

Three-loop pentagonal Wilson loop with Lagrangian insertion

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Employing a cutting-edge bootstrap method, we analytically compute the three-loop pentagonal Wilson loop with Lagrangian insertion in planar $\mathcal{N} = 4$ super-Yang-Mills theory. Via a conjectured duality, this provides the first prediction for the maximally transcendental part of the four-loop five-point all-plus amplitude in pure Yang-Mills theory. Our starting point is an ansatz that encodes the known leading singularities of this object, as well as the relevant function space. The latter has become available only recently, thanks to an analytic computation of all three-loop five-point planar massless Feynman integrals. We determine the coefficients in the ansatz by imposing physical constraints. This includes a near-collinear expansion, which so far has not been applied to this quantity. Taken together, the constraints allow us to uniquely determine the symbol of the answer. We verify the symbol result by an independent integral reduction calculation, which moreover yields the full function-level answer.

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Introduction. Wilson loops play a crucial role in the study of gauge theories. In pure gauge theories, all gauge-invariant information can be expressed in terms of Wilson loops. Moreover, Wilson loops are ubiquitous in QCD as an effective physical description. Examples are soft-gluon resummation, jet physics, and factorization theorems. In planar maximally supersymmetric Yang-Mills theory (sYM), a surprising duality between scattering amplitudes and polygonal Wilson loops has been central to many studies of scattering amplitudes in this theory, such as the discovery of hidden symmetries, a novel operator product expansion, analytic insights into the relevant function space combined with symbol bootstrap approaches, and novel geometric amplitude representations. For recent reviews, see Refs. [1,2]. More recently, it was discovered that a generalization of those Wilson loops—adding a Lagrangian

insertion—conjecturally makes a connection to scattering amplitudes in pure Yang-Mills theory [3]. This opens up the exciting possibility of taking inspiration from the powerful developments in sYM and learning from them for non-supersymmetric scattering amplitudes.

We study the following ratio of vacuum expectation values in sYM theory,

$$F_n(x_1, \dots, x_n; x_0) = \pi^2 \frac{\langle W_n \mathcal{L}(x_0) \rangle}{\langle W_n \rangle}, \quad (1)$$

where the Wilson loops W_n are defined for a null polygon with cusp points $x_1, \dots, x_n$. The edges of this polygon are the momenta of the dual scattering amplitudes. In sYM, F_n is both infrared and ultraviolet finite and therefore can be computed directly in four dimensions. Its integrand is known, in principle, at leading color to all loops from the amplituhedron [4]. Moreover, the full set of leading singularities was initially conjectured in Refs. [3,5] and proven in Ref. [6]. The maximally transcendental part of F_n is conjectured [3] to be dual to the all-plus-helicity amplitude in pure Yang-Mills theory. Thanks to this connection, obtaining perturbative results for F_n also teaches us about the function space needed for Yang-Mills scattering amplitudes.

An attractive way to learn about physical quantities is via the symbol bootstrap. In this method, one sets up an ansatz for the answer. The main ingredients are the expected

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leading singularities and symbols of the transcendental functions. In Ref. [7], the two-loop six-point contribution was bootstrapped in this way, leveraging new insights into the function space [8,9]. However, despite progress [10], determining the three-loop five-point case remained an important challenge. This is due to the previously unknown function space, as well as the technical complexity of handling a large number of multivariable functions. Recent results on the three-loop five-point function space, cf. Ref. [11], have now opened up a new opportunity. In this Letter, we report for the first time on the three-loop results for $n = 5$. In order to achieve this, we follow two complementary approaches.

The first approach employs the symbol bootstrap method. In order to fully determine the answer, we develop novel constraints from a near-collinear expansion, inspired by Ref. [12]. For the purposes of this Letter, we perform a preliminary analysis that uses minimal input about the integrable spectrum of flux-tube excitations [13]. Developing this approach further, toward a complete integrability-based description of Eq. (1), may unlock powerful new constraints on F_n . This could open up novel opportunities to bootstrap this quantity at higher loop orders and to perhaps even compute it at finite coupling. We note that this is the first application of the OPE/near-collinear expansion to Wilson loops with Lagrangian insertion. This is especially significant because the quantity studied is conjecturally dual to the all-plus amplitude in pure Yang-Mills theory, making it much closer to nonsupersymmetric physics than the MHV amplitudes bootstrapped in previous works [14–23].

The second approach is a first-principles calculation. We use the latest developments in integral reduction techniques in order to relate the known integrand of F_5 at three loops, cf. Ref. [24], to the results for Feynman integrals from Ref. [11]. This approach allows us to verify the symbol result obtained from the bootstrap method and, moreover, yields the full function-level answer.

In this way, we are able to determine the answer in two completely complementary ways. This is the first physical application of the analytic three-loop five-point Feynman integrals.

This Letter is organized as follows. We briefly introduce the Wilson loop with Lagrangian insertion in Sec. II and discuss what is known about its leading singularities and the relevant function space. In Sec. III, we compute the near-collinear expansion of this quantity. Based on those results, we calculate the three-loop pentagonal Wilson loop with Lagrangian insertion in Sec. IV, via the symbol bootstrap method. In Sec. V, we discuss properties of the result. In Sec. VI, we independently verify our symbol result through a direct calculation based on integral reduction. Finally, the summary and outlook are given in Sec. VII.

Perturbative structure. We work in the weak coupling perturbative expansion and in the large N_c limit,

$$F_n = \sum_{L \geq 0} (g^2)^{L+1} F_n^{(L)}, \quad g^2 = \frac{g_{\text{YM}}^2 N_c}{16}. \quad (2)$$

The Born level results $F_n^{(0)}$ and the one-loop corrections $F_n^{(1)}$ have been computed for arbitrary n in [3]. The perturbative results for four and five cusp cases have been obtained up to three and two loops in Refs. [25–27] and in [3,5], respectively. Due to the dual conformal symmetry of sYM, the quantity depends on $3n - 11$ cross-ratios [28], which is the same number of kinematic variables as an n massless particle scattering process in generic theories, such as QCD. Thanks to the amplitude-Wilson loop duality [29–31] at the level of loop integrands [32], the loop integrand of $F_n^{(L)}$ can be constructed from the (integrand of the logarithm of the) $(L + 1)$ -loop MHV amplitude. The latter is known up to six loops for the five-particle case [24].

Let us focus on the case $n = 5$ from now on. The L -loop contribution to this quantity can be written as

$$F_5^{(L)} = \sum_{i=0}^5 r_i g_i^{(L)}, \quad (3)$$

with the leading singularities r_i given in Ref. [10]. The $g_i^{(L)}$ are expected to be pure functions of transcendental weight $2L$. Since in the following we focus on the five-particle case, we will denote $F = F_5$ for simpler notation.

Let us discuss in more detail what is known about the function space g_i at three loops. Recently, all three-loop, five-point, planar massless Feynman integrals have been calculated analytically in Refs. [11,33], using the canonical differential equation method [34]. It turns out that the result for all planar massless Feynman integrals involves 56 symbol letters, confirming a conjecture made in Ref. [10].

The results of Ref. [11] allow us to extract the specific weight-six symbol space needed for describing $F^{(3)}$. We organize the symbols according to their transformation properties under the D_5 dihedral group. In order to achieve this, we use finite field computational tools [35,36]; see also Refs. [37,38] for related methods. We find 2220 linearly independent weight-six symbols. It turns out that the number of symbols required to construct $F^{(3)}$ is slightly different, as we explain presently. Note that $F^{(3)}$ contains both the genuine three-loop integrals and products of lower-loop five-point integrals. Taking these into account gives a total of 4729 symbols.

This number can be reduced by considering the conjectured duality relation with all-plus amplitudes [3]. This relation constrains the function space because it relates certain quantities obtained from products to other quantities that are expressed in terms of three-loop integrals only. Before using this information in order to write a bootstrap ansatz for Eq. (3), let us first discuss constraints that come from a near-collinear expansion of the Wilson loop contour.

Let us discuss the OPE picture in more detail, in order to make further quantitative predictions. We consider single-particle flux-tube excitations and label them by their type. In the space-time picture, they correspond to field insertions in the large-spin single-trace operators [54] which are holographically dual to excitations of the GKP string [55]. Their integrable spectrum is parametrized by rapidity u . An excitation of type $\mathbf{a}$ carries energy $E_{\mathbf{a}}(u)$, momentum $p_{\mathbf{a}}(u)$, and $U(1)$ charge $m_{\mathbf{a}}$, corresponding to the conformal symmetries of the reference square. Their contribution to the ratio G is as follows,

$$G_{\mathbf{a}} = \int_{-\infty}^{+\infty} \frac{du}{2\pi} \hat{\mu}_{\mathbf{a}}(u) Q_{\mathbf{a}}(u, Z), \quad (12)$$

where

$$\hat{\mu}_{\mathbf{a}}(u) = e^{-E_{\mathbf{a}}(u)\tau + ip_{\mathbf{a}}(u)\sigma + i\phi m_{\mathbf{a}}\mu_{\mathbf{a}}(u)}, \quad (13)$$

and the exponential factor describes propagation of the type $\mathbf{a}$ excitation through the reference square, with the measure $\mu_{\mathbf{a}}(u)$. The transition form factor $Q_{\mathbf{a}}$ is a Taylor series in Z , and it describes the transition of the excitation in the presence of the Lagrangian operator.

The gluon excitations $\mathbf{a} = F, \bar{F}$ are the simplest to analyze [14]. They have the lowest energy $E_F(u) = 1 + O(g^2)$. Thus, they are the leading contribution of order T^1 in the near-collinear limit, cf. Eq. (10). They do not mix with the multiparticle excitations. In addition, $p_F(u) = 2u + O(g^2)$ and $\mu_F(u) = O(g^2)$ [40].

On the one hand, the spectrum of flux-tube excitations is integrable; their energies, momenta, and measures have been calculated at finite coupling [13], and they are known at any perturbative order. On the other hand, we can glean information on $Q_{\mathbf{a}}$ from the known perturbative data on $G^{(L)}$ with $L \leq 2$. Comparing the OPE expansion, Eq. (10), with the single-gluon contributions given in Eq. (12), one finds perturbative expansions of Q_F and $Q_{\bar{F}}$ up to order $(g^2)^{L-1}$. Using these, we can calculate, from Eq. (12), the logarithmically enhanced contributions $T^1 \log^{\ell'}(T)$ in the expansion at higher loops, i.e., for $G^{(L+\ell')}$ with $\ell' \leq \ell' \leq \ell' + L$.

For example, from the Born-level equation (11), we find

$$Q_{\bar{F}}(u, Z) = \frac{Z}{g^2} \left(u^2 + \frac{1}{4} \right) + O(g^0), \quad (14)$$

which is sufficient to calculate the leading logarithms $T^1 \log^L(T)$ of $G^{(L)}$ at any L . The prediction is

$$G^{(L)} = -\frac{TFZ}{2L!} \log^L(T) \int_{-\infty}^{+\infty} \frac{du}{2\pi} \frac{[E_{\frac{3}{2}}^{(1)}(u)]^L e^{2iu\sigma}}{\cosh(\pi u)}, \quad (15)$$

where $E_s^{(1)}(u) = 2\psi(s + iu) + 2\psi(s - iu) - 2\psi(1)$ is the one-loop energy correction for excitations of conformal

spin s [13,56], and we omit terms of order $O(T \log^{L-1}(T))$. Following this approach, we can calculate all logarithmically enhanced contributions $T^1 \log^{\ell'}(T)$ with $1 \leq \ell' \leq 3$ at three loops. For reference, the leading term of the perturbative expansion of the gluon transition is

$$Q_F(u, Z) = Z + O(g^2). \quad (16)$$

We further conjecture an all-loop relation between the transitions

$$Q_{\bar{F}}(u, Z) = \frac{1}{g^2} x \left(u + \frac{i}{2} \right) x \left(u - \frac{i}{2} \right) Q_F(u, Z), \quad (17)$$

where $x(u) = \frac{1}{2}(u + \sqrt{u^2 - 4g^2})$ is the Zhukowsky variable. We find that Eq. (17) is compatible with the two-loop data.

We also considered the OPE contributions from the twist-two (T^2) and twist-three (T^3) single-particle excitations. Multiparticle gluon excitations could mix with them at the level of $(TF)^n \log^1(T)$ and $(T/F)^n \log^0(T)$ OPE terms with twist $n = 2, 3$ in $G^{(3)}$. However, higher powers of $\log(T)$ receive single-particle gluon bound state contributions only, which are under control. Finally, we also considered $T^2 F^0$ terms, which correspond to single-particle twist-two excitations of zero $U(1)$ charge [41].

Bootstrap. We fix the five-cusp quantity at symbol level relying on its physical properties, knowledge about the function space for the relevant Feynman graph topologies, and also conjectures about its analytic properties and the near-collinear OPE.

We construct a weight-six symbol ansatz for $F^{(3)}$, using the symbol space discussed above. We then impose the dihedral symmetries on the symbols,

$$\begin{aligned} g_0^{(3)} &= \rho \circ g_0^{(3)} = \tau \circ g_0^{(3)}, \\ g_1^{(3)} &= \tau \circ \rho \circ g_1^{(3)} \end{aligned} \quad (18)$$

where τ is a cyclic shift and ρ is a reflection, $\tau \circ p_i = p_{i+1}$ and $\rho \circ p_i = p_{6-i}$ at $i = 1, \dots, 5$, and $g_{j+1}^{(3)} = \tau^j \circ g_1^{(3)}$ for $j = 1, \dots, 4$. We find the dimension of the space for $g_0^{(3)}$ and $g_1^{(3)}$ to be 511 and 2403, respectively. Therefore, we have a total of 2914 unknowns at this stage. In order to fix them, we require the following conditions:

- (i) In both the collinear limit $p_4 || p_5$ and in the soft limit $p_5 \rightarrow 0$, we have $F_5 \rightarrow F_4$.
- (ii) The alphabet letters are organized in dimensionless ratios in the symbols.
- (iii) The spurious pole of r_1 at $s_{25} \rightarrow 0$ is suppressed by the vanishing of the accompanying symbol $g_1^{(3)}$.
- (iv) We assume that the conjectured duality to all-plus amplitudes holds. This imposes the constraint that

TABLE I. Counting of the bootstrap constraints on the three-loop ansatz for $F^{(3)}$.

Condition on $F^{(3)}$	Number of constraints
Collinear limit $p_4 p_5$	682
Soft limit $p_5 \rightarrow 0$	237
No spurious poles	1693
Dependence on s_{ij}/s_{kl}	778
Duality to all-plus	1182
Total	2868

the maximally transcendental part of the all-plus amplitude must lie within the function space of three-loop Feynman integrals, without requiring its explicit form. Interestingly, once the bootstrap is successfully completed, it provides a concrete prediction for the maximally transcendental part of the four-loop all-plus amplitude.

In this way, we obtain 2868 independent constraints on the 2914 unknowns in our ansatz, see Table I.

In order to fix the remaining 46 unknowns, we invoke the OPE description of the near-collinear expansion of $F^{(3)}$ at $p_4||p_5$, as discussed in Sec. III. The next-to-leading logarithmic OPE terms $(T/F) \log^1(T)$ in Eq. (10) at three loops fix 39 unknowns. All other single-particle contributions from gluons and their bound states do not provide independent constraints. However, they serve as valuable consistency checks of the bootstrap approach. Finally, we fix the remaining five unknowns by considering the leading logarithmic OPE term $T^2 F^0 \log^3(T)$ for the effective single-particle twist-two excitation $\psi\bar{\psi}$ of zero $U(1)$ charge.

In summary, combining knowledge of the function space, restrictions from the conjectured duality to all-plus amplitudes, physical constraints, and near-collinear conditions, we are able to uniquely fix the bootstrap ansatz. We provide the symbol results for $F^{(L)}$ at $L = 3$ (as well as the lower loop ones, for completeness) in the following repository [57] and as Supplemental Material [58].

Discussion of the result. Note that $F^{(3)}$ is finite and has uniform weight six. Although generic planar three-loop five-point Feynman integrals contain 56 alphabet letters, $F^{(3)}$ contains 30 letters only, namely, 25 two-loop five-point planar letters and five additional three-loop letters that had been predicted in Ref. [10]. For convenience, the relevant letters are listed in the Supplemental Material [58], which includes Refs. [10,59].

It is interesting to study how the symbol letters appear in the symbol of $F^{(3)}$ and to look for patterns across loop orders. We find that the letters appearing in the first three entries coincide with the first three entries appearing at two loops. The novel three-loop letters appear in the fourth entry only; this differs from the individual Feynman integrals, in

which these letters may occur in the fourth, fifth, and sixth entries. The last entries of $g_0^{(3)}$ depend on 19 linear combinations of the letters $w_1, \dots, w_5, w_{11}, \dots, w_{25}$ only. The last entries of $g_1^{(3)}$ depend on 15 linear combinations of the letters $w_{1,\dots,5}, w_8, w_{10}, w_{11,\dots,20}, w_{22}, w_{24}$ only.

Let us also comment on limits of the answer. Note that F_5 depends on five Mandelstam variables (via four dimensionless ratios), so there are many interesting configurations one can consider. Many of these have already been explored in the bootstrap construction. However, one further interesting limit to consider is the multi-Regge limit. This was considered in Sec. 4.5. of Ref. [5] for the two-loop case, where it was found that the symbol of $\log(F/F^{(0)})$ vanishes in that limit, up to two loops. (Note, however, that this relation is not exact, due to beyond-the-symbol terms.) We verify that the same relation holds also at order g^6 .

Direct verification from integral reduction. In this section, we describe a complementary approach to obtaining the three-loop five-point pentagonal Wilson loop with Lagrangian insertion, based on explicit loop integration. This serves as an independent check of the bootstrap construction discussed in Sec. IV and, moreover, provides the full function-level result.

A generic Feynman integral contributing to the Wilson loop can be written as a graph in dual space. The latter corresponds either to products of lower loop graphs (such as the cubic product of pentagons or a product of a one-loop pentagon and a two-loop pentabox integral), which are known from Refs. [60–62], or to genuine three-loop integrals computed in Ref. [11] (or permutations thereof). The reductions are performed using the new SpanningCut feature in the latest version of the package NeatIBP [63–65]. The reduction requires relating a large number of Feynman integrals with complicated numerator insertions to the basis of master integrals, and it represents a computationally demanding calculation.

Although $F^{(3)}$ is finite in four dimensions, each individual Feynman integral develops divergences upon loop integration, of up to order ϵ^{-6} . Therefore, the cancellation of these divergences is an important check of our calculation. Taking the symbol of the final result, we find perfect agreement with the outcome of the symbol bootstrap approach. Beyond the symbol, the IBP reduction yields the full function-level result for $F^{(3)}$, expressed in terms of the canonical master integrals of Ref. [11]. This provides access to numerical evaluation, opening the door to testing the conjectured positivity and complete monotonicity properties [5,10,66].

Summary and Outlook. In this Letter, we computed the pentagonal Wilson loop with a Lagrangian insertion in planar $\mathcal{N} = 4$ sYM theory at three-loop order by

employing a bootstrap approach. An essential new input came from predictions we derived by analyzing the expected structure in a near-collinear expansion. This constitutes the first application of OPE/near-collinear constraints to Wilson loops with Lagrangian insertion, extending the powerful integrability-based bootstrap program—which has been successfully applied to MHV amplitudes in $\mathcal{N} = 4$ sYM [14–23]—to a quantity that is conjecturally dual to the all-plus amplitude in pure Yang-Mills theory and therefore much closer to nonsupersymmetric physics. We independently verified our result by directly reducing the integrand onto the canonical basis from Ref. [11]. This means that we also have access to the full function-level answer, including numerical evaluation. Our result constitutes the first physical quantity computed in the newly uncovered three-loop five-point planar function space.

We anticipate that our results can be extended to function level (i.e., going beyond the proof-of-principle numerical evaluation from Ref. [11]), which will be extremely interesting in the perspective of testing the conjectured positivity [5,10] and complete monotonicity properties [66]. Furthermore, via the conjecture of Ref. [3], our result provides a prediction for the maximally transcendental part of the planar four-loop five-point all-plus amplitude in pure Yang-Mills theory. This prediction is of considerable independent interest, given the recent activity surrounding all-plus amplitudes and their connections to self-dual Yang-Mills theory and the chiral algebra bootstrap [67,68].

Finally, it would be very interesting to develop the near-collinear expansion, or OPE approach, further. We applied it here for the first time to Wilson loops with Lagrangian insertions. While the resulting predictions sufficed to fix the three-loop bootstrap ansatz, considerably stronger constraints should be within reach, and these may ultimately give access to finite-coupling results for the quantities studied here.

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Data availability. The data that support the findings of this article are openly available [57], embargo periods may apply.

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