quad (9)$$

In case (i), $g_0 = g_1 = 0$, applying the discrete sine transform to the above equation gives

$$\left(k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}\right) \widehat{u^h}(\xi) = \widehat{f^h}(\xi) = \hat{f}(\xi) + \sum_{s=\pm 1} s \sum_{m=1}^{\infty} \hat{f}(s\xi + 2mN\pi), \quad \xi/\pi = 1, \dots, N-1.$$

In case (ii), $f = 0$, the solution of (9) can be found in closed form,

$$u^h(x_j) = \frac{g_1 - g_0 \cos k^h}{\sin k^h} \sin(k^h x_j) + g_0 \cos(k^h x_j), \quad x_j = jh, \quad j = 0, 1, \dots, N, \quad (10)$$

where $k^h := \frac{2}{h} \arcsin \frac{kh}{2}$ is the discrete wavenumber. The r.h.s. of (10) is valid if and only if $k^h \notin \mathbb{Z}\pi$ which we assume to hold. The problem (9) is well-posed if and only if $kh \in [2, \infty)$ or $k^h \notin \{1, \dots, N-1\}\pi$. Indeed, (9) can be written as an $(N-1) \times (N-1)$ linear system whose coefficient matrix has the eigenvalues $k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}$ and the eigenvectors $\sin(\xi x_j)$ for $\xi \in \{1, \dots, N-1\}\pi$. The formula (10) permits the grid function u^h to be densely defined in $[0, 1]$. Then the error $e^h(x) := u(x) - u^h(x)$ can be explicitly written as

$$e^h(x) = A_0(x)g_0 + A_1(x)g_1, \quad A_1(x) = \frac{\sin(kx)}{\sin k} - \frac{\sin(k^h x)}{\sin k^h}, \quad A_0(x) = A_1(1-x). \quad (11)$$

We shall first analyze the case (ii), $f = 0$, in subsection 3.1, and then case (i), $g_0 = g_1 = 0$, in the remaining subsections.

3.1 Error for the Dirichlet problem with zero source

From (11), we have

$$\|e^h\| \leq \|A_0\| \cdot |g_0| + \|A_1\| \cdot |g_1| = \|A_1\|(|g_0| + |g_1|).$$

This inequality is sharp by considering $g_0 = 0$ or $g_1 = 0$. So the key is to estimate $\|A_1\|$. We calculate

$$\begin{aligned} \int_0^1 \frac{\sin^2(kx)}{\sin^2 k} dx &= \frac{1}{\sin^2 k} \int_0^1 \frac{1 - \cos(2kx)}{2} dx = \frac{1}{2\sin^2 k} \left(1 - \frac{1}{2k} \sin(2k)\right), \\ \int_0^1 \frac{\sin^2(k^h x)}{\sin^2 k^h} dx &= \frac{1}{2\sin^2 k^h} \left(1 - \frac{1}{2k^h} \sin(2k^h)\right), \\ \int_0^1 \frac{\sin(kx) \sin(k^h x)}{(\sin k) \sin k^h} dx &= \frac{1}{(\sin k) \sin k^h} \frac{1}{2} \int_0^1 \cos((k - k^h)x) - \cos((k + k^h)x) dx \\ &= \frac{1}{2(\sin k) \sin k^h} \left(\frac{\sin(k^h - k)}{k^h - k} - \frac{\sin(k + k^h)}{k + k^h} \right). \end{aligned}$$

Therefore, we have

$$\begin{aligned} \|A_1\|^2 &= \int_0^1 \left[\frac{\sin(kx)}{\sin k} - \frac{\sin(k^h x)}{\sin k^h} \right]^2 dx \\ &= \frac{1}{2\sin^2 k} + \frac{1}{2\sin^2 k^h} - \frac{\cos k}{2k \sin k} - \frac{\cos k^h}{2k^h \sin k^h} - \frac{1}{(\sin k) \sin k^h} \left(\frac{\sin(k^h - k)}{k^h - k} - \frac{\sin(k + k^h)}{k + k^h} \right) \\ &= \frac{1}{(\sin k) \sin k^h} \left[\frac{1}{2} \frac{\sin k^h}{\sin k} + \frac{1}{2} \frac{\sin k}{\sin k^h} - \frac{(\sin k^h) \cos k}{2k} - \frac{(\sin k) \cos k^h}{2k^h} - \frac{\sin(k^h - k)}{k^h - k} + \frac{\sin(k + k^h)}{k + k^h} \right] \\ &=: \frac{1}{(\sin k) \sin k^h} (S_1 + S_2), \end{aligned}$$

where we separated the terms in the brackets into two parts

$$S_1 := \frac{1}{2} \frac{\sin k^h}{\sin k} + \frac{1}{2} \frac{\sin k}{\sin k^h} - \frac{\sin(k^h - k)}{k^h - k}, \quad S_2 := -\frac{(\sin k^h) \cos k}{2k} - \frac{(\sin k) \cos k^h}{2k^h} + \frac{\sin(k + k^h)}{k + k^h}, \quad (12)$$

where S_1 mainly accounts for the dispersion error, and S_2 is small for large k . Note that

$$\begin{aligned} \frac{\sin k^h}{\sin k} &= \frac{\sin(k^h - k + k)}{\sin k} = \frac{\sin(k^h - k) \cos k}{\sin k} + \cos(k^h - k), \\ \frac{\sin k}{\sin k^h} &= \frac{\sin(k - k^h + k^h)}{\sin k^h} = \frac{\sin(k - k^h) \cos k^h}{\sin k^h} + \cos(k - k^h). \end{aligned}$$

So we have

$$S_1 = \frac{1}{2} \sin(k^h - k) (\cot k - \cot k^h) + \cos(k^h - k) - \frac{\sin(k^h - k)}{k^h - k}. \quad (13)$$

We have also

$$\begin{aligned} S_2 &= -\frac{(\sin k^h) \cos k}{2k} - \frac{(\sin k) \cos k^h}{2k^h} + \frac{(\sin k) \cos k^h + (\sin k^h) \cos k}{k + k^h} \\ &= \frac{k^h - k}{2(k + k^h)} \left[\frac{(\sin k) \cos k^h}{k^h} - \frac{(\sin k^h) \cos k}{k} \right] \\ &= \frac{k^h - k}{2(k + k^h)} \left[\frac{(\sin k) \cos k^h - (\sin k^h) \cos k}{k} + \left(\frac{1}{k^h} - \frac{1}{k} \right) (\sin k) \cos k^h \right] \\ &= \frac{k^h - k}{2(k + k^h)} \left[\frac{\sin(k - k^h)}{k} + \frac{k - k^h}{kk^h} (\sin k) \cos k^h \right]. \end{aligned} \quad (14)$$

Lemma 1. Let $\sigma_k := \min_{\xi \in \pi\mathbb{N}} |k - \xi| > 0$. Then $|\sin k| = \sin \sigma_k \in (\frac{2}{\pi}, 1) \sigma_k$.

Proof. Let $n_k \in \mathbb{N}$ be such that $|k - n_k\pi| \leq \frac{\pi}{2}$. Since $\sin x \geq \frac{2}{\pi}x$ for $0 \leq x \leq \frac{\pi}{2}$, we have

$$|\sin k| = \sin |k - n_k\pi| = \sin \sigma_k \in \left(\frac{2}{\pi}, 1\right) \sigma_k,$$

where in the last equation we used the definition of σ_k . $\square$

Lemma 2. Let $k^h := \frac{2}{h} \arcsin \frac{kh}{2}$ and $0 < c < 1$. If $0 < \frac{kh}{2} < 1$, then $\frac{1}{24}k^3h^2 < k^h - k < \frac{\pi-2}{8}k^3h^2$. If in addition $\sigma_k := \min_{\xi \in \pi\mathbb{N}} |k - \xi| > 0$ and $k^3h^2 < \frac{8c\sigma_k}{\pi-2}$, then $k^h - k < c\sigma_k$ and $|\sin k^h| \in (\frac{2(1-c)}{\pi}, 1+c)\sigma_k$.

Proof. Since $x + \frac{x^3}{6} < \arcsin x < x + (\frac{\pi}{2} - 1)x^3$ for $0 < x < 1$, we have $k + \frac{1}{24}k^3h^2 < k^h < k + \frac{\pi-2}{8}k^3h^2 < k + c\sigma_k$. Then $|\xi - k| + |k^h - k| > |\xi - k^h| > |\xi - k| - |k^h - k|$ gives $\min_{\xi \in \pi\mathbb{N}} |\xi - k^h| \in (1 - c, 1 + c)\sigma_k$. So $|\sin k^h| \in (\frac{2(1-c)}{\pi}, 1 + c)\sigma_k$. $\square$

Remark 2. It is important to require k^3h^2 being small for convergence of the finite difference scheme. Otherwise, Lemma 2 says that $k^h - k$ can be large. For example, when k is large and $k^h - k = \pi$, we have $S_1 = -1$, $S_2 < \frac{\pi^2}{4k^3}$ and $\|A_1\| > 1 - \frac{\pi^2}{4k^3}$.

Lemma 3. Under the assumptions of Lemma 2, for S_1 in (13) it holds that

$$\nu(\sigma_k)(k^h - k)^2 < S_1 < \left(\frac{\pi^2}{8(1-c)^2\sigma_k^2} + \frac{1}{6}\right)(k^h - k)^2, \quad (15)$$

where, if $(1+c)\sigma_k > \frac{\pi}{2}$, $\nu(\sigma_k) := \frac{1}{8}$, and if $(1+c)\sigma_k \leq \frac{\pi}{2}$,

$$\nu(\sigma_k) := \max \left\{ \frac{1}{\pi(1+c)^2\sigma_k^2} - \frac{3}{8}, \frac{1}{8} \right\}.$$

Proof. Let $k \in ((n_k^+ - 1)\pi, n_k^+\pi)$ for an integer n_k^+ . By Lemma 2, it holds that $0 < k^h - k < c\sigma_k < \frac{\pi}{2}$. Moreover, $(n_k^+ - 1)\pi + \sigma_k \leq k < k^h < k + c\sigma_k \leq n_k^+\pi - (1-c)\sigma_k$. Hence $(n_k^+ - 1)\pi < k < k^h < n_k^+\pi$, $(n_k^+ - \frac{1}{2})\pi \in (k, k^h)$ only if $(1+c)\sigma_k > \frac{\pi}{2}$, and $\cot k - \cot k^h = \frac{k^h - k}{\sin^2 \tilde{k}}$ for some $\tilde{k} \in (k, k^h)$. Since

$$\max \left\{ x - \frac{1}{6}x^3, \frac{2}{\pi}x \right\} < \sin x < x - \frac{1}{8}x^3, \quad 1 - \frac{1}{2}x^2 < \cos x < 1, \quad \text{for } x \in \left(0, \frac{\pi}{2}\right),$$

it can be deduced from (13) that

$$S_1 < \frac{1}{2} \frac{(k^h - k)^2}{\min\{\sin^2 k, \sin^2 k^h\}} + 1 - \left(1 - \frac{1}{6}(k^h - k)^2\right); \quad \text{and if } (1+c)\sigma_k \leq \frac{\pi}{2},$$

$$S_1 > \frac{1}{2} \frac{2}{\pi} \frac{(k^h - k)^2}{\max\{\sin^2 k, \sin^2 k^h\}} + 1 - \frac{1}{2}(k^h - k)^2 - \left(1 - \frac{1}{8}(k^h - k)^2\right).$$

By Lemma 1 and 2, the two bounds in (15) are obtained. The other lower bound is derived from (12),

$$S_1 > 1 - \left(1 - \frac{1}{8}(k^h - k)^2\right) = \frac{1}{8}(k^h - k)^2,$$

where $0 < k^h - k < \frac{\pi}{2}$, $(n_k^+ - 1)\pi < k < k^h < n_k^+\pi$ and $x + \frac{1}{x} \geq 2$ for $x > 0$ are used. $\square$

Lemma 4. Let $k^h := \frac{2}{h} \arcsin \frac{kh}{2}$ and S_2 given in (14). If $0 < \frac{kh}{2} < 1$, then it holds that

$$-\left(\frac{1}{4k^2} + \frac{1}{4k^3}\right)(k^h - k)^2 < S_2 < \left(\frac{1}{4k^2} + \frac{1}{4k^3}\right)(k^h - k)^2.$$

Proof. The conclusion follows directly from $k^h > k > 0$, $|\sin x| \leq |x|$, $|\sin x| \leq 1$ and $|\cos x| \leq 1$. $\square$

Theorem 1 (L^2 Error for $f = 0$). *Under the assumptions of Lemma 2, for the L^2 -norm of A_1 in (11), it holds that*

$$\frac{1}{24\sigma_k\sqrt{1+c}}\sqrt{\nu(\sigma_k) - \frac{1}{4k^2} - \frac{1}{4k^3}k^3h^2} < \|A_1\| < \frac{\pi(\pi-2)}{16\sigma_k\sqrt{1-c}}\sqrt{\frac{\pi^2}{8(1-c)^2\sigma_k^2} + \frac{1}{6} + \frac{1}{4k^2} + \frac{1}{4k^3}k^3h^2},$$

where $\sigma_k = \min_{\xi \in \pi\mathbb{N}} |k - \xi| > 0$, $k^3h^2 \frac{(\pi-2)}{8\sigma_k} < c < 1$ and $\nu(\sigma_k)$ is defined in Lemma 3. Moreover, the error $e^h = u - u^h$ satisfies $\|e^h\| \leq \|A_1\|(|g_0| + |g_1|)$ with equality attained when $g_0 = 0$ or $g_1 = 0$, and the relative error satisfies

$$\frac{\|e^h\|}{\|u\|} \leq \frac{\sqrt{2}|\sin k|}{\sqrt{1 - \frac{\sin 2k}{2k}}} \|A_1\|$$

with equality attained when $g_0 = 0$ or $g_1 = 0$. Note also that $|\sin k| \asymp \sigma_k$ by Lemma 1.

Proof. The absolute error estimate is obtained by combining Lemmas 1, 2, 3 and 4. The relative error estimate follows from

$$\|u\| \geq \left| |g_1| \cdot \left\| \frac{\sin(kx)}{\sin k} \right\| - |g_0| \cdot \left\| \frac{\sin(k(1-x))}{\sin k} \right\| \right|$$

with equality attained when $g_0 = 0$ or $g_1 = 0$. $\square$

It is also interesting to estimate the H^1 -semi-norm of $A_1(x)$ in (11). Some calculations lead to

$$|A_1|_1^2 = \int_0^1 \left(k \frac{\cos(kx)}{\sin k} - k^h \frac{\cos(k^h x)}{\sin k^h} \right)^2 dx = \frac{kk^h}{\sin k \sin k^h} (\tilde{S}_1 + \tilde{S}_2),$$

where we introduced

$$\tilde{S}_1 := \frac{1}{2} \frac{k \sin k^h}{k^h \sin k} + \frac{1}{2} \frac{k^h \sin k}{k \sin k^h} - \frac{\sin(k^h - k)}{k^h - k}, \quad \tilde{S}_2 := \frac{(\sin k^h) \cos k}{2k^h} + \frac{(\sin k) \cos k^h}{2k} - \frac{\sin(k + k^h)}{k + k^h}. \quad (16)$$

More calculations as previously done for S_1 and S_2 yield

$$\begin{aligned} \tilde{S}_1 = & \frac{1}{2} \sin(k^h - k) (\cot k - \cot k^h) + \cos(k^h - k) - \frac{\sin(k^h - k)}{k^h - k} \\ & + (k^h - k) \left[-(\sin(k^h - k)) \left(\frac{\cot k}{2k^h} + \frac{\cot k^h}{2k} \right) + (\cos(k^h - k)) \frac{k^h - k}{2kk^h} \right], \end{aligned} \quad (17)$$

$$\tilde{S}_2 = \frac{k^h - k}{2(k + k^h)} \left[\frac{\sin(k - k^h)}{k} + \frac{k^h - k}{kk^h} (\sin k^h) \cos k \right]. \quad (18)$$

Lemma 5. *Under the assumptions of Lemma 2, for $\tilde{S}_1$ in (17) it holds that*

$$\tilde{\nu}(\sigma_k, k)(k^h - k)^2 < \tilde{S}_1 < \left(\frac{\pi^2}{8(1-c)^2\sigma_k^2} + \frac{1}{6} + \frac{\pi(2-c)}{4\sigma_k(1-c)k} + \frac{1}{2k^2} \right) (k^h - k)^2,$$

where, if $(1+c)\sigma_k > \frac{\pi}{2}$, $\tilde{\nu}(\sigma_k, k) := \frac{1}{8}$, and if $(1+c)\sigma_k \leq \frac{\pi}{2}$,

$$\tilde{\nu}(\sigma_k, k) := \max \left\{ \frac{1}{\pi(1+c)^2\sigma_k^2} - \frac{3}{8} - \frac{\pi(2-c)}{4\sigma_k(1-c)k} + \frac{2-c^2\sigma_k^2}{8k^2}, \frac{1}{8} \right\}.$$

Proof. The lower bound $\frac{1}{8}(k^h - k)^2$ is derived from (16) similarly to the proof of Lemma 3. For the other bounds, note that the first line of (17) equals S_1 , and by Lemma 1 and 2 the remaining line satisfies

$$\begin{aligned} & (k^h - k) \left[-(\sin(k^h - k)) \left(\frac{\cot k}{2k^h} + \frac{\cot k^h}{2k} \right) + (\cos(k^h - k)) \frac{k^h - k}{2kk^h} \right] \\ & \in (k^h - k)^2 \left(-\frac{\pi(2-c)}{4\sigma_k(1-c)k} + \frac{1 - \frac{1}{2}(k^h - k)^2}{2kk^h}, \frac{\pi(2-c)}{4\sigma_k(1-c)k} + \frac{1}{2k^2} \right). \end{aligned}$$

We conclude by using $k^h - k < c\sigma_k$, $k^h = \frac{2}{h} \arcsin \frac{kh}{2} < \frac{\pi}{2}k < 2k$ and Lemma 3. $\square$

Lemma 6. Let $k^h := \frac{2}{h} \arcsin \frac{kh}{2}$ and $\tilde{S}_2$ be given in (18). If $0 < \frac{kh}{2} < 1$, then it holds that

$$-\left(\frac{1}{4k^2} + \frac{1}{4k^3}\right)(k^h - k)^2 < \tilde{S}_2 < \left(\frac{1}{4k^2} + \frac{1}{4k^3}\right)(k^h - k)^2.$$

Proof. The conclusion follows directly from $k^h > k > 0$, $|\sin x| \leq |x|$, $|\sin x| \leq 1$ and $|\cos x| \leq 1$. $\square$

Theorem 2 (H^1 error for $f = 0$). Under the assumptions of Lemma 2, for A_1 in (11), we have

$$\frac{1}{24\sigma_k\sqrt{1+c}}\sqrt{\tilde{\nu}(\sigma_k, k) - \frac{1}{4k^2} - \frac{1}{4k^3}k^4h^2} < |A_1|_1 < \frac{\pi(\pi-2)}{16\sigma_k\sqrt{1-c}}\sqrt{\frac{\pi^2}{4(1-c)^2\sigma_k^2} + \frac{1}{3} + \frac{\pi(2-c)}{2\sigma_k(1-c)k} + \frac{3}{2k^2} + \frac{1}{2k^3}k^4h^2},$$

where $\sigma_k = \min_{\xi \in \pi\mathbb{N}} |k - \xi| > 0$, $k^3h^2 \frac{(\pi-2)}{8\sigma_k} < c < 1$, and $\tilde{\nu}(\sigma_k, k)$ is defined in Lemma 5. Moreover, the error $e^h = u - u^h$ satisfies $|e^h|_1 \leq |A_1|_1(|g_0| + |g_1|)$ with equality attained when $g_0 = 0$ or $g_1 = 0$, and the relative error satisfies

$$\frac{|e^h|_1}{|u|_1} \leq \frac{\sqrt{2}|\sin k|}{\sqrt{1 + \frac{\sin 2k}{2k}}} \cdot \frac{|A_1|_1}{k}$$

with equality attained when $g_0 = 0$ or $g_1 = 0$. Note also that $|\sin k| \asymp \sigma_k$ by Lemma 1.

Proof. The conclusion is obtained by combining Lemmas 1, 2, 5, 6, and $k^h = \frac{2}{h} \arcsin \frac{kh}{2} < \frac{\pi}{2}k < 2k$. $\square$

3.2 Well-posedness of the classical 3-point centered scheme

The discretized problem is well-posed if and only if $\lambda^h(\xi) := k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2} \neq 0$ for $\xi \in \{1, \dots, N-1\}\pi$. Given that the continuous problem (1) is well-posed, we can expect for *all* sufficiently small h that the discretized problem is also well-posed. A corresponding upper bound for h is:

Lemma 7. Suppose $\sigma_k := \min_{\xi \in \pi\mathbb{N}} |k - \xi| > 0$. Let $n_k^+ \in \mathbb{N}$ such that $(n_k^+ - 1)\pi < k < n_k^+\pi$. If

$$0 < h = \frac{1}{N} < h_k := 2\sqrt{3\sigma_k} / \left(\frac{\sigma_k}{2} + n_k^+\pi\right)^{3/2} = O(\sqrt{\sigma_k}k^{-3/2}), \quad (19)$$

or $k(kh)^2/\sigma_k \ll 1$ (as found in [9] for general FEMs), then

$$\sigma_k^h := \min_{(\xi/\pi)=1, \dots, N-1} \left| k - \frac{2}{h} \sin \frac{\xi h}{2} \right| \geq \frac{\sigma_k}{2}, \quad (20)$$

and $\lambda^h := k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2} \geq \max\{2k - \frac{\sigma_k}{2}, k + \frac{\sigma_k}{2}\} \frac{\sigma_k}{2}$.

Proof. If $\frac{2}{h} \sin \frac{\xi h}{2} \geq n_k^+\pi$ or $\frac{2}{h} \sin \frac{\xi h}{2} \leq (n_k^+ - 1)\pi$, then $\left| k - \frac{2}{h} \sin \frac{\xi h}{2} \right| \geq \sigma_k$. If $\xi < k$, then

$$\frac{2}{h} \sin \frac{\xi h}{2} \leq \xi < k \text{ and } \left| k - \frac{2}{h} \sin \frac{\xi h}{2} \right| = k - \frac{2}{h} \sin \frac{\xi h}{2} \geq k - \xi = |k - \xi| \geq \sigma_k.$$

We need only to consider the case $(n_k^+ - 1)\pi < \frac{2}{h} \sin \frac{\xi h}{2} < n_k^+\pi$ and $\xi \geq n_k^+\pi$. It suffices to show that $n_k^+\pi - \frac{2}{h} \sin \frac{\xi h}{2} < \frac{\sigma_k}{2}$, which is equivalent to

$$\frac{\xi h}{2} - \sin \frac{\xi h}{2} < \frac{\sigma_k h}{4} + \frac{\xi h - n_k^+\pi h}{2}.$$

It is thus enough to show that $\theta - \sin \theta < \sigma_k h/4$ for $\theta = \xi h/2$. Since $\sin \theta > \theta - \frac{\theta^3}{3!}$ for $\theta \in (0, \pi/2)$, it suffices to show $\frac{\theta^3}{3!} < \sigma_k h/4$, which is equivalent to $\sin \theta < \sin \sqrt[3]{3\sigma_k h/2} =: \sin v$. Since $\sin \theta < n_k^+\pi h/2$ and $\sin v > v - \frac{v^3}{3!}$, it is enough to show that $n_k^+\pi h/2 < v - \frac{v^3}{3!}$, which is

$$n_k^+\pi h/2 < \sqrt[3]{3\sigma_k h/2} - (\sigma_k h/4).$$

Solving the inequality for h gives the conclusion. $\square$

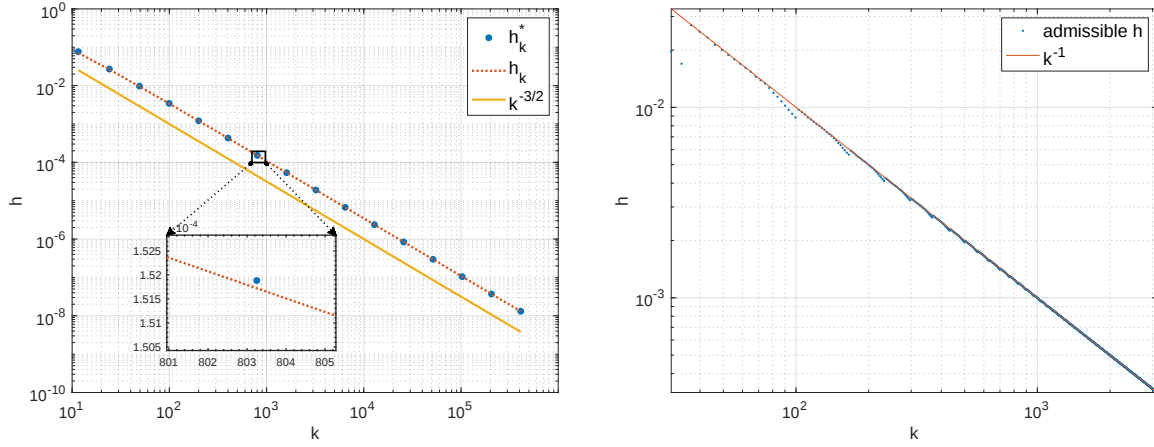


Figure 1: Admissible mesh size h for well-posedness of (9). Left: Upper bounds h_k (19) and h_k^* (21) so that all smaller h verifies (20) with $\sigma_k = 1$. Right: Existence of $h = O(k^{-1})$ verifying (20) with $\sigma_k = 1$.

Remark 3. If we define $h_k^* > 0$ as the largest reciprocal of an integer such that

$$\min_{(\xi/\pi)=1, \dots, N-1} \left| k - \frac{2}{h} \sin \frac{\xi h}{2} \right| \geq \frac{\sigma_k}{2} \quad (21)$$

for all $h = 1/N \in (0, h_k^*)$, then h_k^* is likely of the same order in k as the upper bound h_k in (19) is. This is illustrated on the left of Fig. 1. But Lemma 7 does not prohibit using larger mesh size. The existence of a mesh size $h \sim k^{-1}$ that verifies $\sigma_k^h \geq \sigma_k/2$ is shown on the right of Fig. 1.

3.3 Aliasing error of the classical 3-point centered scheme

From now on, we assume that $\lambda^h \neq 0$. Then the derivative of the partial error e_1^h in (3) is

$$\begin{aligned} (e_1^h)'(x) &= \sum_{(\xi/\pi)=1}^{N-1} \left(\hat{u}(\xi) - \widehat{u^h}(\xi) \right) \xi \cos(\xi x) = (E_1^h)'(x) - (E_2^h)'(x) \\ &:= \sum_{(\xi/\pi)=1}^{N-1} \left(\frac{\xi}{\lambda} - \frac{\xi}{\lambda^h} \right) \hat{f}(\xi) \cos(\xi x) - \sum_{(\xi/\pi)=1}^{N-1} \frac{\xi}{\lambda^h} \sum_{s=\pm 1} s \sum_{m=1}^{\infty} \hat{f}(s\xi + 2mN\pi) \cos(\xi x). \end{aligned} \quad (22)$$

To estimate E_2^h , we first note that

$$\left| \sum_{m=1}^{\infty} \hat{f}(\pm\xi + 2mN\pi) \right| \leq \sqrt{\sum_{m=1}^{\infty} \frac{1}{(\pm\xi + 2mN\pi)^{2p}}} \cdot \sqrt{\sum_{m=1}^{\infty} |(\pm\xi + 2mN\pi)^p \hat{f}(\pm\xi + 2mN\pi)|^2}, \quad (23)$$

and for $0 \leq \xi \leq (N-1)\pi$ that

$$\sum_{m=1}^{\infty} \frac{1}{(\pm\xi + 2mN\pi)^{2p}} \leq \frac{1}{(\pm\xi + 2N\pi)^{2p}} + \frac{1}{2N\pi} \int_{\pm\xi + 2N\pi}^{\infty} \frac{1}{t^{2p}} dt \leq \frac{2p}{2p-1} \frac{1}{((\frac{3}{2} \pm \frac{1}{2})N\pi)^{2p}}. \quad (24)$$

We can then estimate

$$\begin{aligned}
|E_2^h|_1^2 &= \sum_{(\xi/\pi)=1}^{N-1} \frac{\xi^2}{|\lambda^h|^2} \left| \sum_{s=\pm 1} \sum_{m=1}^{\infty} \hat{f}(s\xi + 2mN\pi) \right|^2 \\
&\leq \max_{\xi \in \{1, \dots, N-1\}\pi} \frac{\xi^2}{|\lambda^h|^2} \sum_{(\xi/\pi)=1}^{N-1} \left| \sum_{s=\pm 1} \sum_{m=1}^{\infty} \hat{f}(s\xi + 2mN\pi) \right|^2 \\
&\leq 2 \max_{\xi \in \{1, \dots, N-1\}\pi} \frac{\xi^2}{|\lambda^h|^2} \sum_{(\xi/\pi)=1}^{N-1} \left[\left| \sum_{m=1}^{\infty} \hat{f}(\xi + 2mN\pi) \right|^2 + \left| \sum_{m=1}^{\infty} \hat{f}(-\xi + 2mN\pi) \right|^2 \right].
\end{aligned}$$

Therefore, for $p \geq 1$, using (24), we have

$$|E_2^h|_1 \leq 2 \max_{\xi \in \{1, \dots, N-1\}\pi} \frac{\xi}{|\lambda^h|} \frac{h^p}{\pi^p} |f_{\text{high}}|_p. \quad (25)$$

Lemma 8. Suppose $k > \pi$, $0 < \frac{kh}{2} \leq C_\mu < 1$, and there is a sequence of $h = \frac{1}{N}$ going to zero such that

$$\tilde{\sigma}_k := \min_{\xi, h} \left| k - \frac{2}{h} \sin \frac{\xi h}{2} \right| > 0 \text{ over } \xi \in \{1, \dots, N-1\}\pi \text{ and the sequence of } h \text{ going to zero.}$$

Then, for $\lambda^h = k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}$, the H^1 -semi-norm of the aliasing error E_2^h in (22) satisfies

$$|E_2^h|_1 \leq \frac{(kh)^p}{\tilde{\sigma}_k \pi^{p-1}} k^{-p} |f_{\text{high}}|_p. \quad (26)$$

Proof. Based on (25), it suffices to find an upper bound of

$$\frac{\xi}{|\lambda^h|} = \frac{\xi}{|k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}|} \quad \text{over } \xi \in \{1, \dots, N-1\}\pi.$$

Denote $\theta_k := \arcsin \frac{kh}{2}$ and $\theta := \frac{\xi h}{2}$. Then

$$\frac{\xi}{|\lambda^h|} = \frac{h}{2} \frac{\theta}{|\sin^2 \theta_k - \sin^2 \theta|} =: \frac{h}{2} \phi(\theta) \quad \text{for } \theta \in \{1, \dots, N-1\} \frac{\pi h}{2} =: \Theta.$$

When $\theta < \theta_k$, the function $\phi(\theta)$ increases with θ . Let $\theta_- := \max\{\theta \in \Theta : \theta < \theta_k\}$. So

$$\phi(\theta) \leq \frac{\theta_-}{\sin^2 \theta_k - \sin^2 \theta_-} \leq \frac{2}{h\tilde{\sigma}_k} \cdot \frac{\theta_-}{\sin \theta_k + \sin \theta_-} \leq \frac{2}{h\tilde{\sigma}_k} \cdot \frac{\theta_-}{\frac{2}{\pi}\theta_k + \frac{2}{\pi}\theta_-} < \frac{\pi}{2h\tilde{\sigma}_k} \quad \text{when } \theta \in \Theta \cap (0, \theta_k).$$

When $\theta > \theta_k$, the function $\phi(\theta)$ has the derivative

$$\phi'(\theta) = \frac{\sin^2 \theta - \sin^2 \theta_k - \theta \sin(2\theta)}{(\sin^2 \theta - \sin^2 \theta_k)^2}.$$

So any stationary point θ_c of ϕ satisfies $\sin^2 \theta_c - \sin^2 \theta_k - \theta_c \sin(2\theta_c) = 0$ and

$$\phi(\theta_c) = \frac{\theta_c}{\sin^2 \theta_c - \sin^2 \theta_k} = \frac{1}{\sin(2\theta_c)}.$$

Let $\theta_+ := \min\{\theta \in \Theta : \theta > \theta_k\}$ and $\theta_{\max} := \max \Theta$. If $\theta_+ < \frac{\pi}{4}$, then the numerator of $\phi'(\theta_+)$ satisfies

$$\sin^2 \theta_+ - \sin^2 \theta_k - \theta_+ \sin(2\theta_+) = \sin(2\tilde{\theta})(\theta_+ - \theta_k) - \theta_+ \sin(2\theta_+) < 0,$$

because by the mean value theorem $\tilde{\theta} < \theta_+$. Note that the derivative of the numerator of $\phi'(\theta)$ is $-2\theta \cos(2\theta)$. So if $\theta_+ < \frac{\pi}{4}$, then $\phi' < 0$ on $[\theta_+, \frac{\pi}{4}]$. Therefore, no matter $\theta_+ < \frac{\pi}{4}$ or not, any stationary point θ_c of ϕ in $[\theta_+, \theta_{\max}]$ must satisfy $\theta_c \geq \frac{\pi}{4}$. It follows that

$$\phi(\theta_c) \leq \frac{1}{\sin(2\theta_{\max})} = \frac{1}{\sin((N-1)\pi h)} = \frac{1}{\sin(\pi h)} \leq \frac{1}{2h}.$$

Since $k > \pi$, the numerator of $\phi'(\theta_{\max})$ satisfies

$$\sin^2 \frac{\pi h}{2} - \sin^2 \theta_k - (1-h) \frac{\pi}{2} \sin(\pi h) < \frac{\pi^2 h^2}{4} - \frac{k^2 h^2}{4} - (1-h)\pi h < 0.$$

Note that

$$\phi(\theta_+) = \frac{\theta_+}{\sin^2 \theta_k - \sin^2 \theta_+} \leq \frac{2}{h\tilde{\sigma}_k} \cdot \frac{\theta_+}{\sin \theta_k + \sin \theta_+} < \frac{2}{h\tilde{\sigma}_k} \cdot \frac{\theta_+}{\sin \theta_+} < \frac{\pi}{h\tilde{\sigma}_k}.$$

So we obtain

$$\max_{\theta \in \Theta} \phi(\theta) < \max\left\{\frac{\pi}{h\tilde{\sigma}_k}, \frac{1}{2h}\right\} = \frac{\pi}{h\tilde{\sigma}_k}, \quad \text{and} \quad \max_{\xi \in \{1, \dots, N-1\}} \frac{\xi}{|\lambda^h|} < \frac{\pi}{2\tilde{\sigma}_k}.$$

Substituting this into (25) gives the conclusion. $\square$

Remark 4. By Lemma 8 the second part $(E_2^h)'$ of $(e_1^h)'$ in (22) is controlled, similarly to $(e_2^h)'$ in (4), by source f_{high} not resolved by the grid, when $k > \pi$, $\frac{kh}{2} \leq C_\mu < 1$ and $\tilde{\sigma}_k > 0$. But $|E_2^h|_1$ behaves as $O((kh)^p/\tilde{\sigma}_k)$, much larger than $|e_2^h|_1 = O(h(kh)^p)$, if $|f_{\text{high}}|_p = O(k^p)$.

The L^2 -norm of the aliasing error can also be derived. Recall that

$$\begin{aligned} e_1^h(x) &= \sum_{(\xi/\pi)=1}^{N-1} \left(\hat{u}(\xi) - \widehat{u^h}(\xi) \right) \sin(\xi x) = E_1^h(x) - E_2^h(x) \\ &= \sum_{(\xi/\pi)=1}^{N-1} \left(\frac{1}{\lambda} - \frac{1}{\lambda^h} \right) \hat{f}(\xi) \sin(\xi x) - \sum_{(\xi/\pi)=1}^{N-1} \frac{1}{\lambda^h} \sum_{s=\pm 1} \sum_{m=1}^{\infty} \hat{f}(s\xi + 2mN\pi) \sin(\xi x). \end{aligned} \quad (27)$$

Lemma 9. Suppose $k > \pi$, $0 < \frac{kh}{2} \leq C_\mu < 1$, and there is a sequence of $h = \frac{1}{N}$ going to zero such that

$$\tilde{\sigma}_k := \min_{\xi, h} \left| k - \frac{2}{h} \sin \frac{\xi h}{2} \right| > 0 \text{ over } \xi \in \{1, \dots, N-1\}\pi \text{ and the sequence of } h \text{ going to zero.}$$

Then, for $\lambda^h = k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}$, the L^2 -norm of the aliasing error E_2^h in (27) satisfies

$$\|E_2^h\| \leq \frac{2h(kh)^{p-1}}{\tilde{\sigma}_k \pi^p} k^{-p} |f_{\text{high}}|_p.$$

Proof. Based on (23) and (24), we have

$$\begin{aligned} \|E_2^h\|^2 &= \sum_{(\xi/\pi)=1}^{N-1} \frac{1}{|\lambda^h|^2} \left| \sum_{s=\pm 1} \sum_{m=1}^{\infty} \hat{f}(s\xi + 2mN\pi) \right|^2 \\ &\leq \max_{\xi \in \{1, \dots, N-1\}\pi} \frac{1}{|\lambda^h|^2} \sum_{(\xi/\pi)=1}^{N-1} \left| \sum_{s=\pm 1} \sum_{m=1}^{\infty} \hat{f}(s\xi + 2mN\pi) \right|^2 \\ &\leq 2 \max_{\xi \in \{1, \dots, N-1\}\pi} \frac{1}{|\lambda^h|^2} \sum_{(\xi/\pi)=1}^{N-1} \left[\left| \sum_{m=1}^{\infty} \hat{f}(\xi + 2mN\pi) \right|^2 + \left| \sum_{m=1}^{\infty} \hat{f}(-\xi + 2mN\pi) \right|^2 \right]. \end{aligned}$$

Therefore, for $p \geq 1$, using (24), we get

$$\|E_2^h\| \leq 2 \max_{\xi \in \{1, \dots, N-1\}\pi} \frac{1}{|\lambda^h|} \frac{h^p}{\pi^p} |f_{\text{high}}|_p.$$

Note that

$$\frac{1}{|\lambda^h|} = \frac{1}{|k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}|} = \frac{1}{|k - \frac{2}{h} \sin \frac{\xi h}{2}|} \frac{1}{|k + \frac{2}{h} \sin \frac{\xi h}{2}|} \leq \frac{1}{\tilde{\sigma}_k k}.$$

Combining the above two inequalities gives the conclusion. $\square$

Remark 5. By Lemma 9, the L^2 -norm of the aliasing error is $O\left(\frac{(kh)^p}{\tilde{\sigma}_k k}\right)$ if $|f_{\text{high}}|_p = O(k^p)$. This can be compared to the H^1 -semi-norm of the aliasing error which is $O\left(\frac{(kh)^p}{\tilde{\sigma}_k}\right)$; see Lemma 8.

3.4 Absolute error estimates of the classical 3-point centered scheme

We now turn to estimate the first part of $(e_1^h)'$ given in (3) and (22),

$$(E_1^h)'(x) = \sum_{(\xi/\pi)=1}^{N-1} \left(\frac{\xi}{\lambda} - \frac{\xi}{\lambda^h} \right) \hat{f}(\xi) \cos(\xi x), \quad (28)$$

the only part of $(e^h)' = (E_1^h)' - (E_2^h)' + (e_2^h)'$ controlled by the grid well-resolved source f_{low} . Since

$$\|E_1^h\|_1^2 = \frac{1}{2} \sum_{(\xi/\pi)=1}^{N-1} \left| \frac{\xi}{\lambda} - \frac{\xi}{\lambda^h} \right|^2 |\hat{f}(\xi)|^2 \leq \|f_{\text{low}}\|^2 \max_{\xi \in \{1, \dots, N-1\}\pi} \left| \frac{\xi}{\lambda} - \frac{\xi}{\lambda^h} \right|^2, \quad (29)$$

we need only to find the maximum of

$$\psi(\xi) := \left| \frac{\xi}{\lambda} - \frac{\xi}{\lambda^h} \right| = \left| \frac{\xi}{k^2 - \xi^2} - \frac{\xi}{k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}} \right| = \frac{h}{2} \left| \frac{\theta}{\mu^2 - \theta^2} - \frac{\theta}{\mu^2 - \sin^2 \theta} \right| =: \frac{h}{2} \phi(\theta) \quad (30)$$

for $\mu := kh/2$ and $\theta := \xi h/2$.

Remark 6. The inequality in (29) is sharp. Let $\xi_* := \arg \max_{\xi \in \{1, \dots, N-1\}\pi} \psi(\xi)$. Then the inequality holds with equality if $f_{\text{low}} = \hat{f}(\xi_*) \sin(\xi_* x)$. In the convergence test, one usually takes a fixed f as $h \rightarrow 0$. So the sharpness may be perturbed if ξ_* depends on h . This is not an issue, if ξ_* is independent of h or if ξ_* varies slightly around a fixed number, which is the case for ξ_* being the continuous frequencies ξ closest to k , or their discrete counterparts $\frac{2}{h} \sin \frac{\xi h}{2}$ closest to k , as we shall see in Lemma 10. However, for the case $\xi_* = (N-1)\pi$ which we shall also see in Lemma 10, the sharpness will require a changing f at higher and higher frequency as $h \rightarrow 0$. In that case, we will derive an alternate estimate to (29) using the smoothness of a fixed f .

Lemma 10. Suppose $k > 2\pi$, $\mu := \frac{kh}{2} \leq C_\mu < 1$, $\sigma_k := \min_{\xi \in \pi\mathbb{N}} |k - \xi| > 0$, and there is a sequence of $h = \frac{1}{N}$ ($N \geq 4$) going to zero such that

$$\tilde{\sigma}_k := \min_{\xi, h} \left| k - \frac{2}{h} \sin \frac{\xi h}{2} \right| > 0 \text{ over } \xi \in \{1, \dots, N-1\}\pi \text{ and the sequence of } h \text{ going to zero.}$$

Let $k^h := \frac{2}{h} \arcsin \frac{kh}{2}$, $\xi_{\max} = (N-1)\pi$, and $k_\pm \in \pi\mathbb{N}$ (resp. $k_\pm^h \in \pi\mathbb{N}$) be the closest points such that $k_- < k < k_+$ (resp. $k_-^h < k^h < k_+^h$). Then, $k_+ < \xi_{\max}$, and

$$\max_{\xi \in \{1, \dots, N-1\}\pi} \psi(\xi) = \max\{\psi(k_-), \psi(k_+), \psi(k_-^h), \psi(k_+^h), \psi(\xi_{\max})\},$$

where ψ is given in (30), $\psi(k_\pm^h)$ can be removed if $k_\pm^h \geq \xi_{\max}$, and k_+ (resp. k_-^h) equals k_+^h (resp. k_-) when $\pi\mathbb{N} \cap (k, k^h) = \emptyset$. Moreover, we have

$$\begin{aligned} \frac{k^3 h^2}{(240\sigma_- + k^3 h^2)6\sigma_-} &< \psi(k_-) < \frac{k^3 h^2}{(24\sigma_- + k^3 h^2)2\sigma_-}, \\ \frac{1}{15} \frac{(k + \sigma_+)^3 h^2}{\sigma_+ (4\sigma_-^h + k^3 h^2)} &< \psi(k_+) < \frac{2}{3} \frac{k^3 h^2}{\sigma_-^h \sigma_+ \sqrt{1 - C_\mu^2}}, \end{aligned} \quad \text{if } \pi\mathbb{N} \cap (k, k^h) \neq \emptyset,$$

$$\frac{(1 - \frac{\pi^2}{80} C_\mu^2)(k + \sigma_+)^3 h^2}{12\sigma_-^h(4\sigma_+ + k^3 h^2)} < \psi(k_-^h) < \frac{\pi^4}{384} \frac{k^3 h^2}{\sigma_-^h \sigma_+ \sqrt{1 - C_\mu^2}}, \quad \text{if } \pi\mathbb{N} \cap (k, k^h) \neq \emptyset,$$

$$\frac{(1 - \frac{(1+\pi)^2}{80} C_\mu^2)(k + \sigma_+^h)^3 h^2}{3(4\sigma_+^h + k^3 h^2)^2} < \psi(k_+^h) < \frac{(1 + \pi)^4}{16} \frac{k^3 h^2}{\sigma_+^h(24\sigma_+^h + k^3 h^2) \cos(\theta_\mu + \frac{\sigma_+^h h}{2})}, \quad \text{if } C_\mu < \cos \frac{\sigma_+^h h}{2},$$

$$\frac{h}{\pi} \left(\frac{9\pi^2}{64} - 1 \right) < \psi(\xi_{\max}) < \frac{4(\pi^2 - 4)\pi h}{(\cos^2 \frac{\pi h}{2} - C_\mu^2)(9\pi^2 - 64)}, \quad \text{if } C_\mu < \cos \frac{\pi h}{2},$$

where $\sigma_\pm := |k - k_\pm| \geq \sigma_k = \min\{\sigma_-, \sigma_+\}$, $\sigma_\pm^h := |k^h - k_\pm^h| \geq \tilde{\sigma}_k$ and $\theta_\mu := \arcsin C_\mu$.

Remark 7. Note that $\pi\mathbb{N} \cap (k, k^h) \neq \emptyset$ if and only if $k_+ < k^h$. Using $\mu^3/6 < \arcsin \mu - \mu < (\pi - 2)\mu^3/2$ for $0 < \mu < 1$, we find a sufficient condition for $k_+ \geq k^h$ is that $k^3 h^2 \leq 8\sigma_+ / (\pi - 2)$ and a sufficient condition for $k_+ < k^h$ is that $k^3 h^2 > 24\sigma_+$.

Remark 8. On the one hand, if $k^3 h^2 \gtrsim \sigma_-$, then the lower bound of $\psi(k_-)$ is greater than a positive constant times $1/\sigma_-$, independent of k and h , no matter how small kh is. On the other hand, if $k^3 h^2 < C$, then based on Lemma 10 we can find the bounds

$$\frac{k^3 h^2}{(240\sigma_- + C)6\sigma_-} < \psi(k_-) < \frac{k^3 h^2}{48\sigma_-}.$$

In particular, if $k^3 h^2 \lesssim \sigma_k$ and $\sigma_- = \sigma_k$, then $\psi(k_-) \asymp k^3 h^2 / \sigma_k^2$. If $\sigma_+ = \sigma_k$ and the assumptions of Lemma 2 hold, then $\sigma_+^h \asymp \sigma_k$ and $\psi(k_+^h) \asymp k^3 h^2 / \sigma_k^2$.

Proof of Lemma 10. Let $\Theta := \{1, \dots, N-1\} \frac{\pi h}{2}$, $\theta_k := \arcsin \mu$, $\theta_{\max} := \frac{h}{2} \xi_{\max} = \frac{\pi}{2}(1-h)$, $\mu_\pm := \frac{h}{2} k_\pm$, and $\theta_\pm := \frac{h}{2} k_\pm^h$. We first show that $\sigma_\pm^h \geq \tilde{\sigma}_k$. Indeed, by the mean value theorem, it holds

$$|k^h - k_\pm^h| = \frac{2}{h} \left| \arcsin \frac{kh}{2} - \frac{k_\pm^h h}{2} \right| = \frac{2}{h} |\theta_k - \theta_\pm| \geq \frac{2}{h} |\sin \theta_k - \sin \theta_\pm| = \left| k - \frac{2}{h} \sin \frac{k_\pm^h h}{2} \right|.$$

Recall the definition of ϕ in (30). When $0 < \theta < \mu$, the function

$$\phi(\theta) = \frac{(\theta^2 - \sin^2 \theta)\theta}{(\mu^2 - \theta^2)(\mu^2 - \sin^2 \theta)}$$

is increasing because the numerator is increasing and the denominator is decreasing. Indeed, $(\theta^2 - \sin^2 \theta)' = 2\theta - \sin(2\theta) > 0$. So the max $\phi(\theta)$ over $[0, \mu_-]$ is attained at $\theta = \mu_-$.

When $\mu < \theta < \theta_k$, we have

$$\phi(\theta) = \frac{\theta}{\theta^2 - \mu^2} + \frac{\theta}{\mu^2 - \sin^2 \theta} = \frac{1}{2} \left(\frac{1}{\theta - \mu} + \frac{1}{\theta + \mu} \right) + \frac{1}{2\mu} \left(\frac{\theta}{\mu - \sin \theta} + \frac{\theta}{\mu + \sin \theta} \right).$$

Note that $1/(\theta \pm \mu)$ is convex for $\theta \in (\mu, \infty)$. We calculate

$$\left(\frac{\theta}{\mu \pm \sin \theta} \right)' = \frac{1}{\mu \pm \sin \theta} - \frac{\pm \theta \cos \theta}{(\mu \pm \sin \theta)^2}, \quad \left(\frac{\theta}{\mu \pm \sin \theta} \right)'' = \frac{\mp 2 \cos \theta \pm \theta \sin \theta}{(\mu \pm \sin \theta)^2} + \frac{2\theta \cos^2 \theta}{(\mu \pm \sin \theta)^3}.$$

Since $1 \geq \mu = \sin \theta_k > \sin \theta > 0$ and $\theta > 0$, we have

$$\frac{2 \cos \theta}{(\mu - \sin \theta)^2} > \frac{2 \cos \theta}{(\mu + \sin \theta)^2}, \quad \frac{2\theta \cos^2 \theta}{(\mu - \sin \theta)^3} \geq \frac{\theta \sin \theta}{(\mu - \sin \theta)^2}.$$

Hence, ϕ is convex for $\theta \in (\mu, \theta_k)$. If $\mu_+ \leq \theta_-$ (that is, $\Theta \cap (\mu, \theta_k) \neq \emptyset$), then $\phi(\theta)$ for $\theta \in [\mu_+, \theta_-]$ attains its maximum at either μ_+ or θ_- .

When $\theta_k < \theta < \frac{\pi}{2}$, we have

$$\phi(\theta) = \frac{\theta}{\sin^2 \theta - \mu^2} - \frac{\theta}{\theta^2 - \mu^2} \text{ has no local maximum for } \theta_k < \theta < \frac{\pi}{2} \text{ and } 0 < \mu < 1. \quad (31)$$

The proof can be found in Appendix A. Hence, $\phi(\theta)$ on $\theta \in [\theta_+, \theta_{\max}]$ attains its maximum at either θ_+ or $\theta_{\max}$ when $\theta_+ < \theta_{\max}$ (otherwise, there is no such interval to consider). Note that if $\mu \leq C_\mu < \frac{1}{2}$ and $k > \pi$ then it holds that $\theta_+ < \theta_{\max}$. Indeed, we have $h < \frac{1}{\pi} < \frac{2}{\pi + \sigma_+^h}$ so $\sin(\theta_{\max} - \frac{\sigma_+^h h}{2}) = \cos(\frac{\pi + \sigma_+^h}{2} h) > 1 - \frac{(\pi + \sigma_+^h)^2}{8} h^2 > \frac{1}{2} > \sin \theta_k$.

Next, we shall estimate the candidates for $\max \phi(\theta)$. Using $\sin x > x - \frac{1}{3!}x^3$ for $x \in (0, \frac{\pi}{2})$ and $\mu - \mu_- = \frac{\sigma_- h}{2} > 0$, we have

$$\begin{aligned} \phi(\mu_-) &= \frac{\mu_- - \sin \mu_-}{\mu - \sin \mu_-} \cdot \frac{\mu_- + \sin \mu_-}{\mu + \sin \mu_-} \cdot \frac{\mu_-}{\mu + \mu_-} \cdot \frac{1}{\mu - \mu_-} \\ &< \frac{\mu_- - (\mu_- - \frac{1}{3!}\mu_-^3)}{\mu - (\mu_- - \frac{1}{3!}\mu_-^3)} \cdot 1 \cdot \frac{1}{2} \cdot \frac{2}{\sigma_- h} < \frac{\mu_-^3}{3\sigma_- h + \mu_-^3} \cdot \frac{1}{\sigma_- h} = \frac{k^3 h}{(24\sigma_- + k^3 h^2)\sigma_-}. \end{aligned}$$

Note that $\sigma_- < \pi < \frac{k}{2}$ implies $\mu < 2\mu - \sigma_- h = 2\mu_-$. Using also $x - \frac{1}{3!}x^3 < \sin x < x - \frac{1}{3!}x^3 + \frac{1}{5!}x^5$ for $x \in (0, \frac{\pi}{2})$ and $\mu_- < \mu < 1$, we get

$$\begin{aligned} \phi(\mu_-) &> \frac{\mu_- - (\mu_- - \frac{1}{3!}\mu_-^3 + \frac{1}{5!}\mu_-^5)}{\mu - (\mu_- - \frac{1}{3!}\mu_-^3 + \frac{1}{5!}\mu_-^5)} \cdot \frac{\mu_- + \mu_- - \frac{1}{3!}\mu_-^3}{\mu + \mu_- - \frac{1}{3!}\mu_-^3} \cdot \frac{1}{3} \cdot \frac{2}{\sigma_- h} \\ &= \frac{\mu_-^3(1 - \frac{1}{20}\mu_-^2)}{3\sigma_- h + \mu_-^3(1 - \frac{1}{20}\mu_-^2)} \cdot \frac{\mu_- + \mu_- - \frac{1}{3!}\mu_-^3}{\mu + \mu_- - \frac{1}{3!}\mu_-^3} \cdot \frac{1}{3} \cdot \frac{2}{\sigma_- h} \\ &> \frac{\mu_-^3(1 - \frac{1}{20})}{3\sigma_- h + \frac{\mu_-^3}{2^3}(1 - \frac{1}{20})} \cdot \frac{\mu_- + \mu_- - \frac{1}{3!}\mu_-}{2\mu_- + \mu_- - \frac{1}{3!}\mu_-} \cdot \frac{1}{3} \cdot \frac{2}{\sigma_- h} > \frac{k^3 h}{(240\sigma_- + k^3 h^2)3\sigma_-}. \end{aligned}$$

If $\mu_+ < \theta_k$ i.e. $\Theta \cap (\mu, \theta_k) \neq \emptyset$, then $\phi(\mu_+)$ and $\phi(\theta_-)$ need to be counted as candidates for the maximum. Since $\theta_k = \arcsin \mu$, we know $\sin \mu_+ < \mu$, and

$$\phi(\mu_+) = \frac{\mu_+ - \sin \mu_+}{\mu - \sin \mu_+} \cdot \frac{\mu_+ + \sin \mu_+}{\mu + \sin \mu_+} \cdot \frac{\mu_+}{\mu + \mu_+} \cdot \frac{1}{\mu_+ - \mu}.$$

Using $1 > C_\mu \geq \mu = \sin \theta_k$, $\mu_+ \leq \theta_- < \theta_k$ and $\sigma_-^h h/2 = \theta_k - \theta_- < \pi h/2$ we find

$$\begin{aligned} \mu - \sin \mu_+ &= \sin \theta_k - \sin \mu_+ > (\theta_k - \mu_+) \cos \theta_k \geq \left(\frac{\sigma_-^h h}{2} + \theta_- - \mu_+ \right) \sqrt{1 - C_\mu^2}, \\ \mu - \sin \mu_+ &= \sin \theta_k - \sin \mu_+ < \theta_k - \mu_+ = (\theta_k - \theta_-) + (\theta_- - \mu_+). \end{aligned}$$

Note that $\theta_k > \theta_- \geq \mu_+ > \mu$ and $\arcsin x - x < x^3$ for $0 < x < 1$. So

$$0 \leq \theta_- - \mu_+ < \theta_k - \mu = \arcsin \mu - \mu < \mu^3.$$

Using $x - \frac{x^3}{3!} + \frac{x^5}{5!} > \sin x > x - \frac{x^3}{3!}$ for $x \in (0, \pi/2)$ and $\mu < \mu_+ < 2\mu < 2$ (for $\mu > \pi h/2 > \mu_+ - \mu$), we have

$$\frac{2\mu_+^3}{15} < \frac{\mu_+^3}{6} \left(1 - \frac{\mu_+^2}{20} \right) < \mu_+ - \sin \mu_+ < \frac{\mu_+^3}{6} < \frac{4}{3}\mu^3.$$

Combining all this, we obtain

$$\frac{2}{15} \frac{(k + \sigma_+)^3 h}{\sigma_+ (4\sigma_-^h + k^3 h^2)} = \frac{2}{15} \frac{\mu_+^3}{\frac{\sigma_-^h h}{2} + \mu^3} \cdot \frac{1}{\sigma_+ h} < \phi(\mu_+) < \frac{4}{3} \frac{\mu^3}{\frac{\sigma_-^h h}{2} \sqrt{1 - C_\mu^2}} \cdot \frac{4}{\sigma_+ h} = \frac{4}{3} \frac{k^3 h}{\sigma_-^h \sigma_+ \sqrt{1 - C_\mu^2}}.$$

If $\theta_- > \mu$ i.e. $\Theta \cap (\mu, \theta_k) \neq \emptyset$, $\phi(\theta_-)$ is a candidate for $\max \phi$. For $\mu = \sin \theta_k$ and $\theta_k > \theta_-$, we have

$$\phi(\theta_-) = \frac{\theta_- - \sin \theta_-}{\mu - \sin \theta_-} \cdot \frac{\theta_- + \sin \theta_-}{\mu + \sin \theta_-} \cdot \frac{\theta_-}{\mu + \theta_-} \cdot \frac{1}{\theta_- - \mu}.$$

Using $1 > C_\mu \geq \mu = \sin \theta_k$ and $\sigma_-^h h/2 = \theta_k - \theta_-$, we find

$$\frac{\sigma_-^h h}{2} = \theta_k - \theta_- > \mu - \sin \theta_- = \sin \theta_k - \sin \theta_- > (\theta_k - \theta_-) \cos \theta_k \geq \frac{\sigma_-^h h}{2} \sqrt{1 - C_\mu^2}.$$

Using $x - \frac{x^3}{3!} + \frac{x^5}{5!} > \sin x > x - \frac{x^3}{3!}$ for $x \in (0, \frac{\pi}{2})$ and $\mu + \frac{h}{2}\sigma_+ \leq \theta_- < \frac{\pi}{2}\mu$ (for $\theta_- < \theta_k < \frac{\pi}{2} \sin \theta_k$), we have

$$\frac{(1 - \frac{\pi^2}{80} C_\mu^2)(\mu + \frac{h}{2}\sigma_+)^3}{6} < \frac{\theta_-^3}{6} \left(1 - \frac{\theta_-^2}{20}\right) < \theta_- - \sin \theta_- < \frac{\theta_-^3}{6} < \frac{\pi^3}{48} \mu^3.$$

Combining all this and using also $\theta_- - \mu = \theta_- - \mu_+ + \mu_+ - \mu < \mu^3 + \frac{\sigma_+^h}{2}$, we obtain

$$\frac{(1 - \frac{\pi^2}{80} C_\mu^2)(k + \sigma_+)^3 h}{6\sigma_-^h(4\sigma_+ + k^3 h^2)} < \phi(\theta_-) < \frac{\pi^3}{48} \frac{\mu^3}{\frac{\sigma_-^h h}{2} \sqrt{1 - C_\mu^2}} \cdot \frac{\pi}{2} \cdot 1 \cdot \frac{2}{\sigma_+ h} = \frac{\pi^4}{192} \frac{k^3 h}{\sigma_-^h \sigma_+ \sqrt{1 - C_\mu^2}}.$$

If $\theta_+ < \theta_{\max}$, then θ_+ needs to be considered. For $\mu = \sin \theta_k$ and $\theta_k < \theta_+$, we have

$$\phi(\theta_+) = \frac{\theta_+ - \sin \theta_+}{\sin \theta_+ - \mu} \cdot \frac{\theta_+ + \sin \theta_+}{\mu + \sin \theta_+} \cdot \frac{\theta_+}{\mu + \theta_+} \cdot \frac{1}{\theta_+ - \mu}.$$

Using $1 > C_\mu \geq \mu = \sin \theta_k$, $\sigma_+^h h/2 = \theta_+ - \theta_k < \pi h/2 < \frac{kh}{4} = \frac{\mu}{2}$ and $C_\mu = \sin \theta_\mu < \cos(\sigma_+^h h/2)$ (so that $\theta_\mu + \frac{\sigma_+^h h}{2} < \frac{\pi}{2}$), we find

$$\theta_+ - \mu > \sin \theta_+ - \mu = \sin \theta_+ - \sin \theta_k > (\theta_+ - \theta_k) \cos \theta_+ > \frac{\sigma_+^h h}{2} \cos \left(\theta_\mu + \frac{\sigma_+^h h}{2} \right).$$

Using $x - \frac{x^3}{3!} + \frac{x^5}{5!} > \sin x > x - \frac{x^3}{3!}$ for $x \in (0, \frac{\pi}{2})$ and $\mu + \frac{\sigma_+^h h}{2} \leq \theta_+ = \frac{\sigma_+^h h}{2} + \theta_k < (\frac{1}{2} + \frac{\pi}{2})\mu$, we have

$$\frac{(1 - \frac{(1+\pi)^2}{80} C_\mu^2)(\mu + \frac{\sigma_+^h h}{2})^3}{6} < \frac{\theta_+^3}{6} \left(1 - \frac{\theta_+^2}{20}\right) < \theta_+ - \sin \theta_+ < \frac{\theta_+^3}{6} < \frac{(1+\pi)^3}{48} \mu^3.$$

Note that $\frac{h}{2}\sigma_+^h + \frac{\mu^3}{6} < \theta_+ - \mu = (\theta_+ - \theta_k) + (\theta_k - \mu) < \frac{h}{2}\sigma_+^h + \mu^3$. Combining all this, we get

$$\begin{aligned} \phi(\theta_+) &< \frac{(1+\pi)^3}{48} \frac{\mu^3}{\frac{\sigma_+^h h}{2} \cos(\theta_\mu + \frac{\sigma_+^h h}{2})} \left(\frac{1}{2} + \frac{\pi}{2}\right) \frac{6}{3h\sigma_+^h + \mu^3} \\ &= \frac{(1+\pi)^4}{8} \frac{k^3 h}{\sigma_+^h(24\sigma_+^h + k^3 h^2) \cos(\theta_\mu + \frac{\sigma_+^h h}{2})}, \\ \phi(\theta_+) &> \frac{(1 - \frac{(1+\pi)^2}{80} C_\mu^2)(\mu + \frac{\sigma_+^h h}{2})^3}{12(\frac{h}{2}\sigma_+^h + \mu^3)^2} = \frac{(1 - \frac{(1+\pi)^2}{80} C_\mu^2)(k + \sigma_+^h)^3 2h}{3(4\sigma_+^h + k^3 h^2)^2}. \end{aligned}$$

For $\mu = \sin \theta_k$ and $\theta_k < \theta_{\max}$, we have

$$\phi(\theta_{\max}) = \frac{\theta_{\max}^2 - \sin^2 \theta_{\max}}{\sin^2 \theta_{\max} - \mu^2} \cdot \frac{\theta_{\max}}{\theta_{\max}^2 - \mu^2}.$$

Note that $\sin^2 \theta_{\max} = \cos^2 \frac{\pi h}{2} > (1 - \frac{\pi^2 h^2}{8})^2 > 1 - \frac{\pi^2 h^2}{4}$, $\theta_{\max}^2 = \frac{\pi^2}{4}(1 - 2h + h^2)$. So

$$\frac{9\pi^2}{64} - 1 < \theta_{\max}^2 - \sin^2 \theta_{\max} < \frac{\pi^2}{4} - 1,$$

where to get the first inequality we used the assumption $0 < h \leq \frac{1}{4}$. We have also

$$\frac{2}{\pi} < \frac{1}{\theta_{\max}} < \frac{\theta_{\max}}{\theta_{\max}^2 - \mu^2} < \frac{\pi}{2} \left(\frac{9\pi^2}{64} - 1 \right)^{-1},$$

where for the second inequality the assumption $0 < h \leq \frac{1}{4}$ is used. Note that

$$1 > \sin^2 \theta_{\max} - \mu^2 > \cos^2 \frac{\pi h}{2} - C_\mu^2.$$

Combining all this and using the assumption $C_\mu < \cos \frac{\pi h}{2}$, we get

$$\frac{2}{\pi} \left(\frac{9\pi^2}{64} - 1 \right) < \phi(\theta_{\max}) < \left(\frac{\pi^2}{4} - 1 \right) \left(\cos^2 \frac{\pi h}{2} - C_\mu^2 \right)^{-1} \frac{\pi}{2} \left(\frac{9\pi^2}{64} - 1 \right)^{-1}.$$

We conclude by multiplying $\frac{h}{2}$ with ϕ to get ψ (30). $\square$

From Lemma 10 and Remark 8, we can see that, when $k^3 h$ is greater than a certain constant it holds that $\psi(\xi_{\max}) < \max \psi$, and the error is of order $k^3 h^2$ for a fixed f in the worst case; otherwise, $\max \psi = \psi(\xi_{\max})$ will be of order h . As discussed in Remark 6, in the case of $\max \psi = \psi(\xi_{\max})$ i.e. $k^3 h$ less than a certain constant, we will derive an alternate estimate using the smoothness of f .

Before doing that, we first check whether the smoothness of f improves the convergence order of $\psi(k_-)$ (the discussion of $\psi(k_+)$, $\psi(k_\pm^h)$ would be similar). If $f \in H_0^1(0, 1)$, then the estimate (29) can be modified to

$$|E_1^h|_1^2 = \frac{1}{2} \sum_{(\xi/\pi)=1}^{N-1} \left| \frac{1}{\lambda} - \frac{1}{\lambda^h} \right|^2 |\xi \hat{f}(\xi)|^2 \leq |f_{\text{low}}|_1^2 \max_{\xi \in \{1, \dots, N-1\}\pi} \left| \frac{1}{\lambda} - \frac{1}{\lambda^h} \right|^2. \quad (32)$$

So we need only to find the maximum of

$$\psi_e(\xi) := \left| \frac{1}{\lambda} - \frac{1}{\lambda^h} \right| = \left| \frac{1}{k^2 - \xi^2} - \frac{1}{k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}} \right| = \frac{h^2}{4} \left| \frac{1}{\mu^2 - \theta^2} - \frac{1}{\mu^2 - \sin^2 \theta} \right| =: \frac{h^2}{4} \phi_e(\theta). \quad (33)$$

The subscript 'e' indicates the quantity is mainly useful for the evanescent modes with $\xi > k_+^h$, which we shall see as follows. For $\theta \in (0, \mu)$, we have

$$\phi_e(\theta) = \frac{1}{\mu^2 - \theta^2} - \frac{1}{\mu^2 - \sin^2 \theta}, \quad \phi_e'(\theta) = \frac{2\theta(\mu^2 - \sin^2 \theta)^2 - (\mu^2 - \theta^2)^2 \sin(2\theta)}{(\mu^2 - \theta^2)^2 (\mu^2 - \sin^2 \theta)^2} > 0.$$

So $\max_{(0, \mu_-]} \phi_e = \phi_e(\mu_-)$. The estimate of $\phi_e(\mu_-)$ needs only a small modification of the estimate of $\phi(\mu_-)$ in the proof of Lemma 10. More precisely, the term $1/(\mu + \mu_-)$ is used now instead of $\mu_-/(\mu + \mu_-)$. We already know $\mu_- < \mu < 2\mu_-$. So $\frac{1}{2\mu_-} < 1/(\mu + \mu_-) < \frac{2}{3\mu_-}$ replaces $\frac{1}{3} < \mu_-/(\mu + \mu_-) < \frac{1}{2}$ and gives

$$\frac{k^2}{(240\sigma_- + k^3 h^2)\sigma_-} < \phi_e(\mu_-) < \frac{\mu^2}{3\sigma_- h + \mu^3} \cdot \frac{4}{3\sigma_- h} = \frac{8k^2}{(24\sigma_- + k^3 h^2)3\sigma_-}.$$

Hence, in terms of ψ_e we have

$$\frac{k^2 h^2}{(240\sigma_- + k^3 h^2)4\sigma_-} < \psi_e(k_-) < \frac{2k^2 h^2}{(24\sigma_- + k^3 h^2)3\sigma_-}.$$

The upper bound says that $\psi_e(k_-)$ converges to zero no slower than of order $k^2 h^2$. This has no difference in h to the order $k^3 h^2$ of $\psi(k_-)$, but it has one order less in k . However, does this really mean $|E_1^h|_1$ converges at the same speed? Note that to make the inequality (32) sharp, or more precisely here make the estimate for E_1^h restricted to $\xi \in [\pi, k_-]$ sharp, we need to take f_{low} along $\sin(k_- x)$ whose derivative will contribute to $|f_{\text{low}}|_1$ with an extra factor k . In other words, when the frequency k_- is active, $|E_1^h|_1$ is still of order $k^3 h^2$, not improved by the smoothness of f . This is actually observed in numerical experiments. Let $f(x) = C(\sin(10\pi x) + \sin(20\pi x) + \sin(40\pi x) + \sin(80\pi x))$ with C such that $\|f\| = 1$, and $k \in \{10, 20, 40, 80\}\pi + 1$. For each k , we use a very fine mesh with $N \approx 8k^2$ to get a reference solution, and a sequence of doubly refined meshes starting with $N \approx k$ to compute the H^1 -semi-norm of the errors. The results are shown in Figure 2 which corroborates the order $k^3 h^2$. For example, at a fixed h , the marked points from low to high correspond to successively doubled k 's, and form roughly a geometric

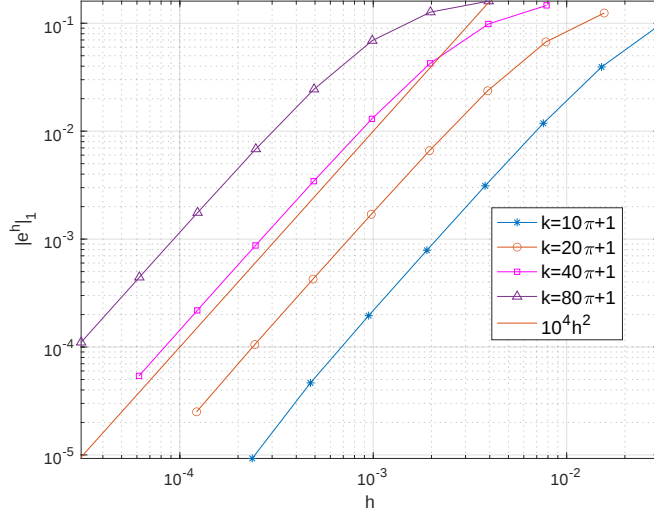


Figure 2: Errors in the H^1 -semi-norm for $f(x) = C(\sin(10\pi x) + \sin(20\pi x) + \sin(40\pi x) + \sin(80\pi x))$.

progression with the common ratio eight. Also, there are pairs of marked points, approximately at the same height but on different curves, which correspond to k -values in a ratio of 4 (or $\frac{1}{4}$) and h -values in a ratio of $\frac{1}{8}$ (or 8).

Having understood that we would not gain more from smoothness of f for the propagating modes (i.e. with $\xi \leq k_+^h$), and in the need of a better estimate when $k^3 h$ is sufficiently small (so that $\max \psi = \psi(\xi_{\max})$ which is merely of order h), we derive the following alternate estimates. By the way, we show all the evanescent modes (i.e. with $\xi > k_+^h$) can not converge faster than of order h^2 .

Lemma 11. *Under the assumptions of Lemma 10 and using the notation therein, it holds that*

$$\max_{\xi \in \{1, \dots, N-1\}\pi} \psi_e = \max\{\psi_e(k_-), \psi_e(k_+), \psi_e(k_-^h), \psi_e(k_+^h), \psi_e(\xi_{\max})\},$$

where the function ψ_e is defined in (33). Moreover, ψ_e is convex on $(k, \frac{\pi}{h}]$. Let ξ_e be the unique minimal point of ψ_e over $(k, \frac{\pi}{h}]$. Then

$$\begin{aligned} \frac{k^2 h^2}{(240\sigma_- + k^3 h^2)4\sigma_-} &< \psi_e(k_-) < \frac{2k^2 h^2}{(24\sigma_- + k^3 h^2)3\sigma_-}, \\ \frac{1}{15} \frac{(k + \sigma_+)^2 h^2}{\sigma_+ (4\sigma_-^h + k^3 h^2)} &< \psi_e(k_+) < \frac{1}{3} \frac{k^2 h^2}{\sigma_-^h \sigma_+ \sqrt{1 - C_\mu^2}}, & \text{if } \pi\mathbb{N} \cap (k, k^h) \neq \emptyset, \\ \frac{(1 - \frac{\pi^2}{80} C_\mu^2)(k + \sigma_+)^2 h^2}{3\sigma_-^h (2 + \pi)(4\sigma_+ + k^3 h^2)} &< \psi_e(k_-^h) < \frac{\pi^4}{768} \frac{k^2 h^2}{\sigma_-^h \sigma_+ \sqrt{1 - C_\mu^2}}, & \text{if } \pi\mathbb{N} \cap (k, k^h) \neq \emptyset, \\ \frac{(1 - \frac{(1+\pi)^2}{80} C_\mu^2)(k + \sigma_+^h)^2 h^2}{3(4\sigma_+^h + k^3 h^2)^2} &< \psi_e(k_+^h) < \frac{(1 + \pi)^4 k^2 h^2}{32\sigma_+^h (24\sigma_+^h + k^3 h^2) \cos(\theta_\mu + \frac{\sigma_+^h h}{2})}, & \text{if } C_\mu < \cos \frac{\sigma_+^h h}{2}, \\ \frac{(9\pi^2 - 64)h^2}{64\pi^2} &< \psi_e(\xi_{\max}) < \frac{4(\pi^2 - 4)h^2}{(\cos^2 \frac{\pi h}{2} - C_\mu^2)(9\pi^2 - 64)}, & \text{if } C_\mu < \cos \frac{\pi h}{2}, \\ \frac{h^2}{18} &< \psi_e(\xi_e) < \psi_e(\xi_{\max}). \end{aligned}$$

Remark 9. Lemma 11 gives the better and exact order h^2 for the evanescent modes, compared to Lemma 10. It can be seen also from Lemma 11 that the propagating modes usually converge slower

than the evanescent modes because the ψ_e at the former frequencies have the extra factor k^2 . We propose to use (32) and Lemma 11 only when $k^3 h$ is sufficiently small (so that $\max \psi = \psi(\xi_{\max})$; see Lemma 10). In that case, the estimates of Lemma 11 can be further improved, but we will not make more efforts here.

Remark 10. Lemma 11 is useful also for the L^2 -norm of E_1^h because

$$\|E_1^h\|^2 = \frac{1}{2} \sum_{(\xi/\pi)=1}^{N-1} \left| \frac{1}{\lambda} - \frac{1}{\lambda^h} \right|^2 |\hat{f}(\xi)|^2 \leq \|f_{\text{low}}\|^2 \max_{\xi \in \{1, \dots, N-1\}\pi} \left| \frac{1}{\lambda} - \frac{1}{\lambda^h} \right|^2.$$

Hence, the exact order of $\|E_1^h\|$ is $k^2 h^2$.

Proof of Lemma 11. Recall the notation used in the proof of Lemma 10. The estimate of $\psi_e(k_-)$ has been given in the above discussion, along with the result $\max_{(0, k_-]} \psi_e = \psi_e(k_-)$.

When $\mu < \theta < \theta_k$, we have

$$\phi_e(\theta) = \frac{1}{\theta^2 - \mu^2} + \frac{1}{\mu^2 - \sin^2 \theta} = \frac{1}{2\mu} \left(\frac{1}{\theta - \mu} - \frac{1}{\theta + \mu} \right) + \frac{1}{2\mu} \left(\frac{1}{\mu - \sin \theta} + \frac{1}{\mu + \sin \theta} \right).$$

To show that ϕ_e is convex on (μ, θ_k) , we calculate

$$2\mu\phi_e''(\theta) = \frac{2}{(\theta - \mu)^3} - \frac{2}{(\theta + \mu)^3} - \frac{\sin \theta}{(\mu - \sin \theta)^2} + \frac{\sin \theta}{(\mu + \sin \theta)^2} + \frac{2 \cos^2 \theta}{(\mu - \sin \theta)^3} + \frac{2 \cos^2 \theta}{(\mu + \sin \theta)^3}.$$

Using $0 < \sin \theta < \mu < \theta < \frac{\pi}{2}$, we find

$$\frac{2}{(\theta - \mu)^3} > \frac{2}{(\theta + \mu)^3}, \quad \frac{2 \cos^2 \theta}{(\mu - \sin \theta)^3} > \frac{\sin \theta}{(\mu - \sin \theta)^2} \Leftarrow \sin \theta + \sin^2 \theta < 2.$$

Hence, $\phi_e'' > 0$ on (μ, θ_k) . So the candidates for $\max \phi_e$ on (μ, θ_k) are $\phi_e(\mu_+)$ and $\phi_e(\theta_-)$ if $\mu_+ < \theta_k$. The estimate of $\phi_e(\mu_+)$ is quite similar to the estimate of $\phi(\mu_+)$ in the proof of Lemma 10. We need only to replace $\mu_+ / (\mu + \mu_+)$ there with $1 / (\mu + \mu_+)$ here. Since $0 < \mu < \mu_+$, we find

$$\frac{1}{2\mu_+} < \frac{1}{\mu + \mu_+} < \frac{1}{2\mu} \quad \text{instead of} \quad \frac{1}{2} < \frac{\mu_+}{\mu + \mu_+} < 1$$

should be used. Therefore, we get

$$\frac{1}{15} \frac{(k + \sigma_+)^2 h^2}{\sigma_+ (4\sigma_-^h + k^3 h^2)} < \psi_e(k_+) < \frac{1}{3} \frac{k^2 h^2}{\sigma_-^h \sigma_+ \sqrt{1 - C_\mu^2}}, \quad \text{if } \pi\mathbb{N} \cap (k, k^h) \neq \emptyset.$$

In a similar way, noting that $\mu + \theta_- < \mu_+ + \theta_k < \mu_+ + \frac{\pi}{2}\mu$ and using

$$\frac{2}{(2 + \pi)\mu_+} < \frac{1}{\mu + \theta_-} < \frac{1}{2\mu} \quad \text{instead of} \quad \frac{1}{2} < \frac{\theta_-}{\mu + \theta_-} < 1,$$

we find

$$\frac{(1 - \frac{\pi^2}{80} C_\mu^2)(k + \sigma_+)^2 h^2}{3\sigma_-^h (2 + \pi)(4\sigma_+ + k^3 h^2)} < \psi_e(k_-^h) < \frac{\pi^4}{768} \frac{k^2 h^2}{\sigma_-^h \sigma_+ \sqrt{1 - C_\mu^2}}, \quad \text{if } \pi\mathbb{N} \cap (k, k^h) \neq \emptyset.$$

When $\theta_k < \theta < \frac{\pi}{2}$, with $\mu = \sin \theta_k$ we have that

$$\phi_e(\theta) = \frac{1}{\sin^2 \theta - \mu^2} - \frac{1}{\theta^2 - \mu^2} \text{ has no local maximum for } \theta \in (\theta_k, \frac{\pi}{2}) \text{ and } 0 < \mu < 1. \quad (34)$$

The proof can be found in Appendix B. So the candidates for $\max \phi_e$ on $\Theta \cap (\theta_k, \theta_{\max}]$ are $\phi_e(\theta_+)$ (if $\theta_+ < \theta_{\max}$) and $\phi_e(\theta_{\max})$. To estimate $\phi_e(\theta_+)$, we can again modify the estimates of $\phi(\theta_+)$ in the proof of Lemma 10. Using

$$\frac{1}{2\theta_+} < \frac{1}{\mu + \theta_+} < \frac{1}{2\mu} \quad \text{instead of} \quad \frac{1}{2} < \frac{\theta_+}{\mu + \theta_+} < 1,$$

we can find

$$\frac{(1 - \frac{(1+\pi)^2}{80} C_\mu^2)(k + \sigma_+^h)^2 h^2}{3(4\sigma_+^h + k^3 h^2)^2} < \psi_e(k_+^h) < \frac{(1 + \pi)^4 k^2 h^2}{32\sigma_+^h (24\sigma_+^h + k^3 h^2) \cos(\theta_\mu + \frac{\sigma_+^h h}{2})}, \text{ if } C_\mu < \cos \frac{\sigma_+^h h}{2}.$$

For $\mu = \sin \theta_k$ and $\theta_k < \theta_{\max}$, we have

$$\phi_e(\theta_{\max}) = \frac{\theta_{\max}^2 - \sin^2 \theta_{\max}}{\sin^2 \theta_{\max} - \mu^2} \cdot \frac{1}{\theta_{\max}^2 - \mu^2}.$$

Recall from the proof of Lemma 10,

$$\frac{9\pi^2}{64} - 1 < \theta_{\max}^2 - \sin^2 \theta_{\max} < \frac{\pi^2}{4} - 1, \quad 1 > \sin^2 \theta_{\max} - \mu^2 > \cos^2 \frac{\pi h}{2} - C_\mu^2.$$

Since $\theta_{\max}^2 = \frac{\pi^2}{4}(1 - 2h + h^2)$, $0 < \mu < 1$ and $0 < h \leq \frac{1}{4}$, we find

$$\frac{\pi^2}{4} > \theta_{\max}^2 - \mu^2 > \frac{9\pi^2}{64} - 1.$$

Combining this and using the assumption $C_\mu < \cos \frac{\pi h}{2}$, we obtain

$$\left(\frac{9\pi^2}{64} - 1\right) \frac{4}{\pi^2} < \phi_e(\theta_{\max}) < \left(\frac{\pi^2}{4} - 1\right) \left(\cos^2 \frac{\pi h}{2} - C_\mu^2\right)^{-1} \left(\frac{9\pi^2}{64} - 1\right)^{-1}.$$

Denote $\theta_e := \xi_e h/2$. To find the minimal point θ_e of ϕ_e on $[\theta_k, \frac{\pi}{2}]$, we calculate

$$\phi_e'(\theta) = -\frac{\sin(2\theta)}{(\sin^2 \theta - \mu^2)^2} + \frac{2\theta}{(\theta^2 - \mu^2)^2}, \quad \phi_e'\left(\frac{\pi}{2}\right) > 0, \quad \lim_{\theta \rightarrow \theta_k + 0} \phi_e'(\theta) < 0.$$

Since ϕ_e is convex in $[\theta_k, \frac{\pi}{2}]$ and $\theta_e = \arg \min_{[\theta_k, \pi/2]} \phi_e$, we have $\phi_e'(\theta_e) = 0$, from which we find

$$\frac{1}{\sin^2 \theta_e - \mu^2} = \sqrt{\frac{2\theta_e}{\sin(2\theta_e)}} \cdot \frac{1}{\theta_e^2 - \mu^2}.$$

Substituting this into $\phi_e(\theta_e)$, and using $\frac{x}{\sin x} > 1 + \frac{x^2}{6}$ for $0 < x < \pi$ and $\sqrt{1+x} > 1 + \frac{x}{3}$ for $0 < x < 3$, we get

$$\phi_e(\theta_e) = \left(\sqrt{\frac{2\theta_e}{\sin(2\theta_e)}} - 1\right) \frac{1}{\theta_e^2 - \mu^2} > \frac{4\theta_e^2}{18} \cdot \frac{1}{\theta_e^2} = \frac{2}{9}.$$

Multiplying ϕ_e with $\frac{h^2}{4}$ gives the conclusion for ψ_e . $\square$

Putting all the results on the downsampling, aliasing and operator errors together, we have an estimate of the total error in the H^1 -semi-norm and L^2 -norm.

Theorem 3 (Absolute error with nonzero f). *Suppose the problem (1) has $k > 2\pi$, $\sigma_k := \min_{\xi \in \pi\mathbb{N}} |k - \xi| > 0$, $f \in H_0^p(0, 1)$ with $p \geq 1$, $g_0 = g_1 = 0$. Suppose $0 < \frac{kh}{2} \leq C_\mu < \cos \frac{\pi h}{2}$, and there is a sequence of $h = \frac{1}{N}$ ($N \geq 4$) going to zero such that*

$$\tilde{\sigma}_k := \min_{\xi, h} \left| k - \frac{2}{h} \sin \frac{\xi h}{2} \right| > 0 \text{ over } \xi \in \{1, \dots, N-1\}\pi \text{ and the sequence of } h \text{ going to zero.}$$

Let f be decomposed as (6). Then the finite difference scheme (9) has a unique solution u^h . Moreover,

$$|u - u^h|_1 \leq \left(\frac{h(kh)^p}{\pi^2 - 4C_\mu^2} + \frac{(kh)^p}{\tilde{\sigma}_k} \right) \pi^{1-p} k^{-p} |f_{\text{high}}|_p + |E_1^h|_1,$$

$$\|u - u^h\| \leq \left(\frac{h^2(kh)^p}{\pi^2 - 4C_\mu^2} + \frac{2(kh)^p}{\tilde{\sigma}_k k} \right) \pi^{-p} k^{-p} |f_{\text{high}}|_p + \|E_1^h\|,$$

with E_1^h given in (28), and equality is attained when $f_{\text{high}} = 0$. In turn, E_1^h satisfies

$$\frac{h^2}{18} |f_{\text{low},e}|_1 \leq |E_1^h|_1 \leq \min\{C(k, h) \|f_{\text{low}}\|, C_e(k, h) |f_{\text{low}}|_1\}, \quad \frac{h^2}{18} \|f_{\text{low},e}\| \leq \|E_1^h\| \leq C_e(k, h) \|f_{\text{low}}\|,$$

where $f_{\text{low},e} := \sum_{(\xi/\pi)=\lceil kh/\pi \rceil}^{N-1} \hat{f}(\xi) \sin(\xi x)$, $kh := \frac{2}{h} \arcsin \frac{kh}{2}$, the upper bounds are attainable, and there exist positive constants $C_1, C_2, c, c_e, \tilde{C}$ and $\tilde{C}_e$ independent of k and h such that, when $k^3 h^2 < C_1 \sigma_k$ it holds that

$$ck^3 h^2 / \sigma_k^2 < C(k, h) < \tilde{C} k^3 h^2 / \sigma_k^2, \quad c_e k^3 h^2 / \sigma_k^2 < k C_e(k, h) < \tilde{C}_e k^3 h^2 / \sigma_k^2,$$

and when $k^3 h^2 > C_2 \max(\sigma_k, \sigma_-^h)$ it holds that $C(k, h)$ or $k C_e(k, h)$ is greater than a positive constant times $1/\sigma_k$, where σ_-^h is defined in Lemma 10.

Remark 11. Here $C_e(k, h)$ is multiplied with k because $|E_1^h|_1 \leq C_e(k, h) |f_{\text{low}}|_1$ holds with equality when $f_{\text{low}} = \sin(\xi x)$ for some $\xi \in \pi\mathbb{N}$ satisfying $|\xi - k| < \pi$ and in this case $|f_{\text{low}}|_1$ is of order k . Note that the upper bound is attained when f is chosen dependently on k and as a result $|f|_p = O(k^p)$.

Proof. The proof is obtained by combining (3), (7), (8), Lemma 8, Lemma 9, (22), (29), Lemma 10, (32) and Lemma 11. $\square$

3.5 Relative error estimates of the classical 3-point centered scheme

To estimate the relative error, we recall the solution u of (1) and the solution u^h of (9) in case (i), $g_0 = g_1 = 0$, are

$$u(x) = \sum_{\xi \in \pi\mathbb{N}} \frac{\hat{f}(\xi)}{k^2 - \xi^2} \sin(\xi x), \quad u^h(x) = \sum_{(\xi/\pi)=1}^{N-1} \frac{\widehat{f^h}(\xi)}{k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}} \sin(\xi x),$$

$$\widehat{f^h}(\xi) = \hat{f}(\xi) + \sum_{s=\pm 1} s \sum_{m=1}^{\infty} \hat{f}(s\xi + 2mN\pi), \quad \text{for } \xi \in \{1, \dots, N-1\}\pi.$$

We have already shown that $f_{\text{high}} = \sum_{(\xi/\pi)=N+1}^{\infty} \hat{f}(\xi) \sin(\xi x)$ causes the downsampling error (7) and aliasing error (26). Let us see how they behave in the relative sense.

Lemma 12. Suppose $k > \frac{4\pi}{\pi - \sqrt{16 - \pi^2}} \approx 18.88$, $0 < \frac{kh}{2} \leq C_\mu < 1$. Then, for $p \geq 1$, the downsampling error e_2^h in (3) satisfies

$$\frac{\|e_2^h\|}{\|u\|} < \frac{(kh)^p}{\pi^p} \frac{k^{-p} |f_{\text{high}}|_p}{\|f_{\text{low}}\|}, \quad \frac{|e_2^h|_1}{|u|_1} < \frac{(kh)^{p-1}}{\pi^{p-1}} \frac{k^{-p} |f_{\text{high}}|_p}{k^{-1} |f_{\text{low}}|_1}.$$

Remark 12. Recall from Remark 1 that as $N \rightarrow \infty$ we have $f_{\text{high}} \rightarrow 0$ and $f_{\text{low}} \rightarrow f$ for a fixed $f \in H_0^p(0, 1)$. So the relative errors converge faster than the displayed powers of h . But if $|f_{\text{high}}|_p = O(k^p)$ and $kh = O(1)$, then Lemma 12 says the relative error is bounded in L^2 and H^1 .

Remark 13. Compared to the absolute errors of downsampling (7) and (8), the exponents of h here are decreased by two. This is caused by the fact that f_{low} depends on h and the bound for u_{low} becomes sharp only for increasingly oscillatory f (see the following proof). If f and k are fixed, then u is fixed and the relative error should be of the same order in h as the absolute error is.

Proof of Lemma 12. By Parseval's identity, we have

$$\frac{\|e_2^h\|^2}{\|u\|^2} = \frac{\sum_{(\xi/\pi)=N}^{\infty} \frac{1}{|k^2 - \xi^2|^2} |\hat{f}(\xi)|^2}{\left(\sum_{(\xi/\pi)=1}^{N-1} + \sum_{(\xi/\pi)=N}^{\infty} \right) \frac{1}{|k^2 - \xi^2|^2} |\hat{f}(\xi)|^2} = \frac{\|e_2^h\|^2}{\|u_{\text{low}}\|^2 + \|e_2^h\|^2}.$$

Note that

$$\|e_2^h\| \leq \max_{\xi \geq N\pi} \frac{1}{|k^2 - \xi^2| \cdot |\xi|^p} |f_{\text{high}}|_p, \quad \|u_{\text{low}}\| \geq \min_{\xi \in \{1, \dots, N-1\}\pi} \frac{1}{|k^2 - \xi^2|} \|f_{\text{low}}\|.$$

We consider the case of $(N-1)^2\pi^2 - k^2 > k^2 - \pi^2 > 0$. This is guaranteed by $\frac{2}{h} > k > \frac{4\pi}{\pi - \sqrt{16 - \pi^2}}$:

$$(N-1)^2\pi^2 - k^2 > k^2 - \pi^2 \Leftrightarrow ((N-1)^2 + 1)\pi^2 > 2k^2 \Leftrightarrow ((1-h)^2 + h^2)\pi^2 > 8 \Leftrightarrow h < \frac{2}{k} < \frac{\pi - \sqrt{16 - \pi^2}}{2\pi}.$$

In this case, we have

$$\min_{\xi \in \{1, \dots, N-1\}\pi} \frac{1}{|k^2 - \xi^2|} = \frac{1}{(N-1)^2\pi^2 - k^2}, \quad \max_{\xi \geq N\pi} \frac{1}{|k^2 - \xi^2| \cdot |\xi|^p} = \frac{1}{N^2\pi^2 - k^2} \frac{1}{N^p\pi^p}.$$

Therefore, it holds that

$$\frac{\|e_2^h\|}{\|u\|} \leq \frac{\|e_2^h\|}{\|u_{\text{low}}\|} \leq \frac{(N-1)^2\pi^2 - k^2}{N^2\pi^2 - k^2} \frac{1}{N^p\pi^p} \frac{|f_{\text{high}}|_p}{\|f_{\text{low}}\|} < \frac{h^p}{\pi^p} \frac{|f_{\text{high}}|_p}{\|f_{\text{low}}\|}.$$

For the H^1 -semi-norm of e_2^h , we note that

$$|e_2^h|_1 \leq \max_{\xi \geq N\pi} \frac{1}{|k^2 - \xi^2| \cdot |\xi|^{p-1}} |f_{\text{high}}|_p, \quad |u_{\text{low}}|_1 \geq \min_{\xi \in \{1, \dots, N-1\}\pi} \frac{1}{|k^2 - \xi^2|} |f_{\text{low}}|_1.$$

The estimation of the relative error is similar to the previous one in the L^2 -norm. $\square$

Lemma 13. Suppose $k > \frac{4\pi}{\pi - \sqrt{16 - \pi^2}} \approx 18.88$, $0 < \frac{kh}{2} \leq C_\mu < 1$, and there exists a sequence of $h = \frac{1}{N}$ going to zero such that

$$\tilde{\sigma}_k := \min_{\xi, h} \left| k - \frac{2}{h} \sin \frac{\xi h}{2} \right| > 0 \text{ over } \xi \in \{1, \dots, N-1\}\pi \text{ and the sequence of } h \text{ going to zero.}$$

Then, for $\lambda^h = k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}$ and $p \geq 2$, the aliasing error E_2^h in (27) satisfies

$$\frac{\|E_2^h\|}{\|u\|} < \frac{2k(kh)^{p-2}}{\tilde{\sigma}_k \pi^{p-2}} \frac{k^{-p} |f_{\text{high}}|_p}{\|f_{\text{low}}\|}, \quad \frac{|E_2^h|_1}{|u|_1} < \frac{k(kh)^{p-2}}{\tilde{\sigma}_k \pi^{p-3}} \frac{k^{-p} |f_{\text{high}}|_p}{k^{-1} |f_{\text{low}}|_1}.$$

Proof. We invoke Lemma 9 and Lemma 8 for bounds of E_2^h , and recall from the proof of Lemma 12 that

$$\|u_{\text{low}}\| \geq \min_{\xi \in \{1, \dots, N-1\}\pi} \frac{1}{|k^2 - \xi^2|} \|f_{\text{low}}\|, \quad |u_{\text{low}}|_1 \geq \min_{\xi \in \{1, \dots, N-1\}\pi} \frac{1}{|k^2 - \xi^2|} |f_{\text{low}}|_1,$$

$$\min_{\xi \in \{1, \dots, N-1\}\pi} \frac{1}{|k^2 - \xi^2|} = \frac{1}{(N-1)^2\pi^2 - k^2}.$$

Combining all this gives the upper bounds for $\|E_2^h\|/\|u_{\text{low}}\| \geq \|E_2^h\|/\|u\|$ and $|E_2^h|_1/|u_{\text{low}}|_1 \geq |E_2^h|_1/|u|_1$. $\square$

Now we start estimating the relative error due to operator discretization. That is, for E_1^h in (27),

$$\frac{\|E_1^h\|^2}{\|u\|^2} = \frac{\sum_{(\xi/\pi)=1}^{N-1} \left| \frac{1}{\lambda} - \frac{1}{\lambda^h} \right|^2 |\hat{f}(\xi)|^2}{\|u\|^2} = \sum_{(\xi/\pi)=1}^{N-1} w^h(\xi) \frac{|\lambda(\xi) - \lambda^h(\xi)|^2}{|\xi^p \lambda^h(\xi)|^2}, \quad (35)$$

where the weight function $w^h(\xi)$ is given by

$$w^h(\xi) := \frac{|\xi^p \hat{u}(\xi)|^2}{\|u\|^2} = \frac{|\xi^p \hat{f}(\xi)|^2}{|\lambda(\xi)|^2 \|u\|^2}, \quad \text{and} \quad \sum_{(\xi/\pi)=1}^{N-1} w^h(\xi) = \frac{|u_{\text{low}}|_p^2}{\|u\|^2}. \quad (36)$$

Note that as $h = \frac{1}{N} \rightarrow 0$, $|u_{\text{low}}|_p \rightarrow |u|_p$. It can be deduced from (35) and (36) that

$$\frac{\|E_1^h\|}{\|u\|} \leq \frac{|u_{\text{low}}|_p}{\|u\|} \max_{\xi \in \{1, \dots, N-1\}\pi} \left| \frac{\lambda - \lambda^h}{\xi^p \lambda^h} \right|, \quad (37)$$

which holds with equality if and only if $\hat{f}(\xi) = 0$ for $\xi \in \{\pi, \dots, (N-1)\pi\} \setminus \{\xi_*\}$ where $\{\xi_*\}$ is the maximizer set of $|\lambda - \lambda^h|/|\xi^p \lambda^h|$ over $\xi \in \{1, \dots, N-1\}\pi$. So, if ξ_* does not change with N , then the equality holds for the fixed $f(x) = \sin(\xi_* x)$ and $|u_{\text{low}}|_p/\|u\| = \xi_*^p$. Our intention is to find, for a given wavenumber k , a source f independent of the mesh size $h = 1/N$ (but f may depend on k) such that the upper bound is attainable. We will see that $p = 2$ is an appropriate choice.

The relative error in the H^1 -semi-norm can be analyzed in a similar way. Specifically, we have

$$\frac{|E_1^h|_1^2}{|u|_1^2} = \frac{\sum_{(\xi/\pi)=1}^{N-1} \left| \frac{1}{\lambda} - \frac{1}{\lambda^h} \right|^2 |\xi \hat{f}(\xi)|^2}{|u|_1^2} = \sum_{(\xi/\pi)=1}^{N-1} \frac{|\xi^{p+1} \hat{f}(\xi)|^2}{|\lambda(\xi)|^2 |u|_1^2} \cdot \frac{|\lambda(\xi) - \lambda^h(\xi)|^2}{|\xi^p \lambda^h(\xi)|^2},$$

which leads to

$$\frac{|E_1^h|_1}{|u|_1} \leq \frac{|u_{\text{low}}|_{p+1}}{|u|_1} \max_{\xi \in \{1, \dots, N-1\}\pi} \left| \frac{\lambda - \lambda^h}{\xi^p \lambda^h} \right|. \quad (38)$$

So for both the L^2 - and H^1 -norms it is essential to find the same maximum.

Lemma 14. Suppose $2\pi < k \notin \pi\mathbb{N}$, $\frac{kh}{2} \leq C_\mu \leq \frac{3}{4}$ and a sequence of $h = \frac{1}{N} < \frac{1}{2\pi}$ satisfying

$$\tilde{\sigma}_k := \min_{\xi, h} \left| k - \frac{2}{h} \sin \frac{\xi h}{2} \right| > 0 \text{ over } \xi \in \{1, \dots, N-1\}\pi \text{ and the sequence of } h \text{ going to zero.}$$

Let $\xi_{\max} := (N-1)\pi$, $k_-^h := \frac{2}{h} \arcsin \frac{kh}{2}$, $k_\pm^h \in \pi\mathbb{N}$ such that $k_-^h < k^h < k_+^h$ and $k_+^h - k_-^h = \pi$. Denote $\tilde{\sigma}_\pm^h := |k - \frac{2}{h} \sin \frac{k_\pm^h}{2}|$. Let $\lambda := k^2 - \xi^2$, $\lambda^h := k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}$ and $\psi_{\text{rel}}(\xi) := \left| \frac{\lambda - \lambda^h}{\xi^2 \lambda^h} \right|$. Then $\max_{\xi \in \{1, \dots, N-1\}\pi} \psi_{\text{rel}}(\xi)$ is attained at one of k_-^h , k_+^h and $\xi_{\max}$ with

$$\frac{1}{196\tilde{\sigma}_-^h} kh^2 < \psi_{\text{rel}}(k_-^h) < \frac{\pi^3}{48(2+\pi)\tilde{\sigma}_-^h} kh^2, \quad \frac{1}{64\tilde{\sigma}_+^h} kh^2 < \psi_{\text{rel}}(k_+^h) < \frac{3\pi}{32\tilde{\sigma}_+^h} kh^2, \quad \frac{9}{100} h^2 < \psi_{\text{rel}}(\xi_{\max}) < \frac{2}{3} h^2,$$

where $\pi \geq \tilde{\sigma}_\pm^h \geq \tilde{\sigma}_k$.

Proof. Let $\mu := \frac{kh}{2}$, $\theta := \frac{\xi h}{2}$. We find $\psi_{\text{rel}}(\xi) = \frac{h^2}{4} \cdot \frac{\theta^2 - \sin^2 \theta}{\theta^2 |\mu^2 - \sin^2 \theta|} =: \frac{h^2}{4} \phi_{\text{rel}}(\theta)$. When $\sin \theta < \mu$,

$$\phi_{\text{rel}}(\theta) = \frac{1 - \frac{\sin^2 \theta}{\theta^2}}{\mu^2 - \sin^2 \theta} \text{ increases with } \theta \text{ for } 0 < \theta < \frac{\pi}{2} \text{ and } \sin \theta < \mu.$$

So k_-^h is the unique maximizer of $\psi_{\text{rel}}(\xi)$ on $(0, k_-^h]$. When $\sin \theta > \mu$, we have

$$\phi_{\text{rel}}(\theta) = \frac{\theta^2 - \sin^2 \theta}{\theta^2 (\sin^2 \theta - \mu^2)} \text{ has no local maximum for } 0 < \theta_k := \frac{h}{2} k^h = \arcsin \mu < \theta < \frac{\pi}{2}.$$

Indeed, we calculate

$$\theta^3 (\sin^2 \theta - \mu^2)^2 \phi'_{\text{rel}}(\theta) = -2 (\theta^3 \sin \theta \cos \theta - \sin^4 \theta + \mu^2 \sin^2 \theta - \theta \mu^2 \sin \theta \cos \theta)$$

and a critical point $\theta_0 \in (\arcsin \mu, \frac{\pi}{2})$ of ϕ_{rel} is a root of

$$\mu^2 = \frac{\theta^3 \cos \theta - \sin^3 \theta}{\theta \cos \theta - \sin \theta} =: v(\theta). \quad (39)$$

By calculations, we find

$$(\theta \cos \theta - \sin \theta)^2 v'(\theta) = (\theta - \sin \theta)(\theta + \sin \theta) (\theta \sin^2 \theta + 3\theta \cos^2 \theta - 3 \sin \theta \cos \theta) > 0,$$

because $(\theta \sin^2 \theta + 3\theta \cos^2 \theta - 3 \sin \theta \cos \theta)' = 4 \sin^2 \theta - 4\theta \sin \theta \cos \theta > 0$ for $\theta \in (0, \frac{\pi}{2})$. Hence, $v'(\theta) > 0$ and there is at most one critical point of ϕ_{rel} . Suppose $\theta_0 \in (\arcsin \mu, \frac{\pi}{2})$ is a critical point of ϕ_{rel} . By substitution with (39), we find

$$\theta_0^5 (\theta_0^2 - \sin^2 \theta_0) \phi_{rel}''(\theta_0) = 2 \sin \theta_0 \cos \theta_0 (\tan \theta_0 - \theta_0) (3\theta_0 + \theta_0 \tan^2 \theta_0 - 3 \tan \theta_0) > 0,$$

because $(3\theta + \theta \tan^2 \theta - 3 \tan \theta)' = 2 \tan \theta (\theta \sec^2 \theta - \tan \theta) > 0$ for $\theta \in (0, \frac{\pi}{2})$. That means θ_0 can only be a local minimum.

It remains to estimate all the candidates $\phi_{rel}(\theta_-)$, $\phi_{rel}(\theta_+)$ and $\phi_{rel}(\theta_{\max})$ for $\max \phi_{rel}$, where $\theta_{\pm} := \frac{k_{\pm}^h h}{2}$ and $\theta_{\max} := \frac{(N-1)\pi h}{2}$, corresponding to $\psi_{rel}(\xi)$ at $\xi = k_{\pm}^h, \xi_{\max}$. Note that $\frac{h}{2}\pi > \frac{h}{2}|k^h - k_{\pm}^h| = |\theta_k - \theta_{\pm}| \geq |\sin \theta_k - \sin \theta_{\pm}| = \frac{h}{2} \left| k - \frac{2}{h} \sin \frac{k_{\pm}^h h}{2} \right| = \frac{h}{2} \tilde{\sigma}_{\pm}^h \geq \frac{h}{2} \tilde{\sigma}_k$, $k_{-}^h < k^h = \frac{2}{h} \arcsin \frac{k h}{2} < \frac{\pi}{2} k$, $k_{-}^h > k^h - \pi > k - \pi > \frac{k}{2}$, and $k < k_{+}^h < k^h + \pi < \frac{\pi}{2} k + \frac{1}{2} k < 3k$. These are useful in the following.

First, at θ_- , we have

$$\phi_{rel}(\theta_-) = \frac{\theta_-^2 - \sin^2 \theta_-}{\theta_-^2 (\sin^2 \theta_k - \sin^2 \theta_-)} = \left(1 - \frac{\sin \theta_-}{\theta_-}\right) \left(1 + \frac{\sin \theta_-}{\theta_-}\right) \frac{1}{\sin \theta_k - \sin \theta_-} \cdot \frac{1}{\sin \theta_k + \sin \theta_-}.$$

Note that $x - \frac{x^3}{6} < \sin x < x - \frac{x^3}{8}$ and $x < \frac{\pi}{2} \sin x$ for $x \in (0, \frac{\pi}{2})$. We get

$$\phi_{rel}(\theta_-) < \frac{1}{24} (k_{-}^h)^2 h^2 \cdot 2 \cdot \frac{2}{h \tilde{\sigma}_{-}^h} \cdot \frac{\pi}{(k + k_{-}^h) h} < \frac{\pi^3}{12(2 + \pi) \tilde{\sigma}_{-}^h} k,$$

$$\phi_{rel}(\theta_-) > \frac{1}{32} (k_{-}^h)^2 h^2 \cdot 1 \cdot \frac{2}{h \tilde{\sigma}_{-}^h} \cdot \frac{2}{h(k + k_{-}^h)} > \frac{1}{48 \tilde{\sigma}_{-}^h} k.$$

Second, at θ_+ , we have

$$\phi_{rel}(\theta_+) = \frac{\theta_+^2 - \sin^2 \theta_+}{\theta_+^2 (\sin^2 \theta_+ - \sin^2 \theta_k)} = \left(1 - \frac{\sin \theta_+}{\theta_+}\right) \left(1 + \frac{\sin \theta_+}{\theta_+}\right) \frac{1}{\sin \theta_+ - \sin \theta_k} \cdot \frac{1}{\sin \theta_k + \sin \theta_+}.$$

Similar to the estimate of $\phi_{rel}(\theta_-)$, we get

$$\phi_{rel}(\theta_+) < \frac{1}{24} (k_{+}^h)^2 h^2 \cdot 2 \cdot \frac{2}{h \tilde{\sigma}_{+}^h} \cdot \frac{\pi}{(k + k_{+}^h) h} < \frac{3\pi}{8 \tilde{\sigma}_{+}^h} k,$$

$$\phi_{rel}(\theta_+) > \frac{1}{32} (k_{+}^h)^2 h^2 \cdot 1 \cdot \frac{2}{h \tilde{\sigma}_{+}^h} \cdot \frac{2}{h(k + k_{+}^h)} > \frac{1}{16 \tilde{\sigma}_{+}^h} k.$$

Finally, at $\theta_{\max} = \frac{\pi}{2}(1 - h)$, we have

$$\phi_{rel}(\theta_{\max}) = \frac{\theta_{\max}^2 - \sin^2 \theta_{\max}}{\theta_{\max}^2 (\sin^2 \theta_{\max} - \sin^2 \theta_k)} = \frac{\frac{\pi^2}{4}(1 - h)^2 - \cos^2 \frac{\pi h}{2}}{\frac{\pi^2}{4}(1 - h)^2 (\cos^2 \frac{\pi h}{2} - \frac{k^2 h^2}{4})}.$$

From the assumption $0 < h < \frac{1}{2\pi}$, using also $\cos x > 1 - \frac{1}{2}x^2$ for $x \in (0, \frac{\pi}{2})$ we have $\cos^2 \frac{\pi h}{2} = \frac{1}{2}(1 + \cos(\pi h)) > 1 - \frac{\pi^2 h^2}{4} > \frac{15}{16}$. Combining this with the assumption $\frac{k h}{2} < \frac{3}{4}$ gives

$$\frac{9}{25} = 1 - \frac{4}{\pi^2(\frac{3}{\pi} - \frac{1}{2\pi})^2} < \sec^2 \frac{\pi h}{2} - \frac{4}{\pi^2(1 - h)^2} < \phi_{rel}(\theta_{\max}) < \frac{1}{\cos^2 \frac{\pi h}{2} - \frac{k^2 h^2}{4}} < \frac{8}{3}.$$

To conclude for ψ_{rel} , we need only to multiply ϕ_{rel} with $\frac{h^2}{4}$. □

Now we can summarize the relative error.

Theorem 4 (Relative error with nonzero f). *Suppose the problem (1) has $k > \frac{4\pi}{\pi - \sqrt{16 - \pi^2}} \approx 18.88$, $\sigma_k := \min_{\xi \in \pi\mathbb{N}} |k - \xi| > 0$, $f \in H_0^p(0, 1)$ with $p \geq 2$, $g_0 = g_1 = 0$. Suppose $0 < \frac{kh}{2} \leq C_\mu \leq \frac{3}{4}$, and there is a sequence of $h = \frac{1}{N}$ going to zero such that*

$$\tilde{\sigma}_k := \min_{\xi, h} \left| k - \frac{2}{h} \sin \frac{\xi h}{2} \right| > 0 \text{ over } \xi \in \{1, \dots, N-1\}\pi \text{ and the sequence of } h \text{ going to zero.}$$

Let $k^h := \frac{2}{h} \arcsin \frac{kh}{2}$, $k_\pm^h \in \pi\mathbb{N}$ such that $k_-^h < k^h < k_+^h$ and $k_+^h - k_-^h = \pi$. Let f be decomposed as in (6). Then the finite difference scheme (9) has a unique solution u^h . Moreover,

$$\begin{aligned} \frac{\|u - u^h\|}{\|u\|} &\leq \left(\frac{(kh)^p}{\pi^p} + \frac{2k(kh)^{p-2}}{\tilde{\sigma}_k \pi^{p-2}} \right) \frac{k^{-p} |f_{\text{high}}|_p}{\|f_{\text{low}}\|} + \frac{\|E_1^h\|}{\|u\|}, \\ \frac{|u - u^h|_1}{|u|_1} &\leq \left(\frac{k(kh)^{p-1}}{\pi^{p-1}} + \frac{k(kh)^{p-2}}{\tilde{\sigma}_k \pi^{p-2}} \right) \frac{k^{-p} |f_{\text{high}}|_p}{k^{-1} |f_{\text{low}}|_1} + \frac{|E_1^h|_1}{|u|_1}, \end{aligned}$$

with E_1^h given in (28), and equality is attained when $f_{\text{high}} = 0$. In turn, E_1^h satisfies

$$\frac{\|E_1^h\|}{\|u\|} \leq \frac{k^{-2} |u_{\text{low}}|_2}{\|u\|} k^2 C_{\text{rel}}(k, h), \quad \frac{|E_1^h|_1}{|u|_1} \leq \frac{k^{-3} |u_{\text{low}}|_3}{k^{-1} |u|_1} k^2 C_{\text{rel}}(k, h),$$

where the upper bounds are attained when $\hat{f}(\xi) = 0$ for all $\xi \in \{1, \dots, N-1\}\pi$ but one of $k_\pm^h$, and there exist positive constants c_{rel} and $\tilde{C}_{\text{rel}}$ independent of k , $\tilde{\sigma}_k^h$ and h such that

$$c_{\text{rel}} k^3 h^2 / \tilde{\sigma}_k^h < k^2 C_{\text{rel}}(k, h) < \tilde{C}_{\text{rel}} k^3 h^2 / \tilde{\sigma}_k^h,$$

where $\tilde{\sigma}_k^h = \min\{\tilde{\sigma}_\pm^h\}$, and $\tilde{\sigma}_\pm^h$ are defined in Lemma 14. In particular, when the upper bounds for E_1^h relative to u are attained, e.g. $f(x) = 2 \sin(k_\pm^h x)$, we have

$$u = \frac{f}{k^2 - (k_\pm^h)^2}, \quad \|u\| = \frac{\|f\|}{k^2 - (k_\pm^h)^2}, \quad |u|_p = |u_{\text{low}}|_p = \frac{\|f\| (k_\pm^h)^p}{k^2 - (k_\pm^h)^2},$$

and hence the exact order of the relative errors are $k^3 h^2 / \tilde{\sigma}_k^h$, or more precisely

$$\frac{\|E_1^h\|}{\|u\|} = \frac{|E_1^h|_1}{|u|_1} = (k_\pm^h)^2 C_{\text{rel}}(k, h) \in (k_\pm^h)^2 k h^2 (\tilde{\sigma}_k^h)^{-1} (c_{\text{rel}}, \tilde{C}_{\text{rel}}).$$

Proof. The proof is obtained by combining Lemma 12, Lemma 13, (37) (38) and Lemma 14. $\square$

Remark 14. Under the assumptions of Lemma 2, we have $k_- < k < k_+$ for some $k_\pm \in \pi\mathbb{N}$ and $k_+ - k_- = \pi$. Then $k_\pm^h = k_\pm$, and for $0 < c < 1$ from Lemma 2, $k > 6\pi$, it holds that

$$\begin{aligned} \tilde{\sigma}_-^h &= \left| k - \frac{2}{h} \sin \frac{k_-^h h}{2} \right| \in \left(k - k_-, k - k_- + \frac{1}{24} k_-^3 h^2 \right) \subset (k - k_-) \left(1, 1 + \frac{c}{3} \right), \\ \tilde{\sigma}_+^h &= \left| k - \frac{2}{h} \sin \frac{k_+^h h}{2} \right| \in \left(k_+ - k - \frac{1}{24} k_+^3 h^2, k_+ - k \right) \subset (k_+ - k) \left(1 - \frac{7^3 c}{6^3 3}, 1 \right). \end{aligned}$$

So $\tilde{\sigma}_k^h = \min\{\tilde{\sigma}_\pm^h\}$ in Theorem 4 is of the same order as $\sigma_k = \min\{|k - k_\pm|\}$.

4 Visual analysis of dispersion correction schemes

We have already seen from (2), (10) and Section 3.1 that for the zero source problem the discretization error is essentially in the discrete wavenumber k^h . This becomes the motivation of dispersion correction. In 1D, k^h is simply a constant depending on kh for a given linear scheme, and the error in k^h can be completely removed; see e.g. [5, 16].

For the classical 3-point centered scheme (9), one possibility adopted in [16] is to modify the wavenumber k to be used in the scheme (9) and get the new scheme

$$(\tilde{k}^2 - \frac{2}{h^2})u^h(x_j) + \frac{1}{\tilde{h}^2}u^h(x_{j-1}) + \frac{1}{\tilde{h}^2}u^h(x_{j+1}) = f(x_j), \quad u^h(x_0) = g_0, \quad u^h(x_N) = g_1. \quad (40)$$

When $f = 0$, the solution of (40) is given by (10) which is copied here,

$$u^h(x_j) = \frac{g_1 - g_0 \cos k^h}{\sin k^h} \sin(k^h x_j) + g_0 \cos(k^h x_j), \quad x_j = jh, \quad j = 0, 1, \dots, N,$$

but with $k^h := \frac{2}{h} \arcsin \frac{\tilde{k}h}{2}$ ($\tilde{k}$ replacing k). The idea is to let $k^h = k$ by well choosing $\tilde{k}$. That is, solve

$$\frac{2}{h} \arcsin \frac{\tilde{k}h}{2} = k \quad \text{to find} \quad \tilde{k} = \frac{2}{h} \sin \frac{kh}{2}.$$

Then, the discretization error of the new scheme vanishes when $f = 0$. An error analysis when $f \neq 0$ is given by [11] using the framework “consistency + stability $\Rightarrow$ convergence”, which shows the maximum error is bounded from above by $(\frac{1}{\tilde{k}} \|f''\|_{L^\infty} + k^2 \|f\|_{L^\infty})h^2$ up to a constant factor.

Another possibility adopted by [5] is to scale the discrete Laplacian but retain the original wavenumber k . This amounts to multiply the left hand side (only) of (40) with $\frac{k^2}{\tilde{k}^2}$ and get

$$\left(k^2 - \frac{k^2}{\tilde{k}^2} \frac{2}{h^2}\right)u^h(x_j) + \frac{k^2}{\tilde{k}^2} \frac{1}{h^2}u^h(x_{j-1}) + \frac{k^2}{\tilde{k}^2} \frac{1}{h^2}u^h(x_{j+1}) = f(x_j), \quad u^h(x_0) = g_0, \quad u^h(x_N) = g_1. \quad (41)$$

When $f = 0$, the scheme (41) is equivalent to (40). The original work of [5] is in the finite element framework with the source treated by integral. The idea is to “eliminate the phase lag $k - k^h$ for as many right-hand sides as possible”, not only for $f = 0$ but also for piecewise constant f . For a different problem than (1) with the right boundary condition being $u' - iku = 0$, it was shown in [5] that the H^1 -semi-norm of the error is bounded from above by $h\|f\|_{H^1}$ up to a constant factor.

Remark 15. If we multiply f (only) in (40) with $\frac{\tilde{k}^2}{k^2}$, then we obtain a scheme equivalent to (41).

As we have seen, the 1D dispersion correction is determined up to a constant factor. If we follow a third approach proposed by [42] originally for 2D and 3D problems, then we would get

$$\left(k^2 - \frac{k^2}{\tilde{k}^2} \frac{2}{h^2}\right)u^h(x_j) + \frac{k^2}{\tilde{k}^2} \frac{1}{h^2}u^h(x_{j-1}) + \frac{k^2}{\tilde{k}^2} \frac{1}{h^2}u^h(x_{j+1}) = \frac{kh}{2} \cot \frac{kh}{2} f(x_j), \quad u^h(x_0) = g_0, \quad u^h(x_N) = g_1. \quad (42)$$

To evaluate the three dispersion free schemes (40), (41) and (42), we use the Fourier analysis as a visual tool. Since the downsampling and aliasing errors are smaller (for smooth f) than the operator error, we will focus on the latter. The operator symbols of (40), (41) and (42), that map u^h to f^h , are

$$\lambda_k^h := \tilde{k}^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}, \quad \lambda_\Delta^h := k^2 - \frac{k^2}{\tilde{k}^2} \frac{4}{h^2} \sin^2 \frac{\xi h}{2}, \quad \lambda_{\Delta,f}^h := \frac{2}{kh} \tan \frac{kh}{2} \lambda_\Delta^h, \quad \xi \in \{1, \dots, N-1\}\pi \text{ for } h = \frac{1}{N}. \quad (43)$$

Recall that the continuous symbol is $\lambda = k^2 - \xi^2$, and the symbol errors are defined as

$$\psi := \left| \frac{\xi}{\lambda} - \frac{\xi}{\lambda^h} \right|, \quad \psi_e := \left| \frac{1}{\lambda} - \frac{1}{\lambda^h} \right|, \quad \psi_{rel} := \left| \frac{\lambda - \lambda^h}{\xi^2 \lambda^h} \right|, \quad \xi \in \{1, \dots, N-1\}\pi \text{ for } h = \frac{1}{N}, \quad (44)$$

where λ^h is the discrete symbol. For the classical centered scheme, $\lambda^h = k^2 - \frac{4}{h^2} \sin^2 \frac{\xi h}{2}$. For the scheme (40), (41) or (42), it is λ_k^h , λ_Δ^h or $\lambda_{\Delta,f}^h$ in (43). From (29), (32), (37) and (38), it is essentially the symbol error ψ , ψ_e or ψ_{rel} that determines the convergence in terms of absolute/relative error in the L^2 - or H^1 -semi-norm.

Figure 3 shows the symbol errors ψ_e (44) for the four schemes under h -refinement. We see that the dispersion free schemes have lower maxima of ψ_e than the classical one, at the price of larger ψ_e at smaller ξ (roughly $< \frac{5}{6}k$ or $< \frac{2}{3}k$). We also see that the scheme (42) modifying both the discrete Laplacian and the source performs the best. The order of $\max \psi_e$ is h^2 , which corroborates Lemma 11.

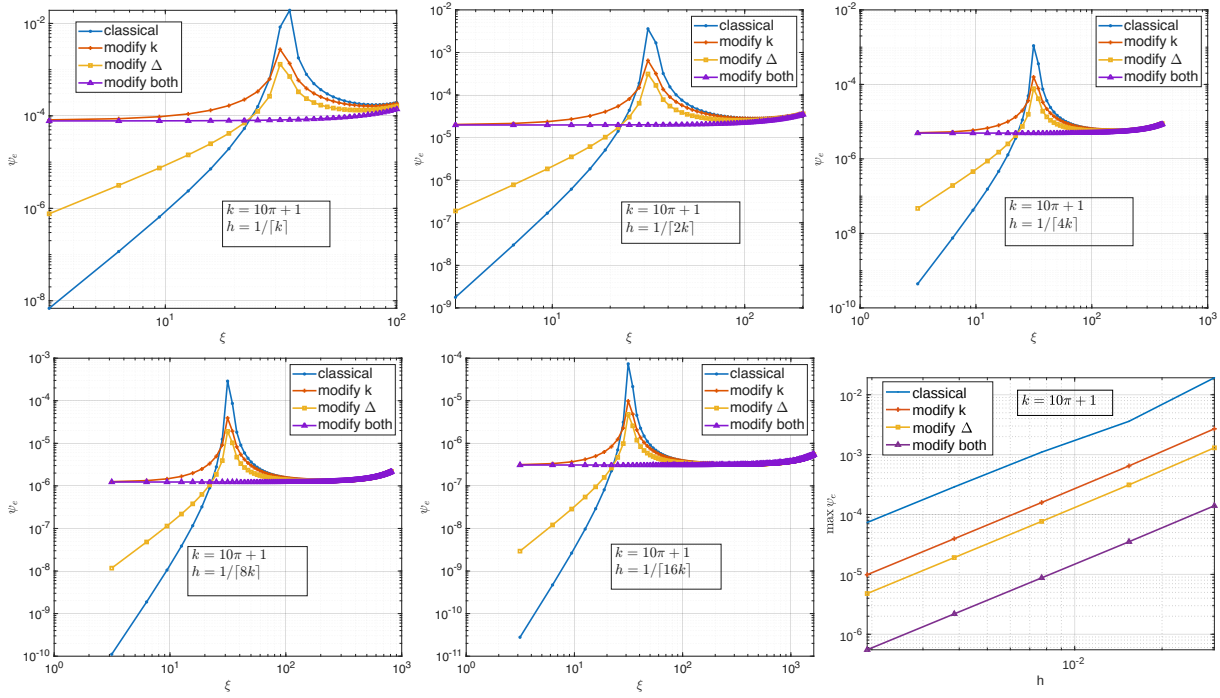


Figure 3: Symbol errors ψ_e (44) for the classical (9) & dispersion free (40), (41), (42): h -refinement

Next, the influence of the wavenumber k is demonstrated, see Figure 4 in which k is quadrupled while kh is halved. This clearly shows that the classical scheme can not converge in this setting with k^3h^2 fixed. This corresponds to the order k^3h^2 proved in Lemma 10. Figure 4 shows also that the schemes (40) and (41) have the symbol error of order k^2h^2 which translates to the same order of $|u - u^h|_1$ by (29), while the scheme (42) is even better and of ² order $k^{3/2}h^2$.

Next, the relative symbol error ψ_{rel} is visualized in Figure 5 where kh is fixed while k is doubled. According to (38), $\max \psi_{rel}$ has to be multiplied with $|u_{low}|_3/|u|_1$ to give the upper bound of $|u - u^h|_1/|u|_1$, and when the upper bound is attained, $|u_{low}|_3/|u|_1$ may contribute some powers of k (see Theorem 4). For the classical scheme, we see from Figure 5 that ψ_{rel} is of order kh^2 which corroborates Lemma 14. For the dispersion free schemes (40) and (42), the relative symbol error ψ_{rel} does not decrease with h (while kh is fixed) at the first frequency $\xi = \pi$, which slows down also the convergence at the other low frequencies. The dispersion free scheme (41) modifying the discrete Laplacian has an almost equidistributed ψ_{rel} over ξ as seen in the figure, and $\max \psi_{rel}$ is attained at $\xi = (N - 1)\pi$ (order k) and is of order h^2 . So the relative error $|u - u^h|_1/|u|_1$ of the scheme (41) is of order k^2h^2 .

Finally, the scaling with σ_k for the relative symbol error ψ_{rel} divided by k^3h^2 is demonstrated in Figure 6 where $k + \sigma_k = 21\pi$, σ_k is halved, and $h = 1/\lceil 1/\sqrt{\sigma_k/k^3} \rceil$. We see that the maximum relative symbol error of the classical scheme is inversely proportional to σ_k , while all the dispersion free schemes are independent of σ_k . In particular, for the third dispersion free scheme from [42], the symbol value near k even decreases linearly with σ_k .

5 Numerical Experiments

We study numerically the scaling with k , h and σ_k . We take $g_0 = g_1 = 0$, $f(x) = \sin(\xi x)$ for some $\xi \in \pi\{1, \dots, \frac{1}{h} - 1\}$. So ξ depends on the finite difference scheme and the error being considered.

First, we fix $\sigma_k = 1$, double $k - \sigma_k$, choose ξ to maximize the absolute error, and let $h = 1/\lceil k^{3/2} \rceil$. The absolute errors are shown in Figure 7, which confirms the results from the visual analysis in section 4.

²This is because the order in h for fixed k must be 2, and it is observed that the scaling $k \rightarrow 4k$, $h \rightarrow h/8$ makes the error scaled by $4^3/8^3 = 2^{-3}$, so that $4^\alpha/8^2 = 2^{-3}$ gives the right exponent $\alpha = \frac{3}{2}$ for k .

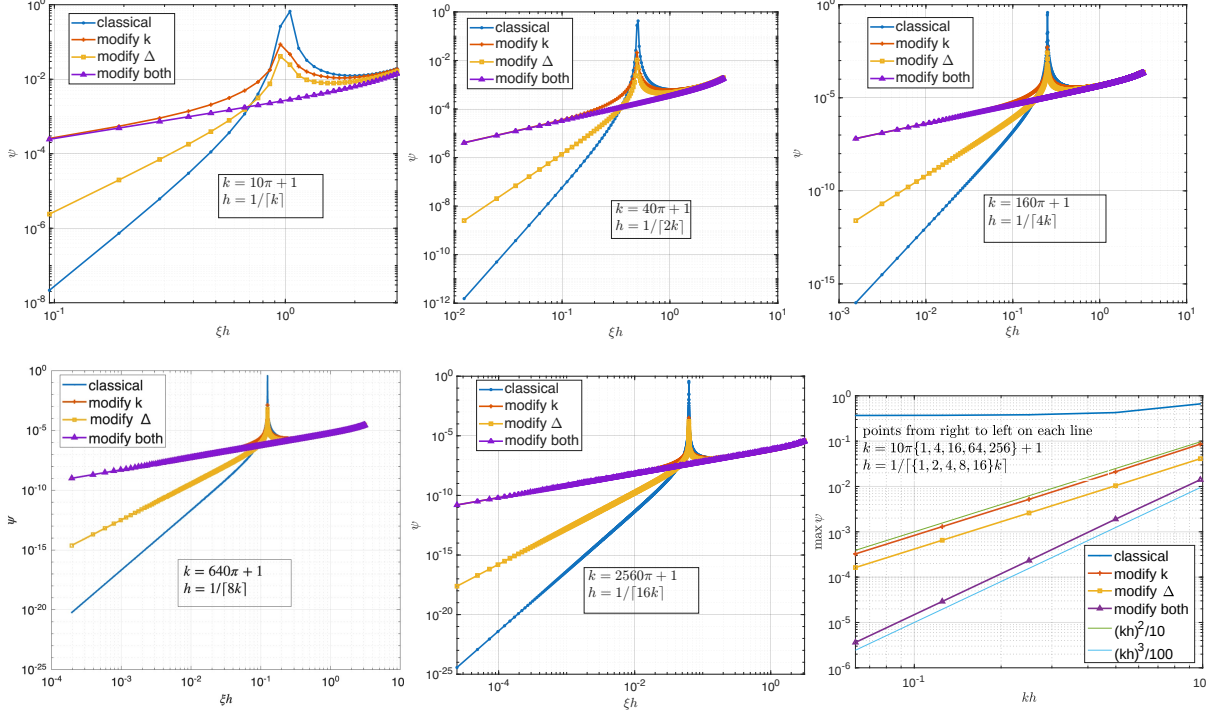


Figure 4: Symbol errors ψ (44) for the classical (9) & dispersion free (40), (41), (42): kh -refinement

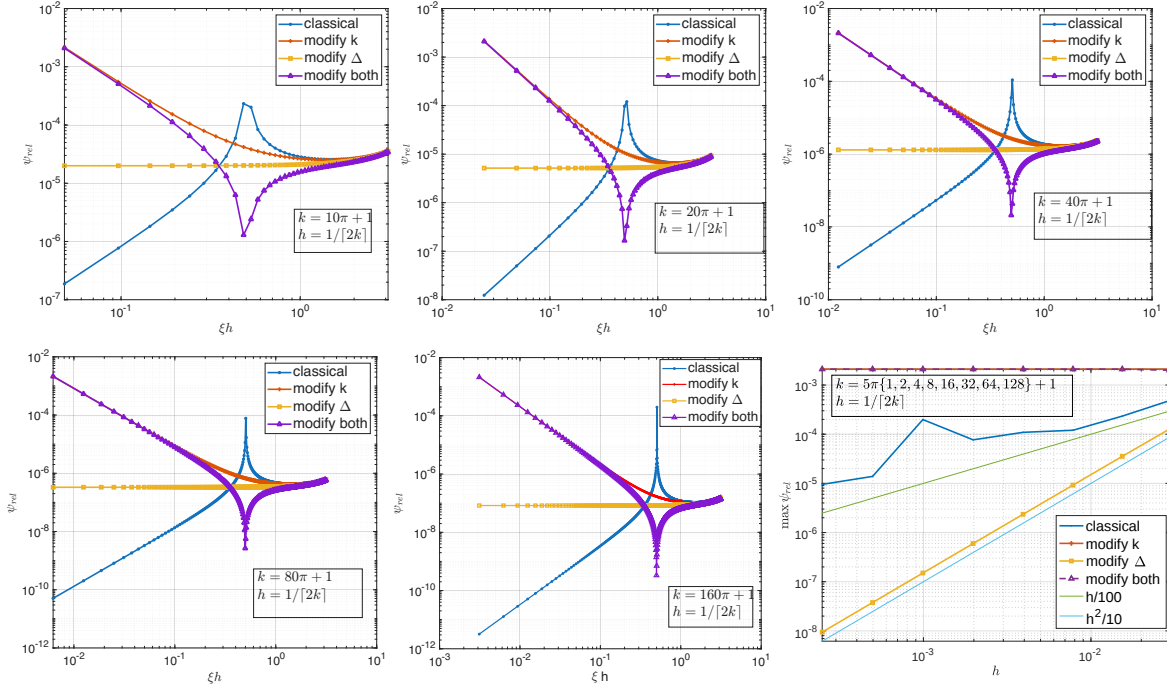


Figure 5: Symbol errors ψ_{rel} (44) for the classical (9) & dispersion free (40), (41), (42): kh fixed

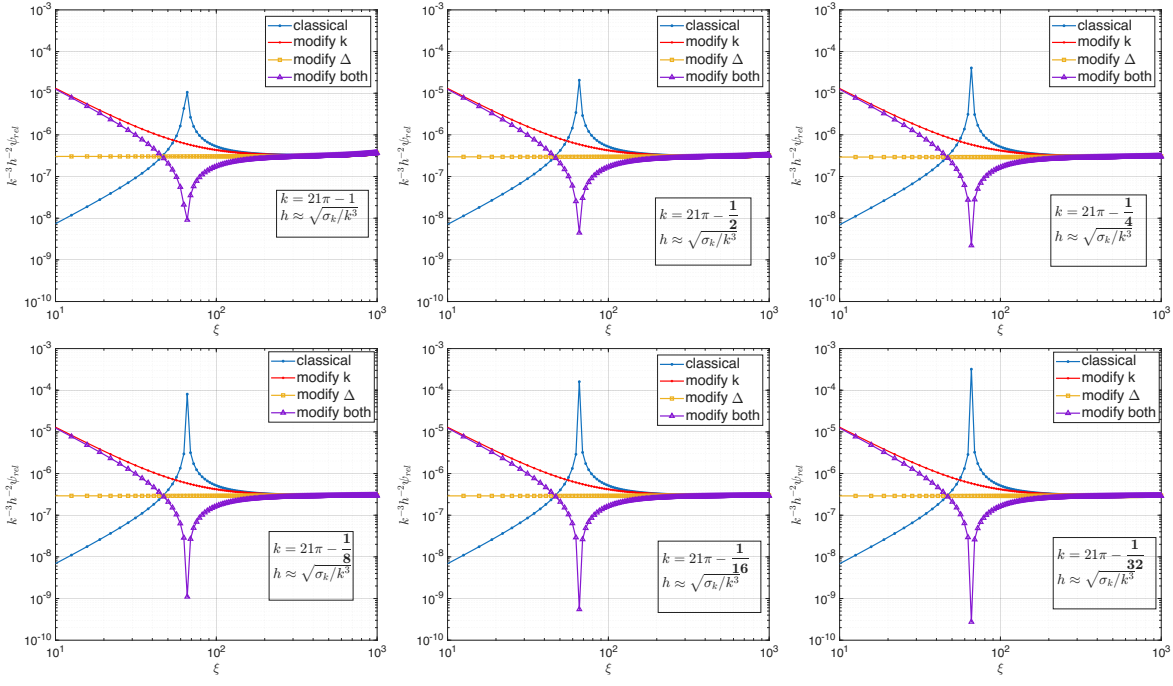


Figure 6: Divided symbol errors $\frac{\psi_{rel}}{k^3 h^2}$ (44) for the classical (9) & dispersion free (40), (41), (42)

One needs to be careful to read the scaling shown in the figure. For example, the L^2 error of (42) in Figure 7 appears to scale as $(kh)^6$ when k doubles and $h \asymp k^{-3/2}$, but since the actual order should be in the form $k^\alpha h^2$, we find $(2 \cdot 2^{-3/2})^6 = 2^\alpha \cdot (2^{-3/2})^2$ gives $\alpha = 0$. Then in Figure 8, we study the dependence on σ_k , which corroborates Theorem 3 and the results from the visual analysis in section 4.

In the same settings as for the absolute errors, we numerically compute the relative errors. But note that the estimates (37) and (38) depend on $|u|_{p+2}/|u|_p$ for $p = 0, 1$. In particular, when $\sigma_k = 1$, $h \asymp k^{-3/2}$ and $f(x) = \sin(\pi(1 - \frac{1}{h})x)$, we have $|u|_{p+2}/|u|_p \asymp k^3$, and we observed the numerical relative errors of order $k^3 h^2 = O(1)$ for all the finite difference schemes. Also, for the scheme (40) and (42), taking $f(x) = \sin(\pi x)$ results $O(1)$ relative errors. Therefore, we shall assume here $f(x) = \sin(\xi x)$ with $\xi \asymp k$. First, the scaling with k and h is shown in Figure 9. Then we study the dependence on σ_k in Figure 10, which corroborates Theorem 4 as well as the results from the visual analysis in section 4.

6 Conclusions and Discussions

Based on Fourier decomposition, we analyzed the classical centered finite difference method for the Helmholtz equation in 1D with Dirichlet conditions. Such results have been considered standard for the closely related finite element method. Our estimates are guaranteed by two-sided bounds on the attainable worst case, and the lower bounds are the main novelty. That is, for each wavenumber k , we can choose a source term to maximize the error order in k , and the maximal error is bounded from below and above. The distance σ_k of k to the square-root of the spectrum of the continuous negative Laplacian is revealed in the error estimates. We also used the Fourier decomposition for evaluating three dispersion free finite difference methods, which was impossible by the dispersion analysis (because all have zero dispersion error).

There are some limitations of the proposed approach in this work. First, it only works on uniform grids of simple geometry. Second, with radiation boundary conditions the generalized Fourier decomposition based on the Sturm-Liouville problem will lead to a non-orthogonal basis, and the current approach does not work directly. It might be interesting to try the singular value decomposition i.e. consider the least-squared $(\mathcal{L}^* \mathcal{L})$ Sturm-Liouville problem, which diagonalises the Helmholtz operator with two orthogonal bases. Third, it works only for constant coefficient problems.

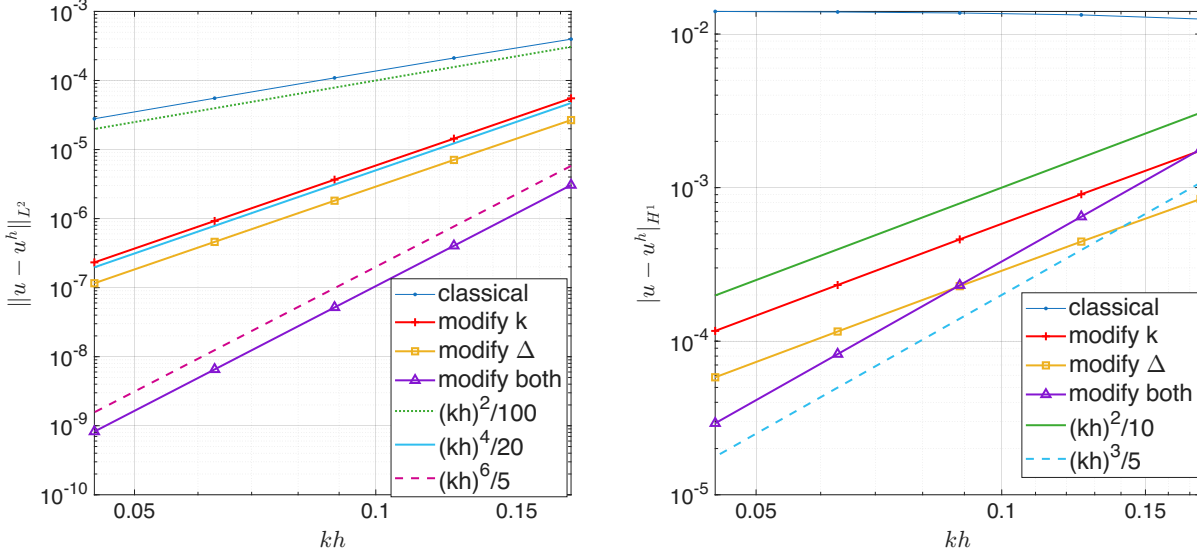


Figure 7: Numerical absolute errors with $g_0 = g_1 = 0$, $f = \sin(\xi x)$, $k = 10\pi \cdot 2^{0.4} + 1$, $h = 1/\lceil k^{3/2} \rceil$, and $\xi = k - 1$ for the classical (9) & dispersion free (40), (41), but $\xi = \pi(\frac{1}{h} - 1)$ for (42). In this setting, the scalings shown are only apparent and must be reinterpreted in the form $k^\alpha h^2$ because all the schemes are second order in h for fixed k . For example, comparing $(2k \cdot 2^{-3/2}h)^3 = (2 \cdot 2^{-3/2})^3(kh)^3$ and $(2k)^\alpha(2^{-3/2}h)^2 = 2^{\alpha-3}k^\alpha h^2$, we obtain $-3/2 = \alpha - 3$ or $\alpha = 3/2$. See also the footnote 2 for Figure 4.

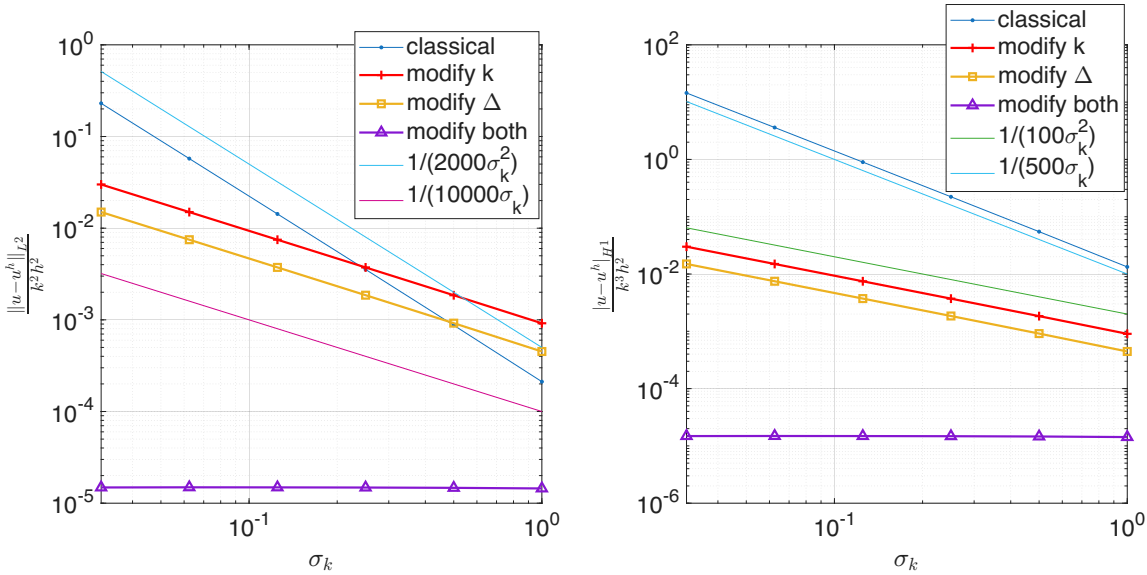


Figure 8: Numerical absolute errors (divided by $k^2 h^2$ on the left and $k^3 h^2$ on the right) against $\sigma_k = \text{dist}(k, \pi\mathbb{N})$ with $k^3 h^2 \approx \sigma_k$, $k = 20\pi + \sigma_k$, $f = \sin(20\pi x)$ and $g_0 = g_1 = 0$ for the classical (9) & dispersion free (40), (41), (42)

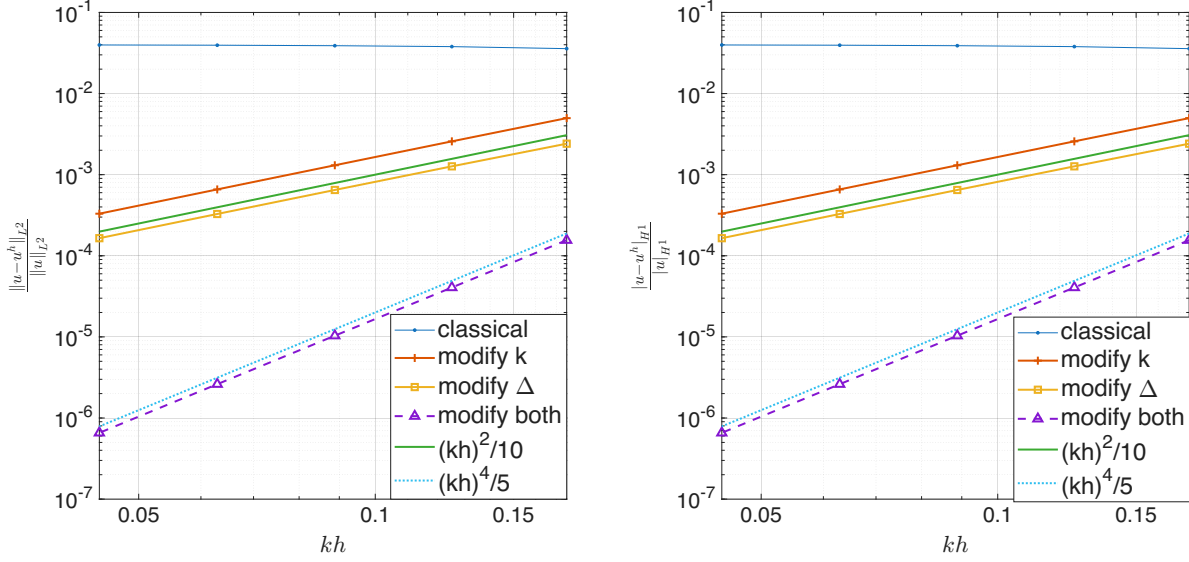


Figure 9: Numerical relative errors with $g_0 = g_1 = 0$, $f = \sin(\xi x)$, $k = 10\pi \cdot 2^{0:4} + 1$, $h = 1/\lceil k^{3/2} \rceil$, and $\xi = k - 1$ for the classical (9) & dispersion free (40), (41), (42). The L^2 - and H^1 -semi-norm relative errors are equal in this case. In this setting, the scalings shown are only apparent and must be reinterpreted in the form $k^\alpha h^2$ because all the schemes are second order in h for fixed k . For example, comparing $(2k \cdot 2^{-3/2}h)^4 = (2 \cdot 2^{-3/2})^4 (kh)^4$ and $(2k)^\alpha (2^{-3/2}h)^2 = 2^{\alpha-3} k^\alpha h^2$, we obtain $-2 = \alpha - 3$ or $\alpha = 1$.

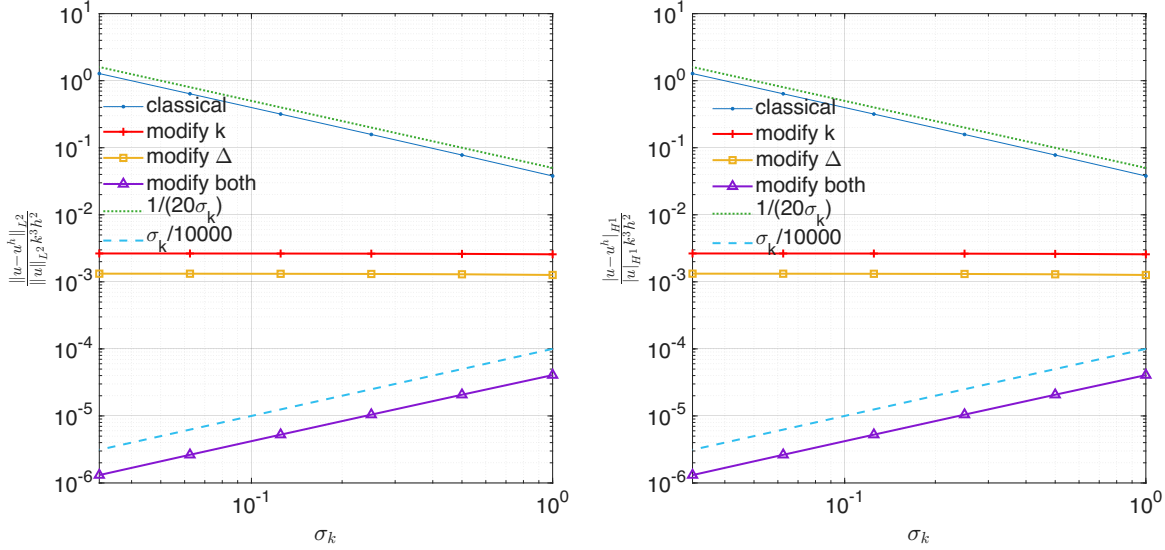


Figure 10: Numerical relative errors (divided by $k^3 h^2$) against $\sigma_k = \text{dist}(k, \pi\mathbb{N})$ with $k^3 h^2 \approx \sigma_k$, $k = 20\pi + \sigma_k$, $f = \sin(20\pi x)$ and $g_0 = g_1 = 0$ for the classical (9) & dispersion free (40), (41). The L^2 - and H^1 -semi-norm relative errors are equal in this case.

However, the proposed approach provides a new tool for quantitatively evaluating linear schemes, in complement to dispersion analysis. The latter considers only the zero source case and does not lead to error estimates. In other words, the approach can be thought of as a quantitative tool for finite difference methods in analogy to the local (or rigorous) Fourier analysis for multigrid methods. It will be helpful for evaluating and designing finite difference methods for the Helmholtz equation. Some ideas have been presented in [15] which inspired this work.

For future work, it is interesting to consider models in 2D/3D with simple geometries and analyze some compact high-order schemes, which is more challenging e.g. in finding the maximum of a multivariate symbol. Moreover, it is worthwhile to try optimizing discretization parameters based on the Fourier decomposition.

We note that wavenumber explicit error estimates have been well developed for low and high order finite element methods. A parallel development for finite difference methods would be good to have, given that they are actually used in applications (e.g. [43]) for *variable coefficient* Helmholtz problems. The variational theory of finite difference methods developed in [30] may be useful.

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Data Availability

Data publicly available at <https://bitbucket.org/mathbuddy/fourierfdm1d>

Conflict of interest

The authors declare that they have no conflict of interest.

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A Proof of the claim (31)

The claim (31) is

$$\phi(\theta) = \frac{\theta}{\sin^2 \theta - \mu^2} - \frac{\theta}{\theta^2 - \mu^2} \text{ has no local maximum for } \theta_k < \theta < \frac{\pi}{2} \text{ and } 0 < \mu < 1,$$

where $\theta_k := \arcsin \mu$. The following is a proof.

Proof. We calculate

$$\phi'(\theta) = \frac{2\theta^2}{(\theta^2 - \mu^2)^2} - \frac{1}{\theta^2 - \mu^2} + \frac{1}{\sin^2 \theta - \mu^2} - \frac{2\theta \sin \theta \cos \theta}{(\sin^2 \theta - \mu^2)^2} =: \frac{\mathcal{P}(\theta)}{(\sin^2 \theta - \mu^2)^2 (\theta^2 - \mu^2)^2}.$$

Let $\nu = \mu^2$. Then a critical point θ_* of $\phi(\theta)$ is the root of

$$\mathcal{P}(\theta) = -2\theta^5 \sin \theta \cos \theta + \theta^4 \sin^2 \theta + \theta^2 \sin^4 \theta + (-\theta^4 + 4\theta^3 \sin \theta \cos \theta - 4\theta^2 \sin^2 \theta + \sin^4 \theta) \nu + (3\theta^2 - \sin^2 \theta - 2\theta \sin \theta \cos \theta) \nu^2 = 0.$$

The above equation is quadratic in ν . By calculation, we find

$$\nu = \frac{\theta^4 - \sin^4 \theta - 4\theta^3 \sin \theta \cos \theta + 4\theta^2 \sin^2 \theta \pm \frac{1}{4\sqrt{2}}(2\theta^2 + \cos(2\theta) - 1)\sqrt{t}}{2(3\theta^2 - \sin \theta(\sin \theta + 2\theta \cos \theta))} =: w_{\pm}(\theta),$$

where

$$t = 128\theta^3 \sin \theta \cos \theta + 8(\theta^2 - \sin^2 \theta)^2.$$

We calculate

$$w_+(\theta) - \sin^2 \theta = \frac{1}{8} \frac{(\theta^2 - \sin^2 \theta)(4\theta^2 - 8\theta \sin(2\theta) + 2\cos(2\theta) - 2 + \sqrt{2t})}{3\theta^2 - \sin \theta(\sin \theta + 2\theta \cos \theta)}.$$

The second factor in the numerator is actually positive, which makes $w_+(\theta) > \sin^2 \theta$. Indeed, we have

$$2t - (4\theta^2 - 8\theta \sin(2\theta) + 2\cos(2\theta) - 2)^2 = 64\theta \sin \theta \cos \theta (6\theta^2 - 2\theta \sin(2\theta) + \cos(2\theta) - 1)$$

and

$$(6\theta^2 - 2\theta \sin(2\theta) + \cos(2\theta) - 1)' = 12\theta - 4\sin(2\theta) - 4\theta \cos(2\theta) > 0 \text{ for } 0 < \theta < \frac{\pi}{2}.$$

So a critical point of ϕ must satisfy $\nu = w_-(\theta)$. We are going to show that $w'_-(\theta) > 0$ for $0 < \theta < \frac{\pi}{2}$. By calculation, we get

$$w'_-(\theta) = \frac{16\theta v(\theta)}{8(3\theta^2 - \sin^2 \theta - 2\theta \sin \theta \cos \theta)^2 \sqrt{t}} \quad \text{with}$$

$$\begin{aligned} v(\theta) = & -16\sqrt{2}\theta^6 + 26\sqrt{2}\theta^6 \sin^2 \theta + 16\sqrt{2}\theta^5 \sin^3 \theta \cos \theta - 36\sqrt{2}\theta^5 \sin \theta \cos \theta - 106\sqrt{2}\theta^4 \sin^4 \theta + \\ & 92\sqrt{2}\theta^4 \sin^2 \theta + 16\sqrt{2}\theta^3 \sin^5 \theta \cos \theta - 24\sqrt{2}\theta^3 \sin^3 \theta \cos \theta + 14\sqrt{2}\theta^2 \sin^6 \theta - 8\sqrt{2}\theta^2 \sin^4 \theta + \\ & 2\sqrt{2}\sin^8 \theta - 4\sqrt{2}\sin^6 \theta - 4\sqrt{2}\sin^5 \theta \cos \theta - \theta^4 \sqrt{t} + 5\theta^4 \sqrt{t} \sin^2 \theta + 2\theta^3 \sqrt{t} \sin \theta \cos \theta - \\ & 4\theta^2 \sqrt{t} \sin^4 \theta - \sqrt{t} \sin^6 \theta + \sqrt{t} \sin^4 \theta - 2\theta \sqrt{t} \sin^3 \theta \cos \theta. \end{aligned}$$

For $0 < \theta \leq 1$, we claim

$$a(\theta) := 8\sqrt{2}\theta^2 - \frac{8\sqrt{2}\theta^4}{3} < \sqrt{t} < \frac{7\theta^6}{30\sqrt{2}} - \frac{8\sqrt{2}\theta^4}{3} + 8\sqrt{2}\theta^2 =: b(\theta). \quad (45)$$

Indeed, $t = 64\theta^3 \sin(2\theta) + 8(\theta - \sin(\theta))^2(\theta + \sin(\theta))^2$ can be enlarged using

$$\begin{aligned} \theta - \sin(\theta) & < \frac{\theta^3}{6} - \frac{\theta^5}{120} + \frac{\theta^7}{5040} \\ \theta + \sin(\theta) & < 2\theta - \frac{\theta^3}{6} + \frac{\theta^5}{120} \\ \sin(2\theta) & < 2\theta - \frac{4\theta^3}{3} + \frac{4\theta^5}{15} - \frac{8\theta^7}{315} + \frac{4\theta^9}{2835} \end{aligned}$$

for $0 < \theta < \frac{\pi}{2}$. Denote the enlarged t as $\tilde{t}$. Then we have

$$\begin{aligned} b(\theta)^2 - \tilde{t} = & \left(\frac{584\theta^{10}}{945} - \frac{2173\theta^{12}}{22680} \right) + \left(\frac{53\theta^{14}}{18900} - \frac{1933\theta^{16}}{11907000} \right) + \left(\frac{19\theta^{18}}{2976750} - \frac{1921\theta^{20}}{11430720000} \right) + \\ & \left(\frac{31\theta^{22}}{11430720000} - \frac{\theta^{24}}{45722880000} \right) > 0 \text{ for } 0 < \theta < 1. \end{aligned}$$

Hence, $\sqrt{t} < b(\theta)$. We can shrink t using

$$\begin{aligned}\theta - \sin(\theta) &> \frac{\theta^3}{6} - \frac{\theta^5}{120} \\ \theta + \sin(\theta) &> 2\theta - \frac{\theta^3}{6} \\ \sin(2\theta) &> 2\theta - \frac{4\theta^3}{3} + \frac{4\theta^5}{15} - \frac{8\theta^7}{315}\end{aligned}$$

for $0 < \theta < \frac{\pi}{2}$. Denote the shrunk t as $\tilde{t}$. Then we have

$$\tilde{t} - a(\theta)^2 = \left(\frac{56\theta^8}{15} - \frac{352\theta^{10}}{189}\right) + \left(\frac{47\theta^{12}}{2025} - \frac{2\theta^{14}}{2025}\right) + \frac{\theta^{16}}{64800} > 0 \text{ for } 0 < \theta < 1.$$

Substituting (45) and

$$\begin{aligned}\theta - \frac{\theta^3}{6} &< \sin \theta < \theta - \frac{\theta^3}{6} + \frac{\theta^5}{120} \\ 1 - \frac{\theta^2}{2} + \frac{\theta^4}{24} - \frac{\theta^6}{720} &< \cos \theta < 1 - \frac{\theta^2}{2} + \frac{\theta^4}{24}\end{aligned}$$

into $v(\theta)$ with upper bounds into negative terms and lower bounds into positive terms, yields

$$\begin{aligned}v(\theta) &> \left(\frac{389\theta^{10}}{90\sqrt{2}} - \frac{1871\theta^{12}}{270\sqrt{2}}\right) + \left(\frac{17071\theta^{14}}{5400\sqrt{2}} - \frac{914\sqrt{2}\theta^{16}}{2025}\right) + \left(\frac{575611\theta^{18}}{2916000\sqrt{2}} - \frac{4573\theta^{20}}{144000\sqrt{2}}\right) + \\ &\quad \left(\frac{140789\theta^{22}}{38880000\sqrt{2}} - \frac{1263749\theta^{24}}{4199040000\sqrt{2}}\right) + \left(\frac{58373\theta^{26}}{3110400000\sqrt{2}} - \frac{49411\theta^{28}}{55987200000\sqrt{2}}\right) + \\ &\quad \left(\frac{17221\theta^{30}}{559872000000\sqrt{2}} - \frac{139\theta^{32}}{186624000000\sqrt{2}}\right) + \left(\frac{\theta^{34}}{89579520000\sqrt{2}} - \frac{7\theta^{36}}{89579520000000\sqrt{2}}\right) > 0\end{aligned}$$

for $0 < \theta < \sqrt{\frac{1167}{1871}}$. Note that $\sqrt{\frac{1167}{1871}} > \frac{7}{10}$. For $\frac{7}{10} \leq \theta \leq \frac{\pi}{2}$, we make use of interval arithmetic in Mathematica to show $v(\theta) > 0$. The code is given below.

```
a = 7/10; b = Pi/2; n = 100; (*Number of subdivisions*) subintervals = Subdivide[a, b, n];
allIntervalsPositive = True; (*Check each subinterval*)
For[i = 1, i <= n, i++,
  smallInt = Interval[{subintervals[[i]], subintervals[[i + 1]]}];
  vSmallInt = v[smallInt];
  If[Min[vSmallInt] <= 0, allIntervalsPositive = False; Break[];];
If[allIntervalsPositive, Print["v(x) > 0 in [", a, ", ", b, "]",
  Print["Potential root found in subinterval: ", smallInt]]
```

In summary, $w'_-(\theta) > 0$ on $\theta \in (0, \frac{\pi}{2})$. Therefore, in $\theta \in (0, \frac{\pi}{2})$, $\nu = w_-(\theta)$ has at most one root, and $\phi(\theta)$ has at most one critical point. Note that $\mathcal{P}(\theta = \arcsin \mu) = -2\theta(\theta - \sin \theta)^2 \sin \theta(\theta + \sin \theta)^2 \cos \theta < 0$ for $0 < \mu < 1$, and $\mathcal{P}(\theta = \frac{\pi}{2}) = -\frac{1}{16}(\mu^2 - 1)((16 - 12\pi^2)\mu^2 + \pi^4 + 4\pi^2) > 0$ for $0 < \mu < 1$. So $\phi(\theta)$ in $\theta_k < \theta < \frac{\pi}{2}$ is decreasing before the only critical point and then increasing after. That means $\phi(\theta)$ has no local maximum in $\theta_k < \theta < \frac{\pi}{2}$. $\square$

B Proof of the claim (34)

We first copy the claim (34) here:

$$\phi_e(\theta) = \frac{1}{\sin^2 \theta - \mu^2} - \frac{1}{\theta^2 - \mu^2} \text{ has no local maximum for } \theta \in (\theta_k, \frac{\pi}{2}) \text{ and } 0 < \mu < 1,$$

where $\theta_k := \arcsin \mu$. Then we give the proof as follows.

Proof. We calculate

$$\phi'_e(\theta) = \frac{2\theta}{(\theta^2 - \mu^2)^2} - \frac{2\sin\theta\cos\theta}{(\sin^2\theta - \mu^2)^2} =: 2\frac{\mathcal{P}(\theta)}{(\theta^2 - \mu^2)^2(\mu^2 - \sin^2\theta)^2}.$$

Let $\nu = \mu^2$. Then a critical point θ_* of $\phi_e(\theta)$ is the root of

$$\mathcal{P}(\theta) = -\theta^4\sin\theta\cos\theta + \theta\sin^4\theta + (2\theta^2\sin\theta\cos\theta - 2\theta\sin^2\theta)\nu + (\theta - \sin\theta\cos\theta)\nu^2 = 0$$

By solving for ν from the above equation, we find θ_* must satisfy one of the following equations

$$\nu = \frac{\theta\sin^2\theta - \theta^2\sin\theta\cos\theta \pm \sqrt{\theta}\sqrt{\sin\theta\cos\theta}(\theta^2 - \sin^2\theta)}{\theta - \sin\theta\cos\theta} =: w_{\pm}(\theta).$$

We calculate and use $x > \sin x > 0$ for $0 < x < \pi$ to find

$$w_+(\theta) - \sin^2\theta = 2\frac{\theta^2 - \sin^2\theta}{\theta - \sin\theta\cos\theta} \left(\sqrt{2\theta}\sqrt{\sin(2\theta)} - \sin(2\theta) \right) > 0.$$

So the only equation that θ_* needs to satisfy is $\nu = w_-(\theta)$. We claim that $w'_-(\theta) > 0$ and thus $w_-(\theta)$ is increasing for $0 < \theta < \frac{\pi}{2}$. This will be shown for $0 < \theta \leq 1$ and $1 \leq \theta < \frac{\pi}{2}$ separately. We calculate

$$\begin{aligned} & \left(2\sqrt{\theta}\sqrt{\sin\theta\cos\theta}(\sin\theta\cos\theta - \theta)^2 \right) w'_-(\theta) \\ &= 2\theta^{3/2}\sin^2\theta\cos^2\theta\sqrt{\sin\theta\cos\theta} - 2\theta^{7/2}\cos^2\theta\sqrt{\sin\theta\cos\theta} - 2\theta^{3/2}\sin^4\theta\sqrt{\sin\theta\cos\theta} + \\ & \quad 2\theta^{7/2}\sin^2\theta\sqrt{\sin\theta\cos\theta} + 2\theta^{5/2}\sin\theta\cos\theta\sqrt{\sin\theta\cos\theta} + \theta^4\sin^2\theta - \theta^4\cos^2\theta - \theta^3\sin\theta\cos^3\theta + \\ & \quad \theta^3\sin^3\theta\cos\theta - 3\theta^3\sin\theta\cos\theta - \theta^2\sin^4\theta + 10\theta^2\sin^2\theta\cos^2\theta - 3\theta\sin^3\theta\cos^3\theta - \sin^4\theta\cos^2\theta - \\ & \quad \theta\sin^5\theta\cos\theta - \theta\sin^3\theta\cos\theta - 2\sqrt{\theta}\sin^3\theta\cos\theta\sqrt{\sin\theta\cos\theta} =: v(\theta). \end{aligned}$$

We note that $v(\theta)$ is a sum of positive terms and negative terms.

For $0 < \theta \leq 1$, we first show that

$$\sqrt{\theta} - \frac{\theta^{5/2}}{3} + \frac{\theta^{9/2}}{90} - \frac{\theta^{13/2}}{180} < \sqrt{\sin\theta\cos\theta} < \sqrt{\theta} - \frac{\theta^{5/2}}{3} + \frac{\theta^{9/2}}{90}, \quad (46)$$

or equivalently

$$a(\theta) := 2\theta - \frac{4\theta^3}{3} + \frac{4\theta^5}{15} - \frac{\theta^7}{27} + \frac{31\theta^9}{4050} - \frac{\theta^{11}}{4050} + \frac{\theta^{13}}{16200} < \sin(2\theta) < 2\theta - \frac{4\theta^3}{3} + \frac{4\theta^5}{15} - \frac{2\theta^7}{135} + \frac{\theta^9}{4050} =: b(\theta).$$

By Maclaurin series, we can show for $0 < \theta \leq 1$ that

$$c(\theta) := 2\theta - \frac{4\theta^3}{3} + \frac{4\theta^5}{15} - \frac{8\theta^7}{315} + \frac{4\theta^9}{2835} - \frac{8\theta^{11}}{155925} < \sin(2\theta) < 2\theta - \frac{4\theta^3}{3} + \frac{4\theta^5}{15} - \frac{8\theta^7}{315} + \frac{4\theta^9}{2835} =: d(\theta)$$

We note for $0 < \theta \leq 1$ that

$$c(\theta) - a(\theta) = \left(\frac{11\theta^7}{945} - \frac{59\theta^9}{9450} \right) + \left(\frac{61\theta^{11}}{311850} - \frac{\theta^{13}}{16200} \right) > 0, \quad b(\theta) - d(\theta) = \frac{2\theta^7}{189} - \frac{11\theta^9}{9450} > 0.$$

We substitute (46) and

$$\begin{aligned} \theta - \frac{\theta^3}{6} + \frac{\theta^5}{120} - \frac{\theta^7}{5040} &< \sin\theta < \theta - \frac{\theta^3}{6} + \frac{\theta^5}{120} \\ 1 - \frac{\theta^2}{2} + \frac{\theta^4}{24} - \frac{\theta^6}{720} &< \cos\theta < 1 - \frac{\theta^2}{2} + \frac{\theta^4}{24} \end{aligned}$$

into $v(\theta)$ with upper bounds into negative terms and lower bounds into positive terms, and get

$$v(\theta) > \left(\frac{92\theta^{10}}{315} - \frac{7619\theta^{12}}{37800} \right) + \left(\frac{5207\theta^{14}}{85050} - \frac{678781\theta^{16}}{63504000} \right) + \left(\frac{267361\theta^{18}}{228614400} - \frac{9557\theta^{20}}{120960000} \right) + \left(\frac{11827\theta^{22}}{4572288000} \right) + \\ \left(\frac{299807\theta^{24}}{5761082880000} - \frac{2240017\theta^{26}}{230443315200000} \right) + \left(\frac{78433\theta^{28}}{172832486400000} - \frac{57977\theta^{30}}{5530639564800000} \right) + \\ \left(\frac{73\theta^{32}}{592568524800000} - \frac{\theta^{34}}{1185137049600000} \right) > 0 \quad \text{for } 0 < \theta \leq 1.$$

Therefore, $w'_-(\theta) > 0$ for $0 < \theta \leq 1$.

For $1 \leq \theta < \frac{\pi}{2}$, we make use of interval arithmetic in Mathematica. The code is similar to that in Appendix A. Running the code, we get the result `v(x)>0 in [1,Pi/2]`. Hence, $w'_-(\theta) > 0$ for $1 \leq \theta < \frac{\pi}{2}$.

Now we have proved w_- is increasing in $\theta \in (0, \frac{\pi}{2})$. So $\nu = w_-(\theta)$ has at most one root in $\theta \in (0, \frac{\pi}{2})$. That is, $\phi_e(\theta)$ has at most one critical point in $\theta \in (0, \frac{\pi}{2})$. Note that

$$\mathcal{P}(\theta = \arcsin \mu) = -(\theta - \sin \theta)^2 \sin \theta (\theta + \sin \theta)^2 \cos \theta < 0 \text{ and } \mathcal{P}(\theta = \frac{\pi}{2}) = \frac{\pi}{2}(\nu - 1)^2 > 0.$$

So $\phi'_e(\theta)$ is negative before the only critical point of ϕ_e and positive after for $\theta \in (\arcsin \mu, \frac{\pi}{2})$. The only critical point of ϕ_e is a local minimum. That shows ϕ_e for $\theta \in (\arcsin \mu, \frac{\pi}{2})$ has no local maximum. $\square$