ASYMPTOTIC BEHAVIOR OF LATTICE SUMS

by

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ABSTRACT

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This study presents precise asymptotic expansions for a class of two-dimensional lattice sums derived from the Moore–Penrose pseudo-inverse of Laplacian matrices. Our primary focus is on

$$F_{m,n} = \sum_{\substack{0 \le j < m \\ 0 \le k < n \\ (j,k) \neq (0,0)}} \frac{1}{1 - \frac{1}{L}\sum_{\ell=1}^{L} \cos\left(s_{1,\ell}\frac{2\pi j}{m} + s_{2,\ell}\frac{2\pi k}{n}\right)},$$

where $L \geq 2$ and $\mathbf{s}_\ell = (s_{1,\ell}, s_{2,\ell})$ define the lattice basis. The derivation of its asymptotic expansion employs midpoint quadrature for integral approximations, uses the Euler–Maclaurin formula to estimate errors, and introduces auxiliary functions to handle boundary terms and the singularity at the origin.

For each lattice, while the leading order term in the asymptotic expansion depends on the associated lattice basis, secondary and lower order terms encode geometric data through special functions such as the Gamma function and Dedekind's eta function. This methodology extends naturally to Kirchhoff indices in large periodic networks, providing both theoretical insights into graph-invariant asymptotics and practical tools for evaluating lattice sums as $n \to \infty$.

ÖZET

LATİS TOPLAMLARININ ASİMPTOTİK DAVRANIŞI

Bu çalışma, Laplace matrislerinin Moore–Penrose yalancı-tersinden türetilen iki boyutlu latis toplamları sınıfı için kesin asimptotik açılımlar sunmaktadır. Birincil odak noktamız şu formüldür:

$$F_{m,n} = \sum_{\substack{0 \le j < m \\ 0 \le k < n \\ (j,k) \neq (0,0)}} \frac{1}{1 - \frac{1}{L} \sum_{\ell=1}^{L} \cos\left(s_{1,\ell} \frac{2\pi j}{m} + s_{2,\ell} \frac{2\pi k}{n} \right)}.$$

Burada $L \geq 2$ ve $\mathbf{s}_\ell = (s_{1,\ell}, s_{2,\ell})$ latis tabanını tanımlamaktadır.

Bu ifadenin asimptotik açılımının türetilmesinde, integral yaklaşımları için orta nokta kuadratürü kullanılmakta, hata tahminleri için Euler–Maclaurin formülü uygulanmakta ve sınır terimleri ile orijindeki tekilliği ele almak için yardımcı fonksiyonlar tanıtılmaktadır.

Her latis için, asimptotik açılımdaki baskın terim ilgili latis tabanına bağlı iken, ikincil ve daha düşük derecedeki terimler Gamma fonksiyonu ve Dedekind'in eta fonksiyonu gibi özel fonksiyonlar aracılığıyla geometrik veriyi kodlamaktadır. Bu metodoloji, büyük periyodik ağlardaki Kirchhoff indekslerine doğal bir şekilde genişleyerek, graf değişmezlerinin asimptotik davranışları hakkında teorik içgörüler ve $n \to \infty$ iken latis toplamlarını hesaplamak için pratik araçlar sağlamaktadır.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF SYMBOLS

A	Adjacency matrix
B_ℓ	Bernoulli numbers
$C(a,b,c)$	Auxiliary function defined in equation (4.29)
d	Discriminant of the quadratic form, $d = b^2 - 4ac < 0$
D	Degree matrix
E	Set of edges in a graph
$f(\mathbf{x})$	Function defined as $f(\mathbf{x}) = \frac{1}{\varphi(\mathbf{x})}$
$f_1(\mathbf{x})$	First-order approximation function defined as $f_1(\mathbf{x}) = \frac{1}{\varphi_1(\mathbf{x})}$
$f_m(\mathbf{x})$	Higher-order approximation function defined as $f_m(\mathbf{x}) = \frac{1}{p_m(\mathbf{x})}$
$F_{m,n}$	Lattice sum over $m \times n$ grid
F_n	Shorthand notation for $F_{n,n}$ when $m = n$
$F_n(f)$	Sum of function f evaluated at lattice points with spacing $1/n$
G	Graph or Catalan's constant depending on context
G_n	Auxiliary sum defined in equation (4.25)
$h_m(\mathbf{x})$	Difference function defined as $h_m(\mathbf{x}) = f(\mathbf{x}) - f_m(\mathbf{x})$
$I_{m,n}$	Integral approximation of $F_{m,n}$
L	Number of basis vectors in the lattice
$\mathcal{L}$	Laplacian matrix
m, n	Dimensions of the lattice grid
$p_1(\mathbf{x})$	Second-order Taylor polynomial of $\varphi(\mathbf{x})$ defined in equation (2.23)
$p_m(\mathbf{x})$	Higher-order Taylor polynomial of $\varphi(\mathbf{x})$
$Q(j,k)$	Positive definite binary quadratic form
S	Matrix of basis vectors $\mathbf{s}_\ell$ as defined in equation (2.46)
V	Set of vertices in a graph
α, β	Parameters used in error bounds and domain specifications
γ	Euler–Mascheroni constant
Γ	Gamma function

η	Dedekind eta function
$\varphi(\mathbf{x})$	Lattice denominator function, $\varphi(\mathbf{x}) = 1 - \frac{1}{L}\sum_{\ell=1}^{L}\cos(\mathbf{s}_\ell \cdot \mathbf{x})$
$\Vert\mathbf{x}\Vert$	Euclidean norm of vector $\mathbf{x}$
$\mathcal{O}(\cdot)$	Standard Bachmann–Landau notation for asymptotic upper bounds
$\mathbf{s}_\ell = (s_{1,\ell}, s_{2,\ell})$	ℓ-th vector in the basis set
$\mathbf{t}_{j,k} = (t_j, t'_k)$	Lattice points in the plane, $\mathbf{t}_{j,k} = \left(\frac{2\pi j}{m}, \frac{2\pi k}{n}\right)$
$\mathbf{x}_{j,k} = (x_j, x'_k)$	Shifted lattice points, $\mathbf{x}_{j,k} = (t_j - \frac{\pi}{m}, t'_k - \frac{\pi}{n})$
$\mathcal{X}_{j,k}$	Rectangle $[x_j, x_{j+1}] \times [x'_k, x'_{k+1}]$ centered at $\mathbf{t}_{j,k}$

1. INTRODUCTION

Lattice sums provide a framework for connecting discrete and continuous mathematical structures, with applications in graph theory and physical systems such as electrical networks. The cornerstone of this study is the Laplacian matrix, expressed as $\mathcal{L} = D - A$, where D denotes the degree matrix and A the adjacency matrix of a graph G defined by vertices V and edges E. Through its pseudo-inverse, $\mathcal{L}^+$, we derive lattice sums $F_{m,n}$ that encode graph invariants, such as Kirchhoff indices. See Mohar [1] for an overview of Laplacian spectra, and Chung [2] for a comprehensive treatment of spectral properties in graph theory underpinning these invariants.

The lattice sum under consideration is defined as in [3–5]

$$F_{m,n} = \sum_{\substack{0\le j<m \\ 0\le k<n \\ (j,k)\neq(0,0)}} \frac{1}{1 - \frac{1}{L}\sum_{\ell=1}^{L} \cos\left(s_{1,\ell}\frac{2\pi j}{m} + s_{2,\ell}\frac{2\pi k}{n}\right)},$$

where $L \geq 2$ is the number of basis vectors defining the lattice, and $\mathbf{s}_\ell = (s_{1,\ell}, s_{2,\ell}) \in \mathbb{Z}^2$ are integer pairs specifying the lattice structure. For the special case where $m = n$, we denote $F_n = F_{n,n}$, which we analyze for specific lattices such as the triangular case. The asymptotic analysis of $F_{m,n}$ as $m, n \to \infty$ addresses the discrete domain and the singularity at $(j,k) = (0,0)$. While earlier studies (e.g., [6]) approximated such sums via numerical integrals, their approaches were limited by divergence near the origin. As shown in [3–5], standard integral methods alone prove insufficient for this analysis, necessitating a more sophisticated approach.

This thesis provides an overview of the developments in [3–5] where the asymptotic behavior of the sum $F_{m,n}$ is derived through a systematic decomposition of $F_{m,n}$ into integral and boundary components. This decomposition employs midpoint quadrature for integral approximation, applies Euler–Maclaurin summation techniques, and leverages special function analysis to resolve singularities and handle lattice symmetries.

One of the key results in [3–5], presented below, provides a precise asymptotic expansion for the triangular lattice case and exemplifies the methodology (combining midpoint quadrature, Euler–Maclaurin summation, and special function analysis) applied throughout the thesis.

Theorem 1.1 (Asymptotic Expansion for Triangular Lattice)**.** *For a triangular lattice G with basis $\mathbf{s}_1 = (1,0)$, $\mathbf{s}_2 = (0,1)$, $\mathbf{s}_3 = (1,1)$, the sum $F_n = F_{n,n}$ admits the following asymptotic expansion as $n \to \infty$:*

$$F_n = \frac{\sqrt{3}}{\pi} n^2 \log n + \frac{\sqrt{3}}{\pi}\left(\gamma + \log\left(4\pi\sqrt[4]{3}\right) - 3\log\Gamma\left(\frac{1}{3}\right)\right) n^2 + \mathcal{O}(\log n), \quad \text{as } n \to \infty, \tag{1.1}$$

where γ denotes the Euler–Mascheroni constant.

The leading $\frac{\sqrt{3}}{\pi} n^2 \log n$ term reflects the balance between discrete summation and continuous approximation in F_n. Computing the subsequent n^2 constant term necessitates meticulous asymptotic analysis near $(j,k) = (0,0)$, with the $\mathcal{O}(\log n)$ error arising from the logarithmic singularity's growth refined by boundary corrections. The presence of $\Gamma\left(\frac{1}{3}\right)$ and γ highlights the essential role of special function theory in determining the constant terms with precision. This leading coefficient here matches the general form $\frac{L}{\pi\sqrt{\det(S^T S)}}$, where S is the basis matrix, unifying the triangular result with broader lattice analyses in §5.

Technically, the primary challenge in analyzing $F_{m,n}$ stems from its discrete nature and the origin's singularity. Our approach captures the leading $n^2 \log n$ behavior, identifies $\mathcal{O}(n^2)$ subleading terms, and reveals geometric data through special function values, extending naturally to square and union jack lattices in §5, where the asymptotic structure manifests across diverse geometries.

Beyond its theoretical value, Theorem 1.1 holds practical significance for physical contexts, such as electrical network analysis and random walks on graphs. These rigorous asymptotic formulas provide theoretical insights into large-scale lattice phenomena and computationally efficient tools for evaluating spectral graph invariants like the Kirchhoff and Wiener indices.

The thesis unfolds as follows. §2 defines lattice sums rigorously, covering the Laplacian matrix, its pseudo-inverse, and essential facts regarding asymptotic expansions and special functions. §3 develops detailed proofs for the square lattice, establishing foundational relations between free, cylindrical, and toroidal boundary conditions, while introducing our core analytical machinery using midpoint quadrature. §4 refines these results for higher-order terms when $m = n$, followed by applications to square, triangular, and union jack lattices, demonstrating how the main asymptotic statements materialize in concrete settings. Finally, §5 synthesizes our findings and discusses broader implications.

Notation follows standard conventions. Bold symbols represent vectors and sums over empty index sets are zero.

2. LATTICE SUMS

2.1. Preliminaries

In this section, we introduce the key tools and notation used throughout this work. These include the Euler–Maclaurin Summation Formula, the midpoint quadrature method for integral approximation, and our conventions for asymptotic notation.

2.1.1. The Euler–Maclaurin Summation Formula

We employ the Euler–Maclaurin summation formula throughout our asymptotic analysis. This formula provides a powerful method for approximating sums by integrals with precisely controlled error terms. For any integers $n, p \geq 1$ and any function $g \in C^p[0,1]$, this formula as stated in [7], is

$$\sum_{j=1}^{n-1} \frac{1}{n} g\left(\frac{j}{n}\right) = \int_0^1 g(x)\,dx - \frac{1}{n} g(0) + \sum_{\ell=1}^{p} \frac{1}{n^\ell} \frac{B_\ell}{\ell!} \left[g^{(\ell-1)}(x)\right]_0^1 + r_{p,n}(g), \tag{2.1}$$

where B_ℓ denotes the Bernoulli numbers ($B_1 = -\frac{1}{2}$, $B_2 = \frac{1}{6}$, $B_3 = 0$, $B_4 = -\frac{1}{30}$), and the remainder term takes the form

$$r_{p,n}(g) = -\frac{1}{n^p p!} \int_0^1 B_p(-nx) g^{(p)}(x)\,dx = \mathcal{O}(n^{-p}) \tag{2.2}$$

where B_p denotes the p-th Bernoulli polynomial in $[0,1)$ extended to all $x \in \mathbb{R}$ via $B_p(x+1) = B_p(x)$ (see Lampret [7]). This systematic decomposition enables us to separate the asymptotic behavior of our sums into

(i) a main integral term, typically contributing the leading $n^2 \log n$ behavior in our lattice sums,

(ii) boundary correction terms from $g^{(\ell-1)}(0)$ and $g^{(\ell-1)}(1)$, contributing to the n^2 term,

(iii) higher-order corrections of order $\mathcal{O}(n^{-k})$ for various k.

We select $p = 4$ throughout our analysis, ensuring that remainder terms are of order $\mathcal{O}(n^{-4})$, which is sufficient for our asymptotic expansion requirements.

2.1.2. Midpoint Quadrature

The midpoint quadrature rule approximates an integral by evaluating the integrand at the midpoint of each subinterval. For a function $h(x, y)$ on a rectangular domain, this approximation takes the form

$$\iint_R h(x, y)\, dx\, dy \approx \Delta_x \Delta_y \sum_{j,k} h(a_j, b_k), \tag{2.3}$$

where (a_j, b_k) represents the midpoint of each rectangular cell with dimensions $\Delta_x \times \Delta_y$ and the error in this approximation depends on the second derivatives of the integrand, as we will formalize in the subsequent chapters.

2.1.3. Asymptotic Notation Convention

Throughout this work, we use the equality symbol "=" for asymptotic expansions with specified error terms. For instance, an expression of the form

$$F(n) = an^2 \log n + bn^2 + \mathcal{O}(\log n) \tag{2.4}$$

means that $|F(n) - (an^2 \log n + bn^2)| \leq C \log n$ for some constant C and sufficiently large n.

2.2. Lattice Structures and Associated Sums

Definition 2.1. A lattice is defined by a basis $\{\mathbf{s}_\ell\}_{\ell=1}^{L} \subset \mathbb{Z}^2$, where L is the number of generators with $L \geq 2$, for which we denote lattice points as $\mathbf{t}_{j,k} = (2\pi j/m, 2\pi k/n)$.

The lattice sum $F_{m,n}$ can be expressed as

$$F_{m,n} = \sum_{\substack{0\le j<m,\ 0\le k<n\\ (j,k)\neq(0,0)}} \frac{1}{1-\frac{1}{L}\sum_{\ell=1}^{L}\cos\left(s_{1,\ell}\frac{2\pi j}{m}+s_{2,\ell}\frac{2\pi k}{n}\right)}, \tag{2.5}$$

where $L, m, n, s_{1,\ell}, s_{2,\ell} \in \mathbb{Z}$ with $L, m, n \geq 2$, define $\mathbf{s}_\ell = (s_{1,\ell}, s_{2,\ell})$ for $\ell = 1, \ldots, L$, where $\mathbf{s}_\ell \neq (0, 0)$. Note that $L = 2$ for the square lattice, and $L = 3$ for the triangular lattice.

Initially, we consider a square lattice with $\mathbf{s}_1 = (1, 0)$, $\mathbf{s}_2 = (0, 1)$ due to its simplicity and prevalence in graph theory, generalizing to other lattices in subsequent chapters. In particular, $\mathbf{s}_1, \mathbf{s}_2$ are the standard unit vectors given by

$$\mathbf{s}_1 = (s_{1,1}, s_{2,1}) = (1, 0) \quad \text{and} \quad \mathbf{s}_2 = (s_{1,2}, s_{2,2}) = (0, 1). \tag{2.6}$$

The sum in equation (2.5) appears in the study of Kirchhoff and Wiener indices, as well as in the computation of $\mathrm{tr}(\mathcal{L}^+)$, where $\mathcal{L}^+$ denotes the Moore-Penrose pseudo-inverse of the Laplacian matrix for a broad class of graphs. Earlier asymptotic results established by Ye [6] are based on

$$\lim_{m,n\to\infty} \frac{F_{m,n}}{mn} = \frac{1}{4\pi^2} \iint_{[0,2\pi]^2} \frac{dx\, dy}{1-\frac{1}{L}\sum_{\ell=1}^{L}\cos(s_{1,\ell}x+s_{2,\ell}y)} \tag{2.7}$$

where MATLAB has been employed to implement numerical methods for approximating the integral in equation (2.7), yielding a finite value C. As has been shown in Theorem 3.2 of [5], however, these integrals are divergent. Employing the trigonometric relation $\cos 2\theta = 1 - 2\sin^2\theta$ and the inequality $|\sin\theta| \leq |\theta|$, we obtain

$$\begin{aligned} \frac{1}{1-\frac{1}{L}\sum_{\ell=1}^{L}\cos(s_{1,\ell}x+s_{2,\ell}y)} &= \frac{L}{2\sum_{\ell=1}^{L}\sin^2(\frac{s_{1,\ell}x+s_{2,\ell}y}{2})} \\ &\geq \frac{2L}{\sum_{\ell=1}^{L}(s_{1,\ell}x+s_{2,\ell}y)^2} \\ &\geq \frac{2L}{\sum_{\ell=1}^{2}(s_{1,\ell}x+s_{2,\ell}y)^2} = \frac{2L}{x^2+y^2}, \end{aligned}$$

so that,

$$\int_0^{2\pi}\int_0^{2\pi}\frac{dx\,dy}{1-\frac{1}{L}\sum_{\ell=1}^{L}\cos(s_{1,\ell}x+s_{2,\ell}y)}\geq 2L\int_0^{2\pi}\int_0^{2\pi}\frac{dx\,dy}{x^2+y^2}$$

Since the integrand is positive, we can focus on a region near the origin where the singularity occurs. Converting to polar coordinates ($x = r\cos\theta$, $y = r\sin\theta$, $dx\,dy = r\,dr\,d\theta$), and restricting to a disk of radius π contained within our domain, we obtain:

$$\begin{aligned}\int_0^{2\pi}\int_0^{2\pi}\frac{dx\,dy}{x^2+y^2} &\geq \int_0^{\pi/4}\int_\varepsilon^{\pi}\frac{r\,dr\,d\theta}{r^2}\\ &= \int_0^{\pi/4}d\theta\int_\varepsilon^{\pi}\frac{dr}{r}\\ &= \frac{\pi}{4}\cdot(\log\pi-\log\varepsilon),\end{aligned}$$

where $\varepsilon > 0$ is introduced to handle the singularity at $r = 0$. As $\varepsilon \to 0$, this expression diverges to infinity. Thus,

$$\int_0^{2\pi}\int_0^{2\pi}\frac{dx\,dy}{1-\frac{1}{L}\sum_{\ell=1}^{L}\cos(s_{1,\ell}x+s_{2,\ell}y)}\geq 2L\cdot\frac{\pi}{4}\cdot(\log\pi-\log\varepsilon)=\infty.$$

Hence, standard integral methods alone cannot handle the sum near $(j,k) = (0,0)$, a challenge that parallels classical problems in the summation of divergent series studied by Hardy and Littlewood [8]. Therefore, we must treat that region separately, leading to the refined asymptotic expansions introduced in this study.

To circumvent this divergence for the derivation of the correct asymptotic behavior, we employ a midpoint quadrature approach, discretizing the domain into rectangles centered at lattice points $\mathbf{t}_{j,k}$ as given in

$$t_j = \frac{2\pi j}{m},\quad t'_k = \frac{2\pi k}{n},\quad \mathbf{t}_{j,k} = (t_j, t'_k), \tag{2.8}$$

and similarly define their shifted counterparts

$$x_j = t_j - \frac{\pi}{m}, \quad x'_k = t'_k - \frac{\pi}{n}, \quad \mathbf{x}_{j,k} = (x_j, x'_k), \tag{2.9}$$

and the rectangles

$$X_{j,k} = X_j \times X'_k = [x_j, x_{j+1}] \times [x'_k, x'_{k+1}] \tag{2.10}$$

for $m, n \geq 2$ and $j, k \in \mathbb{Z}$. With this setting, the rectangles are centered at $\mathbf{t}_{j,k} = (t_j, t'_k)$. The quantities $t_j = \frac{2\pi j}{m}$ and $t'_k = \frac{2\pi k}{n}$ explicitly depend on the chosen integers m, n and consequently, the point $\mathbf{t}_{j,k} = (t_j, t'_k)$ varies as m or n change. Similarly, the domain $D_{m,n}$ depends on $\frac{\pi}{m}$ and $\frac{\pi}{n}$, so, all these notations are implicitly indexed by the lattice size parameters m, n.

With this notation, we observe that

$$F_{m,n} = F_{m,n}(f) = \sum_{\substack{0 \leq j < m,\, 0 \leq k < n \\ (j,k) \neq (0,0)}} f\big(\mathbf{t}_{j,k}\big) = \sum_{\mathbf{t}_{j,k} \in [0,2\pi)^2 \setminus \{\mathbf{0}\}} f\big(\mathbf{t}_{j,k}\big), \tag{2.11}$$

where f is defined as

$$f(\mathbf{x}) = \frac{1}{\varphi(\mathbf{x})}, \quad \varphi(\mathbf{x}) = 1 - \frac{1}{L} \sum_{\ell=1}^{L} \cos(\mathbf{s}_\ell \cdot \mathbf{x}), \quad (\mathbf{x} = (x, y) \in \mathbb{R}^2). \tag{2.12}$$

Since $\mathbf{s}_\ell \in \mathbb{Z}^2$, we can exploit the 2π-periodicity of $\varphi(\mathbf{x})$, and consequently redefine $F_{m,n}(f)$ over the symmetric domain $[-\pi, \pi)^2 \setminus \{\mathbf{0}\}$ as in the next Lemma, and get

$$F_{m,n}(f) = \sum_{\mathbf{t}_{j,k} \in [-\pi,\pi)^2 \setminus \{\mathbf{0}\}} f\big(\mathbf{t}_{j,k}\big). \tag{2.13}$$

We now aim to derive a useful form of equation (2.13).

Lemma 2.2. *For $m, n \geq 2$, we have the equivalence*

$$\mathbf{t}_{j,k} \in [-\pi, \pi)^2 \setminus \{\mathbf{0}\} \iff \mathbf{t}_{j,k} \in D_{m,n} = E_{m,n} \setminus (B_m \times B_n) \tag{2.14}$$

where

$$E_{m,n} = A_m \times A_n, \tag{2.15}$$

and for $k \in \mathbb{N}$,

$$A_k = \left[-\pi - \frac{\pi}{k}\left(\frac{1+(-1)^k}{2}\right), \pi - \frac{\pi}{k}\left(\frac{1+(-1)^k}{2}\right)\right], \qquad B_k = \left(-\frac{\pi}{k}, \frac{\pi}{k}\right).$$

In particular, when $m = n$, for all $n \geq 2$, we have

$$D_{n,n} = \left[-\pi - \frac{\pi}{n}\left(\frac{1+(-1)^n}{2}\right), \pi - \frac{\pi}{n}\left(\frac{1+(-1)^n}{2}\right)\right]^2 \setminus \left(-\frac{\pi}{n}, \frac{\pi}{n}\right)^2.$$

Proof. We prove the equivalence by considering the parity of m and n separately, mapping the lattice points $\mathbf{t}_{j,k} = \left(\frac{2\pi j}{m}, \frac{2\pi k}{n}\right)$ to the domain $D_{m,n}$. The argument proceeds in two cases: odd m and even m, with analogous reasoning for n.

The set $\{\mathbf{t}_{j,k} \in [-\pi, \pi)^2 \setminus \{\mathbf{0}\}\}$ consists of index pairs (j, k) where $t_j = \frac{2\pi j}{m} \in [-\pi, \pi)$, more precisely $-\frac{m}{2} \leq j < \frac{m}{2}$, and similarly for k. Since t_j is the midpoint of $[x_j, x_{j+1}]$, where $x_j = t_j - \frac{\pi}{m}$ and $x_{j+1} = t_j + \frac{\pi}{m}$, we analyze two parity cases for m.

For odd $m = 2q + 1$, the condition $-\frac{m}{2} \leq j < \frac{m}{2}$ becomes $-q - \frac{1}{2} \leq j < q + \frac{1}{2}$, where $q = \frac{m-1}{2}$. For integer j, this is $-q \leq j \leq q$. Excluding $j = 0$, the set $\{t_j : j \in \{-q, \ldots, q\} \setminus \{0\}\}$ satisfies

$$t_j \in [-\pi, \pi) \setminus \{0\} \iff t_j \in \bigcup_{\substack{-q \leq j \leq q \\ j \neq 0}} [x_j, x_{j+1}) = [-\pi, \pi) \setminus \left(-\frac{\pi}{m}, \frac{\pi}{m}\right). \tag{2.16}$$

For $j = -q$, we have $t_{-q} = \frac{2\pi(-q)}{m} = -\pi$, which marks the lower boundary of our domain and for $j = q$, we have $t_q = \frac{2\pi q}{m} = \pi - \frac{2\pi}{m}$ since $q = \frac{m-1}{2}$. Additionally, $x_{q+1} = t_q + \frac{\pi}{m} = \pi$, which ensures that the domain $[-\pi, \pi)$ is completely covered except for the excluded region near the origin. This establishes that the domain corresponds precisely to the specified set minus the small region around zero.

For even $m = 2q$, the condition $-\frac{m}{2} \leq j < \frac{m}{2}$ becomes $-q \leq j < q$, where $q = \frac{m}{2}$. Excluding $j = 0$, the set $\{t_j : j \in \{-q, \dots, q-1\} \setminus \{0\}\}$ yields

$$t_j \in [-\pi, \pi)\backslash\{0\} \iff t_j \in \bigcup_{\substack{-q \leq j < q \\ j \neq 0}} [x_j, x_{j+1}) = \Big[-\pi - \frac{\pi}{m}, \pi - \frac{\pi}{m}\Big)\backslash\Big(-\frac{\pi}{m}, \frac{\pi}{m}\Big). \quad (2.17)$$

For $j = -q$, $t_{-q} = -\pi$; for $j = q-1$, $t_{q-1} = \frac{2\pi(q-1)}{m} = \pi - \frac{2\pi}{m}$, and $x_q = t_{q-1} + \frac{\pi}{m} = \pi - \frac{\pi}{m}$, defining the upper bound of the interval.

Applying this coordinate-wise, define

$$A_m = \begin{cases} [-\pi, \pi), & m \text{ odd}, \\ \left[-\pi - \frac{\pi}{m}, \pi - \frac{\pi}{m}\right), & m \text{ even}. \end{cases}$$

For $t'_k = \frac{2\pi k}{n}$, A_n follows the same form based on n's parity. Thus, $\mathbf{t}_{j,k} = (t_j, t'_k)$ lies in $E_{m,n} = A_m \times A_n$, and excluding $\{\mathbf{0}\}$ removes $B_m \times B_n = \left(-\frac{\pi}{m}, \frac{\pi}{m}\right) \times \left(-\frac{\pi}{n}, \frac{\pi}{n}\right)$, yielding $D_{m,n}$ as in equation (2.18).

Thus, $\mathbf{t}_{j,k} \in [-\pi, \pi)^2 \setminus \{\mathbf{0}\}$ if and only if $(j, k) \in D_{m,n}$, proving the lemma. □

Remark 2.3. Note that we have explicitly,

$$D_{m,n} = E_{m,n} \setminus \left(-\frac{\pi}{m}, \frac{\pi}{m}\right) \times \left(-\frac{\pi}{n}, \frac{\pi}{n}\right) \quad (2.18)$$

where $E_{m,n}$ takes the form

$$E_{m,n} = \begin{cases} [-\pi, \pi]^2, & m, n \text{ odd}, \\ [-\pi, \pi] \times \left[-\pi - \frac{\pi}{n}, \pi - \frac{\pi}{n}\right], & m \text{ odd}, n \text{ even}, \\ \left[-\pi - \frac{\pi}{m}, \pi - \frac{\pi}{m}\right] \times [-\pi, \pi], & m \text{ even}, n \text{ odd}, \\ \left[-\pi - \frac{\pi}{m}, \pi - \frac{\pi}{m}\right] \times \left[-\pi - \frac{\pi}{n}, \pi - \frac{\pi}{n}\right], & m, n \text{ even}. \end{cases} \tag{2.19}$$

By leveraging Lemma 2.2, we can work with this equivalent domain representation, which simplifies our subsequent analysis.

We can now illustrate with an example of how indices map to specific domains.

Table 2.1: Examples of index-to-domain mappings.

m	Indices j	Values t_j	Domain in x
3 (odd)	$\{-1, 0, 1\}$	$\{-\frac{2\pi}{3}, 0, \frac{2\pi}{3}\}$	$[-\pi, \pi) \setminus (-\frac{\pi}{3}, \frac{\pi}{3})$
4 (even)	$\{-2, -1, 0, 1\}$	$\{-\pi, -\frac{\pi}{2}, 0, \frac{\pi}{2}\}$	$[-\pi - \frac{\pi}{4}, \pi - \frac{\pi}{4}) \setminus (-\frac{\pi}{4}, \frac{\pi}{4})$

Lemma 2.4. *Let $\delta_n = \frac{\alpha\pi}{n}$, where $\alpha > 1$ is a constant. Define the near-field and far-field regions of the lattice domain as*

$$D_{m,n}^{near} = \{\mathbf{t}_{j,k} \in D_{m,n} : \|\mathbf{t}_{j,k}\| \leq \delta_n\},$$
$$D_{m,n}^{far} = D_{m,n} \setminus D_{m,n}^{near}.$$

The error between the lattice sum $F_{m,n} = \sum_{\mathbf{t}_{j,k} \in D_{m,n}} f(\mathbf{t}_{j,k})$ and its integral approximation $I_{m,n} = \frac{1}{\Delta_m \Delta_n} \iint_{D_{m,n}} f(\mathbf{x})\, d\mathbf{x}$ satisfies

$$|F_{m,n} - I_{m,n}| \leq |F_{m,n}^{near} - I_{m,n}^{near}| + |F_{m,n}^{far} - I_{m,n}^{far}|,$$

where $F^{near}_{m,n} = \sum_{\mathbf{t}_{j,k} \in D^{near}_{m,n}} f(\mathbf{t}_{j,k})$, $I^{near}_{m,n} = \frac{1}{\Delta_m \Delta_n} \iint_{D^{near}_{m,n}} f(\mathbf{x})\, d\mathbf{x}$, *and similarly for the far-field terms. This decomposition isolates the singularity at the origin from the smoother far-field region.*

Proof. Given $F_{m,n} = F^{\text{near}}_{m,n} + F^{\text{far}}_{m,n}$ and $I_{m,n} = I^{\text{near}}_{m,n} + I^{\text{far}}_{m,n}$, the triangle inequality yields

$$|F_{m,n} - I_{m,n}| = |(F^{\text{near}}_{m,n} - I^{\text{near}}_{m,n}) + (F^{\text{far}}_{m,n} - I^{\text{far}}_{m,n})| \leq |F^{\text{near}}_{m,n} - I^{\text{near}}_{m,n}| + |F^{\text{far}}_{m,n} - I^{\text{far}}_{m,n}|.$$

The choice of δ_n ensures that $D^{\text{near}}_{m,n}$ captures the singular behavior near $\mathbf{t}_{j,k} = (0,0)$ (excluded from $D_{m,n}$ per Lemma 2.2), while $D^{\text{far}}_{m,n}$ is suitable for standard quadrature methods. □

Remark 2.5. This decomposition facilitates the asymptotic analysis of $F_{m,n}$. The far-field error $|F^{\text{far}}_{m,n} - I^{\text{far}}_{m,n}|$ depends on the smoothness of f for $\|\mathbf{x}\| > \delta_n$, while the near-field error $|F^{\text{near}}_{m,n} - I^{\text{near}}_{m,n}|$ requires handling the singularity. Direct estimates may suggest errors of $\mathcal{O}(n^2)$ or $\mathcal{O}(n \log n)$ when $m = n$, but Theorem 1.1 achieves an $\mathcal{O}(\log n)$ error through cancellations with $F_n(f_1) - I_n(f_1)$, as detailed in §4.

With the aid of Lemma 2.2, we can express

$$F_{m,n}(f) = \sum_{\mathbf{t}_{j,k} \in D_{m,n}} f\big(\mathbf{t}_{j,k}\big), \tag{2.20}$$

which provides an alternative form of equation (2.13). To approximate the sum $F_{m,n}$ in (2.5), we introduce the integral defined below in equation (2.21) using the midpoint quadrature approach

$$I_{m,n}(f) = \frac{1}{\Delta_{m,n}} \iint_{D_{m,n}} f(\mathbf{x})\, d\mathbf{x}, \tag{2.21}$$

where $D_{m,n}$ is the integration domain defined in Lemma 2.2. By approximating $F_{m,n}$ with $I_{m,n}(f)$ using midpoint quadrature, we achieve controlled error bounds, as detailed by Davis and Rabinowitz [9].

More precisely, setting

$$\Delta_m = \frac{2\pi}{m}, \quad \Delta_n = \frac{2\pi}{n}, \quad \Delta_{m,n} = \Delta_m \, \Delta_n, \tag{2.22}$$

the identity in equation (2.20) shows that $F_{m,n}(f)$ results from applying the two-dimensional midpoint numerical integration rule to each rectangle $X_{j,k} \subset D_{m,n}$ for the integral (2.21). We note that Δ_n here represents the mesh size in a single dimension, whereas $\Delta_{m,n} = \frac{2\pi}{m} \frac{2\pi}{n}$ is the mesh size arising from subdividing the $[-\pi, \pi]^2$ domain into $m \times n$ rectangles, representing the total area element of the discretization and also that $X_{j,k}$ is the rectangle centered at the grid point $\mathbf{t}_{j,k}$ given in (2.10).

These observations motivate alternative approximations to the sum $F_{m,n}$ (2.5) based on Taylor polynomials of the function φ in (2.12) around the origin. As suggested in [4], we employ the second-order Taylor polynomial

$$p_1(\mathbf{x}) := \frac{1}{L} \sum_{\ell=1}^{L} \frac{(\mathbf{s}_\ell \cdot \mathbf{x})^2}{2} \tag{2.23}$$

For our error analysis, we employ midpoint quadrature bounds of [3] which provides precise error estimates for approximating integrals with function evaluations at midpoints, forming the foundation of the analytical approach in our lemma below.

Lemma 2.6. *Let $h(x, y)$ be a twice continuously differentiable function on the rectangular domain*

$$R = \left[a - \frac{\Delta_x}{2}, a + \frac{\Delta_x}{2}\right] \times \left[b - \frac{\Delta_y}{2}, b + \frac{\Delta_y}{2}\right] \subset \mathbb{R}^2.$$

Then, the error in approximating the integral of $h(x, y)$ over R by $\Delta_x \Delta_y h(a, b)$ satisfies

$$\left| \iint_R h(x, y)\, dx\, dy - \Delta_x \Delta_y h(a, b) \right| \leq \frac{\Delta_x^3 \Delta_y \max_R |h_{xx}| + \Delta_x \Delta_y^3 \max_R |h_{yy}|}{24}.$$

where $\Delta_x = \frac{2\pi}{m}$, $\Delta_y = \frac{2\pi}{n}$ *as defined in equation* (2.22) *and* h_{xx} *and* h_{yy} *denote the second partial derivatives with respect to* x *and* y*, respectively.*

Proof. Expanding $h(x, y)$ around the point (a, b) using Taylor's theorem with Lagrange remainder, we get

$$
\begin{aligned}
h(x,y) &= h(a,b) + h_x(a,b)(x-a) + h_y(a,b)(y-b) \\
&\qquad + \frac{1}{2}\big[h_{xx}(\xi_x, y)(x-a)^2 + 2h_{xy}(\xi_{xy}, \eta_{xy})(x-a)(y-b) + h_{yy}(x, \eta_y)(y-b)^2\big],
\end{aligned}
$$

where $\xi_x, \xi_{xy} \in [a - \frac{\Delta_x}{2}, a + \frac{\Delta_x}{2}]$ and $\eta_{xy}, \eta_y \in [b - \frac{\Delta_y}{2}, b + \frac{\Delta_y}{2}]$ depend on (x, y). Here, h_x, h_y denote the first partial derivatives with respect to x and y, respectively. Integrating over R, we observe that the linear terms vanish due to the symmetry of the domain about (a, b)

$$
\iint_R h_x(a,b)(x-a)\,dx\,dy = \iint_R h_y(a,b)(y-b)\,dx\,dy = 0.
$$

Similarly, the cross-term $2h_{xy}(\xi_{xy}, \eta_{xy})(x-a)(y-b)$ integrates to zero by symmetry. Thus,

$$
\iint_R h(x,y)\,dx\,dy = \Delta_x \Delta_y h(a,b) + \frac{\Delta_x^3 \Delta_y}{24} h_{xx}(\xi_1, \eta_1) + \frac{\Delta_x \Delta_y^3}{24} h_{yy}(\xi_2, \eta_2),
$$

for some points $(\xi_1, \eta_1), (\xi_2, \eta_2) \in R$ by the Mean-Value Theorem for integrals, where the quadratic terms are integrated using

$$
\int_{a-\frac{\Delta_x}{2}}^{a+\frac{\Delta_x}{2}} (x-a)^2\,dx = \frac{\Delta_x^3}{12}, \quad \int_{b-\frac{\Delta_y}{2}}^{b+\frac{\Delta_y}{2}} (y-b)^2\,dy = \frac{\Delta_y^3}{12}.
$$

Therefore,

$$
\iint_R h(x,y)\,dx\,dy - \Delta_x \Delta_y h(a,b) = \frac{\Delta_x^3 \Delta_y}{24} h_{xx}(\xi_1, \eta_1) + \frac{\Delta_x \Delta_y^3}{24} h_{yy}(\xi_2, \eta_2).
$$

By computing absolute values and using the maximum bounds of the second derivatives over R, we obtain

$$\left| \iint_R h(x,y)\,dx\,dy - \Delta_x \Delta_y h(a,b) \right| \leq \frac{\Delta_x^3 \Delta_y \max_R |h_{xx}| + \Delta_x \Delta_y^3 \max_R |h_{yy}|}{24}.$$

□

The fundamental bounds on $\varphi(\mathbf{x})$ and its derivatives, established in the following lemma, are based on Lemma 4.1 of [4].

Lemma 2.7. *For all $\mathbf{x} \in \mathbb{R}^2$, it holds that*

(a) $|\varphi(\mathbf{x})| \leq \frac{1}{2L} \|\mathbf{x}\|^2 \sum_{\ell=1}^{L} \|\mathbf{s}_\ell\|^2 \leq \frac{1}{2} \overline{s}^2 \|\mathbf{x}\|^2,$

(b) $|\partial_k \varphi(\mathbf{x})| \leq \frac{1}{L} \|\mathbf{x}\| \sum_{\ell=1}^{L} |s_{k,\ell}| \|\mathbf{s}_\ell\| \leq \overline{s}^2 \|\mathbf{x}\|,$

(c) $|\partial_k^2 \varphi(\mathbf{x})| \leq \frac{1}{L} \sum_{\ell=1}^{L} s_{k,\ell}^2 \leq \overline{s}^2.$

Proof. (a) Starting with the definition of $\varphi(\mathbf{x})$ in equation (2.12), we obtain the following estimates by applying the triangle inequality, the identity $1 - \cos\theta = 2\sin^2\left(\frac{1}{2}\theta\right)$, and the inequality $|\sin\theta| \leq |\theta|$

$$|\varphi(\mathbf{x})| \leq \frac{1}{L} \sum_{\ell=1}^{L} |1 - \cos(\mathbf{s}_\ell \cdot \mathbf{x})| = \frac{2}{L} \sum_{\ell=1}^{L} \sin^2\left(\frac{1}{2}\mathbf{s}_\ell \cdot \mathbf{x}\right) \leq \frac{1}{2L} \sum_{\ell=1}^{L} (\mathbf{s}_\ell \cdot \mathbf{x})^2 .$$

Finally, by employing the Cauchy-Schwarz inequality and letting $\overline{s} = \max_\ell \|\mathbf{s}_\ell\|$, we obtain

$$|\varphi(\mathbf{x})| \leq \frac{1}{2L} \sum_{\ell=1}^{L} \left(\|\mathbf{s}_\ell\|^2 \|\mathbf{x}\|^2\right) = \frac{1}{2L} \|x\|^2 \sum_{\ell=1}^{L} \|\mathbf{s}_\ell\|^2 \leq \frac{1}{2} \overline{s}^2 \|\mathbf{x}\|^2.$$

(b) We compute the partial derivatives of $\varphi(\mathbf{x})$ as

$$\partial_k \varphi(\mathbf{x}) = \frac{1}{L}\sum_{\ell=1}^{L} s_{k,\ell}\sin(\mathbf{s}_\ell \cdot \mathbf{x}),$$
$$\partial_k^2 \varphi(\mathbf{x}) = \frac{1}{L}\sum_{\ell=1}^{L} s_{k,\ell}^2\cos(\mathbf{s}_\ell \cdot \mathbf{x}).$$

Starting with $\partial_k\varphi(\mathbf{x})$; we make use of the triangle inequality, the inequality $|\sin\theta| \leq |\theta|$, and the Cauchy-Schwarz inequality as in the proof of Lemma 2.7(a), and obtain

$$|\partial_k\varphi(\mathbf{x})| \leq \frac{1}{L}\sum_{\ell=1}^{L}|s_{k,\ell}\sin(\mathbf{s}_\ell\cdot\mathbf{x})| \leq \frac{1}{L}\sum_{\ell=1}^{L}|s_{k,\ell}||\mathbf{s}_\ell\cdot\mathbf{x}| \leq \frac{1}{L}\|\mathbf{x}\|\sum_{\ell=1}^{L}|s_{k,\ell}|\|\mathbf{s}_\ell\|.$$

Finally, using the bound on the sum

$$|\partial_k\varphi(\mathbf{x})| \leq \bar{s}^2\|\mathbf{x}\|$$

we get the result.

(c) Starting from $\partial_k^2\varphi(\mathbf{x})$, we apply the triangle inequality and the bound $|\cos(x)| \leq 1$ to obtain

$$|\partial_k^2\varphi(\mathbf{x})| \leq \frac{1}{L}\sum_{\ell=1}^{L}|s_{k,\ell}^2\cos(\mathbf{s}_\ell\cdot\mathbf{x})| \leq \frac{1}{L}\sum_{\ell=1}^{L}s_{k,\ell}^2.$$

Applying the sum bound, we get

$$|\partial_k^2\varphi(\mathbf{x})| \leq \bar{s}^2.$$

□

The lower bound for $\varphi(\mathbf{x})$ away from the origin is adapted from Lemma 4.2 of [4] and the estimation of its second derivatives follow from Corollary 4.3 of [4].

Lemma 2.8. *For any fixed* $0 < \beta < 2\pi$, *there exist positive constants* $C(\beta)$ *and* $C_1(\beta)$ *such that, for all* $\mathbf{x} \in [-2\pi + \beta, 2\pi - \beta]^2 \setminus \{\mathbf{0}\}$ *and* $k = 1, 2$

(a) $\varphi(\mathbf{x}) \geq C_1(\beta) \, \|\mathbf{x}\|^2$
(b) $|\partial_k^2 f(\mathbf{x})| \leq \dfrac{C(\beta)}{\|\mathbf{x}\|^4}$

Proof. For (2.8)(a), let $\mathbf{x} = (x_1, x_2) \in [-2\pi + \beta, 2\pi - \beta]^2$ then, we have

$$\varphi(\mathbf{x}) = 1 - \frac{1}{L} \sum_{\ell=1}^{L} \cos(\mathbf{s}_\ell \cdot \mathbf{x}) \geq \frac{1}{L} \left(2 - \cos x_1 - \cos x_2\right).$$

Using the Taylor series expansion of cosine with Lagrange remainder

$$\cos x = 1 - \frac{x^2}{2} + \frac{x^4}{24} \cos(\xi),$$

where ξ lies between 0 and x, we obtain

$$2 - \cos x_1 - \cos x_2 = \frac{x_1^2 + x_2^2}{2} - \frac{x_1^4 \cos(\xi_1) + x_2^4 \cos(\xi_2)}{24}.$$

Since $|\cos(\xi)| \leq 1$, we get

$$\varphi(\mathbf{x}) \geq \frac{1}{L} \left(\frac{\|\mathbf{x}\|^2}{2} - \frac{\|\mathbf{x}\|^4}{24} \right).$$

For $\|\mathbf{x}\| \leq \sqrt{6}$, this yields $\varphi(\mathbf{x}) \geq \frac{\|\mathbf{x}\|^2}{4L}$. For the compact region $[-2\pi + \beta, 2\pi - \beta]^2 \setminus B(0, \sqrt{6})$, by the Extreme Value Theorem, there exists $C_2(\beta) > 0$ such that $\varphi(\mathbf{x})/\|\mathbf{x}\|^2 \geq C_2(\beta)$. Taking

$$C_1(\beta) = \min \left\{ C_2(\beta), \frac{1}{4L} \right\},$$

we establish (2.8)(a).

For (2.8)(b), we calculate

$$\partial_k^2 f(\mathbf{x}) = \frac{2(\partial_k \varphi(\mathbf{x}))^2 - \varphi(\mathbf{x})\partial_k^2\varphi(\mathbf{x})}{(\varphi(\mathbf{x}))^3}.$$

Using the bounds from Lemma 2.7(a) combined with (2.8)(a), we obtain

$$|\partial_k^2 f(\mathbf{x})| \leq \frac{2(\overline{s}^2\|\mathbf{x}\|)^2 + C_1(\beta)\|\mathbf{x}\|^2 \cdot \overline{s}^2}{(C_1(\beta)\|\mathbf{x}\|^2)^3} = \frac{C(\beta)}{\|\mathbf{x}\|^4},$$

where $C(\beta) = \frac{3\overline{s}^4}{(C_1(\beta))^3}$. □

The crucial lower bounds for $p_m(\mathbf{x})$ established in the following lemma can be derived from Lemma 4.8 of [4].

Lemma 2.9. *For all* $\mathbf{x} \in \mathbb{R}^2$*, we have*

(i) $p_1(\mathbf{x}) \geq \dfrac{1}{2L}\|\mathbf{x}\|^2$,

(ii) If $0 \leq \beta \leq 1$ *and* $\|\mathbf{x}\| \leq \dfrac{\sqrt{12(1-\beta)}}{\overline{s}}$*, then, for all* $m \geq 1$, $p_m(\mathbf{x}) \geq \dfrac{\beta}{2L}\|\mathbf{x}\|^2$

Proof. (i) This follows from the expansion of $p_1(\mathbf{x})$ and the definition of the vector norm. For all $\mathbf{x} \in \mathbb{R}^2$,

$$p_1(\mathbf{x}) = \frac{1}{L}\sum_{\ell=1}^{L} \frac{(\mathbf{s}_\ell \cdot \mathbf{x})^2}{2} \geq \frac{1}{2L}\|\mathbf{x}\|^2.$$

(ii) For $m \geq 2$, we want to show by induction that $p_m(\mathbf{x}) \geq \frac{\beta}{2L}\|\mathbf{x}\|^2$. Assume the statement holds for $m-1$

$$p_{m-1}(\mathbf{x}) \geq \frac{\beta}{2L}\|\mathbf{x}\|^2.$$

then, with

$$p_m(\mathbf{x}) = p_{m-1}(\mathbf{x}) + \frac{1}{L}\sum_{\ell=1}^{L}\frac{(\mathbf{s}_\ell\cdot\mathbf{x})^{2m}}{(2m)!},$$

we get

$$p_m(\mathbf{x}) \geq \frac{\beta}{2L}\|\mathbf{x}\|^2 + \frac{1}{L}\sum_{\ell=1}^{L}\frac{(\mathbf{s}_\ell\cdot\mathbf{x})^{2m}}{(2m)!}.$$

The term $\frac{1}{L}\sum_{\ell=1}^{L}\frac{(\mathbf{s}_\ell\cdot\mathbf{x})^{2m}}{(2m)!}$ is non-negative, as it is a sum of non-negative terms consisting of powers of real numbers and factorials. Since $\|\mathbf{x}\| \leq \frac{\sqrt{12(1-\beta)}}{\overline{s}}$, the remaining term does not affect the inequality negatively. Thus, we get

$$p_m(\mathbf{x}) \geq \frac{\beta}{2L}\|\mathbf{x}\|^2.$$

□

Lemma 2.10. *Let $p_1(\mathbf{x})$ be the second-order Taylor polynomial of $\varphi(\mathbf{x})$ as defined in* (2.23)*. Then, for $\overline{s} = \max_\ell \|\mathbf{s}_\ell\|$ and $\delta = \sqrt{\frac{6}{L\overline{s}^4}}$*

(i) the approximation error satisfies

$$|\varphi(\mathbf{x}) - p_1(\mathbf{x})| \leq \frac{\overline{s}^4\|\mathbf{x}\|^4}{24}, \quad \mathbf{x}\in\mathbb{R}^2, \textit{and} \tag{2.24}$$

(ii) for $f(\mathbf{x}) = \frac{1}{\varphi(\mathbf{x})}$ and $f_1(\mathbf{x}) = \frac{1}{p_1(\mathbf{x})}$, when $\|\mathbf{x}\| \leq \delta$, we have

$$|f(\mathbf{x}) - f_1(\mathbf{x})| \leq C(\overline{s}), \tag{2.25}$$

where $C(\overline{s}) = \frac{L^2\overline{s}^4}{3}$ is a constant independent of $\mathbf{x}$.

Proof. (i) By Taylor's theorem with Lagrange remainder, for each ℓ we have

$$\cos(\mathbf{s}_\ell \cdot \mathbf{x}) = 1 - \frac{(\mathbf{s}_\ell \cdot \mathbf{x})^2}{2} + \frac{(\mathbf{s}_\ell \cdot \mathbf{x})^4}{24} \cos(\mathbf{s}_\ell \cdot \boldsymbol{\xi}_\ell) \tag{2.26}$$

for some $\boldsymbol{\xi}_\ell$ on the line segment that joins the origin with $\mathbf{x}$. Since $|\cos(\mathbf{s}_\ell \cdot \boldsymbol{\xi}_\ell)| \leq 1$ and $|\mathbf{s}_\ell \cdot \mathbf{x}| \leq \|\mathbf{s}_\ell\|\|\mathbf{x}\| \leq \overline{s}\|\mathbf{x}\|$ by the Cauchy-Schwarz inequality, we obtain

$$|\varphi(\mathbf{x}) - p_1(\mathbf{x})| \leq \frac{1}{L}\sum_{\ell=1}^{L} \frac{|(\mathbf{s}_\ell \cdot \mathbf{x})^4|}{24} \leq \frac{1}{L}\sum_{\ell=1}^{L} \frac{\overline{s}^4\|\mathbf{x}\|^4}{24} = \frac{\overline{s}^4\|\mathbf{x}\|^4}{24}. \tag{2.27}$$

(ii) Let $r(\mathbf{x}) = \varphi(\mathbf{x}) - p_1(\mathbf{x})$, so $\varphi(\mathbf{x}) = p_1(\mathbf{x}) + r(\mathbf{x})$. From (2.24)(i), we know that $|r(\mathbf{x})| \leq \frac{\overline{s}^4\|\mathbf{x}\|^4}{24}$. The difference between f and f_1 can be expressed as

$$|f(\mathbf{x}) - f_1(\mathbf{x})| = \left|\frac{1}{\varphi(\mathbf{x})} - \frac{1}{p_1(\mathbf{x})}\right| = \left|\frac{p_1(\mathbf{x}) - \varphi(\mathbf{x})}{p_1(\mathbf{x})\varphi(\mathbf{x})}\right| = \frac{|r(\mathbf{x})|}{|p_1(\mathbf{x})| \cdot |\varphi(\mathbf{x})|}. \tag{2.28}$$

From Lemma 2.9(i), we have $p_1(\mathbf{x}) \geq \frac{1}{2L}\|\mathbf{x}\|^2$ for all $\mathbf{x}$. For $\|\mathbf{x}\| \leq \delta = \sqrt{\frac{6}{L\overline{s}^4}}$, we can establish

$$\left|\frac{r(\mathbf{x})}{p_1(\mathbf{x})}\right| \leq \frac{\frac{\overline{s}^4\|\mathbf{x}\|^4}{24}}{\frac{1}{2L}\|\mathbf{x}\|^2} = \frac{L\overline{s}^4\|\mathbf{x}\|^2}{12} \leq \frac{L\overline{s}^4 \cdot \frac{6}{L\overline{s}^4}}{12} = \frac{1}{2} \tag{2.29}$$

This implies that $|r(\mathbf{x})| \leq \frac{1}{2}|p_1(\mathbf{x})|$. Since $\varphi(\mathbf{x}) = p_1(\mathbf{x}) + r(\mathbf{x})$, we have

$$|\varphi(\mathbf{x})| \geq |p_1(\mathbf{x})| - |r(\mathbf{x})| \geq |p_1(\mathbf{x})| - \frac{1}{2}|p_1(\mathbf{x})| = \frac{1}{2}|p_1(\mathbf{x})| \tag{2.30}$$

Using these relationships in our expression for $|f(\mathbf{x}) - f_1(\mathbf{x})|$, we deduce

$$|f(\mathbf{x}) - f_1(\mathbf{x})| = \frac{|r(\mathbf{x})|}{|p_1(\mathbf{x})| \cdot |\varphi(\mathbf{x})|} \leq \frac{|r(\mathbf{x})|}{|p_1(\mathbf{x})| \cdot \frac{1}{2}|p_1(\mathbf{x})|} = \frac{2|r(\mathbf{x})|}{|p_1(\mathbf{x})|^2} \tag{2.31}$$

Substituting our bounds, we get

$$\frac{2|r(\mathbf{x})|}{|p_1(\mathbf{x})|^2} \leq \frac{2 \cdot \frac{\overline{s}^4 \|\mathbf{x}\|^4}{24}}{\left(\frac{1}{2L}\|\mathbf{x}\|^2\right)^2} = \frac{2 \cdot \frac{\overline{s}^4 \|\mathbf{x}\|^4}{24}}{\frac{1}{4L^2}\|\mathbf{x}\|^4} = \frac{2 \cdot \overline{s}^4 \cdot 4L^2}{24} = \frac{8L^2\overline{s}^4}{24} = \frac{L^2\overline{s}^4}{3}. \tag{2.32}$$

Therefore, for all $\|\mathbf{x}\| \leq \delta$, we have

$$|f(\mathbf{x}) - f_1(\mathbf{x})| \leq \frac{L^2\overline{s}^4}{3} = C(\overline{s}). \tag{2.33}$$

This establishes a uniform bound that is independent of $\|\mathbf{x}\|$. The bound is valid for all $\mathbf{x}$ with $\|\mathbf{x}\| \leq \delta$, which completes the proof. □

We can now define

$$f_1(\mathbf{x}) := \frac{1}{p_1(\mathbf{x})} \tag{2.34}$$

as an approximation of f in (2.12). This leads to the alternative approximations of $F_{m,n}(f)$ in the form

$$F_{m,n}(f_1) := \sum_{\mathbf{t}_{j,k} \in D_{m,n}} f_1(\mathbf{t}_{j,k}) \quad \text{and} \quad I_{m,n}(f_1) := \frac{1}{\Delta_{m,n}} \iint_{D_{m,n}} f_1(\mathbf{x})\, d\mathbf{x}. \tag{2.35}$$

The following lemma which establishes uniform bounds on sums of maximum values, follows the approach outlined in Lemma 3.3 of Ecevit and Boysal [5]. This technique enables us to systematically control error terms when converting between discrete sums and continuous integrals.

Lemma 2.11. *For all integers $m, n \geq 2$, it holds that*

$$\frac{\Delta_{m,n}}{mn} \sum_{\mathbf{t}_{j,k} \in D_{m,n}} \max_{\mathbf{x} \in X_{j,k}} \frac{1}{\|\mathbf{x}\|^4} \leq 3\left(\frac{m}{n} + \frac{n}{m}\right)^2.$$

Proof. Using the notation established in (2.8)–(2.10) and applying (2.8), we obtain

$$
\begin{aligned}
\sum_{\mathbf{t}_{j,k}\in D_{m,n}} \max_{\mathbf{x}\in X_{j,k}} \frac{\Delta_{m,n}}{\|\mathbf{x}\|^4} &\le \sum_{\substack{|j|\le \frac{m}{2}\\ |k|\le \frac{n}{2}\\ (j,k)\neq(0,0)}} \max_{\mathbf{x}\in X_{j,k}} \frac{\Delta_{m,n}}{\|\mathbf{x}\|^4} \\
&\le \sum_{\substack{1\le j\le \frac{m}{2}\\ 1\le k\le \frac{n}{2}}} \max_{\mathbf{x}\in X_{j,k}} \frac{4\Delta_{m,n}}{\|\mathbf{x}\|^4} + \sum_{1\le j\le \frac{m}{2}} \max_{\mathbf{x}\in X_{j,0}} \frac{2\Delta_{m,n}}{\|\mathbf{x}\|^4} + \sum_{1\le k\le \frac{n}{2}} \max_{\mathbf{x}\in X_{0,k}} \frac{2\Delta_{m,n}}{\|\mathbf{x}\|^4} \\
&\le \sum_{\substack{2\le j\le \frac{m}{2}\\ 2\le k\le \frac{n}{2}}} \max_{\mathbf{x}\in X_{j,k}} \frac{4\Delta_{m,n}}{\|\mathbf{x}\|^4} + \sum_{1\le j\le \frac{m}{2}} \max_{\mathbf{x}\in X_{j,0}} \frac{6\Delta_{m,n}}{\|\mathbf{x}\|^4} + \sum_{1\le k\le \frac{n}{2}} \max_{\mathbf{x}\in X_{0,k}} \frac{6\Delta_{m,n}}{\|\mathbf{x}\|^4} \\
&= \sum_{\substack{2\le j\le \frac{m}{2}\\ 2\le k\le \frac{n}{2}}} \frac{4\Delta_{m,n}}{\|\mathbf{x}_{j,k}\|^4} + \sum_{1\le j\le \frac{m}{2}} \frac{6\Delta_{m,n}}{x_j^4} + \sum_{1\le k\le \frac{n}{2}} \frac{6\Delta_{m,n}}{(x_k')^4}. \qquad (2.36)
\end{aligned}
$$

For the first sum, we can bound each term in the summation by integrating the function $\frac{4}{\|\mathbf{x}\|^4}$ over corresponding rectangles. Since this function is decreasing as $\|\mathbf{x}\|$ increases, and $\mathbf{x}_{j,k}$ is the center of rectangle $X_{j,k}$, we observe

$$
\begin{aligned}
&\sum_{\substack{2\le j\le \frac{m}{2}\\ 2\le k\le \frac{n}{2}}} \frac{4\Delta_{m,n}}{\|\mathbf{x}_{j,k}\|^4} \;\le\; \sum_{\substack{2\le j\le \frac{m}{2}\\ 2\le k\le \frac{n}{2}}} \int_{X_{j-1,k-1}} \frac{4}{\|\mathbf{x}\|^4}\,d\mathbf{x} \;\le\; \int_{[0,\pi]^2\setminus\left[0,\frac{\pi}{m}\right]\times\left[0,\frac{\pi}{n}\right]} \frac{4}{\|\mathbf{x}\|^4}\,d\mathbf{x} \\
&\le \int_0^{\frac{\pi}{4}} \int_{\sqrt{\frac{\pi^2}{m^2}+\frac{\pi^2}{n^2}}}^{\sqrt{2}\,\pi} \frac{4}{r^4}\, r\,dr\,d\theta \;\le\; \frac{1}{2\pi}\,\frac{m^2n^2}{m^2+n^2} \;\le\; \frac{1}{4\pi}\,\frac{(m^2+n^2)^2}{m^2+n^2} \;=\; \frac{m^2+n^2}{4\pi}. \qquad (2.37)
\end{aligned}
$$

For the boundary terms, we have

$$
\begin{aligned}
\sum_{1\le j\le \frac{m}{2}} \frac{6\Delta_{m,n}}{x_j^4} &= \frac{6\Delta_{m,n}}{x_1^4} + \sum_{2\le j\le \frac{m}{2}} \frac{6\Delta_{m,n}}{x_j^4} = \frac{6\Delta_{m,n}}{x_1^4} + 6\Delta_n \sum_{2\le j\le \frac{m}{2}} \frac{\Delta_m}{x_j^4} \\
&\le \frac{6\Delta_{m,n}}{x_1^4} + 6\Delta_n \sum_{2\le j\le \frac{m}{2}} \int_{x_{j-1}}^{x_j} \frac{1}{t^4}\,dt \le \frac{6\Delta_{m,n}}{x_1^4} + 6\Delta_n \int_{\frac{\pi}{m}}^{\pi} \frac{1}{t^4}\,dt \le \frac{28}{\pi^2}\frac{m^3}{n}, \qquad (2.38)
\end{aligned}
$$

and analogously,

$$\sum_{1 \le k \le \frac{n}{2}} \frac{6\Delta_{m,n}}{(x'_k)^4} \le \frac{28}{\pi^2} \frac{n^3}{m}. \tag{2.39}$$

Combining (2.37)–(2.39) in (2.36), we obtain

$$\Delta_{m,n} \sum_{\mathbf{t}_{j,k} \in D_{m,n}} \max_{\mathbf{x} \in X_{j,k}} \frac{1}{\|\mathbf{x}\|^4} \le \frac{m^2 + n^2}{4\pi} + \frac{28}{\pi^2} \left(\frac{m^3}{n} + \frac{n^3}{m} \right). \tag{2.40}$$

Dividing (2.40) by mn, noting $\frac{m^2+n^2}{mn} = \frac{m}{n} + \frac{n}{m}$, as well as observing that

$$\frac{m}{n} + \frac{n}{m} \le \left(\frac{m}{n} + \frac{n}{m} \right)^2$$

and

$$\frac{m^2}{n^2} + \frac{n^2}{m^2} \le \left(\frac{m}{n} + \frac{n}{m} \right)^2,$$

we arrive at

$$\frac{\Delta_{m,n}}{mn} \sum_{\mathbf{t}_{j,k} \in D_{m,n}} \max_{\mathbf{x} \in X_{j,k}} \frac{1}{\|\mathbf{x}\|^4} \le \left(\frac{1}{4\pi} + \frac{28}{\pi^2} \right) \left(\frac{m}{n} + \frac{n}{m} \right)^2 \approx 2.92 \left(\frac{m}{n} + \frac{n}{m} \right)^2 < 3 \left(\frac{m}{n} + \frac{n}{m} \right)^2,$$

which establishes the claimed inequality. $\square$

For the square lattice case, when m and n are not necessarily equal, the functions f in (2.12) and f_1 in (2.34) take the explicit forms

$$f(\mathbf{x}) = \frac{1}{\varphi(\mathbf{x})} = f(x, y) = \frac{1}{1 - \frac{1}{2}(\cos x + \cos y)} \tag{2.41}$$

and

$$f_1(\mathbf{x}) = f_1(x, y) = \frac{4}{x^2 + y^2}, \tag{2.42}$$

where $p_1(\mathbf{x}) = \frac{1}{2}(x^2 + y^2)$ from (2.21) with $L = 2$. In the continuous domain, $f_1(\mathbf{x}) = \frac{4}{x^2+y^2}$ as defined in equation (2.42), while in the discrete sum $F_{m,n}(f_1)$, we use $f_1(\mathbf{t}_{j,k}) = \frac{4}{(2\pi j/m)^2+(2\pi k/n)^2}$ to account for lattice spacing, consistent with the scaling in §3.

Let us note that the asymptotic behavior investigated here need not be limited to $F_{m,n}$. To prepare for the next theorem, we first establish the connection between the lattice sum $F_{m,n}$ and the Kirchhoff index. The Kirchhoff index $Kf(G)$ of a graph G, defined as the sum of effective resistances between all vertex pairs in an electrical network interpretation, can be expressed in terms of $F_{m,n}$ for square lattices. In particular, for lattices with free ($P_m \square P_n$), cylindrical ($P_m \square C_n$), and toroidal ($C_m \square C_n$) boundary conditions (see [6, 10, 11]), we have

$$Kf(P_m \square P_n) = \frac{mn}{4} F^{\text{free}}_{m,n} = \frac{mn}{4} \sum_{\substack{0 \le j < m \\ 0 \le k < n \\ (j,k) \ne (0,0)}} \frac{1}{1 - \frac{1}{2}(\cos \frac{\pi j}{m} + \cos \frac{\pi k}{n})}, \tag{2.43}$$

$$Kf(P_m \square C_n) = \frac{mn}{4} F^{\text{cyl}}_{m,n} = \frac{mn}{4} \sum_{\substack{0 \le j < m \\ 0 \le k < n \\ (j,k) \ne (0,0)}} \frac{1}{1 - \frac{1}{2}(\cos \frac{\pi j}{m} + \cos \frac{2\pi k}{n})}, \tag{2.44}$$

$$Kf(C_m \square C_n) = \frac{mn}{4} F^{\text{tor}}_{m,n} = \frac{mn}{4} \sum_{\substack{0 \le j < m \\ 0 \le k < n \\ (j,k) \ne (0,0)}} \frac{1}{1 - \frac{1}{2}(\cos \frac{2\pi j}{m} + \cos \frac{2\pi k}{n})}, \tag{2.45}$$

where $F^{\text{free}}_{m,n}, F^{\text{cyl}}_{m,n}, F^{\text{tor}}_{m,n}$ denote the lattice sums under each boundary condition.

In this work, we analyze the relationship between $F^{\text{tor}}_{m,n}(f)$ and $I_{m,n}(f)$, alongside algebraic identities linking $F^{\text{free}}_{m,n}$ and $F^{\text{cyl}}_{m,n}$ to $F^{\text{tor}}_{m,n}$, including their leading asymptotic terms. Physically, $F_{m,n}$ relates to the Kirchhoff index, which quantifies total effective resistance and corresponds to the trace of the Laplacian pseudo-inverse, $\mathrm{tr}(\mathcal{L}^+)$. The asymptotic results in this work thus enable estimation of this index for large periodic networks, with applications in network design and random walk analysis (cf. [10, 11]).

The following theorems form a cohesive framework for our asymptotic analysis. Theorem 2.12 establishes the universal scaling behavior of lattice sums across different boundary conditions, Theorem 2.13 identifies the precise leading coefficient in the asymptotic expansion for square domains, and Theorem 2.15 quantifies the approximation error when using our decomposition approach. Together, these results provide a complete characterization of the asymptotic behavior of lattice sums, with progressively refined error bounds. As shown in Theorem 1.1 of Ecevit and Boysal [5], the Kirchhoff index for a square lattice with different boundary conditions exhibits universal asymptotic behavior. The following theorem establishes this universal asymptotic behavior of the Kirchhoff indices, demonstrating consistent scaling across boundary conditions for large lattices.

Theorem 2.12 (Universal Asymptotic Behavior)**.** *For $0 < \alpha \leq \beta$ and each $F_{m,n}$ in the set*

$$\{F^{free}_{m,n}, F^{cyl}_{m,n}, F^{tor}_{m,n}\},$$

there exists a constant $C_{\alpha,\beta} > 0$ such that

$$\left|\frac{F_{m,n}}{mn\log(mn)} - \frac{1}{\pi}\right| \leq \frac{C_{\alpha,\beta}}{\log(mn)}$$

for all $m, n \geq 2$ with $\alpha \leq \frac{m}{n} \leq \beta$. Additionally, for fixed $\alpha, \beta > 0$ with $\alpha \leq \beta$,

$$\lim_{r\to\infty} \sup_{\substack{m,n\geq r \\ \alpha\leq \frac{m}{n}\leq\beta}} \left|\frac{F_{m,n}}{mn\log(mn)} - \frac{1}{\pi}\right| = 0$$

uniformly over m, n satisfying the ratio condition, and for all $k \in \mathbb{N}$, we have

$$\lim_{m\to\infty} \frac{F_{m,km}}{m(km)\log(m(km))} = \lim_{n\to\infty} \frac{F_{kn,n}}{(kn)n\log((kn)n)} = \frac{1}{\pi}.$$

For the special case $m = n$, we define $F_n = F_{n,n}$ for a simplified notation and set the following theorem which establishes the universal asymptotic behavior and follows from the framework developed in Theorem 3.2 of [4].

Theorem 2.13. *(Asymptotic Equivalence) If $\Sigma_n \in \{F_n(f), F_n(f_1), I_n(f), I_n(f_1)\}$, then,*

$$\Sigma_n = \frac{L}{\pi\sqrt{\det(S^T S)}}\, n^2 \log n + \mathcal{O}(n^2)$$

as $n \to \infty$, where L is the number of generators in the lattice and S is the matrix of basis vectors defined by

$$S = \begin{bmatrix} s_{1,1} & \cdots & s_{1,\ell} & \cdots & s_{1,L} \\ s_{2,1} & \cdots & s_{2,\ell} & \cdots & s_{2,L} \end{bmatrix}^T \tag{2.46}$$

with each row of S corresponding to a lattice generator $\mathbf{s}_\ell = (s_{1,\ell}, s_{2,\ell})$ as defined in §2. The matrix $S^T S$ defined in Equation (2.46) encodes the geometry of the lattice, and its determinant affects the leading coefficient in the asymptotic expansion.

Remark 2.14. Theorem 2.13's dominant term $\frac{L}{\pi\sqrt{\det(S^T S)}} n^2 \log n$ exceeds the $\mathcal{O}(n^2)$ error, as $\frac{n^2}{n^2 \log n} = \frac{1}{\log n} \to 0$ when $n \to \infty$. This asymptotic relationship holds uniformly for non-degenerate lattices ($\det(S^T S) > 0$).

The key error bound presented in the following theorem is stated by Theorem 3.3 of [4].

Theorem 2.15. *We have*

$$F_n(f) - I_n(f) + I_n(f_1) - F_n(f_1) = \mathcal{O}(\log n) \text{ as } n \to \infty. \tag{2.47}$$

This theorem provides our key error estimate, demonstrating that the asymptotic behavior of $F_n(f)$ can be accurately determined through the more tractable quantities

$I_n(f)$, $I_n(f_1)$, and $F_n(f_1)$. The $\mathcal{O}(\log n)$ error term arises from careful handling of the singularity near the origin, using the decomposition approach introduced in Lemma 2.4 and further refined through cancellation effects.

The error is negligible compared to the leading term, as $\frac{\log n}{n^2 \log n} = \mathcal{O}(n^{-2}) \to 0$ when $n \to \infty$. This confirms the asymptotic validity of our approximation approach. The error term reflects the second-order Taylor series expansion of $\varphi(\mathbf{x})$ used in f_1 as defined in equation (2.23), valid asymptotically as $\mathbf{x} \to 0$. This approximation introduces errors of order $\mathcal{O}(\|\mathbf{x}\|^2)$ near the origin, which integrate to $\mathcal{O}(\log n)$ due to the logarithmic singularity, as will be shown in the subsequent chapters.

The theorems above describe the asymptotic behavior of these sums and integrals to high orders. In particular, Theorem 2.13 for asymptotic equivalence, establishes that the leading terms in the asymptotic expansions of $F_n(f)$, $I_n(f)$, $F_n(f_m)$, and $I_n(f_m)$ as $n \to \infty$ are identical. This is followed by Theorem 2.15 for approximation and error bounds, which demonstrates that as $n \to \infty$, $F_n(f)$ can be approximated by a combination of $F_n(f_m)$ and $I_n(f_m)$ with an error term of order $\mathcal{O}(\log n)$ when $m = 1$ and $\mathcal{O}(1)$ when $m > 1$. The error term reflects the second-order Taylor series expansion of $\varphi(\mathbf{x})$ used in f_1 as defined in equation (2.23), valid asymptotically as $\mathbf{x} \to 0$.

Proofs of Theorems 2.13 and 2.15 are given in the subsequent chapters. For the triangular lattice, we apply (2.47) to simplify the approach, consistent with [3]. This equation allows us to rewrite $F_n(f)$, the original lattice sum in a powerful reformulation, since $I_n(f)$ is the continuous integral approximation that can be evaluated using standard techniques such as polar coordinates and special functions, $I_n(f_1)$ is the integral of the approximant function, often having a simple closed form, and $F_n(f_1)$ is the sum of the approximant function, which is more tractable than the original sum. For the triangular lattice in particular, this approach allows us to calculate $I_n(f)$ directly through explicit integration, determine $I_n(f_1)$ using simpler quadratic forms, evaluate $F_n(f_1)$ using number-theoretic techniques and combine these results to obtain the asymptotic expansion for $F_n(f)$ with error $\mathcal{O}(\log n)$. This creates a systematic pathway to determine the asymptotic behavior without having to directly analyze the more complex original sum. In this path, we explore the asymptotic properties of $I_n(f_1)$ and $F_n(f_1)$ across general planar lattices. Although the integral $I_n(f)$ varies with the specific lattice, its explicit computation is feasible for any prescribed lattice structure.

As established in §2.1, the Euler–Maclaurin summation formula (2.1) serves as a foundational tool in our asymptotic analysis, providing a systematic framework for transforming discrete sums into integral representations with precisely controlled error terms as shown in equation (2.2). For any integers n, $p \geq 1$ and function $g \in C^p[0,1]$, this formula decomposes the sum into main integral contributions, boundary correction terms, and rigorously bounded remainders. The selection of $p = 4$ throughout our work ensures remainder terms of order $\mathcal{O}(n^{-4})$, which proves sufficient for our asymptotic regime. When applied to specific functions such as those encountered in §4.4.1, this decomposition yields the precise asymptotic expansions with controlled error terms that form the technical core of Theorems 2.13 and 2.15.

Concerning $F_n(f_1)$ and $I_n(f_1)$, let us define

$$a := \sum_{\ell=1}^{L} s_{1,\ell}^2, \quad b := 2\sum_{\ell=1}^{L} s_{1,\ell}s_{2,\ell}, \quad c := \sum_{\ell=1}^{L} s_{2,\ell}^2, \tag{2.48}$$

where $a, b, c \in \mathbb{Z}$ and $d = -4\det(S^T S)$ (see (2.46)).

Under this notation, we present the asymptotic behavior of $F_n(f_1)$ and $I_n(f_1)$, where this result corresponds to Theorem 3.6 of [4].

Theorem 2.16. *For the function $F_n(f_1)$, $n \to \infty$, we have*

$$\begin{aligned} F_n(f_1) = \frac{2L}{\pi\sqrt{|d|}} n^2 \log n + \frac{L}{\pi^2\sqrt{|d|}} \Bigg[& 2\pi\left(\gamma - \log 2\right) - 4\pi \log|\eta(\mu)| \\ & + \left(\frac{\pi}{2} - \arctan\left(\frac{c-a}{\sqrt{|d|}}\right)\right) \log\left(\frac{c}{a}\right) - C(a,b,c) \Bigg] n^2 \end{aligned}$$

$$+\frac{L}{\pi^2}\left[\frac{1}{3}\left(\frac{1}{a-b+c}+\frac{1}{a+b+c}+\frac{\pi}{\sqrt{|d|}}\right)\right.$$
$$\left.-\frac{1+(-1)^n}{2}\left(\frac{\pi}{\sqrt{|d|}}+\frac{2}{a-b+c}\right)\right]+\mathcal{O}\left(\frac{\log n}{n^2}\right) \tag{2.49}$$

where $\mu = \frac{-b+\sqrt{|d|}i}{2c}$ *and* $|\eta(\mu)|$ *is as presented in Apostol [12], §3.*

The following theorem presents the asymptotic expansion of $I_n(f_1)$, following the analysis given in Theorem 3.7 of [4].

Theorem 2.17. *For odd* n*,*

$$I_n(f_1) = \frac{2L}{\pi\sqrt{|d|}}\, n^2 \log n.$$

For even n*, as* $n \to \infty$*,*

$$I_n(f_1) = \frac{2L}{\pi\sqrt{|d|}}\, n^2 \log n - \left(\frac{L}{\pi\sqrt{|d|}} + \frac{2L}{\pi^2}\frac{1}{a-b+c}\right) + \mathcal{O}\left(\frac{1}{n^2}\right).$$

The proof of Theorem 2.16 is presented in §4.4.2, while that of Theorem 2.17 appears in §4.2. In relation to the proof of Theorem 2.17, it is worth observing that, with a, b, and c defined as in Equation (2.48), we find

$$f_1(x,y) = \frac{1}{p_1(x,y)} = \frac{2L}{ax^2+bxy+cy^2}. \tag{2.50}$$

3. SQUARE LATTICE

Having established the general framework for lattice sums in §2, we now specialize our analysis to the important case of the square lattice. The techniques developed here—particularly the handling of boundary conditions and the relationship between discrete sums and continuous integrals will form the foundation for our treatment of higher-order terms and more complex lattice geometries in subsequent chapters. This chapter focuses on applying our framework to the square lattice, establishing exact relations as will be given in Theorem 3.1 and uniform asymptotic estimates in Theorem 3.2. We begin by deriving an exact relation between the sums $F^{\mathrm{free}}_{m,n}$ and $F^{\mathrm{cyl}}_{m,n}$ to $F^{\mathrm{tor}}_{m,n}$, where "free," "cyl," and "tor" denote free, cylindrical, and toroidal boundary conditions, respectively. The relationship between lattice sums with different boundary conditions was derived in Theorem 2.3 of Ecevit and Boysal [5] given by

Theorem 3.1. *For all $m, n \geq 2$, the sums $F^{free}_{m,n}$ and $F^{cyl}_{m,n}$ are related to $F^{tor}_{m,n}$ through the identities*

$$F^{free}_{m,n} = \frac{1}{4}F^{tor}_{2m,2n} + \frac{1}{2}\big(B^{sum}_1(2m) + B^{sum}_1(2n) - B^{sum}_2(2m) - B^{sum}_2(2n)\big) - \frac{7}{8} \tag{3.1}$$

and

$$F^{cyl}_{m,n} = \frac{1}{2}F^{tor}_{2m,n} + B^{sum}_1(n) - B^{sum}_2(n) - \frac{1}{2}, \tag{3.2}$$

where

$$B^{sum}_1(m) = \frac{m^2-1}{6}, \quad B^{sum}_2(m) = \frac{m}{2\sqrt{2}}\left(\frac{1}{(3+2\sqrt{2})^m - 1} - \frac{1}{(3-2\sqrt{2})^m - 1}\right) - \frac{1}{2}.$$

Proof. Since the derivation of (3.2) follows an analogous path, we only prove (3.1). The proof proceeds by separating terms in $F^{\mathrm{tor}}_{2m,2n}$ to isolate boundary contributions, applying index shifts to exploit symmetry, and computing residues via the contour integral method. We begin by isolating the boundary terms (where $j = 0$ or $k = 0$) in $F^{\text{tor}}_{2m,2n}$ to obtain

$$F^{\text{tor}}_{2m,2n} = \sum_{\substack{1\le j<2m\\1\le k<2n}} \frac{1}{1-\frac{1}{2}\left(\cos\left(\frac{2\pi j}{2m}\right)+\cos\left(\frac{2\pi k}{2n}\right)\right)} + 2\tilde{B}^{\text{sum}}_1(2m) + 2\tilde{B}^{\text{sum}}_1(2n), \tag{3.3}$$

where $\tilde{B}^{\text{sum}}_1(m)$ represents the sum along a single axis

$$\tilde{B}^{\text{sum}}_1(m) = \sum_{j=1}^{m-1} \frac{1}{1-\cos\left(\frac{2\pi j}{m}\right)}.$$

To utilize symmetry properties, we perform an index shift $j \to -j + 2m$. Under this transformation, $\cos\left(\frac{2\pi j}{2m}\right)$ becomes $\cos\left(\pi - \frac{\pi j}{m}\right) = -\cos\left(\frac{\pi j}{m}\right)$, which allows us to define the new auxiliary sum

$$\tilde{B}^{\text{sum}}_2(m) = \sum_{j=1}^{m-1} \frac{1}{3-\cos\left(\frac{2\pi j}{m}\right)}.$$

For the specific case of $m = 2m'$ where m' is the original parameter, this gives

$$\tilde{B}^{\text{sum}}_2(2m) = 2\sum_{j=1}^{m-1} \frac{1}{3-\cos\left(\frac{\pi j}{m}\right)} + \frac{1}{4}.$$

After performing similar index shifts for both coordinates and combining the resulting expressions, we can reorganize the sum in (3.3) according to different regions of the (j, k) lattice. In particular, we separate the terms where j and k are both in $\{1, 2, \ldots, m-1\}$ and $\{1, 2, \ldots, n-1\}$ respectively, and account for the symmetry in the cosine terms. This leads to

$$F^{\text{tor}}_{2m,2n} = \sum_{\substack{1\le j<m\\1\le k<n}} \frac{4}{1-\frac{1}{2}\left(\cos\left(\frac{\pi j}{m}\right)+\cos\left(\frac{\pi k}{n}\right)\right)} + 2\big(\tilde{B}^{\text{sum}}_1(2m) + \tilde{B}^{\text{sum}}_1(2n) + \tilde{B}^{\text{sum}}_2(2m) + \tilde{B}^{\text{sum}}_2(2n)\big) - \frac{1}{2}. \tag{3.4}$$

For the free boundary condition sum, we observe that $\tilde{B}_1^{\mathrm{sum}}(2m) = 2\sum_{j=1}^{m-1} \frac{1}{1-\cos\frac{\pi j}{m}} + \frac{1}{2}$. This allows us to express

$$F_{m,n}^{\mathrm{free}} = \sum_{\substack{1\le j<m\\1\le k<n}} \frac{1}{1-\frac{1}{2}\left(\cos\frac{\pi j}{m}+\cos\frac{\pi k}{n}\right)} + \tilde{B}_1^{\mathrm{sum}}(2m) + \tilde{B}_1^{\mathrm{sum}}(2n) - 1. \tag{3.5}$$

Comparing equations (3.4) and (3.5), we derive

$$F_{m,n}^{\mathrm{free}} = \frac{1}{4}\,F_{2m,2n}^{\mathrm{tor}} + \frac{1}{2}(\tilde{B}_1^{\mathrm{sum}}(2m) + \tilde{B}_1^{\mathrm{sum}}(2n) - \tilde{B}_2^{\mathrm{sum}}(2m) - \tilde{B}_2^{\mathrm{sum}}(2n)) - \frac{7}{8}. \tag{3.6}$$

To complete the proof, we need to establish the identities

$$\tilde{B}_1^{\mathrm{sum}}(m) = B_1^{\mathrm{sum}}(m) \quad \text{and} \quad \tilde{B}_2^{\mathrm{sum}}(m) = B_2^{\mathrm{sum}}(m) \quad (m \ge 2). \tag{3.7}$$

Since the derivation of the first identity is straightforward, we focus on establishing the second identity in (3.7). We begin by rewriting

$$\tilde{B}_2^{\mathrm{sum}}(m) = \sum_{\zeta^m=1,\zeta\ne1} \frac{1}{3-\frac{\zeta+\zeta^{-1}}{2}} = -2\sum_{\zeta^m=1} \frac{\zeta}{\zeta^2-6\zeta+1} - \frac{1}{2},$$

where ζ ranges over the m-th roots of unity excluding 1. To evaluate this sum, we apply the residue theorem on the extended complex plane. We consider the meromorphic differential

$$G(z)dz = \frac{z}{z^2-6z+1}\cdot\frac{1}{z^m-1}\cdot\frac{1}{z}\,dz,$$

which has poles at

- $z = 0$ (from the $\frac{1}{z}$ factor),
- $z = r_1 = 3+2\sqrt{2}$ and $z = r_2 = 3-2\sqrt{2}$ (roots of $z^2-6z+1=0$),
- and the m-th roots of unity (from the $\frac{1}{z^m-1}$ factor).

By the residue theorem, the sum of all residues equals zero. Calculating the residues at each pole and rearranging, we obtain

$$\sum_{\zeta^m=1} \frac{\zeta}{\zeta^2 - 6\zeta + 1} = -m(\mathrm{Res}_{z=r_1} G(z)dz + \mathrm{Res}_{z=r_2} G(z)dz).$$

The residues at r_1 and r_2 can be computed as

$$\mathrm{Res}_{z=r_i} G(z)dz = \frac{r_i}{(r_i)^m - 1} \cdot \frac{1}{r_i'}, \quad i = 1, 2$$

where r_i' is the derivative of $z^2 - 6z + 1$ evaluated at r_i. Computing these residues explicitly and substituting back yields exactly the formula for $B_2^{\mathrm{sum}}(m)$ given in the theorem statement. Thus, $\tilde{B}_2^{\mathrm{sum}}(m) = B_2^{\mathrm{sum}}(m)$, completing the proof. □

In connection with which we have the following result derived as Theorem 2.1 of Ecevit and Boysal [5],

Theorem 3.2. *For the toroidal boundary conditions, we obtain the uniform estimate*

$$\frac{|F_{m,n}^{\mathrm{tor}} - I_{m,n}|}{mn} \leq C \left(\frac{m}{n} + \frac{n}{m}\right)^3, \tag{3.8}$$

where the constant $C > 0$ is independent of both m and n, with $m, n \geq 2$.

Proof. Applying the midpoint quadrature error bound from Lemma 2.6, we obtain

$$\begin{aligned} |F_{m,n}^{\mathrm{tor}} - I_{m,n}| &\leq \sum_{\mathbf{t}_{j,k} \in D_{m,n}} \left| f\left(\mathbf{t}_{j,k}\right) - \frac{1}{\Delta_{m,n}} \int_{X_{j,k}} f(\mathbf{x})\, d\mathbf{x} \right| \\ &\leq \frac{1}{24} \sum_{\mathbf{t}_{j,k} \in D_{m,n}} \left(\Delta_m^2 \max_{\mathbf{x} \in X_{j,k}} |\partial_1^2 f(\mathbf{x})| + \Delta_n^2 \max_{\mathbf{x} \in X_{j,k}} |\partial_2^2 f(\mathbf{x})| \right), \end{aligned}$$

where $\Delta_m = \frac{2\pi}{m}$ and $\Delta_n = \frac{2\pi}{n}$ are the mesh sizes, and $\Delta_{m,n} = \frac{4\pi^2}{mn}$, Substituting these values and factoring out $\Delta_{m,n} = \Delta_m \Delta_n$, we get

$$
\begin{aligned}
|F^{\text{tor}}_{m,n} - I_{m,n}| &\leq \frac{1}{24} \sum_{\mathbf{t}_{j,k} \in D_{m,n}} \big(\Delta_m^2 \Delta_n \cdot \frac{1}{\Delta_n} \max_{\mathbf{x} \in X_{j,k}} |\partial_1^2 f(\mathbf{x})| + \Delta_n^2 \Delta_m \cdot \frac{1}{\Delta_m} \max_{\mathbf{x} \in X_{j,k}} |\partial_2^2 f(\mathbf{x})| \big) \\
&= \frac{1}{24} \sum_{\mathbf{t}_{j,k} \in D_{m,n}} \big(\frac{n}{m} \Delta_{m,n} \max_{\mathbf{x} \in X_{j,k}} |\partial_1^2 f(\mathbf{x})| + \frac{m}{n} \Delta_{m,n} \max_{\mathbf{x} \in X_{j,k}} |\partial_2^2 f(\mathbf{x})| \big).
\end{aligned}
$$

From Lemma 2.8(b), we have the bound $|\partial_k^2 f(\mathbf{x})| \leq \frac{C(\beta)}{\|\mathbf{x}\|^4}$ for $k = 1, 2$, which allows us to write

$$
\begin{aligned}
|F^{\text{tor}}_{m,n} - I_{m,n}| &\leq \frac{1}{24} \sum_{\mathbf{t}_{j,k} \in D_{m,n}} \big(\frac{n}{m} \Delta_{m,n} \frac{C(\beta)}{\min_{\mathbf{x} \in X_{j,k}} \|\mathbf{x}\|^4} + \frac{m}{n} \Delta_{m,n} \frac{C(\beta)}{\min_{\mathbf{x} \in X_{j,k}} \|\mathbf{x}\|^4} \big) \\
&= \frac{C(\beta)}{24} \left(\frac{n}{m} + \frac{m}{n} \right) \Delta_{m,n} \sum_{\mathbf{t}_{j,k} \in D_{m,n}} \max_{\mathbf{x} \in X_{j,k}} \frac{1}{\|\mathbf{x}\|^4}.
\end{aligned}
$$

Dividing both sides by mn and using $\Delta_{m,n} = \frac{4\pi^2}{mn}$, we get

$$
\begin{aligned}
\frac{|F^{\text{tor}}_{m,n} - I_{m,n}|}{mn} &\leq \frac{C(\beta)}{24} \left(\frac{n}{m} + \frac{m}{n} \right) \frac{\Delta_{m,n}}{mn} \sum_{\mathbf{t}_{j,k} \in D_{m,n}} \max_{\mathbf{x} \in X_{j,k}} \frac{1}{\|\mathbf{x}\|^4} \\
&= \frac{C(\beta) \cdot 4\pi^2}{24} \left(\frac{n}{m} + \frac{m}{n} \right) \frac{1}{(mn)^2} \sum_{\mathbf{t}_{j,k} \in D_{m,n}} \max_{\mathbf{x} \in X_{j,k}} \frac{1}{\|\mathbf{x}\|^4}.
\end{aligned}
$$

Now we apply Lemma 2.11, which gives us

$$
\frac{\Delta_{m,n}}{mn} \sum_{\mathbf{t}_{j,k} \in D_{m,n}} \max_{\mathbf{x} \in X_{j,k}} \frac{1}{\|\mathbf{x}\|^4} \leq 3 \left(\frac{m}{n} + \frac{n}{m} \right)^2.
$$

Substituting this bound, we obtain

$$
\begin{aligned}
\frac{|F^{\text{tor}}_{m,n} - I_{m,n}|}{mn} &\leq \frac{C(\beta) \cdot 4\pi^2}{24} \left(\frac{n}{m} + \frac{m}{n} \right) \cdot 3 \left(\frac{m}{n} + \frac{n}{m} \right)^2 \\
&= \frac{C(\beta) \cdot 4\pi^2 \cdot 3}{24} \left(\frac{m}{n} + \frac{n}{m} \right)^3 = \frac{C(\beta) \cdot \pi^2}{2} \left(\frac{m}{n} + \frac{n}{m} \right)^3.
\end{aligned}
$$

Setting $C = \frac{C(\beta)\cdot\pi^2}{2}$, which is independent of m and n, we obtain the desired uniform estimate

$$\frac{|F^{\mathrm{tor}}_{m,n} - I_{m,n}|}{mn} \leq C\left(\frac{m}{n} + \frac{n}{m}\right)^3,$$

completing the proof. □

Following the approach in Theorem 2.2 of Ecevit and Boysal [5], we decompose the domain $D_{m,n}$ and apply the error estimates as

Theorem 3.3. *There exists a constant C such that, for all $m, n \geq 2$,*

$$\frac{|I_{m,n} - A_{m,n}|}{mn} \leq C$$

where

$$A_{m,n} = \frac{1}{\pi} mn\,\log(mn) + \frac{4mn}{\pi^2}\log\left(\frac{m}{n}\right)\left(\frac{\pi}{4} - \arctan\frac{b_m}{b_n}\right) \tag{3.9}$$

with

$$b_m = \tan\left(\frac{\pi}{2m}\right) \qquad (m \in \mathbb{N}).$$

Proof. We proceed by introducing a sequence of approximating integrals that progressively approach $A_{m,n}$, then bounding the difference between consecutive approximations.

First, an auxiliary integral is introduced for the proof as

$$I^1_{m,n} = \frac{mn}{4\pi^2}\iint_{R_{m,n}} \frac{dx\,dy}{1 - \frac{1}{2}(\cos x + \cos y)}.$$

Subsequently, we establish bounds for the difference between $I_{m,n}$ and $I^1_{m,n}$, analyze the asymptotic behavior of $I^1_{m,n}$, and combine these results to obtain the desired estimate. The set $(D_{m,n} \setminus R_{m,n}) \cup (R_{m,n} \setminus D_{m,n})$ is a subset of $R = [-\frac{3\pi}{2}, \frac{3\pi}{2}]^2 \setminus [-\frac{\pi}{2}, \frac{\pi}{2}]^2$, and the integrand is bounded on R regardless of the values of m and n. These ensure the existence of a constant C such that, for all $m, n \geq 2$,

$$\left| I_{m,n} - I^1_{m,n} \right| \leq C\, mn. \tag{3.10}$$

Concerning $I^1_{m,n}$, observe that the integrand is even with respect to both x and y, and $R_{m,n}$ is symmetric with respect to the coordinate axes. Thus,

$$I^1_{m,n} = \frac{mn}{\pi^2} \iint_{R^+_{m,n}} \frac{dx\, dy}{1 - \frac{1}{2}(\cos x + \cos y)} = \frac{4mn}{\pi^2} \iint_{P_{m,n}} \frac{du\, dv}{u^2 + v^2 + 2u^2v^2}$$

where $R^+_{m,n}$ denotes the segment of $R_{m,n}$

$$R_{m,n} = [-\pi, \pi]^2 \setminus \left[-\frac{\pi}{m}, \frac{\pi}{m}\right] \times \left[-\frac{\pi}{n}, \frac{\pi}{n}\right]$$

located in the first quadrant, and

$$P_{m,n} = [0, \infty)^2 \setminus ([0, b_m] \times [0, b_n]);$$

the second identity follows from the transformation

$$\begin{cases} x = 2 \arctan u \\ y = 2 \arctan v \end{cases}$$

which maps the infinite first quadrant to $[0, \pi/2]^2$. Conversion to polar coordinates and use of the substitution $t = \sqrt{2}\, r \cos\theta \sin\theta$ for the radial integral yield

$$I^1_{m,n} = \frac{4mn}{\pi^2} \left[\int_0^{\arctan \frac{b_n}{b_m}} \int_{\frac{b_m}{\cos\theta}}^{\infty} + \int_{\arctan \frac{b_n}{b_m}}^{\frac{\pi}{2}} \int_{\frac{b_n}{\sin\theta}}^{\infty} \right] \frac{r\, dr\, d\theta}{r^2 + 2r^4 \cos^2\theta \sin^2\theta}$$

$$= \frac{4mn}{\pi^2}\left[\int_0^{\arctan\frac{b_n}{b_m}}\int_{\sqrt{2}b_m\sin\theta}^{\infty} + \int_{\arctan\frac{b_n}{b_m}}^{\frac{\pi}{2}}\int_{\sqrt{2}b_n\cos\theta}^{\infty}\right]\Big(\frac{1}{t} - \frac{t}{t^2+1}\Big)dt\,d\theta$$

$$= \frac{2mn}{\pi^2}\left[\int_0^{\arctan\frac{b_n}{b_m}}\log\left(\frac{1+2b_m^2\sin^2\theta}{2b_m^2\sin^2\theta}\right)d\theta \right.$$
$$\left. + \int_{\arctan\frac{b_n}{b_m}}^{\frac{\pi}{2}}\log\left(\frac{1+2b_n^2\cos^2\theta}{2b_n^2\cos^2\theta}\right)d\theta\right].$$

Since $\log(1+x) \leq x$ on $[0,\infty)$ and $\tan x \leq 2x$ on $[0,\frac{\pi}{4}]$, for $m \geq 2$ there holds

$$\left|\log\left(\frac{1+2b_m^2\sin^2\theta}{2b_m^2\sin^2\theta}\right) + \log(b_m^2\sin^2\theta)\right| = \left|\log\left(\frac{1+2b_m^2\sin^2\theta}{2}\right)\right|$$
$$\leq \log 2 + \log(1+2b_m^2) \leq \log 2 + 2b_m^2 = \log 2 + 2\tan^2\left(\frac{\pi}{2m}\right) \leq \log 2 + \frac{2\pi^2}{m^2} < 6.$$

An analogous estimate holds for the second integrand. Consequently, if we introduce a second approximation focusing on the dominant logarithmic terms

$$I_{m,n}^2 = -\frac{2mn}{\pi^2}\left[\int_0^{\arctan\frac{b_n}{b_m}}\log\left(b_m^2\sin^2\theta\right)d\theta + \int_{\arctan\frac{b_n}{b_m}}^{\frac{\pi}{2}}\log\left(b_n^2\cos^2\theta\right)d\theta\right],$$

then, for all $m,n \geq 2$, we can bound the difference

$$\left|I_{m,n}^1 - I_{m,n}^2\right| \leq \frac{2mn}{\pi^2}\left(\frac{6\pi}{2} + \frac{6\pi}{2}\right) = \frac{12}{\pi}mn. \tag{3.11}$$

Moreover, since

$$0 < -\int_0^{\arctan\frac{b_n}{b_m}}\log(\sin^2\theta)\,d\theta < -\int_0^{\frac{\pi}{2}}\log(\sin^2\theta)\,d\theta = \pi\,\log 2$$

and

$$0 < -\int_{\arctan\frac{b_m}{b_n}}^{\frac{\pi}{2}}\log(\cos^2\theta)\,d\theta < -\int_0^{\frac{\pi}{2}}\log(\cos^2\theta)\,d\theta = \pi\,\log 2,$$

for all $m, n \geq 2$, there holds

$$\left|I^2_{m,n} - I^3_{m,n}\right| \leq \frac{2mn}{\pi^2}\,(\pi\,\log 2 + \pi\,\log 2) = \frac{\log 16}{\pi}\,mn, \tag{3.12}$$

where we introduce a third approximation, that isolates the $\log(b_m^2)$ and $\log(b_n^2)$ terms,

$$\begin{aligned} I^3_{m,n} &= -\frac{2mn}{\pi^2}\left[\int_0^{\arctan\frac{b_n}{b_m}} \log(b_m^2)\,d\theta + \int_{\arctan\frac{b_n}{b_m}}^{\frac{\pi}{2}} \log(b_n^2)\,d\theta\right] \\ &= -\frac{4mn}{\pi^2}\left(\log(b_m)\,\arctan\frac{b_n}{b_m} + \log(b_n)\,\arctan\frac{b_m}{b_n}\right). \end{aligned}$$

Additionally, $\log(\tan x) = \log(x + \mathcal{O}(x^3)) = \log x + \log(1 + \mathcal{O}(x^2)) = \log x + \mathcal{O}(x^2)$ as $x \to 0^+$, and there exists a constant C such that

$$\begin{aligned} \left|\log(b_m) + \log m\right| &\leq \left|\log(b_m) - \log\left(\frac{\pi}{2m}\right)\right| + \left|\log\left(\frac{\pi}{2m}\right) + \log m\right| \\ &= \left|\log\left(\tan\left(\frac{\pi}{2m}\right)\right) - \log\left(\frac{\pi}{2m}\right)\right| + \log\left(\frac{\pi}{2}\right) \leq \frac{C}{m^2} + \log\left(\frac{\pi}{2}\right) \end{aligned}$$

for all $m \geq 2$. Consequently, there exists a constant C such that, for all $m, n \geq 2$,

$$\left|I^3_{m,n} - I^4_{m,n}\right| \leq C\,mn \tag{3.13}$$

where our fourth approximation which replaces $\log(b_m)$ with $\log(m)$ (and similarly for n) is

$$I^4_{m,n} = \frac{4mn}{\pi^2}\left(\log(m)\,\arctan\frac{b_n}{b_m} + \log(n)\,\arctan\frac{b_m}{b_n}\right);$$

direct substitution entails that in fact $I^4_{m,n} = A_{m,n}$. By combining inequalities (3.10)–(3.13) and setting $C = C_1 + \frac{12}{\pi} + \frac{\log 16}{\pi} + C_4$, we establish that for all $m, n \geq 2$:

$$\left|I_{m,n} - A_{m,n}\right| \leq C\,mn, \tag{3.14}$$

which completes the proof. $\square$

3.1. Proof of Theorem 2.12

Proof of Theorem 2.12

With $A_{m,n}$ as in Theorem 3.3, equation (3.9), given constants $0 < \alpha \leq \beta$, we need to establish the asymptotic relationship between $F_{m,n}$ and $mn\log(mn)$.

Let us begin by recalling the error bounds from Theorem 3.2:

$$\frac{|F^{\text{tor}}_{m,n} - I_{m,n}|}{mn} \leq C\left(\frac{m}{n} + \frac{n}{m}\right)^3 \tag{3.15}$$

This bounds the difference between the discrete sum $F^{\text{tor}}_{m,n}$ and its integral approximation $I_{m,n}$. From Theorem 3.3, we have the approximation error

$$\frac{|I_{m,n} - A_{m,n}|}{mn} \leq C \tag{3.16}$$

where C is a constant independent of m and n. By applying the triangle inequality, we can combine these results

$$\frac{\left|F^{\text{tor}}_{m,n} - A_{m,n}\right|}{mn} \leq \frac{\left|F^{\text{tor}}_{m,n} - I_{m,n}\right|}{mn} + \frac{|I_{m,n} - A_{m,n}|}{mn} \leq C\left(\frac{m}{n} + \frac{n}{m}\right)^3 + C.$$

Under the constraint $\alpha \leq \frac{m}{n} \leq \beta$, the ratio terms are bounded as

$$\left(\frac{m}{n} + \frac{n}{m}\right)^3 \leq \left(\beta + \frac{1}{\alpha}\right)^3. \tag{3.17}$$

Thus, there exists a constant $C'_{\alpha,\beta}$ dependent only on α and β such that

$$\frac{\left|F^{\text{tor}}_{m,n} - A_{m,n}\right|}{mn} \leq C'_{\alpha,\beta}. \tag{3.18}$$

Also, from the definition of $A_{m,n}$ in (3.9), we can bound the difference between $A_{m,n}$ and the leading term $\frac{1}{\pi}mn\log(mn)$. In particular, the second term in (3.9) is bounded when $\alpha \leq \frac{m}{n} \leq \beta$, since both $\log\left(\frac{m}{n}\right)$ and $\arctan\frac{b_m}{b_n}$ are bounded. This yields

$$\frac{\left|A_{m,n} - \frac{1}{\pi}\, mn\, \log(mn)\right|}{mn} \leq \frac{3}{\pi}\, \max\left\{\left|\log\alpha\right|, \left|\log\beta\right|\right\}. \tag{3.19}$$

This in turn will imply Theorem 2.12 from inequalities (3.18) and (3.19) when $F_{m,n} = F^{\rm tor}_{m,n}$. In fact, (3.18) combined with (3.1) gives us, for all $m, n \geq 2$,

$$\begin{aligned}
\frac{\left|F^{\rm free}_{m,n} - \frac{1}{4}\, A_{2m,2n}\right|}{mn} &\leq \frac{\left|F^{\rm tor}_{2m,2n} - A_{2m,2n}\right|}{4mn} \\
&+ \frac{\left|\frac{1}{2}\left(B_1(2m) + B_1(2n) - B_2(2m) - B_2(2n)\right) - \frac{7}{8}\right|}{mn} \\
&\leq C'_{\alpha,\beta} + \frac{1}{3}\, \frac{m^2+n^2}{mn} \leq C'_{\alpha,\beta} + \frac{1}{3}\left(\frac{1}{\alpha} + \beta\right)
\end{aligned}$$

where we applied the bound $0 \leq \frac{1}{2}\left(B^{\rm sum}_1(2m) + B^{\rm sum}_1(2n) - B^{\rm sum}_2(2m) - B^{\rm sum}_2(2n)\right) - \frac{7}{8} \leq (m^2+n^2)/3$.

As above, this estimate, (3.19) implies Theorem 2.12 for $F_{m,n} = F^{\rm free}_{m,n}$. The proof for $F_{m,n} = F^{\rm cyl}_{m,n}$ is similarly based on (3.18) and (3.2).

$\square$

4. HIGHER-ORDER ASYMPTOTIC BEHAVIOR OF $F_{m,n}(f)$ WHEN $m = n$

Here, we refine our asymptotic analysis for square domains ($m = n$), illustrating the application of the theorems derived, to three lattice types.

4.1. Lemmata

We initially analyze the function φ in (2.12) together with its partial derivatives

$$\partial_k \varphi(\mathbf{x}) = \frac{1}{L} \sum_{\ell=1}^{L} s_{k,\ell} \sin(\mathbf{s}_\ell \cdot \mathbf{x}) \quad \text{and} \quad \partial_k^2 \varphi(\mathbf{x}) = \frac{1}{L} \sum_{\ell=1}^{L} s_{k,\ell}^2 \cos(\mathbf{s}_\ell \cdot \mathbf{x}), \tag{4.1}$$

where $\partial_k = \dfrac{\partial}{\partial x_k}$, for $k = 1, 2$. The crucial bounds on second derivatives of f(x) presented in the following lemma build upon techniques developed in Boysal, Ecevit, and Yildirim, Corollary 4.9 [4], and further extended in Ecevit and Boysal [5]. Lemma 3.2 of [5] provides the framework for controlling the singularity at the origin, while the specific form of these bounds follows the approach of [4].

Lemma 4.1 (Bounds on Second Derivatives)**.** *Let $\beta \in (0, 1)$ be fixed, and let $\Omega_\beta = \{\mathbf{x} \in \mathbb{R}^2 : 0 < \|\mathbf{x}\| \le \frac{\sqrt{12(1-\beta)}}{\overline{s}}\}$. Then, there exists a constant $C_3(\beta) > 0$ such that for all $\mathbf{x} \in \Omega_\beta$,*

$$|\partial_k^2 f(\mathbf{x})| \le \frac{C_3(\beta)}{\|\mathbf{x}\|^4},$$

where the constant $C_3(\beta)$ is explicitly given by

$$C_3(\beta) = \frac{3\overline{s}^4}{C_1(\beta)^3},$$

with the constant $C_1(\beta)$ as in (2.2).

Proof. Let $\mathbf{x} \in \Omega_\beta$. By the chain rule,

$$\partial_k^2 f(\mathbf{x}) = \frac{2(\partial_k \varphi(\mathbf{x}))^2 - \varphi(\mathbf{x})\partial_k^2 \varphi(\mathbf{x})}{(\varphi(\mathbf{x}))^3}.$$

Using the uniform bounds from Lemma 2.7(b) and Lemma 2.7(c) for all $\mathbf{x} \in \Omega_\beta$ and $k = 1, 2$, and the lower bound from Lemma (2.8)(a), we get,

$$|\partial_k^2 f(\mathbf{x})| \leq \frac{2(\overline{s}^2\|\mathbf{x}\|)^2 + C_1(\beta)\|\mathbf{x}\|^2\overline{s}^2}{(C_1(\beta)\|\mathbf{x}\|^2)^3} = \frac{3\overline{s}^4}{C_1(\beta)^3}\frac{1}{\|\mathbf{x}\|^4}.$$

□

Taylor series approximation derivations of φ itself and its first- and second-order partial derivatives around the origin follow, all of which are derived following the approach in Lemma 4.4 of [4].

Lemma 4.2. *For all $\mathbf{x} \in \mathbb{R}^2$, all $m \geq 0$, and $k = 1, 2$, we have*

$$\begin{aligned}
\varphi(\mathbf{x}) &= \frac{1}{L}\sum_{\ell=1}^{L}\Big\{\sum_{j=1}^{m}\frac{(-1)^{j+1}(\mathbf{s}_\ell\cdot\mathbf{x})^{2j}}{(2j)!} + \frac{(-1)^m(\mathbf{s}_\ell\cdot\mathbf{x})^{2m+2}}{(2m+2)!}\cos(\mathbf{s}_\ell\cdot\mathbf{p})\Big\},\\
\partial_k\varphi(\mathbf{x}) &= \frac{1}{L}\sum_{\ell=1}^{L}s_{k,\ell}\Big\{\sum_{j=1}^{m}\frac{(-1)^{j+1}(\mathbf{s}_\ell\cdot\mathbf{x})^{2j-1}}{(2j-1)!} + \frac{(-1)^m(\mathbf{s}_\ell\cdot\mathbf{x})^{2m+1}}{(2m+1)!}\cos(\mathbf{s}_\ell\cdot\mathbf{q})\Big\},\\
\partial_k^2\varphi(\mathbf{x}) &= \frac{1}{L}\sum_{\ell=1}^{L}s_{k,\ell}^2\Big\{1 + \sum_{j=1}^{m}\frac{(-1)^{j}(\mathbf{s}_\ell\cdot\mathbf{x})^{2j}}{(2j)!} + \frac{(-1)^{m+1}(\mathbf{s}_\ell\cdot\mathbf{x})^{2m+2}}{(2m+2)!}\cos(\mathbf{s}_\ell\cdot\mathbf{r})\Big\}
\end{aligned}$$

for some $\mathbf{p}, \mathbf{q}, \mathbf{r} \in \mathbb{R}^2$ which depend on m and $\mathbf{x}$ and also lie on the line segment that joins the origin with $\mathbf{x}$.

Proof. To prove this lemma, we make use of the Taylor series expansion of $\cos(\mathbf{s}\cdot\mathbf{x})$. For $\mathbf{s} = (s_1, s_2) \in \mathbb{R}^2$, the expansion is

$$\cos(\mathbf{s}\cdot\mathbf{x}) = \sum_{j=0}^{\infty}\frac{(-1)^j(\mathbf{s}\cdot\mathbf{x})^{2j}}{(2j)!},$$

yielding

$$\partial_k \cos(\mathbf{s}\cdot\mathbf{x}) = -s_k \sin(\mathbf{s}\cdot\mathbf{x}).$$

Similarly, using the Taylor series expansion of $\sin(\mathbf{s}\cdot\mathbf{x})$

$$\sin(\mathbf{s}\cdot\mathbf{x}) = \sum_{j=0}^{\infty} \frac{(-1)^j(\mathbf{s}\cdot\mathbf{x})^{2j+1}}{(2j+1)!}.$$

we get

$$\partial_k \cos(\mathbf{s}\cdot\mathbf{x}) = -s_k \sum_{j=0}^{\infty} \frac{(-1)^j(\mathbf{s}\cdot\mathbf{x})^{2j+1}}{(2j+1)!}.$$

Taking the second derivative,

$$\partial_k^2 \cos(\mathbf{s}\cdot\mathbf{x}) = -s_k^2 \cos(\mathbf{s}\cdot\mathbf{x}),$$

we get,

$$\partial_k^2 \cos(\mathbf{s}\cdot\mathbf{x}) = s_k^2 \sum_{j=0}^{\infty} \frac{(-1)^j(\mathbf{s}\cdot\mathbf{x})^{2j}}{(2j)!}.$$

We can then write $\varphi(\mathbf{x})$ and its derivatives after these expansions as

$$\varphi(\mathbf{x}) = \frac{1}{L}\sum_{\ell=1}^{L}\left\{\sum_{j=1}^{m} \frac{(-1)^{j+1}(\mathbf{s}_\ell\cdot\mathbf{x})^{2j}}{(2j)!} + \frac{(-1)^m(\mathbf{s}_\ell\cdot\mathbf{x})^{2m+2}}{(2m+2)!}\cos(\mathbf{s}_\ell\cdot\mathbf{p})\right\},$$

where $\mathbf{p}$ lies on the line segment connecting the origin and $\mathbf{x}$.

The first derivative is

$$\partial_k\varphi(\mathbf{x}) = \frac{1}{L}\sum_{\ell=1}^{L} s_{k,\ell}\left\{\sum_{j=1}^{m} \frac{(-1)^{j+1}(\mathbf{s}_\ell\cdot\mathbf{x})^{2j-1}}{(2j-1)!} + \frac{(-1)^m(\mathbf{s}_\ell\cdot\mathbf{x})^{2m+1}}{(2m+1)!}\cos(\mathbf{s}_\ell\cdot\mathbf{q})\right\},$$

where $\mathbf{q}$ is similarly defined as $\mathbf{p}$.

The second derivative is

$$\partial_k^2\varphi(\mathbf{x}) = \frac{1}{L}\sum_{\ell=1}^{L} s_{k,\ell}^2 \left\{1 + \sum_{j=1}^{m} \frac{(-1)^j(\mathbf{s}_\ell\cdot\mathbf{x})^{2j}}{(2j)!} + \frac{(-1)^{m+1}(\mathbf{s}_\ell\cdot\mathbf{x})^{2m+2}}{(2m+2)!}\cos(\mathbf{s}_\ell\cdot\mathbf{r})\right\},$$

where $\mathbf{r}$ also lies on the line segment that joins the origin with $\mathbf{x}$. We obtain required expressions by choosing $n = 2m+1$ for φ and $\partial_k^2\varphi$, and $n = 2m$ for $\partial_k\varphi$. □

Noting that, for $m \geq 1$,

$$\partial_k p_m(\mathbf{x}) = \frac{1}{L}\sum_{\ell=1}^{L} s_{k,\ell}\sum_{j=1}^{m}\frac{(-1)^{j+1}(\mathbf{s}_\ell\cdot\mathbf{x})^{2j-1}}{(2j-1)!},$$

and

$$\partial_k^2 p_m(\mathbf{x}) = \frac{1}{L}\sum_{\ell=1}^{L} s_{k,\ell}^2\left\{1 + \sum_{j=1}^{m-1}\frac{(-1)^j(\mathbf{s}_\ell\cdot\mathbf{x})^{2j}}{(2j)!}\right\}.$$

Lemma 4.2 yields the following corollary, where the relationship between $\varphi(\mathbf{x})$ its Taylor polynomial $p_m(\mathbf{x})$ corresponds to Corollary 4.5 of [4].

Corollary 4.3. *For all $m \geq 1$, all $\mathbf{x} \in \mathbb{R}^2$, and $k = 1, 2$, we have*

$$\varphi(\mathbf{x}) = p_m(\mathbf{x}) + \frac{1}{L}\frac{(-1)^m}{(2m+2)!}\sum_{\ell=1}^{L}(\mathbf{s}_\ell\cdot\mathbf{x})^{2m+2}\cos(\mathbf{s}_\ell\cdot\mathbf{p}), \tag{4.2}$$

$$\partial_k\varphi(\mathbf{x}) = \partial_k p_m(\mathbf{x}) + \frac{1}{L}\frac{(-1)^m}{(2m+1)!}\sum_{\ell=1}^{L} s_{k,\ell}(\mathbf{s}_\ell\cdot\mathbf{x})^{2m+1}\cos(\mathbf{s}_\ell\cdot\mathbf{q}),$$

$$\partial_k^2\varphi(\mathbf{x}) = \partial_k^2 p_m(\mathbf{x}) + \frac{1}{L}\frac{(-1)^m}{(2m)!}\sum_{\ell=1}^{L} s_{k,\ell}^2(\mathbf{s}_\ell\cdot\mathbf{x})^{2m}\cos(\mathbf{s}_\ell\cdot\mathbf{r}).$$

In each remainder term, by the mean-value form of Taylor's theorem, the point $\mathbf{p}, \mathbf{q}, \mathbf{r}$ in $\mathbb{R}^2$, which is also dependent on m and $\mathbf{x}$, and, when applicable, on k, is guaranteed *to lie on the line segment that joins the origin with* $\mathbf{x}$*. We keep this consistent notation in all three expansions.*

Proof. The Taylor polynomial and its derivative with respect to x_k can be expressed as

$$p_m(\mathbf{x}) = \frac{1}{L}\sum_{\ell=1}^{L}\sum_{j=1}^{m}\frac{(-1)^{j+1}}{(2j)!}(\mathbf{s}_\ell\cdot\mathbf{x})^{2j}, \tag{4.3}$$

$$\partial_k p_m(\mathbf{x}) = \frac{1}{L}\sum_{\ell=1}^{L}\sum_{j=1}^{m}\frac{(-1)^{j+1}2j}{(2j)!}(\mathbf{s}_\ell\cdot\mathbf{x})^{2j-1}s_{k,\ell}. \tag{4.4}$$

The remainder term in our expansion takes the form

$$R(\mathbf{x}) = \frac{1}{L}\sum_{\ell=1}^{L}\frac{(-1)^m}{(2m+2)!}(\mathbf{s}_\ell\cdot\xi_\ell(\mathbf{x}))^{2m+2}\cos(\mathbf{s}_\ell\cdot\xi_\ell(\mathbf{x})), \tag{4.5}$$

with $\xi_\ell(\mathbf{x})$ lying on the line segment that joins the origin with $\mathbf{x}$. Hence, to take a derivative with respect to x_k of $R(\mathbf{x})$ we need to apply the chain rule such that

$$\begin{aligned}\frac{\partial}{\partial x_k}&\Big((\mathbf{s}_\ell\cdot\xi_\ell(\mathbf{x}))^{2m+2}\cos(\mathbf{s}_\ell\cdot\xi_\ell(\mathbf{x}))\Big)\\ &= (2m+2)\left(\mathbf{s}_\ell\cdot\xi_\ell(\mathbf{x})\right)^{2m+1}\cos\left(\mathbf{s}_\ell\cdot\xi_\ell(\mathbf{x})\right)\cdot\frac{\partial}{\partial x_k}\left(\mathbf{s}_\ell\cdot\xi_\ell(\mathbf{x})\right)\\ &\quad-\left(\mathbf{s}_\ell\cdot\xi_\ell(\mathbf{x})\right)^{2m+2}\sin\left(\mathbf{s}_\ell\cdot\xi_\ell(\mathbf{x})\right)\cdot\frac{\partial}{\partial x_k}\left(\mathbf{s}_\ell\cdot\xi_\ell(\mathbf{x})\right).\end{aligned}$$

Since $\xi_\ell(\mathbf{x})$ is itself a function of $\mathbf{x}$, applying the chain rule once more, we can show that

$$\frac{\partial}{\partial x_k}(\mathbf{s}_\ell\cdot\xi_\ell(\mathbf{x})) = s_{k,\ell}\cdot\frac{\partial\xi_\ell(\mathbf{x})}{\partial x_k}.$$

By Taylor's theorem, we know that the remainder term is already implicitly bounded. This allows us to apply the Mean Value Theorem, according to which an intermediate point η_ℓ exists on the line segment that joins the origin with $\mathbf{x}$ such that

$$\frac{\partial R(\mathbf{x})}{\partial x_k} = \frac{1}{L}\sum_{\ell=1}^{L} \frac{(-1)^m}{(2m+1)!} s_{k,\ell}(\mathbf{s}_\ell \cdot \eta_\ell)^{2m+1} \cos(\mathbf{s}_\ell \cdot \eta_\ell).$$

Proceeding, we can further simplify this to introduce a single point $\mathbf{q}$ such that

$$\frac{\partial R(\mathbf{x})}{\partial x_k} = \frac{1}{L}\sum_{\ell=1}^{L} \frac{(-1)^m}{(2m+1)!} s_{k,\ell}(\mathbf{s}_\ell \cdot \mathbf{x})^{2m+1} \cos(\mathbf{s}_\ell \cdot \mathbf{q})$$

where $\mathbf{q}$ is yet another intermediate point between $\mathbf{0}$ and $\mathbf{x}$, depending on m, $\mathbf{x}$, and k. However, the second derivative of $p_m(\mathbf{x})$ is still simple to compute since it is a polynomial form of terms

$$\frac{\partial^2 p_m(\mathbf{x})}{\partial x_k^2} = \sum_{j=1}^{m} \frac{(-1)^{j+1}}{L} \sum_{\ell=1}^{L} \frac{2j(2j-1)(\mathbf{s}_\ell \cdot \mathbf{x})^{2j-2} s_{k,\ell}^2}{(2j)!}.$$

Next, we compute the second derivative of $(R(\mathbf{x})$. Again, carefully applying the chain rule, we see that

$$\begin{aligned}
&\frac{\partial^2}{\partial x_k^2}\left((\mathbf{s}_\ell \cdot \xi_\ell(\mathbf{x}))^{2m+2} \cos(\mathbf{s}_\ell \cdot \xi_\ell(\mathbf{x}))\right) \\
&\quad = \frac{\partial}{\partial x_k}\left((2m+2)(\mathbf{s}_\ell \cdot \xi_\ell(\mathbf{x}))^{2m+1} \cos(\mathbf{s}_\ell \cdot \xi_\ell(\mathbf{x})) \cdot \frac{\partial}{\partial x_k}(\mathbf{s}_\ell \cdot \xi_\ell(\mathbf{x}))\right) \\
&\qquad - \frac{\partial}{\partial x_k}\left((\mathbf{s}_\ell \cdot \xi_\ell(\mathbf{x}))^{2m+2} \sin(\mathbf{s}_\ell \cdot \xi_\ell(\mathbf{x})) \cdot \frac{\partial}{\partial x_k}(\mathbf{s}_\ell \cdot \xi_\ell(\mathbf{x}))\right).
\end{aligned}$$

We then differentiate each term according to the chain rule, do the simplifications, and finally apply the Mean Value Theorem to get

$$\frac{\partial^2 R(\mathbf{x})}{\partial x_k^2} = \frac{1}{L}\sum_{\ell=1}^{L} \frac{(-1)^m}{(2m)!} s_{k,\ell}^2(\mathbf{s}_\ell \cdot \mathbf{x})^{2m} \cos(\mathbf{s}_\ell \cdot \mathbf{r})$$

where $\mathbf{r}$ is another point along the line segment that joins the origin with $\mathbf{x}$. □

Bulding upon the above corollary, we arrive at the estimates that follow.

Corollary 4.4. *For all* $\mathbf{x} \in \mathbb{R}^2$, *we have*

$$|\varphi(\mathbf{x}) - p_m(\mathbf{x})| \leq \frac{\overline{s}^{2m+2}}{(2m+2)!}\|\mathbf{x}\|^{2m+2}, \tag{4.6}$$

$$|\partial_k\varphi(\mathbf{x}) - \partial_k p_m(\mathbf{x})| \leq \frac{\overline{s}^{2m+2}}{(2m+1)!}\|\mathbf{x}\|^{2m+1}, \tag{4.7}$$

$$|\partial_k^2\varphi(\mathbf{x}) - \partial_k^2 p_m(\mathbf{x})| \leq \frac{\overline{s}^{2m+2}}{(2m)!}\|\mathbf{x}\|^{2m}. \tag{4.8}$$

Proof. We employ Corollary 4.3, the triangle inequality, and the Cauchy-Schwarz inequality to have

$$\begin{aligned}|\varphi(\mathbf{x}) - p_m(\mathbf{x})| &\leq \frac{1}{L}\frac{1}{(2m+2)!}\|\mathbf{x}\|^{2m+2}\sum_{\ell=1}^{L}\|\mathbf{s}_\ell\|^{2m+2} \\ &\leq \frac{1}{(2m+2)!}\|\mathbf{x}\|^{2m+2}\max_\ell\|\mathbf{s}_\ell\|^{2m+2} = \frac{\overline{s}^{2m+2}}{(2m+2)!}\|\mathbf{x}\|^{2m+2}.\end{aligned}$$

This proves (4.6).

For (4.7), differentiating with respect to k, applying the triangle inequality and bounding by the maximum $\overline{s}$, we get

$$|\partial_k\varphi(\mathbf{x}) - \partial_k p_m(\mathbf{x})| \leq \frac{1}{L}\frac{1}{(2m+1)!}\|\mathbf{x}\|^{2m+1}\sum_{\ell=1}^{L}|s_{k,\ell}|\|\mathbf{s}_\ell\|^{2m+1}.$$

With the inequalities

$$\sum_{\ell=1}^{L}|s_{k,\ell}|\|\mathbf{s}_\ell\|^{2m+1} \leq \sum_{\ell=1}^{L}\|\mathbf{s}_\ell\|^{2m+1}, \leq L\overline{s}^{2m+1}.$$

we obtain,

$$|\partial_k\varphi(\mathbf{x}) - \partial_k p_m(\mathbf{x})| \leq \frac{\overline{s}^{2m+1}}{(2m+1)!}\|\mathbf{x}\|^{2m+1}.$$

establishing (4.7).

For(4.8), differentiate again

$$|\partial_k^2\varphi(\mathbf{x}) - \partial_k^2 p_m(\mathbf{x})| \leq \frac{1}{L}\frac{1}{(2m)!}\|\mathbf{x}\|^{2m}\sum_{\ell=1}^{L} s_{k,\ell}^2\|\mathbf{s}_\ell\|^{2m}.$$

Using the Cauchy-Schwarz inequality in its vector form,

$$\sum_{\ell=1}^{L} s_{k,\ell}^2\|\mathbf{s}_\ell\|^{2m} \leq \left(\sum_{\ell=1}^{L} s_{k,\ell}^2\right)^{1/2}\left(\sum_{\ell=1}^{L}\|\mathbf{s}_\ell\|^{2m}\right)^{1/2},$$

and bounding each term as

$$\left(\sum_{\ell=1}^{L} s_{k,\ell}^2\right)^{1/2} \leq \overline{s}, \quad \left(\sum_{\ell=1}^{L}\|\mathbf{s}_\ell\|^{2m}\right)^{1/2} \leq \overline{s},$$

we get

$$|\partial_k^2\varphi(\mathbf{x}) - \partial_k^2 p_m(\mathbf{x})| \leq \frac{\overline{s}^2}{(2m)!}\|\mathbf{x}\|^{2m}.$$

This completes the proof of (4.8). So, the corollary holds for all $m \geq 1$, $\mathbf{x} \in \mathbb{R}^2$, and $k = 1, 2$. □

The bounds for the Taylor polynomial and its derivatives given in the following lemma correspond to Lemma 4.7 of [4].

Lemma 4.5. *The following bounds hold for the Taylor polynomial $p_m(\mathbf{x})$ and its derivatives. For any $C_4 > 0$, and for all $m \geq 1$, $\mathbf{x} \in \mathbb{R}^2$ with $\|\mathbf{x}\| \leq C_4$, and $k = 1, 2$*

(i) the Taylor polynomial $p_m(\mathbf{x})$ satisfies

$$|p_m(\mathbf{x})| \leq \frac{1}{L}\|\mathbf{x}\|^2 \sum_{\ell=1}^{L}\sum_{j=1}^{m} \frac{\|\mathbf{s}_\ell\|^{2j} C_4^{2j-2}}{(2j)!} \leq \frac{\cosh(\overline{s}\, C_4)-1}{C_4^2}\|\mathbf{x}\|^2, \tag{4.9}$$

(ii) the first-order partial derivative is bounded as

$$|\partial_k p_m(\mathbf{x})| \leq \frac{1}{L}\|\mathbf{x}\| \sum_{\ell=1}^{L} |s_{k,\ell}| \sum_{j=1}^{m} \frac{\|\mathbf{s}_\ell\|^{2j-1} C_4^{2j-2}}{(2j-1)!} \leq \frac{\overline{s}\, \sinh(\overline{s}\, C_4)}{C_4}\|\mathbf{x}\|, \tag{4.10}$$

(iii) the second-order partial derivative is bounded as

$$|\partial_k^2 p_m(\mathbf{x})| \leq \frac{1}{L}\sum_{\ell=1}^{L} s_{k,\ell}^2 \Big\{1 + \sum_{j=1}^{m-1} \frac{\|\mathbf{s}_\ell\|^{2j} C_4^{2j}}{(2j)!}\Big\} \leq \overline{s}^2 \cosh(\overline{s}\, C_4). \tag{4.11}$$

Proof. Recalling that $p_m(\mathbf{x})$ is the $2m$-th order Taylor polynomial of the function

$$\varphi(\mathbf{x}) = 1 - \frac{1}{L}\sum_{\ell=1}^{L} \cos(\mathbf{s}_\ell \cdot \mathbf{x}),$$

given by

$$p_m(\mathbf{x}) = \frac{1}{L}\sum_{\ell=1}^{L}\sum_{j=1}^{m} \frac{(-1)^{j+1}(\mathbf{s}_\ell \cdot \mathbf{x})^{2j}}{(2j)!},$$

we prove each inequality separately.

(i) Using the triangle inequality, Lemma 2.9(1), and the inequality

$$|(\mathbf{s}_\ell \cdot \mathbf{x})^{2j}| \leq \|\mathbf{x}\|^{2j}\|\mathbf{s}_\ell\|^{2j}, \tag{4.12}$$

which follows from the Cauchy-Schwarz inequality, we get the following estimates

$$|p_m(\mathbf{x})| \leq \frac{1}{L}\sum_{\ell=1}^{L}\sum_{j=1}^{m}\frac{|(\mathbf{s}_\ell\cdot\mathbf{x})^{2j}|}{(2j)!} \leq \frac{1}{L}\|\mathbf{x}\|^2\sum_{\ell=1}^{L}\sum_{j=1}^{m}\frac{\|\mathbf{s}_\ell\|^{2j}}{(2j)!}.$$

Next, we recognize that the series $\sum_{j=1}^{\infty}\frac{\|\mathbf{s}_\ell\|^{2j}C_4^{2j-2}}{(2j)!}$ is a part of the exponential series, related to the hyperbolic cosine function

$$\sum_{j=1}^{\infty}\frac{x^{2j}}{(2j)!} = \cosh(x) - 1.$$

Thus, if $\overline{s} = \max_\ell \|\mathbf{s}_\ell\|$, we have

$$\sum_{j=1}^{m}\frac{\|\mathbf{s}_\ell\|^{2j}C_4^{2j-2}}{(2j)!} \leq \frac{\cosh(\overline{s}C_4) - 1}{C_4^2}.$$

Hence, we conclude as

$$|p_m(\mathbf{x})| \leq \frac{\cosh(\overline{s}C_4) - 1}{C_4^2}\|\mathbf{x}\|^2.$$

(ii) We now obtain the following estimates by applying the triangle inequality, the Cauchy-Schwarz inequality, and the inequality $|(\mathbf{s}_\ell\cdot\mathbf{x})^{2j-1}| \leq \|\mathbf{x}\|^{2j-1}\|\mathbf{s}_\ell\|^{2j-1}$

$$|\partial_k p_m(\mathbf{x})| \leq \frac{1}{L}\|\mathbf{x}\|\sum_{\ell=1}^{L}|s_{k,\ell}|\sum_{j=1}^{m}\frac{\|\mathbf{s}_\ell\|^{2j-1}C_4^{2j-2}}{(2j-1)!} \leq \frac{\overline{s}\,\sinh(\overline{s}\,C_4)}{C_4}\|\mathbf{x}\|,$$

where we used the series expansion of the hyperbolic sine function

$$\sum_{j=1}^{\infty}\frac{x^{2j-1}}{(2j-1)!} = \sinh(x).$$

(iii) We obtain the following estimates by applying the triangle inequality, the Cauchy-Schwarz inequality, and the inequality $|(\mathbf{s}_\ell\cdot\mathbf{x})^{2j}| \leq \|\mathbf{x}\|^{2j}\|\mathbf{s}_\ell\|^{2j}$

$$|\partial_k^2 p_m(\mathbf{x})| \leq \frac{1}{L}\sum_{\ell=1}^{L} s_{k,\ell}^2 \left(1 + \sum_{j=1}^{m-1} \frac{\|\mathbf{s}_\ell\|^{2j} C_4^{2j}}{(2j)!}\right) \leq \overline{s}^2 \cosh(\overline{s}\, C_4),$$

where we used the series expansion of the hyperbolic cosine function

$$\sum_{j=1}^{\infty} \frac{x^{2j}}{(2j)!} = \cosh(x) - 1.$$

□

Corollary 4.6. *(i) For a given $C_4 > 0$, there exists a constant $C_4' > 0$, depending only on C_4 such that*

$$|\partial_k^2 f_1(\mathbf{x})| \leq \frac{C_4'}{\|\mathbf{x}\|^4},$$

provided that $0 < \|\mathbf{x}\| \leq C_4$, where, $\partial_k^2 f_1(\mathbf{x}) = \frac{\partial^2 f_1}{\partial x_k^2}$ denotes the second partial derivative with respect to the k-th component.

(ii) Given a fixed $\beta \in (0,1)$, there exists a constant $C_5(\beta) > 0$ satisfying $|\partial_k^2 f_m(\mathbf{x})| \leq \frac{C_5(\beta)}{\|\mathbf{x}\|^4}$ for all $m \geq 1$ and for $0 < \|\mathbf{x}\| \leq \frac{\sqrt{12(1-\beta)}}{\overline{s}}$, where $\overline{s} = \max_\ell \|\mathbf{s}_\ell\|$.

Proof. (i) We begin by expressing the second partial derivative of $f_1(\mathbf{x})$ with respect to x_k as

$$\partial_k^2 f_1(\mathbf{x}) = \frac{2(\partial_k p_1(\mathbf{x}))^2 - p_1(\mathbf{x})\, \partial_k^2 p_1(\mathbf{x})}{(p_1(\mathbf{x}))^3}.$$

Applying the triangle inequality, we obtain

$$|\partial_k^2 f_1(\mathbf{x})| \leq \frac{2|\partial_k p_1(\mathbf{x})|^2 + |p_1(\mathbf{x})|\, |\partial_k^2 p_1(\mathbf{x})|}{|p_1(\mathbf{x})|^3}.$$

Now we make use of Lemma 4.5(3) and Lemma 2.9(1) in the inequality of $|\partial_k^2 f_1(\mathbf{x})|$ and get

$$|\partial_k^2 f_1(\mathbf{x})| \leq \frac{2\left(\frac{\overline{s}\,\sinh(\overline{s}\,C_4)}{C_4}\|\mathbf{x}\|\right)^2 + \frac{\cosh(\overline{s}\,C_4)-1}{C_4^2}\,\|\mathbf{x}\|^2\;\overline{s}^2\,\cosh(\overline{s}\,C_4)}{\left(\frac{1}{2L}\|\mathbf{x}\|^2\right)^3}.$$

Subsequent simplification yields

$$|\partial_k^2 f_1(\mathbf{x})| \leq \frac{8\,L^3\,\overline{s}^2}{C_4^2}\left[3\cosh^2(\overline{s}\,C_4) - \cosh(\overline{s}\,C_4) - 2\right]\,\frac{1}{\|\mathbf{x}\|^4}.$$

We can write the constant in the above inequality as C_4' by

$$C_4' = \frac{8\,L^3\,\overline{s}^2}{C_4^2}\left[3\cosh^2(\overline{s}\,C_4) - \cosh(\overline{s}\,C_4) - 2\right].$$

So, we are now able to show that $|\partial_k^2 f_1(\mathbf{x})| \leq \frac{C_4'}{\|\mathbf{x}\|^4}$ for $0 < \|\mathbf{x}\| \leq C_4$, where C_4' depends only on C_4. Using the derivative rules for composed functions, we can express $\partial_k^2 f_m(\mathbf{x})$ in terms of $p_m(\mathbf{x})$ and its derivatives. For $f_m(\mathbf{x}) = \frac{1}{p_m(\mathbf{x})}$, we have

$$\partial_k f_m(\mathbf{x}) = -\frac{\partial_k p_m(\mathbf{x})}{(p_m(\mathbf{x}))^2} \tag{4.13}$$

$$\partial_k^2 f_m(\mathbf{x}) = -\frac{\partial_k^2 p_m(\mathbf{x})}{(p_m(\mathbf{x}))^2} + \frac{2(\partial_k p_m(\mathbf{x}))^2}{(p_m(\mathbf{x}))^3} \tag{4.14}$$

From Lemma 4.5, we have bounds on $p_m(\mathbf{x})$ and its derivatives as

$$|p_m(\mathbf{x})| \leq \frac{\cosh(\overline{s}\,C_4) - 1}{C_4^2}\|\mathbf{x}\|^2,$$

$$|\partial_k p_m(\mathbf{x})| \leq \frac{\overline{s}\,\sinh(\overline{s}\,C_4)}{C_4}\|\mathbf{x}\|,$$

and

$$|\partial_k^2 p_m(\mathbf{x})| \leq \overline{s}^2 \cosh(\overline{s}\, C_4).$$

Additionally, from Lemma 2.9(2), we have the lower bound

$$p_m(\mathbf{x}) \geq \frac{\beta}{2L}\|\mathbf{x}\|^2, \tag{4.15}$$

for $\|\mathbf{x}\| \leq \frac{\sqrt{12(1-\beta)}}{\overline{s}}$. Substituting these bounds into the expression for $\partial_k^2 f_m(\mathbf{x})$ and simplifying yields the desired result

$$|\partial_k^2 f_m(\mathbf{x})| \leq \frac{C_5(\beta)}{\|\mathbf{x}\|^4}, \tag{4.16}$$

where $C_5(\beta)$ is the constant defined as

$$C_5(\beta) = \frac{8, L^3, \overline{s}^4}{\beta^3(1-\beta)}\left[3\cosh^2(\sqrt{12(1-\beta)}) - \cosh(\sqrt{12(1-\beta)}) - 2\right].$$

(ii) For $f_m(\mathbf{x})$, we follow a similar approach. The second partial derivative satisfies the recursive relation

$$\partial_k^2 f_m(\mathbf{x}) = \frac{2(\partial_k p_m(\mathbf{x}))^2 - p_m(\mathbf{x})\,\partial_k^2 p_m(\mathbf{x})}{(p_m(\mathbf{x}))^3}, \tag{4.17}$$

valid for all $\mathbf{x}$ in the domain of definition. Applying the triangle inequality, we get

$$|\partial_k^2 f_m(\mathbf{x})| \leq \frac{2|\partial_k p_m(\mathbf{x})|^2 + |p_m(\mathbf{x})|\,|\partial_k^2 p_m(\mathbf{x})|}{|p_m(\mathbf{x})|^3}.$$

We apply the bound from Lemma 4.5(3) and Lemma 2.9(2) again and substitution yields

$$|\partial_k^2 f_m(\mathbf{x})| \leq \frac{2\left(\frac{\bar{s}\,\sinh(\bar{s}\,C_4)}{C_4}\|\mathbf{x}\|\right)^2 + \frac{\cosh(\bar{s}\,C_4)-1}{C_4^2}\,\|\mathbf{x}\|^2\;\bar{s}^2\;\cosh(\bar{s}\,C_4)}{\left(\frac{\beta}{2L}\|\mathbf{x}\|^2\right)^3}.$$

Simplifying, we get

$$|\partial_k^2 f_m(\mathbf{x})| \leq \frac{8\,L^3\,\bar{s}^2}{\beta^3\,C_4^2}\left[3\cosh^2(\bar{s}\,C_4) - \cosh(\bar{s}\,C_4) - 2\right]\frac{1}{\|\mathbf{x}\|^4}.$$

Now, we choose $C_4 = \frac{\sqrt{12(1-\beta)}}{\bar{s}}$ which satisfies the condition in Lemma 2.9. This leads to

$$\begin{aligned}|\partial_k^2 f_m(\mathbf{x})| \leq \frac{8\,L^3\,\bar{s}^4}{\beta^3}&\left[3\cosh^2\left(\sqrt{12(1-\beta)}\right) - \cosh\left(\sqrt{12(1-\beta)}\right) - 2\right]\\ &\times\frac{1}{12(1-\beta)}\,\frac{1}{\|\mathbf{x}\|^4}.\end{aligned}$$

We define $C_5(\beta)$ as the constant factor in this inequality as

$$C_5(\beta) = \frac{8L^3\bar{s}^4}{\beta^3}\left[3\cosh^2(\sqrt{12(1-\beta)}) - \cosh(\sqrt{12(1-\beta)}) - 2\right]\frac{1}{12(1-\beta)}.$$

Therefore, we have shown that $|\partial_k^2 f_m(\mathbf{x})| \leq \frac{C_5(\beta)}{\|\mathbf{x}\|^4}$ for all $m \geq 1$ for $0 < \|\mathbf{x}\| \leq \frac{\sqrt{12(1-\beta)}}{\bar{s}}$, where $C_5(\beta)$ depends only on β, where

$$C_5(\beta) = \frac{8L^3\bar{s}^4}{\beta^3}\cdot\frac{\sinh^2(\sqrt{12(1-\beta)})}{(1-\beta)} + \frac{2\bar{s}^2L^3}{\beta^3}\cdot\cosh(\sqrt{12(1-\beta)})$$

For typical values such as $\beta = 0.5$, this yields approximately $C_5(0.5) \approx 500L^3\bar{s}^4$, which remains finite for all legitimate lattice structures where L and $\bar{s}$ are bounded. □

Lemma 4.7. *For $\beta \in (0,1)$, there exists $C_6(\beta) > 0$ such that for all $m \geq 1$ and $\mathbf{x} \in \mathbb{R}^2$ with $0 < \|\mathbf{x}\| \leq \frac{\sqrt{12(1-\beta)}}{\bar{s}}$*

$$|\partial_k^2 h_m(\mathbf{x})| \leq C_6(\beta)\|\mathbf{x}\|^{2m-4}$$

for $k = 1, 2$ where $h_m(\mathbf{x}) = f(\mathbf{x}) - f_m(\mathbf{x})$.

Proof. Given $f(\mathbf{x}) = \frac{1}{\varphi(\mathbf{x})}$ and $f_m(\mathbf{x}) = \frac{1}{p_m(\mathbf{x})}$, we define $h_m(\mathbf{x}) = f_m(\mathbf{x}) - f(\mathbf{x}) = \frac{p_m(\mathbf{x})-\varphi(\mathbf{x})}{\varphi(\mathbf{x})p_m(\mathbf{x})}$. Our goal is to bound its second partial derivative with respect to x_k. Applying the quotient rule, we compute

$$\partial_k^2 h_m(\mathbf{x}) = \frac{\partial_k^2 p_m(\mathbf{x}) - \partial_k^2\varphi(\mathbf{x})}{\varphi(\mathbf{x})p_m(\mathbf{x})} - \frac{(\partial_k p_m(\mathbf{x}) - \partial_k\varphi(\mathbf{x}))(\partial_k\varphi(\mathbf{x})p_m(\mathbf{x}) + \varphi(\mathbf{x})\partial_k p_m(\mathbf{x}))}{[\varphi(\mathbf{x})p_m(\mathbf{x})]^2},$$

which, with algebraic simplification, expands into

$$\begin{aligned}\partial_k^2 h_m(\mathbf{x}) = &\frac{2[\partial_k\varphi(\mathbf{x})]^2[p_m(\mathbf{x}) - \varphi(\mathbf{x})](p_m^2(\mathbf{x}) + p_m(\mathbf{x})\varphi(\mathbf{x}) + \varphi^2(\mathbf{x}))}{\varphi^3(\mathbf{x})p_m^3(\mathbf{x})}\\ &+ \frac{2[\partial_k\varphi(\mathbf{x}) - \partial_k p_m(\mathbf{x})][\partial_k\varphi(\mathbf{x}) + \partial_k p_m(\mathbf{x})]}{p_m^3(\mathbf{x})}\\ &+ \frac{\partial_k^2\varphi(\mathbf{x})[\varphi(\mathbf{x}) - p_m(\mathbf{x})][\varphi(\mathbf{x}) + p_m(\mathbf{x})]}{\varphi^2(\mathbf{x})p_m^2(\mathbf{x})} + \frac{\partial_k^2 p_m(\mathbf{x}) - \partial_k^2\varphi(\mathbf{x})}{p_m^2(\mathbf{x})}.\end{aligned} \tag{4.18}$$

To bound the absolute value, we apply the triangle inequality to each term and get

$$\begin{aligned}|\partial_k^2 h_m(\mathbf{x})| \leq &\frac{2[\partial_k\varphi(\mathbf{x})]^2|p_m(\mathbf{x}) - \varphi(\mathbf{x})|(p_m^2(\mathbf{x}) + p_m(\mathbf{x})\varphi(\mathbf{x}) + \varphi^2(\mathbf{x}))}{|\varphi(\mathbf{x})|^3|p_m(\mathbf{x})|^3}\\ &+ \frac{2|\partial_k\varphi(\mathbf{x}) - \partial_k p_m(\mathbf{x})|(|\partial_k\varphi(\mathbf{x})| + |\partial_k p_m(\mathbf{x})|)}{|p_m(\mathbf{x})|^3}\\ &+ \frac{|\partial_k^2\varphi(\mathbf{x})||\varphi(\mathbf{x}) - p_m(\mathbf{x})|(\varphi(\mathbf{x}) + p_m(\mathbf{x}))}{|\varphi(\mathbf{x})|^2|p_m(\mathbf{x})|^2} + \frac{|\partial_k^2 p_m(\mathbf{x}) - \partial_k^2\varphi(\mathbf{x})|}{|p_m(\mathbf{x})|^2}.\end{aligned} \tag{4.19}$$

We now substitute established bounds from prior results. Lemma 2.7(a) and (b) provide bounds on $|\varphi(\mathbf{x})|$ and $|\partial_k\varphi(\mathbf{x})|$, and Lemma 2.8(a) gives the lower bound for $\varphi(\mathbf{x})$, while Lemma 4.5 and Lemma 2.9 address the Taylor polynomial $p_m(\mathbf{x})$. Corollary 4.4; in particular, inequality (4.6), estimates the difference between $\varphi(\mathbf{x})$ and $p_m(\mathbf{x})$. These bounds facilitate the subsequent analysis of the lattice sum approximations. Applying the bounds from Corollary 4.4, in particular equation (4.6) for $|\varphi(\mathbf{x})-p_m(\mathbf{x})|$, we obtain a combined expression. After careful reduction, this results in

$$\begin{aligned}|\partial_k^2 h_m(\mathbf{x})| \le{}& \frac{32L^3\overline{s}^{2m+6}[\cosh(\overline{s}\,C_4)-1]C_4^2}{\beta^3 C_1^3(\beta)}\|\mathbf{x}\|^{2m-4} + \frac{32L^3\overline{s}^{2m+5}[\overline{s}C_4+\sinh(\overline{s}\,C_4)]}{\beta^3 C_1^3(\beta)}\|\mathbf{x}\|^{2m-4}\\ &+\frac{16L^3\overline{s}^{2m+6}[\overline{s}^2C_4^2+2(\cosh(\overline{s}\,C_4)-1)C_4^2]}{\beta^3 C_1^2(\beta)}\|\mathbf{x}\|^{2m-4} + \frac{16L^3\overline{s}^{2m+4}}{\beta^3 C_1^2(\beta)}\|\mathbf{x}\|^{2m-4}\\ ={}& \frac{L^3\overline{s}^{2m+4}}{\beta^3}\|\mathbf{x}\|^{2m-4}\left[\frac{32\overline{s}^2[\cosh(\overline{s}\,C_4)-1]C_4^2}{C_1^3(\beta)} + \frac{32\overline{s}[\overline{s}C_4+\sinh(\overline{s}\,C_4)]}{C_1^3(\beta)}\right.\\ &\left.+\frac{16\overline{s}^2[\overline{s}^2C_4^2+2(\cosh(\overline{s}\,C_4)-1)C_4^2]}{C_1^2(\beta)} + \frac{16}{C_1^2(\beta)}\right].\end{aligned}$$

Defining the constant

$$\begin{aligned}C_6(\beta) = \frac{L^3\overline{s}^{2m+4}}{\beta^3}&\left[\frac{32\overline{s}^2[\cosh(\overline{s}\,C_4)-1]C_4^2}{C_1^3(\beta)} + \frac{32\overline{s}[\overline{s}C_4+\sinh(\overline{s}\,C_4)]}{C_1^3(\beta)}\right.\\ &\left.+\frac{16\overline{s}^2[\overline{s}^2C_4^2+2(\cosh(\overline{s}\,C_4)-1)C_4^2]}{C_1^2(\beta)} + \frac{16}{C_1^2(\beta)}\right],\end{aligned}\tag{4.20}$$

we conclude

$$|\partial_k^2 h_m(\mathbf{x})| \le C_6(\beta)\|\mathbf{x}\|^{2m-4},$$

establishing the desired bound. □

For comparing the sums and integrals we will have, we need the asymptotic estimates for radial sums presented in the lemma below that utilize the results from Lemma 4.11 of [4].

Lemma 4.8. *Given $\alpha \in \mathbb{R}$, we have, as $n \to \infty$,*

$$\Delta_n^2 \sum_{\mathbf{t}_{j,k}\in D_n} \max_{\mathbf{x}\in X_{j,k}} \frac{1}{\|\mathbf{x}\|^\alpha} = \begin{cases}\mathcal{O}(n^{\alpha-2}), & \alpha > 2,\\ \mathcal{O}(\log n), & \alpha = 2,\\ \mathcal{O}(1), & \alpha < 2.\end{cases}\tag{4.21}$$

Proof. Define $S_n = \Delta_n^2 \sum_{\mathbf{t}_{j,k}\in D_n} \max_{\mathbf{x}\in X_{j,k}} \frac{1}{\|\mathbf{x}\|^\alpha}$. We begin by noting that for $\alpha > 0$, the function $\frac{1}{\|\mathbf{x}\|^\alpha}$ decreases as $\|\mathbf{x}\|$ increases. Since $\mathbf{t}_{j,k}$ is the midpoint of rectangle $X_{j,k}$, we have $\|\mathbf{t}_{j,k}\| \le \|\mathbf{x}\|$ for any $\mathbf{x}$ in the corners of $X_{j,k}$. Therefore, $\max_{\mathbf{x}\in X_{j,k}} \frac{1}{\|\mathbf{x}\|^\alpha} \le \frac{1}{\|\mathbf{t}_{j,k}\|^\alpha}$, which implies

$$S_n \le \Delta_n^2 \sum_{\mathbf{t}_{j,k}\in D_n} \frac{1}{\|\mathbf{t}_{j,k}\|^\alpha}.$$

We proceed by considering three cases,

(i) For $\alpha > 2$, we have

$$\frac{1}{\|\mathbf{t}_{j,k}\|^\alpha} = \left(\frac{n}{2\pi}\right)^\alpha \frac{1}{(j^2+k^2)^{\alpha/2}}.$$

Therefore,

$$\Delta_n^2 \sum_{\mathbf{t}_{j,k}\in D_n} \frac{1}{\|\mathbf{t}_{j,k}\|^\alpha} = \left(\frac{n}{2\pi}\right)^\alpha \Delta_n^2 \sum_{\mathbf{t}_{j,k}\in D_n} \frac{1}{(j^2+k^2)^{\alpha/2}}.$$

We can approximate the sum using a double integral as

$$\sum_{\mathbf{t}_{j,k}\in D_n} \frac{1}{(j^2+k^2)^{\alpha/2}} \approx \int_1^n \int_1^n \frac{dx\,dy}{(x^2+y^2)^{\alpha/2}}.$$

Define $S_n = \sum_{\mathbf{t}_{j,k}\in D_n} f(\mathbf{t}_{j,k})$, then, for $\alpha > 2$, the integral is bounded by

$$\int_1^n \int_1^n \frac{dx\,dy}{(x^2+y^2)^{\alpha/2}} \le \int_1^n \int_1^n \frac{dx\,dy}{x^\alpha} = \int_1^n \frac{dx}{x^\alpha} \int_1^n dy = \mathcal{O}(n^{2-\alpha}).$$

Hence,

$$S_n \le \left(\frac{n}{2\pi}\right)^\alpha \Delta_n^2 \mathcal{O}(n^{2-\alpha}) = \mathcal{O}(n^{\alpha-2}).$$

(ii) For $\alpha = 2$, we consider the sum

$$\sum_{\mathbf{t}_{j,k} \in D_n} \frac{1}{(j^2 + k^2)}.$$

We approximate this sum using an integral

$$\sum_{\mathbf{t}_{j,k} \in D_n} \frac{1}{(j^2 + k^2)} \approx \int_1^n \int_1^n \frac{dx\, dy}{x^2 + y^2}.$$

The integral for $\alpha = 2$ is bounded by

$$\int_1^n \int_1^n \frac{dx\, dy}{x^2 + y^2} \leq 4 \int_1^n \frac{dy}{y} \int_1^y \frac{dx}{x^2} = 4 \int_1^n \frac{dy}{y} \left(-\frac{1}{x}\Big|_1^y \right) = 4 \int_1^n \frac{1 - \frac{1}{y}}{y}\, dy = \mathcal{O}(\log n).$$

Thus,

$$S_n \leq \Delta_n^2 \mathcal{O}(\log n) = \mathcal{O}(\log n).$$

(iii) For $\alpha < 2$, we approximate the sum using a double integral over the domain $[1, n]^2$

$$\sum_{\mathbf{t}_{j,k} \in D_n} \frac{1}{(j^2 + k^2)^{\alpha/2}} \approx \int_1^n \int_1^n \frac{dx\, dy}{(x^2 + y^2)^{\alpha/2}}.$$

By evaluating the integral, we find that it converges to $\mathcal{O}(1)$ for $\alpha < 2$. Hence,

$$S_n = \Delta_n^2 \sum_{\mathbf{t}_{j,k} \in D_n} \frac{1}{\|\mathbf{t}_{j,k}\|^{\alpha}} = \mathcal{O}(1).$$

The integral is bounded by

$$\int_1^n \int_1^n \frac{dx\, dy}{(x^2 + y^2)^{\alpha/2}} \leq \int_1^n \int_1^n \frac{dx\, dy}{x^{\alpha}} = \int_1^n \frac{dx}{x^{\alpha}} \int_1^n dy.$$

Since $\alpha < 2$, the integral $\int_1^n \frac{dx}{x^\alpha}$ converges as $n \to \infty$, implying that the overall integral is $\mathcal{O}(1)$. Hence,

$$S_n \leq \Delta_n^2 \mathcal{O}(1) = \mathcal{O}(1).$$

□

With these bounds established, we now quantify the leading asymptotic behavior of sums and integrals involving f and f_1.

4.2. Asymptotic Behavior of $I_n(f_1)$

Having analyzed the discrete sum $F_n(f_1)$ in the previous section, we now turn our attention to its continuous counterpart, the integral $I_n(f_1)$. This integral plays a crucial role in our asymptotic analysis, as the difference between $F_n(f)$ and $I_n(f)$ contributes to the overall error term in Theorem 2.15. To proceed with the proof of Theorem 2.17, we begin by applying the definition of f_1 from equation (2.50).

Proof. (*of Theorem 2.17*)

By (2.50)

$$I_n(f_1) = \frac{1}{\Delta_n^2} \iint_{D_n} f_1 \, dx \, dy = \frac{1}{\Delta_n^2} \iint_{D_n} \frac{2L}{ax^2 + bxy + cy^2} dx \, dy$$

where a, b, c are as in (2.48). Since $f_1(x, y) = f_1(y, x)$. We now define the following sets to decompose the domain D_n

$$E(R) := \Big([0, R] \times [-R, R]\Big) \setminus \Big([0, \frac{\pi}{n}] \times [-\frac{\pi}{n}, \frac{\pi}{n}]\Big),$$
$$E_n := [\pi - \frac{\pi}{n}, \pi + \frac{\pi}{n}] \times [-\pi - \frac{\pi}{n}, -\pi + \frac{\pi}{n}],$$

where $E(R)$ represents the half-plane domain excluding a small rectangle, and E_n denotes the boundary region at the corners of D_n. These sets allow us to express $D_n \approx E(\pi) \cup E_n$ for odd n, with appropriate adjustments for even n, facilitating integration over regions more amenable to analysis. The explicit form of D_n in (2.19) enables us to write

$$I_n(f_1) = \frac{1}{\Delta_n^2} \begin{cases} 2 \iint_{E(\pi)} f_1 \, dx \, dy, & n \text{ is odd}, \\ \left(\iint_{E(\pi + \frac{\pi}{n})} + \iint_{E(\pi - \frac{\pi}{n})} - \iint_{E_n} \right) f_1 \, dx \, dy, & n \text{ is even}. \end{cases} \tag{4.22}$$

Indeed, for $R > \frac{\pi}{n}$, the transformation to polar coordinates yields the double integral

$$\begin{aligned} \iint_{E(R)} f_1 \, dx \, dy &= \int_{-\frac{\pi}{2}}^{-\frac{\pi}{4}} \int_{-\frac{\pi}{n \sin\theta}}^{-\frac{R}{\sin\theta}} \frac{2L}{a\cos^2\theta + b\cos\theta\sin\theta + c\sin^2\theta} \frac{1}{r} dr d\theta \\ &+ \int_{-\frac{\pi}{4}}^{\frac{\pi}{4}} \int_{\frac{\pi}{n \cos\theta}}^{\frac{R}{\cos\theta}} \frac{2L}{a\cos^2\theta + b\cos\theta\sin\theta + c\sin^2\theta} \frac{1}{r} dr d\theta \\ &+ \int_{\frac{\pi}{4}}^{\frac{\pi}{2}} \int_{\frac{\pi}{n \sin\theta}}^{\frac{R}{\sin\theta}} \frac{2L}{a\cos^2\theta + b\cos\theta\sin\theta + c\sin^2\theta} \frac{1}{r} dr d\theta \\ &= \log\left(\frac{n\,R}{\pi}\right) \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{2L}{a\cos^2\theta + b\cos\theta\sin\theta + c\sin^2\theta} d\theta \\ &= \log\left(\frac{n\,R}{\pi}\right) \frac{4L}{\sqrt{|d|}} \arctan\left(\frac{b + 2c\,\tan\theta}{\sqrt{|d|}}\right)\Big|_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \\ &= \log\left(\frac{n\,R}{\pi}\right) \frac{4L\pi}{\sqrt{|d|}} = \log\left(\frac{n\,R}{\pi}\right) \frac{2L\pi}{\sqrt{\det(S^T S)}}. \end{aligned} \tag{4.23}$$

Using(4.22), we obtain

$$I_n(f_1) = \frac{L}{\pi\sqrt{\det(S^T S)}} n^2 \, \log n$$

when n is odd, and

$$I_n(f_1) = \frac{L}{\pi\sqrt{\det(S^T S)}} n^2 \left(\log n + \frac{1}{2} \log\left(1 - \frac{1}{n^2}\right)\right) - \frac{1}{\Delta_n^2} \iint_{E_n} f_1 \, dx \, dy$$

when n is even. As for the very last integral, since $\partial_1^2 f_1, \partial_2^2 f_1 \asymp 1$ on E_n, Lemma 2.6 gives

$$\frac{1}{\Delta_n^2} \iint_{E_n} f_1 \, dx \, dy = f_1(-\pi, \pi) + \mathcal{O}\left(\frac{1}{n^2}\right) = \frac{2L}{\pi^2} \frac{1}{a-b+c} + \mathcal{O}\left(\frac{1}{n^2}\right).$$

□

4.3. Proof of Theorem 2.13

Let $S = \{F_n(f),\ F_n(f_1),\ I_n(f),\ I_n(f_1)\}$. We aim to show that for all pairs $A, B \in S$, the difference $|A - B| = \mathcal{O}(n^2)$ as $n \to \infty$.

We first consider the difference between the sum $F_n(f)$ and the integral $I_n(f)$. By Corollary 4.6(1), this difference can be bounded as

$$|F_n(f) - I_n(f)| \leq \frac{C_4'}{12} \Delta_n^2 \sum_{\mathbf{t}_{j,k} \in D_n} \max_{\mathbf{x} \in X_{j,k}} \frac{1}{\|\mathbf{x}\|^4}, \text{ by Corollary 4.6(1)} \tag{4.24}$$

where C_4' is a positive constant independent of n. By using Lemma 4.8, in particular the case for $\alpha > 2$ in equation (4.21),we can bound the sum over $1/\|\mathbf{x}\|^4$ as

$$\sum_{\mathbf{t}_{j,k} \in D_n} \frac{1}{\|\mathbf{t}_{j,k}\|^4} = \sum_{\mathbf{t}_{j,k} \in D_n} \frac{1}{(j^2 + k^2)^2} = \mathcal{O}(n^2).$$

So, plugging this back into the inequality, we get

$$|F_n(f) - I_n(f)| = \mathcal{O}(n^2).$$

Now let us examine the difference between the sums $F_n(f)$ and $F_n(f_1)$. We need to bound the difference $|f(\mathbf{x}) - f_1(\mathbf{x})|$. By Lemma 2.10(ii), we have the uniform bound

$$|f(\mathbf{x}) - f_1(\mathbf{x})| \leq C'(\overline{s})$$

for $\|\mathbf{x}\| \leq \delta$, where $C'(\overline{s}) = \frac{3L^2}{\overline{s}^4}$ is a constant. For points $\mathbf{t}_{j,k}$ far from the origin, the difference is also bounded. Thus, for all $\mathbf{t}_{j,k} \in D_n$, we can assume $|f(\mathbf{t}_{j,k}) - f_1(\mathbf{t}_{j,k})|$ is bounded by some constant $C_{\max}$. Therefore,

$$|F_n(f) - F_n(f_1)| \leq \sum_{\mathbf{t}_{j,k} \in D_n} |f(\mathbf{t}_{j,k}) - f_1(\mathbf{t}_{j,k})| \leq \sum_{\mathbf{t}_{j,k} \in D_n} C_{\max} = C_{\max} \cdot |D_n|.$$

Since $|D_n|$, the number of lattice points in D_n, is $\mathcal{O}(n^2)$, we conclude

$$|F_n(f) - F_n(f_1)| \leq C_{\max} \cdot \mathcal{O}(n^2) = \mathcal{O}(n^2).$$

Next, consider the difference between the integrals $I_n(f)$ and $I_n(f_1)$. By Corollary 4.6(2), the difference $f(\mathbf{x}) - f_1(\mathbf{x})$ behaves as $\mathcal{O}(\|\mathbf{x}\|^2)$, so

$$|f(\mathbf{x}) - f_1(\mathbf{x})| \leq C_6 \|\mathbf{x}\|^2$$

by Corollary 4.6(1). Substituting this into the integral difference

$$|I_n(f) - I_n(f_1)| = \left| \iint_{D_n} (f(\mathbf{x}) - f_1(\mathbf{x}))\, d\mathbf{x} \right| \leq C_6 \iint_{D_n} \|\mathbf{x}\|^2\, d\mathbf{x}.$$

By Lemma 4.8(3) (in particular, the case for $\alpha < 2$ in equation (4.21)) to compute the integral

$$\iint_{D_n} \|\mathbf{x}\|^2\, d\mathbf{x} = \mathcal{O}(n^2),$$

we conclude

$$|I_n(f) - I_n(f_1)| = \mathcal{O}(n^2).$$

For any remaining pair A and B in S, we use the triangle inequality

$$|A - B| \leq |A - C| + |B - C|.$$

Since individual terms are $\mathcal{O}(n^2)$, we conclude

$$|A - B| = \mathcal{O}(n^2).$$

We have used corollary 4.6, Corollary 4.4, Lemma 2.9 and Lemma 4.8 to show that the difference between any two elements in the set S is $\mathcal{O}(n^2)$. This covers all $\binom{4}{2} = 6$ possible pairs in S, including sums vs. integrals and different functions. Thus, for all pairs $A, B \in S$, we have

$$|A - B| = \mathcal{O}(n^2).$$

Thus, having established that $|F_n(f) - F_n(f_1)|$, $|F_n(f_1) - I_n(f_1)|$, and $|I_n(f_1) - I_n(f)|$ are all $\mathcal{O}(n^2)$, the leading term in the asymptotic expansion must be the same for all these quantities. From Theorem 2.17, we know that $I_n(f_1) = \frac{L}{\pi\sqrt{\det(S^T S)}} n^2 \log n + \mathcal{O}(n^2)$, which we will examine in detail later. Therefore, all quantities in the set S must share this same leading term, proving the theorem.

4.4. The Sum $F_n(f_1)$

The asymptotic behavior of the sum

$$F_n(f_1) := F_{n,n}(f_1) = \sum_{\mathbf{t}_{j,k} \in D_{n,n}} f_1(\mathbf{t}_{j,k})$$

will be our focus now. In our analysis, we first relate this sum to the auxiliary sum G_n:

$$G_n := \sum_{j,k=1}^{n-1} \left(\frac{1}{aj^2 - bjk + ck^2} + \frac{1}{aj^2 + bjk + ck^2} \right), \tag{4.25}$$

where a, b, and c are positive constants satisfying $b^2 < 4ac$.

Definition 4.9. The positive definite binary quadratic form is defined as

$$Q(j,k) = aj^2 + bjk + ck^2,$$

with discriminant $d := b^2 - 4ac < 0$, where $a, b, c \in \mathbb{R}$ and $a, c > 0$.

The quadratic form $Q(j,k) = aj^2 + bjk + ck^2$ in equation (4.25) can be expressed in matrix form as

$$Q(j,k) = \begin{bmatrix} j & k \end{bmatrix} \begin{bmatrix} a & b/2 \\ b/2 & c \end{bmatrix} \begin{bmatrix} j \\ k \end{bmatrix}. \tag{4.26}$$

The condition $d = b^2 - 4ac < 0$ ensures that the matrix in (4.26) has positive eigenvalues, which guarantees that $Q(j,k) > 0$ for all real pairs $(j,k) \neq (0,0)$. Consequently, the quadratic form remains positive for all integer pairs $(j,k) \neq (0,0)$, confirming its positive definiteness under the conditions $a, c > 0$.

In order to analyze the asymptotic behavior of the sum G_n defined in equation (4.25), we need to introduce a complex parameter that encodes the geometry of the lattice. This parameter is defined by

$$\mu = \frac{-b + \sqrt{|d|}i}{2c}. \tag{4.27}$$

The parameter μ has a geometric interpretation; it represents the ratio of the two periods of a complex lattice in the upper half-plane. For different lattice types, we observe the following.

- For the Square Lattice, we have $\mu = i$, corresponding to orthogonal basis vectors with equal length.
- For the Triangular Lattice, we have $\mu = \frac{-1+i\sqrt{3}}{2}$, corresponding to basis vectors with angle $\pi/3$
- For the Union Jack Lattice, we have $\mu = i$ (with scaled coefficients), reflecting its square structure with diagonal connections.

The parameter μ lies in the upper half-plane ($\Im(\mu) > 0$) due to the positive definiteness of the quadratic form, which enables the application of modular transformation properties when evaluating the Dedekind eta function $\eta(\mu)$. This will be crucial when expressing our asymptotic results, as outlined in Theorem 2.16

4.4.1. The Sum G_n

For G_n as in the sum in (4.25), we have the following theorem, where the precise asymptotic expansion presented corresponds to Theorem 3.4 of [4].

Theorem 4.10. *As $n \to \infty$, we have*

$$\begin{aligned} G_n\,(= G_{n,Q}) = \frac{2\pi}{\sqrt{|d|}} \log n &+ \left[\frac{2\pi}{\sqrt{|d|}}\gamma - \frac{\pi^2}{6}\left(\frac{1}{a} + \frac{1}{c}\right) - \frac{4\pi}{\sqrt{|d|}} \log|\eta(\mu)| \right. \\ &\quad \left. + \frac{1}{\sqrt{|d|}} \left(\left(\frac{\pi}{2} - \arctan\left(\frac{c-a}{\sqrt{|d|}}\right)\right) \log\left(\frac{c}{a}\right) - C(a,b,c) \right) \right] \\ &+ \left(\frac{1}{a} + \frac{1}{c} - \frac{\pi}{\sqrt{|d|}} \right) \frac{1}{n} \\ &+ \left[\frac{1}{2}\left(\frac{1}{a} + \frac{1}{c}\right) + \frac{1}{12}\left(\frac{1}{a-b+c} + \frac{1}{a+b+c} \right) - \frac{\pi}{6\sqrt{|d|}} \right] \frac{1}{n^2} \end{aligned} \tag{4.28}$$

$$+\left[\frac{1}{6}\left(\frac{1}{a}+\frac{1}{c}\right)+\frac{1}{12}\left(\frac{1}{a-b+c}+\frac{1}{a+b+c}\right)\right]\frac{1}{n^3}+\mathcal{O}\left(\frac{\log n}{n^4}\right)$$

where η *represents the Dedekind eta function and, while* Cl_2 *stands for the Clausen function, defined by*

$$\mathrm{Cl}_2(\theta)=\sum_{k=1}^{\infty}\frac{\sin(k\theta)}{k^2}\qquad(\theta\in\mathbb{R}),$$

see [13];

$$\begin{aligned}C(a,b,c):=\mathrm{Cl}_2\left(\pi-2\arctan\left(\frac{2a-b}{\sqrt{|d|}}\right)\right)+\mathrm{Cl}_2\left(\pi-2\arctan\left(\frac{2a+b}{\sqrt{|d|}}\right)\right)\\+\mathrm{Cl}_2\left(\pi-2\arctan\left(\frac{2c-b}{\sqrt{|d|}}\right)\right)+\mathrm{Cl}_2\left(\pi-2\arctan\left(\frac{2c+b}{\sqrt{|d|}}\right)\right).\end{aligned}\tag{4.29}$$

Theorem 4.10 provides the complete asymptotic expansion for G_n with explicit error bounds. The connection to our original lattice sum $F_n(f_1)$ comes through the relationship $F_n(f_1)=\frac{Ln^2}{2\pi^2}[G_n+\text{boundary terms}]$, where the boundary terms arise from the lattice points along the coordinate axes. By carefully accounting for these boundary contributions, we will derive the asymptotic behavior of $F_n(f_1)$ in Theorem 2.16.

Remark 4.11. Given that G_n remains unchanged when a and c are swapped, this result must exhibit the same symmetry. The sole apparently asymmetric term in Equation (4.28) is

$$-\frac{4\pi}{\sqrt{|d|}}\log|\eta(\mu)|+\frac{\pi}{2\sqrt{|d|}}\log\frac{c}{a}.$$

Nevertheless, swapping a and c leaves the value unaltered, owing to the transformation

$$\eta\Big(-\frac{1}{\tau}\Big)=(-i\tau)^{\frac{1}{2}}\eta(\tau),$$

valid for any τ with $\Im\tau > 0$, adopting the principal branch where $1^{\frac{1}{2}} = 1$. The invariance under the substitution of b with $-b$ arises from the equality $|\eta(\mu)| = |\eta(-\overline{\mu})|$.

We give the proof of Theorem 4.10 along with an analysis of the asymptotic behavior of the auxiliary functions. The parameter μ is given by (4.27) where the imaginary unit i enables the appropriate handling of the discriminant's square root, maintaining the structure required for transformations. The terms involving μ and $\overline{\mu}$ contain imaginary components; however, it is important to note that these imaginary parts cancel out when combined in the summation. This cancellation ensures that the contributions to G_n are real-valued. For instance, logarithmic differences such as

$$\log(n + \mu j) - \log(n + \overline{\mu} j)$$

yield a factor of $2i$ due to logarithmic identities. Summing these contributions absorbs the imaginary component, resulting in purely real-valued arctangent terms.

Using the summation identity for the digamma function defined as $\psi(z) = \frac{d}{dz} \ln \Gamma(z) = \frac{\Gamma'(z)}{\Gamma(z)}$ from [14],

$$\sum_{k=1}^{n-1} \frac{1}{k+z} = \psi(n+z) - \psi(1+z), \qquad (-z \notin \mathbb{N}), \tag{4.30}$$

we decompose the sum G_n as

$$\begin{aligned} G_n = \frac{i}{\sqrt{|d|}} \sum_{j=1}^{n-1} \frac{1}{j} \Big(&\psi(n+\mu j) - \psi(1+\mu j) - \psi(n+\overline{\mu} j) + \psi(1+\overline{\mu} j) \\ &- \psi(n-\mu j) + \psi(1-\mu j) + \psi(n-\overline{\mu} j) - \psi(1-\overline{\mu} j) \Big) \end{aligned} \tag{4.31}$$

where μ is defined by equation (4.27).To handle large arguments in the digamma functions, we apply the asymptotic expansion

$$\psi(z) = \log z - \frac{1}{2z} - \frac{1}{12z^2} + \mathcal{O}\left(\frac{1}{|z|^4}\right), \quad \text{as } |z| \to \infty, \ |\arg(z)| < \pi - \beta, \tag{4.32}$$

where $\beta > 0$ is a small positive constant and the condition $|\arg(z)| < \pi - \beta$ is satisfied for $z = n + \mu j$ and $z = n - \mu j$. This is because $\Im(\mu j) = \frac{\sqrt{|d|}j}{2c}$ is bounded relative to n for $1 \leq j \leq n-1$, ensuring that $\arg(n+\mu j)$ and $\arg(n-\mu j)$ remain within the required range for sufficiently large n. Using recurrence and reflection formulas

$$\psi(1+z) = \psi(z) + \frac{1}{z}, \quad \psi(1-z) = \psi(z) + \pi\cot(\pi z),$$

we proceed to simplify G_n as

$$\begin{aligned} G_n = \frac{i}{\sqrt{|d|}} \sum_{j=1}^{n-1} \frac{1}{j} \Bigg(& \log(n+\mu j) - \log(n+\overline{\mu} j) - \log(n-\mu j) + \log(n-\overline{\mu} j) \\ & - \frac{1}{2}\left(\frac{1}{n+\mu j} - \frac{1}{n+\overline{\mu} j} - \frac{1}{n-\mu j} + \frac{1}{n-\overline{\mu} j} \right) \\ & - \frac{1}{12}\left(\frac{1}{(n+\mu j)^2} - \frac{1}{(n+\overline{\mu} j)^2} - \frac{1}{(n-\mu j)^2} + \frac{1}{(n-\overline{\mu} j)^2} \right) \\ & + \pi\cot(\pi\mu j) - \pi\cot(\pi\overline{\mu} j) - \frac{1}{\mu j} + \frac{1}{\overline{\mu} j} \Bigg) + \mathcal{O}\left(\frac{\log n}{n^4}\right). \end{aligned} \tag{4.33}$$

To further simplify, we express logarithmic terms in terms of arctangent functions using the identity

$$\log(x+iy) - \log(x-iy) = 2i\arctan\left(\frac{y}{x}\right),$$

transforming the logarithmic differences into real-valued arctangent expressions

$$\begin{aligned} G_n = \frac{i}{\sqrt{|d|}} \sum_{j=1}^{n-1} \frac{1}{j} \Bigg(& 2i\arctan\left(\frac{\sqrt{|d|}j}{2c-bj}\right) + 2i\arctan\left(\frac{\sqrt{|d|}j}{2c+bj}\right) \\ & - \frac{1}{2}\left(\frac{(\overline{\mu}-\mu)j}{|n+\mu j|^2} + \frac{(\overline{\mu}-\mu)j}{|n-\mu j|^2} \right) \\ & - \frac{1}{12}\left(\frac{2(\overline{\mu}-\mu)nj + (\overline{\mu}^2-\mu^2)j^2}{|n+\mu j|^4} + \frac{2(\overline{\mu}-\mu)nj - (\overline{\mu}^2-\mu^2)j^2}{|n-\mu j|^4} \right) \\ & + 2i\pi\left(\frac{e^{2i\pi\mu j}}{1-e^{2i\pi\mu j}} + \frac{e^{-2i\pi\overline{\mu} j}}{1-e^{-2i\pi\overline{\mu} j}} + 1 \right) \\ & + \left(\frac{1}{\overline{\mu}} - \frac{1}{\mu}\right)\frac{1}{j} \Bigg) + \mathcal{O}\left(\frac{\log n}{n^4}\right). \end{aligned}$$

This results in

$$\begin{aligned}
G_n = -\frac{2}{\sqrt{|d|}} \sum_{j=1}^{n-1} \frac{1}{j} \Bigg(& \arctan\left(\frac{\sqrt{|d|}\frac{j}{n}}{2c - b\frac{j}{n}}\right) + \arctan\left(\frac{\sqrt{|d|}\frac{j}{n}}{2c + b\frac{j}{n}}\right)\Bigg) \\
& - \frac{1}{2n} \sum_{j=1}^{n-1} \frac{1}{j} \Big(\frac{1}{a\left(\frac{j}{n}\right)^2 - b\frac{j}{n} + c} + \frac{1}{a\left(\frac{j}{n}\right)^2 + b\frac{j}{n} + c} \Big) \\
& - \frac{1}{12n^2} \sum_{j=1}^{n-1} \frac{1}{j^2} \Big(\frac{2c - b\frac{j}{n}}{\left(a\left(\frac{j}{n}\right)^2 - b\frac{j}{n} + c\right)^2} + \frac{2c + b\frac{j}{n}}{\left(a\left(\frac{j}{n}\right)^2 + b\frac{j}{n} + c\right)^2} \Big) \\
& + \frac{4\pi}{\sqrt{|d|}} \Re\left(\sum_{j=1}^{n-1} \frac{1}{j} \frac{e^{2i\pi\mu j}}{1 - e^{2i\pi\mu j}}\right) + \frac{2\pi}{\sqrt{|d|}} \sum_{j=1}^{n-1} \frac{1}{j} \\
& - \frac{1}{a} \sum_{j=1}^{n-1} \frac{1}{j^2} + \mathcal{O}\left(\frac{\log n}{n^4}\right).
\end{aligned} \tag{4.34}$$

We express G_n in terms of auxiliary functions $\mathcal{G}_k$ as

$$G_n = -\frac{2}{\sqrt{|d|}}\mathcal{G}_1 - \frac{1}{2n}\mathcal{G}_2 - \frac{1}{12n^2}\mathcal{G}_3 + \frac{4\pi}{\sqrt{|d|}}\mathcal{G}_4 + \frac{2\pi}{\sqrt{|d|}}\mathcal{G}_5 - \frac{1}{a}\mathcal{G}_6 + \mathcal{O}\left(\frac{\log n}{n^4}\right)$$

where

$$\begin{aligned}
\mathcal{G}_1 &= \sum_{j=1}^{n-1} \frac{1}{j} \left(\arctan \frac{\sqrt{|d|}j}{2c - bj} + \arctan \frac{\sqrt{|d|}j}{2c + bj} \right), \\
\mathcal{G}_2 &= \sum_{j=1}^{n-1} \frac{1}{j} \left(\frac{1}{a\left(\frac{j}{n}\right)^2 - b\frac{j}{n} + c} + \frac{1}{a\left(\frac{j}{n}\right)^2 + b\frac{j}{n} + c} \right), \\
\mathcal{G}_3 &= \sum_{j=1}^{n-1} \frac{1}{j^2} \left(\frac{2c - b\frac{j}{n}}{\left(a\left(\frac{j}{n}\right)^2 - b\frac{j}{n} + c\right)^2} + \frac{2c + b\frac{j}{n}}{\left(a\left(\frac{j}{n}\right)^2 + b\frac{j}{n} + c\right)^2} \right), \\
\mathcal{G}_4 &= \Re\left(\sum_{j=1}^{n-1} \frac{1}{j} \frac{e^{2i\pi\mu j}}{1 - e^{2i\pi\mu j}}\right), \\
\mathcal{G}_5 &= \sum_{j=1}^{n-1} \frac{1}{j}, \\
\mathcal{G}_6 &= \sum_{j=1}^{n-1} \frac{1}{j^2}.
\end{aligned}$$

Indeed, each $\mathcal{G}_k$ captures a specific aspect of the asymptotic behavior. In detail,

- $\mathcal{G}_1$ captures the main logarithmic growth through arctangent integrals.
- $\mathcal{G}_2$ represents first-order boundary corrections.
- $\mathcal{G}_3$ accounts for second-order corrections in the denominator.
- $\mathcal{G}_4$ connects to the Dedekind eta function, encoding lattice geometry.
- $\mathcal{G}_5$ is the harmonic sum contributing to the constant term.
- $\mathcal{G}_6$ is the sum of reciprocal squares, related to $\zeta(2) = \pi^2/6$.

To derive the asymptotic behavior of $\mathcal{G}_1$, we define a continuous function $g_1(x)$ such that

$$g_1(x) = g_-(x) + g_+(x), \quad \text{where} \quad g_\pm(x) = \frac{1}{x}\arctan\left(\frac{\sqrt{|d|}x}{2c \pm bx}\right).$$

This allows us to approximate $\mathcal{G}_1$ by

$$\mathcal{G}_1 \approx \sum_{j=1}^{n-1} \frac{1}{n} g_1\left(\frac{j}{n}\right).$$

Applying the Euler–Maclaurin summation formula (2.1) with $p = 4$, we express this sum as

$$\sum_{j=1}^{n-1} \frac{1}{n} g_1\left(\frac{j}{n}\right) = \int_0^1 g_1(x)\,dx - \frac{g_1(0)}{2n} + \sum_{\ell=1}^{p} \frac{1}{n^\ell}\frac{B_\ell}{\ell!}\left[g_1^{(\ell-1)}(x)\right]_0^1 + r_{p,n}(g_1),$$

ensuring that the remainder term $r_{4,n}(g_1)$ is of order $\mathcal{O}(n^{-4})$. For each function $g_\pm(x)$, we can express the arctangent term as

$$\arctan\left(\frac{\sqrt{|d|}x}{2c \pm bx}\right) = \Im \log\left(1 + \frac{2ax - b \pm i\sqrt{|d|}x}{2c \pm bx}\right).$$

This identity follows from the fact that for complex numbers $z = a + bi$, we have $\arctan(b/a) = \Im \log(a + bi)$. Setting $a = 2c \pm bx$ and $b = \sqrt{|d|}x$ gives the desired result, connecting the arctangent term to the imaginary part of a logarithmic expression and facilitating integration by parts. To handle the singularity at $x = 0$, we employ a limiting procedure

$$\int_0^1 g_1(x)\,dx = \lim_{\epsilon \to 0} \int_\epsilon^1 g_1(x)\,dx$$

Using the dilogarithmic identity $\int_0^1 \frac{\log x}{x+w}\,dx = -\mathrm{Li}_2\left(-\frac{1}{w}\right)$, we express the integral as

$$\int_0^1 g_1(x)\,dx = \Im\left[\mathrm{Li}_2\left(\frac{b+\sqrt{|d|}i}{2c}\right) - \mathrm{Li}_2\left(\frac{-b+\sqrt{|d|}i}{2c}\right)\right].$$

To convert this to real values, we apply Kummer's formula

$$\begin{aligned}\mathrm{Li}_2(re^{i\theta}) = &\int_0^r \frac{\log(1-2x\cos\theta+x^2)}{2x}\,dx \\ &+ i\left[\omega\log r + \frac{1}{2}\big(\mathrm{Cl}_2(2\theta)+\mathrm{Cl}_2(2\omega)-\mathrm{Cl}_2(2\theta+2\omega)\big)\right],\end{aligned}$$

where $\omega = \arctan\left(\frac{r\sin\theta}{1-r\cos\theta}\right)$. With $r = \sqrt{\frac{a}{c}}$ and $\theta_\pm = \arctan\left(\frac{b}{\sqrt{|d|}}\right) \pm \frac{\pi}{2}$, we obtain the real-valued form

$$\int_0^1 g_1(x)\,dx = \left(\frac{\pi}{2} - \arctan\left(\frac{c-a}{\sqrt{|d|}}\right)\right)\log\sqrt{\frac{a}{c}} + \frac{1}{2}C(a,b,c), \tag{4.35}$$

where $C(a,b,c)$ is the auxiliary function defined in (4.29). For boundary corrections, we examine the behavior at $x = 0$ and $x = 1$. For the boundary values at the origin, we have

$$g_\pm(0) = \frac{\sqrt{|d|}}{2c}, \quad g'_\pm(0) = \mp\frac{\sqrt{|d|}b}{4c^2}, \quad g''_\pm(0) = \frac{\sqrt{|d|}(b^2-4ac)}{8c^3} \tag{4.36}$$

which are essential for our error analysis. At $x = 1$, we calculate

$$g_\pm(1) = \arctan\left(\frac{\sqrt{|d|}}{2c\pm b}\right), \quad g'_\pm(1) = \frac{\sqrt{|d|}}{2(a\pm b+c)} - \arctan\left(\frac{\sqrt{|d|}}{2c\pm b}\right),$$

Combining the main integral, boundary corrections, and higher-order terms, we obtain the complete asymptotic representation of $\mathcal{G}_1$

$$\begin{aligned}\mathcal{G}_1 = &\left(\frac{\pi}{2} - \arctan\left(\frac{c-a}{\sqrt{|d|}}\right)\right)\log\sqrt{\frac{a}{c}} + \frac{1}{2}C(a,b,c)\\ &+ \frac{1}{2n}\left(\frac{\sqrt{|d|}}{c} + \frac{\pi}{2} - \arctan\left(\frac{c-a}{\sqrt{|d|}}\right)\right)\\ &+ \frac{1}{12n^2}\left(\frac{\sqrt{|d|}}{2}\left(\frac{1}{a-b+c} + \frac{1}{a+b+c}\right) - \frac{\pi}{2} + \arctan\left(\frac{c-a}{\sqrt{|d|}}\right)\right)\\ &+ \mathcal{O}\left(\frac{1}{n^4}\right). \end{aligned} \tag{4.37}$$

To approximate $\mathcal{G}_2$, we start with its original summation expression

$$\mathcal{G}_2 = \sum_{j=1}^{n-1}\frac{1}{j}\left(\frac{1}{n+\mu j} - \frac{1}{n+\overline{\mu}j} - \frac{1}{n-\mu j} + \frac{1}{n-\overline{\mu}j}\right),$$

where $\mu = \frac{-b+\sqrt{|d|}i}{2c}$ and $\overline{\mu}$ is its complex conjugate. This structure suggests that $\mathcal{G}_2$ can be approximated more efficiently by defining a function $g_2(x)$ that captures the quadratic relationships in the terms of $\mathcal{G}_2$. Thus, we define the function

$$g_2(x) = \frac{1}{ax^2-bx+c} + \frac{1}{ax^2+bx+c},$$

where a, b, and c are parameters from the quadratic form $Q(j,k) = aj^2+bjk+ck^2$, with discriminant $d = b^2-4ac < 0$, ensuring that Q is positive definite. This definition of $g_2(x)$ encapsulates the structure of the individual terms in $\mathcal{G}_2$ and allows us to express $\mathcal{G}_2$ as

$$\mathcal{G}_2 = \sum_{j=1}^{n-1}\frac{1}{j}\cdot g_2\left(\frac{j}{n}\right) + \mathcal{O}\left(\frac{1}{n^2}\right).$$

Applying the Euler–Maclaurin formula (2.1) with $p = 4$ to this expression yields

$$\sum_{j=1}^{n-1} \frac{1}{j} \cdot g_2\left(\frac{j}{n}\right) = \frac{n}{\Delta_n} \int_0^1 g_2(x)\, dx - \frac{g_2(0)}{2}$$
$$+ \sum_{\ell=1}^{4} \frac{B_\ell}{\ell!} \Delta_n^{\ell-1} \left[g_2^{(\ell-1)}(0) + (-1)^{\ell-1} g_2^{(\ell-1)}(1) \right] + \mathcal{O}\left(\Delta_n^4\right),$$

where $\Delta_n = \frac{1}{n}$. The principal contribution comes from the integral term as

$$\int_0^1 g_2(x)\, dx = \int_0^1 \left(\frac{1}{ax^2 - bx + c} + \frac{1}{ax^2 + bx + c} \right) dx.$$

For analytical purposes, we decompose this integral into its constituent components as

$$\int_0^1 \frac{1}{ax^2 - bx + c}\, dx + \int_0^1 \frac{1}{ax^2 + bx + c}\, dx.$$

Each of these integrals converges because $ax^2 \pm bx + c$ remains positive over $[0, 1]$ due to the discriminant $d < 0$. Furthermore, both terms behave as constants divided by c near $x = 0$, so the integrals converge smoothly over the interval. To simplify the expression, we use symmetry in b and rewrite the sum under our change of variables as

$$\int_0^1 g_2(x)\, dx = 2 \int_0^1 \frac{c}{(ax^2 + c)^2 - b^2x^2}\, dx, \tag{4.38}$$

where the denominator structure reflects the underlying quadratic form. Evaluating this integral yields

$$\int_0^1 g_2(x)\, dx = \frac{2}{\sqrt{|d|}} \left(\frac{\pi}{2} - \arctan\left(\frac{c - a}{\sqrt{|d|}} \right) \right),$$

where the arctangent term accounts for the asymmetry in b and adjusts the result based on a and c. To further refine the approximation, we address the boundary corrections at $x = 0$ and $x = 1$. At $x = 0$, we evaluate

$$g_2(0) = \frac{2}{c},$$

which provides a boundary correction term of

$$-\frac{g_2(0)}{2n} = -\frac{1}{n} \cdot \frac{1}{c}.$$

At $x = 1$, we compute

$$g_2(1) = \frac{1}{a-b+c} + \frac{1}{a+b+c},$$

giving a boundary correction of

$$\frac{g_2(1)}{2n} = \frac{1}{2n}\left(\frac{1}{a-b+c} + \frac{1}{a+b+c}\right).$$

Thus, combining these, the boundary corrections at $x = 0$ and $x = 1$ contribute

$$-\frac{1}{2n}\left(\frac{2}{c} + \frac{1}{a-b+c} + \frac{1}{a+b+c}\right).$$

To achieve further precision, we also include a higher-order correction term at $\mathcal{O}(1/n^2)$, which comes from evaluating the second derivatives of $g_2(x)$ at $x = 0$ and $x = 1$. These terms provide an additional correction of

$$-\frac{1}{12n^2}\left(\frac{2a-b}{(a-b+c)^2} + \frac{2a+b}{(a+b+c)^2}\right),$$

accounting for second-order boundary effects. Combining the integral, boundary corrections, and higher-order terms, we arrive at the refined approximation for $\mathcal{G}_2$ as

$$\begin{aligned}\mathcal{G}_2 = \frac{2}{\sqrt{|d|}}\left(\frac{\pi}{2} - \arctan\left(\frac{c-a}{\sqrt{|d|}}\right)\right) - \frac{1}{2n}\left(\frac{2}{c} + \frac{1}{a-b+c} + \frac{1}{a+b+c}\right) \\ - \frac{1}{12n^2}\left(\frac{2a-b}{(a-b+c)^2} + \frac{2a+b}{(a+b+c)^2}\right) + \mathcal{O}\left(\frac{1}{n^4}\right).\end{aligned}$$

For $\mathcal{G}_3$, beginning with the initial form, we have

$$\mathcal{G}_3 = \sum_{j=1}^{n-1} \frac{1}{j^2}\left(\frac{1}{(n+\mu j)^2} + \frac{1}{(n+\overline{\mu} j)^2} + \frac{1}{(n-\mu j)^2} + \frac{1}{(n-\overline{\mu} j)^2}\right),$$

where $\mu = \frac{-b+\sqrt{|d|}i}{2c}$ and $\overline{\mu}$ is its complex conjugate. We approximate $\mathcal{G}_3$ by defining

$$g_3(x) = \frac{2c-bx}{(ax^2-bx+c)^2} + \frac{2c+bx}{(ax^2+bx+c)^2},$$

which represents the structure of each term in $\mathcal{G}_3$ and enables us to rewrite $\mathcal{G}_3$ as

$$\mathcal{G}_3 \approx \sum_{j=1}^{n-1} \frac{1}{j^2} g_3\left(\frac{j}{n}\right).$$

Applying the Euler–Maclaurin summation formula directly to $\sum_{j=1}^{n-1} \frac{1}{j^2} g_3\left(\frac{j}{n}\right)$, we treat it as

$$\sum_{j=1}^{n-1} \frac{1}{j^2} g_3\left(\frac{j}{n}\right) \approx n\int_0^1 \frac{g_3(x)}{x^2}\,dx - \frac{f(0)+f(1)}{2} + \sum_{\ell=1}^{p} \frac{B_\ell}{\ell!}\left(f^{(\ell-1)}(1) - f^{(\ell-1)}(0)\right) + r_{p,n}(f),$$

where $f(x) = \frac{1}{x^2} g_3(x)$ and B_ℓ denotes the Bernoulli numbers. This integral and the boundary terms provide the primary approximation for $\mathcal{G}_3$. To compute the main term, we evaluate

$$\int_0^1 \frac{g_3(x)}{x^2}\, dx = \int_0^1 \frac{1}{x^2} \left(\frac{2c - bx}{(ax^2 - bx + c)^2} + \frac{2c + bx}{(ax^2 + bx + c)^2} \right) dx.$$

Due to the $\frac{1}{x^2}$ term, this integral introduces both logarithmic and constant terms near $x = 0$. Expanding each term asymptotically for small x or performing partial fraction decomposition, we find

$$\int_0^1 f(x)\, dx = \frac{1}{a - b + c} + \frac{1}{a + b + c} + \frac{2}{\sqrt{|d|}} \left(\frac{\pi}{2} - \arctan \frac{c - a}{\sqrt{|d|}} \right).$$

Calculating boundary corrections at $x = 0$ and $x = 1$, we evaluate derivatives of $f(x) = \frac{1}{x^2} g_3(x)$ as required by the Euler–Maclaurin approach (2.1). At $x = 0$, we find

$$g_3(0) = \frac{4}{c}, \quad f(0) = \frac{4}{x^2 c},$$

which contributes a correction term

$$-\frac{f(0)}{2n^2} = -\frac{1}{n^2} \cdot \frac{2}{c}.$$

At $x = 1$, we compute

$$g_3(1) = \frac{2c - b}{(a - b + c)^2} + \frac{2c + b}{(a + b + c)^2}, \quad f(1) = g_3(1),$$

providing a boundary correction of

$$\frac{g_3(1)}{2n^2} = \frac{1}{2n^2} \left(\frac{2c - b}{(a - b + c)^2} + \frac{2c + b}{(a + b + c)^2} \right).$$

These boundary terms will combine into the total correction by utilizing

$$-\frac{1}{2n^2}\left(\frac{4}{c}+\frac{2c-b}{(a-b+c)^2}+\frac{2c+b}{(a+b+c)^2}\right).$$

To achieve maximal precision, we include higher-order boundary corrections by evaluating the second derivatives of $f(x)=\frac{1}{x^2}g_3(x)$ at $x=0$ and $x=1$. This yields a correction at $\mathcal{O}(1/n^3)$ as follows

$$-\frac{1}{12n^3}\left(\frac{2(2a-b)}{(a-b+c)^3}+\frac{2(2a+b)}{(a+b+c)^3}\right).$$

Combining the integral, boundary corrections, and higher-order terms, we obtain the final expression

$$\begin{aligned}\mathcal{G}_3 = &\frac{1}{a-b+c}+\frac{1}{a+b+c}\\ &+\frac{2}{\sqrt{|d|}}\left(\frac{\pi}{2}-\arctan\left(\frac{c-a}{\sqrt{|d|}}\right)\right)\\ &-\frac{1}{2n^2}\left(\frac{4}{c}+\frac{2c-b}{(a-b+c)^2}+\frac{2c+b}{(a+b+c)^2}\right)\\ &-\frac{1}{12n^3}\left(\frac{2(2a-b)}{(a-b+c)^3}+\frac{2(2a+b)}{(a+b+c)^3}\right)+\mathcal{O}\left(\frac{1}{n^4}\right)\end{aligned}$$

For $\mathcal{G}_4$, we employ a different approach utilizing the properties of Dedekind's eta function. Beginning with the sum representation

$$\mathcal{G}_4=\sum_{j=1}^{n-1}\frac{1}{j}\frac{e^{2i\pi\mu j}}{1-e^{2i\pi\mu j}}, \tag{4.39}$$

where μ is defined by equation (4.27), we proceed by setting $q:=e^{2i\pi\mu}$ with $|q|=e^{-\pi\sqrt{|d|}/c}$. Rewriting $\mathcal{G}_4$ in terms of q, we obtain

$$\mathcal{G}_4=\sum_{j=1}^{n-1}\frac{1}{j}\frac{q^j}{1-q^j}. \tag{4.40}$$

Given $|q| < 1$, we extend the sum to infinity with an error term

$$\sum_{j=1}^{n-1} \frac{1}{j} \frac{q^j}{1-q^j} = \sum_{j=1}^{\infty} \frac{1}{j} \frac{q^j}{1-q^j} + \mathcal{O}(|q|^n). \tag{4.41}$$

Expanding $\frac{1}{1-q^j}$ as a geometric series, we find

$$\sum_{j=1}^{\infty} \frac{1}{j} \frac{q^j}{1-q^j} = \sum_{j=1}^{\infty} \sum_{k=0}^{\infty} \frac{1}{j} (q^{k+1})^j. \tag{4.42}$$

Interchanging the order of summation for this convergent infinite series, we establish the identity

$$\sum_{j=1}^{\infty} \frac{1}{j} \frac{q^j}{1-q^j} = -\sum_{k=0}^{\infty} \log(1-q^{k+1}), \tag{4.43}$$

which we can equivalently write as

$$\sum_{j=1}^{\infty} \frac{1}{j} \frac{q^j}{1-q^j} = -\log\left(\prod_{k=0}^{\infty} (1-q^{k+1}) \right). \tag{4.44}$$

The interchange of summation order of (4.43) is justified by absolute convergence of the series when $|q| < 1$, which follows from $\|q^j/(1-q^j)\| < Cq^j$ for some constant C and all $j \geq 1$. This identity follows from the logarithmic series expansion $-\log(1-x) = \sum_{j=1}^{\infty} \frac{x^j}{j}$ for $|x| < 1$, applied term by term. Now, recall the classical identity for the Dedekind eta function defined in [12]

$$\eta(\tau) = q^{1/24} \prod_{k=1}^{\infty} (1-q^k), \quad q = e^{2\pi i \tau}. \tag{4.45}$$

Using this identity with $\tau = \mu$, we can express our infinite sum in closed form as

$$\sum_{j=1}^{\infty} \frac{1}{j} \frac{q^j}{1-q^j} = -\log\left(q^{-1/24} \eta(\mu) \right). \tag{4.46}$$

Taking the real part and accounting for the error term, we obtain

$$\mathcal{G}_4 = -\Re\left(\log\left(q^{-1/24}\eta(\mu)\right)\right) + \mathcal{O}(|q|^n). \tag{4.47}$$

Simplifying further, we get

$$\mathcal{G}_4 = -\left(\frac{\pi\sqrt{|d|}}{24c} + \log|\eta(\mu)|\right) + \mathcal{O}(|q|^n). \tag{4.48}$$

For $\mathcal{G}_5$, we start with the harmonic series

$$\mathcal{G}_5 = \sum_{j=1}^{n-1} \frac{1}{j},$$

which approximates $\log n + \gamma$, where γ is the Euler–Mascheroni constant. Extending the series slightly and including corrections, we find

$$\mathcal{G}_5 = \log n + \gamma - \frac{1}{2n} - \frac{1}{12n^2} + \mathcal{O}\left(\frac{1}{n^4}\right).$$

Finally, to derive $\mathcal{G}_6$, we use formulas (6.4.3) and (6.4.12) from Abramowitz and Stegun [14], §6.4, for series sums. Given

$$\mathcal{G}_6 = \sum_{j=1}^{n-1} \frac{1}{j^2},$$

we approximate it using integrals and correction terms for improved accuracy. The main term from the integral $\int_1^n \frac{1}{x^2}\,dx$ is

$$\int_1^n \frac{1}{x^2}\,dx = \left[-\frac{1}{x}\right]_1^n = 1 - \frac{1}{n}.$$

Adding higher-order correction terms, formula 6.4.3 of [14] provides $\frac{1}{2n^2}$ and $\frac{1}{12n^3}$, yielding

$$\sum_{j=1}^{n-1} \frac{1}{j^2} \approx 1 - \frac{1}{n} + \frac{1}{2n^2} + \frac{1}{12n^3}.$$

Incorporating the constant term $\frac{\pi^2}{6}$ (since $\sum_{j=1}^{\infty} \frac{1}{j^2} = \frac{\pi^2}{6}$), we find that the auxiliary sum admits the asymptotic expansion

$$\mathcal{G}_6 = \frac{\pi^2}{6} - \frac{1}{n} - \frac{1}{2n^2} - \frac{1}{6n^3} + \mathcal{O}\left(\frac{1}{n^5}\right), \tag{4.49}$$

as $n \to \infty$.

The error term in our final asymptotic expansion is determined by the behavior of $\mathcal{G}_6$ in equation (4.49), combined with the contributions from equation (4.37).

Completing our asymptotic analysis, we conclude that the final expressions for $\mathcal{G}_4$, $\mathcal{G}_5$, and $\mathcal{G}_6$ are

$$\mathcal{G}_4 = -\left(\frac{\pi\sqrt{|d|}}{24c} + \log|\eta(\mu)|\right) + \mathcal{O}(|q|^n),$$

$$\mathcal{G}_5 = \log n + \gamma - \frac{1}{2n} - \frac{1}{12n^2} + \mathcal{O}\left(\frac{1}{n^4}\right),$$

$$\mathcal{G}_6 = \frac{\pi^2}{6} - \frac{1}{n} - \frac{1}{2n^2} - \frac{1}{6n^3} + \mathcal{O}\left(\frac{1}{n^5}\right).$$

4.4.2. Analysis of the Sum $F_n(f_1)$

Proof of Theorem 2.16

Proof. The asymptotic behavior of $F_n(f_1)$, as shown in this theorem, generalizes the results in Theorem 3.6 given in [4].

Examining the sum $F_n(f_1)$ with parameters a, b, and c as defined in (2.48), we establish a connection with the function described in (2.50). The structure of the domain D_n depends on the parity of n, as specified in Lemma 2.2 and the explicit forms of D_n in Remark 2.3. For clarity, we express this in terms of integer indices as

$$F_n(f_1) = \frac{Ln^2}{2\pi^2} \times \begin{cases} \displaystyle\sum_{\substack{-(n-1)/2 \le j,k \le (n-1)/2 \\ (j,k) \neq (0,0)}} \frac{1}{aj^2+bjk+ck^2}, & \text{if } n \text{ is odd,} \\ \displaystyle\sum_{\substack{-n/2 \le j,k \le (n-2)/2 \\ (j,k) \neq (0,0)}} \frac{1}{aj^2+bjk+ck^2}, & \text{if } n \text{ is even.} \end{cases}$$

To exploit the symmetry properties of the quadratic form, we reformulate our sum in terms of three auxiliary components

$$F_n(f_1) = \begin{cases} \dfrac{Ln^2}{\pi^2}(G_{\frac{n+1}{2}} + H_a + H_c), & n \text{ odd} \\ \dfrac{Ln^2}{\pi^2}(G_{\frac{n+2}{2}} + H_a + H_c - \frac{1}{2}U_{\frac{n}{2}}) + \dfrac{2L}{\pi^2}(\frac{1}{a+b+c} - \frac{1}{a} - \frac{1}{c}), & n \text{ even} \end{cases}$$

Through appropriate manipulation, this expression can be reformulated as

$$F_n(f_1) = \begin{cases} \dfrac{Ln^2}{\pi^2}\left(G_{\frac{n+1}{2}} + \left(\frac{1}{a} + \frac{1}{c}\right) H_{\frac{n+1}{2}}\right), & n \text{ odd,} \\ \dfrac{Ln^2}{\pi^2}\left(G_{\frac{n+2}{2}} + \left(\frac{1}{a} + \frac{1}{c}\right) H_{\frac{n+2}{2}} - \frac{1}{2}U_{\frac{n}{2}}\right) + \dfrac{2L}{\pi^2}\left(\frac{1}{a+b+c} - \frac{1}{a} - \frac{1}{c}\right), & n \text{ even.} \end{cases} \tag{4.50}$$

In this context, H_n exhibits the structure

$$H_n = \mathcal{G}_6 = \sum_{j=1}^{n-1} \frac{1}{j^2} = \frac{\pi^2}{6} - \frac{1}{n} - \frac{1}{2n^2} - \frac{1}{6n^3} + \mathcal{O}\left(\frac{1}{n^5}\right). \tag{4.51}$$

Additionally, we define the auxiliary sum

$$\begin{aligned} U_n &= \sum_{j=1}^{n} \left(\frac{1}{aj^2 + bjn + cn^2} + \frac{1}{aj^2 - bjn + cn^2} + \frac{1}{an^2 + bnj + cj^2} + \frac{1}{an^2 - bnj + cj^2} \right) \\ &= \frac{1}{n} \sum_{j=1}^{n} \frac{1}{n} \left(\frac{1}{a\left(\frac{j}{n}\right)^2 + b\frac{j}{n} + c} + \frac{1}{a\left(\frac{j}{n}\right)^2 - b\frac{j}{n} + c} \right. \\ &\quad \left. + \frac{1}{a + b\frac{j}{n} + c\left(\frac{j}{n}\right)^2} + \frac{1}{a - b\frac{j}{n} + c\left(\frac{j}{n}\right)^2} \right). \end{aligned}$$

Analyzing U_n requires the Euler-Maclaurin summation approach. In particular, with $p = 4$ and the function

$$g(x) = \frac{1}{ax^2 + bx + c} + \frac{1}{ax^2 - bx + c} + \frac{1}{a + bx + cx^2} + \frac{1}{a - bx + cx^2}.$$

We note key properties

$$g(0) = 2\left(\frac{1}{a} + \frac{1}{c}\right), \quad g'(0) = 0, \quad \text{and} \quad g(1) = -g'(1) = 2\left(\frac{1}{a - b + c} + \frac{1}{a + b + c}\right).$$

Moreover, we have

$$\begin{aligned} \int_0^1 g(x)\,dx &= \frac{2}{\sqrt{|d|}} \left(\arctan\left(\frac{2a + b}{\sqrt{|d|}}\right) + \arctan\left(\frac{2a - b}{\sqrt{|d|}}\right) \right. \\ &\quad \left. + \arctan\left(\frac{2c + b}{\sqrt{|d|}}\right) + \arctan\left(\frac{2c - b}{\sqrt{|d|}}\right) \right) \\ &= \frac{2\pi}{\sqrt{|d|}}. \end{aligned}$$

This analysis yields

$$U_n = \frac{2\pi}{\sqrt{|d|}}\frac{1}{n} + \left(\frac{1}{a-b+c} + \frac{1}{a+b+c} - \frac{1}{a} - \frac{1}{c}\right)\frac{1}{n^2} \\ - \frac{1}{6}\left(\frac{1}{a-b+c} + \frac{1}{a+b+c}\right)\frac{1}{n^3} + \mathcal{O}\left(\frac{1}{n^5}\right). \tag{4.52}$$

By combining equations (4.28), (4.51), and (4.52) within the framework of (4.50), we arrive at the desired result. □

4.4.3. Examples

Example 4.12 (Square Lattice)**.** For the square lattice, the sum F_n takes the explicit form

$$F_n = F_n(f) = \sum_{\substack{j,k=0 \\ (j,k)\neq(0,0)}}^{n-1} \frac{1}{1 - \frac{1}{2}\left(\cos\left(\frac{2\pi j}{n}\right) + \cos\frac{2\pi k}{n}\right)}. \tag{4.53}$$

Applying Theorem 2.15, in particular equation (2.47), we obtain the asymptotic expansion,

$$F_n = \frac{2}{\pi}n^2 \log n + \frac{1}{\pi}\Big(2\gamma + \log\big(\frac{32\pi}{\Gamma(1/4)^4}\big)\Big)n^2 + \mathcal{O}(\log n). \tag{4.54}$$

This is demonstrated using Theorems 2.16 and 2.17 with parameters $L = 2, a = 1, b = 0, c = 1$ for the square lattice. The asymptotic expansion in equation (4.54) follows directly from the error bound in Theorem 2.15, equation (2.47) as

$$F_n(f_1) = \frac{2}{\pi}n^2 \log n + \frac{2}{\pi}\left(\gamma - 2\log|\eta(i)| - \frac{2G}{\pi} - \log 2\right)n^2 + \mathcal{O}(\log n), \tag{4.55}$$

and

$$I_n(f_1) = \frac{2}{\pi}n^2 \log n + \mathcal{O}(1). \tag{4.56}$$

The integral $I_n(f_1)$ admits the asymptotic expansion

$$I_n(f_1) = \frac{2}{\pi}n^2 \log n + \frac{1}{\pi}\left(3\log 2 - 2\log \pi + \frac{4G}{\pi}\right) n^2 + \mathcal{O}(1), \tag{4.57}$$

as derived below where G denotes Catalan's constant. Since $\eta(i) = \dfrac{\Gamma(\frac{1}{4})}{2\pi^{\frac{3}{4}}}$, [15] use of equations (4.55), (4.56) and (4.57) in Theorem 2.15, in particular equation (2.47), gives (4.54).

To prove equation (4.57), we begin with the integral expression given in (2.21). Although the integration domain D_n varies with the parity of n, since f in Equation (2.11) exhibits 2π-periodicity in each of its arguments, $I_n(f)$ can be reformulated as

$$I_n(f) = \frac{1}{\Delta_n^2} \iint_{R_n} f(\mathbf{x})\, d\mathbf{x} \tag{4.58}$$

where the integration region R_n is given by $R_n = [-\pi, \pi]^2 \setminus [-\frac{\pi}{n}, \frac{\pi}{n}]^2$ for all n.

For the square lattice (4.58) takes on the form

$$I_n(f) = \frac{n^2}{4\pi^2} \iint_{R_n} \frac{1}{1 - \frac{1}{2}(\cos x + \cos y)}\, dx\, dy.$$

Exploiting the symmetry of the region R_n and the even nature of the integrand with respect to both x and y, we obtain

$$I_n(f) = \frac{n^2}{\pi^2} \iint_{R_n^+} \frac{1}{1 - \frac{1}{2}(\cos x + \cos y)}\, dx\, dy,$$

where $R_n^+ = [0, \pi]^2 \setminus [0, \frac{\pi}{n}]^2$. Substituting $\tan\frac{x}{2} = u \geq 0$ and $\tan\frac{y}{2} = v \geq 0$ in equation (4.58) we obtain the Jacobian determinant

$$dx\, dy = \frac{4\, du\, dv}{(1 + u^2)^2(1 + v^2)^2}$$

and the transformed integrand

$$1-\frac{1}{2}(\cos x+\cos y)=1-\frac{1}{2}\left(\frac{1-u^2}{1+u^2}+\frac{1-v^2}{1+v^2}\right)=\frac{u^2+v^2+2u^2v^2}{(1+u^2)(1+v^2)}$$

This gives us

$$I_n(f)=\frac{4n^2}{\pi^2}\iint_{P_n}\frac{1}{u^2+v^2+2u^2v^2}\,du\,dv,$$

with $P_n=[0,\infty)^2\setminus[0,b_n]^2$ and $b_n=\tan\left(\frac{\pi}{2n}\right)$. Transitioning to polar coordinates and subsequently employing the substitution $r\sin(2\alpha)=\sqrt{2}t$ in the inner integral leads us to the final result

$$\begin{aligned}I_n(f)&=\frac{8n^2}{\pi^2}\int_0^{\pi/4}\int_{\frac{b_n}{\cos\alpha}}^{\infty}\frac{r\,dr\,d\alpha}{r^2+2r^4\cos^2\alpha\sin^2\alpha}=\frac{8n^2}{\pi^2}\int_0^{\pi/4}\int_{\sqrt{2}b_n\sin\alpha}^{\infty}\frac{dt\,d\alpha}{t(1+t^2)}\\&=\frac{4n^2}{\pi^2}\int_0^{\pi/4}\log\left(\frac{t^2}{1+t^2}\right)\Big|_{\sqrt{2}b_n\sin\alpha}^{\infty}d\alpha=\frac{4n^2}{\pi^2}\int_0^{\pi/4}\log\left(\frac{1+2b_n^2\sin^2\alpha}{2b_n^2\sin^2\alpha}\right)d\alpha.\end{aligned}\tag{4.59}$$

Since

$$\log\Big(\frac{1+2b_n^2\sin^2\alpha}{2b_n^2\sin^2\alpha}\Big)=-\log(2b_n^2\sin^2\alpha)+\mathcal{O}\big(\frac{1}{n^2}\big)$$

and

$$\int_0^{\pi/4}\log(\sin\alpha)\,d\alpha=-\frac{\pi}{4}\log 2-\frac{G}{2},$$

where G is Catalan's constant

$$G=\sum_{k=0}^{\infty}\frac{(-1)^k}{(2k+1)^2}=0.915965594177219\ldots,\tag{4.60}$$

using $\log(\tan x)=\log(x)+\mathcal{O}(x^2)$ as $x\to0^+$, we get

$$\int_0^{\pi/4}\log\Big(\frac{1+2b_n^2\sin^2\alpha}{2b_n^2\sin^2\alpha}\Big)\,d\alpha=-\frac{\pi}{4}\log(2b_n^2)+G+\frac{\pi}{2}\log 2+\mathcal{O}\big(\frac{1}{n^2}\big)$$

$$= \frac{\pi}{2}\log n + \big(\frac{3\pi}{4}\log 2 - \frac{\pi}{2}\log\pi + G\big) + \mathcal{O}\big(\frac{1}{n^2}\big),$$

and equation (4.57) follows.

Example 4.13 (Triangular Lattice)**.** For the triangular lattice case, we analyze the sum that serves as the triangular-lattice analogue of the square-lattice sum in equation (4.53)

$$F_n = F_n(f) = \sum_{\substack{0\le j,k<n\\(j,k)\neq(0,0)}} \frac{1}{1-\frac{1}{3}\big(\cos\frac{2\pi j}{n}+\cos\frac{2\pi k}{n}+\cos\frac{2\pi(j+k)}{n}\big)}. \tag{4.61}$$

The lattice geometry is encoded by three generators ($L = 3$) through the matrix

$$S = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}^T, \quad S^TS = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix},$$

yielding $\det(S^TS) = 3$. Near the origin, the Taylor series expansion of the denominator function gives the quadratic form

$$\varphi(\mathbf{x}) \approx \frac{1}{3}(x_1^2 + x_1x_2 + x_2^2), \tag{4.62}$$

corresponding to parameters $a = b = c = 1$. This follows from expanding the cosine terms in the denominator of (4.61) and collecting the second-order terms. Thus, the discriminant $d = -3$ is negative, confirming that the quadratic form is positive definite, with $|d| = 3$ in the notation of §4.1. This structure determines the universal coefficient $\frac{L}{\pi\sqrt{|d|}} = \frac{3}{\pi\sqrt{3}} = \frac{\sqrt{3}}{\pi}$, appearing in all asymptotic expansions.

By Theorems 2.16 and 2.17, in particular equations (2.49) and (4.56), we obtain

$$F_n(f_1) = \frac{\sqrt{3}}{\pi}\, n^2\log n + \frac{\sqrt{3}}{\pi}\big(\gamma - \log 2 - 2\log|\eta(\mu)|\big)\, n^2 + \mathcal{O}(1), \tag{4.63}$$

$$I_n(f_1) = \frac{\sqrt{3}}{\pi}\, n^2\log n \; + \; \mathcal{O}(1), \tag{4.64}$$

where the parameter $\mu = \frac{-b+\sqrt{|d|}i}{2c}$ defined by equation (4.27) encodes the triangular lattice geometry. The integral analysis follows equations (4.58)–(4.59), with a key transformation arising from

$$\int_0^{\pi/4} \log\left(\frac{1+2b_n^2\sin^2\alpha}{2b_n^2\sin^2\alpha}\right) d\alpha, \quad b_n = \tan\left(\frac{\pi}{2n}\right). \tag{4.65}$$

Using the first-order approximation $\tan(x) \approx x$ for small x, we have $b_n^2 \approx \frac{\pi^2}{4n^2}$. For large n, we can expand the logarithmic term as

$$\begin{aligned}\log\left(\frac{1+2b_n^2\sin^2\alpha}{2b_n^2\sin^2\alpha}\right) &= \log\left(\frac{1}{2b_n^2\sin^2\alpha}+1\right) &(4.66)\\ &= -\log(2b_n^2\sin^2\alpha) + \mathcal{O}\left(\frac{1}{n^2}\right). &(4.67)\end{aligned}$$

Decomposing the logarithm further, we get

$$\begin{aligned}-\log(2b_n^2\sin^2\alpha) &= -\log(2) - \log(b_n^2) - \log(\sin^2\alpha) &(4.68)\\ &= -\log(2) - \log\left(\frac{\pi^2}{4n^2}\right) - \log(\sin^2\alpha) &(4.69)\\ &= -\log(2) + \log(n^2) - \log\left(\frac{\pi^2}{4}\right) - \log(\sin^2\alpha). &(4.70)\end{aligned}$$

Using the identity [16]

$$\int_0^{\pi/4} \log(\sin\alpha)\, d\alpha = -\frac{\pi}{4}\log 2 - \frac{G}{2}, \tag{4.71}$$

where G denotes Catalan's constant, and integrating term by term, we get

$$\begin{aligned}\int_0^{\pi/4} \log\left(\frac{1+2b_n^2\sin^2\alpha}{2b_n^2\sin^2\alpha}\right) d\alpha &= -\frac{\pi}{4}\log(2b_n^2) + G + \frac{\pi}{2}\log 2 + \mathcal{O}\left(\frac{1}{n^2}\right) &(4.72)\\ &= \frac{\pi}{2}\log n + \left(\frac{3\pi}{4}\log 2 - \frac{\pi}{2}\log\pi + G\right) + \mathcal{O}\left(\frac{1}{n^2}\right). &(4.73)\end{aligned}$$

This integral evaluation contributes to the final expression

$$I_n(f) = \frac{\sqrt{3}}{\pi} n^2 \log n + \frac{\sqrt{3}}{\pi} \left(\log\left(\frac{24}{\pi^2}\right) + \frac{4G}{\pi} \right) n^2 + \mathcal{O}(1) \tag{4.74}$$

Consequently,

$$I_n(f) = \frac{\sqrt{3}}{\pi}\, n^2\, \log n + \frac{\sqrt{3}}{\pi} \Big(\log\big(\tfrac{24}{\pi^2}\big) + \tfrac{4G}{\pi} \Big)\, n^2 + \mathcal{O}(1).$$

For odd versus even n, boundary corrections contribute terms of order $\mathcal{O}(1)$ or $\mathcal{O}\big(\frac{\log n}{n^2}\big)$, as can be seen in the domain characterization of Lemma 2.2 and the explicit forms of D_n in equation (2.18) of Remark 2.3. Applying the difference identity from Theorem 2.15, equation (2.47),

$$F_n \;=\; I_n(f) \;-\; I_n(f_1) \;+\; F_n(f_1) \;+\; \mathcal{O}(\log n),$$

we substitute the expressions for $I_n(f)$, $I_n(f_1)$, and $F_n(f_1)$. The leading $n^2 \log n$ terms from $I_n(f)$ and $F_n(f_1)$ contribute equally, while $I_n(f_1)$ has the opposite sign. The constant terms combine to yield

$$F_n = \frac{\sqrt{3}}{\pi}\, n^2 \log n + \frac{\sqrt{3}}{\pi} \Big(\gamma + \log\big(4\pi \sqrt[4]{3}\big) - 3 \log \Gamma\big(\frac{1}{3}\big) \Big) n^2 + \mathcal{O}(\log n). \tag{4.75}$$

This confirms Theorem 1.1, in particular the error bound of order $\mathcal{O}(\log n)$ established in equation (2.47). The connection between the Dedekind eta function term in $F_n(f_1)$ and the Gamma function in the final result comes from the identity [14]

$$\eta\left(\frac{-1 + i\sqrt{3}}{2}\right) = \frac{3^{1/8}}{\sqrt{2\pi}} \Gamma\left(\frac{1}{3}\right)^{3/2},$$

which allows us to rewrite

$$-2 \log |\eta(\mu)| = -2 \log \left| \frac{3^{1/8}}{\sqrt{2\pi}} \Gamma\left(\frac{1}{3}\right)^{3/2} \right| = -\frac{1}{4} \log 3 + \log(2\pi) - 3 \log \Gamma\left(\frac{1}{3}\right)$$

Substituting this into equation (4.63) and combining with the other terms leads precisely to equation (4.75).

The special function $\Gamma\left(\frac{1}{3}\right)$ arises from these boundary and constant-term evaluations, mirroring the role of $\Gamma\left(\frac{1}{4}\right)$ in the square lattice case (equation (4.54)). This underscores the distinct geometric structures; the triangular lattice's coefficient $\frac{\sqrt{3}}{\pi}$ contrasts with the square lattice's $\frac{2}{\pi}$, yet both exhibit the universal $n^2 \log n$ growth with coefficients following the general form $\frac{L}{\pi\sqrt{\det(S^T S)}}$.

Example 4.14 (Union Jack Lattice)**.** The sum associated with the Union Jack Lattice is

$$F_n(f) = \sum_{\substack{j,k=0 \\ (j,k)\neq(0,0)}}^{n-1} \frac{1}{1 - \frac{1}{4}\left(\cos\left(\frac{2\pi j}{n}\right) + \cos\frac{2\pi k}{n} + \cos\frac{2\pi(j-k)}{n} + \cos\frac{2\pi(j+k)}{n}\right)}. \tag{4.76}$$

For this case, we get

$$\varphi(\mathbf{x}) = 1 - \frac{1}{4}(\cos x_1 + \cos x_2 + \cos(x_1 - x_2) + \cos(x_1 + x_2)), \tag{4.77}$$

and

$$S = \begin{bmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & -1 & 1 \end{bmatrix}^T, \quad S^T S = \begin{bmatrix} 3 & 0 \\ 0 & 3 \end{bmatrix}, \tag{4.78}$$

so that $\sqrt{\det(S^T S)} = 3$. Applying Theorem 2.16, equation (2.49), and Theorem 2.17 with $a = c = 3$, $b = 0$, and $d = 4ac - b^2 = 36$, we obtain

$$F_n(f_1) = \frac{4}{3\pi} n^2 \log n + \frac{4}{3\pi}\left(\gamma - \log 2 - 2\log|\eta(i)| - \frac{2G}{\pi}\right) n^2 + \mathcal{O}(1)$$

and

$$I_n(f_1) = \frac{4}{3\pi} n^2 \log n + \mathcal{O}(1).$$

Following the integral analysis in the Square Lattice example (4.57) through the same procedure between (4.58) and (4.59) yields

$$\begin{aligned}
I_n(f) &= \frac{n^2}{4\pi^2}\iint_{R_n} \frac{dx\,dy}{1-\frac{1}{4}(\cos x+\cos y+\cos(x-y)+\cos(x+y))} \\
&= \frac{n^2}{\pi^2}\iint_{R_n^+} \frac{dx\,dy}{1-\frac{1}{4}(\cos x+\cos y+\cos(x-y)+\cos(x+y))} \\
&= \frac{8n^2}{\pi^2}\iint_{P_n} \frac{du\,dv}{3u^2+3v^2+2u^2v^2} \\
&= \frac{16n^2}{\pi^2}\int_0^{\pi/4}\int_{\frac{b_n}{\cos\alpha}}^{\infty} \frac{r\,dr\,d\alpha}{3r^2+2r^4\cos^2\alpha\sin^2\alpha}. \\
&= \frac{16n^2}{\pi^2}\int_0^{\pi/4}\int_{\sqrt{2}b_n\sin\alpha}^{\infty} \frac{dt\,d\alpha}{t(3+t^2)} \quad \left(\text{with } r\sin(2\alpha)=\sqrt{2}t \text{ and } dr=\frac{dt}{\sqrt{2}\sin(2\alpha)}\right) \\
&= \frac{16n^2}{\pi^2}\int_0^{\pi/4}\int_{\sqrt{2}b_n\sin\alpha}^{\infty} \frac{1}{t}\cdot\frac{1}{3+t^2}\,dt\,d\alpha \\
&= \frac{16n^2}{\pi^2}\int_0^{\pi/4}\left[\frac{1}{6}\log\left(\frac{3+t^2}{t^2}\right)\right]_{\sqrt{2}b_n\sin\alpha}^{\infty} d\alpha \\
&= \frac{8n^2}{3\pi^2}\int_0^{\pi/4}\log\left(\frac{3+2b_n^2\sin^2\alpha}{2b_n^2\sin^2\alpha}\right) d\alpha.
\end{aligned}$$

For large n, we approximate $\tan(x)\approx x$ for small x, giving $b_n \approx \frac{\pi}{2n}$ and $b_n^2 \approx \frac{\pi^2}{4n^2}$. Since $\frac{3}{2b_n^2\sin^2\alpha} \gg 1$, we expand

$$\begin{aligned}
\log\left(\frac{3+2b_n^2\sin^2\alpha}{2b_n^2\sin^2\alpha}\right) &= \log\left(\frac{3}{2b_n^2\sin^2\alpha}+1\right) \\
&= \log\left(\frac{3}{2b_n^2\sin^2\alpha}\right)+\mathcal{O}\left(\frac{1}{n^2}\right) \\
&= \log(3)-\log(2)-\log(b_n^2)-\log(\sin^2\alpha)+\mathcal{O}\left(\frac{1}{n^2}\right) \\
&= \log\left(\frac{6}{\pi^2}\right)+\log(n^2)-\log(\sin^2\alpha)+\mathcal{O}\left(\frac{1}{n^2}\right).
\end{aligned}$$

Using the identity $\int_0^{\pi/4}\log(\sin\alpha)\,d\alpha = -\frac{\pi}{4}\log 2-\frac{G}{2}$ where G is Catalan's constant, and noting that $\log(\sin^2\alpha)=2\log(\sin\alpha)$, we get

$$\int_0^{\pi/4}\log\left(\frac{3+2b_n^2\sin^2\alpha}{2b_n^2\sin^2\alpha}\right) d\alpha = \frac{\pi}{4}\log\left(\frac{6}{\pi^2}\right)+\frac{\pi}{4}\log(n^2)+\frac{\pi}{2}\log 2+G+\mathcal{O}\left(\frac{1}{n^2}\right)$$

$$= \frac{\pi}{2}\log n + \left(\frac{\pi}{4}\log\left(\frac{6}{\pi^2}\right) + \frac{\pi}{2}\log 2 + G\right) + \mathcal{O}\left(\frac{1}{n^2}\right).$$

This integral evaluation yields the expression

$$I_n(f) = \frac{4}{3\pi}n^2\log n + \frac{2n^2}{3\pi}\left(\log\left(\frac{24}{\pi^2}\right) + \frac{4G}{\pi}\right) + \mathcal{O}(1). \tag{4.79}$$

Applying Theorem 2.15, equation (2.47), we substitute the expressions for $I_n(f)$, $I_n(f_1)$, and $F_n(f_1)$. The leading $n^2\log n$ terms contribute with appropriate signs, while the constant terms combine to yield

$$\begin{aligned}
F_n(f) = {} & \frac{4}{3\pi}n^2\log n + \frac{2n^2}{3\pi}\left(\log\left(\frac{24}{\pi^2}\right) + \frac{4G}{\pi}\right) - \frac{4}{3\pi}n^2\log n \\
& + \frac{4}{3\pi}n^2\log n + \frac{4}{3\pi}\left(\gamma - \log 2 - 2\log|\eta(i)| - \frac{2G}{\pi}\right)n^2 + \mathcal{O}(\log n) \\
= {} & \frac{4}{3\pi}n^2\log n + \frac{2n^2}{3\pi}\left[\log\left(\frac{24}{\pi^2}\right) + \frac{4G}{\pi} + 2\gamma - 2\log 2 - 4\log|\eta(i)| - \frac{4G}{\pi}\right] + \mathcal{O}(\log n).
\end{aligned}$$

The Catalan constant terms cancel out, and using the identity $\eta(i) = \frac{\Gamma(1/4)}{2\pi^{3/4}}$, we have

$$\begin{aligned}
-4\log|\eta(i)| &= -4\log\left|\frac{\Gamma(1/4)}{2\pi^{3/4}}\right| \\
&= -4\log\Gamma(1/4) + 4\log(2\pi^{3/4}) \\
&= -4\log\Gamma(1/4) + 4\log 2 + 3\log\pi.
\end{aligned}$$

Substituting this expression and combining all logarithmic terms gives

$$\begin{aligned}
F_n(f) &= \frac{4}{3\pi}n^2\log n + \frac{2n^2}{3\pi}\left[2\gamma + \log\left(\frac{24}{\pi^2}\right) + 2\log 2 - 4\log\Gamma(1/4) + 3\log\pi\right] + \mathcal{O}(\log n) \\
&= \frac{4}{3\pi}n^2\log n + \frac{2n^2}{3\pi}\left[2\gamma + \log\left(\frac{24\cdot 4\cdot\pi^3}{\pi^2\cdot\Gamma(1/4)^4}\right)\right] + \mathcal{O}(\log n) \\
&= \frac{4}{3\pi}n^2\log n + \frac{2}{3\pi}\Big(2\gamma + \log\big(\frac{96\pi}{\Gamma(1/4)^4}\big)\Big)n^2 + \mathcal{O}(\log n).
\end{aligned}$$

This confirms the pattern established by the square and triangular lattice cases, with the leading term coefficient $\frac{4}{3\pi}$ following the universal form $\frac{L}{\pi\sqrt{\det(S^T S)}}$, where $L = 4$ and $\sqrt{\det(S^T S)} = 3$.

The results in this section confirms the universal pattern established in Theorem 2.13, where the leading coefficient follows the form $\frac{L}{\pi\sqrt{\det(S^T S)}}$. The special function terms in the $\mathcal{O}(n^2)$ coefficient encode the specific geometric properties of the lattice, while the error term of $\mathcal{O}(\log n)$ arises from the careful treatment of the singularity near the origin as shown in the proof of Theorem 2.15.

5. CONCLUSION

This thesis establishes asymptotic expansions for lattice sums $F_{m,n}$, leveraging midpoint quadrature, Euler–Maclaurin summation, and special function analysis to bridge their discrete lattice structure with continuous approximations. The proofs systematically address boundary terms and singularities, achieving error bounds of $\mathcal{O}(\log n)$ as exemplified in Theorem 1.1.

Through detailed computations for square, triangular, and union jack lattices, we confirm the universal leading term coefficient $\frac{L}{\pi\sqrt{\det(S^T S)}} n^2 \log n$, where S is the basis matrix and L is the number of generators. Subleading terms, involving special functions like $\Gamma(\frac{1}{4})$, $\Gamma(\frac{1}{3})$, and Catalan's constant G, encode lattice-specific geometry. Each example highlights distinct aspects of the general theory and confirms the universal nature of the $n^2 \log n$ term. Boundary analysis and singularity handling prove critical for precision across all cases.

Furthermore, these asymptotic expansions extend across diverse lattices, linking discrete sums to continuous approximations with a dominant $n^2 \log n$ term. By isolating singularities and integrating approximations with boundary corrections, we establish a robust toolset for handling lattice sums across varied graphs and boundary conditions. As shown, these findings clarify the $\mathcal{O}(n^2 \log n)$ scaling while unveiling finer structures through special function constants, equipping researchers with tools for analyzing higher-dimensional lattices and refining error bounds in Network Theory.

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APPENDIX A: SPECIAL FUNCTIONS AND ASYMPTOTIC COEFFICIENTS COMPARISON FOR LATTICE TYPES

A.1. Special Functions

In our analysis of lattice sums, several special functions play crucial roles. This appendix provides a rigorous treatment of these functions, emphasizing their mathematical properties and connections to lattice geometry.

A.1.1. Dedekind eta Function

The Dedekind eta function $\eta(\tau)$ is defined for $\Im(\tau) > 0$ by

$$\eta(\tau) = q^{1/24} \prod_{n=1}^{\infty} (1 - q^n), \quad q = e^{2\pi i \tau}, \tag{A.1}$$

as given in Apostol [12], §3, the modular transformations of which

$$\eta(\tau + 1) = e^{\pi i/12} \eta(\tau), \tag{A.2}$$

$$\eta(-1/\tau) = \sqrt{-i\tau}\, \eta(\tau), \tag{A.3}$$

have been derived in [12], § 3.4.

Special values relevant to lattice sums, in particular

$$\eta(i) = \frac{\Gamma(1/4)}{2\pi^{3/4}} \quad \text{(square lattice)}, \tag{A.4}$$

$$\eta\left(\frac{-1 + i\sqrt{3}}{2}\right) = \frac{3^{1/8}}{\sqrt{2\pi}} \Gamma\left(\frac{1}{3}\right)^{3/2} \quad \text{(triangular lattice)}, \tag{A.5}$$

have been computed via theta relations in Borwein et al. [15], Section 4.2.

In this study, in Theorem 2.16, $\eta(\mu)$ encodes lattice geometry through μ. For the square lattice, $\log|\eta(i)| = \log\left(\frac{\Gamma(1/4)}{2\pi^{3/4}}\right)$ in equation (4.54) reflects four-fold symmetry; for the triangular lattice, $\mu = \frac{-1+i\sqrt{3}}{2}$ appears in equation (4.75).

A.1.2. Dilogarithm and Clausen Functions

The dilogarithm is defined by

$$\mathrm{Li}_2(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^2}, \quad |z| \leq 1, \tag{A.6}$$

with analytic continuation to $\mathbb{C} \setminus [1, \infty)$, and $\mathrm{Li}_2(1) = \frac{\pi^2}{6}$, per Lewin [13], §1.

The Clausen function is

$$\mathrm{Cl}_2(\theta) = \Im(\mathrm{Li}_2(e^{i\theta})) = \sum_{k=1}^{\infty} \frac{\sin(k\theta)}{k^2}, \tag{A.7}$$

converging uniformly for $\theta \in [0, 2\pi)$, as in Kirillov [17], §2.

These functions contribute to the constant $C(a, b, c)$ (equation (4.29)), part of the $\mathcal{O}(n^2)$ term in Theorem 2.16, with a, b, c from equation (2.48).

A.1.3. Gamma Function and Constants

The Gamma function is defined for $\Re(z) > 0$ by

$$\Gamma(z) = \int_0^{\infty} t^{z-1} e^{-t}\, dt, \tag{A.8}$$

with analytic continuation to $\mathbb{C} \setminus \{0, -1, -2, \ldots\}$, per Abramowitz and Stegun [14], § 6.1. For special values, we start with,

$$\Gamma\left(\frac{1}{4}\right) = \frac{2\pi^{3/4}}{\eta(i)} \approx 3.6256 \quad \text{for the square lattice,} \tag{A.9}$$

$$\Gamma\left(\frac{1}{3}\right) = \left(\frac{\sqrt{2\pi}}{3^{1/8}}\eta\left(\frac{-1+i\sqrt{3}}{2}\right)\right)^{2/3} \approx 2.6789 \quad \text{for the triangular lattice,} \tag{A.10}$$

which are found in [14], § 6.1.33.

Catalan's constant appears in square and union jack lattice expansions

$$G = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^2} = -\int_0^{\pi/4} \log(\sin\theta)\, d\theta \approx 0.915966, \tag{A.11}$$

derived in Borwein et al. [15], p. 147.

The Euler–Mascheroni constant emerges from harmonic sums

$$\gamma \approx 0.57721, \quad \sum_{j=1}^{n-1} \frac{1}{j} = \log n + \gamma + \mathcal{O}\left(\frac{1}{n}\right), \tag{A.12}$$

as stated by Lagarias [19], §4.

A.1.4. Asymptotic Relevance

Our asymptotic expansions connect to these functions through the leading term

$$\frac{L}{\pi\sqrt{\det(S^T S)}} n^2 \log n,$$

where S is defined in equation (2.46). The constant terms include contributions from γ (Theorem 4.10), $\log|\eta(\mu)|$ (Theorem 2.16), and Γ values (equations (4.54) and (4.75)). For example, in the square lattice, γ and G combine to determine the $\mathcal{O}(n^2)$ coefficient in equation (4.54), with the error term $\mathcal{O}(\log n)$ arising from the analysis of near-field and far-field regions as decomposed in Lemma 2.4, combined with cancellation effects.

The interplay between these functions is central to our analysis, enabling precise expansions across lattice types. For additional properties and computational tools (e.g., numerical evaluation via software), see Gradshteyn and Ryzhik [16] and NIST DLMF [18].

A.2. Comparison of Asymptotic Coefficients Across Different Lattice Types

Table A.1 confirms the universal pattern for the leading coefficient $\frac{L}{\pi\sqrt{\det(S^TS)}}$. For the square lattice, $L = 2$ and $\det(S^TS) = 1$, yielding $\frac{2}{\pi}$. For the triangular lattice, $L = 3$ and $\det(S^TS) = 3$, giving $\frac{\sqrt{3}}{\pi}$. For the union jack lattice, $L = 4$ and $\det(S^TS) = 9$, resulting in $\frac{4}{3\pi}$.

Despite the different lattice geometries, all cases exhibit a universal $n^2 \log n$ growth pattern, confirming the robustness of our asymptotic analysis framework.

Table A.1: Comparison of asymptotic coefficients across different lattice types.

Lattice Type	Leading Coefficient	Main Constant Term	Error Term
Square	$\frac{2}{\pi}$	$\frac{2\gamma}{\pi} + \frac{1}{\pi}\log\left(\frac{32\pi}{\Gamma(1/4)^4}\right)$	$\mathcal{O}(\log n)$
Triangular	$\frac{\sqrt{3}}{\pi}$	$\frac{\sqrt{3}}{\pi}\left(\gamma + \log(4\pi\sqrt[4]{3}) - 3\log\Gamma(\frac{1}{3})\right)$	$\mathcal{O}(\log n)$
Union Jack	$\frac{4}{3\pi}$	$\frac{2}{3\pi}\left(2\gamma + \log\left(\frac{96\pi}{\Gamma(1/4)^4}\right)\right)$	$\mathcal{O}(\log n)$