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MULTIVARIATE FOURIER TRANSFORM METHODS OVER SIMPLEX AND SUPER-SIMPLEX DOMAINS*[1)]

Jiachang Sun
(*Institute of Software, Chinese Academy of Sciences, Beijing 100080, China*)

Dedicated to the 70th birthday of Professor Lin Qun

Abstract

In this paper we propose the well-known Fourier method on some non-tensor product domains in R^d, including simplex and so-called super-simplex which consists of $(d+1)!$ simplices. As two examples, in 2-D and 3-D case a super-simplex is shown as a parallel hexagon and a parallel quadrilateral dodecahedron, respectively. We have extended most of concepts and results of the traditional Fourier methods on multivariate cases, such as Fourier basis system, Fourier series, discrete Fourier transform (DFT) and its fast algorithm (FFT) on the super-simplex, as well as generalized sine and cosine transforms (DST, DCT) and related fast algorithms over a simplex. The relationship between the basic orthogonal system and eigen-functions of a Laplacian-like operator over these domains is explored.

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1. Introduction

It is well known that the univariate Fourier transform and its tensor product form in high dimension have been played a key role in applied mathematics and scientific computations in many fields. Unfortunately, in high dimension the tensor product approach has to be limited to domains which can transformed into a box. With theoretical interests and application drives for developing more efficient grid generation and fast solver for numerical PDE, there have been increasing interests in how to extend Fourier methods into irregular domains. Since simplex is one of the simplest non-box domains, it seems more attention has being paid to the multivariate orthogonal polynomials on simplex [1, 3, 4, 5, 10, 11, 12, 13]. In this paper we also study so-called generalized sine and cosine transform and related fast transforms on a simplex.

As is well-known a simplex is a natural extension of an interval $[0, 1]$ in $1-D$. However, besides simplex there is another kind of domain partition which is really important for high dimension case. In 2-D and 3-D case, they are parallel hexagon and parallel dodecahedrons which can be taken as a natural extension of the symmetry interval $[-1, -1]$ instead of a general interval $[0, 1]$. In application point of views, this kind of domain partitions exist in nature almost everywhere. As a well-known example, the shape of honeycombs is a hexagon instead of quadrilaterals. There are many parallel dodecahedron shapes in natural crystals.

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Mathematically, it is worth to note that besides a box partition with d-directions, such a super-simplex partitions $d+1$-directions can also form a tiling in $\mathbb{R}^d$. However, a pure simplex partition can not form a tiling if only shifting operators are allowed.

The most important issue of the generalization of Fourier transform for non-box domains is the construction of the orthogonal bases. There is an intrinsic relationship between Fourier basis and the Laplacian-like operator. As is well known, the eigen-decompositions of the Laplacian-like operator usually result in the orthogonal exponential bases on box domains, instead of orthogonal polynomials. To construct orthogonal bases in our case, in this paper we adopt eigen-decompositions of the differential operators with periodic boundary conditions over the super-simplex domain or with zero Dirichlet and zero Neumann boundary conditions. The idea and algorithms may be useful for spectral methods and preconditioning algorithms for numerical PDE solvers for non separable problems and over more wide non tensor-product partitions.

The remainder of this paper is organized as follows. In §2, after introducing some homogeneous coordinates, we present a tiling of the $d+1$-direction partition in $\mathbb{R}^d$. In §3, we construct a basis and investigate its some properties, such as periodicity, orthogonality and completeness. Then we study the related Fourier series and its convergence. We put our focus on exploring the intrinsic relationship between the above basic system and eigenfunctions of a Laplacian-Like PDE operator. On the analogy of univariate case, so-called generalized sine (HSin) and cosine functions (HCos) are defined in the whole space, especially on a simplex in §4. Finally we investigate the generalized Fourier transform (HFT) and propose a fast discrete Fourier transform (HFFT) on §5.

2. Notations and Definitions

Suppose vectors $\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_d$ are linear independent in $\mathbb{R}^d$ and G is the Gram matrix

$$G(\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_d) = \begin{pmatrix} \mathbf{e}_1\cdot\mathbf{e}_1 & \mathbf{e}_1\cdot\mathbf{e}_2 & ... & \mathbf{e}_1\cdot\mathbf{e}_d \\ \mathbf{e}_2\cdot\mathbf{e}_1 & \mathbf{e}_2\cdot\mathbf{e}_2 & ... & \mathbf{e}_2\cdot\mathbf{e}_d \\ ... & ... & ... & ... \\ \mathbf{e}_d\cdot\mathbf{e}_1 & \mathbf{e}_d\cdot\mathbf{e}_2 & ... & \mathbf{e}_d\cdot\mathbf{e}_d \end{pmatrix} = [\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_d]^T[\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_d] \tag{2.1}$$

where the notation $\mathbf{e}_1\cdot\mathbf{e}_2 = \mathbf{e}_1'\mathbf{e}_2$ denotes the inner product of $\mathbf{e}_1$ and $\mathbf{e}_2$ in $\mathbb{R}^d$.

We define a set of vectors as

$$[\mathbf{n}_1, \mathbf{n}_2, ..., \mathbf{n}_d] = [\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_d][G(\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_d)]^{-1}. \tag{2.2}$$

Then two vector sets $\{\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_d\}$ and $\{\mathbf{n}_1, \mathbf{n}_2, ..., \mathbf{n}_d\}$ are bi-orthogonal in the sense

$$[\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_d]^T[\mathbf{n}_1, \mathbf{n}_2, ..., \mathbf{n}_d] = [\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_d]^T[\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_d][G(\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_d)]^{-1} = I.$$

Moreover, we define the $(d+1)$-th direction vector

$$\mathbf{n}_{d+1} = -\sum_{\mu=1}^{d}\mathbf{n}_\mu. \tag{2.3}$$

Hence there are totally $2\binom{d+1}{d-1} = d(d+1)$ hyperplanes via the $d+1$ directions $\mathbf{n}_1, ..., \mathbf{n}_d, \mathbf{n}_{d+1}$. Now we lift the space $\mathbb{R}^d$ to $\mathbb{R}^{\binom{d+1}{2}}$. Set

$$\mathbf{n}_{\nu,\nu} = \mathbf{n}_\nu \quad (\nu = 1, ...d), \qquad \mathbf{n}_{\mu,\nu} = \mathbf{n}_\nu - \mathbf{n}_\mu \quad (1 \le \mu < \nu \le d). \tag{2.4}$$

For each point $P \in \mathbb{R}^d$, we introduce its $\binom{d+1}{2}$ affine coordinates by taking its corresponding vector projections in the space $\mathbb{R}^d$ as

$$t_{\nu,\nu} = t_\nu = \mathbf{P}\cdot\mathbf{n}_\nu \quad (\nu = 1, ...d), \qquad t_{\mu,\nu} = \mathbf{P}\cdot\mathbf{n}_{\mu,\nu} \quad (1 \le \mu < \nu \le d) \tag{2.5}$$

with the similar relations to (2.4) $t_{\mu,\nu} = t_\nu - t_\mu \quad (1 \le \mu < \nu \le d)$.

Later we denote $\mathbf{P} \in \sigma_d$ in $\mathbb{R}^{\binom{d+1}{2}}$ by means

$$\sigma_d := \{\mathbf{P} = (t_{\mu,\nu}) \in \mathbb{R}^{\binom{d+1}{2}} | t_{\nu,\nu} = t_\nu \quad (\nu = 1, ..., d), \quad t_{\mu,\nu} = t_\nu - t_\mu \quad (1 \le \mu < \nu \le d)\}. \tag{2.6}$$

and the integer point set by

$$\Lambda := \{\mathbf{j} \,|\mathbf{j} = (j_{\mu,\nu}) \in \sigma_d, j_\nu \in \mathbb{Z}, \nu = 1, ...d\}. \tag{2.7}$$

Taking the origin point as the center, we define a basic d-D domain Ω_o to be a semi-open parallel polyhedron as follows

Definition 2.1. *A semi-open super-simplex and a super-simplex in $\mathbb{R}^d$ is defined as*

$$\Omega_o = \{P | P = (t_{\mu,\nu}) \in \sigma_d, \quad -1 \le t_{\mu,\nu} < 1 \quad (1 \le \mu \le \nu \le d)\} \tag{2.8}$$

and

$$\Omega = \{P | P = (t_{\mu,\nu}) \in \sigma_d, \quad -1 \le t_{\mu,\nu} \le 1, \quad (1 \le \mu \le \nu \le d)\} \tag{2.9}$$

respectively, where σ_d is defined in (2.6).

It is easy to know a super-simplex Ω defined in (2.8) is the closed set of Ω_o and has $d(d+1)$ hyperplanes and $2(2^d - 1)$ vertices in $\mathbb{R}^d$.

As two examples, the basic domain Ω shows a parallel hexagon in 2-D in Figure 2.1 or a parallel quadrilateral dodecahedron in 3-D in Figure 2.2, respectively. For sake of symmetry, in $2-D$ case we always take $t_1 + t_2 + t_3 = 0$, see [6],[9].

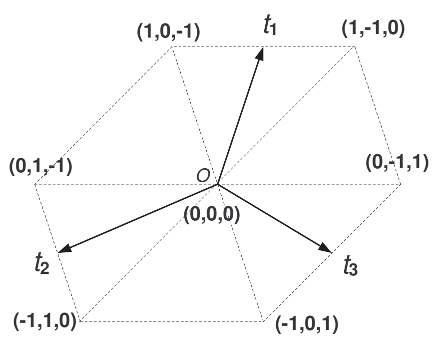

Figure 2.1: Parallel hexagon in 2-D

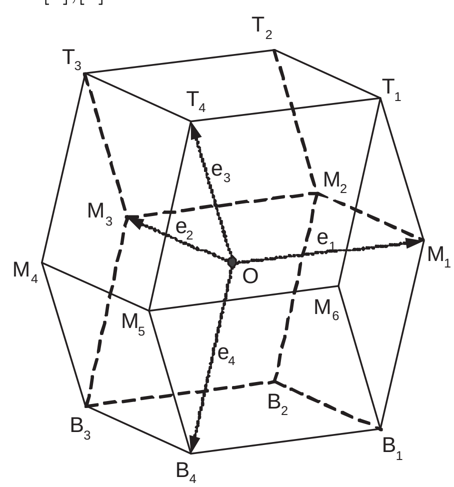

Figure 2.2: Parallel dodecahedron in 3-D

To make a tiling in $\mathbb{R}^d$ via the semi-open basic domain Ω_o, we introduce following definition.

Definition 2.2. *A shifting semi-open super-simplex $\Omega_Q \in \mathbb{R}^d$ is defined as*

$$\Omega_Q(P) = \{P | P - Q \in \Omega_o, Q \in \Theta\} \tag{2.10}$$

where the integer point set

$$\Theta := \{Q | Q = (k_{\mu,\nu}) \in \Lambda, \quad \sum_{\nu=1}^{d} k_{\nu,\nu} \equiv 0 \quad (mod \quad d+1)\} \tag{2.11}$$

Now we turn to study so-called tiling property of the super-simplex partition.

Theorem 2.1. *[Tiling] The set of all Ω_Q with $Q \in \Theta$, defined in (2.11), forms a tiling in $\mathbb{R}^d$ in the sense*

$$\bigcup_{Q \in \Theta} \Omega_Q = \mathbb{R}^d \qquad and \qquad \Omega_{Q_1} \bigcap_{Q_1 \ne Q_2} \Omega_{Q_2} = \varnothing. \tag{2.12}$$

Proof. For any given point $P \in \mathbb{R}^d$, its first d affine coordinates in (2.5) can be expressed as

$$t_\nu = j_\nu + r_\nu, \quad j_\nu \in \mathbb{Z}, \quad 0 \le r_\nu < 1 \qquad \nu = 1, ...d.$$

Without loss of generality we may assume $r_1 \ge r_2 \ge ... \ge r_d$, and

$$-d \le js = \sum_{\nu=1}^{d} j_\nu \le 0 \quad (mod \quad d+1).$$

We may define the first d affine coordinates for $Q = (k_1, k_2, k_3, ..., k_d, ...) \in \Theta$ as

$$(k_1, k_2, k_3, ..., k_d) = \begin{cases} (j_1, j_2, j_3, ..., j_d), & js \equiv 0 \quad (mod \quad d+1) \\ (j_1+1, j_2, j_3..., j_d), & js \equiv -1 \quad (mod \quad d+1) \\ (j_1+1, j_2+1, j_3, ..., j_d), & js \equiv -2 \quad (mod \quad d+1) \\ \cdots & \cdots \\ (j_1+1, j_2+1, ..., j_{d-1}+1, j_d), & js \equiv 1-d \quad (mod \quad d+1) \\ (j_1+1, j_2+1, ..., j_{d-1}+1, j_d+1), & js \equiv -d \quad (mod \quad d+1) \end{cases}$$

Thus $P - Q \in \Omega_o$, we have proved the first part of the theorem. Next, suppose the second part of (2.12) is not true. There would be a point $P \in \mathbb{R}^d$ belong to two different domains Ω_{Q_1} and Ω_{Q_2} at the same time. Then for each $1 \le \mu \le \nu \le d$ there would be

$$-2 < t_{\mu,\nu}(Q_1) - t_{\mu,\nu}(Q_2) = (t_{\mu,\nu}(Q_1) - t_{\mu,\nu}(P)) - (t_{\mu,\nu}(Q_2) - t_{\mu,\nu}(P)) < 2, \quad 1 \le \mu \le \nu \le d.$$

This means all absolute values of each coordinates for $Q = Q_1 - Q_2 \in \Theta$ must be less than 2. However, from the definitions (2.8) and (2.10) the inequalities can not be true unless $Q_1 \equiv Q_2$. The proof has been completed.

The following Lemma is obvious in geometry point of views.

Lemma 2.1. *Domain Ω can be decomposed into $d+1$ cubes in $\mathbb{R}^d$*

$$\Omega = \bigcup_{\nu=1}^{d+1} \Omega_\nu \tag{2.13}$$

where Ω_ν's are cubes defined as

$$\Omega_\nu = \{P | \ 0 \le t_{\mu,\nu} \le 1 \quad 1 \le \mu < \nu, \quad or \quad -1 \le t_{\nu,\mu} \le 0, \quad \mu \ge \nu\}, \qquad \nu = 1, ..., d.$$
$$\Omega_{d+1} = \{P | \ 0 \le t_{\mu,\mu} = t_\mu \le 1, \quad \mu = 1, ..., d.\}. \tag{2.14}$$

Therefore, though the basic Ω is not a tensor-product domain, however, it is belongs to piece-wise tensor product domains in the sense that it can be taken as a union of $d+1$ cubes. This means there are $d+1$ cubes which are all across the original and consist of d direction among the $d+1$ directions. The union set of the $d+1$ cubes is just the basic d-D domain. This fact will be useful to prove some properties later.

Corollary 2.1. *The super-simplex domain $\Omega \in \mathbb{R}^d$ can be decomposed into $(d+1)!$ simplices with the same volume, a typical one among them can be expressed as*

$$\Omega_S = \{P \in \Omega_{d+1} | \ 0 \le t_1 \le ... \le t_d \le 1\}. \tag{2.15}$$

This is why we call Ω as a super-simplex in $\mathbb{R}^d$.

Finally we introduce following homogeneous coordinates

$$\bar{t}_\mu = (d+1)t_\mu - \sum_{\nu=1}^{d} t_\nu, \quad (\mu = 1, ..., d), \quad \bar{t}_{d+1} = -\sum_{\mu=1}^{d} \bar{t}_\mu = -\sum_{\mu=1}^{d} t_\mu, \tag{2.16}$$

and the related integer sets

$$\bar{j}_\nu = (d+1)j_\nu - \sum_{\mu=1}^{d} j_\mu \qquad (\nu = 1, ..., d), \qquad \bar{j}_{d+1} = -\sum_{\mu=1}^{d} j_\mu = -\sum_{\mu=1}^{d} \bar{j}_\mu. \tag{2.17}$$

Then the Ω in (2.9) and Λ in (2.7) can also be expressed as

$$\Omega = \{P|P = (\bar{t}_1, ..., \bar{t}_d, \bar{t}_{d+1}) \in \sigma_d, -1 \le t_{\mu,\nu} \le 1 \ (1 \le \mu \le \nu \le d)\},$$
$$\Lambda = \{\mathbf{j} \ |\mathbf{j} = (\bar{j}_1, ..., \bar{j}_d, \bar{j}_{d+1}) \in \sigma_d, j_\nu \in \mathbb{Z}, \nu = 1, ...d\}. \tag{2.18}$$

Definition 2.3. *Given integer vector* $\mathbf{j} \in \Lambda$ *in (2.7) and* $\mathbf{P} \in \sigma_d$ *in (2.6), the inner product in* $\mathbb{R}^{\binom{d+1}{2}}$ *is defined by*

$$\mathbf{j} \cdot \mathbf{P} = \sum_{1 \le \mu \le \nu \le d} j_{\mu,\nu} t_{\mu,\nu}. \tag{2.19}$$

The following lemma can be verified by a straightforward computation and it is useful later.

Lemma 2.2. *The inner product* $\mathbf{j} \cdot \mathbf{P}$ *in* $\mathbb{R}^{\binom{d+1}{2}}$ *can also be written to following various forms*

$$\mathbf{j} \cdot \mathbf{P} = \sum_{\nu=1}^{d} \bar{j}_\nu t_\nu = \sum_{\nu=1}^{d} j_\nu \bar{t}_\nu = \frac{1}{d+1} \sum_{\nu=1}^{d+1} \bar{j}_\nu \bar{t}_\nu,$$

or

$$\mathbf{j} \cdot \mathbf{P} = \sum_{\mu<\nu} \bar{j}_\mu t_{\mu,\nu} - \bar{j}_{d+1} t_\nu - \sum_{\mu>\nu} \bar{j}_\mu t_{\nu,\mu}, \quad \nu = 1, ..., d$$

where $\bar{t}_\nu$ *and* $\bar{j}_\nu$ *(*$\nu = 1, ..., d+1$*) are defined in (2.17) and (2.16).*

3. An Orthogonal Function System on the Basic Domain

Definition 3.1. *The generalized Fourier functions in the space* $\mathbb{R}^d$ *are defined as*

$$g_{\mathbf{j}}(P) = e^{i\frac{2\pi}{d+1}\mathbf{j}\cdot\mathbf{P}} \tag{3.1}$$

where the inner product $\mathbf{j} \cdot \mathbf{P}$ *is understood in* $\mathbb{R}^{\binom{d+1}{2}}$ *as Definition 2.3.*

In particular, on an integer node $P = (k_{\mu,\nu}) \in \sigma_d, k_\nu \in \mathbb{Z}$, the function $g_{\mathbf{j}}(P)$ can only take $d+1$ possible values which all are the roots of $z^{d+1} = 1$.

Theorem 3.1. *[Periodicity] For any integer node* $Q \in \Theta$*, defined in (2.11), then for all integer vector* $\mathbf{j} \in \Lambda$ *in (2.7)*

$$g_{\mathbf{j}}(P+Q) = g_{\mathbf{j}}(P), \qquad for \quad all \quad P. \tag{3.2}$$

Proof. It only needs to note that

$$g_{\mathbf{j}}(P+Q) = e^{i\frac{2\pi}{d+1}j\cdot(P+Q)} = g_{\mathbf{j}}(P)e^{i\frac{2\pi}{d+1}j\cdot Q}$$

where

$$j \cdot Q = (d+1)\sum_{\nu=1}^{d} j_\nu k_\nu - \sum_{\mu=1}^{d} j_\mu \sum_{\mu=1}^{d} k_\mu.$$

From (2.11), for $Q \in \Theta$, $\sum_{\mu=1}^{d} k_\mu = 0 \quad (mod \quad d+1)$. Hence, $e^{i\frac{2\pi}{d+1}j\cdot Q} = 1$.

Thus, we may study the function focused on the basic domain Ω later.

Corollary 3.1. *$Q = (k_{\mu,\nu}) \in \Theta$ is called to be a minimum periodicity of function $g_{\mathbf{j}}(P)$ if*

$$\sum_{1\le\mu\le\nu\le d} k^2_{\mu,\nu} = 2(d+1). \tag{3.3}$$

Proof. Among $d(d+1)$ neighboring nodes $Q \in \Theta$ of Ω there are only two different cases. $2d$ neighbor points among them are $k_\nu = \pm(1+\delta_{\nu,\mu})(\nu,\mu = 1,...d)$. And other $d(d-1)$ neighbor nodes are $k_\mu = \pm 1, \quad k_\nu = \mp 1$ $(1 \le \mu < \nu \le d)$, others $k_\lambda = 0, \quad (\lambda \ne \mu, \quad \lambda \ne \nu, \quad \lambda = 1,...,d)$. Both integer nodes satisfy the condition (3.3).

Lemma 3.1. *[Normalization of Integral] For any integer vector $\mathbf{j} \in \Lambda$*

$$\int_\Omega g_{\mathbf{j}}(P)dP = C_\Omega \ \delta_{|\mathbf{j}|,0}. \tag{3.4}$$

where C_Ω is the volume of Ω.

Proof. The equality (3.4) is trivial if $\mathbf{j}$ is a zero vector. Otherwise from (2.14), the integral domain can be decomposed into $d+1$ boxes in $\mathbb{R}^d$. By Lemma 2.1 and Lemma 2.2, we have

$$I(\mathbf{j}) := \int_\Omega g_{\mathbf{j}}(P)dP = \sum_{\nu=1}^{d+1} I_\nu(j), \tag{3.5}$$

where for $\nu = 1,...,d$

$$I_\nu(\mathbf{j}) = \int_{\Omega_\nu} \exp\{\frac{2\pi i}{d+1}(\sum_{\mu<\nu} \bar{j}_\mu t_{\mu,\nu} - \bar{j}_{d+1}t_\nu - \sum_{\mu>\nu} \bar{j}_\mu t_{\nu,\mu}\}dP$$

$$= \{\prod_{\mu<\nu}\int_0^1 e^{\frac{2\pi i}{d+1}\bar{j}_\mu t_{\mu,\nu}}dP\}\int_{-1}^0 e^{-\frac{2\pi i}{d+1}\bar{j}_{d+1}t_\nu}dP\{\prod_{\mu>\nu}\int_{-1}^0 e^{-\frac{2\pi i}{d+1}\bar{j}_\mu t_{\nu,\mu}}dP\},$$

and

$$I_{d+1}(\mathbf{j}) = \int_{\Omega_{d+1}} \exp\{\frac{2\pi i}{d+1}(\sum_{\mu=1}^d \bar{j}_\mu t_\mu)\}dP = \prod_{\mu=1}^d \int_0^1 e^{\frac{2\pi i}{d+1}\bar{j}_\mu t_\mu}dP.$$

If all $\bar{j}_\nu \ne 0$, from (2.17), $e^{i\frac{2\pi}{d+1}\bar{j}_\nu} = e^{i\frac{2\pi}{d+1}\bar{j}_{d+1}}$ for $\nu = 1,...,d$. Hence we have

$$I_\nu(\mathbf{j}) = (\frac{2\pi i}{d+1})^{-d}\ \{\prod_{1\le\mu\ne\nu\le d} \bar{j}_\mu\}^{-1}(\bar{j}_{d+1})^{-1}(e^{\frac{2\pi i}{d+1}\bar{j}_{d+1}} - 1)^d$$

and

$$I_{d+1}(\mathbf{j}) = (\frac{2\pi i}{d+1})^{-d}\{\prod_{\mu=1}^d \bar{j}_\mu\}^{-1}(e^{\frac{2\pi i}{d+1}\bar{j}_{d+1}} - 1)^d.$$

Therefore, if all $\bar{j}_\nu \ne 0$

$$I(\mathbf{j}) = (\frac{2\pi i}{d+1})^{-d}\{\prod_{\mu=1}^{d+1} \bar{j}_\mu\}^{-1}(e^{i\frac{2\pi i}{d+1}\bar{j}_{d+1}} - 1)^d \sum_{\nu=1}^{d+1} \bar{j}_\nu = 0.$$

because of $\sum_{\nu=1}^{d+1} \bar{j}_\nu = 0$. Otherwise, if some, not all, $\bar{j}_\nu = 0$, the above derivation is still valid by excluding these zero terms. The proof is completed.

Based on the above Lemma we can obtain the following orthogonality theorem directly.

Theorem 3.2. *[Orthogonality] For* $\mathbf{j}$, $\mathbf{k}$ $\in \Lambda$

$$< g_{\mathbf{j}}, g_{\mathbf{k}} >_{\Omega} = C_{\Omega}\delta_{|j-k|,0} \tag{3.6}$$

where the inner product on Ω

$$< f, g >_{\Omega} = \int_{\Omega} f(P)\bar{g}(P)dp$$

and C_{Ω} *is the volume of* Ω.

Proof. It is only need to point that

$$< g_{\mathbf{j}}, g_{\mathbf{k}} >_{\Omega} = \int_{\Omega} g_{\mathbf{j}-\mathbf{k}}(P)dP.$$

Theorem 3.3. *[Completeness] The set of* $g_{\mathbf{j}}(P)$ *forms a complete orthogonal system in the space* $C(\Omega(\mathbb{R}^d))$.

We can prove the above basic theorem based on the following well-known Stone-Weierstrass theorem.

Lemma 3.2 (Stone-Weierstrass [2]). *Let* S *be a compact set and* A *an algebra (over* C*) of complex valued continuous functions on* S*. Assume that* A *separates points, contains the constants, and is itself conjugate. Then the uniform closure of* A *is equal to the algebra of all complex valued continuous functions on* S*.*

Since Ω is a centrally symmetric domain in $\mathbb{R}^d$ and the multiple Fourier functions $g_{\mathbf{j}}(P)$ are complex. It is easy to see that $V = \text{Span}\{g_{\mathbf{j}}(P), \mathbf{j} \in \Lambda\}$ forms an algebra of complex valued functions on Ω, which contains the constants, and is self-conjugate.

From Theorem 3.1 we know that $g_{\mathbf{j}}(P_1) = g_{\mathbf{j}}(P_2)$ if and only if $Q = P_1 - P_2 \in \Theta$. So V separates all the inner points of Ω. As for the boundary points of Ω, we can view the points P_1 and P_2 as the "same" point in the sense of congruence if $P_1 - P_2 \in \Theta$. In this way, V separates the points of Ω and by Lemma 3.2, we arrive at the following lemma.

Lemma 3.3. *Let* $C_p(\Omega) = \{f \in C(\Omega) : \ f(P_1) = f(P_2), \forall P_1 - P_2 \in \Theta\}$ *and* $L^q_p(\Omega) = \{f \in L^q(\Omega) : \ f(P_1) = f(P_2), \forall P_1 - P_2 \in \Theta\}$*. Then* V *is dense in* $C_p(\Omega)$ *and in* $L^q_p(\Omega), 1 \leq q < \infty$.

Therefore, the density of V in $C_p(\Omega)$ is an immediate result of Lemma 3.2. Since $C(\Omega)$ is dense in $L^q(\Omega)$, we deduce that V is also dense in $L^q_p(\Omega)$. The completeness of the orthogonal system has been proved.

Hence, once we have a complete orthogonal basis, it is reasonable to define its generalized Fourier series as

Definition 3.2. *For a function* $f(P) \in L(\Omega)$*, the related generalized Fourier series (HFS) are defined as*

$$f(P) \sim \sum_{\mathbf{j}\in\Lambda} \gamma_{\mathbf{j}} \ \ g_{\mathbf{j}}(P), \qquad \gamma_{\mathbf{j}} = \frac{1}{c_{\Omega}} < f(P), g_{\mathbf{j}}(P) >_{\Omega} . \tag{3.7}$$

As a consequence of Theorem 3.3, by the density of V in $L^q_p(\Omega)$, we deduce that

Lemma 3.4. *Let* $f \in L(\Omega)$*. If for any* $\mathbf{j} \in \Lambda$*,* $\gamma_{\mathbf{j}} = 0$*, then* $f = 0$ *.a.e.*

Corollary 3.2. *For a d-D continuous function* $f(P) \in C_{\Omega}(\mathbb{R}^d)$ *with periodicity* Ω *, if its all coefficients* $\gamma_{\mathbf{j}}$ *are zeros, the function* $f(P)$ *must equal to zero itself.*

There are different ways to define a partial sum of the generalized Fourier series in high dimension case. To match our domain partition, we define

Definition 3.3.

$$S_n[f](P) = \sum_{\mathbf{j}\ \in \Lambda_n} \gamma_{\mathbf{j}} \quad g_{\mathbf{j}}(P) \tag{3.8}$$

where

$$\Lambda = \bigcup_{n=0}^{\infty} \Lambda_n \quad with \quad \Lambda_n := \{\mathbf{j}\ \in \Lambda \mid -n \leq j_{\nu,\mu} \leq n,\ 1 \leq \nu \leq \mu \leq d\}. \tag{3.9}$$

Remark. Almost all results of the traditional Fourier series with its convergence rate can be extended to the general domain Ω case, just like the case of traditional Fourier series with tensor product over box domains. Below we list some of them. In 2-D arbitrary triangle domain case, the related proofs are shown in [8]. The detailed proofs for general case will be published elsewhere later.

Proposition 3.1. *For $f(P) \in C^1_\Omega(\mathbb{R}^d)$, the HFS (3.7) converges uniformly.*

Proposition 3.2. *If a bounded function $|f(P)| \leq M$ is periodic over the basic domain Ω, then there is an upper estimation of its finite Fourier series*

$$|S_n[f]| \leq CM(\ln n)^d \tag{3.10}$$

where C is a constant.

Proposition 3.3. *Let $f \in C^k_\Omega$ and $|D^k(f)| \leq M_k$, then following error estimate holds*

$$|S_n[f] - f| \leq CM_k(\ln n)^d n^{-k} \tag{3.11}$$

where C is a constant.

Finally we explore the intrinsic relationship between the above basic functions system and eigenfunctions of a second order elliptic operator with periodic boundary conditions over domains consist of the $d+1$ direction mesh.

Define an elliptic operator in $\mathbb{R}^d$

$$\mathcal{L} = -d \sum_{1\leq\nu<\mu\leq d+1} \left(\frac{\partial}{\partial \bar{t}_\nu} - \frac{\partial}{\partial \bar{t}_\mu}\right)^2 \tag{3.12}$$

where $d+1$ homogeneous variables $\bar{t}_\nu (\nu = 1, ..., d+1)$, defined in (2.16), are taken to be independent each other in this case.

By Lemma 2.2, $g_{\mathbf{j}}(P)$ can be expressed as

$$g_{\mathbf{j}}(P) = \exp\left\{\frac{2\pi i}{(d+1)^2} \sum_{\nu=1}^{d+1} \bar{j}_\nu \bar{t}_\nu\right\}.$$

It is easy to verify that

$$\mathcal{L} g_{\mathbf{j}}(P) = \lambda_j g_{\mathbf{j}}(P) \tag{3.13}$$

where

$$\lambda_j = \left(\frac{2\pi}{(d+1)^2}\right)^2 \sum_{1\leq\nu<\mu\leq d+1} (\bar{j}_\nu - \bar{j}_\mu)^2 = \frac{4\pi^2}{(d+1)^2}\left\{\sum_{1\leq\nu<\mu\leq d} (j_\nu - j_\mu)^2 + \sum_{\nu=1}^{d} j_\nu^2\ \right\}. \tag{3.14}$$

In fact, from (2.17), we know

$$\sum_{1\leq\nu<\mu\leq d+1} (\bar{j}_\nu - \bar{j}_\mu)^2 = \sum_{1\leq\nu<\mu\leq d} ((d+1)j_\nu - (d+1)j_\mu)^2 + \sum_{1\leq\nu<d+1} ((d+1)\bar{j}_\nu)^2.$$

The elliptic operator in (3.12) may have various forms in different coordinates. In terms of the affine coordinates $[t_1, ..., t_d]$, from (2.16) $t_\nu = \frac{1}{d+1}(\bar{t}_\nu - \bar{t}_{d+1})$ $(\nu = 1, ..., d)$ and

$$\sum_{1\le\nu<\mu\le d}(\frac{\partial}{\partial\bar{t}_\nu} - \frac{\partial}{\partial\bar{t}_\mu})^2 + \sum_{1\le\nu\le d}(\frac{\partial}{\partial\bar{t}_\nu} - \frac{\partial}{\partial\bar{t}_{d+1}})^2 = \frac{1}{(d+1)^2}\{\sum_{1\le\nu\le\mu\le d}(\frac{\partial}{\partial t_\nu} - \frac{\partial}{\partial t_\mu})^2$$

$$+ \sum_{1\le\nu\le d}(\frac{\partial}{\partial t_\nu} + \sum_{\mu=1}^{d}\frac{\partial}{\partial t_\mu})^2\}.$$

Then

$$\mathcal{L} = -\frac{d}{(d+1)^2}\{\sum_{1\le\nu\le\mu\le d}(\frac{\partial}{\partial t_\nu} - \frac{\partial}{\partial t_\mu})^2 + \sum_{1\le\nu\le d}(\frac{\partial}{\partial t_\nu} + \sum_{\mu=1}^{d}\frac{\partial}{\partial t_\mu})^2\}$$

or

$$\mathcal{L} = -[\frac{\partial}{\partial t_1}, ..., \frac{\partial}{\partial t_d}]M_d[\frac{\partial}{\partial t_1}, ..., \frac{\partial}{\partial t_d}]^T, \quad M_d = \frac{d}{d+1}(\mathbf{I}_d + \mathbf{e}\mathbf{e}^T) = d((d+1)\mathbf{I}_d - \mathbf{e}\mathbf{e}^T)^{-1} \tag{3.15}$$

where I_d is the identity matrix of order d and $\mathbf{e} = (1, ..., 1)$.

Back to a Cartesian coordinates system, we assume

$$\mathbf{P} = [x_1, ..., x_d] = [t_1, ..., t_d]\ J, \quad J = [\mathbf{e}_1, ..., \mathbf{e}_d].$$

where J is a Jacobian matrix, then $[\frac{\partial}{\partial t_1}, ..., \frac{\partial}{\partial t_d}] = [\frac{\partial}{\partial x_1}, ..., \frac{\partial}{\partial x_d}]\ J$.

Therefore in the Cartesian coordinates system, the operator can be written as

$$\mathcal{L} = -[\frac{\partial}{\partial x_1}, ..., \frac{\partial}{\partial x_d}]JM_dJ'[\frac{\partial}{\partial x_1}, ..., \frac{\partial}{\partial x_d}]^T. \tag{3.16}$$

In particularly, $-\mathcal{L} = \Delta$ becomes the Laplace operator if we take

$$(\mathbf{e}_\mu, \mathbf{e}_\mu) = 1, \quad (\mu = 1, ..., d), \quad (\mathbf{e}_\nu, \mathbf{e}_\mu) = -\frac{1}{d}, \quad (1 \le \nu \ne \mu \le d). \tag{3.17}$$

In fact, in the special case we have

$$J'J = G(\mathbf{e}_1, ..., \mathbf{e}_d) = \frac{1}{d}((d+1)\mathbf{I}_d - \mathbf{e}\mathbf{e}^T) = M_d^{-1}$$

where $G(\mathbf{e}_1, ..., \mathbf{e}_d))$ is the Gram matrix defined in (2.1). Hence $JM_dJ' = I_d$. In (3.18) case, the corresponding 2-D and 3-D domains Ω show a regular parallel hexagon in Figure 2.1 and a rhombic dodecahedron in 3-D in Figure 2.2, respectively.

Moreover, if we take

$$(\mathbf{e}_\mu, \mathbf{e}_\mu) = 1, \quad (\mu = 1, ..., d), \quad (\mathbf{e}_\nu, \mathbf{e}_\mu) = \cos\alpha, \quad (1 \le \nu \ne \mu \le d). \tag{3.18}$$

Denote $G(\alpha) := \mathbf{I}_d + \cos\alpha\mathbf{e}\mathbf{e}^T$. Since

$$(\mathbf{I}_d + \mathbf{e}\mathbf{e}^T)(\mathbf{I}_d + \cos\alpha\mathbf{e}\mathbf{e}^T) = \mathbf{I}_d + (1 + d\cos\alpha)\mathbf{e}\mathbf{e}^T$$

Then the condition number becomes

$$cond((\mathbf{I}_d + \mathbf{e}\mathbf{e}^T)(\mathbf{I}_d + \cos\alpha\mathbf{e}\mathbf{e}^T)) = \max(1 + d(1 + d\cos\alpha), \frac{1}{1 + d(1 + d\cos\alpha)})$$

In general, therefore, it is reasonable to call $\mathcal{L}$ in (3.12) to be a Laplacian-like operator.

Combining above derivation with the completeness theorem 3.3 leads to the following theorem

Theorem 3.4. *The generalized Fourier functions $g_j(P)$ in (3.1) form an orthogonal and complete eigen-decomposition of the Laplacian-like eigen problem (3.12)-(3.13) with $d+1$-direction periodic boundary conditions on the hyper-dodecahedron domain Ω in (2.18). Moreover, the corresponding eigenvalues are listed in (3.14) with the range $\mathbf{j} \in \Lambda$ in (2.7) .*

4. Generalized Sine and Cosine Functions in $\mathbb{R}^d$

Analogy with 1-D case, now we define generalized sine and cosine functions with periodicity Q from complex Fourier function g_{j} in (3.1) with $d+1$ direction parameters (2.17) in $\mathbb{R}^d$.

At first we observe that for any point $P = [\bar{t}_1, ..., \bar{t}_{d+1}] \in \mathbb{R}^d$, there are totally $(d+1)!$ points which can be obtained by permutation the order from the $d+1$ original parameters . They can be divided into two permutation sets, depending on the permutation number is even or odd.

Definition 4.1. *$[\bar{t}_{\nu_1}, ..., \bar{t}_{\nu_{d+1}}] \in V_+$ or $[\bar{t}_{\nu_1}, ..., \bar{t}_{\nu_{d+1}}] \in V_-$ if the vector is an even or odd permutation of $[\bar{t}_1, ..., \bar{t}_{d+1}]$, respectively.*

Hence, all points can also be divided into two groups.

Definition 4.2. *$\bigwedge_+(P) := \{\bar{P} | \bar{P} \sim [\bar{t}_{\nu_1}, ..., \bar{t}_{\nu_{d+1}}] \in V_+[\bar{t}_1, ..., \bar{t}_{d+1}]\}$ and $\bigwedge_-(P) := \{\bar{P} | \bar{P} \sim [\bar{t}_{\nu_1}, ..., \bar{t}_{\nu_{d+1}}] \in V_-[\bar{t}_1, ..., \bar{t}_{d+1}]\}$.*

Thus, we may define generalized sine and cosine functions as follows

Definition 4.3. *For each point $P \in \mathbb{R}^d$ and index $\mathbf{j} \in \Lambda$,*

$$HSin_{\mathbf{j}}(P) := \frac{1}{(d+1)!i} \{ \sum_{\bar{P}_+ \in \bigwedge_+(P)} g_{\mathrm{j}}(\bar{P}_+) - \sum_{\bar{P}_- \in \bigwedge_-(P)} g_{\mathrm{j}}(\bar{P}_-) \} \tag{4.1}$$

and

$$HCos_{\mathbf{j}}(P) := \frac{1}{(d+1)!} \{ \sum_{\bar{P}_+ \in \bigwedge_+(P)} g_{\mathrm{j}}(\bar{P}_+) + \sum_{\bar{P}_- \in \bigwedge_-(P)} g_{\mathrm{j}}(\bar{P}_-) \}. \tag{4.2}$$

where $g_{\mathrm{j}}(P)$ is the Fourier functions defined in (3.1).

Then, $HSin_{\mathbf{j}}(P) = HSin_{\mathbf{k}}(P)$, if $\mathbf{j} \in \bigwedge_+(\mathbf{k})$; $HSin_{\mathbf{j}}(P) = -HSin_{\mathbf{k}}(P)$, if $\mathbf{j} \in \bigwedge_-(\mathbf{k})$, $HCos_{\mathbf{j}}(P) = HCos_{\mathbf{k}}(P)$, if $\mathbf{j} \in \bigwedge_+(\mathbf{k}) \bigcup \bigwedge_-(\mathbf{k})$.

Definition 4.4. *Two vectors in Λ is called $\mathbf{j} \equiv \mathbf{k}$ (mod$\bigwedge$) if and only if $\mathbf{j} \in \bigwedge_+(\mathbf{k}) \bigcup \bigwedge_-(\mathbf{k})$.*

Lemma 4.1. *For all $\mathbf{j} \in \Lambda$ and all point $P \in \mathbb{R}^d$*

$$||HSin_{\mathbf{j}}(P)|| \le 1, \quad ||HCos_{\mathbf{j}}(P)|| \le 1, \quad ||HSin_{\mathbf{j}}^2(P) + HCos_{\mathbf{j}}^2(P)|| \le 1. \tag{4.3}$$

Proof. The first two inequalities are obvious since $dim(\bigwedge_+(P)) = dim(\bigwedge_-(P)) = \frac{(d+1)!}{2}$. Moreover, because

$$\frac{1}{4}((d+1)!)^2 (HSin_{\mathbf{j}}^2(P) + HCos_{\mathbf{j}}^2(P)) = \sum_{\bar{P}_+ \in \bigwedge_+(P)} g_{\mathrm{j}}(\bar{P}_+) \sum_{\bar{P}_- \in \bigwedge_-(P)} g_{\mathrm{j}}(\bar{P}_-).$$

On the righthand side there are totally $((d+1)!/2)^2$ terms in which the absolute value of each term is not exceed to 1. It leads to the third inequality in (4.3).

The last two inequalities in (4.3) are sharp since both equalities hold on the origin point and several integer points. However, the first inequality is not sharp in general.

The following results on periodicity and orthogonality of $HSin$ and $HCos$ can be derived from Theorem 3.1 Theorem 3.2 on $g_{\mathrm{j}}(P)$ directly.

Lemma 4.2. *For any integer point $Q \in \Theta$ defined in (2.11), for all integer vector $\mathbf{j}$*

$$HSin_{\mathrm{j}}(P+Q) = HSin_{\mathrm{j}}(P), \quad HCos_{\mathrm{j}}(P+Q) = HCos_{\mathrm{j}}(P), \qquad for \;\; all \;\; P. \tag{4.4}$$

Besides, any $Q \in \Theta$ satisfying the condition (3.3) is their minimum periodicity.

Lemma 4.3. *If* $\mathbf{j} \neq \mathbf{k}$ *(mod$\bigwedge$), then*

$$< HSin_{\mathbf{j}},\ HSin_{\mathbf{k}} >_{\Omega}= 0, \quad < HCos_{\mathbf{j}},\ HCos_{\mathbf{k}} >_{\Omega}= 0. \tag{4.5}$$

Besides, for any pair $\mathbf{j}, \mathbf{k} \in \Lambda$

$$< HSin_{\mathbf{j}},\ HCos_{\mathbf{k}} >_{\Omega}= 0. \tag{4.6}$$

Theorem 4.1. *HSin functions vanish on all hyperplanes with* $t_{\nu,\mu}$*=integer, i.e.*

$$HSin_{\mathbf{j}}(P) = 0, \quad if \quad t_{\nu,\mu} = integer, \quad (1 \leq \nu \leq \mu \leq d). \tag{4.7}$$

Proof. It is only need to prove that the function can be decomposed several terms which vanish on all the above hyperplanes. In fact, due to the location symmetry of $\mathbf{j}$ and P in the basic function $g_{\mathbf{j}}$, $HSin_{\mathbf{j}}(P)$ can also be written as

$$\frac{(d+1)!}{2} HSin_{\mathbf{j}}(P) = \frac{1}{2i}\{ \sum_{\mathbf{j}\ \in \bigwedge_{+}(\mathbf{j})} g_{\mathbf{j}}(P) - \sum_{\mathbf{j}\ \in \bigwedge_{-}(\mathbf{j})} g_{\mathbf{j}}(P)\}. \tag{4.8}$$

At first we keep the last index in $\bigwedge_{+}(\mathbf{j})$ to be $\bar{j}_{d+1}$, for any permutation $\mathbf{j}_{+} \ \in \bigwedge_{+}(\mathbf{j})$, we can find a $\mathbf{j}_{-} \ \in \bigwedge_{-}(\mathbf{j})$ via exchanging the first index and last index only, suppose the first index is, say, $\bar{j}_1$, since (2.16), $\bar{j}_1 - \bar{j}_{d+1} = (d+1)j_1$, $\bar{t}_1 - \bar{t}_{d+1} = (d+1)t_1$, then

$$\begin{aligned} g_{\mathbf{j}_{+}}(P) - g_{\mathbf{j}_{-}}(P) &= e^{i\frac{2\pi}{(d+1)^2}\sum_{\nu=2}^{d}\bar{j}_\nu \bar{t}_\nu}\{e^{i\frac{2\pi}{(d+1)^2}(\bar{j}_1\bar{t}_1 + \bar{j}_{d+1}\bar{t}_{d+1}\ )} - e^{i\frac{2\pi}{(d+1)^2}(\bar{j}_{d+1}\bar{t}_1 + \bar{j}_1\bar{t}_{d+1}\ )}\} \\ &= 2ie^{i\frac{2\pi}{(d+1)^2}\sum_{\nu=2}^{d}\bar{j}_\nu \bar{t}_\nu} e^{i\frac{\pi}{(d+1)^2}(\bar{j}_1 + \bar{j}_{d+1})(\bar{t}_1 + \bar{t}_{d+1})} \sin j_1 t_1 \pi \end{aligned}$$

and

$$\frac{1}{2i}\{g_{\mathbf{j}_{+}}(P) - g_{\mathbf{j}_{-}}(P)\} = \exp\{\frac{2\pi i}{(d+1)^2}\sum_{\nu\neq 1}^{d}\bar{j}_\nu \bar{t}_\nu\} \exp\{\frac{\pi i}{(d+1)^2}\sum_{\nu\neq 1}^{d}\bar{j}_\nu \sum_{\nu\neq 1}^{d}\bar{t}_\nu\} \sin j_1 t_1 \pi. \tag{4.9}$$

Hence, in this special case

$$\frac{1}{2i}\{g_{\mathbf{j}_{+}}(P) - g_{\mathbf{j}_{-}}(P)\} = f_1(\bar{t}_2, ..., \bar{t}_d) \sin j_1 t_1 \pi.$$

Thus, we may decompose the generalized sine function (4.1) into $\binom{d+1}{2}$ terms where each term has a factor $\sin j_{\nu,\mu} t_1 \pi$ $(1 \leq \nu \leq \mu \leq d)$

$$HSin_{\mathbf{j}}(P) = \sum_{1\leq\nu\leq\mu\leq d} f_{\nu,\mu}(\bar{t}_2, ..., \bar{t}_d) \sin j_{\nu,\mu} t_{11} \pi$$

where

$$j_{\nu,\nu} = j_\nu, \quad (\nu = 1, ..., d), \quad j_{\nu,\mu} = j_\nu - j_\mu, \quad (1 \leq \nu < \mu \leq d).$$

Therefore, we assert that functions HSin vanish on hyperplanes with $t_1 = t_{11}$=integer. With similar derivation we can prove the left cases of (4.7).
As an example, for 2-D case, we have

$$\begin{aligned} HSin_{\mathbf{j}}(P) &= \frac{1}{3}\{e^{\frac{\pi i}{3}\bar{j}_2\bar{t}_2} \sin j_1 t_1 \pi + e^{\frac{\pi i}{3}\bar{j}_1\bar{t}_2} \sin j_2 t_1 \pi + e^{\frac{\pi i}{3}\bar{j}_3\bar{t}_2} \sin(j_1 - j_2) t_1 \pi\} \\ &= \frac{1}{3}\{e^{\frac{\pi i}{3}\bar{j}_2\bar{t}_1} \sin j_1 t_2 \pi + e^{\frac{\pi i}{3}\bar{j}_1\bar{t}_1} \sin j_2 t_2 \pi + e^{\frac{\pi i}{3}\bar{j}_3\bar{t}_1} \sin(j_1 - j_2) t_2 \pi\} \\ &= \frac{1}{3}\{e^{\frac{\pi i}{3}\bar{j}_2\bar{t}_3} \sin j_1 (t_1 - t_2) \pi + e^{\frac{\pi i}{3}\bar{j}_1\bar{t}_3} \sin j_2 (t_1 - t_2) \pi + e^{\frac{\pi i}{3}\bar{j}_3\bar{t}_3} \sin(j_1 - j_2)(t_1 - t_2) \pi\} \end{aligned}$$

and

$$HCos_{\mathbf{j}}(P) = \frac{1}{3}\{e^{\frac{\pi i}{3}\bar{j}_2\bar{t}_2} \cos j_1 t_1 \pi + e^{\frac{\pi i}{3}\bar{j}_1\bar{t}_2} \cos j_2 t_1 \pi + e^{\frac{\pi i}{3}\bar{j}_3\bar{t}_2} \cos(j_1 - j_2) t_1 \pi\}$$

$$= \frac{1}{3}\{e^{\frac{\pi i}{3}\bar{j}_2\bar{t}_1}\cos j_1 t_2\pi + e^{\frac{\pi i}{3}\bar{j}_1\bar{t}_1}\cos j_2 t_2\pi + e^{\frac{\pi i}{3}\bar{j}_3\bar{t}_1}\cos(j_1 - j_2)t_2\pi\}$$

$$= \frac{1}{3}\{e^{\frac{\pi i}{3}\bar{j}_2\bar{t}_3}\cos j_1 t_{12}\pi + e^{\frac{\pi i}{3}\bar{j}_1\bar{t}_3}\cos j_2 t_{12}\pi + e^{\frac{\pi i}{3}\bar{j}_3\bar{t}_3}\cos j_{12} t_{12}\pi\}.$$

Along with a similar way, in general $d-$ dimension case, the generalized cosine function $HCos_{\mathbf{j}}(P)$ can be decomposed into $\binom{d+1}{2}$ terms. Each term involves a factor $\cos j_{\nu,\mu} t_1\pi$ such that

$$HCos_{\mathbf{j}}(P) = HCos_{\mathbf{j}}(t_1, \bar{t}_2, ..., \bar{t}_d) = \sum_{1\le\nu\le\mu\le d} f_{\nu,\mu}(\bar{t}_2, ..., \bar{t}_d)\cos j_{\nu,\mu} t_1\pi.$$

Note that the term $f_{\nu,\mu}(\bar{t}_2, ..., \bar{t}_d)$ before $\cos j_1 t_1\pi$ do not depend on the variable t_1. Therefore, as a function depends on d variables $(t_1, \bar{t}_2, ..., \bar{t}_d)$, we know that the partial differential functions $\frac{\partial HCos_{\mathbf{j}}(t_1,\bar{t}_2,...,\bar{t}_d)}{\partial t_1}$ vanish on hyperplanes with $t_1 = integer$.

In general, for each $\lambda = 1, ..., d$, since the d variables $(\bar{t}_1, ..., \bar{t}_{\lambda-1}, t_\lambda, \bar{t}_{\lambda+1}, ..., \bar{t}_d)$ are independent, hence, there are additive separable decompositions of $HCos_{\mathbf{j}}(P)$ such that

$$HCos_{\mathbf{j}}(P) = HCos_{\mathbf{j}}(\bar{t}_1, ..., \bar{t}_{\lambda-1}, t_\lambda, \bar{t}_{\lambda+1}, ..., \bar{t}_d)$$
$$= \sum_{1\le\nu\le\mu\le d} f_{\nu,\mu}(\bar{t}_1, ..., \bar{t}_{\lambda-1}, \bar{t}_{\lambda+1}, ..., \bar{t}_d)\cos j_{\nu,\mu} t_\lambda\pi.$$

Analogically, for each $(1 \le l < m \le d)$, the d variables $(\bar{t}_1, ..., \bar{t}_{l-1}, \bar{t}_{l+1}, t_{lm}, \bar{t}_{m-1}, \bar{t}_{m+1}, ..., \bar{t}_d, \bar{t}_{d+1})$ are independent, hence, there are additive separable decompositions of $HCos_{\mathbf{j}}(P)$ such that

$$HCos_{\mathbf{j}}(P) = HCos_{\mathbf{j}}(\bar{t}_1, ..., \bar{t}_{l-1}, \bar{t}_{l+1}, t_{lm}, \bar{t}_{m-1}, \bar{t}_{m+1}, ..., \bar{t}_d, \bar{t}_{d+1})$$
$$= \sum_{1\le\nu\le\mu\le d} f_{\nu,\mu}(\bar{t}_1, ..., \bar{t}_{l-1}, \bar{t}_{l+1}, \bar{t}_{m-1}, \bar{t}_{m+1}, ..., \bar{t}_d, \bar{t}_{d+1})\cos j_{\nu,\mu} t_{lm}\pi.$$

The above derivations lead to the following assertion

Theorem 4.2.

$$\frac{\partial HCos_{\mathbf{j}}(P)}{\partial t_{\nu,\mu}}|_{t_{\nu,\mu}=integer} = 0, \quad (1 \le \nu \le \mu \le d). \tag{4.10}$$

In geometry, for each $1 \le \nu \le \mu \le d$, $t_{\nu,\mu}$ represents a direction connecting a vertex and the barycenter of corresponding simplex. Hence, the above identities (4.10) may be called Neumann boundary conditions on a simplex.

In the sense of mod$\bigwedge$, the number of index is reduced by a factor $(d+1)!$. Hence, for functions $HSin_{\mathbf{j}}(P)$ and $HCos_{\mathbf{j}}(P)$ we can reduced the defined domain from Ω to one of its $(d+1)!$ simplex, e.g. Ω_S in (2.15) and reduced the index vector range $\mathbf{j}$ from Λ to

$$\Xi := \{\mathbf{j} \in \Lambda \mid 0 < \bar{j}_1 \le \bar{j}_2 \le \cdots \le \bar{j}_d\}, \tag{4.11}$$

or

$$\Xi^+ := \{\mathbf{j} \in \Lambda \mid 0 \le \bar{j}_1 \le \bar{j}_2 \le \cdots \le \bar{j}_d\}. \tag{4.12}$$

for $HSin_{\mathbf{j}}(P)$ and $HCos_{\mathbf{j}}(P)$, respectively.

Finally, we obtain following conclusions

Theorem 4.3. *The generalized sine family $HSin_{\mathbf{j}}(P)$ in (4.1) and the generalized cosine family $HCos_{\mathbf{j}}(P)$ in (4.2) form an orthogonal complete eigen-decomposition of eigen problem (3.13) with zero boundary conditions or with zero Neumann boundary conditions (4.10) along a given simplex (2.15) respectively. Moreover, their corresponding eigenvalues are also listed in (3.14) for $\mathbf{j} \in \Xi$ or $\mathbf{j} \in \Xi^+$, respectively .*

Similarly to univariate case, now we may define so-called generalized sine transform and cosine transform as follows

Definition 4.5. *For a $f \in L(\Omega_S)$, its generalized sine transform (HCT) is defined as*

$$f(P) \sim \sum_{\mathbf{j} \in \Xi^+} \alpha_{\mathbf{j}} \quad HCos_{\mathbf{j}}(P), \qquad \alpha_{\mathbf{j}} = \frac{1}{c_{\Omega_S}} < f(P), HCos_{\mathbf{j}}(P) >_{\Omega_S} \tag{4.13}$$

and its generalized cosine transform (HST) is defined as

$$f(P) \sim \sum_{\mathbf{j} \in \Xi} \beta_{\mathbf{j}} \quad HSin_{\mathbf{j}}(P), \qquad \beta_{\mathbf{j}} = \frac{1}{c_{\Omega_S}} < f(P), HSin_{\mathbf{j}}(P) >_{\Omega_S} \tag{4.14}$$

where c_{Ω_S} is the volume of the simplex Ω_S and Ξ and Ξ^+ are defined in (4.11) and (4.12), respectively.

Analogy to the proof of Theorem 3.3, we obtain the following results:

Theorem 4.4. *For all $\mathbf{j} \in \Xi$, the set of $HSin_{\mathbf{j}}(P)$ and $HCos_{\mathbf{j}}(P)$ form complete orthogonal system in the space $C(\Omega_S(\mathbb{R}^d))$, respectively.*

Lemma 4.4. *Let $f \in L(\Omega_S)$. If all coefficients of its HST or HCT vanish, i.e. all $\alpha_{\mathbf{j}} = 0$ or all $\beta_{\mathbf{j}} = 0$, then $f = 0$ .a.e.*

Corollary 4.1. *For a d-D continuous function $f(P) \in C_{\Omega_S}$ with zero boundary values along Ω_S , if its all coefficients $\beta_{\mathbf{j}}$ are zeros, the function $f(P)$ must equal to zero itself.*

5. Discrete Fourier Transform (HFT) and Fast Fourier Transform (HFFT) over $\Omega(\mathbb{R}^d)$

Now we consider so-called discrete Fourier transform. Set discrete sets

$$\Lambda_N := \{\mathbf{k} \in \Lambda \mid -N \leq k_{\nu,\mu} \leq N-1, \ 1 \leq \nu \leq \mu \leq d\}. \tag{5.1}$$

where Λ is defined in (2.7). In 3-D case, a picture for Λ_2 is shown in Figure 5.3.

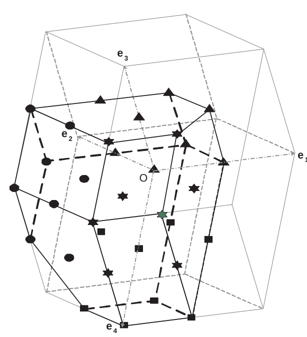

Figure 5.3: A discrete set Λ_2 in 3-D

Just like the decomposition (2.13) in continuous case, there is a decomposition for discrete case

$$\Lambda_N := \bigcup_{\nu=1}^{d+1} \Lambda_{N,\nu}$$

where

$$\Lambda_{N,\nu} = \{\mathbf{k} \in \Lambda \mid 1 \le k_{\mu,\nu} \le N, \quad 1 \le \mu < \nu, \quad or \quad 1-N \le k_{\nu,\mu} \le 0, \quad \mu \ge \nu\}, \qquad \nu = 1, ..., d.$$

$$\Lambda_{N,d+1} = \{\mathbf{k} \in \Lambda \mid 1 \le k_{\mu,\mu} \le N, \quad \mu = 1, ..., d.\}. \tag{5.2}$$

Hence, we have

Lemma 5.1.

$$dim\ \Lambda_N = \sum_{\nu=1}^{d+1} dim\ \Lambda_{N,\nu} = (d+1)N^d.$$

Definition 5.1. *Given $(d+1)N^d$ data $\{f_\mathbf{k}\}$ with $\mathbf{k} \in \Lambda_N$, for $\mathbf{j} \in \Lambda_N$ the generalized discrete Fourier transform (HDFT) is defined as*

$$F_\mathbf{j} = \sum_{\mathbf{k} \in \Lambda_N} g^N_{\mathbf{j},\mathbf{k}} f_\mathbf{k}\ , \quad g^N_{\mathbf{j},\mathbf{k}} \ = \ e^{\frac{2\pi i}{(d+1)N}\mathbf{j}\cdot\mathbf{k}} \tag{5.3}$$

and the related inverse discrete Fourier transform (HIDFT) is defined as

$$f_\mathbf{j} = \frac{1}{(d+1)N^d} \sum_{\mathbf{k} \in \Lambda_N} \bar{g}^N_{\mathbf{j},\mathbf{k}} F_\mathbf{k}\ , \quad \bar{g}^N_{\mathbf{j},\mathbf{k}} = e^{-\frac{2\pi i}{(d+1)N}\mathbf{j}\cdot\mathbf{k}} \tag{5.4}$$

Remark. The definition of the above inverse transform is reasonable and unique, because by using the similar derivation of Lemma 3.1 we know

$$\sum_{\mathbf{k} \in \Lambda_N} g^N_{\mathbf{j_1},\mathbf{k}} \bar{g}^N_{\mathbf{j_2},\mathbf{k}} = (d+1)N^d \delta_{|\mathbf{j_1}-\mathbf{j_2}|,0}. \tag{5.5}$$

The corresponding matrix form of the HDFT and HIDFT become

$$\mathbf{F} = G_N\ \mathbf{f}, \quad G_N = (\ g^N_{\mathbf{j},\mathbf{k}}\ ) \tag{5.6}$$

and

$$\mathbf{f} = G_N^{-1}\ \mathbf{F}, \quad G_N^{-1} = \frac{1}{(d+1)N^d}(\ \bar{g}^N_{\mathbf{j},\mathbf{k}}\ ). \tag{5.7}$$

It is obvious that the working amount is $O(N^{2d})$ in magnitude by direct matrix multiplication. It is too expansive for applications.

In the case of $d = 2$ and $d = 3$ we have proposed and implemented a corresponding fast algorithm called HFFT ([9], [14]). The HFFT algorithm can also be extended on our general d-dimension case based on the following Lemma listed below. Let us start from the case $N = 2n$.

Lemma 5.2. *For $N = 2n$ there is a factorization for G_N in terms of smaller G_n in $\mathbb{R}^d$:*

$$G_N = P_N^{-1}(T_{2,d} \bigotimes I_{(d+1)n^d}) D_N (I_{2^d} \bigotimes G_n) Q_N \tag{5.8}$$

where $T_{2,d}$, defined below in (5.16), is a constant matrix of order 2^d and I_m is the identity matrix with an indicated order m , notation $\bigotimes$ is so-called Krönecker product, D_N, defined in (5.15), is a diagonal matrix of order $(d+1)N^d$, P_N and Q_N are two permutation matrices of order $(d+1)N^d$ which represent domain decomposition on the left-side for $\mathbf{F}$ and multi-color reordering on the right-hand for $\mathbf{f}$, respectively.

Proof. By using periodicity of function $g^N_{\mathbf{j},\mathbf{k}}$ we first extend the data from Λ_N to Λ_N^* defined as

$$\Lambda_N^* := \{\mathbf{k} \in \Lambda \mid -N \le k_{\nu,\mu} \le N,\ 1 \le \nu \le \mu \le d\}.$$

In order to do multi-color reordering, we take two 2^d integer points as

$$\mathbf{P}_\nu = \sum_{l=1}^{d} \nu_l \mathbf{e}^{[l]} \in \Lambda, \quad \mathbf{Q}_\nu = \sum_{l=1}^{d} \nu_l (\mathbf{e}^{[l]} + \sum_{l=1}^{d} \mathbf{e}^{[l]}) \in \Theta, \quad (\nu_1, ..., \nu_d = 0, 1). \tag{5.9}$$

where $\mathbf{e}^{[l]}$ is l-th coordinate unit vector in $\mathbb{R}^n$. In terms of vectors in $\mathbb{R}^{\binom{d+1}{2}}$, it is easy to know their inner product

$$(\mathbf{e}^{[m]}, \mathbf{e}^{[n]}) = 3\delta_{n,m} - 1, \quad (\mathbf{e}^{[m]}, \sum_{n=1}^{d} \mathbf{e}^{[n]}) = 3 - d \ \ (m = 1, ..., d). \tag{5.10}$$

Moreover,

$$(\mathbf{P}_\nu, \mathbf{Q}_\nu) = \sum_{n,m=1}^{d} (3\delta_{n,m} + (2-d))\nu_n \mu_m. \tag{5.11}$$

Denote

$$\Lambda_N^{[2]}(P_\nu) = \{\mathbf{k} \ |2\mathbf{k} + \mathbf{P}_\nu \in \Lambda_N^*\}.$$

then the original data can be decomposed into 2^d parts by multi-color reordering

$$\{f_\mathbf{k} | \mathbf{k} \in \Lambda_N\} = \bigcup_{\nu_1,...,\nu_d=0}^{1} \{f_\mathbf{k} | \mathbf{k} \in \Lambda_N^{[2]}(P_\nu)\} = \bigcup_{\nu_1,...,\nu_d=0}^{1} \{f_{2\mathbf{k}+\mathbf{P}_\nu} | \mathbf{k} \in \Lambda_n\} \tag{5.12}$$

where all $f_{2\mathbf{k}+\mathbf{P}_\nu}$ represent data $f_\mathbf{k} \in \Lambda_N^{[2]}(P_\nu)$ via a suitable reordering the subscript $\mathbf{k}$.

Similarly, based on the periodic extension the functional data also can be divided into 2^d parts via domain decomposition

$$\{F_\mathbf{j} | \mathbf{j} \in \Lambda_N\} = \bigcup_{\mu_1,...,\mu_d=0}^{1} \{F_\mathbf{j} | \mathbf{j} \in \Lambda_n(nQ_\mu)\} = \bigcup_{\mu_1,...,\mu_d=0}^{1} \{F_{\mathbf{j}+n\mathbf{Q}_\mu} | \mathbf{j} \in \Lambda_n\} \tag{5.13}$$

where all $F_{\mathbf{j}+\mathbf{n}\mathbf{Q}_\mu}$ represent data $F_\mathbf{j} \in \Lambda_n(nQ_\mu)$ via a suitable reordering the subscript $\mathbf{j}$. A simple example in 2-D is shown in Figure 5.4-5.5 and Figure 5.6 [9].

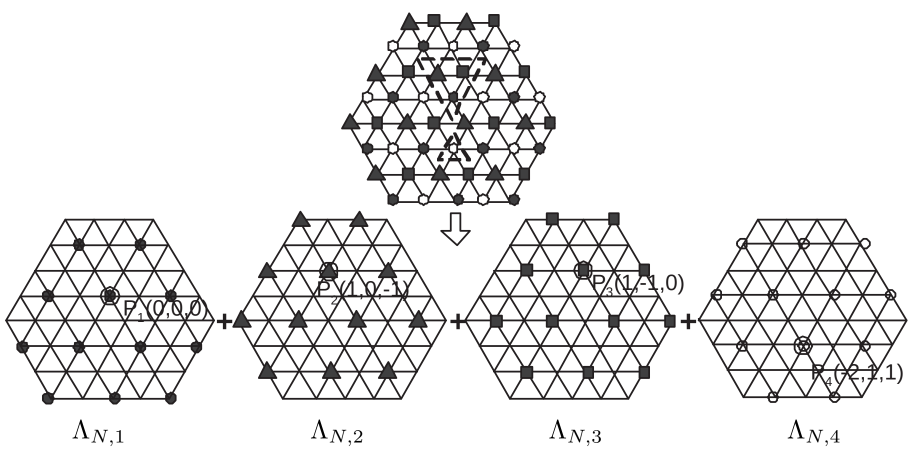

Figure 5.4: 2-D Odd-even reordering Λ_{2n}

Since (2.11),(2.17)and (5.3) we know $g^n_{n\mathbf{Q}_\mu,\mathbf{k}} = 1$, hence

$$g^N_{\mathbf{j}+n\mathbf{Q}_\mu,2\mathbf{k}+\mathbf{P}_\nu} = g^N_{n\mathbf{Q}_\mu,2\mathbf{k}} \cdot g^N_{n\mathbf{Q}_\mu,\mathbf{P}_\nu} \cdot g^N_{\mathbf{j},\mathbf{P}_\nu} \cdot g^N_{\mathbf{j},2\mathbf{k}} = g^2_{\mathbf{Q}_\mu,\mathbf{P}_\nu} \cdot g^N_{\mathbf{j},\mathbf{P}_\nu} \cdot g^n_{\mathbf{j},\mathbf{k}}.$$

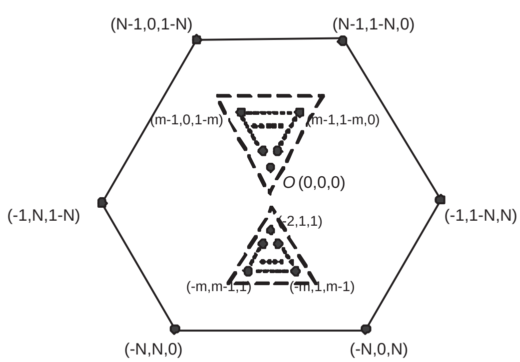

Figure 5.5: 2-D Multi-color reordering

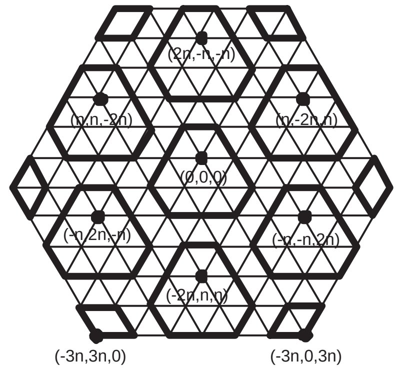

Figure 5.6: 2-D Domain-decomposition

Substituting (5.12) and (5.13) into (5.3) leads to

$$F_{\mathbf{j}+n\mathbf{Q}_\mu} = \sum_{\nu_1,\ldots,\nu_d=0}^{1} \sum_{\mathbf{k}\,\in\Lambda_n(\mathbf{P}_\nu)} g^N_{\mathbf{j}+n\mathbf{Q}_\mu,2\mathbf{k}+\mathbf{P}_\nu} f_{\mathbf{k}} = \sum_{\nu_1,\ldots,\nu_d=0}^{1} g^2_{\mathbf{Q}_\mu,\mathbf{P}_\nu}\cdot g^N_{\mathbf{j},\mathbf{P}_\nu} \sum_{\mathbf{k}\,\in\Lambda_n(\mathbf{P}_\nu)} g^n_{\mathbf{j},\mathbf{k}} f_{\mathbf{k}}. \quad (5.14)$$

where the first two terms are independent on $\mathbf{k}$

$$g^2_{\mathbf{Q}_\mu,\mathbf{P}_\nu} = \exp\{\frac{\pi i}{d+1}(\mathbf{P}_\nu,\mathbf{Q}_\mu)\}, \quad g^N_{\mathbf{j},\mathbf{P}_\nu} = \exp\{\frac{2\pi i}{(d+1)N}\sum_{l=1}^{d} j_l\nu_l\}.$$

Denote a 2^d order matrix by $T_{2,d} = (g^2_{\mathbf{Q}_\mu,\mathbf{P}_\nu})$, and a $(d+1)N^d$ order diagonal matrix by

$$D_N = (\exp\{\frac{2\pi i}{(d+1)N}\sum_{l=1}^{d} j_l\nu_l\})_{\mathbf{j}\in\Lambda_n,(\nu_1,\ldots\nu_d=0,1)} \quad (5.15)$$

By (5.11), $T_{2,d}$ can be expressed to

$$T_{2,d} = (\exp\{\frac{\pi i}{d+1}(\sum_{n,m=1}^{d}(3\delta_{n,m}+(2-d))\nu_n\mu_m)\})_{(\nu_1,\ldots\nu_d=0,1)\times(\mu_1,\ldots,\mu_d=0,1)} \quad (5.16)$$

In particulary, for $d=2$

$$T_{2,2} = ((-1)^{\nu_1\mu_1+\nu_2\mu_2})_{-0\le\nu_1,\nu_2,\mu_1,\mu_2\le 1} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} = T_2 \bigotimes T_2 \quad (5.17)$$

where matrix $T_2 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ appears in the usual 1-D FFT algorithm.

Take P_N and Q_N to be two suitable permutation matrices of order $(d+1)N^d$ which represent domain decomposition on the left-side for $\mathbf{F}$ and multi-color reordering on the right-hand for $\mathbf{f}$, respectively. Substituting the above matrices into (5.14) leads to the matrix form (5.8). Hence we have proved the above Lemma 5.2.

Furthermore, we have

Corollary 5.1. *For a general case $N = N_0 2^m$ the transform matrix G_N can be represented by G_{N_0} via the following factorization*

$$G_N =(\prod_{l=1}^{m}\{(I_{2^{d(l-1)}} \bigotimes P^{-1}_{N2^{1-l}})(I_{2^{d(l-1)}} \bigotimes (T_{2,d} \bigotimes I_{(d+1)(2^{-l}N)^d})(I_{2^{d(l-1)}} \bigotimes D_{N2^{1-l}})\})$$
$$(I_{2^{md}} \bigotimes G_{N_0})(\prod_{l=1}^{m}\{I_{2^{d(m-l)}} \bigotimes Q_{N2^{l-m}}\}), \tag{5.18}$$

where $P_{N2^{1-l}}$ and $Q_{N2^{l-m}}$ $(l = 1, ..., m)$ are related l-step permutation operators on function data $F_{\mathbf{j}}$ and original data $f_{\mathbf{k}}$, respectively, $D_{N2^{1-l}}$ are the corresponding diagonal matrices.

Moreover, there is analogue factorization for more general case $N = N_0 n^m$.

Corollary 5.2. *If $N = N_0 n^m$, then*

$$G_N =(\prod_{l=1}^{m}\{(I_{n^{d(l-1)}} \bigotimes P^{-1}_{Nn^{1-l}})(I_{n^{d(l-1)}} \bigotimes (T_{n,d} \bigotimes I_{(d+1)(n^{-l}N)^d})(I_{n^{d(l-1)}} \bigotimes D_{Nn^{1-l}})\})$$
$$(I_{n^{md}} \bigotimes G_{N_0})(\prod_{l=1}^{m}\{I_{n^{d(m-l)}} \bigotimes Q_{Nn^{l-m}}\}), \tag{5.19}$$

where $T_{n,d}$ is a constant matrix of order n^d

$$T_{n,d} = (\exp\{\frac{2\pi i}{n(d+1)}(\mathbf{P}_\nu, \mathbf{Q}_\mu)\})_{(\nu_1,\dots\nu_d=0,\dots,n-1)\times(\mu_1,\dots,\mu_d=0,\dots,n-1)}. \tag{5.20}$$

Therefore, the following theorem is a natural consequence of the above corollary.

Theorem 5.1. *The HFFT factorization formula (5.19) can reduce the computation complexity of matrix multiplication (5.7) from $O(N^{2d})$ to $O(N^d LogN)$.*

Similar to the above HDFT in(5.3), we may also define so-called generalized discrete sine (HDST) and discrete cosine transform (HDCT) over Ω_S.

Let $\Xi_N = \Lambda_N \bigcap \Xi$ and $\Xi_N^+ = \Lambda_N \bigcap \Xi^+$. It is not hard to know the amount of nodes for Ξ_N and Ξ_N^+ equal to the freedom number of the corresponding $(n-1-d)$-degree and n-degree polynomials in $\mathbb{R}^d$, i.e.

$$dim\Xi_N(\mathbb{R}^d) = \binom{N-1}{d}, \quad dim\Xi_N^+(\mathbb{R}^d) = \binom{N+d}{d}.$$

Definition 5.2. *Given $\binom{N-1}{d}$ data $\{f_{\mathbf{k}}\}$ with $\mathbf{k} \in \Xi_N$ $(N \geq d+1)$, for $\mathbf{j} \in \Xi_N$ the generalized discrete sine transform (HDST) and its inverse transform can be defined as*

$$HS_{\mathbf{j}}\ [f] = \sum_{\mathbf{k}\ \in \Xi_N} HSin^N_{\mathbf{j},\mathbf{k}}\ f_{\mathbf{k}} \tag{5.21}$$

and

$$HS^{-1}_{\mathbf{j}}\ [f] = \frac{1}{\binom{N-1}{d}} \sum_{\mathbf{k}\ \in \Xi_N} HSin^N_{\mathbf{j},\mathbf{k}}\ f_{\mathbf{k}} \tag{5.22}$$

respectively, where $HSin^N_{\mathbf{j},\mathbf{k}}$ is defined in (4.1).

Definition 5.3. *Given $\binom{N+d}{d}$ data $\{f_{\mathbf{k}}\}$ with $\mathbf{k} \in \Xi_N^+$, for $\mathbf{j} \in \Xi_N^+$ the generalized discrete cosine transform (HDCT)and its inverse transform can be defined as*

$$HC_{\mathbf{j}}\ [f] = \sum_{\mathbf{k}\ \in \Xi_N^+} HCos^N_{\mathbf{j},\mathbf{k}}\ f_{\mathbf{k}} \tag{5.23}$$

and

$$HC_{\mathbf{j}}^{-1}\ [f] = \frac{1}{\binom{N+d}{d}} \sum_{\mathbf{k}\ \in \Xi_N^+} HCos_{\mathbf{j},\mathbf{k}}^N\ f_{\mathbf{k}} \tag{5.24}$$

respectively, where $HCos_{\mathbf{j},\mathbf{k}}^N$ *is defined in (4.2).*

The above fast algorithms (5.19) designed for HFFT can be moved to the case of HDST and HDCT. One may also design the fast transform special for HDST or HDCT. Recently some fast algorithms have been designed and implemented in $2-D$ [9]. and $3-D$ case [14] And this approach has been applied to construct so-called approximate eigen-decomposition preconditioners for solving numerical PDE problems [7]. This approach may become a useful tools of spectral methods and preconditioning algorithm for numerical PDE solvers.

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