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A GENERALIZED EULER-MACLAURIN FORMULA FOR THE HURWITZ ZETA FUNCTION

EUGENIO P. BALANZARIO

(Communicated by Stanislav Jakubec)

ABSTRACT. We use an evaluation of the Mellin transform of a Fourier series in terms of some Dirichlet series in order to generalize the classical Euler-Maclaurin formula for the numerical evaluation of the Riemann zeta function.

§1. Introduction

In this note we consider the Hurwitz zeta function defined initially by

$$\zeta(s,a) = \sum_{j=0}^{\infty} \frac{1}{(j+a)^s} \quad \text{for} \quad 0 < a \le 1 \quad \text{and} \quad \sigma := \Re e(s) > 1.$$
 (1)

In §2 below, the Mellin transform of a Fourier series $\Delta(x)$ is evaluated in terms of Dirichlet series. Let $\ell \geq 1$. For $0 < \sigma < 1$ we have

$$\left\{\int_{1/\ell}^{\infty} \frac{\Delta(x)}{x^s} \,\mathrm{d}x\right\} + \int_{0}^{1/\ell} \frac{\Delta(x)}{x^s} \,\mathrm{d}x = \chi_1(s) \sum_{j=1}^{\infty} \frac{a_j}{j^{1-s}} + \chi_2(s) \sum_{j=1}^{\infty} \frac{b_j}{j^{1-s}} \,, \quad (2)$$

where a_j and b_j are the Fourier coefficients of $\Delta(x)$ and we have written $\left\{ \int_{1/\ell}^{\infty} x^{-s} \Delta(x) \, dx \right\}$ to represent the continuation to $\sigma > 0$ of the integral inside the brackets (defined for $\sigma > 1$). See equations (7) for the definitions of $\chi_1(s)$ and $\chi_2(s)$. Then use this evaluation (2) in order to obtain a generalization of the Euler-Maclaurin formula for the numerical evaluation of the Riemann zeta function, see [1; Chap. 6] for example.

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EUGENIO P. BALANZARIO

\S 2. Mellin transform of a Fourier series

Now we state the main result of this section and then we prove it in a series of lemmas.

THEOREM 1. With $e(x) = e^{2\pi i x}$, consider the Fourier series

$$\Delta(x) = \sum_{j \in \mathbb{Z}} c_j e(jx) = c_0 + 2 \sum_{j=1}^{\infty} \left\{ a_j \cos(2\pi jx) + b_j \sin(2\pi jx) \right\}$$
(3)

where

$$a_{j} = \frac{c_{j} + c_{-j}}{2} = \int_{-1/2}^{+1/2} \Delta(x) \cos(2\pi j x) \, \mathrm{d}x \,,$$

$$b_{j} = \frac{c_{-j} - c_{j}}{2 \,\mathrm{i}} = \int_{-1/2}^{+1/2} \Delta(x) \sin(2\pi j x) \, \mathrm{d}x \,.$$
(4)

Assume $c_j \ll 1/|j|$ as $|j| \to \infty$. Let ℓ be a real number greater than or equal to one. For $s = \sigma + \mathrm{i}t$ such that $\sigma > 1$, define

$$z(s) = \int_{1/\ell}^{\infty} x^{-s} \Delta(x) \, \mathrm{d}x \,. \tag{5}$$

Then z(s) has an analytic (resp. meromorphic) continuation to the half plane $\sigma > 0$ if $c_0 = 0$ (resp. if $c_0 \neq 0$). Now define for $\sigma > 0$ the two Dirichlet series

$$\mathcal{Z}_1(s) = \sum_{j=1}^{\infty} \frac{a_j}{j^s} , \qquad \mathcal{Z}_2(s) = \sum_{j=1}^{\infty} \frac{b_j}{j^s} ,$$
 (6)

and for all s the two χ functions

$$\begin{aligned} \chi_1(s) &= 2(2\pi)^{s-1} \Gamma(1-s) \sin\left(\frac{\pi s}{2}\right), \\ \chi_2(s) &= 2(2\pi)^{s-1} \Gamma(1-s) \cos\left(\frac{\pi s}{2}\right). \end{aligned} \tag{7}$$

Finally, for $0 < \sigma < 1$, define $\mathcal{E}(s) = -\int_{0}^{1/\ell} x^{-s} \Delta(x) \, \mathrm{d}x$. If $0 < \sigma < 1$, then $z(s) = \chi_1(s)\mathcal{Z}_1(1-s) + \chi_2(s)\mathcal{Z}_2(1-s) + \mathcal{E}(s)$. (8)

Since $c_j \ll 1/|j|$ as $|j| \to \infty$, then we can integrate term by term the Fourier series in (5) to obtain ∞

$$z(s) = \sum_{j \in \mathbb{Z}} c_j \int_{1/\ell} x^{-s} e(jx) \, \mathrm{d}x \,. \tag{9}$$

In the next lemma we evaluate the individual terms in the sum in (9). While we prove the lemma for $\sigma > 0$, we actually use it for $\sigma > 1$.

LEMMA 1. Let α and ℓ be positive real numbers. Let $s = \sigma + it$ be such that $\sigma > 0$. Let

$$\Gamma(1-s, i\alpha) = \int_{L(\alpha)} z^{-s} e^{-z} dz, \quad and \quad \Gamma(1-s, -i\alpha) = \int_{\overline{L}(\alpha)} z^{-s} e^{-z} dz$$

where $L(\alpha) = \{x + i\alpha : 0 \le x < \infty\}$ is a horizontal line segment and $\overline{L}(\alpha)$ is the complex conjugate of $L(\alpha)$, so that $\overline{L}(\alpha) = \{x - i\alpha : 0 \le x < \infty\}$. Then we have

$$\int_{1/\ell}^{\infty} x^{-s} e^{-i\alpha x} dx = e\left(\pm\frac{s-1}{4}\right) \alpha^{s-1} \Gamma(1-s,\pm\frac{i\alpha}{\ell}), \qquad (10)$$

$$\int_{1/\ell}^{\infty} x^{-s} e^{+i\alpha x} dx = e\left(-\frac{s-1}{4}\right)\alpha^{s-1}\Gamma\left(1-s,-\frac{i\alpha}{\ell}\right).$$
(11)

Proof. Let us denote by I_1 the integral (10). We consider a contour C by starting at $z = 1/\ell$, and then moving to the right along the real axis until we reach z = R, where R is a large real number. Then we turn around the origin in the negative direction until we meet the vertical line passing through $z = 1/\ell$. Finally, we move upwards along this vertical line until we reach the starting point. It is clear that

$$\int\limits_C z^{-s} e^{-i\alpha z} dz = 0.$$

Denote by C_2 the circle segment making up C, so that $C_2 = \{Re^{-i\theta} : 0 \le \theta \le \pi/2 + o(1)\}$. Let $\theta^* = \log R/\alpha R$. By splitting C_2 according to whether $\theta^* \le \theta \le \pi/2$ or $0 \le \theta \le \theta^*$ we obtain

$$\int_{C_2} z^{-s} e^{-i\alpha z} dz \ll R^{1-\sigma} \left(e^{-\alpha R \sin \theta^*} + \frac{\log R}{\alpha R} \right) \to 0$$

when $R \to \infty$. Thus, I_1 is equal to

$$-\operatorname{i} \int_{0}^{\infty} \left(\frac{1}{\ell} - \operatorname{i} y\right)^{-s} \operatorname{e}^{-\operatorname{i} \alpha \left(\frac{1}{\ell} - \operatorname{i} y\right)} \, \mathrm{d} y = e\left(\frac{s-1}{4}\right) \operatorname{e}^{-\operatorname{i} \alpha/\ell} \int_{0}^{\infty} \left(y + \frac{\mathrm{i}}{\ell}\right)^{-s} \operatorname{e}^{-\alpha y} \, \mathrm{d} y$$
$$= e\left(\frac{s-1}{4}\right) \operatorname{e}^{-\operatorname{i} \alpha/\ell} \int_{0}^{\infty} \left(\frac{y}{\alpha} + \frac{\mathrm{i}}{\ell}\right)^{-s} \operatorname{e}^{-y} \frac{1}{\alpha} \, \mathrm{d} y$$
$$= e\left(\frac{s-1}{4}\right) \alpha^{s-1} \int_{L(\alpha/\ell)} z^{-s} \operatorname{e}^{-z} \, \mathrm{d} z \, .$$

A similar argument proves formula (11).

Assume $\sigma > 1$. From (9) and Lemma 1, we see that z(s) is equal to

$$\begin{aligned} \frac{c_0 \ell^{s-1}}{s-1} + (2\pi)^{s-1} \sum_{j=1}^{\infty} \frac{1}{j^{1-s}} \Big[e\Big(-\frac{s-1}{4}\Big) \Gamma\Big(1-s, -\frac{2\pi i j}{\ell}\Big) c_j \\ + e\Big(\frac{s-1}{4}\Big) \Gamma\Big(1-s, \frac{2\pi i j}{\ell}\Big) c_{-j} \Big] \end{aligned}$$

With $c^{\pm} = c_{\pm j}$ and $\alpha^{\pm} = e(\pm (s-1)/4)\Gamma(1-s,\pm 2\pi i j/\ell)$, we can write the expression inside the square brackets as

$$\alpha^{-} \cdot c^{+} + \alpha^{+} \cdot c^{-} = (\alpha^{+} + \alpha^{-}) \cdot \frac{c^{+} + c^{-}}{2} + (-\alpha^{+} + \alpha^{-}) \cdot \frac{c^{+} - c^{-}}{2}.$$

Hence we obtain

$$z(s) = \frac{c_0 \ell^{s-1}}{s-1} + (2\pi)^{s-1} \sum_{j=1}^{\infty} \frac{1}{j^{1-s}} \left[a_j A_j(s) - ib_j B_j(s) \right]$$
(12)

where for $j \in \mathbb{N}$, we have set

$$A_j(s) = e\left(-\frac{s-1}{4}\right)\Gamma\left(1-s, -\frac{2\pi i j}{\ell}\right) + e\left(\frac{s-1}{4}\right)\Gamma\left(1-s, \frac{2\pi i j}{\ell}\right),\tag{13}$$

$$B_j(s) = e\left(-\frac{s-1}{4}\right)\Gamma\left(1-s, -\frac{2\pi\,\mathrm{i}\,j}{\ell}\right) - e\left(\frac{s-1}{4}\right)\Gamma\left(1-s, \frac{2\pi\,\mathrm{i}\,j}{\ell}\right),\tag{14}$$

and a_i , b_i are as in (4).

LEMMA 2. The sum on the right hand side of (12) represents an analytic function on $\sigma > 0$. Thus, if $c_0 = 0$, then z(s) does not have singularities in this half plane, while if $c_0 \neq 0$, then z(s) has a simple pole at s = 1 with residue equal to c_0 .

P r o o f. Notice first that the incomplete gamma functions of Lemma 1 are analytic functions of its first argument. By a theorem of Weierstrass on the uniform convergence of analytic functions, it suffices to show that the infinite series in (12) converges uniformly on compact subsets of the complex plane. Now notice that for any positive real number α

$$|\Gamma(1-s,\pm \mathrm{i}\,\alpha)| \le \int_{0}^{\infty} |x-\mathrm{i}\,\alpha|^{-\sigma} \,\mathrm{e}^{-x} \,\mathrm{d}x \le \left(\frac{1}{\alpha}\right)^{\sigma}.$$

Putting $\alpha = 2\pi j/\ell$ with $j \in \mathbb{N}$ and $\ell > 1$ fixed, we see that our infinite series is bounded by

$$\cosh\!\left(\tfrac{\pi t}{2}\right) \sum_{j=1}^{\infty} \frac{1}{j^{1-\sigma}} \!\left(\frac{\ell}{2\pi j}\right)^{\sigma} \!\left(|c_{j}| + |c_{-j}|\right) \ll \sum_{j=1}^{\infty} \frac{|c_{j}| + |c_{-j}|}{j} < \infty$$

where the implied constant in \ll depends both on σ and t.

The next step is to change the path of integration in the gamma functions from the horizontal line segments L and L from Lemma 1 by a path first along the imaginary axis and then along the real axis.

LEMMA 3. Let $A_j(s)$ and $B_j(s)$ be as in (13) and (14) respectively. If s is such that $0 < \sigma < 1$, then

$$\begin{split} A_j(s) &= 2\Gamma(1\!-\!s)\sin\!\left(\frac{\pi s}{2}\right) + \mathcal{A}_j(s)\,,\\ -\,\mathrm{i}B_j(s) &= 2\Gamma(1\!-\!s)\cos\!\left(\frac{\pi s}{2}\right) + \mathcal{B}_j(s)\,, \end{split}$$

where the reminder terms $\mathcal{A}_{i}(s)$ and $\mathcal{B}_{i}(s)$ are respectively

$$-\frac{2}{(2\pi j)^{s-1}} \int_{0}^{1/\ell} \cos(2\pi jy) y^{-s} \, \mathrm{d}y \qquad and \qquad -\frac{2}{(2\pi j)^{s-1}} \int_{0}^{1/\ell} \sin(2\pi jy) y^{-s} \, \mathrm{d}y.$$

P r o o f. We will prove only the assertion for $B_i(s)$, the evaluation of $A_i(s)$ being similar. It is easy to see that the integral of $e^{-z} z^{-s}$ along a finite vertical line segment tends to zero as we move this segment horizontally to the right. Hence, we can write $\Gamma(1-s, -2\pi i j/\ell) = \Gamma(1-s) + I_1(s)$ where

$$I_1(s) = \int_{C_1} e^{-z} z^{-s} dz$$
(15)

and C_1 is the line segment which goes from $-2\pi i j/\ell$ to 0. Then we have

$$e\left(-\frac{s-1}{4}\right) \cdot I_{1}(s) = e\left(-\frac{s-1}{4}\right) \int_{-2\pi j/\ell}^{0} e^{-iy} (iy)^{-s} i dy$$

= $-e\left(-\frac{s-1}{4}\right) \cdot (-i)^{-s+1} \int_{0}^{2\pi j/\ell} e^{iy} y^{-s} dy = -\int_{0}^{2\pi j/\ell} e^{iy} y^{-s} dy.$

We also write $\Gamma(1-s, 2\pi i j/\ell) = \Gamma(1-s) + I_2(s)$ where $I_2(s)$ is as in (15) with C_1 replaced by $C_2;$ the line segment which goes from $2\pi\,\mathrm{i}j/\ell$ to the origin.

As before, we now obtain

$$e\left(\frac{s-1}{4}\right) \cdot I_2(s) = -\int_{0}^{2\pi j/\ell} e^{-iy} y^{-s} dy.$$

Thus $B_j(s)$ equals

$$\Gamma(1-s)\left[e\left(-\frac{s-1}{4}\right) - e\left(\frac{s-1}{4}\right)\right] - \int_{0}^{2\pi j/\ell} \left(e^{iy} - e^{-iy}\right) y^{-s} \, \mathrm{d}y$$
$$= 2\,\mathrm{i}\Gamma(1-s)\cos\left(\frac{\pi s}{2}\right) - \frac{2\,\mathrm{i}}{(2\pi j)^{s-1}} \int_{0}^{1/\ell} \sin(2\pi jy) y^{-s} \, \mathrm{d}y.$$

Now we are ready to prove Theorem 1.

The term in square brackets in the last expression is equal to

$$\begin{aligned} \mathcal{E}(s) &= -c_0 \int_0^{1/\ell} x^{-s} \, \mathrm{d}x - \sum_{j=1}^\infty \frac{1}{(2\pi j)^{1-s}} \bigg\{ \frac{2a_j}{(2\pi j)^{s-1}} \int_0^{1/\ell} \cos(2\pi jx) x^{-s} \, \mathrm{d}x \\ &+ \frac{2b_j}{(2\pi j)^{s-1}} \int_0^{1/\ell} \sin(2\pi jx) x^{-s} \, \mathrm{d}x \bigg\} \\ &= -\int_0^{1/\ell} x^{-s} \bigg\{ c_0 + 2\sum_{j=1}^\infty a_j \cos(2\pi jx) + b_j \sin(2\pi jx) \bigg\} \, \mathrm{d}x \\ &= -\int_0^{1/\ell} x^{-s} \Delta(x) \, \mathrm{d}x \,. \end{aligned}$$

§3. Euler-Maclaurin formula

Now we apply Theorem 1 in order to obtain the following generalization of the Euler-Maclaurin formula for the numerical evaluation of the Riemann zeta function.

THEOREM 2. Let $\Delta(x)$ be a periodic function of $x \in \mathbb{R}$ with period one. Assume that $\int_{0}^{1} \Delta(x) \, dx = 1$. Let $0 < a \le 1$ and for $x \in \mathbb{R}$ let $\Delta_{a}(x) = \Delta(x-a)$. Let

$$\Delta_{a}(x) = 1 + 2\sum_{j=1}^{\infty} \{\alpha_{j}(a)\cos(2\pi jx) + \beta_{j}(a)\sin(2\pi jx)\}$$
(16)

be the Fourier series expansion of $\Delta_a(x)$. For $x \in [0,1)$ and $n \in \mathbb{N}$, let

$$\begin{split} B_0(x) &= \Delta(x)\,,\\ B_n(x) &= \int\limits_0^x B_{n-1}(y)\,\,\mathrm{d} y + \int\limits_0^1 (y-1) B_{n-1}(y)\,\,\mathrm{d} y\,. \end{split}$$

For $x \in [a, a+1)$ let $B_n(x; a) = B_n(x-a)$ and extend the domain of definition of $B_n(x; a)$ so that it is a periodic function of $x \in \mathbb{R}$ of period one. Let $\chi_1(s)$ and $\chi_1(s)$ be as in (7). Let η be a positive integer and let J be a nonnegative integer. Let $\zeta(s, a)$ be the Hurwitz zeta function. If $0 < \sigma < 1$, then we have

$$\begin{split} \zeta(s,a) &= \sum_{j=0}^{\eta-1} \frac{1}{(j+a)^s} + \chi_1(s) \sum_{j=1}^{\infty} \frac{\alpha_j(a)}{j^{1-s}} + \chi_2(s) \sum_{j=1}^{\infty} \frac{\beta_j(a)}{j^{1-s}} \\ &\quad - \int_{1-a}^{1} \frac{\Delta(x)}{(x+a-1)^s} \, \mathrm{d}x - \sum_{j=0}^{\eta-1} \int_{0}^{1} \frac{\Delta(x)}{(x+j+a)^s} \, \mathrm{d}x \\ &\quad + \sum_{j=0}^{J-1} (s)_j \frac{B_{j+1}(a^-;a)}{(\eta+a)^{s+j}} - (s)_J \int_{\eta+a}^{\infty} \frac{B_J(x;a)}{x^{s+J}} \, \mathrm{d}x \\ (s)_J &= \prod_{\ell=0}^{J-1} (s+\ell) \,. \end{split}$$

Proof. Let $0 < a \le 1$. Let $\sigma > 1$. Notice first that

where

$$\zeta(s,a) = \int_a^\infty x^{-s} \Delta_a(x) \, \mathrm{d}x - \int_{a^-}^\infty x^{-s} \, \mathrm{d}B_1(x;a) \, .$$

Let η be a positive integer. Then we have

$$\begin{split} \zeta(s,a) &= \int_{a}^{\infty} x^{-s} \Delta_{a}(x) \, \mathrm{d}x - \int_{a^{-}}^{\eta+a^{-}} x^{-s} \, \mathrm{d}B_{1}(x;a) - \int_{\eta+a^{-}}^{\infty} x^{-s} \, \mathrm{d}B_{1}(x;a) \\ &= \sum_{j=0}^{\eta-1} \frac{1}{(j+a)^{s}} + \int_{a}^{\infty} \frac{\Delta_{a}(x)}{x^{s}} \, \mathrm{d}x - \int_{a}^{\eta+a} \frac{\Delta_{a}(x)}{x^{s}} \, \mathrm{d}x - \int_{\eta+a^{-}}^{\infty} x^{-s} \, \mathrm{d}B_{1}(x;a) \, . \end{split}$$

Let $0 < \sigma < 1$. From Theorem 1, we obtain

$$\left\{ \int_{a}^{\infty} \frac{\Delta_a(x)}{x^s} \, \mathrm{d}x \right\} - \int_{a}^{\eta+a} \frac{\Delta_a(x)}{x^s} \, \mathrm{d}x$$
$$= \chi_1(s) \sum_{j=1}^{\infty} \frac{\alpha_j(a)}{j^{1-s}} + \chi_2(s) \sum_{j=1}^{\infty} \frac{\beta_j(a)}{j^{1-s}} - \int_{0}^{\eta+a} \frac{\Delta_a(x)}{x^s} \, \mathrm{d}x \, .$$

We can write the last integral as

$$\int_{1-a}^{1} \frac{\Delta(x)}{(x+a-1)^s} \, \mathrm{d}x + \sum_{j=0}^{\eta-1} \int_{0}^{1} \frac{\Delta(x)}{(x+j+a)^s} \, \mathrm{d}x$$

Let J be a nonnegative integer. Integrating by parts we obtain

$$-\int_{\eta+a^{-}}^{\infty} x^{-s} \, \mathrm{d}B_1(x;a) = \sum_{j=0}^{J-1} (s)_j \frac{B_{j+1}(a^-;a)}{(\eta+a)^{s+j}} - (s)_J \int_{\eta+a}^{\infty} \frac{B_J(x;a)}{x^{s+J}} \, \mathrm{d}x \, .$$

This finishes the proof of Theorem 2.

§4. Example

When $\Delta(x)$ is piecewise of polynomial form, then integrals of the form $\int_{\alpha}^{1} \Delta(x)(x+\beta)^{-s} dx$ can be explicitly evaluated when $\alpha \in \{0, 1-a\}$ and $\beta \ge 0$. In this section we exploit this observation and consider a concrete case of Theorem 2 above.

Let $\Delta(x) = -6x(x-1)$. The Fourier coefficients of $\Delta_a(x)$ in (16) are

$$\alpha_j(a) = -\frac{3}{j^2\pi^2}\cos(2aj\pi) \qquad \text{and} \qquad \beta_j(a) = -\frac{3}{j^2\pi^2}\sin(2aj\pi)\,.$$

For $\sigma < 1$ we have

$$\int_{1-a}^{1} \frac{\Delta(x)}{(x+a-1)^s} \, \mathrm{d}x = \frac{6a^{2-s}(s+2a-3)}{(s-1)(s-2)(s-3)}$$

On the other hand $\int_{0}^{1} \Delta(x)(x+j+a)^{-s} dx$ is equal to

$$\frac{6(s+2j+2a-1)}{(s-1)(s-2)(s-3)}(j+a+1)^{2-s} - \frac{6(-s+2j+2a+3)}{(s-1)(s-2)(s-3)}(j+a)^{2-s}$$

Writing B_i in place of $B_i(a^-; a)$, we obtain

$$B_1 = \frac{1}{2}, \ B_2 = \frac{1}{10}, \ B_3 = 0, \ B_4 = \frac{-1}{560}, \ B_5 = 0, \ B_6 = \frac{13}{302400}, \dots$$

With this data, numerical computation of the Hurwitz zeta function is feasible. The degree of accuracy in these computations is given by an upper bound for

$$(s)_J \int\limits_{\eta+a}^{\infty} rac{B_J(x;a)}{x^{s+J}} \mathrm{d}x$$

This upper bound is easily computed once $B_J(x; a)$ has been calculated.

J	$.5+29\mathrm{i}$	$.5 + 325 \mathrm{i}$	$.5 + 1305 \mathrm{i}$
0	0.0945295	0.0282984	0.0141243
1	0.0185811	0.0056396	0.0028177
2	0.0003278	0.0001011	0.0000506
4	0.0000078	0.0000024	0.0000012

TABLE	1.
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In Table 1 above, we display the numerical value of the error when $\zeta(s, 1/3)$ is computed with the data corresponding to $\Delta(x) = -6x(x-1)$. In Table 1, we have always set $\eta = [t]$ where t is the imaginary part of s = 0.5 + it. Thus for example, we see that when J = 4, the error is of order 10^{-6} for the above values of s.

Many choices for $\Delta(x)$ are possible besides -6x(x-1). For example, we can set $\Delta(x) = c_n x^n (x-1)^n$, where *n* is a natural number and c_n is such that $\int_0^1 \Delta(x) \, dx = 1$. In this case, if *n* is large enough, then $\Delta(x)$ will have many continuous derivatives and hence the Fourier coefficients will converge fast to zero. This will make the infinite series multiplying the terms $\chi_1(s)$ and $\chi_2(s)$ rapidly convergent. Notice however that if *n* is large, then other terms in the formula approximating the Hurwitz zeta function become more complex.

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