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ACCURATE CALCULATION OF FUNCTIONS USED IN A MODEL OF THE NEMATIC BEHAVIOR OF SELF-ASSEMBLING SYSTEMS

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ABSTRACT. An algorithm used to evaluate double sums arising in a model describing the nematic phase behavior of surfactant solutions is demonstrated to yield approximations accurate to within a tenth of a percent. When direct summation would converge slowly, an asymptotic result is employed based on a double application of the Euler-Maclaurin sum formula.

1. INTRODUCTION

A model formulated by Herzfeld [3] provides a description of the liquid crystalline phase behavior of various protein and surfactant solutions. This model uses a lattice description of excluded volume effects and a phenomenological description of the reversible assembly of amphiphilic molecules into rod-like and plate-like aggregates of arbitrary size, which spontaneously align at sufficiently high concentrations. The predicted state of the system is the one which minimizes the free energy functional derived from the model. Locating this minimum when plate-like aggregates are present requires evaluation of the following four functions for $0 < P, \mathscr{P}, Q < 1$ (P, $\mathscr{P}$ and Q may be very close to 1):

$$G(P, \mathscr{P}, Q) = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} P^m \mathscr{P}^n Q^{mn}, \tag{1.1a}$$

$$G_1(P, \mathscr{P}, Q) = \sum_m\sum_n mP^m \mathscr{P}^n Q^{mn}, \tag{1.1b}$$

$$G_2(P, \mathscr{P}, Q) = \sum_m\sum_n nP^m \mathscr{P}^n Q^{mn} = G_1(\mathscr{P}, P, Q), \tag{1.1c}$$

$$G_3(P, \mathscr{P}, Q) = \sum_m\sum_n mnP^m \mathscr{P}^n Q^{mn}, \tag{1.1d}$$

cf. [3, 5, 6]. Here and below, summations whose limits are unspecified are understood to run from 0 to ∞. An algorithm developed by Berger and Herzfeld

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for evaluating the functions in (1.1) is given in [6] and has been used to study the phase behavior of surfactant solutions [5, 6].

In this paper we demonstrate that the overall algorithm, assuming exact arithmetic, gives values for G, G_1, G_2 and G_3 with relative error (error/exact value) bounded by $1/1000$. While the analysis below assumes infinite precision arithmetic, the algorithm itself incorporates asymptotic expansions for certain expressions involving the exponential integral function $\mathrm{Ei}(z)$ when cancellation of terms might otherwise cause serious loss of accuracy. We next display Table 1 to indicate the sensitivity of the values of the G functions to small changes in P, $\mathscr{P}$ and Q.

TABLE 1. Some values of the G functions.

P	$\mathscr{P}$	Q	G	G_1	G_2	G_3
.9999	.9999	.999999999	9.16E7	8.44E11	8.44E11	7.20E15
.9999	.9999	1	10.0E7	10.0E11	10.0E11	10.0E15
.9999	.999999	.999999999	2.02E9	7.98E12	7.99E14	1.22E18
.9999	.999999	1	10.0E9	100.E12	100.E14	100.E18

In §2 we give a complete description of the algorithm, in preparation for the proof of accuracy which then follows.

2. ALGORITHM FOR EVALUATING (1.1)

Let $0 < P, \mathscr{P}, Q < 1$. If either P or $\mathscr{P}$ is less than .64, or Q is smaller than .95, a direct partial summation is used to determine the functions in (1.1). Otherwise, a double application of the Euler-Maclaurin summation formula is employed. For direct partial summation, it is useful to rearrange the sums in (1.1) into the "herringbone pattern" $\sum_l T_l$, where T_l designates the sum over the pairs (m, n) in the half-line at and to the right of (l, l) and in the half-line above (l, l); e.g., for a given nonnegative integer L,

$$G(P, \mathscr{P}, Q) = \sum_{l=0}^{L} H(P, \mathscr{P}, Q, l) + E(P, \mathscr{P}, Q, L), \tag{2.1a}$$

where

$$\begin{aligned} H(P, \mathscr{P}, Q, l) &= \sum_{m=l}^{\infty} P^m \mathscr{P}^l Q^{ml} + \sum_{n=l}^{\infty} P^l \mathscr{P}^n Q^{ln} - P^l \mathscr{P}^l Q^{l^2} \\ &= P^l \mathscr{P}^l Q^{l^2}[(1 - PQ^l)^{-1} + (1 - \mathscr{P}Q^l)^{-1} - 1], \end{aligned} \tag{2.1b}$$

$$E(P, \mathscr{P}, Q, L) = \sum_{m=L+1}^{\infty} \sum_{n=L+1}^{\infty} P^m \mathscr{P}^n Q^{mn}. \tag{2.1c}$$

Similar expressions are valid for G_i, H_i, and E_i, $i = 1, 2, 3$. Recall that by differentiating $\sum_i z^i = (1 - z)^{-1}$ and then multiplying by z, one has $\sum_i iz^i = z(1 - z)^{-2}$ (further iterations of this procedure are used below), and so the H_i can be easily evaluated in closed form.

The approximate value for G is the first term on the right side of (2.1a). We next indicate how to choose L so that E will be as small as required. Define

$$K = L + 1, \qquad \rho = \rho(L) = P^K \mathscr{P}^K Q^{K^2} \tag{2.2}$$

and observe that

$$\begin{aligned} E(P, \mathscr{P}, Q, L) &= \rho \sum_{m=K}^{\infty} \sum_{n=K}^{\infty} (PQ^K)^{m-K} (\mathscr{P}Q^K)^{n-K} Q^{(m-K)(n-K)} \\ &= \rho \sum_i \sum_j (PQ^K)^i (\mathscr{P}Q^K)^j Q^{ij} = \rho G(PQ^K, \mathscr{P}Q^K, Q). \end{aligned} \tag{2.3}$$

Since G is an increasing function of P, $\mathscr{P}$ and Q, $G(PQ^K, \mathscr{P}Q^K, Q) < G(P, \mathscr{P}, Q)$, and so the relative error $E(P, \mathscr{P}, Q, L)/G(P, \mathscr{P}, Q)$ is bounded by ρ. For $P < .64$ or $\mathscr{P} < .64$ or $Q < .95$, this may be made quite small (e.g., smaller than $1/1000$) without having to take L very large. Note that $\rho(l)$ occurs in $H(P, \mathscr{P}, Q, l+1)$, so there is essentially no additional cost in computing the current value of ρ as l is successively increased until ρ satisfies a given stopping criterion.

In similar fashion one has

$$\begin{aligned} G_i(P, \mathscr{P}, Q) = \sum_{l=0}^{L} H_i(P, \mathscr{P}, Q, l) &+ K\rho G(PQ^K, \mathscr{P}Q^K, Q) \\ &+ \rho G_i(PQ^K, \mathscr{P}Q^K, Q), \qquad \text{for } i = 1, 2. \end{aligned} \tag{2.4}$$

To evaluate $G_1(P, \mathscr{P}, Q)$, we initially calculate the value of the first term on the right side of (2.4), with L the first integer for which ρ is less than or equal to half of whatever relative error tolerance $\tau > 0$ is prescribed. The value of the second term on the right side of (2.4) is then added in, with $G(PQ^K, \mathscr{P}Q^K, Q)$ calculated to within a relative error of $\tau/2$ as described above. The same procedure is used for G_2. Finally, for G_3 one has

$$\begin{aligned} G_3(P, \mathscr{P}, Q) = \sum_{l=0}^{L} H_3(P, \mathscr{P}, Q, l) &+ K^2 \rho G(PQ^K, \mathscr{P}Q^K, Q) \\ &+ K\rho G_1(PQ^K, \mathscr{P}Q^K, Q) + K\rho G_2(PQ^K, \mathscr{P}Q^K, Q) \\ &+ \rho G_3(PQ^K, \mathscr{P}Q^K, Q). \end{aligned} \tag{2.5}$$

To compute G_3 using (2.5), L is the first integer for which $\rho \le \tau/2$, and then G, G_1 and G_2 at $(PQ^K, \mathscr{P}Q^K, Q)$ are obtained to within a relative error of $\tau/2$ as described above.

As P, $\mathscr{P}$ and Q all approach 1, these "herringbone" sums require an increasingly large number of terms. Therefore, when

$$P \ge .64, \qquad \mathscr{P} \ge .64 \qquad \text{and} \qquad Q \ge .95, \tag{2.6}$$

we employ the Euler-Maclaurin summation formula (with 3 correction terms) as described below. The selection of the constants .64 and .95 in (2.6) (while somewhat arbitrary) was guided by the error analysis which follows.

2.1. Use of the Euler-Maclaurin formula. When (2.6) obtains, we will make repeated use of the summation formula

$$\sum_{k=0}^{\infty} f(k) = \int_0^{\infty} f(s)\,ds + \frac{f(0)}{2} - \frac{f^{(1)}(0)}{12} + \frac{f^{(3)}(0)}{720} + \tilde{r}, \tag{2.7}$$

where $f(s)$ is any "well-behaved" function on $[0, \infty)$ and $\tilde{r}$ denotes the remainder term, see, e.g., [4]. Analysis of the remainder terms when using (2.7) to evaluate (1.1) (confirmed by numerical experiments) indicates that in general it is essential to arrange to apply (2.7) to (1.1) only at points $(P, \mathscr{P}, Q)$ with

$$\ln Q/\ln P \le 1/4 \qquad \text{and} \qquad \ln Q/\ln \mathscr{P} \le 1/4. \tag{2.8}$$

This is easily accomplished by always doing preliminary herringbone sums with $L = 3$ ($K \equiv L + 1 = 4$) and using equations (2.1), (2.3), (2.4) and (2.5) to reduce evaluation of G, G_1, G_2 and G_3 at $(P, \mathscr{P}, Q)$ to evaluation at $(\tilde{P}, \tilde{\mathscr{P}}, Q) = (PQ^4, \mathscr{P}Q^4, Q)$ for which (2.8) is obviously valid. If either PQ^4 or $\mathscr{P}Q^4$ is less than .64, herringbone sums are used to obtain the G functions at $(\tilde{P}, \tilde{\mathscr{P}}, Q)$, otherwise (2.7) is employed, as we now describe. For simplicity in the notation, we drop the tilde over P and $\mathscr{P}$ when it should be clear from the context whether the original $(P, \mathscr{P}, Q)$ point or $(\tilde{P}, \tilde{\mathscr{P}}, Q)$ is under consideration (in particular it is to be understood that (2.7) is only applied to $(\tilde{P}, \tilde{\mathscr{P}}, Q)$).

Assume (2.6) and (2.8) are valid, and use the convention that sums and integrals whose limits are unspecified are understood to run from 0 to ∞. To determine $G(P, \mathscr{P}, Q)$ using the Euler-Maclaurin formula, define

$$f(x, y) = P^x \mathscr{P}^y Q^{xy} = \exp(x \ln P + y \ln \mathscr{P} + xy \ln Q) \tag{2.9}$$

and apply (2.7) to f considered as a function of x, obtaining

$$\begin{aligned} \sum_m P^m \mathscr{P}^y Q^{my} = \int f(x, y)\,dx + \mathscr{P}^y/2 - (\ln P + y \ln Q)\mathscr{P}^y/12 \\ + (\ln P + y \ln Q)^3 \mathscr{P}^y/720 + r(y) \qquad \text{for } y \ge 0. \end{aligned} \tag{2.10}$$

Bounds on the remainder r are obtained in the next section. Now sum both sides of (2.10) over $y = 0, 1, 2, \ldots$ and get

$$G(P, \mathscr{P}, Q) = \sum_n \int f(x, n)\,dx + A + \sum_n r(n), \tag{2.11}$$

where A denotes terms which are evaluated in closed form after straightforward albeit lengthy algebra. Since $f(x, y) > 0$ and the relevant series and integrals are convergent, we have

$$\sum_n \int f(x, n)\,dx = \int \sum_n f(x, n)\,dx. \tag{2.12}$$

Now apply (2.7) to the right side of (2.12) to find

$$\begin{aligned}\sum_n \int f(x,n)\,dx &= \iint f(x,y)\,dy\,dx \\ &+ \int \left[f(x,0)/2 - f_y(x,0)/12 + f_{yyy}(x,0)/720\right] dx \\ &+ \int s(x)\,dx,\end{aligned} \tag{2.13}$$

where s is the remainder term. Let

$$I(P,\mathscr{P},Q) \equiv \iint f(x,y)\,dy\,dx, \tag{2.14}$$

and let B denote the second summand on the right side of (2.13), which is evaluated in closed form. We then have

$$G(P,\mathscr{P},Q) = I + A + B + \sum_n r(n) + \int s(x)\,dx. \tag{2.15}$$

We approximate G by $I+A+B$ (the calculation of I is described immediately below), and in the next section we show that the remainder terms in (2.15) lead to a relative error of at most $1/1000$.

The same approach leads to

$$G_i(P,\mathscr{P},Q) = I_i + A_i + B_i + \sum_n r_i(n) + \int s_i(x)\,dx \qquad \text{for } i = 1, 2, 3 \tag{2.16}$$

with the notation corresponding to that in (2.15) (A_i and B_i are evaluated in closed form and r_i and s_i are remainder terms) and where

$$\begin{aligned}I_1(P,\mathscr{P},Q) &\equiv \iint xf(x,y)\,dx\,dy = P\,I_P(P,\mathscr{P},Q),\\ I_2(P,\mathscr{P},Q) &\equiv \iint yf(x,y)\,dx\,dy = \mathscr{P}\,I_{\mathscr{P}}(P,\mathscr{P},Q),\\ I_3(P,\mathscr{P},Q) &\equiv \iint xyf(x,y)\,dx\,dy = Q\,I_Q(P,\mathscr{P},Q),\end{aligned} \tag{2.17}$$

with f as in (2.9) and with I_P denoting the partial derivative of I with respect to P etc. The last equality in each line of (2.17) is justified by taking difference quotients approximating I_P, $I_{\mathscr{P}}$, I_Q and using the mean value theorem and then the Lebesgue dominated convergence theorem. The complete algebraic expressions for $A+B$, A_1+B_1, and A_3+B_3 are given in the Appendix and in the listing of the computer program SUM2D (available from the author) which implements the algorithm for evaluating G, G_1, G_2 and G_3. In the program, when (2.16) is being applied, $G_2(P,\mathscr{P},Q) = G_1(\mathscr{P},P,Q)$ is actually obtained by calculating the approximate value of $G_1(\mathscr{P},P,Q)$ via (2.16).

2.2. Evaluation of I, I_1, I_2 and I_3. We have

$$\begin{aligned} I(P, \mathscr{P}, Q) &= \int_y \exp(y \ln \mathscr{P}) \left\{ \int_x \exp[(\ln P + y \ln Q)x]\, dx \right\} dy \\ &= \int -(\ln P + y \ln Q)^{-1} \exp(y \ln \mathscr{P})\, dy. \end{aligned} \tag{2.18}$$

Now set

$$\lambda = \ln P \ln \mathscr{P} / \ln Q \tag{2.19}$$

and use the change of variables $s = \lambda + y \ln \mathscr{P}$ in (2.18) to find

$$\begin{aligned} I(P, \mathscr{P}, Q) &= \int_{-\infty}^{\lambda} (e^{-\lambda} / \ln Q) e^s s^{-1}\, ds \\ &= (e^{-\lambda} / \ln Q) \mathrm{Ei}(\lambda) = \lambda e^{-\lambda} \mathrm{Ei}(\lambda) / (\ln P \ln \mathscr{P}), \end{aligned} \tag{2.20}$$

where

$$\mathrm{Ei}(z) = \int_{-\infty}^{z} t^{-1} \exp(t)\, dt \qquad \text{for } z < 0 \tag{2.21}$$

is the exponential integral function (cf. formula 8.211 of [2], and page 228 of [1] where $\mathrm{E}_1(w) = -\mathrm{Ei}(-w)$ for $w > 0$). From (2.20) and (2.17) we have

$$\begin{aligned} I_1(P, \mathscr{P}, Q) &= \{-I(P, \mathscr{P}, Q) \ln \mathscr{P} + 1/\ln P\} / \ln Q, \\ I_2(P, \mathscr{P}, Q) &= \{-I(P, \mathscr{P}, Q) \ln P + 1/\ln \mathscr{P}\} / \ln Q, \\ I_3(P, \mathscr{P}, Q) &= \{I(P, \mathscr{P}, Q)\lambda - I(P, \mathscr{P}, Q) - 1/\ln Q\} / \ln Q. \end{aligned} \tag{2.22}$$

For $-1 < \lambda < 0$, the formula 5.1.53 on page 231 of [1] is used to obtain $\mathrm{Ei}(\lambda)$ and thereafter I, I_1, I_2 and I_3. For $-59 < \lambda \leq -1$ formula 5.1.56 of [1] is used to evaluate $\lambda \exp(-\lambda)\mathrm{Ei}(\lambda)$ and thereby I, I_1, I_2 and I_3 ($\mathrm{Ei}(\lambda)$ and $\exp(-\lambda)\mathrm{Ei}(\lambda)$ may be obtained using a special function library routine, if available, e.g., MMDEI in IMSL). In order to avoid serious loss of significant digits from cancellation of terms in (2.22) (particularly in I_3) as $-\lambda$ becomes large, for $\lambda \leq -59$ we use the asymptotic expansion for $\lambda \exp(-\lambda)\mathrm{Ei}(\lambda)$ coming from formula 8.215 of [2] (note there the $\exp(-x)$ factor also is to apply to R_n), viz.

$$\lambda e^{-\lambda} \mathrm{Ei}(\lambda) = \sum_{k=0}^{n-1} \frac{k!}{\lambda^k} + E_n, \qquad \text{where } |E_n| \leq n!/|\lambda|^n. \tag{2.23}$$

From (2.23), (2.20) and (2.22) one can obtain the following approximations to be used for $\lambda \leq -59$ (cf. §3.6):

$$\begin{aligned} I(P, \mathscr{P}, Q) &\approx (1 + 1/\lambda + 2/\lambda^2 + 6/\lambda^3)/(\ln P \ln \mathscr{P}), \\ I_1(P, \mathscr{P}, Q) &\approx D/[(\ln P)^2 \ln \mathscr{P}], \\ &\qquad \text{where } D \equiv -1 - 2/\lambda - 6/\lambda^2 - 24/\lambda^3, \\ I_2(P, \mathscr{P}, Q) &\approx D/[(\ln \mathscr{P})^2 \ln P], \\ I_3(P, \mathscr{P}, Q) &\approx (1 + 4/\lambda + 18/\lambda^2 + 96/\lambda^3)/(\ln P \ln \mathscr{P})^2. \end{aligned} \tag{2.24}$$

In the next section we prove

Theorem 2.1. *The algorithm described in this section* (*with* $\tau = 1/1000$ *when herringbone sums are used*) *gives values for* G, G_1, G_2 *and* G_3 *with relative error* (*error*/*exact value*) *no larger than* $1/1000$.

It should be pointed out that the above result assumes there is no round-off error in the calculations. The expansions in (2.24) deal with the situation where it was seen that finite precision arithmetic threatened to introduce significant errors. Note, however, that we are not claiming to treat all the limitations of finite machine precision. In particular, there would be computational difficulties if the arithmetic $z = 1 - P$, or $z = 1 - \mathscr{P}$, or $z = 1 - Q$ loses "too many" significant digits. Error estimates which are sharper than those stated in Theorem 2.1 are given in Lemma 3.5 in §3.3, and in §3.5.

Values of G, G_1, G_2 and G_3 from SUM2D on test cases with $P \geq .64$, $\mathscr{P} \geq .64$, $Q \geq .95$ were consistent to within 0.1% with those obtained by "brute force" use of the herringbone sum option (with $\tau = 1/10000$) in SUM2D.

3. Proof of Theorem 2.1

We demonstrate the accuracy claimed in Theorem 2.1 by obtaining bounds for: the remainder terms in the Euler-Maclaurin summations, the errors in the approximations used for the exponential integral function, and the errors in the asymptotic expansions used for I, I_1, I_2 and I_3 when $\lambda \leq -59$. We first give a bound (suitable for our specific applications) for the remainder term in the form of the Euler-Maclaurin sum formula given in (2.7).

3.1. A Bound for the remainder in (2.7). We will be using (2.7) with $f(s)$ of the form e^{as} or se^{as} with a some negative constant. The following result, which follows directly from, e.g., pages 177-179 of [4], will serve our requirements.

Lemma 3.1. *Assume* $f(s)$ *is in* $C^6[0, \infty)$, *the sum and integral in* (2.7) *are absolutely convergent,* $f^{(i)}(s) \to 0$ *as* $s \to \infty$ *for* $i = 1$ *and* 3, *and* $f^{(6)}(s) \in L^1(0, \infty)$. *Then the remainder term* $\tilde{r}$ *in* (2.7) *is bounded by*

$$|\tilde{r}| \leq \frac{2B_6(0)}{6!} \int_0^\infty \left|f^{(6)}(s)\right| ds \tag{3.1}$$

where $B_6(x)$ *is the sixth Bernoulli polynomial* $(B_6(0) = 1/42)$.

Proof. See problem 22 on page 179 of [4], let $m = 2$, note from problems 19 and 20 that $|B_6(s) - B_6(0)| \leq 2B_6(0)$, and then let $r \to \infty$. □

As an immediate consequence one has

Corollary 3.2. *Suppose, in addition to the hypotheses of Lemma* 3.1, f *satisfies*

$$\int_0^\infty \left|f^{(6)}(s)\right| ds \leq C_5 \left|f^{(5)}(0)\right|. \tag{3.2}$$

Then

$$|\tilde{r}| \leq 2C_5 \frac{B_6(0)}{6!} \left|f^{(5)}(0)\right| = 2C_5 \frac{\left|f^{(5)}(0)\right|}{30240}. \tag{3.3}$$

If $f(s) = e^{as}$, then $f^{(6)}$ has one sign on $[0, \infty)$ and C_5 in (3.2) is 1 (in this case a sharper bound for $|\tilde{r}|$ is available, cf. [4, p. 154], but we will not require it here). We also have

Remark 3.3. If $f(s) = se^{as}$ with a some negative constant, then (3.2) is valid when

$$C_5 = \tilde{K}_5 \equiv 1 + \frac{2e^{-6}}{5}. \tag{3.4}$$

Proof. One may verify by induction that

$$f^{(k)}(s) = (a^k s + ka^{k-1})e^{as} \qquad \text{for } k = 0, 1, \ldots, \tag{3.5}$$

and so

$$f^{(6)}(s) = 0 \qquad \text{only at the point } p = -6/a. \tag{3.6}$$

Then

$$\int_0^\infty \left|f^{(6)}(s)\right| ds = -\int_0^p f^{(6)}(s)\, ds + \int_p^\infty f^{(6)}(s)\, ds = f^{(5)}(0) - 2f^{(5)}(p), \tag{3.7}$$

from which the result quickly follows. □

For future use, we define

$$K_5 = 5\tilde{K}_5 = 5 + 2e^{-6} \tag{3.8a}$$

and note that when $f(s) = s\exp(as)$,

$$\tilde{K}_5 \left|f^{(5)}(0)\right| = K_5 a^4. \tag{3.8b}$$

We are now in a position to estimate the remainder terms in (2.15) and (2.16).

3.2. Bounds on the Euler-Maclaurin remainders in (2.15) and (2.16). We first treat the remainder terms for $G(P, \mathscr{P}, Q)$. Recalling the notation in (2.9), (2.10), (2.13) and (2.15), and Corollary 3.2 and the sentence below it, we have

$$|r(n)| \le 2|\ln P + n\ln Q|^5 \mathscr{P}^n/30240 \qquad \text{for } n = 0, 1, 2, \ldots, \tag{3.9a}$$

$$|s(x)| \le 2|\ln \mathscr{P} + x\ln Q|^5 e^{x\ln P}/30240 \qquad \text{for } x \ge 0. \tag{3.9b}$$

For convenience, we introduce the notation

$$\delta = 1/30240. \tag{3.9c}$$

We next calculate a bound for $\int |s(x)|\, dx$, making use of the formula

$$\int_0^\infty x^k e^{ax}\, dx = (-1)^{k+1} k!/a^{k+1} \qquad \text{for } a < 0 \text{ and } k = 0, 1, 2, \ldots, \tag{3.10}$$

see, e.g., 4.2.55 in [1]. From (2.6), $\mathscr{P} \ge .64$, so $|\ln \mathscr{P}| \le 1/2$, and setting $c = \ln Q/\ln P$, we have

$$\begin{aligned} \int |s(x)|\, dx &\le 2\delta \int (1/2 + x|\ln Q|)^5 e^{x\ln P}\, dx \\ &= 2\delta(1/32 + 5c/16 + 5c^2/2 + 15c^3 + 60c^4 + 120c^5)/|\ln P|. \end{aligned} \tag{3.11}$$

From (2.8), $c \le 1/4$, and noting that

$$|\ln z| = \sum_{n=1}^{\infty}(1-z)^n/n > 1-z \qquad \text{for } 0 < z < 1, \tag{3.12}$$

we obtain

$$\int |s(x)|\,dx \le 2\delta(54.5/64)/|\ln P| \le 2\delta/(1-P) \le 2\delta G(P, \mathscr{P}, Q), \tag{3.13}$$

with the last inequality following from (2.1) with $L = 0$.

We next provide a bound for $\sum_n |r(n)|$ by dominating this sum with an integral. For each positive integer n, $|r(n)|$ is bounded by

$$2\delta \int_{n-1}^{n} |\ln P + n \ln Q|^5 \mathscr{P}^n\,dy \le 2\delta \int_{n-1}^{n} |\ln P + \ln Q + y \ln Q|^5 \mathscr{P}^y\,dy, \tag{3.14a}$$

since the inequality is valid for the integrands when $n - 1 \le y \le n$. Recalling (2.6) and the resulting fact that $|\ln P| + |\ln Q| \le .44629 + .05130 \le 1/2$, (3.14a) implies

$$\begin{aligned} \sum_n |r(n)| &= |r(0)| + \sum_{n=1}^{\infty} |r(n)| \\ &\le 2\delta |\ln P|^5 + 2\delta \int_0^{\infty} (1/2 + y|\ln Q|)^5 \mathscr{P}^y\,dy. \end{aligned} \tag{3.14b}$$

As above, the last term in (3.14b) is bounded by $2\delta G(P, \mathscr{P}, Q)$. From (2.1), for P and $\mathscr{P} \ge .64$, $G(P, \mathscr{P}, Q) \ge 2/.36 - 1 \ge 4$. Since $|\ln P| \le 1/2$, one has $|\ln P|^5 \le 1/32 \le G(P, \mathscr{P}, Q)/128$, and so from (3.13) and (3.14),

$$\begin{aligned} \sum_n |r(n)| + \int |s(x)|\,dx &\le 4\tfrac{1}{64} G(P, \mathscr{P}, Q)/30240 \\ &\le (.00014) G(P, \mathscr{P}, Q). \end{aligned} \tag{3.15}$$

3.2.1. Bounds on r_1 and s_1. Estimates for the remainder terms in (2.16) generally follow a similar pattern. We start with r_1 and s_1. For r_1, apply (2.7) and §3.1 to $f(s) = \mathscr{P}^n s \exp(as)$ with $a = \ln P + n \ln Q$, and obtain

$$|r_1(n)| \le 2\delta K_5 |\ln P + n \ln Q|^4 \mathscr{P}^n \qquad \text{for } n = 0, 1, 2, \ldots. \tag{3.16}$$

Analogous to (3.14),

$$\begin{aligned} \sum_n |r_1(n)| &\le 2\delta K_5 \int |\ln P + \ln Q + y \ln Q|^4 \mathscr{P}^y\,dy + 2\delta K_5 |\ln P|^4 \\ &\le 2\delta K_5 \int (1/2 + y|\ln Q|)^4 \mathscr{P}^y\,dy + 2\delta K_5 |\ln P|^4 \\ &\le 2\delta K_5 (42/64)/|\ln \mathscr{P}| + \delta K_5/8. \end{aligned} \tag{3.17}$$

To obtain an error bound relative to G_1 we use

Lemma 3.4. *One has* $G_1(P, \mathscr{P}, Q) \geq 2/|\ln \mathscr{P}| \geq 4$ *when* (2.6) *and* (2.8) *are valid.*

Proof. We have

$$(3.18)\qquad \begin{aligned} G_1(P, \mathscr{P}, Q) &\geq \sum_{m=1}^{5} mP^m \sum_n (\mathscr{P}Q^m)^n = \sum_{m=1}^{5} \frac{mP^m}{1-\mathscr{P}Q^m} \\ &\geq \sum_{m=1}^{5} \frac{m(.64)^m}{1-\mathscr{P}Q^m}. \end{aligned}$$

Now using (2.8),

$$(3.19a)\qquad 1-\mathscr{P}Q^m < |\ln(\mathscr{P}Q^m)| = |\ln \mathscr{P}| + m|\ln Q| \leq |\ln \mathscr{P}|(1+m/4),$$

and so

$$(3.19b)\qquad (1-\mathscr{P}Q^m)^{-1} > |\ln \mathscr{P}|^{-1} 4/(4+m).$$

Substituting this in (3.18) and performing the arithmetic yields the first inequality of the lemma, and recalling that $|\ln \mathscr{P}| \leq 1/2$ gives the second. □

Equation (3.17) together with Lemma 3.4 and the fact that $K_5 < 5.005$ shows that

$$(3.20)\qquad \begin{aligned} \sum_n |r_1(n)| &\leq (\delta K_5(21/32) + \delta K_5/32) G_1(P, \mathscr{P}, Q) \\ &\leq (.00012) G_1(P, \mathscr{P}, Q). \end{aligned}$$

Turning our attention to $s_1(x)$,

$$(3.21)\qquad |s_1(x)| \leq 2\delta|\ln \mathscr{P} + x\ln Q|^5 xP^x \qquad \text{for } x \geq 0,$$

and so

$$(3.22)\qquad \int |s_1(x)|\,dx \leq 2\delta|\ln P|^{-2}(222/64).$$

Taking the terms in (1.1b) with $n = 0$, 1, 2 and 3, and using (3.19) gives

$$(3.23)\qquad G_1(P, \mathscr{P}, Q) \geq |\ln P|^{-2}(.64 + .249 + .105 + .046) \geq |\ln P|^{-2}.$$

Then (3.22) and (3.23) imply

$$(3.24)\qquad \int |s_1(x)|\,dx \leq G_1(P, \mathscr{P}, Q)\delta(111/16) < (.00023)G_1(P, \mathscr{P}, Q).$$

Since $G_2(P, \mathscr{P}, Q)$ is obtained by computing $G_1(\mathscr{P}, P, Q)$, the relative error bounds for the approximation of $G_1(P, \mathscr{P}, Q)$ apply as well to $G_2(P, \mathscr{P}, Q)$.

3.2.2. Bounds on r_3 and s_3. The same approach as above leads to

$$(3.25)\qquad \begin{aligned} \sum_n |r_3(n)| &\leq 2\delta K_5 \int (y+1)(1/2 + y|\ln Q|)^4 \mathscr{P}^y\,dy \\ &\leq 2\delta K_5 \left(\tfrac{42}{64}|\ln \mathscr{P}|^{-1} + 2\tfrac{3}{32}(\ln \mathscr{P})^{-2}\right), \end{aligned}$$

$$(3.26) \quad \int |s_3(x)|\,dx \le 2\delta K_5 \int x(1/2 + x|\ln Q|)^4 P^x\,dx \le 2\delta K_5 (2\tfrac{3}{32}(\ln P)^{-2}).$$

We now show how the above estimates lead to bounds on the relative error in the values for the G functions.

3.3. Consequences of the bounds on the Euler-Maclaurin remainder terms. Recall the discussion between (2.8) and (2.9). The estimates we have obtained so far enable us to demonstrate

Lemma 3.5. *Assume both* $(P, \mathscr{P}, Q)$ *and* $(\tilde{P}, \tilde{\mathscr{P}}, Q)$ *satisfy* (2.6), *in which case the Euler-Maclaurin formula is used to obtain the G functions at* $(\tilde{P}, \tilde{\mathscr{P}}, Q)$. *Assume there is no error in the evaluation of the terms* I, I_1, I_2 *and* I_3 *(i.e., all the error comes from the Euler-Maclaurin remainder terms). Then the relative error in the calculated value of* $G(P, \mathscr{P}, Q)$ *is at most* .00014, *the relative error in the calculated values for* $G_1(P, \mathscr{P}, Q)$ *and* $G_2(P, \mathscr{P}, Q)$ *is no larger than* .00035, *and* .0005002 *bounds the relative error in the computed value of* $G_3(P, \mathscr{P}, Q)$.

Proof. Note the basic facts that: if the relative error in an approximation v to some value V is τ, and c is a constant, then the relative error in cv approximating cV is τ; if the relative errors in $v_1, \dots, v_n$ approximating the positive quantities $V_1, \dots, V_n$ are all bounded by τ, then the relative error in $v_1 + \cdots + v_n$ approximating $V_1 + \cdots + V_n$ is likewise bounded by τ; and if V is the sum of positive quantities V_1 and V_2, approximated by values v_1 (with relative error τ_1) and v_2 (with error e_2), then the relative error in $v_1 + v_2 \approx V$ is bounded by $\tau_1 + e_2/V$. The estimate for G follows from (2.1a), (2.3), (2.15) and (3.15), and the estimate for G_1 is a consequence of (2.4), (2.16), (3.15), (3.20) and (3.24). The result for G_2 then also follows, noting the last sentence of §3.2.1.

The bound for the error in G_3 is a bit more complex. From (2.5), (2.16) and the above, a bound for the relative error, τ_3, in $G_3(P, \mathscr{P}, Q)$ is given by

$$(3.27) \quad \tau_3 \le .00035 + P^4\mathscr{P}^4Q^{16}\left(\sum_n |r_3(n)| + \int |s_3(x)|\,dx\right) \Big/ G_3(P, \mathscr{P}, Q).$$

Equations (3.25) and (3.26), and the fact that $|\ln\tilde{\mathscr{P}}| \le 1/2$, give

$$(3.28) \quad \begin{aligned} \sum_n |r_3(n)| + \int |s_3(x)|\,dx &\le 2\delta K_5\{(\tfrac{42}{128} + 2\tfrac{3}{32})(\ln\tilde{\mathscr{P}})^{-2} + 2\tfrac{3}{32}(\ln\tilde{P})^{-2}\} \\ &\le .000802(\ln\tilde{\mathscr{P}})^{-2} + .0007(\ln\tilde{P})^{-2}. \end{aligned}$$

Taking the terms in (1.1d) with $n = 1$, 2, 3 and 4, and then using (3.12) and setting $\rho = P^4\mathscr{P}^4Q^{16}$ shows that

$$(3.29a) \quad G_3(P, \mathscr{P}, Q) > 10\rho(1 - PQ^4)^{-2} = 10\rho(1 - \tilde{P})^{-2} > 10\rho(\ln\tilde{P})^{-2}.$$

Since G_3 is symmetric in P and $\mathscr{P}$, it is also true that

$$(3.29b) \quad G_3(P, \mathscr{P}, Q) > 10P^4\mathscr{P}^4Q^{16}(1 - \tilde{\mathscr{P}})^{-2} > 10P^4\mathscr{P}^4Q^{16}(\ln\tilde{\mathscr{P}})^{-2}.$$

Then (3.27), (3.28) and (3.29) give

$$\tau_3 \leq .00035 + .0000802 + .00007 = .0005002 \tag{3.30}$$

and we have the result. □

3.4. Bounds on the errors in I, I_1, I_2 and I_3. We now obtain bounds on the contribution to the relative error in G, G_1, G_2 and G_3 from the errors in I, I_1, I_2 and I_3 in the three cases $-1 < \lambda < 0$, $-59 < \lambda \leq -1$, and $\lambda \leq -59$, and thereby complete the proof of Theorem 2.1. Note from (2.22) that $I_2(P, \mathscr{P}, Q) = I_1(\mathscr{P}, P, Q)$, so results for I_2 follow immediately from those for I_1.

3.4.1. Bounds when $-1 < \lambda < 0$. From formula 5.1.53 of [1], the error in $\mathrm{Ei}(z)$ is bounded by 2×10^{-7}. The function $\mathrm{Ei}(z)$ is decreasing on $(-\infty, 0)$, hence on $(-1, 0)$, $|\mathrm{Ei}(\lambda)| \geq |\mathrm{Ei}(-1)| > .21$ (for the latter see, e.g., [1 or 2]). Thus,

$$\begin{aligned} &\text{the error in } \mathrm{Ei}(\lambda) < (2 \times 10^{-7}/.21).21 < 1 \times 10^{-6}\mathrm{Ei}(\lambda) \\ &\qquad\qquad\qquad\qquad\qquad\qquad \text{for } -1 < \lambda < 0. \end{aligned} \tag{3.31}$$

Setting $R_{mn} = \{(x, y) : m \leq x \leq m+1,\ n \leq y \leq n+1\}$, we also have

$$\begin{aligned} I(P, \mathscr{P}, Q) &= \sum_m \sum_n \int_{R_{mn}} f(x, y)\,dx\,dy \\ &\leq \sum_m \sum_n \int_{R_{mn}} P^m \mathscr{P}^n Q^{mn}\,dx\,dy = G(P, \mathscr{P}, Q). \end{aligned} \tag{3.32}$$

Hence from (2.20),

$$\text{the error in } I < 1 \times 10^{-6} I \leq 1 \times 10^{-6} G \qquad \text{for } -1 < \lambda < 0. \tag{3.33}$$

Bound for I_1. From (2.22), (3.33) and (2.20)

$$\begin{aligned} \text{the error in } I_1 &\leq (\text{the error in } I) \ln \mathscr{P} / \ln Q \\ &< 1 \times 10^{-6} I \ln \mathscr{P} / \ln Q \qquad \text{for } -1 < \lambda < 0, \end{aligned} \tag{3.34a}$$

$$I_1 = 1/(\ln P \ln Q) - I \ln \mathscr{P} / \ln Q = (1 - \lambda e^{-\lambda}\mathrm{Ei}(\lambda))/(\ln P \ln Q). \tag{3.34b}$$

Since we wish to obtain a relative error bound for the error in I_1, we next extract a lower bound for I_1. From formula 8.212.4 of [2] with $\lambda = -x$ (which may be verified using the change of variable $w = \lambda + \ln t$) we have

$$\lambda e^{-\lambda}\mathrm{Ei}(\lambda) = \int_0^1 \frac{\lambda}{\lambda + \ln t}\,dt \qquad \text{for } \lambda < 0, \tag{3.35a}$$

and thus the facts that

$$\lambda e^{-\lambda}\mathrm{Ei}(\lambda) \text{ is a decreasing function of } \lambda \text{ for } \lambda < 0, \tag{3.35b}$$

$$0 < \lambda e^{-\lambda}\mathrm{Ei}(\lambda) < 1 \qquad \text{for } \lambda < 0. \tag{3.35c}$$

From page 250 of [1], the value at $\lambda = -1$ of $\lambda e^{-\lambda}\mathrm{Ei}(\lambda) = -\lambda e^{-\lambda}\mathrm{E}_1(-\lambda)$ is less than .6, so from (3.34b) and (3.35b)

$$I_1 \geq .4/(\ln P \ln Q) \quad \text{and} \quad I_1^{-1} \leq (\ln P \ln Q)/.4 \qquad \text{for } -1 < \lambda < 0, \tag{3.36}$$

and so

$$\text{(3.37)}\qquad \begin{aligned} \text{the error in } I_1 &< [(1\times 10^{-6} I \ln \mathscr{P}/\ln Q) I_1^{-1}] I_1 \\ &\le 2.5\times 10^{-6}\lambda e^{-\lambda}\mathrm{Ei}(\lambda) I_1 \le 1.5\times 10^{-6} I_1 \qquad \text{for } -1<\lambda<0. \end{aligned}$$

Our bound for the error in I_1 will be completed using the following result.

Lemma 3.6. *Assume* (2.6) *and* (2.8) *are valid. Then*

$$I_1(P, \mathscr{P}, Q) < 3G_1(P, \mathscr{P}, Q).$$

Equation (3.37) and Lemma 3.6 give the estimate

$$\text{(3.38)}\qquad \text{the error in } I_1 < 4.5\times 10^{-6} G_1 \qquad \text{for } -1<\lambda<0.$$

The pattern of the demonstration of (3.38) will be repeated throughout this section.

Proof of Lemma 3.6. We have $I_1 \le \sum_m \sum_n (m+1) P^m \mathscr{P}^n Q^{mn} = G_1 + G$. Now $G = (1-\mathscr{P})^{-1} + \sum_{m>0}\sum_n P^m \mathscr{P}^n Q^{mn} < (1-\mathscr{P})^{-1} + G_1$, and

$$\begin{aligned} |\ln z| &= \sum_{i=1}^{\infty} (1-z)^i/i < (1-z) + \sum_{i=2}^{\infty} (1-z)^i/2 \\ &= (1-z) + \frac{(1-z)^2}{2z} \qquad \text{for } 0<z<1, \end{aligned}$$

and so

$$\text{(3.39)}\quad |\ln z| \le (1-z) + (1-z)(.36/1.28) \le 4(1-z)/3 \qquad \text{for } .64 \le z < 1.$$

Since (2.6) is being assumed, (3.39) implies that

$$\text{(3.40)}\qquad (1-\mathscr{P})^{-1} \le 4|\ln \mathscr{P}|^{-1}/3,$$

and this together with Lemma 3.4 and the above gives

$$\text{(3.41)}\quad G(P, \mathscr{P}, Q) < 2G_1(P, \mathscr{P}, Q) \qquad \text{when (2.6) and (2.8) are valid},$$

and hence $I_1 < 3G_1$.

Bound for I_3 when $-1<\lambda<0$. Estimating the relative error in I_3 follows the same pattern of obtaining an upper bound for the error in I_3 and a lower bound for the value of I_3. From (2.22) and (2.20),

$$\text{(3.42)}\qquad \begin{aligned} \text{the error in } I_3 &\le 2(\text{the error in } \mathrm{Ei}(\lambda)) e^{-\lambda}/(\ln Q)^2 \\ &\le (4\times 10^{-7} e (\ln Q)^{-2} I_3^{-1}) I_3. \end{aligned}$$

We next determine a lower bound for I_3, which then gives an upper limit on the size of I_3^{-1}. Again from (2.22) and (2.20),

$$\text{(3.43a)}\quad I_3(P, \mathscr{P}, Q) = k(\lambda)/(\ln Q)^2 \qquad \text{and thus} \qquad I_3^{-1} = (\ln Q)^2/k(\lambda),$$

where

$$\text{(3.43b)}\qquad k(\lambda) \equiv \lambda e^{-\lambda}\mathrm{Ei}(\lambda) - e^{-\lambda}\mathrm{Ei}(\lambda) - 1.$$

We will demonstrate below that

$$k(\lambda) = \int_0^\infty \frac{te^{-t}}{(t-\lambda)^2}\, dt, \tag{3.43c}$$

which shows that $k(\lambda)$ is a positive increasing function for $-\infty < \lambda < 0$. Thus, using, e.g., Table 5.6 on page 250 of [1],

$$k(\lambda) \ge k(-1) > .1926 \qquad \text{for } -1 < \lambda < 0. \tag{3.44}$$

Equations (3.42), (3.43) and (3.44) give

$$\text{the error in } I_3 \le (4 \times 10^{-7} e/.1926) I_3 \le 5.66 \times 10^{-6} I_3. \tag{3.45}$$

We also prove below

Lemma 3.7. *Assume* (2.6) *and* (2.8) *are valid. Then*

$$I_3(P, \mathscr{P}, Q) < 12 G_3(P, \mathscr{P}, Q).$$

This together with (3.45) gives the estimate

$$\text{the error in } I_3(P, \mathscr{P}, Q) \le 6.8 \times 10^{-5} G_3(P, \mathscr{P}, Q) \qquad \text{for } -1 < \lambda < 0. \tag{3.46}$$

Proof of (3.43c). From formula 8.212.3 of [2] (which may be verified by integration by parts and a simple change of variable),

$$\lambda e^{-\lambda}\mathrm{Ei}(\lambda) - 1 = \int_0^\infty \frac{\lambda e^{-t}}{(t-\lambda)^2}\, dt. \tag{3.47}$$

Starting from (2.21) with t replaced by w, and then using the change of variable $w = \lambda - t$,

$$\mathrm{Ei}(\lambda) = \int_{-\infty}^{\lambda} \frac{e^w}{w}\, dw = \int_0^\infty \frac{e^\lambda e^{-t}}{\lambda - t}\, dt = \int_0^\infty \frac{(\lambda - t) e^\lambda e^{-t}}{(t-\lambda)^2}\, dt \tag{3.48}$$

so

$$-e^{-\lambda}\mathrm{Ei}(\lambda) = \int_0^\infty \frac{(t-\lambda)e^{-t}}{(t-\lambda)^2}\, dt, \tag{3.49}$$

and summing (3.47) and (3.49) gives the desired result, (3.43c). □

Proof of Lemma 3.7. Bounding the integrand for I_3 over each R_{mn} results in

$$\begin{aligned} I_3(P, \mathscr{P}, Q) \le{}& G_3(P, \mathscr{P}, Q) + G_2(P, \mathscr{P}, Q) \\ &+ G_1(P, \mathscr{P}, Q) + G(P, \mathscr{P}, Q). \end{aligned} \tag{3.50}$$

Also,

$$\begin{aligned} G_1(P, \mathscr{P}, Q) &= P(1-P)^{-2} + \sum_m \sum_{n>0} m P^m \mathscr{P}^n Q^{mn} \\ &< P(1-P)^{-2} + G_3(P, \mathscr{P}, Q) \end{aligned} \tag{3.51}$$

and similarly

$$G(P, \mathscr{P}, Q) < (1-P)^{-1} + (1-\mathscr{P})^{-1} + G_3(P, \mathscr{P}, Q). \tag{3.52}$$

Performing the same type of computation as used to obtain (3.23),

$$G_3(P,\mathscr{P},Q) > \sum_{n=1}^{3} n\mathscr{P}^n \sum_m m(PQ^n)^m > (.249+.210+.138)|\ln P|^{-2} \tag{3.53}$$
$$= .597|\ln P|^{-2} \qquad \text{when (2.6) and (2.8) are valid.}$$

Since $P \geq .64$, one has $|\ln P| \leq .44629$, and (3.53) and (3.39) with $z = P$ give

$$G_3(P,\mathscr{P},Q) > |\ln P|^{-1}.597/.44629 > 4|\ln P|^{-1}/3 \geq (1-P)^{-1}. \tag{3.54}$$

Interchanging P and $\mathscr{P}$ in (3.54) yields

$$G_3(P,\mathscr{P},Q) > (1-\mathscr{P})^{-1}, \tag{3.55}$$

and so

$$G(P,\mathscr{P},Q) < 3G_3(P,\mathscr{P},Q). \tag{3.56}$$

Also from (3.53) and (3.39) with $z = P$,

$$3G_3(P,\mathscr{P},Q) > 1.791|\ln P|^{-2} > 16|\ln P|^{-2}/9 > P/(1-P)^2, \tag{3.57}$$

and therefore

$$G_1(P,\mathscr{P},Q) < 4G_3(P,\mathscr{P},Q), \tag{3.58}$$

and, interchanging P and $\mathscr{P}$ in (3.58), $G_2 < 4G_3$. Equations (3.50), (3.56) and (3.58) give the result. □

3.4.2. Bounds when $-59 < \lambda \leq -1$. The approach for obtaining these estimates follows a course similar to the above. From formula 5.1.56 of [1], the error ζ in $\lambda e^{-\lambda}\mathrm{Ei}(\lambda)$ is less than 2×10^{-8} for $-59 < \lambda \leq -1$, and from Table 5.6 of [1] and (3.35b), $\lambda e^{-\lambda}\mathrm{Ei}(\lambda) \geq .5963$ for $\lambda \leq -1$, hence

$$\zeta < (2 \times 10^{-8}/.5963)\lambda e^{-\lambda}\mathrm{Ei}(\lambda) \leq 3.4 \times 10^{-8}\lambda e^{-\lambda}\mathrm{Ei}(\lambda). \tag{3.59}$$

Therefore, from (2.20) and (3.32),

$$\text{the error in } I < 3.4 \times 10^{-8} I \leq 3.4 \times 10^{-8} G. \tag{3.60}$$

The error in I_1 is bounded by the error in I times $\ln\mathscr{P}/\ln Q$, and

$$I_1^{-1} \leq \ln P \ln Q/(1-\xi),$$

where ξ is the value of $\lambda e^{-\lambda}\mathrm{Ei}(\lambda)$ at $\lambda = -59$. We conservatively bound ξ from above by the value of $\lambda e^{-\lambda}\mathrm{Ei}(\lambda)$ at $\lambda = 1/.015$ given in Table 5.2 of [1] (one could obtain a somewhat sharper bound, if desired, by using formula 5.1.55 of [1] at $\lambda = -59$), which leads to $(1-\xi) \geq .0145$, and so

$$\text{the error in } I_1 \leq (3.4 \times 10^{-8} I \ln\mathscr{P}/\ln Q)(\ln P \ln Q/.0145)I_1 \tag{3.61}$$
$$\leq 2.4 \times 10^{-6} I_1 \leq 7.2 \times 10^{-6} G_1,$$

using (3.35c) and Lemma 3.6.

The error in I_3 is bounded by twice the error in I times $\lambda/\ln Q$, while $I_3^{-1} \leq (\ln Q)^2/k(-59)$. Again using Table 5.2 of [1], .00021 is a conservative lower bound for $k(-59)$, and this together with (3.60) and (3.35c) gives

$$\text{the error in } I_3 \leq (6.8 \times 10^{-8}/.00021)I_3 \leq 3.24 \times 10^{-4} I_3. \tag{3.62}$$

Lemma 3.7 is no longer adequate to obtain the desired result, but recall we are actually applying (3.62) to $(\tilde{P}, \tilde{\mathscr{P}}, Q)$ in the context of (2.5) (with $K = 4$). Thus our next step is to bound the error in $\rho G_3(\tilde{P}, \tilde{\mathscr{P}}, Q)$ in terms of $G_3(P, \mathscr{P}, Q)$ when $\lambda \le -1$. From (2.16) applied at the point $(\tilde{P}, \tilde{\mathscr{P}}, Q)$, and setting $\tilde{G}_3 = G_3(\tilde{P}, \tilde{\mathscr{P}}, Q)$ and $G_3 = G_3(P, \mathscr{P}, Q)$, and similarly with $\tilde{I}_3$ and I_3,

$$\begin{aligned} \text{the error in } \rho\tilde{G}_3/G_3 = \rho(&\text{the error in } \tilde{I}_3)/G_3 \\ &+ \rho\left(\sum_n r_3(n) + \int s_3(x)\,dx\right)\Big/ G_3. \end{aligned} \tag{3.63}$$

Now from (3.28) and (3.29), the last term in (3.63) is bounded by .0001502, while (2.16) and inspection of the signs of the terms in the expression for A_3+B_3 in the Appendix gives

$$\begin{aligned} \tilde{G}_3 = \tilde{I}_3 + &\sum_n r_3(n) + \int s_3(x)\,dx \\ &- \frac{\tilde{\mathscr{P}}}{12(1-\tilde{\mathscr{P}})^2} - \frac{1}{12(\ln \tilde{P})^2} + \text{positive terms}. \end{aligned} \tag{3.64a}$$

Again using (3.29), (3.64a) gives

$$\rho\tilde{I}_3/G_3 \le \rho\tilde{G}_3/G_3 + .0001502 + 1/60. \tag{3.64b}$$

Since all the terms on the right side of (2.5) are positive, $\rho\tilde{G}_3/G_3 \le 1$ and

$$\rho\tilde{I}_3/G_3 \le 1 + .0001502 + 1/60 \le 1.017. \tag{3.65}$$

Then (3.62) at $(\tilde{P}, \tilde{\mathscr{P}}, Q)$, (3.63) and (3.65) yield

$$\text{the error in } \rho\tilde{G}_3/G_3 \le .00032951 + .0001502 \le .00048. \tag{3.66}$$

3.4.3. Bounds when $\lambda \le -59$. We first note that repeated integration by parts in (2.21) leads to (2.23), and to the fact that the sign of E_n in (2.23) is the same as the sign of the first omitted term, viz., $n!/\lambda^n$. Let e_0 be the value which, when added to the approximation for I in the right side of (2.24), gives I exactly, and similarly with e_1 for I_1, and e_3 for I_3. Then the same algebra which gives (2.24) shows that e_0 and e_1 have the same sign as, and are bounded by the magnitude of $24\lambda^{-4}/(\ln P \ln \mathscr{P})$ and $-120\lambda^{-4}/[(\ln P)^2 \ln \mathscr{P}]$, respectively; and e_3 is the sum of two terms with the same signs as, and bounded by the magnitudes of $720\lambda^{-4}/(\ln P \ln \mathscr{P})^2$ and $-120\lambda^{-4}/(\ln P \ln \mathscr{P})^2$. The error in I, when $\lambda \le -59$, is thus bounded by $2 \times 10^{-6}/(\ln P \ln \mathscr{P})$, while

$$I \ge (1 - 1/59 - 6/59^3)/(\ln P \ln \mathscr{P}) \ge .983/(\ln P \ln \mathscr{P}). \tag{3.67}$$

Thus,

$$\text{the error in } I \le 2.04 \times 10^{-6} I \le 2.04 \times 10^{-6} G. \tag{3.68}$$

Analogous calculations lead to

(3.69a) $\qquad$ the error in $I_1 \leq 1.04 \times 10^{-5} I_1 \leq 3.12 \times 10^{-5} G_1$,

(3.69b) $\qquad$ the error in $I_3 \leq 6.46 \times 10^{-5} I_3$.

Comparing (3.69b) with (3.62), we see that (3.66) is also valid for $\lambda \leq -59$.

3.5. Proof of Theorem 2.1. Assume both $(P, \mathscr{P}, Q)$ and $(\tilde{P}, \tilde{\mathscr{P}}, Q)$ satisfy (2.6). The results and method of proof of Lemma 3.5, together with the bounds on the error in I, I_1, I_2 and I_3 in §3.4 demonstrate that: the relative error in $G(P, \mathscr{P}, Q)$ is bounded by .00014204, the relative error in $G_1(P, \mathscr{P}, Q)$ (and G_2) is bounded by .0003812, and .0008612 bounds the relative error in $G_3(P, \mathscr{P}, Q)$. (We have retained extra digits in various constants to make it easier to follow the calculations of the bounds.) □

3.6. Closing remarks. The value $\lambda_a = -59$, beyond which (2.24) is used, was determined as that λ at which rough estimates for the errors in I_3 using (2.22) and using (2.24) were equal; the estimates being, respectively,

$$(\text{the error in } I)\lambda/\ln Q \approx (2 \times 10^{-8}/(\ln P \ln \mathscr{P}))\lambda/\ln Q = 2 \times 10^{-8}(\ln Q)^{-2}$$

and

$$840\lambda^{-4}(\ln P \ln \mathscr{P})^{-2} = 840\lambda^{-6}(\ln Q)^{-2}.$$

The resulting λ_a is $-58.958 \approx -59$. If the accuracy of the evaluation of $\lambda e^{-\lambda}\mathrm{Ei}(\lambda)$ is increased, a corresponding value of λ_a should be used, and corresponding error estimates can be readily obtained with the methods developed in §3.

Appendix. Closed form expressions for the quantities $A + B$, $A_1 + B_1$ and $A_3 + B_3$ in equations (2.15), (2.16).

$$\begin{aligned} A + B = {} & \frac{1}{2(1-\mathscr{P})} - \frac{\ln P}{12(1-\mathscr{P})} - \frac{\mathscr{P}\ln Q}{12(1-\mathscr{P})^2} + \frac{(\ln P)^3}{720(1-\mathscr{P})} \\ & + \frac{\mathscr{P}(\ln P)^2 \ln Q}{240(1-\mathscr{P})^2} + \frac{\mathscr{P}\ln P\,(\ln Q)^2}{240(1-\mathscr{P})^2} + \frac{\mathscr{P}^2 \ln P\,(\ln Q)^2}{120(1-\mathscr{P})^3} \\ & + \frac{(\ln Q)^3}{720}\left[\frac{\mathscr{P}}{(1-\mathscr{P})^2} + \frac{6\mathscr{P}^2}{(1-\mathscr{P})^3} + \frac{6\mathscr{P}^3}{(1-\mathscr{P})^4}\right] \\ & - \frac{1}{2\ln P} + \frac{\ln \mathscr{P}}{12\ln P} - \frac{\ln Q}{12(\ln P)^2} - \frac{(\ln \mathscr{P})^3}{720\ln P} \\ & + \frac{(\ln \mathscr{P})^2 \ln Q}{240(\ln P)^2} - \frac{\ln \mathscr{P}\,(\ln Q)^2}{120(\ln P)^3} + \frac{(\ln Q)^3}{120(\ln P)^4}, \end{aligned}$$

$$A_1 + B_1 = -\frac{1}{12(1-\mathscr{P})} + \frac{(\ln P)^2}{240(1-\mathscr{P})} + \frac{\mathscr{P}\ln P \ln Q}{120(1-\mathscr{P})^2} + \frac{\mathscr{P}(\ln Q)^2}{240(1-\mathscr{P})^2}$$
$$+ \frac{\mathscr{P}^2(\ln Q)^2}{120(1-\mathscr{P})^3} + \frac{1}{2(\ln P)^2} - \frac{\ln \mathscr{P}}{12(\ln P)^2} + \frac{\ln Q}{6(\ln P)^3}$$
$$+ \frac{(\ln \mathscr{P})^3}{720(\ln P)^2} - \frac{\ln Q\,(\ln \mathscr{P})^2}{120(\ln P)^3} + \frac{\ln \mathscr{P}\,(\ln Q)^2}{40(\ln P)^4} - \frac{(\ln Q)^3}{30(\ln P)^5},$$

$$A_3 + B_3 = -\frac{\mathscr{P}}{12(1-\mathscr{P})^2} + \frac{\mathscr{P}(\ln P)^2}{240(1-\mathscr{P})^2} + \frac{\mathscr{P}\ln P \ln \mathscr{P}}{120(1-\mathscr{P})^2} + \frac{\mathscr{P}^2 \ln P \ln Q}{60(1-\mathscr{P})^3}$$
$$+ \frac{\mathscr{P}(\ln Q)^2}{240(1-\mathscr{P})^2} + \frac{\mathscr{P}^2(\ln Q)^2}{40(1-\mathscr{P})^3} + \frac{\mathscr{P}^3(\ln Q)^2}{40(1-\mathscr{P})^4} - \frac{1}{12(\ln P)^2}$$
$$+ \frac{(\ln \mathscr{P})^2}{240(\ln P)^2} - \frac{\ln \mathscr{P} \ln Q}{60(\ln P)^3} + \frac{(\ln Q)^2}{40(\ln P)^4}.$$

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