THE FIRST AND SECOND MOMENT FOR THE LENGTH OF THE PERIOD OF THE CONTINUED FRACTION EXPANSION FOR $\sqrt{d}$

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Abstract. Let d be any positive and non square integer. We prove an upper bound for the first two moments of the length $T(d)$ of the period of the continued fraction expansion for $\sqrt{d}$. This allows to improve the existing results for the large deviations of $T(d)$.

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1. Introduction and results

Let $d \in \mathbb{N}$. Let $T(d)$ be the length of the minimal positive period for the simple continued fraction expansion for $\sqrt{d}$ when d is not a square, otherwise let $T(d) = 0$. Sierpiński [8, p. 293] (see also [9, p. 315]) noticed that Lagrange's argument proving the periodicity of this representation actually proves that $T(d) \leq 2d$. Hickerson [2] noticed that this argument shows that $T(d) \leq g(d)$, where

$$g(d) := \#\big\{(m, q) \in \mathbb{N}^2 \colon m < \sqrt{d},\ |q - \sqrt{d}| < m, q \mid (d - m^2)\big\},$$

and used this bound to prove that $T(d) \leq g(d) \leq d^{1/2+\log 2/\log\log d+O(\log\log\log d/(\log\log d)^2))}$. He also proved that $g(d) = \Omega(\sqrt{d})$. In the same years both Hirst [3] (for squarefree d, only) and Podsypanin [5, 6] (for any d) independently proved that $T(d) \ll \sqrt{d}\log d$; Hirst as a consequence of a different formula computing $g(d)$ allowing a stronger bound for $g(d)$, and Podsypanin via a connection between $T(d)$ and the residue at 1 of the Dedekind zeta function associated with the field $\mathbb{Q}[\sqrt{d}]$. The same connection was independently noticed also by Stanton, Sudler and Willams [10] who proved that $T(d) \leq c\sqrt{d}\log d$ for a smaller value of the constant c, later further improved by Cohn [1]. This connection also shows that in case the Generalized Riemann Hypothesis holds for quadratic fields, then the upper bound improves to $T(d) \ll \sqrt{d}\log\log d$ (see [5, 6]), in agreement with the heuristic and numerical investigations in [11]. Cohn [1] also proved that $T(d) = \Omega(\sqrt{d}/\log\log d)$.
At first it was believed that $T(d) \ll \sqrt{d}$, but nowadays the general sentiment has changed, in spite of the fact that all proven results are still compatible with such a strong upper bound. For sure $T(d)$ strongly oscillates, passing from values as small as 1 (for $d = m^2 + 1$, any m) and 2 (for $d = m^2 + 2m/a$, any m and any $a|2m$, $a \neq 2m$) to as large as $\sqrt{d}/\log\log d$ infinitely often by Cohn's theorem. This suggests to try to bound in some way the number of d where $T(d)$ is exceptionally large, in some sense. Let

$$D(x, \alpha) := \{d \in (x, 2x] \colon T(d) > \alpha\sqrt{d}\}.$$

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Rockett and Szüsz [7] used the connection with the residue of the Dedekind zeta function to prove that

$$\#D(x,\alpha) \leq \frac{c+o(1)}{\log^2\alpha}\,x \qquad \text{as } x\to\infty \tag{1}$$

for a suitable but undetermined constant c.

In this paper we extract some more information from the bound $T(d) \leq g(d)$, via an explicit computation of the first two moments for g. In fact, we prove the following facts.

Theorem 1. *Let $x > 1$, then*

$$\sum_{d\leq x} g(d) = c_1 x^{3/2} - 2x - 2\sqrt{x} + \theta(x + 4\sqrt{x}), \tag{2}$$

where $c_1 := \frac{4}{3}\log 2 = 0.9241\ldots$ and $\theta = \theta(x) \in [0,1]$, and

$$\sum_{d\leq x} g(d)^2 \leq 11.9\,x^2 + 5\,x^{3/2}\log^2(4e^4x). \tag{3}$$

A modification of the argument proving (3) allows to strengthen its conclusion and prove that $\sum_{d\leq x} g(d)^2 \leq 8x^2 + O(x^{3/2}\log^4 x)$ as x diverges: we do not provide the details for this improvement, but we describe the basic steps at the end of Section 3.
From the inequality $T(d) \leq g(d)$ we deduce that:

Corollary 1. *Let $x > 1$, then*

$$\sum_{d\leq x} T(d) \leq c_1 x^{3/2} \quad \text{and} \quad \sum_{d\leq x} T(d)^2 \leq 11.9\,x^2 + 5\,x^{3/2}\log^2(4e^4x)$$

where $c_1 := \frac{4}{3}\log 2 = 0.9241\ldots$. Moreover,

$$\sum_{x<d\leq 2x} T(d) \leq c_2 x^{3/2} + O(\sqrt{x}) \quad \text{and} \quad \sum_{x<d\leq 2x} T(d)^2 \leq 47\,x^2 + O(x^{3/2}\log^2 x)$$

as $x\to\infty$, where $c_2 := \frac{8\sqrt{2}-4}{3}\log 2 = 1.6898\ldots$.

Proof. Only the last claim is not immediate. It follows noticing that $\sum_{x<d\leq 2x} g(d)^2 = \sum_{d\leq 2x} g(d)^2 - \sum_{d\leq x} g(d)^2$, that $\sum_{x<d\leq 2x} g(d)^2 \leq 47.6\,x^2 + O(x^{3/2}\log^2 x)$ by (3), and that $\sum_{d\leq x} g(d)^2 \geq c_1^2\,x^2 + O(x^{3/2})$ by the Cauchy–Schwarz inequality and (2). □

The bounds in Corollary 1 allow to improve (1) in the following way.

Corollary 2. *Let $\alpha > 0$ and $x > 1$. Then*

$$\#D(x,\alpha) \leq \frac{c_2+o(1)}{\alpha}\,x \quad \text{and} \quad \#D(x,\alpha) \leq \frac{47+o(1)}{\alpha^2}\,x,$$

where $c_2 := \frac{8\sqrt{2}-4}{3}\log 2 = 1.6898\ldots$.

The claims are not trivial for $\alpha > c_2$ and $\alpha > \sqrt{47}$, respectively; the first claim supersedes the second one when $\alpha \in (\sqrt{47}, 47/c_2)$.

We have some comments about these results:

- For the second moment we have not determined the asymptotic behaviour, but the order we have found is the correct one since, as we have already noticed, the Cauchy–Schwarz inequality and (2) show that
$$\sum_{d\le x} g(d)^2 \ge (c_1^2 + o(1))x^2 \quad \text{as } x \to \infty.$$
- In similar way, Hölder's inequality shows that every moment $M_{g,r}$ satisfies the lower-bound
$$M_{g,r}(x) := \sum_{d\le x} g(d)^r \ge (c_1^r + o_r(1))x^{r/2+1} \quad \text{as } x \to \infty.$$
For some time we have cultivated the hope to prove that this is the correct order also for $r \ge 3$. In fact, we have succeeded to prove that the analogue of the U term appearing in the proof of (3) (see Section 3) is $\ll_r x^{r/2+1}$ for every r. However, the analogue of the V term resisted to every attempt to bound it nontrivially, and numerically, for $r = 3$, it seems that it grows as $x^{5/2}\log x$, not as $x^{5/2}$. As a consequence, the idea that the order of $M_{g,r}(x)$ is $x^{r/2+1}$ is probably incorrect, and a behaviour of type $M_{g,r}(x) \asymp_r x^{r/2+1}(\log x)^{r-2}$ appears to be a better conjecture.
- An upper bound of that type can be proved for the moments of T, since
$$\begin{aligned} M_{T,r}(x) := \sum_{d\le x} T(d)^r &= \sum_{d\le x} T(d)^{r-2}T(d)^2 \\ &\ll_r x^{(r-2)/2}(\log x)^{r-2} \sum_{d\le x} T(d)^2 \ll_r x^{r/2+1}(\log x)^{r-2} \end{aligned}$$
for every $r \ge 2$, by the bound for $T(d)$ and Corollary 1. (This argument cannot by applied for the moments of g since the bound $\sqrt{d}\log d$ is proved for $g(d)$ only when d is squarefree). However, the moments for T are probably smaller. In fact, computations support the conjecture that the orders of both the mean value $\frac{1}{x}\sum_{d\le x} T(d)$ and the mean second moment $\overline{M}_{T,2}(x) := \frac{1}{x}\sum_{d\le x} T(d)^2$ are $o(\sqrt{x})$ and $o(x)$, respectively, so that probably the bounds in Corollary 1 are not the sharpest ones. More precisely, their graphs suggest that they behave as $\sqrt{x}/(\log x)^{0.6}$, and as $x/(\log x)^{0.8}$ respectively: see Figure 1.

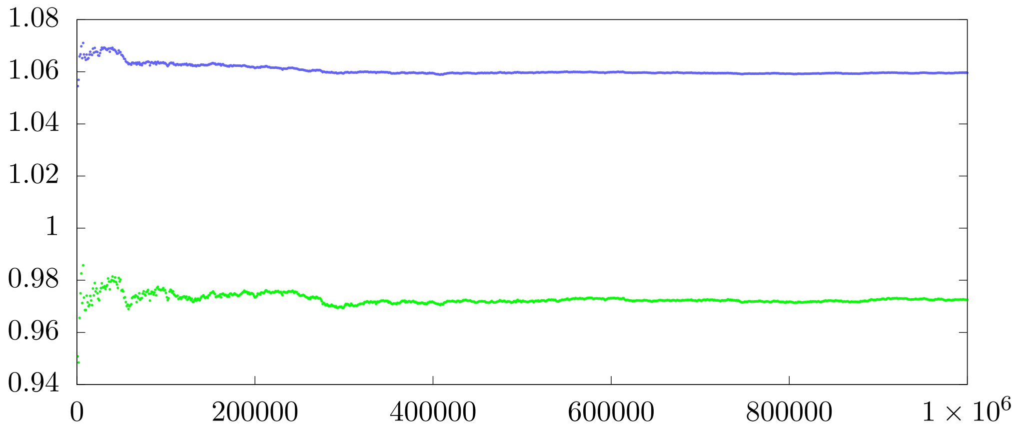

FIGURE 1: Graphs of $\left(\frac{1}{x}\sum_{d\le x} T(d)\right)/\left(\sqrt{x}/(\log x)^{0.6}\right)$ (upper) and of $\left(\frac{1}{x}\sum_{d\le x} T(d)^2\right)/\left(x/(\log x)^{0.8}\right)$ (lower).

- The numerical evidence also shows that when restricted to prime values of d, the mean value $\frac{1}{\pi(x)}\sum_{d\le x, d\,\mathrm{prime}} T(d)$ and the mean second moment $\frac{1}{\pi(x)}\sum_{d\le x, d\,\mathrm{prime}} T(d)^2$ have the orders $\sqrt{x}$ and x, respectively: see Figure 2. If correct, the comparison with what happens for the unrestricted means shows that, essentially, the largest values for $T(d)$ come from prime numbers.

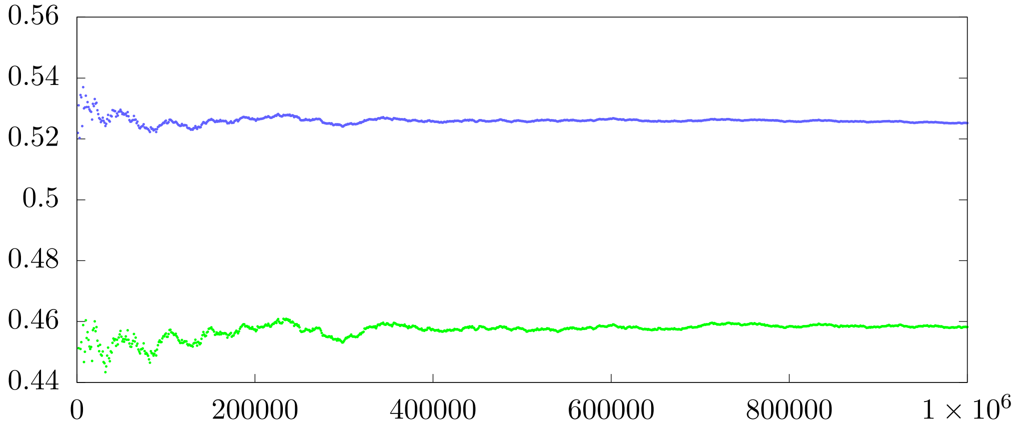

FIGURE 2: Graphs of $\big(\frac{1}{\pi(x)}\sum_{d\le x,\, d\,\mathrm{prime}} T(d)\big)/\sqrt{x}$ (upper) and of $\big(\frac{1}{\pi(x)}\sum_{d\le x,\, d\,\mathrm{prime}} T(d)^2\big)/x$ (lower).

- Finally, we mention here that very recently M. A. Korolev has announced via a preprint in arXiv [4] that $\sum_{d\le x} g(d)^2 = (c_0 + O_\varepsilon(x^{-1/108+\varepsilon}))x^2$ with $c_0 = 1.2\dots$. As a consequence, the asymptotic behaviour for the second moment of g is now known.

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2. Proof of Equation (2)

2.1. **Preliminary results.** By its definition

$$g(d) = \#\big\{(m,q)\in\mathbb{N}^2\colon m<\sqrt{d},\ |q-\sqrt{d}|<m,\ \text{and } \exists k\in\mathbb{Z} \text{ with } d=m^2+kq\big\}.$$

The strict inequalities in the definition of $g(d)$ require m, q, k and d to be at least 1. Let thus $\mathbb{N}_1 := \{n\in\mathbb{N}\colon n\ge 1\}$. Then

$$g(d) = \#G(d),$$

where

$$G(d) := \big\{(m,q,k)\in\mathbb{N}_1^3\colon d=m^2+kq, |q-m|<\sqrt{d}<q+m\big\}$$

that squaring becomes

$$= \big\{(m,q,k)\in\mathbb{N}_1^3\colon d=m^2+kq, q-2m<k<q+2m\big\}.$$

The sets $G(d)$ are disjoint because of the condition $d = m^2 + kq$. Hence

$$\sum_{d\le x} g(d) = \#\bigcup_{d\le x} G(d) = \#\big\{(m,q,k)\in\mathbb{N}_1^3\colon m^2+kq\le x, q-2m<k<q+2m\big\}. \tag{4}$$

For future reference, we notice that if (m,q,k) belongs to this set then $m \le \sqrt{x-kq} < \sqrt{x}$ and, with $d := m^2+kq$, from the initial definition of $G(d)$ we have $q < \sqrt{d}+m \le \sqrt{x}+m$. We need also the following lemma.

Lemma 1. *Let $y \ge 1$ be an integer. Then there exists $\theta = \theta(y) \in [0,1]$ such that:*

$$\sum_{q=y+1}^{2y} \frac{1}{q} = \log 2 - \frac{1}{4y+2\theta}.$$

Proof. Applying the third order Euler–McLaurin formula we get

$$\begin{aligned}
\sum_{q=y+1}^{2y} \frac{1}{q} &= \sum_{q=y}^{2y} \frac{1}{q} - \frac{1}{y} \\
&= \int_y^{2y} \frac{\mathrm{d}q}{q} - \frac{1}{y} + \frac{1}{2}\Big[\frac{1}{2y}+\frac{1}{y}\Big] - \frac{1}{12}\Big[\frac{1}{(2y)^2}-\frac{1}{y^2}\Big] - \int_y^{2y}\frac{B_3(x)}{x^4}\,\mathrm{d}x \\
&= \log 2 - \frac{1}{4y} + \frac{1}{16y^2} - \int_y^{2y}\frac{B_3(x)}{x^4}\,\mathrm{d}x,
\end{aligned}$$

where, denoting $\{x\}$ the fractional part of x, $B_3(x) := \{x\}^3 - 3\{x\}^2/2 + \{x\}/2$. The claim follows since $B_3(x) \in [-1/20, 1/20]$. □

2.2. **Proof of** (2)**.** In all the following computations, each summation index (i.e. m, q or k) is implicitly at least equal to 1. Furthermore, to ease the notations, we set $y := \lceil\sqrt{x}\rceil - 1$, hence $y < \sqrt{x} \le y+1$, and the symbol θ denotes a quantity which is not a constant, i.e. does not necessarily assume the same value in every instance, but is always in $[0,1]$.

From (4) and the lines below we have

$$\sum_{d\le x} g(d) = \sum_{m<\sqrt{x}}\Bigg[\sum_{q<\sqrt{x}-m}\ \sum_{k<q+2m} 1 + \sum_{\sqrt{x}-m\le q<\sqrt{x}+m}\ \sum_{k\le(x-m^2)/q} 1 - \sum_{2m<q<\sqrt{x}+m}\ \sum_{k\le q-2m} 1\Bigg],$$

i.e.,

$$= \sum_{m<\sqrt{x}}\Big[\sum_{q<\sqrt{x}-m}(q+2m-1) + \sum_{\sqrt{x}-m\le q<\sqrt{x}+m}\Big(\frac{x-m^2}{q}-\theta\Big) - \sum_{2m<q<\sqrt{x}+m}(q-2m)\Big],$$

where θ depends on x, m and q but is in $[0,1]$. The sums $\sum_{q<\sqrt{x}-m} q$ and $\sum_{2m<q<\sqrt{x}+m}(q-2m)$ cancel out. This gives

$$\begin{aligned}
&= \sum_{m<\sqrt{x}}\Big[\sum_{q<\sqrt{x}-m}(2m-1) + \sum_{\sqrt{x}-m\le q<\sqrt{x}+m}\frac{x-m^2}{q} - 2\theta m\Big] \\
&= \sum_{m<\sqrt{x}}\Big[(2m-1)(y-m) + \sum_{\sqrt{x}-m\le q<\sqrt{x}+m}\frac{x-m^2}{q}\Big] - \theta y(y+1).
\end{aligned}$$

We exchange the summation order in the second sum. For this we observe that $m < \sqrt{x}$ means that $m \leq y$, hence $q < \sqrt{x} + m \leq \sqrt{x} + y$ implies that $q \leq 2y$. Moreover, the assumption $\sqrt{x} - m \leq q < \sqrt{x} + m$ gives $\sqrt{x} - q \leq m$ when $\sqrt{x} - q$ is positive, and $q - \sqrt{x} < m$ otherwise. This gives

$$= \sum_{m<\sqrt{x}} (2m-1)(y-m) + \Big[\sum_{q<\sqrt{x}} \sum_{\sqrt{x}-q\leq m<\sqrt{x}} + \sum_{\sqrt{x}\leq q\leq 2y} \sum_{q-\sqrt{x}<m<\sqrt{x}} \Big] \frac{x-m^2}{q} - \theta y(y+1).$$

In terms of y, the ranges become

$$= \sum_{m\leq y} (2m-1)(y-m) + \Big[\sum_{q\leq y} \sum_{y-q<m\leq y} + \sum_{y<q\leq 2y} \sum_{q-y\leq m\leq y} \Big] \frac{x-m^2}{q} - \theta y(y+1).$$

Recalling that $\sum_{k=1}^N k^2 = N(N+1)(2N+1)/6$, after some algebra we get

$$= -\frac{2}{3}y^2 + \frac{y}{6} + (2y+1)\Big(x - \frac{y^2+y}{3}\Big) \sum_{y<q\leq 2y} \frac{1}{q} - \theta y(y+1).$$

By Lemma 1 this is

$$= -\frac{2}{3}y^2 + \frac{y}{6} + (2y+1)\Big(x - \frac{y^2+y}{3}\Big)\Big(\log 2 - \frac{1}{4y+2\widetilde{\theta}}\Big) - \theta y(y+1),$$

for some $\theta, \widetilde{\theta} \in [0,1]$. This is $\frac{4}{3}(\log 2)x^{3/2} + R$ with $R = O(x)$. With elementary computations one shows that $-2x - 2\sqrt{x} \leq R \leq -x + 2\sqrt{x}$.

3. Proof of Equation (3)

From the computations at the beginning of 2.1 we have that $g(d)^2 = \#(G(d)\times G(d))$ and $G(d)$ are disjoint, so that

$$\sum_{d\leq x} g(d)^2 = \#\big\{(m_1,q_1,k_1,m_2,q_2,k_2) \in \mathbb{N}_1^6 \colon m_1^2 + k_1q_1 = m_2^2 + k_2q_2,\ m_1^2 + k_1q_1 \leq x \text{ and } q_i - 2m_i < k_i < q_i + 2m_i\ \forall i\big\}.$$

Thus,

$$\sum_{d\leq x} g(d)^2 = \sum_{\substack{m_1,m_2\colon\\ m_i<\sqrt{x}}} \sum_{\substack{q_1,q_2\colon\\ q_i<\sqrt{x}+m_i}} \sum_{\substack{k_1,k_2\colon\\ |q_i-k_i|<2m_i\\ m_1^2+k_1q_1=m_2^2+k_2q_2\\ m_1^2+k_1q_1\leq x}} 1$$

that we estimate with

$$\leq \sum_{\substack{m_1,m_2\colon\\ m_i<\sqrt{x}}} \sum_{\substack{q_1,q_2\colon\\ q_i\leq\sqrt{x}+m_i}} \sum_{\substack{k_1,k_2\colon\\ 0<k_i\leq 2\sqrt{x}-q_i\\ m_1^2+k_1q_1=m_2^2+k_2q_2}} 1$$

because $|q_i - k_i| < 2m_i$ and $m_i^2 + k_iq_i \leq x$ imply that $k_i \leq (x - m_i^2)/q_i \leq 2\sqrt{x} - q_i$: the resulting bound is a bit loose, but it is independent of m_i, and this is very useful for the

computation.
We notice that

$$\sum_{\substack{k_1,k_2:\\0<k_1\le\beta_1\\0<k_2\le\beta_2\\m_1^2+k_1q_1=m_2^2+k_2q_2}} 1 \le \Big(1+\min\Big(\frac{D\beta_1}{q_2},\frac{D\beta_2}{q_1}\Big)\Big)\chi_D(m_1^2,m_2^2)$$

where $D := \gcd(q_1,q_2)$ and $\chi_D(m_1^2,m_2^2)=1$ when $m_1^2=m_2^2 \pmod D$, 0 otherwise.

Proof. Let $D := \gcd(q_1,q_2)$. From the Chinese remainder theorem, there exist k_1 and $k_2 \in \mathbb{Z}$ such that $m_1^2+k_1q_1=m_2^2+k_2q_2$ if and only if $D \mid m_1^2-m_2^2$. In that case they are of the form $k_1 = a+\ell\frac{q_2}{D}$, $k_2 = b+\ell\frac{q_1}{D}$, where (a,b) is one solution and $\ell\in\mathbb{Z}$. The assumption that k_1 is in $(0,\beta_1]$ implies that ℓ is in $(-aD/q_2,(\beta_1-a)D/q_2]$ and there are at most $1+\beta_1D/q_2$ integers in this interval.
The similar argument for k_2 gives the other upper bound for the number of solutions. □

As a consequence we have that

$$\sum_{d\le x} g(d)^2 \le \sum_{\substack{m_1,m_2:\\m_i<\sqrt{x}}}\ \sum_{\substack{q_1,q_2:\\q_i\le\sqrt{x}+m_i}} D\min\Big(\frac{2\sqrt{x}-q_1}{q_2},\frac{2\sqrt{x}-q_2}{q_1}\Big)\chi_D(m_1^2,m_2^2)$$
$$+\sum_{\substack{m_1,m_2:\\m_i<\sqrt{x}}}\ \sum_{\substack{q_1,q_2:\\q_i\le\sqrt{x}+m_i}} \chi_D(m_1^2,m_2^2) =: U+V.$$

Firstly we estimate the contribution of the U term. We have

$$U=\sum_{\substack{q_1,q_2:\\q_i<2\sqrt{x}}} D\min\Big(\frac{2\sqrt{x}-q_1}{q_2},\frac{2\sqrt{x}-q_2}{q_1}\Big)\sum_{\substack{m_1,m_2:\\\max(1,q_i-\sqrt{x})\le m_i<\sqrt{x}}}\chi_D(m_1^2,m_2^2).$$

We split the computation according to the value of D. So, letting $q_1' := q_1/D$, $q_2' := q_2/D$, and $L := 2\sqrt{x}/D$ we get

$$=\sum_{D\le 2\sqrt{x}} D \sum_{\substack{q_1',q_2':\\q_i'<L\\\gcd(q_1',q_2')=1}} \min\Big(\frac{L-q_1'}{q_2'},\frac{L-q_2'}{q_1'}\Big)\sum_{\substack{m_1,m_2:\\\max(1,Dq_i'-\sqrt{x})\le m_i<\sqrt{x}}}\chi_D(m_1^2,m_2^2). \tag{5}$$

The next lemma allows to estimate the innermost sum.

Lemma 2. *Let $D\in\mathbb{N}$, $D\ge 1$, then*

$$\sum_{m_1,m_2\in\mathbb{Z}/D\mathbb{Z}}\chi_D(m_1^2,m_2^2)=c(D)D$$

where c is the multiplicative map with

$$c(p^k) := \begin{cases} k & \text{if } p=2,\\ 1+k-k/p & \text{otherwise.}\end{cases}$$

Proof. By the Chinese remainder theorem $\chi_D(m_1^2, m_2^2) = 1$ if and only if $m_1^2 - m_2^2 = 0 \pmod{p^k}$ for every $p^k \| D$ so that it is sufficient to prove the result when $D = p^k$ is a power of a prime p.
If $n \in \mathbb{Z}$, we denote $\overline{n}$ the class of n in $\mathbb{Z}/p^k\mathbb{Z}$. Let $A := (\mathbb{Z}/p^k\mathbb{Z})^2$ and $P := \{(\overline{m_1}, \overline{m_2}) \in A \colon \overline{m_1}^2 = \overline{m_2}^2\}$. To prove the lemma, we need to check that P has $c(p^k)p^k$ elements. Let $f \colon A \longrightarrow A$ be the map defined by

$$f(\alpha, \beta) := (\alpha + \beta, \alpha - \beta),$$

and let $m \colon A \longrightarrow \mathbb{Z}/p^k\mathbb{Z}$ be the multiplication map: $m(\overline{a}, \overline{b}) = \overline{a}\overline{b}$. We thus have

$$(\overline{m_1}, \overline{m_2}) \in P \iff m(f(\overline{m_1}, \overline{m_2})) = \overline{0}.$$

Let $Z := m^{-1}(\overline{0})$. Let $(\overline{a}, \overline{b}) \in Z$. There are p^k such pairs with $\overline{a} = \overline{0}$. Otherwise, for any $u \in [0, k-1]$, there are $p^{k-u} - p^{k-u-1}$ classes $\overline{a}$ such that $p^u \| a$; then $p^{k-u} \mid b$, and there are p^u such classes; there are therefore $p^k - p^{k-1}$ pairs $(\overline{a}, \overline{b}) \in Z$ with $p^u \| a$. Summing over u, and adding the case with $\overline{a} = \overline{0}$, we get that Z has $p^k + k(p^k - p^{k-1})$ elements.
If p is odd, then f is invertible with inverse

$$g(\overline{a}, \overline{b}) = \Big(\frac{\overline{a} + \overline{b}}{\overline{2}}, \frac{\overline{a} - \overline{b}}{\overline{2}}\Big),$$

therefore P and Z have the same number of elements.
If $p = 2$, things are slightly more complicated because 2 is not invertible anymore. To have $(\overline{m_1}, \overline{m_2}) \in P$, we need to have m_1 and m_2 of the same parity. Let E be the subset of $(\mathbb{Z}/2^k\mathbb{Z})^2$ made of pairs $(\overline{m_1}, \overline{m_2})$ where m_1 and m_2 have the same parity. Then $F := f(E)$ is the set of pairs $(\overline{2a}, \overline{2b})$ and

$$f^{-1}\big(f(\overline{m_1}, \overline{m_2})\big) = \Big\{(\overline{m_1}, \overline{m_2}), \big(\overline{m_1 + 2^{k-1}}, \overline{m_2 + 2^{k-1}}\big)\Big\}.$$

We have $P = f^{-1}(Z \cap F)$ and therefore the cardinality of P is twice that of $Z \cap F$. If $(\overline{a}, \overline{b}) \in Z \backslash F$, then a or b is odd. In that case $\overline{a}$ or $\overline{b}$ is invertible so that the other one is $\overline{0}$. There are thus $2 \cdot 2^{k-1}$ elements in $Z \backslash F$, therefore $k(2^k - 2^{k-1}) = k2^{k-1}$ elements in $Z \cap F$. Therefore P has $k2^k$ elements. □

According to the previous lemma we have that

$$\sum_{\substack{m_1, m_2 \colon \\ \max(1, q_i - \sqrt{x}) \le m_i < \sqrt{x}}} \chi_D(m_1^2, m_2^2) \le c(D)D \prod_{i=1,2} \Big(\frac{\min(\sqrt{x}, 2\sqrt{x} - q_i)}{D} + 1\Big)$$
$$\le c(D)D \prod_{i=1,2} \big(\min(L/2, L - q_i') + 1\big),$$

and from (5), with the suppression of the assumption $\gcd(q_1', q_2') = 1$, we get

$$U \le \sum_{D \le 2\sqrt{x}} c(D)D^2 \sum_{\substack{q_1', q_2' \colon \\ q_i' < L}} \prod_{i=1,2} \big(\min(L/2, L - q_i') + 1\big) \min\Big(\frac{L - q_1'}{q_2'}, \frac{L - q_2'}{q_1'}\Big). \tag{6}$$

The function $f(q_1', q_2') := \prod_{i=1,2} \big(\min(L/2, L - q_i') + 1\big) \min\big(\frac{L - q_1'}{q_2'}, \frac{L - q_2'}{q_1'}\big)$ decreases in each argument when $q_1', q_2' \in [1, L]$, so the corresponding integral extended to the region $[0, L] \times$

$[0, L]$ provides an upper bound for the sum. Moreover, we further introduce the new variables a, b such that $q_1' =: aL = 2\sqrt{x}a/D$, $q_2' =: bL = 2\sqrt{x}b/D$, yielding

$$U \leq \sum_{D\leq 2\sqrt{x}} c(D)D^2\Big[\Big(\frac{2\sqrt{x}}{D}\Big)^4 A + \Big(\frac{2\sqrt{x}}{D}\Big)^3 B + \Big(\frac{2\sqrt{x}}{D}\Big)^2 C\Big],$$

where

$$A := \int_{a,b\in(0,1]} \min\Big(\frac{1}{2}, 1-a\Big)\min\Big(\frac{1}{2}, 1-b\Big)\min\Big(\frac{1-a}{b}, \frac{1-b}{a}\Big)\,\mathrm{d}a\,\mathrm{d}b = \frac{7}{6}\log 2 - \frac{37}{72},$$
$$B := \int_{a,b\in(0,1]} \Big(\min\Big(\frac{1}{2}, 1-a\Big) + \min\Big(\frac{1}{2}, 1-b\Big)\Big)\min\Big(\frac{1-a}{b}, \frac{1-b}{a}\Big)\,\mathrm{d}a\,\mathrm{d}b = \frac{19}{6}\log 2 - \frac{11}{12},$$
$$C := \int_{a,b\in(0,1]} \min\Big(\frac{1-a}{b}, \frac{1-b}{a}\Big)\,\mathrm{d}a\,\mathrm{d}b = 2\log 2.$$

Hence the bound says

$$U \leq 16Ax^2\sum_{D=1}^{+\infty}\frac{c(D)}{D^2} + 8Bx^{3/2}\sum_{D\leq 2\sqrt{x}}\frac{c(D)}{D} + 4Cx\sum_{D\leq 2\sqrt{x}} c(D),$$

that we estimate with

$$\leq 16Ax^2\sum_{D=1}^{+\infty}\frac{c(D)}{D^2} + 8(B+C)x^{3/2}\sum_{D\leq 2\sqrt{x}}\frac{c(D)}{D},$$

because $D \leq 2\sqrt{x}$.

We can evaluate explicitly the series, since $F(s) := \sum_{n=1}^{+\infty} c(n)n^{-s} = \frac{4^s-2^s+1}{4^s-2^s-1}\frac{\zeta(s)^2}{\zeta(s+1)}$ for $\mathrm{Re}(s) > 1$. Thus,

$$\sum_{D=1}^{+\infty}\frac{c(D)}{D^2} = F(2) = \frac{13}{14}\frac{\zeta(2)^2}{\zeta(3)} = 2.090\ldots$$

To bound the sum we introduce both the Dirichlet series $H(s) =: \sum_{n=1}^{+\infty} h(n)n^{-s}$ such that $F(s) =: H(s)\zeta(s)^2$, so that

$$H(s) = \Big(1 - \frac{1/2}{2^s} + \frac{3/2^2}{2^{2s}} + \frac{3/2^3}{2^{3s}} + \cdots\Big)\prod_{p\,\mathrm{odd}}\Big(1 - \frac{1/p}{p^s}\Big),$$

and the series $\widetilde{H}(s) := \sum_{n=1}^{+\infty} |h(n)|n^{-s}$, so that

$$\widetilde{H}(s) = \Big(1 + \frac{1/2}{2^s} + \frac{3/2^2}{2^{2s}} + \frac{3/2^3}{2^{3s}} + \cdots\Big)\prod_{p\,\mathrm{odd}}\Big(1 + \frac{1/p}{p^s}\Big) = \frac{4^{s+1}+2}{4^{s+1}-1}\frac{\zeta(s+1)}{\zeta(2s+2)}.$$

Thus,

$$\sum_{D\leq 2\sqrt{x}}\frac{c(D)}{D} = \sum_{u\leq 2\sqrt{x}}\frac{h(u)}{u}\sum_{v\leq 2\sqrt{x}/u}\frac{d(v)}{v},$$

where $d(v)$ counts the divisors of v. Since $\sum_{v\leq w}\frac{d(v)}{v} \leq \frac{1}{2}\log^2(e^2 w)$ for every w (by partial summation from $\sum_{v\leq w} d(v) \leq w\log w + w$, which is weaker than what is known about the mean value for the divisor function, but which is sufficient for our purposes), we get

$$\begin{aligned}\sum_{D\leq 2\sqrt{x}}\frac{c(D)}{D}&\leq\sum_{u\leq 2\sqrt{x}}\frac{|h(u)|}{2u}\log^2(2e^2\sqrt{x})\leq\frac{\widetilde{H}(1)}{2}\log^2(2e^2\sqrt{x})\\&=\frac{3}{5}\frac{\zeta(2)}{\zeta(4)}\log^2(2e^2\sqrt{x})\leq 0.228\log^2(4e^4x).\end{aligned}$$

Thus,

$$U\leq 9.9\,x^2+4.87\,x^{3/2}\log^2(4e^4x). \tag{7}$$

Lastly we estimate the contribution of the V term. We bound it trivially, i.e. substituting $\chi_D(m_1^2,m_2^2)$ with 1. However, to improve the conclusion, we retain the remark that when m_1 and m_2 have different parity, then q_1 and q_2 cannot be both even. In this way we get that

$$\begin{aligned}V&=\sum_{\substack{m_1,m_2:\\ m_i<\sqrt{x}}}\sum_{\substack{q_1,q_2:\\ q_i\leq\sqrt{x}+m_i}}\chi_D(m_1^2,m_2^2)\leq\sum_{\substack{m_1,m_2:\\ m_i\leq\sqrt{x}}}\sum_{\substack{q_1,q_2:\\ q_i\leq\sqrt{x}+m_i}}1-\sum_{\substack{m_1,m_2:\\ m_1\neq m_2 \pmod 2\\ m_i\leq\sqrt{x}}}\sum_{\substack{q_1,q_2:\\ q_i\text{ even}\\ q_i\leq\sqrt{x}+m_i}}1\\&\leq\Big[\sum_{m\leq\sqrt{x}}(\sqrt{x}+m)\Big]^2-2\sum_{\substack{m_1\leq\sqrt{x}\\ m_1\text{ even}}}\sum_{\substack{m_2\leq\sqrt{x}\\ m_2\text{ odd}}}\frac{(\sqrt{x}+m_1-2)}{2}\frac{(\sqrt{x}+m_2-2)}{2}\\&\leq\Big[\sum_{m\leq\sqrt{x}}(\sqrt{x}+m)\Big]^2-\frac{1}{2}\sum_{u\leq\frac{\sqrt{x}}{2}}(2u+\sqrt{x}-2)\sum_{v\leq\frac{\sqrt{x}+1}{2}}(2v+\sqrt{x}-3).\end{aligned}$$

After some computations we get that

$$V\leq\frac{63}{32}x^2+\frac{51}{16}x^{3/2}-\frac{111}{32}x+\frac{57}{16}\sqrt{x}-\frac{5}{4}\leq\frac{63}{32}x^2+\frac{51}{16}x^{3/2}. \tag{8}$$

Adding (7) and (8) we get the claim since $\frac{51}{16}x^{3/2}\leq 0.13\,x^{3/2}\log^2(4e^4x)$ for every $x\geq 1$.

Retaining the coprimality condition in (6) the main term in (7) appears divided by $\zeta(2)$, at the cost of error terms of size $O(x^{3/2}\log^4 x)$. Also (8) can be improved a bit using the result in Lemma 2 and keeping the resulting coprimality condition. The combined effect of these two improvements gives the bound $8x^2+O(x^{3/2}\log^4 x)$ mentioned after Theorem 1.

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