

Projection to the Set of Shift Orthogonal Functions*

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Abstract

This paper presents a fast algorithm for projecting a given function to the set of shift orthogonal functions (i.e. set containing functions with unit L^2 norm that are orthogonal to their prescribed shifts). The algorithm can be parallelized easily and its computational complexity is bounded by $O(M \log(M))$, where M is the number of coefficients used for storing the input. To derive the algorithm, a particular class of basis called Shift Orthogonal Basis Functions are introduced and some theory regarding them is developed.

1 Introduction

Let $\Omega = [0, L_1] \times \cdots \times [0, L_d]$ be a bounded, periodic domain. Let $\mathbf{w} = (w_1, \dots, w_d) \in \mathbb{R}_+^d$ be a basis of a d -dimensional lattice, and define

$$\Gamma_{\mathbf{w}} = \{\mathbf{jw} := (j_1 w_1, \dots, j_d w_d) \mid \mathbf{j} = (j_1, \dots, j_d) \in \mathbb{Z}^d\}. \quad (1)$$

Note that to make the boundary of Ω periodic, we require that L_i be divisible by w_i , for $i = 1, \dots, d$. Endow Ω with the usual inner product

$$\langle f, g \rangle = \int_{\Omega} f^* g \, d\mathbf{x}.$$

For any function $f(\mathbf{x}) \in L^2(\Omega)$, we say f is *shift orthogonal*, if it satisfies *shift orthogonality constraints*:

$$\int_{\Omega} f(\mathbf{x})^* f(\mathbf{x} - \mathbf{jw}) \, d\mathbf{x} = \delta_{\mathbf{j}0} \quad \text{for all } \mathbf{jw} \in \Gamma_{\mathbf{w}}. \quad (2)$$

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Shift orthogonality constraints arise naturally in many applications of science and engineering. However, due to the numerical and theoretical challenges in imposing the shift orthogonality constraints, these constraints have not received much attention in the literature.

The main contribution of this paper is to propose a very fast algorithm for finding a shift orthogonal functions that is closest in L^2 norm to a given function (i.e. projection to the set of shift orthogonal functions). Note that shift orthogonal functions constitute a set and not a vector space. There are many potential applications for the algorithm described in this paper. As an example, in section 5 we demonstrate how the algorithm increases the speed in computing CPWs described in [4]. Further applications of the algorithm will be investigated in subsequent research projects.

In order to devise the algorithm we introduce the notion of Shift Orthogonal Basis Functions (SOBFs) and develop some theory for them. For one dimensional periodic domain $[0, L_1]$ we call a family of functions

$$\{\xi_j^i(x)\}_{i=0, j=0}^{i=\infty, j=L_1/w_1-1},$$

with $\xi_j^i(x) = \xi_0^i(x - jw_1)$, *Shift Orthogonal Basis Functions (SOBFs)* if they form a complete orthonormal set of basis for space $L^2([0, L_1])$. We refer to superscript index i as the *depth index*, and subscript index j as the *shift index*. For higher dimensional periodic domains, we call a complete set of basis SOBFs if they are formed from the tensor product of one dimensional SOBFs. Section 4 describes a concrete example of SOBFs with certain nice properties.

It turns out that SOBFs have been of interest to quantum mechanics and signal analysis communities (i.e. although, the orthonormal basis considered in these literatures are usually defined in domain \mathbb{R}^d , instead of periodic bounded domains). In [10, 9], a numerical example of SOBFs, called phase space Wannier functions, are provided that are exponentially localized in time and frequency domain and for which the matrix of the Laplacian operator is near-diagonal (i.e. see [9, equations 2.1, 2.3 and 2.5]). Reference [8] provides a simple description of certain SOBFs, called Wilson basis, whose Fourier transform have specific bimodal form (see [8, equations 1.9a and 1.9b]). An explicit example of Wilson basis with exponential decay in time and frequency domain is also constructed in [8] using rapidly converging superpositions of Gaussians (i.e. however, the Laplacian matrix is no longer near-diagonal for this basis). Other examples of Wilson basis are presented in [12] and [11].

The remainder of this paper consists of the following: Section 2 develops some theory regarding SOBFs that is used in devising the fast algorithm. Section 3 contains the description of the fast algorithm and highlights some of its important properties including its computational complexity. Section 4 describes a concrete example of SOBFs, which we call Shift Orthogonal Plane Waves (SOPWs), that have certain nice properties. Section 5 gives an application of the fast algorithm in generating CPWs. Section 6 presents some concluding remarks. Appendices A, B and C contain proofs for properties of SOPWs mentioned in section 4.

2 Shift Orthogonal Basis Functions (SOBFs)

This section develops some theory for SOBFs in multidimensional domains. Some of this theory also appears in [3]. For the ease of exposition, the concepts are illustrated for 2D domain. The results to other dimensions can be extended in the trivial way.

By scaling, it is assumed without loss of generality that $\Omega = [0, L_1] \times [0, L_2]$ and the length of the shift in each coordinate is unit length (i.e. L_1 and L_2 are replaced by L_1/w_1 and L_2/w_2 , respectively). Because SOBFs in 1D form an orthonormal set of basis, tensor product can be used to form orthonormal set of basis for 2D. That is, any function $f \in L^2(\Omega)$ can be expressed by

$$f(x_1, x_2) = \sum_{i_1, i_2=1}^{\infty} \sum_{j_1=0, j_2=0}^{L_1-1, L_2-1} a_{j_1, j_2}^{i_1, i_2} \xi_{j_1}^{i_1}(x_1) \xi_{j_2}^{i_2}(x_2). \quad (3)$$

Remark 2.1 In what follows i_1 and i_2 and their primes (i.e. $i_1', i_2'',$ etc.) take value from $1, 2, \dots$. Indices j_1, s_1 and their primes take value from $\{0, \dots, L_1 - 1\}$. Indices j_2 and s_2 and their primes take value from $\{0, 1, \dots, L_2 - 1\}$. Also addition and subtraction for indices j_1, s_1 and their primes are performed in module L_1 . Similarly, addition and subtraction for indices j_2, s_2 and their primes are performed in module L_2 .

Note that

$$\begin{aligned} f(x_1 - s_1, x_2 - s_2) &= \sum_{i_1, i_2=1}^{\infty} \sum_{j_1=0, j_2=0}^{L_1-1, L_2-1} a_{j_1, j_2}^{i_1, i_2} \xi_{j_1}^{i_1}(x_1 - s_1) \xi_{j_2}^{i_2}(x_2 - s_2) \\ &= \sum_{i_1, i_2=1}^{\infty} \sum_{j_1=0, j_2=0}^{L_1-1, L_2-1} a_{j_1, j_2}^{i_1, i_2} \xi_{j_1+s_1}^{i_1}(x_1) \xi_{j_2+s_2}^{i_2}(x_2) \\ &= \sum_{i_1, i_2=1}^{\infty} \sum_{j_1=0, j_2=0}^{L_1-1, L_2-1} a_{j_1-s_1, j_2-s_2}^{i_1, i_2} \xi_{j_1}^{i_1}(x_1) \xi_{j_2}^{i_2}(x_2). \end{aligned} \quad (4)$$

Also, suppose

$$g(x_1, x_2) = \sum_{i_1, i_2=1}^{\infty} \sum_{j_1=0, j_2=0}^{L_1-1, L_2-1} b_{j_1, j_2}^{i_1, i_2} \xi_{j_1}^{i_1}(x_1) \xi_{j_2}^{i_2}(x_2).$$

Because SOBFs in 2D form an orthonormal set:

$$\int g(x_1, x_2)^* f(x_1 - s_1, x_2 - s_2) \, d\mathbf{x} = \sum_{i_1, i_2=1}^{\infty} \sum_{j_1=0, j_2=0}^{L_1-1, L_2-1} b_{j_1, j_2}^{i_1, i_2}{}^* a_{j_1-s_1, j_2-s_2}^{i_1, i_2}. \quad (5)$$

We use a specific multi-index notation

$$(i_1, i_2; j_1, j_2)_{i_1=1, i_2=1, j_1=0, j_2=0}^{i_1=\infty, i_2=\infty, j_1=L_1-1, j_2=L_2-1},$$

to refer to the entries of an infinite dimensional vector. To be rigorous, there is a (non-unique) one-to-one and onto mapping

$$\rho : \mathbb{N} \times \mathbb{N} \times \{0, \dots, L_1 - 1\} \times \{0, \dots, L_2 - 1\} \rightarrow \mathbb{N}.$$

Indeed, by $(i_1, i_2; j_1, j_2)$, we mean $\rho((i_1, i_2; j_1, j_2))$; however, to avoid cumbersome notation, we just use $(i_1, i_2; j_1, j_2)$ to refer to the positive integer instead. As it will be seen shortly, i_1 and j_1 are related to depth index and shift index for the first coordinate, respectively. Similarly, i_2 and j_2 are related to the depth index and shift index for the second coordinate, respectively. We also use multi-index notation

$$(s_1, s_2)_{s_1=0, s_2=0}^{s_1=L_1-1, s_2=L_2-1},$$

to refer to the entries of a vector of length $L_1 L_2$. Again, to be rigorous, there is a (non-unique) one-to-one and onto mapping

$$\tilde{\rho} : \{0, \dots, L_1 - 1\} \times \{0, \dots, L_2 - 1\} \rightarrow \{1, 2, \dots, L_1 L_2\}.$$

Indeed, by (s_1, s_2) , we mean $\tilde{\rho}((s_1, s_2))$; however, to avoid cumbersome notation, we just use (s_1, s_2) to refer to the elements of $\{1, \dots, L_1 L_2\}$.

In view of (3), function f can be represented in SOBFs basis using infinite dimensional vector

$$\mathbf{SOBF}(f)(i_1, i_2; j_1, j_2) := a_{j_1, j_2}^{i_1, i_2}. \quad (6)$$

Also for any infinite dimensional vector $a \in \mathbb{C}^{\mathbb{N}}$, define

$$\mathbf{ISOBF}(a) := \sum_{i_1, i_2=1}^{\infty} \sum_{j_1=0, j_2=0}^{L_1-1, L_2-1} a(i_1, i_2; j_1, j_2) \xi_{j_1}^{i_1}(x_1) \xi_{j_2}^{i_2}(x_2). \quad (7)$$

For any infinite dimensional vector v and all pairs (s_1, s_2) , define transformation $S(s_1, s_2)$ in the following way:

$$\tilde{v} = S(s_1, s_2)v \quad \text{if and only if} \quad \tilde{v}(i_1, i_2; j_1, j_2) = v(i_1, i_2; j_1 - s_1, j_2 - s_2).$$

Note that from (4),

$$\mathbf{SOBF}(f(x_1 - s_1, x_2 - s_2)) = S(s_1, s_2)\mathbf{SOBF}(f(x_1, x_2)).$$

In view of (5), for $s_1, s'_1 = 0, \dots, L_1 - 1$ and $s_2, s'_2 = 0, \dots, L_2 - 1$:

$$\langle g(x_1 - s_1, x_2 - s_2), f(x_1 - s'_1, x_2 - s'_2) \rangle = \langle S(s_1, s_2)\mathbf{SOBF}(g), S(s'_1, s'_2)\mathbf{SOBF}(f) \rangle. \quad (8)$$

Define Set of Shift Orthogonal as follow:

$$\begin{aligned} \mathbf{SSO} &= \{v \in \mathbb{C}^{\mathbb{N}} : \langle v, S(s_1, s_2)v \rangle = \delta_{0s_1} \delta_{0s_2} \text{ for all } s_1 \text{ and } s_2\} \\ &= \{v \in \mathbb{C}^{\mathbb{N}} : \langle S(s'_1, s'_2)v, S(s_1, s_2)v \rangle = \delta_{s'_1 s_1} \delta_{s'_2 s_2} \text{ for all } s_1, s'_1, s_2 \text{ and } s'_2\}. \end{aligned}$$

Observe that \mathcal{SSO} is only a set and not a subspace. Moreover, equation (8) implies that $f(x_1, x_2)$ is shift orthogonal if and only if $\mathbf{SOBF}(f) \in \mathcal{SSO}$ (i.e. see theorem 2.2).

Define \mathcal{B} -transform to be operator $\mathcal{B} : \mathbb{C}^{\mathbb{N}} \rightarrow \mathbb{C}^{\mathbb{N}}$ defined by

$$\mathcal{B}(v)(i_1, i_2; j_1, j_2) = \sum_{\ell_1, \ell_2} e^{i2\pi(\frac{j_1}{L_1}, \frac{j_2}{L_2}) \cdot (\ell_1, \ell_2)} v(i_1, i_2; \ell_1, \ell_2). \quad (9)$$

The intuition for \mathcal{B} -transform is that for every fixed i_1 and i_2 , if $v(i_1, i_2; : , :)$ and $\mathcal{B}(v)(i_1, i_2; : , :)$ are thought as $L_1 \times L_2$ matrices then

$$\mathcal{B}(v)(i_1, i_2; : , :) = L_1 L_2 \mathcal{F}_{2D}^{-1}(v(i_1, i_2; : , :)),$$

where \mathcal{F}_{2D}^{-1} is the 2D discrete inverse Fourier transform. The inverse of \mathcal{B} -transform, $\mathcal{B}^{-1} : \mathbb{C}^{\mathbb{N}} \rightarrow \mathbb{C}^{\mathbb{N}}$, is

$$\mathcal{B}^{-1}(v)(i_1, i_2; j_1, j_2) = \frac{1}{L_1 L_2} \sum_{\ell_1, \ell_2} e^{-i2\pi(\frac{j_1}{L_1}, \frac{j_2}{L_2}) \cdot (\ell_1, \ell_2)} v(i_1, i_2; \ell_1, \ell_2).$$

Similar to the above, \mathcal{B}^{-1} -transform can be written as

$$\mathcal{B}^{-1}(v)(i_1, i_2; : , :) = \frac{1}{L_1 L_2} \mathcal{F}_{2D}(v(i_1, i_2; : , :)),$$

where \mathcal{F}_{2D} is the 2D discrete Fourier transform.

The importance of \mathcal{B} -transform appears in the following two theorems:

Theorem 2.2 *For given function f , the followings are equivalent:*

1. f is shift orthogonal.
2. $\mathbf{SOBF}(f) \in \mathcal{SSO}$.
3. for all $(j_1, j_2) \in \{0, \dots, L_1 - 1\} \times \{0, \dots, L_2 - 1\}$,

$$\|\mathcal{B}(\mathbf{SOBF}(f))(: , : ; j_1, j_2)\|_2 = 1.$$

Theorem 2.3 *For given functions f and g , the followings are equivalent:*

1. for all $s_1, s'_1 = 0, \dots, L_1 - 1$ and $s_2, s'_2 = 0, \dots, L_2 - 1$,

$$\langle g(x_1 - s_1, x_2 - s_2), f(x_1 - s'_1, x_2 - s'_2) \rangle = 0.$$

2. for all $s_1 = 0, \dots, L_1 - 1$ and $s_2 = 0, \dots, L_2 - 1$,

$$\langle \mathbf{SOBF}(g), S(s_1, s_2) \mathbf{SOBF}(f) \rangle = 0.$$

3. for all $j_1 = 0, \dots, L_1 - 1$ and $j_2 = 0, \dots, L_2 - 1$,

$$\left\langle \mathcal{B}(\mathbf{SOBF}(g))(\cdot, \cdot; j_1, j_2), \mathcal{B}(\mathbf{SOBF}(f))(\cdot, \cdot; j_1, j_2) \right\rangle = 0.$$

In order to prove the above two theorems, we need to introduce some more notations and concepts. We use multi-index notation to define matrices in the following way: Identify entries of matrix A by $A(\cdot|\cdot)$, where the index to the left of “|” determines the row number of the entry and the index to the right of “|” determines the column number of the entry. Let W be the $L_1 L_2 \times L_1 L_2$ matrix defined by

$$W(s_1, s_2|j_1, j_2) = \frac{1}{\sqrt{L_1 L_2}} e^{-i2\pi(\frac{s_1}{L_1}, \frac{s_2}{L_2}) \cdot (j_1, j_2)}.$$

Let W_∞ to be infinite dimensional square matrix defined by

$$W_\infty(i_1, i_2; s_1, s_2|i'_1, i'_2; j_1, j_2) = \frac{1}{\sqrt{L_1 L_2}} e^{-i2\pi(\frac{s_1}{L_1}, \frac{s_2}{L_2}) \cdot (j_1, j_2)} \delta_{i_1 i'_1} \delta_{i_2 i'_2}.$$

Finally, for any infinite dimensional vector v , let $\text{circ}(v)$ be the $L_1 L_2 \times \mathbb{N}$ matrix defined by

$$\text{circ}(v)(s_1, s_2|i_1, i_2; j_1, j_2) = (S(s_1, s_2)v)(i_1, i_2; j_1, j_2) = v(i_1, i_2; j_1 - s_1, j_2 - s_2).$$

Note that W and W_∞ are unitary matrix (i.e. although the latter is infinite dimensional and by unitary we mean that $W_\infty W_\infty^\dagger$ is infinite dimensional diagonal matrix whose diagonal entries are one). To see this, observe that for example,

$$\begin{aligned} & (W_\infty W_\infty^\dagger)(i_1, i_2; s_1, s_2|i'_1, i'_2; s'_1, s'_2) \\ &= \sum_{i''_1, i''_2} \sum_{s''_1, s''_2} W_\infty(i_1, i_2; s_1, s_2|i''_1, i''_2; s''_1, s''_2) W_\infty^\dagger(i''_1, i''_2; s''_1, s''_2|i'_1, i'_2; s'_1, s'_2) \\ &= \sum_{i''_1, i''_2} \sum_{s''_1, s''_2} W_\infty(i_1, i_2; s_1, s_2|i''_1, i''_2; s''_1, s''_2) \overline{W_\infty(i'_1, i'_2; s'_1, s'_2|i''_1, i''_2; s''_1, s''_2)} \\ &= \sum_{i''_1, i''_2} \sum_{s''_1, s''_2} \frac{1}{\sqrt{L_1 L_2}} e^{-i2\pi(\frac{s_1}{L_1}, \frac{s_2}{L_2}) \cdot (s''_1, s''_2)} \delta_{i_1 i''_1} \delta_{i_2 i''_2} \frac{1}{\sqrt{L_1 L_2}} e^{i2\pi(\frac{s'_1}{L_1}, \frac{s'_2}{L_2}) \cdot (s''_1, s''_2)} \delta_{i'_1 i''_1} \delta_{i'_2 i''_2} \\ &= \sum_{i''_1} \delta_{i_1 i''_1} \delta_{i'_1 i''_1} \sum_{i''_2} \delta_{i_2 i''_2} \delta_{i'_2 i''_2} \sum_{s''_1, s''_2} \frac{1}{L_1 L_2} e^{i2\pi(\frac{s'_1 - s_1}{L_1}, \frac{s'_2 - s_2}{L_2}) \cdot (s''_1, s''_2)} \\ &= \delta_{i_1 i'_1} \delta_{i_2 i'_2} \delta_{s_1 s'_1} \delta_{s_2 s'_2}. \end{aligned}$$

Another important property that W and W_∞ have is that if $\text{circ}(v)$ is multiplied on left by W and on right by W_∞^\dagger , then

$$(W \text{circ}(v) W_\infty^\dagger)(s_1, s_2|i_1, i_2; j_1, j_2) = \delta_{s_1 j_1} \delta_{s_2 j_2} \mathcal{B}(v)(i_1, i_2; j_1, j_2). \quad (10)$$

To see the above, note that

$$\begin{aligned}
& (W \text{circ}(v) W_\infty^\dagger)(s_1, s_2 | i_1, i_2; j_1, j_2) \\
&= \sum_{j'_1, j'_2} \sum_{i'_1, i'_2, s'_1, s'_2} W(s_1, s_2 | j'_1, j'_2) \text{circ}(v)(j'_1, j'_2 | i'_1, i'_2; s'_1, s'_2) W_\infty^\dagger(i'_1, i'_2; s'_1, s'_2 | i_1, i_2; j_1, j_2) \\
&= \sum_{j'_1, j'_2} \sum_{i'_1, i'_2} \sum_{s'_1, s'_2} \frac{e^{-i2\pi(\frac{s'_1}{L_1}, \frac{s'_2}{L_2}) \cdot (j'_1, j'_2)}}{\sqrt{L_1 L_2}} v(i'_1, i'_2; s'_1 - j'_1, s'_2 - j'_2) \frac{e^{i2\pi(\frac{j_1}{L_1}, \frac{j_2}{L_2}) \cdot (s'_1, s'_2)}}{\sqrt{L_1 L_2}} \delta_{i_1 i'_1} \delta_{i_2 i'_2} \\
&= \sum_{j'_1, j'_2} \sum_{\ell_1, \ell_2} \frac{e^{-i2\pi(\frac{s_1}{L_1}, \frac{s_2}{L_2}) \cdot (j'_1, j'_2)}}{\sqrt{L_1 L_2}} v(i_1, i_2; \ell_1, \ell_2) \frac{e^{i2\pi(\frac{j_1}{L_1}, \frac{j_2}{L_2}) \cdot (\ell_1 + j'_1, \ell_2 + j'_2)}}{\sqrt{L_1 L_2}} \\
&= \sum_{j'_1, j'_2} \frac{1}{L_1 L_2} e^{i2\pi(\frac{j_1 - s_1}{L_1}, \frac{j_2 - s_2}{L_2}) \cdot (j'_1, j'_2)} \sum_{\ell_1, \ell_2} v(i_1, i_2; \ell_1, \ell_2) e^{i2\pi(\frac{j_1}{L_1}, \frac{j_2}{L_2}) \cdot (\ell_1, \ell_2)} \\
&= \delta_{s_1 j_1} \delta_{s_2 j_2} \mathcal{B}(v)(i_1, i_2; j_1, j_2),
\end{aligned}$$

where (9) was used for the last equality. Equality (10) is very significant: it shows how $\text{circ}(v)$ can be turned into a “pseudo-diagonal” matrix using unitary matrices W and W_∞ . Equation (10) is used extensively, in the remainder of this section.

Finally, for any two infinite dimensional vectors a and b :

$$(\text{circ}(b) \text{circ}(a)^\dagger)(s_1, s_2 | j_1, j_2) = \overline{\langle S(s_1, s_2) b, S(j_1, j_2) a \rangle}. \quad (11)$$

For observe that

$$\begin{aligned}
& (\text{circ}(b) \text{circ}(a)^\dagger)(s_1, s_2 | j_1, j_2) \\
&= \sum_{i_1, i_2, j'_1, j'_2} \text{circ}(b)(s_1, s_2 | i_1, i_2; j'_1, j'_2) \text{circ}(a)^\dagger(i_1, i_2; j'_1, j'_2 | j_1, j_2) \\
&= \sum_{i_1, i_2, j'_1, j'_2} \text{circ}(b)(s_1, s_2 | i_1, i_2; j'_1, j'_2) \overline{\text{circ}(a)(j_1, j_2 | i_1, i_2; j'_1, j'_2)} \\
&= \sum_{i_1, i_2, j'_1, j'_2} (S(s_1, s_2) b)(i_1, i_2; j'_1, j'_2) \overline{(S(j_1, j_2) a)(i_1, i_2; j'_1, j'_2)} \\
&= \overline{\langle S(s_1, s_2) b, S(j_1, j_2) a \rangle}.
\end{aligned}$$

Now we are ready to prove theorem 2.2 and 2.3.

Proof of theorem 2.2: The equivalence of 1 and 2 follows easily from (8) (i.e. with $g = f$) and the definition of \mathcal{SSO} . It remains to prove the equivalence between 2 and 3:

Set $v = \mathbf{SOBF}(f)$. Equation (11) (i.e. with $a = b = v$) implies that $v \in \mathcal{SSO}$ if and only if $(\text{circ}(v) \text{circ}(v)^\dagger)(s_1, s_2 | j_1, j_2) = \delta_{s_1 j_1} \delta_{s_2 j_2}$ for all s_1, j_1, s_2 and j_2 (i.e. matrix $\text{circ}(v) \text{circ}(v)^\dagger$ is the $L_1 L_2 \times L_1 L_2$ identity matrix).

Next let

$$V = W \text{circ}(v) W_\infty^\dagger.$$

Compute VV^\dagger in two ways: On one hand, because W_∞ is unitary

$$VV^\dagger = W \text{circ}(v) W_\infty^\dagger W_\infty \text{circ}(v)^\dagger W^\dagger = W \text{circ}(v) \text{circ}(v)^\dagger W^\dagger. \quad (12)$$

On the other hand, (10) yields that

$$\begin{aligned} & VV^\dagger(s_1, s_2 | j_1, j_2) \\ &= \sum_{i_1, i_2, j'_1, j'_2} V(s_1, s_2 | i_1, i_2; j'_1, j'_2) V^\dagger(i_1, i_2; j'_1, j'_2 | j_1, j_2) \\ &= \sum_{i_1, i_2, j'_1, j'_2} V(s_1, s_2 | i_1, i_2; j'_1, j'_2) \overline{V(j_1, j_2 | i_1, i_2; j'_1, j'_2)} \\ &= \sum_{i_1, i_2, j'_1, j'_2} \mathcal{B}(v)(i_1, i_2; j'_1, j'_2) \delta_{s_1 j'_1} \delta_{s_2 j'_2} \overline{\mathcal{B}(v)(i_1, i_2; j'_1, j'_2) \delta_{j_1 j'_1} \delta_{j_2 j'_2}} \\ &= \sum_{i_1, i_2} |\mathcal{B}(v)(i_1, i_2; j_1, j_2)|^2 \delta_{s_1 j_1} \delta_{s_2 j_2} \\ &= \|\mathcal{B}(v)(\cdot, \cdot; j_1, j_2)\|_2^2 \delta_{s_1 j_1} \delta_{s_2 j_2}. \end{aligned} \quad (13)$$

Now if $\text{circ}(v) \text{circ}(v)^\dagger$ is the identity matrix (i.e. $v \in \mathcal{SSO}$), then from (12) and W being unitary, one concludes that VV^\dagger is the identity matrix. Hence, by (13), it must be the case that

$$\|\mathcal{B}(v)(\cdot, \cdot; j_1, j_2)\|_2 = 1,$$

for all $(j_1, j_2) \in \{0, \dots, L_1 - 1\} \times \{0, \dots, L_2 - 1\}$.

Conversely, if the above holds, then by (13), VV^\dagger is the identity matrix. Therefore, because W is a unitary matrix, $W^\dagger VV^\dagger W$ would be the identity matrix as well. Equation (12), yields that

$$W^\dagger VV^\dagger W = \text{circ}(v) \text{circ}(v)^\dagger.$$

Hence, $\text{circ}(v) \text{circ}(v)^\dagger$ is the identity matrix, which implies $v \in \mathcal{SSO}$. ■

Proof of theorem 2.3: The equivalence of 1 and 2 follows easily from (8) and the fact that

$$\langle \mathbf{SOBF}(g), S(s_1, s_2) \mathbf{SOBF}(f) \rangle = 0 \quad \text{for all } s_1 \text{ and } s_2,$$

is equivalent to

$$\langle S(s_1, s_2) \mathbf{SOBF}(g), S(s'_1, s'_2) \mathbf{SOBF}(f) \rangle = 0 \quad \text{for all } s_1, s'_1, s_2 \text{ and } s'_2. \quad (14)$$

It remains to show that (14) is equivalent to 3. Let $b = \mathbf{SOBF}(g)$ and $a = \mathbf{SOBF}(f)$. Equation (11), yields that (14) is equivalent to $(\text{circ}(b) \text{circ}(a)^\dagger)(s_1, s_2 | j_1, j_2) = 0$ for all s_1, j_1, s_2 and j_2 (i.e. matrix $\text{circ}(b) \text{circ}(a)^\dagger$ is the $L_1 L_2 \times L_1 L_2$ zero matrix).

Next let

$$B = W \text{circ}(b) W_\infty^\dagger \quad \text{and} \quad A = W \text{circ}(a) W_\infty^\dagger.$$

Compute BA^\dagger in two ways: On one hand, because W_∞ is unitary

$$BA^\dagger = W \text{circ}(b) W_\infty^\dagger W_\infty \text{circ}(a)^\dagger W^\dagger = W \text{circ}(b) \text{circ}(a)^\dagger W^\dagger. \quad (15)$$

On the other hand, (10) yields that

$$\begin{aligned}
& BA^\dagger(s_1, s_2 | j_1, j_2) \\
&= \sum_{i_1, i_2, j'_1, j'_2} B(s_1, s_2 | i_1, i_2; j'_1, j'_2) A^\dagger(i_1, i_2; j'_1, j'_2 | j_1, j_2) \\
&= \sum_{i_1, i_2, j'_1, j'_2} B(s_1, s_2 | i_1, i_2; j'_1, j'_2) \overline{A(j_1, j_2 | i_1, i_2; j'_1, j'_2)} \\
&= \sum_{i_1, i_2, j'_1, j'_2} \mathcal{B}(b)(i_1, i_2; j'_1, j'_2) \delta_{s_1 j'_1} \delta_{s_2 j'_2} \overline{\mathcal{B}(a)(i_1, i_2; j'_1, j'_2) \delta_{j_1 j'_1} \delta_{j_2 j'_2}} \\
&= \sum_{i_1, i_2} \mathcal{B}(b)(i_1, i_2; j_1, j_2) \overline{\mathcal{B}(a)(i_1, i_2; j_1, j_2) \delta_{s_1 j_1} \delta_{s_2 j_2}} \\
&= \langle \mathcal{B}(b)(\cdot, \cdot; j_1, j_2), \mathcal{B}(a)(\cdot, \cdot; j_1, j_2) \rangle \delta_{s_1 j_1} \delta_{s_2 j_2}. \tag{16}
\end{aligned}$$

Now if $\text{circ}(b)\text{circ}(a)^\dagger$ is the zero matrix, then (15) implies that BA^\dagger is the zero matrix. Hence, by (16), it must be the case that

$$\langle \mathcal{B}(b)(\cdot, \cdot; j_1, j_2), \mathcal{B}(a)(\cdot, \cdot; j_1, j_2) \rangle = 0,$$

for all $(j_1, j_2) \in \{0, \dots, L_1 - 1\} \times \{0, \dots, L_2 - 1\}$.

Conversely, if the above holds, then by (16), BA^\dagger is the zero matrix. Therefore, $W^\dagger BA^\dagger W$ would also be the zero matrix. Equation (15) yields that

$$W^\dagger BA^\dagger W = \text{circ}(b)\text{circ}(a)^\dagger.$$

Hence, $\text{circ}(b)\text{circ}(a)^\dagger$ is the zero matrix, which implies (14). \blacksquare

For any function $g \in L^2(\Omega)$, let Πg denote the projection of g into the set of shift orthogonal functions; that is,

$$\Pi g := \underset{f}{\operatorname{argmin}} \|g - f\|_2 \quad \text{subject to } f \text{ being shift orthogonal.}$$

Indeed using SOBFs basis,

$$\Pi g = \mathbf{ISOBF}(Proj_{\mathcal{SSO}}(\mathbf{SOBF}(g))),$$

where for any $b \in \mathbb{C}^{\mathbb{N}}$,

$$Proj_{\mathcal{SSO}}(b) := \underset{v}{\operatorname{argmin}} \|b - v\|_2 \quad \text{subject to } v \in \mathcal{SSO}.$$

Observe that in the above two definitions the minimum arguments are not necessarily unique, and Πg and $Proj_{\mathcal{SSO}}(b)$ are sets.

Define operator $\Theta : \mathbb{C}^{\mathbb{N}} \rightarrow \mathbb{C}^{\mathbb{N}}$ by

$$\Theta(v)(\cdot, \cdot; j_1, j_2) = \begin{cases} \vec{e} & \text{if } v(\cdot, \cdot; j_1, j_2) = \vec{0} \\ \frac{v(\cdot, \cdot; j_1, j_2)}{\|v(\cdot, \cdot; j_1, j_2)\|_2} & \text{otherwise,} \end{cases}$$

where \vec{e} is a fixed infinite dimensional real vector with unit L^2 norm.

Lemma 2.4 For any $b \in \mathbb{C}^{\mathbb{N}}$,

$$\mathcal{B}^{-1}(\Theta(\mathcal{B}(b))) \in Proj_{SSO}(b).$$

Proof: Suppose $v \in SSO$ and set

$$p = \mathcal{B}(b) \quad \text{and} \quad q = \mathcal{B}(v).$$

Note that,

$$\begin{aligned} \|b - v\|_2^2 &= \frac{1}{L_1 L_2} \|\text{circ}(b) - \text{circ}(v)\|_F^2 = \frac{1}{L_1 L_2} \|W \text{circ}(b) W_\infty^\dagger - W \text{circ}(v) W_\infty^\dagger\|_F^2 \\ &= \frac{1}{L_1 L_2} \|\mathcal{B}(b) - \mathcal{B}(v)\|_2^2 = \frac{1}{L_1 L_2} \|p - q\|_2^2, \end{aligned}$$

where equalities similar to (10) were used for the second last inequality. Now minimizing $\|p - q\|_2$ amounts to solving $L_1 L_2$ subproblems: for every $j_1 = 0, \dots, L_1 - 1$ and $j_2 = 0, \dots, L_2 - 1$, solve

$$\text{argmin}_{i_1, i_2} \sum |p(i_1, i_2; j_1, j_2) - q(i_1, i_2; j_1, j_2)|^2 \quad \text{subject to} \quad \sum_{i_1, i_2} |q(i_1, i_2; j_1, j_2)|^2 = 1. \quad (17)$$

The constraints in the above subproblems are due to $v \in SSO$ and equivalence of 2 and 3 in theorem 2.2. The solutions to the above subproblems are exactly

$$\begin{cases} q(:, :, j_1, j_2) = p(:, :, j_1, j_2) / \|p(:, :, j_1, j_2)\|_2 & \text{if } \|p(:, :, j_1, j_2)\|_2 \neq 0 \\ \text{any infinite dimensional complex vector with unit } L^2 \text{ norm} & \text{if } \|p(:, :, j_1, j_2)\|_2 = 0, \end{cases}$$

that is, projection of $p(:, :, j_1, j_2)$ into an infinite dimensional ball of radius 1. In particular, set $q = \Theta(p)$ (i.e. choose a fixed real valued vector in the second case above), in which case, $v = \mathcal{B}^{-1}(\Theta(p))$ would be an element of $Proj_{SSO}(b)$. \blacksquare

Remark 2.5 Theorem 2.2 in paper [2] and definition of operator Θ , yields that if infinite dimensional vector b is real valued, then $\mathcal{B}^{-1}(\Theta(\mathcal{B}(b)))$ is also real valued. This is why in the case $v(:, :, j_1, j_2) = \vec{0}$, we assign to operator Θ the fixed infinite dimensional vector \vec{e} ; which is real valued and has unit L^2 norm. Indeed, (as it is apparent in the proof of lemma 2.4) had we defined operator Θ to output all infinite dimensional (complex) vector of unit L^2 norm in the case $v(:, :, j_1, j_2) = \vec{0}$, then $\mathcal{B}^{-1}(\Theta(\mathcal{B}(b)))$ would have been a set equal to $Proj_{SSO}(b)$; however, some elements of $\mathcal{B}^{-1}(\Theta(\mathcal{B}(b)))$ would have been complex valued.

3 Fast Algorithm for Projection to the Space of Shift Orthogonal Functions

For computational purposes, only a finite number of SOBFs basis are used to represent a function. In this section, assume that for the first coordinate all SOBFs basis whose depth

Three dimensional version of algorithm 1 is:

Algorithm 2: Projection to $\mathcal{SSO}(N_1N_2N_3)$

Input: \vec{b}

Output: $\vec{v} = Proj_{\mathcal{SSO}(N_1N_2N_3)}(\vec{b})$

```

1 for  $i_1 = 1, \dots, N_1, i_2 = 1, \dots, N_2$  and  $i_3 = 1, \dots, N_3$  do
2    $\lfloor p(i_1, i_2, i_3; \cdot, \cdot, \cdot) = L_1L_2L_3\mathcal{F}_{3D}^{-1}(b(i_1, i_2, i_3; \cdot, \cdot, \cdot))$ ; //  $p = \mathcal{B}(b)$ .
3 for  $j_1 = 0, \dots, L_1 - 1, j_2 = 0, \dots, L_2 - 1$  and  $j_3 = 0, \dots, L_3 - 1$  do
4   if  $\|p(\cdot, \cdot, \cdot; j_1, j_2, j_3)\|_2 \neq 0$  then
5      $\lfloor q(\cdot, \cdot, \cdot; j_1, j_2, j_3) = p(\cdot, \cdot, \cdot; j_1, j_2, j_3) / \|p(\cdot, \cdot, \cdot; j_1, j_2, j_3)\|_2$ ; //  $q = \mathcal{B}(v)$ .
6   else
7      $\lfloor q(\cdot, \cdot, \cdot; j_1, j_2, j_3) = \vec{\mathbf{1}} / \sqrt{N_1N_2N_3}$ .
8 for  $i_1 = 1, \dots, N_1, i_2 = 1, \dots, N_2$  and  $i_3 = 1, \dots, N_3$  do
9    $\lfloor v(i_1, i_2, i_3; \cdot, \cdot, \cdot) = \frac{1}{L_1L_2L_3}\mathcal{F}_{3D}(q(i_1, i_2, i_3; \cdot, \cdot, \cdot))$ ; //  $v = \mathcal{B}^{-1}(q)$ .
```

Finally, the one dimensional version of algorithm 1 for domain $\Omega = [0, L]$ (i.e. again using appropriate scaling, it is assumed that the length of the shift is 1) and

$$g(x) \approx \sum_{i=1}^N \sum_{j=0}^{L-1} b_j^i \xi_j^i(x),$$

is the following:

Algorithm 3: Projection to $\mathcal{SSO}(N)$

Input: \vec{b}

Output: $\vec{v} = Proj_{\mathcal{SSO}(N)}(\vec{b})$

```

1 for  $i = 1, \dots, N$  do
2    $\lfloor p(i; \cdot) = L\mathcal{F}_{1D}^{-1}(b(i; \cdot))$ ; //  $p = \mathcal{B}(b)$ .
3 for  $j = 0, \dots, L - 1$  do
4   if  $\|p(\cdot; j)\|_2 \neq 0$  then
5      $\lfloor q(\cdot; j) = p(\cdot; j) / \|p(\cdot; j)\|_2$ ; //  $q = \mathcal{B}(v)$ .
6   else
7      $\lfloor q(\cdot; j) = \vec{\mathbf{1}} / \sqrt{N}$ .
8 for  $i = 1, \dots, N$  do
9    $\lfloor v(i; \cdot) = \frac{1}{L}\mathcal{F}_{1D}(q(i; \cdot))$ ; //  $v = \mathcal{B}^{-1}(q)$ .
```

3.1 Computational Complexity and Important Features of the Algorithm

This sections describes the computational complexity of algorithm 1 and highlights some of the important properties of this algorithm. The results stay the same for domains with dimensions other than $d = 2$.

Let $M = L_1 L_2 N_1 N_2$ be the size of input vector \vec{b} ; which indicates the number of coefficients used to represent the given function. Algorithm 1 consists of three “for” loops. Each iteration in the first and the last “for” loop can be computed using $O(L_1 L_2 \log(L_1 L_2))$ operations via inverse Fast Fourier Transform and Fast Fourier Transform, respectively. Each iteration in the second “loop” can be done using $O(N_1 N_2)$. Therefore, algorithm 1 can be performed using

$$N_1 N_2 O(L_1 L_2 \log(L_1 L_2)) + L_1 L_2 O(N_1 N_2) + N_1 N_2 O(L_1 L_2 \log(L_1 L_2))$$

operations, which leads to computational complexity of

$$O(M \log(L_1 L_2)) < O(M \log(M)).$$

Furthermore, note that each of the “for” loops in algorithms 1 can be done in parallel. This enhances the speed of the algorithm even further and makes it suitable for inputs with large dimensions.

Another nice property of algorithm 1 is that for real valued input vector \vec{v} , it outputs a real valued vector $Proj_{SSO(N_1 N_2)}(\vec{b})$ (i.e. recall remark 2.5). The importance of this property is that if function g and SOBFs $\{\xi_{j_1}^{i_1}(x_1)\xi_{j_2}^{i_2}(x_2)\}$ are real valued then **SOBF**(g) would be a real valued vector, and therefore using algorithm 1, the projected Πg would also be real valued.

4 An interesting example of SOBFs: Shift Orthogonal Plane Waves (SOPWs)

This section provides an example of real valued SOBFs with certain nice properties called Shift Orthogonal Plane Waves (SOPWs). As it will be seen shortly, SOPWs are suitable for numerical computation because there exist an exact prescription of them in terms of Fourier basis. Therefore, functions can be expanded in terms of SOPWs very efficiently using FFT and its inverse.

Consider 1D domain $\Omega = [0, L]$ with periodic boundary and by scaling (i.e. replacing L by L/w) assume that $w = 1$. Furthermore, suppose that L is even. This assumption is made so that the formulas provided in this section are easier to express. Nevertheless, the assumption that L is even is not very restrictive as the parity of L is not significant in many applications.

Recall that functions

$$\phi_n(x) = \frac{1}{\sqrt{L}} e^{i2\pi n x/L} \quad \text{for } n \in \mathbb{Z}, \quad (19)$$

as well as

$$\left\{ \frac{1}{\sqrt{L}}, \frac{2}{\sqrt{2L}} \cos(2\pi n x/L), \frac{2}{\sqrt{2L}} \sin(2\pi n x/L) \right\}_{n=1}^{\infty} \quad (20)$$

form orthonormal basis for $L^2(\Omega)$. Denote the L -th roots of unity by

$$\omega_j = e^{i2\pi j/L} \quad \text{for } j = 0, \dots, L-1.$$

Shift Orthogonal Plane Waves (SOPWs) are denoted by

$$\{\theta_j^i(x)\}_{i=1, j=0}^{i=\infty, j=L-1},$$

and defined in the following way: set

$$\theta_j^1(x) = \frac{1}{\sqrt{L}} \sum_{|n| < \frac{L}{2}} \omega_j^{-n} \phi_n(x) + \frac{1}{\sqrt{2L}} \sum_{|n| = \frac{L}{2}} \omega_j^{-n} \phi_n(x) \quad (21)$$

$$\theta_j^k(x) = \frac{1}{\sqrt{L}} \sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} (\text{sgn}(n)i)^{k-1} \omega_j^{-n} \phi_n(x) + \frac{1}{\sqrt{2L}} \sum_{|n| = \frac{(k-1)L}{2}, \frac{kL}{2}} (\text{sgn}(n)i)^{k-1} \omega_j^{-n} \phi_n(x) \quad (22)$$

Figure 1 plots SOPWs given by equations (21) and (22) with depth index ranging from 1 to 6 and shift index equal to $L/2$.

Using the expression

$$\frac{1}{L} \sum_{n=k}^{k+L-1} \omega_j^n = \delta_{j0}, \quad (23)$$

and after some calculations one can verify that for $n \geq 1$,

$$\phi_0(x) = \frac{1}{\sqrt{L}} \sum_{j=0}^{L-1} \theta_j^1(x), \quad (24)$$

$$\phi_n(x) = \frac{(-\text{sgn}(n)i)^{k-1}}{\sqrt{L}} \sum_{j=0}^{L-1} \omega_j^n \theta_j^k(x) \quad \text{for } \frac{(k-1)L}{2} < |n| < \frac{kL}{2}, \quad (25)$$

$$\phi_n(x) = \frac{(-\text{sgn}(n)i)^{k-1}}{\sqrt{2L}} \left(\sum_{j=0}^{L-1} \omega_j^n \theta_j^k(x) - \text{sgn}(n)i \sum_{j=0}^{L-1} \omega_j^n \theta_j^{k+1}(x) \right) \quad \text{for } |n| = \frac{kL}{2}. \quad (26)$$

First note that $\theta_j^i(x) = \theta_0^i(x-j)$. Moreover, it is straightforward using identity (23) to verify that $\{\theta_j^i\}_{i=1, j=0}^{i=\infty, j=L-1}$ form an orthonormal set. Finally, $\{\theta_j^i\}_{i=1, j=0}^{i=\infty, j=L-1}$ is complete in $L^2(\Omega)$ because of relations (24), (25), (26) and completeness of $\{\phi_n\}_{n=-\infty}^{n=\infty}$. Hence, the set of SOPWs defined by (21) and (22) is an example of SOBFs.

Equations (21) and (22) can be re-written to represent SOPWs $\{\theta_j^i\}_{i=1, j=0}^{i=\infty, j=L-1}$ in terms of (20):

$$\theta_j^1(x) = \frac{1}{L} + \sum_{n=1}^{L/2-1} \frac{2}{L} \cos\left(\frac{2\pi n(x-j)}{L}\right) + \frac{\sqrt{2}}{L} \cos\left(\frac{2\pi(L/2)(x-j)}{L}\right),$$

$$\theta_j^k(x) = \frac{2}{L} \sum_{\frac{(k-1)L}{2} < n < \frac{kL}{2}} (-1)^{\frac{k}{2}} \sin\left(\frac{2\pi n(x-j)}{L}\right) + \frac{\sqrt{2}}{L} \sum_{n = \frac{(k-1)L}{2}, \frac{kL}{2}} (-1)^{\frac{k}{2}} \sin\left(\frac{2\pi n(x-j)}{L}\right) \quad \text{for } k \text{ even,}$$

$$\theta_j^k(x) = \frac{2}{L} \sum_{\frac{(k-1)L}{2} < n < \frac{kL}{2}} (-1)^{\frac{k-1}{2}} \cos\left(\frac{2\pi n(x-j)}{L}\right) + \frac{\sqrt{2}}{L} \sum_{n = \frac{(k-1)L}{2}, \frac{kL}{2}} (-1)^{\frac{k-1}{2}} \cos\left(\frac{2\pi n(x-j)}{L}\right) \quad \text{for } k \text{ odd,}$$

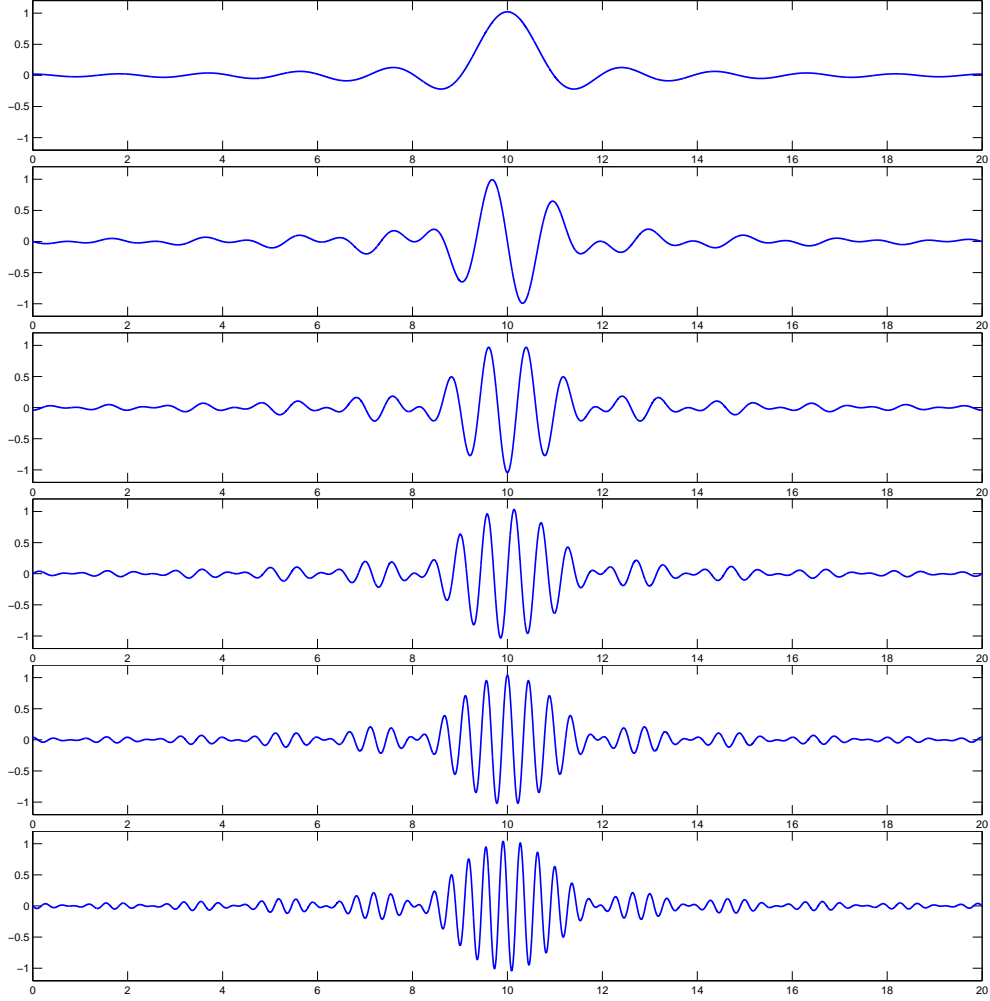


Figure 1: From top to bottom, the first 6 SOPWs given by equations (21) and (22) with distinct depth index and shift index equal to $L/2$.

and in closed form:

$$\theta_j^1(x) = \frac{1}{L} \frac{\sin(2\pi(\frac{L-1}{2})(x-j)/L)}{\sin(\pi(x-j)/L)} + \frac{\sqrt{2}}{L} \cos\left(\frac{2\pi(L/2)(x-j)}{L}\right),$$

$$\theta_j^k(x) = \frac{2}{L} (-1)^{\frac{k}{2}} \sin\left(\frac{2\pi(\frac{kL}{2} - \frac{L}{4})(x-j)}{L}\right) \left[\frac{\sin(\pi(\frac{L}{2} - 1)(x-j)/L)}{\sin(\pi(x-j)/L)} + \sqrt{2} \cos\left(\frac{\pi(x-j)}{2}\right) \right] \quad \text{for } k \text{ even,}$$

$$\theta_j^k(x) = \frac{2}{L} (-1)^{\frac{k-1}{2}} \cos\left(\frac{2\pi(\frac{kL}{2} - \frac{L}{4})(x-j)}{L}\right) \left[\frac{\sin(\pi(\frac{L}{2} - 1)(x-j)/L)}{\sin(\pi(x-j)/L)} + \sqrt{2} \cos\left(\frac{\pi(x-j)}{2}\right) \right] \quad \text{for } k \text{ odd.}$$

Equations (21), (22) and equations (24), (25), (26) suggest that FFT can be used to switch between Fourier basis and SOPWs efficiently and easily. This is very important for computational purposes as it provides an efficient method to represent functions in terms of SOPWs.

Another important property of the SOPWs is that θ_j^i are the solutions to a specific

variational problem. This is shown in appendix A. The final important property of θ_j^i is that for any i and j

$$\partial_{xx}\theta_j^i \in \text{span}\{\theta_k^i\}_{k=0}^{L-1}.$$

This can be seen by direct computation (see appendix C) or using Euler-Lagrange equations for the variational problem (i.e. see appendix B).

A disadvantage that SOPWs have, in comparison to Fourier basis (19) is that SOPWs are not eigenfunctions of the derivative operator. Nevertheless, it is shown in appendix C that for any i and j ,

$$\partial_x\theta_j^i \in \text{span}\{\theta_k^{i-1}, \theta_k^i, \theta_k^{i+1}\}_{k=0}^{L-1}.$$

5 Application to solving CPWs

This section outlines how the projection algorithm described in section 3 is used to compute Compressed Plain Waves (CPWs) (i.e. see [4]). The shift orthogonality constraints in the construction of CPWs makes their computation challenging and numerically inefficient. However, applying the projection algorithm circumvents these difficulties.

Basic compressed plane waves $\{\psi^n\}_{n=1}^\infty$ are defined by:

$$\begin{aligned} \psi^1(\mathbf{x}) = \operatorname{argmin}_\psi & \frac{1}{\mu} \int_\Omega |\psi(\mathbf{x})| \, d\mathbf{x} + \int_\Omega \psi(\mathbf{x}) \hat{H}_0 \psi \, d\mathbf{x} \\ \text{s.t.} & \int_\Omega \psi(\mathbf{x}) \psi(\mathbf{x} - \mathbf{j}\mathbf{w}) \, d\mathbf{x} = \delta_{\mathbf{j}0}, \quad \mathbf{j} \in \mathbb{Z}^d, \end{aligned} \quad (27)$$

where $\hat{H}_0 = -\frac{1}{2}\Delta$. The higher modes can be recursively defined as:

$$\begin{aligned} \psi^{n+1}(\mathbf{x}) = \operatorname{argmin}_\psi & \frac{1}{\mu} \int_\Omega |\psi(\mathbf{x})| \, d\mathbf{x} + \int_\Omega \psi \hat{H}_0 \psi(\mathbf{x}) \, d\mathbf{x} \\ \text{s.t.} & \begin{cases} \int_\Omega \psi(\mathbf{x}) \psi(\mathbf{x} - \mathbf{j}\mathbf{w}) \, d\mathbf{x} = \delta_{\mathbf{j}0}, & \mathbf{j} \in \mathbb{Z}^d \\ \int_\Omega \psi(\mathbf{x}) \psi^i(\mathbf{x} - \mathbf{j}\mathbf{w}) \, d\mathbf{x} = 0, & i = 1, \dots, n. \end{cases} \end{aligned} \quad (28)$$

To simplify our discussion, we only consider $\Omega = [0, L_1] \times [0, L_2]$, in 2D with periodic boundary conditions; the algorithms below can be straightforwardly extended to other dimensions. We use SOPWs given by equations (21) and (22) as the SOBFs used in section 3. In particular, we expand the given function g in terms of SOPWs:

$$g(x_1, x_2) = \sum_{i_1, i_2=1}^{N_1, N_2} \sum_{j_1=0, j_2=0}^{L_1-1, L_2-1} b_{j_1, j_2}^{i_1, i_2} \theta_{j_1}^{i_1}(x_1) \theta_{j_2}^{i_2}(x_2).$$

Operators **SOPW** and **ISOPW** are defined in the similar way to definitions (6) and (7):

$$\mathbf{SOPW}(g)(i_1, i_2; j_1, j_2) := b_{j_1, j_2}^{i_1, i_2},$$

and

$$\mathbf{ISOPW}(b) := \sum_{i_1, i_2=1}^{N_1, N_2} \sum_{j_1=0, j_2=0}^{L_1-1, L_2-1} b_{j_1, j_2}^{i_1, i_2} \theta_{j_1}^{i_1}(x_1) \theta_{j_2}^{i_2}(x_2).$$

Other examples of SOBFs could also be used. For this application, SOPWs were chosen mainly due to the efficiency in calculating the result of operators **SOPW** and **ISOPW** from Fourier coefficient (i.e. recall from section 4 that FFT and its inverse provide an efficient procedure to switch between representation of a function in Fourier basis ϕ_n 's and its representation in SOPWs θ_j^i 's).

By introducing an auxiliary variable $u = \psi, v = \psi$, the constrained optimization problem is equivalent to the following problem:

$$\begin{aligned} \psi^1 &= \operatorname{argmin}_{\psi, u} \frac{1}{\mu} \int |u(\mathbf{x})| \, d\mathbf{x} + \int \psi \hat{H}_0 \psi \, d\mathbf{x} \\ \text{s.t. } u &= \psi, v = \psi \quad \& \quad \int v(\mathbf{x})v(\mathbf{x} - \mathbf{j}\mathbf{w}) \, d\mathbf{x} = \delta_{\mathbf{j}0}, \quad \mathbf{j} \in \mathbb{Z}^2, \end{aligned} \quad (29)$$

which can be solved by an algorithm based on the Bregman iteration (i.e. see [13, 14, 15]).

Algorithm 4: Solving the first CPW using the projection algorithm

- 1 Initialize $u^0 = v^0 = \psi^{1,0}, D^0 = B^0 = 0$.
 - 2 **while** “not converged” **do**
 - 3 $\psi^{1,k} =$
 $\operatorname{argmin}_{\psi} \int \psi \hat{H}_0 \psi \, d\mathbf{x} + \frac{\lambda}{2} \int (\psi - u^{k-1} + D^{k-1})^2 \, d\mathbf{x} + \frac{r}{2} \int (\psi - v^{k-1} + B^{k-1})^2 \, d\mathbf{x};$
 - 4 $v^k = \operatorname{argmin}_v \frac{r}{2} \int (\psi^{1,k} - v + B^{k-1})^2 \, d\mathbf{x}, \text{ s.t. } \int v(\mathbf{x})v(\mathbf{x} - \mathbf{j}\mathbf{w}) \, d\mathbf{x} = \delta_{\mathbf{j}0}, \quad \mathbf{j} \in \mathbb{Z}^2;$
 - 5 $u^k = \operatorname{argmin}_u \frac{1}{\mu} \int |u| \, d\mathbf{x} + \frac{\lambda}{2} \int (\psi^{1,k} - u + D^{k-1})^2 \, d\mathbf{x};$
 - 6 $D^k = D^{k-1} + \psi^{1,k} - u^k;$
 - 7 $B^k = B^{k-1} + \psi^{1,k} - v^k.$
-

All the above sub-optimization problems can be efficiently solved as follows:

$$(\hat{H}_0 + \lambda + r)\psi^{1,k} = \lambda(u^{k-1} - D^{k-1}) + r(v^{k-1} - B^{k-1}) \quad (30)$$

$$v^k = \mathbf{ISOPW}(\operatorname{Proj}_{\mathcal{SSO}(N_1, N_2)}(\mathbf{SOPW}(\psi^{1,k} + B^{k-1}))) \quad (31)$$

$$u^k = \operatorname{sgn}(\psi^{1,k} + D^{k-1}) \max(0, |\psi^{1,k} + D^{k-1}| - \frac{1}{\lambda\mu}) \quad (32)$$

Similarly, ψ^{n+1} is obtained by solving the optimization problem (28) efficiently. Suppose that the first n levels $\Psi^n = \{\psi^1, \dots, \psi^n\}$ are already constructed and let $a^m =$

SOPW(ψ^m), $m = 1, \dots, n$. In this case, the goal is to find v^k satisfying

$$v^k = \operatorname{argmin}_v \int (\psi^{n+1,k} - v + B^{k-1})^2 d\mathbf{x}, \text{ s.t. } \begin{cases} \int v(\mathbf{x})v(\mathbf{x} - \mathbf{j}\mathbf{w}) d\mathbf{x} = \delta_{\mathbf{j}0}, & \mathbf{j} \in \mathbb{Z}^2 \\ \int v(\mathbf{x})\psi^m(\mathbf{x} - \mathbf{j}\mathbf{w}) d\mathbf{x} = 0, & m = 1, \dots, n. \end{cases} \quad (33)$$

Define

$$\mathcal{S}(\Psi^n) = \operatorname{span}\{S(s_1, s_2)a^m\}_{s_1=0, s_2=0, m=1}^{s_1=L_1-1, s_2=L_2-1, m=n}.$$

Using the SOPWs basis, the above problem is equivalent to solving the following problem in SOPWs frequency space:

$$\operatorname{Proj}_{\mathcal{SSO}(N_1N_2) \cap \mathcal{S}(\Psi^n)^\perp}(b) := \operatorname{argmin} \|b - v\|_2 \quad \text{s.t.} \quad v \in \mathcal{SSO}(N_1N_2) \cap \mathcal{S}(\Psi^n)^\perp. \quad (34)$$

Vector b is given and the objective is to find vector v closest to b that is shift orthogonal and perpendicular to a^1 to a^n .

Theorems 2.2 and 2.3 yield that in order to solve problem (34), for each j_1 and j_2 one needs to find vector z_{j_1, j_2} that is closest to $\mathcal{B}(b)(:, :, j_1, j_2)$, perpendicular to $\mathcal{B}(a^m)(:, :, j_1, j_2)$ for $m = 1, \dots, n$, and lives on the unit sphere. Moreover note that, again by theorems 2.2 and 2.3, $\{\mathcal{B}(a^m)(:, :, j_1, j_2)\}_{m=1}^{m=n}$ form an orthonormal set of vectors for each j_1 and j_2 , because elements of Ψ^n are constructed such that they are shift orthogonal and orthogonal to shift span of each other. Hence, z_{j_1, j_2} can be computed in two steps:

- $z_{j_1, j_2} = \mathcal{B}(b)(:, :, j_1, j_2) - \sum_{m=1}^n \langle \mathcal{B}(a^m)(:, :, j_1, j_2), \mathcal{B}(b)(:, :, j_1, j_2) \rangle \mathcal{B}(a^m)(:, :, j_1, j_2)$,
- $z_{j_1, j_2} = z_{j_1, j_2} / \|z_{j_1, j_2}\|_2 \quad (\text{if } \|z_{j_1, j_2}\|_2 \neq 0)$.

In summary:

Algorithm 5: Projection to $\mathcal{SSO}(N_1N_2) \cap \mathcal{S}(\Psi^n)^\perp$

Input: b, a^1, \dots, a^n

Output: $v = \operatorname{Proj}_{\mathcal{SSO}(N_1N_2) \cap \mathcal{S}(\Psi^n)^\perp}(b)$

- 1 **for** $i_1 = 1, \dots, N_1$ **and** $i_2 = 1, \dots, N_2$ **do**
 - 2 $\lfloor \mathcal{B}(b)(i_1, i_2; : , :) = L_1 L_2 \mathcal{F}_{2D}^{-1}(b(i_1, i_2; : , :))$
 - 3 **for** $j_1 = 0, \dots, L_1 - 1$ **and** $j_2 = 0, \dots, L_2 - 1$ **do**
 - 4 $z_{j_1, j_2} = \mathcal{B}(b)(:, :, j_1, j_2) - \sum_{m=1}^n \langle \mathcal{B}(a^m)(:, :, j_1, j_2), \mathcal{B}(b)(:, :, j_1, j_2) \rangle \mathcal{B}(a^m)(:, :, j_1, j_2)$
 - 5 **if** $\|z_{j_1, j_2}\|_2 \neq 0$ **then**
 - 6 $\lfloor \mathcal{B}(v)(:, :, j_1, j_2) = z_{j_1, j_2} / \|z_{j_1, j_2}\|_2$
 - 7 **else**
 - 8 $\lfloor \mathcal{B}(v)(:, :, j_1, j_2) = \text{a unit real vector orthogonal to } \{\mathcal{B}(a)(:, :, j_1, j_2)\}_{m=1}^{m=n}$.
 - 9 **for** $i_1 = 1, \dots, N_1$ **and** $i_2 = 1, \dots, N_2$ **do**
 - 10 $\lfloor v(i_1, i_2; : , :) = \frac{1}{L_1 L_2} \mathcal{F}_{2D}(\mathcal{B}(v)(i_1, i_2; : , :))$
-

Therefore, the following algorithm is used to solve for ψ^{n+1} :

Algorithm 6: Solving the $n+1$ -th BCPW using the projection algorithm

- 1 Initialize $u^0 = v^0 = \psi^{n+1,0}, D^0 = B^0 = 0$.
 - 2 **while** “not converged” **do**
 - 3 $\psi^{n+1,k}$ solves $(\hat{H}_0 + \lambda + r)\psi^{n+1,k} = \lambda(u^{k-1} - D^{k-1}) + r(v^{k-1} - B^{k-1})$;
 - 4 $v^k = \mathbf{ISOPW}(Proj_{\mathcal{SSO}(N_1 N_2) \cap \mathcal{S}(\Psi^n)^\perp}(\mathbf{SOPW}(\psi^{n+1,k} + B^{k-1})))$;
 - 5 $u^k = \text{sgn}(\psi^{1,k} + D^{k-1}) \max(0, |\psi^{n+1,k} + D^{k-1}| - \frac{1}{\lambda\mu})$;
 - 6 $D^k = D^{k-1} + \psi^{n+1,k} - u^k$;
 - 7 $B^k = B^{k-1} + \psi^{n+1,k} - v^k$.
-

Figure 2 plots the first four BCPWs in 1D using the proposed algorithms. These results are very consistent with the results in [4]. Table 1, highlights the computational speed gained by using the new procedure outlined in this section.

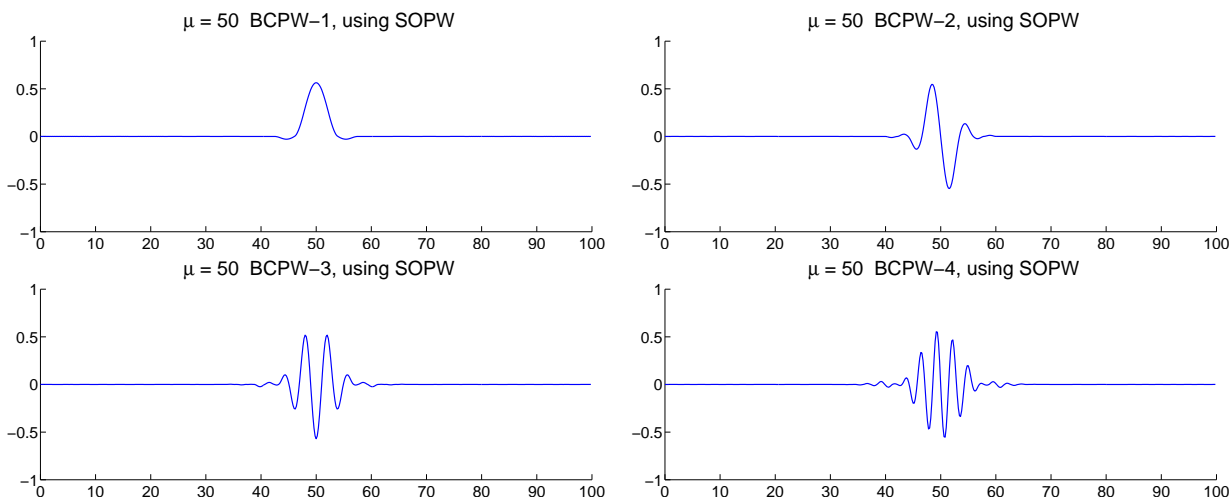


Figure 2: The first 4 one-dimensional BCPWs obtained by using the new procedure.

6 Conclusion

This paper presents a fast algorithm for finding a closest shift orthogonal function to a given function. The algorithm can be easily implemented using FFT and has computational complexity bounded by $M \log(M)$, where M is the number of coefficients used to store the input function.

The algorithm described here is very useful for problems with shift orthogonality constraints. As an example, the application of the algorithm in computing Compressed Plain Waves (CPWs) is shown.

# of points	Algorithm proposed in [4]					The new procedure				
	ψ^1	ψ^2	ψ^3	ψ^4	total	ψ^1	ψ^2	ψ^3	ψ^4	total
500	23.05	29.39	21.40	9.42	83.26	0.30	1.47	0.44	0.28	2.49
1000	53.11	116.30	81.28	29.99	280.68	0.71	3.48	1.23	0.66	6.08

Table 1: CPU time consumption (seconds) for computing the first 4 one-dimensional BCPWs using SOPWs and FFT with the same accuracy.

A Variational Origin of SOPWs

Here, it is shown that in $1D$, if there is no L^1 term in the definition of CPWs (i.e. $\mu = \infty$) then they are essentially the same as SOPWs given by (21) and (22). Let $\Omega = [0, L]$ (where L is even) and by scaling assume that $w = 1$. For any function ψ define

$$\mathcal{J}_\infty(\psi) := \int_\Omega \psi \hat{H}_0 \psi \, dx. \quad (35)$$

As before, $\hat{H}_0 = -\frac{1}{2}\partial_{xx}$. It is clear that \hat{H}_0 has eigenfunctions $\phi_n(x) = \frac{1}{\sqrt{L}}e^{i2\pi nx/L}$ with corresponding eigenvalue $\lambda_n = 2(\pi n/L)^2$, $n = 0, \pm 1, \pm 2, \dots$. Note that BCPWs $\{\theta^i\}_{i=1}^{i=\infty}$ when there is no L^1 term (i.e. $\mu = \infty$) are defined in the following way:

$$\begin{aligned} \psi^1 &= \underset{\psi}{\operatorname{argmin}} \mathcal{J}_\infty(\psi) \quad \text{s.t.} \quad \int \psi(x)\psi(x-j)dx = \delta_{j0}, \\ \psi^k &= \underset{\psi}{\operatorname{argmin}} \mathcal{J}_\infty(\psi) \quad \text{s.t.} \quad \begin{cases} \int \psi(x)\psi(x-j)dx = \delta_{j0}, \\ \int \psi(x)\psi^i(x-j)dx = 0 \quad \text{for } i = 1, \dots, k-1. \end{cases} \end{aligned} \quad (36)$$

The main result of this section is the following theorem, which implies $\{\psi^i\}_{i=1}^{i=\infty}$ are indeed SOPWs $\{\theta^i\}_{i=1}^{i=\infty}$:

Theorem A.1 *One set of solutions to problem (36) are*

$$\theta^1(x) = \frac{1}{\sqrt{L}} \sum_{|n| < \frac{L}{2}} \phi_n(x) + \frac{1}{\sqrt{2L}} \sum_{|n| = \frac{L}{2}} \phi_n(x),$$

and, for $k > 1$

$$\theta^k(x) = \frac{1}{\sqrt{L}} \sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} (\operatorname{sgn}(n)i)^{k-1} \phi_n(x) + \frac{1}{\sqrt{2L}} \sum_{|n| = \frac{(k-1)L}{2}, \frac{kL}{2}} (\operatorname{sgn}(n)i)^{k-1} \phi_n(x)$$

Proof: Since ϕ_n 's form complete set, for any function $\theta(x) \in L^2$ we can write

$$\theta(x) = \sum_{n=-\infty}^{\infty} a(n)\phi_n(x). \quad (37)$$

Consequently,

$$\mathcal{J}_\infty(\theta) = \sum_{n=-\infty}^{\infty} |a(n)|^2 \lambda_n = \sum_{n=1}^{\infty} (|a(n)|^2 + |a(-n)|^2) \lambda_n, \quad (38)$$

and shift orthogonality constraints yield that

$$\begin{aligned} \delta_{j0} &= \int \theta^*(x) \theta(x-j) dx = \sum_{n=-\infty}^{\infty} |a(n)|^2 e^{-i2\pi jn/L} \\ &= |a(0)|^2 + \sum_{n=1}^{\infty} (|a(n)|^2 + |a(-n)|^2) \cos(2\pi jn/L) - i \sum_{n=1}^{\infty} (|a(n)|^2 - |a(-n)|^2) \sin(2\pi jn/L). \end{aligned} \quad (39)$$

Therefore, for $\theta(x)$ to be feasible (i.e satisfy shift orthogonality constraints), it must be the case that $|a(n)| = |a(-n)|$ for all $n \geq 1$. Note that changing the phase value of $a(n)$ and $a(-n)$ does not change the value of the objective function (38). Thus, the phase factor of $a(n)$ and $a(-n)$ can be chosen in such a way that

$$a(-n) = a^*(n), \quad \text{for } n = 1, 2, \dots \quad (40)$$

The above conditions guarantee that $\theta(x)$ is real valued. Hence, there always exist a real valued minimizers for variational problem (36). In view of (40), equations (38) and (39) can be re-written: objective function becomes

$$\mathcal{J}_\infty(\theta) = 2 \sum_{n=1}^{\infty} |a(n)|^2 \lambda_n, \quad (41)$$

and shift orthogonality constraints yield that for $j = 0, 1, \dots, L-1$,

$$\delta_{j0} = |a(0)|^2 + 2 \sum_{n=1}^{\infty} |a(n)|^2 \cos(2\pi jn/L). \quad (42)$$

Lets first find θ^1 . To that end, the goal is to find $\{a(n)\}_{n=0}^{\infty}$ that minimizes (41) and satisfies (42) for $j = 0, \dots, L-1$. Set

$$\begin{cases} c(0) = |a(0)|^2 \\ c(n) = 2|a(n)|^2 \end{cases} \quad \text{for } n = 1, 2, \dots \quad (43)$$

Let M be the $L \times L$ matrix whose (j, n) -th entry is $\cos(2\pi jn/L)$ for $j, n = 0, \dots, L-1$. Form infinite dimensional matrix A by concatenating infinitely many copies of M side by side, that is

$$A = [M|M|\dots].$$

Therefore, to find θ^1 , one needs to solve the following optimization problem:

$$\underset{c}{\operatorname{argmin}} \lambda^T c \quad \text{s.t.} \quad Ac = b, c \geq 0, \quad (44)$$

where

$$\lambda^T = [\lambda_0, \lambda_1, \dots], \quad c^T = [c(0), c(1), \dots], \quad \text{and} \quad b^T = [1, \underbrace{0, \dots, 0}_{L-1}].$$

Observe that matrix M is not invertible. However, it can be partitioned in the following way: Let $\vec{1} = M(:, 1)$, $M_L = M(:, 2 : L/2 - 1)$, $\vec{e} = M(:, L/2)$ and $M_R = M(:, L/2 + 1 : L - 1)$. Then

$$A = [\vec{1}|M_L|\vec{e}|M_R|\vec{1}|M_L|\vec{e}|M_R|\dots].$$

The strategy is to guess the solution to problem (44) and then verify (i.e. using the dual formulation of (44)) that it is indeed the optimal solution. For this purpose we first prove the following three lemmas:

Lemma A.2 *The $L \times (L/2 - 1)$ matrices $[\vec{1}|M_L|\vec{e}]$ and $[\vec{e}|M_R|\vec{1}]$ have full rank.*

Proof: First observe that matrix $[\vec{e}|M_R|\vec{1}]$ is formed from matrix $[\vec{1}|M_L|\vec{e}]$ if the columns are arranged in the opposite order. Thus it suffices to only show $[\vec{1}|M_L|\vec{e}]$ has full rank. For contrary assume the opposite that $[\vec{1}|M_L|\vec{e}]$ is not full rank, then there exist nontrivial set of constants $\{k_n\}_{n=0}^{n=L/2}$ such that

$$\sum_{n=0}^{L/2} k_n \cos(2\pi jn/L) = 0 \quad \text{for } j = 0, \dots, L - 1.$$

The above system of equations implies that

$$\sum_{n=0}^{L-1} k'_n e^{-i2\pi jn/L} = 0 \quad \text{for } j = 0, \dots, L - 1, \quad (45)$$

where

$$k'_n = \begin{cases} k_n & \text{for } n = 0 \text{ and } L/2, \\ k_n/2 & \text{for } 0 < n < L/2, \\ k_{L-n}/2 & \text{for } L/2 < n \leq L - 1. \end{cases}$$

However, system of equations (45) implies that the columns of the $L \times L$ Discrete Fourier Transform matrix are linearly dependent; which contradicts invertibility of the DFT matrix. ■

Lemma A.3 *For $k \geq 1$ and $j = 0, \dots, L - 1$:*

$$\frac{1}{L} \cos(\pi j(k - 1)) + \frac{2}{L} \sum_{\frac{(k-1)L}{2} < n < \frac{kL}{2}} \cos(2\pi jn/L) + \frac{1}{L} \cos(\pi jk) = \delta_{j0}.$$

Proof: If $j = 0$ the result is clear. For $j = 1, \dots, L - 1$:

$$\begin{aligned}
& \frac{1}{L} \cos(\pi j(k-1)) + \frac{2}{L} \sum_{\frac{(k-1)L}{2} < n < \frac{kL}{2}} \cos(2\pi jn/L) + \frac{1}{L} \cos(\pi jk) = \\
&= \frac{1}{L} \cos(\pi j(k-1)) + \frac{2}{L} \sum_{\frac{(k-1)L}{2} < n < \frac{kL}{2}} \frac{1}{2} [\cos(2\pi jn/L) + \cos(2\pi j(kL-n)/L)] + \frac{1}{L} \cos(\pi jk) = \\
&= \frac{1}{L} \sum_{\frac{(k-1)L}{2} \leq n < \frac{(k+1)L}{2}} \cos(2\pi jn/L) = \frac{1}{L} \operatorname{Re} \left\{ \sum_{n=(k-1)L/2}^{(k+1)L/2-1} e^{i2\pi jn/L} \right\} = \\
&= \frac{1}{L} \operatorname{Re} \left\{ e^{i\pi j(k-1)} \left(\frac{1 - e^{i2\pi jL/L}}{1 - e^{i2\pi j/L}} \right) \right\} = 0.
\end{aligned}$$

The result follows. ■

Lemma A.4 Assume that there exist vector $y \in \mathbb{R}^L$ and infinite dimensional vector s such that

$$A^T y + s = \lambda, \quad s \geq 0.$$

If c is feasible for problem (44), then

$$\lambda^T c \geq y^T b.$$

Furthermore, if additionally s and c satisfy complementary slackness property $s^T c = 0$, then c is the solution to problem (44).

Proof: Observe that for any feasible c in problem (44),

$$\lambda^T c = (A^T y + s)^T c = y^T A c + s^T c = y^T b + s^T c \geq y^T b,$$

where the last inequality is from nonnegativity of s and c . Hence, the minimum value of the objective function in problem (44) is $y^T b$. Moreover, the minimum is achieved if c is feasible and satisfies $s^T c = 0$. ■

Now returning to optimization problem (44), set

$$c^T = \left[\frac{1}{L}, \underbrace{\frac{2}{L}, \dots, \frac{2}{L}}_{L/2-1}, \frac{1}{L}, 0, 0, \dots \right],$$

and find y that satisfies

$$[\vec{1}|M_L|\vec{e}]^T y = [\lambda_0, \dots, \lambda_{L/2}]^T.$$

Such y exist because by lemma A.2 matrix $[\vec{1}|M_L|\vec{e}]$ is full rank. Finally, set

$$s = \lambda - A^T y.$$

Lemma A.3 implies that c is feasible for problem (44). Moreover, it is straightforward to verify that

$$s^T = \underbrace{[0, \dots, 0]}_{L/2+1}, \lambda_{\frac{L}{2}+1} - \lambda_{\frac{L}{2}-1}, \lambda_{\frac{L}{2}+2} - \lambda_{\frac{L}{2}-2}, \dots, \lambda_L - \lambda_0, \lambda_{L+1} - \lambda_1, \dots \\ \dots, \lambda_{\frac{3L}{2}+1} - \lambda_{\frac{L}{2}-1}, \lambda_{\frac{3L}{2}+2} - \lambda_{\frac{L}{2}-2}, \dots, \lambda_{2L} - \lambda_0, \lambda_{2L+1} - \lambda_1, \dots] \geq 0.$$

Thus, by lemma A.4, c is the solution of problem (44). Hence, in view of (43),

$$\begin{cases} |a(n)| = 1/\sqrt{L} & \text{for } n = \pm 1, \dots, \pm(\frac{L}{2} - 1), \\ |a(\pm \frac{L}{2})| = 1/\sqrt{2L} \\ |a(n)| = 0 & \text{otherwise.} \end{cases}$$

Note that any phase values for $a(n)$ as long as (40) holds is acceptable. If all the phase factors are set to equal to 1, then

$$\theta^1(x) = \frac{1}{\sqrt{L}} \sum_{|n| < \frac{L}{2}} \phi_n(x) + \frac{1}{\sqrt{2L}} \sum_{|n| = \frac{L}{2}} \phi_n(x).$$

Next, lets find θ^2 . For $j = 0, \dots, L - 1$, define

$$\theta_j^1(x) := \theta^1(x - j).$$

Observe that from relationships (24) and (25) (i.e. with $k = 1$),

$$\{\phi_n\}_{n=-L/2+1}^{n=L/2-1} \subset \text{span}\{\theta_j^1\}_{j=0}^{j=L-1}.$$

In particular, orthogonality to previous CPWs constraints in problem (36), imply that if θ^2 is expanded in the form (37), it is necessary (but not sufficient) that $a(0) = \dots = a(\pm(\frac{L}{2} - 1)) = 0$. Let θ^* be the solution of problem

$$\min_{\theta} \mathcal{J}_{\infty}(\theta) \quad \text{s.t.} \quad \int \theta(x)\theta(x - j)dx = \delta_{j0}, \quad (46)$$

with an additional constraint that if θ^* is expanded in the form (37), then $a(n) = 0$ for $|n| < L/2$. Using the same arguments as before, one concludes that to find a candidate for θ^* it is required to solve an optimization problem similar to (44); however, this time

$$\lambda^T = [\lambda_{\frac{L}{2}}, \lambda_{\frac{L}{2}+1}, \dots], \quad c^T = [c(\frac{L}{2}), c(\frac{L}{2} + 1), \dots], \quad \text{and} \quad M = [\vec{e}^T M_R | \vec{1} | M_L].$$

Repeating the same line of logic as before, the optimal solution is still

$$c^T = [\frac{1}{L}, \underbrace{\frac{2}{L}, \dots, \frac{2}{L}}_{L/2-1}, \frac{1}{L}, 0, 0, \dots].$$

Hence, for θ^* ,

$$\begin{cases} |a(\pm\frac{L}{2})| = |a(\pm L)| = 1/\sqrt{2L} \\ |a(n)| = 1/\sqrt{L} \\ |a(n)| = 0 \end{cases} \quad \begin{array}{l} \text{for } n = \pm(\frac{L}{2} + 1), \dots, \pm(L - 1), \\ \text{otherwise.} \end{array}$$

Now observe that θ^* is not necessarily the same as θ^2 , as θ^2 satisfies stricter constraints (i.e. orthogonality to $\{\theta_j^1\}_{j=0}^{L-1}$) than θ^* . Nevertheless, there is a particular choice of phases for $a(n)$'s for which

$$\theta^*(x) = \frac{1}{\sqrt{L}} \sum_{\frac{L}{2} < |n| < L} (\text{sgn}(n)i)\phi_n(x) + \frac{1}{\sqrt{2L}} \sum_{|n|=\frac{L}{2}, L} (\text{sgn}(n)i)\phi_n(x).$$

It is easy to verify that the above function is indeed orthogonal to set $\{\theta_j^1\}_{j=0}^{L-1}$. Therefore,

$$\theta^2(x) = \frac{1}{\sqrt{L}} \sum_{\frac{L}{2} < |n| < L} (\text{sgn}(n)i)\phi_n(x) + \frac{1}{\sqrt{2L}} \sum_{|n|=\frac{L}{2}, L} (\text{sgn}(n)i)\phi_n(x).$$

Continue the above procedure to find the subsequent BCPWs: for example if θ^3 is expanded in the form (37), it is necessary (but not sufficient) that $a(n) = 0$, for $|n| < L$. For from relationships (24), (25) (i.e. with $k = 1, 2$) and (26) (i.e. with $k = 1$):

$$\{\phi_n\}_{n=-(L-1)}^{n=L-1} \subset \text{span}\{\theta_j^1, \theta_j^2\}_{j=0}^{j=L-1},$$

and from the orthogonality to previous CPWs constraints in problem (36).

Let θ^* be the solution of problem (46) with an additional constraint that if it is expanded in the form (37), then $a(n) = 0$ for $|n| < L$. We conclude that for θ^* ,

$$\begin{cases} |a(\pm L)| = |a(\pm\frac{3L}{2})| = 1/\sqrt{2L} \\ |a(n)| = 1/\sqrt{L} \\ |a(n)| = 0 \end{cases} \quad \begin{array}{l} \text{for } n = \pm(L + 1), \dots, \pm(\frac{3L}{2} - 1), \\ \text{otherwise.} \end{array}$$

Note that θ^* is already orthogonal to the space spanned by all shifts of function θ^1 . To make θ^* orthogonal to the space spanned by all shifts of function θ^2 (and therefore, derive a formula for θ^3), a particular choice of phase factors for $a(n)$'s are chosen. Consequently,

$$\theta^3(x) = \frac{1}{\sqrt{L}} \sum_{L < |n| < \frac{3L}{2}} (-1)\phi_n(x) + \frac{1}{\sqrt{2L}} \sum_{|n|=L, \frac{3L}{2}} (-1)\phi_n(x).$$

B Laplacian of the SOPWs

Here, it is shown that for any set of solutions to the variational problem (36):

$$\partial_{xx}\theta_j^k \in \text{span}\{\theta_\ell^k\}_{\ell=0}^{\ell=L-1},$$

where $\theta_j^k(x) := \theta^k(x - j)$. Observe that it suffices to show that

$$\partial_{xx}\theta^k \in \text{span}\{\theta_\ell^k\}_{\ell=0}^{L-1}.$$

From the theory of variational calculus with constraints (i.e. see for example [6, Chapter 8]) at the k -th step (i.e. when θ_j^i for $i = 1, \dots, k - 1$ are already determined), if θ^k is the solution to the variational problem (36), then it is the weak solution of the Euler-Lagrange equation

$$\Delta\theta^k = \sum_{i=1}^k \sum_{j=0}^{L-1} \lambda_j^i \theta_j^i, \quad (47)$$

where constants λ_j^i are the Lagrange multipliers corresponding to the orthonormality constraints:

$$\int \theta^k(x) \theta_j^k(x) dx = \delta_{j0} \quad \text{and} \quad \int \theta^k(x) \theta_j^i(x) dx = 0 \quad \text{for } i = 1, \dots, k - 1.$$

It remains to show that $\lambda_j^i = 0$ for all $i < k$. Fix $n < k$ and $\ell \in \{0, \dots, L - 1\}$. Multiply both sides of (47) by θ_ℓ^n , integrate over the domain $[0, L]$, and use orthonormalities of $\{\theta_j^i\}_{i=1, j=0}^{i=k, j=L-1}$ and integration by parts to conclude that

$$\lambda_\ell^n = \int \Delta\theta^k(x) \theta_\ell^n(x) dx = \int \theta^k(x) \Delta\theta_\ell^n(x) dx = \int \theta_{L-\ell}^k(x) \Delta\theta^n(x) dx. \quad (48)$$

Next, observe that θ^n must satisfy a similar equation to (47); that is,

$$\Delta\theta^n = \sum_{i=1}^n \sum_{j=0}^{L-1} \gamma_j^i \theta_j^i.$$

From definition of θ^k in (36) and because $n < k$, one concludes that $\theta_{L-\ell}^k$ is orthogonal to $\{\theta_j^i\}_{i=1, j=0}^{i=n, j=L-1}$. Therefore, multiplying the above equation by $\theta_{L-\ell}^k$ and integrating over the domain, yields that

$$\int \theta_{L-\ell}^k \Delta\theta^n(x) dx = 0.$$

The above equation and equation (48) imply that $\lambda_\ell^n = 0$ as was to be shown.

C First and Second Derivative of SOPWs

Here, formulas for the first and second derivatives of SOPWs, defined by (21) and (22), are presented. These results are important in determining the matrix elements of the derivative and Laplacian operator when SOPWs basis are used.

The first derivative of of SOPWs are given by the following theorem:

Theorem C.1 (First Derivatives) For $k = 1, 2, \dots$ and $\ell = 0, \dots, L - 1$,

$$\partial_x \theta_\ell^k = \frac{\pi}{L} \left[-(k-1) \sum_j (-1)^{(k-1)(j-\ell)} \theta_j^{k-1} + \sum_j a(j-\ell) \theta_j^k + k \sum_j (-1)^{k(j-\ell)} \theta_j^{k+1} \right],$$

where

$$a(j-\ell) = \begin{cases} 0 & \text{if } j-\ell = 0, \\ (-1)^k (2k-1) \cot(\pi(j-\ell)/L) & \text{if } j-\ell \text{ is odd,} \\ \cot(\pi(j-\ell)/L) & \text{otherwise,} \end{cases}$$

and dummy variable j takes its values values from $\{0, 1, \dots, L-1\}$.

The second derivative of SOPWs are given by the following theorem:

Theorem C.2 (Second Derivatives) For $k = 1, 2, \dots$ and $\ell = 0, \dots, L - 1$,

$$\partial_{xx} \theta_\ell^k = \frac{-\pi^2}{L^2} \sum_j b(j-\ell) \theta_j^k$$

where

$$b(j-\ell) = \begin{cases} (k^2 - k + 1/3)L^2 + 2/3 & \text{if } j-\ell = 0, \\ (-1)^k (4k-2) \csc^2(\pi(j-\ell)/L) & \text{if } j-\ell \text{ is odd,} \\ 2 \csc^2(\pi(j-\ell)/L) & \text{otherwise,} \end{cases}$$

and dummy variable j takes its values from $\{0, 1, \dots, L-1\}$.

Recall that $\omega_j = e^{i2\pi j/L}$. The following lemma is essential in the proof of the above theorems:

Lemma C.3 For positive integer k , even L and $j = 0, \dots, L-1$:

$$\sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} n \omega_j^n = \begin{cases} 0 & \text{if } j = 0, \\ \frac{-i}{2} L (-1)^k (2k-1) \cot(\pi j/L) & \text{if } j \text{ is odd,} \\ \frac{-i}{2} L \cot(\pi j/L) & \text{otherwise,} \end{cases}$$

and

$$\sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} n^2 \omega_j^n = \begin{cases} \frac{1}{12} (L-2)L[(3k^2 - 3k + 1)L - 1] & \text{if } j = 0, \\ \frac{L}{2} (-1)^k (2k-1) \csc^2(\pi j/L) - (-1)^k (2k-1) \frac{L^2}{4} & \text{if } j \text{ is odd,} \\ \frac{L}{2} \csc^2(\pi j/L) - (k^2 + (k-1)^2) \frac{L^2}{4} & \text{otherwise,} \end{cases}$$

Proof: It is easy to verify the case $j = 0$, so we assume $j \neq 0$. Let

$$c(x) = \sum_{\frac{(k-1)L}{2} < n < \frac{kL}{2}} \cos(nx).$$

Then

$$\sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} n \omega_j^n = \sum_{\frac{(k-1)L}{2} < n < \frac{kL}{2}} n (\omega_j^n - \bar{\omega}_j^n) = 2i \sum_{\frac{(k-1)L}{2} < n < \frac{kL}{2}} n \sin\left(\frac{2\pi n j}{L}\right) = (-2i) c'\left(\frac{2\pi j}{L}\right),$$

and

$$\sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} n^2 \omega_j^n = \sum_{\frac{(k-1)L}{2} < n < \frac{kL}{2}} n^2 (\omega_j^n + \bar{\omega}_j^n) = 2 \sum_{\frac{(k-1)L}{2} < n < \frac{kL}{2}} n^2 \cos\left(\frac{2\pi n j}{L}\right) = (-2) c''\left(\frac{2\pi j}{L}\right).$$

It is well known (i.e. for example see [7, page 290]) that

$$c(x) = \frac{\sin\left(\left(\frac{L}{2} - 1\right)x/2\right)}{\sin(x/2)} \cos\left(\frac{(2k-1)}{4} Lx\right).$$

The rest of the proof follows from straightforward but tedious calculations: one finds close formulas for $c'(x)$ and $c''(x)$, substitutes $x = 2\pi j/L$ and simplifies. In particular, table 2 is helpful in simplifying. \blacksquare

$j \pmod 4$	$\cos\left(\frac{\pi j(2k-1)}{2}\right)$	$\sin\left(\frac{\pi j(2k-1)}{2}\right)$	$\cos\left(\frac{\pi j(L/2-1)}{L}\right)$	$\sin\left(\frac{\pi j(L/2-1)}{L}\right)$
0	1	0	$\cos(\pi j/L)$	$-\sin(\pi j/L)$
1	0	$(-1)^{k+1}$	$\sin(\pi j/L)$	$\cos(\pi j/L)$
2	-1	0	$-\cos(\pi j/L)$	$\sin(\pi j/L)$
3	0	$(-1)^k$	$-\sin(\pi j/L)$	$-\cos(\pi j/L)$

Table 2: Trigonometry identities for integers k, j and even positive number L .

The proof of theorems C.1 and C.2 are very similar. The idea of the proof is simple: write SOPWs basis in terms of Fourier basis using formulas (21) and (22), take appropriate number of derivatives, and then use formulas (25) and (26) to write back the result in terms of the SOPWs basis.

Proof of theorem C.1: First observe that because $\theta_\ell^k(x) = \theta_0^k(x - \ell)$, it suffices to find $\partial_x \theta_0^k$ and then by shifting, the corresponding formulas for SOPWs with other shift indices follow easily. Now using formulas (21) and (22),

$$\begin{aligned} \partial_x \theta_0^k &= \frac{1}{\sqrt{L}} \sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} (\text{sgn}(n)i)^{k-1} \partial_x \phi_n + \frac{1}{\sqrt{2L}} \sum_{|n| = \frac{(k-1)L}{2}, \frac{kL}{2}} (\text{sgn}(n)i)^{k-1} \partial_x \phi_n \\ &= \frac{1}{\sqrt{L}} \sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} (\text{sgn}(n)i)^{k-1} \left(\frac{i2\pi n}{L}\right) \phi_n + \frac{1}{\sqrt{2L}} \sum_{|n| = \frac{(k-1)L}{2}, \frac{kL}{2}} (\text{sgn}(n)i)^{k-1} \left(\frac{i2\pi n}{L}\right) \phi_n. \end{aligned} \tag{49}$$

Now from equations (25) and using lemma C.3,

$$\begin{aligned}
& \frac{1}{\sqrt{L}} \sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} (\operatorname{sgn}(n)i)^{k-1} \left(\frac{i2\pi n}{L}\right) \phi_n \\
&= \frac{1}{\sqrt{L}} \sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} (\operatorname{sgn}(n)i)^{k-1} \left(\frac{i2\pi n}{L}\right) \frac{(-\operatorname{sgn}(n)i)^{k-1}}{\sqrt{L}} \sum_{j=0}^{L-1} \omega_j^n \theta_j^k \\
&= \frac{i2\pi}{L^2} \sum_{j=0}^{L-1} \left(\sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} n \omega_j^n \right) \theta_j^k \\
&= \frac{\pi}{L} \sum_{j=0}^{L-1} a(j) \theta_j^k, \tag{50}
\end{aligned}$$

where

$$a(j) = \begin{cases} 0 & \text{if } j = 0, \\ (-1)^k (2k - 1) \cot(\pi j/L) & \text{if } j \text{ is odd,} \\ \cot(\pi j/L) & \text{otherwise.} \end{cases}$$

On the other hand, equation (26) implies that for $|n| = \frac{kL}{2}$,

$$\phi_n(x) = \frac{(-\operatorname{sgn}(n)i)^{k-1}}{\sqrt{2L}} \left(\sum_{j=0}^{L-1} (-1)^{kj} \theta_j^k(x) - \operatorname{sgn}(n)i \sum_{j=0}^{L-1} (-1)^{kj} \theta_j^{k+1}(x) \right). \tag{51}$$

Therefore,

$$\begin{aligned}
& \frac{1}{\sqrt{2L}} \sum_{|n|=\frac{kL}{2}} (\operatorname{sgn}(n)i)^{k-1} \left(\frac{i2\pi n}{L}\right) \phi_n \\
&= \frac{1}{2L} \left(\frac{i2\pi}{L}\right) \sum_{|n|=\frac{kL}{2}} \left(n \sum_{j=0}^{L-1} (-1)^{kj} \theta_j^k - |n|i \sum_{j=0}^{L-1} (-1)^{kj} \theta_j^{k+1} \right) \\
&= \frac{\pi}{L} k \sum_{j=0}^{L-1} (-1)^{kj} \theta_j^{k+1}. \tag{52}
\end{aligned}$$

Again, equation (26) implies that for $|n| = \frac{(k-1)L}{2}$,

$$\phi_n(x) = \frac{(-\operatorname{sgn}(n)i)^{k-2}}{\sqrt{2L}} \left(\sum_{j=0}^{L-1} (-1)^{(k-1)j} \theta_j^{k-1}(x) - \operatorname{sgn}(n)i \sum_{j=0}^{L-1} (-1)^{(k-1)j} \theta_j^k(x) \right). \tag{53}$$

Therefore,

$$\begin{aligned}
& \frac{1}{\sqrt{2L}} \sum_{|n|=\frac{(k-1)L}{2}} (\operatorname{sgn}(n)i)^{k-1} \left(\frac{i2\pi n}{L}\right) \phi_n \\
&= \frac{1}{2L} \left(\frac{i2\pi}{L}\right) \sum_{|n|=\frac{(k-1)L}{2}} \left(|n|i \sum_{j=0}^{L-1} (-1)^{(k-1)j} \theta_j^{k-1} + n \sum_{j=0}^{L-1} (-1)^{(k-1)j} \theta_j^k \right) \\
&= -\frac{\pi}{L} (k-1) \sum_{j=0}^{L-1} (-1)^{(k-1)j} \theta_j^{k-1}. \tag{54}
\end{aligned}$$

Substituting (50), (52) and (54) into equation (49) yields that

$$\partial_x \theta_0^k = \frac{\pi}{L} \left[-(k-1) \sum_{j=0}^{L-1} (-1)^{(k-1)j} \theta_j^{k-1} + \sum_{j=0}^{L-1} a(j) \theta_j^k + k \sum_{j=0}^{L-1} (-1)^{kj} \theta_j^{k+1} \right].$$

This completes the proof. \blacksquare

Proof of theorem C.2: Again observe that because $\theta_\ell^k(x) = \theta_0^k(x - \ell)$, it suffices to find $\partial_{xx} \theta_0^k$ and then by shifting, the corresponding formulas for SOPWs with other shift indices follow easily. Now using formulas (21) and (22),

$$\begin{aligned}
& \partial_{xx} \theta_0^k \\
&= \frac{1}{\sqrt{L}} \sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} (\operatorname{sgn}(n)i)^{k-1} \partial_{xx} \phi_n + \frac{1}{\sqrt{2L}} \sum_{|n|=\frac{(k-1)L}{2}, \frac{kL}{2}} (\operatorname{sgn}(n)i)^{k-1} \partial_{xx} \phi_n \\
&= \frac{1}{\sqrt{L}} \sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} (\operatorname{sgn}(n)i)^{k-1} \left(\frac{-4\pi^2 n^2}{L^2}\right) \phi_n + \frac{1}{\sqrt{2L}} \sum_{|n|=\frac{(k-1)L}{2}, \frac{kL}{2}} (\operatorname{sgn}(n)i)^{k-1} \left(\frac{-4\pi^2 n^2}{L^2}\right) \phi_n. \tag{55}
\end{aligned}$$

Now from equations (25) and using lemma C.3,

$$\begin{aligned}
& \frac{1}{\sqrt{L}} \sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} (\operatorname{sgn}(n)i)^{k-1} \left(\frac{-4\pi^2 n^2}{L^2}\right) \phi_n \\
&= \frac{1}{\sqrt{L}} \sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} (\operatorname{sgn}(n)i)^{k-1} \left(\frac{-4\pi^2 n^2}{L^2}\right) \frac{(-\operatorname{sgn}(n)i)^{k-1}}{\sqrt{L}} \sum_{j=0}^{L-1} \omega_j^n \theta_j^k \\
&= \frac{-4\pi^2}{L^3} \sum_{j=0}^{L-1} \left(\sum_{\frac{(k-1)L}{2} < |n| < \frac{kL}{2}} n^2 \omega_j^n \right) \theta_j^k \\
&= \frac{-\pi^2}{L^2} \sum_{j=0}^{L-1} \tilde{b}(j) \theta_j^k, \tag{56}
\end{aligned}$$

where

$$\tilde{b}(j) = \begin{cases} (L-2)[(3k^2 - 3k + 1)L - 1]/3 & \text{if } j = 0, \\ (-1)^k(4k-2)\csc^2(\pi j/L) - (-1)^k(2k-1)L & \text{if } j \text{ is odd,} \\ 2\csc^2(\pi j/L) - (k^2 + (k-1)^2)L & \text{otherwise.} \end{cases}$$

On the other hand, from (51),

$$\begin{aligned} & \frac{1}{\sqrt{2L}} \sum_{|n|=\frac{kL}{2}} (\operatorname{sgn}(n)i)^{k-1} \left(\frac{-4\pi^2 n^2}{L^2}\right) \phi_n \\ &= \frac{1}{2L} \left(\frac{-4\pi^2}{L^2}\right) \sum_{|n|=\frac{kL}{2}} \left(n^2 \sum_{j=0}^{L-1} (-1)^{kj} \theta_j^k - n^2 \operatorname{sgn}(n)i \sum_{j=0}^{L-1} (-1)^{kj} \theta_j^{k+1} \right) \\ &= \frac{-\pi^2}{L^2} k^2 L \sum_{j=0}^{L-1} (-1)^{kj} \theta_j^k. \end{aligned} \tag{57}$$

Also from (53),

$$\begin{aligned} & \frac{1}{\sqrt{2L}} \sum_{|n|=\frac{(k-1)L}{2}} (\operatorname{sgn}(n)i)^{k-1} \left(\frac{-4\pi^2 n^2}{L^2}\right) \phi_n \\ &= \frac{1}{2L} \left(\frac{-4\pi^2}{L^2}\right) \sum_{|n|=\frac{(k-1)L}{2}} \left(n^2 \operatorname{sgn}(n)i \sum_{j=0}^{L-1} (-1)^{(k-1)j} \theta_j^{k-1} + n^2 \sum_{j=0}^{L-1} (-1)^{(k-1)j} \theta_j^k \right) \\ &= \frac{-\pi^2}{L^2} (k-1)^2 L \sum_{j=0}^{L-1} (-1)^{(k-1)j} \theta_j^k. \end{aligned} \tag{58}$$

Substituting (56), (57) and (58) into equation (55) and simplifying yields that

$$\partial_{xx} \theta_0^k = \frac{-\pi^2}{L^2} \sum_{j=0}^{L-1} b(j) \theta_j^k.$$

This completes the proof. ■

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