THE PSEUDOINVERSE OF THE LAPLACIAN MATRIX: ASYMPTOTIC BEHAVIOR OF ITS TRACE

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(Received August 10, 2022; accepted November 7, 2022)

Abstract. In this paper we are concerned with the asymptotic behavior of

$$\text{tr}(L^+_{sq}) = \frac{1}{4} \sum_{j,k=0}^{n-1} \frac{1}{1 - \frac{1}{2}(\cos \frac{2\pi j}{n} + \cos \frac{2\pi k}{n})},$$

the trace of the pseudoinverse of the Laplacian matrix related with the square lattice, as $n \to \infty$. The method we developed for such sums in former papers depends on the use of Taylor approximations for the summands. It was shown that the error term depends on whether the Taylor polynomial used is of degree two or higher. Here we carry this out for the square lattice with a fourth degree Taylor polynomial and thereby obtain a result with an improved error term which is perhaps the most precise one can hope for.

1. Introduction

This paper is a continuation of our articles [2] and [3] where certain sums involving the cosine function were asymptotically evaluated over the triangular, the square and the modified union jack lattices. Here we present the most precise calculation possible within the framework set up in [3] in the case of the square lattice. The sums studied in [2] and [3] are realized as the trace $\text{tr}(L^+)$ of the pseudoinverse $L^+$ of the Laplacian matrix $L$ which is a fundamental object in spectral theory of graphs, networks, grids, and arithmetic of curves (see e.g. [5–10,13]). In certain cases (see [7,8]), $\text{tr}(L^+)$ arises as the only nontrivial term in the calculation of intrinsic graph invariants such as the Kirchhoff index and the tau constant.

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This research is supported by Boğaziçi University Research Fund Grant Number 13387.

Key words and phrases: lattice sum, elementary classical function, asymptotic approximation.

Mathematics Subject Classification: primary 33B10, 41A60.
For a variety of lattices endowed with periodic boundary conditions, $\text{tr}(\mathcal{L}^+)$ can be expressed in terms of a sum of the form [3]

\begin{equation}
F_n = \sum_{j,k=0}^{n-1} \frac{1}{1 - \frac{1}{L} \sum_{\ell=1}^{L} \cos(s_{\ell} \cdot t_{j,k})}
\end{equation}

where $L \geq 2$ is an integer, $s_{\ell} = (s_{1,\ell}, s_{2,\ell}) \in \mathbb{Z}^2 \setminus \{0\}$ for $\ell = 1, \ldots, L$ with $s_1 = (1, 0)$ and $s_2 = (0, 1)$, and $t_{j,k} = (t_j, t_k) = \left(\frac{2\pi j}{n}, \frac{2\pi k}{n}\right)$ for $j, k \in \mathbb{Z}$. For instance, for the square, triangular, and modified union jack lattices, it is known that (see [13])

\begin{align*}
\text{tr}(\mathcal{L}_{\text{sq}}^+) &= \frac{1}{4} F_n^{\text{sq}} = \frac{1}{4} \sum_{j,k=0}^{n-1} \frac{1}{1 - \frac{1}{2} \left(\cos \frac{2\pi j}{n} + \cos \frac{2\pi k}{n}\right)}, \\
\text{tr}(\mathcal{L}_{\text{tr}}^+) &= \frac{1}{6} F_n^{\text{tr}} = \frac{1}{6} \sum_{j,k=0}^{n-1} \frac{1}{1 - \frac{1}{3} \left(\cos \frac{2\pi j}{n} + \cos \frac{2\pi k}{n} + \cos \frac{2\pi (j+k)}{n}\right)}, \\
\text{tr}(\mathcal{L}_{\text{muj}}^+) &= \frac{1}{8} F_n^{\text{muj}} \\
&= \frac{1}{8} \sum_{j,k=0}^{n-1} \frac{1}{1 - \frac{1}{4} \left(\cos \frac{2\pi j}{n} + \cos \frac{2\pi k}{n} + \cos \frac{2\pi (j-k)}{n} + \cos \frac{2\pi (j+k)}{n}\right)}.
\end{align*}

Former studies on $F_n$ were either outright wrong ([14] gives purported approximate values for divergent integrals) or quite rough (the estimates of [7] do not even capture the asymptotic value of $F_n$) – whence arose the need to do correct and precise calculations. The asymptotic behavior of the sum $F_n^{\text{tr}}$ associated with the triangular lattice was studied in [2]. There it was shown that

\begin{equation}
F_n^{\text{tr}} = \frac{\sqrt{3}}{\pi} n^2 \log n + \frac{\sqrt{3}}{\pi} \left(\gamma + \log \left(\frac{4\pi \sqrt{3}}{\Gamma\left(\frac{3}{4}\right)}\right)n^2 + \mathcal{O}(\log n)\right) \text{ as } n \to \infty,
\end{equation}

where $\gamma$ is Euler’s constant. The approach in [2] was generalized in [3] to develop methods for obtaining the asymptotic behavior of the general sum $F_n$ of (1.1) within errors of $\mathcal{O}(\log n)$ and $\mathcal{O}(1)$ as $n \to \infty$. They are based on the asymptotic analyses of integrals of $f$ and sums and integrals of $f_m$, where

\begin{equation}
f(x) = \frac{1}{\psi(x)} \text{ with } \psi(x) = 1 - \frac{1}{L} \sum_{\ell=1}^{L} \cos(s_{\ell} \cdot x), \quad x = (x, y) \in \mathbb{R}^2,
\end{equation}

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and

\begin{equation}
(1.4) \quad f_m(x) = \frac{1}{p_m(x)} \quad \text{with} \quad p_m(x) = \frac{1}{L} \sum_{\ell=1}^{L} \sum_{j=1}^{m} \frac{(-1)^{j+1}(s_{\ell} \cdot x)^{2j}}{(2j)!} \quad (m \geq 1);
\end{equation}

\(p_m\) is the \(2m\)-th order Taylor polynomial approximation of \(\psi\) around the origin. As shown in [3], the use of \(f_m\) allows for the determination of the asymptotic expansion with an error term of \(O(\log n)\) for \(m = 1\), and \(O(1)\) for any larger value of \(m\). The ideal choice is therefore \(f_2\). However, working with \(f_2\) demands significantly more delicate analyses compared to \(f_1\). In fact, the examples provided in [3] are based on the use of \(f_1\) for proving

\begin{equation}
(1.5) \quad F_n^{sq} = \frac{2}{\pi} n^2 \log n + \frac{2}{\pi} \left( \gamma + \log \left( \frac{4\sqrt{2\pi}}{\Gamma(\frac{1}{4})^2} \right) \right) n^2 + O(\log n),
\end{equation}

and

\begin{equation}
(1.6) \quad F_n^{muj} = \frac{4}{3\pi} n^2 \log n + \frac{4}{3\pi} \left( \gamma + \log \left( \frac{4\sqrt{6\pi}}{\Gamma(\frac{1}{4})^2} \right) \right) n^2 + O(\log n),
\end{equation}

as \(n \to \infty\). In this paper we use \(f_2\) for the first time and prove the following:

**Theorem 1.1.** As \(n \to \infty\), we have

\begin{equation}
(1.7) \quad F_n^{sq} = \frac{2}{\pi} n^2 \log n + \frac{2}{\pi} \left( \gamma + \log \left( \frac{4\sqrt{2\pi}}{\Gamma(\frac{1}{4})^2} \right) \right) n^2 + O(1).
\end{equation}

The motivation behind Theorem 1.1 comes from numerical evidence. Note that the asymptotic expansions (1.2), (1.5), and (1.6) are all in the form

\[F_n = an^2 \log n + bn^2 + O(\log n)\]

for some constants \(a\) and \(b\). The errors

\begin{equation}
(1.8) \quad E_n = F_n - (an^2 \log n + bn^2)
\end{equation}

displayed in Figure 1 suggest that, in fact,

\[F_n = an^2 \log n + bn^2 + O(1)\]

with \(E_n \approx -0.12\), \(E_n \approx -0.25\), \(E_n \approx -0.37\) as \(n \to \infty\) for the sums associated with the square, triangular, and modified union jack lattices respectively.

As stated above, the estimate given in Theorem 1.1 is as precise as it can get within the analytical framework developed in [3]. Even if one may...
Aspire to carry out an exact algebraic calculation involving cyclotomic fields (at least in some special cases such as \( n \) running through the sequence of primes, or the sequence of powers of 2), the question of how one would obtain the value of \( F_n \), or merely its asymptotic value, from the resulting algebraic numbers remains.

The paper is organized as follows. In Section 2 we revisit the method developed in [3] for studying the asymptotic behavior of the general sum (1.1) as \( n \to \infty \). In the same section, we also take on the sum \( F_{n}^{\text{sq}} \) corresponding to the square lattice, and deferring the technical details to Sections 3 and 4, present the proof of Theorem 1.1. In these latter sections we study the asymptotic behavior of \( I_n^\beta(f_2) \) and \( F_n^\beta(f_2) \) (an integral and a sum related with \( f_2 \)) when \( F_n = F_{n}^{\text{sq}} \).

2. The setup

As shown in [3], using the \( 2\pi \)-periodicity of \( \psi \) in both of its arguments, the sum \( F_n \) in (1.1) can be recast as

\[
F_n = F_n(f) = \sum_{t_{j,k} \in D_n} f(t_{j,k}) \quad \text{with} \quad D_n = \bigcup_{t_{j,k} \in [-\pi,\pi]^2 \setminus \{0\}} X_{j,k}
\]

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where \( X_{j,k} = X_j \times X_k \) with \( X_j = [x_j, x_{j+1}] \) and \( x_j = t_j - \frac{\pi}{n} \) for \( j \in \mathbb{Z} \). Explicitly

\[
D_n = \begin{cases} 
[-\pi, \pi]^2 \setminus [\frac{-\pi}{n}, \frac{\pi}{n}]^2, & n \text{ odd}, \\
[-\pi - \frac{\pi}{n}, \pi - \frac{\pi}{n}]^2 \setminus [-\frac{\pi}{n}, \frac{\pi}{n}]^2, & n \text{ even}.
\end{cases}
\]

A first approximation to \( F_n(f) \) is the integral

\[
I_n(f) = \frac{1}{2\Delta_n^2} \iint_{D_n} f(x) \, dx, \quad \Delta_n = \frac{2\pi}{n},
\]

since \( F_n(f) \) can be obtained from \( I_n(f) \) by applying the product cubature rule, with both factors coming from the midpoint rule, on each of the rectangles \( X_{j,k} \) in \( D_n \). Other possible approximations are

\[
F_n(f_m) = \sum_{t_{j,k} \in D_n} f_m(t_{j,k}), \quad I_n(f_m) = \frac{1}{2\Delta_n^2} \iint_{D_n} f_m(x) \, dx,
\]

and these are not problematic when \( m = 1 \) since \( p_1(x) = 0 \) only for \( x = 0 \). However, when \( m > 1 \), \( p_m \) may also vanish at some other points in \( [-\pi, \pi] \times [-\pi, \pi] \), and therefore \( D_n \) will have to be restricted to a smaller region (see [3, Remark 1]). Given a fixed \( \beta \in (0, 1) \), \( p_m (m \geq 1) \) is never zero on

\[
(2.1) \quad D_n^{\beta} = \bigcup_{|t_j|,|t_k| \leq \frac{\sqrt{n(1-\beta)}}{2}} X_{j,k} \quad (\overline{s} = \max_{1 \leq \ell \leq L} \| s_\ell \|),
\]

and

\[
F_n^{\beta}(f_m) = \sum_{t_{j,k} \in D_n^{\beta}} f_m(t_{j,k}), \quad I_n^{\beta}(f_m) = \frac{1}{2\Delta_n^2} \iint_{D_n^{\beta}} f_m(x) \, dx
\]

provide alternative approximations to \( F_n(f) \). The main results of [3] for the determination of the asymptotic behavior of \( F_n(f) \) are Theorems A and B:

**Theorem A.** If

\[
\Sigma_n \in \{ F_n(f), F_n^{\beta}(f), F_n(f_1), F_n^{\beta}(f_m), I_n(f), I_n^{\beta}(f), I_n(f_1), I_n^{\beta}(f_m) \}
\]

for some fixed \( \beta \in (0, 1) \) and \( m \geq 1 \), then

\[
\Sigma_n = \frac{|\Phi|}{\pi \sqrt{\det(S^T S)}} n^2 \log n + O(n^2)
\]

as \( n \to \infty \) where

\[
S = \begin{bmatrix} 
s_{1,1} & \ldots & s_{1,\ell} & \ldots & s_{1,|\Phi|} \\
s_{2,1} & \ldots & s_{2,\ell} & \ldots & s_{2,|\Phi|}
\end{bmatrix}^T.
\]
Theorem B. As \( n \to \infty \), we have
\[
F_n(f) - I_n(f) + I_n(f_1) - F_n(f_1) = O(\log n),
\]
and, for any fixed \( \beta \in (0, 1) \),
\[
F_n(f) - I_n(f) + I_n^\beta(f_m) - F_n^\beta(f_m) = \begin{cases} O(\log n), & m = 1, \\ O(1), & m \geq 2. \end{cases}
\]

The asymptotic behavior of \( I_n(f_1) \) and \( F_n(f_1) \) were derived in the general setting of the sum (1.1) with respective error terms of \( O\left(\frac{1}{n^2}\right) \) and \( O\left(\frac{\log n}{n^2}\right) \) in [3]. That of the integral \( I_n(f) \) was derived up to an error term of \( O(1) \) when \( F_n(f) \) pertains to the triangular lattice in [2], and when it corresponds to the square and modified union jack lattices in [3]. Using (2.2), the asymptotic behavior of \( F_n(f) \) in these three cases were obtained within errors of \( O(\log n) \).

As is apparent from (2.3), however, the ideal choice for the methods developed in [3] is \( m = 2 \) as it yields the optimal error bound of \( O(1) \) with the least possible effort. On the other hand, working with \( I_n^\beta(f_2) \) and \( F_n^\beta(f_2) \) is significantly more challenging in the general setting of the sum (1.1) when compared to \( I_n(f_1) \) and \( F_n(f_1) \). This is because, in addition to the significantly more difficult analyses, the former demands working with the factorization of a polynomial of degree four (namely \( p_2 \)) so as to obtain a partial fraction decomposition of \( f_2 \) to begin with, whereas the latter involves \( p_1 \) which is a polynomial of degree two only.

With this in mind, in this paper we study the asymptotic behavior of \( I_n^\beta(f_2) \) and \( F_n^\beta(f_2) \) associated with the sum \( F_n = F_n(f) = F_n^{sq} \) corresponding to the square lattice. Let us note that in this case (cf. (1.3), (1.4), and (2.1))
\[
f(x) = \frac{1}{\psi(x)} = \frac{1}{1 - \frac{1}{2}(\cos x + \cos y)},
\]
\[
f_1(x) = \frac{1}{p_1(x)} = \frac{4}{x^2 + y^2}, \quad f_2(x) = \frac{1}{p_2(x)} = \frac{4}{x^2 + y^2 - \frac{1}{12}(x^4 + y^4)},
\]
and \( \sigma = 1 \). For the calculations and analyses that follow, we choose
\[
\beta = 1 - \frac{\pi^2}{20} \in (0, 1)
\]
so that
\[
D_n^\beta = \bigcup_{|t_j|,|t_k| \leq \frac{\pi}{n}} X_{j,k} = [-\beta_n, \beta_n]^2 \setminus \left(-\frac{\pi}{n}, \frac{\pi}{n}\right)^2
\]

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where
\[(2.5) \quad \beta_n = \frac{\pi}{2} \left(1 + \frac{2 - n_0}{n}\right) \quad \text{with} \quad n \equiv n_0 \pmod{4}, \quad n_0 \in \{0, 1, 2, 3\}.\]

Observe that the second identity in (2.4) is a consequence of
\[(2.6) \quad |t_j| \leq \frac{\pi}{2} \iff |j| \leq \frac{n-n_0}{4} \iff -\frac{\pi}{n} \leq \frac{n-n_0}{4} - \frac{\pi}{n}.\]

**Proof of Theorem 1.1.** As was shown in [3], for the square lattice we have
\[(2.7) \quad I_n(f) = \frac{2}{\pi} n^2 \log n + \frac{1}{\pi} \left(\log \left(\frac{8}{\pi^2}\right) + \frac{4G}{\pi}\right) n^2 + O(1)\]
where $G$ is Catalan’s constant. In Section 3, we show that
\[(2.8) \quad I_\beta_n(f_2) = a_0 n^2 \log n + a_1 n^2 + a_2 n + O(1)\]
by explicitly determining the constants $a_j$. In Section 4, we prove that
\[(2.9) \quad F_\beta_n(f_2) = b_0 n^2 \log n + b_1 n^2 + b_2 n + O(1)\]
without making the constants $b_j$ explicit. (The proof of (2.9) given in Section 4 is based on a decomposition of $F_n(f_2)$ into six pieces followed by a study of their asymptotic behavior. For three of them the coefficients will be given explicitly.) In fact, we do not need the explicit values of these constants since the use of (2.7), (2.8), and (2.9) in (2.3) implies that
\[F_n(f) = c_0 n^2 \log n + c_1 n^2 + c_2 n + O(1)\]
for some constants $c_j$ and this, in turn, implies through (1.5) that these constants must be as given in (1.7). Thus Theorem 1.1 follows.

**3. Asymptotic behavior of $I_\beta_n(f_2)$**

In this section we prove the following for the asymptotic behavior of $I_\beta_n(f_2)$.

**Proposition 3.1.** As $n \to \infty$, we have
\[I_\beta_n(f_2) = \frac{2}{\pi} n^2 \log n + \frac{1}{\pi} \left(\log \left(\frac{8}{\pi^2}\right) + \frac{4G}{\pi}\right) n^2 + O(1)\]
\[+ \frac{96}{\pi^2 \mu} \left(2 \sqrt{\frac{\nu+1}{\nu-1}} \arctan \sqrt{\frac{\nu+1}{\nu-1}} + \frac{1}{\sqrt{\nu}} \log \left(\frac{\sqrt{\nu+1}}{\sqrt{\nu-1}}\right)\right) (2-n_0)n + O(1),\]
where, denoting the Clausen function by $\text{Cl}_2$,

\[
\lambda = \text{Cl}_2(2 \arctan \rho) - \text{Cl}_2(\pi + 2 \arctan \rho) + \left(\frac{\pi}{2} + 2 \arctan \rho\right) \log(\rho)
\]

\[
- \text{Cl}_2\left(\frac{\pi}{2} + \arccos\left(\frac{\nu - 1}{\nu + 1}\right)\right) - \text{Cl}_2\left(\frac{\pi}{2} - \arccos\left(\frac{\nu - 1}{\nu + 1}\right)\right),
\]

and

\[
\mu = \sqrt{24^2 + 48\pi^2 - \pi^4}, \quad \nu = \frac{\mu + 24}{\pi^2}, \quad \rho = \nu - \sqrt{\nu^2 - 1}.
\]

Note that $\mu \approx 30.86$, $\nu \approx 5.56$, $\rho \approx 0.09$.

The proof of Proposition 3.1 is based on several lemmas.

**Lemma 3.2.** As $n \to \infty$, we have

\[
I_{\beta n}(f_2) = \frac{2}{\pi} n^2 \log n + \frac{2}{\pi} \left(\frac{2G}{\pi} + \log \frac{\sqrt{6}}{\pi} - \frac{1}{\pi} (J_{n,1} + J_{n,2})\right)n^2 + O(1)
\]

with

\[
J_{n,1} = \int_0^{\pi/2} \log(2u_n - 1 - \cos \theta) \, d\theta, \quad J_{n,2} = \int_0^{\pi/2} \log\left(\cos \theta + 1 - \frac{1}{u_n}\right) \, d\theta
\]

where

\[
u_n = \alpha_n + \sqrt{\alpha_n^2 - \frac{1}{2}} \quad \text{with} \quad \alpha_n = \frac{\beta_n^2 + 6}{2\beta_n^2}.
\]

**Proof.** Considering $I_{\beta n}(f_1)$ first, switching to polar coordinates, we compute

\[
I_{\beta n}(f_1) = \frac{1}{\Delta_n^2} \int\int_{D_n^\beta} f_1 \, dx \, dy = \frac{4}{\Delta_n^2} \int\int_{D_n^\beta} \frac{dx \, dy}{x^2 + y^2}
\]

\[
= \frac{16}{\Delta_n^2} \int\int_{[0,\beta_n]^2 \setminus [0,\pi]^2} \frac{dx \, dy}{x^2 + y^2} = \frac{32}{\Delta_n^2} \int_0^{\frac{\beta_n}{\cos \theta}} \frac{1}{r} dr \, d\theta = \frac{8\pi}{\Delta_n^2} \log \frac{n \beta_n}{\pi},
\]

so that

\[
I_{\beta n}(f_1) = \frac{2}{\pi} n^2 \log n - \frac{\log 4}{\pi} n^2 + \frac{2(2 - n_0)}{\pi} n + O(1).
\]

Similarly, writing $\eta^2(\theta) = \cos^4 \theta + \sin^4 \theta$, we have

\[
I_{\beta n}(f_2) = \frac{1}{\Delta_n^2} \int\int_{D_n^\beta} f_2 \, dx \, dy = \frac{4}{\Delta_n^2} \int\int_{D_n^\beta} \frac{dx \, dy}{x^2 + y^2 - \frac{1}{12}(x^4 + y^4)}
\]
\[
\begin{align*}
\text{THE PSEUDOINVERSE OF THE LAPLACIAN MATRIX} & \quad \text{417} \\
& \quad \frac{16}{\Delta_n^2} \int \int_{[0,\beta_n]^2 \setminus [0,\gamma_n]^2} \frac{dx \, dy}{x^2 + y^2 - \frac{1}{12}(x^4 + y^4)} = \frac{32}{\Delta_n^2} \int_0^{\pi/4} \int_{\cos \theta}^{\beta_n \cos \theta} \frac{dr \, d\theta}{r - \frac{\eta^2(\theta)}{12} r^3} \\
& \quad = \frac{32}{\Delta_n^2} \int_0^{\pi/4} \int_{\cos \theta}^{\beta_n \cos \theta} \left( \frac{1}{r} + \frac{r \eta^2(\theta)}{12 - r^2 \eta^2(\theta)} \right) dr \, d\theta,
\end{align*}
\]
and therefore
\[(3.4)\]
\[
I_n^\beta(f_2) = I_n^\beta(f_1) + \frac{16}{\Delta_n^2} \int_0^{\pi/4} \left( \log \left( 12 - \left( \frac{\alpha_n \eta(\theta)}{\cos \theta} \right)^2 \right) - \log \left( 12 - \left( \frac{\beta_n \eta(\theta)}{\cos \theta} \right)^2 \right) \right) d\theta.
\]
We have
\[(3.5)\]
\[
\frac{16}{\Delta_n^2} \int_0^{\pi/4} \log \left( 12 - \left( \frac{\pi \eta(\theta)}{\cos \theta} \right)^2 \right) d\theta = \frac{16}{\Delta_n^2} \int_0^{\pi/4} \left( \log 12 + \mathcal{O} \left( \frac{1}{n^2} \right) \right) d\theta = \frac{\log 12}{\pi} n^2 + \mathcal{O}(1).
\]
On the other hand, using
\[
\int_0^\theta \log(\cos \phi) \, d\phi = -\theta \log 2 + \frac{1}{2} \text{Cl}_2(\pi - 2\theta)
\]
([12, p. 306, Formula 5]), we have
\[(3.6)\]
\[
\int_0^{\pi/4} \log \left( 12 - \left( \frac{\beta_n \eta(\theta)}{\cos \theta} \right)^2 \right) d\theta = \int_0^{\pi/4} \left[ \log(12 \cos^2 \theta - \beta_n^2 \eta^2(\theta)) - 2 \log(\cos \theta) \right] d\theta
\]
\[
= \int_0^{\pi/4} \log \left( 12 \cos^2 \theta - \beta_n^2 \eta^2(\theta) \right) d\theta + \frac{\pi \log 2 - 2G}{2}.
\]
Since \( \eta^2(\theta) = 2 \cos^4 \theta - 2 \cos^2 \theta + 1 \), we have
\[
12 \cos^2 \theta - \beta_n^2 \eta^2(\theta) = -2\beta_n^2 \left( \cos^4 \theta - 2\alpha_n \cos^2 \theta + \frac{1}{2} \right)
\]
\[
= \frac{\beta_n^2}{2} \left( 2 \left( \alpha_n + \sqrt{\alpha_n^2 - \frac{1}{2}} \right) - 2 \cos^2 \theta \right) \left( 2 \cos^2 \theta - 2 \left( \alpha_n - \sqrt{\alpha_n^2 - \frac{1}{2}} \right) \right)
\]
\[
= \frac{\beta_n^2}{2} (2u_n - 1 - \cos 2\theta) (\cos 2\theta + 1 - \frac{1}{u_n}),
\]
\[\text{Analysis Mathematica 49, 2023}\]
so that
\[
\int_0^{\pi/4} \log(12 \cos^2 \theta - \beta_n^2 \eta^2(\theta)) \, d\theta = \frac{\pi}{4} \log \left( \frac{\beta_n^2}{2} \right) + \int_0^{\pi/4} \log \left( (2u_n - 1 - \cos 2\theta) \left( \cos 2\theta + 1 - \frac{1}{u_n} \right) \right) \, d\theta
\]
\[
= \frac{\pi}{4} \log \left( \frac{\beta_n^2}{2} \right) + \frac{1}{2} \int_0^{\pi/2} \log(2u_n - 1 - \cos \theta) \, d\theta
\]
\[
+ \frac{1}{2} \int_0^{\pi/2} \log \left( \cos \theta + 1 - \frac{1}{u_n} \right) \, d\theta.
\]
Using this last identity in (3.6) and then using (3.3), (3.5) and (3.6) in (3.4), we obtain (3.1). □

To understand the asymptotic behavior of the integrals $J_{n,1}$ and $J_{n,2}$ in (3.2), we note that
\[
\alpha_n = \frac{1}{2} + \frac{3}{\beta_n^2} = \frac{1}{2} + \frac{12}{\pi^2} \left( 1 + \frac{1}{2 - n_0} \right)^2 = \frac{1}{2} + \frac{12}{\pi^2} \left( 2 - n_0 \right) + O \left( \frac{1}{n^2} \right),
\]
\[
\sqrt{\alpha_n^2 - \frac{1}{2}} = \mu \left( \frac{24}{2\pi^2} - \frac{24 + \pi^2}{\mu} \right) + O \left( \frac{1}{n^2} \right),
\]
so that
\[
2u_n - 1 = \nu - \frac{48(\nu + 1)}{\mu} \frac{2 - n_0}{n} + O \left( \frac{1}{n^2} \right) \quad (\nu \approx 5.6),
\]
and
\[
1 - \frac{1}{u_n} = \frac{\nu - 1}{\nu + 1} - \frac{96}{\mu(\nu + 1)} \frac{2 - n_0}{n} + O \left( \frac{1}{n^2} \right) \quad \left( \frac{\nu - 1}{\nu + 1} \approx 0.7 \right).
\]
We need to study the following integrals to understand $J_{n,1}$ and $J_{n,2}$:
\[
J_1(\tau_n) = \int_0^{\pi/2} \log(\tau_n - \cos \theta) \, d\theta \quad \text{with} \quad \tau_n = 2u_n - 1 \approx 5.6,
\]
\[
J_2(\tau_n) = \int_0^{\pi/2} \log(\cos \theta + \tau_n) \, d\theta \quad \text{with} \quad \tau_n = 1 - \frac{1}{u_n} \approx 0.7.
\]
For either case we write
\[
\tau_n = a + \frac{b(n)}{n} + O \left( \frac{1}{n^2} \right)
\]
where $b(n)$ is bounded.

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Lemma 3.3. If the sequence \(\{\tau_n\}\) satisfies (3.9) with \(a > 1\), then as \(n \to \infty\) we have

\[
J_1(\tau_n) = J_{11}(a) + J_{12}(a) \frac{b(n)}{n} + \mathcal{O}\left(\frac{1}{n^2}\right)
\]

where

\[
J_{11}(a) = \text{Cl}_2\left(\pi + 2 \arctan (a - \sqrt{a^2 - 1})\right) - \text{Cl}_2\left(2 \arctan (a - \sqrt{a^2 - 1})\right)
\]

\[
\left(\frac{\pi}{2} + 2 \arctan (a - \sqrt{a^2 - 1})\right) \log (a - \sqrt{a^2 - 1}) - \frac{\pi}{2} \log 2
\]

and

\[
J_{12}(a) = \frac{2}{\sqrt{a^2 - 1}} \arctan\left(\sqrt{\frac{a + 1}{a - 1}}\right).
\]

Proof. For \(a > 1\), we have

\[
J_1(\tau_n) = \int_0^{\pi/2} \log (a - \cos \theta) \, d\theta + \int_0^{\pi/2} \log \left(1 + \frac{b(n)}{a - \cos \theta} + \mathcal{O}\left(\frac{1}{n^2}\right)\right) \, d\theta
\]

\[
= I_1(a) + \frac{b(n)}{n} I_2(a) + \mathcal{O}\left(\frac{1}{n^2}\right)
\]

where

\[
I_1(a) = \int_0^{\pi/2} \log (a - \cos \theta) \, d\theta \quad \text{and} \quad I_2(a) = \int_0^{\pi/2} \frac{d\theta}{a - \cos \theta}.
\]

To complete the proof, we show that \(I_1(a) = J_{11}(a)\) and \(I_2(a) = J_{12}(a)\). For the former, we make use of [12, p. 308, Formula 39]

\[
\int_0^\phi \log(1 - 2r \cos \theta + r^2) \, d\theta = \text{Cl}_2(2\phi + 2\omega) - \text{Cl}_2(2\phi) - \text{Cl}_2(2\omega) - 2\omega \log r \quad (0 < r < 1),
\]

where \(\omega = \arg(1 - re^{-i\phi})\). To this end, we set \(r = a - \sqrt{a^2 - 1}\) so that \(a = \frac{1 + r^2}{2r}\) and therefore (using \(\text{Cl}_2(\pi) = 0\))

\[
I_1(a) = \int_0^{\pi/2} \log \left(\frac{1 + r^2}{2r} - \cos \theta\right) \, d\theta
\]

\[
= \int_0^{\pi/2} \log(1 - 2r \cos \theta + r^2) \, d\theta - \frac{\pi}{2} \log 2r = J_{11}(a).
\]
As for $I_2(a)$, we have

$$I_2(a) = \frac{2}{\sqrt{a^2 - 1}} \arctan\left(\sqrt{\frac{a+1}{a-1}} \tan \frac{\theta}{2}\right)\bigg|_{\theta=0}^{\pi/2} = J_{12}(a).$$

This finishes the proof. □

**Lemma 3.4.** If the sequence $\{\tau_n\}$ satisfies (3.9) with $a \in (0, 1)$, then as $n \to \infty$ we have

$$J_2(\tau_n) = J_{21}(a) + J_{22}(a) \frac{b(n)}{n} + \mathcal{O}\left(\frac{1}{n^2}\right)$$

where

$$J_{21}(a) = \Cl_2\left(\frac{\pi}{2} + \arccos a\right) + \Cl_2\left(\frac{\pi}{2} - \arccos a\right) - \frac{\pi}{2} \log 2$$

and

$$J_{22}(a) = \frac{1}{\sqrt{1-a^2}} \log\left(\frac{1 + \sqrt{1-a^2}}{a}\right).$$

**Proof.** For $a > 0$, we have

$$J_2(\tau_n) = \int_0^{\pi/2} \log(\cos \theta + a) \, d\theta + \int_0^{\pi/2} \log \left(1 + \frac{b(n)}{n} \frac{1}{\cos \theta + a}\right) \, d\theta
$$

$$= I_3(a) + \frac{b(n)}{n} I_4(a) + \mathcal{O}\left(\frac{1}{n^2}\right),$$

where

$$I_3(a) = \int_0^{\pi/2} \log(\cos \theta + a) \, d\theta \quad \text{and} \quad I_4(a) = \int_0^{\pi/2} \frac{d\theta}{\cos \theta + a}.$$

Considering $I_3(a)$, we recall [12, p. 308, Formula 36]

$$\int_0^\varphi \log(1 + \sec \phi \cos \theta) \, d\theta = \Cl_2(\pi + \phi - \varphi) + \Cl_2(\pi - \phi - \varphi) - \varphi \log(2 \cos \phi).$$

Therefore, for $a \in (0, 1)$, setting $a = \cos \phi$, we have

$$I_3(a) = \frac{\pi}{2} \log a + \int_0^{\pi/2} \log(1 + \sec \phi \cos \theta) \, d\theta = J_{21}(a).$$
For $I_4(a)$, we have

$$I_4(a) = \frac{1}{\sqrt{1 - a^2}} \left( \log \left( 1 + \sqrt{\frac{1 - a}{1 + a}} \tan \frac{\theta}{2} \right) - \log \left( 1 - \sqrt{\frac{1 - a}{1 + a}} \tan \frac{\theta}{2} \right) \right) \bigg|_{\theta = 0} = J_{22}(a).$$

This completes the proof. □

**Proof of Proposition 3.1.** In light of Lemma 3.2, equations (3.7), (3.8) and (3.9), and Lemmas 3.3 and 3.4, we have

$$I^{\beta}_{n}(f_2) = \frac{2}{\pi} n^2 \log n + \frac{2}{\pi} \left( \frac{2G}{\pi} + \log \frac{\sqrt{6}}{\pi} - \frac{1}{\pi} \left( J_{11}(\nu) + J_{21}(\frac{\nu - 1}{\nu + 1}) \right) \right) n^2$$

$$+ \frac{96}{\pi^2 \mu} \left( (\nu + 1)J_{12}(\nu) + \frac{2}{\nu + 1} J_{22}(\frac{\nu - 1}{\nu + 1}) \right) (2 - n_0)n + O(1).$$

Simplifying this expression we obtain Proposition 3.1. □

**4. Asymptotic behavior of $F^\beta_n(f_2)$**

In this section we prove the following for the asymptotic behavior of $F^\beta_n(f_2)$.

**Proposition 4.1.** As $n \to \infty$, we have

$$F^\beta_n(f_2) = \frac{2}{\pi} n^2 \log n + \alpha(n_0)n^2 + \beta(n_0)n + O(1)$$

for some constants $\alpha(n_0)$ and $\beta(n_0)$ where $n_0$ is as defined in (2.5).

The plan of the proof is as follows. First we set

$$N = \frac{n - n_0}{4},$$

$$A_k = \sqrt{1 + 4 \frac{\pi^2 k^2}{3n^2}} \left( 1 - \frac{\pi^2 k^2}{3n^2} \right), \quad B_k = \frac{3n^2}{2\pi^2} (1 + A_k), \quad C_k = \frac{3n^2}{2\pi^2} (A_k - 1),$$

and, in Subsection 4.1, we utilize a partial fraction decomposition along with the functional relations and the asymptotic behavior of the digamma function [15] to show the following.
LEMMA 4.2. As \( n \to \infty \), we have

\[
R_n^\beta(f_2) = \frac{2n^2}{\pi^2} \left( R_{n,1} - 2R_{n,2} + R_{n,3} + \pi R_{n,4} + 2\pi R_{n,5} + Q_{n} \right) + O(1)
\]

where

\[
R_{n,1} = \sum_{k=1}^{N} \frac{1}{N} \frac{1}{A_k} \frac{N}{\sqrt{B_k}} \log \left( \frac{1 + \frac{N}{\sqrt{B_k}}}{1 - \frac{N}{\sqrt{B_k}}} \right), \quad R_{n,2} = \sum_{k=1}^{N} \frac{1}{N} \frac{1}{A_k} \arctan\left( \frac{\sqrt{C_k}}{N} \right),
\]

\[
R_{n,3} = \sum_{k=1}^{N} \frac{1}{A_k} \frac{k^2 + N^2 - \frac{\pi^2}{3n^2}(k^4 + N^4)}{1 - e^{-2\pi \sqrt{C_k}}}, \quad R_{n,4} = \sum_{k=1}^{N} \frac{1}{A_k} \frac{1}{\sqrt{C_k}},
\]

\[
R_{n,5} = \sum_{k=1}^{N} \frac{1}{A_k} \frac{e^{-2\pi \sqrt{C_k}}}{1 - e^{-2\pi \sqrt{C_k}}}, \quad Q_{n} = \sum_{k=1}^{N} \frac{1}{k^2 - \frac{\pi^2}{3n^2} k^4}.
\]

In Subsection 4.2 we estimate the summands in \( R_{n,j} \). In Subsections 4.3-4.7 we use these estimates to study the asymptotic behavior of \( R_{n,j} \) and \( Q_{n} \) and prove that

LEMMA 4.3. As \( n \to \infty \), we have

\[
R_{n,\ell} = \alpha_{\ell} + \beta_{\ell}(n_0) \frac{1}{n} + \gamma_{\ell}(n_0) \frac{1}{n^2} + O\left( \frac{1}{n^3} \right), \quad \ell = 1, 2,
\]

\[
R_{n,3} = \beta_3 \frac{1}{n} + O\left( \frac{1}{n^2} \right),
\]

\[
R_{n,4} = \log n + \alpha_4(n_0) + \beta_4(n_0) \frac{1}{n} + \gamma_4(n_0) \frac{1}{n^2} + O\left( \frac{\log n}{n^3} \right),
\]

\[
R_{n,5} = \log \left( \frac{2\pi \frac{3}{4}}{\sqrt{\pi} \Gamma\left( \frac{1}{4} \right)} \right) + O\left( \frac{1}{n^2} \right),
\]

\[
Q_{n} = \frac{\pi^2}{6} + \left( \frac{\pi}{2\sqrt{3}} \log \left( \frac{4\sqrt{3} + \pi}{4\sqrt{3} - \pi} \right) - 4 \right) \frac{1}{n} + O\left( \frac{1}{n^2} \right),
\]

for some constants \( \alpha_{\ell}, \beta_{\ell}, \) and \( \gamma_{\ell} \) some of which depend on \( n_0 \).

The use of (4.7)–(4.11) in (4.3) proves Proposition 4.1. In principle, the constants in (4.7) and (4.9) can be computed explicitly. As will be apparent from the derivations that follow, however, this would require the evaluation of some nontrivial integrals. The constant \( \beta_3 \) in (4.8) is given explicitly at the end of Subsection 4.4.

Concerning the proof of Lemma 4.3, let us mention that the study of the sums \( R_{n,1} \) and \( R_{n,2} \) in Subsection 4.3 leading to the asymptotic relation

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(4.7) is based on further decompositions of these sums and utilization of the following version of the Euler-Maclaurin formula due to Lampret [11].

**Theorem C.** For any \( N, p \in \mathbb{N} \) and any function \( g \in C^p[0,1] \),

\[
\sum_{k=1}^{N} \frac{1}{N} g\left(\frac{k}{N}\right) = \int_{0}^{1} g(x) \, dx + \frac{1}{N} (g(1) - g(0)) + \sum_{\ell=1}^{p} \frac{1}{N^\ell} \frac{B_\ell}{\ell!} \left[ g^{(\ell-1)}(x) \right]_{0}^{1} + r_{p,N}(g),
\]

where \( B_\ell \) are the Bernoulli numbers (\( B_1 = -\frac{1}{2}, B_2 = \frac{1}{6}, B_3 = 0, B_4 = -\frac{1}{30}, \ldots \)), and

\[
r_{p,N}(g) = -\frac{1}{N^p} \frac{1}{p!} \int_{0}^{1} B_p(-Nx) g^{(p)}(x) \, dx
\]

with \( B_p(x) \) being the \( p \)-th Bernoulli polynomial in \([0,1]\) extended to all \( x \in \mathbb{R} \) via \( B_p(x+1) = B_p(x) \).

The study of \( R_{n,4} \) in Subsection 4.5 resulting in the asymptotic relation (4.9) is similar but additionally involves a singularity extraction technique. As for \( R_{n,5} \), a different and more delicate analytical approach is utilized in Subsection 4.6 to prove the relation (4.10). Concerning \( R_{n,3} \) and \( Q_n \), in Subsections 4.4 and 4.7, we employ partial fraction decompositions along with the functional relations and the asymptotic behavior of the digamma function and prove relations (4.8) and (4.11).

**4.1. Proof of Lemma 4.2.** With \( N \) as defined in (4.1), we see from (2.4) that \( t_{j,k} \in D_n^\beta \) if and only if \( |j|, |k| \leq N \) and \((j,k) \neq (0,0)\) (see (2.6)). Accordingly

\[
(4.12) \quad F_n^\beta(f_2) = \sum_{t_{j,k} \in D_n^\beta} f_2(t_{j,k}) = \frac{n^2}{\pi^2} \sum_{|j|,|k| \leq N} \frac{1}{j^2 + k^2 - \frac{\pi^2}{3N^2} (j^4 + k^4)}
\]

\[
\quad = \frac{4n^2}{\pi^2} \left( \sum_{k=1}^{N} \frac{1}{k^2 - \frac{\pi^2}{3N^2} k^4} + \sum_{j,k=1}^{N} \frac{1}{j^2 + k^2 - \frac{\pi^2}{3N^2} (j^4 + k^4)} \right)
\]

\[
\quad = \frac{4n^2}{\pi^2} (Q_n + R_n), \quad \text{say (see (4.6))}.
\]

Considering the sum \( R_n \), we use the partial fraction decomposition

\[
(4.13) \quad \frac{1}{x^2 - ax^4 + b} = \frac{1}{2A\sqrt{B}} \left( \frac{1}{x + \sqrt{B}} - \frac{1}{x - \sqrt{B}} \right) + \frac{i}{2A\sqrt{C}} \left( \frac{1}{x + i\sqrt{C}} - \frac{1}{x - i\sqrt{C}} \right)
\]
(valid for \(a, b > 0\) with \(A = \sqrt{1 + 4ab}, \ B = \frac{1+A}{2a}, \ \text{and} \ C = \frac{A-1}{2a} = \frac{2b}{1+A}\) for the parameters \(x = j, \ a = \frac{\pi^2}{3n^2}, \ b = k^2 - \frac{\pi^2}{3n^2}k^4, \ \text{and the relation} [1, \ \text{Formula 6.3.6}]\)

\[
\sum_{j=1}^{N} \frac{1}{j+a} = \psi(N + 1 + a) - \psi(1 + a), \quad (a \not\in -N),
\]

for the digamma function to evaluate the sum with respect to \(j\) to have

\[
R_n = \sum_{k=1}^{N} \frac{\psi(N+1+\sqrt{B_k}) - \psi(1+\sqrt{B_k}) - \psi(N+1-\sqrt{B_k}) + \psi(1-\sqrt{B_k})}{2A_k\sqrt{B_k}} \\
+ i \sum_{k=1}^{N} \frac{\psi(N+1+i\sqrt{C_k}) - \psi(1+i\sqrt{C_k}) - \psi(N+1-i\sqrt{C_k}) + \psi(1-i\sqrt{C_k})}{2A_k\sqrt{C_k}}
\]

where \(A_k, \ B_k, \ \text{and} \ C_k\) are as defined in (4.2). Next we use the functional relations [1, Formulas 6.3.5, 6.3.7]

\[
\psi(1+z) = \psi(z) + \frac{1}{z} \quad \text{and} \quad \psi(1-z) = \psi(z) + \pi \cot \pi z
\]

for the digamma function to write

\[
\psi(N + 1 + \sqrt{B_k}) = \psi(\sqrt{B_k} + N) + \frac{1}{\sqrt{B_k} + N},
\]

\[
\psi(N + 1 - \sqrt{B_k}) = \psi(\sqrt{B_k} - N) + \pi \cot \pi (\sqrt{B_k} - N),
\]

\[
\psi(1 + \sqrt{B_k}) - \psi(1 - \sqrt{B_k}) = \frac{1}{\sqrt{B_k}} - \pi \cot \pi \sqrt{B_k},
\]

\[
\psi(N + 1 + i\sqrt{C_k}) = \psi(N + i\sqrt{C_k}) + \frac{1}{N + i\sqrt{C_k}},
\]

\[
\psi(N + 1 - i\sqrt{C_k}) = \psi(N - i\sqrt{C_k}) + \frac{1}{N - i\sqrt{C_k}},
\]

\[
\psi(1 + i\sqrt{C_k}) - \psi(1 - i\sqrt{C_k}) = \frac{1}{i\sqrt{C_k}} - \pi \cot \pi i\sqrt{C_k},
\]

and use the fact that the cotangent function is \(\pi\)-periodic to have

\[
R_n = \sum_{k=1}^{N} \frac{1}{2A_k\sqrt{B_k}} \left( \psi(\sqrt{B_k} + N) - \psi(\sqrt{B_k} - N) + \frac{1}{\sqrt{B_k} + N} - \frac{1}{\sqrt{B_k}} \right)
\]
\[ + i \sum_{k=1}^{N} \frac{1}{2A_k \sqrt{C_k}} \left( \psi(N + i \sqrt{C_k}) - \psi(N - i \sqrt{C_k}) \right) \]

\[ - \frac{2i \sqrt{C_k}}{C_k + N^2} - \frac{1}{i \sqrt{C_k}} + \pi \cot \pi i \sqrt{C_k} \).\]

For \( 1 \leq k \leq N \), the estimates

\[ (4.18) \quad 1 < A_k < \frac{13}{10}, \quad \frac{3n^2}{\pi^2} < B_k < \frac{7n^2}{2\pi^2}, \]

\[ \frac{69k^2}{100} < C_k < k^2, \quad \frac{3n}{10} < \sqrt{B_k} \pm N < \frac{17n}{20} \]

are easily shown to hold, and they allow us to employ the asymptotic expansion [1, Formula 6.3.18]

\[ (4.19) \quad \psi(z) = \log z - \frac{1}{2z} - \frac{1}{12z^2} + \mathcal{O}(\frac{1}{|z|^4}), \quad \text{as } |z| \to \infty \text{ with } |\arg z| < \pi - \delta, \]

in (4.17) to deduce

\[ R_n = \sum_{k=1}^{N} \frac{1}{2A_k \sqrt{B_k}} \left( \log \left( \frac{\sqrt{B_k} + N}{\sqrt{B_k} - N} \right) + \frac{\sqrt{B_k}}{B_k - N^2} - \frac{1}{\sqrt{B_k}} \right) \]

\[ + i \sum_{k=1}^{N} \frac{1}{2A_k \sqrt{C_k}} \left( 2i \arctan \frac{\sqrt{C_k}}{N} - \frac{i \sqrt{C_k}}{C_k + N^2} - \frac{1}{i \sqrt{C_k}} + \pi \cot \pi i \sqrt{C_k} \right) \]

\[ + \mathcal{O}(\frac{1}{n^2}), \]

which we rewrite as

\[ (4.20) \quad R_n = \frac{1}{2} \sum_{k=1}^{N} \frac{1}{N} \frac{1}{A_k} \frac{N}{\sqrt{B_k}} \log \left( \frac{1 + \frac{N}{\sqrt{B_k}}}{1 - \frac{N}{\sqrt{B_k}}} \right) - \sum_{k=1}^{N} \frac{1}{N} \frac{1}{A_k} \frac{N}{\sqrt{B_k}} \frac{\arctan(\frac{\sqrt{C_k}}{N})}{\sqrt{C_k}} \]

\[ + \frac{1}{2} \sum_{k=1}^{N} \frac{1}{A_k} \left( \frac{1}{B_k - N^2} + \frac{1}{C_k + N^2} \right) - \frac{1}{2} \sum_{k=1}^{N} \frac{1}{A_k} \left( \frac{1}{B_k} + \frac{1}{C_k} \right) \]

\[ + \frac{1}{2} \sum_{k=1}^{N} \pi i \cot \pi i \sqrt{C_k} \frac{\pi \cot \pi i \sqrt{C_k}}{A_k \sqrt{C_k}} + \mathcal{O}(\frac{1}{n^2}). \]
Next, in (4.20), we use (4.2) in the third and fourth sums and the definition of the cotangent function in the last sum to obtain

\[
R_n = \frac{1}{2} \sum_{k=1}^{N} \frac{1}{N} A_k \sqrt{B_k} \log \left( \frac{1 + \frac{N}{\sqrt{B_k}}}{1 - \frac{N}{\sqrt{B_k}}} \right) - \sum_{k=1}^{N} \frac{1}{N} \arctan \left( \frac{\sqrt{C_k}}{N} \right)
\]

\[
+ \frac{1}{2} \sum_{k=1}^{N} k^2 + N^2 - \frac{\pi^2}{3n^2} (k^4 + N^4) - \frac{1}{2} Q_n
\]

\[
+ \frac{\pi}{2} \sum_{k=1}^{N} \frac{1}{A_k \sqrt{C_k}} + \pi \sum_{k=1}^{N} \frac{1}{A_k \sqrt{C_k}} e^{-2\pi \sqrt{C_k}} + O\left( \frac{1}{n^2} \right)
\]

\[
= \frac{1}{2} R_{n,1} - R_{n,2} + \frac{1}{2} R_{n,3} - \frac{1}{2} Q_n + \frac{\pi}{2} R_{n,4} + \pi R_{n,5} + O\left( \frac{1}{n^2} \right)
\]

(see (4.4)–(4.6)). Finally, we use (4.21) in (4.12) to get (4.3), and this completes the proof of Lemma 4.2.

**4.2. Approximation of the summands.** Here we study the asymptotic behavior of the summands in \( R_{n,j} \) for \( j = 1, 2, 4 \). To this end, we introduce the notation

\[
a_k = \frac{\pi}{4 \sqrt{3}} \frac{k}{N}, \tag{4.22}
\]

\[
\frac{1}{N_0} = \begin{cases} \frac{n_0}{4} \frac{1}{N}, & n_0 \in \{1, 2, 3\}, \\ 0, & n_0 = 0, \end{cases} \tag{4.23}
\]

and use (4.1) in (4.2) to write

\[
A_k = \sqrt{1 + \frac{4a_k^2}{(1 + \frac{1}{N_0})^2} \left( 1 - \frac{a_k^2}{(1 + \frac{1}{N_0})^2} \right)}
\]

(note that \( 0 < a_k < \frac{1}{2} \)). For a constant \( 0 < a < \frac{1}{2} \),

\[
\Psi(x) = \sqrt{1 + \frac{4a^2}{(1 + x)^2} \left( 1 - \frac{a^2}{(1 + x)^2} \right)}
\]

is smooth on the interval \((-\frac{1}{2}, \infty)\). We set

\[
A = \sqrt{1 + 4a^2(1 - a^2)}.
\]

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By Taylor’s theorem with remainder, we have

\[
\frac{1}{\Psi(x)} = \frac{1}{A} \left\{ 1 - \frac{4a^2(2a^2 - 1)}{A^2} x + \frac{2a^2(8a^6 + 4a^4 + 10a^2 - 3)}{A^4} x^2 + \mathcal{O}(x^3) \right\},
\]

\[
\sqrt{1 + \Psi(x)} = \sqrt{1 + A} \left\{ 1 + \frac{2a^2(2a^2 - 1)}{A(1 + A)} x \right\},
\]

\[
+ \frac{a^2}{A^2(1 + A)} \left( \frac{(2a^2 - 3)(12a^4 - 1)}{A} - \frac{2a^2(2a^2 - 1)^2}{1 + A} \right) x^2 + \mathcal{O}(x^3) \right\},
\]

\[
\frac{1}{\sqrt{1 + \Psi(x)}} = \frac{1}{\sqrt{1 + A}} \left\{ 1 - \frac{2a^2(2a^2 - 1)}{A(1 + A)} x \right\},
\]

\[
+ \frac{a^2}{A^2(1 + A)} \left( \frac{6a^2(2a^2 - 1)^2}{1 + A} - (2a^2 - 3)(12a^4 - 1) \right) x^2 + \mathcal{O}(x^3) \right\}
\]

which are valid on \((-\frac{1}{2}, \infty)\). Setting

\[
A_k = \sqrt{1 + 4a_k^2 (1 - a_k^2)},
\]

and implementing these Taylor approximations for \(a = a_k\) and \(x = \frac{1}{N_0}\), we obtain

\[
(4.24) \quad \frac{1}{A_k} = \alpha_{k,1} \left\{ 1 + \beta_{k,1} \frac{1}{N_0} + \gamma_{k,1} \frac{1}{N_0^2} + \mathcal{O}\left( \frac{1}{N_0^3} \right) \right\}
\]

with

\[
\alpha_{k,1} = \frac{1}{A_k}, \quad \beta_{k,1} = -\frac{4a_k^2(2a_k^2 - 1)}{A_k^2}, \quad \gamma_{k,1} = \frac{2a_k^2(8a_k^6 + 4a_k^4 + 10a_k^2 - 3)}{A_k^4},
\]

\[
\sqrt{1 + A_k} = \alpha_{k,2} \left\{ 1 + \beta_{k,2} \frac{1}{N_0} + \gamma_{k,2} \frac{1}{N_0^2} + \mathcal{O}\left( \frac{1}{N_0^3} \right) \right\}
\]

with

\[
\alpha_{k,2} = \sqrt{1 + A_k}, \quad \beta_{k,2} = \frac{2a_k^2(2a_k^2 - 1)}{A_k(1 + A_k)},
\]

\[
\gamma_{k,2} = \frac{a_k^2}{A_k^2(1 + A_k)} \left( \frac{(2a_k^2 - 3)(12a_k^4 - 1)}{A_k} - \frac{2a_k^2(2a_k^2 - 1)^2}{1 + A_k} \right),
\]

and

\[
(4.25) \quad \frac{1}{\sqrt{1 + A_k}} = \alpha_{k,3} \left\{ 1 + \beta_{k,3} \frac{1}{N_0} + \gamma_{k,3} \frac{1}{N_0^2} + \mathcal{O}\left( \frac{1}{N_0^3} \right) \right\}
\]
with
\[
\alpha_{k,3} = \frac{1}{\sqrt{1 + A_k}}, \quad \beta_{k,3} = -\beta_{k,2},
\]
\[
\gamma_{k,3} = \frac{a_k^2}{A_k^2(1 + A_k)} \left( \frac{6a_k^2(2a_k^2 - 1)^2}{1 + A_k} - \frac{(2a_k^2 - 3)(12a_k^4 - 1)}{A_k} \right).
\]

Since
\[
\frac{1}{1 + \frac{1}{N_0}} = 1 - \frac{1}{N_0} + \frac{1}{N_0^2} + \mathcal{O}\left(\frac{1}{N_0^3}\right),
\]
(4.25) entails
\[
\frac{N}{\sqrt{B_k}} = \frac{2\pi}{\sqrt{6}} \frac{1}{1 + A_k} \frac{N}{n} = \frac{\pi}{2\sqrt{6}} \frac{1}{1 + A_k} \frac{1}{1 + \frac{1}{N_0}}
\]
\[
= \alpha_{k,4} \left\{ 1 + \beta_{k,4} \frac{1}{N_0} + \gamma_{k,4} \frac{1}{N_0^2} + \mathcal{O}\left(\frac{1}{N_0^3}\right) \right\}
\]
with
\[
\alpha_{k,4} = \frac{\pi}{2\sqrt{6}} \alpha_{k,3}, \quad \beta_{k,4} = \beta_{k,3} - 1, \quad \gamma_{k,4} = 1 - \beta_{k,3} + \gamma_{k,3},
\]
so that
\[
1 + \frac{N}{\sqrt{B_k}} = (1 + \alpha_{k,4}) \left\{ 1 + \frac{\alpha_{k,4}}{1 + \alpha_{k,4}} \left( \beta_{k,4} \frac{1}{N_0} + \gamma_{k,4} \frac{1}{N_0^2} + \mathcal{O}\left(\frac{1}{N_0^3}\right) \right) \right\}.
\]
Therefore
\[
\log \left( 1 + \frac{N}{\sqrt{B_k}} \right) = \log(1 + \alpha_{k,4}) \pm \frac{\alpha_{k,4} \beta_{k,4}}{1 + \alpha_{k,4}} \frac{1}{N_0}
\]
\[
+ \left( \frac{\alpha_{k,4} \gamma_{k,4}}{1 + \alpha_{k,4}} - \frac{1}{2} \left( \frac{\alpha_{k,4} \beta_{k,4}}{1 + \alpha_{k,4}} \right)^2 \right) \frac{1}{N_0^2} + \mathcal{O}\left(\frac{1}{N_0^3}\right).
\]
Accordingly, (4.27) implies
\[
\log \left( \frac{1 + \frac{N}{\sqrt{B_k}}}{1 - \frac{N}{\sqrt{B_k}}} \right) = \log(\alpha_{k,5}) + \beta_{k,5} \frac{1}{N_0} + \gamma_{k,5} \frac{1}{N_0^2} + \mathcal{O}\left(\frac{1}{N_0^3}\right)
\]
with
\[
\alpha_{k,5} = \frac{1 + \alpha_{k,4}}{1 - \alpha_{k,4}}, \quad \beta_{k,5} = \frac{2\alpha_{k,4} \beta_{k,4}}{1 - \alpha_{k,4}^2}, \quad \gamma_{k,5} = \frac{2\alpha_{k,4} \gamma_{k,4}}{1 - \alpha_{k,4}^2} + \frac{2\alpha_{k,4}^3 \beta_{k,4}^2}{(1 - \alpha_{k,4}^2)^2}.
\]

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Next, using (4.2), we have
\[ C_k = \frac{3n^2}{2\pi^2} (A_k - 1) = \frac{3n^2 A_k^2 - 1}{2\pi^2 (1 + A_k)} = \frac{2}{1 + A_k} k^2 \left( 1 - \frac{\pi^2k^2}{3n^2} \right) \]
so that, by (4.22) and (4.23),
\[(4.29) \quad \frac{\sqrt{C_k}}{N} = \frac{\sqrt{2}}{N} \frac{k}{\sqrt{1 + A_k}} \sqrt{1 - \frac{\pi^2k^2}{3n^2}} = \frac{\sqrt{2}}{N} \frac{k}{\sqrt{1 + A_k}} \sqrt{1 - \frac{a_k^2}{(1 + \frac{1}{N})^2}}. \]
In (4.29), using (4.25) along with the Taylor approximation
\[ \sqrt{1 - \frac{a_k^2}{(1 + x)^2}} = \sqrt{1 - a_k^2} \left\{ 1 + \frac{a_k^2}{1 - a_k^2} x + \frac{a_k^2(2a_k^2 - 3)}{2(1 - a_k^2)^2} x^2 + \mathcal{O}(x^3) \right\} \]
(which is valid on \((-\frac{1}{2}, \infty)\) when \(0 < a < \frac{1}{2}\)), we deduce
\[(4.30) \quad \frac{\sqrt{C_k}}{N} = \alpha_{k,6} \left\{ 1 + \beta_{k,6} \frac{1}{N_0} + \gamma_{k,6} \frac{1}{N_0^2} + \mathcal{O}\left(\frac{1}{N_0^3}\right) \right\} \]
with
\[ \alpha_{k,6} = \frac{\sqrt{2}}{N} \frac{k}{\sqrt{1 + A_k}} \frac{\sqrt{1 - a_k^2}}{1 - a_k^2}, \quad \beta_{k,6} = \beta_{k,3} + \frac{a_k^2}{1 - a_k^2}, \]
\[ \gamma_{k,6} = \gamma_{k,3} + \beta_{k,3} a_k^2 + \frac{a_k^2(2a_k^2 - 3)}{2(1 - a_k^2)^2}. \]
In light of (4.30), using the Taylor approximation \((\alpha \neq 0, x > -1)\)
\[ \frac{\arctan(\alpha(1+x))}{\alpha(1+x)} = \frac{\arctan \alpha}{\alpha} (1 - x + x^2) + \frac{1}{1 + \alpha^2} x - \frac{1 + 2\alpha^2}{(1 + \alpha^2)^2} x^2 + \mathcal{O}(x^3), \]
we therefore get
\[(4.31) \quad \frac{\arctan(\frac{\sqrt{C_k}}{N})}{\frac{\sqrt{C_k}}{N}} = \alpha_{k,7} \left\{ 1 + \beta_{k,7} \frac{1}{N_0} + \gamma_{k,7} \frac{1}{N_0^2} \right\} + \beta'_{k,7} \frac{1}{N_0} + \gamma'_{k,7} \frac{1}{N_0^2} + \mathcal{O}\left(\frac{1}{N_0^3}\right) \]
with
\[ \alpha_{k,7} = \frac{\arctan \alpha_{k,6}}{\alpha_{k,6}}, \quad \beta_{k,7} = -\beta_{k,6}, \quad \gamma_{k,7} = \beta_{k,6}^2 - \gamma_{k,6} \]
and

\[
\beta'_{k,7} = \frac{\beta_{k,6}}{1 + \alpha_{k,6}^2}, \quad \gamma'_{k,7} = \frac{\gamma_{k,6}}{1 + \alpha_{k,6}^2} - \frac{\beta_{k,6}^2(1 + 2\alpha_{k,6}^2)}{(1 + \alpha_{k,6}^2)^2}.
\]

Concerning the summand in \(R_{n,1}\), we combine (4.24), (4.26) and (4.28) to get

\[
\frac{1}{A_k} \frac{N}{\sqrt{B_k}} \log \left( \frac{1 + \frac{N}{\sqrt{B_k}}}{1 - \frac{N}{\sqrt{B_k}}} \right) = \alpha_{k,8} + \beta_{k,8} \frac{1}{N_0} + \gamma_{k,8} \frac{1}{N_0^2} + \mathcal{O}\left( \frac{1}{N_0^3} \right)
\]

with

\[
\alpha_{k,8} = \alpha_{k,1} \alpha_{k,4} \log(\alpha_{k,5}), \quad \beta_{k,8} = \alpha_{k,1} \alpha_{k,4} ((\beta_{k,1} + \beta_{k,4}) \log(\alpha_{k,5}) + \beta_{k,5}), \\
\gamma_{k,8} = \alpha_{k,1} \alpha_{k,4} ((\beta_{k,1} \beta_{k,4} + \gamma_{k,1} + \gamma_{k,4}) \log(\alpha_{k,5}) + (\beta_{k,1} + \beta_{k,4}) \beta_{k,5} + \gamma_{k,5}).
\]

For the summand in \(R_{n,2}\), we use (4.24) and (4.31) to obtain

\[
\frac{1}{A_k} \arctan\left( \frac{\sqrt{\alpha_{k}}}{\sqrt{N}} \right) = \alpha_{k,9} + \beta_{k,9} \frac{1}{N_0} + \gamma_{k,9} \frac{1}{N_0^2} + \mathcal{O}\left( \frac{1}{N_0^3} \right)
\]

with

\[
\alpha_{k,9} = \alpha_{k,1} \alpha_{k,7}, \quad \beta_{k,9} = \alpha_{k,1} (\alpha_{k,7} (\beta_{k,1} + \beta_{k,7}) + \beta'_{k,7}), \\
\gamma_{k,9} = \alpha_{k,1} ((\beta_{k,1} \beta_{k,7} + \gamma_{k,1} + \gamma_{k,7}) \alpha_{k,7} + \beta_{k,1} \beta'_{k,7} + \gamma'_{k,7}).
\]

As for the term \(\frac{1}{A_k \sqrt{C_k}}\) appearing in \(R_{n,4}\) and \(R_{n,5}\), we use (4.30) to deduce

\[
\frac{1}{A_k \sqrt{C_k}} = \frac{1}{k} \alpha_{k,10} \left\{ 1 + \beta_{k,10} \frac{1}{N_0} + \gamma_{k,10} \frac{1}{N_0^2} + \mathcal{O}\left( \frac{1}{N_0^3} \right) \right\}
\]

with

\[
\alpha_{k,10} = \frac{\sqrt{1 + A_k}}{\sqrt{2} \sqrt{1 - \alpha_{k}^2}}, \quad \beta_{k,10} = -\beta_{k,6}, \quad \gamma_{k,10} = \beta_{k,6}^2 - \gamma_{k,6},
\]

and we combine (4.24) with (4.34) to obtain

\[
\frac{1}{A_k \sqrt{C_k}} = \frac{1}{k} \alpha_{k,11} \left\{ 1 + \beta_{k,11} \frac{1}{N_0} + \gamma_{k,11} \frac{1}{N_0^2} + \mathcal{O}\left( \frac{1}{N_0^3} \right) \right\}
\]

with

\[
\alpha_{k,11} = \alpha_{k,1} \alpha_{k,10}, \quad \beta_{k,11} = \beta_{k,1} + \beta_{k,10}, \quad \gamma_{k,11} = \beta_{k,1} \beta_{k,10} + \gamma_{k,1} + \gamma_{k,10}.
\]
4.3. Asymptotic behavior of $R_{n,1}$ and $R_{n,2}$. Concerning the asymptotic behavior of $R_{n,1}$ and $R_{n,2}$, here we prove (4.7). In view of (4.21), we see that (4.32) and (4.33) imply for $\ell = 1, 2$

\begin{equation}
(4.36) \quad R_{n,\ell} = \sum_{k=1}^{N} \frac{1}{N} \mu_{\ell,1}(\frac{k}{N}) + \frac{1}{N_0} \sum_{k=1}^{N} \frac{1}{N} \mu_{\ell,2}(\frac{k}{N}) + \frac{1}{N_0^2} \sum_{k=1}^{N} \frac{1}{N} \mu_{\ell,3}(\frac{k}{N}) + O\left(\frac{1}{N_0^3}\right) = R_{n,\ell,1} + \frac{1}{N_0} R_{n,\ell,2} + \frac{1}{N_0^2} R_{n,\ell,3} + O\left(\frac{1}{N_0^3}\right), \quad \text{say,}
\end{equation}

where the functions $\mu_{1,1}(x)$, $\mu_{1,2}(x)$, $\mu_{1,3}(x)$ are obtained by replacing $\frac{k}{N}$ with $x$ in $\alpha_{k,8}$, $\beta_{k,8}$, and $\gamma_{k,8}$ respectively, and $\mu_{2,1}(x)$, $\mu_{2,2}(x)$, $\mu_{2,3}(x)$ are similarly obtained from $\alpha_{k,9}$, $\beta_{k,9}$, and $\gamma_{k,9}$ respectively. The functions $\mu_{\ell,j}(x)$ $(1 \leq \ell \leq 2$ and $1 \leq j \leq 3)$ so obtained are smooth in the interval $[0,1]$, and therefore Theorem C applies to each of the sums $R_{n,\ell,j}$ $(1 \leq \ell \leq 2$ and $1 \leq j \leq 3)$) to yield

\begin{equation}
(4.37) \quad R_{n,\ell,j} = a_{\ell,j} + b_{\ell,j} \frac{1}{N} + c_{\ell,j} \frac{1}{N^2} + O\left(\frac{1}{N^3}\right)
\end{equation}

for some constants $a_{\ell,j}$, $b_{\ell,j}$, and $c_{\ell,j}$. Since $\frac{1}{N_0} = \frac{n_0}{4N}$, and

\begin{equation}
(4.38) \quad \frac{1}{N} = \frac{4}{n - n_0} = \frac{4}{n} \left(1 - \frac{n_0}{n}\right) = \frac{4}{n} \left(1 + \frac{n_0}{n} + \left(\frac{n_0}{n}\right)^2\right) + O\left(\frac{1}{n^4}\right),
\end{equation}

use of (4.37) in (4.36) implies (4.7) for $\ell = 1, 2$.

4.4. Asymptotic behavior of $R_{n,3}$. Here we study $R_{n,3}$ and prove the asymptotic relation (4.8). To this end, we employ (4.13) for the parameters $x = k$, $a = \frac{\pi^2}{3n^2}$, $b = N^2 - \frac{\pi^2}{3n^2} N^4$ and then apply (4.14) to deduce

\begin{align*}
R_{n,3} &= \frac{\psi(N + 1 + \sqrt{B_N}) - \psi(1 + \sqrt{B_N}) - \psi(N + 1 - \sqrt{B_N}) + \psi(1 - \sqrt{B_N})}{2A_N\sqrt{B_N}} \\
&\quad + i \frac{\psi(N + 1 + i\sqrt{C_N}) - \psi(1 + i\sqrt{C_N}) - \psi(N + 1 - i\sqrt{C_N}) + \psi(1 - i\sqrt{C_N})}{2A_N\sqrt{C_N}}.
\end{align*}

We then use (4.16) and the $\pi$-periodicity of the cotangent function to obtain

\begin{align*}
R_{n,3} &= \frac{1}{2A_N\sqrt{B_N}} \left( \psi(\sqrt{B_N} + N) - \psi(\sqrt{B_N} - N) + \frac{1}{\sqrt{B_N} + N} - \frac{1}{\sqrt{B_N}} \right) \\
&\quad + \frac{i}{2A_N\sqrt{C_N}} \left( \psi(N + i\sqrt{C_N}) - \psi(N - i\sqrt{C_N}) \\
&\quad - 2i\sqrt{C_N} \left( \frac{1}{C_N + N^2} - \frac{1}{i\sqrt{C_N}} + \pi \cot \pi i\sqrt{C_N} \right) \right).
\end{align*}
Use of (4.18) for \( k = N \) shows that the terms, aside from those involving the digamma and the cotangent functions, are of size \( \mathcal{O}(\frac{1}{N^2}) \). For the cotangent term, employing (4.18) for \( k = N \) we obtain

\[
\pi \cot \pi i\sqrt{C_N} = -i\pi - i\pi \frac{2e^{-2\pi \sqrt{C_N}}}{1 - e^{-2\pi \sqrt{C_N}}} = -i\pi + \mathcal{O}(e^{-\pi N}).
\]

Accordingly,

\[
R_{n,3} = \frac{\psi(\sqrt{B_N} + N) - \psi(\sqrt{B_N} - N)}{2AN\sqrt{B_N}} + i \frac{\psi(N + i\sqrt{C_N}) - \psi(N - i\sqrt{C_N}) - i\pi}{2AN\sqrt{C_N}} + \mathcal{O}\left(\frac{1}{N^2}\right).
\]

Then we use the asymptotic expansion (4.19) (in the form \( \psi(z) = \log z + \mathcal{O}(\frac{1}{z}) \)) along with (4.18) for \( k = N \) to get

\[
R_{n,3} = \frac{1}{2AN\sqrt{B_N}} \log \left(\frac{\sqrt{B_N} + N}{\sqrt{B_N} - N}\right) + \frac{1}{2AN\sqrt{C_N}} \left(\pi - 2\arctan\left(\frac{\sqrt{C_N}}{N}\right)\right) + \mathcal{O}\left(\frac{1}{N^2}\right)
\]

\[
= \frac{1}{2N} \frac{1}{AN\sqrt{B_N}} \log \left(1 + \frac{N}{\sqrt{B_N}}\right) - \frac{1}{N} \frac{1}{AN\sqrt{C_N}} \arctan\left(\frac{\sqrt{C_N}}{N}\right) + \frac{\pi}{2} \frac{1}{2N\sqrt{C_N}}
\]

\[
+ \mathcal{O}\left(\frac{1}{N^2}\right) = R_{n,3,1} - R_{n,3,2} + R_{n,3,3} + \mathcal{O}\left(\frac{1}{N^2}\right), \quad \text{say.}
\]

By use of (4.32), (4.33), and (4.35), we have

\[
R_{n,3,1} = \frac{1}{2N} \alpha_{N,8} + \mathcal{O}\left(\frac{1}{N^2}\right), \quad R_{n,3,2} = \frac{1}{N} \alpha_{N,9} + \mathcal{O}\left(\frac{1}{N^2}\right),
\]

\[
R_{n,3,3} = \frac{\pi}{2N} \alpha_{N,11} + \mathcal{O}\left(\frac{1}{N^2}\right)
\]

so that

\[
R_{n,3} = \frac{\alpha_{N,8} - 2\alpha_{N,9} + \pi \alpha_{N,11}}{2} \frac{1}{N} + \mathcal{O}\left(\frac{1}{N^2}\right).
\]

Using (4.38) in (4.39), we conclude

\[
R_{n,3} = 2(\alpha_{N,8} - 2\alpha_{N,9} + \pi \alpha_{N,11}) \frac{1}{n} + \mathcal{O}\left(\frac{1}{n^2}\right).
\]
Noting that $\alpha_{N,j}$, $\beta_{N,j}$, and $\gamma_{N,j}$ are in fact constants,

$$\alpha_{N,8} = \frac{\pi}{2\sqrt{6}} \frac{1}{\sqrt{1 + A_N}} \log \left( \frac{2\sqrt{6}\sqrt{1 + A_N} + \pi}{2\sqrt{6}\sqrt{1 + A_N} - \pi} \right),$$

$$\alpha_{N,9} = \frac{2\sqrt{6}}{\sqrt{48 - \pi^2}} \frac{\sqrt{1 + A_N}}{A_N} \arctan \left( \frac{\sqrt{48 - \pi^2}}{2\sqrt{6}\sqrt{1 + A_N}} \right),$$

$$\alpha_{N,11} = \frac{2\sqrt{6}}{\sqrt{48 - \pi^2}} \frac{\sqrt{1 + A_N}}{A_N},$$

where

$$A_N = \sqrt{1 + \frac{\pi^2}{12} \left( 1 - \frac{\pi^2}{48} \right)},$$

(4.40) delivers (4.8) with $\beta_3 = 2(\alpha_{N,8} - 2\alpha_{N,9} + \pi\alpha_{N,11}).$

4.5. Asymptotic behavior of $R_{n,4}$. Here we consider $R_{n,4}$ in (4.5) and prove the asymptotic relation (4.9). First we observe that

$$\alpha_{k,11} = \frac{\sqrt{1 + A_k}}{\sqrt{2}\sqrt{1 - a_k^2 A_k}}$$

is bounded for $1 \leq k \leq N$ so that the use of (4.22) in (4.35) entails

$$R_{n,4} = \sum_{k=1}^{N} \frac{1}{k} \alpha_{k,11} + \frac{1}{N_0} \sum_{k=1}^{N} \frac{1}{k} \alpha_{k,11} \beta_{k,11} + \frac{1}{N_0^2} \sum_{k=1}^{N} \frac{1}{k} \alpha_{k,11} \gamma_{k,11} + O \left( \frac{\log N}{N_0^3} \right)$$

$$= \sum_{k=1}^{N} \frac{1}{k} \alpha_{k,11} + \frac{\pi}{4\sqrt{3}} \frac{1}{N_0} \sum_{k=1}^{N} \frac{1}{N} \alpha_{k,11} \beta_{k,11} \frac{a_k}{a_k}$$

$$+ \frac{\pi}{4\sqrt{3}} \frac{1}{N_0^2} \sum_{k=1}^{N} \frac{1}{N} \alpha_{k,11} \gamma_{k,11} \frac{a_k}{a_k} + O \left( \frac{\log N}{N_0^3} \right)$$

$$= R_{n,4,1} + \frac{\pi}{4\sqrt{3}} \frac{1}{N_0} R_{n,4,2} + \frac{\pi}{4\sqrt{3}} \frac{1}{N_0^2} R_{n,4,3} + O \left( \frac{\log N}{N_0^3} \right), \text{ say.}$$

For $R_{n,4,1}$, we note that

$$\alpha_{k,11} = \mu \left( \frac{k}{N} \right)$$

(4.42)
where

\[
\mu(x) = \frac{\sqrt{1 + \sqrt{1 + \frac{\pi^2}{12}x^2(1 - \frac{\pi^2}{48}x^2)}}}{\sqrt{2 \sqrt{1 - \frac{\pi^2}{48}x^2} \sqrt{1 + \frac{\pi^2}{12}x^2(1 - \frac{\pi^2}{48}x^2)}}}
\]

The function \( \mu \) admits a convergent Taylor series expansion valid in an interval containing \([-1, 1]\) which is

\[
(4.43) \quad \mu(x) = 1 - \frac{\pi^2}{48}x^2 + \frac{11\pi^4}{4608}x^4 - \frac{41\pi^6}{221184}x^6 + O(x^8).
\]

Therefore, the function

\[
\mu_1(x) = \frac{\mu(x) - 1}{x}
\]

is smooth on the interval \([0, 1]\). This motivates us to write

\[
R_{n,4,1} = \sum_{k=1}^{N} \frac{1}{k} \alpha_{k,11} = \sum_{k=1}^{N} \frac{1}{k} \mu \left( \frac{k}{N} \right) = \sum_{k=1}^{N} \frac{1}{k} + \sum_{k=1}^{N} \frac{1}{N} \mu \left( \frac{k}{N} \right) - \frac{1}{N}
\]

\[
= \sum_{k=1}^{N} \frac{1}{k} + \sum_{k=1}^{N} \frac{1}{N} \mu_1 \left( \frac{k}{N} \right).
\]

By the well-known formula (see, for example, [1, Formulas 6.3.2, 6.3.18])

\[
\sum_{k=1}^{N} \frac{1}{k} = \log N + \gamma + \frac{1}{2N} - \frac{1}{12N^2} + O \left( \frac{1}{N^4} \right),
\]

and the application of Theorem C to the second sum giving

\[
\sum_{k=1}^{N} \frac{1}{N} \mu_1 \left( \frac{k}{N} \right) = d_1 + d_2 \frac{1}{N} + d_3 \frac{1}{N^2} + O \left( \frac{1}{N^3} \right)
\]

for some constants \( d_j \), we have

\[
(4.44) \quad R_{n,4,1} = \log N + a_{4,1} + b_{4,1} \frac{1}{N} + c_{4,1} \frac{1}{N^2} + O \left( \frac{1}{N^3} \right)
\]

for some constants \( a_{4,1}, b_{4,1}, \) and \( c_{4,1} \). As for \( R_{n,4,2} \) and \( R_{n,4,3} \), we note that \( \beta_{k,11} \) and \( \gamma_{k,11} \) contain \( a_k \) (in fact \( a_k^2 \)) as a factor:

\[
(4.45) \quad \frac{\beta_{k,11}}{a_k^2} = \frac{2(1 - 2a_k^2)(2 + A_k)}{A_k^2(1 + A_k)} - \frac{1}{1 - a_k^2}.
\]

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and

\[
\gamma_{k,11} = \frac{2(8a_k^6 + 4a_k^4 + 10a_k^2 - 3)}{\mathcal{A}_k^4} - \frac{8a_k^6 + 4a_k^4 + 10a_k^2 - 3}{\mathcal{A}_k^3(1 + A_k)}
- \frac{2a_k^2(2a_k^2 - 1)^2}{\mathcal{A}_k^2(1 + A_k)^2} - \frac{2a_k^2(2a_k^2 - 1)}{\mathcal{A}_k(1 + A_k)(1 - a_k^2)} + \frac{4a_k^2(2a_k^2 - 1)}{\mathcal{A}_k^2(1 - a_k^2)} + \frac{3}{2(1 - a_k^2)^2}.
\]

The importance of this observation is that both $\beta_{k,11}$ and $\gamma_{k,11}$ are of the form $\mu\left(\frac{k}{N}\right)$ for smooth functions $\mu$ on $[0,1]$. Since $\alpha_{k,11}$ also has the same form, we conclude for $j = 2,3$ that

\[
R_{n,4,j} = \sum_{k=1}^{N} \frac{1}{N} \mu_j\left(\frac{k}{N}\right)
\]

for appropriately defined smooth functions $\mu_j$ on the interval $[0,1]$. Therefore Theorem C applies to both of these sums to yield for $j = 2,3$

\[
R_{n,4,j} = a_{4,j} + b_{4,j} \frac{1}{N} + c_{4,j} \frac{1}{N^2} + O\left(\frac{1}{N^3}\right)
\]

for some constants $a_{4,j}$, $b_{4,j}$, and $c_{4,j}$. Using (4.44) and (4.47) in (4.41) and then making use of (4.23) and (4.38), we deduce (4.9).

4.6. Asymptotic behavior of $R_{n,5}$. Here we prove (4.10) for the asymptotic behavior of $R_{n,5}$. To this end, we first show the following.

**Lemma 4.4.** As $n \to \infty$, we have

\[
R_{n,5} = \sum_{1 \leq k \leq \log N} \frac{1}{k} \alpha_{k,11} e^{-2\pi \sqrt{C_k} (p+1)} + O\left(\frac{1}{N^2}\right).
\]

**Proof.** We use (4.22) in (4.35) to write

\[
R_{n,5} = \sum_{k=1}^{N} \frac{1}{A_k \sqrt{C_k}} e^{-2\pi \sqrt{C_k} / (1 - e^{-2\pi \sqrt{C_k}})} = \sum_{k=1}^{N} \frac{1}{k} \alpha_{k,11} e^{-2\pi \sqrt{C_k} / (1 - e^{-2\pi \sqrt{C_k}})}
+ \frac{\pi}{4\sqrt{3}} \sum_{k=1}^{N} \alpha_{k,11} \left\{ \frac{1}{NN_0} \beta_{k,11} + \frac{1}{NN_0^2} \gamma_{k,11} + \frac{1}{k} O\left(\frac{1}{N_0^3}\right) \right\} e^{-2\pi \sqrt{C_k} / (1 - e^{-2\pi \sqrt{C_k}})}.
\]

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From (4.42), (4.45), and (4.46), we see that $\alpha_{k,11}$, $\frac{\beta_{k,11}}{a_k}$, and $\frac{\gamma_{k,11}}{a_k}$ are bounded for $1 \leq k \leq N$. Moreover, since $\frac{k}{2} < \frac{\sqrt{k}}{10}k < \sqrt{\frac{N}{k}}$,

$$0 < \sum_{k=1}^{N} \frac{1}{k} \frac{e^{-2\pi \sqrt{C_k}}}{1 - e^{-2\pi \sqrt{C_k}}} < \sum_{k=1}^{N} \frac{e^{-2\pi \sqrt{C_k}}}{1 - e^{-2\pi \sqrt{C_k}}} < \sum_{k=1}^{\infty} \frac{e^{-\pi k}}{1 - e^{-\pi k}} < \infty.$$ 

Therefore (4.49) implies

$$R_{n,5} = \sum_{k=1}^{N} \frac{1}{k} \alpha_{k,11} \frac{e^{-2\pi \sqrt{C_k}}}{1 - e^{-2\pi \sqrt{C_k}}} + O\left(\frac{1}{NN_0}\right) + O\left(\frac{1}{NN_0^2}\right) + O\left(\frac{1}{N^3}\right)$$

which, in turn, gives

(4.50) 

$$R_{n,5} = \sum_{k=1}^{N} \frac{1}{k} \alpha_{k,11} \frac{e^{-2\pi \sqrt{C_k}}}{1 - e^{-2\pi \sqrt{C_k}}} + O\left(\frac{1}{N^2}\right).$$

Since $\frac{k}{2} < \sqrt{\frac{N}{k}}$, we have

(4.51) 

$$0 < \sum_{k=1}^{\log N} \frac{1}{k} \frac{e^{-2\pi \sqrt{C_k}}}{1 - e^{-2\pi \sqrt{C_k}}} < \sum_{k=1}^{\log N} \frac{1}{k} \frac{e^{-\pi k}}{1 - e^{-\pi k}} < \sum_{k=1}^{\log N} \frac{e^{-\pi k}}{1 - e^{-\pi k}} \leq \frac{e^{-\pi \log N}}{(1 - e^{-\pi})^2} = \frac{N^{-\pi}}{(1 - e^{-\pi})^2}.$$

Accordingly, since $\alpha_{k,11}$ is bounded, using (4.51) in (4.50), we obtain

(4.52) 

$$R_{n,5} = \sum_{1 \leq k \leq \log N} \frac{1}{k} \alpha_{k,11} \frac{e^{-2\pi \sqrt{C_k}}}{1 - e^{-2\pi \sqrt{C_k}}} + O\left(\frac{1}{N^2}\right).$$

Note further that

$$\sum_{1 \leq k \leq \log N} \frac{1}{k} \alpha_{k,11} \frac{e^{-2\pi \sqrt{C_k}}}{1 - e^{-2\pi \sqrt{C_k}}} = \sum_{1 \leq k \leq \log N} \frac{1}{k} \alpha_{k,11} e^{-2\pi \sqrt{C_k}(p+1)}$$

$$= \sum_{1 \leq k \leq \log N} \frac{1}{k} \alpha_{k,11} e^{-2\pi \sqrt{C_k}(p+1)}.$$
and, using $\frac{k^2}{2} < \sqrt{C_k}$,

$$0 < \sum_{1 \leq k \leq \log N, \; p > \log N} \frac{1}{k} e^{-2\pi \sqrt{C_k}(p+1)} < \sum_{1 \leq k \leq \log N} e^{-\pi k(p+1)} \leq \sum_{1 \leq k \leq \log N} \frac{e^{-\pi k(1+\log N)}}{1 - e^{-\pi k}}$$

$$< \sum_{k=1}^{\infty} \frac{e^{-\pi k(1+\log N)}}{1 - e^{-\pi}} = \frac{1}{1 - e^{-\pi}} \left( e^{(eN)(1+\log N)} - 1 \right) \leq \frac{e^{-\pi}}{(1 - e^{-\pi})^2} N^{-\pi}.$$ 

Therefore, since $\alpha_{k,11}$ is bounded, (4.52) gives (4.48). This completes the proof. □

To further simply the relation given in Lemma 4.4, we estimate $\alpha_{k,11}$ and the term in the exponent in (4.48), and prove the following.

**Lemma 4.5.** As $n \to \infty$, we have

(4.53) \[ R_{n,5} = \sum_{1 \leq k \leq \log N} \frac{1}{k} e^{-2\pi k(p+1)} + O\left(\frac{1}{N^2}\right). \]

**Proof.** From (4.42) and (4.43), we have for $1 \leq k \leq \log N$

(4.54) \[ \alpha_{k,11} = 1 - \frac{\pi^2}{48 N^2} + O\left(\frac{\log^4 N}{N^4}\right). \]

On the other hand, from (4.30), we have

(4.55) \[ -2\pi \sqrt{C_k} = -2\pi \frac{\sqrt{2} \sqrt{1 - a_k^2}}{\sqrt{1 + A_k}} k \left\{ 1 + \beta_{k,6} \frac{1}{N_0} + \gamma_{k,6} \frac{1}{N_0^2} + O\left(\frac{1}{N_0^3}\right) \right\}. \]

Replacing $\frac{k}{N}$ by $x$ in $\frac{\sqrt{2} \sqrt{1 - a_k^2}}{\sqrt{1 + A_k}}$, we obtain the function

$$\mu(x) = \frac{\sqrt{2} \sqrt{1 - \frac{\pi^2}{48} x^2}}{\sqrt{1 + \sqrt{1 + \frac{\pi^2}{12} x^2(1 - \frac{\pi^2}{48} x^2)}}}$$

for which Taylor’s theorem with remainder delivers

$$\mu(x) = 1 - \frac{\pi^2}{48} x^2 + O(x^4), \quad \text{for } x \in \left[ -\frac{4\sqrt{3}}{\pi}, \frac{4\sqrt{3}}{\pi} \right].$$

Therefore, for $1 \leq k \leq \log N$, we have

$$-2\pi \frac{\sqrt{2} \sqrt{1 - a_k^2}}{\sqrt{1 + A_k}} = \left\{ -2\pi + \frac{\pi^3}{24} \frac{k^2}{N^2} + O\left(\frac{\log^4 N}{N^4}\right) \right\}.$$
Using this in (4.55) and recalling (4.22), we obtain for $1 \leq k \leq \log N$

\begin{equation}
2 \pi \sqrt{C_k}(p+1) = \left\{ 2 \pi - \frac{\pi^3 k^2}{24 N^2} + \mathcal{O}\left(\frac{\log^4 N}{N^4}\right) \right\} \times \left\{ 1 + \frac{\pi^2 \beta_{k,6}}{48 a_k^2 N^2 N_0} + \frac{\pi^2 \gamma_{k,6}}{48 a_k^2 N^2 N_0^2} + \mathcal{O}\left(\frac{1}{N^3}\right) \right\} k(p+1).
\end{equation}

Note that

\begin{align*}
\frac{\beta_{k,6}}{a_k^2} &= \frac{2(1-2a_k^2)}{\mathcal{A}_k(1+\mathcal{A}_k)} + \frac{1}{1-a_k^2}, \\
\frac{\gamma_{k,6}}{a_k^2} &= \frac{1}{\mathcal{A}_k^2(1+\mathcal{A}_k)} \left( \frac{6a_k^2(2a_k^2-1)^2}{1+\mathcal{A}_k} - \frac{(2a_k^2 - 3)(12a_k^4 - 1)}{\mathcal{A}_k} \right) + \frac{2a_k^2 - 1 - 2a_k^2}{\mathcal{A}_k(1+\mathcal{A}_k)} + \frac{2a_k^2 - 3}{2(1-a_k^2)^2}
\end{align*}

are bounded for $1 \leq k \leq N$. Therefore, for $1 \leq k \leq \log N$ and $0 \leq p \leq \log N$, we have

\begin{equation}
\beta_{k,6} k^j (p+1) = \frac{\pi^2 \beta_{k,6}}{48 a_k^2 N^2 N_0} k^{j+2} (p+1) = \mathcal{O}\left(\frac{\log^j N}{N^2}\right), \quad j \in \mathbb{N},
\end{equation}

and this also holds when $\beta_{k,6}$ is replaced with $\gamma_{k,6}$. Note also that

\begin{equation}
\exp\left(\frac{\log^j N}{N^\alpha N_0^\beta}\right) = 1 + \mathcal{O}\left(\frac{\log^j N}{N^\alpha + \beta}\right), \quad \text{for } j, \alpha, \beta \geq 0, \ \alpha + \beta > 0,
\end{equation}

where we have used $e^x = 1 + x + \mathcal{O}(x^2) = 1 + \mathcal{O}(x)$ for $x = o(1)$. Therefore, in light of (4.56), use of (4.57) and (4.58) implies for $1 \leq k \leq \log N$ and $0 \leq p \leq \log N$ that

\begin{equation}
e^{-2\pi \sqrt{C_k}(p+1)} = e^{-2\pi k(p+1)} e^{\frac{\pi^3 k^3}{24 N^2} (p+1)} \left( 1 + \mathcal{O}\left(\frac{\log^4 N}{N^3}\right) \right) = e^{-2\pi k(p+1)} \left( 1 + \frac{\pi^3 k^3}{24 N^2} (p+1) + \mathcal{O}\left(\frac{\log^8 N}{N^4}\right) \right) \left( 1 + \mathcal{O}\left(\frac{\log^4 N}{N^3}\right) \right) = e^{-2\pi k(p+1)} \left\{ 1 + \frac{\pi^3 k^3}{24 N^2} (p+1) + \mathcal{O}\left(\frac{\log^4 N}{N^3}\right) \right\}.
\end{equation}
Finally, using (4.54) and (4.59), we obtain for $1 \leq k \leq \log N$ and $0 \leq p \leq \log N$ that

\[
(4.60) \quad \frac{1}{k} \alpha_{k,11} e^{-2\pi \sqrt{k}(p+1)} = \frac{1}{k} e^{-2\pi k(p+1)} \left\{ 1 - \frac{\pi^2 k^2}{48 N^2} + \frac{\pi^3 k^3}{24 N^2} (p + 1) + \mathcal{O}\left(\frac{\log^4 N}{N^3}\right) \right\}.
\]

Moreover, since the double series

\[
\sum_{k \geq 1, \ p \geq 0} e^{-2\pi k(p+1)} k^\alpha (1 + p)^\beta
\]

converges for any $\alpha, \beta \in \mathbb{R}$, use of (4.60) entails

\[
\sum_{1 \leq k \leq \log N \atop 0 \leq p \leq \log N} \frac{1}{k} \alpha_{k,11} e^{-2\pi \sqrt{k}(p+1)} = \sum_{1 \leq k \leq \log N \atop 0 \leq p \leq \log N} \frac{1}{k} e^{-2\pi k(p+1)} + \mathcal{O}\left(\frac{1}{N^2}\right),
\]

and therefore (4.48) yields (4.53). This completes the proof. □

Finally, we establish the following relation.

**Lemma 4.6.** As $n \to \infty$, there holds

\[
(4.61) \quad R_{n,5} = \sum_{k=1}^{\infty} \frac{1}{k} \frac{e^{-2\pi k}}{1 - e^{-2\pi k}} + \mathcal{O}\left(\frac{1}{n^2}\right).
\]

**Proof.** Since

\[
\sum_{1 \leq k \leq \log N \atop 0 \leq p \leq \log N} \frac{1}{k} e^{-2\pi k} - \sum_{1 \leq k \leq \log N \atop p > \log N} \frac{1}{k} e^{-2\pi k(p+1)} = \sum_{1 \leq k \leq \log N \atop p > \log N} \frac{1}{k} e^{-2\pi k(p+1)}
\]

and

\[
0 < \sum_{1 \leq k \leq \log N \atop p > \log N} \frac{1}{k} e^{-2\pi k(p+1)} < \sum_{1 \leq k \leq \log N \atop p > \log N} e^{-2\pi k(p+1)}
\]

\[
\leq \sum_{1 \leq k \leq \log N} \frac{e^{-2\pi k(1+\log N)}}{1 - e^{-2\pi k}} < \sum_{k=1}^{\infty} \frac{e^{-2\pi k(1+\log N)}}{1 - e^{-2\pi}} \leq \frac{e^{-2\pi}}{(1 - e^{-2\pi})^2} N^{-2\pi},
\]

(4.53) implies

\[
(4.62) \quad R_{n,5} = \sum_{1 \leq k \leq \log N} \frac{1}{k} \frac{e^{-2\pi k}}{1 - e^{-2\pi k}} + \mathcal{O}\left(\frac{1}{N^2}\right).
\]

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Further, since
\[
0 < \sum_{k > \log N} \frac{1}{k} \frac{e^{-2\pi k}}{1 - e^{-2\pi k}} < \sum_{k > \log N} \frac{e^{-2\pi k}}{1 - e^{-2\pi}} \leq \frac{N^{-2\pi}}{(1 - e^{-2\pi})^2}
\]
(4.62) entails
\[
R_{n,5} = \sum_{k=1}^{\infty} \frac{1}{k} \frac{e^{-2\pi k}}{1 - e^{-2\pi k}} + \mathcal{O}\left(\frac{1}{N^2}\right).
\]
Therefore (4.61) follows from (4.63) with the aid of (4.38).

As for the proof of (4.10), we note for \( q = e^{-2\pi} \)
\[
\sum_{k=1}^{\infty} \frac{1}{k} \frac{e^{-2\pi k}}{1 - e^{-2\pi k}} = \sum_{k=1}^{\infty} \sum_{m=0}^{\infty} \frac{1}{k} (q^{m+1})^k = -\sum_{m=0}^{\infty} \sum_{k=1}^{\infty} \frac{-1}{k} (q^{m+1})^k
\]
\[
= -\sum_{m=0}^{\infty} \log(1 - q^{m+1}) = -\log\left(\prod_{m=0}^{\infty} (1 - q^{m+1})\right)
\]
\[
= -\log((q; q)_{\infty}) = -\log(q^{-\frac{\pi}{2}} \eta(i)),
\]
where \((q; q)_{\infty}\) is the \(q\)-Pochhammer symbol and \(\eta\) is the Dedekind eta-function [15]. Since \(\eta(i) = \frac{\Gamma(\frac{1}{2})}{2\pi^{\frac{1}{2}}}\), use of (4.64) in (4.61) proves (4.10).

### 4.7. Asymptotic behavior of \( Q_n \)

Here we study \( Q_n \) in (4.6) and establish (4.11). To this end, we use partial fractions to write
\[
Q_n = \frac{\pi}{2\sqrt{3n}} \sum_{k=1}^{N} \left( \frac{1}{k + \frac{\sqrt{3n}}{\pi}} - \frac{1}{k - \frac{\sqrt{3n}}{\pi}} \right) + \sum_{k=1}^{N} \frac{1}{k^2} = \frac{\pi}{2\sqrt{3n}} Q_{n,1} + \sum_{k=1}^{N} \frac{1}{k^2},
\]
say. For \( Q_{n,1} \), we utilize (4.14) to obtain
\[
Q_{n,1} = \psi\left(N + 1 + \frac{\sqrt{3n}}{\pi}\right) - \psi\left(1 + \frac{\sqrt{3n}}{\pi}\right) - \psi\left(N + 1 - \frac{\sqrt{3n}}{\pi}\right) + \psi\left(1 - \frac{\sqrt{3n}}{\pi}\right).
\]
Next we employ (4.15) to write
\[
\psi\left(N + 1 + \frac{\sqrt{3n}}{\pi}\right) = \psi\left(\frac{\sqrt{3n}}{\pi} + N\right) + \frac{1}{\sqrt{3n} + N},
\]
\[
\psi\left(N + 1 - \frac{\sqrt{3n}}{\pi}\right) = \psi\left(\frac{\sqrt{3n}}{\pi} - N\right) + \pi \cot \pi\left(\frac{\sqrt{3n}}{\pi} - N\right),
\]

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\[
\psi\left(1 + \frac{\sqrt{3}n}{\pi}\right) - \psi\left(1 - \frac{\sqrt{3}n}{\pi}\right) = \frac{1}{\sqrt{3n}} - \pi \cot \frac{\sqrt{3n}}{\pi},
\]

and use the \(\pi\)-periodicity of the cotangent function to have

\[
Q_{n,1} = \psi\left(\frac{\sqrt{3}n}{\pi} + N\right) - \psi\left(\frac{\sqrt{3}n}{\pi} - N\right) + O\left(\frac{1}{n}\right).
\]

Then we apply (4.19) (in the form \(\psi(z) = \log z + O\left(\frac{1}{z}\right)\)) to deduce

\[
Q_{n,1} = \log\left(\frac{\sqrt{3n}}{\pi} + N\right) + O\left(\frac{1}{n}\right).
\]

Since

\[
\frac{\sqrt{3n}}{\pi} + N = \frac{\sqrt{3n}}{\pi} + \frac{n-n_0}{4} = 4\sqrt{3} + \pi \left(1 - \frac{\pi n_0}{4\sqrt{3} + \pi}\right) - \frac{1}{4},
\]

\[
\frac{\sqrt{3n}}{\pi} - N = \frac{\sqrt{3n}}{\pi} - \frac{n-n_0}{4} = 4\sqrt{3} - \pi \left(1 + \frac{\pi n_0}{4\sqrt{3} - \pi}\right),
\]

(4.66) entails

\[
Q_{n,1} = \log\left(\frac{4\sqrt{3} + \pi}{4\sqrt{3} - \pi}\right) + O\left(\frac{1}{n}\right).
\]

Finally, from [1, formulas 6.4.3, 6.4.12], we have

\[
\sum_{k=1}^{N} \frac{1}{k^2} = \frac{\pi^2}{6} - \frac{1}{N} + O\left(\frac{1}{N^2}\right) = \frac{\pi^2}{6} - \frac{4}{n} + O\left(\frac{1}{n^2}\right).
\]

Accordingly, use of (4.67) and (4.68) in (4.65) proves (4.11).

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