PROPERTIES OF DISCRETE DELTA FUNCTIONS AND LOCAL CONVERGENCE OF THE IMMERSED BOUNDARY METHOD

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Abstract. Many problems involving internal interfaces can be formulated as partial differential equations with singular source terms. Numerical approximation to such problems on a regular grid necessitates suitable regularizations of delta functions. We study the convergence properties of such discretizations for constant coefficient elliptic problems using the immersed boundary method as an example. We show how the order of the differential operator, order of the finite difference discretization, and properties of the discrete delta function all influence the local convergence behavior. In particular, we show how a recently introduced property of discrete delta functions - the smoothing order - is important in the determination of local convergence rates.

Key words. immersed boundary method, discrete delta function, smoothing order, moment order

1. Introduction. There are many problems in applied mathematics in which the field variables of interest (velocity field, temperature field, etc.) possess discontinuities within its domain of definition. Problems of fluid structure interaction, two phase fluid flow, phase transition and image analysis are prime examples. Such problems can often be recast in terms of partial differential equations (PDE) with singular sources. The PDE is often discretized on a uniform grid using standard methods. The singular source terms are regularized in an appropriate way so that its presence can be felt by the underlying grid. This strategy, first introduced in the immersed boundary method by Peskin [18, 17, 14], has since been adopted as an essential component in numerous interface computations including front-tracking methods [23, 19] and level-set methods [16, 20].

The convergence properties of such methods have been the topic of many papers [15, 22, 24, 3, 10, 12] but a theoretical understanding is still largely lacking. This is in contrast to the immersed interface method, a closely related method, for which a detailed theoretical understanding is emerging [2, 13]. The goal of this paper is to analytically study this problem extending previous results that were confined to the two-dimensional Stokes problem with spectral discretization [15]. Here, we study the multi-dimensional case for general elliptic problems with general discretizations of the differential operators and focus on the pointwise convergence properties. This study was in part motivated by observations in [15] of better-than-expected convergence rates for particular choices of discrete delta functions (see Section 5).

Consider the following model problem:

$$Lu = f,\ f = \int F(\boldsymbol{\theta})\delta(\mathbf{x} - \mathbf{X}(\boldsymbol{\theta}))d\boldsymbol{\theta}, \tag{1.1}$$

where L is some elliptic operator, f is a singular source term and u is the solution. The singular source term f is given as a measure, often supported on a manifold (or immersed structure) of non-zero codimension. In the above, the immersed structure has a global coordinate system θ, and the position of this structure is given by $\mathbf{X}(\theta)$. The quantity $F(\theta)$ gives the strength of the measure at each given point on the manifold and $\delta(\mathbf{x} - \mathbf{X}(\theta))$ is the delta function centered at $\mathbf{X}(\theta)$. Let

$$L_h u_h = f_h \tag{1.2}$$

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be the numerical approximation to this problem where h is the grid spacing, L_h is the finite difference discretization of L, f_h is a suitable regularization of the singular measure f and u_h is the approximate solution. One way of discretizing f_h is to let

$$f_h(\mathbf{x}) = \int_{\text{disc}} F(\boldsymbol{\theta})\delta_h(\mathbf{x} - \mathbf{X}(\boldsymbol{\theta}))d\boldsymbol{\theta} \tag{1.3}$$

where $\int_{\text{disc}} \cdot d\boldsymbol{\theta}$ is some discretization of the integral and δ_h is a suitable regularization of the delta function. In this paper, we perform a careful analysis on how the order of the differential operator, the order of the finite difference discretization and properties of the regularized or discrete delta functions influence convergence properties of numerical approximations.

In section 2 we introduce the model problem. We consider the constant coefficient elliptic problem (1.1) in a periodic domain. Periodicity will allow us to use Fourier methods to estimate the error. Consider the Green's function $G(\mathbf{x} - \mathbf{X}) = G_{\mathbf{x}}(\mathbf{X})$. for (1.1). The exact solution u can be written as:

$$u(\mathbf{x}) = \int G_{\mathbf{x}}(\mathbf{X}(\boldsymbol{\theta}))F(\boldsymbol{\theta})d\boldsymbol{\theta}. \tag{1.4}$$

In a similar fashion, we may write u_h as:

$$u_h(\mathbf{x}) = \int_{\text{disc}} \widehat{G}_{h,\mathbf{x}}(\mathbf{X}(\boldsymbol{\theta}))F(\boldsymbol{\theta})d\boldsymbol{\theta}, \tag{1.5}$$

where $\widehat{G}_{h,\mathbf{x}}(\mathbf{X})$ is the discrete analogue of the continuous Green's function $G_{\mathbf{x}}(\mathbf{X})$ (see (2.10), where $\widehat{G}_{h,\mathbf{x}} = \mathcal{I}G_{h,\mathbf{x}}$). We may thus write the error $u - u_h$ as follows:

$$\begin{aligned} u(\mathbf{x}) - u_h(\mathbf{x}) &= E_Q(\mathbf{x}) + E_{IB}(\mathbf{x}), \\ E_Q(\mathbf{x}) &= \int G_{\mathbf{x}}(\mathbf{X}(\boldsymbol{\theta}))F(\boldsymbol{\theta})d\boldsymbol{\theta} - \int_{\text{disc}} G_{\mathbf{x}}(\mathbf{X}(\boldsymbol{\theta}))F(\boldsymbol{\theta})d\boldsymbol{\theta} \\ E_{IB}(\mathbf{x}) &= \int_{\text{disc}} \left(G_{\mathbf{x}}(\mathbf{X}(\boldsymbol{\theta})) - \widehat{G}_{h,\mathbf{x}}(\mathbf{X}(\boldsymbol{\theta}))\right) F(\boldsymbol{\theta})d\boldsymbol{\theta}. \end{aligned} \tag{1.6}$$

We shall call the term E_Q the quadrature error and E_{IB} the immersed boundary error. The quadrature error E_Q depends on the discretization used to describe the immersed structure. For points $\mathbf{x}$ not on the immersed structure, a bound on the quadrature error can often be easily obtained by elementary considerations. Indeed, in [22], the authors do not consider the error E_Q at all, and simply examine the difference:

$$\widetilde{E}_{IB}(\mathbf{x}) = \int \left(G_{\mathbf{x}}(\mathbf{X}(\boldsymbol{\theta})) - \widehat{G}_{h,\mathbf{x}}(\mathbf{X}(\boldsymbol{\theta}))F(\boldsymbol{\theta}))\right) d\theta. \tag{1.7}$$

The estimation of E_{IB} (or $\widetilde{E}_{IB}$) is far more subtle. Indeed, the technical contribution of this paper is in the estimation of the quantity:

$$\mathcal{E}_{IB} = G_{\mathbf{x}}(\mathbf{X}) - \widehat{G}_{h,\mathbf{x}}(\mathbf{X}). \tag{1.8}$$

We point out that our analysis is also closely related to the method of regularized Stokeslets, as proposed in [6, 7].

In section 3, we discuss properties of discrete delta functions that are important in examining the error $\mathcal{E}_{IB}$. The discrete delta function is required to satisfy discrete moment condition, the importance of which has been discussed by many authors [22, 15]. We shall see that the smoothing order, first introduced in [4] is also important in establishing error bounds for $\mathcal{E}_{IB}$. The smoothing order is a generalization of the even-odd condition that has been imposed on discrete delta functions to avoid the checker-board instability associated with central-differencing operators [17]. As we shall see, the smoothing order has the effect of "smoothing out" the high frequency errors and preventing Gibbs-type phenomena from corrupting convergence.

Section 4 is the technical core of this paper. Here, we establish bounds on $\mathcal{E}_{IB}$ depending on the order of the finite difference discretization q, the moment order m, the smoothing order s, the order the differential operator n_0 and the dimension n. We shall see that the estimate for $\mathcal{E}_{IB}$ depends strongly on whether $\mathbf{x}$ and $\mathbf{X}$ share the same coordinate values (i.e., if $\mathbf{x} = (x_1, \cdots, x_n)$ and $\mathbf{X} = (X_1, \cdots, X_n)$, $x_k = X_k$ for some values of k). This *grid line effect* is diminished if the discrete delta function has high smoothing order.

In Section 5, we consider the two-dimensional Stokes problem and see that the estimates that we obtain for pointwise convergence are optimal by examining the convergence rates for different choices of discrete delta functions, some of which are newly introduced in this paper.

2. Model problem. Let $\mathbb{U} = (\mathbb{R}/2\pi\mathbb{Z})^n$, where each coordinate runs from 0 to 2π. Consider a connected bounded domain in $\mathbb{R}^d, d \leq n$ whose closure we denote by Θ. We consider the following problem:

$$Lu(\mathbf{x}) = f(\mathbf{x}),\ f(\mathbf{x}) = \int_\Theta F(\boldsymbol{\theta}) \left(\delta(\mathbf{x} - \mathbf{X}(\boldsymbol{\theta})) - (2\pi)^{-n}\right) d\boldsymbol{\theta}. \tag{2.1}$$

Here L is a constant coefficient linear elliptic differential operator. We shall later specify the exact scope of differential operators we consider. $\mathbf{X}(\boldsymbol{\theta})$ is a continuous map from Θ to $\mathbb{R}^n$ and $F(\boldsymbol{\theta})$ is a function defined on Θ with values in $\mathbb{R}$. We denote the image of $\mathbf{X} : \Theta \to \mathbb{U}$ by Γ which we shall refer to as the immersed structure or boundary, although Γ may not necessarily be a (hyper)surface of codimension 1. The constant factor $1/(2\pi)^n$ is subtracted to make sure that the above problem has a solution, given that it is posed on a periodic domain. We seek the unique solution that satisfies $\int_\mathbb{U} u(\mathbf{x})d\mathbf{x} = 0$. We write the solution u as an integral over Θ:

$$u(\mathbf{x}) = \int_\Theta G(\mathbf{x} - \mathbf{X}(\boldsymbol{\theta}))F(\boldsymbol{\theta})d\boldsymbol{\theta}. \tag{2.2}$$

In the above, the Green's function $G(\mathbf{x})$ can be written as

$$\begin{aligned} G(\mathbf{x}) &= \frac{1}{(2\pi)^n} \sum_{\mathbf{k}\in Z^n} \mathcal{Q}(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{x}), \\ \mathcal{Q}(\mathbf{k}) &= \begin{cases} \frac{1}{\mathcal{A}(\mathbf{k})} & \text{when} \quad \mathbf{k} \in \mathbb{Z}^n, \mathbf{k} \neq \mathbf{0}, \\ 0 & \text{when} \quad \mathbf{k} = \mathbf{0}, \end{cases} \end{aligned} \tag{2.3}$$

where $\mathcal{A}(\mathbf{k})$ is the Fourier multiplier corresponding to the operator L. We have assumed that $\mathcal{A}(\mathbf{k}) \neq 0$ for $\mathbf{k} \neq 0$, and here, we are using the ellipticity of L. When L is the Laplacian, for example, $\mathcal{A}(\mathbf{k}) = -|\mathbf{k}|^2$ where $|\mathbf{k}|$ is the Euclidean norm of $\mathbf{k}$. Note that, in general, the above expression for G is only valid in the sense of distribution.

We discretize the problem by laying a uniform Cartesian grid with mesh width h on $\mathbb{U}$. The discretization of the immersed structure Γ can be performed in many ways, and much of the subsequent analysis does not depend the choice of discretization. For definiteness, we shall adopt the following discretization on Γ: we lay a uniform Cartesian grid with mesh width $\Delta\theta$ on Θ to obtain a curvilinear coordinate system on Γ. The discretized equations can be written as follows:

$$L_h u_h(\mathbf{x}) = f_h(\mathbf{x}),\ f_h(\mathbf{x}) = \sum_{\boldsymbol{\theta}\in\mathcal{G}_\theta} F(\boldsymbol{\theta})\left(\delta_h(\mathbf{x}-\mathbf{X}(\boldsymbol{\theta})) - (2\pi)^{-n}\right)(\Delta\theta)^d. \tag{2.4}$$

Here L_h is a finite difference discretization or spectral discretization of L, and $\mathbf{x}\in\mathcal{G}_h$, the set of Cartesian grid points on $\mathbb{U}$. For definiteness, we have chosen a simple quadrature rule to discretize the integral representation of f. The resulting sum is over grid points in Θ which we denote by $\mathcal{G}_\theta$. We shall refer to a point $\mathbf{X}(\boldsymbol{\theta}), \boldsymbol{\theta}\in\mathcal{G}_\theta$ as an immersed boundary point. The function $\delta_h(\mathbf{x})$ is a regularization of the Dirac delta function, which we shall refer to as a *discrete delta functions* whose properties are the topic of section 3. We write u_h as

$$u_h(\mathbf{x}) = \sum_{\mathbf{y}\in\mathcal{G}_h} G_h(\mathbf{x}-\mathbf{y}) f_h(\mathbf{y}) h^n, \tag{2.5}$$

where $G_h(\mathbf{x})$ is given by:

$$\begin{aligned} G_h(\mathbf{x}) &= \frac{1}{(2\pi)^n}\sum_{\mathbf{k}\in\mathbb{Z}^n} \mathcal{Q}_h(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{x}),\ \mathbf{k}=(k_1,\cdots,k_n),\\ \mathcal{Q}_h(\mathbf{k}) &= \begin{cases} \frac{1}{\mathcal{A}_h(\mathbf{k})} & \text{when } \mathcal{A}_h(\mathbf{k})\neq 0, \text{ and } -\pi\le k_l h<\pi, \text{ for all } 1\le l\le n,\\ 0 & \text{otherwise.}\end{cases} \end{aligned} \tag{2.6}$$

Here, $\mathcal{A}_h(\mathbf{k})$ is the Fourier multiplier corresponding to the operator L_h. We have assumed that the operator L_h is translation invariant so that such a Fourier representation is possible (translation invariance is true for practically all finite difference discretizations of constant coefficient PDEs). If L_h is the five point Laplacian in two dimensions, for example, $\mathcal{A}_h(\mathbf{k}) = -4(\sin^2(kh/2)+\sin^2(lh/2))/h^2, \mathbf{k}=(k,l)$. We point out that, if (2.4) is uniquely solvable under the constraint $\sum_{\mathbf{x}\in\mathcal{G}_h} u_h(\mathbf{x})h^n = 0$, then $\mathbf{k}=\mathbf{0}$ is the only point in $\mathcal{K}_h$ for which $\mathcal{A}_h(\mathbf{k})=0$, and thus, the above is indeed the solution to (2.4) under this constraint.

We shall make one technical modification to (2.6). We assume that

$$\mathcal{Q}_h(\mathbf{k}) = 0, \mathbf{k}=(k_1,\cdots,k_n) \text{ if } |k_l h|\ge\pi \text{ for some } l. \tag{2.7}$$

This amounts to replacing $-\pi\le k_l h<\pi$ with $-\pi<k_l h<\pi$ in the definition of $\mathcal{Q}_h$ in (2.6). This modification will not make any difference if the number of grid points in each coordinate direction is odd ($2\pi/h$ is odd) or if the smoothing order of the discrete delta function is greater than or equal to 1 (see below). We note that it is indeed possible to state all results to follow even if we do not make this modification, and the results will be essentially the same. Without this modification, however, some statements and proofs to follow will be longer and more laborious without addition of new ideas.

Our convergence results to follow will pertain to conditions on $\mathcal{Q}(\mathbf{k})$ and $\mathcal{Q}_h(\mathbf{k})$ and not on $\mathcal{A}(\mathbf{k})$ or $\mathcal{A}_h(\mathbf{k})$. Note also that (2.5) and (2.6) make sense for any $\mathbf{x}\in\mathbb{U}$, not just grid points $\mathcal{G}_h$. We shall henceforth view u_h and G_h as functions of $\mathbf{x}\in\mathbb{U}$.

Let us further rewrite (2.5). Substitute the expression for f_h in (2.4) into (2.5). After changing the order of summation, we find

$$u_h(\mathbf{x}) = \sum_{\theta \in \mathcal{G}_\theta} \left(\sum_{\mathbf{y} \in \mathcal{G}_h} G_{h,\mathbf{x}}(\mathbf{y}) \delta_h(\mathbf{y} - \mathbf{X}(\boldsymbol{\theta})) h^n \right) F(\boldsymbol{\theta})(\Delta\theta)^d, \tag{2.8}$$

where we used the notation $G_{h,\mathbf{x}}(\mathbf{y}) = G_h(\mathbf{x} - \mathbf{y})$. For a function q defined on the grid $\mathcal{G}_h$, define

$$(\mathcal{I}q)(\mathbf{Y}) = \sum_{\mathbf{y} \in \mathcal{G}_h} q(\mathbf{y}) \delta_h(\mathbf{y} - \mathbf{Y}) h^n \tag{2.9}$$

where $\mathbf{Y} \in \mathbb{U}$. The function $\mathcal{I}q$ defined on $\mathbb{U}$ may be seen as an interpolant of the grid function q obtained using the discrete delta function δ_h. With this, we may write (2.8) as:

$$u_h(\mathbf{x}) = \sum_{\boldsymbol{\theta} \in \mathcal{G}_\theta} (\mathcal{I}G_{h,\mathbf{x}})(\mathbf{X}(\boldsymbol{\theta})) F(\boldsymbol{\theta})(\Delta\theta)^d. \tag{2.10}$$

The function $\mathcal{I}G_{h,\mathbf{x}}$ corresponds to $\widehat{G}_{h,\mathbf{x}}$ in (1.5). We would like to estimate the difference $u - u_h$. Write $u - u_h$ as follows:

$$\begin{aligned} u(\mathbf{x}) - u_h(\mathbf{x}) &= E_Q(\mathbf{x}) + E_{IB}(\mathbf{x}) \\ E_Q(\mathbf{x}) &= \int_\Theta G_{\mathbf{x}}(\mathbf{X}(\boldsymbol{\theta})) F(\boldsymbol{\theta}) d\theta - \sum_{\boldsymbol{\theta} \in \mathcal{G}_\theta} G_{\mathbf{x}}(\mathbf{X}(\boldsymbol{\theta})) F(\boldsymbol{\theta})(\Delta\theta)^d, \\ E_{IB}(\mathbf{x}) &= \sum_{\boldsymbol{\theta} \in \mathcal{G}_\theta} \mathcal{E}_{IB}(\mathbf{X}(\boldsymbol{\theta})) F(\boldsymbol{\theta})(\Delta\theta)^d, \quad \mathcal{E}_{IB}(\mathbf{X}, \mathbf{x}) = (G_{\mathbf{x}} - \mathcal{I}G_{h,\mathbf{x}})(\mathbf{X}). \end{aligned} \tag{2.11}$$

In the above, we used the notation $G_{\mathbf{x}}(\mathbf{y}) = G(\mathbf{x} - \mathbf{y})$. The first term E_Q is the *quadrature error*. Since $G_{\mathbf{x}}(\mathbf{y})$ is just the (continuous) Green's function whose properties are well-known, the estimation of the error E_Q falls within the purview of the (classical) theory of numerical quadrature, and will not be the focus of this paper. When $\mathbf{x} \notin \Gamma$, the estimation of this error is particularly simple, as we shall see in Section 5. The second term E_{IB} is the error that comes from the Cartesian discretization of $\mathbb{U}$ and the regularization of the delta function. We call E_{IB} the *immersed boundary error*. The main technical contribution of this paper is to estimate $\mathcal{E}_{IB}(\mathbf{X}, \mathbf{x})$. Before we proceed, we discuss relevant properties of discrete delta functions.

3. Discrete delta function and smoothing order. In this section, we discuss properties of delta function regularizations. In particular, we introduce the *smoothing order* of discrete delta functions. We assume that δ_h has the form

$$\delta_h(\mathbf{x}) = \frac{1}{h^n} \prod_{i=1}^n \phi\left(\frac{x_i}{h}\right), \ \mathbf{x} = (x_1, \cdots, x_n)^T \tag{3.1}$$

for some function ϕ defined on the real line. Functions ϕ commonly used satisfy a subset of the following conditions.

- ϕ has compact support. We let $r_\phi > 0$ be the smallest real number such that the following holds:

$$\phi(r) \neq 0 \text{ only if } -r_\phi \leq r \leq r_\phi. \tag{3.2}$$

- ϕ satisfies moment conditions. When ϕ satisfies

$$\sum_{k\in\mathbb{Z}} \phi(k-r) = 1 \qquad \text{if } j=0 \tag{3.3}$$

$$\sum_{k\in\mathbb{Z}} (k-r)^j \phi(k-r) = 0 \qquad \text{if } j>0 \tag{3.4}$$

  for all $r \in \mathbb{R}$, ϕ is said to satisfy the j-th order moment condition. If ϕ has compact support, the above sums contain only finitely many terms. If ϕ satisfies moment conditions up to order $m-1$, we shall say, following [22], that ϕ is of *moment order* m.
- We shall say that ϕ is of *smoothing order* $s \geq 1$ if the following condition is met. There is a function $\psi(r)$ of compact support such that

$$\phi(r) = \frac{1}{2^s} \sum_{l=0}^{s} \binom{s}{l} \psi(r-l). \tag{3.5}$$

  where $\binom{s}{l}$ is the binomial coefficient. In other words, ϕ is of smoothing order s if it is a discrete convolution of a compactly supported function ψ against the binomial distribution $B(s,1/2)$, generated by tossing a fair coin s times. We shall say that ϕ is of smoothing order 0 if it has compact support.
- ϕ satisfies the *sum of squares* condition:

$$\forall r \in \mathbb{R}, \sum_{l\in\mathbb{Z}} \phi(l-r)^2 = \text{const.} \tag{3.6}$$

- ϕ is continuous.

The first condition is for computational efficiency and is satisfied by all discrete delta functions used in practice. It ensures that each immersed boundary point only communicates with a finite number of grid points independent of the mesh spacing h. This condition also implies that the sums appearing in the definitions of moment and smoothing order contain only finitely many terms. In addition to r_ϕ, it is useful to introduce the following constant. Denote by a_ϕ the smallest half integer (i.e. $2a_\phi$ is an integer) such that

$$\phi(r) \neq 0 \text{ only if } -a_\phi \leq r < a_\phi. \tag{3.7}$$

If ϕ is right continuous, then a_ϕ is just the smallest half integer such that $a_\phi \geq r_\phi$. The constants r_ϕ and a_ϕ are, of course, different in general. However, for most functions ϕ used in practice $r_\phi = a_\phi$. We shall always assume that ϕ is compactly supported.

The sum of squares condition and the continuity condition will not play a big role in this paper. We shall assume ϕ is continuous nevertheless, which, together with the assumption of compact support, implies that ϕ is bounded. The motivation for the sum of squares condition is discussed in [17], and there is interesting numerical evidence to suggest its importance in specific contexts [4, 5].

The moment condition ensures accuracy of interpolation operations performed with discrete delta functions. This is expressed in the following result, which can be found in many places (for example [22]).

LEMMA 3.1. *Denote by $\mathcal{P}_m$ the set of polynomials of degree less than m. A function ϕ of compact support is of moment order $m \geq 1$ if and only if it satisfies the* *following condition:*

$$\forall r \in \mathbb{R} \text{ and } \forall g \in \mathcal{P}_m,\ \sum_{k\in\mathbb{Z}} g(k)\phi(k-r) = g(r). \tag{3.8}$$

Proof. Assume ϕ is of moment order m. Then,

$$\begin{aligned}\sum_{k\in\mathbb{Z}} g(k)\phi(k-r) &= \sum_{k\in\mathbb{Z}}\left(\sum_{n=0}^{m-1}\frac{g^{(j)}(r)}{j!}(k-r)^j\right)\phi(k-r)\\ &= \sum_{n=0}^{m-1}\frac{g^{(j)}(r)}{j!}\left(\sum_{k\in\mathbb{Z}}(k-r)^j\phi(k-r)\right) = g(r).\end{aligned} \tag{3.9}$$

Since ϕ is compactly supported, we may change the order of summation in the second equality. We used the moment conditions (3.3) and (3.4) in the last equality.

If ϕ satisfies (3.8), one may take $g(k) = (k-r)^j, 0 \le j \le m-1$ to obtain the moment conditions (3.3) and (3.4). □

We now turn to the third condition. This condition has not received much discussion in the literature (but see [4]). As will be seen in Section 4, the smoothing order has the effect of removing high frequency errors. This can be roughly explained as follows. Equation (3.5) states that a discrete delta function of smoothing order s is a linear combination of translates of the binomial distribution $B(s, 1/2)$. The binomial distribution $B(s = 1, 1/2)$, seen as a grid function, is equal to $1/2$ at two grid points and is zero elsewhere. As s increases, the binomial distribution $B(s, 1/2)$ approaches a Gaussian (central limit theorem). The binomial distribution thus becomes "smoother" with larger s; its discrete Fourier transform has smaller contributions from high frequency components (see Lemma 4.3 and the remarks following its proof). The smoothing order thus suppresses high frequency errors. This effect is loosely analogous to the difference between the Dirichlet kernel and the Fejér kernel in the convergence of Fourier series. Use of the Dirichlet kernel suffers from the Gibbs phenomenon, whereas the Fejér kernel does not.

Note first that if ϕ is of smoothing order $s \ge 1$, it is also of smoothing order $s' < s$ since:

$$\phi(r) = \frac{1}{2^s}\sum_{l=0}^{s}\binom{s}{l}\psi(r-l) = \frac{1}{2^{s-1}}\sum_{l=0}^{s-1}\binom{s-1}{l}\left(\frac{1}{2}(\psi(r-l-1)+\psi(r-l))\right). \tag{3.10}$$

We now state the following characterization of smoothing order. Define

$$\psi^{(k)}(r) = 2\sum_{l=0}^{\infty}(-1)^l\psi^{(k-1)}(r-l),\ k \ge 1, \tag{3.11}$$

where we take $\psi^{(0)} = \phi$.

LEMMA 3.2. *Suppose ϕ has compact support. The function ϕ is of smoothing order s if and only if $\psi^{(k)}, 0 \le k \le s$ are compactly supported. If ϕ is of smoothing order $s \ge 1$, the function ψ in (3.5) is equal to $\psi^{(s)}$, and its support is contained in the interval $[-r_\phi, r_\phi - s]$. In particular, ψ is uniquely determined by ϕ. If ϕ is continuous (or bounded) so is ψ.*

Proof. When $s = 0$, the claim is trivial.

Suppose $s = 1$. Let $\psi^{(1)}$ be compactly supported. It is easy to see that $\phi(r) = \psi^{(1)}(r) + \psi^{(1)}(r-1)$. The function ϕ is therefore of smoothing order 1. Suppose in turn that ϕ is of smoothing order 1. If $r < -r_\phi$, $\psi^{(1)}(r)$ is clearly equal to 0. If $r > r_\phi - 1$, we have

$$\begin{aligned}
\psi^{(1)}(r) &= 2\sum_{l=0}^{\infty}(-1)^l\phi(r-l) = 2\sum_{l\in\mathbb{Z}}(-1)^l\phi(r-l) \\
&= 2\sum_{l\in\mathbb{Z}}(-1)^l(\psi(r-l)+\psi(r-l-1)) \\
&= 2\sum_{l\in\mathbb{Z}}(-1)^l(\psi(r-l)-\psi(r-l)) = 0
\end{aligned} \tag{3.12}$$

where we used the fact that $\phi(r) = 0$ for $r > r_\phi$ in the second equality and (3.5) with $s = 1$ in the third equality. We now show that $\psi(r) = \psi^{(1)}(r)$. The function $\varphi = \psi - \psi^{(1)}$ is of compact support, and satisfies the following:

$$\varphi(r) + \varphi(r-1) = 0. \tag{3.13}$$

Suppose the smallest closed interval on which $\varphi(r)$ is supported is $a \le r \le b$. Then, the support of $\varphi(r-1)$ is contained in $a+1 \le r \le b+1$, and therefore, $\varphi(r) = 0$ for $a \le r < a+1$. This contradicts the minimality assumption of $a \le r \le b$ unless $\varphi(r)$ is identically equal to 0.

Suppose ϕ is of smoothing order $s \ge 2$. Then, it is of smoothing order 1, so there is a function $\psi^{(1)}$ such that

$$\begin{aligned}
\phi(r) &= \frac{1}{2}\left(\psi^{(1)}(r) + \psi^{(1)}(r-1)\right) \\
&= \frac{1}{2}\left(\frac{1}{2^{s-1}}\sum_{l=0}^{s-1}\binom{s-1}{l}\psi(r-l) + \frac{1}{2^{s-1}}\sum_{l=0}^{s-1}\binom{s-1}{l}\psi(r-l-1)\right) \\
&= \frac{1}{2}\left(\tilde{\psi}(r) + \tilde{\psi}(r-1)\right).
\end{aligned} \tag{3.14}$$

By uniqueness of this decomposition for functions of smoothing order 1, we have

$$\psi^{(1)}(r) = \tilde{\psi}(r) = \frac{1}{2^{s-1}}\sum_{l=0}^{s-1}\binom{s-1}{l}\psi(r-l). \tag{3.15}$$

This shows that $\psi^{(1)}(r)$ is of smoothing order $s-1$. We now iterate this argument $k \le s$ times to conclude that $\psi^{(k)}$ is of smoothing order $s-k$ and

$$\psi^{(k)}(r) = \begin{cases} \frac{1}{2^{s-k}}\sum_{l=0}^{s-k}\binom{s-k}{l}\psi(r-l) & \text{if } 0 \le k \le s-1, \\ \psi(r) & \text{if } k = s. \end{cases} \tag{3.16}$$

This shows that $\psi = \psi^{(s)}$ and ψ is therefore uniquely determined by ϕ. The statement about the support of ψ is clear from the above proof. Equation (3.11) shows that $\psi^s = \psi$ can be written as a linear combination of integer translates of ϕ. Therefore, ψ is continuous (bounded) if and only if ϕ is continuous (bounded). □

According to the above lemma, ϕ is of smoothing order 1 if and only if the following holds:

$$\sum_{l\in\mathbb{Z}}(-1)^l\phi(r-l) = 0. \tag{3.17}$$

This can be written as

$$\sum_{k:\text{odd}} \phi(r-k) = \sum_{k:\text{even}} \phi(r-k). \tag{3.18}$$

In this sense, we can view the smoothing order as being a generalization of the above *even-odd* condition. This condition was originally introduced to avoid the "checker-board" type instability that manifests itself when using the central difference operator for the discretization of divergence and gradient operators in the Navier Stokes equations [17]. Our main motivation for introducing the smoothing order, however, is that it plays an important role in determining the error $\mathcal{E}_{IB}$. In Appendix A, we discuss an equivalent characterization of the smoothing order due to [4]

We say that ϕ is of class (m,s) if it is of moment order m and smoothing order s. We shall always assume $m \geq 1$ and that ϕ is compactly supported and bounded. This raises the question as to whether such ϕ exist. We can prove the following. Recall that r_ϕ was defined in (3.2).

LEMMA 3.3. *There are no functions ϕ of class (m,s) such that $2r_\phi < m+s$. There is a unique right continuous function of class (m,s) such that $2r_\phi = m+s$.*

Proof. We first prove a statement in terms of a_ϕ of (3.7) instead of r_ϕ. By Lemma 3.1, a function ϕ of compact support is of moment order m if and only if the following holds:

$$\forall r \in \mathbb{R} \text{ and } \forall g \in \mathcal{P}_m,\ \sum_{k\in\mathbb{Z}} g(k)\phi(r-k) = g(r). \tag{3.19}$$

Here, $\mathcal{P}_m$ is the space of polynomials of degree less than m. We shall often regard $\mathcal{P}_m$ as a vector space over $\mathbb{R}$. For convenience, we have changed the sign in the argument of ϕ, and the equivalence of the above with (3.8) is trivial. We may rewrite the above as follows:

$$\forall 0 \leq r < 1 \text{ and } \forall g \in \mathcal{P}_m,\ \sum_{k=0}^{2a_\phi-1} g(k)\phi(-a_\phi+r+k) = g(a_\phi - r). \tag{3.20}$$

If $s \geq 1$ substitute (3.5) in the above sum,

$$\begin{aligned} &\sum_{k=0}^{2a_\phi-1} g(k)\left(\frac{1}{2^s}\sum_{l=0}^{s}\binom{s}{l}\psi(-a_\phi+r+k-l)\right)\\ &=\sum_{k=0}^{2a_\phi-s-1}\left(\frac{1}{2^s}\sum_{l=0}^{s}\binom{s}{l}g(k+l)\right)\psi(-a_\phi+r+k) = g(a_\phi-r). \end{aligned} \tag{3.21}$$

In rearranging this sum, we used the fact that $\psi(-a_\phi+r+k-l)=0$ if $k-l<0$ or if $k-l \geq 2a_\phi - s$. This follows since the support of $\psi(r)$ is non-zero only if $-a_\phi \leq r < a_\phi - s$ (see Lemma 3.2). If $s \geq 1$ let

$$\psi_k(r) = \psi(-a_\phi+k+r),\ 0 \leq r < 1, 0 \leq k \leq 2a_\phi - s - 1. \tag{3.22}$$

If $s=0$, we let $\psi=\phi$ in the above expression. For $s \geq 1$, define the linear operator $\mathcal{L}_s$ mapping $\mathcal{P}_m$ to itself:

$$(\mathcal{L}_s g)(x) = \frac{1}{2^s}\sum_{l=0}^{s}\binom{s}{l}g(x+l),\ g(x) \in \mathcal{P}_m. \tag{3.23}$$

For $s = 0$, we let $\mathcal{L}_s$ be the identity. Using (3.21), (3.22) and (3.23), we may write (3.20) in the following fashion:

$$\forall 0 \leq r < 1 \text{ and } \forall g \in \mathcal{P}_m, \quad \sum_{k=0}^{2a_\phi - s - 1} (\mathcal{L}_s g)(k)\psi_k(r) = g(a_\phi - r). \tag{3.24}$$

The operator $\mathcal{L}_s$ is invertible on $\mathcal{P}_m$. This can be seen as follows. Take m polynomials $g_0, \cdots, g_{m-1}$ such that g_l is a degree l polynomial. These m polynomials form a basis of $\mathcal{P}_m$. It is clear from (3.23) that the polynomial $\mathcal{L}_s g_l$ is a degree l polynomial as well. Therefore, $\mathcal{L}_s$ maps a set of basis vectors to a set of basis vectors, and thus, $\mathcal{L}_s$ is invertible. We may thus further rewrite (3.24).

$$\forall 0 \leq r < 1 \text{ and } \forall g \in \mathcal{P}_m, \quad \sum_{k=0}^{2a_\phi - s - 1} g(k)\psi_k(r) = (\mathcal{L}_s^{-1} g)(a_\phi - r). \tag{3.25}$$

In order for the above to hold, we need only check this relation for m linearly independent polynomials in $\mathcal{P}_m$. Let

$$g_0(k) = 1, \; g_l(k) = k(k-1)\cdots(k-l+1) \text{ for } 0 \leq l \leq m-1. \tag{3.26}$$

The above condition is equivalent to

$$\sum_{k=0}^{2a_\phi - s - 1} g_l(k)\psi_k(r) = (\mathcal{L}_s^{-1} g_l)(a_\phi - r). \tag{3.27}$$

This can be rewritten in the following matrix form:

$$\begin{aligned} G\boldsymbol{\psi} = \mathbf{h}, \; \boldsymbol{\psi} &= (\psi_0(r), \cdots, \psi_{2a_\phi - s - 1}(r))^T, \\ \mathbf{h} &= ((\mathcal{L}_s^{-1} g_0)(a_\phi - r), \cdots, (\mathcal{L}_s^{-1} g_{m-1})(a_\phi - r))^T. \end{aligned} \tag{3.28}$$

where G is a $m \times (2a_\phi - s)$ matrix. It is easy to see that G is an upper triangular matrix with non-zero diagonal entries. Let us view (3.28) as an equation for $\boldsymbol{\psi}$. Suppose $m \leq 2a_\phi - s$. Then, G is full rank, and thus, there is a solution to (3.28). In particular, if $m = 2a_\phi - s$, there is a single solution to (3.28). The solution is clearly a piecewise polynomial, and this means that $2r_\phi = 2a_\phi = m + s$ in this case.

If $m \geq 2a_\phi - s$, all elements of the last $m - (2a_\phi - s)$ rows of the matrix G are 0. On the other hand, the last $m - (2a_\phi - s)$ entries of the vector $\mathbf{h}$ are not equal to 0, since a non-zero polynomial cannot vanish identically on an interval. Therefore, a compactly supported function of class (m, s) can exist only if $2a_\phi \geq m + s$.

Now, suppose $2r_\phi < m + s$, which implies that $2a_\phi \leq m + s$. We know that there are no functions of class (m, s) such that $2a_\phi \leq m + s - 1$. We therefore assume that $2a_\phi = m + s$. But if this is so, $2r_\phi = m + s$ as we saw above, which is a contradiction.

Finally, suppose $2r_\phi = m + s$ and that ϕ is right continuous. Then, $2a_\phi = m + s$, and we have already seen that there is only one function ϕ of class (m, s) such that $2a_\phi = m + s$. □

It is straightforward to modify the above proof to show that there are at most two functions of class (m, s) such that $2r_\phi = m + s$, one right continuous and the other left continuous. It is not necessarily true that these functions are continuous (in which case the two functions will coincide).

Let us say that a function ϕ of class (m, s) is of class $(m, s, \sigma, 2r_\phi), \sigma = 1(0)$ if the sum of squares condition is (not) satisfied and ϕ has support of $2r_\phi$. We have written a MATLAB routine that automatically generates a continuous function of class $(m, s, \sigma, m + s + \sigma)$ if such a function exists. Experimentation suggests that there is at most one such continuous function for any m, s, σ (when $\sigma = 0$, this is a direct consequence of Lemma 3.3). We conjecture that there is a unique continuous function of class $(m, s, \sigma, m + s + \sigma)$ if and only if m is even. When m is odd, there is no such continuous function. Similar observations have been made in the case of $s = 0, 1$ and/or $\sigma = 0, 1$ [22, 17, 21, 4]. It is not difficult to show that the unique function of class $(m, 0, 0, m)$ is indeed continuous if m is even, the proof of which we omit (although this result seems to be new). We shall test various discrete delta functions that belong to these classes in our computational convergence study, many of which are new.

4. Estimate of $\mathcal{E}_{IB}(\mathbf{X}, \mathbf{x})$. In this section, we estimate $\mathcal{E}_{IB}(\mathbf{X}, \mathbf{x})$ defined in (2.11). In [15] and [22], the authors estimate this error by writing

$$\mathcal{E}_{IB} = (G_{\mathbf{x}} - \mathcal{I}G_{\mathbf{x}}) + \mathcal{I}(G_{\mathbf{x}} - G_{h,\mathbf{x}}), \tag{4.1}$$

and estimating the two errors separately. We have found that there is a cancellation of errors that cannot be captured if we estimate $\mathcal{E}_{IB}$ in this way. We shall instead estimate $\mathcal{E}_{IB}$ directly.

Let us first rewrite $(\mathcal{I}G_{h,\mathbf{x}})(\mathbf{X})$. Let $\mathbf{X} = (X_1, \cdots, X_n)$. Write X_i as follows:

$$X_i = (R_i + r_i)h, \; R_i \in \mathbb{Z} \text{ and } \begin{cases} 0 \le r_i < 1 & \text{if } 2a_\phi \text{ is even,} \\ -1/2 \le r_i < 1/2 & \text{if } 2a_\phi \text{ is odd.} \end{cases} \tag{4.2}$$

Consider a Cartesian grid point $\mathbf{y} = (y_1, \cdots, y_n)$. For each $i = 1, \cdots, n$, let $l_i = \frac{y_i}{h} - R_i$, so $y_i = (l_i + R_i)h$. Then we have

$$\delta_h(\mathbf{y} - \mathbf{X}(\theta)) = \frac{1}{h^n} \prod_{i=1}^n \phi\left(\frac{1}{h}(y_i - X_i)\right) = \frac{1}{h^n} \prod_{i=1}^n \phi(l_i - r_i) \tag{4.3}$$

Now, consider the expression $(\mathcal{I}G_{h,\mathbf{x}})(\mathbf{X})$. Using (2.6), (2.9) and (3.1), we have

$$\begin{aligned} (\mathcal{I}G_{h,\mathbf{x}})(\mathbf{X}) &= \frac{1}{(2\pi)^n} \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathcal{Q}_h(\mathbf{k}) \tilde{\rho}(h, \mathbf{k}, \mathbf{X}) \exp(i\mathbf{k} \cdot (\mathbf{x} - \mathbf{X})), \\ \tilde{\rho}(h, \mathbf{k}, \mathbf{X}) &= \sum_{\mathbf{y} \in \mathcal{G}_h} \exp(-i\mathbf{k} \cdot (\mathbf{y} - \mathbf{X})) \prod_{\ell=1}^n \phi\left(\frac{y_\ell - X_\ell}{h}\right). \end{aligned} \tag{4.4}$$

We may further simplify $\tilde{\rho}$ as follows:

$$\begin{aligned} \tilde{\rho}(h, \mathbf{k}, \mathbf{X}) &= \sum_{\mathbf{y} \in \mathcal{G}_h} \prod_{\ell=1}^n \left(\phi\left(\frac{y_\ell - X_\ell}{h}\right) \exp(-ik_\ell(y_\ell - X_\ell))\right) \\ &= \sum_{\mathbf{l} \in \mathbb{Z}^n} \prod_{\ell=1}^n \left(\phi\left(l_\ell - r_\ell\right) \exp(-ihk_\ell(l_\ell - r_\ell))\right) \\ &= \prod_{\ell=1}^n \left(\sum_{l_\ell \in \mathbb{Z}} \left(\phi\left(l_\ell - r_\ell\right) \exp(-ihk_\ell(l_\ell - r_\ell))\right)\right) \end{aligned} \tag{4.5}$$

where $\mathbf{k} = (k_1, \cdots, k_n)$ and $\mathbf{l} = (l_1, \cdots, l_n)$. In replacing the summation in $\mathcal{G}_h$ to $\mathbb{Z}^n$ in the second equality, we assumed that h is small enough so that the support of δ_h is smaller than $\mathbb{U}$. Define

$$\begin{aligned} \rho_{\mathbf{r}}(\mathbf{t}) &= \prod_{i=1}^{n} \rho_{r_i}(t_i), \ \mathbf{t} = (t_1, \cdots, t_n) \in \mathbb{R}^n, \\ \rho_r(t) &= \begin{cases} \sum_{l=a_-}^{a_+} \phi(l-r) \exp(-i(l-r)t) & \text{if } |t| < \pi, \\ 0 & \text{otherwise .} \end{cases} \end{aligned} \tag{4.6}$$

where $\mathbf{r} = (r_1, \cdots, r_n)$, $a_\pm = \pm(a_\phi + 1/2)$ if $2a_\phi$ is an odd number and $a_\pm = \pm a_\phi$ if $2a_\phi$ is an even number. From (4.4), (4.5) and (4.6) it follows that

$$(\mathcal{I}G_{h,\mathbf{x}})(\mathbf{X}) = \frac{1}{(2\pi)^n} \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathcal{Q}_h(\mathbf{k}) \rho_{\mathbf{r}}(h\mathbf{k}) \exp(i\mathbf{k} \cdot (\mathbf{x} - \mathbf{X})). \tag{4.7}$$

We shall often suppress the dependence of $\rho_{\mathbf{r}}$ on $\mathbf{r}$ and simply write ρ, since all of our estimates will be independent of $\mathbf{r}$.

Recalling the definition of $G_{\mathbf{x}}$ in (2.3), we see that

$$\begin{aligned} \mathcal{E}_{IB}(\mathbf{X}, \mathbf{x}) &= G_{\mathbf{x}}(\mathbf{X}) - (\mathcal{I}G_{h,\mathbf{x}})(\mathbf{X}) \\ &= \frac{1}{(2\pi)^n} \sum_{\mathbf{k} \in \mathbb{Z}^n} \left(\mathcal{Q}(\mathbf{k}) - \rho(h\mathbf{k}) \mathcal{Q}_h(\mathbf{k}) \right) \exp(i\mathbf{k} \cdot \mathbf{z}) \end{aligned} \tag{4.8}$$

where $\mathbf{z} = \mathbf{x} - \mathbf{X}$. Our task is thus to estimate the above quantity.

In order to estimate $\mathcal{E}_{IB}$, we must specify properties satisfied by $\mathcal{Q}$ and $\mathcal{Q}_h$. For this purpose, we introduce the following grid operators. Let $\mathcal{Y}(\mathbf{t})$ be a function of $\mathbf{t} = (t_1, \cdots, t_n) \in \mathbb{R}^n$. For $i = 1, \cdots, n$, let $\hat{\mathbf{e}}_i$ denote the i^{th} unit coordinate vector in $\mathbb{R}^n$. Let

$$\mathcal{T}_i \mathcal{Y}(\mathbf{t}) = \mathcal{Y}(\mathbf{t} - \hat{\mathbf{e}}_i), \quad \mathcal{D}_i \mathcal{Y}(\mathbf{t}) = \mathcal{Y}(\mathbf{t}) - \mathcal{T}_i \mathcal{Y}(\mathbf{t}). \tag{4.9}$$

The operator $\mathcal{T}_i$ is the i-th translation operator and $\mathcal{D}_i$ the i-th difference operator. Let $\boldsymbol{\alpha} = (\alpha_1, \cdots, \alpha_n)$ be a multi-index so that the α_i are nonnegative integers. Define

$$\mathcal{T}^{\boldsymbol{\alpha}} = \prod_{i=1}^{n} \mathcal{T}_i^{\alpha_i}, \quad \mathcal{D}^{\boldsymbol{\alpha}} = \prod_{i=1}^{n} \mathcal{D}_i^{\alpha_i}, \tag{4.10}$$

with the understanding that $\mathcal{T}_i^0$ and $\mathcal{D}_i^0$ are the identity. Note that the operators $\mathcal{T}$ and $\mathcal{D}$ are commutative. We also have the following product formula. Let $\mathcal{X}(\mathbf{t})$ and $\mathcal{Y}(\mathbf{t})$ be two functions of $\mathbf{t} \in \mathbb{R}^n$. Then,

$$\mathcal{D}^{\boldsymbol{\alpha}}(\mathcal{X}\mathcal{Y}) = \sum_{\boldsymbol{\beta}+\boldsymbol{\gamma}=\alpha} \left(\prod_{i=1}^{n} \binom{\alpha_i}{\beta_i} \right) \left(\mathcal{T}^{\boldsymbol{\beta}} \mathcal{D}^{\boldsymbol{\gamma}} \mathcal{X} \right) \left(\mathcal{D}^{\boldsymbol{\beta}} \mathcal{Y} \right) \tag{4.11}$$

where $\boldsymbol{\alpha} = (\alpha_1, \cdots, \alpha_n), \boldsymbol{\beta} = (\beta_1, \cdots, \beta_n)$ and $\boldsymbol{\gamma}$ are n-dimensional multi-indices.

We record the following elementary relation between differencing and differentiation. To state this, we introduce the following notation:

$$\mathbf{I}_{\mathbf{t},\boldsymbol{\alpha}} = I_{t_1,\alpha_1} \times I_{t_2,\alpha_2} \times \cdots \times I_{t_n,\alpha_n}, \ I_{t_i,\alpha_i} = [t_i - \alpha_i, t_i]. \tag{4.12}$$

We shall say that $\boldsymbol{\alpha} \geq \boldsymbol{\beta}$ if for all i, $\alpha_i \geq \beta_i$.

Lemma 4.1. *Let $\mathcal{V}(\mathbf{t})$ be defined on an open set $\Sigma \subseteq \mathbb{R}^n$. Let $\mathbf{y} \in \Sigma$ and $\boldsymbol{\sigma} = (\sigma_1, \cdots, \sigma_n)$ be a multi-index such that $\mathbf{I}_{\mathbf{y},\boldsymbol{\sigma}} \subseteq \Sigma$. Furthermore, suppose that for any $\mathbf{x} \in \mathbf{I}_{\mathbf{y},\boldsymbol{\sigma}}$ and for any multi-index $\boldsymbol{\alpha} \leq \boldsymbol{\sigma}$, the $\boldsymbol{\alpha}$ partial derivative $\frac{\partial^{\boldsymbol{\alpha}}\mathcal{V}(\mathbf{x})}{\partial \mathbf{x}^{\boldsymbol{\alpha}}}$ exists and is uniformly continuous on $\mathbf{I}_{\mathbf{y},\boldsymbol{\sigma}}$. Then for any multi-index $\boldsymbol{\alpha} \leq \boldsymbol{\sigma}$, we have*

$$\mathcal{D}^{\boldsymbol{\alpha}}\mathcal{V}(\mathbf{y}) = \frac{\partial^{\boldsymbol{\alpha}}\mathcal{V}}{\partial \mathbf{x}^{\boldsymbol{\alpha}}}(\zeta_{\mathbf{y}}) \tag{4.13}$$

where $\zeta_{\mathbf{y}}$ is an interior point in $\mathbf{I}_{\mathbf{y},\boldsymbol{\sigma}}$.

Proof. This is a direct consequence from the mean value theorem. □

We can now state our assumptions on $\mathcal{Q}$ and $\mathcal{Q}_h$ For $\mathcal{Q}(\mathbf{k})$ we let

$$|\mathcal{D}^{\boldsymbol{\alpha}}\mathcal{Q}(\mathbf{k})| \leq C_{\boldsymbol{\alpha}} |\mathbf{k}|^{-|\boldsymbol{\alpha}|-n_0}, \ |\boldsymbol{\alpha}| = \sum_{i=1}^{n} \alpha_i, \ \boldsymbol{\alpha} = (\alpha_1, \cdots, \alpha_n), \tag{4.14}$$

where n_0 is some constant. The constant n_0 corresponds to the order of the differential operator in question. In the case of the Laplacian, $n_0 = 2$.

Take a n-dimensional multi-index $\boldsymbol{\beta}$ and let $q > 0$. We say that $\mathcal{Q}_h$ is of *order* $(\boldsymbol{\beta}, q)$ if, for any n-dimensional multi-index $\boldsymbol{\alpha} \leq \boldsymbol{\beta}$ and sufficiently small h, we have

$$|\mathcal{D}^{\boldsymbol{\alpha}} (\mathcal{Q}(\mathbf{k}) - \mathcal{Q}_h(\mathbf{k}))| \leq C_\alpha |h\mathbf{k}|^q |\mathbf{k}|^{-|\boldsymbol{\alpha}|-n_0} \text{ for all } \mathbf{k} \text{ such that } \mathbf{I}_{\mathbf{k},\boldsymbol{\alpha}} \in \mathcal{J}_{\pi/h}, \tag{4.15}$$

where C_α are positive constants that do not depend on h or $\mathbf{k}$, and the set $\mathcal{J}_c, c > 0$ is given by

$$\mathcal{J}_c = \{\mathbf{t} = (t_1, \cdots, t_n) \in \mathbb{R}^n | \forall i = 1, \cdots, n, |t_i| < c\}. \tag{4.16}$$

We shall denotes its closure by $\bar{\mathcal{J}}_c$.

The exponent q is the order of the finite difference scheme. Indeed, the above condition says that if $\mathbf{k}$ is small in magnitude, the difference between $\mathcal{Q}$ and $\mathcal{Q}_h$ is proportional to h^q. The presence of the factor $|\mathbf{k}|^{-|\alpha|-n_0}$ implies that $\mathcal{Q}_h$ must behave like $\mathcal{Q}$ when $|\mathbf{k}|$ is on the order of $1/h$ when $\boldsymbol{\alpha} \leq \boldsymbol{\beta}$.

This condition is satisfied by many, if not most finite difference discretization L_h of L. For example, if L is homogeneous, $\mathcal{Q}_h(\mathbf{k})/\mathcal{Q}(\mathbf{k})$ is usually a function only of $h\mathbf{k}$, which we denote by $\Lambda(h\mathbf{k})$. In this case a sufficient condition for $\mathcal{Q}_h$ to be of order $(\boldsymbol{\beta}, q)$ is

$$\left| \frac{\partial^{\boldsymbol{\alpha}}(1 - \Lambda(\mathbf{y}))}{\partial \mathbf{y}} \right| \leq C |\mathbf{y}|^{q-|\boldsymbol{\alpha}|} \text{ for } \boldsymbol{\alpha} \leq \boldsymbol{\beta} \text{ and } |y_i| \leq \pi, \mathbf{y} = (y_1, \cdots, y_n). \tag{4.17}$$

where $C > 0$ is a constant that only depends on Λ and $\boldsymbol{\alpha}$. It can be shown that $\mathcal{Q}_h$ corresponding to many finite difference schemes used in practice are of order $(\boldsymbol{\beta}, q)$ for any $\boldsymbol{\beta}$ (i.e., (4.15) is satisfied by all $\boldsymbol{\alpha}$). In this case, we could simply say that $\mathcal{Q}_h$ is of order q. The results to follow will nonetheless be stated in terms of the order $(\boldsymbol{\beta}, q)$ since this condition can be checked easily by performing a finite number of calculations.

Consider the Laplacian L in two dimensions and let L_h be the standard five-point discretization of L. For this problem, $\mathcal{Q}(\mathbf{k}) = -|\mathbf{k}|^2 = -(k^2 + l^2)$ where $\mathbf{k} = (k, l) \in \mathbb{Z}^2$. In this case we have

$$\Lambda(h\mathbf{k}) = \frac{\mathcal{Q}_h(\mathbf{k})}{\mathcal{Q}(\mathbf{k})} = \frac{h^2(k^2 + l^2)}{4\left((\sin(kh/2))^2 + (\sin(lh/2))^2\right)}. \tag{4.18}$$

We thus have

$$1-\Lambda(h\mathbf{k})=1-\frac{|h\mathbf{k}|^2}{|h\mathbf{k}|^2+\mathcal{O}(|h\mathbf{k}|^4)}=\mathcal{O}(|h\mathbf{k}|^2). \tag{4.19}$$

Thus, $q=2$ and this is the same as the order of discretization of L_h. It is not difficult to check that (4.17) holds for any multi-index $\boldsymbol{\beta}$.

We would now like to estimate $\mathcal{E}_{IB}$. In view of (4.8), the most straightforward way to estimate this quantity would be

$$|\mathcal{E}_{IB}|\leq\frac{1}{(2\pi)^n}\sum_{\mathbf{k}\in\mathbb{Z}^n}\left|(\mathcal{Q}(\mathbf{k})-\rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k}))\right|. \tag{4.20}$$

The right hand side, unfortunately, is usually not convergent. In the case of the Laplacian, for example, the right hand side is a lattice sum of terms that behave like $1/|\mathbf{k}|^2$ for large $|\mathbf{k}|$, and if $n\geq 2$, this is not convergent. The non-convergence of the right hand side is not all that surprising. Indeed, when $\mathbf{z}=\mathbf{x}-\mathbf{X}=0$, $\mathcal{E}_{IB}=G_{\mathbf{x}}(\mathbf{X})-\mathcal{I}G_{h,\mathbf{x}}(\mathbf{X})$ cannot be convergent since $G_{\mathbf{x}}(\mathbf{X})=G(\mathbf{x}-\mathbf{X})$, the continuous Green's function, is infinite, whereas the numerical approximation, $\mathcal{I}G_{h,\mathbf{x}}(\mathbf{X})$ is finite. If a meaningful estimate of $\mathcal{E}_{IB}$ can be obtained at all, such an estimate will only be valid if $\mathbf{z}=\mathbf{x}-\mathbf{X}\neq 0$. This implies that we must take advantage of cancellations of oscillatory of complex exponentials.

We first introduce a smooth cut-off of the continuous Green's function G. Let $\chi_0(t),t\in\mathbb{R}$ be a smooth function such that

$$\chi_0(t)=\begin{cases}1 & \text{if } |t|\leq 1,\\ 0 & \text{if } |t|\geq 2.\end{cases} \tag{4.21}$$

For $\mathbf{t}=(t_1,t_2,\cdots,t_n)\in\mathbb{R}^n$, let $\chi(\mathbf{t})=\prod_{i=1}^n\chi_0(t_i)$. Pick a positive integer $N>0$ and let

$$\tilde{G}_N(\mathbf{z})=\frac{1}{(2\pi)^n}\sum_{\mathbf{k}\in\mathbb{Z}^n}\chi\left(\frac{\mathbf{k}}{N}\right)\mathcal{Q}(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{z}). \tag{4.22}$$

Instead of $\mathcal{E}_{IB}$, we shall obtain an estimate for

$$\mathcal{E}_{IB}^N(\mathbf{X},\mathbf{x})=\tilde{G}_N(\mathbf{z})-(\mathcal{I}G_{h,\mathbf{x}})(\mathbf{X}). \tag{4.23}$$

This expression is easier to handle since $\mathcal{E}_{IB}^N$ is now a finite sum in terms of Fourier series and we thus do not have to worry about questions of summability. For this to work, we must show that $\tilde{G}_N(\mathbf{z})\to G(\mathbf{z})$ as $N\to\infty$.

Lemma 4.2. *Assume that $\mathcal{Q}$ satisfies* (4.14). *Then for any $\mathbf{z}\in\mathbb{R}^n,\mathbf{z}\neq\mathbf{0}$, $\tilde{G}_N(\mathbf{z})\to G(\mathbf{z})$ as $N\to\infty$.*

Proof. We first prove that $\{\tilde{G}_N(\mathbf{z})\}$ is a Cauchy sequence. Pick a multi-index $\boldsymbol{\alpha}=(\alpha_1,\cdots,\alpha_n)$ such that $-n_0+n-|\boldsymbol{\alpha}|<0$ and if $z_i=0$ let $\alpha_i=0$ for all $i=1,2,\cdots,n$. At least one of the z_i is not zero since $\mathbf{z}\neq 0$, and thus, $|\boldsymbol{\alpha}|$ can be made as large as we want. Take the difference between $\tilde{G}_M(\mathbf{z})$ and $\tilde{G}_N(\mathbf{z})$, $M>N$

and use summation by parts in the $\boldsymbol{\alpha}$ direction.

$$\begin{aligned}
&|\tilde{G}_M(\mathbf{z}) - \tilde{G}_N(\mathbf{z})| \\
\leq& \frac{1}{(2\pi)^n \prod_{i=1}^n |1-e^{iz_i}|^{\alpha_i}} \sum_{\mathbf{k}\in\mathbb{Z}^n} \left| \mathcal{D}^{\boldsymbol{\alpha}} \left(\left(\chi\left(\frac{\mathbf{k}}{M}\right) - \chi\left(\frac{\mathbf{k}}{N}\right) \right) \mathcal{Q}(\mathbf{k}) \right) \right| \\
\leq& C \left(\sum_{\mathbf{k}\in\mathcal{A}_{M,N}} \left| \mathcal{D}^{\boldsymbol{\alpha}} \left(\chi\left(\frac{\mathbf{k}}{M}\right) \mathcal{Q}(\mathbf{k}) \right) \right| + \sum_{\mathbf{k}\in\mathcal{B}_N} \left| \mathcal{D}^{\boldsymbol{\alpha}} \left(\chi\left(\frac{\mathbf{k}}{N}\right) \mathcal{Q}(\mathbf{k}) \right) \right| \right)
\end{aligned} \tag{4.24}$$

where C is a constant that depends only on $\mathbf{z}$. We used $\left|1-e^{iz_i}\right|^{\alpha_i} \neq 0$. The sets $\mathcal{A}_{M,N}, \mathcal{B}_N$ are given by

$$\begin{aligned}
\mathcal{A}_{M,N} &= \{\boldsymbol{k}\in\mathbb{Z}^n : \boldsymbol{I}_{\boldsymbol{k},\boldsymbol{\alpha}} \nsubseteq \mathbb{R}^n\backslash\mathcal{J}_{2M} \text{ and } \boldsymbol{I}_{\boldsymbol{k},\boldsymbol{\alpha}} \nsubseteq \bar{\mathcal{J}}_N\}, \\
\mathcal{B}_N &= \{\boldsymbol{k}\in\mathbb{Z}^n : \boldsymbol{I}_{\boldsymbol{k},\boldsymbol{\alpha}} \nsubseteq \mathbb{R}^n\backslash\mathcal{J}_{2N} \text{ and } \boldsymbol{I}_{\boldsymbol{k},\boldsymbol{\alpha}} \nsubseteq \bar{\mathcal{J}}_N\}.
\end{aligned}$$

From the definition of χ and Lemma 4.1, for any n-dimensional multi-index $\boldsymbol{\tau} \leq \boldsymbol{\alpha}$, we have

$$\left| \mathcal{D}^{\boldsymbol{\tau}} \chi\left(\frac{\mathbf{k}}{M}\right) \right| \leq c_{\boldsymbol{\tau},\chi} \frac{1}{M^{|\boldsymbol{\tau}|}} \tag{4.25}$$

where $c_{\boldsymbol{\tau},\chi} > 0$ is a constant that depends only on the $C^{|\tau|}$ norm of χ. Then from (4.14) and the product formula (4.11), for $\mathbf{k}\in\mathcal{A}_{M,N}$, we have

$$\left| \mathcal{D}^{\boldsymbol{\alpha}} \left(\chi\left(\frac{\mathbf{k}}{M}\right) \mathcal{Q}(\mathbf{k}) \right) \right| \leq c_{\boldsymbol{\alpha}} |\mathbf{k}|^{-|\boldsymbol{\alpha}|-n_0} \tag{4.26}$$

where $c_{\boldsymbol{\alpha}} > 0$ is a constant that does not depend on $\mathbf{k}$. Similarly, when $\mathbf{k}\in\mathcal{B}_N$, we have

$$\left| \mathcal{D}^{\boldsymbol{\alpha}} \left(\chi\left(\frac{\mathbf{k}}{N}\right) \mathcal{Q}(\mathbf{k}) \right) \right| \leq c_{\boldsymbol{\alpha}} \frac{1}{N^{|\alpha|}} |\mathbf{k}|^{-n_0} \tag{4.27}$$

where $c_{\boldsymbol{\alpha}} > 0$ is a constant that does not depend on $\mathbf{k}$. Then

$$\begin{aligned}
|\tilde{G}_M(\mathbf{z}) - \tilde{G}_N(\mathbf{z})| \leq& C \left(\sum_{\mathbf{k}\in\mathcal{A}_{M,N}} |\mathbf{k}|^{-|\boldsymbol{\alpha}|-n_0} + \frac{1}{N^{|\alpha|}} \sum_{\mathbf{k}\in\mathcal{B}_N} |\mathbf{k}|^{-n_0} \right) \\
\leq& C \left(\int_{\frac{N}{2}}^{\frac{5M}{2}} r^{-|\boldsymbol{\alpha}|-n_0+n-1} dr + \frac{1}{N^{|\boldsymbol{\alpha}|}} \int_{\frac{N}{2}}^{\frac{5N}{2}} r^{-n_0+n-1} dr \right) \\
\leq& C N^{-n_0+n-|\boldsymbol{\alpha}|}(1+\log N),
\end{aligned} \tag{4.28}$$

where the constants C may be different. We shall hence forth choose not to keep track of constants if not necessary. Since $-n_0+n-|\boldsymbol{\alpha}|<0$ by assumption, $\{\tilde{G}_N(\mathbf{z})\}$ is a Cauchy sequence for all $\mathbf{z}\neq 0$. Hence it must converge pointwise to a function denoted by $\tilde{G}(\mathbf{z})$. On the other hand, from we know that $\tilde{G}_N(\mathbf{z})$ converges to $G(\mathbf{z})$ in the sense of distribution. Thus, $\tilde{G}(\mathbf{z}) = G(\mathbf{z})$. ▯

Our next task is to establish bounds on $\mathcal{E}_{IB}^N$. Like the proof of the above lemma, our main tool is summation by parts. It is thus important to examine the the differences of $\rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k})$. We first examine the derivatives of ρ_r defined in (4.6).

Lemma 4.3. *Consider ϕ in (4.6). Suppose ϕ has compact support. We have*

$$\left|\rho_r^{(k)}(t)\right| \leq C_k,\ k \geq 0,\ |t| < \pi,\ |r| < 1. \tag{4.29}$$

Suppose ϕ is of moment order m. We have

$$|\rho_r(t) - 1| \leq C_0 t^m,\ \text{and}\ \left|\rho_r^{(k)}(t)\right| \leq C_k t^{m-k},\ 1 \leq k \leq m, |t| < \pi, |r| < 1. \tag{4.30}$$

Suppose ϕ is of smoothing order s. We have

$$|\rho_r(t - \pi)| \leq C_\pi (t - \pi)^s\ \text{and}\ |\rho_r(t + \pi)| \leq C_\pi (t + \pi)^s\ \text{for}\ t \in \mathbb{R}, |r| < 1. \tag{4.31}$$

In the above, C_0, C_k and C_π are positive constants that depend only on ϕ.

Proof. Inequality (4.29) is immediate from the definition of ρ_r in (4.6).

For any $|t| \leq \pi$, we have,

$$\begin{aligned} \exp(-i(l-r)t) &= \sum_{n=0}^{m-1} (l-r)^n \frac{(-it)^n}{n!} + t^m R_m(l-r,t), \\ R_m(l-r,t) &= \frac{(-i(l-r))^m}{(m-1)!} \int_0^1 \left((1-s)^{m-1} \exp(-i(l-r)ts)\right) ds. \end{aligned} \tag{4.32}$$

Substituting this into (4.6) and using the moment conditions (3.3) and (3.4) (ϕ is of moment order m by assumption), we get

$$\rho_r(t) = 1 + t^m \sum_{l=a_-}^{a_+} \phi(l-r) R_m(l-r,t). \tag{4.33}$$

We thus have

$$|\rho_r(t) - 1| \leq t^m \sum_{l=a_-}^{a_+} |\phi(l-r)|\, |R_m(l-r,t)| \leq C_0 t^m. \tag{4.34}$$

From the boundedness of ϕ and the expression for R_m in (4.32), we see that the constant C_0 may be chosen independent of $|r| < 1$. This is the first inequality in (4.30). Differentiating (4.33) k times and proceeding in a similar fashion, we obtain the rest of (4.30).

Substituting (3.5) into (4.6), we have, for $|t| \leq \pi$,

$$\begin{aligned} \rho_r(t) &= \sum_{l=a_-}^{a_+} \left(\sum_{j=0}^{s} \frac{1}{2^s} \binom{s}{j} \psi(l-r-j) \right) \exp(-i(l-r)t) \\ &= \sum_{l=a_-}^{a_+-s} \left(\sum_{j=0}^{s} \frac{1}{2^s} \binom{s}{j} \exp(-i(l+j-r)t) \right) \psi(l-r) \\ &= \left(\sum_{l=a_-}^{a_+-s} \exp(-i(l+s/2-r)t) \psi(l-r) \right) (\cos(t/2))^s. \end{aligned} \tag{4.35}$$

In the second equality, we used Lemma 3.2 (ψ has support between $[-r_\phi, r_\phi - s]$ and thus the summation bounds are a_- and $a_+ - s$). Hence $\rho_r(t), t \in \mathbb{R}$ can be written as

$$\begin{aligned} &\rho_r(t) = \varphi_r(t)\sigma(t),\ \varphi_r(t) = \sum_{l=a_-}^{a_+-s} \exp(-i(l+s/2-r)t)\psi(l-r) \\ &\sigma(t) = \begin{cases} (\cos(t/2))^s & \text{if } |t| \leq \pi, \\ 0 & \text{otherwise.} \end{cases} \end{aligned} \tag{4.36}$$

Inequality (4.31) is now immediate. □

Before we proceed, we comment on the significance of the above result. In view of (4.7), $\rho(h\mathbf{k})$ may be viewed as a cutoff function for $\mathcal{Q}_h(\mathbf{k})$. Note that $\mathcal{Q}_h(\mathbf{k})$ has, in general, a jump discontinuity at $k_i = \pm\pi/h$ (see (2.6)). A cutoff function should ideally be equal to 1 for small values of the frequency $\mathbf{k}$, and smooth out the discontinuity at $k_i = \pm\pi/h$. The above lemma states that this is indeed the case. Close to $\mathbf{k} = 0$, $\rho(h\mathbf{k})$ is close to 1 given (4.30). Close to $k_i = \pm\pi/h$, multiplication by $\rho(h\mathbf{k})$ will eliminate any discontinuity given (4.31). The moment order, therefore, controls the accuracy in the low frequency range, and the smoothing order suppresses Gibbs type phenomena that may corrupt convergence.

We now state two lemmas, Lemma 4.4 and Lemma 4.5 that state the above intuition in precise terms. The first deals with the difference $\mathcal{Q}(\mathbf{k}) - \rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k})$ for small values of the wave number $\mathbf{k}$. Here, the difference is dictated by the order of $\mathcal{Q}_h$ and the moment order of ϕ.

Lemma 4.4. *Suppose $\mathcal{Q}$ satisfies (4.14), $\mathcal{Q}_h$ is of order $(\boldsymbol{\alpha}, q)$ (see (4.15)) and ϕ in the definition of (4.6) is of moment order m. Take $\mathbf{k} \in \mathbb{Z}^n$ such that $I_{\mathbf{k},\boldsymbol{\alpha}} \subset \mathcal{J}_{\pi/h}$. Then, for sufficiently small h, we have*

$$|\mathcal{D}^{\boldsymbol{\alpha}} (\mathcal{Q}(\mathbf{k}) - \rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k}))| \leq C\, |h\mathbf{k}|^{\min(m,q)}\, |\mathbf{k}|^{-|\alpha|-n_0}, \tag{4.37}$$

where C is a constant that does not depend on h or $\mathbf{k}$.

Proof. We first show that, for any n-dimensional multi-index $\boldsymbol{\beta}$,

$$\left|\mathcal{D}^{\beta}(1-\rho(h\mathbf{k}))\right| \leq C_{\boldsymbol{\beta}}\, |h\mathbf{k}|^m\, |\mathbf{k}|^{-|\boldsymbol{\beta}|}. \tag{4.38}$$

where $C_{\boldsymbol{\beta}}$ only depends on $\boldsymbol{\beta}$ and not on h or $\mathbf{k}$. When $\boldsymbol{\beta} = \mathbf{0} = (0, \cdots, 0)$, the above is an immediate consequence of (4.30). Let $\boldsymbol{\beta} \neq \mathbf{0}$. Then,

$$\left|\mathcal{D}^{\beta}(1-\rho(h\mathbf{k}))\right| = \prod_{i=1}^{n} \left|\mathcal{D}_i^{\beta_i}\rho_{r_i}(hk_i)\right|, \tag{4.39}$$

where $\mathbf{k} = (k_1, \cdots, k_n)$ and $\boldsymbol{\beta} = (\beta_1, \cdots, \beta_n)$. It suffices to show that

$$\left|\mathcal{D}_i^{\beta_i}\rho_{r_i}(hk_i)\right| \leq \begin{cases} C_{\beta_i} & \text{if } \beta_i = 0, \\ C_{\beta_i}\, |hk_i|^m\, k_i^{-\beta_i} & \text{if } 1 \leq \beta_i \leq m, \\ C_{\beta_i} h^{\beta_i} & \text{if } \beta_i > m, \end{cases} \tag{4.40}$$

where C_{β_i} are positive constant that do not depend on h or $\mathbf{k}$. The case $\beta_i = 0$ is trivial. The case $1 \leq \beta_i \leq m$ is an immediate consequence of (4.30) and Lemma 4.1. The case $\beta_i > m$ follows from (4.29) and Lemma 4.1. Noting that $|k_i| \leq |\mathbf{k}|$, and that $|hk_i| < \pi$, we obtain (4.38).

Write $\mathcal{Q}(\mathbf{k}) - \rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k})$ as follows:

$$\mathcal{Q}(\mathbf{k}) - \rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k}) = \mathcal{Q}(\mathbf{k}) - \mathcal{Q}_h(\mathbf{k}) + \mathcal{Q}_h(\mathbf{k})(1-\rho(h\mathbf{k})). \tag{4.41}$$

Now, from (4.14) and (4.15), so long as $\boldsymbol{\beta} \le \boldsymbol{\alpha}$, we have

$$\left|\mathcal{D}^{\boldsymbol{\beta}}\mathcal{Q}_h(\mathbf{k})\right| \le \left|\mathcal{D}^{\boldsymbol{\beta}}\mathcal{Q}(\mathbf{k})\right| + \left|\mathcal{D}^{\boldsymbol{\beta}}(\mathcal{Q}(\mathbf{k}) - \mathcal{Q}_h(\mathbf{k}))\right| \le C_{\boldsymbol{\beta}} \left|\mathbf{k}\right|^{-|\boldsymbol{\beta}|-n_0} \tag{4.42}$$

where $C_{\boldsymbol{\beta}}$ is a constant that does not depend on h or $\mathbf{k}$ and we used the fact that $|h\mathbf{k}| \le \sqrt{n}\pi$ by the assumption that $I_{\mathbf{k},\boldsymbol{\alpha}} \subset \mathcal{J}_{\pi/h}$. Given (4.38) and the product formula, we have

$$\left|\mathcal{D}^{\boldsymbol{\alpha}}(\mathcal{Q}_h(\mathbf{k})(1-\rho(h\mathbf{k})))\right| \le C_{\boldsymbol{\alpha}} \left|h\mathbf{k}\right|^m \left|\mathbf{k}\right|^{-|\boldsymbol{\alpha}|-n_0}. \tag{4.43}$$

Using (4.41), (4.15) and the above inequality, we obtain the desired inequality. □

The next lemma examines the effect of the smoothing order on the error for wave numbers in the vicinity of $k_i = \pm\pi/h$. To state this lemma, we define the following. For any $\mathbf{k} \in \mathbb{Z}^n$ and a multi-index $\boldsymbol{\alpha}$, consider $\mathbf{I}_{\mathbf{k},\boldsymbol{\alpha}} = I_{k_1,\alpha_1} \times \cdots \times I_{k_n,\alpha_n}$. Let $j = i_1, \cdots, i_l$ be all the coordinate directions for which

$$\frac{\pi}{h} \in I_{k_j,\alpha_j} \text{ or } -\frac{\pi}{h} \in I_{k_j,\alpha_j}. \tag{4.44}$$

We denote this integer l by $\zeta_h(\mathbf{k},\boldsymbol{\alpha})$ (see (4.12)). Clearly, $0 \le \zeta_h(\mathbf{k},\boldsymbol{\alpha}) \le n$. It is also clear that $\zeta_h(\mathbf{k},\boldsymbol{\alpha}) \ne 0$ if and only if

$$\mathbf{I}_{\mathbf{k},\boldsymbol{\alpha}} \not\subset \mathcal{J}_{\pi/h} \text{ and } \mathbf{I}_{\mathbf{k},\boldsymbol{\alpha}} \not\subset \mathbb{R}^n \backslash \bar{\mathcal{J}}_{\pi/h}. \tag{4.45}$$

Lemma 4.5. *Let $\mathcal{Q}_h(\mathbf{k})$ be of order $(\boldsymbol{\alpha}, q)$ (see (4.15)) and ϕ (used to define ρ) be of smoothing order s. Suppose $\boldsymbol{\alpha} \le \boldsymbol{\alpha}_0 = (s+1, \cdots, s+1)$. Let $\mathbf{k} \in \mathbb{Z}^n$ satisfying $l = \zeta_h(\mathbf{k},\boldsymbol{\alpha}) \ne 0$. Then,*

$$\left|\mathcal{D}^{\boldsymbol{\alpha}}(\rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k}))\right| \le Ch^{n_0+|\boldsymbol{\alpha}|-l} \tag{4.46}$$

where C is a constant that depends only on $\boldsymbol{\alpha}$ and not on h or $\mathbf{k}$.

Proof. Without loss of generality, we assume that $j = 1, \cdots, l$ are the coordinate directions for which (4.44) holds. Let $\boldsymbol{\alpha} = (\alpha_1, \cdots, \alpha_n)$. Define the n-dimensional multi-index $\boldsymbol{\alpha}' = (0, \cdots, 0, \alpha_{l+1}, \cdots, \alpha_n)$. Write ρ as

$$\rho(h\mathbf{k}) = \prod_{i=1}^{l} \rho_{r_i}(hk_i) \prod_{i=l+1}^{n} \rho_{r_i}(hk_i) = \rho^1(h\mathbf{k})\rho^2(h\mathbf{k}). \tag{4.47}$$

We have

$$\begin{aligned} \left|\mathcal{D}^{\boldsymbol{\alpha}}(\rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k}))\right| &= \left|\mathcal{D}^{\boldsymbol{\alpha}-\boldsymbol{\alpha}'}\left(\rho^1(h\mathbf{k})\mathcal{D}^{\boldsymbol{\alpha}'}\left(\rho^2(h\mathbf{k})\mathcal{Q}_h(\mathbf{k})\right)\right)\right| \\ &\le C_{\boldsymbol{\alpha}} \sum_{\boldsymbol{\beta} \le \alpha - \alpha'} \left|\rho^1(h(\mathbf{k}-\boldsymbol{\beta}))\right| \left|\mathcal{D}^{\boldsymbol{\alpha}'}\left(\rho^2(h(\mathbf{k}-\boldsymbol{\beta}))\mathcal{Q}_h(\mathbf{k}-\boldsymbol{\beta})\right)\right|. \end{aligned} \tag{4.48}$$

In the equality, we used the fact that ρ^1 does not depend on the last $n-l$ coordinates. The inequality follows from the definition of the differencing operator, where $C_{\boldsymbol{\alpha}}$ is a combinatorial coefficient that only depends on $\boldsymbol{\alpha}$. For $\boldsymbol{\beta} = (\beta_1, \cdots, \beta_n) \le \boldsymbol{\alpha} - \boldsymbol{\alpha}'$, $k_i - \beta_i \in I_{k_i,\alpha_i}$. Given (4.44), if $1 \le i \le l$, we have

$$\left|(k_i - \beta_i)h - \pi\right| \le h\left|\boldsymbol{\alpha}\right| \text{ or } \left|(k_i - \beta_i)h + \pi\right| \le h\left|\boldsymbol{\alpha}\right|. \tag{4.49}$$

Therefore, from (4.31) and (4.47),

$$\left|\rho^1(h(\mathbf{k}-\boldsymbol{\beta}))\right| \leq C_{\boldsymbol{\alpha}} h^{ls}. \tag{4.50}$$

Note that

$$\mathbf{I}_{\mathbf{k}-\boldsymbol{\beta},\boldsymbol{\alpha}'} \in \mathcal{J}_{\pi/h} \text{ or } \mathbf{I}_{\mathbf{k}-\boldsymbol{\beta},\boldsymbol{\alpha}'} \in \mathbb{R}^n \backslash \mathcal{J}_{\pi/h}. \tag{4.51}$$

If the latter is true,

$$\left|\mathcal{D}^{\boldsymbol{\alpha}'}\left(\rho^2(h(\mathbf{k}-\boldsymbol{\beta}))\mathcal{Q}_h(\mathbf{k}-\boldsymbol{\beta})\right)\right| = 0 \tag{4.52}$$

since $\mathcal{Q}_h = 0$ in $\mathbb{R}^n \backslash \mathcal{J}_{\pi/h}$. If the former is true, we may estimate this quantity by an argument similar to Lemma 4.4. For $\boldsymbol{\gamma} \leq \boldsymbol{\alpha} - \boldsymbol{\alpha}'$ we have:

$$\mathcal{D}^{\gamma}(\rho^2(h(\mathbf{k}-\boldsymbol{\beta}))) \leq C_{\boldsymbol{\gamma}} h^{|\boldsymbol{\gamma}|} \tag{4.53}$$

where we used (4.29) and Lemma 4.1. Combining this with (4.42) using the product formula and noting that $1/(2h) < |\mathbf{k}|$, we get

$$\left|\mathcal{D}^{\boldsymbol{\alpha}'}\left(\rho^2(h(\mathbf{k}-\boldsymbol{\beta}))\mathcal{Q}_h(\mathbf{k}-\boldsymbol{\beta})\right)\right| \leq C_{\boldsymbol{\alpha}} h^{|\boldsymbol{\alpha}-\boldsymbol{\alpha}'|+n_0}. \tag{4.54}$$

Combining this with (4.50) and noting that $|\boldsymbol{\alpha}'| \leq l(s+1)$ by the assumption that $\boldsymbol{\alpha} \leq \boldsymbol{\alpha}_0$, we obtain the desired inequality. □

THEOREM 4.6. *Assume that ϕ is of class (m,s) for some integer $m \geq 1$ and $s \geq 0$. Let $\mathcal{Q}$ satisfy (4.14) and let $\mathcal{Q}_h$ be of order $(\boldsymbol{\alpha}, q)$ (see (4.15)) where $\boldsymbol{\alpha} = (\alpha_1, \cdots, \alpha_n)$ satisfies $\boldsymbol{\alpha} \leq \boldsymbol{\alpha_0} = (s+1, \cdots, s+1)$ and $|\boldsymbol{\alpha}| > n - n_0$. For sufficiently small h, we have*

$$|\mathcal{E}_{IB}(\mathbf{X},\mathbf{x})| \leq \begin{cases} C\left(\prod_{i=1}^n |\sin(z_i/2)|^{-\alpha_i}\right) h^{\min(m,q,\mu)} & \text{if } \min(m,q) \neq \mu, \\ C\left(\prod_{i=1}^n |\sin(z_i/2)|^{-\alpha_i}\right) h^{\mu} \log h^{-1} & \text{if } \min(m,q) = \mu, \end{cases} \tag{4.55}$$

where $\mu = n_0 + |\boldsymbol{\alpha}| - n$ and $C > 0$ is a constant that does not depend on $h, \mathbf{k}$ or $\mathbf{z} = \mathbf{x} - \mathbf{X} = (z_1, \cdots, z_n)$. The expression $|\sin(z_i/2)|^{-\alpha_i}$ should be understood in the following sense: if $z_i = 0$, $|\sin(z_i/2)|^0 = 1$ and $|\sin(z_i/2)|^{-\alpha_i} = \infty$ if $\alpha_i > 0$.

Proof. We assume $\alpha_i = 0$ if $z_i = 0$. Otherwise the inequality is trivial. We shall obtain an estimate for $\mathcal{E}_{IB}^N$ defined in (4.23). Take $N > 4/h$ in (4.23). Using summation by parts in the direction indicated by $\boldsymbol{\alpha}$, and taking absolute values, we have

$$\begin{aligned} \left|\mathcal{E}_{IB}^N(\mathbf{X},\mathbf{x})\right| &= \left|\frac{1}{(2\pi)^n}\sum_{\mathbf{k}\in\mathbb{Z}^n}\left(\chi\left(\frac{\mathbf{k}}{N}\right)\mathcal{Q}(\mathbf{k}) - \rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k})\right)\exp(i\mathbf{k}\cdot\mathbf{z})\right| \\ &\leq \frac{1}{(2\pi)^n}\left(\prod_{i=1}^n |\sin(z_i/2)|^{-\alpha_i}\right)\sum_{\mathbf{k}\in\mathbb{Z}^n}\left|\mathcal{D}^{\boldsymbol{\alpha}}\left(\chi\left(\frac{\mathbf{k}}{N}\right)\mathcal{Q}(\mathbf{k}) - \rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k})\right)\right|. \end{aligned} \tag{4.56}$$

We divide the above summation over $\mathbb{Z}^n$ into the following disjoint sets:

$$\begin{aligned} \mathcal{S}_0 &= \{\mathbf{k} \in \mathbb{Z}^n | \mathbf{I}_{\mathbf{k},\boldsymbol{\alpha}} \subset \mathbb{R}^n \backslash \mathcal{J}_{2N}\}, \\ \mathcal{S}_1 &= \{\mathbf{k} \in \mathbb{Z}^n | \mathbf{I}_{\mathbf{k},\boldsymbol{\alpha}} \subset \mathbb{R}^n \backslash \bar{\mathcal{J}}_{\pi/h}, \mathbf{I}_{\mathbf{k},\boldsymbol{\alpha}} \not\subset \mathbb{R}^n \backslash \mathcal{J}_{2N}\}, \\ \mathcal{S}_2 &= \{\mathbf{k} \in \mathbb{Z}^n | \mathbf{I}_{\mathbf{k},\boldsymbol{\alpha}} \subset \mathcal{J}_{\pi/h}\}, \\ \mathcal{S}_3 &= \{\mathbf{k} \in \mathbb{Z}^n | \mathbf{I}_{\mathbf{k},\boldsymbol{\alpha}} \not\subset \mathcal{J}_{\pi/h}, \mathbf{I}_{\mathbf{k},\boldsymbol{\alpha}} \not\subset \mathbb{R}^n \backslash \bar{\mathcal{J}}_{\pi/h}\}. \end{aligned}$$

It is clear that $\mathbb{Z}^n$ is a disjoint union of $\mathcal{S}_0, \mathcal{S}_1, \mathcal{S}_2$ and $\mathcal{S}_3$. Note first that the sum over $\mathcal{S}_0$ is 0 since $\chi(\mathbf{k}/N) = 0$ and $\rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k}) = 0$ when $\mathbf{k} \in \mathcal{S}_0$.

Let us now consider the sum over $\mathcal{S}_1$. When $\mathbf{k} \in \mathcal{S}_1$, for any n-dimensional multi-index $\boldsymbol{\tau} \leq \boldsymbol{\alpha}$, we have, similarly to (4.25),

$$\left|\mathcal{D}^{\boldsymbol{\tau}} \chi\left(\frac{\mathbf{k}}{N}\right)\right| \leq C\frac{1}{N^{|\boldsymbol{\tau}|}} \leq C\frac{1}{|k|^{\boldsymbol{\tau}}}$$

where we used the fact that $\mathbf{k}$ is of magnitude at most order N. Using (4.14) and the product formula, we have

$$\left|\mathcal{D}^{\boldsymbol{\alpha}}\left(\chi\left(\frac{\mathbf{k}}{N}\right)\mathcal{Q}(\mathbf{k})\right)\right| \leq C|\mathbf{k}|^{-|\boldsymbol{\alpha}|-n_0}$$

for $\mathbf{k} \in \mathcal{S}_1$. Therefore,

$$\begin{aligned}\sum_{\mathbf{k}\in\mathcal{S}_1}\left|\mathcal{D}^{\boldsymbol{\alpha}}\left(\chi\left(\frac{\mathbf{k}}{N}\right)\mathcal{Q}(\mathbf{k}) - \rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k})\right)\right| &= \sum_{\mathbf{k}\in\mathcal{S}_1}\left|\mathcal{D}^{\boldsymbol{\alpha}}\left(\chi\left(\frac{\mathbf{k}}{N}\right)\mathcal{Q}(\mathbf{k})\right)\right| \\ \leq C\sum_{\mathbf{k}\in\mathcal{S}_1}|\mathbf{k}|^{-|\boldsymbol{\alpha}|-n_0} \leq C\int_{\frac{\pi}{2h}}^{\frac{5\sqrt{n}N}{2}} r^{-|\boldsymbol{\alpha}|-n_0+n-1}dr \leq Ch^{\mu},\end{aligned} \tag{4.57}$$

where we used $\rho(h\mathbf{k})Q_h(\mathbf{k}) = 0$ given $\mathbf{I}_{\mathbf{k},\boldsymbol{\alpha}} \not\subset \mathbb{R}^n\backslash\bar{\mathcal{J}}_{\pi/h}$.

Let us now consider the sum over $\mathcal{S}_2$.

$$\begin{aligned}&\sum_{\mathbf{k}\in\mathcal{S}_1}\left|\mathcal{D}^{\boldsymbol{\alpha}}\left(\chi\left(\frac{\mathbf{k}}{N}\right)\mathcal{Q}(\mathbf{k}) - \rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k})\right)\right| \\ &\leq \sum_{\mathbf{k}\in\mathcal{S}_1} C\left|h\mathbf{k}\right|^{\min(m,q)}|\mathbf{k}|^{-|\boldsymbol{\alpha}|-n_0} \leq C\int_1^{1/h}(hr)^{\min(m,q)}r^{-|\boldsymbol{\alpha}|-n_0+n-1}dr \\ &= \begin{cases} Ch^{\min(m,q,\mu)} & \text{if } \min(m,q) \neq \mu, \\ Ch^{\mu}\log h^{-1} & \text{if } \min(m,q) = \mu. \end{cases}\end{aligned} \tag{4.58}$$

where we used the fact that $\chi(\mathbf{k}/N) = 1$ for $\mathbf{k} \in \mathcal{J}_{\pi/h}$ and Lemma 4.4 in the first inequality.

We finally consider the sum over $\mathcal{S}_3$. As we saw in the discussion preceding Lemma 4.5, the set $\mathcal{S}_3$ can be characterized as the subset of $\mathbf{k} \in \mathbb{Z}^n$ for which $\zeta_h(\mathbf{k}, \boldsymbol{\alpha}) \neq 0$. Let

$$\mathcal{S}_3^l = \{\mathbf{k} \in \mathbb{Z}^n | \zeta_h(\mathbf{k}, \boldsymbol{\alpha}) = l\}. \tag{4.59}$$

Clearly $\mathcal{S}_3$ is the disjoint union of the sets $\mathcal{S}_3^l, l = 1, \cdots, n$. Now,

$$\begin{aligned}\mathcal{M}_l = &\sum_{\mathbf{k}\in\mathcal{S}_3^l}\left|\mathcal{D}^{\boldsymbol{\alpha}}\left(\chi\left(\frac{\mathbf{k}}{N}\right)\mathcal{Q}(\mathbf{k}) - \rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k})\right)\right| \\ \leq &\sum_{\mathbf{k}\in\mathcal{S}_3^l}|\mathcal{D}^{\boldsymbol{\alpha}}\mathcal{Q}(\mathbf{k})| + |\mathcal{D}^{\boldsymbol{\alpha}}(\rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k}))|.\end{aligned} \tag{4.60}$$

Given (4.14) and the fact that $|\mathbf{k}| > 1/(2h)$ for $\mathbf{k} \in \mathcal{S}_3$, we have $|\mathcal{D}^{\boldsymbol{\alpha}}\mathcal{Q}(\mathbf{k})| \leq Ch^{|\boldsymbol{\alpha}|+n_0}$. Combining this with Lemma 4.5, we have

$$\mathcal{M}_l \leq Ch^{n_0+|\boldsymbol{\alpha}|-l}\left|\mathcal{S}_3^l\right| \tag{4.61}$$

where $\left|\mathcal{S}_3^l\right|$ is the number of $\mathbf{k}$ lattice points that belong to $\mathcal{S}_3^l$. Clearly, $\left|\mathcal{S}_3^l\right|$ scales like h^{l-n}. Therefore,

$$\begin{aligned}&\sum_{\mathbf{k}\in\mathcal{S}_3}\left|\mathcal{D}^{\boldsymbol{\alpha}}\left(\chi\left(\frac{\mathbf{k}}{N}\right)\mathcal{Q}(\mathbf{k})-\rho(h\mathbf{k})\mathcal{Q}_h(\mathbf{k})\right)\right|\\ =&\sum_{l=1}^{n}\mathcal{M}_l\leq\sum_{l=1}^{n}Ch^{n_0+|\boldsymbol{\alpha}|-l}\cdot h^{l-n}\leq Ch^{\mu}.\end{aligned}\tag{4.62}$$

Combining (4.57), (4.58), (4.62) and (4.56), we obtain (4.55) except that we have $\mathcal{E}_{IB}^N$ in place of $\mathcal{E}_{IB}$. By Lemma 4.2, we may take the limit as $N\to\infty$ to obtain the desired estimate. □

5. Application to the 2D stationary Stokes problem. In this section we consider the problem of a one-dimensional force generator immersed in a two-dimensional periodic Stokes fluid. We shall consider two discretization schemes, a second order discretization and a spectral discretization. We address local convergence properties of the velocity field. This problem was discussed previously in [15]. The theory in [15] was developed only for the spectral discretization. The theory was only able to explain pointwise convergence rates up to order 2, a significant underestimate for certain choices of discrete delta function as we shall see below.

5.1. Theory. We consider the problem on a periodic domain $\mathbb{U}=(\mathbb{R}/2\pi\mathbb{Z})^2$. The immersed boundary $\mathbf{X}(\theta)$ parametrized by $\theta\in\Theta=\mathbb{R}/(2\pi\mathbb{Z})$ defines a simple closed curve Γ in $\mathbb{U}$. The equations are

$$\Delta\mathbf{u}=\nabla p-\mathbf{f},\quad \nabla\cdot\mathbf{u}=0,\tag{5.1}$$

$$\mathbf{f}=\int_{-\pi}^{\pi}\mathbf{F}(\theta)\left(\delta(\mathbf{x}-\mathbf{X}(\theta))-(2\pi)^{-2}\right)d\theta,\quad \int_{\mathbb{U}}\mathbf{u}d\mathbf{x}=0,\tag{5.2}$$

where $\mathbf{u}$ is the velocity field and p is the pressure. Here $\mathbf{F}$ is the force along the boundary and δ is the Dirac delta function. This problem is different from the model problem described in Section 2 in that the unknowns functions are vector-valued. We shall apply our theory componentwise. The discretized equations using Immersed Boundary discretization are

$$L_h\mathbf{u}_h=\mathbf{D}_hp_h-\mathbf{f}_h,\quad \mathbf{D}_h\cdot\mathbf{u}_h=0,\tag{5.3}$$

$$\mathbf{f}_h=\sum_{\theta_m\in\mathcal{G}_\theta}\mathbf{F}(\theta_m)(\delta_h(\mathbf{x}-\mathbf{X}(\theta_m))-(2\pi)^{-2})\Delta\theta,\quad \sum_{\mathbf{x}\in\mathcal{G}_h}\mathbf{u}_h(\mathbf{x})h^2=0,\tag{5.4}$$

where L_h and D_h are discretizations of the Laplacian and the gradient/divergence operators respectively and δ_h is the discrete delta function. We lay a uniform grid in $\Theta=[-pi,\pi]$ so that $\theta_m=m\Delta\theta$. As in the scalar model problem, the velocity field for the continuous problem can be written as follows:

$$\begin{aligned}&\mathbf{u}(\mathbf{x})=\int_{-\pi}^{\pi}G(\mathbf{x}-\mathbf{X}(\theta))\mathbf{F}(\theta)d\theta,\\ &G(\mathbf{x})=\frac{1}{(2\pi)^2}\sum_{|\mathbf{k}|\neq0,\mathbf{k}\in\mathbb{Z}^2}\mathcal{Q}(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{x}),\ \mathcal{Q}(\mathbf{k})=\frac{1}{|\mathbf{k}|^2}\cdot\frac{1}{|\mathbf{k}|^2}\begin{pmatrix}l^2 & -kl\\ -kl & k^2\end{pmatrix},\end{aligned}\tag{5.5}$$

where $\mathbf{k} = (k, l)$. The matrix valued function $G(\mathbf{x})$ is nothing other than the Stokeslet for the two-dimensional periodic domain. The discrete solution can be written as

$$\begin{aligned} \mathbf{u}_h(\mathbf{x}) &= \sum_{\theta_m \in \mathcal{G}_\theta} (\mathcal{I}G_{h,\mathbf{x}})(\mathbf{X}(\theta_m))\mathbf{F}(\theta_m)\Delta\theta, \\ G_h(\mathbf{x}) &= \frac{1}{(2\pi)^2} \sum_{\mathbf{k}\in\mathbb{Z}^2} \mathcal{Q}_h(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{x}). \end{aligned} \tag{5.6}$$

The Fourier multiplier $\mathcal{Q}_h$ is different depending on the discretization scheme. For the spectral discretization, we take

$$\mathcal{Q}_h^{\mathrm{spec}}(\mathbf{k}) = \begin{cases} \mathcal{Q}(\mathbf{k}) & \text{if } 0 < |k| < \pi/h \text{ and } 0 < |l| < \pi/h, \\ 0 & \text{otherwise.} \end{cases} \tag{5.7}$$

For the second order discretization of the Stokes problem, we take L_h to be the standard five-point discretization of the Laplacian and $\mathbf{D}_h$ to be the central differencing operator. In this case, the discrete matrix problem has a four dimensional null-space (if $2\pi/h$ is even) that correspond to checkerboard patterns. In order to make the problem solvable, $\mathbf{f}_h$ must be in the range of the discretized operator. The standard way to accomplish this in the immersed boundary context is to use a discrete delta function that satisfies the even-odd condition, i.e., smoothing order 1. The discretized solution is further constrained not to contain Fourier components that correspond to the null space. This allows us to uniquely solve the problem. The corresponding discrete Green's function has the following form:

$$\begin{aligned} \mathcal{Q}_h^{\mathrm{2nd}}(\mathbf{k}) &= h^2 \hat{L}_{kl}^{-1} \left(D_k^2 + D_l^2\right)^{-1} \begin{pmatrix} D_l^2 & -D_k D_l \\ -D_k D_l & D_k^2 \end{pmatrix}, \\ \hat{L}_{kl} &= 4\left(\sin(kh/2)^2 + \sin(lh/2)^2\right), \quad D_k = \sin(kh), \end{aligned} \tag{5.8}$$

when $0 < |k| < \pi/h$ and $0 < |l| < \pi/h$ and 0 otherwise.

We want to estimate the error between $\mathbf{u}$ and $\mathbf{u}_h$ at a certain point $\mathbf{x} \notin \Gamma$. In order to do so, we split this error into two parts, the quadrature error and the immersed boundary error.

$$\begin{aligned} (\mathbf{u} - \mathbf{u}_h)(\mathbf{x}) &= \mathbf{E}_Q(\mathbf{x}) + \mathbf{E}_{IB}(\mathbf{x}) \\ \mathbf{E}_Q(\mathbf{x}) &= \int_{-\pi}^{\pi} G_{\mathbf{x}}(\mathbf{X}(\theta))\mathbf{F}(\theta)d\theta - \sum_{\theta_m\in\mathcal{G}_\theta} G_{\mathbf{x}}(\mathbf{X}(\theta_m))\mathbf{F}(\theta_m)\Delta\theta \\ \mathbf{E}_{IB}(\mathbf{x}) &= \sum_{\theta_m\in\mathcal{G}_\theta} \boldsymbol{\mathcal{E}}_{IB}(\mathbf{X}(\theta_m), \mathbf{x})\mathbf{F}(\theta_m)\Delta\theta,\ \boldsymbol{\mathcal{E}}_{IB}(\mathbf{X}, \mathbf{x}) = (G_{\mathbf{x}} - (\mathcal{I}G_{h,\mathbf{x}}))(\mathbf{X}) \end{aligned} \tag{5.9}$$

The only difference between (2.11) and the above is that $\mathbf{F}$ has values in $\mathbb{R}^2$ and that the Green's function G, G_h are matrix valued. The interpolation operator $\mathcal{I}$ acts componentwise. Assume $\mathbf{F}(\theta)$ and $\mathbf{X}(\theta)$ are C^k functions. Note that the quadrature rule we use, the trapezoidal rule, is a k-th order quadrature rule for C^k periodic functions [1, 11, 9, 25]. When $\mathbf{x} \notin \Gamma$, the integrand in the integral in (5.9) is a C^k function (note that it is *not* a C^k function if $\mathbf{x} \in \Gamma$ since the Green's function has a singularity there). The quadrature error $\mathbf{E}_Q(\mathbf{x})$,

$$|\mathbf{E}_Q(\mathbf{x})| \le C(\Delta\theta)^k \tag{5.10}$$

where C is a constant that depends on the k-th derivative of the integrand, and thus on $\mathbf{X}(\theta), \mathbf{F}(\theta)$ and $\mathbf{x}$. The immersed boundary error can be bounded by

$$|\mathbf{E}_{IB}(\mathbf{x})| \leq \left(\max_{\theta\in\Theta} |\mathbf{F}(\theta)|\right) \sum_{\theta_m \in \mathcal{G}_\theta} |\boldsymbol{\mathcal{E}}_{IB}(\mathbf{X}(\theta_m), \mathbf{x})| \, \Delta\theta. \tag{5.11}$$

The estimation of this error thus rests on the estimation of $|\boldsymbol{\mathcal{E}}_{IB}|$, for which we can use the results of the previous section. In the case of the spectral scheme, we can directly apply Theorem 4.6 componentwise with $q = \infty, n = 2, n_0 = 2$. In the case of the second order scheme, we cannot directly apply Theorem 4.6. This is due to the fact that $\mathcal{Q}_h^{\text{2nd}}$ has a singularity as $\mathbf{k} = (k,l) \to \pm(\pi/h, \pi/h), \pm(\pi/h, -\pi/h)$. These four singularities correspond to null spaces of the second order discretization of the Stokes problem. We can obtain the following bound nonetheless thanks to the fact that the smoothing order is greater than or equal to 1.

Proposition 5.1. *Consider $\boldsymbol{\mathcal{E}}_{IB}^{2nd}(\mathbf{X}, \mathbf{x})$, the difference $\boldsymbol{\mathcal{E}}_{IB}$ for the second order differencing scheme. Suppose the discrete delta function is class (m, s) where both m and s are greater than or equal to 1. Suppose $\mathbf{z} = \mathbf{x} - \mathbf{X} = (z_1, z_2) \neq (0, 0)$. We have the following estimate. For multi-index $\boldsymbol{\alpha} = (\alpha_1, \alpha_2), |\boldsymbol{\alpha}| = 2$, we have*

$$\left|\mathcal{E}_{IB}^{2nd}(\mathbf{X}, \mathbf{x})\right| \leq C \left(\Pi_{i=1}^2 |\sin(z_i/2)|^{-\alpha_i}\right) h^2 \log(h^{-1}), \tag{5.12}$$

where the above is understood in the same sense as Theorem 4.6

Proof. We only sketch the proof. Note that in the proof of Theorem 4.6, The conditions on $\mathcal{Q}_h$ and ρ were used only insofar as they imply (4.37) and (4.46) of Lemma 4.4 and 4.5. It can be shown that $\rho(h\mathbf{k})\mathcal{Q}_h^{\text{2nd}}(\mathbf{k})$ satisfies (4.37) and (4.46) nevertheless. Note that

$$\begin{aligned}\rho(h\mathbf{k})\mathcal{Q}_h^{\text{2nd}}(\mathbf{k}) =& h^2\varphi_1(hk)\varphi_2(hl)\hat{L}_{kl}^{-1} \\ & (\cos(kh/2))^s(\cos(lh/2))^s \left(D_k^2 + D_l^2\right)^{-1} \begin{pmatrix} D_l^2 & -D_kD_l \\ -D_kD_l & D_k^2 \end{pmatrix}\end{aligned} \tag{5.13}$$

where we used expression (4.36). If $s \geq 1$, the factor $(\cos(kh/2))^s(\cos(lh/2))^s$ tames the singularity introduced by D_k and D_l $\mathbf{k} = (k,l) \to \pm(\pi/h, \pi/h), \pm(\pi/h, -\pi/h)$ so that the function $\rho(h\mathbf{k})\mathcal{Q}_h^{\text{2nd}}(\mathbf{k})$ is a C^2 function of $\mathbf{k}$. This may be used to show that (4.37) and (4.46) are satisfied. The rest of the proof is the same as Theorem 4.6. ◻

We may now obtain an estimate for $\mathbf{u}(\mathbf{x}) - \mathbf{u}_h(\mathbf{x}), \mathbf{x} \notin \Gamma$. We start with the second order scheme. For any point $\mathbf{X}(\theta_m)$, according to Proposition 5.1, we have

$$\begin{aligned}\left|\boldsymbol{\mathcal{E}}_{IB}^{\text{2nd}}(\mathbf{X}(\theta_m), \mathbf{x})\right| \leq& Ch^2\log(h^{-1}) \min\left(|\sin(x - X(\theta_m))|^{-2}, |\sin(y - Y(\theta_m))|^{-2}\right) \\ \leq& C'h^2\log(h^{-1}) \, |\mathbf{x} - \mathbf{X}(\theta_m)|^{-2}\end{aligned} \tag{5.14}$$

where $\mathbf{x} = (x, y)$ and $\mathbf{X} = (X, Y)$ and C, C' are positive constants that do not depend on h or θ_m. From (5.9), (5.10), (5.11) and (5.14), we have

$$|\mathbf{u}(\mathbf{x}) - \mathbf{u}_h(\mathbf{x})| \leq Ch^2 \log(h^{-1}) + C(\Delta\theta)^k. \tag{5.15}$$

where the constants depend on $\mathbf{X}, \mathbf{F}$ and $\mathbf{x}$. In fact, the same argument shows the following. Suppose $\mathcal{U} \subset \mathbb{U}$ is an open set such that its closure has no intersection with Γ. Then,

$$\|u - u_h\|_{L^\infty(\mathcal{U})} \leq Ch^2\log(h^{-1}) + C(\Delta\theta)^k. \tag{5.16}$$

where $L^\infty(\mathcal{U})$ denotes the L^∞ norm in $\mathcal{U}$. If we take $\Delta\theta = Ch$ (i.e., refine $\Delta\theta$ proportionally to h), then we get second order for any point $\mathbf{x} \notin \Gamma$ if $\mathbf{F}$ and $\mathbf{X}$ are C^2 functions.

Now, consider convergence for the spectral scheme. Let the discrete delta function be of class (m, s). In Theorem 4.6, we must take $q = \infty, n = n_0 = 2$. Thus, the convergence rate of $\boldsymbol{\mathcal{E}}_{IB}^{\text{spec}}$ ($\boldsymbol{\mathcal{E}}_{IB}$ for the spectral scheme) is dictated by the smaller of $\mu = |\boldsymbol{\alpha}|$ and m where $\boldsymbol{\alpha}$ is under the restriction that $\boldsymbol{\alpha} \leq (s+1, s+1)$.

Let us consider the case $s = 0$. We have the restriction $\boldsymbol{\alpha} = (\alpha_1, \alpha_2) \leq (1, 1)$. We thus have two kinds of bounds for $\boldsymbol{\mathcal{E}}_{IB}^{\text{spec}}$:

$$
\begin{aligned}
&|\boldsymbol{\mathcal{E}}_{IB}^{\text{spec}}(\mathbf{X}(\theta_m), \mathbf{x})| \leq Ch\,|\mathbf{x} - \mathbf{X}(\theta_m)|^{-1} \text{ for } m \geq 1,\\
&|\boldsymbol{\mathcal{E}}_{IB}^{\text{spec}}(\mathbf{X}(\theta_m), \mathbf{x})| \leq Ch^2 \log(h^{-1})\,|x - X(\theta_m)|^{-1}\,|y - Y(\theta_m)|^{-1} \text{ for } m \geq 2.
\end{aligned}
\tag{5.17}
$$

The first bound can be obtained by combining the bounds for $\boldsymbol{\alpha} = (0, 1)$ and $\boldsymbol{\alpha} = (1, 0)$ and the second comes from the bound for $\boldsymbol{\alpha} = (1, 1)$. Take any point $\mathbf{x} \notin \Gamma$. When $m = 1$, we can only obtain a first order bound. The error estimate is

$$
|\mathbf{u}(\mathbf{x}) - \mathbf{u}_h(\mathbf{x})| \leq Ch + C(\Delta\theta)^k. \tag{5.18}
$$

Let $m \geq 2$. We would like to use the second bound in (5.17) since this would give us a faster convergence rate. However, we cannot do this in general because there may be points $\mathbf{X}(\theta_m)$ on the immersed boundary for which $x = X(\theta_m)$ or $y = Y(\theta_m)$. Therefore, we are forced to use the first bound in (5.17) and thus, our bound remains first order. Thus, when $s = 0$, we can only obtain a first order bound whatever the moment order may be.

We can obtain better bounds, however, if $\mathbf{x}$ is located in a favorable place with respect to the immersed structure. Suppose $\mathbf{x}$ happens to be a *corner point*: there are no points $\mathbf{X}(\theta_m)$ for which $x = X(\theta_m)$ or $y = Y(\theta_m)$. For such points, we can obtain the bound (5.17). It is also possible to obtain better bounds when $\mathbf{x} \notin \Gamma$ is a *non-tangent point*: the two lines parallel to the coordinate axes going through the point $\mathbf{x}$ is not tangent to the curve Γ. In this case, the error $u - u_h$ behaves like $h(h + \Delta\theta) + (\Delta\theta)^k$ up to possible logarithmic factors [15].

Now suppose $m \leq s+1$. Then, we can obtain the following bounds for any point in $\mathbf{x} \notin \Gamma$:

$$
|\mathbf{u}(\mathbf{x}) - \mathbf{u}_h(\mathbf{x})| \leq
\begin{cases}
Ch^2 \log(h^{-1}) + C(\Delta\theta)^k & \text{if } m = 2,\\
Ch^m + C(\Delta\theta)^k & \text{if } m \neq 2.
\end{cases}
\tag{5.19}
$$

What these considerations suggest is that when $m > s+1$, we may see differences in convergence rate depending on the location of $\mathbf{x} \in \Gamma$ relative to the grid and the immersed boundary Γ. In other words, if there is a mismatch in m and s ($m > s+1$), we expect to see grid effects.

5.2. Computational demonstration. In this section we demonstrate computational results for the velocity field of the 2-D Stokes problem discussed above. We perform computational experiments for different choices of discrete delta functions.

We must specify our model problem. Take the coordinates in $\mathbb{U}$ to be $[0, 2\pi) \times [0, 2\pi)$. We let $\mathbf{X}(\theta)$ and $\mathbf{F}(\theta)$ to be the following:

$$
\mathbf{X}(\theta) = \frac{\pi}{12}\begin{pmatrix} 12 + (6 + \cos(3\theta))\cos\theta \\ 12 + (6 + \cos(3\theta))\sin\theta \end{pmatrix}, \quad \mathbf{F}(\theta) = \begin{pmatrix} 1 + \sin\theta \\ 1 + \cos\theta \end{pmatrix}. \tag{5.20}
$$

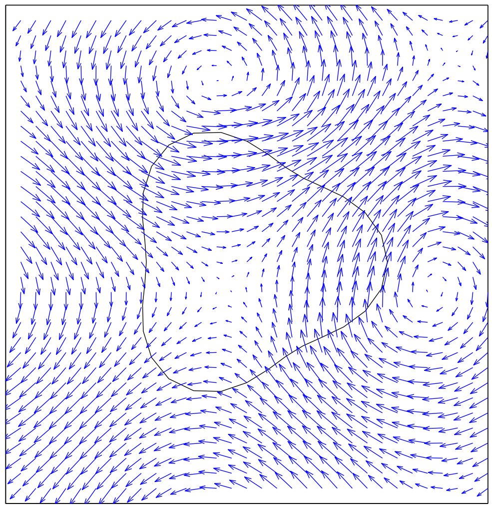

FIG. 5.1. *Plot of the velocity field obtained by solving the model problem* (5.20).

The position of the immersed boundary and the resulting velocity field is plotted in Figure 5.1.

The discrete delta functions we use are plotted in Figure 5.2, each of which is the unique continuous discrete delta function of class $(m, s, \sigma, 2r_\phi)$ (see end of Section 3). Of the discrete delta functions listed, those of class $(4, 3, 0, 7)$, $(4, 2, 1, 7)$, $(4, 3, 1, 8)$, $(6, 5, 0, 11)$ and $(6, 5, 1, 12)$ seem to be new. We do not list the explicit formulae for all of these discrete delta functions, since the algebraic expressions are long and tedious.

In order to examine local convergence rates, we compute the following quantity at $\mathbf{x}$ on the $N \times N$ grid:

$$r^N(\mathbf{x}) = \log_2\left(\frac{\left|\mathbf{u}^N(\mathbf{x}) - \mathbf{u}^{2N}(\mathbf{x})\right|}{\left|\mathbf{u}^{2N}(\mathbf{x}) - \mathbf{u}^{4N}(\mathbf{x})\right|}\right). \tag{5.21}$$

We let $M = 4N, M\Delta\theta = 2\pi$ so that $\Delta\theta$ is refined proportionally to h. We take $N = 256$ in all our calculations.

In Figure 5.3, we plot the computed pointwise convergence rate $r^N(\mathbf{x})$ as a function of $\mathbf{x}$ for a few of the discrete delta functions when the spectral discretization is used. We see that for the cases $(m, s, \sigma, 2r_\phi) = (2, 1, 1, 4)$ and $(4, 3, 1, 8)$ the pointwise convergence rate is uniformly 2 or 4 if the point is away from the immersed boundary. When $(m, s, \sigma, 2r_\phi) = (4, 0, 0, 4)$ and $(4, 1, 1, 6)$, however, we see that there are prominent grid effects. At corner points, which do not share the x or y coordinate with any immersed boundary point, we see convergence of order approximately 2 and 4 respectively, which again is in agreement with our theory.

In Table 5.1, we examine all 16 discrete delta functions. For the discrete delta functions of classes $(2, 1, 1, 4)$ and $(4, 1, 1, 6)$ we test convergence both for the second order and spectral schemes. We calculate the mean of r^N over points in the $N \times N$ grid that are at least two mesh points away from the support of the discrete delta function. We denote this quantity by $\bar{r}^N$. Also listed is the mean deviation σ_r^N, the average of $\left|r^N(\mathbf{x}) - \bar{r}^N\right|$ over tested grid points $\mathbf{x}$. Along with the computed rate, we also list the theoretically predicted rate, modulo logarithmic factors, at general

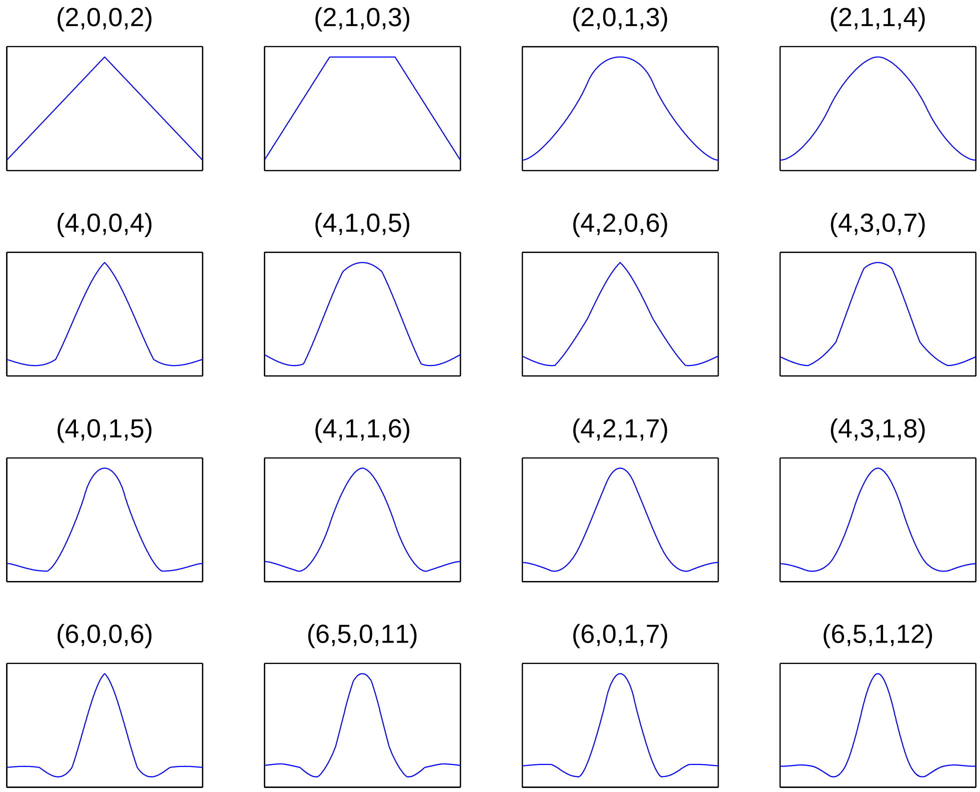

FIG. 5.2. *Plots of discrete delta functions of class* $(m, s, \sigma, 2r_\phi)$ *(see end of Section 3) used in computational experiments.*

points, non-tangent points and corner points. We see a broad agreement with the theory we developed. The average rate of convergence is approximately in between the theoretical rate for the non-tangent points and the corner points, since these two classes of points, together, make up almost all of the grid points. When $m < s + 1$, σ_r^N is large indicating a large grid effect as was seen in Figure 5.3. When $m = s + 1$, we observe clean m-order pointwise convergence.

6. Conclusion. In this paper, we have established bounds for the error $\mathcal{E}_{IB}$ and discussed how this quantity depends on the properties of the discrete delta function and the discretization of the differential operator. The moment order and the order of the discretization determines accuracy for low frequency components whereas the high frequency errors were controlled by the smoothing order. The optimality of the somewhat elaborate expressions obtained in Section 4 were tested for the two-dimensional Stokes problem. The observed convergence rates are in line with the predicted rates. We observe prominent grid effects when there is a mismatch between the moment order and smoothing order. This result highlights the role played by the smoothing order in determining the rate of convergence of immersed boundary type methods. This also says that the smoothing order is potentially important in suppressing grid effects in immersed boundary computations, a hitherto unrecognized role.

It has been conjectured in [22, 8] that a finite difference scheme with order q

m	s	σ	$2r_\phi$	q	gen.	n.t.	cor.	$\bar{r}^{256}$	σ_r^{256}
2	1	1	4	2	2	2	2	2.003	0.022
4	1	1	6	2	2	3	4	2.004	0.029
2	0	0	2	∞	1	2	2	2.024	0.263
2	1	0	3	∞	2	2	2	2.001	0.054
2	0	1	3	∞	1	2	2	1.996	0.080
2	1	1	4	∞	2	2	2	2.002	0.010
4	0	0	4	∞	1	2	2	2.202	0.896
4	1	0	5	∞	2	3	4	3.386	0.929
4	2	0	6	∞	3	4	4	4.027	0.212
4	3	0	7	∞	4	4	4	4.029	0.153
4	0	1	5	∞	1	2	2	2.211	0.987
4	1	1	6	∞	2	3	4	3.502	0.809
4	2	1	7	∞	3	4	4	4.017	0.106
4	3	1	8	∞	4	4	4	4.000	0.039
6	0	0	6	∞	1	2	2	2.197	0.899
6	5	0	11	∞	6	6	6	6.079	0.246
6	0	1	7	∞	1	2	2	2.203	0.987
6	5	1	12	∞	6	6	6	6.026	0.095

TABLE 5.1

A table of computed convergence rates. m: moment order, s: smoothing order, σ: sum of squares condition, $2r_\phi$: size of support, q: order of discretization of Stokes problem, gen.: predicted convergence rate at general points, n.t.: predicted convergence rate at non-tangent points, cor.: predicted convergence rate at corner points, $\bar{r}^{256}$: average pointwise rate, σ_r^{256}: mean deviation of pointwise rate.

with discrete delta functions of moment order m lead to local convergence of order $\min(m, q)$ based on numerical examples. Our results show that this is not necessarily true, although this is indeed true if the smoothing order is high enough. It is certainly possible, that additional properties of the finite difference scheme may lead to the conjectured rate. We plan to address this in a future publication.

In this paper, we only applied our estimates for $\mathcal{E}_{IB}$ to the problem of local convergence for the two-dimensional Stokes problem. Our estimate on $\mathcal{E}_{IB}$ applies to higher dimensional problems that are of general elliptic type. It is thus possible to apply this to other problems in higher dimensions. We can also apply these estimates to the question of global convergence: L^p error estimates. This L^∞ error estimate for the Stokes problem in two dimensions with a spectral discretization was treated in [15]. Such results will be obtained using the results of the current paper and will be a subject of an upcoming publication.

Appendix A. An Alternative Characterization of the Smoothing Order. The smoothing order is in fact also equivalent to the following condition, which is reminiscent of the characterization of the moment condition given in Lemma 3.1.

LEMMA A.1. *Let ϕ be a non-zero function of compact support. Denote by $\mathcal{P}_s$ the set of polynomials of degree less than s. The function ϕ is of smoothing order $s \geq 1$ if and only if it satisfies the following condition:*

$$\forall r \in \mathbb{R} \text{ and } \forall g \in \mathcal{P}_s,\ \sum_{k\in\mathbb{Z}} (-1)^k g(k)\phi(r-k) = 0. \tag{A.1}$$

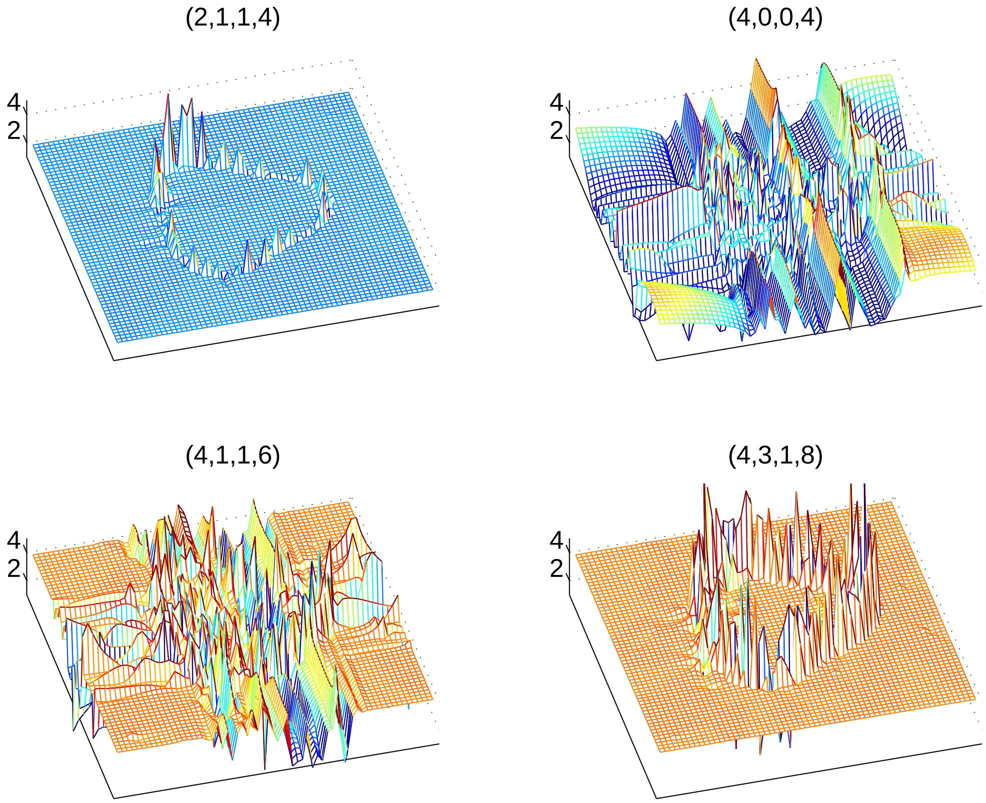

FIG. 5.3. *A plot of $r^{256}(\mathbf{x})$ plotted every 4 grid points in both coordinate directions. Note that the convergence rate is uniformly 2 and 4 respectively away from the immersed boundary for discrete delta functions of classes $(2,1,1,4)$ and $(4,3,1,8)$. For the cases $(4,0,0,4)$ and $(4,1,1,6)$ cases, we see prominent grid effects, although at corner points, we see approximate 2nd and 4th order convergence respectively.*

Proof. We first rewrite condition (A.1). Define

$$\phi_k(r) = \phi(-a_\phi + k + r),\ 0 \le k \le 2a_\phi - 1,\ 0 \le r < 1. \tag{A.2}$$

where a_ϕ was defined in (3.7). We may now rewrite the condition (A.1) as

$$\forall 0 \le r < 1 \text{ and } \forall g \in \mathcal{P}_s,\ \sum_{k=0}^{2a_\phi - 1} (-1)^k g(k)\phi_k(r) = 0. \tag{A.3}$$

The function ϕ satisfies condition (A.3), if and only if (A.3) is true for s polynomials, $g_0, \cdots, g_{s-1}$ that form a basis of $\mathcal{P}_s$, seen as a vector space over $\mathbb{R}$. Let

$$g_0(k) = 1,\ g_l(k) = k(k-1)\cdots(k-l+1), 1 \le l \le s-1. \tag{A.4}$$

The above polynomials clearly form a basis of $\mathcal{P}_s$. We thus consider the s relations:

$$\sum_{k=0}^{2a_\phi - 1} (-1)^k g_l(k)\phi_k(r) = 0,\ 0 \le l \le s-1. \tag{A.5}$$

We rewrite this in matrix form:

$$M\boldsymbol{\phi} = 0, \ \boldsymbol{\phi} = (\phi_0, \cdots, \phi_{2a_\phi - 1})^T. \tag{A.6}$$

where M is an $s \times 2a_\phi$ matrix. It is easily seen that M is an upper triangular matrix with non-zero entries along the diagonal. This implies that M is full rank. Thus, (A.6), seen as an equation for $\boldsymbol{\phi}$, can only have a solution if $2a_\phi \geq s$. If $2a_\phi = s$, $\boldsymbol{\phi} = \mathbf{0}$ and this contradicts the assumption that ϕ is non-zero. We therefore assume $2a_\phi > s$.

Since M is full rank, the kernel of M is of dimension $2a_\phi - s$. We now show that the kernel of M is spanned by the following $2a_\phi - s$ linearly independent vectors:

$$\mathbf{v}_l = \Big(\underbrace{0, \cdots, 0}_{l}, \binom{s}{0}, \binom{s}{1}, \cdots, \binom{s}{s}, \underbrace{0, \cdots, 0}_{2a_\phi - s - l - 1}\Big)^T, \ 0 \leq l \leq 2a_\phi - s - 1. \tag{A.7}$$

We must show that each of these vectors is in the null space of M. All elements of the vector $M\mathbf{v}_l$ are of the following form:

$$\sum_{k=0}^{s} (-1)^k \binom{s}{k} g(k) \tag{A.8}$$

where $g \in \mathcal{P}_s$. It suffices to show that (A.8) is zero for any $g \in \mathcal{P}_s$. We must check that (A.8) is zero for a set of basis vectors of $\mathcal{P}_s$, and for this purpose, we again use the polynomials g_l defined in (A.4). Consider the binomial formula:

$$(1+t)^s = \sum_{k=0}^{s} \binom{s}{k} t^k. \tag{A.9}$$

Differentiate the above l times with respect to t:

$$s(s-1)\cdots(s-l+1)(1+t)^{s-l} = \sum_{k=l}^{s} \binom{s}{k} g_l(k) t^{k-l}. \tag{A.10}$$

Substituting $t = -1$, we see that (A.8) is 0 for $g = g_l$.

Thus, $\boldsymbol{\phi}$ can be written as linear combinations of $\mathbf{v}_l, 0 \leq l \leq 2a_\phi - s - 1$.

$$\boldsymbol{\phi}(r) = \sum_{l=0}^{2a_\phi - s - 1} \varphi_l(r) \mathbf{v}_l, \tag{A.11}$$

where $\varphi_l(r)$ are functions defined for $0 \leq r < 1$. Define $\psi(r)$ as

$$\psi(r) = \begin{cases} 0 & \text{if } r < -a_\phi \\ 2^s \varphi_l(r + a_\phi - l) & \text{if } -a_\phi + l \leq r < -a_\phi + l + 1, \ 0 \leq l \leq 2a_\phi - s - 1 \\ 0 & \text{if } r \geq a_\phi - s. \end{cases} \tag{A.12}$$

Recalling the definition of $\boldsymbol{\phi}$ in (A.6), it is easily seen that expression (A.11) is nothing other than (3.5) written in a different way. □

In [4], the author introduces the following conditions that generalize the even-odd condition. A function ϕ satisfies the alternating moment condition of order p if it satisfies the condition

$$\sum_{k \in \mathbb{Z}} (-1)^k (r-k)^j \phi(r-k) = 0 \text{ for } j \geq 0 \tag{A.13}$$

for all $r \in \mathbb{R}$. It is immediate from the above lemma that a non-zero function ϕ of compact support is of smoothing order $s \geq 1$ if and only if it satisfies the alternating moment conditions up to order $s-1$.

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