J. Math. Anal. Appl. 463 (2018) 134–160

Contents lists available at ScienceDirect

Journal of Mathematical Analysis and Applications

www.elsevier.com/locate/jmaa

A lattice sum involving the cosine function

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ARTICLE INFO

Article history:
Received 19 May 2017
Available online 13 March 2018
Submitted by B.C. Berndt

Keywords:
Lattice sum
Elementary classical functions
Asymptotic approximation

ABSTRACT

In this article we prove that, as $n \to \infty$,

$$\sum_{j,k=1}^{n-1} \frac{1}{3 - \cos\frac{2\pi j}{n} - \cos\frac{2\pi k}{n} - \cos\frac{2\pi(j+k)}{n}} \sim \frac{n^2 \log n}{\sqrt{3}\pi}.$$

We also obtain the secondary term of size $\asymp n^2$ to be followed by an error term of size $O(\log n)$. In this work, results and techniques from classical analysis involving roles by several special functions, from number theory, and from numerical analysis are needed.

1. Introduction

The sum

$$S_n := \sum_{j,k=1}^{n-1} \frac{1}{3 - \cos\frac{2\pi j}{n} - \cos\frac{2\pi k}{n} - \cos\frac{2\pi(j+k)}{n}} \quad (n \geq 2) \tag{1.1}$$

$$= \frac{1}{2} \sum_{j,k=1}^{n-1} \frac{1}{\sin^2\frac{\pi j}{n} + \sin^2\frac{\pi k}{n} + \sin^2\frac{\pi(j+k)}{n}} \tag{1.2}$$

and other sums and integrals of similar types have been significant in studies of lattice Green's functions which arise in many problems in condensed matter physics, random walks on lattices and the calculation of the resistance of resistor networks (see e.g. [7] and [16]), and in studies of metrized graphs [6]. Since even the order of magnitude of S_n as $n \to \infty$ wasn't known, in this paper we study this sum.

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https://doi.org/10.1016/j.jmaa.2018.03.014

It is not difficult to obtain the non-trivial lower bound

$$S_n > \frac{n^2 \log n}{4\pi^2} + O(n^2) \tag{1.3}$$

by using

$$\sin^2 \theta \le \theta^2, \quad \forall \theta \in \mathbb{R} \tag{1.4}$$

in (1.2). To get an upper bound one can employ a result due to Montgomery [11]:

$$(\sin \pi\theta)^{-2} \le (\pi||\theta||)^{-2} + c, \; ||\theta|| := \min(\theta - \lfloor \theta \rfloor, \lceil \theta \rceil - \theta), \;\; c := 1 - \frac{4}{\pi^2}, \quad \forall \theta \in \mathbb{R}. \tag{1.5}$$

Upon plugging (1.5) in (1.2), in all of its occurrences the constant c may be neglected if we are just trying to determine the order of magnitude of S_n. This leads to

$$S_n \ll n^2 \log n, \tag{1.6}$$

which in conjunction with (1.3) gives the order of magnitude of S_n:

$$S_n \asymp n^2 \log n. \tag{1.7}$$

Our main result is

Theorem. *As $n \to \infty$,*

$$\sum_{j,k=1}^{n-1} \frac{1}{3 - \cos\frac{2\pi j}{n} - \cos\frac{2\pi k}{n} - \cos\frac{2\pi(j+k)}{n}} = \frac{n^2 \log n}{\sqrt{3}\pi} + \frac{n^2}{\sqrt{3}\pi}\Big(\gamma - \frac{\sqrt{3}\pi}{6} + \log(4\pi\sqrt[4]{3}) - 3\log\Gamma\big(\frac{1}{3}\big)\Big) + O\big(\log n\big), \tag{1.8}$$

where γ is Euler's constant.

The following two sections contain two proofs for the asymptotic value of S_n. The rest of the paper is for obtaining the secondary term and the error term. We achieve this by first relating S_n to an integral by the methods of numerical analysis (which is the main cause of the error term $O(\log n)$ in (1.8)), and then carrying out the evaluations of the terms which appear in the relation. It is desirable to obtain a more precise version of (1.8). In fact, since the summands are algebraic numbers in the cyclotomic field obtained by adjoining a primitive n-th root of unity to $\mathbb{Q}$, due to the symmetry involved in the sum the precise value of S_n must be a rational number ($S_2 = \frac{1}{4}$, $S_3 = \frac{10}{9}$, $S_4 = \frac{44}{16}$, $S_5 = \frac{58}{11}$, $S_6 = \frac{1577}{180}, \ldots$) We wonder whether a method for determining this rational number for any given n can be developed.

2. Proof of the asymptotic value

We first observe that by applying changes of variables the summation variables in (1.2) may be brought into the domain $0 < |j|, |k| \le \frac{n}{2}$ without changing the summands. (For example, for the portion $0 < j \le \frac{n}{2}$, $\frac{n}{2} < k < n$, $\frac{n}{2} < j + k \le n$ we take $k - n$ as our new k and leave j unchanged.) This will allow us to use Taylor expansion around the origin. First we deal with those j, k pairs which are not close to the origin. If $j^2 + k^2 \ge \frac{n^2}{72}$, say, then $\max(\frac{|j|}{n}, \frac{|k|}{n}) \ge \frac{1}{12}$. Hence each such summand will satisfy

$$\frac{1}{\sin^2\frac{\pi j}{n}+\sin^2\frac{\pi k}{n}+\sin^2\frac{\pi(j+k)}{n}} \le \frac{1}{\sin^2\frac{\pi}{12}} = \frac{4}{2-\sqrt{3}}. \tag{2.1}$$

The number of such summands is $< n^2$, so that the contribution of those j, k pairs which are far from the origin is

$$\sum_{\substack{-\frac{n}{2}\le j,k\le \frac{n}{2} \\ j^2+k^2\ge \frac{n^2}{72}}} \frac{1}{\sin^2\frac{\pi j}{n}+\sin^2\frac{\pi k}{n}+\sin^2\frac{\pi(j+k)}{n}} = O(n^2). \tag{2.2}$$

For the j, k pairs satisfying $0 < |j|+|k| \le \frac{n}{6}$ (which are all in the disk $j^2+k^2 \le \frac{n^2}{36}$) we have by Taylor's theorem for functions of two variables ([3], p. 152)

$$\sin^2\pi x+\sin^2\pi y+\sin^2\pi(x+y) = 2\pi^2(x^2+xy+y^2)+R_3(x,y), \tag{2.3}$$

with

$$\begin{aligned} R_3(x,y) = -8\pi^4\Big\{&\frac{x^4}{4!}\big[\cos 2\pi x+\cos 2\pi(x+y)\big]_{p^*}+\frac{x^3y}{3!}\big[\cos 2\pi(x+y)\big]_{p^*} \\ +&\frac{x^2y^2}{2!2!}\big[\cos 2\pi(x+y)\big]_{p^*}+\frac{xy^3}{3!}\big[\cos 2\pi(x+y)\big]_{p^*}+\frac{y^4}{4!}\big[\cos 2\pi y+\cos 2\pi(x+y)\big]_{p^*}\Big\} \end{aligned} \tag{2.4}$$

where p^* is a point on the line segment joining $(0,0)$ and (x,y). We see that

$$R_3(\frac{j}{n},\frac{k}{n}) = \delta_{j,k}\cdot\frac{2\pi^4}{3n^4}(j^2+|jk|+k^2)^2 \quad \text{for some } \delta_{j,k}\in[-1,1]. \tag{2.5}$$

Now, by formulas (2.2)–(2.5), we have

$$\begin{aligned} S_n &= \frac{1}{2}\sum_{\substack{j,k \\ 0<|j|+|k|\le\frac{n}{6}}} \frac{1}{\sin^2\frac{\pi j}{n}+\sin^2\frac{\pi k}{n}+\sin^2\frac{\pi(j+k)}{n}} + O(n^2) \\ &= \frac{1}{2}\sum_{\substack{j,k \\ 0<|j|+|k|\le\frac{n}{6}}} \frac{1}{\frac{2\pi^2}{n^2}(j^2+jk+k^2)+R_3(\frac{j}{n},\frac{k}{n})} + O(n^2) \\ &= \frac{n^2}{4\pi^2}\sum_{\substack{j,k \\ 0<|j|+|k|\le\frac{n}{6}}} \frac{1}{(j^2+jk+k^2)}\cdot\frac{1}{1+\delta_{j,k}\frac{\pi^2}{3}\frac{(j^2+|jk|+k^2)^2}{n^2(j^2+jk+k^2)}} + O(n^2). \end{aligned} \tag{2.6}$$

Now we notice that

$$1 \le \frac{(j^2+|jk|+k^2)}{(j^2+jk+k^2)} \le 3, \tag{2.7}$$

and

$$\frac{j^2+|jk|+k^2}{n^2} \le \frac{(|j|+|k|)^2}{n^2} \le \frac{1}{36} \quad \text{for } |j|+|k|\le\frac{n}{6},$$

so that

$$\frac{\pi^2}{3}\frac{(j^2+|jk|+k^2)^2}{n^2(j^2+jk+k^2)} \le \frac{\pi^2}{36} < 1,$$

and the expansion

$$\frac{1}{1+\delta_{j,k}\cdot\frac{\pi^2}{3}\frac{(j^2+|jk|+k^2)^2}{n^2(j^2+jk+k^2)}} = 1+\sum_{m=1}^{\infty}\left(\delta_{j,k}\frac{\pi^2}{3}\frac{(j^2+|jk|+k^2)^2}{n^2(j^2+jk+k^2)}\right)^m$$

is valid and we plug it in (2.6). Then we have

$$\begin{aligned} S_n &= \frac{n^2}{4\pi^2}\sum_{\substack{j,k\\ 0<|j|+|k|\le\frac{n}{6}}}\frac{1}{j^2+jk+k^2} \\ &+ \frac{n^2}{4\pi^2}\sum_{\substack{j,k\\ 0<|j|+|k|\le\frac{n}{6}}}\frac{1}{j^2+jk+k^2}\sum_{m=1}^{\infty}\left(\delta_{j,k}\frac{\pi^2}{3}\frac{(j^2+|jk|+k^2)^2}{n^2(j^2+jk+k^2)}\right)^m + O(n^2). \end{aligned} \tag{2.8}$$

Now by (2.7) we see that

$$\begin{aligned} \sum_{m=1}^{\infty}\left(\delta_{j,k}\frac{\pi^2}{3}\frac{(j^2+|jk|+k^2)^2}{n^2(j^2+jk+k^2)}\right)^m &\le \sum_{m=1}^{\infty}\left(3\pi^2\frac{j^2+jk+k^2}{n^2}\right)^m \\ &= \frac{3\pi^2}{n^2}(j^2+jk+k^2)\sum_{m=0}^{\infty}\left(3\pi^2\frac{j^2+jk+k^2}{n^2}\right)^m. \end{aligned}$$

Hence the second term on the right hand side of (2.8) is majorized by

$$\begin{aligned} &\frac{3}{4}\sum_{\substack{j,k\\ 0<|j|+|k|\le\frac{n}{6}}}\sum_{m=0}^{\infty}\left(3\pi^2\cdot\frac{j^2+jk+k^2}{n^2}\right)^m \\ &< \frac{3}{4}\sum_{\substack{j,k\\ 0<|j|+|k|\le\frac{n}{6}}}\sum_{m=0}^{\infty}\left(\frac{\pi^2}{12}\right)^m = \frac{9}{12-\pi^2}\sum_{\substack{j,k\\ 0<|j|+|k|\le\frac{n}{6}}}1 = O(n^2). \end{aligned}$$

Thus (2.8) simplifies into

$$\begin{aligned} S_n &= \frac{n^2}{4\pi^2}\sum_{\substack{j,k\\ 0<|j|+|k|\le\frac{n}{6}}}\frac{1}{j^2+jk+k^2} + O(n^2) \\ &= \frac{n^2}{2\pi^2}\Big(\sum_{\substack{0\le j,k\le\frac{n}{6}\\ 0<j+k\le\frac{n}{6}}}\frac{1}{j^2+jk+k^2} + \sum_{\substack{0\le j,k\le\frac{n}{6}\\ 0<j+k\le\frac{n}{6}}}\frac{1}{j^2-jk+k^2}\Big) + O(n^2) \\ &= \frac{n^2}{2\pi^2}\Big(\sum_{1\le j,k\le\frac{n}{6}}\frac{1}{j^2+jk+k^2} + \sum_{1\le j,k\le\frac{n}{6}}\frac{1}{j^2-jk+k^2}\Big) + O(n^2). \end{aligned} \tag{2.9}$$

Observing that

$$\begin{aligned} \sum_{1\le j,k\le\frac{n}{6}}\frac{1}{j^2\pm jk+k^2} &= \sum_{k=1}^{\frac{n}{6}}\Big(\sum_{j=1}^{\infty}\frac{1}{j^2\pm jk+k^2} - \sum_{j>\frac{n}{6}}\frac{1}{j^2\pm jk+k^2}\Big) \\ &= \sum_{k=1}^{\frac{n}{6}}\Big(\sum_{j=1}^{\infty}\frac{1}{j^2\pm jk+k^2} - O(\frac{1}{n})\Big), \end{aligned} \tag{2.10}$$

we can cast (2.9) into

$$S_n = \frac{n^2}{2\pi^2}\sum_{k=1}^{\frac{n}{6}}\sum_{j=1}^{\infty}\Big(\frac{1}{j^2+jk+k^2}+\frac{1}{j^2-jk+k^2}\Big)+O(n^2). \tag{2.11}$$

Expanding into partial fractions we have

$$S_n = \frac{n^2}{2\pi^2}\sum_{k=1}^{\frac{n}{6}}\sum_{j=1}^{\infty}\frac{i}{\sqrt{3}j}\Big(\frac{1}{j+ke^{\frac{\pi}{3}i}}-\frac{1}{j+ke^{-\frac{\pi}{3}i}}+\frac{1}{j-ke^{-\frac{\pi}{3}i}}-\frac{1}{j-ke^{\frac{\pi}{3}i}}\Big)+O(n^2). \tag{2.12}$$

The sum over j is evaluated in terms of the digamma function (see §6.8 of [1]) and we have

$$\begin{aligned} S_n &= \frac{n^2}{2\sqrt{3}\pi^2}\sum_{k=1}^{\frac{n}{6}}\frac{i}{k}\big(-\psi(1+ke^{\frac{\pi}{3}i})+\psi(1+ke^{-\frac{\pi}{3}i})-\psi(1-ke^{-\frac{\pi}{3}i})+\psi(1-ke^{\frac{\pi}{3}i})\big)+O(n^2)\\ &= \frac{n^2}{2\sqrt{3}\pi^2}\sum_{k=1}^{\frac{n}{6}}\frac{i}{k}\big(-2i\Im\psi(1+ke^{\frac{\pi}{3}i})+2i\Im\psi(1-ke^{\frac{\pi}{3}i})\big)+O(n^2)\\ &= \frac{n^2}{\sqrt{3}\pi^2}\sum_{k=1}^{\frac{n}{6}}\frac{1}{k}\Im\big[\psi(1+ke^{\frac{\pi}{3}i})-\psi(1-ke^{\frac{\pi}{3}i})\big]+O(n^2), \end{aligned} \tag{2.13}$$

since $\psi(\overline{z})=\overline{\psi(z)}$ (for this and other formulas involving the digamma function see §6.3 of [1]). In the last summand there is a quantity of the form $\psi(z)-\psi(2-z)$. The recurrence formula $\psi(z+1)=\psi(z)+\frac{1}{z}$, turns this into $\psi(z)-\psi(1-z)-\frac{1}{1-z}$. Then by the reflection formula $\psi(1-z)=\psi(z)+\pi\cot\pi z$ this quantity is expressed as $-\pi\cot\pi z-\frac{1}{1-z}$. Hence (2.13) becomes

$$\begin{aligned} S_n &= \frac{n^2}{\sqrt{3}\pi^2}\sum_{k=1}^{\frac{n}{6}}\frac{1}{k}\Im\Big[-\pi\cot(\pi(1+ke^{\frac{\pi}{3}i}))+\frac{1}{ke^{\frac{\pi}{3}i}}\Big]+O(n^2)\\ &= -\frac{n^2}{\sqrt{3}\pi}\sum_{k=1}^{\frac{n}{6}}\frac{1}{k}\Im\cot(\pi(1+ke^{\frac{\pi}{3}i}))+O(n^2). \end{aligned} \tag{2.14}$$

Now

$$\cot(\pi(1+ke^{\frac{\pi}{3}i})) = \begin{cases} \cot\left(\frac{\sqrt{3}\pi k}{2}i\right) = -i\coth\left(\frac{\sqrt{3}\pi k}{2}\right) & \text{if } k \text{ is even},\\ -\tan\left(\frac{\sqrt{3}\pi k}{2}i\right) = -i\tanh\left(\frac{\sqrt{3}\pi k}{2}\right) & \text{if } k \text{ is odd}, \end{cases}$$

so that

$$\begin{aligned} S_n &= \frac{n^2}{\sqrt{3}\pi}\Big(\sum_{\substack{1\le k\le \frac{n}{6}\\ k:\text{ odd}}}\frac{1}{k}\tanh\Big(\frac{\sqrt{3}\pi k}{2}\Big)+\sum_{\substack{1\le k\le \frac{n}{6}\\ k:\text{ even}}}\frac{1}{k}\coth\Big(\frac{\sqrt{3}\pi k}{2}\Big)\Big)+O(n^2)\\ &= \frac{n^2}{\sqrt{3}\pi}\Big(\sum_{\substack{1\le k\le \frac{n}{6}\\ k:\text{ odd}}}\frac{1}{k}\cdot\frac{1-e^{-\sqrt{3}\pi k}}{1+e^{-\sqrt{3}\pi k}}+\sum_{\substack{1\le k\le \frac{n}{6}\\ k:\text{ even}}}\frac{1}{k}\cdot\frac{1+e^{-\sqrt{3}\pi k}}{1-e^{-\sqrt{3}\pi k}}\Big)+O(n^2)\\ &= \frac{n^2}{\sqrt{3}\pi}\sum_{k=1}^{\frac{n}{6}}\frac{1}{k}\cdot\big(1+O(e^{-\sqrt{3}\pi k})\big)+O(n^2) \end{aligned}$$

$$
\begin{aligned}
&= \frac{n^2}{\sqrt{3}\pi}\Big(\sum_{k=1}^{\frac{n}{6}} \frac{1}{k} + O\Big(\sum_{k=1}^{\frac{n}{6}} \frac{e^{-\sqrt{3}\pi k}}{k}\Big)\Big) + O(n^2) \\
&= \frac{n^2}{\sqrt{3}\pi}\Big([\log\frac{n}{6} + \gamma + O(\frac{1}{n})] + O\Big(\sum_{k=1}^{\frac{n}{6}} e^{-\sqrt{3}\pi k}\Big)\Big) + O(n^2) \\
&\sim \frac{n^2 \log n}{\sqrt{3}\pi}.
\end{aligned}
\tag{2.15}
$$

We remark that the calculation of the infinite series in (2.11) can also be done by using the residue theorem. For fixed non-zero integer k, let

$$
f_k(z) := \frac{1}{(z + ke^{\frac{\pi}{3}i})(z - ke^{\frac{2\pi}{3}i})} \frac{1}{1 - e^{2\pi z i}}.
$$

Then $f_k(z)$ has simple poles at $-ke^{\frac{\pi}{3}i}$, $ke^{\frac{2\pi}{3}i}$, and at all integers, and it has no pole at infinity. Then, by residue theorem on the extended complex plane (see, for example, §5.3 of Chapter III of [4]), the total residue is zero, that is,

$$
\operatorname*{Res}_{z=-ke^{\frac{\pi}{3}i}} f_k(z) + \operatorname*{Res}_{z=ke^{\frac{2\pi}{3}i}} f_k(z) + \sum_{m\in\mathbb{Z}} \operatorname*{Res}_{z=m} f_k(z) = 0.
$$

Evaluating the residues, we have

$$
\frac{1}{k(e^{\frac{\pi}{3}i} + e^{\frac{2\pi}{3}i})}\Big(\frac{1}{1 - e^{2\pi k e^{\frac{2\pi}{3}i} i}} - \frac{1}{1 - e^{-2\pi k e^{\frac{\pi}{3}i} i}}\Big) + \sum_{m\in\mathbb{Z}} \frac{1}{m^2 + mk + k^2} \frac{-1}{2\pi i e^{2\pi m i}} = 0.
$$

Then

$$
\sum_{m\in\mathbb{Z}} \frac{1}{m^2 + mk + k^2} = \frac{2\pi i}{k(e^{\frac{\pi}{3}i} + e^{\frac{2\pi}{3}i})}\Big(\frac{1}{1 - e^{2\pi k e^{\frac{2\pi}{3}i} i}} - \frac{1}{1 - e^{-2\pi k e^{\frac{\pi}{3}i} i}}\Big),
$$

so that

$$
\sum_{m\in\mathbb{Z}\setminus\{0\}} \frac{1}{m^2 + mk + k^2} = \frac{2\pi}{\sqrt{3}k}\Big(\frac{1}{1 - e^{2\pi k e^{\frac{2\pi}{3}i} i}} - \frac{1}{1 - e^{-2\pi k e^{\frac{\pi}{3}i} i}}\Big) - \frac{1}{k^2},
$$

and plugging this in (2.11) we obtain (2.14).

3. A number theoretic approach for the asymptotic value

For basic facts used in this section we refer the reader to [2]. The denominators in (2.9) are norms of certain algebraic integers in $\mathbb{Q}(\sqrt{-3})$. The set $\{1, e^{\frac{\pi}{3}i}\}$ is an integral basis for the ring of integers of $\mathbb{Q}(\sqrt{-3})$ seen as a vector space over $\mathbb{Z}$. We have

$$
j^2 + jk + k^2 = N_{\mathbb{Q}(\sqrt{-3})/\mathbb{Q}}(j + ke^{\frac{\pi}{3}i}).
\tag{3.1}
$$

We will relate the sums in (2.9) to the Dedekind zeta-function of the field

$$
\zeta_{\mathbb{Q}(\sqrt{-3})}(s) := \sum_{\mathfrak{a}} \frac{1}{N(\mathfrak{a})^s}, \quad (\Re s > 1),
\tag{3.2}
$$

where the norm is relative to the field extension $\mathbb{Q}(\sqrt{-3})/\mathbb{Q}$ and $\mathfrak{a}$ runs through all non-zero integral ideals of $\mathbb{Q}(\sqrt{-3})$. This Dedekind zeta-function factors as

$$\zeta_{\mathbb{Q}(\sqrt{-3})}(s) = \zeta(s)L(s,\chi), \tag{3.3}$$

where $\zeta(s)$ is the Riemann zeta-function and

$$L(s,\chi) = \sum_{m=1}^{\infty} \frac{\chi(m)}{m^s} \tag{3.4}$$

is the Dirichlet L-function associated with the character $\chi \pmod 3$ defined on the integers as

$$\chi(m) = \begin{cases} 0 & \text{if } m \equiv 0 \pmod 3 \\ 1 & \text{if } m \equiv 1 \pmod 3 \\ -1 & \text{if } m \equiv 2 \pmod 3. \end{cases} \tag{3.5}$$

Since the field $\mathbb{Q}(\sqrt{-3})$ has class number 1, all of its ideals are principal ideals (and the unique factorization property holds for its ring of integers). Take a principal ideal $\big(j + ke^{\frac{\pi}{3}i}\big)$. Multiplying this ideal by the numbers $(e^{\frac{\pi}{3}i})^\ell$, $\ell = 0, 1, \ldots, 5$, doesn't change the ideal since $e^{\frac{\pi}{3}i}$ is a unit, and therefore doesn't change the norm either. Then for $\ell = 0, 1, \ldots, 5$ for the same value of the norm we obtain the representations j^2+jk+k^2, $(-k)^2+(-k)(j+k)+(j+k)^2$, $(-(j+k))^2+(-(j+k))j+j^2$, $(-j)^2+(-j)(-k)+(-j)^2$, $k^2+k(-(j+k))+(-(j+k))^2$, $(j+k)^2+(j+k)(-j)+(-j)^2$ respectively. So there is a cyclic process in which the ordered pair (j,k) goes to $(k,-(j+k))$, which in turn goes to $(-(j+k),j)$ and this is mapped back to (j,k). Hence each such principal ideal $\big(j + ke^{\frac{\pi}{3}i}\big)$ gives rise to its norm written in three ways as denominators in (2.9). In the particular case of an ideal with $jk = 0$, say the ideal (j) where $j \neq 0$, the set of ordered pairs arising in this process consists of $(j,0)$, $(0,-j)$ and $(-j,j)$. Of these the first two won't lead to representations which appear as denominators in (2.9) since the cases with $jk = 0$ are not included there, so these have to be subtracted. Thus we obtain, for $\Re s > 1$,

$$\begin{aligned}\sum_{j,k=1}^{\infty} \Big(\frac{1}{(j^2+jk+k^2)^s} + \frac{1}{(j^2-jk+k^2)^s}\Big) &= 3\zeta_{\mathbb{Q}(\sqrt{-3})}(s) - 2\zeta(2s) \\ &= 3\zeta(s)L(s,\chi) - 2\zeta(2s). \end{aligned}\tag{3.6}$$

Now note that instead of the sums in the last line of (2.9) we may consider

$$\sum_{m=1}^{\frac{n^2}{12}} \frac{f(m)}{m}, \tag{3.7}$$

where $f(m)$ is the number of ways m can be expressed as $j^2 \pm jk + k^2$, $j,k \geq 1$, within an error of $O(1)$ because passing to (3.7) involves a difference of $O(n^2)$ terms each of which is of size $O\big(\frac{1}{n^2}\big)$. This error is absorbed by the error term $O(n^2)$ in the last line of (2.9). We evaluate (3.7) as

$$3L(1,\chi)\log(\frac{n^2}{12}) + O(1) = 3\frac{\pi}{3^{\frac{3}{2}}}\log(\frac{n^2}{12}) + O(1) = \frac{2\pi}{\sqrt{3}}\log n + O(1), \tag{3.8}$$

using a Tauberian theorem for Dirichlet series from [12]. Thus, returning to (2.9), we find

$$S_n = \frac{n^2\log n}{\sqrt{3}\pi} + O(n^2). \tag{3.9}$$

4. Relating the sum S_n to an integral

With the calculations of the preceding sections we could only determine the asymptotic value of S_n. We wish to calculate the secondary main term of the value of S_n as $n \to \infty$. For this purpose we begin by relating the sum S_n to a certain double integral.

When one encounters a sum such as (1.1), one would perhaps be tempted to express it as a Riemann integral. In particular, for (1.1) with a large n the first impulse might be to think of it as a Riemann sum with the square $(0, 2\pi) \times (0, 2\pi)$ chopped into little squares of side length $\frac{2\pi}{n}$, and express the sum as

$$\left(\frac{n}{2\pi}\right)^2 \int_0^{2\pi}\int_0^{2\pi} \frac{d\theta\, d\phi}{3 - \cos\theta - \cos\phi - \cos(\theta+\phi)}. \tag{4.1}$$

However, this integral is divergent. This is in accordance with what we already know from (1.3), for if the integral in (4.1) were convergent then that would imply $S_n = O(n^2)$. The divergence is caused by the behaviour of the integrand at the corners of the square.

The integral

$$I_n := \left(\frac{n}{2\pi}\right)^2 \int_{\frac{\pi}{n}}^{\frac{\pi(2n-1)}{n}} \int_{\frac{\pi}{n}}^{\frac{\pi(2n-1)}{n}} \frac{d\theta\, d\phi}{3 - \cos\theta - \cos\phi - \cos(\theta+\phi)} \tag{4.2}$$

is appropriate for our purpose. The endpoints in this integral have been determined so as to make the midpoints of the subintervals to be constructed below coincide with the points in the summands of (1.1) (see (4.9) and (4.5)).

In order to establish a relation between S_n and I_n we begin with a lemma.

Lemma. *For a twice continuously differentiable function $h(x, y)$ on the domain $R = [a - \frac{\Delta_x}{2}, a + \frac{\Delta_x}{2}] \times [b - \frac{\Delta_y}{2}, b + \frac{\Delta_y}{2}] \subset \mathbb{R}^2$, we have*

$$\left| \iint_R h(x,y)\, dx\, dy - \Delta_x\, \Delta_y\, h(a,b) \right| \le \frac{\Delta_x^3\, \Delta_y \max_R |h_{xx}| + \Delta_x\, \Delta_y^3 \max_R |h_{yy}|}{24}. \tag{4.3}$$

Proof. We first write

$$\begin{aligned}\iint_R h(x,y)\, dx\, dy - \Delta_x\, \Delta_y\, h(a,b) &= \int_{b-\frac{\Delta_y}{2}}^{b+\frac{\Delta_y}{2}} \Big(\int_{a-\frac{\Delta_x}{2}}^{a+\frac{\Delta_x}{2}} h(x,y)\, dx - \Delta_x h(a,y) \Big) dy \\ &\quad + \Delta_x \Big(\int_{b-\frac{\Delta_y}{2}}^{b+\frac{\Delta_y}{2}} h(a,y) dy - \Delta_y h(a,b) \Big).\end{aligned}$$

To the quantities inside parentheses on the right-hand side we can apply the midpoint rule (see, e.g., (9.5)–(9.6) of [14])

$$\int_a^b H(x) dx = (b-a)\, H\!\left(\frac{a+b}{2}\right) + \frac{(b-a)^3}{24} H''(\xi) \quad \text{for some } \xi \in (a,b) \tag{4.4}$$

valid for a twice continuously differentiable H. Hence we have

$$\iint\limits_R h(x,y)\,dx\,dy - \Delta_x\,\Delta_y\,h(a,b) = \frac{\Delta_x^3}{24}\int\limits_{b-\frac{\Delta_y}{2}}^{b+\frac{\Delta_y}{2}} h_{xx}(a'(y),y)\,dy + \frac{\Delta_x\,\Delta_y^3}{24}h_{yy}(a,b')$$

for some $a'(y) \in [a - \frac{\Delta_x}{2}, a + \frac{\Delta_x}{2}]$ and $b' \in [b - \frac{\Delta_y}{2}, b + \frac{\Delta_y}{2}]$, and (4.3) follows immediately. □

Let $f(x,y) = \dfrac{1}{3 - \cos x - \cos y - \cos(x+y)}$, and $t_j = \frac{2\pi j}{n}$, $(j \in \mathbb{Z})$, so that

$$S_n = \sum_{0<t_j,t_k<2\pi} f(t_j,t_k) = \sum_{\substack{-\pi<t_j,t_k\le\pi \\ t_j\neq 0, t_k\neq 0}} f(t_j,t_k) = \mathcal{F}_{n,1} + \mathcal{F}_{n,2},\ \text{say}, \tag{4.5}$$

with

$$\mathcal{F}_{n,1} := \sum_{0<|t_j|,|t_k|\le\frac{1}{2}} f(t_j,t_k) \qquad \text{and} \qquad \mathcal{F}_{n,2} := S_n - \mathcal{F}_{n,1}. \tag{4.6}$$

As $x^2 + xy + y^2$ is the first non-zero term in the Taylor expansion of the denominator of f about the origin, it is relevant to consider also the sum

$$\mathcal{G}_{n,1} := \sum_{0<|t_j|,|t_k|\le\frac{1}{2}} g(t_j,t_k) \qquad \text{where} \qquad g(x,y) := \frac{1}{x^2+xy+y^2}. \tag{4.7}$$

We define

$$h := f - g \quad \text{and} \quad \mathcal{H}_{n,1} := \mathcal{F}_{n,1} - \mathcal{G}_{n,1} \tag{4.8}$$

and set

$$x_j = \frac{2\pi j}{n} - \frac{\pi}{n}, \quad X_j = [x_j, x_{j+1}], \quad \Delta = x_{j+1} - x_j = \frac{2\pi}{n}, \quad (j \in \mathbb{Z}). \tag{4.9}$$

Note that $t_j = \frac{x_{j+1}+x_j}{2}$. Also set

$$D_{n,1} = \bigcup_{0<|t_j|,|t_k|\le\frac{1}{2}} X_j \times X_k, \quad D_{n,2} = \Big(\bigcup_{\substack{-\pi<t_j,t_k\le\pi \\ t_j\neq 0, t_k\neq 0}} X_j \times X_k\Big)\backslash D_{n,1}. \tag{4.10}$$

We now write

$$\iint\limits_{D_{n,1}} h(x,y)\,dxdy - \Delta^2\mathcal{H}_{n,1} = \sum_{0<|t_j|,|t_k|\le\frac{1}{2}} \Big(\iint\limits_{X_j\times X_k} h(x,y)\,dxdy - \Delta^2 h(t_j,t_k)\Big)$$

and appeal to the Lemma to deduce that

$$\Big|\iint\limits_{D_{n,1}} h(x,y)\,dxdy - \Delta^2\mathcal{H}_{n,1}\Big| \le \frac{\Delta^4}{24}\sum_{0<|t_j|,|t_k|\le\frac{1}{2}} (M_{j,k}^1 + M_{j,k}^2) \tag{4.11}$$

where $M^1_{j,k} := \max\limits_{X_j \times X_k} |h_{xx}|$, $M^2_{j,k} := \max\limits_{X_j \times X_k} |h_{yy}|$. In order to estimate $h_{xx} = f_{xx} - g_{xx}$, we calculate

$$f_{xx} = \frac{f^N}{f^D}, \quad g_{xx} = \frac{g^N}{g^D}, \tag{4.12}$$

where

$$\begin{aligned} f^N &= 2\left(\sin x + \sin(x+y)\right)^2 - \left(\cos x + \cos(x+y)\right)\left(3 - \cos x - \cos y - \cos(x+y)\right); \\ f^D &= u^3, \qquad u(x,y) = 3 - \cos x - \cos y - \cos(x+y); \\ g^N &= 6\left(x^2 + xy\right); \quad g^D = v^3, \quad v(x,y) = x^2 + xy + y^2. \end{aligned} \tag{4.13}$$

By trigonometric identities f^N can be re-expressed as

$$\begin{aligned} f^N = \frac{1}{2}\Big(&- 5\cos(x+y) + \cos(x-y) + \cos(x+2y) - 2\cos(2x+y) \\ &- \cos 2(x+y) + 6 - 5\cos x - \cos(2x) + 6\cos y\Big). \end{aligned} \tag{4.14}$$

Let $\mathbf{p} = (x,y)$ and $\mathbf{0} = (0,0)$. We now apply Taylor's theorem as in (2.3), but with the fourth order remainder, to f^N and to u, and find after pedestrian calculations

$$f^N(\mathbf{p}) = g^N(\mathbf{p}) + R^N(\mathbf{p},\mathbf{p}') \qquad \text{and} \qquad u(\mathbf{p}) = v(\mathbf{p}) + R^D(\mathbf{p},\mathbf{p}'') \tag{4.15}$$

for some $\mathbf{p}' = (x',y')$ and $\mathbf{p}'' = (x'',y'')$ between $\mathbf{0}$ and $\mathbf{p}$, where

$$\begin{aligned} R^N(\mathbf{p},\mathbf{p}') = R^N_4(\mathbf{p},\mathbf{p}') = \frac{1}{48}\Big(&- 5(x+y)^4\cos(x'+y') + (x-y)^4\cos(x'-y') \\ &+ (x+2y)^4\cos(x'+2y') - 2(2x+y)^4\cos(2x'+y') \\ &- (2x+2y)^4\cos(2x'+2y') - x^4(5\cos x' + 16\cos 2x') + 6y^4\cos y'\Big), \end{aligned} \tag{4.16}$$

and

$$R^D(\mathbf{p},\mathbf{p}'') = R^D_4(\mathbf{p},\mathbf{p}'') = -\frac{1}{24}\left(x^4\cos x'' + (x''+y'')^4\cos(x''+y'') + y^4\cos y''\right). \tag{4.17}$$

Note that

$$f^D(\mathbf{p}) = \left(g^D(\mathbf{p}) + R^D(\mathbf{p},\mathbf{p}'')\right)^3. \tag{4.18}$$

It follows that

$$h_{xx} = f_{xx} - g_{xx} = \frac{g^N + R^N(\mathbf{p},\mathbf{p}')}{(v + R^D(\mathbf{p},\mathbf{p}''))^3} - \frac{g^N}{v^3} = \frac{h^N}{h^D} \tag{4.19}$$

where

$$h^N = v^3 R^N(\mathbf{p},\mathbf{p}') - g^N R^D(\mathbf{p},\mathbf{p}'')(3v^2 + 3vR^D(\mathbf{p},\mathbf{p}'') + R^D(\mathbf{p},\mathbf{p}'')^2) \tag{4.20}$$

and

$$h^D = (v + R^D(\mathbf{p},\mathbf{p}''))^3 v^3. \tag{4.21}$$

Writing $x = |\mathbf{p}|\cos\theta$ and $y = |\mathbf{p}|\sin\theta$, we have

$$|R^N(\mathbf{p},\mathbf{p}')| \le \frac{5(x+y)^4 + (x-y)^4 + (x+2y)^4 + 2(2x+y)^4 + (2x+2y)^4 + 21x^4 + 6y^4}{48};$$

and from this we deduce

$$|R^N(\mathbf{p},\mathbf{p}')| \le 4|\mathbf{p}|^4. \tag{4.22}$$

The estimates

$$|R^D(\mathbf{p},\mathbf{p}'')| \le \frac{|\mathbf{p}|^4}{4}, \qquad |v| \le \frac{3}{2}|\mathbf{p}|^2, \qquad |g^N| \le 3(1+\sqrt{2})|\mathbf{p}|^2 \tag{4.23}$$

are found in a similar way. Using (4.22) and (4.23) in (4.20), we see

$$|h^N(\mathbf{p})| \le 28|\mathbf{p}|^{10}, \quad (|\mathbf{p}| \le 1). \tag{4.24}$$

We have from

$$v \ge \frac{|\mathbf{p}|^2}{2}, \tag{4.25}$$

$$v + R^D(\mathbf{p},\mathbf{p}'') \ge \frac{|\mathbf{p}|^2}{2} - \frac{|\mathbf{p}|^4}{4} \ge \frac{|\mathbf{p}|^2}{4}, \quad (|\mathbf{x}| \le 1). \tag{4.26}$$

Use of (4.25) and (4.26) in (4.21) yields

$$|h^D(\mathbf{p})| \ge \frac{|\mathbf{p}|^{12}}{8^3}, \quad (|\mathbf{x}| \le 1). \tag{4.27}$$

Combining (4.24) and (4.27), and setting $C = 7 \cdot 4^7$, we obtain

$$|h_{xx}(\mathbf{p})| \le \frac{C}{|\mathbf{p}|^2}, \quad (0 < |\mathbf{p}| \le 1). \tag{4.28}$$

It follows that, for all sufficiently large n,

$$\begin{aligned}
\sum_{\substack{0<|t_j|,|t_k| \\ t_j^2+t_k^2 \le \frac{1}{2}}} \max_{X_j \times X_k} |h_{xx}| &\le C \sum_{\substack{0<|t_j|,|t_k| \\ t_j^2+t_k^2 \le \frac{1}{2}}} \max_{X_j \times X_k} \frac{1}{|\mathbf{p}|^2} = 4C \sum_{\substack{0<t_j,t_k \\ t_j^2+t_k^2 \le \frac{1}{2}}} \frac{1}{x_j^2 + x_k^2} \\
&= 4C\Big\{ \sum_{\substack{0<t_k \\ t_1^2+t_k^2 \le \frac{1}{2}}} \frac{2}{x_1^2 + x_k^2} + \frac{1}{\Delta^2} \sum_{\substack{t_1<t_j,t_k \\ t_j^2+t_k^2 \le \frac{1}{2}}} \frac{1}{x_j^2 + x_k^2}\Delta^2 \Big\} \\
&\le 4C\Big\{ \sum_{k=1}^{\infty} \frac{2}{x_1^2 + x_k^2} + \frac{1}{\Delta^2} \int_0^{\frac{\pi}{2}} \int_{\frac{\pi}{n}}^{1} \frac{1}{r^2}\, r dr d\theta \Big\} \\
&= 4C\Big\{ \frac{2n^2}{\pi^2} \sum_{k=1}^{\infty} \frac{1}{1+(2k-1)^2} + \frac{1}{\Delta^2}\frac{\pi}{2}(\log n - \log \pi) \Big\}
\end{aligned}$$

and therefore

$$\sum_{\substack{0<|t_j|,|t_k| \\ t_j^2+t_k^2\le\frac{1}{2}}} \max_{X_j\times X_k} |h_{xx}| = O(n^2\log n). \tag{4.29}$$

Clearly the same estimate holds with h_{yy} in place of h_{xx}, so that using (4.29) in (4.11) gives

$$\iint\limits_{D_{n,1}} h(x,y)\,dxdy - \Delta^2\mathcal{H}_{n,1} = O(\frac{\log n}{n^2}), \tag{4.30}$$

which we rewrite as

$$\Delta^2\mathcal{F}_{n,1} = \iint\limits_{D_{n,1}} f(x,y)\,dxdy - \iint\limits_{D_{n,1}} g(x,y)\,dxdy + \Delta^2\mathcal{G}_{n,1} + O(\log n/n^2). \tag{4.31}$$

Considering next the remainder $\mathcal{F}_{n,2}$ in (4.6), we note that the same argument leading to (4.11) delivers

$$\Big|\iint\limits_{D_{n,2}} f(x,y)\,dxdy - \Delta^2\mathcal{F}_{n,2}\Big| \le \frac{\Delta^4}{24}\sum_{(t_j,t_k)\in D_{n,2}} (\max_{X_j\times X_k}|f_{xx}| + \max_{X_j\times X_k}|f_{yy}|). \tag{4.32}$$

These maxima are $O(1)$ in $D_{n,2}$ and there are $O(n^2)$ summands, so that

$$\iint\limits_{D_{n,2}} f(x,y)\,dxdy - \Delta^2\mathcal{F}_{n,2} = O(\Delta^4 n^2) = O(\frac{1}{n^2}). \tag{4.33}$$

Using (4.31) and (4.33) in (4.6), we obtain

$$\begin{aligned}\Delta^2 S_n &= \iint\limits_{D_{n,1}\cup D_{n,2}} f(x,y)\,dxdy - \iint\limits_{D_{n,1}} g(x,y)\,dxdy + \Delta^2\mathcal{G}_{n,1} + O(\frac{\log n}{n^2}) \\ &= \int_{\frac{\pi}{n}}^{2\pi-\frac{\pi}{n}}\int_{\frac{\pi}{n}}^{2\pi-\frac{\pi}{n}} f(x,y)\,dxdy - \iint\limits_{D_{n,1}} g(x,y)\,dxdy + \Delta^2\mathcal{G}_{n,1} + O(\frac{\log n}{n^2}) \end{aligned} \tag{4.34}$$

by the periodicity of f in x and y. Let

$$\mathcal{G}'_{n,1} = \sum_{0<|t_j|,|t_k|<2\pi} g(t_j,t_k) \quad \text{and} \quad D'_{n,1} = \bigcup_{0<|t_j|,|t_k|<2\pi} X_j\times X_k. \tag{4.35}$$

The inequality (4.32) continues to hold with $D_{n,2}$, f, and $\mathcal{F}_{n,2}$ replaced by $D'_{n,1}\backslash D_{n,1}$, g, and $\mathcal{G}'_{n,1}-\mathcal{G}_{n,1}$, so that just as (4.32) implies (4.33), we have

$$\iint\limits_{D'_{n,1}\backslash D_{n,1}} g(x,y)\,dxdy - \Delta^2(\mathcal{G}'_{n,1}-\mathcal{G}_{n,1}) = O(\frac{1}{n^2}). \tag{4.36}$$

Plugging this into (4.34), we obtain

$$\Delta^2 S_n = \int_{\frac{\pi}{n}}^{2\pi-\frac{\pi}{n}}\int_{\frac{\pi}{n}}^{2\pi-\frac{\pi}{n}} f(x,y)\,dxdy - \iint\limits_{D'_{n,1}} g(x,y)\,dxdy + \Delta^2\mathcal{G}'_{n,1} + O(\frac{\log n}{n^2}). \tag{4.37}$$

Writing

$$G(x,y) = g(x,y) + g(-x,y), \tag{4.38}$$

we have

$$\iint\limits_{D'_{n,1}} g(x,y)\,dxdy = 2\int\limits_{\frac{\pi}{n}}^{2\pi-\frac{\pi}{n}}\int\limits_{\frac{\pi}{n}}^{2\pi-\frac{\pi}{n}} G(x,y)\,dxdy, \tag{4.39}$$

and

$$\mathcal{G}'_{n,1} = \sum_{0<|t_j|,|t_k|<2\pi} g(t_j,t_k) = 2\sum_{0<t_j,t_k<2\pi} G(t_j,t_k) = 2\sum_{j,k=1}^{n-1} G(t_j,t_k). \tag{4.40}$$

Using (4.39) and (4.40) in (4.37), we reach

$$\begin{aligned} S_n &= I_n + 2\Big(\frac{n}{2\pi}\Big)^2\Big[\sum_{j,k=1}^{n-1}\Big(\frac{1}{j^2+jk+k^2}+\frac{1}{j^2-jk+k^2}\Big) \\ &\quad - \int\limits_{\frac{\pi}{n}}^{\frac{\pi(2n-1)}{n}}\int\limits_{\frac{\pi}{n}}^{\frac{\pi(2n-1)}{n}}\Big(\frac{1}{x^2+xy+y^2}+\frac{1}{x^2-xy+y^2}\Big)\,dxdy\Big] + O(\log n) \\ &= I_n + 2\Big(\frac{n}{2\pi}\Big)^2\Big[G_n - I_G\Big] + O(\log n), \quad \text{say.} \end{aligned} \tag{4.41}$$

There are now two ways to complete the evaluation of the right-hand side of (4.41): Either evaluate the double sum and the double integral separately or take them together. For the latter alternative there is an Euler–Maclaurin summation formula for double series due to Riesel which is very handy except that the error terms were not specified in [15]. It is possible to develop a version of this formula which includes estimates for the errors, but we won't take this way here since in our particular example including more terms (involving higher order derivatives) leads to worse results as a comparison with the direct numerical calculations for S_n reveals. This stems from the fact that the higher order derivatives of the particular function in the summand assume very large values near the corner of the region which is close to the origin. Therefore in the following sections we will calculate the three terms appearing on the right hand-side of (4.41) separately.

5. Evaluation of $I_n = \big(\frac{n}{2\pi}\big)^2 \int\limits_{\frac{\pi}{n}}^{\frac{\pi(2n-1)}{n}}\int\limits_{\frac{\pi}{n}}^{\frac{\pi(2n-1)}{n}} \frac{d\theta\, d\phi}{3-\cos\theta-\cos\phi-\cos(\theta+\phi)}$

In the domain of integration of I_n for the portion $\theta,\ \phi \in [\pi, \frac{(2n-1)\pi}{n}]$ we use $2\pi-\theta$, $2\pi-\phi$ and see that this portion is the same as the portion $\theta,\ \phi \in [\frac{\pi}{n},\pi]$. What remains of the square is twice the portion $\theta \in [\frac{\pi}{n},\pi]$, $\phi \in [\pi, \frac{(2n-1)\pi}{n}]$ (because of symmetry of the integrand and of the regions with respect to θ and ϕ). Changing ϕ to $2\pi-\phi$ brings the domain of integration to $\theta,\ \phi\in[\frac{\pi}{n},\pi]$, but also alters the integrand by making the denominator $3-\cos\theta-\cos\phi-\cos(\theta-\phi)$. Thus we have

$$I_n = 2 \cdot \frac{n^2}{4\pi^2} \int_{\frac{\pi}{n}}^{\pi} \int_{\frac{\pi}{n}}^{\pi} \Big(\frac{1}{3 - \cos\theta - \cos\phi - \cos(\theta + \phi)} + \frac{1}{3 - \cos\theta - \cos\phi - \cos(\theta - \phi)} \Big) \, d\theta \, d\phi. \tag{5.1}$$

Putting $u = \tan\frac{\theta}{2}$, $v = \tan\frac{\phi}{2}$ transforms (5.1) to

$$I_n = \frac{n^2}{\pi^2} \int_{\tan\frac{\pi}{2n}}^{\infty} \int_{\tan\frac{\pi}{2n}}^{\infty} \frac{u^2 + v^2 + u^2v^2}{(u^2 + v^2 + u^2v^2)^2 - u^2v^2} \, du \, dv. \tag{5.2}$$

We switch to polar coordinates by putting $u = r\cos\alpha$, $v = r\sin\alpha$ and have

$$I_n = \frac{2n^2}{\pi^2} \int_{\alpha=0}^{\frac{\pi}{4}} \int_{r=\frac{\tan\frac{\pi}{2n}}{\sin\alpha}}^{\infty} \frac{1 + r^2\cos^2\alpha\sin^2\alpha}{r\big((1 + r^2\cos^2\alpha\sin^2\alpha)^2 - (\cos\alpha\sin\alpha)^2\big)} \, dr \, d\alpha. \tag{5.3}$$

Letting $\beta = 2\alpha$ we re-write (5.3) as

$$I_n = \frac{n^2}{\pi^2} \int_{\beta=0}^{\frac{\pi}{2}} \int_{r=\frac{\sqrt{2}\tan\frac{\pi}{2n}}{\sqrt{1-\cos\beta}}}^{\infty} \frac{1 + r^2\frac{\sin^2\beta}{4}}{r\big((1 + r^2\frac{\sin^2\beta}{4})^2 - \frac{\sin^2\beta}{4}\big)} \, dr \, d\beta. \tag{5.4}$$

Now we define a new variable $t := \frac{r\sin\beta}{\sqrt{2}}$ for fixed β. Then

$$I_n = \frac{n^2}{\pi^2} \int_{\beta=0}^{\frac{\pi}{2}} \int_{t=\frac{\tan\frac{\pi}{2n}\sin\beta}{\sqrt{1-\cos\beta}}}^{\infty} \frac{1 + \frac{t^2}{2}}{t\big((1 + \frac{t^2}{2})^2 - \frac{\sin^2\beta}{4}\big)} \, dt \, d\beta. \tag{5.5}$$

Reversing the order of integration gives

$$I_n = \frac{n^2}{\pi^2} \Big(\int_{t=\sqrt{2}\tan\frac{\pi}{2n}}^{\infty} \int_{\beta=0}^{\frac{\pi}{2}} + \int_{t=\tan\frac{\pi}{2n}}^{\sqrt{2}\tan\frac{\pi}{2n}} \int_{\beta=\arccos\left((\frac{t}{\tan\frac{\pi}{2n}})^2-1\right)}^{\frac{\pi}{2}} \Big) \frac{1 + \frac{t^2}{2}}{t\big((1 + \frac{t^2}{2})^2 - \frac{\sin^2\beta}{4}\big)} \, d\beta \, dt. \tag{5.6}$$

The integral with respect to β has the evaluation

$$\int \frac{1}{1 - \frac{\sin^2\beta}{a^2}} \, d\beta = \frac{a\arctan\left(\frac{\sqrt{a^2-1}\tan\beta}{a}\right)}{\sqrt{a^2 - 1}} + C, \quad (a > 1), \tag{5.7}$$

where C is a constant of integration. We will employ (5.7) with $a = 2(1 + \frac{t^2}{2})$ in (5.6), so that

$$\int_0^{\frac{\pi}{2}} \frac{d\beta}{1 - \frac{\sin^2\beta}{(2(1+\frac{t^2}{2}))^2}} = \frac{(1 + \frac{t^2}{2})\pi}{\sqrt{(1 + t^2)(3 + t^2)}},$$

and

$$\int_{\arccos\left((\frac{t}{\tan\frac{\pi}{2n}})^2-1\right)}^{\frac{\pi}{2}} \frac{d\beta}{1-\frac{\sin^2\beta}{(2(1+\frac{t^2}{2}))^2}} = \frac{(1+\frac{t^2}{2})\pi}{\sqrt{(1+t^2)(3+t^2)}}$$
$$-\frac{2+t^2}{\sqrt{(1+t^2)(3+t^2)}}\arctan\left(\frac{\sqrt{(1+t^2)(3+t^2)}}{2+t^2}\tan\left(\arccos\left((\frac{t}{\tan\frac{\pi}{2n}})^2-1\right)\right)\right).$$

Since $\tan(\arccos u) = \frac{\sqrt{1-u^2}}{u}$, we have

$$\tan\left(\arccos\left((\frac{t}{\tan\frac{\pi}{2n}})^2-1\right)\right) = \frac{t}{\tan\frac{\pi}{2n}}\frac{\sqrt{2-(\frac{t}{\tan\frac{\pi}{2n}})^2}}{(\frac{t}{\tan\frac{\pi}{2n}})^2-1}.$$

Using these (5.6) becomes

$$I_n = \frac{n^2}{\pi^2}\int_{\tan\frac{\pi}{2n}}^{\infty}\frac{\pi}{t\sqrt{(1+t^2)(3+t^2)}}\,dt \tag{5.8}$$
$$-\frac{n^2}{\pi^2}\int_{\tan\frac{\pi}{2n}}^{\sqrt{2}\tan\frac{\pi}{2n}}\frac{2}{t\sqrt{(1+t^2)(3+t^2)}}\arctan\left(\frac{t}{\tan\frac{\pi}{2n}}\frac{\sqrt{(1+t^2)(3+t^2)}}{2+t^2}\frac{\sqrt{2-(\frac{t}{\tan\frac{\pi}{2n}})^2}}{(\frac{t}{\tan\frac{\pi}{2n}})^2-1}\right)dt.$$

We can easily estimate the very last integral for $n \geq 3$. The arctan takes values in $[0, \frac{\pi}{2}]$, the factor before arctan is of size $\asymp \frac{1}{t} \asymp \frac{1}{\tan\frac{\pi}{2n}}$, and the interval of integration is of length $\asymp \tan\frac{\pi}{2n}$. Hence this integral is bounded, and (5.8) simplifies to

$$I_n = \frac{n^2}{\pi^2}\int_{\tan\frac{\pi}{2n}}^{\infty}\frac{\pi}{t\sqrt{(1+t^2)(3+t^2)}}\,dt + O(n^2). \tag{5.9}$$

The substitution $\tan\nu = \sqrt{\frac{1+t^2}{3+t^2}}$ transforms the last integral to

$$\frac{n^2}{\pi}\int_{\arctan\sqrt{\frac{1+\tan^2\frac{\pi}{2n}}{3+\tan^2\frac{\pi}{2n}}}}^{\frac{\pi}{4}}\frac{1}{4\sin^2\nu-1}\,d\nu.$$

Now letting $\tan\frac{\nu}{2} = x$ the last integral becomes

$$-\frac{2n^2}{\pi}\int_{\tan\left(\frac{1}{2}\arctan\sqrt{\frac{1+\tan^2\frac{\pi}{2n}}{3+\tan^2\frac{\pi}{2n}}}\right)}^{\tan\frac{\pi}{8}}\frac{1+x^2}{x^4-14x^2+1}\,dx$$
$$= -\frac{2n^2}{\pi}\int_{\frac{\sqrt{4+2\tan^2\frac{\pi}{2n}}-\sqrt{3+\tan^2\frac{\pi}{2n}}}{\sqrt{1+\tan^2\frac{\pi}{2n}}}}^{\sqrt{2}-1}\frac{1+x^2}{x^4-14x^2+1}\,dx \tag{5.10}$$

$$= -\frac{2n^2}{\pi}\int_{\varpi_n}^{\sqrt{2}-1}\frac{1+x^2}{x^4-14x^2+1}\,dx, \quad \text{say.}$$

Note that, using $\sqrt{1+y} = 1+\frac{y}{2}-\frac{y^2}{8}+O(y^3)$ for small y and the Taylor–Maclaurin series $\tan w = w+\frac{w^3}{3}+O(w^5)$ for small $|w|$, for n large enough we see (with $t := \tan\frac{\pi}{2n}$ for convenience)

$$\begin{aligned}
\varpi_n &:= \frac{\sqrt{4+2\tan^2\frac{\pi}{2n}}-\sqrt{3+\tan^2\frac{\pi}{2n}}}{\sqrt{1+\tan^2\frac{\pi}{2n}}} = \frac{2\sqrt{1+\frac{t^2}{2}}-\sqrt{3}\sqrt{1+\frac{t^2}{3}}}{\sqrt{1+t^2}} \\
&= \frac{2\big(1+\frac{t^2}{4}-\frac{t^4}{32}+O(t^6)\big)-\sqrt{3}\big(1+\frac{t^2}{6}-\frac{t^4}{72}+O(t^6)\big)}{1+\frac{t^2}{2}-\frac{t^4}{8}+O(t^6)} \\
&= \Big((2-\sqrt{3})+\big(\frac{3-\sqrt{3}}{6}\big)t^2+\big(\frac{-9+2\sqrt{3}}{144}\big)t^4+O(t^6)\Big)\cdot\Big(1-\frac{t^2}{2}+\frac{3t^4}{8}+O(t^6)\Big) \\
&= (2-\sqrt{3})+\big(\frac{-3+2\sqrt{3}}{6}\big)t^2+\big(\frac{63-40\sqrt{3}}{144}\big)t^4+O(t^6) \\
&= (2-\sqrt{3})\cdot\Big(1+\frac{1}{8\sqrt{3}}\frac{\pi^2}{n^2}+\frac{6-\sqrt{3}}{2304}\frac{\pi^4}{n^4}+O(\frac{1}{n^6})\Big) > 2-\sqrt{3} > 0
\end{aligned} \tag{5.11}$$

Returning to (5.10), we expand the integrand into partial fractions to have

$$\begin{aligned}
&-\frac{n^2}{2\sqrt{3}\pi}\int_{\varpi_n}^{\sqrt{2}-1}\Big(\frac{1}{x-(2+\sqrt{3})}-\frac{1}{x+(2+\sqrt{3})}-\frac{1}{x-(2-\sqrt{3})}+\frac{1}{x+(2-\sqrt{3})}\Big)\,dx \\
&= -\frac{n^2}{2\sqrt{3}\pi}\big(\log(\varpi_n-(2-\sqrt{3}))+O(1)\big) = -\frac{n^2}{2\sqrt{3}\pi}\log\big(\frac{\pi^2}{n^2}\frac{2-\sqrt{3}}{8\sqrt{3}}+O(\frac{1}{n^4})\big)+O(n^2) \qquad (5.12) \\
&= \frac{n^2\log n}{\sqrt{3}\pi}+O(n^2),
\end{aligned}$$

where we have made use of (5.11) twice in the penultimate line. Inserting this in (5.9), we obtain

$$I_n = \frac{n^2\log n}{\sqrt{3}\pi}+O(n^2). \tag{5.13}$$

We are interested in the estimation of the $O(n^2)$ term in (5.12) (in order to get an explicit secondary main term instead of leaving it as just $O(n^2)$ as in (5.13)) although there still remains the problem of calculating the second integral in (5.8) more precisely. The precise evaluation of the first line of (5.12) is

$$= -\frac{n^2}{2\sqrt{3}\pi}\Big(\log(2+\sqrt{3})+\log\big(\frac{\varpi_n+2+\sqrt{3}}{(\varpi_n+2-\sqrt{3})(2+\sqrt{3}-\varpi_n)}\big)+\log(\varpi_n-(2-\sqrt{3}))\Big), \tag{5.14}$$

where the very last term gives the main contribution of size $n^2\log n$ and the first two terms give $O(n^2)$. To calculate the expression in (5.14) we write from (5.11)

$$\varpi_n = 2-\sqrt{3}+\epsilon_n, \quad \epsilon_n = (2-\sqrt{3})\cdot\Big(\frac{1}{8\sqrt{3}}\frac{\pi^2}{n^2}+\frac{6-\sqrt{3}}{2304}\frac{\pi^4}{n^4}+O(\frac{1}{n^6})\Big). \tag{5.15}$$

Then

$$\log\Big(\frac{\varpi_n+2+\sqrt{3}}{(\varpi_n+2-\sqrt{3})(2+\sqrt{3}-\varpi_n)}\Big)=\log\Big(\frac{2+\sqrt{3}}{\sqrt{3}}\Big)-\Big(\frac{9+4\sqrt{3}}{12}\Big)\epsilon_n+O(\epsilon_n^2)$$
$$=\log\Big(\frac{2+\sqrt{3}}{\sqrt{3}}\Big)-\frac{6-\sqrt{3}}{96\sqrt{3}}\frac{\pi^2}{n^2}+O(\frac{1}{n^4}),$$

and

$$\log\epsilon_n=-2\log n+\log\Big(\frac{(2-\sqrt{3})\pi^2}{8\sqrt{3}}\Big)+\frac{2\sqrt{3}-1}{96}\frac{\pi^2}{n^2}+O(\frac{1}{n^4}),$$

so that (5.14) becomes

$$\frac{n^2}{\sqrt{3}\pi}\Big(\log n-\frac{1}{2}\log\Big(\frac{2+\sqrt{3}}{24}\pi^2\Big)+O(\frac{1}{n^4})\Big). \tag{5.16}$$

Thus, denoting the second term on the right-hand side of (5.8) by

$$R_n:=-\frac{n^2}{\pi^2}\int\limits_{\tan\frac{\pi}{2n}}^{\sqrt{2}\tan\frac{\pi}{2n}}\frac{2}{t\sqrt{(1+t^2)(3+t^2)}}\arctan\left(\frac{t}{\tan\frac{\pi}{2n}}\frac{\sqrt{(1+t^2)(3+t^2)}}{2+t^2}\frac{\sqrt{2-(\frac{t}{\tan\frac{\pi}{2n}})^2}}{(\frac{t}{\tan\frac{\pi}{2n}})^2-1}\right)dt, \tag{5.17}$$

(it was seen between (5.8) and (5.9) that $R_n=O(n^2)$), we have obtained

$$I_n=\frac{n^2\log n}{\sqrt{3}\pi}-\frac{n^2}{2\sqrt{3}\pi}\log\Big(\frac{2+\sqrt{3}}{24}\pi^2\Big)+R_n+O(\frac{1}{n^2}). \tag{5.18}$$

To understand R_n we begin by letting $w=\frac{t}{\tan\frac{\pi}{2n}}$, so that (5.17) becomes

$$R_n=-\frac{n^2}{\pi^2}\int\limits_1^{\sqrt{2}}\frac{2}{w\sqrt{(1+(w\tan\frac{\pi}{2n})^2)(3+(w\tan\frac{\pi}{2n})^2)}}$$
$$\times\arctan\left(\frac{w\sqrt{2-w^2}}{w^2-1}\frac{\sqrt{(1+(w\tan\frac{\pi}{2n})^2)(3+(w\tan\frac{\pi}{2n})^2)}}{2+(w\tan\frac{\pi}{2n})^2}\right)dw. \tag{5.19}$$

As in (5.11) we calculate

$$\sqrt{(1+(w\tan\frac{\pi}{2n})^2)(3+(w\tan\frac{\pi}{2n})^2)}=\sqrt{3}\Big(1+\frac{w^2}{6}\frac{\pi^2}{n^2}+O(\frac{1}{n^4})\Big),$$
$$\frac{\sqrt{(1+(w\tan\frac{\pi}{2n})^2)(3+(w\tan\frac{\pi}{2n})^2)}}{2+(w\tan\frac{\pi}{2n})^2}=\frac{\sqrt{3}}{2}\Big(1+\frac{w^2}{24}\frac{\pi^2}{n^2}+O(\frac{1}{n^4})\Big),$$

and we can re-write (5.19) as

$$R_n=-\frac{n^2}{\pi^2}\int\limits_1^{\sqrt{2}}\frac{2}{\sqrt{3}w}\Big(1-\frac{w^2}{6}\frac{\pi^2}{n^2}+O(\frac{1}{n^4})\Big)$$
$$\times\arctan\left(\frac{w\sqrt{2-w^2}}{w^2-1}\frac{\sqrt{3}}{2}\Big(1+\frac{w^2}{24}\frac{\pi^2}{n^2}+O(\frac{1}{n^4})\Big)\right)dw. \tag{5.20}$$

Now since

$$\arctan(a + a\epsilon) = \arctan(a) + \frac{a\epsilon}{1+a^2} + O\Big(\frac{\epsilon^2(1+a^3)}{(1+a^2)^2}\Big)$$

with

$$a = \frac{\sqrt{3}}{2}\frac{w\sqrt{2-w^2}}{w^2-1}, \qquad \epsilon = \frac{w^2}{24}\frac{\pi^2}{n^2} + O(\frac{1}{n^4}),$$

valid for $a \in [0, \infty)$ and formally valid even for $w = 1^+$, we express (5.20) as

$$\begin{aligned} R_n = &-\frac{n^2}{\pi^2}\int_1^{\sqrt{2}} \frac{2}{\sqrt{3}w}\Big(1 - \frac{w^2}{6}\frac{\pi^2}{n^2} + O(\frac{1}{n^4})\Big) \\ &\times \Big[\arctan\Big(\frac{\sqrt{3}}{2}\frac{w\sqrt{2-w^2}}{w^2-1}\Big) + \frac{w^3(w^2-1)\sqrt{2-w^2}}{4\sqrt{3}\big((w^2-1)^2+3\big)}\frac{\pi^2}{n^2} + O(\frac{1}{n^4})\Big] \\ = &-\frac{n^2}{\pi^2}\int_1^{\sqrt{2}} \frac{2}{\sqrt{3}w}\arctan\Big(\frac{\sqrt{3}}{2}\frac{w\sqrt{2-w^2}}{w^2-1}\Big)\,dw \\ &+ \int_1^{\sqrt{2}}\Big[\frac{w}{3\sqrt{3}}\arctan\Big(\frac{\sqrt{3}}{2}\frac{w\sqrt{2-w^2}}{w^2-1}\Big) - \frac{1}{6}\frac{w^2(w^2-1)\sqrt{2-w^2}}{(w^2-1)^2+3}\Big]\,dw + O(\frac{1}{n^2}). \end{aligned} \tag{5.21}$$

By the last sentence of §4 we need to evaluate only the term of size $\asymp n^2$ in R_n. We let $w^2 = \dfrac{2}{1+u^2}$ and then integrate by parts ($\dfrac{2u}{1+u^2}\,du = d(\log(1+u^2))$) to have

$$\begin{aligned} \int_1^{\sqrt{2}} \frac{2}{\sqrt{3}w}\arctan\Big(\frac{\sqrt{3}}{2}\frac{w\sqrt{2-w^2}}{w^2-1}\Big)\,dw &= \int_0^1 \frac{2u}{\sqrt{3}(1+u^2)}\arctan\Big(\frac{\sqrt{3}u}{1-u^2}\Big)\,du \\ &= \frac{\pi\log 2}{2\sqrt{3}} - \int_0^1 \frac{(1+u^2)\log(1+u^2)}{u^4+u^2+1}\,du. \end{aligned} \tag{5.22}$$

By expanding into partial fractions we have

$$\begin{aligned} &-\int_0^1 \frac{(1+u^2)\log(1+u^2)}{u^4+u^2+1}\,du = \\ &\frac{i}{2\sqrt{3}}\int_0^1 [\log(1+ui) + \log(1-ui)]\Big[\frac{-1}{u+e^{\frac{2\pi}{3}i}} + \frac{1}{u+e^{-\frac{\pi}{3}i}} + \frac{1}{u+e^{-\frac{2\pi}{3}i}} + \frac{-1}{u+e^{\frac{\pi}{3}i}}\Big]\,du \\ &= \frac{1}{\sqrt{3}}\Im\int_0^1 \frac{\log(1+ui)}{u+e^{\frac{2\pi}{3}i}} - \frac{\log(1+ui)}{u+e^{-\frac{\pi}{3}i}} - \frac{\log(1+ui)}{u+e^{-\frac{2\pi}{3}i}} + \frac{\log(1+ui)}{u+e^{\frac{\pi}{3}i}}\,du \\ &= \frac{1}{\sqrt{3}}\Im\int_0^i \frac{\log(1+v)}{v+e^{-\frac{5\pi}{6}i}} - \frac{\log(1+v)}{v+e^{\frac{\pi}{6}i}} - \frac{\log(1+v)}{v+e^{-\frac{\pi}{6}i}} + \frac{\log(1+v)}{v+e^{\frac{5\pi}{6}i}}\,dv. \end{aligned} \tag{5.23}$$

Let L be the line segment from 0 to i. In (5.23) we have four integrals of the type $\int\limits_L \frac{\log(1+v)}{v+b}\,dv$. (There are formulas in [10] for such integrals but the conditions for the applicability of those formulas were not stated clearly, and in fact they are not applicable in some cases relevant to us.) With the values of b in (5.23) it is valid to separate the logarithm into two parts and write

$$\log(1+v) = \begin{cases} \log(v+b) + \log(1+\frac{1-b}{v+b}) & \text{if } |v+b| > |1-b| \ \forall v \in L \\ \log(1-b) + \log(1+\frac{v+b}{1-b}) & \text{if } |v+b| < |1-b| \ \forall v \in L \end{cases}$$
$$= \begin{cases} \log(v+b) + \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m}\Big(\frac{1-b}{v+b}\Big)^m & \text{if } |v+b| > |1-b| \ \forall v \in L \\ \log(1-b) + \sum_{m=1}^{\infty} \frac{(-1)^{m+1}}{m}\Big(\frac{v+b}{1-b}\Big)^m & \text{if } |v+b| < |1-b| \ \forall v \in L. \end{cases} \tag{5.24}$$

Now we integrate term by term and find

$$\int\limits_L \frac{\log(1+v)}{v+b}\,dv = \tag{5.25}$$
$$\begin{cases} \frac{1}{2}\big(\log^2(b+i) - \log^2 b\big) + \mathrm{Li}_2\big(\frac{b-1}{b+i}\big) - \mathrm{Li}_2\big(\frac{b-1}{b}\big) & \text{if } |v+b| > |1-b| \ \forall v \in L \\ \log(1-b)\log\big(\frac{b+i}{b}\big) + \mathrm{Li}_2\big(\frac{b}{b-1}\big) - \mathrm{Li}_2\big(\frac{b+i}{b-1}\big) & \text{if } |v+b| < |1-b| \ \forall v \in L, \end{cases}$$

where (see [17])

$$\mathrm{Li}_2(z) := -\int\limits_0^z \frac{\log(1-u)}{u}\,du, \quad \big(z \in \mathbb{C}\setminus[1,\infty),\ \arg(1-z) \in (-\pi,\pi)\big) \tag{5.26}$$
$$= \sum_{k=1}^{\infty} \frac{z^k}{k^2}, \quad (|z| \le 1). \tag{5.27}$$

Using (5.25) in (5.23) (for the first and fourth terms in (5.23) the second case of (5.25) applies, for the second and third terms the first case of (5.25) applies) the imaginary part in (5.23) is evaluated as

$$-\frac{\pi}{2}\log\big(\frac{1+\sqrt{3}}{\sqrt{2}}\big) - \frac{5\pi}{24}\log 3$$
$$- \Im\big[\mathrm{Li}_2\big(\frac{1-i}{1+\sqrt{3}}\big) + \mathrm{Li}_2\big(\frac{1+i}{3+\sqrt{3}}\big) + \mathrm{Li}_2\big(\frac{-(1+i)}{1+\sqrt{3}}\big) + \mathrm{Li}_2\big(\frac{\sqrt{3}(1-i)}{1+\sqrt{3}}\big)\big]. \tag{5.28}$$

Now we use, with $\omega = \arg(1 - re^{-\theta i})$,

$$\Im\mathrm{Li}_2(re^{i\theta}) = \omega\log r + \frac{1}{2}[\mathrm{Cl}_2(2\theta) + \mathrm{Cl}_2(2\omega) - \mathrm{Cl}_2(2\theta+2\omega)], \quad (0 < r < 1), \tag{5.29}$$

a formula due to Kummer (see (5.2)–(5.5) in [10]), where

$$\mathrm{Cl}_2(\theta) := \Im\mathrm{Li}_2(e^{i\theta}) = \sum_{k=1}^{\infty} \frac{\sin k\theta}{k^2} \tag{5.30}$$

is Clausen's function. The result of these calculations, in which we use

$$\mathrm{Cl}_2(-\theta) = -\mathrm{Cl}_2(\theta), \qquad 2\mathrm{Cl}_2\big(\frac{\pi}{3}\big) = 3\mathrm{Cl}_2\big(\frac{2\pi}{3}\big), \tag{5.31}$$

is

$$\int_1^{\sqrt{2}} \frac{2}{\sqrt{3}w} \arctan\Big(\frac{\sqrt{3}}{2}\frac{w\sqrt{2-w^2}}{w^2-1}\Big)\, dw = \frac{\pi}{\sqrt{3}} \log(\sqrt{3}-1) + \frac{5}{3\sqrt{3}}\mathrm{Cl}_2\big(\frac{\pi}{3}\big). \tag{5.32}$$

To complete this section we find the value of the integral in the last line of (5.21). Letting $w^2 - 1 = x$ turns this integral into

$$\frac{1}{6\sqrt{3}} \int_0^1 \arctan\Big(\frac{\sqrt{3}}{2}\frac{\sqrt{1-x^2}}{x}\Big)\, dx - \frac{1}{12}\int_0^1 \frac{x\sqrt{1-x^2}}{(x^2+3)}\, dx,$$

which upon letting $x = \cos\theta$ becomes

$$\frac{1}{6\sqrt{3}} \int_0^{\pi/2} \sin\theta \arctan\Big(\frac{\sqrt{3}}{2}\tan\theta\Big) d\theta - \frac{1}{12}\int_0^{\pi/2} \frac{\cos\theta\sin^2\theta}{4-\sin^2\theta}\, d\theta.$$

Using integration by parts in the first integral here we have

$$\frac{1}{6\sqrt{3}}\Big[-\cos\theta\arctan\Big(\frac{\sqrt{3}}{2}\tan\theta\Big)\Big|_0^{\pi/2} + \int_0^{\pi/2}\cos\theta\frac{2\sqrt{3}}{4-\sin^2\theta}d\theta\Big] - \frac{1}{12}\int_0^{\pi/2}\frac{\cos\theta\sin^2\theta}{4-\sin^2\theta}d\theta,$$

which simplifies to

$$\frac{1}{3}\int_0^{\pi/2}\frac{\cos\theta}{4-\sin^2\theta}d\theta - \frac{1}{12}\int_0^{\pi/2}\frac{\cos\theta\sin^2\theta}{4-\sin^2\theta}d\theta = \frac{1}{12}\int_0^{\pi/2}\cos\theta d\theta = \frac{1}{12}.$$

Hence

$$\int_1^{\sqrt{2}} \Big[\frac{w}{3\sqrt{3}}\arctan\Big(\frac{\sqrt{3}}{2}\frac{w\sqrt{2-w^2}}{w^2-1}\Big) - \frac{1}{6}\frac{w^2(w^2-1)\sqrt{2-w^2}}{(w^2-1)^2+3}\Big]\, dw = \frac{1}{12}. \tag{5.33}$$

Combining (5.18), (5.21), (5.32), and (5.33) we reach

$$I_n = \frac{n^2\log n}{\sqrt{3}\pi} + \frac{n^2}{\sqrt{3}\pi}\Big(\log\big(\frac{2\sqrt{3}}{\pi}\big) - \frac{5}{3\pi}\mathrm{Cl}_2\big(\frac{\pi}{3}\big)\Big) + \frac{1}{12} + O\big(\frac{1}{n^2}\big). \tag{5.34}$$

6. Evaluation of $G_n := \sum_{j,k=1}^{n-1}\big(\frac{1}{j^2+jk+k^2} + \frac{1}{j^2-jk+k^2}\big)$

In this section we consider the sum G_n which occurs in (4.41). Expanding the summand into partial fractions as in (2.12) we have

$$\sum_{j=1}^{n-1}\Big(\frac{1}{j^2+jk+k^2}+\frac{1}{j^2-jk+k^2}\Big)$$
$$=\frac{i}{\sqrt{3}k}\Big(\sum_{j=1}^{\infty}-\sum_{j=n}^{\infty}\Big)\Big(\frac{1}{j+ke^{\frac{\pi}{3}i}}-\frac{1}{j+ke^{-\frac{\pi}{3}i}}+\frac{1}{j-ke^{-\frac{\pi}{3}i}}-\frac{1}{j-ke^{\frac{\pi}{3}i}}\Big).$$

In the sum $\sum_{j=n}^{\infty}$ we replace j by $j+n-1$ so that we shift the sum to start from 1. Then as in (2.13) we have the expression in terms of the digamma function

$$\sum_{j=1}^{n-1}\Big(\frac{1}{j^2+jk+k^2}+\frac{1}{j^2-jk+k^2}\Big)$$
$$=\frac{i}{\sqrt{3}k}\Big[-\psi(1+ke^{\frac{\pi}{3}i})+\psi(1+ke^{-\frac{\pi}{3}i})-\psi(1-ke^{-\frac{\pi}{3}i})+\psi(1-ke^{\frac{\pi}{3}i})$$
$$+\psi(n+ke^{\frac{\pi}{3}i})-\psi(n+ke^{-\frac{\pi}{3}i})+\psi(n-ke^{-\frac{\pi}{3}i})-\psi(n-ke^{\frac{\pi}{3}i})\Big]$$
$$=\frac{2}{\sqrt{3}k}\Im\big[\psi(1+ke^{\frac{\pi}{3}i})+\psi(1-ke^{-\frac{\pi}{3}i})-\psi(n+ke^{\frac{\pi}{3}i})-\psi(n-ke^{-\frac{\pi}{3}i})\big].$$

Therefore

$$G_n=\frac{2}{\sqrt{3}}\sum_{k=1}^{n-1}\frac{\Im\big(\psi(1+ke^{\frac{\pi}{3}i})+\psi(1-ke^{-\frac{\pi}{3}i})\big)}{k}-\frac{\Im\big(\psi(n+ke^{\frac{\pi}{3}i})+\psi(n-ke^{-\frac{\pi}{3}i})\big)}{k}$$
$$=\frac{2}{\sqrt{3}}(G_{n,1}-G_{n,2}),\quad \text{say.} \tag{6.1}$$

We use the recurrence and reflection formulas for the digamma function, as was done in passing to (2.14), to have

$$G_{n,1}=-\frac{\sqrt{3}}{2}\sum_{k=1}^{n-1}\frac{1}{k^2}+\pi\sum_{k=1}^{n-1}\frac{1}{k}\Im\cot\Big(\frac{\pi k}{e^{i\pi/3}}\Big).$$

Since $\cot z=i\dfrac{e^{2iz}+1}{e^{2iz}-1}$ the last term simplifies into

$$\sum_{k=1}^{n-1}\frac{1}{k}\Im\cot\Big(\frac{\pi k}{e^{i\pi/3}}\Big)=\sum_{k=1}^{n-1}\frac{1}{k}+2\sum_{k=1}^{n-1}\frac{1}{k}\frac{q^k}{1-q^k},\qquad (q=-e^{-\sqrt{3}\pi}),$$

so that

$$G_{n,1}=\pi\sum_{k=1}^{n-1}\frac{1}{k}-\frac{\sqrt{3}}{2}\sum_{k=1}^{n-1}\frac{1}{k^2}+2\pi\sum_{k=1}^{n-1}\frac{1}{k}\frac{q^k}{1-q^k}. \tag{6.2}$$

For the first two terms of the right-hand side of (6.2) we employ

$$\sum_{k=1}^{n-1}\frac{1}{k}=-\frac{1}{n}+\sum_{k=1}^{n}\frac{1}{k}=-\frac{1}{n}+\Big(\log n+\gamma+\frac{1}{2n}-\frac{1}{12n^2}+O\Big(\frac{1}{n^4}\Big)\Big) \tag{6.3}$$

from p. 560 of [8], and

$$\sum_{k=1}^{n-1}\frac{1}{k^2}=\frac{\pi^2}{6}-\frac{1}{n}-\frac{1}{2n^2}-\frac{1}{6n^3}+O\big(\frac{1}{n^5}\big) \tag{6.4}$$

which is written by combining (6.4.3) and (6.4.12) of [1]. As for the last member of (6.2), by the alternating series test we have

$$\sum_{k=1}^{n-1}\frac{1}{k}\frac{q^k}{1-q^k}=\sum_{k=1}^{\infty}\frac{1}{k}\frac{q^k}{1-q^k}+O\Big(\frac{1}{ne^{\sqrt{3}\pi n}}\Big), \tag{6.5}$$

(the last infinite series is an instance of the quantum dilogarithm $\mathrm{Li}_2(x;q)=\sum_{k=1}^{\infty}\frac{1}{k}\frac{x^k}{1-q^k}$, see [17]), and then

$$\begin{aligned}\sum_{k=1}^{\infty}\frac{1}{k}\frac{q^k}{1-q^k}&=\sum_{k=1}^{\infty}\sum_{m=0}^{\infty}\frac{1}{k}(q^{m+1})^k=-\sum_{m=0}^{\infty}\sum_{k=1}^{\infty}\frac{-1}{k}(q^{m+1})^k=-\sum_{m=0}^{\infty}\log(1-q^{m+1})\\&=-\log\Big(\prod_{m=0}^{\infty}(1-q^{m+1})\Big)=:-\log\left((q;q)_\infty\right)\end{aligned} \tag{6.6}$$

where $(q;q)_\infty$ is the q-Pochhammer symbol. Writing $q=e^{2\pi\tau i}$, for $\Im\tau>0$, $(q;q)_\infty$ is related to the Dedekind eta-function as $(q;q)_\infty=q^{-\frac{1}{24}}\eta(\tau)$. To $q=-e^{-\sqrt{3}\pi}$ there corresponds $\tau=e^{\frac{\pi}{3}i}$. We can evaluate $\eta\big(e^{\frac{\pi}{3}i}\big)$ by the result given in [13] on the Chowla–Selberg formula [5] employing the facts that $e^{\frac{\pi}{3}i}$ is in the field $\mathbb{Q}(\sqrt{-3})$ which has class number 1 and x^2+xy+y^2 is the only reduced binary quadratic form of discriminant -3. Hence we obtain

$$\prod_{m=0}^{\infty}\Big(1-\big(-e^{-\sqrt{3}\pi}\big)^{m+1}\Big)=\frac{3^{\frac{1}{8}}e^{\frac{\sqrt{3}\pi}{24}}\Big(\Gamma\big(\frac{1}{3}\big)\Big)^{\frac{3}{2}}}{2\pi}. \tag{6.7}$$

Plugging the results of (6.3)–(6.7) in (6.2), we obtain

$$\begin{aligned}G_{n,1}&=\pi\log n+\Big(\pi\gamma-\frac{\sqrt{3}\pi^2}{6}+2\pi\log\frac{2\pi}{3^{\frac{1}{8}}}-3\pi\log\Gamma\big(\frac{1}{3}\big)\Big)\\&\quad+\frac{\sqrt{3}-\pi}{2n}+\frac{3\sqrt{3}-\pi}{12n^2}+\frac{\sqrt{3}}{12n^3}+O\big(\frac{1}{n^4}\big).\end{aligned} \tag{6.8}$$

In $G_{n,2}$ of (6.1) we use (6.3.18) of [1],

$$\psi(z)=\log z-\frac{1}{2z}-\frac{1}{12z^2}+O\big(\frac{1}{z^4}\big)$$

(see [8] for a discussion about this asymptotic) with $z=n\pm ke^{\frac{\pi}{3}i}$. This leads to

$$\begin{aligned}G_{n,2}&=\sum_{k=1}^{n-1}\frac{1}{k}\arctan\big(\frac{\sqrt{3}kn}{n^2-k^2}\big)+\frac{\sqrt{3}}{4}\sum_{k=1}^{n-1}\Big(\frac{1}{n^2+nk+k^2}+\frac{1}{n^2-nk+k^2}\Big)\\&\quad+\frac{\sqrt{3}}{12}\sum_{k=1}^{n-1}\Big(\frac{n+\frac{k}{2}}{(n^2+nk+k^2)^2}+\frac{n-\frac{k}{2}}{(n^2-nk+k^2)^2}\Big)+O\big(\frac{\log n}{n^4}\big).\end{aligned} \tag{6.9}$$

We are going to evaluate these sums by applying the following version of the Euler–Maclaurin summation formula due to Lampret [9]: For any integers n, $p \geq 1$ and any function $f \in C^p[a,b]$,

$$h\sum_{k=0}^{n-1} f(a+kh) = \int_a^b f(x)\,dx + \sum_{j=1}^{p} h^j \frac{B_j}{j!}\left[f^{(j-1)}(x)\right]_a^b + r_p(a,b,n), \tag{6.10}$$

where B_j are the Bernoulli numbers, $h = \dfrac{b-a}{n}$, and

$$r_p(a,b,n) = -\frac{h^p}{p!}\int_a^b B_p\big(\frac{a-x}{h}\big) f^{(p)}(x)\,dx \tag{6.11}$$

with $B_p(x)$, the p-th Bernoulli polynomial in $[0,1)$ extended to all $x \in \mathbb{R}$ via $B_p(x+1) = B_p(x)$. Expressing the first sum in (6.9) as

$$-\frac{\sqrt{3}}{n} + \sum_{k=0}^{n-1} \frac{1}{n}\Big(\frac{1}{\frac{k}{n}} \arctan\big(\frac{\sqrt{3}\frac{k}{n}}{1-(\frac{k}{n})^2}\big)\Big) \tag{6.12}$$

for this application we take $a = 0, b = 1, h = \dfrac{1}{n}, p = 4, f(x) = \dfrac{1}{x}\arctan\big(\dfrac{\sqrt{3}x}{1-x^2}\big)$ (we can take $f(0) = \sqrt{3}$, $f(1) = \dfrac{\pi}{2}, f'(0) = 0, f'(1) = \dfrac{2}{\sqrt{3}} - \dfrac{\pi}{2}$ by considering limits as $x \to 0^+$ and $x \to 1^-$). Then

$$r_4(0,1,n) = -\frac{1}{24n^4}\int_0^1 B_4(-nx) f^{(\mathrm{iv})}(x)\,dx, \tag{6.13}$$

and since $f^{(\mathrm{iv})}(x)$ remains bounded on $[0,1]$ (the values at the endpoints determined by limits), we have

$$\sum_{k=1}^{n-1} \frac{1}{k}\arctan\big(\frac{\sqrt{3}kn}{n^2-k^2}\big) = \int_0^1 \frac{1}{x}\arctan\big(\frac{\sqrt{3}x}{1-x^2}\big)\,dx - \frac{\frac{\sqrt{3}}{2}+\frac{\pi}{4}}{n} + \frac{\frac{1}{6\sqrt{3}}-\frac{\pi}{24}}{n^2} + O\big(\frac{1}{n^4}\big). \tag{6.14}$$

Now, integration by parts gives

$$\int_0^1 \frac{1}{x}\arctan\big(\frac{\sqrt{3}x}{1-x^2}\big)\,dx = -\sqrt{3}\int_0^1 \frac{(1+x^2)\log x}{x^4+x^2+1}\,dx, \tag{6.15}$$

an integral similar to the one in (5.23). Expanding into partial fractions as in (5.23), we arrive at

$$\int_0^1 \frac{1}{x}\arctan\big(\frac{\sqrt{3}x}{1-x^2}\big)\,dx = -\Im\int_0^1 \log(x)\Big(\frac{1}{x+e^{-\frac{\pi}{3}i}} + \frac{1}{x+e^{-\frac{2\pi}{3}i}}\Big)\,dx. \tag{6.16}$$

Now, integration by parts gives

$$\begin{aligned}\int_0^1 \frac{\log x}{x+b}\,dx &= \frac{1}{b}\int_0^1 \frac{\log x}{1+\frac{x}{b}}\,dx = (\log x)\log(1+\frac{x}{b})\Big|_0^1 - \int_0^1 \frac{\log(1+\frac{x}{b})}{x}\,dx \\ &= -\int_0^1 \frac{\log(1+\frac{x}{b})}{x}\,dx = -\int_0^{-\frac{1}{b}} \frac{\log(1-u)}{u}\,du. \end{aligned} \tag{6.17}$$

For $-\frac{1}{b} \in \mathbb{C} \setminus [1, \infty)$, the last integral is evaluated by (5.26). Thus we find that

$$\int_0^1 \frac{1}{x} \arctan\big(\frac{\sqrt{3}x}{1-x^2}\big)\, dx = -\Im\big(\mathrm{Li}_2(-e^{\frac{\pi}{3}i}) + \mathrm{Li}_2(-e^{\frac{2\pi}{3}i})\big) = \frac{5}{3}\mathrm{Cl}_2(\frac{\pi}{3}), \tag{6.18}$$

and by (6.14) that

$$\sum_{k=1}^{n-1} \frac{1}{k} \arctan\big(\frac{\sqrt{3}kn}{n^2-k^2}\big) = \frac{5}{3}\mathrm{Cl}_2(\frac{\pi}{3}) - \frac{\frac{\sqrt{3}}{2}+\frac{\pi}{4}}{n} + \frac{\frac{1}{6\sqrt{3}}-\frac{\pi}{24}}{n^2} + O(\frac{1}{n^4}). \tag{6.19}$$

We rewrite the second sum of (6.9) as

$$-\frac{2}{n^2} + \frac{1}{n}\sum_{k=0}^{n-1} \frac{1}{n}\Big(\frac{1}{1+\frac{k}{n}+(\frac{k}{n})^2} + \frac{1}{1-\frac{k}{n}+(\frac{k}{n})^2}\Big). \tag{6.20}$$

To apply (6.10), we take $a = 0, b = 1, h = \dfrac{1}{n}, p = 4, f(x) = \dfrac{1}{1+x+x^2} + \dfrac{1}{1-x+x^2}$. Then $f(0) = 2$, $f(1) = \dfrac{4}{3}, f'(0) = 0, f'(1) = -\dfrac{4}{3}$, $f'''(x)$ and $f^{(\mathrm{iv})}(x)$ are bounded on $[0, 1]$, and the expression in (6.20) is equal to

$$\frac{1}{n}\int_0^1 \Big(\frac{1}{1+x+x^2} + \frac{1}{1-x+x^2}\Big)\, dx - \frac{5}{3n^2} - \frac{1}{9n^3} + O(\frac{1}{n^5}).$$

The last integral is evaluated by first expanding the integrand into partial fractions as $\dfrac{\pi}{\sqrt{3}}$, hence we find

$$\sum_{k=1}^{n-1} \Big(\frac{1}{n^2+nk+k^2} + \frac{1}{n^2-nk+k^2}\Big) = \frac{\pi}{\sqrt{3}n} - \frac{5}{3n^2} - \frac{1}{9n^3} + O(\frac{1}{n^5}). \tag{6.21}$$

Similarly, the last sum of (6.9) is rewritten as

$$-\frac{2}{n^3} + \frac{1}{n^2}\sum_{k=0}^{n-1} \frac{1}{n}\Big(\frac{1+\frac{k}{2n}}{(1+\frac{k}{n}+(\frac{k}{n})^2)^2} + \frac{1-\frac{k}{2n}}{(1-\frac{k}{n}+(\frac{k}{n})^2)^2}\Big) \tag{6.22}$$

To apply (6.10), we take $a = 0, b = 1, h = \dfrac{1}{n}, p = 2, f(x) = \dfrac{1+\frac{x}{2}}{(1+x+x^2)^2} + \dfrac{1-\frac{x}{2}}{(1-x+x^2)^2}$. Then $f(0) = 2$, $f(1) = \dfrac{2}{3}, f'(0) = 0, f'(1) = -\dfrac{16}{9}$, $f''(x)$ is bounded on $[0, 1]$, and the expression in (6.22) is equal to

$$\frac{1}{n^2}\int_0^1 \Big(\frac{1+\frac{x}{2}}{(1+x+x^2)^2} + \frac{1-\frac{x}{2}}{(1-x+x^2)^2}\Big)\, dx - \frac{4}{3n^3} + O(\frac{1}{n^4}).$$

The last integral is easily evaluated as $\dfrac{4+\sqrt{3}\pi}{6}$, so that

$$\sum_{k=1}^{n-1} \Big(\frac{n+\frac{k}{2}}{(n^2+nk+k^2)^2} + \frac{n-\frac{k}{2}}{(n^2-nk+k^2)^2}\Big) = \frac{4+\sqrt{3}\pi}{6n^2} - \frac{4}{3n^3} + O(\frac{1}{n^4}). \tag{6.23}$$

Putting (6.19), (6.21) and (6.23) together in (6.9), we have

$$G_{n,2} = \frac{5}{3}\mathrm{Cl}_2(\frac{\pi}{3}) - \frac{\sqrt{3}}{2n} - \frac{11\sqrt{3}}{36n^2} - \frac{5\sqrt{3}}{36n^3} + O(\frac{\log n}{n^4}), \tag{6.24}$$

and (6.24) and (6.8) plugged in (6.1) gives

$$\begin{aligned} G_n = \frac{2\pi}{\sqrt{3}}\log n + \Big(\frac{2\pi\gamma}{\sqrt{3}} - \frac{\pi^2}{3} + \frac{4\pi}{\sqrt{3}}\log\frac{2\pi}{3^{\frac{1}{8}}} - 2\sqrt{3}\pi\log\Gamma\big(\frac{1}{3}\big) - \frac{10}{3\sqrt{3}}\mathrm{Cl}_2(\frac{\pi}{3})\Big) \\ + \frac{2-\frac{\pi}{\sqrt{3}}}{n} + \frac{\frac{10}{9} - \frac{\pi}{6\sqrt{3}}}{n^2} + \frac{\frac{4}{9}}{n^3} + O(\frac{\log n}{n^4}). \end{aligned} \tag{6.25}$$

7. Evaluation of $I_G := -\int_{\frac{\pi}{n}}^{\frac{\pi(2n-1)}{n}}\int_{\frac{\pi}{n}}^{\frac{\pi(2n-1)}{n}} \Big(\frac{1}{x^2+xy+y^2} + \frac{1}{x^2-xy+y^2}\Big)\,dxdy$

In this section upon evaluating I_G of (4.41) we will finish the proof of the theorem. In I_G the region of integration is symmetric with respect to the line $x = y$, the integrand is invariant under the interchange of x and y, and as in (2.12) the integrand can be expanded into partial fractions, so that we have

$$\begin{aligned} I_G &= \frac{2i}{\sqrt{3}}\int_{\frac{\pi}{n}}^{2\pi-\frac{\pi}{n}}\int_{\frac{\pi}{n}}^{y}\frac{1}{y}\Big(\frac{1}{x+ye^{\frac{\pi}{3}i}} - \frac{1}{x+ye^{-\frac{\pi}{3}i}} + \frac{1}{x-ye^{-\frac{\pi}{3}i}} - \frac{1}{x-ye^{\frac{\pi}{3}i}}\Big)\,dx\,dy \\ &= \frac{2i}{\sqrt{3}}\int_{\frac{\pi}{n}}^{2\pi-\frac{\pi}{n}}\frac{1}{y}\Big[\log(x+ye^{\frac{\pi}{3}i}) - \log(x+ye^{-\frac{\pi}{3}i}) \\ &\qquad + \log(x-ye^{-\frac{\pi}{3}i}) - \log(x-ye^{\frac{\pi}{3}i})\Big]_{x=\frac{\pi}{n}}^{x=y}\,dy \\ &= \frac{2i}{\sqrt{3}}\int_{\frac{\pi}{n}}^{2\pi-\frac{\pi}{n}}\frac{1}{y}\Big[2i\mathrm{Arg}(1+e^{\frac{\pi}{3}i}) + 2i\mathrm{Arg}(1-e^{-\frac{\pi}{3}i}) \\ &- \big(\log(1+\frac{n}{\pi}ye^{\frac{\pi}{3}i}) - \log(1+\frac{n}{\pi}ye^{-\frac{\pi}{3}i}) + \log(1-\frac{n}{\pi}ye^{-\frac{\pi}{3}i}) - \log(1-\frac{n}{\pi}ye^{\frac{\pi}{3}i})\big)\Big]\,dy \\ &= -\frac{2\pi}{\sqrt{3}}\log(2n-1) + \frac{2i}{\sqrt{3}}\Big[\mathrm{Li}_2(-\frac{ne^{\frac{\pi}{3}i}}{\pi}y) - \mathrm{Li}_2(-\frac{ne^{-\frac{\pi}{3}i}}{\pi}y) \\ &\qquad + \mathrm{Li}_2(\frac{ne^{-\frac{\pi}{3}i}}{\pi}y) - \mathrm{Li}_2(\frac{ne^{\frac{\pi}{3}i}}{\pi}y)\Big]_{\frac{\pi}{n}}^{2\pi-\frac{\pi}{n}} \qquad (7.1) \\ &= -\frac{2\pi}{\sqrt{3}}\log(2n-1) + \frac{2i}{\sqrt{3}}\Big[L(2\pi-\frac{\pi}{n}) - L(\frac{\pi}{n})\Big], \text{ say,} \end{aligned}$$

where to pass to the penultimate member (5.26) is employed. We see that

$$\begin{aligned} L(\frac{\pi}{n}) &= \mathrm{Li}_2(-e^{\frac{\pi}{3}i}) - \mathrm{Li}_2(-e^{-\frac{\pi}{3}i}) + \mathrm{Li}_2(e^{-\frac{\pi}{3}i}) - \mathrm{Li}_2(e^{\frac{\pi}{3}i}) \\ &= -2i\Im\mathrm{Li}_2(-e^{-\frac{\pi}{3}i}) - 2i\Im\mathrm{Li}_2(e^{\frac{\pi}{3}i}) = -2i\big(\mathrm{Cl}_2(\frac{2\pi}{3}) + \mathrm{Cl}_2(\frac{\pi}{3})\big) = -\frac{10i}{3}\mathrm{Cl}_2(\frac{\pi}{3}) \end{aligned} \tag{7.2}$$

by (5.31). Next, in

$$L(2\pi - \frac{\pi}{n}) = \mathrm{Li}_2(-(2n-1)e^{\frac{\pi}{3}i}) - \mathrm{Li}_2(-(2n-1)e^{-\frac{\pi}{3}i}) + \mathrm{Li}_2((2n-1)e^{-\frac{\pi}{3}i}) - \mathrm{Li}_2((2n-1)e^{\frac{\pi}{3}i})$$

the arguments of the dilogarithm are not on the ray $[0, \infty)$ allowing us to apply the inversion formula

$$\mathrm{Li}_2(z) = -\mathrm{Li}_2(\frac{1}{z}) - \frac{\pi^2}{6} - \frac{1}{2}\log^2(-z), \tag{7.3}$$

so that these values of the dilogarithm are expressed in terms of the values of the dilogarithm at the reciprocal points which are inside the unit disk. Hence we have

$$\begin{aligned} L(2\pi - \frac{\pi}{n}) &= -\mathrm{Li}_2(\frac{-1}{(2n-1)e^{\frac{\pi}{3}i}}) + \mathrm{Li}_2(\frac{-1}{(2n-1)e^{-\frac{\pi}{3}i}}) - \mathrm{Li}_2(\frac{1}{(2n-1)e^{-\frac{\pi}{3}i}}) \\ &+ \mathrm{Li}_2(\frac{1}{(2n-1)e^{\frac{\pi}{3}i}}) - \frac{1}{2}\log^2((2n-1)e^{\frac{\pi}{3}i}) + \frac{1}{2}\log^2((2n-1)e^{-\frac{\pi}{3}i}) \\ &- \frac{1}{2}\log^2(-(2n-1)e^{-\frac{\pi}{3}i}) + \frac{1}{2}\log^2(-(2n-1)e^{\frac{\pi}{3}i}). \end{aligned}$$

The logarithm terms here add up to $-2\pi(\log(2n-1))i$ using the principal branch of the logarithm. For the values of the dilogarithm we use (5.31). Hence we have

$$\begin{aligned} L(2\pi - \frac{\pi}{n}) &= -2\pi(\log(2n-1))i \\ &\quad - 2\sqrt{3}i\sum_{m=0}^{\infty}\Big(\frac{1}{(6m+1)^2(2n-1)^{6m+1}} - \frac{1}{(6m+5)^2(2n-1)^{6m+5}}\Big) \\ &= -2\pi(\log(2n-1))i - \frac{2\sqrt{3}}{2n-1}i + O(\frac{1}{(2n-1)^5}). \end{aligned} \tag{7.4}$$

Combining (7.1), (7.3) and (7.4), we obtain

$$\begin{aligned} I_G &= \frac{2\pi}{\sqrt{3}}\log(2n-1) - \frac{20}{3\sqrt{3}}\mathrm{Cl}_2(\frac{\pi}{3}) + \frac{4}{2n-1} + O(\frac{1}{n^5}) \\ &= \frac{2\pi}{\sqrt{3}}\log n + (\frac{2\pi\log 2}{\sqrt{3}} - \frac{20}{3\sqrt{3}}\mathrm{Cl}_2(\frac{\pi}{3})) + \frac{2-\frac{\pi}{\sqrt{3}}}{n} + \frac{1-\frac{\pi}{4\sqrt{3}}}{n^2} + \frac{\frac{1}{2}-\frac{\pi}{12\sqrt{3}}}{n^3} + O(\frac{1}{n^4}). \end{aligned} \tag{7.5}$$

8. Conclusion

Putting the results (5.34), (6.25) and (7.5) together gives

$$\begin{aligned} I_n + 2(\frac{n}{2\pi})^2\Big[G_n - I_G\Big] &= \frac{n^2\log n}{\sqrt{3}\pi} + \frac{n^2}{\sqrt{3}\pi}\Big(\gamma - \frac{\sqrt{3}\pi}{6} + \log(4\pi\sqrt[4]{3}) - 3\log\Gamma(\frac{1}{3})\Big) \\ &+ \Big(\frac{1}{12} + \frac{1}{18\pi^2} + \frac{1}{24\sqrt{3}\pi}\Big) + \frac{\frac{1}{24\sqrt{3}\pi} - \frac{1}{36\pi^2}}{n} + O(\frac{\log n}{n^2}), \end{aligned} \tag{8.1}$$

and from (4.41) we obtain the result announced in our Theorem.

The referee informed us that the total of the terms of magnitude smaller than n^2 seems to converge numerically to $\frac{1}{12}$ as $n \to \infty$. So in the final form of our paper we gave the terms of size $o(\log n)$ in §5–7 even though there is an error of $O(\log n)$ term from §4. Now that the constant term is seen to be different from $\frac{1}{12}$, it becomes clear that the difference between S_n and the quantity in (8.1) is $\gg 1$. This points to the limitation of the methods of this paper.

Acknowledgments

We thank the referee for carefully reading the paper and for the remark about the convergence of the smaller terms. To include the smaller terms we made some changes in the arguments of §6 which in fact led to a simpler presentation. Although it is not manifest in the final version of this paper, we have made use of MAPLE, WolframAlpha and Wikipedia while studying for this article.

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