SPARSE VARIANCE FOR PRIMES IN ARITHMETIC PROGRESSION

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Abstract. An analogue of the Montgomery-Hooley asymptotic formula is established for the variance of the number of primes in arithmetic progressions, in which the moduli are restricted to the values of a polynomial.

1. Introduction

The distribution of primes is a fundamental problem in the theory of numbers. Our concern here is with the error terms that arise in the prime number theorem for arithmetic progressions. Let ϕ denote Euler's totient, and define the relevant quantity $E(x;k,l)$ for real $x \geq 2$, and coprime natural numbers k and l, through the equation

$$\sum_{\substack{p\leq x\\ p\equiv l \bmod k}} \log p = \frac{x}{\phi(k)} + E(x;k,l).$$

Montgomery [8] obtained an asymptotic formula for the variance

$$V(x,y) = \sum_{k\leq y} \sum_{\substack{l=1\\ (l,k)=1}}^{k} |E(x;k,l)|^2$$

that was promptly refined by Hooley [5], and now takes the shape

$$V(x,y) = xy\log y + cxy + O(x^{1/2}y^{3/2} + x^2(\log x)^{-A}). \tag{1}$$

Here, the coefficient c is a certain real constant, the exponent A is a preassigned positive real number, and the relation (1) holds uniformly for $1 \leq y \leq x$. In this range, the asymptotic formula (1) implies the upper bound

$$V(x,y) \ll xy\log x + x^2(\log x)^{-A} \tag{2}$$

which is known as the Barban-Davenport-Halberstam theorem. If one singles out an individual progression l modulo k from the mean $V(x,y)$, then one recovers from the bound (2) the Siegel-Walfisz theorem, the latter asserting that the estimate

$$E(x;k,l) \ll x(\log x)^{-A/2}$$

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holds uniformly in k and l. Although it seems difficult to improve this last bound, the asymptotic formula for $V(x,y)$ shows that in mean square, the average size of $E(x;k,l)$ is about the square-root of $(x\log x)/k$.

One might ask whether conclusions similar to those described above are possible for thinner averages, for example with the moduli k restricted to the values of a polynomial. This was studied recently by Mikawa and Peneva [7], who obtained a result analogous to the Barban-Davenport-Halberstam theorem. More precisely, let $f\in\mathbb{Q}[t]$ denote an integer-valued polynomial of degree $d\ge 2$, with positive leading coefficient and derivative f'. Then, there exist real numbers y_1 such that the inequalities $f(y)\ge 2$ and $f'(y)\ge 1$ hold for all $y\ge y_1$. Denote the smallest such y_1 with $y_1\ge 1$ by $y_0(f)$. We may now define

$$V_f(x,y)=\sum_{y_0(f)<k\le y} f'(k)\sum_{\substack{l=1\\(l,f(k))=1}}^{f(k)} |E(x;f(k),l)|^2. \tag{3}$$

In this notation, the aforementioned estimate of Mikawa and Peneva asserts that whenever $A\ge 1$ is a real number, then there is a $B\ge 1$ such that, uniformly for $f(y)\le x(\log x)^{-B}$, one has

$$V_f(x,y)\ll x^2(\log x)^{-A}. \tag{4}$$

We note here that Theorem 2 of [7] relates to a variant of $V_f(x,y)$, with the weight $f'(k)$ in (3) replaced by $k^{-1}\phi(f(k))$. However, as is easily checked, the bound (4) above is equivalent to the conclusion in [7]. Our purpose in this paper is to establish a version of the Montgomery-Hooley asymptotic formula for $V_f(x,y)$.

Theorem. *Let f be an integer-valued polynomial of degree $d\ge 2$, with positive leading coefficient. Then, whenever $f(y)\le x$, one has*

$$V_f(x,y)=xf(y)\log f(y)+C(f)xf(y)+O\big(x^{1/2}f(y)^{3/2}+x^2(\log x)^{-A}\big),$$

wherein $C(f)$ denotes a certain real number depending only on f.

A new approach[1] to the Montgomery-Hooley theorem was developed by Goldston and Vaughan [3] and Vaughan [10]. In contrast with previous work that depended on the additive theory of primes, the evaluation of $V(x,y)$ is now linked to the problem of finding an asymptotic formula for the number of solutions of the equation $p_1-p_2=hk$ in primes p_1,p_2 not exceeding x, and natural numbers h and k with $k\le y$. This may be viewed as a ternary additive problem that is well within the competence of the circle method. Moreover, the primes enter the scene only through an application of the Siegel-Walfisz theorem. Vinogradov's estimate for exponential sums over primes is not required since the minor arc analysis can be performed primarily with the product hk. Following these patterns, we are led to consider the equation $p_1-p_2=hf(k)$, and again, a treatment by the circle method is possible. A detailed discussion of this equation is to be found in §§3 and 4, following a preparatory analysis in the next section. Reflecting a similar problem in the work of Vaughan [10], the treatment of the major arcs invokes certain auxiliary averages of multiplicative functions that are supplied in §§5 and 6, thereby completing the proof of the theorem.

There is an extensive literature relating to improvements of the error term in the asymptotic formula (1) that are subject to the truth of the Riemann hypothesis for Dirichlet

[1]For historical comments on the genesis of this method, the curious reader is directed to p. 118 of [3].

L-functions (see, in particular, Hooley [5], [6], Friedlander and Goldston [2], Goldston and Vaughan [3] and Vaughan [11]). Likewise, in the conclusion of our theorem above, the term $x^2(\log x)^{-A}$ may be replaced conditionally by $x^{2-\delta(d)}$, where $\delta(d)$ is a positive real number the size of which is determined by the maximal savings available for Weyl sums involving a degree d polynomial. We spare the reader any details.

Our methods are rather flexible. One may replace the primes with other sequences of interest, and functions can be substituted for the polynomial f with growth more rapid than any polynomial. For example, by working along the lines of Brüdern and Perelli [1], it should be possible to deduce an asymptotic formula for $V_f(x,y)$ when $f(k) = [\exp((\log k)^\gamma)]$, and γ is any positive number smaller than 3/2.

2. Two preparatory steps

Our initial advance on the analysis of the variance $V_f(x,y)$ involves the isolation of a term accessible to the circle method, and this is the objective of this section. Fix the value of $A \geq 1$ for the rest of the paper, and choose a permissible value of $B = B(A)$ so that the asymptotic relation (4) holds uniformly for $f(y) \leq x(\log x)^{-B}$. An inspection of [7] reveals that one may take $B = 2^{4d}A$. When x is sufficiently large, there is a unique solution y to the equation $f(y) = x(\log x)^{-B}$ that we denote by $y_1 = y_1(x)$. As a truncated analogue of the sum $V_f(x,y)$ defined in (3), we define

$$V_f'(x,y) = \sum_{y_1<k\leq y} f'(k) \sum_{\substack{l=1\\(l,f(k))=1}}^{f(k)} |E(x;f(k),l)|^2. \tag{5}$$

Then in view of the definition (3) and the estimate (4), it is easily verified that

$$V_f(x,y) = V_f'(x,y) + O(x^2(\log x)^{-A}). \tag{6}$$

We have removed small values of k from $V_f(x,y)$ mainly for technical convenience. To do so, we had to invoke the work of Mikawa and Peneva [7], but it would be possible, and perhaps more coherent, to cover small k by our method. However, a critical step for small k would depend on the ideas of section 2.2 in [7], and that we would have need to duplicate in any case. In the interest of brevity, we therefore prefer to work temporarily with $V_f'(x,y)$.

In the next step, we open the square in (5). Let

$$\vartheta(x;k,l) = \sum_{\substack{p\leq x\\p\equiv l \bmod k}} \log p$$

and

$$\Phi_f(z,y) = \sum_{z<k\leq y} \frac{f'(k)}{\phi(f(k))}. \tag{7}$$

Then it follows from (5) that

$$V_f'(x,y) = S_1 - 2xS_2 + x^2\Phi_f(y_1,y), \tag{8}$$

where

$$S_1 = \sum_{y_1<k\le y} f'(k) \sum_{\substack{l=1\\(l,f(k))=1}}^{f(k)} \vartheta(x;f(k),l)^2,$$

$$S_2 = \sum_{y_1<k\le y} \frac{f'(k)}{\phi(f(k))} \sum_{\substack{l=1\\(l,f(k))=1}}^{f(k)} \vartheta(x;f(k),l).$$

By the Prime Number Theorem, one finds that

$$\sum_{\substack{l=1\\(l,f(k))=1}}^{f(k)} \vartheta(x;f(k),l) = \sum_{\substack{p\le x\\ p\nmid f(k)}} \log p = x + O(x(\log x)^{-3A}).$$

Consequently, using only straightforward estimates, one discovers that whenever $f(y)\le x$, one has

$$S_2 = x\Phi_f(y_1,y) + O(x(\log x)^{2-3A}). \tag{9}$$

Similarly, one may derive the relation

$$\sum_{\substack{l=1\\(l,f(k))=1}}^{f(k)} \vartheta(x;f(k),l)^2 = \sum_{\substack{p_1\le x\\ p_1\nmid f(k)}} \sum_{\substack{p_2\le x\\ p_2\nmid f(k)\\ p_1\equiv p_2 \bmod f(k)}} (\log p_1)(\log p_2).$$

Here we separate the diagonal terms with $p_1=p_2$ from the off-diagonal ones. Note that the conditions $p_1|f(k)$ and $p_1\equiv p_2 \bmod f(k)$ imply that $p_1=p_2$. We may therefore ignore the constraint $p_j\nmid f(k)$ $(j=1,2)$ when considering the off-diagonal terms. In this way, by symmetry, we derive the formula

$$\sum_{\substack{l=1\\(l,f(k))=1}}^{f(k)} \vartheta(x;f(k),l)^2 = \sum_{\substack{p\le x\\ p\nmid f(k)}} (\log p)^2 + 2 \sum\sum_{\substack{p_1<p_2\le x\\ p_1\equiv p_2 \bmod f(k)}} (\log p_1)(\log p_2).$$

We next reintroduce the terms with $p|f(k)$, and sum over k. Then, much as in the analysis leading to the relation (9), we find that

$$S_1 = 2S_0 + \sum_{y_1<k\le y} f'(k) \sum_{p\le x} (\log p)^2 + O(x(\log x)^2), \tag{10}$$

where

$$S_0 = \sum_{y_1<k\le y} f'(k) \sum\sum_{\substack{p_1<p_2\le x\\ p_1\equiv p_2 \bmod f(k)}} (\log p_1)(\log p_2). \tag{11}$$

On applying partial summation within (10), and substituting the outcome together with (8) and (9) into (6), we obtain our final formula

$$V_f(x,y) = 2S_0 - x^2\Phi_f(y_1,y) + f(y)\sum_{p\le x}(\log p)^2 + O(x^2(\log x)^{-A}). \tag{12}$$

3. The circle method

In this section we apply the circle method to evaluate the sum S_0 defined in equation (11). With this objective in view, we rewrite the congruence condition $p_1 \equiv p_2 \bmod f(k)$ in (11) in the form $p_2 - p_1 = hf(k)$, with $h \in \mathbb{Z}$. In addition, we observe that the supplementary condition $h \geq 1$ is equivalent to the summation condition $p_1 < p_2$ imposed in the second summation of (11). Consequently, on writing

$$T_f(\alpha) = \sum_{y_1 < k \leq y} f'(k) \sum_{h \leq x/f(k)} e(\alpha h f(k)), \tag{13}$$

$$U(\alpha) = \sum_{p \leq x} (\log p) e(\alpha p), \tag{14}$$

we may use orthogonality to infer from (11) that

$$S_0 = \int_0^1 T_f(\alpha) |U(\alpha)|^2 \, d\alpha.$$

We analyse this integral by splitting the range of integration into major and minor arcs. The dissection depends on the absolute constant $D \geq 1$ that arises in Lemma 1 below. Let $C = 4d^3DB$, and write $Q = (\log x)^C$. Let $\mathfrak{M}$ denote the union of the pairwise disjoint intervals $|\alpha - a/q| \leq Q/x$ with $1 \leq a \leq q \leq Q$ and $(a,q) = 1$. Let $\mathfrak{m} = [Q/x, 1 + Q/x] \setminus \mathfrak{M}$. The contribution from the minor arcs is controlled with the aid of the bound

$$\sup_{\alpha \in \mathfrak{m}} |T_f(\alpha)| \ll x (\log x)^{-2A} \tag{15}$$

that we establish in a moment. Equipped with (15) and the elementary estimate

$$\int_0^1 |U(\alpha)|^2 \, d\alpha = \sum_{p \leq x} (\log p)^2 \ll x \log x,$$

we infer that

$$S_0 = S_{\mathfrak{M}} + O(x^2 (\log x)^{1-2A}), \tag{16}$$

where

$$S_{\mathfrak{M}} = \int_{\mathfrak{M}} T_f(\alpha) |U(\alpha)|^2 \, d\alpha. \tag{17}$$

The major arc contribution $S_{\mathfrak{M}}$ will be discussed in §4. In the remainder of this section, we briefly sketch a proof of (15). This bound of Weyl's type is certainly familiar territory for workers in the field, but a suitable reference does not seem to be available. The argument below is streamlined so as to confirm (15) with little effort, but when one seeks for the strongest possible bounds, one can do rather better, in particular when d is small. This is of no relevance for us, but an analysis of $V_f(x, y)$ under GRH is sensitive to this comment.

Let $y_0 \leq z_0 \leq z$, and consider the weighted Weyl sum

$$S(\beta; z_0, z) = \sum_{z_0 < n \leq z} f'(n) e(\beta f(n)).$$

Lemma 1. *There is an absolute constant $D \geq 1$ with the property that whenever $\beta \in \mathbb{R}$, and b and r are coprime natural numbers with $|r\beta - b| \leq 1/r$, one has*

$$S(\beta; z_0, z) \ll z^d(\log z)\big((r + z^d|r\beta - b|)^{-1} + z^{-1} + (r + z^d|r\beta - b|)z^{-d}\big)^{1/(Dd^3)}.$$

Proof. When k is a natural number, let $J_{s,k}(P)$ denote the number of integral solutions of the simultaneous equations

$$\sum_{i=1}^{s}(x_i^j - y_i^j) = 0 \qquad (1 \leq j \leq k),$$

with $1 \leq x_i, y_i \leq P$ $(1 \leq i \leq s)$. Then, by Theorem 7.4 of Vaughan [9], for example, there exists an absolute constant $D \geq 1$ such that whenever $s \geq \frac{1}{2}Dk^3$, one has $J_{s,k}(P) \ll P^{2s-k(k+1)/2}$. Applying Theorem 5.2 of Vaughan [9] in conjunction with partial summation, we deduce that

$$S(\beta; z_0, z) \ll z^d(\log z)(r^{-1} + z^{-1} + rz^{-d})^{1/(Dd^3)}.$$

The conclusion of the lemma now follows from a familiar transference principle (see, for example, Exercise 2 of Chapter 2 of Vaughan [9]). □

We are now ready to deduce (15). Let $y(h)$ be the upper bound for k determined by the simultaneous conditions $k \leq y$ and $f(k) \leq x/h$. Then $f(y(h)) = \min\{f(y), x/h\}$. Reversing the order of summation in (13) yields

$$T_f(\alpha) = \sum_{h \leq (\log x)^B} S(\alpha h; y_1, y(h)). \tag{18}$$

Suppose that $\alpha \in \mathfrak{m}$. For any integer h with $1 \leq h \leq (\log x)^B$, we apply Dirichlet's theorem to find coprime integers $r = r(h)$ and $b = b(h)$ with

$$1 \leq r \leq y(h)^{d-2/3} \quad \text{and} \quad |\alpha hr - b| \leq y(h)^{-d+2/3}.$$

The validity of the simultaneous conditions $hr \leq Q$ and $|\alpha - b/(hr)| \leq Q/x$ would imply that $\alpha \in \mathfrak{M}$, whence for each h, at least one of these inequalities fails. If $hr > Q$, then $r > (\log x)^{C-B}$, and an application of Lemma 1 with $\beta = \alpha h$ yields

$$S(\alpha h; y_1, y(h)) \ll x(\log x)(r^{-1} + y(h)^{-2/3})^{1/(Dd^3)} \ll x(\log x)^{1+(B-C)/(Dd^3)}.$$

If $hr \leq Q$ but $|\alpha - b/(hr)| > Q/x$, meanwhile, then in like manner Lemma 1 gives

$$S(\alpha h; y_1, y(h)) \ll x(\log x)Q^{-1/(Dd^3)} \ll x(\log x)^{1-C/(Dd^3)}.$$

Summing over natural numbers h with $h \leq (\log x)^B$, we deduce (15) from (18).

4. The major arcs

We move on to analyse the major arc contribution $S_{\mathfrak{M}}$ to S_0, and subsequently incorporate the conclusions of the previous section in order to obtain an asymptotic formula for S_0. For $\alpha \in \mathfrak{M}$, one may write $\alpha = \beta + a/q$ for some $\beta \in \mathbb{R}$ with $|\beta| \leq Q/x$, and coprime integers a and q with $1 \leq a \leq q \leq Q$. Then, by (14) and Lemma 3.1 of Vaughan [9], one has

$$U(\alpha) = \frac{\mu(q)}{\phi(q)}J(\beta) + O(x(\log x)^{-5C}),$$

where

$$J(\beta) = \sum_{n \le x} e(\beta n).$$

The trivial upper bound $T_f(\alpha) \ll x \log x$ (which is available from (13)) and (17) now suffice to confirm that

$$S_{\mathfrak{M}} = \sum_{q \le Q} \frac{\mu(q)^2}{\phi(q)^2} \sum_{\substack{a=1\\(a,q)=1}}^{q} \int_{-Q/x}^{Q/x} T_f(\beta + a/q) |J(\beta)|^2 \, d\beta + O(x^2 (\log x)^{-C}).$$

We would like to extend the sum over all natural numbers q here. It is convenient to do this in two steps. In the first of these steps, we extend the range for q above to $q \le x^{1/(2d)}$. For this, we note that the intervals $|\alpha - a/q| \le Q/x$ with $1 \le a \le q \le x^{1/(2d)}$ and $(a, q) = 1$ are pairwise disjoint. When a and q are coprime natural numbers with $1 \le a \le q$ and $Q < q \le x^{1/(2d)}$, and $|\beta| \le Q/x$, one has $\beta + a/q \in \mathfrak{m}$. Therefore, on recalling (15), for any such β, a and q, one has

$$|T_f(\beta + a/q)| \le \sup_{\alpha \in \mathfrak{m}} |T_f(\alpha)| \ll x(\log x)^{-2A}.$$

Combining this estimate with the elementary inequality

$$\int_{-Q/x}^{Q/x} |J(\beta)|^2 \, d\beta \le \int_{-1/2}^{1/2} |J(\beta)|^2 \, d\beta = [x],$$

we deduce that

$$S_{\mathfrak{M}} = \sum_{q \le x^{1/(2d)}} \frac{\mu(q)^2}{\phi(q)^2} \sum_{\substack{a=1\\(a,q)=1}}^{q} \int_{-Q/x}^{Q/x} T_f(\beta + a/q) |J(\beta)|^2 \, d\beta + O(x^2 (\log x)^{1-2A}). \tag{19}$$

Before extending the range for q even further, we complete the integral in (19) to $|\beta| \le \frac{1}{2}$. In this range for β, one has $J(\beta) \ll |\beta|^{-1}$, so that another application of the trivial bound $T_f(\alpha) \ll x \log x$ in combination with straightforward estimates yields the upper bound

$$\sum_{q \le x^{1/(2d)}} \frac{\mu(q)^2}{\phi(q)^2} \sum_{\substack{a=1\\(a,q)=1}}^{q} \int_{Q/x \le |\beta| \le \frac{1}{2}} |T_f(\beta + a/q) J(\beta)^2| \, d\beta$$
$$\ll x(\log x) \sum_{q \le x} \frac{1}{\phi(q)} \int_{Q/x}^{1/2} \beta^{-2} \, d\beta \ll x^2 (\log x)^{2-C}.$$

Hence, we may indeed extend the integration in (19) to $[-\frac{1}{2}, \frac{1}{2}]$ with the introduction of acceptable errors. However, by orthogonality and (13), one has

$$\begin{aligned}
\int_{-1/2}^{1/2} T_f(\beta + a/q) |J(\beta)|^2 \, d\beta &= \sum_{y_1 < k \le y} f'(k) \sum_{h \le x/f(k)} \sum_{\substack{n_1 \le x\ n_2 \le x\\ n_2 - n_1 = hf(k)}} \sum e\left(\frac{ahf(k)}{q}\right) \\
&= \sum_{y_1 < k \le y} f'(k) \sum_{h \le x/f(k)} e\Big(\frac{ahf(k)}{q}\Big)([x] - hf(k)).
\end{aligned}$$

In the last sum, we may replace $[x]$ by x, introducing an error bounded by $O(x\log x)$ into this identity. We summarize and inject these results into (19) to infer that

$$S_{\mathfrak{M}} = M_0 + O(x^2(\log x)^{-A}), \tag{20}$$

where

$$M_0 = \sum_{q\le x^{1/(2d)}} \frac{\mu(q)^2}{\phi(q)^2} \sum_{y_1<k\le y} f'(k) \sum_{h\le x/f(k)} c_q(hf(k))(x-hf(k)),$$

in which we have written

$$c_q(n) = \sum_{\substack{a=1\\(a,q)=1}}^{q} e\Big(\frac{an}{q}\Big)$$

for Ramanujan's sum.

Recall that $y(h)$ was defined through the equation $f(y(h)) = \min\{f(y), x/h\}$. In the definition of M_0, we exchange the order of summation of h and k and then sort k according to residue classes modulo q. Then

$$M_0 = \sum_{q\le x^{1/(2d)}} \frac{\mu(q)^2}{\phi(q)^2} \sum_{h\le x/f(y_1)} \sum_{a=1}^{q} c_q(hf(a)) \sum_{\substack{y_1<k\le y(h)\\ k\equiv a \bmod q}} f'(k)(x-hf(k)). \tag{21}$$

For small q, Euler's summation formula readily yields an asymptotic formula for the innermost sum, with a main term independent of a. It is then possible to sum $c_q(hf(a))$ over a. This process will largely disentangle the sum in (21). Two lemmata make this analysis precise.

Lemma 2. *With x, y and h in the ranges as above, and uniformly in q, one has*

$$\sum_{\substack{y_1<k\le y(h)\\ k\equiv a \bmod q}} f'(k)(x-hf(k)) = \frac{1}{q}\int_{f(y_1)}^{f(y(h))} (x-ht)\,dt + O(xy^{d-1}+y^{2d-1}h).$$

Proof. Observe first that by Euler's summation formula, if $g:[X,Y]\to\mathbb{R}$ is continuously differentiable, then

$$\sum_{\substack{X<k\le Y\\ k\equiv a \bmod q}} g(k) = \frac{1}{q}\int_X^Y g(t)\,dt + E, \tag{22}$$

where the implicitly defined real number E satisfies the bound

$$|E| \le \int_X^Y |g'(t)|\,dt + |g(X)| + |g(Y)|.$$

For the application at hand, we take $g(t) = f'(t)(x-hf(t))$, and put $X = y_1$ and $Y = y(h)$. Note, in particular, that $x - hf(t) = O(x)$ for all relevant choices of t, and hence $g(t) \ll y^{d-1}x$ for $X \le t \le Y$. Also, one has $g'(t) = f''(t)(x-hf(t)) - hf'(t)^2$. Then it follows that

$$E \ll xy^{d-1} + y^{2d-1}h. \tag{23}$$

Finally, by substitution one obtains

$$\int_{y_1}^{y(h)} f'(t)(x-hf(t))\,dt = \int_{f(y_1)}^{f(y(h))} (x-h\tau)\,d\tau. \tag{24}$$

The conclusion of the lemma follows by collecting together (22), (23) and (24). □

In advance of the statement of the next lemma, for each natural number m, we define $\rho(m)$ to be the number of solutions of the congruence $f(a) \equiv 0 \bmod m$.

Lemma 3. *For any $h \in \mathbb{N}$, the sum*

$$w_h(q) = \frac{1}{q}\sum_{a=1}^{q} c_q(hf(a))$$

is a multiplicative function of q. When p is a prime, one has

$$w_h(p) = \begin{cases} p-1, & \text{when } p|h, \\ \rho(p)-1, & \text{when } p \nmid h. \end{cases}$$

Proof. Since $c_q(n)$ is multiplicative as a function of q (see, for example, Theorem 272 of Hardy and Wright [4]), it suffices to apply the Chinese Remainder Theorem to the sum over a in order to confirm the multiplicativity of $w_h(q)$. Next, when p is a prime, we apply the definition of $c_q(n)$ and orthogonality to obtain the relation

$$w_h(p) = \frac{1}{p}\sum_{l=1}^{p-1}\sum_{a=1}^{p} e\Big(\frac{lhf(a)}{p}\Big) = \mathrm{card}\{1 \le a \le p :\ hf(a) \equiv 0 \bmod p\} - 1,$$

and the lemma follows at once. □

We inject the asymptotic formula supplied by Lemma 2 into (21). This introduces an error term

$$\sum_{q \le x^{1/(2d)}} \frac{\mu(q)^2}{\phi(q)^2} \sum_{h \le x/f(y_1)} q\phi(q)(xy^{d-1} + y^{2d-1}h) \ll x^{2-1/(2d)+\varepsilon},$$

so that we now have

$$M_0 = \sum_{q \le x^{1/(2d)}} \frac{\mu(q)^2}{\phi(q)^2} \sum_{h \le x/f(y_1)} w_h(q) \int_{f(y_1)}^{f(y(h))} (x - ht)\,dt + O(x^{2-1/(2d)+\varepsilon}). \tag{25}$$

We next exchange the order of summation and complete the sum over q. By Lemma 3, the multiplicative function $w_h(q)\mu(q)^2$ is non-negative and bounded by $O((q,h)q^{\varepsilon})$. This implies that

$$\sum_{q \le x^{1/(2d)}} \frac{\mu(q)^2}{\phi(q)^2} w_h(q) = W(h) + O(h^{\varepsilon} x^{-1/(2d)}),$$

with

$$W(h) = \sum_{q=1}^{\infty} \frac{\mu(q)^2}{\phi(q)^2} w_h(q) = \frac{h}{\phi(h)} \prod_{p \nmid h} \left(1 + \frac{\rho(p)-1}{(p-1)^2}\right). \tag{26}$$

A trivial estimate for the integral in (25) shows it to be $O(f(y)x)$, and this suffices here to conclude that

$$M_0 = \sum_{h \le x/f(y_1)} W(h) \int_{f(y_1)}^{f(y(h))} (x - ht)\,dt + O(x^{2-1/(2d)+\varepsilon}).$$

The derivative of $t(x-\frac{1}{2}ht)$ with respect to t is $x-ht$, and we have $f(y(h))=f(y)$ when $h\le x/f(y)$, and $f(y(h))=x/h$ when $h>x/f(y)$. Hence, if we compute the integral and split the sum over h at $x/f(y)$ when appropriate, we readily find that

$$M_0=\tfrac{1}{2}\big(f(y_1)^2\Theta_f(x/f(y_1))-f(y)^2\Theta_f(x/f(y))\big)+O(x^{2-1/(2d)+\varepsilon}) \tag{27}$$

where

$$\Theta_f(H)=\sum_{h\le H}\frac{W(h)}{h}(H-h)^2. \tag{28}$$

We summarize the analysis based on the application of the circle method by combining (16), (20) and (27), thereby obtaining the formula

$$2S_0=f(y_1)^2\Theta_f(x/f(y_1))-f(y)^2\Theta_f(x/f(y))+O(x^2(\log x)^{-A}), \tag{29}$$

and thus we enter the opening phase of the endgame.

5. An exercise in multiplicative number theory

In view of the relations (29) and (12), the evaluation of $V_f(x,y)$ is reduced to the deduction of appropriate asymptotic formulae for the functions Φ_f and Θ_f, defined in (7) and (28), respectively. This is accomplished largely by a series of exercises in multiplicative number theory. We begin with an analysis of the Dirichlet series associated with the function $W(h)/h$, restricting attention for the time being to the situation wherein $\rho(2)\ge 1$. An inspection of (26) shows that the series

$$D(s)=\sum_{n=1}^{\infty}W(n)n^{-1-s}$$

converges absolutely in the half-plane $\mathrm{Re}\,(s)>0$, and that $W(h)/W(1)$ is multiplicative. Hence, for $\mathrm{Re}\,(s)>0$, one has

$$D(s)=W(1)\prod_p D_p(s) \tag{30}$$

with

$$D_p(s)=1+\left(1+\frac{\rho(p)-1}{(p-1)^2}\right)^{-1}\sum_{l=1}^{\infty}\phi(p^l)^{-1}p^{-ls}. \tag{31}$$

Notice here that since $\rho(p)\ge 0$, the Euler factor $D_p(s)$ is defined for all values of p, with the exception of $p=2$ in the special case $\rho(2)=0$. It is for this reason that we isolate the latter situation below.[2]

The Euler product (30) yields an analytic continuation of $D(s)$ to a meromorphic function on the half-plane $\mathrm{Re}\,(s)>-2$. In order to see this, it will be convenient to write $\xi=p^{-1-s}$, and define the real number $\lambda=\lambda(p)$ by means of the identity

$$\left(1+\frac{\rho(p)-1}{(p-1)^2}\right)^{-1}=1-\frac{\lambda(p)}{p^2}. \tag{32}$$

[2] We are grateful to the referee for prompting our separate treatment of this case.

It is apparent from the relation defining $\lambda(p)$ that $0 \le \lambda \ll 1$, wherein the implicit constant depends only on f. We may rearrange the Euler factors into the shape

$$D_p(s) = 1 + \frac{p}{p-1}\left(1 - \frac{\lambda}{p^2}\right)\frac{\xi}{1-\xi},$$

and consequently,

$$\begin{aligned} (1-\xi)D_p(s) &= 1 + \frac{\xi}{p-1}\left(1 - \frac{\lambda}{p}\right), \\ \left(1 - \frac{\xi}{p}\right)(1-\xi)D_p(s) &= 1 + \left(\frac{\xi}{p}\right)\frac{1-\lambda}{p-1} - \left(\frac{\xi}{p}\right)^2\frac{p}{p-1}\left(1 - \frac{\lambda}{p}\right), \\ \frac{(1-\xi/p)(1-\xi)}{1-\xi^2/p^2}D_p(s) &= 1 + \left(\frac{\xi/p}{1+\xi/p}\right)\left(\frac{1-\lambda}{p-1}\right). \end{aligned}$$

On recalling (30), and rewriting ξ as p^{-1-s} again, the previous formulae transform into the relations

$$\frac{D(s)}{W(1)} = \zeta(s+1)E_1(s) = \zeta(s+1)\zeta(s+2)E_2(s) = \frac{\zeta(s+1)\zeta(s+2)}{\zeta(2s+4)}E_3(s), \tag{33}$$

where we have written

$$E_1(s) = \prod_p \left(1 + \frac{p^{-s}}{p(p-1)}\left(1 - \frac{\lambda(p)}{p}\right)\right), \tag{34}$$

$$E_2(s) = \prod_p \left(1 + \frac{p^{-s}}{p^2(p-1)}(1-\lambda(p)) - \frac{p^{-2s}}{p^3(p-1)}\left(1 - \frac{\lambda(p)}{p}\right)\right), \tag{35}$$

$$E_3(s) = \prod_p \left(1 + \frac{1-\lambda(p)}{(p-1)(1+p^{s+2})}\right). \tag{36}$$

Here ζ denotes Riemann's zeta function, and the product E_j converges absolutely and locally uniformly in the half-plane $\mathrm{Re}\,(s) > -(j+1)/2$ for $j = 1, 2, 3$. In particular, the relations recorded in (33) provide the analytic continuation of $D(s)$ to the half-plane $\mathrm{Re}\,(s) > -2$. In the half-plane $\mathrm{Re}\,(s) \ge -3/2$, meanwhile, the only singularities of $D(s)$ are simple poles at $s = 0$ and $s = -1$.

Returning now to (28), we deduce from one of Perron's formulae that

$$\Theta_f(H) = \frac{1}{\pi i}\int_{2-i\infty}^{2+i\infty} \frac{D(s)H^{s+2}}{s(s+1)(s+2)}\,ds. \tag{37}$$

Observe that from (36), one finds that the function $E_3(s)$ is holomorphic and uniformly bounded in $\mathrm{Re}\,(s) \ge -3/2$. Invoking only standard estimates for the zeta factors in (33), one can move the line of integration on the right hand side of (37) to $\mathrm{Re}\,(s) = -3/2$. The reader may care to inspect the analysis on p. 141 of Goldston and Vaughan [3] for the necessary ideas, though in the present circumstances one should not use the Riemann hypothesis. One may also compare the discussion on p. 791 of Vaughan [10]. If $R(z)$ is the residue of the integrand in (37) at $s = z$, then it follows that

$$\tfrac{1}{2}\Theta_f(H) = R(0) + R(-1) + O(H^{1/2}). \tag{38}$$

We compute $R(0)$ explicitly by using (33) and (34) along with the familiar expansion

$$\frac{\zeta(1+s)}{s}=\frac{1}{s^2}+\frac{\gamma}{s}+O(1).$$

A short calculation then reveals that

$$R(0)=\tfrac{1}{2}c(f)H^2\log H+\Gamma_0H^2, \tag{39}$$

where

$$c(f)=W(1)\prod_p\left(1+\frac{1-\lambda(p)p^{-1}}{p(p-1)}\right) \tag{40}$$

and $\Gamma_0=\Gamma_0(f)$ is a certain real number, the precise value of which is not relevant to our subsequent discussion. Another short calculation leads from (26) and (32) to the alternative formulae

$$\begin{aligned}c(f)&=\prod_p\left(1+\frac{\rho(p)-1}{(p-1)^2}\right)\left(1+\frac{1-\lambda(p)p^{-1}}{p(p-1)}\right)\\&=\prod_p\left(1+\frac{\rho(p)}{p(p-1)}\right)=\sum_{n=1}^\infty\frac{\mu(n)^2\rho(n)}{n\phi(n)}.\end{aligned} \tag{41}$$

In the latter form, this constant will play an important role later.

A similar technique may be applied to evaluate $R(-1)$. In this instance we use (33) and (35) and then reach the transitional formula

$$R(-1)=-W(1)E_2(-1)\zeta(0)H\log H+\Gamma_{-1}H, \tag{42}$$

where $\Gamma_{-1}=\Gamma_{-1}(f)$ is another real number, the precise value of which is again of little importance in what follows. We remark, however, that $\Gamma_{-1}(f)$ could be made just as explicit as $c(f)$. Observe next that $\zeta(0)=-1/2$, and so on applying (26), (32) and (35), we find that the Euler factors of $W(1)$ and $E_2(-1)$ combine to give the formula

$$\begin{aligned}W(1)E_2(-1)&=\prod_p\left(1+\frac{\rho(p)-1}{(p-1)^2}\right)\left(1+\frac{1-\lambda(p)}{p(p-1)}-\frac{1-\lambda(p)p^{-1}}{p(p-1)}\right)\\&=\prod_p\left(1+\frac{\rho(p)-1}{(p-1)^2}\right)\left(1-\frac{\lambda(p)}{p^2}\right)=1.\end{aligned}$$

We may therefore conclude that

$$R(-1)=\tfrac{1}{2}H\log H+\Gamma_{-1}H. \tag{43}$$

On substituting (39) and (43) into (38), we obtain the expansion

$$\Theta_f(H)=c(f)H^2\log H+2\Gamma_0H^2+H\log H+2\Gamma_{-1}H+O(H^{1/2}),$$

which may be incorporated into (29), leading to the asymptotic formula

$$\begin{aligned}2S_0=c(f)x^2\log\left(\frac{f(y)}{f(y_1)}\right)&-xf(y)\log\left(\frac{x}{f(y)}\right)-2\Gamma_{-1}xf(y)\\&+O\big(x^{1/2}f(y)^{3/2}+x^2(\log x)^{-A}\big).\end{aligned} \tag{44}$$

This completes the evaluation of the expression S_0 defined in equation (11).

We turn our attention now to the situation with $\rho(2) = 0$. Here, as a consequence of (26), one sees that $W(h) = 0$ whenever h is odd, and moreover that for all natural numbers m one has

$$\frac{W(2m)}{W(2)} = \frac{m}{\phi(2m)} \prod_{\substack{p|m \\ p>2}} \left(1 + \frac{\rho(p)-1}{(p-1)^2}\right)^{-1}.$$

Define

$$\rho_0(p) = \begin{cases} 2, & \text{when } p = 2, \\ \rho(p), & \text{when } p > 2. \end{cases}$$

In the remainder of this section, we adopt the convention that the decoration of a symbol with a subscript 0 is to be interpreted as indicating that the definition of that symbol is to be modified by replacing $\rho(p)$ by $\rho_0(p)$ throughout. We now find that $W(2) = W_0(1)$ and

$$\frac{W(2m)}{W_0(1)} = \prod_{p|m} \left(1 + \frac{\rho_0(p)-1}{(p-1)^2}\right)^{-1} \left(\frac{p}{p-1}\right).$$

In particular, it follows that $W(2m)/W_0(1)$ is a multiplicative function of m. With the Dirichlet series $D(s)$ defined as before, we again find that $D(s)$ converges absolutely in the half-plane $\mathrm{Re}\,(s) > 0$. Hence, for $\mathrm{Re}\,(s) > 0$, one has

$$D(s) = 2^{-1-s} \sum_{m=1}^{\infty} W(2m) m^{-1-s} = W_0(1) 2^{-1-s} \prod_p D_{p,0}(s), \tag{45}$$

with $D_{p,0}(s)$ defined via (31).

We may now execute the argument following (31) to establish that the analogue of (33) holds, save that in present circumstances $D(s)/W(1)$ is replaced by $2^{1+s}D(s)/W_0(1)$. It follows, in particular, that the analogue of the asymptotic relation (38) holds. A modest calculation reveals that

$$R_0(0) = \tfrac{1}{4} c_0(f) H^2 \log H + \Gamma_0 H^2, \tag{46}$$

where $c_0(f)$ is defined via (40), and $\Gamma_0 = \Gamma_0(f)$ is a certain (but different) real number, the precise value of which is again of no importance in what follows. In addition, as a consequence of the argument underlying (41), we have

$$c_0(f) = \prod_p \left(1 + \frac{\rho_0(p)}{p(p-1)}\right) = 2 \prod_{p>2} \left(1 + \frac{\rho(p)}{p(p-1)}\right) = 2c(f). \tag{47}$$

So far as $R(-1)$ is concerned, the modification to the formula (33) leaves the relation (42) essentially unchanged, save that Γ_{-1} will need adjustment invisible in the ensuing discussion. We therefore deduce as before that the analogue of (43) holds, whence on substituting (46) and (43) into (38) we conclude that

$$\Theta_f(H) = \tfrac{1}{2} c_0(f) H^2 \log H + 2\Gamma_0 H^2 + H \log H + 2\Gamma_{-1} H + O(H^{1/2}).$$

Incorporating this, as before, into (29), and recalling (47), we arrive at the asymptotic formula (44). In this way, we have established the asymptotic relation (44) in all circumstances.

6. Another exercise in multiplicative number theory

Our treatment of the sum Φ_f defined in equation (7) takes the convolution

$$\frac{q}{\phi(q)} = \sum_{r|q} \frac{\mu(r)^2}{\phi(r)}$$

as the starting point. By reversing the order of summation, we obtain

$$\sum_{y_0(f)<k\le z} \frac{f(k)}{\phi(f(k))} = \sum_{r\le f(z)} \frac{\mu(r)^2}{\phi(r)} \sum_{\substack{y_0(f)<k\le z\\ f(k)\equiv 0 \bmod r}} 1 = \sum_{r\le f(z)} \frac{\mu(r)^2}{\phi(r)} \Big(\frac{\rho(r)}{r} z + O(\rho(r)) \Big).$$

Since $\rho(p) \le d$ for primes p large enough in terms of f, we now deduce from (41) that

$$\sum_{y_0(f)<k\le z} \frac{f(k)}{\phi(f(k))} = c(f)z + O((\log z)^d).$$

This relation may be summed by parts against the differentiable factor $f'(t)/f(t)$. For large t, one has

$$\frac{d}{dt}(f'(t)/f(t)) \ll t^{-2},$$

and consequently we are led to the asymptotic formula

$$\sum_{y_0(f)<k\le z} \frac{f'(k)}{\phi(f(k))} = c(f)\log f(z) + \tilde{c}(f) + O\left(\frac{(\log z)^d}{z} \right),$$

where $\tilde{c}(f)$ is a real number, the value of which, yet again, plays no role in our conclusions. Substituting this formula into the definition (7), we infer that whenever $x^{1/d}(\log x)^{-B} \le y \le x^{1/d}$, one has

$$\Phi_f(y_1, y) = c(f) \log \left(\frac{f(y)}{f(y_1)} \right) + O(x^{-1/d}(\log x)^{B+d}). \tag{48}$$

We now substitute (44) and (48) into the asymptotic relation (12), thereby deducing that

$$V_f(x,y) = xf(y)\log f(y) + f(y) \left(\sum_{p\le x} (\log p)^2 - x\log x \right) - 2\Gamma_{-1} x f(y) + O(x^{1/2} f(y)^{3/2} + x^2(\log x)^{-A}).$$

By the Prime Number Theorem and partial summation, we therefore arrive at the asymptotic formula

$$V_f(x,y) = xf(y)\log f(y) - (2\Gamma_{-1}+1)xf(y) + O(x^{1/2}f(y)^{3/2} + x^2(\log x)^{-A}),$$

and this confirms the conclusion of our theorem with $C(f) = -(2\Gamma_{-1}+1)$.

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