A Sieve Auxiliary Function

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Dedicated to Professor Heini Halberstam, on the occasion of his retirement.

Abstract. In the sieve theories of Rosser-Iwaniec and Diamond-Halberstam-Richert, the upper and lower bound sieve functions (F and f, respectively) satisfy a coupled system of differential-difference equations with retarded arguments. To aid in the study of these functions, Iwaniec introduced a conjugate difference-differential equation with an advanced argument, and gave a solution, q, which is analytic in the right half-plane. The analysis of the bounding sieve functions, F and f, is facilitated by an adjoint integral inner-product relation which links the local behaviour of $F - f$ with that of the sieve auxiliary function, q. In addition, q plays a fundamental role in determining the sieving limit of the combinatorial sieve, and hence in determining the boundary conditions of the sieve functions, F and f. The sieve auxiliary function, q, has been tabulated previously, but these data were not supported by numerical analysis, due to the prohibitive presence of high-order partial derivatives arising from the numerical quadrature methods used [15, 17]. In this paper, we develop additional representations of q. Certain of these representations are amenable to detailed error analysis. We provide this error analysis, and as a consequence, we indicate how q-values guaranteed to at least seven decimal places can be tabulated.

1. Introduction

In his seminal paper, Rosser's Sieve [11], Iwaniec introduced a pair of difference-differential equations which have been studied more recently by Diamond, Halberstam, and Richert [3–10], and by Wheeler [17, 18]. The equations appear as auxiliary equations in connection with the problem of estimating

$$S(\mathscr{A}, \mathscr{P}, x) := \#\{a \in \mathscr{A} : \gcd(a, \prod_{\substack{p<x \\ p\in\mathscr{P}}} p) = 1\},$$

where $\mathscr{P}$ is a set of primes and $\mathscr{A}$ is a finite set of integers. In the sieve theories of Rosser-Iwaniec and Diamond-Halberstam-Richert, the equations take the form

$$(uq_\kappa(u))' = \kappa q_\kappa(u) + \kappa q_\kappa(u+1) \tag{1.1}$$

and

$$(up_\kappa(u))' = \kappa p_\kappa(u) - \kappa p_\kappa(u+1), \tag{1.2}$$

where u, κ are real and positive. The parameter κ denotes the dimension of the sieve, or sifting density, and is a measure of the average number of residue classes per prime in the sequence being sifted. Iwaniec gave solutions to (1.1) and (1.2) involving the so-called complementary exponential integral [14, p.40] defined by

$$\operatorname{Ein}(z) := \int_0^z \frac{1-e^{-t}}{t}\, dt.$$

The solutions are

$$q_\kappa(u) = \frac{\Gamma(2\kappa)}{2\pi i} \int z^{-2\kappa} e^{uz} e^{\kappa \operatorname{Ein}(-z)}\, dz \tag{1.3}$$

and

$$p_\kappa(u) = \int_0^\infty e^{-xu-\kappa \operatorname{Ein}(x)}\, dx, \tag{1.4}$$

where in (1.3), the contour starts at $-\infty$, hugging the negative real axis, then circles the origin in the positive direction before returning to $-\infty$. In this paper, we focus on the problems presented by the function q_κ, since p_κ, being the Laplace transform of a positive function, is relatively simple to deal with. In [7], it is shown that the solutions (1.3), (1.4) are unique, subject to mild polynomial-like growth conditions at infinity. In Section 2 below, we prove that (1.3) is the unique solution in a class of functions representable as a Laplace/Mellin transform. In Section 3, an asymptotic expansion is derived, and a few properties of the coefficients are proved. In Section 4, we give a representation of q_κ in terms of an operator that arises in other contexts. Finally, it is of some interest to have values of q_κ tabulated. We take up this problem in Section 5. We remark that this paper is based in significant part on the author's Ph.D. thesis [2].

2. The Function $q_\kappa(u)$

The difference-differential equation (1.1) can be rewritten in the form

$$\left(u^{1-\kappa} q_\kappa(u)\right)' = \kappa u^{-\kappa} q_\kappa(u+1),$$

so that the value of the function at u is given by an integral involving the function at larger values of the argument. Since integration is a smoothing operation, one expects repeated integrations to yield a C^∞ solution, given only mild assumptions on the behaviour of the function at infinity. In fact, it is easy to see that Iwaniec's solution (1.3) is analytic in the right half-plane and that $q_\kappa(u)$ as given by (1.3) is asymptotic to $u^{2\kappa-1}$ as u tends to infinity.

In [7], the solution (1.3) is shown to be unique in the class of normalized polynomial-like functions. In other words, (1.3) is the unique solution to (1.1) which satisfies $q_\kappa(u) \sim u^b$ as $u \to \infty$, for some constant b (and hence we must have $b = 2\kappa - 1$). In the sequel, we shall prove a uniqueness result of a somewhat different kind, which shows that (1.3) is unique in a class of functions representable as a Laplace/Mellin transform. For this task, it is profitable to view $q_\kappa(s)$ as a function of the complex variable κ, with s lying in the right half-plane, although for sieve applications, we are primarily concerned with positive real values of the parameters. But first, we need to recast (1.3) as an integral over the positive real axis.

Proposition 2.1. *Let n be a non-negative integer, and suppose $\Re(n+1-2\kappa) > 0$. Then*

$$q_\kappa(s) = \frac{(-1)^n}{\Gamma(n+1-2\kappa)} \int_0^\infty x^{n-2\kappa} \left(\frac{\partial}{\partial x}\right)^n e^{-sx} e^{\kappa \operatorname{Ein}(x)}\, dx, \quad \Re(s) > 0. \tag{2.1}$$

Remark. If κ is real and small enough so that $n = 0$ or $n = 1$ is permissible (i.e. $\kappa < 1/2$ in the former case, $\kappa < 1$ in the latter) then one can use the representation (2.1) to compute $q_\kappa(u)$ quite easily. However, as n increases, the higher order partial derivatives rapidly become cumbersome, and so for larger values of κ, the method of Section 5 is preferrable.

Proof Sketch. The case $n = 0$ can be found in Iwaniec [11, p.184]. Te Riele [15, p.6] and Wheeler [17, p.73] derive (2.1) from the $n = 0$ case by performing repeated integration by parts on the latter. One can also obtain (2.1) directly from (1.3), integrating by parts n times. The integrated terms all vanish due to the presence of e^{sz} as a factor in every derivative of $e^{sz}e^{\kappa \operatorname{Ein}(-z)}$. One can then collapse the contour onto the negative real axis, and after some minor simplifications, (2.1) results. See [2, p.12] for details.

We are now ready to prove that (2.1) is the unique solution to (1.1) in the class of functions representable as a Laplace/Mellin transform. For convenience, the following notation will be used. Let $\mathscr{G}$ denote the set of functions g such that $g^{(n)} \in L^1[0, \infty]$ for $n = 0, 1, 2, 3$ and for which $g^{(n)}$ vanishes at both zero and infinity for $n = 0, 1, 2$. Also, for each real $B \geqslant 0$, put

$$\mathscr{F}_B := \{f : y \mapsto e^{-By} f(y) \in \mathscr{G}\}.$$

Theorem 1 (Uniqueness). *Let n be the least non-negative integer such that $\Re(2\kappa) < n+1$. Then up to multiplication by an arbitrary function of κ,*

$$q_\kappa(s) := \frac{(-1)^n}{\Gamma(n+1-2\kappa)} \int_0^\infty x^{n-2\kappa} \left(\frac{\partial}{\partial x}\right)^n e^{-sx} e^{\kappa \operatorname{Ein}(x)}\, dx, \quad \Re s > 0 \tag{2.2}$$

is the unique solution to the difference-differential equation

$$(sq_\kappa(s))' = \kappa q_\kappa(s) + \kappa q_\kappa(s+1)$$

which satisfies

$$q_\kappa(s) \text{ is an entire function of } \kappa, \tag{2.3}$$

$$\exists B \geqslant 0 \text{ such that } q_\kappa(s) = \int_0^\infty e^{-sy} f_\kappa(y)\, dy, \quad \Re(2\kappa) < -2, \quad \Re(s) > 0, \tag{2.4}$$

for some $f_\kappa \in \mathscr{F}_B$.

Remark. Note that f_κ can be very general. Of course, if $f_\kappa(x) \sim \dfrac{x^{-2\kappa}}{\Gamma(1-2\kappa)}$ as $x \to 0+$, then (2.4) would imply that $q_\kappa(u) \sim u^{2\kappa-1}$ as $u \to \infty$, but we do not assume this.

Proof. Suppose that (2.4) holds for some $B \geqslant 0$. We shall show that necessarily, $f_\kappa(x) = x^{-2\kappa} e^{\kappa \operatorname{Ein}(x)}$ up to an arbitrary constant multiple (depending on κ), and that (2.2) follows. The Laplace inversion theorem guarantees that for any $c > B$, we have

$$f_\kappa(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{sx} q_\kappa(s)\, ds, \quad x > 0. \tag{2.5}$$

Our approach is to differentiate (2.5) with respect to x and then use the difference-differential equation satisfied by q_κ to obtain a differential equation for f_κ that can be solved explicitly. But first, we must justify differentiating (2.5) under the integral sign. We require the following lemmata.

Lemma 2.1. *Suppose (2.4) holds for some $B \geqslant 0$ and $f_\kappa \in \mathscr{F}_B$. Let $\Re(s) > B$. Then*

$$q_\kappa(s) = \frac{1}{s^p} \int_0^\infty e^{-sy} f_\kappa^{(p)}(y)\, dy, \quad p = 0, 1, 2, 3.$$

Proof. Integrate (2.4) by parts repeatedly. In each case, the integrated term vanishes by the hypotheses on f_κ and the definition of $\mathscr{G}$.

Lemma 2.2. *Suppose (2.4) holds for some* $B \geqslant 0$*. Let* $c > B$*. Then for all* $x > 0$*, the function*

$$F(x) := \int_{c-i\infty}^{c+i\infty} e^{sx} q_\kappa(s)\, ds \quad \textit{satisfies} \quad F'(x) = \int_{c-i\infty}^{c+i\infty} e^{sx} s\, q_\kappa(s)\, ds.$$

Proof. For positive integers n, define

$$F_n(x) := \int_{c-in}^{c+in} e^{sx} q_\kappa(s)\, ds, \quad x > 0.$$

It is clear that for each n, F_n' exists, is continous, and is given by

$$F_n'(x) = \int_{c-in}^{c+in} e^{sx} s\, q_\kappa(s)\, ds, \quad x > 0.$$

Let

$$G(x) := \int_{c-i\infty}^{c+i\infty} e^{sx} s\, q_\kappa(s)\, ds, \quad x > 0.$$

We shall show that the sequence F_n' converges uniformly to G on compact intervals. Let $0 < a < M$ and for now, make the restriction $x \in [a, M]$. By Lemma 2.1,

$$\begin{aligned}
|G(x) - F_n'(x)| &\leqslant \left| \int_{c+in}^{c+i\infty} e^{sx} s\, q_\kappa(s)\, ds \right| + \left| \int_{c-i\infty}^{c-in} e^{sx} s\, q_\kappa(s)\, ds \right| \\
&\ll e^{cM} \left| \int_{c+in}^{c+i\infty} s\, q_\kappa(s)\, ds \right| \\
&= e^{cM} \left| \int_{c+in}^{c+i\infty} \int_0^\infty e^{-sy} f_\kappa'''(y)\, dy\, \frac{ds}{s^2} \right| \\
&= e^{cM} \int_n^\infty \left| \int_0^\infty e^{-cy} f_\kappa'''(y) e^{-ity}\, dy \right| \frac{dt}{c^2+t^2} \\
&\leqslant e^{cM} \int_n^\infty \int_0^\infty |e^{-cy} f_\kappa'''(y)|\, dy\, \frac{dt}{c^2+t^2}. \qquad (2.6)
\end{aligned}$$

Now by the assumption $f_\kappa \in \mathscr{F}_B$, we have that $y \mapsto e^{-cy} f_\kappa'''(y) \in L^1[0, \infty]$. Thus the inner integral in (2.6) is finite, and as $n \to \infty$, it follows that $|G(x) - F_n'(x)| \to 0$ independently of $x \in [a, M]$. In other words, $F_n' \to G$ uniformly on $[a, M]$, and hence G is continuous there. Furthermore, by uniform convergence,

$$\int_a^x G(y)\, dy = \lim_{n\to\infty} \int_a^x F_n'(y)\, dy = \lim_{n\to\infty} (F_n(x) - F_n(a)) = F(x) - F(a).$$

By continuity of G and the fundamental theorem of calculus, $F'(x) = G(x)$ holds for all $x \in [a, M]$. Finally, since $0 < a < M$ were arbitrary, the lemma is proved.

Continuing with the proof of Theorem 1 we therefore have

$$\begin{aligned} f_\kappa'(x) &= \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{sx} s\, q_\kappa(s)\, ds \\ &= \frac{e^{sx} s q_\kappa(s)}{2\pi i x}\bigg|_{c-i\infty}^{c+i\infty} - \frac{1}{2\pi i x}\int_{c-i\infty}^{c+i\infty} e^{sx}\,(s\, q_\kappa(s))'\, ds. \end{aligned}$$

We claim the integrated term vanishes. Writing $s = c + iT$, we have

$$\lim_{T\to\infty}\left|e^{(c+iT)x}(c+iT)q_\kappa(c+iT)\right| = e^{cx}\lim_{T\to\infty}\left|\int_0^\infty e^{-(c+iT)y} f_\kappa'(y)\, dy\right| = 0,$$

by the Riemann-Lebesgue lemma. Therefore,

$$\begin{aligned} x f_\kappa'(x) &= -\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{sx}\,(s q_\kappa(s))'\, ds \\ &= -\frac{\kappa}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{sx} q_\kappa(s)\, ds - \frac{\kappa}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{sx} q_\kappa(s+1)\, ds \\ &= -\kappa f_\kappa(x) - \kappa e^{-x}\int_{c+1-i\infty}^{c+1+i\infty} e^{sx} q_\kappa(s)\, ds \\ &= -\kappa f_\kappa(x) - \kappa e^{-x} f_\kappa(x). \end{aligned}$$

Solving the separable first order differential equation for f_κ yields

$$f_\kappa(x) = A_\kappa\, x^{-2\kappa} e^{\kappa\,\mathrm{Ein}(x)}, \tag{2.7}$$

where A_κ is a constant depending only on κ. For convenience, put $C_\kappa = A_\kappa\,\Gamma(1-2\kappa)$. Since the difference-differential equation (1.1) satisfied by q_κ is homogeneous, i.e. insensitive to multiplication by an arbitrary function of κ, we may take $C_\kappa = 1$ without loss of generality. Also, note that f_κ as given by (2.7) does indeed lie in the set $\mathscr{F}$ for $\Re(2\kappa) < -2$, as stipulated. Thus we have shown that up to multiplication by an arbitrary function of κ,

$$q_\kappa(s) = \frac{1}{\Gamma(1-2\kappa)}\int_0^\infty x^{-2\kappa} e^{-sx} e^{\kappa\,\mathrm{Ein}(x)}\, dx, \quad \Re(2\kappa) < -2, \quad \Re s > 0. \tag{2.8}$$

However (2.8) is an analytic function of κ for $\Re(2\kappa) < 1$, so in fact, (2.8) provides an analytic continuation of $q_\kappa(s)$ to the open left half-plane $\Re(2\kappa) < 1$. To complete the proof of Theorem 1, we need to analytically continue q_κ to an entire function of κ. We now set

$$F_\kappa(x) = e^{-sx} e^{\kappa \operatorname{Ein}(x)}, \qquad G_\kappa(x) = x^{-2k}$$

and integrate (2.8) by parts n times, using the formula

$$\int_0^\infty F_\kappa(x) G_\kappa(x)\, dx = \sum_{j=0}^{n-1} (-1)^j F_\kappa^{(j)}(x)\, G_\kappa^{(-j-1)}(x) \Big|_0^\infty + (-1)^n \int_0^\infty F_\kappa^{(n)}(x)\, G_\kappa^{(-n)}(x)\, dx.$$

We claim the integrated terms all vanish. To see this, note that

$$G_\kappa^{(-j-1)}(x) = \frac{x^{j+1-2\kappa}}{(1-2\kappa)_{j+1}}.$$

Furthermore, since $F_\kappa(x)$ is an entire function of x,

$$\lim_{x\to 0+} F_\kappa^{(j)}(x) G_\kappa^{(-j-1)}(x) = F_\kappa^{(j)}(0) \lim_{x \to 0+} \frac{x^{j+1-2\kappa}}{(1-2\kappa)_{j+1}} = 0,$$

for $\Re(2\kappa) < 1$ and j a non-negative integer. On the other hand, e^{-sx} is a factor of every term in $F_\kappa^{(j)}(x)$, whereas for $x > 0$,

$$\left| \left(\frac{\partial}{\partial x} \right)^r e^{\kappa \operatorname{Ein}(x)} \right| \ll e^{\varepsilon x},$$

for every $r > 0$, $\varepsilon > 0$. Thus

$$\lim_{x \to \infty} G_\kappa^{(-j-1)}(x) F_\kappa^{(j)}(x) = 0.$$

It follows that for $\Re s > 0$,

$$\begin{aligned} q_\kappa(s) &= \frac{(-1)^n}{(1-2\kappa)_n\, \Gamma(1-2\kappa)} \int_0^\infty x^{n-2\kappa} \left(\frac{\partial}{\partial x} \right)^n e^{-sx} e^{\kappa \operatorname{Ein}(x)}\, dx \\ &= \frac{(-1)^n}{\Gamma(n+1-2\kappa)} \int_0^\infty x^{n-2\kappa} \left(\frac{\partial}{\partial x} \right)^n e^{-sx} e^{\kappa \operatorname{Ein}(x)}\, dx, \quad \Re(2\kappa) < 1. \end{aligned} \tag{2.9}$$

Now observe that (2.9) actually gives an analytic continuation of $q_\kappa(s)$ to the half-plane $\Re(2\kappa) < n + 1$, which completes the proof.

3. The Asymptotic Expansion

Recalling (1.3) again, if 2κ is a positive integer, then the branch point in the integrand at $z = 0$ becomes a pole, and we can collapse the horizontal portions of the contour onto the negative real axis, so that

$$q_\kappa(u) = \frac{\Gamma(2\kappa)}{2\pi i} \oint_{|z|=1} z^{-2\kappa} e^{uz} e^{\kappa \operatorname{Ein}(-z)}\, dz = \left(\frac{\partial}{\partial z}\right)^{2\kappa-1} e^{uz} e^{\kappa \operatorname{Ein}(-z)} \bigg|_{z=0}.$$

This suggests that when 2κ is not a positive integer, we define the fractional derivative $(\partial/\partial z)^{2\kappa-1}$ by means of

$$\left(\frac{\partial}{\partial z}\right)^{2\kappa-1} e^{uz} e^{\kappa \operatorname{Ein}(-z)} \bigg|_{z=0} := q_\kappa(u) = \frac{\Gamma(2\kappa)}{2\pi i} \int_{\leftrightarrows\circlearrowleft} z^{-2\kappa} e^{uz} e^{\kappa \operatorname{Ein}(-z)}\, dz.$$

In other words, for general κ, it may be profitable to view $q_\kappa(u)$ as a fractional derivative. Thus, in some sense, soon to be made precise,

$$q_\kappa(u) \sim \left(\frac{\partial}{\partial z}\right)^{2\kappa-1} e^{uz} e^{\kappa \operatorname{Ein}(-z)} \bigg|_{z=0}.$$

For example, applying Leibniz's rule to the above yields the formal expansion

$$\begin{aligned} q_\kappa(u) &\sim \sum_{n=0}^{\infty} \binom{2\kappa-1}{n} \left(\frac{\partial}{\partial z}\right)^{n} e^{\kappa \operatorname{Ein}(-z)} \bigg|_{z=0} \cdot \left(\frac{\partial}{\partial z}\right)^{2\kappa-1-n} e^{uz} \bigg|_{z=0} \\ &= \sum_{n=0}^{\infty} \binom{2\kappa-1}{n} b_n(\kappa)\, u^{2\kappa-1-n}, \end{aligned} \tag{3.1}$$

which, in view of our previous remarks, gives a true equality when 2κ is a positive integer. Here, $b_n(\kappa)$ is the nth degree polynomial in κ defined by

$$b_n(\kappa) := \left(\frac{\partial}{\partial z}\right)^{n} e^{\kappa \operatorname{Ein}(-z)} \bigg|_{z=0} \tag{3.2}$$

and the fractional derivative of e^{uz} is given, of course, by

$$\left(\frac{\partial}{\partial z}\right)^{2\kappa-1-n} e^{uz} \bigg|_{z=0} = \frac{\Gamma(2\kappa-n)}{2\pi i} \int_{\leftrightarrows\circlearrowleft} z^{n-2\kappa} e^{uz}\, dz = u^{2\kappa-1-n}.$$

It turns out that (3.1) is a valid asymptotic expansion for u-values tending to positive infinity.

Theorem 2. *Let $b_n(\kappa)$ be defined as in (3.2), κ real. Then the asymptotic expansion*

$$q_\kappa(u) \sim \sum_{n=0}^{\infty} \binom{2\kappa-1}{n} b_n(\kappa)\, u^{2\kappa-1-n}, \quad u \to \infty$$

is valid.

Proof Sketch. The asymptotic expansion with remainder after n terms appears in essentially the above guise in both [11, p.183] and [17, p.37]. The main idea is to expand $e^{\kappa\,\mathrm{Ein}(-z)}$ into its Taylor series, and then use Hankel's contour formula for the reciprocal of the gamma function. For an analysis of the size of the remainder term in (3.1) see [2, Chapter 8, Theorem 6].

It is interesting to deduce some properties of the coefficients $b_n(\kappa)$ of the asymptotic expansion provided by Theorem 2. Rewriting (3.2) in the form

$$e^{\kappa\,\mathrm{Ein}(-z)} = \sum_{n=0}^{\infty} \frac{z^n}{n!} b_n(\kappa), \tag{3.3}$$

it is immediate that $b_0(\kappa) = 1$. For positive integers n, we have the following recurrence formula which gives $b_n(\kappa)$ in terms of $b_0(\kappa)$, $b_1(\kappa)$, $\ldots, b_{n-1}(\kappa)$.

Proposition 3.1. *If n is a positive integer and $b_n(\kappa)$ is given by (3.3), then*

$$b_n(\kappa) = -\frac{\kappa}{n} \sum_{j=0}^{n-1} \binom{n}{j} b_j(\kappa).$$

Proof. Applying the operator $z \cdot d/dz$ to (3.3), one obtains

$$\sum_{n=0}^{\infty} n b_n(\kappa) \frac{z^n}{n!} = -\kappa\,(e^z - 1)\, e^{\kappa\,\mathrm{Ein}(-z)}.$$

The result now follows on comparing coefficients of $z^n/n!$.

For concreteness, the first few b polynomials are listed below.

$$b_0 = 1, \quad b_1 = -\kappa, \quad b_2 = \kappa^2 - \kappa/2, \quad b_3 = -\kappa^3 + 3\kappa^2/2 - \kappa/3.$$

The following result shows a connection with the Bernoulli numbers, defined by

$$\frac{z}{e^z - 1} = \sum_{n=0}^{\infty} \frac{z^n}{n!} B_n, \quad |z| < 2\pi.$$

Theorem 3. *Let α be an arbitrary constant. Then for all non-negative integers n,*

$$\sum_{j=0}^{n-2} \binom{n}{j} b_{j+1}(\alpha) B_{n-j} = (n/2 - \alpha)\, b_n(\alpha) - b_{n+1}(\alpha).$$

Remark. The sum on the left vanishes when $n = 0, 1$. For general n, $b_n(\alpha)$ is a polynomial in α of degree n. Thus the coefficients of α^n and of α^{n+1} on the right hand side both must vanish.

Proof. Let $[z^n/n!]F(z)$ denote the coefficient of $z^n/n!$ in the analytic function $F(z)$. We proceed by developing

$$Q_n(u, \alpha) := \left(\frac{\partial}{\partial z}\right)^n e^{uz} e^{\alpha\,\mathrm{Ein}(-z)}\bigg|_{z=0} = [z^n/n!]\, e^{uz} e^{\alpha\,\mathrm{Ein}(-z)}$$

as a Fourier series in u on $]0, 1[$. Note that $b_n(\alpha) = Q_n(0, \alpha)$. We require the following

Lemma 3.1. *Let α be an arbitrary constant. Then for all non-negative integers n,*

$$Q_n(1, \alpha) = (1 - n/\alpha)\, Q_n(0, \alpha) = (1 - n/\alpha)\, b_n(\alpha).$$

Proof. By definition,

$$\begin{aligned} Q_n(1, \alpha) &= [z^n/n!]\, e^z e^{\alpha\,\mathrm{Ein}(-z)} \\ &= [z^n/n!]\, (e^z - 1)\, e^{\alpha\,\mathrm{Ein}(-z)} + [z^n/n!]\, e^{\alpha\,\mathrm{Ein}(-z)} \\ &= n \left[\frac{z^{n-1}}{(n-1)!}\right] \left(\frac{e^z - 1}{z}\right) e^{\alpha\,\mathrm{Ein}(-z)} + b_n(\alpha) \\ &= -\frac{n}{\alpha} \left[\frac{z^{n-1}}{(n-1)!}\right] \frac{d}{dz} e^{\alpha\,\mathrm{Ein}(-z)} + b_n(\alpha) \\ &= (1 - n/\alpha)\, b_n(\alpha). \end{aligned}$$

Returning to the proof of Theorem 3, we will compute the Fourier coefficients of $Q_n(u, \alpha)$. We note that $Q_n(u, \alpha)$ is sufficiently smooth to be representable as the sum of its Fourier series for $0 < u < 1$. Since

$$\alpha \int_0^1 e^{uz} e^{\alpha\,\mathrm{Ein}(-z)}\, du = \alpha \left(\frac{e^z - 1}{z}\right) e^{\alpha\,\mathrm{Ein}(-z)} = -\frac{d}{dz}\, e^{\alpha\,\mathrm{Ein}(-z)}$$

and

$$\alpha\int_0^1 e^{uz}e^{\alpha\,\mathrm{Ein}(-z)}e^{-2\pi imu}\,du = \frac{\alpha\, e^{\alpha\,\mathrm{Ein}(-z)}}{z-2\pi im}\,(e^z-1)$$
$$= -\frac{z}{z-2\pi im}\cdot\frac{d}{dz}\,e^{\alpha\,\mathrm{Ein}(-z)},$$

it follows that for $0<u<1$,

$$\alpha Q_n(u,\alpha) = -\left[\frac{z^n}{n!}\right]\frac{d}{dz}\,e^{\alpha\,\mathrm{Ein}(-z)} - \sum_{m\neq 0} e^{2\pi imu}\left[\frac{z^n}{n!}\right]\frac{z}{z-2\pi im}\cdot\frac{d}{dz}\,e^{\alpha\,\mathrm{Ein}(-z)}$$
$$= -b_{n+1}(\alpha) + \sum_{m\neq 0} e^{2\pi imu}\sum_{j=0}^{n-1}\binom{n}{j}b_{j+1}(\alpha)\frac{(n-j)!}{(2\pi im)^{n-j}}.$$

When $u=0$, the Fourier series converges to the arithmetic mean of the function evaluated at the two end-points $u=0,1$. Thus applying Lemma 3.1, we have

$$-\sum_{m\neq 0}\sum_{j=0}^{n-1}\binom{n}{j}b_{j+1}(\alpha)\frac{(n-j)!}{(2\pi im)^{n-j}} = -\frac{\alpha}{2}Q_n(0,\alpha) - \frac{\alpha}{2}Q_n(1,\alpha) - b_{n+1}(\alpha)$$
$$= -\frac{\alpha}{2}b_n(\alpha) - \frac{\alpha}{2}\left(1-\frac{n}{\alpha}\right)b_n(\alpha) - b_{n+1}(\alpha)$$
$$= (n/2-\alpha)\,b_n(\alpha) - b_{n+1}(\alpha).$$

The result now follows on applying Euler's famous evaluation of the Riemann zeta function in the form

$$-\sum_{m\neq 0}\frac{(n-j)!}{(2\pi im)^{n-j}} = \begin{cases} B_{n-j}, & n-j\geqslant 2,\\ 0, & n-j=1.\end{cases}$$

Next, we analyze the behaviour of $b_n(\kappa)$ for large n. Since the generating function $e^{\kappa\,\mathrm{Ein}(-z)}$ is entire, it follows by Hadamard's root test that $\limsup_{n\to\infty}\sqrt[n]{|\,b_n(\kappa)/n!\,|} < 1/R$ for every $R>0$, i.e. $\limsup_{n\to\infty}\sqrt[n]{|\,b_n(\kappa)/n!\,|}=0$. However, since this information does not reveal how quickly or how slowly $|\,b_n(\kappa)/n!\,|$ tends to zero, we seek a concrete upper bound.

Theorem 4. *Let $\kappa>0$. Then, for all non-negative integers n, we have*

$$\left|\frac{b_n(\kappa)}{n!}\right| \leqslant \left(\frac{e}{\log(1+n/\kappa)}\right)^n. \tag{3.4}$$

A somewhat more precise inequality is given by

$$\left|\frac{b_n(\kappa)}{n!}\right| \leqslant \exp\left\{\kappa\int_0^L t^{-1}\left(e^t-1\right)\,dt\right\}\Big/\left\{\log(1+n/\kappa)\right\}^n, \tag{3.5}$$

where $L := \log(1 + n/\kappa)$.

Proof. For any $r > 0$, Cauchy's inequality gives

$$\left|\frac{b_n(\kappa)}{n!}\right| \leqslant r^{-n} \max_{|z|=r} \left|e^{\kappa \operatorname{Ein}(-z)}\right|.$$

Now on the circle $|z| = r$,

$$\left|e^{\kappa \operatorname{Ein}(-z)}\right| = \left|\exp\left\{-\kappa \sum_{n=1}^{\infty} \frac{z^n}{n!\,n}\right\}\right| \leqslant \exp\left\{\kappa \sum_{n=1}^{\infty} \frac{r^n}{n!\,n}\right\} = \exp\left\{\kappa \int_0^r \frac{e^t - 1}{t}\,dt\right\}.$$

Thus

$$\left|\frac{b_n(\kappa)}{n!}\right| \leqslant \inf_{r>0} r^{-n} \exp\left\{\kappa \int_0^r t^{-1}\left(e^t - 1\right)\,dt\right\} = \inf_{r>0} r^{-n} e^{-\kappa \operatorname{Ein}(-r)}. \tag{3.6}$$

Minimizing with respect to $r > 0$, we find on taking the logarithmic derivative that $\kappa r^{-1}(e^r - 1) - r^{-1}n = 0$ so that $r = \log(1 + n/\kappa) = L$. The inequality (3.5) now follows on substituting the optimal value of r into (3.6). If we use the fact that

$$\int_0^r \frac{e^t - 1}{t}\,dt = \sum_{n=1}^{\infty} \frac{r^n}{n!\,n} \leqslant e^r - 1,$$

then (3.5) with $r = L$ yields

$$\left|\frac{b_n(\kappa)}{n!}\right| \leqslant \frac{\exp\{\kappa(1 + n/\kappa - 1)\}}{\log^n(1 + n/\kappa)} = \left(\frac{e}{\log(1 + n/\kappa)}\right)^n,$$

which is (3.4).

Improvements. Put $M(r) := \max_{|z|=r} \left|e^{\kappa \operatorname{Ein}(-z)}\right|$. Our proof of (3.4) used the inequality

$$M(r) = \max_{|z|=r} \left|\exp\left\{-\kappa \sum_{n=1}^{\infty} \frac{z^n}{n!\,n}\right\}\right| \leqslant \exp\left\{\kappa \sum_{n=1}^{\infty} \frac{r^n}{n!\,n}\right\}, \tag{3.7}$$

which at first glance may appear wasteful, since at no point on the circle $|z| = r$ do we have $\arg(z^n) = \pi$ for every positive integer n. However, an attractive argument of Andrew Odlyzko [13] shows that the estimate (3.7) cannot be substantially improved. Consider $z = x + \pi i$, where $x > 0$ is large. The main contribution to the sum comes from terms with n close to x, and for such terms,

$$z^n = x^n \left(1 + \frac{\pi i}{x}\right)^n \sim x^n e^{\pi i} = -x^n, \quad x \to \infty.$$

Thus it would seem that any significant improvement on Theorem 4 cannot be based on Cauchy's inequality. However, if one considers the Cauchy integral formula

$$\frac{b_n(\kappa)}{n!} = \frac{1}{2\pi i} \oint_{|z|=r} z^{-n-1} e^{\kappa \operatorname{Ein}(-z)}\, dz,$$

one observes that $\left|e^{\kappa \operatorname{Ein}(-z)}\right|$ is close to its maximum $M(r)$ for only a small portion of z-values on the circle. This suggests that Theorem 4 can be improved using saddle-point asymptotics. Using this approach, the author was able to improve on Theorem 4 by the factor $(2\pi(\kappa+n)\log(1+n/\kappa))^{-1/2}$. See [2, Chapter 9, Theorem 8] for details.

4. An Operator Representation

We begin this section with an informal argument which should help motivate what follows. Let $f(z)$ be a formal power series in z and let $D = d/du$. Since $D^n e^{uz} = z^n e^{uz}$ for all non-negative integers n, it follows by linearity that the equation $f(z)\, e^{uz} = f(D)\, e^{uz}$ holds, at least in the formal sense. If we now apply this observation to the contour representation (1.3) with $f(z) := e^{\kappa \operatorname{Ein}(-z)}$, we obtain

$$\begin{aligned} q_\kappa(u) &= \frac{\Gamma(2\kappa)}{2\pi i} \int_{\leftrightarrows\circlearrowleft} z^{-2\kappa} e^{\kappa \operatorname{Ein}(-D)} e^{uz}\, dz \\ &= e^{\kappa \operatorname{Ein}(-D)} \frac{\Gamma(2\kappa)}{2\pi i} \int_{\leftrightarrows\circlearrowleft} z^{-2\kappa} e^{uz}\, dz \\ &= e^{\kappa \operatorname{Ein}(-D)}\, u^{2\kappa-1}. \end{aligned} \tag{4.1}$$

Pulling the differential operator outside the integral requires justification, and we shall do this shortly. But for the moment, a few remarks about (4.1) are in order. Recalling the power series representation for Ein, we may write

$$\operatorname{Ein}(-D) = -\sum_{n=1}^{\infty} \frac{D^n}{n!\, n}$$

and hence expanding the operator into powers of D, we formally obtain the expression

$$q_\kappa(u) \sim \sum_{n=0}^{\infty} b_n(\kappa) \frac{D^n}{n!} u^{2\kappa-1} = \sum_{n=0}^{\infty} \binom{2\kappa-1}{n} b_n(\kappa)\, u^{2\kappa-1-n} \tag{4.2}$$

in agreement with Theorem 2. In particular, the $n = 0$ term gives the known asymptotic formula $q_\kappa(u) \sim u^{2\kappa-1}$ as $u \to \infty$.

Next, we point out that the differential operator $\mathrm{Ein}(-D)$ can be recast in the form of an integral operator. For the sake of brevity, we put $T := \mathrm{Ein}(-D)$. Recalling the integral representation for Ein, we have

$$T := \mathrm{Ein}(-D) = \int_0^1 \frac{1-e^{tD}}{t}\, dt.$$

Now if f is analytic in a disk centred at u with radius $r > 0$, and $|t| < r$, then Taylor's theorem gives

$$e^{tD} f(u) = \sum_{n=0}^{\infty} \frac{t^n}{n!} D^n f(u) = \sum_{n=0}^{\infty} \frac{t^n}{n!} f^{(n)}(u) = f(u+t).$$

Thus for those functions f which are analytic in a disk centred at u with radius $r \geqslant 1$,

$$Tf(u) = \int_0^1 \left(1 - e^{tD}\right) f(u) \frac{dt}{t} = \int_0^1 \frac{f(u) - f(u+t)}{t}\, dt. \tag{4.3}$$

Now the integral on the far right of (4.3) makes sense if f is integrable on $[u, u+1]$ and for some $\varepsilon > 0$, we have $|f(u) - f(u+t)| \ll t^\varepsilon$ as $t \to 0+$. For such f, we can define $Tf(u)$ by (4.3), and if T is defined this way, then $Tf(u)$ makes sense for a larger class of functions than merely those functions which are analytic in a suitably large disk centred at u. Thus there is no need to view T as a power series in D in order to determine $Tf(u)$. In the case of interest, $f(u) = u^{2\kappa-1}$ and (4.1) becomes

$$q_\kappa(u) = e^{\kappa T} u^{2\kappa-1} = \sum_{n=0}^{\infty} \frac{\kappa^n}{n!} T^n u^{2\kappa-1} \tag{4.4}$$

and so it makes sense to study the iterated integral operator T^n. We shall take this up after first proving the representation (4.4) rigorously.

Theorem 5. *Let $D := d/du$ and $T := \mathrm{Ein}(-D)$. Then for any complex number κ, and real $u > 0$,*

$$q_\kappa(u) = e^{\kappa T} u^{2\kappa-1} = \sum_{n=0}^{\infty} \frac{\kappa^n}{n!} T^n u^{2\kappa-1}.$$

Aside. In sieve applications, we are concerned primarily with positive real values of κ, and $\kappa > 1$ in particular.

Proof. Fix κ and consider the function of the complex variable w defined by

$$g_w(u) := \int_{\rightleftarrows\!\circlearrowleft} z^{-2\kappa} e^{uz} e^{w\,\mathrm{Ein}(-z)}\,dz, \quad u > 0.$$

By Taylor's theorem,

$$g_w(u) = \sum_{n=0}^{\infty} \frac{w^n}{n!} \left(\frac{\partial}{\partial w}\right)^n g_w(u)\Big|_{w=0}.$$

On the other hand, from (1.3) and the definition of $g_w(u)$,

$$q_\kappa(u) = \frac{\Gamma(2\kappa)}{2\pi i}\, g_w(u)\Big|_{w=\kappa}.$$

Thus,

$$q_\kappa(u) = \frac{\Gamma(2\kappa)}{2\pi i} \sum_{n=0}^{\infty} \frac{\kappa^n}{n!} \left(\frac{\partial}{\partial w}\right)^n g_w(u)\Big|_{w=0}$$

and it remains only to show that for all non-negative integers n,

$$T^n u^{2\kappa-1} = \frac{\Gamma(2\kappa)}{2\pi i} \left(\frac{\partial}{\partial w}\right)^n g_w(u)\Big|_{w=0}. \tag{4.5}$$

For $n = 0$, we have

$$\frac{\Gamma(2\kappa)}{2\pi i}\, g_0(u) = \frac{\Gamma(2\kappa)}{2\pi i} \int_{\rightleftarrows\!\circlearrowleft} z^{-2\kappa} e^{uz}\,dz = u^{2\kappa-1} = T^0 u^{2\kappa-1}.$$

Suppose now that (4.5) holds up to $n-1$, where n is a positive integer. Then

$$\begin{aligned}
&\frac{\Gamma(2\kappa)}{2\pi i}\left(\frac{\partial}{\partial w}\right)^n g_w(u)\bigg|_{w=0}\\
&=\frac{\Gamma(2\kappa)}{2\pi i}\int z^{-2\kappa}e^{uz}\left(\operatorname{Ein}(-z)\right)^n\,dz\\
&=\frac{\Gamma(2\kappa)}{2\pi i}\int z^{-2\kappa}e^{uz}\left(\operatorname{Ein}(-z)\right)^{n-1}\int_0^1\frac{1-e^{tz}}{t}\,dt\,dz\\
&=\int_0^1\frac{1}{t}\,\frac{\Gamma(2\kappa)}{2\pi i}\int z^{-2\kappa}e^{uz}\left(1-e^{tz}\right)\left(\operatorname{Ein}(-z)\right)^{n-1}\,dz\,dt\\
&=\int_0^1 t^{-1}\{T^{n-1}u^{2\kappa-1}-T^{n-1}(u+t)^{2\kappa-1}\}\,dt\\
&=T^n u^{2\kappa-1},
\end{aligned}$$

by induction.

Having proved the representation (4.4), it is natural to ask how rapidly the series of T-iterates converges to the function q_κ. To this end, we prove the following

Theorem 6. *Let $\kappa>0$, $u>0$, and let n be a non-negative integer satisfying $n>2\kappa-1$. Define*

$$S_n := q_\kappa(u)-\sum_{j=0}^{n-1}\frac{\kappa^j}{j!}T^j\,u^{2\kappa-1}.$$

Then as $n\to\infty$, we have, with $c:=\operatorname{Ein}(1)=0.796599\ldots$,

$$S_n \ll_\kappa \frac{\kappa^n}{n!}+\kappa^n\left(\frac{e^c}{u}\right)^{n/\log n}\left(\frac{\log n}{n}\right)^n\Gamma\left(\frac{n}{\log n}+1-2\kappa\right)u^{2\kappa-1}.$$

Remark. If $2\kappa\geqslant 1$, then Stirling's formula provides the simplification

$$S_n \ll_\kappa \frac{\kappa^n}{n!}+\kappa^n\left(\frac{e^c}{ue}\right)^{n/\log n}\left(\frac{\log n}{n}\right)^{n(1-1/\log n+1/2n)}u^{2\kappa-1}.$$

Proof. We have

$$\begin{aligned} S_n &= \sum_{j=n}^{\infty} \frac{\kappa^j}{j!} T^j\, u^{2\kappa-1} = \sum_{j=n}^{\infty} \frac{\Gamma(2\kappa)}{2\pi i} \left(\frac{\partial}{\partial w}\right)^j g_w(u)\Big|_{w=0} \\ &= \sum_{j=n}^{\infty} \frac{\kappa^j}{j!} \frac{\Gamma(2\kappa)}{2\pi i} \int_{\leftrightarrows\circlearrowleft} z^{-2\kappa} e^{uz}\, \mathrm{Ein}^j(-z)\, dz \\ &= \frac{\Gamma(2\kappa)}{2\pi i} \int_{\leftrightarrows\circlearrowleft} z^{-2\kappa} e^{uz} \sum_{j=n}^{\infty} \frac{\kappa^j}{j!}\, \mathrm{Ein}^j(-z)\, dz. \end{aligned}$$

Since $n > 2\kappa - 1$ and $\sum_{j=n}^{\infty} \frac{\kappa^j}{j!}\, \mathrm{Ein}^j(-z) \ll |z|^n$ as $z \to 0$, we may collapse the contour onto the real half-line, obtaining

$$S_n = \pi^{-1}\Gamma(2\kappa)\, \sin(2\pi\kappa) \int_0^{\infty} x^{-2\kappa} e^{-ux} \sum_{j=n}^{\infty} \frac{\kappa^j}{j!}\, \mathrm{Ein}^j(x)\, dx.$$

Let

$$\begin{aligned} I_n &:= \int_0^1 x^{-2\kappa} e^{-ux} \sum_{j=n}^{\infty} \frac{\kappa^j}{j!}\, \mathrm{Ein}^j(x)\, dx, \\ J_n &:= \int_1^{\infty} x^{-2\kappa} e^{-ux} \sum_{j=n}^{\infty} \frac{\kappa^j}{j!}\, \mathrm{Ein}^j(x)\, dx. \end{aligned}$$

Note that for any $y \geqslant 0$,

$$\sum_{j=n}^{\infty} \frac{y^j}{j!} = \frac{y^n}{n!}\left(1 + \frac{y}{n+1} + \frac{y^2}{(n+1)(n+2)} + \cdots\right) \leqslant \frac{y^n}{n!} e^y.$$

Thus, as $0 \leqslant \mathrm{Ein}(x) \leqslant x$, we have

$$I_n \leqslant \frac{\kappa^n}{n!} \int_0^1 x^{n-2\kappa} e^{-ux} e^{\kappa x}\, dx \leqslant \frac{\kappa^n}{n!} \cdot \frac{e^{\kappa}}{n+1-2\kappa}. \tag{4.6}$$

With I_n now satisfactorily estimated, we turn to J_n. Recall the formula [14, p.40]

$$\mathrm{Ein}(x) = \log x + \gamma + \mathrm{E}_1(x), \quad x > 0,$$

where E_1 denotes the exponential integral defined by

$$\mathrm{E}_1(x) = \int_x^{\infty} e^{-t} \frac{dt}{t}, \quad x > 0,$$

and γ denotes Euler's constant. To estimate J_n, we use $\mathrm{Ein}(x) \leqslant \log x + \gamma + \mathrm{E}_1(1) \leqslant \log x + c$, where $c := \mathrm{Ein}(1) = 0.7965995\ldots \leqslant 1$. Thus,

$$J_n \leqslant \int_1^\infty x^{-2\kappa} e^{-ux} \sum_{j=n}^\infty \frac{(\kappa\alpha)^j}{j!}\, dx, \tag{4.7}$$

where $\alpha := \alpha(x) = c + \log x$. We now estimate the sum $\sum_{j=n}^\infty \frac{(\kappa\alpha)^j}{j!}$. Let $r > \kappa$. Then

$$\sum_{j=n}^\infty \frac{(\kappa\alpha)^j}{j!} = \sum_{j=n}^\infty \left(\frac{\kappa}{r}\right)^j \frac{(\alpha r)^j}{j!} \leqslant \left(\frac{\kappa}{r}\right)^n \sum_{j=0}^\infty \frac{(\alpha r)^j}{j!} = \left(\frac{\kappa}{r}\right)^n e^{\alpha r}. \tag{4.8}$$

Substituting (4.8) into the estimate (4.7) for J_n yields

$$\begin{aligned} J_n &\leqslant \left(\frac{\kappa}{r}\right)^n \int_1^\infty x^{-2\kappa} e^{-ux} e^{\alpha r}\, dx \\ &= \left(\frac{\kappa}{r}\right)^n e^{cr} \int_1^\infty x^{r-2\kappa} e^{-ux}\, dx \\ &\leqslant \left(\frac{\kappa}{r}\right)^n e^{cr} \frac{\Gamma(r+1-2\kappa)}{u^{r+1-2\kappa}}. \end{aligned} \tag{4.9}$$

For fixed $r > \max(\kappa, 2\kappa - 1)$, it is clear from (4.9) that $\lim_{n\to\infty} J_n = 0$. For example, taking $r = 2\kappa$ and using $c = \mathrm{Ein}(1) < 1$, we see that $J_n \leqslant e^{2\kappa} u^{-1} 2^{-n}$. But one can do better by choosing r more carefully, say by minimizing the right hand side of (4.9) with respect to r. By taking the logarithmic derivative, the optimal r is seen to satisfy

$$c - n/r + \psi(r + 1 - 2\kappa) - \log u = 0,$$

or

$$n = r\{\psi(r + 1 - 2\kappa) + c - \log u\}, \tag{4.10}$$

where as customary, $\psi = \Gamma'/\Gamma$. Inverting (4.10) and using the fact that $\psi(r + 1 - 2\kappa) \sim \log r$ as $r \to \infty$, we find that r is approximately $n/\log n$. With this choice, (4.9) yields

$$J_n \leqslant \kappa^n \left(\frac{e^c}{u}\right)^{n/\log n} \left(\frac{\log n}{n}\right)^n \Gamma\left(\frac{n}{\log n} + 1 - 2\kappa\right) u^{2\kappa-1}. \tag{4.11}$$

The theorem now follows on combining (4.6) with (4.11) and absorbing the factors which are independent of n into the $\ll_\kappa$ constant.

We now return to study the integral operator T and its iterates in more detail. Recall that for $f \in L^1[u, u+1]$ satisfying some Lipschitz condition at u, we may define

$$Tf(u) = \int_0^1 \frac{f(u) - f(u+t)}{t}\, dt, \tag{4.12}$$

which is consistent with the definition of T as a differential operator for f analytic at u. We also note that the representation (4.12) has occurred in important contexts outside sieve theory. For example,

$$\begin{aligned} T(\log u) &= -\int_0^1 \frac{\log(u+t) - \log u}{t}\, dt = -\int_0^1 \log(1+t/u)\, \frac{dt}{t}, \quad w = -t/u \\ &= -\int_0^{-1/u} \log(1-w)\, \frac{dw}{w} \\ &= \mathrm{Li}_2\left(-1/u\right), \end{aligned}$$

where

$$\mathrm{Li}_2(z) := -\int_0^z \log(1-w)\, \frac{dw}{w} = \sum_{n=1}^{\infty} \frac{z^n}{n^2}, \quad |z| < 1,$$

is the ubiquitous dilogarithm. For $f \in C^1[u, u+1]$, we can integrate (4.12) by parts. Thus

$$Tf(u) = \{f(u) - f(u+t)\} \log t \Big|_0^1 + \int_0^1 f'(u+t) \log t\, dt. \tag{4.13}$$

But

$$\begin{aligned} \lim_{t \to 0+} \{f(u) - f(u+t)\} \log t = \lim_{t \to 0+} \frac{f(u) - f(u+t)}{t} \cdot t \log t = f'(u) \lim_{t \to 0+} t \log t \\ = 0. \end{aligned}$$

Thus (4.13) becomes

$$Tf(u) = \int_0^1 f'(u+t) \log t\, dt. \tag{4.14}$$

Since $\int_0^1 \log t\, dt = -1$, it follows that Tf can be viewed as a weighted average of $-f'$. More generally, for n a positive integer, one can show that

$$T^n f(u) = \int_{[0,1]^n} f^{(n)}(u + t_1 + \cdots + t_n) \log t_1 \cdots \log t_n\, dt_1 \cdots dt_n$$

if $f \in C^n[u, u+1]$.

The integrands in the representations (4.12) and (4.14) both contain apparent singularities at the origin. We develop an additional representation in which the corresponding singularity is hidden. Again, assume f possesses the requisite derivatives.

Proposition 4.1. *Let $f \in C^1[u, u+1]$. Then $Tf(u) = -\int_0^1 \int_0^1 f'(u+st)\, ds\, dt$. More generally, if n is any positive integer and $f \in C^n[u, u+1]$, then*

$$T^n f(u) = (-1)^n \int_{[0,1]^n} \int_{[0,1]^n} f^{(n)}(u + s_1 t_1 + \cdots + s_n t_n)\, ds_1 \cdots ds_n\, dt_1 \cdots dt_n.$$

Proof. By definition

$$\begin{aligned} Tf(u) &= \int_0^1 \frac{f(u) - f(u+t)}{t}\, dt = -\int_0^1 \int_u^{u+t} f'(x)\, dx\, \frac{dt}{t} \\ &= -\int_0^1 \int_0^t f'(u+r)\, dr\, \frac{dt}{t} \\ &= -\int_0^1 \int_0^1 f'(u+st)\, ds\, dt. \qquad (4.15) \end{aligned}$$

The general case is handled inductively.

Note that the apparent singularity at the origin has been hidden. Also, (4.15) shows that Tf is a weighted average of $-f'$ over the unit square.

5. Numerical Analysis

Here, we give a detailed numerical analysis of a Simpson's rule-based scheme for computing $q_\kappa(u)$ for the range $1 \leqslant \kappa < 3$, $1 \leqslant u \leqslant 6$. Following Iwaniec [11], we set

$$e^{\kappa \operatorname{Ein}(-z)} = \sum_{j=0}^{n} b_j(\kappa)\, \frac{z^j}{j!} + S_n(-z)$$

and rewrite (1.3) (via Hankel's formula for $1/\Gamma$) in the form

$$q_\kappa(u) = \sum_{j=0}^{n} \binom{2\kappa - 1}{j} b_j(\kappa) u^{2\kappa-1-j} + \frac{\Gamma(2\kappa)}{2\pi i} \int_{\mathcal{H}} z^{-2\kappa} e^{uz}\, S_n(-z)\, dz.$$

Next, since $|S_n(-z)| \ll |z|^{n+1}$ as $z \to 0$, the integral around the circular portion tends to 0 with the radius, as long as $n+1 > 2\kappa - 1$. Here $1 \leqslant \kappa < 3$, so we require $n \geqslant 4$. Then the contour may be collapsed onto the negative real axis, and after routine calculations, one obtains

$$\text{(5.1)} \quad q_\kappa(u) = \sum_{j=0}^{4} \binom{2\kappa-1}{j} b_j(\kappa)\, u^{2\kappa-j-1} + \frac{\sin(2\pi\kappa)}{\pi}\,\Gamma(2\kappa) \int_0^\infty x^{-2\kappa} e^{-ux}\{e^{\kappa\,\mathrm{Ein}(x)} - P(x)\}\,dx,$$

where $P(x) := \sum_{j=0}^{4} (-1)^j\, b_j(\kappa)\, \frac{x^j}{j!}$ is the fourth-degree Maclaurin polynomial for $e^{\kappa\,\mathrm{Ein}(x)}$. We use the representation (5.1) to compute $q_\kappa(u)$ for various values of κ, u. We have written C code to perform these computations, but to guarantee their accuracy, an accompanying error analysis is necessary. Since $\binom{2\kappa-1}{j} b_j(\kappa)$ is a polynomial in κ for non-negative integers j, we regard computations of the summation term in (5.1) as exact and henceforth focus exclusively on the computational problems that the integral in (5.1) presents. To avoid additional complications in the corresponding error analysis, we do not make use of any numerical integration packages. For the same reason, we avoid using built-in special functions such as the incomplete gamma function. The only non-elementary function we do use is the complete gamma function, since we are satisfied that its implementation gives the correct answers to within the number of significant digits specified.

Let $I = I_1 + I_2 + I_3 - I_4$ denote the integral in (5.1), where

$$I_1 := \int_0^1 x^{-2\kappa} e^{-ux}\{e^{\kappa\,\mathrm{Ein}(x)} - P(x)\}\,dx, \qquad I_2 := \int_1^{20} x^{-2\kappa} e^{-ux} e^{\kappa\,\mathrm{Ein}(x)}\,dx$$

$$I_3 := \int_{20}^\infty x^{-2\kappa} e^{-ux} e^{\kappa\,\mathrm{Ein}(x)}\,dx, \qquad I_4 := \int_1^\infty x^{-2\kappa} e^{-ux} P(x)\,dx.$$

In I_3, we have chosen 20 as the lower limit of integration so as to make the integral negligible in the rectangle of interest, namely $1 \leqslant \kappa < 3$, $1 \leqslant u \leqslant 6$. See Theorem 7 below for details. In I_1, we have chosen 1 as the upper limit of integration in order to make computation via Taylor series expansion feasible. It turns out (Theorem 9) that at least 35 terms are needed to make the error negligible. Accordingly, we approximate the braced expression in I_1 by its Taylor polynomial of degree 35. By definition of $P(x)$, the lowest degree term in this polynomial has x to the fifth power. We then approximate I_1 by incomplete gamma functions. Complementary incomplete gamma functions are used to approximate I_4. This leaves I_2, which we treat by splitting up the interval $[1, 20]$ into appropriate subintervals and then applying Simpson's rule.

Theorem 7. *Again, let*

$$\mathrm{E}_1(x) := \int_x^\infty \frac{e^{-t}}{t}\,dt, \quad x > 0$$

denote the exponential integral [1, p.228], [14, p.40]. *Then,*

$$I_3 \leqslant u^{-1}\,20^{-\kappa} e^{\kappa\gamma} e^{\kappa\,\mathrm{E}_1(20)} e^{-20u}. \tag{5.3}$$

Furthermore, on any rectangle $1 \leqslant u_1 \leqslant u \leqslant u_2 \leqslant 6$, $1 \leqslant \kappa_1 \leqslant \kappa \leqslant \kappa_2 \leqslant 3$, *we have*

$$I_3 \leqslant u_1^{-1}\,20^{-\kappa_1} e^{\kappa_1\gamma} e^{\kappa_1\,\mathrm{E}_1(20)} e^{-20u_1} \leqslant 0.184 \times 10^{-9}, \quad \textit{with } u_1 = \kappa_1 = 1. \tag{5.4}$$

Proof. We apply once more the relationship [14, p.40]

$$\mathrm{Ein}(x) = \log x + \gamma + \mathrm{E}_1(x), \quad x > 0,$$

where γ denotes Euler's constant. Thus,

$$I_3 = \int_{20}^\infty x^{-2\kappa} e^{-ux} e^{\kappa\,\mathrm{Ein}(x)}\,dx = \int_{20}^\infty x^{-\kappa} e^{-ux} e^{\kappa(\gamma+\mathrm{E}_1(x))}\,dx.$$

Note that the factors $x^{-\kappa}$ and $e^{\kappa(\gamma+\mathrm{E}_1(x))}$ in the integrand are decreasing functions of x. Therefore,

$$I_3 \leqslant 20^{-\kappa} e^{\kappa(\gamma+\mathrm{E}_1(20))} \int_{20}^\infty e^{-ux}\,dx,$$

which gives (5.3). Since $\gamma + \mathrm{E}_1(20) - \log 20 < 0$, the expression on the right in (5.3) is decreasing in κ and u, from which (5.4) follows.

We can compute values of $\mathrm{Ein}(x)$ for $x > 1$ using $\mathrm{Ein}(x) = \log x + \gamma + \mathrm{E}_1(x)$, and a continued fraction which can approximate E_1 to within any specified amount. Our approximation is based on a continued fraction expansion for the complementary incomplete gamma function [1, p.263], [16, p.356]

$$\Gamma(a,u) := \int_u^\infty t^{a-1} e^{-t}\,dt = \cfrac{e^{-u}u^a}{u + \cfrac{1-a}{1 + \cfrac{1}{u + \cfrac{2-a}{1 + \cfrac{2}{u + \cfrac{3-a}{1 + \cfrac{3}{u + \ddots}}}}}}} \tag{5.5}$$

defined for all a and $u > 0$. Note that $\mathrm{E}_1(x) = \Gamma(0, x)$ for $x > 0$.

We now wish to determine the error committed in using an approximation E_1^* in place of E_1 in the evaluation of I_2.

Theorem 8. *Let $0 < \varepsilon < 0.048$ be given and suppose that $|\,\mathrm{E}_1^*(x) - \mathrm{E}_1(x)| < \varepsilon$ for $1 \leqslant x \leqslant 20$. Let*

$$\Delta I_2 := \left| I_2 - \int_1^{20} x^{-\kappa} e^{-ux} e^{\kappa(\gamma + \mathrm{E}_1^*(x))}\, dx \right|.$$

Then for all $u \geqslant 1$, $\kappa \geqslant 1$,

$$\Delta I_2 \leqslant (e^{\kappa\varepsilon} - 1) e^{\kappa\varepsilon} \{ e^{\kappa(\gamma + \mathrm{E}_1^*(1))} e^{-u} + e^{\kappa(\gamma + \mathrm{E}_1^*(2) - \log 2)} e^{-2u}/(1 - e^{-u}) \}. \tag{5.6}$$

Furthermore, on any rectangle $1 \leqslant u_1 \leqslant u \leqslant u_2 \leqslant 6$, $1 \leqslant \kappa_1 \leqslant \kappa \leqslant \kappa_2 \leqslant 3$, we have

$$\begin{aligned} \Delta I_2 &\leqslant (e^{\kappa_2\varepsilon} - 1) e^{\kappa_2\varepsilon} \{ e^{\kappa_2(\gamma + \mathrm{E}_1^*(1))} e^{-u_1} + e^{\kappa_1(\gamma + \mathrm{E}_1^*(2) - \log 2)} e^{-2u_1}/(1 - e^{-u_1}) \} \\ &\leqslant 0.127 \times 10^{-12}, \qquad \textit{with } \varepsilon = 10^{-14},\ u_1 = \kappa_1 = 1,\ \kappa_3 = 3. \end{aligned} \tag{5.7}$$

Proof. For (5.6) we have

$$\begin{aligned} \Delta I_2 &= \left| \int_1^{20} x^{-\kappa} e^{-ux} e^{\kappa\gamma} (e^{\kappa\,\mathrm{E}_1^*(x)} - e^{\kappa\,\mathrm{E}_1(x)})\, dx \right| \\ &\leqslant \int_1^{20} x^{-\kappa} e^{-ux} e^{\kappa\gamma} e^{\kappa\,\mathrm{E}_1(x)} \left| e^{\kappa(\mathrm{E}_1^*(x) - \mathrm{E}_1(x))} - 1 \right| dx \\ &\leqslant (e^{\kappa\varepsilon} - 1) \sum_{j=1}^{19} j^{-\kappa} e^{-ju} e^{\kappa\gamma} e^{\kappa\,\mathrm{E}_1(j)}, \end{aligned}$$

since the rest of the integrand is decreasing in x. Thus

$$\begin{aligned} \Delta I_2 &\leqslant (e^{\kappa\varepsilon} - 1) \sum_{j=1}^{19} j^{-\kappa} e^{-ju} e^{\kappa\gamma} e^{\kappa\,\mathrm{E}_1^*(j)} e^{\kappa(\mathrm{E}_1(j) - \mathrm{E}_1^*(j))} \\ &\leqslant (e^{\kappa\varepsilon} - 1) e^{\kappa\varepsilon} \sum_{j=1}^{19} j^{-\kappa} e^{-ju} e^{\kappa\gamma} e^{\kappa\,\mathrm{E}_1^*(j)}. \end{aligned}$$

It is easy to show that $\gamma + \mathrm{E}_1(x) - \log x < -0.048$ if $x \geqslant 2$. Thus if $x \geqslant 2$, then $\gamma + \mathrm{E}_1^*(x) - \log x < 0$. It follows that

$$\begin{aligned} \Delta I_2 &\leqslant (e^{\kappa\varepsilon} - 1) e^{\kappa\varepsilon} \{ e^{\kappa(\gamma + \mathrm{E}_1^*(1))} e^{-u} + e^{\kappa(\gamma + \mathrm{E}_1^*(2) - \log 2)} (e^{-2u} + e^{-3u} + \ldots) \} \\ &= (e^{\kappa\varepsilon} - 1) e^{\kappa\varepsilon} \{ e^{\kappa(\gamma + \mathrm{E}_1^*(1))} e^{-u} + e^{\kappa(\gamma + \mathrm{E}_1^*(2) - \log 2)} e^{-2u}/(1 - e^{-u}) \}, \end{aligned}$$

which completes the proof of (5.6). For (5.7), we note that the expression above is majorized by the expression in the statement of (5.7) over the given rectangle. The reason for this is that since $\varepsilon < \gamma$, $\gamma + \mathrm{E}_1^*(x) - \log x > 0$ if $x = 1$, and $\gamma + \mathrm{E}_1^*(x) - \log x < 0$ if $x \geqslant 2$ as we have seen.

Theorem 9. *Let $n \geqslant 6$, and let $R_n(x)$ be the Taylor polynomial of degree n for $e^{\kappa \operatorname{Ein}(x)} - P(x)$. Put $I_1^* = \int_0^1 x^{-2\kappa} e^{-ux} R_n(x)\, dx$. Then*

$$|I_1 - I_1^*| \leqslant \frac{e^{-\kappa \operatorname{Ein}(-r)}}{r^n (r-1)} \int_0^1 x^{n-5} e^{-ux}\, dx \tag{5.8}$$

holds for every $r > 1$. Furthermore, on any rectangle $1 \leqslant u_1 \leqslant u \leqslant u_2 \leqslant 6$, $1 \leqslant \kappa_1 \leqslant \kappa \leqslant \kappa_2 \leqslant 3$, we have

$$|I_1 - I_1^*| \leqslant \frac{e^{-\kappa_2 \operatorname{Ein}(-r)}}{r^n (r-1)} \int_0^1 x^{n-5} e^{-u_1 x}\, dx \tag{5.9}$$

for every $r > 1$.

Note that the integrals can be evaluated exactly in terms of elementary functions. For the full rectangle (i.e. $u_1 = 1, u_2 = 6, \kappa_1 = 1, \kappa_2 = 3$), it is possible to take $r = 2.6, n = 35$ and thereby obtain $|I_1 - I_1^*| \leqslant 0.173... \times 10^{-8}$.

Proof. Let $r > 1$. By definition of I_1^* and $R_n(x)$, we have

$$|I_1 - I_1^*| = \left| \int_0^1 x^{-2\kappa} e^{-ux} \sum_{j=n+1}^{\infty} (-1)^j\, b_j(\kappa)\, \frac{x^j}{j!}\, dx \right|.$$

We now invoke a bound on $|\, b_j(\kappa)/j! \,|$ which was developed in the course of proving Theorem 4. Thus, by inequality (3.6) with $r > 1$, we have

$$\begin{aligned} |I_1 - I_1^*| &\leqslant \int_0^1 x^{-2\kappa} e^{-ux} \sum_{j=n+1}^{\infty} e^{-\kappa \operatorname{Ein}(-r)} \left(\frac{x}{r}\right)^j dx \\ &\leqslant e^{-\kappa \operatorname{Ein}(-r)} \int_0^1 x^{-6} e^{-ux} x^{n+1} \sum_{j=n+1}^{\infty} r^{-j}\, dx \\ &= \frac{e^{-\kappa \operatorname{Ein}(-r)}}{r^n (r-1)} \int_0^1 x^{n-5} e^{-ux}\, dx \end{aligned}$$

which completes the proof of (5.8). Since $-\kappa \operatorname{Ein}(-r) = \kappa \sum_{n=1}^{\infty} \frac{r^n}{n!\, n} > 0$, (5.9) follows from (5.8).

In practice, we take $n = 35$ in Theorem 9 and we compute

$$\begin{aligned} I_1^* &= \sum_{j=5}^{35} (-1)^j \frac{b_j(\kappa)}{j!} \int_0^1 x^{n-2\kappa} e^{-ux}\, dx \\ &= \sum_{j=5}^{35} (-1)^j \frac{b_j(\kappa)}{j!} u^{2\kappa-n-1} \int_0^u t^{n-2\kappa} e^{-t}\, dt \end{aligned}$$

using the incomplete gamma function

$$\gamma(a,u) := \int_0^u t^{a-1} e^{-t}\, dt = u^a \sum_{n=0}^{\infty} \frac{(-u)^n}{n!\,(n+a)},$$

which is defined for all $u > 0$ and $\Re(a) > 0$. We calculate values of $\gamma(a,u)$ using a truncation of the series.

Theorem 10. *Let $6 \leqslant L$ be an integer and let $r > 1$. Then the error committed in computing I_1^* using L terms of the series representation of $\gamma(a,u)$ is less than*

$$\frac{6^{L+1} e^{-\kappa \operatorname{Ein}(-r)}}{(L+1)!\,(L+1)\, r^4\, (r-1).}$$

When $L = 41, r = \frac{3}{2}$, the expression above is $0.3381... \times 10^{-17}$.

Proof. Recall $I_1^* = \sum_{j=5}^{35} (-1)^j \frac{b_j(\kappa)}{j!} u^{2\kappa-j-1} \gamma(j-2\kappa+1, u)$. Put

$$\widetilde{I}_1 = \sum_{j=5}^{35} (-1)^j \frac{b_j(\kappa)}{j!} \sum_{n=0}^{L} \frac{(-u)^n}{n!\,(n+j-2\kappa+1)}.$$

Then

$$|I_1^* - \widetilde{I}_1| \leqslant \sum_{j=5}^{35} \left| \frac{b_j(\kappa)}{j!} \sum_{n=L+1}^{\infty} \frac{(-u)^n}{n!\,(n+j-2\kappa+1)} \right|.$$

Since $1 \leqslant u \leqslant 6$ and $L \geqslant 6$, the terms $\dfrac{u^n}{n!\,(n+j-2\kappa+1)}$ are decreasing to zero, and so by the alternating series test

$$|I_1^* - \widetilde{I}_1| \leqslant \sum_{j=5}^{35} \left| \frac{b_j(\kappa)}{j!} \right| \frac{u^{L+1}}{(L+1)!\,(L+1+j-2\kappa+1)}.$$

Once again invoking inequality (3.6) with $r > 1$, we have

$$\begin{aligned} |I_1^* - \widetilde{I}_1| &\leqslant \frac{6^{L+1}}{(L+1)\,(L+1)!} \sum_{j=5}^{\infty} e^{-\kappa\,\mathrm{Ein}(-r)} r^{-j} \\ &= \frac{6^{L+1} e^{-\kappa\,\mathrm{Ein}(-r)}}{(L+1)!\,(L+1)\,r^4\,(r-1)}. \end{aligned}$$

Recall that $P(x) = \sum_{j=0}^{4} (-1)^j\, b_j(\kappa)\, \frac{x^j}{j!}$ and

$$\begin{aligned} I_4 = \int_1^\infty x^{-2\kappa} e^{-ux} P(x)\,dx &= \sum_{j=0}^{4} (-1)^j\, \frac{b_j(\kappa)}{j!} \int_1^\infty x^{j-2\kappa} e^{-ux}\,dx \\ = \sum_{j=0}^{4} (-1)^j\, \frac{b_j(\kappa)}{j!}\, u^{2\kappa-j-1} \int_u^\infty t^{j-2\kappa} e^{-t}\,dt. \end{aligned}$$

Therefore, we can compute I_4 using the complementary incomplete gamma function (5.5). We have implemented a continued fraction algorithm which computes $\Pi^*(a,u)$, an approximation to $\Pi(a,u) := e^u u^{-a} \Gamma(a,u)$, to within any specified tolerance.

Theorem 11. *Let* $\Pi(a,u) := e^u u^{-a}\Gamma(a,u)$ *and let* Π^* *be a function which satisfies* $|\Pi(a,u) - \Pi^*(a,u)| < 10^{-11}$ *for all values of* $a = j - 2\kappa + 1$, $1 \leqslant \kappa \leqslant 3$, *and* $1 \leqslant u \leqslant 6$. *Put* $I_4^* := \sum_{j=0}^{4} (-1)^j\, \frac{b_j(\kappa)}{j!}\, e^{-u}\Pi^*(j-2\kappa+1,u)$. *Then* $|I_4 - I_4^*| < 4.016... \times 10^{-11}$ *on the full rectangle* $1 \leqslant u \leqslant 6, 1 \leqslant \kappa \leqslant 3$.

Proof. We have

$$\begin{aligned} I_4 &= \sum_{j=0}^{4} (-1)^j\, \frac{b_j(\kappa)}{j!}\, u^{2\kappa-j-1}\Gamma(j-2\kappa+1,u) \\ &= \sum_{j=0}^{4} (-1)^j\, \frac{b_j(\kappa)}{j!}\, e^{-u}\Pi(j-2\kappa+1,u). \end{aligned}$$

Thus, $|I_4 - I_4^*| \leqslant e^{-u} \sum_{j=0}^{4} \left| \frac{b_j(\kappa)}{j!} \right| 10^{-11}$. The remainder of the proof consists in improving our bounds on $|\, b_j(\kappa)/j!\,|$ for $j = 0, 1, 2, 3, 4$.

From Proposition 3.1, we infer that

$$b_0 = 1, \quad b_1 = -\kappa, \quad \frac{b_2}{2!} = \frac{\kappa^2}{2} - \frac{\kappa}{4}, \quad \frac{b_3}{3!} = -\frac{\kappa^3}{6} + \frac{\kappa^2}{4} - \frac{\kappa}{18},$$

$$\frac{b_4}{4!} = \frac{\kappa^4}{24} - \frac{\kappa^3}{8} + \frac{25\kappa^2}{288} - \frac{\kappa}{96}.$$

Thus $|b_0| = 1, |b_1| = |\kappa| \leqslant 3$. Since $b_2'(\kappa) = 2\kappa - 1/2 > 0$ on $[1,3]$, it follows that $b_2(1) \leqslant b_2 \leqslant b_2(3)$ whence $|b_2/2!| \leqslant 15/4$. A similar argument gives $|b_3/3!| \leqslant 29/12$. Unfortunately, b_4 is not monotone on $[1,3]$. However, it is not difficult to show that b_4 has precisely one extremum in $]1,3[$. The extremum is a local minimum and lies in $[1.5, 2.0]$. The graph of $b_4(\kappa)/4!$ is easily shown to be convex on this subinterval and so we construct tangents at $\kappa = 1.5$ and $\kappa = 2.0$ and take the height of their intersection as a possible lower bound on $b_4(\kappa)/4!$. In this way it is easily shown that $|b_4/4!| \leqslant b_4(3)/4! = 3/4$ on $[1,3]$. From this the theorem follows immediately.

It now remains to show how

$$I_2 = \int_1^{20} x^{-2\kappa} e^{-ux} e^{\kappa \operatorname{Ein}(x)}\, dx$$

can be effectively computed. For this, we use Simpson's rule. Recall that the error committed in using Simpson's rule to estimate $\int_a^b r(x)\,dx$ is no more than $M(b-a)^5/2880n^4$, where $M := \max\{|r^{(4)}(x)| : x \in [a,b]\}$, and $a = x_0 < x_1 < \ldots < x_{2n} = b$ are evenly spaced. For our application, we partition the interval $[1, 20]$ into 15 subintervals chosen so that the number of function evaluations needed to commit an error $\leqslant 10^{-10}$ for each subinterval is approximately the same. Thus approximately 60 ($n = 30$ above) function evaluations are needed for each subinterval. If for given κ, u, we put $r(x) = x^{-2\kappa} e^{-ux} e^{\kappa \operatorname{Ein}(x)}$, then each pair of parameter values for κ, u requires a separate computation of I_2.

For each κ, u, and subinterval [a, b], we estimate M and hence determine n so that $M(b-a)^5/2880n^4 < 10^{-10}$. The estimation of the various M values is not as difficult as it may appear, since it so happens that $r^{(4)}$ is decreasing in x for $x \geqslant 1, \kappa > 0, u > 0$. In fact, $r^{(5)}(x) = -x^{-2\kappa} e^{-ux} e^{\kappa \operatorname{Ein}(x)} S(x)/x^5$, where $S(x)$ is a polynomial in x, κ, u, e^{-x} consisting entirely of non-negative terms, a result that can be most easily verified using MAPLE's symbolic capabilities. For a more elegant approach, see [2, p.64]. Thus, it is easy to estimate M and hence to determine the number of function evaluations needed to keep the quadrature error $\leqslant 10^{-10}$ for each subinterval. With 15 subintervals, the total quadrature error is then $\leqslant 15 \times 10^{-10}$. If we combine this error with the error bounds of Theorems 7, 8, 9, and 11, we see that $q_\kappa(u)$ can be computed with an absolute error $\leqslant 0.5 \times 10^{-8}$ if $1 \leqslant u \leqslant 6$, and $1 \leqslant \kappa < 3$.

6. Table of q_κ Values

Based on the methods of Section 5, we have written C code to evaluate the function $q_\kappa(u)$ in the rectangle $1 \leqslant u \leqslant 6$, $1 \leqslant \kappa < 3$. The following table of q_κ values, rounded to seven decimal places, was created using this code. In view of the analysis we have given, the accuracy of these data is guaranteed to within 10^{-7}.

We note that various sieve functions, including q_κ, have been tabulated previously [12, 15, 17]. Although these previous calculations were not supported by numerical analysis, they appear to be in good agreement with our tables.

$u\backslash\kappa$	1.0	1.1	1.2	1.3	1.4
1.0	0.0000000	−0.2463298	−0.4517757	−0.5827670	−0.6070362
1.1	0.1000000	−0.1554682	−0.3861985	−0.5584687	−0.6368735
1.2	0.2000000	−0.0599213	−0.3103561	−0.5184864	−0.6472184
1.3	0.3000000	0.0397676	−0.2252552	−0.4640109	−0.6389713
1.4	0.4000000	0.1431639	−0.1317106	−0.3960188	−0.6128812
1.5	0.5000000	0.2499139	−0.0303940	−0.3153254	−0.5695819
1.6	0.6000000	0.3597240	0.0781317	−0.2226219	−0.5096179
1.7	0.7000000	0.4723479	0.1933882	−0.1185025	−0.4334625
1.8	0.8000000	0.5875756	0.3149645	−0.0034833	−0.3415321
1.9	0.9000000	0.7052267	0.4425035	0.1219827	−0.2341962
2.0	1.0000000	0.8251444	0.5756920	0.2574941	−0.1117856
2.1	1.1000000	0.9471912	0.7142531	0.4026928	0.0254016
2.2	1.2000000	1.0712460	0.8579405	0.5572571	0.1770947
2.3	1.3000000	1.1972009	1.0065331	0.7208959	0.3430465
2.4	1.4000000	1.3249594	1.1598317	0.8933446	0.5230304
2.5	1.5000000	1.4544349	1.3176559	1.0743612	0.7168372
2.6	1.6000000	1.5855488	1.4798409	1.2637237	0.9242733
2.7	1.7000000	1.7182301	1.6462364	1.4612274	1.1451587
2.8	1.8000000	1.8524137	1.8167041	1.6666826	1.3793255
2.9	1.9000000	1.9880400	1.9911164	1.8799134	1.6266165
3.0	2.0000000	2.1250544	2.1693554	2.1007557	1.8868843
3.1	2.1000000	2.2634064	2.3513115	2.3290561	2.1599897
3.2	2.2000000	2.4030493	2.5368827	2.5646710	2.4458019
3.3	2.3000000	2.5439398	2.7259739	2.8074655	2.7441967
3.4	2.4000000	2.6860376	2.9184959	3.0573122	3.0550567

Table 1. Values of $q_\kappa(u)$

$u\backslash\kappa$	1.0	1.1	1.2	1.3	1.4
3.5	2.5000000	2.8293050	3.1143652	3.3140913	3.3782701
3.6	2.6000000	2.9737070	3.3135030	3.5776892	3.7137307
3.7	2.7000000	3.1192105	3.5158354	3.8479984	4.0613372
3.8	2.8000000	3.2657846	3.7212924	4.1249166	4.4209926
3.9	2.9000000	3.4134002	3.9298079	4.4083469	4.7926046
4.0	3.0000000	3.5620300	4.1413192	4.6981965	5.1760844
4.1	3.1000000	3.7116478	4.3557668	4.9943774	5.5713470
4.2	3.2000000	3.8622293	4.5730942	5.2968052	5.9783107
4.3	3.3000000	4.0137512	4.7932477	5.6053993	6.3968969
4.4	3.4000000	4.1661916	5.0161759	5.9200823	6.8270301
4.5	3.5000000	4.3195293	5.2418298	6.2407803	7.2686374
4.6	3.6000000	4.4737447	5.4701628	6.5674220	7.7216485
4.7	3.7000000	4.6288186	5.7011300	6.8999392	8.1859955
4.8	3.8000000	4.7847330	5.9346886	7.2382662	8.6616129
4.9	3.9000000	4.9414706	6.1707975	7.5823395	9.1484370
5.0	4.0000000	5.0990149	6.4094173	7.9320981	9.6464066
5.1	4.1000000	5.2573501	6.6505100	8.2874832	10.1554620
5.2	4.2000000	5.4164612	6.8940393	8.6484378	10.6755454
5.3	4.3000000	5.5763335	7.1399700	9.0149071	11.2066010
5.4	4.4000000	5.7369531	7.3882684	9.3868379	11.7485742
5.5	4.5000000	5.8983068	7.6389019	9.7641788	12.3014121
5.6	4.6000000	6.0603815	7.8918391	10.1468799	12.8650634
5.7	4.7000000	6.2231651	8.1470496	10.5348929	13.4394780
5.8	4.8000000	6.3866455	8.4045041	10.9281711	14.0246072
5.9	4.9000000	6.5508113	8.6641742	11.3266691	14.6204036

Table 1. Values of $q_\kappa(u)$ (continued)

$u\backslash\kappa$	1.5	1.6	1.7	1.8	1.9
1.0	−0.5000000	−0.2527189	0.1194642	0.5692400	1.0130470
1.1	−0.5900000	−0.3981341	−0.0624276	0.3857664	0.8775667
1.2	−0.6600000	−0.5279768	−0.2392354	0.1907910	0.7095828
1.3	−0.7100000	−0.6407309	−0.4075077	−0.0103330	0.5155997
1.4	−0.7400000	−0.7350924	−0.5642137	−0.2127803	0.3017026
1.5	−0.7500000	−0.8099226	−0.7066537	−0.4121459	0.0736383
1.6	−0.7400000	−0.8642136	−0.8323939	−0.6043663	−0.1631256
1.7	−0.7100000	−0.8970635	−0.9392178	−0.7856610	−0.4033546
1.8	−0.6600000	−0.9076573	−1.0250893	−0.9524867	−0.6420132
1.9	−0.5900000	−0.8952530	−1.0881243	−1.1015022	−0.8742366
2.0	−0.5000000	−0.8591695	−1.1265684	−1.2295403	−1.0953091
2.1	−0.3900000	−0.7987782	−1.1387787	−1.3335854	−1.3006458
2.2	−0.2600000	−0.7134953	−1.1232092	−1.4107544	−1.4857782
2.3	−0.1100000	−0.6027764	−1.0783990	−1.4582820	−1.6463414
2.4	0.0600000	−0.4661112	−1.0029623	−1.4735077	−1.7780642
2.5	0.2500000	−0.3030198	−0.8955804	−1.4538653	−1.8767600
2.6	0.4600000	−0.1130491	−0.7549941	−1.3968734	−1.9383194
2.7	0.6900000	0.1042299	−0.5799982	−1.3001275	−1.9587037
2.8	0.9400000	0.3492247	−0.3694364	−1.1612938	−1.9339393
2.9	1.2100000	0.6223233	−0.1221966	−0.9781029	−1.8601125
3.0	1.5000000	0.9238962	0.1627929	−0.7483444	−1.7333655
3.1	1.8100000	1.2542974	0.4865664	−0.4698631	−1.5498923
3.2	2.1400000	1.6138667	0.8501242	−0.1405542	−1.3059353
3.3	2.4900000	2.0029301	1.2544352	0.2416395	−0.9977823
3.4	2.8600000	2.4218014	1.7004388	0.6787316	−0.6217639

Table 1. Values of $q_\kappa(u)$ (continued)

$u\backslash\kappa$	1.5	1.6	1.7	1.8	1.9
3.5	3.2500000	2.8707826	2.1890474	1.1726943	−0.1742506
3.6	3.6600000	3.3501654	2.7211480	1.7254611	0.3483491
3.7	4.0900000	3.8602314	3.2976040	2.3389294	0.9495909
3.8	4.5400000	4.4012534	3.9192567	3.0149622	1.6329963
3.9	5.0100000	4.9734951	4.5869266	3.7553904	2.4020547
4.0	5.5000000	5.5772126	5.3014147	4.5620143	3.2602248
4.1	6.0100000	6.2126543	6.0635033	5.4366053	4.2109358
4.2	6.5400000	6.8800616	6.8739578	6.3809072	5.2575890
4.3	7.0900000	7.5796692	7.7335268	7.3966378	6.4035591
4.4	7.6600000	8.3117055	8.6429433	8.4854900	7.6521950
4.5	8.2500000	9.0763932	9.6029258	9.6491329	9.0068210
4.6	8.8600000	9.8739492	10.6141785	10.8892130	10.4707379
4.7	9.4900000	10.7045851	11.6773922	12.2073550	12.0472238
4.8	10.1400000	11.5685076	12.7932452	13.6051631	13.7395349
4.9	10.8100000	12.4659185	13.9624034	15.0842214	15.5509066
5.0	11.5000000	13.3970153	15.1855212	16.6460949	17.4845536
5.1	12.2100000	14.3619907	16.4632418	18.2923302	19.5436715
5.2	12.9400000	15.3610338	17.7961978	20.0244564	21.7314366
5.3	13.6900000	16.3943295	19.1850117	21.8439855	24.0510070
5.4	14.4600000	17.4620588	20.6302960	23.7524132	26.5055234
5.5	15.2500000	18.5643994	22.1326540	25.7512194	29.0981088
5.6	16.0600000	19.7015255	23.6926798	27.8418686	31.8318700
5.7	16.8900000	20.8736077	25.3109589	30.0258108	34.7098975
5.8	17.7400000	22.0808138	26.9880684	32.3044815	37.7352662
5.9	18.6100000	23.3233083	28.7245773	34.6793027	40.9110356

Table 1. Values of $q_\kappa(u)$ (continued)

$u\backslash\kappa$	2.0	2.1	2.2	2.3	2.4
1.0	1.3333333	1.3908464	1.0499836	0.2185501	−1.1001099
1.1	1.3043333	1.5243262	1.3821575	0.7439733	−0.4513199
1.2	1.2213333	1.5881626	1.6432278	1.2199458	0.1997599
1.3	1.0903333	1.5852899	1.8299174	1.6340082	0.8299406
1.4	0.9173333	1.5193991	1.9406981	1.9763980	1.4191551
1.5	0.7083333	1.3948118	1.9755306	2.2397103	1.9501799
1.6	0.4693333	1.2163857	1.9356654	2.4186357	2.4084172
1.7	0.2063333	0.9894412	1.8234878	2.5097531	2.7817205
1.8	−0.0746667	0.7197033	1.6423938	2.5113625	3.0602523
1.9	−0.3676667	0.4132552	1.3966896	2.4233480	3.2363655
2.0	−0.6666667	0.0765007	1.0915091	2.2470638	3.3045045
2.1	−0.9656667	−0.2838678	0.7327443	1.9852380	3.2611200
2.2	−1.2586667	−0.6608950	0.3269873	1.6418900	3.1045958
2.3	−1.5396667	−1.0473851	−0.1185195	1.2222605	2.8351853
2.4	−1.8026667	−1.4359209	−0.5959269	0.7327492	2.4549552
2.5	−2.0416667	−1.8188800	−1.0968160	0.1808610	1.9677358
2.6	−2.2506667	−2.1884493	−1.6122308	−0.4248418	1.3790769
2.7	−2.4236667	−2.5366372	−2.1327077	−1.0747824	0.6962076
2.8	−2.5546667	−2.8552849	−2.6483007	−1.7584074	−0.0719997
2.9	−2.6376667	−3.1360758	−3.1486047	−2.4642212	−0.9150621
3.0	−2.6666667	−3.3705447	−3.6227762	−3.1798173	−1.8209158
3.1	−2.6356667	−3.5500851	−4.0595517	−3.8919068	−2.7759442
3.2	−2.5386667	−3.6659566	−4.4472651	−4.5863441	−3.7650031
3.3	−2.3696667	−3.7092911	−4.7738629	−5.2481510	−4.7714437
3.4	−2.1226667	−3.6710987	−5.0269181	−5.8615382	−5.7771352

Table 1. Values of $q_\kappa(u)$ (continued)

$u\backslash\kappa$	2.0	2.1	2.2	2.3	2.4
3.5	−1.7916667	−3.5422730	−5.1936439	−6.4099264	−6.7624842
3.6	−1.3706667	−3.3135958	−5.2609050	−6.8759644	−7.7064546
3.7	−0.8536667	−2.9757418	−5.2152288	−7.2415469	−8.5865848
3.8	−0.2346667	−2.5192823	−5.0428162	−7.4878312	−9.3790045
3.9	0.4923333	−1.9346896	−4.7295503	−7.5952520	−10.0584507
4.0	1.3333333	−1.2123398	−4.2610060	−7.5435362	−10.5982823
4.1	2.2943333	−0.3425167	−3.6224581	−7.3117162	−10.9704944
4.2	3.3813333	0.6845856	−2.7988889	−6.8781425	−11.1457315
4.3	4.6003333	1.8788594	−1.7749958	−6.2204963	−11.0933004
4.4	5.9573333	3.2502815	−0.5351981	−5.3158000	−10.7811818
4.5	7.4583333	4.8089097	0.9363567	−4.1404290	−10.1760423
4.6	9.1093333	6.5648813	2.6557865	−2.6701210	−9.2432453
4.7	10.9163333	8.5284105	4.6394688	−0.8799864	−7.9468612
4.8	12.8853333	10.7097863	6.9040356	1.2554829	−6.2496778
4.9	15.0223333	13.1193709	9.4663676	3.7624043	−4.1132096
5.0	17.3333333	15.7675971	12.3435899	6.6674961	−1.4977075
5.1	19.8243333	18.6649676	15.5530666	9.9980699	1.6378328
5.2	22.5013333	21.8220522	19.1123970	13.7820221	5.3356619
5.3	25.3703333	25.2494871	23.0394107	18.0478272	9.6392685
5.4	28.4373333	28.9579729	27.3521639	22.8245302	14.5933716
5.5	31.7083333	32.9582735	32.0689354	28.1417400	20.2439128
5.6	35.1893333	37.2612142	37.2082227	34.0296230	26.6380487
5.7	38.8863333	41.8776811	42.7887388	40.5188963	33.8241440
5.8	42.8053333	46.8186194	48.8294083	47.6408222	41.8517646
5.9	46.9523333	52.0950320	55.3493642	55.4272017	50.7716704

Table 1. Values of $q_\kappa(u)$ (continued)

$u\backslash\kappa$	2.5	2.6	2.7	2.8	2.9
1.0	−2.7500000	−4.3749277	−5.4031157	−5.0933651	−2.6742323
1.1	−2.1292333	−4.0168146	−5.6002049	−6.1323890	−4.7273899
1.2	−1.4230667	−3.4677596	−5.5018414	−6.8127828	−6.4550111
1.3	−0.6639000	−2.7630670	−5.1339481	−7.1330788	−7.8073186
1.4	0.1182667	−1.9381278	−4.5271187	−7.1028117	−8.7521505
1.5	0.8958333	−1.0278948	−3.7153951	−6.7406573	−9.2729269
1.6	1.6436000	−0.0664595	−2.7352620	−6.0728617	−9.3668596
1.7	2.3387667	0.9132980	−1.6248025	−5.1318880	−9.0433475
1.8	2.9609333	1.8800020	−0.4229747	−3.9552308	−8.3225166
1.9	3.4921000	2.8040314	0.8310157	−2.5843615	−7.2338741
2.0	3.9166667	3.6577369	2.0982680	−1.0637805	−5.8150554
2.1	4.2214333	4.4156297	3.3406780	0.5598468	−4.1106475
2.2	4.3956000	5.0545501	4.5213805	2.2384820	−2.1710760
2.3	4.4307667	5.5538166	5.6051508	3.9234466	−0.0515459
2.4	4.3209333	5.8953616	6.5587711	5.5661059	2.1889718
2.5	4.0625000	6.0638529	7.3513685	7.1185086	4.4887136
2.6	3.6542667	6.0468063	7.9547276	8.5339910	6.7840623
2.7	3.0974333	5.8346880	8.3435819	9.7677480	9.0104561
2.8	2.3956000	5.4210094	8.4958864	10.7773759	11.1032698
2.9	1.5547667	4.8024151	8.3930734	11.5233914	12.9986727
3.0	0.5833333	3.9787654	8.0202946	11.9697269	14.6344649
3.1	−0.5079000	2.9532125	7.3666497	12.0842073	15.9508937
3.2	−1.7057333	1.7322733	6.4254038	11.8390077	16.8914526
3.3	−2.9945667	0.3258968	5.1941944	11.2110963	17.4036647
3.4	−4.3564000	−1.2524712	3.6752293	10.1826614	17.4398505

Table 1. Values of $q_\kappa(u)$ (continued)

$u\backslash\kappa$	2.5	2.6	2.7	2.8	2.9
3.5	−5.7708333	−2.9858275	1.8754758	8.7415261	16.9578827
3.6	−7.2150667	−4.8535534	−0.1931574	6.8815496	15.9219285
3.7	−8.6639000	−6.8313594	−2.5136458	4.6030180	14.3031799
3.8	−10.0897333	−8.8912332	−5.0636803	1.9130250	12.0805736
3.9	−11.4625667	−11.0013886	−7.8155053	−1.1741585	9.2415006
4.0	−12.7500000	−13.1262176	−10.7357614	−4.6367217	5.7825066
4.1	−13.9172333	−15.2262444	−13.7853338	−8.4449618	1.7099835
4.2	−14.9270667	−17.2580801	−16.9192046	−12.5609376	−2.9591476
4.3	−15.7399000	−19.1743805	−20.0863101	−16.9381317	−8.1967609
4.4	−16.3137333	−20.9238044	−23.2294023	−21.5211192	−13.9628580
4.5	−16.6041667	−22.4509739	−26.2849130	−26.2452429	−20.2049068
4.6	−16.5644000	−23.6964356	−29.1828233	−31.0362942	−26.8571873
4.7	−16.1452333	−24.5966230	−31.8465346	−35.8102002	−33.8401435
4.8	−15.2950667	−25.0838211	−34.1927441	−40.4727159	−41.0597410
4.9	−13.9599000	−25.0861302	−36.1313225	−44.9191218	−48.4068313
5.0	−12.0833333	−24.5274328	−37.5651946	−49.0339264	−55.7565201
5.1	−9.6065667	−23.3273598	−38.3902232	−52.6905724	−62.9675421
5.2	−6.4684000	−21.4012585	−38.4950944	−55.7511493	−69.8816401
5.3	−2.6052333	−18.6601612	−37.7612061	−58.0661078	−76.3229490
5.4	2.0489333	−15.0107546	−36.0625587	−59.4739802	−82.0973846
5.5	7.5625000	−10.3553503	−33.2656472	−59.8011036	−86.9920362
5.6	14.0062667	−4.5918551	−29.2293566	−58.8613468	−90.7745645
5.7	21.4534333	2.3862568	−23.8048582	−56.4558415	−93.1926025
5.8	29.9796000	10.6899718	−16.8355081	−52.3727157	−93.9731609
5.9	39.6627667	20.4347639	−8.1567475	−46.3868313	−92.8220372

Table 1. Values of $q_\kappa(u)$ (continued)

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