Part IV

Major arcs

Chapter Fourteen

Major arcs: overview and results

Our task, as in Part III, will be to estimate

$$S_\eta(\alpha, x) = \sum_n \Lambda(n) e(\alpha n) \eta(n/x), \tag{14.1}$$

where $\eta : \mathbb{R}^+ \to \mathbb{C}$ is a smooth function, Λ is the von Mangoldt function and $e(t) = e^{2\pi i t}$. Here, we will treat the case of α lying on the major arcs.

We will see how we can obtain good estimates by using smooth functions η based on the Gaussian $e^{-t^2/2}$. This will involve proving new, fully explicit bounds for the Mellin transform of the twisted Gaussian, or, what is the same, bounds on parabolic cylindrical functions in certain ranges. It will also require explicit formulae that are general and strong enough, even for moderate values of x.

Let $\alpha = a/q + \delta/x$. For us, saying that α lies on a major arc will be the same as saying that q and δ are bounded; more precisely, q will be bounded by a constant r and $|\delta|$ will be bounded by a constant times r/q. As is customary on the major arcs, we will express our exponential sum (10.1) as a linear combination of twisted sums

$$S_{\eta,\chi}(\delta/x, x) = \sum_{n=1}^{\infty} \Lambda(n) \chi(n) e(\delta n/x) \eta(n/x), \tag{14.2}$$

for $\chi : \mathbb{Z} \to \mathbb{C}$ a Dirichlet character mod q, i.e., a multiplicative character on $(\mathbb{Z}/q\mathbb{Z})^*$ lifted to $\mathbb{Z}$. (The advantage here is that the phase term is now $e(\delta n/x)$ rather than $e(\alpha n)$, and $e(\delta n/x)$ varies very slowly as n grows.) Our task, then, is to estimate $S_{\eta,\chi}(\delta/x, x)$ for δ small.

Estimates on $S_{\eta,\chi}(\delta/x, x)$ rely on the properties of Dirichlet L-functions $L(s,\chi) = \sum_n \chi(n) n^{-s}$. What is crucial is the location of the zeros of $L(s,\chi)$ in the critical strip $0 \leq \Re s \leq 1$ (a region in which $L(s,\chi)$ can be defined by analytic continuation). In contrast to most previous work, we will not use zero-free regions, which are too narrow for our purposes. Rather, we use a verification of the Generalized Riemann Hypothesis up to bounded height for all conductors $q \leq 400000$ (due to D. Platt [Pla16]).

A key feature of the present work is that it allows one to mimic a wide variety of smoothing functions by means of estimates on the Mellin transform of a single smoothing function – here, the Gaussian $e^{-t^2/2}$.

14.1 RESULTS

Let us first give a bound for exponential sums on the primes using a one-sided Gaussian as the smooth weight.

Theorem 14.1. *Let $\eta : \mathbb{R}^+ \to \mathbb{C}$ be defined by $\eta(t) = \sqrt{2/\pi} \cdot e^{-t^2/2}$. Let χ be a primitive Dirichlet character mod q, $1 \leq q \leq r$, where $r = c \cdot 100000$ with $c = 3$ or $c = 4$.*

Then, for any $x, \delta \in \mathbb{R}$ with $x \geq 10^6$ and $|\delta| \leq 4r/q$,

$$\sum_{n=1}^{\infty} \Lambda(n)\chi(n)e\left(\frac{\delta}{x}n\right)\eta\left(\frac{n}{x}\right) = I_{q=1} \cdot \widehat{\eta}(-\delta) \cdot x + E,$$

where $I_{q=1} = 1$ if $q = 1$, $I_{q=1} = 0$ if $q \neq 1$, and

$$|E| \leq \epsilon_c x + (\kappa_c\sqrt{\delta_0} + 43)\sqrt{x} + 6|\delta|,$$

where $\delta_0 = \max(|\delta|, 4)$, $\epsilon_3 = 3.24 \cdot 10^{-29}$, $\epsilon_4 = 1.26 \cdot 10^{-17}$, $\kappa_3 = 280$ and $\kappa_4 = 242$.

Here we write $\widehat{\eta}(-\delta)$ for $\int_{0^+}^{\infty} \eta(t)e(\delta t)dt$. (Strictly speaking, this is an abuse of language, since the Fourier transform is defined in this way for functions on $\mathbb{R}$, not for functions on $\mathbb{R}^+$.)

As it turns out, smooth weights based on the Gaussian are often better in applications than the Gaussian itself. Here is a result for the smoothing from Part III.

Theorem 14.2. *Let $\eta : \mathbb{R}^+ \to \mathbb{C}$ be defined by $\eta(t) = \sqrt{2/\pi} \cdot 2(e^{-t^2/2} - e^{-2t^2})$. Let χ be a primitive Dirichlet character mod q, $1 \leq q \leq r$, where $r = c \cdot 100000$ with $c = 3$ or $c = 4$.*

Then, for any $x, \delta \in \mathbb{R}$ with $x \geq 10^6$ and $|\delta| \leq 4r/q$,

$$\sum_{n=1}^{\infty} \Lambda(n)\chi(n)e\left(\frac{\delta}{x}n\right)\eta\left(\frac{n}{x}\right) = I_{q=1} \cdot \widehat{\eta}(-\delta) \cdot x + E,$$

where $I_{q=1} = 1$ if $q = 1$, $I_{q=1} = 0$ if $q \neq 1$, and

$$|E| \leq \epsilon_c x + (\kappa_c\sqrt{\delta_0} + 25)\sqrt{x} + 3|\delta|,$$

where $\delta_0 = \max(|\delta|, 4)$, $\epsilon_3 = 9.7 \cdot 10^{-29}$, $\epsilon_4 = 3.76 \cdot 10^{-17}$, $\kappa_3 = 115$ and $\kappa_4 = 100$.

It should be clear that we could obtain an estimate much as in Thm. 14.2 directly from Thm. 14.1 itself. We derive Thm. 14.2 from our general explicit formula simply because doing so results in smaller lower-order terms, while taking next to no additional work.

In much the same way, Thm. 14.1 implies bounds for smoothing functions of the form $\sum_{i=1}^{k} a_i e^{-b_i t^2/2}$, or even $g *_M e^{-t^2/2}$, with g of compact support. Of course, we can also use the general explicit formula to deal with smoothing functions that have

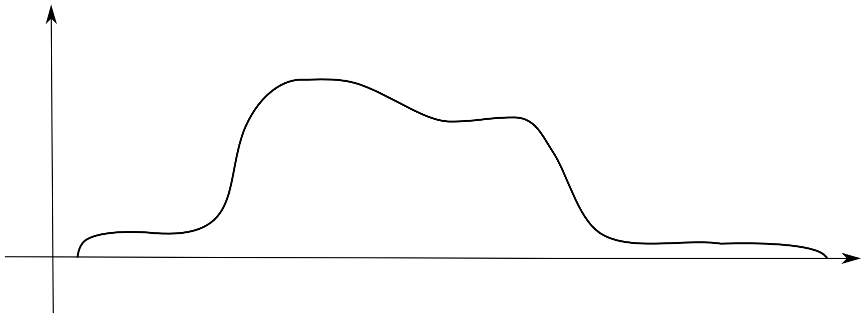

Figure 14.1: A fairly arbitrary $f : \mathbb{R}^+ \to \mathbb{R}$ of compact support

nothing to do with the Gaussian. The advantage of working with the Gaussian is that the estimates from Chapter 15 result in very small values for the constants ϵ_c, as above.

Let us now look at a different kind of modification of the Gaussian smoothing. Say we would like a smoothing that is close in the L^2-norm to some function f of compact support or fast decay – say, the fairly arbitrary function f in Figure 14.1. For instance, in Part V, we will want a smoothing that is close to the function

$$\eta_\circ : t \mapsto \begin{cases} t^3(2-t)^3 e^{-(t-1)^2/2} & \text{for } t \in [0,2], \\ 0 & \text{otherwise,} \end{cases} \tag{14.3}$$

since a function having that shape will make a certain constant optimal. At the same time, we want our smoothing to be based on the one-sided Gaussian, so that we can have very small bounds ϵx.

We will discuss later why a convolution $g(t) *_M e^{-t^2/2}$ would not do. (In brief: approximating given functions f by convolutions is possible, but g could be forced to take enormous values.) We let

$$\eta_+(t) = h_H(t) \cdot \eta_\diamond(t), \tag{14.4}$$

where $\eta_\diamond(t) = te^{-t^2/2}$ and $h_H : (0,\infty) \to \mathbb{R}$ is a band-limited approximation to the function $h : (0,\infty) \to \mathbb{R}$ given by

$$h(t) = \begin{cases} t^2(2-t)^3 e^{t-1/2} & \text{if } t \leq 2, \\ 0 & \text{otherwise.} \end{cases} \tag{14.5}$$

By a *band-limited function*, in the context of the Mellin transform, we mean a function defined as the inverse Mellin transform, taken on the line $\sigma + i\mathbb{R}$, of a function with compact support on $\sigma + i\mathbb{R}$. (A *band-limited function* in the context of the Fourier transform is the inverse Fourier transform of a function with compact support on $\mathbb{R}$.) We can simply take h_H to be the inverse Mellin transform of a truncation of Mh at height H:

$$h_H(x) = \frac{1}{2\pi i} \int_{-iH}^{iH} (Mh)(s) x^{-s} ds. \tag{14.6}$$

This choice makes sense: since the Mellin transform is an isometry, then, among functions defined as inverse Mellin transforms of functions with support on $i \cdot [-H, H]$, the one closest in the L^2 norm to h is h_H.

While Mh_H has no strip of holomorphy, $M\eta_+$ is holomorphic for $\Re s > -1$. We work out the details in Appendix A.2. The main point will be the following. Define $\eta_{\diamondsuit,\delta}(x) = \eta_\diamondsuit(x)e(\delta x)$ and $\eta_{+,\delta}(x) = \eta_+ e(\delta x)$. Then

$$M\eta_{+,\delta}(s) = \frac{1}{2\pi i}\int_{-iH}^{iH} Mh(z) M\eta_{\diamondsuit,\delta}(s-z)dz \tag{14.7}$$

for $\Re s > -1$ (Lemma A.9). In particular, when $t \mapsto \infty^+$, $M\eta_{+,\delta}(\sigma + it)$ decays at least as rapidly as $M\eta_{\diamondsuit,\delta}(\sigma+it)$ does, only delayed by a shift of at most iH. Of course $M\eta_{\diamondsuit,\delta}(s) = M\eta_{\heartsuit,\delta}(s+1)$, where $\eta_{\heartsuit,\delta}(x) = \eta_\heartsuit(x)e(\delta x)$ and $\eta_\heartsuit : (0,\infty) \to \mathbb{R}$ is our favorite function $\eta_\heartsuit(x) = e^{-x^2/2}$.

Theorem 14.3. *Let $\eta(t) = \eta_+(t) = h_H(t)te^{-t^2/2}$, where h_H is as in (14.6). Let χ be a primitive Dirichlet character mod q.*

1. *Let $H = 100$, and assume $q \leq r = 400000$. Then, for any $x, \delta \in \mathbb{R}$ with $x \geq 10^6$ and $|\delta| \leq 4r/q$,*

$$\sum_{n=1}^{\infty} \Lambda(n)\chi(n)e\left(\frac{\delta}{x}n\right)\eta(n/x) = I_{q=1}\cdot\widehat{\eta}(-\delta)\cdot x + E,$$

   where $I_{q=1} = 1$ if $q = 1$, $I_{q=1} = 0$ if $q \neq 1$, and

$$|E| \leq \epsilon_+ x + (78\sqrt{\delta_0} + 23)\sqrt{x} + 2|\delta|,$$

   where $\delta_0 = \max(|\delta|, 4)$ and $\epsilon_+ = 1.93 \cdot 10^{-6}$.

2. *Let $H = 200$, and assume $q' \leq r' = 150000$, where $q' = q/\gcd(q,2)$. Then, for any $x, \delta \in \mathbb{R}$ with $x \geq 10^6$ and $|\delta| \leq 4r'/q'$,*

$$\sum_{n=1}^{\infty} \Lambda(n)\chi(n)e\left(\frac{\delta}{x}n\right)\eta(n/x) = I_{q=1}\cdot\widehat{\eta}(-\delta)\cdot x + E',$$

   where $I_{q=1} = 1$ if $q = 1$, $I_{q=1} = 0$ if $q \neq 1$, and

$$|E'| \leq \epsilon'_+ x + (95\sqrt{\delta_0} + 23)\sqrt{x} + 2|\delta|,$$

   where $\delta_0 = \max(|\delta|, 4)$ and $\epsilon'_+ = 1.81 \cdot 10^{-18}$.

As can be seen, we are giving two sets of bounds in each of our theorems here; they correspond to two sets of choices of parameters. The motivation is in part to leave our options open for later, in part precisely to emphasize that we have some freedom in our choice of parameters, and in part to facilitate comparisons with previous versions of the present work. (Bounds have improved.)

The same method we will use to prove Theorem 14.3 can be used to obtain many other results of the same kind: following the procedure given in §16.2.2, we can bound exponential sums with weights of the form $f_H(t)te^{-t^2/2}$ or $f_H(t)e^{-t^2/2}$, where f_H is a band-limited approximation to just about any continuous function f of fast decay. Having f be C^{k-1} and piecewise C^k, as is the case for our function h with $k = 3$, does help, as it makes the approximation better, by making the tails of $t \mapsto Mh(\sigma+it)$ lighter. The use of $te^{-t^2/2}$ in place of $e^{-t^2/2}$ makes for a wider strip of holomorphy.

The same idea applies if we have estimates for the Mellin transform of some other function $g(t)$ (say, $g(t) = e^{-t}$); we can then follow the same procedure to obtain explicit formulae with weights of the form $f_H(t)g(t)$, approximating a desired weight $f(t)g(t)$.

14.2 MAIN IDEAS

14.2.1 Explicit formulae

An *explicit formula* gives an expression

$$S_{\eta,\chi}(\delta/x, x) = I_{q=1}\widehat{\eta}(-\delta)x - \sum_{\rho} G_\delta(\rho)x^\rho + \text{small error}, \qquad (14.8)$$

where $I_{q=1} = 1$ if $q = 1$ and $I_{q=1} = 0$ otherwise. Here ρ runs over the complex numbers ρ with $L(\rho,\chi) = 0$ and $0 < \Re\rho < 1$ ("non-trivial zeros"). The function G_δ is the Mellin transform of $e(\delta t)\eta(t)$.

The questions are then: where are the non-trivial zeros ρ of $L(s,\chi)$? How fast does $G_\delta(\rho)$ decay as $\Im\rho \to \pm\infty$?

Write $\sigma = \Re s$, $t = \Im s$. The belief is, of course, that $\sigma = 1/2$ for every non-trivial zero (Generalized Riemann Hypothesis), but this is far from proved. Most work to date has used zero-free regions of the form $\sigma \leq 1 - 1/C \log q|t|$, C a constant. These regions are too narrow to yield by themselves estimates of the strength we need. What we will use instead is finite verifications of GRH, i.e., computations proving that, for every Dirichlet character χ of conductor less than some constant r, and for some $T = T_\chi$ that may depend on χ, hypothesis GRH(T) holds: every non-trivial zero $\rho = \sigma + it$ with $|t| \leq T$ satisfies $\Re\sigma = 1/2$.

We will first give explicit formulae for general classes of smoothing functions (§16.1), then specialize to the smoothing functions used in Thms. 14.1–14.3, giving results in terms of the height T up to which GRH has been verified (§16.2). Lastly, we will apply the verification due to Platt, described in §16.3, and thus obtain Thms. 14.1–14.3.

Using a zero-free region or density results to supplement GRH(T), as in [FK15], would result in some gains in the constants ϵ in the terms in ϵx in Thms. 14.1–14.3. We will not go down that route, as our constants ϵ are already much smaller than we need them to be, and the terms proportional to $\sqrt{x}$ dominate when x is not very large. The explicit formula in Prop. 16.6 is general enough that it could be used with zero-free regions or density results if so wished.

What remains to discuss, then, is how to choose η in such a way that $G_\delta(s)$ ($s = \sigma + it$, $\sigma \in [0,1]$) decreases fast enough as $|t|$ increases, so that a functional equation of the form (14.8) and a verification of GRH(T) result in a good estimate.

14.2.2 Choosing smoothing functions

We will discuss at length (§15.2) the issues involved in choosing a smoothing function. Let us go over the main issue briefly.

We should not hope for $G_\delta(s)$ to start decreasing rapidly before $|t|$ is at least as large as a constant times $|\delta|$. Our aim is then to choose η so that $G_\delta(s)$ decreases very rapidly as soon as $t > C|\delta|$, C a moderate constant. We soon find ourselves in a Scylla-and-Charybdis situation, courtesy of the uncertainty principle: roughly speaking, $G_\delta(s)$ cannot decrease faster than exponentially on $|t|/|\delta|$ both for $|\delta| \leq 1$ and for δ large. We discuss this situation in §15.2.

The most delicate case is that of δ large, since then $T/|\delta|$ is small. It turns out we can manage to get decay that is much faster than exponential for δ large, while no slower than exponential for δ small. The idea is to work with smoothing functions based on the (one-sided) Gaussian $e^{-x^2/2}$. Then $G_\delta(s)$ will decay roughly as $e^{-(t/\pi\delta)^2/2}$ for $t = o(\delta^2)$, and as $e^{-(\pi/4)t}$ for larger t. Thus, it is enough for $t > \max(8\pi\delta, 40)$, say, for us to get a factor of roughly about $\min(e^{-32}, e^{-10\pi}) \leq 2.28 \cdot 10^{-14}$, whereas working with an exponential smoothing would have resulted in a factor of about $e^{-8} = 0.00033546\ldots$ under the same assumptions. Since there will be many terms to add, it is clear that $0.00033546\ldots$ would have been much too large.

We will want to work with reasonably precise bounds. The Mellin transform of the twisted Gaussian $e(\delta t)e^{-t^2/2}$ is a parabolic cylinder function $U(a,z)$ with z purely imaginary. Since fully explicit estimates for $U(a,z)$, z imaginary, have not been worked in the literature, we will have to derive them ourselves.

Once we have fully explicit estimates for the Mellin transform of the twisted Gaussian, we are able to use essentially any smoothing function based on the Gaussian $e^{-t^2/2}$.

There remains the question of which specific smoothing functions to choose to work with. In Part III, we used a linear combination of two Gaussians. Later on, in Part V, it will become clear that we want two of our three prime summands to be weighed by a smoothing function of a certain shape. We already spoke briefly in §14.1 of how to approximate a given function $h(t)e^{-t^2/2}$ using a band-limited function h_H. An approximation in L^2 norm makes the most sense in our context, just as an approximation in L^1 norm may be best in some other contexts. We will discuss in Part V why we want our smoothing function to have a specific shape, what are different ways to approach it, and what makes us rule most of them out and follow the one we have chosen.

Chapter Fifteen

The Mellin transform of the twisted Gaussian

15.1 OVERVIEW

15.1.1 Results

Our aim in this chapter is to give fully explicit, yet relatively simple bounds for the Mellin transform $F_\delta(s)$ of $e(\delta x)e^{-x^2/2}$, where δ is arbitrary. The task turns out to be immediately equivalent to that of bounding the parabolic cylinder function $U(a,z)$ for a complex and z purely imaginary. Existing explicit work on $U(a,z)$ treats the case of a and z real, or other cases that are not what we need, and so we must prove bounds on $U(a,z)$ ourselves.

As we shall see, the decay of $F_\delta(s)$ as $\Im s \to \pm\infty$ is quite fast. It would be natural to expect that the bounds we will give will make it easier to choose the Gaussian smoothing in explicit work in number theory, particularly in the context of exponential sums.

Theorem 15.1. *Let $f_\delta(x) = e^{-x^2/2}e(\delta x)$, $\delta \in \mathbb{R}$. Let F_δ be the Mellin transform of f_δ. Let $s = \sigma + it$, $0 \le \sigma \le 2$. Assume $|t| \ge \max(4\pi|\delta|, 40)$. If $\delta \ne 0$ and $\operatorname{sgn}(\delta) \ne \operatorname{sgn}(t)$, then*

$$|F_\delta(s)| \le \left(1 + \frac{c_\sigma}{|t|}\right) \frac{\sqrt{2\pi}|t|^{\sigma-1/2}}{(\max(\sqrt{|t|}, 2\pi|\delta|))^\sigma} \cdot e^{-E(\mathscr{r})|t|}, \tag{15.1}$$

where $\mathscr{r} = |t|/\pi^2\delta^2$, $c_\sigma = 5.6$ for $0 \le \sigma \le 1$, $c_\sigma = 26.94$ for $1 < \sigma \le 2$, and

$$E(\mathscr{r}) = \frac{1}{2}\arccos\frac{1}{\upsilon(\mathscr{r})} - \frac{\upsilon(\mathscr{r}) - 1}{\mathscr{r}} \tag{15.2}$$

$$j(\mathscr{r}) = \sqrt{\mathscr{r}^2 + 1}, \qquad \upsilon(\mathscr{r}) = \sqrt{(1 + j(\mathscr{r}))/2}. \tag{15.3}$$

If $\delta \ne 0$ and $\operatorname{sgn}(\delta) = \operatorname{sgn}(t)$,

$$|F_\delta(s)| \le \left(\kappa_\sigma |t|^{\frac{\sigma-1}{2}} e^{\left(E(\mathscr{r}) - \frac{2}{\mathscr{r}}\right)|t|} + 0.59\right) e^{-\frac{\pi}{2}|t|}, \tag{15.4}$$

where $\kappa_\sigma = 2.56$ for $0 \le \sigma \le 1$ and $\kappa_\sigma = 3.69$ for $1 \le \sigma \le 2$. Under the same conditions, we also have the simpler bound

$$|F_\delta(s)| \le \kappa_\sigma |t|^{\frac{\sigma-1}{2}} e^{-\frac{\pi}{4}|t|}, \tag{15.5}$$

which is also valid for $\delta = 0$ and $\operatorname{sgn}(t)$ arbitrary.

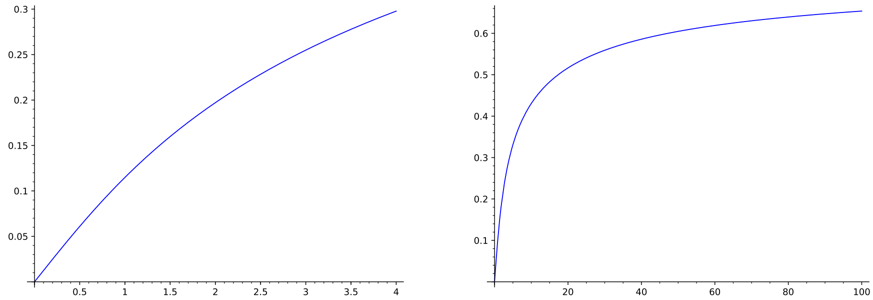

Figure 15.1: The function $E(\mathscr{r})$

See the graph of $E(\mathscr{r})$ (on two ranges) in Figure 15.1.

As we shall see, the choice of smoothing function $\eta(x) = e^{-x^2/2}$ can be easily motivated by the method of stationary phase, but the problem is actually solved by the saddle-point method. One of the challenges here is to keep all expressions explicit and practical.

Our aim has been to give bounds that are strong as soon as $F_\delta(s)$ starts to decay, and not just for $|t|$ very large. As we shall see, decay starts as soon as $|t|$ is larger than $\max(|\delta|, 1)$ or so.

It will become clear that, when $\text{sgn}(\delta) \neq \text{sgn}(t)$, our function $F_\delta(s)$ undergoes a "phase change" when t is about a constant times δ^2, that is, when the parameter $\mathscr{r} = |t|/\pi^2\delta^2$ in the statement of Theorem 15.1 is $\asymp 1$. For $|\delta| \ll |t| \ll \delta^2$, the decay of $F_\delta(s)$ is Gaussian in $|t/\delta|$, but, after $|t|$ increases past δ^2, the decay of $F_\delta(s)$ is exponential in $|t/\delta|$. Our bounds in Theorem 15.1 reflect this fact: since $E(\mathscr{r}) \to 1/8$ for $\mathscr{r} \to 0^+$ and $E(\mathscr{r}) \to \pi/4$ for $\mathscr{r} \to \infty$, the exponent $-E(\mathscr{r})|t|$ is $\sim -\mathscr{r}|t|/8 = -(t/\pi\delta)^2/2$ for $\mathscr{r} \to 0^+$, i.e., for $t = o(\delta^2)$, and it is $\sim -(\pi/4)t$ for $\mathscr{r} \to \infty$.

The upper bound (15.4) for $\text{sgn}(t) = \text{sgn}(\delta)$ is very small: since $E(\mathscr{r}) - 2/\mathscr{r} < \pi/4$ for all $\mathscr{r}$, the bound is always $\ll e^{-\pi t/4}$. It is instructive to compare (15.4) with the true asymptotic for $\delta = 0$: since the Mellin transform of $e^{-x^2/2}$ is $2^{s/2-1}\Gamma(s/2)$, Stirling's formula (Cor. 3.10) gives us that, for $\delta = 0$ and $0 \leq \sigma \leq 1$, $|F_\delta(s)| \sim \sqrt{\pi}|t|^{\frac{\sigma-1}{2}} e^{-\frac{\pi|t|}{4}}$. Thm. 15.1 gives us a bound of exactly the same form, but with a constant $\kappa_\sigma = 2.56$ instead of $\sqrt{\pi}$.

In general, the bounds in Thm. 15.1 are of the right order of magnitude, but the constants in front are not actually optimal. At the end of §15.5.3, we shall discuss in passing how one would go about proving a version of (15.1) with the right constant in front of the main term. The main term in (15.1) is in fact tight for $\mathscr{r} \to 0^+$ and $\mathscr{r} \to \infty$. (The values for c_σ in (15.1) are, on the other hand, far from best.)

Lastly, note that the restriction $0 \leq \sigma \leq 2$ in Theorem 15.1 is not serious, as we can reduce the case of general $s = \sigma + it$ ($s \neq 0, -2, -4, \dots$) to the case $0 \leq \sigma \leq 2$

using integration by parts:

$$\begin{aligned} F_\delta(s) &= \int_0^\infty e(\delta x) e^{-x^2/2} x^{s-1} dx \\ &= -2\pi i \delta \int_0^\infty e(\delta x) e^{-x^2/2} \frac{x^s}{s} dx + \int_0^\infty e(\delta x) e^{-x^2/2} \frac{x^{s+1}}{s} dx \\ &= -\frac{2\pi i \delta}{s} F_\delta(s+1) + \frac{1}{s} F_\delta(s+2), \end{aligned}$$

and so $F_\delta(s+2) = 2\pi i \delta F_\delta(s+1) + s F_\delta(s)$.

15.1.2 Relation to the previous literature

A sketch of a treatment of the Mellin transform of the twisted Gaussian – indeed, of the Mellin transform of the more general function $\exp(-P(x))$, where $P(x)$ is any polynomial – can already be found in [dB81, §6.8–6.9]. The treatment there, like the one here, is based on an application of the saddle-point method. While the initial setup and contours chosen in [dB81, §6.8] are different from the ones here, it ought to be possible to make the approach there explicit as well. Some care should be exercised, however, as [dB81, §6.8] focuses on the case of $|t| \to \infty$, with the coefficients of $P(x)$ held constant. One of the coefficients of our polynomial $P(x)$ is $-2\pi\delta$, and, as we said, we are especially interested in what happens when $|\delta| \ll |t| \ll |\delta|^2$. In fact, faster-than-exponential decay in that range will be crucial in our application later.

Our setup and contours will be more like those in [GST04] and [Tem15, §4.8], which study the parabolic cylinder function $U(a, z)$. As is well known, our Mellin transform $F_\delta(s)$ is closely connected to $U(a, z)$; estimating one is equivalent to estimating the other (see (15.18)). However, [GST04], [Tem15] and several other sources ([TV03], [GST06]) focus on the case of a, z real, whereas we care about a complex and z purely imaginary.

The work of Olver [Olv58], [Olv59], [Olv61], [Olv65] does treat fully general a and z, but it is not explicit. At the same time, the bound in the main theorem [Olv61] does in some sense come close, in that it would only remain to determine the value of the constant k. Starting from the main term there, or from those in [Olv59], one can already see what we have already remarked: if $\operatorname{sgn}(\delta) \neq \operatorname{sgn}(t)$ and $|\delta| \gg 1$, the behavior of F_δ changes when $|t|$ goes past $|\delta|^2$.

We should also comment on applications of the sort we will give, that is, applications to number theory. The Gaussian smoothing $e^{-x^2/2}$ has certainly been used before in number theory; see, notably, Serre's variant (described in [Poi77]) on Odlyzko's work on minorizing discriminants, or Heath-Brown's well-known paper on the fourth power moment of the Riemann zeta function [HB79]. However, we are talking then of non-explicit work; explicit bounds on F_δ were not available.

There has also been work using the Gaussian after a logarithmic change of variables; see, in particular, [Leh66]. In that case, the Mellin transform is simply a Gaussian (as in, e.g., [MV07, Ex. XII.2.9]). However, for δ non-zero, the Mellin transform of a twist $e(\delta x) e^{-(\log x)^2/2}$ decays very slowly, and thus would not be useful to us.

15.2 HOW TO CHOOSE A SMOOTHING FUNCTION?

15.2.1 The method of stationary phase

Let us motivate our choice of smoothing function η. The method of *stationary phase* ([Olv74, §4.11], [Won01, §II.3])) suggests that the main contribution to the integral

$$F_\delta(s) = \int_0^\infty e(\delta x)\eta(x)x^s \frac{dx}{x} \tag{15.6}$$

should come when the phase has derivative 0, as the contribution of parts of the integral where the phase is bounded away from zero can be bounded by repeated integration by parts.

The phase part of (15.6) is

$$e(\delta x)x^{\Im s i} = e^{(2\pi\delta x + t\log x)i}$$

(where we write $s = \sigma + it$); clearly,

$$(2\pi\delta x + t\log x)' = 2\pi\delta + \frac{t}{x} = 0$$

when $x = -t/2\pi\delta$. This equality can hold when $\delta \neq 0$ and $-t/2\pi\delta \geq 0$, i.e., $\mathrm{sgn}(t) \neq \mathrm{sgn}(\delta)$. The contribution of $x = -t/2\pi\delta$ to (15.6) is then

$$\eta(x)e(\delta x)x^{s-1} = \eta\left(\frac{-t}{2\pi\delta}\right) e^{-it} \left(\frac{-t}{2\pi\delta}\right)^{\sigma+it-1} \tag{15.7}$$

multiplied by a "width" approximately equal to a constant divided by

$$\sqrt{|(2\pi i\delta x + t\log x)''|} = \sqrt{|-t/x^2|} = \frac{2\pi|\delta|}{\sqrt{|t|}}.$$

The absolute value of (15.7) is

$$\eta\left(-\frac{t}{2\pi\delta}\right) \cdot \left|\frac{-t}{2\pi\delta}\right|^{\sigma-1}. \tag{15.8}$$

In other words, if $\mathrm{sgn}(t) \neq \mathrm{sgn}(\delta)$ and δ is not too small, asking that $F_\delta(\sigma+it)$ decay rapidly as $|t| \to \infty$ amounts to asking that $\eta(t)$ decay rapidly as $t \to 0$. Thus, if we ask for $F_\delta(\sigma+it)$ to decay rapidly as $|t| \to \infty$ for all moderate δ, we are requesting that

1. $\eta(t)$ decay rapidly as $t \to \infty$,
2. the Mellin transform $F_0(\sigma+it)$ decay rapidly as $t \to \pm\infty$.

Requirement (2) is there because we also need to consider $F_\delta(\sigma+it)$ for δ very small, and, in particular, for $\delta = 0$.

Some readers will recognize the uncertainty principle at work here: one cannot do arbitrarily well in both aspects at the same time. Let us actually derive a precise statement for the uncertainty principle for the Mellin transform in a form fit for our purposes.

15.2.2 An uncertainty principle for the Fourier and Mellin transforms

In its simplest form, the uncertainty principle states that a function and its Fourier transform cannot both have compact support. More generally, the uncertainty principle, or an uncertainty principle, is an inequality showing that a function and its Fourier transform cannot both decay very rapidly.[1]

Let us derive a one-sided uncertainty principle, i.e., a statement that describes how $\widehat{f}$ must behave if $f(x)$ decays rapidly as $x \to \infty$, making no assumptions about $f(x)$ for $x \to -\infty$. One-sided uncertainty principles can already be found in [Naz93] and, later, in [BD06], which refers to [Naz93]; our proof goes along the same lines. (The basic idea of using the Phragmén-Lindelöf principle to prove an uncertainty principle goes back to Hardy [Har33].)

Proposition 15.2. *Let $f : \mathbb{R} \to \mathbb{C}$ be in L^1. Let $r_1 > r_0 > 0$ be such that*

$$|f(x)| \ll e^{-e^{r_1 x}} \qquad \text{as } x \to \infty,$$
$$|\widehat{f}(t)| \ll e^{-\frac{\pi^2}{r_0}|t|} \qquad \text{for all } t \in \mathbb{R}.$$

Then $f(x) = 0$ almost everywhere.

Proof. As in [BD06], we will use the *Bargmann transform* of f, defined to be

$$\mathscr{B}f(z) = e^{\frac{\pi}{2}z^2}\langle f(x), e^{-\pi(x-z)^2}\rangle = e^{\frac{\pi}{2}z^2}\int_{-\infty}^{\infty}\overline{f(x)}e^{-\pi(x-z)^2}dx. \tag{15.9}$$

Since the Fourier transform is an isometry,

$$\mathscr{B}f(z) = e^{\frac{\pi}{2}z^2}\langle \widehat{f}(t), \widehat{e^{-\pi(t-z)^2}}\rangle = e^{-\frac{\pi}{2}z^2}\langle \widehat{f}(t), e^{-\pi(t+iz)^2}\rangle, \tag{15.10}$$

where we use (2.18) in the last equality.

Thus, we have two expressions for $\mathscr{B}f$, one in terms of f and one in terms of $\widehat{f}$. Our assumptions on the decay of f and $\widehat{f}$ will give us two different bounds for $\mathscr{B}f$, useful along different lines on the complex plane. The Phragmén-Lindelöf principle for sectors (Lemma 2.13) will allow us to interpolate between these lines.

Let $r \in (r_0, r_1)$; say $r = (r_0 + r_1)/2$, for concreteness. Define

$$F(z) = e^{-\frac{2\pi z\log z}{r} + \frac{\pi}{2}z^2}\mathscr{B}f(z) \tag{15.11}$$

using the principal branch of the logarithm (i.e., $\log z$ is defined except for z a negative real number).

[1] There are some applications to physics.

First of all, $F(z)$ is bounded on the imaginary line: for $z = i\tau$, $\tau > 0$,

$$\begin{aligned}|F(z)| &= \left|e^{-\frac{2\pi i\tau \log i\tau}{r}} \langle \hat{f}(t), e^{-\pi(t-\tau)^2}\rangle\right| \leq e^{\frac{\pi^2\tau}{r}} \int_{-\infty}^{\infty} |\widehat{f}(t)| e^{-\pi(t-\tau)^2} dt \\ &\ll e^{\frac{\pi^2\tau}{r}} \int_{-\infty}^{\infty} e^{-\frac{\pi^2 t}{r_0} - \pi(t-\tau)^2} dt = e^{\frac{\pi^2\tau}{r}} \int_{-\infty}^{\infty} e^{-\pi\left(t-\tau+\frac{\pi}{2r_0}\right)^2} e^{-\frac{\pi^2\tau}{r_0} + \frac{\pi^3}{(2r_0)^2}} dt \\ &= e^{\frac{\pi^3}{(2r_0)^2}} e^{-\pi^2\left(\frac{1}{r_0}-\frac{1}{r}\right)\tau} \ll e^{-\pi^2\left(\frac{1}{r_0}-\frac{1}{r}\right)\tau}.\end{aligned}$$

and similarly for $\tau < 0$. Thus,

$$F(i\tau) \ll e^{-\pi^2\left(\frac{1}{r_0}-\frac{1}{r}\right)|\tau|} \tag{15.12}$$

for all τ real. (It is clear that $F(z)$ is continuous at 0.)

Let us bound $F(z)$ on the half-line $z = v\tau$, $\tau > 0$, where $v = e^{\epsilon i}$, $\epsilon > 0$ small. By (15.9),

$$F(z) = e^{-\frac{2\pi v\tau(\log\tau + i\epsilon)}{r} + \pi v^2\tau^2} \int_{-\infty}^{\infty} \overline{f(x)} e^{-\pi(x-v\tau)^2} dx.$$

Now $\Re((x-v\tau)^2) = x^2 - 2x\tau\Re v + \Re((v\tau)^2)$, and, for $\tau \geq e$,

$$\Re(v\tau(\log\tau + i\epsilon)) = (\log\tau \cdot \Re v - \epsilon \cdot \Im v)\tau \geq \left(1 - \frac{3}{2}\epsilon^2\right) \tau \log \tau,$$

since $\Re v \geq 1 - \epsilon^2/2$ and $\Im v \leq \epsilon$. Write v_0 for $\Re v$. It is easy to see that

$$\begin{aligned}\Re\left(e^{\pi v^2\tau^2} \int_{-\infty}^{\infty} |f(x)| e^{-\pi(x-v\tau)^2} dx\right) &= \int_{-\infty}^{\infty} |f(x)| e^{-\pi(x^2 - 2x\tau\Re v)} dx \\ &= |f|_1 + \int_0^{\infty} |f(x)| e^{-\pi(x^2-2x\tau\Re v)} dx \\ &\ll 1 + \int_0^{\infty} e^{-e^{r_1 x} - \pi(x^2 - 2x\tau v_0)} dx.\end{aligned}$$

Taking derivatives, we see that $g(x) = e^{r_1 x} + \pi(x^2 - 2x\tau v_0)$ has its minimum for $x \geq 0$ either at $x = 0$ (and then that minimum is 1) or at $x = x_0$, where $r_1 e^{r_1 x_0} = 2\pi(\tau v_0 - x_0)$. Clearly $x_0 \leq \min((\log(2\pi\tau v_0/r_1))/r_1, \tau v_0)$, and so

$$\begin{aligned}g(x_0) &= \frac{2\pi(\tau v_0 - x_0)}{r_1} + \pi(x_0^2 - 2x_0\tau v_0) \\ &\geq -2\pi\tau v_0 x_0 \geq -\frac{2\pi}{r_1}\tau v_0 \log\frac{2\pi\tau v_0}{r_1}.\end{aligned}$$

At the same time,

$$g''(x) = r_1^2 e^{r_1 x} + 2\pi \geq 2\pi \tag{15.13}$$

for all x. Now, since $g'(x_0) = 0$ and $g''(x) \geq 2\pi$ for all x, we have $g(x) \geq g(x_0) + \frac{1}{2}c(x-x_0)^2$ for all x (Taylor expansion). Thus

$$\int_0^{\infty} e^{-e^{r_1 x} - \pi(x^2 - 2x\tau v_0)} dx \leq e^{\frac{2\pi}{r_1}\tau v_0 \log\frac{2\pi\tau v_0}{r_1}} \int_{-\infty}^{\infty} e^{-\pi u^2} du = e^{\frac{2\pi}{r_1}\tau v_0 \log\frac{2\pi\tau v_0}{r_1}}.$$

Hence, for $z = v\tau$, $v = e^{\epsilon i}$,

$$|F(z)| \ll e^{-(1-3\epsilon^2/2)\frac{2\pi}{r}\tau\log\tau + \frac{2\pi}{r_1}\tau v_0 \log\frac{2\pi\tau v_0}{r_1}}. \tag{15.14}$$

Since $r < r_1$, we can set ϵ small enough for $(1-3\epsilon^2/2)/r$ to be larger than $1/r_1$. Then (15.14) gives us that $|F(z)|$ is bounded for $z = v\tau$, $\tau \geq 0$. By symmetry, the same is true for $z = \overline{v}\tau$, $\tau \geq 0$.

(We have not forgotten the case when $g(x)$ has its minimum at $x = 0$. In that case, by $g'(x) \geq 0$ and again by (15.13), $g(x) \geq 1 + \pi x^2$ for all x, and so $\int_0^\infty e^{-g(x)}dx$ is bounded. It follows immediately that $|F(z)|$ is bounded for $z = v\tau, \geq 0$, and thus for $z = \overline{v}\tau$, $\tau \geq 0$, as well.)

Thus, we have that $|F(z)|$ is bounded on four half-lines: $z = i\tau$, $z = v\tau$, $z = \overline{v}\tau$ and $z = -i\tau$, with $\tau > 0$ in each case. By (15.9) and (15.11), $F(z)$ equals a function bounded by $e^{O(|z|^2)}$ times the integral

$$\int_{-\infty}^{\infty} \overline{f(x)} e^{-\pi(x-z)^2} dx.$$

For $x > \Re z + |\Im z|$ or $x < \Re z - |\Im z|$, the exponent $-\pi(x-z)^2$ has negative real part, and so the contribution of such x is bounded by $|f|_1$. For all other x, it is clear that $|x - z|^2 \leq 2|z|^2$, and so their contribution is bounded by $|f|_1 e^{2\pi|z|^2}$. Thus, $|F(z)|$ is bounded by $e^{O(|z|^2)}$. This means that we can apply Phragmén-Lindelöf (Lemma 2.13) to each of the three sectors defined by our four half-lines, since each of these sectors has angle $< \pi/2$. We conclude that $F(z)$ is bounded on the right half-plane $\{z \in \mathbb{C} : \Re z \geq 0\}$.

We will now finish as in [Naz93, §2.3]. Let ϕ be the map $z \mapsto (1+z)/(1-z)$, which takes the unit circle to the imaginary line and the unit disc to the right half-plane. Then $F \circ \phi$ is a bounded holomorphic function on the unit disc S^1. By Jensen's formula (2.35),

$$\frac{1}{r}\int_{rS^1} \log|(F\circ\phi)(z)||dz| \leq \int_{S^1} \log|(F\circ\phi)(z)||dz| \tag{15.15}$$

for every $r \in (0,1)$, where rS^1 is the circle around the origin with radius r.

Assume F is not identically zero on the right half-plane. Then the zeros of F do not have an accumulation point in $\{z \in \mathbb{C} : \Re z > 0\}$. We can thus choose r so that $F \circ \phi$ does not have a zero at distance r from the origin. Then the left side of (15.15) is $> -\infty$, and hence so is the right side. At the same time,

$$\begin{aligned}\int_{S^1} \log|(F\circ\phi)(z)||dz| &= \int_{-i\infty}^{i\infty} \log|F(z)||(\phi^{-1})'(z))||dz| \\ &= \int_{-\infty}^{\infty} \log|F(i\tau)|\frac{2}{1+\tau^2}d\tau,\end{aligned}$$

since $\phi^{-1}(z) = 1 - 2/(z+1)$. By (15.12), $\log|F(i\tau)| \leq -c|\tau| + O(1)$, where $c = \pi^2(1/r_0 - 1/r) > 0$. Hence

$$\int_{-\infty}^{\infty} \log|F(i\tau)|\frac{2}{1+\tau^2}d\tau \leq -2c\int_{-\infty}^{\infty}\frac{|\tau|}{1+\tau^2}d\tau + O(1) = -\infty.$$

Contradiction. Hence F is identically zero on the right half-plane.

By (15.9) and (15.11), $F(i\tau) = e^{\pi^2\tau/r}\widehat{\psi}(-\tau)$, where $\psi(x) = f(x)e^{-\pi x^2}$. Thus, $\widehat{\psi}$ is identically zero. Hence, ψ is zero almost everywhere, and so is f. □

The relation between the Mellin transform and the Fourier transform gives us a one-sided uncertainty principle for the Mellin transform, which is what we actually want.

Proposition 15.3. *Let $\sigma \in \mathbb{R}$, $\phi : (0,\infty) \to \mathbb{C}$ be such that $\phi(x)x^{\sigma-1}$ is in L^1. Let $r, c > 0$ be such that*

$$\begin{aligned} \phi(x) &\ll e^{-x^r} && \text{as } x \to \infty, \\ |M\phi(\sigma + it)| &\ll e^{-c|t|} && \text{for all } t \in \mathbb{R}. \end{aligned} \tag{15.16}$$

If $c > \pi/2r$, then $\phi(x) = 0$ for almost all $x \in \mathbb{R}$.

Proof. Assume $c > \pi/2r$. Let $r_0 = \pi/2c$, $r_1 = (r_0 + r)/2$. Since $\phi(x) \ll e^{-x^r}$ and $r_1 < r$, we clearly have $\phi(x) \ll x^{-\sigma}e^{-x^{r_1}}$ as $x \to \infty$. Thus, for $f(v) = \phi(e^v)e^{v\sigma}$, we see that $f(v) \ll e^{-e^{r_1 v}}$ as $v \to \infty$.

By (2.25) and (15.16),

$$\widehat{f}(t) = M\phi(\sigma - 2\pi it) \ll e^{-2\pi c|t|} = e^{-\frac{\pi^2}{r_0}|t|}.$$

Since $r_0 < r_1$, we apply Prop. 15.2 and obtain that $f(x) = 0$ almost everywhere; hence, $\phi(x) = 0$ almost everywhere. □

Proposition 15.3 is essentially tight: if $\phi(x) = e^{-x^r}$, then, by (3.34), $M\phi(s) = \Gamma(s/r)/r$, and $\Gamma(\sigma + it)$ decays much like $e^{-\pi|t|/2}$ (see (3.44)).

15.2.3 Conclusions. Choice of smoothing function

The precise form of the uncertainty principle relevant here is that given by Proposition 15.3. Once we take it into account, the weight $\eta(x) = e^{-x}$ in Hardy-Littlewood actually looks fairly good: its Mellin transform $\Gamma(\sigma + it)$ decays about as rapidly as it could when $t \to \pm\infty$, namely, roughly as $e^{-\pi|t|/2}$ (see (3.44)). Moreover, for this choice of η, the Mellin transform $F_\delta(s)$ of $\eta(x)e(\delta x)$ can be written explicitly: $F_\delta(s) = \Gamma(s)/(1 - 2\pi i\delta)^s$.

It is not hard to work out an explicit formula[2] (as in Ch. 16) for $\eta(t) = e^{-t}$. However, it is not hard to see that, for $F_\delta(s)$ as above, $F_\delta(1/2 + it)$ decays roughly like $e^{-|t|/2\pi|\delta|}$, just as we expected from (15.8). This is a little too slow for our purposes: we will often have to work with relatively large δ, and we would like to have to check

[2]There may be a minor gap in the literature in this respect. The explicit formula given in [HL22a, Lemma 4] does not make all constants explicit. The constants and trivial-zero terms were fully worked out for $q = 1$ by [Wig20] (cited in [MV07, Exercise 12.1.1.8(c)]; the sign of $\mathrm{hyp}_{\kappa,q}(z)$ there seems to be off). As was pointed out by Landau (see [Har66, p. 628]), [HL22a] seems to neglect the effect of the zeros ρ with $\Re\rho = 0$, $\Im\rho \neq 0$ for χ imprimitive. (The author thanks R. C. Vaughan for this information.)

the zeros of L functions only up to relatively low heights t – say, up to $50|\delta|$. Then $e^{-|t|/2\pi|\delta|} > e^{-8} = 0.00033\ldots$, which is not very small.

We should thus choose a function η that decays considerably faster than an exponential. We still want its Mellin transform to decrease exponentially. Proposition 15.3 tells us that, for the Mellin transform to decrease exponentially, $\eta(x)$ should not decrease faster than e^{-x^r} for some r; moreover, the rate of exponential decay of the Mellin transform will be inversely proportional to r.

We settle for $r = 2$; in other words, we let η be the Gaussian. The decay of the Gaussian smoothing function $\eta(x) = e^{-x^2/2}$ is much faster than exponential. Its Mellin transform is $\Gamma(s/2)$, which decays exponentially as $t = \Im s \to \pm\infty$. (Indeed, it decays as $e^{-\pi|t|/4}$, which, by Prop. 15.3, is optimal given the rate of decay of η.) Moreover, the Mellin transform $F_\delta(s)$ ($\delta \neq 0$), while not an elementary or very commonly occurring function, equals (after a change of variables) a relatively well-studied special function, namely, a parabolic cylinder function $U(a, z)$ (see §4.2.3). This fact is really a decisive factor in our choice of $r = 2$; a back-of-the-envelope calculation should convince the reader that, given Platt's inputs on the zeros of L-functions, a value of r between 3 and 4 would have been optimal.

For $\eta(t) = e^{-x^2/2}$ and δ not too small, the main term of $F_\delta(s)$ will indeed work out to be proportional to $e^{-(t/2\pi\delta)^2/2}$, as the method of stationary phase indicated. Thus, $F_\delta(s)$ will decay much more rapidly than if we had chosen to work with $\eta(x) = e^{-x}$. The "cost" is that the Mellin transform $\Gamma(s/2)$ for $\delta = 0$ now decays like $e^{-\pi|t|/4}$ rather than $e^{-\pi|t|/2}$. This is a cost we can certainly afford.

15.3 THE TWISTED GAUSSIAN: OVERVIEW AND SETUP

We wish to approximate the Mellin transform of a twisted Gaussian $e^{-x^2/2}e(\delta x)$:

$$F_\delta(s) = \int_0^\infty e^{-x^2/2} e(\delta x) x^s \frac{dx}{x}, \tag{15.17}$$

where $\delta \in \mathbb{R}$. It will be immediate from a standard expression (15.21) for the parabolic cylinder function $U(a, z)$ that

$$F_\delta(s) = e^{(\pi i\delta)^2} \Gamma(s) U\left(s - \frac{1}{2}, -2\pi i\delta\right). \tag{15.18}$$

The second argument of U here is purely imaginary. That would not be the case if a Gaussian of non-zero mean were chosen.

15.3.1 Parabolic cylinder functions

As was mentioned in §4.2.3, a parabolic cylinder function is an entire function f such that

$$f'' - \left(\frac{1}{4}z^2 + a\right) f = 0, \tag{15.19}$$

where $a \in \mathbb{C}$ is fixed. It is clear that the space of such functions is at most two-dimensional; as we shall see, it is actually two-dimensional.

Equation (15.19) was first considered by Weber in 1869 [Web69]. Integral representations like the ones we are about to see go back to Whittaker [Whi03].

Lemma 15.4 ([AS64, (19.5.4)], [OLBC10, (12.5.6)]). *Let $a \in \mathbb{C}$. For $c > 0$, the function $z \mapsto U(a, z)$ given by*

$$U(a,z) = \frac{e^{\frac{1}{4}z^2}}{\sqrt{2\pi}i} \int_{c-i\infty}^{c+i\infty} e^{-zu+\frac{u^2}{2}} u^{-a-\frac{1}{2}} du \tag{15.20}$$

satisfies equation (15.19), as does $z \mapsto U(-a, iz)$.

For a fixed and real $z \to +\infty$, $U(a, z) \to 0$ and $|U(-a, +iz)| \to \infty$. Together, $z \mapsto U(a, z)$ and $z \mapsto U(-a, iz)$ span the space of analytic solutions to (15.19).

Since the integrand is holomorphic in u for $\Re u > 0$, the choice of $c > 0$ does not affect the value of the integral.

Proof. Differentiating twice with respect to z, we obtain

$$U'(a,z) = \frac{1}{2} z U(a,z) - U(a-1,z),$$

$$U''(a,z) = \left(\frac{1}{2} + \frac{1}{4}z^2\right) U(a,z) - zU(a-1,z) + U(a-2,z).$$

At the same time, by integration by parts,

$$\int_{c-i\infty}^{c+i\infty} e^{-zu+\frac{u^2}{2}} u^{-a-\frac{1}{2}} du = -\int_{c-i\infty}^{c+i\infty} (u-z) e^{-zu+\frac{u^2}{2}} \frac{u^{-a-\frac{1}{2}}}{-a+\frac{1}{2}} du$$

and so

$$\left(a - \frac{1}{2}\right) U(a,z) = -zU(a-1,z) + U(a-2,z).$$

Hence

$$U''(a,z) = \left(\frac{1}{4}z^2 + a\right) U(a,z),$$

that is, equation (15.19) holds. It is then easy to show that it must also hold for $U(-a, iz)$.

For z with $\Re z \geq 0$, we may shift the contour of integration in (15.20) by $+z$, and obtain

$$\begin{aligned} U(a,z) &= \frac{e^{\frac{1}{4}z^2}}{\sqrt{2\pi}i} \int_{c+z-i\infty}^{c+z+i\infty} e^{-zu+\frac{u^2}{2}} u^{-a-\frac{1}{2}} du \\ &= \frac{e^{-\frac{1}{4}z^2}}{\sqrt{2\pi}i} \int_{c+z-i\infty}^{c+z+i\infty} e^{\frac{(u-z)^2}{2}} u^{-a-\frac{1}{2}} du = \frac{e^{-\frac{1}{4}z^2}}{\sqrt{2\pi}i} \int_{c-i\infty}^{c+i\infty} e^{\frac{u^2}{2}} (u+z)^{-a-\frac{1}{2}} du. \end{aligned}$$

It is thus clear that $U(a,z) \to 0$ for real $z \to +\infty$. For $z = it$ and real $t \to +\infty$, note that $e^{-z^2/4} = e^{t^2/4}$, and that, after a change of variables $u \leftarrow u + z$, we may shift the integral to a contour C consisting of the y axis, except for the segment from $-i$ to i, which gets replaced by the right half of the unit circle. We get:

$$U(-a,it) = \frac{e^{\frac{t^2}{4}}}{\sqrt{2\pi i}} \int_C e^{\frac{(u-it)^2}{2}} u^{a-\frac{1}{2}} du.$$

Then it is clear that, as $t \to \infty$, the contribution of u close to t dominates and exhibits little cancellation. Thus $|U(-a,it)| \to \infty$.

Since $U(a,z)$ and $U(-a,iz)$ display different behavior as $z \to \infty$, they must be linearly independent, and so span the space of solutions to (15.19). □

Lemma 15.5 ([AS64, (19.5.1)], [OLBC10, §12.5]). *For $\Re a > -1/2$,*

$$U(a,z) = \frac{e^{-z^2/4}}{\Gamma\left(\frac{1}{2}+a\right)} \int_0^\infty t^{a-\frac{1}{2}} e^{-\frac{1}{2}t^2 - zt} dt. \tag{15.21}$$

Proof. Write $f_a(z)$ for the function on the right side of (15.21). Differentiating twice with respect to z, we get

$$f_a''(z) = \left(-\frac{1}{2} + \frac{z^2}{4}\right) f_a(z) + \left(a + \frac{1}{2}\right) z f_{a+1}(z) + \left(a+\frac{1}{2}\right)\left(a+\frac{3}{2}\right) f_{a+2}(z).$$

By integration by parts,

$$f_a(z) = z f_{a+1}(z) + \left(a + \frac{3}{2}\right) f_{a+2}(z).$$

Hence

$$f_a''(z) = \left(\frac{1}{4}z^2 + a\right) f_a(z),$$

that is, equation (15.19) holds.

It is easy to see from (15.21) that $f_a(z) \to 0$ for real $z \to +\infty$. Hence, by Lemma 15.4, for any given a, $f_a(z)$ is a multiple of $U(a,z)$. It remains to see which multiple. Let us compare $f_a(0)$ and $U(a,0)$.

By substitution of variables and the definition (3.34) of $\Gamma(s)$,

$$\int_0^\infty t^{a-\frac{1}{2}} e^{-\frac{1}{2}t^2} dt = 2^{\frac{a}{2}-\frac{3}{4}} \int_0^\infty x^{\frac{a}{2}-\frac{3}{4}} e^{-x} dx = 2^{\frac{a}{2}-\frac{3}{4}} \Gamma\left(\frac{a}{2} + \frac{1}{4}\right),$$

and so, by Legendre's duplication formula (3.39),

$$f_a(0) = 2^{\frac{a}{2}-\frac{3}{4}} \frac{\Gamma\left(\frac{a}{2}+\frac{1}{4}\right)}{\Gamma\left(a+\frac{1}{2}\right)} = \sqrt{\pi} \frac{2^{-\frac{a}{2}-\frac{1}{4}}}{\Gamma\left(\frac{a}{2}+\frac{3}{4}\right)}.$$

On the other hand, again by substitution of variables,

$$U(a,0) = \frac{1}{\sqrt{2\pi i}} \int_{c-i\infty}^{c+i\infty} e^{\frac{u^2}{2}} u^{-a-\frac{1}{2}} du = \sqrt{\pi} 2^{-\frac{a}{2}-\frac{1}{4}} \cdot \frac{1}{\sqrt{2\pi i}} \int_{C'} e^z z^{-a/2-3/4} dz,$$

where C' is the image of the line from $c-i\infty$ to $c+i\infty$ under the map $u \mapsto u^2/2$. The contour C' can be shifted to a Hankel contour, as in Lemma 3.8, and so, by the same Lemma,

$$U(a,0) = \sqrt{\pi} \frac{2^{-\frac{a}{2}-\frac{1}{4}}}{\Gamma\left(\frac{a}{2}+\frac{3}{4}\right)} = f_a(0).$$

We conclude that $U(a,z) = f_a(z)$ for all z. □

Remark. The moral here is a familiar one: in a function space with few dimensions, one can hope for striking identities, since they are in some sense forced to exist. Parabolic cylinder functions satisfy a differential equation (15.19) whose dimension we know to be ≤ 2; as is well known and as we have just shown, that bound on the dimension implies that the functions on the right sides of (15.20) and (15.21) are one and the same.

Thus we see one justification of our choice to work with $\exp(x^2/2)$ instead of $\exp(cx^r)$ for some higher power $r > 2$: for higher r, our Mellin transform would lie in a space of higher dimension, in which useful identities would be harder to come by.

15.3.2 Estimates and behavior

The function $U(a,z)$ has been well-studied for a and z real; see, e.g., [Tem10], [Tem15, Ch. 11 and Ch. 30]. Less attention has been paid to the more general case of a and z complex. The most notable exception is by far the work of Olver [Olv58], [Olv59], [Olv61], [Olv65]; he gave asymptotic series for $U(a,z)$, $a, z \in \mathbb{C}$. These were asymptotic series in the sense of Poincaré, and thus not in general convergent. They would likely solve our problem if only they came with error term bounds.

It would seem that all fully explicit error bounds in the literature are either for a and z real, or for a and z outside our range of interest (see both Olver's work and [TV03]). The bounds in [Olv61] involve non-explicit constants. Thus, we will have to find expressions with explicit error bounds ourselves. We will treat the case of z purely imaginary, since it is the one required by our applications. By a standard relation [AS64, §19.4.6], we could reduce the case of z purely imaginary to that of z real; however, we would still need to consider a complex.

To be precise: we need to estimate $U(a,z)$ for $-1/2 \leq \Re a \leq 3/2$ and $|\Im a|$ larger than a constant times $\max(1, |\Im z|)$. By (15.18), these conditions correspond to requiring that $0 \leq \Re s \leq 2$ be within the critical strip, with $|\Im s|$ larger than a constant times $\max(1, |\delta|)$.

We will use the *saddle-point method* (see, e.g., [dB81, §5], [Olv74, §4.7], [Won01, §II.4]) to obtain bounds with an optimal leading-order term and small error terms. (We used the stationary-phase method solely as an exploratory tool.)

What do we expect to obtain? Both the asymptotic expressions in [Olv59] and the bounds in [Olv61] make clear that, if the sign of $t = \Im s$ is different from that of δ, there will be a change in behavior when t gets to be of size about $(2\pi\delta)^2$. This phenomenon is unsurprising, given our discussion using stationary phase: for $|\Im a|$ smaller than a constant times $|\Im z|^2$, the term proportional to $e^{-\pi|t|/4}$ should be dominant, whereas for $|\Im a|$ much larger than a constant times $|\Im z|^2$, the term proportional to $e^{-\frac{1}{2}\left(\frac{t}{2\pi\delta}\right)^2}$ should be dominant.

There is one important difference between the approach we will follow here and that in [Hela]. In [Hela], the integral in (15.17) was estimated by a direct application of the saddle-point method. In the first draft of this book, following a suggestion of N. Temme, and just as in [GST04] or [Tem15, §4.8], identity (15.20) was used instead. Together, (15.18) and (15.20) give us that

$$F_\delta(s) = \frac{e^{-2\pi^2\delta^2}\Gamma(s)}{\sqrt{2\pi i}} \int_{c-i\infty}^{c+i\infty} e^{2\pi i\delta u + \frac{u^2}{2}} u^{-s} du. \tag{15.22}$$

We can use the saddle-point method to estimate the integral in (15.22).

What we will actually do is use the saddle-point method to estimate (15.17) when $\mathrm{sgn}(t) = \mathrm{sgn}(\delta)$ and to estimate (15.22) when $\mathrm{sgn}(t) \neq \mathrm{sgn}(\delta)$. Much of the work – in particular, the computation of the saddle point – will need to be done only once, as it is the same in both cases.

We write

$$\phi(u) = -\frac{u^2}{2} - (2\pi i\delta)u + it\log u \tag{15.23}$$

for u real or complex, so that the integral in (15.22) equals

$$I(s) = \int_{c-i\infty}^{c+i\infty} e^{-\phi(u)} u^{-\sigma} du. \tag{15.24}$$

15.4 THE SADDLE POINT

15.4.1 The saddle-point method

Say we are mountaineers trying to choose a path between two points separated by a mountain chain. A natural approach is to find the lowest possible mountain pass, and take our path to go through it. A mountain pass will be a point that is a local minimum in relation to the mountain range, and a local maximum in relation to our path. The path should be chosen to be perpendicular to the mountain range, so as to cross it rapidly. In other words, a mountain pass looks like a saddle. Assuming differentiable mountains, we see that the gradient of the height must be 0 at the mountain pass. It then suffices to find the points of gradient 0, and see which ones would be valid mountain passes, and which one of them is best in practice.

The idea of the *saddle-point method*, or *method of steepest descent*, is the same. We wish to bound an integral of the form

$$\int_{P_1}^{P_2} f(z)e^{g(z)}dz,$$

where f and g are holomorphic, and P_1, P_2 lie on the complex plane (or possibly at infinity). Due to the exponential, the dominant term is $e^{g(z)}$, and points s where $|g(z)|$ is large contribute much more than those where $|g(z)|$ is not so large. Hence, what we should do is choose a path of integration between P_1 and P_2 so that the largest value of $|g(z)|$ on it is as small as possible. Here $|g(z)|$ corresponds to the height above sea level in the metaphor above. For the gradient of $|g(z)|$ to be 0 at s, it is necessary and sufficient that the complex derivative $g'(z)$ of g at s be 0. Thus, we should find the zeros of $g'(z)$ and choose the one that is the best mountain pass, or *saddle point*.

As we already said, ideally, we ought to go through the saddle point in the direction of *steepest descent*, that is, the direction in which the ascent to and descent from the saddle point s is fastest. Since $g(z) = g(s) + g''(s)(z-s)^2/2 + \dots$, we see that

$$|e^{g(z)}| = |e^{g(s)}||e^{g''(s)(z-s)^2}|\dots = |e^{g(s)}|e^{\Re g''(s)(z-s)^2}\dots$$

Thus, if $w \in \mathbb{C}$ is a unit vector pointing in the direction of steepest descent, $g''(s)w^2$ should be real and negative.

Of course, even after finding the saddle point and the direction of steepest descent, we still have to choose the rest of the path of integration. In order for descent and ascent to be as fast as possible, the path at any point $z \neq s$ should be tangent to the gradient of $\left|e^{g(z)}\right| = e^{\Re g(z)}$ at z. In other words, the path of integration ought to be such that $\Im g(z)$ is constant.

In practice, there are other considerations that can affect our choice of path, including of course the fact that it has to go through P_1 and P_2. What is truly important is that it go through the saddle point. That it go through it in the direction of steepest descent is also highly desirable, as otherwise the constant in front of the main term will not be optimal.[3]

15.4.2 Finding the saddle point

We wish to find a saddle point for the integral in (15.24), that is, a point u at which $\phi'(u) = 0$. Clearly, $\phi'(u) = 0$ if and only if

$$-u - 2\pi i\delta + \frac{it}{u} = 0, \qquad \text{i.e.,} \qquad u^2 - i\ell u - it = 0, \tag{15.25}$$

where $\ell = -2\pi\delta$. The solutions to $\phi'(u) = 0$ are thus

$$u_0 = \frac{i\ell \pm \sqrt{-\ell^2 + 4it}}{2}. \tag{15.26}$$

[3] Some reserve the name "method of steepest descent" for cases in which the direction of steepest descent is chosen, and use "saddle-point method" when that is not necessarily the case. See [Olv70, §1].

The value of $\phi(u)$ at u_0 is

$$\begin{aligned}\phi(u_0) &= -\frac{i\ell u_0 + it}{2} + i\ell u_0 + it\log u_0 \\ &= \frac{i\ell}{2}u_0 + it\log\frac{u_0}{\sqrt{e}}.\end{aligned} \tag{15.27}$$

The second derivative at u_0 is

$$\phi''(u_0) = -\frac{1}{u_0^2}\left(u_0^2 + it\right) = -\frac{1}{u_0^2}(i\ell u_0 + 2it). \tag{15.28}$$

Assign the names $u_{0,+}$, $u_{0,-}$ to the roots in (15.26) according to the sign in front of the square root, where the square root is defined so as to have its argument in the interval $(-\pi/2, \pi/2]$. It is easy to see that $u_{0,+}$ lies on the right half of the plane, whereas $u_{0,-}$ lies on the left half of the plane. We will work with $u_{0,+}$, as it will be feasible to deform our contour of integration (originally going from $c - i\infty$ to $c + i\infty$) so as to go through $u_{0,+}$. We remark that

$$u_{0,+} = \frac{i\ell + |\ell|\sqrt{-1 + \frac{4it}{\ell^2}}}{2} = \frac{\ell}{2}\left(i \pm \sqrt{-1 + \frac{4t}{\ell^2}i}\right) \tag{15.29}$$

where the sign $\pm$ is $+$ if $\ell > 0$ and $-$ if $\ell < 0$. If $\ell = 0$, then $u_{0,+} = (1/\sqrt{2} + i/\sqrt{2})\sqrt{t}$.

We can assume without loss of generality that $t \geq 0$. We will find it convenient to assume $t > 0$, since we can deal with $t = 0$ simply by letting $t \to 0^+$.

15.4.3 The coordinates of the saddle point

We should determine $u_{0,+}$ explicitly, both in rectangular and polar coordinates. Part of the reason why we will need both kinds of coordinates is that we will need to estimate the integrand in (15.24) for $u = u_{0,+}$. The absolute value of the integrand is $\left|e^{-\phi(u_{0,+})}u_{0,+}^{-\sigma}\right| = |u_{0,+}|^{-\sigma}e^{-\Re\phi(u_{0,+})}$, and, by (15.27),

$$\Re\phi(u_{0,+}) = -\frac{\ell}{2}\Im u_{0,+} - \arg(u_{0,+})t. \tag{15.30}$$

If $\ell = 0$, we already know that $\Re u_{0,+} = \Im u_{0,+} = \sqrt{t/2}$, $|u_{0,+}| = \sqrt{t}$ and $\arg u_{0,+} = \pi/4$. Assume, then, that $\ell \neq 0$.

Lemma 15.6. *Let $t, \ell \in \mathbb{R}$, $t > 0$, $\ell \neq 0$. Let $u_{0,+} \in \mathbb{C}$ be as in (15.29). Then*

$$\Re u_{0,+} = \frac{|\ell|}{2}\sqrt{\frac{j(\mathscr{r}) - 1}{2}}, \qquad \Im u_{0,+} = \frac{\ell}{2} + \frac{|\ell|}{2}\sqrt{\frac{j(\mathscr{r}) + 1}{2}}, \tag{15.31}$$

where $j(\mathscr{r}) = (1 + \mathscr{r}^2)^{1/2}$ and $\mathscr{r} = 4t/\ell^2$. Furthermore,

$$|u_{0,+}| = \frac{|\ell|}{\sqrt{2}} \cdot \begin{cases}\sqrt{\upsilon(\mathscr{r})^2 + \upsilon(\mathscr{r})} & \text{if } \ell > 0, \\ \sqrt{\upsilon(\mathscr{r})^2 - \upsilon(\mathscr{r})} & \text{if } \ell < 0,\end{cases} \tag{15.32}$$

$$\arg(u_{0,+}) = \begin{cases} \frac{1}{2}\arccos\frac{-1}{\upsilon(r)} & \text{if } \ell > 0, \\ \frac{1}{2}\arccos\frac{1}{\upsilon(r)} & \text{if } \ell < 0, \end{cases} \tag{15.33}$$

where $\upsilon(r) = \sqrt{(1+j(r))/2}$.

In particular, $\arg(u_{0,+})$ lies in $[0, \pi/2]$, and is close to $\pi/2$ only when $\ell > 0$ and $r \to 0^+$. Notice that $\Re u_{0,+}$ and $\Im u_{0,+}$ are always positive, except for $t = \ell = 0$, in which case $\Re u_{0,+} = \Im u_{0,+} = 0$.

Here and elsewhere, we follow the convention that the images of arcsin and arctan lie in $[-\pi/2, \pi/2]$, whereas the image of arccos lies in $[0, \pi]$.

Proof. Solving a quadratic equation, we see that

$$\sqrt{-1 + \frac{4t}{\ell^2} i} = \sqrt{\frac{j(r)-1}{2}} + i\sqrt{\frac{j(r)+1}{2}}, \tag{15.34}$$

where $j(r) = (1 + r^2)^{1/2}$ and $r = 4t/\ell^2$. Hence

$$\Re u_{0,+} = \pm\frac{\ell}{2}\sqrt{\frac{j(r)-1}{2}}, \qquad \Im u_{0,+} = \frac{\ell}{2}\left(1 \pm \sqrt{\frac{j(r)+1}{2}}\right). \tag{15.35}$$

Here and in what follows, the sign $\pm$ is $+$ if $\ell > 0$ and $-$ if $\ell < 0$. By (15.31),

$$\begin{aligned} |u_{0,+}| &= \frac{|\ell|}{2} \cdot \left|\sqrt{\frac{j(r)-1}{2}} + \left(1 \pm \sqrt{\frac{j(r)+1}{2}}\right) i\right| \\ &= \frac{|\ell|}{2}\sqrt{\frac{j(r)-1}{2} + \frac{j(r)+1}{2} + 1 \pm 2\sqrt{\frac{j(r)+1}{2}}} \\ &= \frac{|\ell|}{2}\sqrt{j(r) + 1 \pm 2\sqrt{\frac{j(r)+1}{2}}} = \frac{|\ell|}{\sqrt{2}}\sqrt{\upsilon(r)^2 \pm \upsilon(r)}. \end{aligned}$$

We now compute the argument of $u_{0,+}$:

$$\begin{aligned} \arg(u_{0,+}) &= \arg\left(\sqrt{\frac{j(r)-1}{2}} + i\left(\pm 1 + \sqrt{\frac{j(r)+1}{2}}\right)\right) \\ &= \arcsin\left(\frac{\pm 1 + \sqrt{\frac{1+j(r)}{2}}}{\sqrt{1 + j(r) \pm 2\sqrt{\frac{1+j(r)}{2}}}}\right) = \arcsin\left(\frac{\sqrt{\pm 1 + \sqrt{\frac{1+j(r)}{2}}}}{\sqrt{2\sqrt{\frac{1+j(r)}{2}}}}\right) \\ &= \arcsin\left(\sqrt{\frac{1}{2}\left(1 \pm \sqrt{\frac{2}{1+j(r)}}\right)}\right) = \frac{\pi}{2} - \frac{1}{2}\arccos\left(\pm\sqrt{\frac{2}{1+j(r)}}\right) \end{aligned} \tag{15.36}$$

by $\cos(\pi - 2\theta) = -\cos 2\theta = 2\sin^2\theta - 1$. Thus, (15.33) holds. □

15.4.4 The direction of steepest descent

It is now time to determine the direction of steepest descent at the saddle-point $u_{0,+}$. Even if we decide to use a contour that goes through the saddle-point in a direction that is not quite optimal, it will be useful to know what the direction w of steepest descent actually is. A contour that passes through the saddle-point making an angle between $-\pi/4+\epsilon$ and $\pi/4-\epsilon$ with w may be acceptable, in that the contribution of the saddle point is then suboptimal by at most a bounded factor depending on ϵ; an angle approaching $-\pi/4$ or $\pi/4$ leads to a contribution that is suboptimal by an unbounded factor, and would thus be less acceptable.

(The line going through the saddle point in the direction of steepest descent is called the *axis* of the saddle point in [dB81].)

Lemma 15.7. *Let $t, \ell \in \mathbb{R}$, $t > 0$, $\ell \neq 0$. Let $\phi : \mathbb{C} \to \mathbb{C}$ be given by*

$$\phi(u) = -\frac{u^2}{2} + \ell i u + it \log u. \tag{15.37}$$

and let $u_{0,+}$ be as in (15.29), so that $\phi'(u_{0,+}) = 0$. The angle that the direction of steepest descent for $-\phi$ at u_0 makes with the y-axis is

$$\begin{cases} \frac{1}{2}\left(\arctan \frac{2v(\mathscr{r})(j(\mathscr{r})-v(\mathscr{r}))}{\mathscr{r}} - \arctan\sqrt{\frac{j(\mathscr{r})-1}{2}}\right) & \text{if } \ell > 0, \\ \frac{1}{2}\left(-\arctan \frac{2v(\mathscr{r})(j(\mathscr{r})+v(\mathscr{r}))}{\mathscr{r}} + \arctan\sqrt{\frac{j(\mathscr{r})-1}{2}}\right) & \text{if } \ell < 0, \end{cases} \tag{15.38}$$

where $\mathscr{r} = 4t/\ell^2$, $j(\mathscr{r}) = (1+\mathscr{r}^2)^{1/2}$ and $v(\mathscr{r}) = \sqrt{(1+j(\mathscr{r}))/2}$.

By "the angle that a vector v makes with the y-axis", we mean $\arg(v) - \pi/2$. It is clear that the direction of steepest descent is defined only modulo π. We care about the direction of steepest descent for $-\phi(u)$ because it is the same as for $e^{-\phi(u)}$.

Proof. Let $w \in \mathbb{C}$ be the unit vector pointing in the direction of steepest descent for $-\phi$, that is, steepest ascent for ϕ. Since $\phi(u) = \phi(u_{0,+}) + \phi''(u_{0,+})(u-u_{0,+})^2 + \cdots$, we see that $w^2\phi''(u_{0,+})$ is real and positive. Thus $\arg(w) = -\arg(\phi''(u_{0,+}))/2 \bmod \pi$. By (15.28),

$$\begin{aligned} \arg(\phi''(u_{0,+})) &= -\pi + \arg(i\ell u_{0,+} + 2it) - 2\arg(u_{0,+}) \bmod 2\pi \\ &= -\frac{\pi}{2} + \arg(\ell u_{0,+} + 2t) - 2\arg(u_{0,+}) \bmod 2\pi. \end{aligned}$$

By (15.31),

$$\begin{aligned} \Re(\ell u_{0,+} + 2t) &= \frac{\ell^2}{2}\left(\pm\sqrt{\frac{j(\mathscr{r})-1}{2}} + \frac{4t}{\ell^2}\right) = \frac{\ell^2}{2}\left(\mathscr{r} \pm \sqrt{\frac{j(\mathscr{r})-1}{2}}\right), \\ \Im(\ell u_{0,+} + 2t) &= \frac{\ell^2}{2}\left(1 \pm \sqrt{\frac{j(\mathscr{r})+1}{2}}\right), \end{aligned}$$

where the sign $\pm$ is $+$ if $\ell > 0$ and $-$ if $\ell < 0$. Noting that $\Re(\ell u_{0,+} + 2t) > 0$, we obtain that $\arg(\ell u_{0,+} + 2t) = \arctan \varpi$, where

$$\varpi = \frac{1 \pm \sqrt{\frac{j(\mathscr{r})+1}{2}}}{\mathscr{r} \pm \sqrt{\frac{j(\mathscr{r})-1}{2}}},$$

and where, as we said before, we define $\arctan$ to have image in $[-\pi/2, \pi/2]$. It is easy to check that $\operatorname{sgn} \varpi = \operatorname{sgn} \ell$. Hence,

$$\arctan \varpi = \pm \frac{\pi}{2} - \arctan \left(\frac{\mathscr{r} \pm \sqrt{\frac{j(\mathscr{r})-1}{2}}}{1 \pm \sqrt{\frac{j(\mathscr{r})+1}{2}}} \right).$$

At the same time,

$$\begin{aligned} \frac{\mathscr{r} \pm \sqrt{\frac{j-1}{2}}}{1 \pm \sqrt{\frac{j+1}{2}}} &= \frac{\left(\mathscr{r} \pm \sqrt{\frac{j-1}{2}}\right)\left(1 \mp \sqrt{\frac{j+1}{2}}\right)}{1 - \frac{j+1}{2}} = \frac{\mathscr{r} \pm \sqrt{2(j-1)} \mp \mathscr{r}\sqrt{2(j+1)}}{1-j} \\ &= \frac{\mathscr{r} \pm \sqrt{\frac{2}{j+1}}\left(\sqrt{j^2-1} - \mathscr{r}\cdot(j+1)\right)}{1-j} = \frac{\mathscr{r} \pm \frac{1}{\upsilon}(\mathscr{r} - \mathscr{r}\cdot(j+1))}{1-j} \\ &= \frac{\mathscr{r}(1 \mp j/\upsilon)}{1-j} = \frac{(-1 \pm j/\upsilon)(j+1)}{\mathscr{r}} = \frac{2\upsilon(-\upsilon \pm j)}{\mathscr{r}}. \end{aligned} \tag{15.39}$$

where we write simply j for $j(\mathscr{r})$. Hence, modulo 2π,

$$\arg(\phi''(u_{0,+})) = -\arctan \frac{2\upsilon(-\upsilon \pm j)}{\mathscr{r}} - 2\arg(u_{0,+}) - \begin{cases} 0 & \text{if } \ell > 0 \\ \pi & \text{if } \ell < 0. \end{cases}$$

Therefore, the direction of steepest descent is

$$\arg(w) = -\frac{\arg(\phi''(u_{0,+}))}{2} = \arg(u_{0,+}) + \frac{1}{2}\arctan \frac{2\upsilon(-\upsilon \pm j)}{\mathscr{r}} + \begin{cases} 0 & \text{if } \ell > 0 \\ \frac{\pi}{2} & \text{if } \ell < 0. \end{cases} \tag{15.40}$$

By (15.33) and $\arccos 1/\upsilon(\mathscr{r}) = \arctan \sqrt{\upsilon(\mathscr{r})^2 - 1} = \arctan \sqrt{(j(\mathscr{r})-1)/2}$, we conclude that

$$\arg(w) = \begin{cases} \frac{\pi}{2} + \frac{1}{2}\left(\arctan \frac{2\upsilon(j-\upsilon)}{\mathscr{r}} - \arctan \sqrt{\frac{j-1}{2}}\right) & \text{if } \ell > 0, \\ \frac{\pi}{2} + \frac{1}{2}\left(-\arctan \frac{2\upsilon(j+\upsilon)}{\mathscr{r}} + \arctan \sqrt{\frac{j-1}{2}}\right) & \text{if } \ell < 0. \end{cases} \tag{15.41}$$

□

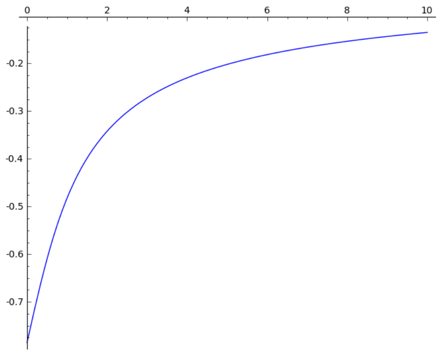

Figure 15.2: Angle between the direction of steepest descent and the y-axis for $\ell < 0$

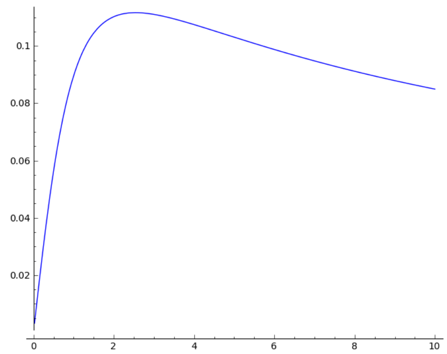

Figure 15.3: Angle between the direction of steepest descent and the y-axis for $\ell > 0$

Figures 15.2 and 15.3 plot the angle that the direction of steepest descent makes with the vertical line, as a function of $\mathscr{r} = 4t/\ell^2$. As can be seen, the direction of steepest descent is nearly vertical for $\ell \geq 0$, assuming, as usual, $t > 0$.

The case $\ell < 0$ of Lemmas 15.6 and 15.7 will never actually be used in the proof of Theorem 15.1. We have worked it out simply for it to orient us in our choices.

15.5 THE INTEGRAL OVER THE CONTOUR

We must now choose the contour of integration. As we mentioned in §15.4.1, the optimal contour should be one on which the phase of the integrand in (15.24) is constant, i.e., $\Im\phi(u)$ is constant.

Writing $u = x + iy$, we obtain from (15.23) that

$$\Im\phi(u) = -xy + \ell x + t \log\sqrt{x^2 + y^2}. \tag{15.42}$$

We would thus be considering the curve $\Im\phi(u) = c$, where c is a constant. Since we need the contour to pass through the saddle point $u_{0,+}$, we set $c = \Im(\phi(u_{0,+}))$. Unfortunately, the curve $\Im\phi(u) = c$ given by (15.42) is rather uncomfortable to work with. Moreover, as we can tell by some plotting or by taking partial derivatives of $\Im\phi(u)$, the curve does not generally go from $O(1) - i\infty$ to $O(1) + i\infty$, but rather takes a sharp bend rightwards as we go upwards past $u_{0,+}$.

Instead, we shall use very simple contours. Recall that we are meant to choose a path $\mathbf{C}$ going through $u_{0,+}$ with the property that

$$\int_{\mathbf{C}} \left| e^{-\phi(u)} u^{-\sigma} du \right| = \int_{\mathbf{C}} e^{-\Re\phi(u)} |u|^{-\sigma} |du|$$

is small. Recall also that we are assuming without loss of generality that $t > 0$. If $\ell = -2\pi\delta$ is positive, then the direction of steepest descent is never far from vertical (see Figure 15.3). Thus, it seems reasonable to let our contour $\mathbf{C}$ be just the vertical line going through $u_{0,+}$.

If $\ell < 0$, then the direction of steepest descent may be far from vertical. Of course we may argue that the bounds we will obtain are so strong that it does not matter much that they are suboptimal, even if it is by a non-constant factor. However, we will later see that there are some additional complications. We will be able to simplify matters while choosing a direction of descent that is close to optimal by rephrasing the problem first.

(For other contexts in which it is convenient and permissible to choose a direction that is not quite that of steepest descent, see, e.g., [Wym64] and [Olv70].)

15.5.1 Approximating $\Re\phi(u)$

Before we settle on our choice of contour $\mathbf{C}$ for $\ell > 0$ and $\ell < 0$, let us show how to bound $\Re\phi(u)$ in a region of the plane. By (15.37),

$$\Re\phi(x+iy) = \frac{y^2 - x^2}{2} - \ell y - t\arg(x+iy). \tag{15.43}$$

Lemma 15.8. *For any $r_0 \geq 0$ and any $r \in [-2r_0, \infty)$,*

$$\arctan r \leq \arctan r_0 + (\arctan' r_0)\cdot(r - r_0). \tag{15.44}$$

Proof. First of all, let us prove that

$$\arctan r + \arctan 2r \geq \frac{3r}{1+r^2} \tag{15.45}$$

for all $r \geq 0$. The derivative of $\arctan r + \arctan 2r - 3r/(1+r^2)$ is

$$\frac{18r^4}{(r^2+1)^2(4r^2+1)},$$

which is ≥ 0. Both sides of (15.45) equal 0 when $r = 0$, and so it follows that (15.45) holds for all $r \geq 0$.

Since $\arctan' r_0 = 1/(1+r_0^2)$, we see from (15.45) that the inequality (15.44) is true for $r = -2r_0$. Now, $\arctan'' r = -2r/(1+r^2)^2$, and so arctan is concave for $r > 0$ and convex for $r < 0$. Concavity implies that (15.44) holds for $r \geq 0$, whereas convexity, together with the fact that (15.44) holds for $r = -2r_0$ and $r = 0$, implies that (15.44) holds for all $-2r_0 \leq r \leq 0$. □

Lemma 15.9. *Let $t, \ell \in \mathbb{R}$, $t > 0$, $\ell \neq 0$. Let $\phi : \mathbb{C} \to \mathbb{C}$ be as in (15.37) and $u_{0,+} \in \mathbb{C}$ be as in (15.29). Let $R = R_1 \cup R_2 \subset \mathbb{C}$, where*

- *R_1 is the quarter-plane $u_{0,+} \cdot ([0,\infty) + i[0,\infty))$,*

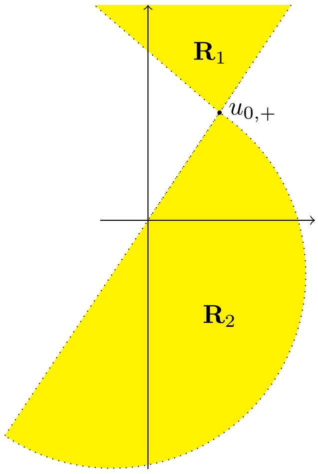

Figure 15.4: Regions R_1 and R_2

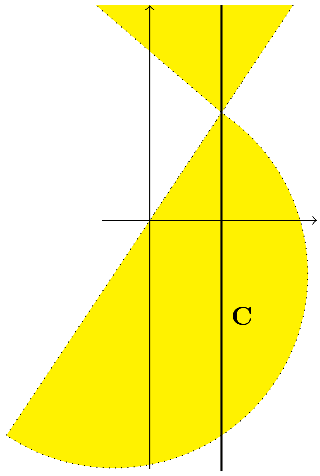

Figure 15.5: Contour $\mathbf{C}$

- *R_2 is a closed half-disk: the half of the disk with center at $-u_{0,+}/2$ and radius $3|u_{0,+}|/2$ lying below the line connecting 0 and $u_{0,+}$.*

  Then, for every $u \in R$,

$$\Re\phi(u) \geq \Re\phi(u_{0,+}) - \Re\frac{(u-u_{0,+})^2}{2}. \tag{15.46}$$

Proof. Let $u \in R$. Consider the line L going through $u_{0,+}$ and u, and let z_0 be the point where the line through the origin orthogonal to L intersects L. By basic Euclidean geometry, z_0 lies on the boundary of the disk D with center at $u_{0,+}/2$ and radius $|u_{0,+}/2|$. Since $u_{0,+}$ lies on the first quadrant, we see that z_0 lies on the half D^- of D lying below the line connecting 0 and $u_{0,+}$. Now, R_2 is the image of D^- under a homothety centered at $u_{0,+}$ with dilation factor 3. We conclude that $L \cap R$ consists of all points z on L that either lie on the upper half of L, meaning the same side of z_0 as $u_{0,+}$, or satisfy $|z - z_0| \leq 2|u_{0,+} - z_0|$.

By (15.37) and the fact that $\phi'(u_{0,+}) = 0$,

$$\begin{aligned}\Re\phi(u) - \Re\phi(u_{0,+}) &= \Re(\phi(u) - (\phi(u_{0,+}) + \phi'(u_{0,+})(u-u_{0,+}))) \\ &= -\Re\frac{(u-u_{0,+})^2}{2} - t(\Im\log u - \Im f(u)),\end{aligned} \tag{15.47}$$

where $f(u) = \log u_{0,+} + (\log' u_{0,+}) \cdot (u - u_{0,+})$. Since $\Im \log u = \arg u$, we see that $u \mapsto \Im f(u)$ is the real-linear approximation to $\arg u$ around $u = u_{0,+}$. The restriction of $\arg(z)$ to L is $\arg z_0 + \arctan l(z)$, where $l(z) = |z - z_0|/|z_0|$ is z lies on the upper half of L and $l(z) = -|z - z_0|/|z_0|$ otherwise. Hence, for u on L,

$$\arg u - \Im f(u) = \arctan l(u) - (\arctan l(u_{0,+}) + (\arctan' l(u_{0,+})) \cdot (l(u) - l(u_{0,+}))).$$

If u is on $L \cap R$, we know that $l(u) \geq -2l(u_{0,+})$. Thus, by Lemma 15.8,

$$\arg u - \Im f(u) < 0.$$

By (15.47), we conclude that

$$\Re\phi(u) - \Re\phi(u_{0,+}) \geq -\Re\frac{(u - u_{0,+})^2}{2}.$$

□

If we use the approximation (15.46) to $\phi(u)$ instead of $\phi(u)$ itself, then the direction of steepest descent actually becomes vertical.

15.5.2 Integral estimates

Let us now estimate some integrals. The method used will be, in essence, a very simple case of the *Laplace method*. (We shall discuss the Laplace method in somewhat greater generality at the end of §15.5.3.) The basic idea is that, in an integral having an exponential factor $e^{f(t)}$ and a non-exponential factor $g(t)$ in the integrand, as in (15.48), we do a Taylor expansion of $g(t)$ around a point t_0 such that $f'(t_0) = 0$, and use an exponential bound on the tails.

Proposition 15.10. *Let $g : \mathbb{R} \to \mathbb{R}$ be $2k$ times differentiable on $\mathbb{R}$, where $k \geq 1$. Let*

$$I = \int_{-\infty}^{\infty} g(t) e^{-\kappa\frac{(t-t_0)^2}{2}} dt \tag{15.48}$$

for some fixed $t_0 \in \mathbb{R}$, $\kappa > 0$. Then

$$I = \sum_{j=0}^{k-1} \frac{\sqrt{2\pi/\kappa}}{(2\kappa)^j j!} g^{(2j)}(t_0) + \mathrm{err}, \tag{15.49}$$

where

$$\frac{\sqrt{2\pi/\kappa}}{(2\kappa)^k k!} \inf_{t\in\mathbb{R}} g^{(2k)}(t) \leq \mathrm{err} \leq \frac{\sqrt{2\pi/\kappa}}{(2\kappa)^k k!} \sup_{t\in\mathbb{R}} g^{(2k)}(t). \tag{15.50}$$

Moreover, if $g^{(2j+1)}(t_0) \leq 0$ for all $0 \leq j < k$, then, for any $\beta > 0$,

$$\mathrm{err} \leq \frac{\sqrt{2\pi/\kappa}}{(2\kappa)^k k!} \sup_{t \geq (1-\beta)t_0} g^{(2k)}(t) + \frac{e^{-\beta(\kappa t_0)^2/2}}{\beta\kappa t_0} \sup_{t\in\mathbb{R}} g(t). \tag{15.51}$$

The condition $g^{(2j+1)}(t_0) \leq 0$ is not indispensable. In its absence, we would have a factor of 2 in front of the second term in the right side of (15.51).

Proof. We can express $g(t)$ by a truncated Taylor series around t_0:

$$g(t) = \sum_{j=0}^{2k-1} \frac{g^{(j)}(t_0)}{j!}(t-t_0)^j + \frac{g^{(2k)}(s)}{(2k)!}(t-t_0)^{2k}$$

for some s between t_0 and t. Hence

$$I = \sum_{j=0}^{2k-1} \frac{g^{(j)}(t_0)}{j!} \int_{-\infty}^{\infty} e^{-\kappa\frac{(t-t_0)^2}{2}}(t-t_0)^j dt + \frac{c}{(2k)!}\int_{-\infty}^{\infty} e^{-\kappa\frac{(t-t_0)^2}{2}}(t-t_0)^{2k} dt$$

for some $c \in [\inf g^{(2k)}(t), \sup g^{(2k)}(t)]$. The terms coming from odd j cancel out:

$$\int_{-\infty}^{\infty} e^{-\kappa\frac{(t-t_0)^2}{2}}(t-t_0)^j dt = \int_{-\infty}^{\infty} e^{-\kappa\frac{t^2}{2}} t^j dt = 0,$$

since $e^{-\kappa t^2/2}t^j$ is an odd function for j odd. For j even,

$$\begin{aligned}\int_{-\infty}^{\infty} e^{-\kappa\frac{(t-t_0)^2}{2}}(t-t_0)^j dt &= \frac{1}{\kappa^{\frac{j+1}{2}}}\int_{-\infty}^{\infty} e^{-u^2/2}u^j du \\ &= \frac{\sqrt{2\pi}}{\kappa^{\frac{j+1}{2}}}(j-1)(j-3)(j-5)\cdots 3\cdot 1 = \frac{j!}{(2\kappa)^{j/2}(j/2)!}\sqrt{2\pi/\kappa}\end{aligned}$$

by induction. Hence (15.49) holds with an error term err bounded as in (15.50).

To obtain the bound in (15.51), start by splitting the integral I:

$$I = \int_{-(1-\beta)t_0}^{\infty} g(t)e^{-\kappa\frac{(t-t_0)^2}{2}} dt + \int_{-\infty}^{-(1-\beta)t_0} g(t)e^{-\kappa\frac{(t-t_0)^2}{2}} dt. \tag{15.52}$$

We bound the first integral on the right side as before. For $j < 2k$ odd, we remark that

$$\begin{aligned}\int_{(1-\beta)t_0}^{\infty} e^{-\kappa\frac{(t-t_0)^2}{2}} g^{(j)}(t_0)(t-t_0)^j dt &= g^{(j)}(t_0)\int_{-\beta t_0}^{\infty} e^{-\kappa\frac{t^2}{2}} t^j dt \\ &= g^{(j)}(t_0)\int_{-\beta t_0}^{\beta t_0} e^{-\kappa\frac{t^2}{2}} t^j dt + g^{(j)}(t_0)\int_{\beta t_0}^{\infty} e^{-\kappa\frac{t^2}{2}} t^j dt < 0\end{aligned}$$

because $g^{(j)}(t_0) < 0$.

The second integral in (15.52) is bounded by $\sup_{t\in\mathbb{R}} g(t)$ times

$$\int_{-\infty}^{-\beta t_0} e^{-\kappa t^2/2} dt \le \frac{1}{\beta\kappa t_0}\int_{-\infty}^{-\beta t_0} \kappa t e^{-\kappa t^2/2} dt = \frac{e^{-\kappa(\beta t_0)^2/2}}{\beta\kappa t_0}.$$

□

Corollary 15.11. *Let $x_0, y_0 > 0$, $l_0 = \sqrt{x_0^2 + y_0^2}$, $\sigma \ge -1$. Let*

$$I_\sigma = \int_{-\infty}^{\infty} \frac{e^{-(y-y_0)^2/2}}{(x_0^2+y^2)^{\sigma/2}} dy. \tag{15.53}$$

Then, if $\sigma \geq 0$,

$$\frac{\sqrt{2\pi}}{l_0^\sigma} - \frac{\sigma\sqrt{2\pi}}{2x_0^{\sigma+2}} \leq I_\sigma \leq \frac{\sqrt{2\pi}}{l_0^\sigma} + \frac{\sigma\sqrt{2\pi}}{e^{3/2}x_0^{\sigma+2}}, \tag{15.54}$$

and, if $-1 \leq \sigma < 0$,

$$\frac{\sqrt{2\pi}}{l_0^\sigma} + \frac{\sigma\sqrt{2\pi}}{e^{3/2}x_0^{\sigma+2}} \leq I_\sigma \leq \frac{\sqrt{2\pi}}{l_0^\sigma} - \frac{\sigma\sqrt{2\pi}}{2x_0^{\sigma+2}}. \tag{15.55}$$

Proof. Let $g(t) = 1/(1+t^2)^{\sigma/2}$. Then

$$I_\sigma = \frac{1}{x_0^\sigma}\int_{-\infty}^{\infty} g(y/x_0)e^{-(y-y_0)^2/2}dy = x_0^{1-\sigma}\int_{-\infty}^{\infty} g(t)e^{-x_0^2\frac{(t-t_0)^2}{2}}dt \tag{15.56}$$

for $t_0 = y_0/x_0$. Thus, by Proposition 15.10 with $\kappa = x_0^2$,

$$I_\sigma = x^{-\sigma}\sqrt{2\pi}g(t_0) + \text{error} = \frac{\sqrt{2\pi}}{l_0^\sigma} + \text{error},$$

where

$$\frac{\sqrt{2\pi}}{2x_0^{\sigma+2}}\inf_{t\in\mathbb{R}} g''(t) \leq \text{error} \leq \frac{\sqrt{2\pi}}{2x_0^{\sigma+2}}\sup_{t\in\mathbb{R}} g''(t).$$

Now

$$g''(t) = \frac{\sigma((\sigma+1)t^2-1)}{(1+t^2)^{\sigma/2+2}},$$

$$g^{(3)}(t) = \frac{-((\sigma+1)t^2-3)\sigma(\sigma+2)t}{(1+t^2)^{\sigma/2+2}}.$$

We can assume $\sigma \neq 0$, as otherwise $g''(t) = 0$ identically, and $\sigma \neq -1$, as it is enough to prove (15.54) and (15.55) for $\sigma \to -1$. Then $g^{(3)}(t) = 0$ when $t = \pm\sqrt{3/(\sigma+1)}$ or $t = 0$. Thus, $g''(t)$ can have local extrema only at those t. When $t \to \pm\infty$, $g''(t) \to 0^+$ if $\sigma > 0$, and $g''(t) \to 0^-$ if $\sigma < 0$. It is then clear that the value $g''(0) = -\sigma$ is the global minimum if $\sigma > 0$, and the global maximum if $\sigma < 0$. It is also clear that, at $t = \pm\sqrt{3/(\sigma+1)}$, $g''(t)$ attains its global maximum if $\sigma > 0$, and its global minimum if $\sigma < 0$. The value of $g''(t)$ for $t = \pm\sqrt{3/(\sigma+1)}$ has absolute value

$$\frac{2|\sigma|}{\left(1+\frac{3}{1+\sigma}\right)^{\frac{\sigma}{2}+2}} = \frac{2|\sigma|}{(f((1+\sigma)/3))^{3/2}} \leq \frac{2|\sigma|}{e^{3/2}},$$

where $f(t) = (1+1/t)^{t+1}$, since $f(t)$ decreases for $t > 0$ and tends to e as $t \to \infty$, as is well-known.

□

Lemma 15.12. *Let* $\sigma \geq 0$. *Define* $g(t) = 1/(1+t^2)^{\sigma/2}$. *Then, for every* $k \geq 0$,

$$|g^{(k)}(t)| \leq \frac{\sigma(\sigma+1)\cdots(\sigma+k-1)}{(1+t^2)^{\frac{\sigma+k}{2}}}.$$

The following elegant proof was kindly contributed by F. Petrov.

Proof. For any a,

$$\frac{1}{(a^2+t^2)^{\sigma/2}} = (t+ai)^{-\sigma/2}(t-ai)^{-\sigma/2}.$$

Differentiating k times, we obtain

$$\left(\frac{1}{(a^2+t^2)^{\sigma/2}}\right)^{(k)} = \sum_{j=0}^{k}\binom{k}{j}\binom{-\sigma/2}{j}\binom{-\sigma/2}{k-j}(t+ai)^{-\sigma/2-j}(t-ai)^{-\sigma/2-(k-j)}.$$

By the triangle inequality, the right side is at most a constant times $(a^2+t^2)^{-(\sigma+k)/2}$. If $a=0$, there is no cancellation, and so the constant is

$$\left|t^{\sigma+k}\left(t^{-\sigma}\right)^{(k)}\right| = \sigma(\sigma+1)\cdots(\sigma+k-1).$$

□

Corollary 15.13. *Let* $x_0, y_0 > 0$, $l_0 = \sqrt{x_0^2+y_0^2}$, $\sigma \geq 0$. *Let* I_σ *be as in (15.53). Then, for any* $k \geq 0$,

$$|I_\sigma| \leq \sqrt{2\pi}\left(\sum_{j=0}^{k-1}\frac{c_{\sigma,j}}{l_0^{\sigma+2j}} + \mathrm{err}\right),$$

where $c_{\sigma,0} = 1$,

$$c_{\sigma,j} = \frac{\sigma(\sigma+1)\cdots(\sigma+2j-1)}{2^j j!} \tag{15.57}$$

for $1 \leq j \leq k$, *and* $\mathrm{err} \leq c_{\sigma,k}/x_0^{\sigma+2k}$. *Moreover, for any* $\beta \in (0,1)$,

$$\mathrm{err} \leq \frac{c_{\sigma,k}}{((1-\beta)l_0)^{\sigma+2k}} + \frac{1/\beta}{\sqrt{2\pi}}\cdot\frac{e^{-\beta^2 y_0^2/2}}{x_0^\sigma y_0}.$$

Proof. We start with (15.56). Then we apply Prop. 15.10 with $\kappa = x_0^2$, and bound the error as in (15.50) and (15.51). Then we bound the derivatives $g^{(2j)}(t)$, $0 \leq j \leq k$, by Lemma 15.12. When using (15.51), we use the easy inequality $(1+((1-\beta)t_0)^2)^{1/2} \geq (1-\beta)(1+t_0^2)^{1/2}$ to bound $|g^{(2k)}(t_0/2)|$ from above. □

15.5.3 The case $\delta < 0$

Let us first consider the case $\delta < 0$, assuming, as usual, that $t > 0$. (In other words, we are in the case $\mathrm{sgn}(t) \neq \mathrm{sgn}(\delta)$.) The variable $\ell = -2\pi\delta$ is obviously positive.

We will choose a vertical path of integration $\mathbf{C}$ through the saddle-point $u_{0,+}$. Above $u_{0,+}$, the contour is in region R, and below $u_{0,+}$, it stays in R for a good while (Figure 15.5).

We may wonder whether the vertical contour $\mathbf{C}$ goes too close to the origin, thus making the factor $|u|^{-\sigma}$ too large. The critical case is that of $\mathscr{r} \to 0^+$, as then $\arg(u_{0,+})$ approaches $\pi/2$. Then, by Lemma 15.6, $x_0 := \Re u_{0,+} \sim |\ell|\mathscr{r}/4 = t/\ell$. As we have implied before, we are interested mainly in the case $t/\ell \gg 1$, as otherwise there is no hope of decay. Thus $x_0 \gg 1$.

When we compare crossing the x-axis at $(x_0, 0)$ with crossing it at some point $(x, 0)$, $x > x_0$, we are comparing $\exp(-\Re\phi(x_0))|x_0|^{-\sigma}$ with $\exp(-\Re\phi(x))|x|^{-\sigma}$, that is to say – by (15.43) – we are comparing $e^{x_0^2/2}|x_0|^{-\sigma}$ with $e^{x^2/2}|x|^{-\sigma}$. It follows easily from $x_0 \gg 1$ and $x > x_0$ that $e^{x_0^2/2}|x_0|^{-\sigma} = O_\sigma(e^{x^2/2}|x|^{-\sigma})$. Thus, even when we take the factor $|u|^{-\sigma}$ into consideration, we find that a vertical contour $\mathbf{C}$ is acceptable.

Before we estimate the path integral, we will prove two easy, useful lemmas.

Lemma 15.14. *Let $t, \ell \in \mathbb{R}^+$. Let $u_{0,+}$ be as in (15.29). Then*

$$\max(\sqrt{t}, \ell) \le |u_{0,+}| \le \max\left(\sqrt{2t}, \frac{3}{2}\ell\right) \quad \textit{and} \quad |\Im u_{0,+}| \ge \max\left(\sqrt{\frac{t}{2}}, \ell\right).$$

Proof. The lower bounds are immediate from (15.31), (15.32) and the inequalities

$$\sqrt{\upsilon(\mathscr{r})^2 + \upsilon(\mathscr{r})} \ge \sqrt{2}, \qquad \sqrt{\frac{j(\mathscr{r}) + 1}{2}} \ge 1,$$

$$\sqrt{\upsilon(\mathscr{r})^2 + \upsilon(\mathscr{r})} > \upsilon(\mathscr{r}) > \sqrt{j(\mathscr{r})/2} > \sqrt{\mathscr{r}/2}.$$

The upper bound on $|u_{0,+}|$ follows from (15.32) and the fact that $\sqrt{(\upsilon(\mathscr{r})^2 + \upsilon(\mathscr{r}))/2} < \frac{3}{2}$ for $\mathscr{r} \le \frac{9}{2}$ (as the inequality holds for $\mathscr{r} = \frac{9}{2}$) and $\sqrt{\upsilon(r)^2 + \upsilon(r)} \le \sqrt{r}$ for $\mathscr{r} \ge \frac{9}{2}$ (as this second inequality holds for $\mathscr{r} = \frac{9}{2}$). □

Lemma 15.15. *Let $t, \ell \in \mathbb{R}^+$. Let $u_{0,+} = x_0 + iy_0$ be as in (15.29). Then*

$$\frac{x_0 y_0}{|u_{0,+}|} \ge \min\left(\frac{2}{3}\frac{t}{\ell}, \frac{\sqrt{t}}{2}\right).$$

Proof. By (15.31) and (15.32), it is enough to show that

$$\sqrt{\frac{j(\mathscr{r}) - 1}{2}} + \frac{\mathscr{r}}{2} \ge \sqrt{\frac{\upsilon(\mathscr{r})^2 + \upsilon(\mathscr{r})}{2}} \cdot \min\left(\frac{2}{3}\mathscr{r}, \sqrt{\mathscr{r}}\right) \tag{15.58}$$

for any $\mathscr{r} \in [0, \infty)$. The proof will proceed as one might expect, namely, by an expansion around $\mathscr{r} = 0$ and an expansion around $\mathscr{r} = \infty$, complemented by the bisection method. [4]

[4] It would be completely reasonable to ask for standard software to do such a proof on its own. Work in this direction does exist: see, e.g., the footnote in [Tuc11, p. 72], referring to the work of Berz and Makino [BM98] on "Taylor models".

Since $\sqrt{\digamma^2+1} \geq 1+\digamma^2/2-\digamma^4/8$ for $0 \leq \digamma \leq \sqrt{8}$, we know that $\sqrt{(j(\digamma)-1)/2+\digamma/2} \geq (\digamma/2)(1-\digamma^2/4)+\digamma/2 = \digamma - \digamma^3/8$; at the same time, $\sqrt{(\upsilon(\digamma)^2+\upsilon(\digamma))/2} \leq 1+3\digamma^2/32$, and so (15.58) holds for $0 \leq \digamma \leq 4/3$.

Similarly, $j(\digamma) = \digamma\sqrt{1+\digamma^2}$ satisfies

$$\digamma\left(1+\frac{1}{2\digamma^2}-\frac{1}{8\digamma^4}\right) \leq j(\digamma) \leq \digamma\left(1+\frac{1}{2\digamma^2}\right)$$

for $\digamma \geq 1/\sqrt{8}$, and so

$$\sqrt{\frac{j(\digamma)-1}{2}} \geq \frac{\sqrt{\digamma}}{2}\left(1-\frac{1}{2\digamma}\right)$$

for $\digamma \geq 1/\sqrt{2}$ and

$$\upsilon(\digamma) = \frac{\sqrt{j(\digamma)+1}}{\sqrt{2}} = \frac{1}{\sqrt{2}}\sqrt{\digamma+1+\frac{1}{2\digamma}} \leq \frac{1}{\sqrt{2}}\left(\sqrt{\digamma}+\frac{1}{2\sqrt{\digamma}}+\frac{1}{8\digamma^{3/2}}\right)$$

for all $\digamma > 0$. Hence

$$\begin{aligned}\sqrt{\frac{\upsilon(\digamma)^2+\upsilon(\digamma)}{2}}\cdot\digamma &\leq \frac{\upsilon(\digamma)+1/2}{\sqrt{2}}\sqrt{\digamma} \leq \left(\sqrt{\digamma}+\frac{1}{\sqrt{2}}+\frac{1}{2\sqrt{\digamma}}+\frac{1}{8\digamma^{3/2}}\right)\frac{\sqrt{\digamma}}{2} \\ &\leq \frac{\digamma}{2}+\frac{\sqrt{\digamma}}{2}\left(1-\frac{1}{2\digamma}\right) = \sqrt{\frac{j(\digamma)-1}{2}}\end{aligned}$$

provided that

$$\frac{1}{4}+\frac{1}{4\sqrt{\digamma}}+\frac{1}{16\digamma} \leq \left(1-\frac{1}{\sqrt{2}}\right)\frac{\sqrt{\digamma}}{2},$$

as is the case for $\digamma \geq 25/4$, say.

We finish by checking (15.58) for $4/3 < \digamma < 25/4$ by bisection. □

Proposition 15.16. *Let $t, \ell, \sigma \in \mathbb{R}$, $t > 0$, $\ell > 0$, $0 \leq \sigma \leq 2$. Assume $t \geq \max(3\ell/2, 6/\sqrt{5})$. Let $\phi : \mathbb{C} \to \mathbb{C}$ be as in (15.37) and $u_{0,+} = x_0 + iy_0 \in \mathbb{C}$ be as in (15.29).*

Then, for any $\beta \in (0,1)$,

$$\left|\int_{x_0-i\infty}^{x_0+i\infty} e^{-\phi(u)}u^{-\sigma}du\right| \leq \left((1+\epsilon_{\sigma,\beta}(t))\frac{\sqrt{2\pi}}{|u_{0,+}|^\sigma}+\frac{2e^{-\beta^2y_0^2/2}}{x_0^\sigma y_0}\right)e^{-\Re\phi(u_{0,+})}$$

where

$$\epsilon_{\sigma,\beta}(t) \leq \frac{\sigma(\sigma+1)}{2t}+\frac{\sigma(\sigma+1)(\sigma+2)(\sigma+3)}{8(1-\beta)^{\sigma+4}t^2}+\frac{0.00104}{t^2}. \tag{15.59}$$

Proof. Clearly,

$$\left|\int_{x_0-i\infty}^{x_0+i\infty} e^{-\phi(u)}u^{-\sigma}du\right| \leq \int_{x_0-i\infty}^{x_0+i\infty} e^{-\Re\phi(u)}|u|^{-\sigma}|du|.$$

By Lemma 15.9,

$$\int_{x_0-2iy_0}^{x_0+i\infty} e^{-\Re\phi(u)}|u|^{-\sigma}|du| = e^{-\Re\phi(u_{0,+})}\int_{x_0-2iy_0}^{x_0+i\infty} e^{-\frac{(y-y_0)^2}{2}}|u|^{-\sigma}|du|. \quad (15.60)$$

We bound the integral on the right of (15.60) by Cor. 15.13 with $k=2$:

$$\begin{aligned}\int_{x_0-2iy_0}^{x_0+i\infty} e^{-\frac{(y-y_0)^2}{2}}|u|^{-\sigma}|du| &\le \int_{-\infty}^{\infty} \frac{e^{-\frac{(y-y_0)^2}{2}}}{(x_0^2+y^2)^{\sigma/2}}dy \\ &\le \sqrt{2\pi}\cdot\left(\frac{1}{l_0^\sigma}+\frac{c_{\sigma,1}}{l_0^{\sigma+2}}+\frac{c_{\sigma,2}}{(l_0/2)^{\sigma+4}}\right)+\frac{2e^{-\beta^2y_0^2/2}}{x_0^\sigma y_0},\end{aligned} \quad (15.61)$$

where $c_{\sigma,j}$ is as in (15.57) and $l_0=\sqrt{x_0^2+y_0^2}=|u_{0,+}|$.

By (15.57) and Lemma 15.14, for any $0<\beta<1$,

$$\frac{c_{\sigma,1}}{l_0^{\sigma+2}} = \frac{\sigma(\sigma+1)/2}{l_0^{\sigma+2}} \le \frac{\sigma(\sigma+1)/2}{t}\cdot\frac{1}{l_0^\sigma},$$

$$\begin{aligned}\frac{c_{\sigma,2}}{((1-\beta)l_0)^{\sigma+4}} &= \frac{\sigma(\sigma+1)(\sigma+2)(\sigma+3)}{8}\cdot\frac{(1-\beta)^{-(\sigma+4)}}{l_0^{\sigma+4}} \\ &\le \frac{\sigma(\sigma+1)(\sigma+2)(\sigma+3)}{8(1-\beta)^{\sigma+4}t^2}\cdot\frac{1}{l_0^\sigma}.\end{aligned}$$

Incidentally, the last term in (15.61) appears only if $y_0 \ge \sqrt{1-(1-\beta)^2}l_0$, as otherwise $x_0 \ge (1-\beta)l_0$, in which case Cor. 15.13 gives us (15.61) without the last term.

It remains to bound the integral going from $x_0-i\infty$ to x_0-2iy_0. By (15.43),

$$\Re\phi(x_0+iy) = \Re\phi(u_{0,+}) + \frac{y^2-y_0^2}{2} + \ell(y_0-y) + t(\arg(x_0+iy_0)-\arg(x_0+iy_0)).$$

Hence, writing $\theta_0=\arg(x_0+iy_0)-\arg(x_0-2iy_0)$, we have

$$\begin{aligned}\int_{x_0-i\infty}^{x_0-2iy_0} e^{-\Re\phi(u)}|u|^{-\sigma}|du| &\le \frac{e^{-\Re\phi(u_{0,+})}}{|u_{0,+}|^\sigma}e^{-\theta_0 t}\int_{-\infty}^{-2y_0} e^{-\frac{y^2-y_0^2}{2}}dy \\ &\le \frac{e^{-\Re\phi(u_{0,+})}}{2y_0|u_{0,+}|^\sigma}e^{-\theta_0 t-\frac{3}{2}y_0^2},\end{aligned}$$

where we bound $|x_0+2y_0 i|$ crudely from below by $|u_{0,+}|$. Since $\ell>0$, we know that $y>x$ (by (15.31)) and so $\theta_0>\pi/4+\arctan 2$. By Lemma 15.14, $2y_0\ge\sqrt{2t}$ and $(3/2)y_0^2\ge 3t/4$. Hence

$$\frac{e^{-\Re\phi(u_{0,+})}}{2y_0|u_{0,+}|^\sigma}e^{-\theta_0 t-\frac{3}{2}y_0^2} \le \sqrt{2\pi}\frac{e^{-\Re\phi(u_{0,+})}}{|u_{0,+}|^\sigma}\frac{1}{t^2}\cdot\frac{t^{3/2}}{2\sqrt{\pi}}e^{-\theta_1 t},$$

where $\theta_1=\pi/4+\arctan 2+3/4$.

It is easy to check that $t^{3/2}e^{-\theta_1 t}$ is decreasing for $t \geq (3/2)/\theta_1$, and that $(3/2)/\theta_1 < 6/\sqrt{5}$. Hence we may replace $t^{3/2}e^{-\theta_1 t}/2\sqrt{\pi}$ with its value $0.00103\ldots$ at $t = 6/\sqrt{5}$.

□

We come to our final bound for $\delta < 0$.

Corollary 15.17. *Let $f_\delta(x) = e^{-x^2/2}e(\delta x)$, $\delta \in \mathbb{R}$. Let F_δ be the Mellin transform of f_δ. Let $s = \sigma + it$, $0 \leq \sigma \leq 2$. Assume $t \geq \max(4\pi|\delta|, 40)$ and $\delta < 0$. Then*

$$|F_\delta(s)| \leq \left(1 + \frac{c_\sigma}{t}\right) \frac{\sqrt{2\pi} t^{\sigma-1/2}}{(\max(\sqrt{t}, 2\pi|\delta|))^\sigma} \cdot e^{-E(\mathscr{r})t}, \tag{15.62}$$

where $\mathscr{r} = t/\pi^2\delta^2$, $c_\sigma = 5.6$ for $0 \leq \sigma \leq 1$, $c_\sigma = 26.94$ for $1 < \sigma \leq 2$, and

$$E(\mathscr{r}) = \frac{1}{2}\arccos\frac{1}{\upsilon(\mathscr{r})} - \frac{\upsilon(\mathscr{r}) - 1}{\mathscr{r}} \tag{15.63}$$

for $j(\mathscr{r}) = \sqrt{\mathscr{r}^2 + 1}$, $\upsilon(\mathscr{r}) = \sqrt{(1 + j(\mathscr{r}))/2}$.

Proof. By (15.22) and (15.24),

$$|F_\delta(s)| = \frac{e^{-2\pi^2\delta^2}|\Gamma(s)|}{\sqrt{2\pi}} \left| \int_{x_0 - i\infty}^{x_0 + i\infty} e^{-\phi(u)} u^{-\sigma} du \right|,$$

where $\phi : \mathbb{C} \to \mathbb{C}$ is as in (15.37) and $u_{0,+} = x_0 + iy_0 \in \mathbb{C}$ is as in (15.29).

By Proposition 15.16 and (15.30),

$$\frac{1}{\sqrt{2\pi}} \left| \int_{x_0 - i\infty}^{x_0 + i\infty} e^{-\phi(u)} u^{-\sigma} du \right| \leq \left(\frac{1 + \epsilon_{\sigma,\beta}(t)}{|u_{0,+}|^\sigma} + \sqrt{\frac{2}{\pi}} \frac{e^{-\beta^2 y_0^2/2}}{x_0^\sigma y_0} \right) e^{\frac{\ell}{2} y_0 + \arg(u_{0,+})t},$$

where $\ell = -2\pi\delta$, and $\epsilon_{\sigma,\beta}(t)$ is bounded as in (15.59).

By Lemma 15.6,

$$e^{-2\pi^2\delta^2} e^{\frac{\ell}{2} y_0} = e^{\frac{\ell^2}{4}(\upsilon(\mathscr{r}) - 1)} = e^{\frac{(\upsilon(\mathscr{r})-1)}{\mathscr{r}} t}, \tag{15.64}$$

where $\mathscr{r} = 4t/\ell^2$. Again by Lemma 15.6,

$$\arg(u_{0,+})t = \left(\frac{1}{2}\arccos\frac{-1}{\upsilon(\mathscr{r})}\right) t = \left(\frac{\pi}{2} - \frac{1}{2}\arccos\frac{1}{\upsilon(\mathscr{r})}\right) t. \tag{15.65}$$

Hence

$$|F_\delta(s)| \leq |\Gamma(s)| e^{\frac{\pi}{2}t} e^{-E(\mathscr{r})t} \left(\frac{1 + \epsilon_{\sigma,\beta}(t)}{|u_{0,+}|^\sigma} + \sqrt{\frac{2}{\pi}} \frac{e^{-\beta^2 y_0^2/2}}{x_0^\sigma y_0} \right), \tag{15.66}$$

where $E(\mathscr{r})$ is as in (15.63). By Corollary 3.10,

$$|\Gamma(s)| e^{\frac{\pi}{2}t} \leq \left(1 + O^*\left(\frac{2}{9t}\right)\right) \cdot \sqrt{2\pi} |t|^{\sigma - 1/2}.$$

Let us now bound and collect our error terms. By Lemma 15.15 and our assumptions on t, we know that $x_0 y_0/|u_{0,+}| \geq 4/3$, and so

$$\sqrt{\frac{2}{\pi}} \frac{e^{-\beta^2 y_0^2/2}}{x_0^\sigma y_0} \leq \frac{\left(\frac{3}{4}\right)^\sigma}{|u_{0,+}|^\sigma} \cdot \sqrt{\frac{2}{\pi}} \frac{e^{-\beta^2 y_0^2/2}}{y_0^{1-\sigma}}.$$

By the bound $y \geq \sqrt{t/2}$ from Lemma 15.14 and the assumption $t \geq 40$, we know that $y_0 \geq \sqrt{20}$. Since $e^{-\beta^2 y_0^2/2} y_0^{\sigma+1}$ is decreasing for $y_0 \geq \sqrt{\sigma+1}/\beta$,

$$\frac{e^{-\beta^2 y_0^2/2}}{y_0^{1-\sigma}} \leq \frac{1}{y_0^2} e^{-20\beta^2/2} 20^{\frac{\sigma+1}{2}} \leq \frac{2e^{-10\beta^2} 20^{\frac{\sigma+1}{2}}}{t} \tag{15.67}$$

provided that $\beta \geq \sqrt{\sigma+1}/\sqrt{20}$.

The term involving β in $\epsilon_{\sigma,\beta}(t)$ is

$$\frac{\sigma(\sigma+1)(\sigma+2)(\sigma+3)}{8(1-\beta)^{\sigma+4} t^2} \leq \frac{\sigma(\sigma+1)(\sigma+2)(\sigma+3)}{8 \cdot 40(1-\beta)^{\sigma+4}} \cdot \frac{1}{t}. \tag{15.68}$$

Therefore, the expression within parenthesis in (15.66) is at most $(1+c_{\beta,\sigma}/t)/|u_{0,+}|^\sigma$, where

$$c_{\beta,\sigma} \leq \sqrt{\frac{160}{\pi}} e^{-10\beta^2} \left(\frac{3}{4}\right)^\sigma 20^{\sigma/2} + \frac{\sigma(\sigma+1)(\sigma+2)(\sigma+3)}{8 \cdot 40(1-\beta)^{\sigma+4}} + \frac{\sigma(\sigma+1)}{2} + \frac{0.00104}{t}.$$

Looking at (15.67) and (15.68) for $\sigma = 1$ and $\sigma = 2$, we see, after a little trial and error, that it makes sense to choose $\beta = 0.4899$ for $0 \leq \sigma \leq 1$ and $\beta = 0.4269$ for $1 < \sigma \leq 2$. Then

$$c_{\beta,\sigma} \leq \begin{cases} 5.34309 & \text{for } 0 \leq \sigma \leq 1 \\ 26.56069 & \text{for } 1 < \sigma \leq 2. \end{cases}$$

Finally,

$$\left(1 + \frac{2}{9t}\right)\left(1 + \frac{c_{\beta,\sigma}}{t}\right) \leq 1 + \left(\frac{2}{9} + \left(1 + \frac{2}{9 \cdot 40}\right) c_\sigma\right)\frac{1}{t} \leq 1 + \frac{c'_\sigma}{t},$$

where $c'_\sigma = 5.595$ for $0 \leq \sigma \leq 1$ and $c'_\sigma = 26.93048$ for $1 < \sigma \leq 2$. We know from Lemma 15.14 that $|u_{0,+}| \geq \max(\sqrt{t}, \ell)$, and so we conclude that

$$|F_\delta(s)| \leq \left(1 + \frac{c'_\sigma}{t}\right) \frac{\sqrt{2\pi} t^{\sigma-1/2}}{(\max(\sqrt{t}, \ell))^\sigma} \cdot e^{-E(r)t}.$$

□

Remarks on a better contour and Laplace's method. In order to obtain a result like Corollary 15.17, but with the right constant in front, we would need to choose a contour going through $u_{0,+}$ in the optimal direction determined in Lemma 15.7. For instance, it can consist of a short straight segment I in that direction, together with two vertical half-lines going up to infinity.

Within the short segment I going through $u_{0,+}$, it is important to work with $\Re\phi(u)$ itself, rather than with the lower bound provided by Lemma 15.9. (On the vertical half-lines, we may use Lemma 15.9.) The integral over I can be determined by the Laplace method, which we are about to outline for our particular case. A more general and detailed description can be found in [dB81, §4].

For u on I, we can write $\Re\phi(u)$ in the form $\kappa_0 + tf_{\rho}(r)$, where r is the parameter in a parametrization $u = u_{0,+} + rv$ of I, with $v \in \mathbb{C}$ of norm proportional to ℓ^2, and hence to t (since $\ell^2 = (4/\rho)t$). Here $\kappa_0 = \Re\phi(u_{0,+})$, and so $f_{\rho}(0) = 0$. We also know that $f'_{\rho}(0) = 0$, since $u_{0,+}$ is a saddle point. It will be useful to assume that I is short enough that r ranges on an interval $[-\tau, \tau]$ with $\tau \ll t^{-1/3}$.

We need to estimate an integral

$$\int_{-\tau}^{\tau} g(r) e^{-tf_{\rho}(r)} dr. \tag{15.69}$$

We can write $f_{\rho}(r) = a_2 r^2 + a_3 r^3 + \ldots$, where $a_i \in \mathbb{C}$ depend on ρ. The main factor in the integrand will be $e^{-a_2 t r^2}$. The remaining factor

$$g(r) \exp(-t(a_3 r^3 + a_4 r^4 + \ldots))$$

can be written as a double power series in the variables tr^3 and r. We would truncate the series at some point. The estimation of the non-truncated terms rests on integrals of the form $\int_{-\infty}^{\infty} P(r, tr^3) e^{-a_2 t r^2} dr$, with P a monomial of bounded degree. We would bound error terms by means of integrals of the form $\int_{-\infty}^{\infty} |r|^k e^{-a_2 t r^2} dr$ and $\int_{-\infty}^{\infty} |tr^3|^k e^{-a_2 t r^2} dr$. See the end of [dB81, §4.4] for details.

The resulting estimate for (15.69) would be of the form $c_0 + c_1/t + \ldots + c_M/t^M + O(C_M/t^{M+1})$, for M of our choice, with c_i and C_M depending on ρ. The final result would be an estimate for $F_\delta(s)$ much like (15.62), but with the right constant in front.

15.5.4 The case $\delta > 0$

If $\delta > 0$, then, as we saw in §15.2.1, the phase is never stationary, and we should expect $F_\delta(s)$ to be small. Indeed, it becomes clear quickly that it is fairly simple to use the saddle-point method to obtain good upper bounds on $F_\delta(s)$ – that is, good enough to suffice for practical purposes.

Let us try, however, to obtain upper bounds of the right order of magnitude, just as for $\delta < 0$. We could proceed much as for $\delta < 0$. Some technical difficulties disappear – for instance, for $u_{0,+}$ defined as before, we obtain from (15.33) that $\arg(u_{0,+}) \in [0, \pi/4]$, and so $\Re u_{0,+} \geq \Im u_{0,+}$, with the consequence that a vertical contour through $u_{0,+}$ never gets much closer to the origin than $u_{0,+}$ itself is. Since we have been working with an integral on the variable u having a factor of $u^{-\sigma}$ in the integrand, it is clear why not approaching the origin is useful.

At the same time, several other difficulties appear. For instance, for $\delta > 0$, a vertical path of integration can be very far from optimal, as we saw in Figure 15.2. There is

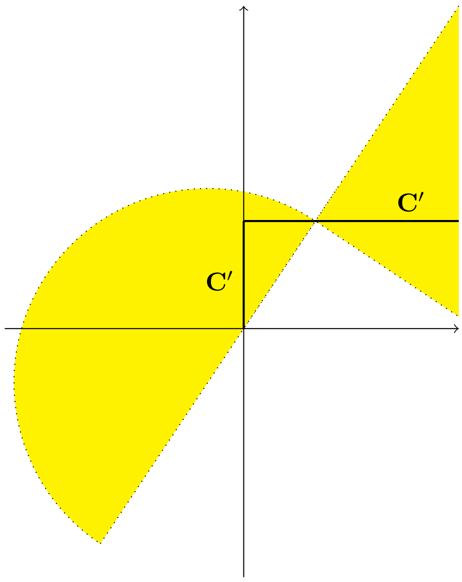

Figure 15.6: Contour $\mathbf{C}'$ for $\delta > 0$, $t > 0$

also the fact that, for $\delta > 0$ and $\ell = -2\pi\delta$, the vertical line through $u_{0,+}$ leaves the shaded region R_2 in Figure 15.4 quite quickly.

Instead, let us proceed as follows. We will use the expression for $U(a, z)$ given by Lemma 15.5, or, what amounts to the same, the expression for $F_\delta(s)$ given by its definition (15.17) as a Mellin transform. We can of course treat the variable t in (15.21) – or the variable x in (15.17) – as a complex variable u. The exponent $-u^2/2-zu$ from (15.21) or (15.17) equals the exponent $-zu + u^2/2$ from (15.20) with sign changed, provided that we also change the sign of z. In other words, we can write

$$F_\delta(s) = \int_0^\infty e^{\phi(u)} u^{\sigma-1} du$$

with $\ell = 2\pi\delta$ rather than $\ell = -2\pi\delta$, where $\phi(u)$ is as in (15.37).

Let $\ell = 2\pi\delta$, then. We will work with a contour $\mathbf{C}'$ starting at the origin and ending at $+\infty$. The saddle point $u_{0,+}$ is exactly as before, for the same value of ℓ. The direction of steepest descent is orthogonal to the one before; thus it will make sense to choose a contour going through $u_{0,+}$ horizontally.

We can readily see that, by Lemma 15.8, and analogously to Lemma 15.9, the bound

$$\Re\phi(u) \le \Re\phi(u_{0,+}) - \Re\frac{(u-u_{0,+})^2}{2} \tag{15.70}$$

holds for u in the region shaded in Figure 15.6, which is simply the region R described in Lemma 15.9 flipped along the line through $u_{0,+}$ and the origin. We can thus allow ourselves to let $\mathbf{C}'$ be the contour starting from the origin, going upwards, and then going to the right horizontally through $u_{0,+}$ up to $+\infty$, as depicted in Figure 15.6.

Let us start by bounding an integral that will appear in a lower-order term. We will treat the range of y close to 0 in Lemma 15.19, since it needs special consideration due to the factor y^{s-1}.

Lemma 15.18. *Let $\ell \geq 0$, $y_0 \geq \max(\ell, 1)$, $s = \sigma + it$, $\sigma \geq 0$. Then,*

$$\int_{\max(\ell,1)}^{y_0} e^{\frac{y^2}{2}-\ell y} y^{s-1} dy \leq 3.31811 \cdot e^{\frac{y_0^2}{2}-\ell y_0} y_0^{\sigma-1}.$$

The constant here is not claimed to be even close to optimal.

Proof. First of all, for any $r > 0$,

$$\int_0^r e^{\frac{y^2}{2}-ry} dy = e^{-\frac{r^2}{2}} \int_0^r e^{\frac{1}{2}(y-r)^2} dy = \sqrt{2} e^{-\frac{r^2}{2}} \int_0^{\frac{r}{\sqrt{2}}} e^{y^2} dy = \sqrt{2} D_+(r/\sqrt{2}), \tag{15.71}$$

where $D_+(x)$ is the Dawson function (4.5). Similarly,

$$\int_1^r e^{\frac{y^2}{2}-ry} dy = \sqrt{2} e^{-\frac{r^2}{2}} \int_0^{\frac{r-1}{\sqrt{2}}} e^{y^2} dy = e^{-r} \sqrt{2e} D_+((r-1)/\sqrt{2}). \tag{15.72}$$

By (4.9), the maximum c_{D_+} of $\sqrt{2} D_+(x)$ is ≤ 0.76516. For $0 \leq r' \leq y_0$,

$$\begin{aligned} \int_{r'}^{y_0} e^{\frac{y^2}{2}-\ell y} dy &= \int_{r'}^{y_0} e^{\frac{(y_0-(y_0-y))^2}{2} - \ell(y_0-(y_0-y))} dy \\ &= e^{\frac{y_0^2}{2}-\ell y_0} \int_0^{y_0-r'} e^{\frac{y^2}{2}-(y_0-\ell)y} dy. \end{aligned} \tag{15.73}$$

For $\sigma \geq 1$, we conclude from (15.71) (with $r = y_0 - \ell$) and (15.73) (with $r' = \ell$) that

$$\left| \int_\ell^{y_0} e^{\frac{y^2}{2}-\ell y} y^{s-1} dy \right| \leq y_0^{\sigma-1} \int_\ell^{y_0} e^{\frac{y^2}{2}-\ell y} dy \leq c_{D_+} e^{\frac{y_0^2}{2}-\ell y_0} y_0^{\sigma-1}. \tag{15.74}$$

Assume now that $0 \leq \sigma < 1$. Using (15.72) instead of (15.71), we see that, for $y_0 \geq \max(\ell, 1) + 1$,

$$\int_{\max(\ell,1)}^{y_0-1} e^{\frac{y^2}{2}-\ell y} y^{\sigma-1} dy \leq e^{1/2-(y_0-\ell)} c_{D_+} e^{\frac{y_0^2}{2}-\ell y_0} \max(\ell,1)^{\sigma-1}.$$

For $r \geq 1$, $r \mapsto e^r r^{\sigma-1}$ is increasing; if $r < 1$, then $e^r < e$. Hence

$$\int_{\max(\ell,1)}^{y_0-1} e^{\frac{y^2}{2}-\ell y} y^{\sigma-1} dy \leq e^{-1/2} c_{D_+} e^{\frac{y_0^2}{2}-\ell y_0} (y_0-1)^{\sigma-1}.$$

At the same time, by (15.73), for any $y_0 \geq 1$,

$$\int_{\max(y_0-1,1)}^{y_0} e^{\frac{y^2}{2}-\ell y} y^{\sigma-1} dy \leq e^{\frac{y_0^2}{2}-\ell y_0} \max(y_0-1,1)^{\sigma-1} \int_0^1 e^{\frac{y^2}{2}-(y_0-\ell)y} dy. \tag{15.75}$$

Since $y_0 \geq \ell$, the integral on the right side of (15.75) is bounded by

$$\int_0^1 e^{\frac{y^2}{2}} dy \leq \sqrt{2} \int_0^{\frac{1}{\sqrt{2}}} e^{x^2} dx = c'_{D_+}, \tag{15.76}$$

where $c'_{D_+} = \sqrt{2e} D_+(1/\sqrt{2}) \leq 1.19496$. Noting that $\max(y_0-1,1)^{\sigma-1} \leq 2y_0^{\sigma-1}$, we conclude that, for $0 \leq \sigma < 1$,

$$\int_{\max(\ell,1)}^{y_0} e^{\frac{y^2}{2}-\ell y} y^{\sigma-1} dy \leq 2\left(\frac{c_{D_+}}{\sqrt{e}} + c'_{D_+}\right) e^{\frac{y_0^2}{2}-\ell y_0} y_0^{\sigma-1}. \tag{15.77}$$

Since the bound (15.74) is stronger than (15.77), we conclude that (15.77) is true for all $\sigma \geq 0$. □

Lemma 15.19. *Let $\ell > 0$, $y_0 \geq \max(\ell, 1)$, $s = \sigma + it$, $0 \leq \sigma \leq 2$, $s \neq 0$. Let*

$$\int_0^{\max(\ell,1)} e^{\frac{y^2}{2}-\ell y} y^{s-1} dy \leq 0.4641 + \frac{3.84369}{|s|}.$$

The condition $\sigma \leq 2$ serves only to simplify an expression; it could be easily removed.

Proof. Since $e^{-\ell}\ell^{\sigma-1} \leq e^{-1}$ for $\ell \geq 1$ and $0 \leq \sigma \leq 2$, we see that, for $\ell \geq 1$,

$$\left| \int_1^{\ell} e^{\frac{y^2}{2}-\ell y} y^{s-1} dy \right| \leq e^{-\ell} c_{D_+} \sqrt{e} \leq c_{D_+}/\sqrt{e}.$$

Let $\ell' = \min(\ell, 1)$. By integration by parts,

$$\int_0^{\ell'} e^{\frac{y^2}{2}-\ell y} y^{s-1} dy = \frac{e^{\frac{(\ell')^2}{2}-\ell\ell'} (\ell')^s}{s} + \frac{\ell}{s}\int_0^{\ell'} e^{\frac{y^2}{2}-\ell y} y^s dy - \frac{1}{s}\int_0^{\ell'} e^{\frac{y^2}{2}-\ell y} y^{s+1} dy.$$

The first term on the right is $\leq 1/|s|$ in absolute value. We may use the bound in (15.76) for the last integral. For the next to last one, we use

$$\int_0^1 e^{\frac{y^2}{2}-\ell y} y^{\sigma} dy \leq \sqrt{e}\int_0^{\infty} e^{-\ell y} dy \leq \frac{\sqrt{e}}{\ell}.$$

Consequently,

$$\left| \int_0^{\ell'} e^{\frac{y^2}{2}-\ell y} y^{s-1} dy \right| \leq \frac{1 + \sqrt{e} + c'_{D_+}}{|s|}.$$

□

Proposition 15.20. *Let $t, \ell, \sigma \in \mathbb{R}$, $t \geq 2$, $\ell > 0$, $0 \leq \sigma \leq 2$. Let $\phi : \mathbb{C} \to \mathbb{C}$ be as in (15.37) and $u_{0,+} = x_0 + iy_0 \in \mathbb{C}$ be as in (15.29). Then*

$$\left|\int_0^\infty e^{\phi(u)} u^{\sigma-1} du\right| \leq \left(1 + \frac{1}{\sqrt{2t}}\right) \frac{\sqrt{2\pi}}{|u_{0,+}|^{1-\sigma}} e^{-\left(\frac{\pi}{2} + \frac{2}{r} - E(r)\right)t} + \left(c_1 e^{\frac{y_0^2}{2} - \ell y_0} y_0^{\sigma-1} + c_{0,s}\right) e^{-\frac{\pi}{2}t}, \tag{15.78}$$

where $E(r)$ is as in (15.2) and

$$c_1 = 3.31811, \qquad c_{0,s} = 0.4641 + \frac{3.84369}{|s|}, \tag{15.79}$$

Proof. We change the contour of integration to the contour $\mathbf{C}'$ defined as the union of the segment $\mathbf{C}'_1$ from 0 to iy_0 and the horizontal ray $\mathbf{C}'_2$ from iy_0 to $+\infty$:

$$F_\delta(s) = \int_{\mathbf{C}'} e^{\phi(u)} u^{\sigma-1} du.$$

On the segment $\mathbf{C}'_1$, the integral equals

$$\int_{\mathbf{C}'_1} e^{\phi(u)} u^{\sigma-1} du = i^\sigma e^{-\frac{\pi}{2}t} \int_0^{y_0} e^{\frac{y^2}{2} - \ell y} y^{s-1} dy.$$

We apply Lemmas 15.18 and 15.19. (By Lemma 15.14 and the assumption $t \geq 2$, we know that the condition $y_0 \geq 1$ is fulfilled.)

By the bound (15.70), which is valid on all of $\mathbf{C}'$,

$$\left|\int_{\mathbf{C}'_2} e^{\phi(u)} u^{\sigma-1} du\right| \leq \int_{\mathbf{C}'_2} e^{\Re\phi(u)} |u|^{\sigma-1} |du| \leq e^{\Re\phi(u_{0,+})} \int_0^\infty e^{-\frac{(x-x_0)^2}{2}} |x + iy_0|^{\sigma-1} dx.$$

Applying Cor. 15.11 with $1-\sigma$ in place of σ, we see that

$$\int_{-\infty}^\infty e^{-\frac{(x-x_0)^2}{2}} |x + iy_0|^{\sigma-1} dx \leq \frac{\sqrt{2\pi}}{l_0^{1-\sigma}} + \frac{c_\sigma}{y_0^{3-\sigma}} \leq \frac{\sqrt{2\pi}}{l_0^{1-\sigma}} \left(1 + \frac{1/\sqrt{2}}{l_0^2}\right),$$

where $l_0 = |x_0 + iy_0| \leq \sqrt{2} y_0$ and

$$c_\sigma = \begin{cases} (1-\sigma)\sqrt{2\pi}/e^{3/2} & \text{if } 0 \leq \sigma \leq 1, \\ (\sigma - 1)\sqrt{2\pi}/2 & \text{if } 1 < \sigma \leq 2; \end{cases}$$

we verify that $c_\sigma 2^{(3-\sigma)/2}$ takes its maximum at $\sigma = 2$ (namely, $1/\sqrt{2}$). By Lemma 15.14, $|l_0| \geq \sqrt{t}$. By (15.30), (15.64) and (15.65),

$$\Re\phi(u_{0,+}) = e^{2\pi^2\delta^2} e^{-\frac{v(r)-1}{r}t} e^{-\left(\frac{\pi}{2} - \frac{1}{2}\arccos\frac{1}{v(r)}\right)t} = e^{-\left(\frac{\pi}{2} + \frac{2}{r} - E(r)\right)t}.$$

□

The following lemma will be useful now and later.

Lemma 15.21. *Let $E(\mathfrak{r})$ be as in (15.2). Then*

$$E'(\mathfrak{r}) = \frac{\upsilon(\mathfrak{r}) - 1}{\mathfrak{r}^2}.$$

Proof. Since $\arccos'(t) = -1/\sqrt{-t^2+1}$,

$$\frac{d}{d\mathfrak{r}} \frac{1}{2} \arccos \frac{1}{\upsilon(\mathfrak{r})} = \frac{\upsilon'(\mathfrak{r})}{2\upsilon^2(\mathfrak{r})} \frac{1}{\sqrt{1 - \frac{1}{\upsilon^2(\mathfrak{r})}}}.$$

Now

$$2\upsilon^2(\mathfrak{r})\sqrt{1 - \frac{1}{\upsilon^2(\mathfrak{r})}} = 2\upsilon(\mathfrak{r})\sqrt{\upsilon^2(\mathfrak{r}) - 1}$$

$$= 2\upsilon(\mathfrak{r})\sqrt{\frac{j(\mathfrak{r}) - 1}{2}} = 2\sqrt{\frac{j^2(\mathfrak{r}) - 1}{4}} = \mathfrak{r}.$$

Hence

$$E'(\mathfrak{r}) = \frac{\upsilon'(\mathfrak{r})}{\mathfrak{r}} - \frac{\upsilon'(\mathfrak{r})}{\mathfrak{r}} + \frac{\upsilon(\mathfrak{r}) - 1}{\mathfrak{r}^2} = \frac{\upsilon(\mathfrak{r}) - 1}{\mathfrak{r}^2}.$$

□

We will simplify the result of Proposition 15.20 by determining the main term. We will assume $t \geq 40$ mainly because we assumed the same in Cor. 15.17; a condition with a much smaller constant than 40 would be enough to give us a good result here.

Corollary 15.22 (to Prop. 15.20)**.** *Let $f_\delta(x) = e^{-x^2/2} e(\delta x)$, $\delta \in \mathbb{R}$. Let F_δ be the Mellin transform of f_δ. Let $s = \sigma + it$, $0 \leq \sigma \leq 2$. Assume $t \geq \max(4\pi|\delta|, 40)$ and $\delta > 0$. Then*

$$|F_\delta(s)| \leq \left(\kappa_\sigma t^{\frac{\sigma-1}{2}} e^{\left(E(\mathfrak{r}) - \frac{2}{\mathfrak{r}}\right)t} + 0.59\right) e^{-\frac{\pi}{2}t}, \tag{15.80}$$

where $\kappa_\sigma = 2.56$ for $0 \leq \sigma \leq 1$ and $\kappa_\sigma = 3.69$ for $1 \leq \sigma \leq 2$, and $E(\mathfrak{r})$ is as in (15.2). Moreover,

$$|F_\delta(s)| \leq \kappa_\sigma t^{\frac{\sigma-1}{2}} e^{-\frac{\pi}{4}t}. \tag{15.81}$$

Proof. We will sweep the term involving c_1 in (15.78) under the rug provided by one term for $\mathfrak{r}$ small and another term for $\mathfrak{r}$ large.

Consider first the case $\mathfrak{r} \leq 4$. By (15.31), $\frac{y_0^2}{2} - \ell y_0 = g(\mathfrak{r}) y_0^2$, where

$$g(\mathfrak{r}) = \frac{1}{2} - \frac{2}{1 + \upsilon(\mathfrak{r})}$$

for $\upsilon(\mathfrak{r})$ as in Lemma 15.6. Since υ is an increasing function, g is also increasing, and so, for $\mathfrak{r} \leq 4$, $g(\mathfrak{r}) \leq g(4) = -0.26909\ldots$. Now, by Lemma 15.14, $y_0 \geq \ell = \sqrt{4t/\mathfrak{r}} \geq \sqrt{4t/4} \geq \sqrt{40}$. Hence, since $0 \leq \sigma \leq 2$,

$$c_1 e^{\frac{y_0^2}{2} - \ell y_0} y_0^{1-\sigma} \leq c_1 e^{g(4) y_0^2} y_0 \leq 0.00044\ldots$$

for c_1 as in (15.79), and so, for $c_{0,s}$ also as in (15.79),

$$c_1 e^{\frac{y_0^2}{2} - \ell y_0} y_0^{1-\sigma} + c_{0,s} \leq 0.56064.$$

By Lemma 15.21, $E'(\mathscr{r}) = (\upsilon(\mathscr{r}) - 1)/\mathscr{r}^2 > 0$, and so E is an increasing function. Hence, $2/\mathscr{r} - E(\mathscr{r})$ is a decreasing function, and thus, for $\mathscr{r} \leq 4$, $2/\mathscr{r} - E(\mathscr{r}) \geq c_0$ for

$$c_0 = 2/4 - E(4) = 0.20216\ldots .$$

Therefore, by Lemma 15.14 and our assumptions $t \geq 2\ell$, $t \geq 40$,

$$\frac{e^{-\left(\frac{2}{\mathscr{r}} - E(\mathscr{r})\right)t}}{|u_{0,+}|^{1-\sigma}} \leq \max\left(\sqrt{2t}, \frac{3}{2}\frac{t}{2}\right) e^{-c_0 t} \leq \frac{3}{2}\frac{40}{2} e^{-40 c_0} = 0.00922\ldots$$

Since $t \geq 40$, we see that

$$\left(1 + \frac{1}{\sqrt{2t}}\right)\sqrt{2\pi} \leq 2.55094 \tag{15.82}$$

for any $\mathscr{r}$. We conclude that, for $\mathscr{r} \leq 4$,

$$|F_\delta(s)| \leq (0.56064 + 0.02355) e^{-\frac{\pi}{2}t} = 0.58419 e^{-\frac{\pi}{2}t}.$$

Consider now $\mathscr{r} > 4$. We can write $\frac{y_0^2}{2} - \ell y_0 = f(\mathscr{r}) t$, where

$$f(\mathscr{r}) = \frac{4}{\mathscr{r}}\left(\frac{1}{2}\left(\frac{1+\upsilon(\mathscr{r})}{2}\right)^2 - \frac{1+\upsilon(\mathscr{r})}{2}\right) = \frac{j(\mathscr{r}) - 1}{4\mathscr{r}} - \frac{1+\upsilon(\mathscr{r})}{\mathscr{r}}$$

and $j(\mathscr{r}) = \sqrt{\mathscr{r}^2 + 1}$, as usual. Since $E'(\mathscr{r}) = (\upsilon(\mathscr{r}) - 1)/\mathscr{r}^2$ and $f'(\mathscr{r}) > ((j(\mathscr{r}) - 1)/4\mathscr{r})' = 1/4j(\mathscr{r}) - (j(\mathscr{r}) - 1)/4\mathscr{r}^2$ we see that

$$\left(E(\mathscr{r}) - \frac{2}{\mathscr{r}} - f(\mathscr{r})\right)' = \frac{\upsilon(\mathscr{r})}{\mathscr{r}^2} + \frac{j(\mathscr{r}) + 3}{4\mathscr{r}^2} - \frac{1}{4j(\mathscr{r})} > \frac{\mathscr{r}}{4\mathscr{r}^2} - \frac{1}{4\mathscr{r}} = 0,$$

since $j(\mathscr{r}) > \mathscr{r}$. Hence, for $\mathscr{r} > 4$,

$$-\left(\frac{2}{\mathscr{r}} - E(\mathscr{r})\right) - f(\mathscr{r}) > c',$$

where $c' = E(4) - 2/4 - f(4) = 0.25275$. Therefore,

$$c_1 e^{\frac{y_0^2}{2} - \ell y_0} y_0^{\sigma - 1} < c_1 \max(1, 2^{\frac{1-\sigma}{2}}) e^{-c' t} \frac{e^{-\left(\frac{2}{\mathscr{r}} - E(\mathscr{r})\right)t}}{|u_{0,+}|^{1-\sigma}} < 0.000191 \frac{e^{-\left(\frac{2}{\mathscr{r}} - E(\mathscr{r})\right)t}}{|u_{0,+}|^{1-\sigma}}. \tag{15.83}$$

We conclude from (15.82) and (15.83) that, for $\mathscr{r} > 4$,

$$\left(1 + \frac{1}{\sqrt{2t}}\right)\frac{\sqrt{2\pi}}{|u_{0,+}|^{1-\sigma}} e^{-\left(\frac{2}{\mathscr{r}} - E(\mathscr{r})\right)t} + c_1 e^{\frac{y_0^2}{2} - \ell y_0} y_0^{\sigma - 1} < 2.55114 \frac{e^{-\left(\frac{2}{\mathscr{r}} - E(\mathscr{r})\right)t}}{|u_{0,+}|^{1-\sigma}}.$$

If $0 \leq \sigma \leq 1$, we simply use the lower bound $|u_{0,+}| \geq \sqrt{t}$ from Lemma 15.14. Say $1 \leq \sigma \leq 2$. It is easy to see that $(\upsilon(\digamma)^2 + \upsilon(\digamma))/\digamma$ is a decreasing function of $\digamma$, and so, by (15.32) and the assumption $\digamma > 4$,

$$|u_{0,+}| \leq \sqrt{\frac{\upsilon(4)^2 + \upsilon(4)}{4}} \frac{|\ell|\sqrt{\digamma}}{\sqrt{2}} = 1.02005\ldots \cdot \sqrt{2t}.$$

Hence, for $1 \leq \sigma \leq 2$, $1/|u_{0,+}|^{1-\sigma} \leq 1.44258 t^{\frac{\sigma-1}{2}}$, and so

$$|F_\delta(s)| \leq k_\sigma t^{\frac{\sigma-1}{2}} e^{-\left(\frac{2}{\digamma} - E(\digamma)\right)t} + 0.5602 e^{-\frac{\pi}{2}t}$$

with $k_\sigma = 2.55114$ for $0 \leq \sigma \leq 1$ and $k_\sigma = 3.68021$ for $1 \leq \sigma \leq 2$.

Therefore, (15.80) holds for $\digamma$ arbitrary. It is clear from (15.2) and (15.3) that, for any $\digamma \geq 0$,

$$E(\digamma) \leq \frac{1}{2} \arccos \frac{1}{\upsilon(\digamma)} \leq \frac{\pi}{4}.$$

Thus (15.81) also holds for any $\digamma$.

□

15.6 CONCLUSION AND FINAL REMARKS

Putting Corollaries 15.17 and 15.22 together, we see that we have proved Theorem 15.1. If $t < 0$, we simply replace t and δ by $-t$ and $-\delta$; $F_\delta(s)$ is then replaced by $\overline{F_\delta(s)}$, and so its absolute value does not change. If $\delta = 0$, we apply Corollary 15.22 with $\delta \to 0^+$.

The following lemma is useful.

Lemma 15.23. *The function $E : [0, \infty) \to [0, \infty)$ in (15.2) is increasing and concave. The function $\digamma \mapsto \digamma E(\digamma)$ is convex.*

Proof. Let j and υ be as in (15.3). By Lemma 15.21,

$$E'(\digamma) = \frac{\upsilon(\digamma) - 1}{\digamma^2} = \frac{(j(\digamma) - 1)/2}{\digamma^2(\upsilon(\digamma) + 1)} = \frac{1}{2(\upsilon(\digamma) + 1)(j(\digamma) + 1)}.$$

Since $j(\digamma)$, $\upsilon(\digamma)$ are non-negative and increasing, it is evident that E' is a non-negative, decreasing function, and thus E is increasing and concave. Since E is increasing, $\digamma \mapsto \digamma E(\digamma)$ is convex. □

Chapter Sixteen

Explicit formulae

An *explicit formula*, in our context, is an expression restating a sum of the form

$$\sum_{n=1}^{\infty} \Lambda(n)\chi(n)g(n/x)$$

in terms of a sum of values $G(\rho)$ of the Mellin transform G of g at the zeros ρ of the L-function $L(s,\chi)$. For us, g will be of the form $g(t) = g_\delta(t) = \eta(t)e(\delta t)$ for some smoothing function η and some $\delta \in \mathbb{R}$. We want a formula whose error terms are good both for δ very close or equal to 0 and for δ farther away from 0. (Indeed, our choice(s) of η will be made so that the transform $G(s) = G_\delta(s)$ of g_δ decays rapidly in both cases.)

We will do as much work as we can for a general smoothing function η. To be precise: we will start by proving a very general explicit formula (Lemma 16.1), valid for a broad class of smoothing functions η. We will then give a very simple estimation of a complex integral (§16.1.3), enabling us to give a simpler explicit formula valid for a still rather large class of continuous smoothing functions (Prop. 16.6). After dealing with a well-known technical issue arising from the residue at $s = 0$ (§16.1.2, §16.1.5) we go on to show how to estimate the contribution of zeros in the critical strip (Lemmas 16.9 and 16.10). We will then be able to prove a form of the explicit formula that yields an estimate given a finite verification of GRH and a bound on the decay of G_δ (Prop. 16.11).

For each function $\eta(t)$, all or almost all we have to do is bound an integral (in Prop. 16.11) and a few norms. The first example we will work out is that of the Gaussian smoothing $\eta(t) = \sqrt{2/\pi} \cdot e^{-t^2/2}$. Then we will treat the smoothing from Part III, namely, $\eta(t) = \sqrt{2/\pi} \cdot 2(e^{-t^2/2} - e^{-2t^2})$.

We will also study the case of a function $\eta(t)$ defined as a multiple $\eta(t) = h_H(t) \cdot te^{-t^2/2}$ of $te^{-t^2/2}$, where $h_H(t)$ is chosen so that $\eta(t)$ will mimic a function of our choice. Bounding norms of $\eta(t)$ then presents some complications, deferred to Appendix A. The effect of the factor $h_H(t)$ will be to convolve the Mellin transform of $te^{-t^2/2}$ by a function of compact support on a vertical line, thus delaying the decay of η by at most a constant shift H.

16.1 A GENERAL EXPLICIT FORMULA

Explicit formulae for general smoothing functions go back at least to Guinand [Gui42] and particularly to Weil [Wei52]. However, explicit work on explicit formulae has usually been done for a specific smoothing chosen from the start. In fact, most explicit work follows the lead of Rosser [Ros41] or Rosser-Schoenfeld [RS75] in choosing a polynomial or piecewise polynomial smoothing. (Repeated integration, as in [RS75] is equivalent to a special case of piecewise polynomial smoothing.) An exception is [Kad05], which starts from Weil's explicit formula and later specifies a smoothing function based on those in [Hea92] and [Ste71]. Another one is [FK15], whose smoothing function is that from [RS03].

16.1.1 The basic explicit formula

Let us start by proving an explicit formula valid whenever the smoothing η and its derivative η' satisfy some mild assumptions.

The basic formula is completely straightforward and essentially standard, as is its proof. Let us just go briefly over the main alternatives, with which the formula here has minor differences.

Weil's explicit formula ([Wei52], included in [Wei09, pp. 48–62]; see also the expositions in [Lan94] and [MV07, §12.2]) expresses the sum of a Mellin transform over zeros of $L(s,\chi)$ in terms of a sum over integers, rather than the other way around. The distinction is not idle, in that the sum over integers is really *two* sums, one involving χ and one involving $\overline{\chi}$. We can eliminate the sum involving $\overline{\chi}$ by assuming our smoothing function $t \mapsto \eta(t/x)$ to vanish on $[0, 1/2]$. However, that will not be the case for our smoothing functions.

The main idea in deriving any explicit formula is to start with an expression giving a sum as integral over a vertical line with an integrand involving a Mellin transform (here, $G_\delta(s)$) and an L-function (here, $L(s,\chi)$). We then shift the line of integration to the left. The stronger our assumptions on our smoothing function, the further left we may shift the line. If we assumed $\eta(t)$ to vanish in a neighborhood of 0, we could proceed as in [IK04, §5.5, Exercise], shifting a line of integration to the far left. (The same holds more generally if $\eta(t)$ is constant in a neighborhood of 0, as in [FK15].) Again, we can make no such assumption.

We will impose some conditions on η that are the same or of the same kind as those in current versions of Weil's explicit formula (see the "Barner conditions" in [Lan94, Ch. XVII, §3], or [MV07, Thm. 12.13]). As usual, when we write that, say, $\eta' t^\sigma$ is in L^1, we mean it in the sense of distributions, i.e., $\|t^\sigma d\eta\| < \infty$. We also recall that by $f(x^+)$ and $f(x^-)$ we mean $\lim_{y\to x^+} f(y)$ and $\lim_{y\to x^-} f(y)$. We write $M\eta$ for the Mellin transform of η, as always, and $M\eta'$ for the Mellin transform of η', where, again, if η is not absolutely continuous, η' is to be understood in the sense of distributions.

Lemma 16.1. *Let $\eta : \mathbb{R}^+ \to \mathbb{C}$ be such that $\eta(t)t^{\sigma_1 - 1}$, $\eta'(t)t^{\sigma_1}$, $\eta'(t)t^{\sigma_0}$ are in L^1 with respect to dt for some $-1 < \sigma_0 < 0$, $\sigma_1 > 1$. Assume that $\eta(t) = (\eta(t^+) + \eta(t^-))/2$ for every $t > 0$.*

Let χ be a Dirichlet character. Then, for any $x \in \mathbb{R}^+$,

$$\sum_{n=1}^{\infty} \Lambda(n)\chi(n)\eta(n/x) = [\chi \textit{ is principal}] \cdot x \int_0^{\infty} \eta(t)dt + \mathrm{Res}_{s=0} \frac{L'(s,\chi)}{L(s,\chi)} \frac{F(s)}{s}$$
$$+ \lim_{T\to\infty} \left(\sum_{\substack{\rho \\ |\Im\rho|\le T}} \frac{F(\rho)}{\rho} \cdot x^{\rho} + \frac{1}{2\pi i} \int_{\sigma_0 - iT}^{\sigma_0 + iT} \frac{L'(s,\chi)}{L(s,\chi)} F(s) \frac{x^s}{s} ds \right), \tag{16.1}$$

where $F(s)$ is the Mellin transform of $\eta'(t)t$, the sum $\sum_\rho$ is taken over zeros ρ of $L(s,\chi)$ with $0 \le \Re\rho \le 1$ and $\rho \ne 0$.

Some remarks are in order.

1. We recall, that, in general, $[\mathbf{true}] = 1$ and $[\mathbf{false}] = 0$.
2. It is to be understood that a hypothetical zero ρ of order k would be counted k times in the sum $\sum_\rho$. As we have remarked before, it is a standard conjecture that every zero ρ of $L(s,\chi)$ has multiplicity 1.
3. We shall see in the proof that the conditions in the lemma imply that $\eta \in L^1$, and thus the first integral in (16.1) is well-defined. In fact, the conditions will imply that $\eta(t)t^{\sigma-1} \in L^1$ for every $\sigma > 0$, and so $M\eta(s)$ is well-defined for $0 < \Re s < \sigma_1$. We could thus replace $F(\rho)/\rho$ in the sum over zeros ρ by the more customary $-M\eta(\rho)$, provided that χ is primitive (as then there are no zeros ρ with $\Re\rho = 0$, $\rho \ne 0$).

Proof. Recall that, for any $u > 0$, the Mellin transform of $x \mapsto \eta(ux)$ is $u^{-s}M\eta$. Hence, for $\Re s > 1$,

$$\frac{L'(s,\chi)}{L(s,\chi)} x^s M\eta(s) = -\sum_n \Lambda(n)\chi(n) n^{-s} x^s M\eta(s)$$
$$= -\sum_n \Lambda(n)\chi(n) \int_0^{\infty} \eta(nt/x) t^{s-1} dt.$$

Since $\eta(t)t^{\sigma_1 - 1} \in L^1$, we see that

$$\sum_n \Lambda(n) \int_0^{\infty} |\eta(nt/x)| t^{\sigma_1-1} dt = \sum_n \Lambda(n)(x/n)^{\sigma_1} \int_0^{\infty} |\eta(t)| t^{\sigma_1-1} dt$$
$$\ll \sum_n \Lambda(n)(x/n)^{\sigma_1} < \infty. \tag{16.2}$$

Hence, by Fubini's theorem, for $\Re s = \sigma_1$,

$$\frac{L'(s,\chi)}{L(s,\chi)} x^s M\eta(s) = -\int_0^{\infty} \sum_n \Lambda(n)\chi(n)\eta(nt/x) t^{s-1} dt. \tag{16.3}$$

Write $S(t) = \sum_n \Lambda(n)\chi(n)\eta(nt/x)$. Again by (16.2), $S(t)t^{\sigma_1-1}$ is in L^1. Hence, the Mellin inversion formula (2.27) applies, and we deduce from (16.3) that

$$\frac{S(t^+)+S(t^-)}{2} = \frac{1}{2\pi i}\cdot \lim_{T\to\infty}\int_{\sigma_1-iT}^{\sigma_1+iT} -\frac{L'(s,\chi)}{L(s,\chi)}x^s M\eta(s)t^{-s}ds.$$

Since $\eta(t) = (\eta(t^+)+\eta(t^-))/2$ for every t, we know that $S(t) = (S(t^+)+S(t^-))/2$. We let $t=1$, and conclude that

$$\sum_n \Lambda(n)\chi(n)\eta(n/x) = \frac{1}{2\pi i}\cdot \lim_{T\to\infty}\int_{\sigma_1-iT}^{\sigma_1+iT} -\frac{L'(s,\chi)}{L(s,\chi)}M\eta(s)x^s ds.$$

What remains is simply to shift the line of integration to $\Re s = -\sigma_0$, using Cauchy's theorem. The rest of the proof consists essentially of a verification that we can do so rigorously. First, we must provide a meromorphic continuation of $M\eta$ up to $\Re s = -\sigma_0$. Let $F(s) = M(t\eta')(s)$. We know that $F(s) = -s\cdot M\eta(s)$ (see (2.33); by integration by parts) for $\Re s = \sigma_1$. Since $\eta'(t)t^{\sigma_0}$ and $\eta'(t)t^{\sigma_1}$ are in L^1, we see that $-F(s)/s$ is a meromorphic continuation of $M\eta(s)$ to $\Re s \in (\sigma_0,\sigma_1)$, continuous on the edges $\Re s = \sigma_0,\sigma_1$, and with at most one pole, viz., at $s=0$.

For f meromorphic, the function $f'(s)/f(s)$ has poles precisely at the zeros and poles of f; the residue of $f'(s)/f(s)$ is k at a zero of f of order k, and $-k$ at a pole of f of order k. We know that $L(s,\chi)$ has a pole at $s=1$ if and only if χ is principal. We also know that $L(s,\chi)$ has no poles and no zeros with $1 < \Re s \leq \sigma_1$ or $\sigma_0 \leq \Re s < 0$, since $\sigma_0 > -1$. Thus, by Cauchy's theorem, if T is such that there are no zeros of $L(s,\chi)$ with imaginary part T or $-T$,

$$\frac{1}{2\pi i}\int_{\mathscr{C}} \frac{L'(s,\chi)}{L(s,\chi)}\frac{F(s)}{s}x^s ds = -1_{\chi=\chi_0}F(1)x - \sum_{\substack{\rho \\ |\Im\rho|\leq T}} \frac{F(\rho)}{\rho}x^\rho + \mathrm{Res}_{s=0}\frac{L'(s,\chi)}{L(s,\chi)}\frac{F(s)}{s},$$

where $\sum_\rho$ goes over the zeros ρ of $L(s,\chi)$ with $0\leq \Re\rho\leq 1$ and $\rho\neq 0$, and $\mathscr{C}$ is the rectangular contour going from $\sigma_1 - iT$ to σ_1+iT and then to σ_0+iT, σ_0-iT and back to $\sigma_1 - iT$. Since $M\eta(s) = -F(s)/s$ for $\Re s = \sigma_1$,

$$\begin{aligned}\int_{\sigma_1-iT}^{\sigma_1+iT} &-\frac{L'(s,\chi)}{L(s,\chi)}M\eta(s)x^s ds \\ &= \int_{\mathscr{C}}\frac{L'(s,\chi)}{L(s,\chi)}\frac{F(s)}{s}x^s ds + \int_{\sigma_0+iT}^{\sigma_1+iT}\frac{L'(s,\chi)}{L(s,\chi)}\frac{F(s)}{s}x^s ds \\ &+ \int_{\sigma_0-iT}^{\sigma_0+iT}\frac{L'(s,\chi)}{L(s,\chi)}\frac{F(s)}{s}x^s ds - \int_{\sigma_0-iT}^{\sigma_1-iT}\frac{L'(s,\chi)}{L(s,\chi)}\frac{F(s)}{s}x^s ds.\end{aligned}$$

Since $\eta(t)t^{\sigma_1-1}\in L^1$, we know that $\eta(t)\cdot 1_{[1,\infty)}$ is in L^1. For $0\leq t\leq 1$,

$$|\eta(t)| \leq |\eta(1)| + \int_t^1 |\eta'(x)|dx,$$

and so, by $t\eta'(t) \in L^1$,

$$\int_0^1 |\eta(t)|dt \leq |\eta(1)| + \int_0^1 |\eta'(x)|x dx < \infty.$$

Hence $\eta \in L^1$. (The same reasoning shows, incidentally, that $\eta(t)t^{\sigma-1} \in L^1$ for every $\sigma > 0$.) We may thus conclude, by (2.33), that

$$F(1) = M(\eta'(t)t)(1) = -M\eta(1) = -\int_{0^+}^\infty \eta(t)dt.$$

We will now show that, for any given $T_0 > 0$, there is a T close to T_0 such that, not only are there no zeros ρ of $L(s,\chi)$ with $|\Im\rho| = T$, but the horizontal integrals

$$\int_{\sigma_0+iT}^{\sigma_1+iT} \frac{L'(s,\chi)}{L(s,\chi)} M\eta(s)x^s ds, \qquad \int_{\sigma_0-iT}^{\sigma_1-iT} \frac{L'(s,\chi)}{L(s,\chi)} M\eta(s)x^s ds$$

are $o(1)$. It will be enough to show that $\max_{s:\sigma_0\leq\Re s\leq\sigma_1,\Im s=T} |L'(s,\chi)/L(s,\chi)|$ is $o(|s|)$, since $|F(s)|$ is bounded for $\sigma_0 \leq \Re s \leq \sigma_1$: we have $|F(s)| \leq |\eta'(t)t^\sigma|_1 \leq |\eta'(t)t^{\sigma_0}|_1 + |\eta'(t)t^{\sigma_1}|_1$ for $\sigma_0 \leq \Re s \leq \sigma_1$. (Here is the reason why we assumed $\eta'(t)t^{\sigma_1} \in L^1$, rather than just assume that $\eta'(t)t^\sigma \in L^1$ for some $\sigma > 0$ and $\eta(t)t^{\sigma_1-1}, \eta(t)t^{\sigma'-1} \in L^1$ for some $\sigma' \in (0,\sigma)$.)

By Lemma 3.19, $L(s,\chi)$ has $\ll \log qT_0$ zeros with imaginary part between T_0 and T_0+1. Then, by the pigeonhole principle, there is an absolute constant $c > 0$ and a $T \in [T_0, T_0+1]$ such that there is no zero of $L(s,\chi)$ or $L(-s,\chi)$ whose ordinate lies in $[T - c/\log qT_0, T + c/\log qT_0]$. We apply Lemma 2.6 with $f(z) = \zeta(\sigma_1 + iT + z)$, $r = \sigma_1 + 1$ and $R = 2\sigma_1 + 3$, say. Thanks to the bound $\log L(s,\chi) \ll \log qT$ from §3.7.2 (valid for $\Re s \geq -4$ and, say, $T_0 \geq 2$), we obtain that

$$\frac{L'(s,\chi)}{L(s,\chi)} = \sum_{\substack{\rho \\ |\Im\rho - T| \leq 2\sigma_1+3}} \frac{1}{s-\rho} + O(\log qT)$$

for $\Im s = T$, $-1 \leq \Re s \leq \sigma_1$, where ρ ranges over the zeros of $L(s,\chi)$. Again by Lemma 3.19, we conclude that $L'(s,\chi)/L(s,\chi) \ll (\log qT)^2$, which is much stronger than the bound we need. It follows that

$$\int_{\sigma_0-iT}^{\sigma_0+iT} \frac{L'(s,\chi)}{L(s,\chi)} \frac{F(s)}{s} x^s ds = \int_{\mathscr{C}} \frac{L'(s,\chi)}{L(s,\chi)} \frac{F(s)}{s} x^s ds + o(1). \tag{16.4}$$

Thus, (16.1) holds at least for an increasing sequence containing at least one T in each interval $[T_0, T_0+1]$ as $T_0 \to \infty$. We apply Lemma 2.6 and Lemma 3.19 again to show that

$$\int_{\sigma_0-i\infty}^{\sigma_0+i\infty} \frac{L'(s,\chi)}{L(s,\chi)} \frac{F(s)}{s} x^s ds = o_{\sigma_0}(1), \qquad \sum_{\substack{\rho \\ |\Im\rho| \in [T_0, T_0+1]}} \frac{F(\rho)}{\rho} x^\rho = o(1).$$

Hence (16.1) holds for general $T \to \infty$. □

Given $f : \mathbb{R}^+ \to \mathbb{R}$ and $\delta \in \mathbb{R}/\mathbb{Z}$, we may of course apply Lemma 16.1 with $\eta(t) = f(t)e(\delta t)$.

16.1.2 The residue at $s = 0$

We should determine the residue

$$\mathrm{Res}_{s=0} \frac{L'(s,\chi)}{L(s,\chi)} \frac{F(s)}{s}$$

appearing in (16.1).

Lemma 16.2. *Let $\eta : \mathbb{R}^+ \to \mathbb{C}$ be such that $\eta \in L^1$ and $\eta'(t)t^\sigma \in L^1$ for σ in some neighborhood of 0. Let $F(s)$ be the Mellin transform of $\eta'(t)t$. Then the Taylor expansion of $F(s)$ around $s = 0$ is*

$$c_0 + c_1 s + c_2 s^2 + \dots$$

with

$$c_0 = \lim_{t\to 0^+} \eta(t), \qquad c_1 = -\int_0^\infty \eta'(t) \log t dt. \tag{16.5}$$

Proof. First of all,

$$F(0) = M(\eta'(t)t)(0) = \int_0^\infty \eta'(t)dt = \lim_{t\to\infty} \eta(t) - \lim_{t\to 0^+} \eta(t).$$

Because $\eta' \in L^1$, $\lim_{t\to\infty} \eta(t)$ exists; because $\eta \in L^1$, it must equal 0. Hence $c_0 = F(0) = \lim_{t\to 0^+} \eta(t)$.

The next coefficient is c_1:

$$\begin{aligned} c_1 = \lim_{s\to 0} \frac{F(s) - F(0)}{s} &= -\lim_{s\to 0} \frac{1}{s} \int_0^\infty \eta'(t)(t^s - 1)dt \\ &= -\int_0^\infty \eta'(t) \lim_{s\to 0} \frac{t^s - 1}{s} dt = -\int_0^\infty \eta'(t) \log t dt. \end{aligned}$$

Here we were able to exchange the limit and the integral because $\eta'(t)t^\sigma$ is in L^1 for σ in a neighborhood of 0. □

Corollary 16.3. *Let χ be a primitive Dirichlet character mod q. Let $\eta : \mathbb{R}^+ \to \mathbb{C}$ be such that $\eta \in L^1$ and $\eta'(t)t^\sigma \in L^1$ for σ in some neighborhood of 0. Define $F(s)$ to be the Mellin transform of $\eta'(t)t$.*

Then the residue

$$\mathrm{Res}_{s=0} \frac{L'(s,\chi)}{L(s,\chi)} \frac{F(s)}{s}$$

equals

$$\left(\lim_{t\to 0^+} \eta(t)\right) \cdot b(\chi) - \begin{cases} \int_0^\infty \eta'(t) \log t \, dt & \text{if } \chi(-1) = 1 \text{ and } q > 1, \\ 0 & \text{otherwise,} \end{cases}$$

where $b(\chi)$ is the constant term in the Laurent expansion of $L'(s,\chi)/L(s,\chi)$ at $s = 0$. Moreover,

$$b(\chi) = \begin{cases} \log \frac{2\pi}{q} + \gamma - \frac{L'(1,\overline{\chi})}{L(1,\overline{\chi})} & \text{if } q > 1, \\ \log 2\pi & \text{if } q = 1. \end{cases}$$

Proof. It is immediate from Lemma 16.2 that the residue equals $c_0 b(\chi) + c_1 b_{-1}(\chi)$, where c_i is as in (16.5) and $b_{-1}(\chi)/s + b(\chi)/s + \ldots$ is the Laurent expansion of $L'(s,\chi)/L(s,\chi)$ at 0. Use (3.68), (3.106) and (3.105). □

16.1.3 The integral for $\Re s = -1/2$.

It is time to estimate the second integral in (16.1). We start by bounding $L'(s,\chi)/L(s,\chi)$ for $\Re s = \sigma_0 < 0$. It will be convenient to fix $\sigma_0 = -1/2$.

Lemma 16.4. *Let χ be a primitive character mod q. Then, for $s = -1/2 + it$,*

$$\left|\frac{L'(s,\chi)}{L(s,\chi)}\right| \leq c + \log q + \frac{1}{2}\log\left(t^2 + \frac{9}{4}\right),$$

where

$$c = \frac{4}{9} + \frac{\pi}{2} + \frac{|\zeta'(3/2)|}{\zeta(3/2)} + \log 2\pi = 5.35835\ldots .$$

Proof. Taking logarithmic derivatives on both sides of the functional equation (3.81), we get that

$$\frac{L'(s,\chi)}{L(s,\chi)} = \log\frac{\pi}{q} - \frac{1}{2}F\left(\frac{s+\kappa}{2}\right) - \frac{1}{2}F\left(\frac{1-s+\kappa}{2}\right) - \frac{L'(1-s,\overline{\chi})}{L(1-s,\overline{\chi})}. \tag{16.6}$$

Using (3.46) and (3.47), it is easy to check that

$$-\frac{1}{2}\left(F\left(\frac{s+\kappa}{2}\right) + F\left(\frac{1-s+\kappa}{2}\right)\right) = -F(1-s) + \log 2 + \frac{\pi}{2}\cot\frac{\pi(s+\kappa)}{2} \tag{16.7}$$

both for $\kappa = 0$ and for $\kappa = 1$, and so

$$\frac{L'(s,\chi)}{L(s,\chi)} = \frac{\pi}{2}\cot\frac{\pi(s+\kappa)}{2} + \log\frac{2\pi}{q} - F(1-s) - \frac{L'(1-s,\overline{\chi})}{L(1-s,\overline{\chi})}. \tag{16.8}$$

Since $\Re s = -1/2$,

$$\left|\cot\frac{\pi(s+\kappa)}{2}\right| = \left|\frac{e^{\mp\frac{\pi}{4}i - \frac{\pi}{2}\tau} + e^{\pm\frac{\pi}{4}i + \frac{\pi}{2}\tau}}{e^{\mp\frac{\pi}{4}i - \frac{\pi}{2}\tau} - e^{\pm\frac{\pi}{4}i + \frac{\pi}{2}\tau}}\right| = 1.$$

By Lemma 3.11 and $|1-s| \geq 3/2$,

$$F(1-s) = \log(1-s) - \frac{1}{2(1-s)} + O^*\left(\frac{1}{4|s|^2}\right) = \log(1-s) + O^*\left(\frac{4}{9}\right).$$

A comparison of Dirichlet series gives

$$\left|\frac{L'(1-s,\overline{\chi})}{L(1-s,\overline{\chi})}\right| \leq \frac{|\zeta'(3/2)|}{|\zeta(3/2)|}. \tag{16.9}$$

Hence

$$\left|\frac{L'(s,\chi)}{L(s,\chi)}\right| \leq \frac{4}{9} + \frac{\pi}{2} + \frac{|\zeta'(3/2)|}{|\zeta(3/2)|} + \left|\log\frac{2\pi}{q}\right| + \frac{1}{2}\log\left(t^2+\frac{9}{4}\right).$$

□

To estimate the second integral in (16.1) for $\sigma_0 = -1/2$, it will clearly be enough to use the following bound. While the proof – based on Plancherel's identity – is simple, one might say that this is the one point in all of §16.1 that is not evident in advance, or at least involves a choice; so far, we have just been doing what one naturally does when trying to prove an explicit formula. (The proof of Weil's explicit formula is substantially different at this point.)

Lemma 16.5. *Let χ be a primitive Dirichlet character mod q. Let $\eta : \mathbb{R}^+ \to \mathbb{C}$ be an absolutely continuous function such that $\eta'(t)t^{-1/2} \in L^1$ and $\eta' \in L^2$. Define $F(s)$ to be the Mellin transform of $\eta'(t)t$.*

Then

$$\frac{1}{2\pi i}\int_{-1/2-i\infty}^{-1/2+i\infty}\left|\frac{L'(s,\chi)}{L(s,\chi)}\frac{F(s)}{s}\right||ds| \leq |\eta'|_2 \cdot (\log q + 6.083). \tag{16.10}$$

It should be clear that we need η to be continuous, or otherwise η' will not be in L^2. We assume more, namely, that η is absolutely continuous, so that η' means the same whether understood as a function or as a distribution, or, in terms of measures, $d\eta = \eta'(x)dx$, i.e., the fundamental theorem of calculus holds for η. See the discussion in §2.3.3.

Proof. By Cauchy-Schwarz, the left side of (16.10) is at most

$$\sqrt{\frac{1}{2\pi}\int_{-\frac{1}{2}-i\infty}^{-\frac{1}{2}+i\infty}\left|\frac{L'(s,\chi)}{L(s,\chi)}\cdot\frac{1}{s}\right|^2|ds|}\cdot\sqrt{\frac{1}{2\pi}\int_{-\frac{1}{2}-i\infty}^{-\frac{1}{2}+i\infty}|F(s)|^2|ds|}.$$

We now apply Plancherel (as in (2.28)), and obtain that

$$\frac{1}{2\pi}\int_{-\frac{1}{2}-i\infty}^{-\frac{1}{2}+i\infty}|F(s)|^2|ds| = \int_0^\infty |\eta'(x)|^2dx. \tag{16.11}$$

By Lemma 16.4 and the triangle inequality,

$$\sqrt{\frac{1}{2\pi}\int_{-\frac{1}{2}-i\infty}^{-\frac{1}{2}+i\infty}\left|\frac{L'(s,\chi)}{L(s,\chi)}\cdot\frac{1}{s}\right|^2|ds|} \tag{16.12}$$

is at most

$$\sqrt{\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{(\log q)^2}{1/4+t^2}dt} + \sqrt{\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{(c+\frac{1}{2}\log\left(t^2+\frac{9}{4}\right))^2}{1/4+t^2}dt}, \tag{16.13}$$

where c is as in Lemma 16.4. The expression under the first square root in (16.13) is simply $(\log q)^2$. The integral under the second square root equals

$$\int_{-C}^{C} \frac{(c + \frac{1}{2}\log(t^2 + \frac{9}{4}))^2}{1/4 + t^2} dt + O^*\left(2\int_{C}^{\infty} \frac{(c_1 + \log t)^2}{c_2 t^2} dt\right) \tag{16.14}$$

for $C > 0$ arbitrary, with $c_1 = c + (1/2)\log(1 + 9/4C^2)$ and $c_2 = 1 + 1/4C^2$. We let $C = 10^8$ and evaluate the first integral in (16.14) numerically (via ARB); it is ≤ 232.4446036. Symbolic integration gives us that the second integral is $\leq 6.16 \cdot 10^{-6}$.

We conclude that the integral under the second square root in (16.13) is at most 232.44462, and so the expression in (16.12) is $\leq \log q + 6.08233$.

□

16.1.4 Explicit formula, second version

We can now state a more worked-out version of Lemma 16.1, under stronger assumptions. We will include a phase $e(\delta t)$, $\delta \in \mathbb{R}/\mathbb{Z}$, since we will need it later.

Proposition 16.6. *Let χ be a primitive Dirichlet character mod q. Let $\delta \in \mathbb{R}/\mathbb{Z}$.*

Let $\eta : \mathbb{R}^+ \to \mathbb{C}$ be an absolutely continuous function such that $\eta' \in L^2$ and $\eta(t)t^\sigma, \eta'(t)t^\sigma, \eta'(t)t^{-1/2} \in L^1$ for some $\sigma > 1$. Write G_δ for the Mellin transform of $\eta_\delta(t) = \eta(t)e(\delta t)$. Then, for any $x \in \mathbb{R}^+$,

$$\sum_{n=1}^{\infty} \Lambda(n)\chi(n)\eta_\delta(n/x) = [q = 1] \cdot \widehat{\eta}(-\delta)x - \lim_{T\to\infty} \sum_{\substack{\rho \\ |\Im\rho| \leq T}} G_\delta(\rho)x^\rho + c_{\eta,\chi,\delta} + \frac{c_{\eta,-,q,\delta}}{\sqrt{x}}, \tag{16.15}$$

where the sum $\sum_\rho$ is taken over the non-trivial zeros of $L(s, \chi)$,

$$|c_{\eta,\chi,\delta}| \leq |\eta(0)b(\chi)| + [q \neq 1] \cdot \int_0^\infty |\eta'_\delta(t)\log t|\, dt, \tag{16.16}$$

$$|c_{\eta,-,q,\delta}| \leq |\eta'_\delta|_2 \cdot (\log q + 6.083)$$

and $b(\chi)$ is the constant term in the Laurent expansion of $L'(s, \chi)/L(s, \chi)$ at $s = 0$.

The term $\int_0^\infty |\eta'_\delta(t)\log t|\, dt$ is actually there only if $q > 1$ and $\chi(-1) = 1$.

Proof. We will apply Lemma 16.1 with $\eta_\delta(t)$ instead of $\eta(t)$. Since η is absolutely continuous, it is bounded on $(0, 1]$, and so $\eta(t)t^\sigma \in L^1$ implies $\eta(t)t^{\sigma'-1} \in L^1$ for every $\sigma' \in (0, \sigma + 1]$. Hence $G_\delta(s)$ is well-defined for $\Re s \in (0, \sigma + 1]$. It also follows that $\eta'_\delta(t)t^{\sigma'} = (\eta'(t) + 2\pi i\delta\eta(t))t^{\sigma'}$ is in L^1 for all $\sigma' \in [-1/2, \sigma]$, and that $G_\delta(s)$ equals the Mellin transform $F_\delta(s)$ of $\eta'_\delta(t)t$ for $\Re s \in (0, \sigma]$. Moreover, since $\eta'_\delta(t)t^{\sigma'} \in L^1$ for σ' in a neighborhood of 0, we know that $\eta'_\delta(t)\log t \in L^1$.

Since η is absolutely continuous and in L^1, it is bounded; being bounded and in L^1, it is in L^2. We also see that $|\eta'_\delta|_2 \leq |\eta'|_2 + 2\pi\delta|\eta|_2$, and so η'_δ is in L^2.

The conditions of Lemma 16.1 are thus fulfilled, and so are those of Corollary 16.3 and Lemma 16.5. We apply them and are done. Since χ is primitive, $L(s,\chi)$ has no zeros with $\Re s = 0$, $s \neq 0$, and thus we need not worry about whether $G_\delta(s)$ is well-defined for $\Re s = 0$. □

Proposition 16.6 leaves us with three tasks: bounding the sum of $G_\delta(\rho)x^\rho$ over all non-trivial zeros ρ with small imaginary part, bounding the sum of $G_\delta(\rho)x^\rho$ over all non-trivial zeros ρ with large imaginary part, and bounding $b(\chi)$. As we already know from (3.99), (3.100) and (3.105), bounding $b(\chi)$ is equivalent to bounding the quotient $\Lambda'(1,\overline{\chi})/\Lambda(1,\overline{\chi})$, or $L'(1,\overline{\chi})/L(1,\overline{\chi})$, and also equivalent to bounding the quantity $B(\chi)$ in the expression (3.97) coming from the Hadamard product for $L(s,\chi)$.

In the end, for our main goal, $b(\chi)$ will not matter, as we will be working with smoothing functions with $\eta(t) = 0$. It is still good to know how to estimate $b(\chi)$.

16.1.5 Bounding $b(\chi)$, or $B(\chi)$, or $L'(1,\chi)/L(1,\chi)$.

There are at least three different ways in which one can go about bounding the quantity $L'(1,\chi)/L(1,\chi)$ (or $\Lambda'(1,\chi)/\Lambda(1,\chi)$, or $B(\chi)$, or $b(\chi)$).

1. We may want to give a bound valid for all Dirichlet characters χ. Now, Lemma 2.6 gives us an expression of the form
$$\frac{L'(s,\chi)}{L(s,\chi)} = \sum_{\rho\in Z} \frac{1}{s-\rho} + \text{error term}, \tag{16.17}$$
where Z is the set of zeros of $L(s,\chi)$ on a disk around $s = 1$ of radius 1, say. It is then clear that the possibility of an exceptional zero poses a problem. The best we can do is use the bound (3.92), which will result on a bound of the form $|L'(1,\chi)/L(1,\chi)| \leq c\sqrt{q}\log^2 q$, for c a small explicit constant.
2. Since we will apply the explicit formula only for functions $L(s,\chi)$ for which we (or rather other people) have verified GRH up to a certain height, we can use an expression such as (16.17) together with our knowledge that $|1-\rho| \geq 1/2$ for every zero ρ of $L(s,\chi)$. Then we obtain a bound of the form $|L'(1,\chi)/L(1,\chi)| \leq C_1 \log q + C_2$, with C_1 and C_2 explicit.
3. For a finite number of characters χ – and we will apply the explicit formula only for a finite number – we can compute $L'(1,\chi)/L(1,\chi)$ directly.

Here (1) is the approach followed in [McC84a, §3] and [BMOR18, §6]. The quality of the resulting bound would be enough for our purposes. At the same time, it is a far larger bound than that resulting from (2) or (3).

In our context, (2) makes sense: we are assuming only that which we will also need elsewhere. One could still object that the strategy is backwards, compared to (3): verifying GRH up a height (even a trivial one) involves evaluating $L(s,\chi)$ at many points; evaluating $L(s,\chi)$ and $L'(s,\chi)$ at a single point $s = 1$ is more direct.

Let us carry out approach (2) in a way that generalizes an elegant answer given by MathOverflow contributor Lucia [Luc].

Lemma 16.7. *Let χ be a primitive Dirichlet character mod $q > 1$. Let $\sigma_0 > 1$. Assume $L(s,\chi)$ satisfies $GRH(\sigma_0/\sqrt{2(\sigma_0-1)})$. Then*

$$\left|\frac{\Lambda'(1,\chi)}{\Lambda(1,\chi)}\right| \leq \left|\frac{\Lambda'(\sigma_0,\chi)}{\Lambda(\sigma_0,\chi)}\right| + 2(\sigma_0-1)\cdot\Re\frac{\Lambda'(\sigma_0,\chi)}{\Lambda(\sigma_0,\chi)}$$

and

$$\left|\frac{L'(1,\chi)}{L(1,\chi)}\right| \leq (\sigma_0-1)\log q + c_0(\sigma_0,\kappa), \tag{16.18}$$

where $\kappa = [\chi(-1) = -1]$ and

$$c_0(\sigma,\kappa) = (1+2(\sigma-1))\left|\frac{\zeta'(\sigma)}{\zeta(\sigma)}\right| + \frac{1}{2}\left(F\left(\frac{\sigma+\kappa}{2}\right) - F\left(\frac{1+\kappa}{2}\right)\right) + (\sigma-1)\left(F\left(\frac{\sigma+\kappa}{2}\right) - \log\pi\right).$$

Thus, for instance, for $\sigma_0 = 4/3$, we assume GRH($\sqrt{8/3}$), and get the bound

$$\left|\frac{L'(1,\chi)}{L(1,\chi)}\right| \leq \frac{1}{3}\log q + \begin{cases} 3.63508 & \text{if } \chi(-1) = 1, \\ 3.76368 & \text{if } \chi(-1) = -1. \end{cases} \tag{16.19}$$

Proof. For any s, we know from (3.97) that

$$\frac{\Lambda'(1,\chi)}{\Lambda(1,\chi)} - \frac{\Lambda'(s,\chi)}{\Lambda(s,\chi)} = \sum_\rho \frac{s-1}{(1-\rho)(s-\rho)},$$

where ρ goes over the non-trivial zeros of $L(s,\chi)$. (This way of canceling out the contribution of $B(\chi)$ is standard.) We want to bound the sum over ρ here in terms of the sum over ρ in (3.102). We can work with $s = \sigma_0 > 1$ real. Then, by (3.102),

$$\Re\frac{\Lambda'(\sigma_0,\chi)}{\Lambda(\sigma_0,\chi)} = \sum_\rho \frac{\sigma_0 - \Re\rho}{|\sigma_0-\rho|^2}.$$

It is clear that, for any real t,

$$\frac{1/2}{|1/2+it|} = \cos\measuredangle ABC \leq \cos\measuredangle AB'C = \frac{\sigma_0 - 1/2}{|\sigma_0 - 1/2 + it|},$$

where A is the point $(1/2, |t|)$, C is the point $(1/2, 0)$, $B = (1,0)$ and $B' = (\sigma_0, 0)$. Hence, for ρ of the form $\rho = 1/2 + it$,

$$\frac{1}{|1-\rho||\sigma_0-\rho|} = \frac{1}{|1/2+it||\sigma_0 - 1/2 - it|} \leq 2\frac{\sigma_0 - 1/2}{|\sigma_0 - (1/2+it)|^2} = 2\frac{\sigma_0 - \Re\rho}{|\sigma_0-\rho|^2}.$$

Now recall that the non-trivial zeros of $L(s,\chi)$ are invariant under the map $\rho \mapsto 1-\overline{\rho}$. For ρ with $\Re\rho \in [0,1]$ and $\Im\rho = t$,

$$\frac{\sigma_0 - \Re\rho}{|\sigma_0-\rho|^2} + \frac{\sigma_0 - \Re(1-\overline{\rho})}{|\sigma_0 - (1-\overline{\rho})|^2} \geq \frac{\sigma_0 - \Re\rho}{|\sigma_0+it|^2} + \frac{\sigma_0 - (1-\Re\rho)}{|\sigma_0+it|^2} = \frac{2\sigma_0 - 1}{\sigma_0^2 + t^2},$$

while $1/(|1-\rho||\sigma_0-\rho|) \leq 1/t^2$. It is clear that $1/t^2 \leq (2\sigma_0-1)/(\sigma_0^2+t^2)$ if $t \geq \sigma_0/\sqrt{2(\sigma_0-1)}$. Hence, if $L(s,\chi)$ fulfills $GRH(\sigma_0/\sqrt{2(\sigma_0-1)})$,

$$\left|\sum_\rho \frac{\sigma_0-1}{(1-\rho)(\sigma_0-\rho)}\right| \leq 2(\sigma_0-1)\sum_\rho \frac{\sigma_0-\Re\rho}{|\sigma_0-\rho|^2} = 2(\sigma_0-1)\Re\frac{\Lambda'(\sigma_0,\chi)}{\Lambda(\sigma_0,\chi)},$$

and so

$$\left|\frac{\Lambda'(1,\chi)}{\Lambda(1,\chi)} - \frac{\Lambda'(\sigma_0,\chi)}{\Lambda(\sigma_0,\chi)}\right| \leq 2(\sigma_0-1)\cdot\Re\frac{\Lambda'(\sigma_0,\chi)}{\Lambda(\sigma_0,\chi)}.$$

By (3.98) (applied twice),

$$\left|\frac{L'(1,\chi)}{L(1,\chi)} - \frac{L'(\sigma_0,\chi)}{L(\sigma_0,\chi)} + \frac{1}{2}\left(F\left(\frac{1+\kappa}{2}\right) - F\left(\frac{\sigma_0+\kappa}{2}\right)\right)\right|$$
$$\leq 2(\sigma_0-1)\cdot\left(\Re\frac{L'(\sigma_0,\chi)}{L(\sigma_0,\chi)} + \frac{1}{2}F\left(\frac{\sigma_0+\kappa}{2}\right) + \frac{1}{2}\log\frac{q}{\pi}\right).$$

Since $-L'(\sigma_0,\chi)/L(\sigma_0,\chi) = \sum_n \Lambda(n)\chi(n)n^{-\sigma_0}$, we see that $|L'(\sigma_0,\chi)/L(\sigma_0,\chi)| \leq -\zeta'(\sigma_0)/\zeta(\sigma_0)$. and so

$$\frac{L'(1,\chi)}{L(1,\chi)} = \frac{L'(\sigma_0,\chi)}{L(\sigma,\chi)} + \frac{1}{2}\left(F\left(\frac{\sigma_0+\kappa}{2}\right) - F\left(\frac{1+\kappa}{2}\right)\right)$$
$$+ (\sigma_0-1)\cdot O^*\left(\log q + 2\left|\frac{\zeta'(\sigma_0)}{\zeta(\sigma_0)}\right| + F\left(\frac{\sigma_0+\kappa}{2}\right) - \log\pi\right).$$

Recalling that F is an increasing function, we reach conclusion (16.18). □

Corollary 16.8. *Let χ be a primitive Dirichlet character mod $q>1$. Let $b(\chi)$ be the constant term in the Laurent expansion of $L'(s,\chi)/L(s,\chi)$ at $s=0$. Assume that $L(s,\chi)$ satisfies GRH($\sqrt{8/3}$). Then*

$$|b(\chi)| \leq \frac{4}{3}\log q + 1.349$$

Proof. Assume first that $q \geq 4$. Then $2\log q > \log 2\pi + \gamma$, and so, by (3.105),

$$|b(\chi)| \leq \log q - (\log 2\pi + \gamma) + \left|\frac{L'(1,\overline{\chi})}{L(1,\overline{\chi})}\right|.$$

Therefore, by Lemma 16.7 with $\sigma_0 = 4/3$,

$$|b(\chi)| \leq \log q - (\log 2\pi + \gamma) + \frac{1}{3}\log q + 3.76368 \leq \frac{4}{3}\log q + 1.34859.$$

Assume now that $1 < q < 4$. Then χ is the only primitive Dirichlet character mod 3. We let ARB compute $L(1,\chi)$ and $L'(1,\chi)$, and we obtain

$$\frac{L'(1,\chi)}{L(1,\chi)} = 0.3682816159\ldots$$

Of course χ is real, and so $\overline{\chi} = \chi$. Hence, by (3.105),

$$|b(\chi)| = -b(\chi) = 0.94819882\ldots < \frac{4}{3}\log 3 + 1.34859.$$

□

There are at least two possible alternatives to Lemma 16.7, that is, other ways to bound $L'(1,\chi)/L(1,\chi)$ assuming GRH(H), H bounded. Let us go over them very briefly.

a) Littlewood (essentially [Lit28]; see also, e.g., [MV07, Thm. 13.3 and Exer. 13.2.1.4]) proved that, under the assumption of GRH, $|L'(1,\chi)/L(1,\chi)| \ll \log\log q$ for χ primitive mod $q > 1$. (In fact, the proof can be made to yield $|L'(1,\chi)/L(1,\chi)| \leq (2+o(1))\log\log q$, and generalizes to Dirichlet characters of number fields [IMS09, Thm. 3].) An explicit version can be extracted from [LLS15, §2]. It seems feasible to modify the proof so as to yield a weaker bound valid under GRH(H), H bounded.
b) Another possibility is to apply Lemma 2.6 (Landau). We would bound $L(s,\chi)$ from above either by a convexity bound (as in [Rad60]) or by combining Pólya-Vinogradov with partial summation. In either case, we would seem to get a bound of the form $|L'(s,\chi)/L(s,\chi)| \leq (4+\epsilon)\log q + c_\epsilon$.

Incidentally, Lemma 16.7 does not "recover" Littlewood's result; under GRH, it gives us only that $|L'(1,\chi)/L(1,\chi)| \leq (1+o(1))\sqrt{\log q}$ (set $\sigma_0 = 1 + 1/\sqrt{\log q}$).

Let us speak briefly of the computational approach. The main issue is that of efficiency. Just as in §4.3.2, it is standard to use a discrete Fourier transform (FFT). See, for instance, [FLM14], or [Lan19], which bounds $L'(1,\chi)/L(1,\chi)$ for all non-principal χ of prime modulus $1 < p \leq 10^6$. A plot in [Lan19] supports the experimental observation in [IMS09] that $|L'(1,\chi)/L(1,\chi)| \leq (1+o(1))\log\log q$ may hold.

As [Lan19] notes, in the case $\chi(-1) = -1$, computing $L'(1,\chi)/L(1,\chi)$ does not require computing $\zeta(s,\alpha)$ as in §4.3.2: one can instead use the classical identities[1] in [Coh07, Prop. 10.3.5 and Cor. 10.3.2] so as to express $L'(0,\chi)$ and $L(0,\chi)$ as linear combinations of values of $\log\Gamma$, and then apply FFT to compute those linear combinations.

16.1.6 Bounding the sum over non-trivial zeros

It now remains to bound the sum $\sum_\rho G_\delta(\rho)x^\rho$ in (16.15). Clearly

$$\left|\sum_{\rho:|\Im\rho|\leq T} G_\delta(\rho)x^\rho\right| \leq \sum_{\rho:|\Im\rho|\leq T} |G_\delta(\rho)|\cdot x^{\Re\rho}.$$

Recall that these are sums over the non-trivial zeros ρ of $L(s,\chi)$.

[1] The identity for $L(0,\chi)$ is equivalent to the Dirichlet class number formula; see [Kan89] for a historical discussion of the identity for $L'(0,\chi)$. Thanks are due to A. Languasco for the latter reference.

We first prove a general lemma on sums of values of functions on the non-trivial zeros of $L(s,\chi)$. The proof involves little more than integration by parts, given the bounds in §3.7.3.3 on the number of zeros $N(T,\chi)$ of $L(s,\chi)$ with $0 \le \Im s \le T$. The error term becomes particularly simple if f is real-valued and decreasing; the statement is then practically identical to that of [Leh66, Lemma 1] (for χ principal), except for the fact that the error term is improved here, or to that of [RS75, Lemma 7] (again for χ principal), except that the error term here is slightly simpler.

Lemma 16.9. *Let $y \ge 1$. Let $f : [y,\infty) \to \mathbb{C}$ be a continuous function such that $f(t)\log t$ and $f'(t)t\log t$ are in L^1. Let χ be a primitive character $\bmod q$, $q \ge 1$. Then*

$$\sum_{\substack{\rho \\ \Im\rho > y}} f(\Im\rho) = \frac{1}{2\pi}\int_y^\infty f(t)\log\frac{qt}{2\pi}dt. \tag{16.20}$$
$$+ O^*\left(|f(y)|g_\chi(y) + \int_y^\infty |f'(t)|g_\chi(t)dt\right),$$

where the sum $\sum_\rho$ is taken over all non-trivial zeros ρ of $L(s,\chi)$, and

$$g_\chi(t) = 0.15\log qt + 3.389 \tag{16.21}$$

If f is real-valued and decreasing, the second line of (16.20) can be replaced by

$$O^*\left(0.15\int_y^\infty \frac{f(t)}{t}dt\right).$$

As usual, when we say that $f'(t)t\log t \in L^1$, we mean it in the sense of distributions, or, what is the same, $t\log t \cdot df(t) \in L^1$.

Proof. As in §3.7.3.3, we let $N(T,\chi)$ count only half of any zero with imaginary part exactly 0 and T. By the functional equation (3.81), ρ is a non-trivial zero of $L(s,\overline{\chi})$ if and only if $1-\rho$ is a non-trivial zero of $L(s,\chi)$. Thus

$$\sum_{\substack{\rho \\ \Im\rho > y}} f(\Im\rho) = \int_{y^+}^\infty f(T)\, dN(T,\chi).$$

Since $f(t)\log t \in L^1$, we know that $\lim_{t\to\infty} f(t)\log t = 0$. Hence, thanks to the estimate given by (3.95) on $N(T,\chi)$, we obtain, for any $T_1 > y$,

$$\begin{aligned}\int_{T_1}^\infty f(T)\, dN(T,\chi) &= -\int_{T_1}^\infty f'(T)(N(T,\chi) - N(y,\chi))dT \\ &= -\int_{T_1}^\infty f'(T)N(T,\chi)dT - f(y)N(y,\chi)\end{aligned}$$

by integration by parts. Also by (3.95),

$$\int_{T_1}^\infty f'(T)N(T,\chi)dT = \int_{T_1}^\infty f'(T)\frac{T}{2\pi}\log\frac{qT}{2\pi e} + O^*\left(\int_{T_1}^\infty |f'(T)|g_\chi(T)dT\right),$$

$$f(T_1)N(T_1,\chi) = f(T_1)\frac{T_1}{2\pi}\log\frac{qT_1}{2\pi e} + O^*(|f(T_1)|g_\chi(T_1)).$$

Integrating by parts again, we obtain that

$$-\int_{T_1}^{\infty} f'(T)\left(\frac{T}{2\pi}\log\frac{qT}{2\pi e} - \frac{T_1}{2\pi}\log\frac{qT_1}{2\pi e}\right)dT = \frac{1}{2\pi}\int_{T_1}^{\infty} f(T)\log\frac{qT}{2\pi}dT.$$

(We can take the upper limit $\to\infty$ of the improper integral along a sequence of values of T for which $f(T)T\log T \to 0$, by $f(t)\log t \in L^1$.) Thus

$$\int_{y^+}^{\infty} f(T)\,dN(T,\chi) = \frac{1}{2\pi}\int_{y^+}^{\infty} f(T)\log\frac{qT}{2\pi}dT + O^*\left(|f(y)|g_\chi(y) + \int_{y^+}^{\infty}|f'(T)|g_\chi(T)dT\right).$$

We conclude that (16.20) holds.

If f is real-valued and decreasing (and so, by $\lim_{t\to\infty} f(t) = 0$, non-negative),

$$|f(y)|g_\chi(y) + \int_y^{\infty}|f'(T)|\cdot g_\chi(T)dT = f(y)g_\chi(y) - \int_y^{\infty} f'(T)g_\chi(T)dT = \int_y^{\infty} f(T)g_\chi'(T)dT = 0.15\int_y^{\infty}\frac{f(T)}{T}dT.$$

by integration by parts once more. □

Let us bound the part of the sum $\sum_\rho G_\delta(\rho)$ corresponding to ρ with $|\Im\rho| \le T_0$. The bound we will give is proportional to $\sqrt{T_0}\log qT_0$, whereas a very naive approach (based on the trivial bound $|G_\delta(\sigma+i\tau)| \le |G_0(\sigma)|$) would give a bound proportional to $T_0\log qT_0$. The proof of our bound is simple; it is based on Cauchy-Schwarz and the fact that the Mellin transform is an isometry.

Lemma 16.10. *Let $\eta:\mathbb{R}_0^+\to\mathbb{R}$ be such that both $\eta(t)$ and $(\log t)\eta(t)$ lie in $L^1\cap L^2$ and $\eta(t)/\sqrt{t}$ lies in L^1 (with respect to dt). Let $\delta\in\mathbb{R}$. Let $G_\delta(s)$ be the Mellin transform of $\eta(t)e(\delta t)$.*

Let χ be a primitive character mod q, $q\ge 1$. Let $T_0 \ge 2\pi e^2/q$. Assume that all non-trivial zeros ρ of $L(s,\chi)$ with $|\Im\rho|\le T_0$ lie on the critical line. Then

$$\sum_{\substack{\rho\text{ non-trivial}\\ |\Im\rho|\le T_0}} |G_\delta(\rho)| \le \left(\frac{|\eta|_2}{\sqrt{\pi}} + 0.3\sqrt{\pi}|\eta(t)\cdot\log(t)|_2\right)\sqrt{T_0}\log qT_0 + \left(6.484\sqrt{\pi}|\eta(t)\log t|_2 - \frac{\log 2\pi\sqrt{e}}{\sqrt{\pi}}|\eta|_2\right)\sqrt{T_0} + \left|\eta(t)t^{-1/2}\right|_1\cdot(0.919\log q + 12.653). \tag{16.22}$$

Proof. The trivial bounds

$$|G_\delta(s)| \leq \int_0^\infty |\eta(t)| t^\sigma \frac{dt}{t} = \left|\eta(t)t^{\sigma-1}\right|_1, \tag{16.23}$$

$$|G'_\delta(s)| = \left|\int_0^\infty (\log t)\eta(t) t^s \frac{dt}{t}\right| \leq \int_0^\infty |(\log t)\eta(t)| t^\sigma \frac{dt}{t} = \left|(\log t)\eta(t)t^{\sigma-1}\right|_1 \tag{16.24}$$

are valid for any $s = \sigma + i\tau$.

Let us bound first the contribution of very low-lying zeros ($|\Im\rho| \leq 1$). By (3.95),

$$N(1,\chi) + N(1,\overline{\chi}) \leq \frac{1}{\pi}\log\frac{q}{2\pi e} + (0.3\log q + 6.778) \leq 0.619\log q + 5.875.$$

Therefore,

$$\sum_{\substack{\rho \text{ non-trivial} \\ |\Im\rho|\leq 1}} |G_\delta(\rho)| \leq \left|\eta(t)t^{-1/2}\right|_1 \cdot (0.619\log q + 5.875). \tag{16.25}$$

Let us now consider zeros ρ with $|\Im\rho| > 1$. Apply Lemma 16.9 with $y = 1$ and

$$f(t) = \begin{cases} |G_\delta(1/2+it)| & \text{if } t \leq T_0, \\ 0 & \text{if } t > T_0. \end{cases}$$

We obtain that, for $T_0 \geq 1$,

$$\sum_{\rho: 1<\Im\rho\leq T_0} f(\Im\rho) = \frac{1}{2\pi}\int_1^{T_0} f(t)\log\frac{qt}{2\pi} dt + O^*\left(|f(1)| g_\chi(1) + \int_1^\infty |f'(t)| g_\chi(t)\, dt\right).$$

We apply Cauchy-Schwarz:

$$\int_1^{T_0} f(t)\log\frac{qt}{2\pi}dt \leq \sqrt{\int_1^{T_0} |f(t)|^2\, dt} \cdot \sqrt{\int_1^{T_0}\left(\log\frac{qt}{2\pi}\right)^2 dt}.$$

Since

$$\int_1^{T_0}\left(\log\frac{qt}{2\pi}\right)^2 dt \leq \frac{2\pi}{q}\int_0^{\frac{qT_0}{2\pi}} (\log t)^2 dt = \left(\left(\log\frac{qT_0}{2\pi}\right)^2 - 2\log\frac{qT_0}{2\pi} + 2\right)\cdot T_0. \quad ,$$

we see, under the assumption $T_0 \geq 2\pi e^2/q$, that

$$\sqrt{\int_1^{T_0}\left(\log\frac{qt}{2\pi}\right)^2 dt} \leq \sqrt{\log^2\frac{qT_0}{2e\pi} + 1}\cdot\sqrt{T_0} \leq \log\frac{qT_0}{2\pi\sqrt{e}}\cdot\sqrt{T_0},$$

since $\sqrt{a^2+1} \leq a + 1/2a \leq a + 1/2$ for $a \geq 1$. Thus, by Cauchy-Schwarz again, we obtain

$$\sum_{\rho: 1 < \Im\rho \leq T_0} f(\Im\rho) \leq \sqrt{\frac{1}{4\pi}\int_0^\infty |G_\delta(1/2+it)|^2 dt} \cdot \sqrt{\frac{T_0}{\pi}} \log \frac{qT_0}{2\pi\sqrt{e}} \\ + |f(1)| g_\chi(1) + \sqrt{\int_1^\infty \left|G_\delta'(1/2+it)\right|^2 dt} \cdot \sqrt{\int_1^\infty |g_\chi(t)|^2 \, dt}, \tag{16.26}$$

since $f(t) = G_\delta(1/2+it)$.

We can estimate the sum over ρ with $-T_0 \leq \Im\rho \leq -1$ in exactly the same way, only with $\overline{\chi}$ instead of χ (since $L(\overline{s},\chi) = \overline{L(s,\overline{\chi})}$) and $f(t) = G_\delta(1/2-it)$ instead of $G_\delta(1/2+it)$. By Plancherel (as in (2.28)),

$$\sqrt{\int_0^\infty |G_\delta(1/2+it)|^2 dt} + \sqrt{\int_0^\infty |G_\delta(1/2-it)|^2 dt} \leq \sqrt{2\int_{-\infty}^\infty |G_\delta(1/2-it)|^2 dt} \\ = \sqrt{4\pi\int_0^\infty |e(\delta t)\eta(t)|^2 dt} = \sqrt{4\pi}|\eta|_2^2.$$

Similarly, since $G_\delta'(s)$ is the Mellin transform of $\log(t)e(\delta t)\eta(t)$ (by (2.33)),

$$\sqrt{\int_1^\infty \left|G_\delta'(1/2+it)\right|^2 dt} + \sqrt{\int_1^\infty \left|G_\delta'(1/2-it)\right|^2 dt} \\ \leq \sqrt{4\pi\int_0^\infty |\log(t)e(\delta t)\eta(t)|^2 dt} = \sqrt{4\pi}|\eta(t)\log(t)|_2.$$

Much as before, since $T_0 \geq 1/q$,

$$\int_1^{T_0} |g_\chi(t)|^2 dt \leq \int_0^{T_0} (0.15\log qt + 3.389)^2 dt \\ \leq \left((0.15\log\frac{qT_0}{e} + 3.389)^2 + 0.15^2\right) T_0$$

and so, since $qT_0 \geq 2\pi e^2$,

$$\sqrt{\int_1^{T_0} |g_\chi(t)|^2 dt} \leq \left(0.15\log\frac{qT_0}{e} + 3.389 + \frac{0.15^2}{2(0.15\log 2\pi e + 3.389)}\right)\sqrt{T_0} \\ \leq (0.15\log qT_0 + 3.242)\sqrt{T_0}.$$

Finally, by (16.23) and (16.21),

$$(|G_\delta(1/2+i)| + |G_\delta(1/2-i)|) \cdot g_\chi(1) \leq \left|\eta(t)t^{-1/2}\right|_1 \cdot (0.3\log q + 6.778).$$

We sum all terms and conclude that (16.22) holds. □

16.1.7 Explicit formula, third version

We can now give our last fairly general explicit formula. As in Prop. 16.6, we will be working with a continuous η that satisfies some more technical conditions. Moreover, we will be assuming that GRH has been checked up to a certain height T. Since we are not otherwise using a zero-free region, it stands to sense that our main error term will be of the form ϵx, where ϵ is a small constant depending on the decay of the Mellin transform G_δ.

Proposition 16.11. *Let χ be a primitive Dirichlet character mod q, $q \geq 1$. Let $\delta \in \mathbb{R}/\mathbb{Z}$. Let $\eta : \mathbb{R}^+ \to \mathbb{C}$ be an absolutely continuous function such that $\eta' \in L^2$ and $\eta(t)t^\sigma, \eta'(t)t^\sigma, \eta'(t)t^{-1/2} \in L^1$ for some $\sigma > 1$. Write G_δ for the Mellin transform of $\eta_\delta(t) = \eta(t)e(\delta t)$.*

Let $T \geq \max(2\pi e^2/q, 5/3)$. Assume that all non-trivial zeros ρ of $L(s,\chi)$ with $|\Im\rho| \leq T$ lie on the critical line. Let $f : (-\infty, -T] \cup [T, \infty) \to [0, \infty)$ be such that $|G_\delta(\sigma + it)| \leq f(t)$ for $0 \leq \sigma \leq 1$, $|t| \geq T$. Assume that $t \mapsto f(t)$, $t \mapsto f(-t)$ are continuous and non-increasing on $[T, \infty)$, and that $f(t)\log t, f'(t)t\log t \in L^1$.

Then, for any $x \in \mathbb{R}^+$,

$$\sum_{n=1}^{\infty} \Lambda(n)\chi(n)\eta_\delta(n/x) = [q=1] \cdot \widehat{\eta}(-\delta)x + O^*\left(\epsilon_{T,q,f} \cdot x\right)$$
$$+ O^*\left(c_{\eta,2}\sqrt{T}\log qT + c_{\eta,1}\sqrt{T} + c_{\eta,1/2,q}\right) \cdot \sqrt{x} + c_{\eta,0,q,\delta} + \epsilon_{T,q,f} + \frac{c_{\eta,-,q,\delta}}{\sqrt{x}}, \quad (16.27)$$

where

$$\epsilon_{T,q,f} = \frac{1}{4\pi}\int_T^\infty (f(t) + f(-t))\log\frac{qt}{2\pi}dt + 0.075\int_T^\infty \frac{f(t)+f(-t)}{t}dt, \quad (16.28)$$

$$c_{\eta,2} = \frac{|\eta|_2}{\sqrt{\pi}} + 0.3\sqrt{\pi}|\eta(t)\log(t)|_2, \qquad c_{\eta,1} = 6.484\sqrt{\pi}|\eta(t)\log t|_2 - \frac{\log 2\pi\sqrt{e}}{\sqrt{\pi}}|\eta|_2, \quad (16.29)$$

$$c_{\eta,1/2,q} = (0.919\log q + 12.653)\left|\eta(t)t^{-1/2}\right|_1, \quad (16.30)$$

$$c_{\eta,0,q,\delta} = \frac{4}{3}\eta(0)\log q + \begin{cases} 1.349|\eta(0)| + |\eta_\delta'(t)\log t|_1 & \text{if } q \neq 1, \\ |\eta(0)|\log 2\pi & \text{if } q = 1, \end{cases} \quad (16.31)$$

$$c_{\eta,-,q,\delta} = (\log q + 6.083)\,|\eta_\delta'|_2\,.$$

Here, as before, we write $\widehat{\eta}(-\delta)$ for $\int_{0^+}^\infty \eta(t)e(\delta t)dt$.

Proof. Apply Prop. 16.6. Recall that $b(\chi) = \log 2\pi$ for $q = 1$ (by Cor. 16.3). If $q \neq 1$, bound $b(\chi)$ by Cor. 16.8, noting that $5/3 > \sqrt{8/3}$.

It remains to bound the sum $\sum_\rho G_\delta(\rho)x^\rho$ in Prop. 16.6. (Given our conditions, the convergence in this sum will be absolute.) By the functional equation, if $\rho = \sigma + it$ is a non-trivial zero of $L(s,\chi)$, so is $1-\overline{\rho} = (1-\sigma)+it$. (They are, of course, the same zero if $\sigma = 1/2$.) Now, for $0 \leq \sigma \leq 1$,

$$x^\sigma + x^{1-\sigma} \leq 1 + x,$$

by convexity of $\sigma \to x^\sigma$. Hence

$$\left|\sum_\rho G_\delta(\rho) x^\rho\right| \leq \sum_\rho |G_\delta(\rho)| \cdot \frac{x+1}{2}.$$

We bound the sum over ρ with $|\Im \rho| > T$ by Lemma 16.9 and Lemma 16.10. □

We could save a factor of $\log T$ in $\epsilon_{T,q,f}$ by using a zero-density estimate, as in [KL14], at the cost of introducing a summand proportional to x^α, $0 < \alpha < 1$.

We will now bound the norms appearing in (16.29)–(16.31) and the integrals in (16.28) for some specific smoothing functions η. Everything else we have done in general.

16.2 EXPLICIT FORMULAE FOR SOME SMOOTHING FUNCTIONS

16.2.1 Decay and norms for the Gaussian

We will now work with smoothing functions $\eta : \mathbb{R}^+ \to \mathbb{R}$ defined by $\eta(x) = e^{-x^2/2}$, or multiples or linear combinations thereof. (For instance, it makes sense to define $\eta : \mathbb{R}^+ \to \mathbb{R}$ by $\eta(x) = \sqrt{2/\pi} \cdot e^{-x^2/2}$, so that $|\eta|_1 = 1$.)

16.2.1.1 Decay

Our main task will be to bound the two integrals in (16.28). The following basic lemma will be useful.

Lemma 16.12. *Let $f_1, f_2, g : [x,\infty) \to \mathbb{R}$ be such that $f_1(t)$ is non-increasing, f_2 and g are absolutely continuous, $\log f_2(t)$ is concave, $g(t)$ is convex, $F(t) = f_1(t) f_2(t) e^{-g(t)}$ satisfies $\lim_{t\to\infty} F(t) = 0$ and $R = g'(x) - f_2'(x)/f_2(x)$ is positive. Then*

$$\int_x^\infty F(t)dt \leq \frac{F(x)}{R}.$$

Proof. Since $\int_x^\infty F(t)dt \leq f_1(x)\int_x^\infty f_2(x)e^{-g(x)}$, we can assume without loss of generality that f_1 is identically 1. Replacing $g(t)$ by $g(t) - \log f_2(t)$, we can assume f_2 is also identically 1. Because $g(t)$ is convex (i.e. $g'(t)$ is increasing),

$$e^{-g(x)} = -\int_x^\infty \left(e^{-g(t)}\right)' dt = \int_x^\infty g'(t)e^{-g(t)}dt \geq g'(x)\int_x^\infty e^{-g(t)}dt,$$

and so $\int_x^\infty e^{-g(t)}dt \leq e^{-g(x)}/g'(x)$, as desired. □

As can be seen from Theorem 15.1, the decay of the Mellin transform $G_\delta(\sigma + it)$ as $|t|$ grows is fast and simple for $\mathrm{sgn}(t) = \mathrm{sgn}(\delta)$, and a little more delicate for $\mathrm{sgn}(t) \neq \mathrm{sgn}(\delta)$. Let us do an estimate for the simple case first.

Lemma 16.13. *Let $\varphi(t) = e^{-\frac{\pi}{4}t}$. Let $q \in \mathbb{Z}^+$. Then, for $T > \max(2\pi e/q, \pi/4)$,*

$$\int_T^\infty \varphi(t) \log \frac{qt}{2\pi} dt \leq \frac{e^{-\frac{\pi}{4}T} \log \frac{qT}{2\pi}}{\frac{\pi}{4} - \frac{1}{T}}, \tag{16.32}$$

$$\int_T^\infty \frac{\varphi(t)}{t} dt \leq \frac{e^{-\frac{\pi}{4}T}}{\frac{\pi}{4}T}. \tag{16.33}$$

Proof. First, apply Lemma 16.12 with $f_1(t) = 1$, $f_2(t) = \log(qt/2\pi)$, $g(t) = \pi t/4$ and $x = T$. The conditions of the lemma are fulfilled because $\log \log t$ is concave for $t \geq 1$ and

$$R = \frac{\pi}{4} - \frac{f_2'(t)}{f_2(t)} = \frac{\pi}{4} - \frac{1}{t \log \frac{qt}{2\pi}} \geq \frac{\pi}{4} - \frac{1}{t} > 0$$

for $t \geq T$. Hence (16.32) holds.

To obtain (16.33), apply Lemma 16.12 with $f_1(t) = 1/t$, $f_2(t) = 1$, $g(t) = \pi t/4$. □

Let us now do the case corresponding to $\mathrm{sgn}(t) \neq \mathrm{sgn}(\delta)$.

Lemma 16.14. *Let $\delta < 0$. Let*

$$\varphi(t) = \left(1 + \frac{c_0}{t}\right) \sqrt{2\pi} \min\left(1, \frac{\sqrt{t}}{2\pi|\delta|}\right) \cdot e^{-E(\mathscr{r})t}, \tag{16.34}$$

where $c_0 \geq 0$, $\mathscr{r} = \mathscr{r}(t) = t/\pi^2\delta^2$ and $E(\mathscr{r})$ is as in (15.2). Let $q \in \mathbb{Z}^+$. Then, for $T \geq \max(2\pi e^2/q, 4\pi|\delta|, 40)$ and $c \geq 0$,

$$\int_T^\infty \varphi(t) \log \frac{q(t+c)}{2\pi} dt \leq \left(1 + \frac{c_0}{T}\right) e^{-E(\mathscr{r}(T))T} \log \frac{q(T+c)}{2\pi} \cdot \begin{cases} 5.927 & \text{if } \mathscr{r} \geq 4, \\ \frac{15.527}{\sqrt{\mathscr{r}}} & \text{if } \mathscr{r} < 4, \end{cases} \tag{16.35}$$

$$\int_T^\infty \frac{\varphi(t)}{t+c} dt \leq \left(1 + \frac{c_0}{T}\right) \frac{e^{-E(\mathscr{r}(T))T}}{T+c} \cdot \begin{cases} 5.6 & \text{if } \mathscr{r} \geq 4, \\ \frac{11.2}{\sqrt{\mathscr{r}}} & \text{if } \mathscr{r} < 4. \end{cases} \tag{16.36}$$

Moreover, $\varphi(t)$ is decreasing for $t \geq T$.

Proof. We let

$$f_1(t) = \sqrt{2\pi}\left(1 + \frac{c_0}{t}\right), \; f_2(t) = \min\left(1, \frac{\sqrt{t}}{2\pi|\delta|}\right) \log \frac{q(t+c)}{2\pi}, \; g(t) = E(\mathscr{r}(t))t,$$

and $x = T$. Since $\log t$ is concave, so is $\min(0, \log t - 2\log 2\pi|\delta|)$; when we consider that $\log \log t$ is concave as well, we see that $\log f_2(t)$ is concave. By Lemma 15.23, $g(t) = \pi^2\delta^2 E(\mathscr{r})\mathscr{r}$ is convex with respect to $\mathscr{r}$ and hence with respect to t.

We apply Lemma 16.12, and obtain

$$\int_T^\infty \varphi(t) \log \frac{q(t+c)}{2\pi} dt \le \frac{1}{R} \varphi(t) \log \frac{q(T+c)}{2\pi},$$

where

$$\begin{aligned} R &= g'(T) - \frac{f_2'(T)}{f_2(T)} = \frac{d}{d\mathscr{r}} E(\mathscr{r})\mathscr{r} - \frac{f_2'(T)}{f_2(T)} \\ &= \frac{1}{2} \arccos \frac{1}{\upsilon(\mathscr{r}(T))} - \frac{1}{(T+c)\log \frac{q(T+c)}{2\pi}} - \begin{cases} 0 & \text{if } T < (2\pi\delta)^2, \\ \frac{1}{2T} & \text{if } T > (2\pi\delta)^2. \end{cases} \end{aligned}$$

If $T = (2\pi\delta)^2$, we use the same expression as for $T > (2\pi\delta)^2$, by continuity.

Consider first the case $T \ge (2\pi\delta)^2$. Then $\mathscr{r}(T) > 4$, and so, since υ is increasing,

$$R \ge \frac{1}{2} \arccos \frac{1}{\upsilon(4)} - \frac{1}{(T+c)\log \frac{q(T+c)}{2\pi}} - \frac{1}{2T} \ge \frac{1}{2} \arccos \frac{1}{\upsilon(4)} - \frac{1}{T} \ge 0.42295,$$

where we have used the condition $T > \max(2\pi e^2/q, 40)$. Hence

$$\frac{1}{R}\sqrt{2\pi} \min\left(1, \frac{\sqrt{t}}{2\pi|\delta|}\right) \le \frac{\sqrt{2\pi}}{R} \le 5.92654.$$

On a different matter: it is clear from (16.34) that $\varphi(t)$ is decreasing for $t \ge (2\pi\delta)^2$, since $E(\mathscr{r})$ is increasing.

Consider now $T < (2\pi\delta)^2$. We know from the proof of Lemma 15.21 that

$$\frac{d}{d\mathscr{r}} \frac{1}{2} \arccos \frac{1}{\upsilon(\mathscr{r})} = \frac{\upsilon'(\mathscr{r})}{\mathscr{r}}.$$

It is easy to verify that $\upsilon'(\mathscr{r})/\mathscr{r}$ is decreasing, and thus $(1/2)\arccos(1/\upsilon(\mathscr{r}))$ is concave. Since $\arccos(1/\upsilon(0)) = 0$, and $T < (2\pi\delta)^2$ means that $\mathscr{r} < 4$, we see that

$$\frac{1}{2} \arccos \frac{1}{\upsilon(\mathscr{r})} \ge \frac{\frac{1}{2}\arccos \frac{1}{\upsilon(4)}}{4} \mathscr{r} \ge 0.11198\mathscr{r}. \tag{16.37}$$

By $T \ge 4\pi\delta$, $T \ge 2\pi e^2/q$ and $c \ge 0$,

$$\frac{1}{(T+c)\log \frac{q(T+c)}{2\pi}} \le \frac{1}{2T} = \frac{\mathscr{r}(T)}{2\mathscr{r}(T)T} = \frac{\mathscr{r}}{2T^2/\pi^2\delta^2} \le \frac{\mathscr{r}}{32}.$$

Hence

$$R \ge \left(0.11198 - \frac{1}{32}\right)\mathscr{r} \ge 0.08072\mathscr{r},$$

and so

$$\frac{1}{R}\sqrt{2\pi} \min\left(1, \frac{\sqrt{t}}{2\pi|\delta|}\right) \le \frac{\sqrt{2\pi}}{R} \cdot \frac{\sqrt{\mathscr{r}}}{2} \le \frac{15.52669}{\sqrt{\mathscr{r}}}.$$

To prove that $\varphi(t)$ is decreasing for $T \leq t < (2\pi\delta)^2$, it is enough to show that $(\log \sqrt{t}e^{-E(\mathscr{r}(t))t})' = 1/2t - g'(t)$ is negative for $t \geq T$. We know from (16.37) that $g'(t) \geq 0.11198\mathscr{r}$, and so, by the assumption $T \geq 4\pi\delta$,

$$g'(t)t \geq 0.11198\frac{t^2}{\pi^2\delta^2} \geq 0.11198 \cdot 4^2 > \frac{1}{2},$$

and so $\varphi(t)$ is decreasing for $T \leq t < (2\pi\delta)^2$.

Let us now prove the second inequality in (16.35). Let

$$f_1(t) = \frac{\sqrt{2\pi}}{t+c}\left(1 + \frac{c_0}{t}\right),\ f_2(t) = \min\left(1, \frac{\sqrt{t}}{2\pi|\delta|}\right),\ g(t) = E(\mathscr{r}(t))t$$

and $x = T$. We apply Lemma 16.12, and obtain

$$\int_T^\infty \frac{\varphi(t)}{t+c}dt \leq \frac{\varphi(t)}{R_1 \cdot (T+c)},$$

where, by Lemma 15.21,

$$R_1 = g'(T) = \frac{d}{d\mathscr{r}}E(\mathscr{r})\mathscr{r} = \frac{1}{2}\arccos\frac{1}{\upsilon(\mathscr{r}(T))}.$$

As we have already seen, for $T \geq (2\pi\delta)^2$,

$$R_1 \geq \frac{1}{2}\arccos\frac{1}{\upsilon(4)} \geq 0.44795,$$

$$\frac{1}{R_1}\sqrt{2\pi}\min\left(1, \frac{\sqrt{t}}{2\pi|\delta|}\right) \leq \frac{\sqrt{2\pi}}{R_1} \leq 5.59578,$$

and, for $T < (2\pi\delta)^2$,

$$R_1 \geq 0.11198\mathscr{r},$$

$$\frac{\sqrt{2\pi}}{R_1}\min\left(1, \frac{\sqrt{t}}{2\pi|\delta|}\right) \leq \frac{\sqrt{2\pi}}{R_1} \cdot \frac{\sqrt{\mathscr{r}}}{2} \leq \frac{11.19231}{\sqrt{\mathscr{r}}}.$$

□

16.2.1.2 Norms

We record a few norms related to the one-sided Gaussian.

Lemma 16.15. *Let $\eta : \mathbb{R}^+ \to \mathbb{R}$ be defined by $\eta(x) = \sqrt{2/\pi} \cdot e^{-x^2/2}$. Then*

$$|\eta|_1 = 1, \quad |\eta|_2 = \sqrt{\frac{2}{\pi}} \cdot \sqrt{\int_0^\infty e^{-x^2}dx} = \frac{1}{\pi^{1/4}}, \tag{16.38}$$

$$|\eta'|_2 = \sqrt{\frac{2}{\pi}} \cdot \sqrt{\int_0^\infty (xe^{-x^2/2})^2 dx} = \frac{1}{\sqrt{2}\cdot\pi^{1/4}}, \tag{16.39}$$

$$|\eta(x)\log(x)|_2 = \sqrt{\frac{2}{\pi}} \cdot \sqrt{\int_0^\infty e^{-x^2} (\log x)^2 dt} \leq 1.11348, \tag{16.40}$$

$$|\eta(x)/\sqrt{x}|_1 = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{e^{-x^2/2}}{\sqrt{x}} dx = \frac{\Gamma(1/4)}{2^{1/4}\sqrt{\pi}} \leq 1.72008, \tag{16.41}$$

$$|\eta(x)\log x|_1 = \sqrt{\frac{2}{\pi}} \cdot \sqrt{\int_0^\infty e^{-x^2/2}\, |\log x| dx} \leq 0.87929, \tag{16.42}$$

$$|\eta'(x)\log x|_1 = \sqrt{\frac{2}{\pi}} \cdot \sqrt{\int_0^\infty x e^{-x^2/2}\, |\log x| dx} \leq 0.40039. \tag{16.43}$$

Hence, for $\delta \in \mathbb{R}$ *and* $\eta_\delta(x) = \eta(x)e(\delta x)$*,*

$$|\eta_\delta'|_2 \leq |\eta'|_2 + 2\pi|\delta||\eta|_2 \leq \frac{1}{\sqrt{2}\cdot \pi^{1/4}} + 2\pi^{3/4}|\delta|, \tag{16.44}$$

$$|\eta_\delta'(x)\log x|_1 \leq |\eta'(x)\log x|_1 + 2\pi|\delta| \cdot |\eta(x)\log x|_1 \leq 0.40039 + 5.52475|\delta|. \tag{16.45}$$

Proof. By symbolic integration for (16.38)–(16.41), rigorous numerical integration for (16.42)–(16.43), and the triangle inequality for (16.44)–(16.45). □

We also record some norms for the smoothing function we used in Part III.

Lemma 16.16. *Let* $\eta : \mathbb{R}^+ \to \mathbb{R}$ *be defined by*

$$\eta(x) = \sqrt{\frac{2}{\pi}} \cdot 2\left(e^{-x^2/2} - e^{-2x^2}\right).$$

Then

$$|\eta|_1 = 1, \quad |\eta|_2 = \frac{\sqrt{6 - 8\sqrt{2/5}}}{\pi^{1/4}} \leq 0.72839, \tag{16.46}$$

$$|\eta'|_2 = \frac{\sqrt{6 - \frac{32}{25}\sqrt{10}}}{\pi^{1/4}} \leq 1.04951, \tag{16.47}$$

$$|\eta(x)\log x|_2 \leq 0.27686, \tag{16.48}$$

$$|\eta(x)/\sqrt{x}|_1 = \frac{\Gamma(1/4)}{\sqrt{\pi}}(2^{3/4} - 2^{1/4}) \leq 1.0076, \tag{16.49}$$

$$|\eta(x)\log x|_1 \leq 0.4155, \tag{16.50}$$

$$|\eta'(x)\log x|_1 \leq 1.10616, \tag{16.51}$$

$$|\eta_\delta'|_2 \leq |\eta'|_2 + 2\pi|\delta|\cdot|\eta|_2 \leq 1.04951 + 4.57661|\delta|, \tag{16.52}$$

$$|\eta_\delta'(x)\log x|_1 \leq |\eta'(x)\log x|_1 + 2\pi|\delta|\cdot|\eta(x)\log x|_1 \leq 1.10616 + 2.61067|\delta|. \tag{16.53}$$

Proof. By symbolic integration for (16.46), (16.47) and (16.49), by rigorous numerical integration for (16.48), (16.50) and (16.51), and by the triangle inequality for (16.52)–(16.53). □

16.2.1.3 Conclusions

We can now state what is really our main result for the Gaussian smoothing. (The version in §14.1 will, as we shall later see, follow from this one, given numerical inputs.)

Proposition 16.17. *Let χ be a primitive Dirichlet character mod q, $q \geq 1$. Let $\delta \in \mathbb{R}$. Let $\eta : \mathbb{R}^+ \to \mathbb{C}$ be defined by $\eta(t) = \sqrt{2/\pi}\cdot e^{-t^2/2}$.*

Let $T \geq \max(2\pi e^2/q, 4\pi|\delta|, 40)$. Assume that all non-trivial zeros ρ of $L(s,\chi)$ with $|\Im\rho| \leq T$ lie on the critical line. Then, for any $x \in \mathbb{R}^+$,

$$\sum_{n=1}^{\infty} \Lambda(n)\chi(n)e\left(\frac{\delta}{x}n\right)\eta\left(\frac{n}{x}\right) = \begin{cases} \widehat{\eta}(-\delta)x + O^*\left(\mathrm{err}_{\eta,\chi}(\delta,x)\right) & \text{if } q = 1, \\ O^*\left(\mathrm{err}_{\eta,\chi}(\delta,x)\right) & \text{if } q > 1, \end{cases} \tag{16.54}$$

where

$$\begin{aligned}\mathrm{err}_{\eta,\chi}(\delta,x) = {} & \left(e^{-E(\digamma(T))T}\cdot\begin{cases}0.44 & \text{if } \digamma \geq 4\\ 1.14/\sqrt{\digamma(T)} & \text{if } \digamma < 4\end{cases} + 0.22e^{-\frac{\pi}{4}T}\right) x\log\frac{qT}{2\pi}\\ & + (1.02\sqrt{T}\log qT + 11.81\sqrt{T} + 1.6\log q + 21.8)\sqrt{x}\\ & + 1.1\log q + 5.6|\delta| + 2 + (\log q + 6.1)(0.6 + 4.8|\delta|)x^{-1/2},\end{aligned} \tag{16.55}$$

with $\digamma = \digamma(t) = t/\pi^2\delta^2$ and $E(\digamma)$ as in (15.2).

Proof. We can assume without loss of generality that $\delta < 0$. (If $\delta = 0$, we let $\delta \to 0^-$.) We define $f(t)$ for $t \geq T$ as $f(t) = \sqrt{2/\pi}\cdot\varphi(t)$, where $\varphi(t)$ is as in (16.34) with $c_0 = 5.6$ and $c = 0$, and $f(t) = \sqrt{2/\pi}\cdot 2.56e^{-(\pi/4)|t|}$ for $t \leq -T$. We apply Proposition 16.11, using Theorem 15.1 to ensure that $f(t)$ is a valid bound for $G_\delta(\sigma+it)$, $0 \leq \sigma \leq 1$, where G_δ is the Mellin transform of $\eta(t)e(\delta t)$.

Let us first bound $\epsilon_{T,q,f}$, starting with the part of (16.28) coming from $f(t)$ rather than $f(-t)$. We apply Lemma 16.14 with $c = 0$ and $c_0 = 5.6$, remembering to multiply by the factor $\sqrt{2/\pi}$ in the definition of $\eta(t)$, and obtain that

$$\frac{1}{4\pi}\int_T^\infty f(t)\log\frac{qt}{2\pi}dt + 0.075\int_T^\infty\frac{f(t)}{t}dt$$

is at most

$$e^{-E(\digamma(T))T}\cdot\begin{cases}0.43\log\frac{qT}{2\pi}+\frac{0.39}{T} & \text{if } \digamma\geq 4,\\ \frac{1.124}{\sqrt{\digamma}}\log\frac{qT}{2\pi}+\frac{0.77}{T\sqrt{\digamma}} & \text{if } \digamma<4.\end{cases}$$

Since $T\geq\max(2\pi e^2/q,40)$, we see that

$$0.43\log\frac{qT}{2\pi}+\frac{0.39}{T}\leq 0.435\log\frac{qT}{2\pi},$$
$$1.124\log\frac{qT}{2\pi}+\frac{0.77}{T}\leq 1.134\log\frac{qT}{2\pi}.$$

We now bound the part coming from $f(-t)$. By Lemma 16.13, $T\geq 40$ and $qT/2\pi\geq e^2$, we obtain

$$\frac{1}{4\pi}\int_T^\infty f(-t)\log\frac{qt}{2\pi}dt+0.075\int_T^\infty\frac{f(-t)}{t}dt$$

is at most

$$\left(0.214\log\frac{qT}{2\pi}+\frac{0.196}{T}\right)e^{-\frac{\pi}{4}T}\leq 0.22\log\frac{qT}{2\pi}e^{-\frac{\pi}{4}T}.$$

It remains to bound the constants in Prop. 16.11. By Lemma 16.15,

$$c_{\eta,2}\leq 1.01586,\quad c_{\eta,1}\leq 11.80604,\quad c_{\eta,1/2,q}\leq 1.58076\log q+21.76418,$$
$$c_{\eta,0,q,\delta}\leq 1.06385\log q+5.52476|\delta|+1.47674,$$
$$c_{\eta,-,q,\delta}\leq(\log q+6.083)(0.53113+4.71947|\delta|).$$

□

Now we give our main result for the smoothing from Part III. We could, of course, deduce an estimate from Prop. 16.17, but considering this smoothing on its own leads to better constants.

Proposition 16.18. *Let χ be a primitive Dirichlet character mod q, $q\geq 1$. Let $\delta\in\mathbb{R}$. Let $\eta:\mathbb{R}^+\to\mathbb{C}$ be defined by $\eta(t)=\sqrt{2/\pi}\cdot 2(e^{-t^2/2}-e^{-2t^2})$.*

Let $T\geq\max(2\pi e^2/q,4\pi|\delta|,40)$. Assume that all non-trivial zeros ρ of $L(s,\chi)$ with $|\Im\rho|\leq T$ lie on the critical line. Then, for any $x\in\mathbb{R}^+$,

$$\sum_{n=1}^{\infty}\Lambda(n)\chi(n)e\left(\frac{\delta}{x}n\right)\eta\left(\frac{n}{x}\right)=\begin{cases}\widehat{\eta}(-\delta)x+O^*\left(\mathrm{err}_{\eta,\chi}(\delta,x)\right) & \text{if } q=1,\\ O^*\left(\mathrm{err}_{\eta,\chi}(\delta,x)\right) & \text{if } q>1,\end{cases}\tag{16.56}$$

where

$$\begin{aligned}\mathrm{err}_{\eta,\chi}(\delta,x)=&\left(e^{-E(\digamma(T))T}\cdot\begin{cases}1.31 & \text{if } \digamma\geq 4\\ 3.41/\sqrt{\digamma(T)} & \text{if } \digamma<4\end{cases}+0.88e^{-\frac{\pi}{4}T}\right)x\log\frac{qT}{2\pi}\\&+(0.56\sqrt{T}\log qT+2.23\sqrt{T}+0.93\log q+12.8)\sqrt{x}\\&+2.7|\delta|+1.2+(\log q+6.1)(1.1+4.6|\delta|)x^{-1/2},\end{aligned}\tag{16.57}$$

with $\digamma=\digamma(t)=t/\pi^2\delta^2$ and $E(\digamma)$ as in (15.2).

Proof. We wish to apply Proposition 16.11. Writing $\eta_0(t)$ for the function $\eta(t)$ in Prop. 16.17, we see we can write our $\eta(t)e(\delta t)$ here as $2(\eta_0(t)e(\delta t) - \eta_0(2t)e(\delta t))$. Hence, the Mellin transform of $\eta(t)e(\delta t)$ here equals $2(G_{0,\delta}(s) - 2^{-s}G_{0,\delta/2})$ in terms of the Mellin transform $G_{0,\delta}$ of $\eta_0(t)e(\delta t)$.

Assuming $\delta < 0$ without loss of generality, just as before, we notice that we can define $f(t) = 4 \cdot \sqrt{2/\pi} \cdot 2.56e^{-(\pi/4)|t|}$ for $t \leq -T$. Let us see what to do for $t \geq T$. A moment's thought shows that the right side of the (15.1), multiplied by $2^{-\sigma}$, takes its maximum for $0 \leq \sigma \leq 1$ at $\sigma = 1$, if δ and t are kept constant and $|t| \geq \max(4\pi|\delta|, 4)$. Hence, $|2^{1-s}G_{0,\delta/2}(\sigma + it)|$ is bounded by $f(t)$ as in (16.34), with $\delta/2$ instead of δ. The bounds in (16.35) and (16.36) decrease as δ decreases. Thus, applying Lemma 16.14 twice, once for $2G_{0,\delta}(s)$ and once for $2^{1-s}G_{0,\delta/2}(s)$, both times with $c = 0$, we obtain a bound for $t \geq 0$ equal to three times the one we obtained for $G_{0,\delta}(s)$ in the proof of Prop. 16.17. Taking totals, we see that

$$\epsilon_{T,q,f} \leq \left(e^{-E(\digamma(T))T} \cdot \begin{cases} 1.305 & \text{if } \digamma \geq 4 \\ 3.402 & \text{if } \digamma \geq 4 \end{cases} + 0.88e^{-\frac{\pi}{4}T} \right) \log \frac{qT}{2\pi}.$$

Now we bound the constants in Prop. 16.11. By Lemma 16.16,

$$c_{\eta,2} \leq 0.55817, \quad c_{\eta,1} \leq 2.22109, \quad c_{\eta,1/2,q} \leq 0.92599 \log q + 12.74917,$$
$$c_{\eta,0,q,\delta} \leq 2.61067|\delta| + 1.10616,$$
$$c_{\eta,-,q,\delta} \leq (\log q + 6.083)(1.04951 + 4.57661|\delta|).$$

□

16.2.2 The case of $\eta_+(t)$

We will work with

$$\eta(t) = \eta_+(t) = h_H(t) \cdot te^{-t^2/2}, \tag{16.58}$$

where h_H is as in (14.6). We recall that h_H is a band-limited approximation to the function h defined in (14.5) – to be more precise, $h_H(it)$ is defined as the inverse Mellin transform of the truncation of $Mh(it)$ to the interval $[-H, H]$.

We are actually defining h, h_H and η in a slightly different way from what was done in the first version of [Hela]. The difference is instructive. There, $\eta(t)$ was defined as $h_H(t)e^{-t^2/2}$, and h_H was a band-limited approximation to a function h defined as in (14.5), but with $t^3(2-t)^3$ instead of $t^2(2-t)^3$. The reason for our new definitions is that now $M\eta(it)$ will be holomorphic on a wider strip, extending up to $\Re s > -1$. Equally to the point, and more or less equivalently, $h'(t)t^\sigma$ will be in L^1 for $\sigma > -1$, and thus the conditions of our general explicit formulae (Lemma 16.1, Prop. 16.6 and Prop. 16.11) will be fulfilled. Were they not – in particular, if we had kept the definition of η and h_H from the first version – we would be able to shift the line of integration only just to the right of $\Re s = 0$. (Since the Mellin transform of $e^{-t^2/2}$ has a pole at $s = 0$, convolving that transform by another function vertically (as in (2.31)) "spreads" the pole nastily on the line $\Re s = 0$.) This issue would not be a serious problem, but it is much more pleasant to be able to use our general procedure, which involves shifting the line of integration to the left of $\Re s = 0$.

As usual, we start by bounding the contribution of zeros with large imaginary part. The procedure is much as before: since $\eta_+(t) = h_H(t) t e^{-t^2/2}$, the Mellin transform $M\eta_+$ is a convolution of $M(te^{-t^2/2})$ and a function of support in $[-H, H]i$, namely, Mh restricted to the imaginary axis. As a consequence, the decay of $M\eta_+$ is (at worst) like the decay of $M(te^{-t^2/2})$, delayed by a shift by H.

Proposition 16.19. *Let $\eta = \eta_+$ be as in (16.58) for some $H \geq 100$. Let χ be a primitive character mod q, $q \geq 1$. Let $\delta \in \mathbb{R}$.*

Let $T = T_0 + H$, where $T_0 \geq \max(2\pi e^2/q, 4\pi|\delta|, 40)$. Assume that all non-trivial zeros ρ of $L(s,\chi)$ with $|\Im \rho| \leq T$ lie on the critical line.

Then, for any $x \in \mathbb{R}^+$,

$$\sum_{n=1}^{\infty} \Lambda(n)\chi(n) e\left(\frac{\delta}{x} n\right) \eta_+(n/x) = \begin{cases} \widehat{\eta_+}(-\delta)x + O^*\left(\mathrm{err}_{\eta_+,\chi}(\delta,x)\right) & \text{if } q = 1, \\ O^*\left(\mathrm{err}_{\eta_+,\chi}(\delta,x)\right) & \text{if } q > 1, \end{cases} \tag{16.59}$$

where

$$\begin{aligned}\mathrm{err}_{\eta_+,\chi}(\delta,x) = &\left(e^{-E(\mathscr{r}(T_0))T_0} \cdot \begin{cases} 1.05 & \text{if } \mathscr{r} \geq 4 \\ 2.72/\sqrt{\mathscr{r}(T_0)} & \text{if } \mathscr{r} < 4 \end{cases} + 0.75 e^{-\frac{\pi}{4}T_0}\right) x \log \frac{qT}{2\pi} \\ &+ (0.566\sqrt{T}\log qT + 1.41\sqrt{T} + 0.84\log q + 11.52)x^{1/2}, \\ &+ 1.6|\delta| + 1.1 + (6.1 \log q)(6 + 2|\delta|)x^{-1/2},\end{aligned} \tag{16.60}$$

with $\mathscr{r} = \mathscr{r}(t) = t/\pi^2\delta^2$ and $E(\mathscr{r})$ is as in (15.2).

Proof. We will apply Proposition 16.11. The first order of business is to bound the integrals in (16.28). Here we take a very simple approach.

By Lemma A.9, the Mellin transform G_δ of $\eta(t)e(\delta t)$ equals

$$\frac{1}{2\pi i}\int_{-iH}^{iH} Mh(z) M\eta_{\heartsuit,\delta}(s+1-z)dz,$$

where $\eta_{\heartsuit,\delta}(t) = e^{-t^2/2}e(\delta t)$. We know from Theorem 15.1 that, for $t \geq T_0$ and $0 \leq \sigma \leq 1$, $|M\eta_{\heartsuit,\delta}(\sigma + 1 + it)| \leq \varphi(t)$, where $\varphi(t)$ is as in (16.34) with $c_0 = 26.94$, and $|M\eta_{\heartsuit,\delta}(\sigma + 1 - it)| \leq 3.69 e^{-\frac{\pi}{4}t}$. Since $t \mapsto \varphi(t)$ is non-increasing, it follows that $|G_\delta(\sigma + it)| \leq f(t)$ for $0 \leq \sigma \leq 1$ and $|t| \geq T$, where

$$f(t) = \frac{1}{2\pi}|Mh(it)|_1 \cdot \begin{cases} \varphi(t-H) & \text{if } t > 0, \\ 3.69 e^{-\frac{\pi}{4}(|t|-H)} & \text{if } t < 0. \end{cases}$$

We apply Lemma 16.14 with $c = H$ and $c_0 = 26.94$, and obtain that

$$\frac{1}{4\pi}\int_T^\infty \varphi(t-H)\log\frac{qt}{2\pi}dt + 0.075\int_{T_0}^\infty \frac{\varphi(t-H)}{t}dt$$

is at most

$$e^{-E(\digamma(T_0))T_0} \cdot \begin{cases} 0.538 \log \frac{qT}{2\pi} + \frac{0.48}{T} & \text{if } \digamma \geq 4, \\ \frac{1.409}{\sqrt{\digamma}} \log \frac{qT}{2\pi} + \frac{0.96}{T\sqrt{\digamma}} & \text{if } \digamma < 4. \end{cases}$$

Since $T \geq \max(2\pi e^2/q, 40)$, we see that

$$0.538 \log \frac{qT}{2\pi} + \frac{0.48}{T} \leq 0.545 \log \frac{qT}{2\pi},$$
$$1.409 \log \frac{qT}{2\pi} + \frac{0.96}{T} \leq 1.422 \log \frac{qT}{2\pi}.$$

Again as in the proof of Prop. 16.17, we apply Lemma 16.13, and see that

$$\frac{1}{4\pi} \int_T^\infty 3.69 e^{-\frac{\pi}{4}(|t|-H)} \log \frac{q(t+H)}{2\pi} dt + 0.075 \int_T^\infty 3.69 \frac{e^{-\frac{\pi}{4}(|t|-H)}}{t} dt$$

is at most

$$\left(0.387 \log \frac{qT}{2\pi} + \frac{0.353}{T}\right) e^{-\frac{\pi}{4}T_0} \leq 0.392 \log \frac{qT}{2\pi} e^{-\frac{\pi}{4}T_0}.$$

By (A.35),

$$\frac{1}{2\pi}|Mh(it)|_1 \leq 1.90966.$$

We conclude that the quantity $\epsilon_{T,q,f}$ defined in Proposition 16.11 is at most

$$\left(e^{-E(\digamma(T_0))T_0} \cdot \begin{cases} 1.041 & \text{if } \digamma \geq 4 \\ 2.716/\sqrt{\digamma(T)} & \text{if } \digamma < 4 \end{cases} + 0.749 e^{-\frac{\pi}{4}T_0}\right) \log \frac{qT}{2\pi}.$$

We may apply Proposition 16.11 because η_+ is absolutely continuous, $\eta_+'(t)$ is in L^2 (by Lemma A.15) and $\eta_+(t)t^2$, $\eta'(t)t^2$ and $\eta_+'(t)t^{-1/2}$ are in L^1 (by Lemmas A.14 and A.17). We bound the norms involving η_+ using the estimates in §A.3. To wit, by (A.43), (A.44), (A.45), and Lemmas A.15 and A.18, and the assumption $H \geq 100$,

$$|\eta_+|_2 \leq 0.80015, \quad |\eta_+(t) \log t|_2 \leq 0.21388, \quad |\eta_+(t)/\sqrt{t}|_1 \leq 0.9099,$$
$$|\eta_+(t) \log t|_1 \leq 0.24522, \quad |\eta_+'(t)|_2 \leq 1.67, \quad |\eta_+'(t) \log t|_1 \leq 1.03.$$

By definition (A.23) and the boundedness of h_H (see §A.2), we know that $\eta_+(0) = 0$.

We can now compute the constants in Proposition 16.11: for $\eta = \eta_+$,

$$\begin{aligned} c_{\eta,2} \log qT + c_{\eta,1} &= \frac{|\eta|_2(\log qT - \log 2\pi\sqrt{e})}{\sqrt{\pi}} + (0.3 \log qT + 6.484)\sqrt{\pi}|\eta(t) \log t|_2 \\ &\leq 0.5652 \log qT + 1.403, \end{aligned}$$

where we have used the assumption that $qT \geq 2\pi e^2 > 2\pi\sqrt{e}$, and

$$c_{\eta,1/2,q} = 0.837 \log q + 11.52,$$
$$c_{\eta,0,q,\delta} = |\eta_\delta'(t) \log t|_1 \leq 2\pi\delta|\eta(t) \log t|_1 + |\eta'(t) \log t|_1 \leq 1.541\delta + 1.03,$$
$$c_{\eta,-,q,\delta} = (\log q + 6.083)(2\pi\delta|\eta(t)|_2 + |\eta'(t)|_2) \leq (\log q + 6.083)(5.03\delta + 1.67).$$

□

16.3 APPLYING GRH(T). CONCLUSIONS.

In §4.3, we discussed D. Platt's numerical verification of GRH up to a given height and conductor (Prop. 4.2) [Pla16]. Let us see what this verification gives us when used as an input to Prop. 16.17.

Proof of Theorem 14.1. We are interested in bounds on $|\operatorname{err}_{\eta,\chi^*}(\delta, x)|$ for $q \le r$ and $|\delta| \le 4r/q$, where $r = c \cdot 100000$, $c = 3$ or $c = 4$. We let $T = 10^8 \max(|\delta|, 4)/4r = \max(250|\delta|/c, 1000/c)$. Thus $qT \le 10^8$.

We apply Prop. 16.17, and write $\varrho = T/\pi^2\delta^2$. The idea now is that there are two ways to bound the exponent $E(\varrho)T$; we will follow one way for $\varrho \le \varrho_0$ and the other one for $\varrho > \varrho_0$, where ϱ_0 will be chosen soon. On the one hand, since $E(\varrho)$ is increasing,

$$E(\varrho)T \ge E(\varrho_0)T \ge E(\varrho_0) \cdot \frac{1000}{c}$$

for $\varrho \ge \varrho_0$. On the other hand, since $E(\varrho)$ is concave (Lemma 15.23), we see that

$$E(\varrho)T \ge \frac{E(\varrho_0)}{\varrho_0}\varrho T = \frac{E(\varrho_0)}{\pi^2\varrho_0}\frac{T^2}{\delta^2} \ge \frac{E(\varrho_0)}{\pi^2\varrho_0}\left(\frac{250}{c}\right)^2$$

for $\varrho \ge \varrho_0$. Our two bounds are equal when

$$\varrho_0 = \frac{c}{1000\pi^2}\left(\frac{250}{c}\right)^2 = \frac{125}{2} \cdot \frac{1}{\pi^2 c},$$

and so that is the value of ϱ_0 we choose. We obtain that, for any ϱ,

$$E(\varrho)T \ge E(\varrho_0) \cdot \frac{1000}{c} \ge \begin{cases} 68.16791 & \text{if } c = 3, \\ 41.62864 & \text{if } c = 4, \end{cases}$$

and so, for $\varrho \ge \varrho_0$,

$$\max\left(0.44, \frac{1.14}{\sqrt{\varrho}}\right) e^{-E(\varrho)T} \le \begin{cases} 1.94863 \cdot 10^{-30} & \text{if } c = 3, \\ 7.5519 \cdot 10^{-19} & \text{if } c = 4. \end{cases}$$

We have to examine the case $\varrho \ge \varrho_0$ more closely, on account of the factor $1/\sqrt{\varrho}$. We can provide an upper bound on this factor, namely,

$$\frac{1}{\sqrt{\varrho}} = \frac{\pi\delta}{\sqrt{T}} = \pi\sqrt{T} \cdot \frac{\delta}{T} \le 10000\pi \cdot \frac{c}{250} = 40\pi c.$$

Hence, for $\varrho \le 0.1$ (say),

$$\frac{1.14}{\sqrt{\varrho}} e^{-E(\varrho)T} \le 1.14 \cdot 40\pi c \cdot e^{-\frac{E(0.1)}{0.1}\left(\frac{250}{\pi c}\right)^2} \le \begin{cases} 2.98987 \cdot 10^{-36} & \text{if } c = 3, \\ 1.970304 \cdot 10^{-19} & \text{if } c = 4. \end{cases}$$

Finally, we use the bisection method (as in §4.1) with 25 iterations, and obtain that, for $0.1 < r < r_0$,

$$\frac{1.14}{\sqrt{r}} e^{-E(r)T} \leq 1.14 \cdot 40\pi c \cdot e^{-\frac{E(r)}{r}\left(\frac{250}{\pi c}\right)^2} \leq \begin{cases} 1.94863 \cdot 10^{-30} & \text{if } c = 3, \\ 7.55189 \cdot 10^{-19} & \text{if } c = 4. \end{cases}$$

Here we can work only with the factor $1.14/\sqrt{r}$ and not with 0.44 because $r_0 < 4$.

It is clear that

$$e^{-\frac{\pi}{4}T} \leq e^{-\frac{\pi}{4}\frac{1000}{4}} \leq 5.33 \cdot 10^{-86}.$$

Recall that $qT_0 \leq 10^8$. We conclude that

$$\left(e^{-E(r(T))T} \cdot \begin{cases} 0.44 & \text{if } r \geq 4 \\ 1.14/\sqrt{r} & \text{if } r < 4 \end{cases} + 0.22 e^{-\frac{\pi}{4}T} \right) \log \frac{qT}{2\pi}$$

is at most

$$\left(\begin{cases} 1.94863 \cdot 10^{-30} & \text{if } c = 3 \\ 7.5519 \cdot 10^{-19} & \text{if } c = 4 \end{cases} + 1.18 \cdot 10^{-86} \right) \log \frac{10^8}{2\pi},$$

which, in turn, is at most

$$\varepsilon_c := \begin{cases} 3.231375 \cdot 10^{-29} & \text{if } c = 3, \\ 1.25232 \cdot 10^{-17} & \text{if } c = 4. \end{cases}$$

As for the second and third lines of (16.55),

$$\begin{aligned} 1.02\sqrt{T} \log qT + 11.81\sqrt{T} &\leq (1.02 \log 10^8 + 11.81)\sqrt{\frac{250 \max(|\delta|, 4)}{c}} \\ &\leq \kappa_c \sqrt{\max(|\delta|, 4)}, \end{aligned}$$

where $\kappa_3 = 279.34$, $\kappa_4 = 241.91$, and

$$1.6 \log q + 21.8 \leq 1.6 \log 400000 + 21.8 \leq 42.5,$$

$$1.1 \log q + 5.6|\delta| + 2 \leq 5.6|\delta| + 14.2,$$
$$(\log q + 6.1)(0.6 + 4.8|\delta|) \leq 91.2|\delta| + 11.4.$$

Hence, assuming $x \geq 10^6$ to simplify, we see that Prop. 16.17 gives us that

$$\begin{aligned} \text{err}_{\eta,\chi}(\delta, x) &\leq \varepsilon_c x + (\kappa_c \sqrt{\max(|\delta|, 4)} + 42.5)\sqrt{x} + (5.6|\delta| + 14.2) + \frac{91.2|\delta| + 11.4}{\sqrt{x}} \\ &\leq \varepsilon_c x + (\kappa_c \sqrt{\max(|\delta|, 4)} + 43)\sqrt{x} + 6|\delta|. \end{aligned}$$

□

Proof of Theorem 14.2. We proceed just as in the proof of Theorem 14.1, setting again $r = c \cdot 100000$ and $T = 10^8 \max(|\delta|, 4)/4r$. The bounds on $e^{-E(\mathscr{r})T}$, $1/\sqrt{\mathscr{r}}$ and $e^{-\pi T/4}$ are as before. We obtain that the first line of the right side of (16.57) is at most

$$\left(\begin{cases} 5.84589 \cdot 10^{-30} & \text{if } c = 3 \\ 2.26557 \cdot 10^{-18} & \text{if } c = 4 \end{cases} + 4.72 \cdot 10^{-86}\right) \cdot \log \frac{10^8}{2\pi},$$

which, in turn, is at most

$$\varepsilon_c := \begin{cases} 9.6942 \cdot 10^{-29} & \text{if } c = 3, \\ 3.75696 \cdot 10^{-17} & \text{if } c = 4. \end{cases}$$

We now bound the second and third lines of (16.57):

$$\begin{aligned} 0.56\sqrt{T}\log qT + 2.23\sqrt{T} &\leq (0.56 \log 10^8 + 2.23)\sqrt{\frac{250 \max(|\delta|, 4)}{c}} \\ &\leq \kappa_c \sqrt{\max(|\delta|, 4)}, \end{aligned}$$

where $\kappa_3 = 114.53$, $\kappa_4 = 99.19$, and

$$0.93 \log q + 12.8 \leq 0.93 \log 400000 + 12.8 \leq 24.8,$$

$$(\log q + 6.1)(1.1 + 4.6|\delta|) \leq 87.4|\delta| + 20.9.$$

Hence, assuming $x \geq 10^6$ to simplify, we see that Prop. 16.18 gives us that

$$\begin{aligned} \operatorname{err}_{\eta,\chi}(\delta, x) &\leq \varepsilon_c x + (\kappa_c \sqrt{\max(|\delta|, 4)} + 24.8)\sqrt{x} + (2.7|\delta| + 1.2) + \frac{87.4|\delta| + 20.9}{\sqrt{x}} \\ &\leq \varepsilon_c x + (\kappa_c \sqrt{\max(|\delta|, 4)} + 25)\sqrt{x} + 3|\delta|. \end{aligned}$$

□

Proof of Theorem 14.3, part 1. Let us work first with the parameters in part 1 of the statement: $H = 100$ and $r = 400000$. We are interested in bounds on $|\operatorname{err}_{\eta,\chi^*}(\delta, x)|$ for $q \leq r$ and $|\delta| \leq 4r/q$. We let $T = T_0 + H$, where

$$T_0 = 6.875 \cdot 10^7 \cdot \frac{\max(|\delta|, 4)}{4r} = \frac{1375}{8} \max\left(\frac{|\delta|}{4}, 1\right).$$

Then $qT \leq 6.875 \cdot 10^7 + Hq$, which is at most 10^8 for $q \leq 312500$, and less than $3.75 \cdot 10^7 + 2Hq$ for $q > 312500$. Hence, T is at most H_q in Proposition 4.2, and so GRH(T) holds.

We apply Prop. 16.19, and write $\mathscr{r} = T_0/\pi^2\delta^2$. Much as before, we note that, for $\mathscr{r} > \mathscr{r}_0$, where $\mathscr{r}_0 > 0$ is arbitrary,

$$E(\mathscr{r})T_0 \geq E(\mathscr{r}_0)T_0 \geq E(\mathscr{r}_0) \cdot \frac{1375}{8},$$

whereas, for $\digamma \leq \digamma_0$,

$$E(\digamma)T_0 \geq \frac{E(\digamma_0)}{\digamma_0}\digamma T_0 = \frac{E(\digamma_0)}{\pi^2\digamma_0}\frac{T_0^2}{\delta^2} \geq \frac{E(\digamma_0)}{\pi^2\digamma_0}\left(\frac{1375}{32}\right)^2.$$

These two bounds are equal when $\digamma_0 = \frac{1375}{128}\pi^{-2}$, and so we choose that value of $\digamma_0$. Then, for any $\digamma \geq \digamma_0$,

$$E(\digamma)T_0 \geq E(\digamma_0)\frac{1375}{8} \geq 21.21593,$$

and so,

$$\max\left(1.05, \frac{2.72}{\sqrt{\digamma}}\right) e^{-E(\digamma)T_0} \leq 1.59299 \cdot 10^{-9}.$$

We have an upper bound on $1/\sqrt{\digamma}$:

$$\frac{1}{\sqrt{\digamma}} = \frac{\pi\delta}{\sqrt{T_0}} = \pi\sqrt{T_0} \cdot \frac{\delta}{T_0} \leq \pi\sqrt{6.875 \cdot 10^7} \cdot \frac{32}{1375} \leq 606.225.$$

Thus, for $\digamma \leq 0.001$,

$$\max\left(1.05, \frac{2.72}{\sqrt{\digamma(T)}}\right) e^{-\frac{E(\digamma)}{\pi^2\digamma}\left(\frac{1375}{32}\right)^2} \leq 1.15275 \cdot 10^{-7}. \qquad (16.61)$$

The bisection method applied to $[0.001, \frac{1375}{128}\pi^{-2}]$ shows that the maximum of the left side of (16.61) on that range is less than $1.15275 \cdot 10^{-7}$.

Since

$$0.75 \cdot e^{-\frac{\pi}{4}T_0} \leq 0.75 \cdot e^{-\frac{\pi}{4}\frac{1375}{8}} \leq 1.7763 \cdot 10^{-59},$$

we conclude that the first line of the right side of (16.60) is at most

$$(1.15275 \cdot 10^{-7} + 1.7763 \cdot 10^{-59}) \cdot \log\frac{1.0875 \cdot 10^8}{2\pi} \leq 1.92126 \cdot 10^{-6}.$$

We bound the other terms in (16.60):

$$\begin{aligned} 0.566\sqrt{T}\log qT + 1.41\sqrt{T} &\leq (0.566\log 108750000 + 1.41)\sqrt{\frac{1375}{32}\max(|\delta|, 4)} \\ &\leq 77.9\sqrt{\max(|\delta|, 4)}, \end{aligned}$$

$$0.84\log q + 11.52 \leq 0.84\log 400000 + 11.52 \leq 22.4,$$

$$(6.1\log q)(6 + 2|\delta|) \leq 473 + 158|\delta|.$$

Hence, assuming $x \geq 10^6$ to simplify, we see that Prop. 16.19 gives us that

$$\mathrm{err}_{\eta_+,\chi}(\delta, x) \leq 1.92126 \cdot 10^{-6}x + (77.9\sqrt{\max(|\delta|, 4)} + 22.5)\sqrt{x} + 2|\delta|.$$

□

Proof of Theorem 14.3, part 2. Let us now work with the parameters in part 2 of the statement: $H = 200$, $r' = 150000$, $q/\gcd(q,2) \leq r'$, $|\delta| \leq 4r'/q'$. We let $T = T_0 + H$, where

$$T_0 = 250 \max\left(\frac{|\delta|}{4}, 1\right),$$

and so $Tq \leq T_0 q + Hq \leq 250 \cdot 2r' + 200 \cdot 2r' \leq 135000000$. By Proposition 4.2, GRH(T) holds.

We apply Prop. 16.19, and write $\mathscr{r} = T_0/\pi^2\delta^2$. Much as before, we note that, for $\mathscr{r} > \mathscr{r}_0$, where $\mathscr{r}_0 > 0$ is arbitrary,

$$E(\mathscr{r})T_0 \geq E(\mathscr{r}_0)T_0 \geq 250E(\mathscr{r}_0),$$

whereas, for $\mathscr{r} \leq \mathscr{r}_0$,

$$E(\mathscr{r})T_0 \geq \frac{E(\mathscr{r}_0)}{\mathscr{r}_0}\mathscr{r}T_0 = \frac{E(\mathscr{r}_0)}{\pi^2\mathscr{r}_0}\frac{T_0^2}{\delta^2} \geq \frac{E(\mathscr{r}_0)}{\pi^2\mathscr{r}_0}\left(\frac{125}{2}\right)^2.$$

The two bounds are equal when $\mathscr{r}_0 = \frac{125}{8}\pi^{-2}$, and so we set $\mathscr{r}_0$ to that value. Then, for any $\mathscr{r} \geq \mathscr{r}_0$, $E(\mathscr{r})T_0 \geq E(\mathscr{r}_0)250$, and so

$$\max\left(1.05, \frac{2.72}{\sqrt{\mathscr{r}}}\right) e^{-E(\mathscr{r})T_0} \leq 1.80186 \cdot 10^{-18}.$$

Now

$$\frac{1}{\sqrt{\mathscr{r}}} = \frac{\pi\delta}{\sqrt{T_0}} = \pi\sqrt{T_0} \cdot \frac{\delta}{T_0} \leq \pi\sqrt{135000000} \cdot \frac{2}{125} \leq 584.033.$$

Thus, for $\mathscr{r} \leq 0.001$,

$$\max\left(1.05, \frac{2.72}{\sqrt{\mathscr{r}(T)}}\right) e^{-\frac{E(\mathscr{r})}{\pi^2\mathscr{r}}\left(\frac{125}{2}\right)^2} \leq 5.46217 \cdot 10^{-19}. \tag{16.62}$$

By the bisection method, we obtain that, for $0.1 < \mathscr{r} < \mathscr{r}_0$,

$$\max\left(1.05, \frac{2.72}{\sqrt{\mathscr{r}(T)}}\right) e^{-\frac{E(\mathscr{r})}{\pi^2\mathscr{r}}\left(\frac{125}{2}\right)^2} \leq 1.8019 \cdot 10^{-18}.$$

We obtain that the first line of the right side of (16.60) is at most

$$(1.8019 \cdot 10^{-18} + 3.9953 \cdot 10^{-86}) \cdot \log\frac{1.35 \cdot 10^8}{2\pi} \leq 1.802 \cdot 10^{-18}.$$

We bound the other terms in (16.60):

$$\begin{aligned} 0.566\sqrt{T}\log qT + 1.41\sqrt{T} &\leq \left(0.566 \log 1.35 \cdot 10^8 + 1.41\right)\sqrt{\frac{125}{2}\max(|\delta|, 4)} \\ &\leq 95\sqrt{\max(|\delta|, 4)}, \end{aligned}$$

$$0.84 \log q + 11.52 \leq 0.84 \log 300000 + 11.52 \leq 22.2,$$
$$(6.1 \log q)(6 + 2|\delta|) \leq 462 + 154|\delta|.$$

Hence, assuming $x \geq 10^6$ to simplify, we see that Prop. 16.19 gives us that

$$\mathrm{err}_{\eta_+,\chi}(\delta, x) \leq 1.802 \cdot 10^{-18} x + \left(95\sqrt{\max(|\delta|, 4)} + 22.3\right)\sqrt{x} + 2|\delta|.$$

□