

## PAIR CORRELATION OF ANGLES BETWEEN RECIPROCAL GEODESICS ON THE MODULAR SURFACE

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**ABSTRACT.** The existence of the limiting pair correlation for angles between reciprocal geodesics on the modular surface is established. An explicit formula is provided, which captures geometric information about the length of reciprocal geodesics, as well as arithmetic information about the associated reciprocal classes of binary quadratic forms. One striking feature is the absence of a gap beyond zero in the limiting distribution, contrasting with the analog Euclidean situation.

### 1. INTRODUCTION

Let  $\mathbb{H}$  denote the upper half-plane and  $\Gamma = \mathrm{PSL}_2(\mathbb{Z})$  the modular group. Consider the modular surface  $X = \Gamma \backslash \mathbb{H}$ , and let  $\Pi : \mathbb{H} \rightarrow X$  be the natural projection. The angles on the upper half plane  $\mathbb{H}$  considered in this paper are the same as the angles on  $X$  between the closed geodesics passing through  $\Pi(i)$ , and the image of the imaginary axis. These geodesics were first introduced in connection with the associated “self-inverse classes” of binary quadratic forms in the classical work of Fricke and Klein [8, p.164], and the primitive geodesics among them were studied recently and called reciprocal geodesics by Sarnak [22]. The aim of this paper is to establish the existence of the pair correlation measure of their angles and to explicitly express it.

For  $g \in \Gamma$ , denote by  $\theta_g \in [-\pi, \pi]$  the angle between the vertical geodesic  $[i, 0]$  and the geodesic ray  $[i, gi]$ . For  $z_1, z_2 \in \mathbb{H}$ , let  $d(z_1, z_2)$  denote the hyperbolic distance, and set

$$\|g\|^2 = 2 \cosh d(i, gi) = a^2 + b^2 + c^2 + d^2, \quad \text{for } g = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathrm{SL}_2(\mathbb{R}).$$

It was proved by Nicholls [16] (see also [17, Theorem 10.7.6]) that for any discrete subgroup  $\Gamma$  of finite covolume in  $\mathrm{PSL}_2(\mathbb{R})$ , the angles  $\theta_\gamma$  are uniformly distributed, in the sense that for any fixed interval  $I \subseteq [-\pi, \pi]$ ,

$$\lim_{R \rightarrow \infty} \frac{\#\{\gamma \in \Gamma : \theta_\gamma \in I, d(i, \gamma i) \leq R\}}{\#\{\gamma \in \Gamma : d(i, \gamma i) \leq R\}} = \frac{|I|}{2\pi}.$$

Effective estimates for the rate of convergence that allow one to take  $|I| \asymp e^{-cR}$  as  $R \rightarrow \infty$  for some constant  $c = c_\Gamma > 0$  were proved for  $\Gamma = \Gamma(N)$  by one of us [1], and in general situations by Risager and Truelsen [20] and by Gorodnik and Nevo [9]. Other related results concerning the uniform distribution of real parts of orbits in hyperbolic spaces were proved by Good [10], and more recently by Risager and Rudnick [19].

The statistics of spacings, such as the pair correlation or the nearest neighbor distribution (also known as the gap distribution) measure the fine structure of sequences of real numbers in a more subtle way than the classical Weyl uniform distribution. Very little is known about the spacing statistics of closed geodesics. In fact, the only result that we are aware of, due to Pollicott and Sharp [18], concerns the correlation of differences of lengths of pairs of closed geodesics on a compact surface of negative curvature, ordered with respect to the word length on the fundamental group.

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This paper investigates the pair correlation of angles  $\theta_\gamma$  with  $d(i, \gamma i) \leq R$ , or equivalently with  $\|\gamma\|^2 \leq Q^2 = e^R \sim 2 \cosh R$  as  $Q \rightarrow \infty$ . As explained in Section 2, these are exactly the angles between reciprocal geodesics on the modular surface.

The Euclidean analog of this problem considers the angles between the line segments connecting the origin  $(0,0)$  with the integral lattice points  $(m,n)$  with  $m^2 + n^2 \leq Q^2$  as  $Q \rightarrow \infty$ . The pair correlation of all lattice point angles (rays are counted with multiplicity) is plotted on the right in Figure 1. When only primitive lattice points are being considered (rays are counted with multiplicity one), the problem reduces to the study of the sequence of Farey fractions with the  $L^2$  norm  $\|m/n\|_2^2 = m^2 + n^2$ . Its pair correlation function is plotted on the left in Figure 1. When Farey fractions are ordered by their denominator, the pair correlation is shown to exist and it is explicitly computed in [5]. A common important feature is the existence of a gap beyond zero for the pair correlation function. This is an ultimate reflection of the fact that the area of a nondegenerate triangle with integer vertices is at least  $1/2$ .

For the hyperbolic lattice centered at  $i$ , it is convenient to start with the (non-uniformly distributed) numbers  $\tan(\theta_\gamma/2)$  with multiplicities, rather than the angles  $\theta_\gamma$  themselves. Employing obvious symmetries explained in Section 3, it is further convenient to restrict to a set of representatives  $\Gamma_{\mathbf{I}}$  consisting of matrices  $\gamma$  such that the point  $\gamma i$  is in the first quadrant in Figure 2. The pair correlation measures of the finite set  $\mathfrak{T}_Q$  of elements  $\tan(\theta_\gamma/2)$  with  $\gamma \in \Gamma_{\mathbf{I}}$  and  $\|\gamma\| \leq Q$  (counted with multiplicities), respectively of the set  $\mathfrak{A}_Q$  of elements  $\theta_\gamma$  with  $\gamma \in \Gamma_{\mathbf{I}}$  and  $\|\gamma\| \leq Q$  (counted with multiplicities) are defined as

$$R_Q^{\mathfrak{T}}(\xi) = \frac{\#\{(\gamma, \gamma') \in \Gamma_{\mathbf{I}}^2 : \|\gamma\|, \|\gamma'\| \leq Q, \gamma' \neq \gamma, 0 \leq \tan(\theta_{\gamma'}/2) - \tan(\theta_\gamma/2) \leq \frac{\xi}{B_Q}\}}{B_Q},$$

$$R_Q^{\mathfrak{A}}(\xi) = \frac{\#\{(\gamma, \gamma') \in \Gamma_{\mathbf{I}}^2 : \|\gamma\|, \|\gamma'\| \leq Q, \gamma' \neq \gamma, 0 \leq \frac{2}{\pi}(\theta_{\gamma'} - \theta_\gamma) \leq \frac{\xi}{B_Q}\}}{B_Q},$$

where  $B_Q \sim \frac{3}{8}Q^2$  denotes the number of elements  $\gamma \in \Gamma_{\mathbf{I}}$  with  $\|\gamma\| \leq Q$ .

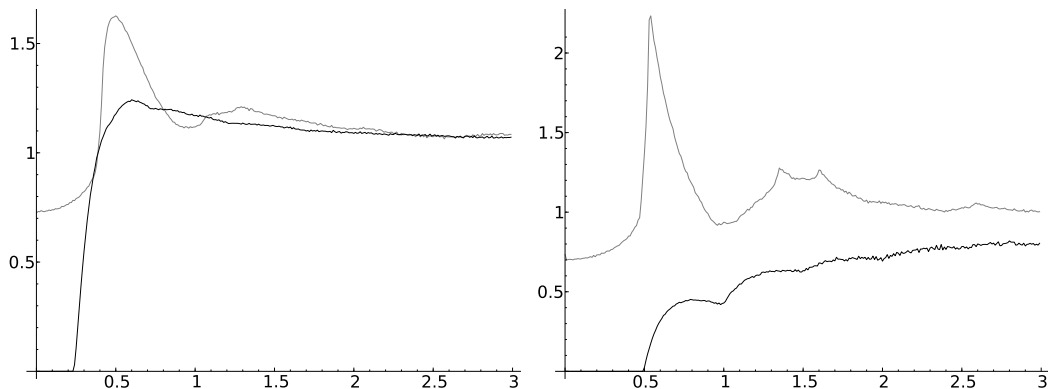


FIGURE 1. The pair correlation functions  $g_2^{\mathfrak{T}}$  (left) and  $g_2^{\mathfrak{A}}$  (right), plotted in grey, compared with the pair correlation function of Farey fractions with  $L^2$  norm, (left) and of the angles (with multiplicities) of lattice points in Euclidean balls (right). The graphs are obtained by counting the pairs in their definition, using  $Q = 4000$  for which  $B_Q = 6000203$ . We used Magma [14] for the numerical computations, and SAGE [21] for plotting the graphs.

One striking feature, shown by numerical calculations in Figure 1, points to the absence of a gap beyond zero in the limiting distribution, in contrast with the Euclidean situation described above.

The main result of this paper is the proof of existence and explicit computation of the pair correlation measures  $R_2^{\mathfrak{S}}$  and  $R_2^{\mathfrak{A}}$ , given by

$$R_2^{\mathfrak{S}}(\xi) = R_2^{\mathfrak{S}}((0, \xi]) := \lim_{Q \rightarrow \infty} R_Q^{\mathfrak{S}}(\xi), \quad R_2^{\mathfrak{A}}(\xi) = R_2^{\mathfrak{A}}((0, \xi]) := \lim_{Q \rightarrow \infty} R_Q^{\mathfrak{A}}(\xi), \quad (1.1)$$

thus answering a question raised in [1].

To give a precise statement consider  $\mathfrak{S}$ , the free semigroup on two generators  $L = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$  and  $R = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ . Repeated application of the Euclidean algorithm shows that  $\mathfrak{S} \cup \{I\}$  coincides with the set of matrices in  $\mathrm{SL}_2(\mathbb{Z})$  with positive entries. The explicit formula for  $R_2^{\mathfrak{S}}(\xi)$  is given as a series of volumes summed over  $\mathfrak{S}$ , plus a finite sum of volumes, and it is stated in Theorem 2 of Section 7. The formula for  $R_2^{\mathfrak{S}}(\xi)$  leads to an explicit formula for  $R_2^{\mathfrak{A}}(\xi)$ , which we state here, partly because the pair correlation function for the angles  $\theta_\gamma$  is more interesting, being equidistributed, and partly because the formula we obtain is simpler.

**Theorem 1.** *The pair correlation measure  $R_2^{\mathfrak{A}}$  exists on  $[0, \infty)$ , and it is given by the  $C^1$  function*

$$R_2^{\mathfrak{A}}\left(\frac{3}{4\pi}\xi\right) = \frac{8}{3\zeta(2)} \left( \sum_{M \in \mathfrak{S}} B_M(\xi) + \sum_{\ell \in [0, \xi/2]} \sum_{K \in [1, \xi/2]} A_{K, \ell}(\xi) \right). \quad (1.2)$$

For  $M \in \mathfrak{S}$ , letting  $U_M = \|M\|^2 / \sqrt{\|M\|^4 - 4}$ ,  $\theta_M$  as above, and  $f_+ = \max(f, 0)$ , we have

$$B_M(\xi) = \frac{\pi}{4} \int_0^{\frac{\pi}{2}} \frac{\left(1/\sqrt{\|M\|^4 - 4} - \sin(2\theta - \theta_M)/\xi\right)_+}{U_M + \cos(2\theta - \theta_M)} d\theta.$$

For integers  $K \in [1, \xi/2]$ ,  $\ell \in [0, \xi/2]$  we have

$$A_{K, \ell}(\xi) = \int_0^{\pi/4} A_{K, \ell}\left(\frac{\xi}{2 \cos^2 t}, t\right) \frac{dt}{\cos^2 t},$$

with  $A_{K, \ell}(\xi, t)$  the area of the region defined by, setting  $e^{i\theta} = (\cos \theta, \sin \theta)$ :

$$\left\{ r e^{i\theta} \in [0, 1]^2 : L_{\ell+1}(e^{i\theta}) > 0, \frac{F_{K, \ell}(\theta)}{\xi} \leq r^2 \leq \frac{\cos^2 t}{\max\{1, L_\ell^2(e^{i\theta}) + L_{\ell+1}^2(e^{i\theta})\}} \right\},$$

where  $F_{K, \ell}(\theta) := \cot \theta + \sum_{i=1}^{\ell} \frac{1}{L_{i-1}(e^{i\theta})L_i(e^{i\theta})} + \frac{L_{\ell+1}(e^{i\theta})}{L_\ell(e^{i\theta})(L_\ell^2(e^{i\theta}) + L_{\ell+1}^2(e^{i\theta}))}$  and the linear forms  $L_i(x, y)$  are defined in terms of the triangle transformation  $T : [0, 1]^2 \rightarrow [0, 1]^2$ ,  $T(x, y) = (y, \lceil \frac{1+x}{y} \rceil y - x)$  by iteration:  $T^i = (L_{i-1}, L_i)$  for  $1 \leq i \leq \ell$  and  $L_{\ell+1} = KL_\ell - L_{\ell-1}$ .

Rates of convergence in (1.1) are effectively described in the proof of Theorem 2 and in Proposition 14.

When  $\xi \leq 2$ , the second sum in (1.2) disappears and the derivative  $B'_M(\xi)$  is explicitly computed in Lemma 16, yielding an explicit formula for the pair correlation density function  $g_2^{\mathfrak{A}}(\xi) = \frac{dR_2^{\mathfrak{A}}(\xi)}{d\xi}$  which matches the graph in Figure 1.

**Corollary 1.** *For  $0 < \xi \leq 2$  we have*

$$g_2^{\mathfrak{A}}\left(\frac{3}{4\pi}\xi\right) = \frac{16}{3\xi^2} \sum_{M \in \mathfrak{S}} \ln \left( \frac{\|M\|^2 + \sqrt{\|M\|^4 - 4}}{\|M\|^2 + \sqrt{\|M\|^4 - 4 - \xi^2}} \right).$$

A formula valid for  $0 < \xi \leq 4$  is given in (8.16) after computing  $A'_{K, 0}(\xi)$ .

The computation is performed in §8.2, and it identifies the first spike in the graph of  $g_2^{\mathfrak{A}}(x)$  at  $x = \frac{3}{4\pi}\sqrt{5}$ . An explicit formula for the pair correlation density  $g_2^{\mathfrak{A}}(x)$  valid for all  $x$ , and also when the point  $i$  is replaced by the other elliptic point  $\rho = e^{\pi i/3}$ , will be given in [4].

Since the series in Corollary 1 is dominated by the absolutely convergent  $\sum_M \xi^2 \|M\|^{-4}$ , we can take the limit as  $\xi \rightarrow 0$ :

$$g_2^{\mathfrak{A}}(0) = \frac{2}{3} \sum_{M \in \mathfrak{S}} \left( \frac{\|M\|^2}{\sqrt{\|M\|^4 - 4}} - 1 \right) = 0.7015\dots$$

Remarkably the previous two formulas, as well as (1.2) for  $\xi \leq 2$ , can be written geometrically as a sum over the primitive closed geodesics  $\mathcal{C}$  on  $X$  which pass through the point  $\Pi(i)$ , where the summand depends only on the length  $\ell(\mathcal{C})$ :

$$g_2^{\mathfrak{A}}(0) = \frac{8}{3} \sum_{\mathcal{C}} \sum_{n \geq 1} \frac{1}{e^{n\ell(\mathcal{C})} - 1}.$$

This is proved in Section 2, where we also give an arithmetic version based on an explicit description of the reciprocal geodesics  $\mathcal{C}$  due to Sarnak [22].

For the rest of the introduction we sketch the main ideas behind the proof, describing also the organization of the article. After reducing to angles in the first quadrant in Section 3, we show that the pair correlation of the quantities  $\Psi(\gamma) = \tan(\theta_\gamma/2)$  is identical to that of  $\Phi(\gamma) = \operatorname{Re}(\gamma i)$ . We are led to estimating the cardinality  $\mathcal{R}_Q^\Phi(\xi)$  of the set

$$\left\{ (\gamma, \gamma') \in \Gamma_{\mathbf{I}}^2 : \|\gamma\|, \|\gamma'\| \leq Q, \gamma' \neq \gamma, 0 \leq \Phi(\gamma') - \Phi(\gamma) \leq \frac{\xi}{B_Q} \right\}.$$

For  $\gamma = \begin{pmatrix} p' & p \\ q' & q \end{pmatrix}$  with nonnegative entries,  $\|\gamma\| \leq Q$ , and  $q, q' > 0$ , consider the associated Farey interval  $[p/q, p'/q']$ , which contains  $\Phi(\gamma)$ . In Section 4, we break the set of pairs  $(\gamma, \gamma')$  above in two parts, depending on whether one of the associated Farey intervals contains the other, or the two intervals intersect at most at one endpoint. In the first case we have  $\gamma = \gamma' M$  or  $\gamma' = \gamma M$  with  $M \in \mathfrak{S}$ , while in the second we have a similar relation depending on the number  $\ell$  of consecutive Farey fractions there are between the two intervals. The first case contributes to the series over  $\mathfrak{S}$  in (1.2), while the second case contributes to the sum over  $K, \ell$ . The triangle map  $T$ , first introduced in [3], makes its appearance in the second case, being related to the denominator of the successor function for Farey fractions.

To estimate the number of pairs  $(\gamma, \gamma M)$  in the first case, a key observation is that for each  $M \in \Gamma$  there exists a function  $\Xi_M(x, y)$ , given by (5.1), such that

$$\Phi(\gamma) - \Phi(\gamma M) = \Xi_M(q', q)$$

for  $\gamma$  as above. Together with estimates for the number of points in two dimensional regions based on bounds on Kloosterman sums (Lemma 7), this allows us to estimate the number of pairs  $(\gamma, \gamma M)$  with fixed  $M \in \mathfrak{S}$ , in terms of the volume of a three dimensional body  $S_{M, \xi}$  given in (7.14). The absence of a gap beyond zero in the pair correlation measure arises as a result of this estimate. The details of the calculation are given in Section 7, giving an explicit formula for  $R_2^{\mathfrak{S}}$  (Theorem 2).

Finally in Section 8 we pass to the pair correlation of the angles  $\theta_\gamma$ , obtaining the formulas of Theorem 1 and Corollary 1.

## 2. RECIPROCAL GEODESICS ON THE MODULAR SURFACE

In this section we recall the definition of reciprocal geodesics and explain how the pair correlation of the angles they make with the imaginary axis is related to the pair correlation considered in the

introduction. We also show that the sums over the semigroup  $\mathfrak{S}$  appearing in the introduction can be expressed geometrically in terms of sums over primitive reciprocal geodesics. A description of the trajectory of reciprocal geodesics on the fundamental domain seems to have first appeared in the classical work of Fricke and Klein [8, p.164], where it is shown that they consist of two closed loops, one the reverse of the other. There the terminology “sich selbst inverse Classe” is used for the equivalence classes of quadratic forms corresponding to reciprocal conjugacy classes of hyperbolic matrices.

Oriented closed geodesics on  $X$  are in one to one correspondence with conjugacy classes  $\{\gamma\}$  of hyperbolic elements  $\gamma \in \Gamma$ . To a hyperbolic element  $\gamma \in \Gamma$  one attaches its axis  $a_\gamma$  on  $\mathbb{H}$ , namely the semicircle whose endpoints are the fixed points of  $\gamma$  on the real axis. The part of the semicircle between  $z_0$  and  $\gamma z_0$ , for any  $z_0 \in a_\gamma$ , projects to a closed geodesic on  $X$ , with multiplicity one if only if  $\gamma$  is a primitive matrix (not a power of another hyperbolic element of  $\Gamma$ ). The group that fixes the semicircle  $a_\gamma$  (or equivalently its endpoints on the real axis) is generated by one primitive element  $\gamma_0$ .

We are concerned with (oriented) closed geodesics passing through  $\Pi(i)$  on  $X$ . Since the axis of a hyperbolic element  $A$  passes through  $i$  if and only if  $A$  is symmetric, the closed geodesics passing through  $\Pi(i)$  correspond to the set  $\mathcal{R}$  of hyperbolic conjugacy classes  $\{\gamma\}$  which contain a symmetric matrix. The latter are exactly the reciprocal geodesics considered by P. Sarnak in [22], where only primitive geodesics are considered.

The reciprocal geodesics can be parameterized in a 2-1 manner by the set  $\mathfrak{S} \subset \Gamma$ , defined in the introduction, which consists of matrices distinct from the identity with nonnegative entries. To describe this correspondence, let  $\mathcal{A} \subset \Gamma$  be the set of symmetric hyperbolic matrices with positive entries. Then we have maps

$$\mathfrak{S} \rightarrow \mathcal{A} \rightarrow \mathcal{R} \tag{2.1}$$

where the first map takes  $\gamma \in \mathfrak{S}$  to  $A = \gamma\gamma^t$ , and the second takes the hyperbolic symmetric  $A$  to its conjugacy class  $\{A\}$ . The first map is bijective, while the second is two-to-one and onto, as it follows from [22]. More precisely, if  $A = \gamma\gamma^t \in \mathcal{A}$  is a primitive matrix, then  $B = \gamma^t\gamma \neq A$  is the only other matrix in  $\mathcal{A}$  conjugate with  $A$ , and  $\{A^n\} = \{B^n\}$  for all  $n \geq 0$ .

Note also that  $\|\gamma\|^2 = \text{Tr}(\gamma\gamma^t)$ , and if  $A$  is hyperbolic with  $\text{Tr}(A) = T$ , then the length of the geodesic associated to  $\{A\}$  is  $2 \ln N(A)$  with  $N(A) = \frac{T + \sqrt{T^2 - 4}}{2}$ .

We need the following:

**Lemma 2.** *Let  $A \in \Gamma$  be a hyperbolic symmetric matrix and let  $\gamma \in \Gamma$  such that  $A = \gamma\gamma^t$ . Then the point  $\gamma i$  is halfway (in hyperbolic distance) between  $i$  and  $Ai$  on the axis of  $A$ .*

*Proof.* We have  $d(i, \gamma i) = d(i, \gamma^t i) = d(\gamma i, Ai)$  where the first equality follows from the hyperbolic distance formula and the second since  $\Gamma$  acts by isometries on  $\mathbb{H}$ . Using formula (3.2), one checks that the angles of  $i, \gamma i$  and  $i, Ai$  are equal, hence  $\gamma i$  is indeed on the axis of  $A$ .  $\square$

We can now explain the connection between the angles  $\theta_\gamma$  in the first and second quadrant in Figure 2, and the angles made by the reciprocal geodesics with the image  $\Pi(i \rightarrow i\infty) = \Pi(i \rightarrow 0)$ . Namely, points in the first and second quadrant are parameterized by  $\gamma i$  with  $\gamma \in \mathfrak{S}$ , and by the lemma the reciprocal geodesic corresponding to  $A = \gamma\gamma^t \in \mathcal{A}$  consists of the loop  $\Pi(i \rightarrow \gamma i)$ , followed by  $\Pi(i \rightarrow \gamma^t i)$  (which is the same as the reverse of the first loop). Therefore to each reciprocal geodesic corresponding to  $A = \gamma\gamma^t \in \mathcal{A}$  correspond two angles, those attached to  $\gamma i$  and  $\gamma^t i$  in Figure 2, measured in the first or second quadrant so that all angles are between 0 and  $\pi/2$ .

In conclusion the angles made by the reciprocal geodesics on  $X$  with the fixed direction  $\Pi(i \rightarrow i\infty)$  consist of the angles in the first quadrant considered before, each appearing twice. Ordering the points  $\gamma i$  in the first quadrant by  $\|\gamma\|$  corresponds to ordering the geodesics by their length.

Therefore the pair correlation measure of the angles of reciprocal geodesics is  $2R_2^{\mathfrak{A}}(\xi/2)$ , where  $R_2^{\mathfrak{A}}$  was defined in the introduction.

The parametrization (2.1) of reciprocal geodesics allows one to rewrite the series appearing in the formula for  $g_2^{\mathfrak{A}}(0)$  in the introduction, as a series over the primitive reciprocal classes  $\mathcal{R}^{\text{prim}}$ :

$$\sum_{M \in \mathfrak{S}} \left( \frac{\|M\|^2}{\sqrt{\|M\|^4 - 4}} - 1 \right) = \sum_{A \in \mathcal{A}} \frac{2}{N(A)^2 - 1} = 4 \sum_{\{\gamma\} \in \mathcal{R}^{\text{prim}}} \sum_{n \geq 1} \frac{1}{N(\gamma)^{2n} - 1},$$

where we have used the fact that for a hyperbolic matrix  $A$  of trace  $T$  we have

$$\sqrt{T^2 - 4} = N(A) - N(A)^{-1} \text{ and } N(A^n) = N(A)^n.$$

One can rewrite the sum further using the arithmetic description of primitive reciprocal geodesics given in [22]. Namely, let  $\mathcal{D}_{\mathcal{R}}$  be the set of nonsquare positive discriminants  $2^\alpha D'$  with  $\alpha \in \{0, 2, 3\}$  and  $D'$  odd divisible only by primes  $p \equiv 1 \pmod{4}$ . Then the set of primitive reciprocal classes  $\mathcal{R}^{\text{prim}}$  decomposes as a disjoint union of finite sets:

$$\mathcal{R}^{\text{prim}} = \bigcup_{d \in \mathcal{D}_{\mathcal{R}}} \mathcal{R}_d^{\text{prim}}$$

with  $|\mathcal{R}_d^{\text{prim}}| = \nu(d)$ , the number of genera of binary quadratic forms of discriminant  $d$ . For  $d \in \mathcal{D}_{\mathcal{R}}$ ,  $\nu(d)$  equals  $2^{\lambda-1}$ , or respectively  $2^\lambda$  depending on whether  $8 \nmid d$ , or respectively  $8 \mid d$ , and  $\lambda$  is the number of distinct odd prime factors of  $d$ . Each class  $\{\gamma\} \in \mathcal{R}_d^{\text{prim}}$  has

$$N(\gamma) = \alpha_d = \frac{u_0 + v_0 \sqrt{d}}{2}$$

with  $(u_0, v_0)$  the minimal positive solution to Pell's equation  $u^2 - dv^2 = 4$ . We then have

$$\sum_{\{\gamma\} \in \mathcal{R}^{\text{prim}}} \sum_{n \geq 1} \frac{1}{N(\gamma)^{2n} - 1} = \sum_{d \in \mathcal{D}_{\mathcal{R}}} \sum_{n \geq 1} \frac{\nu(d)}{\alpha_d^{2n} - 1}.$$

In the same way, by Lemma 12 the pair correlation measure  $R_2^{\mathfrak{S}}(\xi)$  in Theorem 1 can be written for  $\xi \leq 1$  as a sum over classes  $\{\gamma\} \in \mathcal{R}^{\text{prim}}$ , where each summand depends only on  $\xi$  and  $N(\gamma)$ .

### 3. REDUCTION TO THE FIRST QUADRANT

In this section we establish notation in use throughout the paper, and we reduce the pair correlation problem to considering angles in the first quadrant in Figure 2. A similar reduction can be found in [6], in the context of visibility problems for the hyperbolic lattice centered at  $i$ .

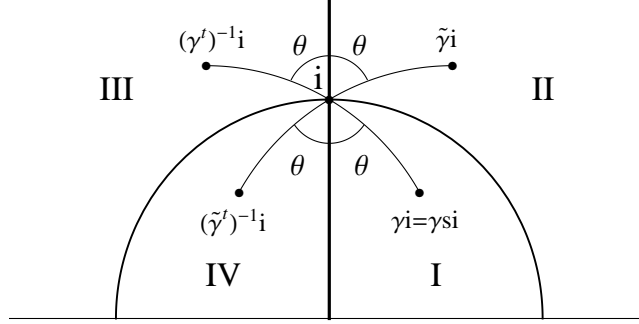
For each  $g = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in SL_2(\mathbb{R})$  define the quantities

$$\begin{aligned} X_g &= a^2 + b^2, & Y_g &= c^2 + d^2, & Z_g &= ac + bd, & T_g &= X_g + Y_g = \|g\|^2, \\ \Phi(g) &= \text{Re}(gi) = \frac{Z_g}{Y_g}, & \epsilon_g &= \frac{1}{2} \left( T_g - \sqrt{T_g^2 - 4} \right). \end{aligned} \quad (3.1)$$

Note that  $X_g Y_g - Z_g^2 = 1$ .

A direct computation yields that the angle  $\theta_g \in [-\pi, \pi]$  between the vertical geodesic  $[i, 0]$  and the geodesic ray  $[i, gi]$  is given by

$$\Psi(g) := \tan \left( \frac{\theta_g}{2} \right) = \frac{X_g - \epsilon_g}{Z_g} = \frac{Z_g}{Y_g - \epsilon_g}. \quad (3.2)$$


 FIGURE 2. Two symmetric geodesics through  $i$ 

The upper half-plane  $\mathbb{H}$  is partitioned into the following four quadrants:

$$\begin{aligned} \mathbf{I} &= \{z \in \mathbb{H} : \operatorname{Re} z > 0, |z| < 1\}, & \mathbf{II} &= \{z \in \mathbb{H} : \operatorname{Re} z > 0, |z| > 1\}, \\ \mathbf{III} &= \{z \in \mathbb{H} : \operatorname{Re} z < 0, |z| > 1\}, & \mathbf{IV} &= \{z \in \mathbb{H} : \operatorname{Re} z < 0, |z| < 1\}. \end{aligned}$$

We denote  $\gamma = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ ,  $\tilde{\gamma} = \begin{pmatrix} d & c \\ b & a \end{pmatrix}$ ,  $s = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ . Let  $\gamma \in \Gamma$ ,  $\gamma \neq I, s$ . For  $\gamma i$  to be in the right half-plane we need  $\operatorname{Re}(\gamma i) > 0$ . This is equivalent with  $ac + bd > 0$  and implies  $ac \geq 0$ ,  $bd \geq 0$  because  $abcd = bc + (bc)^2 \geq 0$ . Since  $ac \geq 0$  without loss of generality we will assume  $a \geq 0$  and  $c \geq 0$  (otherwise consider  $-\gamma$  instead). Without loss of generality assume  $b \geq 0$ ,  $d \geq 0$  as well (otherwise can consider  $\gamma s = \begin{pmatrix} -b & a \\ -d & c \end{pmatrix}$  instead since  $\gamma i = \gamma s i$ ), so we can assume  $\gamma$  has only nonnegative entries.

If  $a, b, c, d \geq 0$  and  $ad - bc = 1$ , then  $\frac{c}{a}$  and  $\frac{d}{b}$  are both  $\leq 1$  or both  $\geq 1$  (since open intervals between consecutive Farey fractions are either nonintersecting or one contains the other). Since  $\gamma i \in \mathbf{I} \iff a^2 + b^2 < c^2 + d^2$ , it follows that both  $\frac{a}{c}$  and  $\frac{b}{d}$  are  $\leq 1$  for  $\gamma i \in \mathbf{I}$ . We conclude that among the eight matrices  $\pm\gamma, \pm\gamma s, \pm\tilde{\gamma}, \pm\tilde{\gamma} s$ , which have symmetric angles (see Figure 2), the one for which  $\gamma i$  is in quadrant  $\mathbf{I}$  can be chosen such that

$$a, b, c, d \geq 0 \quad \text{and} \quad 0 \leq \frac{b}{d} < \frac{a}{c} \leq 1$$

The set of such matrices  $\gamma$  is denoted  $\Gamma_{\mathbf{I}}$ .

Consider the subset  $\mathfrak{R}_Q$  of  $\Gamma_{\mathbf{I}}$  consisting of matrices with entries at most  $Q$ , that is

$$\mathfrak{R}_Q := \left\{ \begin{pmatrix} p' & p \\ q' & q \end{pmatrix} \in \Gamma : 0 \leq p, p', q, q' \leq Q, \frac{p}{q} < \frac{p'}{q'} \leq 1 \right\},$$

and its subset  $\tilde{\mathfrak{R}}_Q$  consisting of those  $\gamma$  with  $\|\gamma\| \leq Q$ . The cardinality  $B_Q$  of  $\tilde{\mathfrak{R}}_Q$  is estimated in Corollary 8 as  $B_Q \sim \frac{3Q^2}{8}$ , in agreement with formula (58) in [22] for the number of reciprocal geodesics of length at most  $x = Q^2$ .

Let  $\mathcal{F}_Q$  be the set of Farey fractions  $p/q$  with  $0 \leq p \leq q \leq Q$  and  $(p, q) = 1$ . The *Farey tessellation* consists of semicircles on the upper half plane connecting Farey fractions  $0 \leq p/q < p'/q' \leq 1$  with  $p'q - pq' = 1$  (see Figure 3). We associate to matrices  $\gamma \in \mathfrak{R}_Q$  with entries as above the arc in the Farey tessellation connecting  $p/q$  and  $p'/q'$ . We clearly have

$$\#\mathfrak{R}_Q = 2\#\mathcal{F}_Q - 3 = \frac{Q^2}{\zeta(2)} + O(Q \ln Q).$$

4. THE COINCIDENCE OF THE PAIR CORRELATIONS OF  $\Phi$  AND  $\Psi$ 

In this section we show that the limiting pair correlations of the sets  $\{\Psi(\gamma)\}$  and  $\{\Phi(\gamma)\}$  ordered by  $\|\gamma\| \rightarrow \infty$  coincide. The proof uses properties of the Farey tessellation, via the correspondence between elements of  $\mathfrak{R}_Q$  and arcs in the Farey tessellation defined at the end of Section 3.

For  $\gamma = \begin{pmatrix} p' & p \\ q' & q \end{pmatrix} \in \mathfrak{R}_Q$ , set  $\gamma_- = \frac{p}{q}$ ,  $\gamma_+ = \frac{p'}{q'}$ . From (3.1), (3.2) we have:

$$\Psi(\gamma) - \Phi(\gamma) = \frac{Z_g}{Y_g(\epsilon_g^{-1}Y_g - 1)} \ll \frac{1}{\|\gamma\|^4}, \quad (4.1)$$

$$\gamma_- < \Phi(\gamma) < \Psi(\gamma) < \gamma_+. \quad (4.2)$$

Denote by  $\mathcal{R}_Q^\Psi(\xi)$ , respectively  $\mathcal{R}_Q^\Phi(\xi)$ , the number of pairs  $(\gamma, \gamma') \in \tilde{\mathfrak{R}}_Q^2$  such that  $0 \leq \Psi(\gamma) - \Psi(\gamma') \leq \frac{\xi}{Q^2}$ , respectively  $0 \leq \Phi(\gamma) - \Phi(\gamma') \leq \frac{\xi}{Q^2}$ . For fixed  $\beta \in (\frac{2}{3}, 1)$ , consider also

$$\mathcal{N}_{Q,\xi,\beta}^\Psi := \left\{ (\gamma, \gamma') \in \tilde{\mathfrak{R}}_Q^2 : |\Psi(\gamma) - \Psi(\gamma')| \leq \frac{\xi}{Q^2}, \|\gamma\| \leq Q^\beta \right\}.$$

and the similarly defined  $\mathcal{N}_{Q,\xi,\beta}^\Phi$ . The trivial inequality

$$\mathcal{R}_Q^\Phi(\xi) \leq 2\mathcal{N}_{Q,\xi,\beta}^\Phi + \#\left\{ (\gamma, \gamma') \in \tilde{\mathfrak{R}}_Q^2 : |\Phi(\gamma) - \Phi(\gamma')| \leq \frac{\xi}{Q^2}, \|\gamma\|, \|\gamma'\| \geq Q^\beta \right\}$$

and the estimate in (4.1) show that there exists a universal constant  $\kappa > 0$  such that

$$\mathcal{R}_Q^\Phi(\xi) \leq 2\mathcal{N}_{Q,\xi,\beta}^\Phi + \#\left\{ (\gamma, \gamma') \in \tilde{\mathfrak{R}}_Q^2 : \gamma \neq \gamma', -\frac{2\kappa}{Q^{3\beta}} \leq \Psi(\gamma) - \Psi(\gamma') \leq \frac{\xi}{Q^2} + \frac{2\kappa}{Q^{3\beta}} \right\},$$

showing that

$$\mathcal{R}_Q^\Phi(\xi) \leq 2\mathcal{N}_{Q,\xi,\beta}^\Phi + \mathcal{R}_Q^\Psi(2\kappa Q^{2-3\beta}) + \mathcal{R}_Q^\Psi(\xi + 2\kappa Q^{2-3\beta}). \quad (4.3)$$

In a similar way we show that

$$\mathcal{R}_Q^\Psi(\xi) \leq 2\mathcal{N}_{Q,\xi,\beta}^\Psi + \mathcal{R}_Q^\Phi(2\kappa Q^{2-3\beta}) + \mathcal{R}_Q^\Phi(\xi + 2\kappa Q^{2-3\beta}). \quad (4.4)$$

We first prove that  $\mathcal{N}_{Q,\xi,\beta}^\Phi$  and  $\mathcal{N}_{Q,\xi,\beta}^\Psi$  are much smaller than  $Q^2$ . For this goal and for latter use, it is important to divide pairs  $(\gamma, \gamma') \in \mathfrak{R}_Q^2$  in three cases, depending on the relative position of their associated arcs in the Farey tessellation (it is well known that two arcs in the Farey tessellation are nonintersecting):

- (i) The arcs corresponding to  $\gamma$  and  $\gamma'$  are *exterior*, i.e.  $\gamma_+ \leq \gamma'_-$  or  $\gamma'_+ \leq \gamma_-$ .
- (ii)  $\gamma' \lesssim \gamma$ , i.e.  $\gamma_- \leq \gamma'_- < \gamma'_+ \leq \gamma_+$ .
- (iii)  $\gamma \lesssim \gamma'$ , i.e.  $\gamma'_- \leq \gamma_- < \gamma_+ \leq \gamma'_+$ .

**Proposition 3.**  $\mathcal{N}_{Q,\xi,\beta}^\Phi \ll Q^{1+\beta} \ln Q$  and  $\mathcal{N}_{Q,\xi,\beta}^\Psi \ll Q^{1+\beta} \ln Q$ .

*Proof.*  $\mathcal{N}_{Q,\xi,\beta}^\Phi$  and  $\mathcal{N}_{Q,\xi,\beta}^\Psi$  are increasing as an effect of enlarging  $\tilde{\mathfrak{R}}_Q$  to  $\mathfrak{R}_Q$ , so for this proof we will replace  $\tilde{\mathfrak{R}}_Q$  by  $\mathfrak{R}_Q$ . We only consider  $\mathcal{N}_{Q,\xi,\beta}^\Phi$  here. The proof for the bound on  $\mathcal{N}_{Q,\xi,\beta}^\Psi$  is identical. Both rely on (4.1) and (4.2).

Denote  $K = \lceil \xi \rceil + 1$ . Upon (4.2) and  $|r' - r| \geq \frac{1}{Q^2}$ ,  $\forall r, r' \in \mathcal{F}_Q$ ,  $r \neq r'$ , it follows that if  $\gamma_+ \leq \gamma'_-$  and  $|\Phi(\gamma') - \Phi(\gamma)| \leq \frac{\xi}{Q^2}$ , then  $\#(\mathcal{F}_Q \cap [\gamma_+, \gamma'_-]) \leq K + 1$ . In particular  $\gamma'_- = \gamma_+$  when  $0 < \xi < 1$ .

We now consider the three cases enumerated before the statement of the proposition.

(i) The arcs corresponding to  $\gamma$  and  $\gamma'$  are exterior. Without loss of generality assume  $\gamma_+ \leq \gamma'_-$ . If  $i$  is such that  $\gamma_+ = \gamma_i$ , the  $i^{\text{th}}$  element of  $\mathcal{F}_Q$ , then  $\gamma'_- = \gamma_{i+r} = \frac{p_{i+r}}{q_{i+r}}$  for some  $0 \leq r < K$ . The equality  $p'_+ q'_- - p'_- q'_+ = 1$  shows that if  $\gamma'_- = \frac{p'_-}{q'_-}$  is fixed, then  $q'_+$  (and therefore  $\gamma'_+ = \frac{p'_+}{q'_+}$ )



is uniquely determined in intervals of length  $\leq q'_-$ . Since  $q'_\pm \leq Q$ , it follows that the number of choices for  $q'_+$  is actually  $\leq \frac{Q}{q'_-} + 1 = \frac{Q}{q_{i+r}} + 1$ .

When  $0 < \xi < 1$  one must have  $\gamma'_- = \gamma_+$ . Knowing  $q_-$  and  $q_+$  would uniquely determine the matrix  $\gamma$ . Then there will be at most  $\frac{Q}{q_+} + 1$  choices for  $\gamma'$ , so the total contribution of this case to  $\mathcal{N}_{Q,\lambda,\beta}^\Phi$  is

$$\leq \sum_{1 \leq q \leq Q^\beta} \sum_{1 \leq q' \leq Q^\beta} \left( \frac{Q}{q} + 1 \right) \ll Q^{1+\beta} \ln Q.$$

When  $\xi \geq 1$  denote by  $q_i, q_{i+1}, \dots, q_{i+K}$  the denominators of  $\gamma_i, \gamma_{i+1}, \dots, \gamma_{i+K}$ . As noticed in [11],  $q_{j+1} = \lceil \frac{Q+q_j}{q_{j+1}} \rceil q_{j+1} - q_j$ . As in [3] consider  $\kappa(x, y) := \lceil \frac{1+x}{y} \rceil$  and  $\mathcal{T}_k = \{(x, y) \in (0, 1]^2 : x + y > 1, \kappa(x, y) = k\}$ . Let  $Q$  large enough so that  $\delta_0 := Q^{\beta-1} < \frac{1}{2K+3}$ . Then  $\frac{q_i}{Q} < \delta_0$  and it is plain (cf. also [3]) that  $\frac{q_{i+1}}{Q} > 1 - \delta_0$  and  $\kappa(\frac{q_i}{Q}, \frac{q_{i+1}}{Q}) = \dots = \kappa(\frac{q_{i+K}}{Q}, \frac{q_{i+K+1}}{Q}) = 2$ . Hence  $(\frac{q_i}{Q}, \frac{q_{i+1}}{Q}) \in \mathcal{T}_1$  and  $(\frac{q_{i+1}}{Q}, \frac{q_{i+2}}{Q}), \dots, (\frac{q_{i+K}}{Q}, \frac{q_{i+K+1}}{Q}) \in \mathcal{T}_2$ , showing in particular that  $\min\{q_{i+1}, \dots, q_{i+K}\} > \frac{Q}{3}$ . Therefore  $\max\{\frac{Q}{q_{i+1}}, \dots, \frac{Q}{q_{i+K}}\} < 3$  and the contribution of this case to  $\mathcal{N}_{Q,\xi,\beta}^\Phi$  is

$$\leq \sum_{1 \leq q \leq Q^\beta} \sum_{1 \leq q' \leq Q^\beta} 4K \ll_\xi Q^{2\beta}.$$

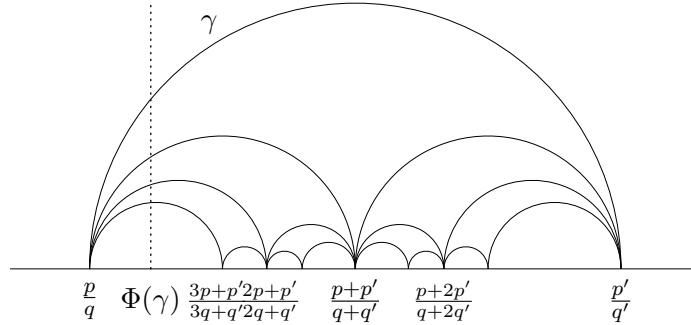


FIGURE 3. The Farey tessellation.

(ii)  $\gamma' \lesssim \gamma$ . Let  $i$  be the unique index for which  $\gamma_i < \Phi(\gamma) < \gamma_{i+1}$  with  $\gamma_i < \gamma_{i+1}$  successive elements in  $\mathcal{F}_Q$ . Since  $|\Phi(\gamma') - \Phi(\gamma)| \leq \frac{\xi}{Q^2}$ , either  $\gamma'_- < \Phi(\gamma) < \gamma'_+$  or there exists  $0 \leq r \leq K$  with  $\gamma'_+ = \gamma_{i-r}$  or with  $\gamma'_- = \gamma_{i+r}$ . In both situations the arc corresponding to the matrix  $\gamma'$  will cross at least one of the vertical lines above  $\gamma_{i-K}, \dots, \gamma_i, \gamma_{i+1}, \dots, \gamma_{i+K}$ . A glance at the Farey tessellation provides an upper bound for this number  $N_{\gamma,K}$  of arcs  $\gamma' \in \mathfrak{R}_Q$ . Actually one sees that the set  $\mathcal{C}_{\gamma,L}$  consisting of  $2 + 2^2 + \dots + 2^L$  arcs obtained from  $\gamma$  by iterating the mediant construction  $L = \lceil \frac{Q}{\min\{q_-, q_+\}} \rceil + 1$  times ( $\gamma$  is not enclosed in  $\mathcal{C}_{\gamma,L}$ ) contains the set  $\{\gamma' \in \mathfrak{R}_Q : \gamma' \lesssim \gamma, \gamma' \neq \gamma\}$ . The former set contains at most  $L$  arcs that are intersected by each vertical direction, and so  $N_{\gamma,K} \leq (2K+1)L$ . Therefore, the contribution of this case to  $\mathcal{N}_{Q,\xi,\beta}^\Phi$  is (first choose  $\gamma$ , then  $\gamma'$ )

$$\leq \sum_{1 \leq q \leq Q^\beta} \sum_{1 \leq q' \leq Q^\beta} (2K+1) \left( \frac{Q}{\min\{q, q'\}} + 1 \right) \ll_\xi Q^{1+\beta} \ln Q.$$

(iii)  $\gamma \lesssim \gamma'$ . We necessarily have  $\gamma = \gamma' M$ , with  $M \in \mathfrak{S}$ . In particular this yields  $\gamma'_\pm \in \mathcal{F}_{Q^\beta}$ . Considering the sub-tessellation defined only by arcs connecting points from  $\mathcal{F}_{Q^\beta}$ , one sees that the number of arcs intersected by a vertical line  $x = \alpha$  with  $\gamma_- = \frac{p}{q} < \alpha < \gamma_+ = \frac{p'}{q'}$ ,  $\gamma = (\gamma_-, \gamma_+) \in \mathcal{F}_{Q^\beta}$  is equal to  $s(q, q')$ , the sum of digits in the continued fraction expansion of  $\frac{q}{q'} < 1$  when  $q < q'$ , and respectively to  $s(q', q)$  when  $q' < q$ . A result from [24] yields in particular that

$$\sum_{0 < q < q' \leq Q^\beta} s(q, q') \ll Q^{2\beta} \ln^2 Q,$$

and therefore

$$\#\{(\gamma, \gamma') \in \mathfrak{R}_{Q^\beta}^2 : \gamma \lesssim \gamma'\} \leq 1 + 2 \sum_{0 < q < q' \leq Q^\beta} s(q, q') \ll Q^{2\beta} \ln^2 Q.$$

This completes the proof of the proposition.  $\square$

Proposition 3 and inequalities (4.3) and (4.4) provide

**Corollary 4.** *For each  $\beta \in (\frac{2}{3}, 1)$ ,*

$$\mathcal{R}_Q^\Psi(\xi) = \mathcal{R}_Q^\Phi(\xi + O(Q^{2-3\beta})) + \mathcal{R}_Q^\Phi(O(Q^{2-3\beta})) + O(Q^{1+\beta} \ln Q).$$

## 5. A DECOMPOSITION OF THE PAIR CORRELATION OF $\{\Phi(\gamma)\}$

To estimate  $\mathcal{R}_Q^\Phi(\xi)$ , recall the correspondence between elements of  $\mathfrak{R}_Q$  and arcs in the Farey tessellation from the end of Section 3. We consider the following two possibilities for the arcs associated to a pair  $(\gamma, \gamma') \in \tilde{\mathfrak{R}}_Q^2$ :

- (i) One of the arcs corresponding to  $\gamma$  and  $\gamma'$  contains the other.
- (ii) The arcs corresponding to  $\gamma$  and  $\gamma'$  are exterior (possibly tangent).

Denoting by  $R_Q^\cap(\xi), R_Q^\cap(\xi)$  the number of pairs in each case we have

$$\mathcal{R}_Q^\Phi(\xi) = R_Q^\cap(\xi) + R_Q^\cap(\xi).$$

**5.1. One of the arcs contains the other.** In this case we have either  $\gamma = \gamma' M$  or  $\gamma' = \gamma M$  with  $M \in \mathfrak{S}$  (see also Figure 4). For each  $M \in \Gamma$  define

$$\Xi_M(x, y) = \frac{xy(Y_M - X_M) + (x^2 - y^2)Z_M}{(x^2 + y^2)(x^2 X_M + y^2 Y_M + 2xy Z_M)}, \quad (5.1)$$

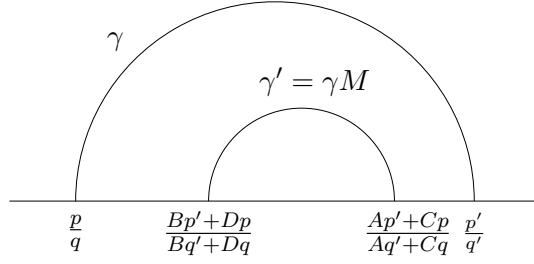
where  $X_M, Y_M, Z_M$  are defined in (3.1). A direct calculation leads for  $\gamma = \left(\frac{p'}{q'}, \frac{p}{q}\right)$  to

$$\Phi(\gamma) - \Phi(\gamma M) = \Xi_M(q', q) \quad (5.2)$$

proving the next statement.

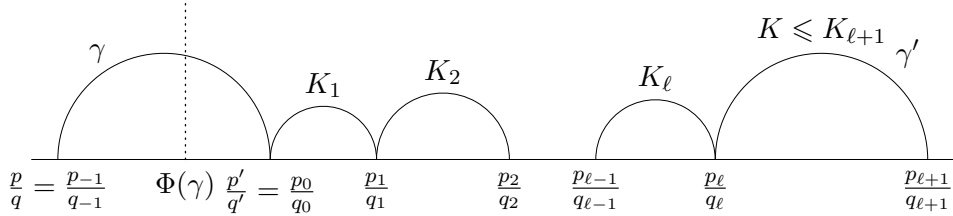
**Lemma 5.** *The number of pairs  $(\gamma, \gamma') \in \tilde{\mathfrak{R}}_Q^2$ ,  $\gamma \neq \gamma'$ , with  $0 \leq \Phi(\gamma) - \Phi(\gamma') \leq \frac{\xi}{Q^2}$  and  $\gamma \lesssim \gamma'$  or  $\gamma' \lesssim \gamma$  (with the notation introduced before Prop. 3) is given by*

$$R_Q^\cap(\xi) = \#\left\{(\gamma, \gamma M) \in \tilde{\mathfrak{R}}_Q^2 : \gamma = \left(\frac{p'}{q'}, \frac{p}{q}\right), M \in \mathfrak{S}, |\Xi_M(q', q)| \leq \frac{\xi}{Q^2}\right\}.$$


 FIGURE 4. The case  $\gamma' \lesssim \gamma$ 

5.2. **Exterior arcs.** In this case we have  $\gamma, \gamma' \in \tilde{\mathfrak{R}}_Q$ ,  $\gamma'_- \geq \gamma_+$ . Let  $\ell \geq 0$  be the number of Farey arcs in  $\mathcal{F}_Q$  connecting the arcs corresponding to  $\gamma, \gamma'$  (see Figure 5). In other words, writing  $\gamma = \left(\frac{p'}{q'}, \frac{p}{q}\right)$ ,  $\gamma' = \left(\frac{p_{\ell+1}}{q_{\ell+1}}, \frac{p_{\ell}}{q_{\ell}}\right)$ , we have that  $\frac{p_0}{q_0} := \frac{p'}{q'}, \frac{p_1}{q_1}, \dots, \frac{p_{\ell}}{q_{\ell}}$  are consecutive elements in  $\mathcal{F}_Q$ . Setting also  $\frac{p_{-1}}{q_{-1}} := \frac{p}{q}$ , it follows that  $q_i = K_i q_{i-1} - q_{i-2}$ , where  $K_i \in \mathbb{N}$ ,  $i = 1, \dots, \ell$ , and  $K_i = \left\lfloor \frac{Q+q_{i-2}}{q_{i-1}} \right\rfloor$  for  $2 \leq i \leq \ell$ .

The fractions  $\frac{p_{\ell}}{q_{\ell}}, \frac{p_{\ell+1}}{q_{\ell+1}}$  are not necessarily consecutive in  $\mathcal{F}_Q$ , but we have  $q_{\ell+1} = K q_{\ell} - q_{\ell-1}$ ,  $K \leq K_{\ell+1} = \left\lfloor \frac{Q+q_{\ell}}{q_{\ell+1}} \right\rfloor$ . It follows that  $\gamma' = \gamma M$  with  $M = \begin{pmatrix} K_1 & 1 \\ -1 & 0 \end{pmatrix} \cdots \begin{pmatrix} K_{\ell} & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} K & 1 \\ -1 & 0 \end{pmatrix}$ .


 FIGURE 5. The case when  $\gamma$  and  $\gamma'$  are exterior

We have  $\ell < \xi$  because

$$\Phi(\gamma') - \Phi(\gamma) > \sum_{i=1}^{\ell} \frac{1}{q_{i-1}q_i} \geq \frac{\ell}{Q^2}.$$

It is also plain to see that

$$\frac{p'}{q'} - \Phi(\gamma) = \frac{q}{q'(q^2 + q'^2)}, \quad \Phi(\gamma') - \frac{p_{\ell}}{q_{\ell}} = \frac{q_{\ell+1}}{q_{\ell}(q_{\ell}^2 + q_{\ell+1}^2)}. \quad (5.3)$$

The last equality in (5.3) and  $q_{\ell}^2 + q_{\ell+1}^2 \leq Q^2$  yield for  $\ell \geq 1$

$$\begin{aligned} \frac{\xi}{Q^2} &\geq \Phi(\gamma') - \Phi(\gamma) \geq \frac{1}{q_{\ell-1}q_{\ell}} + \frac{q_{\ell+1}}{q_{\ell}(q_{\ell}^2 + q_{\ell+1}^2)} \\ &\geq \frac{1}{q_{\ell-1}q_{\ell}} + \frac{Kq_{\ell} - q_{\ell-1}}{q_{\ell}Q^2} = \frac{K}{Q^2} + \frac{Q^2 - q_{\ell-1}^2}{q_{\ell-1}q_{\ell}Q^2} \geq \frac{K}{Q^2} \end{aligned}$$

while if  $\ell = 0$  we have

$$\Phi(\gamma') - \Phi(\gamma) = \frac{K(q'^2 + qq_1)}{(q^2 + q'^2)(q'^2 + q_1^2)} \geq \frac{K}{Q^2},$$

showing that  $K < \xi$ . Notice also that (5.3) yields

$$\Phi(\gamma') - \Phi(\gamma) = \frac{q}{q'(q^2 + q'^2)} + \sum_{i=1}^{\ell} \frac{1}{q_{i-1}q_i} + \frac{q_{\ell+1}}{q_{\ell}(q_{\ell}^2 + q_{\ell+1}^2)}.$$

Let  $\mathcal{T} = \{(x, y) \in (0, 1]^2 : x + y > 1\}$  and consider the map

$$T : (0, 1]^2 \rightarrow \mathcal{T}, \quad T(x, y) = \left( y, \left[ \frac{1+x}{y} \right] y - x \right).$$

Its restriction to  $\mathcal{T}$  is a area-preserving bijection of  $\mathcal{T}$  [3]. Denote  $T^i = (L_{i-1}, L_i)$  and  $K_i = \left[ \frac{1+L_{i-2}}{L_{i-1}} \right]$  if  $i = 0, 1, \dots, \ell$ ,  $K_{\ell+1} = K$ , and  $L_{\ell+1} = KL_{\ell} - L_{\ell-1}$ , so one has

$$\begin{aligned} 0 < L_i(x, y) &\leq 1, \quad i \geq 0, & L_{i-1}(x, y) + L_i(x, y) &> 1, \quad i = 1, \dots, \ell, \\ L_{-1}(x, y) &= x, & L_0(x, y) &= y, \\ L_i(x, y) &= K_i(x, y)L_{i-1}(x, y) - L_{i-2}(x, y), \quad i = 0, 1, \dots, \ell + 1, \\ (q_{i-1}, q_i) &= QT^i\left(\frac{q}{Q}, \frac{q'}{Q}\right) = \left( QL_{i-1}\left(\frac{q}{Q}, \frac{q'}{Q}\right), QL_i\left(\frac{q}{Q}, \frac{q'}{Q}\right) \right), \quad i = 0, 1, \dots, \ell, \\ q_{\ell+1} &= Kq_{\ell} - q_{\ell-1} = Q\left( KL_{\ell}\left(\frac{q}{Q}, \frac{q'}{Q}\right) - L_{\ell-1}\left(\frac{q}{Q}, \frac{q'}{Q}\right) \right). \end{aligned} \tag{5.4}$$

Define also the function

$$\Upsilon_{\ell, K} : (0, 1]^2 \rightarrow (0, \infty), \quad \Upsilon_{\ell, K} = \frac{L_{-1}}{L_0(L_{-1}^2 + L_0^2)} + \sum_{i=1}^{\ell} \frac{1}{L_{i-1}L_i} + \frac{L_{\ell+1}}{L_{\ell}(L_{\ell}^2 + L_{\ell+1}^2)}. \tag{5.5}$$

We proved the following statement.

**Lemma 6.** *The number  $R_Q^{\cap}(\xi)$  of pairs  $(\gamma, \gamma')$  of exterior (possibly tangent) arcs in  $\tilde{\mathfrak{R}}_Q$  for which  $0 < \Phi(\gamma') - \Phi(\gamma) \leq \frac{\xi}{Q^2}$  is given by*

$$R_Q^{\cap}(\xi) = \sum_{\substack{\ell \in [0, \xi) \\ K \in [1, \xi)}} \# \left\{ \begin{array}{l} 0 \leq p \leq q, \quad 0 \leq p' \leq q', \quad p'q - pq' = 1 \\ \begin{pmatrix} p' & p \\ q' & q \end{pmatrix} : p^2 + p'^2 + q^2 + q'^2 \leq Q^2, \quad 0 < Kq_{\ell} - q_{\ell-1} \leq Q \\ p_{\ell}^2 + q_{\ell}^2 + (Kp_{\ell} - p_{\ell-1})^2 + (Kq_{\ell} - q_{\ell-1})^2 \leq Q^2 \\ \Upsilon_{\ell, K}\left(\frac{q}{Q}, \frac{q'}{Q}\right) \leq \xi \end{array} \right\} \tag{5.6}$$

where the sums are over integers in the given intervals, and  $q_{-1} = q, q_0 = q'$ .

## 6. A LATTICE POINT ESTIMATE

**Lemma 7.** *Suppose that  $\Omega$  is a region in  $\mathbb{R}^2$  of area  $A(\Omega)$  and rectifiable boundary of length  $\ell(\partial\Omega)$ . For every integer  $r$  with  $(r, q) = 1$  and  $1 \leq L \leq q$*

$$\mathcal{N}_{\Omega, q, r} := \#\{(a, b) \in \Omega \cap \mathbb{Z}^2 : ab \equiv r \pmod{q}\} = \frac{\varphi(q)}{q^2} A(\Omega) + \mathcal{E}_{\Omega, L, q},$$

where, for each  $\varepsilon > 0$ ,

$$\mathcal{E}_{\Omega, L, q} \ll_{\varepsilon} \frac{q^{1/2+\varepsilon} A(\Omega)}{L^2} + \left(1 + \frac{\ell(\partial\Omega)}{L}\right) \left(\frac{L^2}{q} + q^{1/2+\varepsilon}\right).$$

*Proof.* Replacing  $\mathbb{Z}^2$  by  $L\mathbb{Z}^2$  in the estimate (for a proof see [15, Thm. 5.9])

$$\{(m, n) \in \mathbb{Z}^2 : (m, m+1) \times (n, n+1) \cap \partial\Omega\} \ll 1 + \ell(\partial\Omega),$$

we find that the number of squares  $S_{m,n} = [Lm, L(m+1)] \times [Ln, L(n+1)]$  with  $\mathring{S}_{m,n} \cap \partial\Omega \neq \emptyset$  is  $\ll 1 + \frac{1}{L}\ell(\partial\Omega)$ . Therefore

$$\#\{(m, n) \in \mathbb{Z}^2 : (Lm, L(m+1)) \times (Ln, L(n+1)) \subseteq \Omega\} = \frac{A(\Omega)}{L^2} + O\left(1 + \frac{\ell(\partial\Omega)}{L}\right).$$

Weil's estimates on Kloosterman sums [23] extended to composite moduli in [12] and [7] show that each such square contains  $\frac{\varphi(q)}{q^2}L^2 + O_\varepsilon(q^{1/2+\varepsilon})$  pairs of integers  $(a, b)$  with  $ab \equiv r \pmod{q}$  (see, e.g. [2, Lemma 1.7] for details). Combining these two estimates we find

$$\mathcal{N}_{\Omega, q, r} = \left(\frac{A(\Omega)}{L^2} + O\left(1 + \frac{\ell(\partial\Omega)}{L}\right)\right) \left(\frac{\varphi(q)}{q^2}L^2 + O(q^{1/2+\varepsilon})\right) = \frac{\varphi(q)}{q^2}A(\Omega) + \mathcal{E}_{\Omega, q, L},$$

as desired.  $\square$

**Corollary 8.**  $\#\tilde{\mathfrak{R}}_Q = \frac{3Q^2}{8} + O_\varepsilon(Q^{11/6+\varepsilon})$ .

*Proof.* Note first that one can substitute  $\frac{pq'}{q}$  for  $p' = \frac{1+pq'}{q'}$  in the definition of  $\tilde{\mathfrak{R}}_Q$ , replacing the inequality  $\|\gamma\|^2 \leq Q^2$  by  $(q^2 + q'^2)(q^2 + p^2) \leq Q^2q^2$  without altering the error term. Applying Lemma 7 to  $\Omega_q = \{(u, v) \in [0, q] \times [0, Q] : (q^2 + u^2)(q^2 + v^2) \leq Q^2q^2\}$  and  $L = q^{5/6}$  we infer

$$\#\tilde{\mathfrak{R}}_Q = \sum_{q=1}^Q \frac{\varphi(q)}{q} \cdot \frac{A(\Omega_q)}{q} + O_\varepsilon(Q^{11/6+\varepsilon}).$$

Standard Möbius summation (see, e.g., [2, Lemma 2.3]) applied to the function  $h(q) = \frac{1}{q}A(\Omega_q)$  with  $\|h\|_\infty \leq Q$  and the change of variable  $(q', u, v) = (Qx, Qxy, Qz)$  further yield

$$\#\tilde{\mathfrak{R}}_Q = \frac{Q^2}{\zeta(2)} \text{Vol}(S) + O_\varepsilon(Q^{11/6+\varepsilon}),$$

where

$$S = \{(x, y, z) \in [0, 1]^3 : (1 + y^2)(x^2 + z^2) \leq 1\}.$$

The substitution  $y = \tan \theta$  yields

$$\text{Vol}(S) = \int_0^{\pi/4} \frac{d\theta}{\cos^2 \theta} A(\{(x, z) \in [0, 1]^2 : x^2 + z^2 \leq \cos^2 \theta\}) = \frac{\pi^2}{16},$$

completing the proof of the corollary.  $\square$

The error bound in Corollary 8 can be improved using spectral methods (see Corollary 12.2 in Iwaniec's book [13]). We have given the proof since it is the prototype of applying Lemma 7 to the counting problems of the next section.

## 7. PAIR CORRELATION OF $\{\Phi(\gamma)\}$

The main result of this section is Theorem 2, where we obtain an explicit formula for the pair correlation of the quantities  $\{\Phi(\gamma)\}$  in terms of volumes of three dimensional bodies. The discussion is divided in two cases, as in Section 5.

**7.1. One of the arcs contains the other.** The formula for  $R_Q^{\text{fl}}$  in Lemma 5 provides

$$R_Q^{\text{fl}}(\xi) = \sum_{M \in \mathfrak{S}} \mathcal{N}_{M,Q}(\xi), \quad (7.1)$$

where  $\mathcal{N}_{M,Q}(\xi)$  denotes the number of matrices  $\gamma = \begin{pmatrix} p' & p \\ q' & q \end{pmatrix}$  for which

$$0 \leq p \leq q, \quad 0 \leq p' \leq q', \quad p'q - pq' = 1, \quad |\Xi_M(q', q)| \leq \frac{\xi}{Q^2}, \quad \|\gamma M\| \leq Q. \quad (7.2)$$

The first goal is to replace in (7.2) the inequality  $\|\gamma M\| \leq Q$  by a more tractable one. Taking  $\gamma = \begin{pmatrix} p' & p \\ q' & q \end{pmatrix}$  and substituting  $p = \frac{p'q-1}{q'}$  we write, using the notation (3.1):

$$\|\gamma M\|^2 = \left( \frac{p'^2}{q'^2} + 1 \right) (q'^2 X_M + q^2 Y_M + 2qq' Z_M) + \frac{Y_M}{q'^2} - 2p' \frac{qY_M + q'Z_M}{q'^2}. \quad (7.3)$$

Let  $\tilde{\mathcal{N}}_M(Q, \xi)$  denote the number of integer triples  $(q', q, p')$  such that

$$\begin{cases} 0 \leq p' \leq q' \leq Q, & 0 < q \leq Q, & p'q \equiv 1 \pmod{q'}, \\ |\Xi_M(q', q)| \leq \frac{\xi}{Q^2}, & q'^2 X_M + q^2 Y_M + 2qq' Z_M \leq \frac{Q^2 q'^2}{p'^2 + q'^2}. \end{cases} \quad (7.4)$$

If  $Y_M \leq Q^{2c_0}$  for some constant  $c_0 \in (\frac{1}{2}, 1)$ , then (7.3) yields

$$\mathcal{N}_{M,Q}(\xi) = \tilde{\mathcal{N}}_M(Q(1 + O(Q^{c_0-1})), \xi). \quad (7.5)$$

Next we show that  $\mathcal{N}_{M,Q}(\xi) = 0$  when  $\max\{X_M, Y_M\} \geq Q^{2c_0}$  and  $Q$  is large enough.

**Lemma 9.** *Let  $c_0 \in (\frac{1}{2}, 1)$ . There exists  $Q_0(\xi)$  such that  $\mathcal{N}_{M,Q}(\xi) = 0$  for every  $M \in \mathfrak{S}$  with  $\max\{X_M, Y_M\} \geq Q^{2c_0}$  and  $Q \geq Q_0(\xi)$ .*

*Proof.* We show there are no coprime positive integer lattice points  $(q', q)$  for which

$$|\Xi_M(q', q)| \leq \frac{\xi}{Q^2}, \quad Y_{\gamma M} = q'^2 X_M + q^2 Y_M + 2qq' Z_M \leq Q^2. \quad (7.6)$$

Suppose  $(q', q)$  is such a point, write in polar coordinates  $q'i + q = (q, q') = (r \cos \theta, r \sin \theta)$ ,  $\theta \in (0, \frac{\pi}{2})$ , and consider  $(X, Y, Z) = (X_M, Y_M, Z_M)$ ,  $T = \|M\|^2 = X + Y$ ,  $U_M = \coth \ell(M) = \frac{T}{\sqrt{T^2 - 4}}$ .

Since  $\sin \theta_M = \frac{2Z}{\sqrt{T^2 - 4}}$  and  $\cos \theta_M = \frac{Y - X}{\sqrt{T^2 - 4}}$ , the inequalities in (7.6) can be described as

$$\frac{1}{\xi} \cdot \frac{|\sin(\theta_M - 2\theta)|}{U_M + \cos(\theta_M - 2\theta)} \leq \frac{r^2}{Q^2} \leq \frac{2}{(U_M + \cos(\theta_M - 2\theta))\sqrt{T^2 - 4}}. \quad (7.7)$$

Denoting  $\delta_M = \frac{\theta_M}{2} - \theta$ , from the first and last fraction in (7.7) we infer  $|\sin 2\delta_M| \ll \frac{1}{T}$ . Therefore  $\delta_M$  is close to 0, or to  $\pm \frac{\pi}{2}$ . When  $\delta_M$  is close to 0 we have  $|\tan \delta_M| \ll |\delta_M| \ll |\sin 2\delta_M| \ll \frac{1}{T}$ . When  $\delta_M$  is close to  $\pm \frac{\pi}{2}$  we similarly have  $|\delta_M \mp \frac{\pi}{2}| \ll \frac{1}{T}$ , which we claim is impossible. From

$$\frac{|\tan \delta_M|}{1 + \frac{U_M - 1}{1 + \cos 2\delta_M}} = \frac{|\sin 2\delta_M|}{U_M + \cos 2\delta_M} \leq \frac{\xi}{v^3}$$

it suffices to bound from above  $\frac{U_M - 1}{1 + \cos 2\delta_M}$ , which would imply  $|\tan \delta_M| \ll \xi$ , contradicting  $|\delta_M \mp \frac{\pi}{2}| \ll \frac{1}{T}$ . Since  $Z$  is a positive integer we have  $\sin \theta_M \gg \frac{1}{T}$ . Since  $\cos \theta, \sin \theta > 0$  and  $\theta_M \in (0, \pi)$ , at least one of  $\cos 2\delta_M + \cos \theta_M$  or  $\cos 2\delta_M - \cos \theta_M$  must be nonnegative, showing that  $\cos 2\delta_M \geq -|\cos \theta_M|$ , and so we have

$$1 + \cos 2\delta_M \geq 1 - |\cos \theta_M| = 1 - \sqrt{1 - \sin^2 \theta_M} \gg \frac{1}{T^2}.$$

As  $U_M - 1 \ll \frac{1}{T^2}$ , it follows that  $\frac{U_M - 1}{1 + \cos 2\delta_M} \ll 1$ , proving the claim.

We have thus shown that  $|\delta_M| \leq |\tan \delta_M| \ll \frac{1}{T}$ .

Case I.  $Y > X$ . Then  $0 < \frac{\theta_M}{2} < \frac{\pi}{4}$  and  $Z = \sqrt{XY - 1} < Y$ . Since  $|\delta_M| \ll \frac{1}{T} \ll Q^{-2c_0}$ , it follows that  $0 < \theta < \frac{\pi}{3}$  for large  $Q$ . Employing the formula  $\tan\left(\frac{\theta_M}{2}\right) = \frac{Z}{Y - \epsilon_T}$  we now have

$$\left| \frac{AC + BD}{C^2 + D^2 - \epsilon_T} - \frac{q'}{q} \right| = |\tan \delta_M| \left| 1 + \tan \theta \tan\left(\frac{\theta_M}{2}\right) \right| \ll \frac{1}{T}. \quad (7.8)$$

Combining (7.8) with  $0 < \frac{Z}{Y - \epsilon_T} - \frac{Z}{Y} \ll \frac{1}{T}$  and with  $\left| \frac{Z}{Y} - \frac{A+B}{C+D} \right| \leq \frac{1}{C^2 + D^2} \ll \frac{1}{T}$ , we arrive at

$$\left| \frac{A+B}{C+D} - \frac{q'}{q} \right| \ll \frac{1}{T} \leq Q^{-2c_0}. \quad (7.9)$$

If nonzero, the left-hand side in (7.9) must be  $\geq \frac{1}{q(C+D)}$ . But  $q(C+D) \leq q\sqrt{2(C^2 + D^2)} \leq Q\sqrt{2}$ , and so  $Q^{2c_0} \ll Q$ , contradiction. It remains that  $q = C + D$  and  $q' = A + B$ , which again is not possible because  $Q^{2c_0} \leq (C + D)^2 = q(C + D) \leq Q\sqrt{2}$ .

Case II.  $X > Y$ . Then  $\frac{\pi}{4} < \frac{\theta_M}{2} < \frac{\pi}{2}$  and  $Y \leq \sqrt{XY - 1} = Z$ . As  $|\delta_T| \ll Q^{-2c_0}$ , we must have  $0 < \frac{\pi}{2} - \theta < \frac{\pi}{3}$  for large values of  $Q$ . This time we have

$$\begin{aligned} \left| \frac{Y - \epsilon_T}{Z} - \frac{q}{q'} \right| &= \left| \tan\left(\frac{\pi}{2} - \frac{\theta_M}{2}\right) - \tan\left(\frac{\pi}{2} - \theta\right) \right| \\ &= |\tan \delta_M| \left| 1 + \tan\left(\frac{\pi}{2} - \frac{\theta_M}{2}\right) \tan\left(\frac{\pi}{2} - \theta\right) \right| \leq (1 + \sqrt{3}) |\tan \delta_M| \ll \frac{1}{T}, \end{aligned}$$

which leads (use  $D \geq C \iff B \geq A$ ) to

$$\begin{aligned} \left| \frac{C+D}{A+B} - \frac{q}{q'} \right| &\ll \frac{1}{T} + \frac{\epsilon_T}{Z} + \left| \frac{Y}{Z} - \frac{C+D}{A+B} \right| \ll \frac{1}{T} + \frac{|D-C|}{(A+B)(AC+BD)} \\ &\leq \frac{1}{T} + \frac{1}{(A+B)^2} \leq \frac{1}{T} + \frac{1}{X} \ll \frac{1}{T} \ll Q^{-2c_0}. \end{aligned} \quad (7.10)$$

As in Case I this leads to a contradiction because  $q'(A+B) \leq q'\sqrt{2X} \leq Q\sqrt{2}$  and  $(A+B)^2 \geq Q^{2c_0}$ .  $\square$

In summary, the nonzero contributions to (7.1) can only come from the matrices  $M \in \mathfrak{S}$  with  $\max\{X_M, Y_M\} \leq Q^{2c_0}$ . Next we apply Lemma 7 with  $r = 1$  to the set

$$\Omega = \Omega_{M, q', \xi} = \left\{ (u, v) \in [0, Q] \times [0, q'] : |\Xi_M(q', u)| \leq \frac{\xi}{Q^2}, q'^2 X_M + q^2 Y_M + 2qq' Z_M \leq \frac{Q^2 q^2}{v^2 + q^2} \right\},$$

assuming  $\max\{X_M, Y_M\} \leq Q^{2c_0}$ . We have  $A(\Omega) \leq Q^{1-c_0} q'$ ,  $\ell(\partial\Omega) \ll Q^{1-c_0} + q' \ll Q^{1-c_0}$ ,  $L = q^{5/6}$ , getting  $\mathcal{E}_{\Omega, L, q'} \ll Q^{1-c_0} q'^{-1/6}$  and therefore

$$\tilde{N}_M(Q, \xi) = \sum_{q' \leq Q/\sqrt{X_M}} \frac{\varphi(q')}{q'^2} A(\Omega_{M, q', \xi}) + O_\epsilon \left( \sum_{q' \leq Q/\sqrt{X_M}} Q^{1-c_0} q'^{-1/6+\epsilon} \right). \quad (7.11)$$

A choice of  $\max\{A, B\}$  and  $\max\{C, D\}$  determines  $M$  uniquely, the total contribution of error terms from (7.11) to  $R_Q^{\mathfrak{m}}(\xi)$  is

$$\ll_\xi \sum_{C \leq Q^{c_0}} \sum_{A \leq Q^{c_0}} \sum_{q' \leq Q/A} Q^{1-c_0} q'^{-1/6+\epsilon} \ll Q \sum_{A \leq Q^{c_0}} \left( \frac{Q}{A} \right)^{5/6+\epsilon} \ll Q^{(11+c_0)/6+\epsilon}. \quad (7.12)$$

To estimate the contribution of the main terms we apply Möbius summation to the function  $h_1(q') = \frac{1}{q'} A(\Omega_{M,q',\xi})$  with  $\|h_1\|_\infty \leq Q^{1-c_0}$  and the change of variables  $(q', u, v) = (Qx, Qy, Qxz)$ ,  $(x, y, z) \in [0, 1]^3$ , (7.12) and (7.5), to find

$$\begin{aligned} R_Q^{\text{fl}}(\xi) &= \frac{1}{\zeta(2)} \sum_{\substack{M \in \mathfrak{G} \\ X_M, Y_M \leq Q^{2c_0}}} \left( \int_0^{Q/\sqrt{X_M}} A(\Omega_{M,q',\xi}) \frac{dq'}{q'} + O(Q^{1-c_0} \ln Q) \right) + O_\varepsilon(Q^{(11+c_0)/6+\varepsilon}) \\ &= \frac{Q^2}{\zeta(2)} \sum_{\substack{M \in \mathfrak{G} \\ X_M, Y_M \leq Q^{2c_0}}} \text{Vol}(S_{M,\xi}) + O_\xi(Q^{1+c_0} \ln^2 Q) + O_\varepsilon(Q^{1+c_0+\varepsilon} + Q^{(11+c_0)/6+\varepsilon}), \end{aligned} \quad (7.13)$$

where  $S_{M,\xi}$  is the three dimensional body

$$S_{M,\xi} := \left\{ (x, y, z) \in [0, 1]^3 : |\Xi_M(x, y)| \leq \xi, \quad x^2 X_M + y^2 Y_M + 2xy Z_M \leq \frac{1}{1+z^2} \right\}. \quad (7.14)$$

With  $\eta = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$  notice the equality  $\Xi_{\eta M \eta}(y, x) = -\Xi_M(x, y)$ . Therefore the reflection  $(x, y, z) \mapsto (y, x, z)$  maps  $S_{M,\xi}$  bijectively onto  $S_{\eta M \eta, \xi}$ .

Next we give upper bounds for  $\text{Vol}(S_{M,\xi})$ . Take  $(x, y, z) = (r \cos t, r \sin t, z) \in S_{M,\xi}$ . The proof of (7.9) and (7.10) does not use the integrality of  $q'$  and  $q$ , so denoting  $\omega_M = \frac{C+D}{A+B}$  if  $X_M < Y_M$  and  $\omega_M = \frac{A+B}{C+D}$  if  $Y_M < X_M$  we find  $|\frac{y}{x} - \omega_M| \ll \frac{1}{T}$  in the former case and respectively  $|\frac{x}{y} - \omega_M| \ll \frac{1}{T}$  in the latter case. Writing the area in polar coordinates we find  $r^2 \leq \frac{2}{T}$  and

$$\begin{aligned} \text{Vol}(S_{M,\xi}) &\leq A(\{(x, y) \in [0, 1]^2 : \exists z \in [0, 1], (x, y, z) \in S_{M,\xi}\}) \\ &\leq \frac{1}{2} \int_{\omega_M - \xi T_M^{-1}}^{\omega_M + \xi T_M^{-1}} 2T_M^{-1} dt = \frac{2\xi}{T_M^2} = \frac{2\xi}{\|M\|^4}. \end{aligned} \quad (7.15)$$

The bound (7.15) yields

$$\sum_{M \in \mathfrak{G}} \text{Vol}(S_{M,\xi}) < \infty \quad \text{and} \quad \sum_{\substack{M \in \mathfrak{G} \\ A^2 + B^2 \geq Q^{2c_0}}} \text{Vol}(S_{M,\xi}) \ll_\xi Q^{-2c_0}. \quad (7.16)$$

From (7.13), (7.16) and  $c_0 \in (\frac{1}{2}, 1)$  we infer

$$R_Q^{\text{fl}}(\xi) = \frac{Q^2}{\zeta(2)} \sum_{M \in \mathfrak{G}} \text{Vol}(S_{M,\xi}) + O_\varepsilon(Q^{(11+c_0)/6+\varepsilon}). \quad (7.17)$$

The volume of  $S_{M,\xi}$  can be evaluated in closed form using the substitution  $z = \tan t$ :

$$\text{Vol}(S_{M,\xi}) = \int_0^{\pi/4} B_M(\xi, t) \frac{dt}{\cos^2 t}, \quad (7.18)$$

where  $B_M(\xi, t)$  is the area of the region

$$\left\{ (r \cos \theta, r \sin \theta) \in [0, 1]^2 : \frac{1}{\xi} \cdot \frac{|\sin(2\theta - \theta_M)|}{U_T + \cos(2\theta - \theta_M)} \leq r^2 \leq \frac{1}{\sqrt{T^2 - 4}} \cdot \frac{2 \cos^2 t}{U_T + \cos(2\theta - \theta_M)} \right\}, \quad (7.19)$$

with  $\theta_M \in (0, \frac{\pi}{2})$  having  $\sin \theta_M = \frac{2Z_M}{\sqrt{T^2 - 4}}$  and  $U_T = \frac{T}{\sqrt{T^2 - 4}}$  (for brevity we write  $T = T_M$ ).

The following elementary fact will be useful to prove the differentiability of the volumes as functions of  $\xi$ .



**Lemma 10.** *Assume  $G, H : K \rightarrow \mathbb{R}$  are continuous functions on a compact set  $K \subset \mathbb{R}^k$  and denote  $x_+ = \max\{x, 0\}$ . The formula*

$$V(\xi) := \int_K (\xi - G(v))_+ H(v) dv, \quad \xi \in \mathbb{R},$$

defines a  $C^1$  map on  $\mathbb{R}$  and

$$V'(\xi) = \int_{G < \xi} H(v) dv.$$

Using equation (7.18) we find

$$\text{Vol}(S_{M,\xi}) = \frac{1}{2} \int_0^{\pi/4} dt \int_0^{\pi/2} d\theta \frac{(2/\sqrt{T^2-4} - |\sin(2\theta - \theta_M)|/(\xi \cos^2 t))_+}{U_T + \cos(2\theta - \theta_M)} \quad (7.20)$$

and applying Lemma 10 we obtain:

**Corollary 11.** *The function  $\xi \mapsto \text{Vol}(S_{M,\xi})$  is  $C^1$ .*

For a smaller range for  $\xi$  we have the following explicit formula.

**Lemma 12.** *Suppose that  $\xi \leq Z_M$ . The volume of  $S_{M,\xi}$  only depends on  $\xi$  and  $T = \|M\|^2$ :*

$$\text{Vol}(S_{M,\xi}) = \int_0^{\pi/4} \tan^{-1} \left( \frac{\sqrt{\Delta} - \sqrt{\Delta - 4\xi^2 \cos^4 t}}{2\alpha\xi \cos^2 t} \right) + \frac{1}{2\xi \cos^2 t} \ln \left( 1 - \frac{\sqrt{\Delta} - \sqrt{\Delta - 4\xi^2 \cos^4 t}}{2\alpha} \right) dt,$$

where  $\Delta = T^2 - 4$  and  $\alpha = \frac{T + \sqrt{T^2 - 4}}{2}$ .

*Proof.* The two polar curves in (7.19) intersect for  $|\sin(2\theta - \theta_M)| = \frac{2\xi}{\sqrt{T^2-4}} \cos^2 t$  that is for  $\theta_{\pm} = \frac{\theta_M}{2} \pm \alpha$ , with  $\alpha = \alpha(\xi, t) \in (0, \frac{\pi}{4})$  such that  $\sin 2\alpha = \frac{2\xi}{\sqrt{T^2-4}} \cos^2 t$ . Since  $\sin \theta_M = \frac{2Z}{\sqrt{T^2-4}}$ , the assumption  $\xi \leq Z$  ensures that  $\alpha < \theta_M$ . Thus  $\theta_{\pm} \in [0, \frac{\pi}{2})$ , and a change of variables  $\theta = \frac{\theta_M}{2} + u$  yields

$$B_{M,\xi}(t) = \frac{1}{2} \int_{-\alpha}^{\alpha} \left( \frac{2 \cos^2 t}{\sqrt{T^2-4}} \cdot \frac{1}{U_T + \cos(2u)} - \frac{|\sin(2u)|}{\xi(U_T + \cos(2u))} \right) du.$$

The integrand is even and both integrals can be computed exactly, yielding the formula above.  $\square$

In particular Lemma 12 yields  $\text{Vol}(S_{M,\xi}) \ll \frac{\xi}{T^2}$ , providing an alternative proof for (7.15).

**7.2. Exterior arcs.** Referring to the notation of Sec. 5.2, we first replace the inequalities  $p^2 + p'^2 + q^2 + q'^2 \leq Q^2$  and  $p_\ell^2 + q_\ell^2 + (Kp_\ell - p_{\ell-1})^2 + (Kq_\ell - q_{\ell-1})^2 \leq Q^2$  in (5.6) by simpler ones. Using  $p'q - pq' = 1$  we can replace  $p$  by  $\frac{p'q}{q}$  in the former, while  $p_{\ell-1}$  can be replaced by  $\frac{p_\ell q_{\ell-1}}{q_\ell}$  in the latter. As a result these two inequalities can be substituted in (5.6) by

$$\begin{cases} \left(1 + \frac{p'^2}{q'^2}\right)(q^2 + q'^2) \leq Q^2 \left(1 + O\left(\frac{1}{Q}\right)\right) \\ \left(1 + \frac{p_\ell^2}{q_\ell^2}\right)(q_\ell^2 + (Kq_\ell - q_{\ell-1})^2) \leq Q^2 \left(1 + O\left(\frac{1}{Q}\right)\right). \end{cases} \quad (7.21)$$

Since  $\frac{p_\ell}{q_\ell} = \frac{p'}{q} + O\left(\frac{\ell}{Q}\right)$  and  $q_\ell^2 + (Kq_\ell - q_{\ell-1})^2 \leq 2Q^2$ , the second inequality in (7.21) can be also written as

$$\left(1 + \frac{p'^2}{q'^2}\right)(q_\ell^2 + (Kq_\ell - q_{\ell-1})^2) \leq Q^2 \left(1 + O\left(\frac{1}{Q}\right)\right),$$

leading to

$$R_Q^{\square\square}(\xi) = \sum_{\substack{\ell \in [0, \xi] \\ K \in [1, \xi]}} \sum_{q' < Q} \mathcal{N}_{Q+O(Q^{1/2}), q', K, \ell}^{\square\square}(\xi),$$

where  $\mathcal{N}_{Q, q', K, \ell}^{\square\square}(\xi)$  denotes the number of integer lattice points  $(p', q)$  such that

$$\begin{cases} 0 \leq p' \leq q', & 0 \leq q \leq Q, & p'q \equiv 1 \pmod{q'}, & 0 < Kq\ell - q\ell_{-1} \leq Q \\ \Upsilon_{\ell, K} \left( \frac{q}{Q}, \frac{q'}{Q} \right) \leq \xi, & p'^2 + q'^2 \leq \frac{Q^2 q'^2}{\max\{q^2 + q'^2, q_\ell^2 + (Kq\ell - q\ell_{-1})^2\}}. \end{cases} \quad (7.22)$$

Applying Lemma 7 to the set  $\Omega = \Omega_{q', \ell, K, \xi}^{\square\square}$  of elements  $(u, v)$  for which

$$\begin{cases} u \in [0, Q], & v \in [0, q'], & L_i \left( \frac{u}{Q}, \frac{q'}{Q} \right) > 0, & i = 0, 1, \dots, \ell \\ 0 < KL_\ell \left( \frac{u}{Q}, \frac{q'}{Q} \right) - L_{\ell-1} \left( \frac{u}{Q}, \frac{q'}{Q} \right) \leq 1, & \Upsilon_{\ell, K} \left( \frac{u}{Q}, \frac{q'}{Q} \right) \leq \xi \\ v^2 + q'^2 \leq \frac{Q^2 q'^2}{\max \left\{ u^2 + q'^2, Q^2 L_\ell^2 \left( \frac{u}{Q}, \frac{q'}{Q} \right) + Q^2 \left( KL_\ell \left( \frac{u}{Q}, \frac{q'}{Q} \right) - L_{\ell-1} \left( \frac{u}{Q}, \frac{q'}{Q} \right) \right)^2 \right\}}, \end{cases}$$

with  $A(\Omega) \leq Qq'$ ,  $\ell(\partial\Omega) \ll Q$ ,  $L = q'^{5/6}$ , we find

$$\mathcal{N}_{Q, q', \ell, K}^{\square\square}(\xi) = \frac{\varphi(q')}{q'} \cdot \frac{A(\Omega_{q', \ell, K, \xi}^{\square\square})}{q'} + O_\varepsilon(Qq'^{-1/6+\varepsilon}).$$

This leads in turn to

$$R_Q^{\square\square}(\xi) = \mathcal{M}_Q^{\square\square}(\xi) + O_{\xi, \varepsilon}(Q^{11/16+\varepsilon}),$$

where

$$\mathcal{M}_Q^{\square\square}(\xi) = \sum_{\substack{\ell \in [0, \xi] \\ K \in [1, \xi]}} \sum_{q' \leq Q} \frac{\varphi(q')}{q'} \cdot \frac{A(\Omega_{q', \ell, K, \xi}^{\square\square})}{q'}.$$

For fixed integers  $K \in [1, \xi]$ ,  $\ell \in [0, \xi]$  consider the subset  $T_{K, \ell, \xi}$  of  $[0, 1]^3$  defined as

$$\left\{ (x, y, z) \in [0, 1]^3 : \begin{cases} 0 < L_{\ell+1}(x, y) = KL_\ell(x, y) - L_{\ell-1}(x, y) \leq 1, & \Upsilon_{\ell, K}(x, y) \leq \xi \\ \max \{x^2 + y^2, L_\ell^2(x, y) + L_{\ell+1}^2(x, y)\} \leq \frac{1}{1+z^2} \end{cases} \right\}, \quad (7.23)$$

with  $L_i$  and  $\Upsilon_{\ell, K}$  as in (5.4) and (5.5).

Möbius summation applied to  $h_3(q') = \frac{1}{q'} A(\Omega_{q', \ell, K, \xi}^{\square\square})$  with  $\|h_3\|_\infty \leq Q$ , and the change of variable  $(q', u, v) = (Qx, Qy, Qxz)$ ,  $(x, y, z) \in [0, 1]^3$ , yields

$$\mathcal{M}_Q^{\square\square}(\xi) = \frac{1}{\zeta(2)} \sum_{\substack{\ell \in [0, \xi] \\ K \in [1, \xi]}} \left( \int_0^Q \frac{dq'}{q'} A(\mathcal{M}_{q', \ell, K, \xi}^{\square\square}) + O(Q) \right) = \frac{Q^2}{\zeta(2)} \sum_{\substack{\ell \in [0, \xi] \\ K \in [1, \xi]}} \text{Vol}(T_{K, \ell, \xi}),$$

and so

$$R_Q^{\square\square}(\xi) = \frac{Q^2}{\zeta(2)} \sum_{\substack{\ell \in [0, \xi] \\ K \in [1, \xi]}} \text{Vol}(T_{K, \ell, \xi}) + O_{\xi, \varepsilon}(Q^{11/6+\varepsilon}). \quad (7.24)$$

To show that  $\xi \mapsto \text{Vol}(T_{K,\ell,\xi})$  is  $C^1$  on  $[1, \infty)$ , we change variables  $(x, y, z) = (\cos \theta, \sin \theta, \tan t)$  to obtain

$$\text{Vol}(T_{K,\ell,\xi}) = \int_0^{\pi/4} A_{K,\ell}(\xi, t) \frac{dt}{\cos^2 t}, \quad (7.25)$$

where  $A_{K,\ell}(\xi, t)$  is the area of the region defined by, setting  $e^{i\theta} = (\cos \theta, \sin \theta)$ :

$$\left\{ r e^{i\theta} \in [0, 1]^2 : L_{\ell+1}(e^{i\theta}) > 0, \frac{F_{K,\ell}(\theta)}{\xi} \leq r^2 \leq \frac{\cos^2 t}{\max\{1, L_\ell^2(e^{i\theta}) + L_{\ell+1}^2(e^{i\theta})\}} \right\}$$

with the notations of (5.4) and with

$$F_{K,\ell}(\theta) := \cot \theta + \sum_{i=1}^{\ell} \frac{1}{L_{i-1}(e^{i\theta})L_i(e^{i\theta})} + \frac{L_{\ell+1}(e^{i\theta})}{L_\ell(e^{i\theta})(L_\ell^2(e^{i\theta}) + L_{\ell+1}^2(e^{i\theta}))}.$$

Now notice that  $K_i(x, y) \leq \xi$  when  $1 \leq i \leq \ell$ , as a result of (omitting the arguments of the functions)

$$K_i = \frac{L_i + L_{i-2}}{L_{i-1}} \leq \frac{1}{L_{i-2}L_{i-1}} + \frac{1}{L_{i-1}L_i} < \Upsilon_{\ell,K} \leq \xi.$$

Similarly,  $K_1 = \frac{L_{-1} + L_1}{L_0} \leq \frac{L_{-1}}{L_0} + \frac{1}{L_0 L_1} < \Upsilon_{\ell,K} \leq \xi$ . Thus the projection of  $T_{K,\ell,\xi}$  on the first two coordinates is included into the union of disjoint cylinders  $\mathcal{T}_{\mathbf{k}} := \mathcal{T}_{k_1} \cap T^{-1}\mathcal{T}_{k_2} \cap \dots \cap T^{-\ell+1}\mathcal{T}_{k_\ell}$  with  $\mathcal{T}_{\mathbf{k}} = \{(x, y) : K_1(x, y) = k\}$  and  $\mathbf{k} = (k_1, \dots, k_\ell) \in [1, \xi]^\ell$ . On each set  $\mathcal{T}_{\mathbf{k}}$  all maps  $L_1, \dots, L_\ell, L_{\ell+1}$  are linear, say  $L_i(x, y) = A_i x + B_i y$  where the integers  $A_i, B_i$  depend only on  $k_1, \dots, k_i$  for  $i \leq \ell$  and  $A_{\ell+1}, B_{\ell+1}$  depend only on  $\mathbf{k}$  and  $K$ . Therefore the function  $F_{K,\ell}(\theta)$  is continuous on each region  $\mathcal{T}_{\mathbf{k}}$ , and applying Lemma 10 we conclude that the function  $\xi \mapsto \text{Vol}(T_{K,\ell,\xi})$  is  $C^1$  on  $[1, \infty)$ , being a sum of  $[\xi]^\ell$  volumes, each of which  $C^1$  as functions of  $\xi$ .

**Remark 13.** The region  $T_{K,\ell,\xi}$  can be simplified further. For each integer  $J \in [1, \xi)$ , the map

$$\Psi_J : (u, v) \mapsto (JL_\ell(u, v) - L_{\ell-1}(u, v), L_\ell(u, v))$$

is an area preserving injection on  $\mathcal{T}$ , since it is the composition of  $T^\ell$  in (5.4) followed by the linear transformation  $(u, v) \mapsto (Jv - u, v)$ . Note that under this map (omitting the arguments  $(u, v)$  of the functions below):

$$L_1 \rightarrow \left[ \frac{1 + JL_\ell - L_{\ell-1}}{L_\ell} \right] - (JL_\ell - L_{\ell-1}) = L_{\ell-1}$$

(using  $L_{\ell-1} + L_\ell > 1$ ), and by induction it follows similarly that  $L_i \rightarrow L_{\ell-i}$  for  $0 \leq i \leq \ell$ . Also we have that  $\Psi_J(u, v) = (x, y) \in [0, 1]^2$  if and only if  $x = JL_\ell - L_{\ell-1} \in [0, 1]$  and  $J = \left[ \frac{1+x}{y} \right]$ .

Let us decompose the region  $T_{K,\ell,\xi}$  into a disjoint union of regions  $T_{K,J;\ell,\xi}$ ,  $1 \leq J < \xi$ , obtained by adding the condition  $\left[ \frac{1+x}{y} \right] = J$ . By the discussion of the previous paragraph, the map  $(\Psi_J, \text{Id}_z)$  is a volume preserving bijection taking  $U_{K,J;\ell,\xi}$  onto  $T_{K,J;\ell,\xi}$ , where

$$U_{K,J;\ell,\xi} := \left\{ (x, y, z) \in [0, 1]^3 : \begin{array}{l} x + y > 1, \quad JL_\ell - L_{\ell-1} > 0, \quad KL_0 - L_1 > 0, \quad \Upsilon_{\ell,K,J} \leq \xi, \\ L_0^2 + (KL_0 - L_1)^2 \leq \frac{1}{1+z^2}, \quad L_\ell^2 + (JL_\ell - L_{\ell-1})^2 \leq \frac{1}{1+z^2} \end{array} \right\}.$$

Here  $L_i = L_i(x, y)$  and  $\Upsilon_{\ell,K,J}(x, y) = \frac{JL_\ell - L_{\ell-1}}{L_\ell(L_\ell^2 + (JL_\ell - L_{\ell-1})^2)} + \sum_{i=1}^{\ell} \frac{1}{L_{i-1}L_i} + \frac{KL_0 - L_1}{L_0(L_0^2 + (KL_0 - L_1)^2)}$ .

For  $\alpha \geq 1$ , the transformation  $(\Psi_\alpha, \text{Id}_z)$  maps bijectively the part of  $U_{K,J;\ell,\xi}$  for which  $\left[ \frac{1+L_{\ell-1}}{L_\ell} \right] = \alpha$  onto the part of  $U_{J,K;\ell,\xi}$  for which  $\left[ \frac{1+x}{y} \right] = \alpha$ . Therefore  $\text{Vol}(U_{K,J;\ell,\xi}) = \text{Vol}(U_{J,K;\ell,\xi})$  and the

sum of volumes appearing in (7.26) can be written more symmetrically:

$$\sum_{K \in [1, \xi]} \text{Vol}(T_{K, \ell, \xi}) = \sum_{K, J \in [1, \xi]} \text{Vol}(U_{K, J, \ell, \xi}).$$

As an example of using this formula, if  $1 < \xi \leq 2$  and  $\ell = 1$ , we can only have  $K = J = 1$  and the inequalities  $JL_1 - L_0 > 0$ ,  $KL_0 - L_1 > 0$  cannot be both satisfied, so  $U_{1,1;1,\xi}$  is empty. Therefore the only contribution from the  $T$  bodies in (7.26) comes from  $T_{1,0,\xi}$  if  $\xi \in (1, 2]$ .

We can now prove the main theorem regarding the pair correlation of the quantities  $\{\tan(\theta_\gamma/2)\}$ .

**Theorem 2.** *The pair correlation measure  $R_2^{\mathfrak{S}}$  exists on  $[0, \infty)$ . It is given by the  $C^1$  function*

$$R_2^{\mathfrak{S}}\left(\frac{3}{8}\xi\right) = \frac{8}{3\zeta(2)} \left( \sum_{M \in \mathfrak{S}} \text{Vol}(S_{M,\xi}) + \sum_{\ell \in [0, \xi]} \sum_{K \in [1, \xi]} \text{Vol}(T_{K, \ell, \xi}) \right), \quad (7.26)$$

where the three-dimensional bodies  $S_{M,\xi}$  are defined in (7.14) and the bodies  $T_{K,\ell,\xi}$  are defined in (7.23).

*Proof.* If  $c_0 \in (\frac{1}{2}, 1)$  and  $G(\xi)$  denoting the sum of all volumes in (7.26), by (7.17), (7.24), we infer

$$\mathcal{R}_Q^\Phi(\xi) = \frac{Q^2}{\zeta(2)} G(\xi) + O_{\xi,\varepsilon}(Q^{(11+c_0)/6+\varepsilon}). \quad (7.27)$$

The function  $G$  is  $C^1$  on  $[0, \infty)$  as a result of  $\xi \mapsto \text{Vol}(S_{M,\xi})$  being  $C^1$  on  $[0, \infty)$ , and of  $\xi \mapsto \text{Vol}(T_{K,\ell,\xi})$  being  $C^1$  on  $[1, \infty)$ . Corollary 4 and (7.27) now yield, for  $\beta \in (\frac{2}{3}, 1)$ ,

$$\mathcal{R}_Q^\Psi(\xi) = \frac{Q^2}{\zeta(2)} \left( G(\xi + O(Q^{2-3\beta})) + G(O(Q^{2-3\beta})) \right) + O_{\xi,\varepsilon}(Q^{1+\beta} \ln Q + Q^{(11+c_0)/6+\varepsilon}).$$

Employing again the differentiability of  $G$ , as well as  $G(0) = 0$ , and taking  $\beta = \frac{3}{4}$ ,  $c_0 = \frac{1}{2} + \varepsilon$ , this leads to

$$\mathcal{R}_Q^\Psi(\xi) = \frac{Q^2}{\zeta(2)} G(\xi) + O_{\xi,\varepsilon}(Q^{23/12+\varepsilon}). \quad (7.28)$$

Equality (7.26) now follows from (7.28) and Corollary 8.  $\square$

## 8. PAIR CORRELATION OF $\{\theta_\gamma\}$

In this section we pass to the pair correlation of the angles  $\{\theta_\gamma\}$ , estimating

$$\mathcal{R}_Q^\theta(\xi) := \# \left\{ (\gamma, \gamma') \in \tilde{\mathfrak{R}}_Q^2 : 0 \leq \theta_{\gamma'} - \theta_\gamma \leq \frac{\xi}{Q^2} \right\},$$

thus proving Theorem 1. In §8.2 we also deduce Corollary 1.

**8.1. Proof of Theorem 1.** Define the pair correlation kernel  $F(\xi, t)$  as follows

$$F(\xi, t) = \sum_{M \in \mathfrak{S}} B_M(\xi, t) + \sum_{\substack{\ell \in [0, \xi] \\ K \in [1, \xi]}} A_{K,\ell}(\xi, t). \quad (8.1)$$

where  $B_M(\xi, t)$ ,  $A_{K,\ell}(\xi, t)$  are the areas from (7.18), (7.25), so that by (7.28) we have

$$\mathcal{R}_Q^\Psi(\xi) = \frac{Q^2}{\zeta(2)} \int_0^{\frac{\pi}{4}} F(\xi, t) \frac{dt}{\cos^2(t)} + O_{\xi,\varepsilon}(Q^{(11+c_0)/6+\varepsilon}).$$

**Proposition 14.** *We have the estimate*

$$\mathcal{R}_Q^\theta(\xi) = \frac{Q^2}{\zeta(2)} \int_0^{\frac{\pi}{4}} F\left(\frac{\xi}{2\cos^2 t}, t\right) \frac{dt}{\cos^2 t} + O_{\xi, \varepsilon}(Q^{47/24+\varepsilon}). \quad (8.2)$$

Before giving the proof, note that Theorem 1 follows from the proposition as  $Q \rightarrow \infty$ , taking into account the different normalization in the definition of  $\mathcal{R}_Q^\theta(\xi)$ ,  $R_Q^\theta(\xi)$ , and defining, in view of (8.1) and (8.2):

$$B_M(\xi) := \int_0^{\frac{\pi}{4}} B_M\left(\frac{\xi}{2\cos^2 t}, t\right) \frac{dt}{\cos^2 t}, \quad A_{K, \ell}(\xi) := \int_0^{\frac{\pi}{4}} A_{K, \ell}\left(\frac{\xi}{2\cos^2 t}, t\right) \frac{dt}{\cos^2 t}. \quad (8.3)$$

From the definitions of  $B_M(\xi, t)$ ,  $A_{K, \ell}(\xi, t)$  in the equations following (7.18), (7.25), it is clear that  $B_M(\frac{\xi}{2\cos^2 t}, t) = B_M(\frac{\xi}{2}, 0) \cos^2 t$ ,  $A_{K, 0}(\frac{\xi}{2\cos^2 t}, t) = A_{K, 0}(\frac{\xi}{2}, 0) \cos^2 t$ , hence one has

$$B_M(\xi) = \frac{\pi}{4} B_M\left(\frac{\xi}{2}, 0\right), \quad A_{K, 0}(\xi) = \frac{\pi}{4} A_{K, 0}\left(\frac{\xi}{2}, 0\right), \quad (8.4)$$

which together with (7.20) yields the formula for  $B_M(\xi)$  given in Theorem 1. Note that the range of summation in Theorem 1 restricts to  $K < \xi/2$ ,  $\ell < \xi/2$ , compared to the range in (8.1). Indeed, from the description of  $A_{K, \ell}(\frac{\xi}{2\cos^2 t}, t)$  following (7.25) we see that  $\ell < \Upsilon_{\ell, K} \leq \xi/2$ , while for  $K$  we have  $K < \frac{1}{L_{\ell-1} L_\ell} + \frac{KL_\ell - K_{\ell-1}}{L_\ell} < \Upsilon_{\ell, K} \leq \frac{\xi}{2}$ , and similarly for  $\ell = 0$ .

*Proof.* Consider  $I = [\alpha, \beta]$  with  $N = [Q^d]$ ,  $|I| = N^{-1} \sim Q^{-d}$ ,  $I^+ = [\alpha - Q^{-d'}, \beta + Q^{-d'}]$ ,  $I^- = [\alpha + Q^{-d'}, \beta - Q^{-d'}]$  where  $0 < d = \frac{1}{24} < d' = \frac{1}{12} < 1$ . Partition the interval  $[0, 1)$  into the union of  $N$  intervals  $I_j = [\alpha_j, \alpha_{j+1})$  with  $|I_j| = N^{-1}$  as above. Associate the intervals  $I_j^\pm$  to  $I_j$  as described above. Denote

$$\begin{aligned} \mathfrak{R}_Q^\# &:= \{(\gamma, \gamma') \in \tilde{\mathfrak{R}}_Q^2 : \gamma' \neq \gamma\}, \\ \mathcal{R}_{I, Q}^\theta(\xi) &:= \#\left\{(\gamma, \gamma') \in \mathfrak{R}_Q^\# : 0 \leq \theta_{\gamma'} - \theta_\gamma \leq \frac{\xi}{Q^2}, \Psi(\gamma), \Psi(\gamma') \in I\right\} \\ &\leq \mathcal{R}_{I, Q}^{\theta, \natural}(\xi) := \#\left\{(\gamma, \gamma') \in \mathfrak{R}_Q^\# : 0 \leq \theta_{\gamma'} - \theta_\gamma \leq \frac{\xi}{Q^2}, \Psi(\gamma) \in I\right\}, \\ \mathcal{R}_{I, Q}^\Psi(\xi) &:= \#\left\{(\gamma, \gamma') \in \mathfrak{R}_Q^\# : 0 \leq \Psi(\gamma') - \Psi(\gamma) \leq \frac{\xi}{Q^2}, \Psi(\gamma), \Psi(\gamma') \in I\right\}, \\ \mathcal{R}_{I, Q}^{\Psi, \flat}(\xi) &:= \#\left\{(\gamma, \gamma') \in \mathfrak{R}_Q^\# : 0 \leq \Psi(\gamma') - \Psi(\gamma) \leq \frac{\xi}{Q^2}, \gamma_-, \gamma_+ \in I\right\}, \\ \mathcal{R}_{I, Q}^{\Phi, \flat}(\xi) &:= \#\left\{(\gamma, \gamma') \in \mathfrak{R}_Q^\# : 0 \leq \Phi(\gamma') - \Phi(\gamma) \leq \frac{\xi}{Q^2}, \gamma_-, \gamma_+ \in I\right\}. \end{aligned}$$

Expressing  $\theta_{\gamma'} - \theta_\gamma$  and  $\Psi(\gamma') - \Psi(\gamma)$  by the Mean Value Theorem we find

$$\mathcal{R}_{I, Q}^\Psi\left(\frac{(1+\alpha^2)\xi}{2}\right) \leq \mathcal{R}_{I, Q}^\theta(\xi) \leq \mathcal{R}_{I, Q}^{\Psi, \flat}\left(\frac{(1+\beta^2)\xi}{2}\right). \quad (8.5)$$

**Lemma 15.** *The following estimates hold:*

- (i)  $\sum_{j=1}^N \mathcal{R}_{I_j, Q}^\theta(\xi) \leq \mathcal{R}_Q^\theta(\xi) = \sum_{j=1}^N \mathcal{R}_{I_j, Q}^{\theta, \natural}(\xi) \leq \sum_{j=1}^N \mathcal{R}_{I_j^+, Q}^\theta(\xi) + O(Q^{15/8} \ln^2 Q)$ .
- (ii)  $\mathcal{R}_{I, Q}^\Psi(\xi) = \mathcal{R}_{I, Q}^{\Psi, \flat}(\xi) + O(Q^{1+d'} \ln^2 Q)$ .

*Proof.* The first inequality in (i) is trivial. For the second one note first that the total number of pairs  $(\gamma, \gamma')$  with  $0 \leq \theta_{\gamma'} - \theta_{\gamma} \leq \xi Q^{-2}$  and  $qq' \leq Q^{d'}$ , with  $\gamma_- = \frac{p}{q}$ ,  $\gamma_+ = \frac{p'}{q'}$  is  $\ll_{\xi} Q^d(Q^{d'} \ln Q)(Q \ln Q)$ . For  $\gamma$  with  $qq' > Q^{-d'}$  use  $\Psi(\gamma') - \beta \leq \Psi(\gamma') - \Psi(\gamma) \leq \frac{1}{qq'} \leq Q^{-d'}$ , so  $\Psi(\gamma') \in I_j^+$ . The proof of (ii) is analogous.  $\square$

Returning to the proof of Proposition 14, Lemma 15 and (8.5) yield

$$\sum_{j=1}^N \mathcal{R}_{I_j, Q}^{\Psi} \left( \frac{(1 + \alpha_j^2)\xi}{2} \right) \leq \mathcal{R}_Q^{\theta}(\xi) \leq \sum_{j=1}^N \mathcal{R}_{I_j^+, Q}^{\Psi} \left( \frac{(1 + \alpha_{j+1}^2)\xi}{2} \right) + O_{\varepsilon}(Q^{15/8+\varepsilon}). \quad (8.6)$$

To estimate  $\mathcal{R}_{I, Q}^{\Phi}(\xi)$  we repeat the previous arguments for a short interval  $I$  as above. Adding everywhere the condition  $\gamma_-, \gamma_+ \in I$  we modify  $\mathcal{R}_Q^{\circ}$  by  $\mathcal{R}_{I, Q}^{\circ}$  and  $R_Q^{\circ}$  by  $R_{I, Q}^{\circ}$  in Lemma 5,  $\mathcal{R}_Q^{\square}$  by  $\mathcal{R}_{I, Q}^{\square}$  and  $R_Q^{\square}$  by  $R_{I, Q}^{\square}$  in Lemma 6. The additional condition  $\frac{p}{q}, \frac{p'}{q'} \in I$  is inserted in (7.2). The condition  $0 \leq p' \leq q'$  is replaced by  $q'\alpha \leq p' < q'\beta$  in (7.4), and (7.22), and  $0 \leq p \leq q$  is replaced by  $q\alpha \leq p < q\beta$  in (7.4). The condition  $v \in [0, q']$  is replaced by  $v \in [q'\alpha, q'\beta]$  in the definition of  $\Omega_{M, q', \xi}$ , and  $\Omega_{q', \ell, K, \xi}^{\square}$ . The bodies  $S_{M, \xi}$  and  $T_{K, \ell, \xi}$  are substituted respectively by  $S_{I, M, \xi}$  and  $T_{I, K, \ell, \xi}$  after replacing the condition  $z \in [0, 1]$  in their definition by  $z \in [\alpha, \beta]$ . The analogs of (7.18), and (7.25) hold:

$$\text{Vol}(S_{I, M, \xi}) = \int_I B_M(\xi, t) \frac{dt}{\cos^2 t}, \quad \text{Vol}(T_{I, K, \ell, \xi}) = \int_I A_{K, \ell}(\xi, t) \frac{dt}{\cos^2 t}. \quad (8.7)$$

The approach from Section 7 under the changes specified in the previous paragraph leads to

$$\mathcal{R}_{I, Q}^{\Phi, b}(\xi) = \mathcal{R}_{I, Q}^{\circ}(\xi) + \mathcal{R}_{I, Q}^{\square}(\xi) = \frac{Q^2}{\zeta(2)} \int_{\tan^{-1} I} F(\xi, t) \frac{dt}{\cos^2 t} + O_{\xi, \varepsilon}(Q^{23/12+\varepsilon}), \quad (8.8)$$

with the pair correlation kernel  $F(\xi, t)$  defined by (8.1). We also have

$$\mathcal{R}_{I^+, Q}^{\Phi, b}(\xi) = \mathcal{R}_{I, Q}^{\Phi, b}(\xi) + O_{\xi, \varepsilon}(Q^{23/12+\varepsilon} + Q^{2-d'}). \quad (8.9)$$

The analogs of Lemmas 5, 6 yield upon (8.8) and (8.9)

$$\mathcal{R}_{I, Q}^{\Phi, b}(\xi) = \frac{Q^2}{\zeta(2)} \int_{\tan^{-1} I} F(\xi + O(Q^{-1/3}), t) \frac{dt}{\cos^2 t} + O_{\xi, \varepsilon}(Q^{23/12+\varepsilon}) = \mathcal{R}_{I^+, Q}^{\Phi, b}(\xi). \quad (8.10)$$

The analog of Corollary 4 and (8.10) yield

$$\begin{aligned} \mathcal{R}_{I, Q}^{\Psi, b}(\xi) &= \mathcal{R}_{I, Q}^{\Phi, b}(\xi + O(Q^{-1/4})) + \mathcal{R}_{I, Q}^{\Phi, b}(O(Q^{-1/4})) + O(Q^{7/4+\varepsilon}) \\ &= \frac{Q^2}{\zeta(2)} \int_{\tan^{-1} I} \left( F(\xi + O(Q^{-1/4}), t) + F(O(Q^{-1/4}), t) \right) \frac{dt}{\cos^2 t} + O_{\xi, \varepsilon}(Q^{23/12+\varepsilon}) \\ &= \mathcal{R}_{I^+, Q}^{\Psi, b}(\xi). \end{aligned} \quad (8.11)$$

As shown in Section 7 the function  $F$  is  $C^1$  in  $\xi$ , thus (8.11) gives actually<sup>1</sup>

$$\mathcal{R}_{I, Q}^{\Psi, b}(\xi) = \frac{Q^2}{\zeta(2)} \int_{\tan^{-1} I} F(\xi, t) \frac{dt}{\cos^2 t} + O_{\xi, \varepsilon}(Q^{23/12+\varepsilon}) = \mathcal{R}_{I^+, Q}^{\Psi, b}(\xi). \quad (8.12)$$

Lemma 15 (i), (8.12), and  $F \in C^1[0, \infty)$  yield

$$\mathcal{R}_{I, Q}^{\Psi}(\xi) = \frac{Q^2}{\zeta(2)} \int_{\tan^{-1} I} F(\xi, t) \frac{dt}{\cos^2 t} + O_{\xi, \varepsilon}(Q^{23/12+\varepsilon} + Q^{2-d'}) = \mathcal{R}_{I^+, Q}^{\Psi}(\xi). \quad (8.13)$$

<sup>1</sup>The argument from Section 7 applies before integrating with respect to  $t$  on  $[0, \frac{\pi}{4}]$ , showing that  $F$  is  $C^1$ .

Let also  $\omega_j = \tan^{-1} \alpha_j$ . From (8.13) and (8.5) we further infer

$$\begin{aligned} \frac{Q^2}{\zeta(2)} \int_{\omega_j}^{\omega_{j+1}} F\left(\frac{(1 + \alpha_j^2)\xi}{2}, t\right) \frac{dt}{\cos^2 t} + O_{\xi, \varepsilon}(Q^{23/12+\varepsilon} + Q^{2-d'}) &\leq \mathcal{R}_{I_j, Q}^\theta(\xi) \leq \mathcal{R}_{I_j^+, Q}^\theta(\xi) \\ &\leq \frac{Q^2}{\zeta(2)} \int_{\omega_j}^{\omega_{j+1}} F\left(\frac{(1 + \alpha_{j+1}^2)\xi}{2}, t\right) \frac{dt}{\cos^2 t} + O_{\xi, \varepsilon}(Q^{23/12+\varepsilon} + Q^{2-d'}). \end{aligned} \quad (8.14)$$

Employing also

$$\int_{\omega_j}^{\omega_{j+1}} F\left(\frac{(1 + \alpha_j^2)\xi}{2}, t\right) \frac{dt}{\cos^2 t} = \int_{\omega_j}^{\omega_{j+1}} \left( F\left(\frac{(1 + \tan^2 t)\xi}{2}, t\right) + O(\omega_{j+1} - \omega_j) \right) \frac{dt}{\cos^2 t}$$

and  $(\omega_{j+1} - \omega_j)^2 \leq Q^{-2d}$  we find

$$\mathcal{R}_{I_j, Q}^\theta(\xi) = \frac{Q^2}{\zeta(2)} \int_{\omega_j}^{\omega_{j+1}} F\left(\frac{(1 + \tan^2 t)\xi}{2}, t\right) \frac{dt}{\cos^2 t} + O_{\xi, \varepsilon}(Q^{23/12+\varepsilon}) = \mathcal{R}_{I_j^+, Q}^\theta(\xi). \quad (8.15)$$

Finally Lemma 15 (i) and (8.15) yield (8.2).  $\square$

**8.2. Explicit formula for  $g_2^{\mathfrak{A}}$ .** Next we compute the derivatives  $B'_M(\xi)$ , thus proving Corollary 1. We also obtain the explicit formula (8.16) for  $g_2^{\mathfrak{A}}$  on a larger range than in Corollary 1, after computing the derivative  $A'_{K,0}(\xi)$ .

**Lemma 16.** *For  $M \in \mathfrak{G}$ , let  $T = T_M$ ,  $Z = Z_M$  as in (3.1). The derivative  $B'_M(\xi)$  is given by:*

$$B'_M(\xi) = \begin{cases} \frac{\pi}{4\xi^2} \ln\left(\frac{T + \sqrt{T^2 - 4}}{T + \sqrt{T^2 - 4 - \xi^2}}\right) & \text{if } \xi \leq 2Z \\ \frac{\pi}{8\xi^2} \ln\left(\frac{(T + \sqrt{T^2 - 4})^2(T - \sqrt{T^2 - 4 - \xi^2})}{(4 + 4Z^2)(T + \sqrt{T^2 - 4 - \xi^2})}\right) & \text{if } 2Z \leq \xi \leq \sqrt{T^2 - 4} \\ \frac{\pi}{8\xi^2} \ln\left(\frac{(T + \sqrt{T^2 - 4})^2}{4 + 4Z^2}\right) & \text{if } \xi \geq \sqrt{T^2 - 4}. \end{cases}$$

*Proof.* Using (8.4), we proceed as in the proof of Lemma 12:

$$B_M(\xi) = \frac{\pi}{4\xi} \int_0^{\pi/2} \left( \frac{\xi}{\sqrt{T^2 - 4}} \cdot \frac{1}{U_T + \cos(2\theta - \theta_M)} - \frac{|\sin(2\theta - \theta_M)|}{U_T + \cos(2\theta - \theta_M)} \right)_+ d\theta,$$

where  $U_T = \frac{T}{\sqrt{T^2 - 4}}$  and  $\theta_M \in (0, \frac{\pi}{2})$  has  $\sin \theta_M = \frac{2Z}{\sqrt{T^2 - 4}}$ . Applying Lemma 10, we obtain:

$$B'_M(\xi) = \frac{\pi}{4\xi^2} \int_I \frac{|\sin(2\theta - \theta_M)|}{U_T + \cos(2\theta - \theta_M)} d\theta,$$

with  $I = \left\{ \theta \in (0, \frac{\pi}{2}) : |\sin(2\theta - \theta_M)| < \frac{\xi}{\sqrt{T^2 - 4}} \right\}$ . Clearly  $I = (0, \frac{\pi}{2})$  when  $\xi > \sqrt{T^2 - 4}$ , and if  $\xi \leq \sqrt{T^2 - 4}$ , let  $\alpha = \alpha(\xi) \in (0, \frac{\pi}{4})$  such that  $\sin 2\alpha = \frac{\xi}{\sqrt{T^2 - 4}}$ . Then

$$\xi \leq 2Z \iff \alpha \leq \theta_M/2 \iff I = [\theta_M/2 - \alpha, \theta_M/2 + \alpha],$$

$$2Z \leq \xi \leq \sqrt{T^2 - 4} \iff \alpha \in [\theta_M/2, \pi/4] \iff I = [0, \theta_M/2 + \alpha] \cup [\pi/2 + \theta_M/2 - \alpha, \pi/2],$$

and the integral is easy to compute. The last case appears in the figure below for  $M = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$  and  $\xi = 2.1 \in (2, \sqrt{5})$ .  $\square$

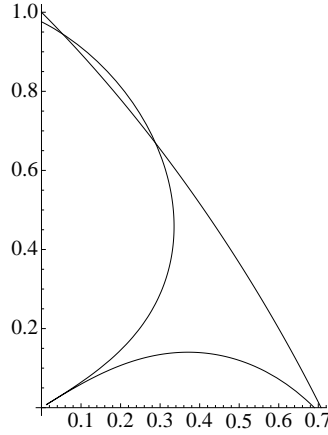


FIGURE 6. The area  $B_M(\xi/2, 0)$  when  $2F \leq \xi \leq \sqrt{T^2 - 4}$ .

A similar computation using (8.4) gives the formula:

$$A'_{K,0}(\xi) = \frac{\pi}{4\xi^2} \cdot \begin{cases} 0 & \text{if } \xi \leq 2K \\ \ln(1 + K^2) + \ln\left(\frac{(1 + x_1^2)(1 + (x_2 - K)^2)}{(1 + x_2^2)(1 + (x_1 - K)^2)}\right) & \text{if } \xi \in [2K, K\sqrt{K^2 + 4}] \\ \ln(1 + K^2) & \text{if } \xi \geq K\sqrt{K^2 + 4}, \end{cases}$$

where  $x_2 > x_1$  are the roots of  $x^2(\xi + 2K) - 2xK(\xi + K) + \xi(K^2 + 1) - 2K = 0$ . By the last paragraph in Remark 13, the body  $T_{1,1,\xi}$  is empty, so  $A_{1,1}(\xi) = 0$ , and we have an explicit formula on a larger range than in the introduction:

$$g_2^{\mathfrak{A}}\left(\frac{3}{4\pi}\xi\right) = \frac{32\pi}{9\zeta(2)} \left( \sum_{M \in \mathfrak{E}} B'_M(\xi) + A'_{1,0}(\xi) \right), \quad 0 < \xi \leq 4. \quad (8.16)$$

We can now explain the presence of the spikes in the graph of  $g_2^{\mathfrak{A}}$  in Figure 1. The function  $B'_M(\xi)$  is not differentiable at  $\xi = 2F$  and  $\sqrt{T^2 - 4}$ , while the function  $A'_{K,0}(\xi)$  is not differentiable at  $\xi = 2K$  and  $\sqrt{(K^2 + 2)^2 - 4}$ . At the point  $\xi = \sqrt{5}$ , two of the functions  $B'_M(\xi)$ , as well as  $A'_{1,0}(\xi)$ , have infinite slopes on the left, which gives the spike on the graph of  $g_2^{\mathfrak{A}}(x)$  at  $x = \frac{3}{4\pi}\sqrt{5}$ .

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