Three-Loop Leading Singularities and BDS Ansatz for Five Particles

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Abstract

We use the leading singularity technique to determine the planar three-loop five-particle amplitude in $\mathcal{N} = 4$ super Yang-Mills in terms of a simple basis of integrals. We analytically compute the integral coefficients for both the parity-even and the parity-odd parts of the amplitude. The parity-even part involves only dual conformally invariant integrals. Using the method of obstructions we numerically evaluate two previously unfixed coefficients which appear in the three-loop BDS ansatz.

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I. INTRODUCTION

Scattering amplitudes in gauge theories are remarkable objects with many properties hidden in the complexity of their Feynman diagram expansion. It is natural to expect the most symmetric gauge theory, $\mathcal{N} = 4$ super-Yang-Mills (SYM), to be especially rich. Two very recent papers [1, 2] have used AdS/CFT to relate and shed light on two particularly remarkable properties of scattering amplitudes in SYM. These properties are dual conformal invariance, first observed for MHV amplitudes in [3] and conjectured to extend to all amplitudes in [4], and an equality between amplitudes and certain lightlike Wilson loops, first established at strong coupling in [5] and at weak coupling in [6, 7]. These developments were pushed forward in a number of papers including [8, 9, 10, 11, 12, 13, 14] and have been reviewed in [15], where a comprehensive set of references may be found.

Much of the recent interest in multi-loop scattering amplitudes has been stimulated by the ABDK/BDS ansatz [16, 17] which suggested that multi-loop MHV amplitudes satisfy a powerful iteration relation implying a simple exponential form for the full all-loop amplitude. Although the ABDK/BDS ansatz was successfully tested for four particles at two [16] and three [17] loops, as well as for five particles at two loops [18, 19], some doubts raised in [20, 21, 22] necessitated an explicit calculation of the two-loop six-particle amplitude [11] which conclusively demonstrated the incompleteness of the BDS ansatz.

Indeed six particles is the earliest that the hypothesized dual conformal symmetry of amplitudes could have allowed BDS to break down; for $n = 4, 5$ the symmetry fixes the form of the amplitude up to a few numerical constants [9, 20]. Beginning at $n = 6$ dual conformal invariance becomes substantially weaker, determining the form of the amplitude only up to an arbitrary function of dual conformally invariant cross-ratios. Nevertheless it was found in parallel work [11, 12] that the amplitude/Wilson loop equality survives at two loops for $n = 6$ despite not being required by dual conformal invariance.

In this paper we study the three-loop BDS ansatz

$$M_n^{(3)}(\epsilon) + \frac{1}{3}(M_n^{(1)}(\epsilon))^3 - M_n^{(1)}(\epsilon)M_n^{(2)}(\epsilon) - f^{(3)}(\epsilon)M_n^{(1)}(3\epsilon) = C^{(3)} + O(\epsilon) \quad (1.1)$$

where $C^{(3)}$ is a previously undetermined numerical constant. In sections II and III we use the leading singularity method [23] to determine the (four-dimensional cut-constructible part of the) 3-loop 5-particle amplitude $M_5^{(3)}$ in terms of a simple basis of integrals. In section IV we
then numerically evaluate enough pieces of these amplitudes (the pieces called ‘obstructions’ in [24, 25]) to determine $C^{(3)} = 17.8241$. Although current developments strongly suggest that the quantity appearing on the right-hand side of (1.1) will in general be non-constant (but still dual conformally invariant) for $n > 5$, there is some utility in knowing the precise number $C^{(3)} = 17.8241$ since for any $n$, whatever appears on the right-hand side of (1.1) must approach this same number in any collinear limit.

II. OUTLINE OF THE CALCULATION

Our goal is to find a compact expression for the planar 3-loop 5-particle amplitude in $\mathcal{N} = 4$ SYM as a linear combination of some basic integrals. Several powerful and related techniques for carrying out calculations such as these include unitarity based methods [26, 27, 28, 29, 30, 31, 32] and more recently, building on [33, 34], maximal cuts [35] and the leading singularity method [23]. For the present calculation we find it convenient to use the leading singularity method (see also [36, 37]) since it allows for all integral coefficients to be determined analytically by solving simple linear equations. In this section we provide a detailed outline of the steps involved in setting up the calculation.

A. Review of the Leading Singularity Method

Suppose we are interested in calculating some $L$-loop scattering amplitude $A$. On the one hand, the amplitude may of course be represented as a sum over Feynman diagrams $F_j$,

$$A(k) = \sum_j \int \prod_{a=1}^L d^d\ell_a \ F_j(k, \ell), \quad (2.1)$$

where $k$ are external momenta and $\ell_a$ are the loop momenta. However it is frequently the case, especially in theories as rich as $\mathcal{N} = 4$ SYM, that directly calculating the sum over Feynman diagrams would be impractical. Rather the calculation proceeds by expressing $A$ as a linear combination of relatively simple integrals in some appropriate basis $\{I_i\}$,

$$A(k) = \sum_i c_i(k) \int \prod_{a=1}^L d^d\ell_a \ I_i(k, \ell), \quad (2.2)$$

and then determining the coefficients $c_i$ by other means.
With the leading singularity method we equate (2.1) and (2.2) and perform the integral
\[ \sum_i c_i(k) \int_{\Gamma} d^4 \ell \, I_i(k, \ell) = \int_{\Gamma} d^4 \ell \sum_j F_j(k, \ell) \] (2.3)
over contours \( \Gamma \in \mathbb{C}^{4L} \) other than the real \( \ell \)-axis. At \( L \) loops each contour is a \( T^{4L} \) inside \( \mathbb{C}^{4L} \). For each contour \( \Gamma \) we obtain one linear equation on the coefficients \( c_i \). Of course if \( \Gamma \) is a random contour then we would generally get the useless equation \( 0 = 0 \), so we should choose contours such that the integral on the right-hand side of (2.3) evaluates the residue on the isolated singularities of Feynman diagrams, which are associated with the locus where internal propagators become on-shell. Since the number of isolated singularities in a generic \( L \)-loop diagram can be as high as \( 2^L \) (simple diagrams can have fewer isolated singularities), the leading singularity method gives rise to an exponentially large (in \( L \)) number of linear equations for the coefficients \( c_i \). We note that the homogeneous part of these linear equations (the left-hand side of (2.3)) depends only on the set of integrals \( \{I_i\} \) and the choice of contours, while the details of which particular helicity configuration is under consideration enters only into the inhomogeneous terms on the right-hand side.

B. Integration Strategy: Collapse and Expand

Here we briefly review from \( [23, 34, 35, 36, 37] \) the integration rules which make it simple to evaluate the contour integrals appearing in (2.3) in the cases relevant to the present calculation. Let us focus on a box with loop momentum \( p \) and external momenta \( k_i \). The box may be sitting inside a higher-loop diagram, in which case the \( k_i \) may involve other loop momenta. The sum over Feynman diagrams contains poles at the locus
\[ S = \{ p \in \mathbb{C}^4 : p^2 = 0, \ (p - k_1)^2 = 0, \ (p - k_{12})^2 = 0 , \ (p + k_4)^2 = 0 \}, \] (2.4)
which, for generic \( k_i \), consists of two distinct points. To each of these points there is an associated contour \( \Gamma_p \) such that integrating \( p \) over \( \Gamma_p \) calculates the residue at the associated point.

The residue of a one-loop amplitude at one of these poles is computed by removing the four internal propagators and evaluating the product of on-shell tree amplitudes at the four corners (summed over all helicities of internal states). In the simplest application, when all four \( k_i \) satisfy \( k_i^2 = 0 \), this product evaluates on either contour \( \Gamma_p \) to a four-particle tree
amplitude, leading to the ‘collapse rule’ graphically depicted as

\[
\int_{\Gamma_p} d^4 p \quad \left( \begin{array}{c}
k_1 \\
n \\
k_3 \\
k_4 \\
k_2 \\
k_3 \\
k_1 \\
k_2 \\
k_4 \\
k_1 \\
k_3 \\
k_4 \\
\end{array} \right) = \quad \left( \begin{array}{c}
k_4 \\
k_3 \\
k_2 \\
k_1 \\
k_4 \\
k_3 \\
k_1 \\
k_2 \\
k_4 \\
k_1 \\
k_3 \\
k_4 \\
\end{array} \right) .
\]

The figure on the left indicates the sum over that subset of all one-loop Feynman diagrams in which all four of the indicated propagators are present. Of course it may as well be the sum over all one-loop Feynman diagrams since those that do not contain all four of the indicated propagators contribute zero to the residue.

When one of the \( k_i^2 \) is non-zero, the result (2.5) holds on only one of the two \( \Gamma_p \) contours, while the integral over the other contour gives zero. Given a helicity assignment for the external particles it is a simple matter to determine which of the two solutions leads to the non-zero result.

It is frequently the case that after collapsing a box in some loop momentum \( p \) there are less than four exposed propagators in some other loop momentum, which would apparently indicate a codimension 1 singularity rather than an isolated singularity. In this case one can use the ‘expand rule’

\[
\left( \begin{array}{c}
k_2 \\
n \\
k_3 \\
k_4 \\
k_1 \\
k_2 \\
k_3 \\
k_1 \\
k_4 \\
k_1 \\
k_2 \\
k_3 \\
\end{array} \right) = \quad \left( \begin{array}{c}
k_1 \\
k_2 \\
k_3 \\
k_4 \\
k_1 \\
k_2 \\
k_3 \\
k_1 \\
k_4 \\
k_1 \\
k_3 \\
k_4 \\
\end{array} \right) + \text{terms non-singular at } (k_1 + k_2)^2 = 0
\]

\[
\left( \begin{array}{c}
k_1 \\
k_2 \\
k_3 \\
k_4 \\
k_1 \\
k_2 \\
k_3 \\
k_1 \\
k_4 \\
k_1 \\
k_3 \\
k_4 \\
\end{array} \right) = \quad \left( \begin{array}{c}
k_2 \\
k_3 \\
k_1 \\
k_4 \\
k_2 \\
k_3 \\
k_1 \\
k_4 \\
k_1 \\
k_2 \\
k_3 \\
k_4 \\
\end{array} \right) + \text{terms non-singular at } (k_2 + k_3)^2 = 0
\]

to expose additional propagators inside a tree amplitude. The choice of how to expand is correlated with the choice of integration contour for the next loop momentum. In the example shown here, the terms isolated on the first line are those which survive a contour integration around the singularity at \( (k_1 + k_2)^2 = 0 \) while the second expansion displays those terms isolated by a contour integration around the singularity at \( (k_2 + k_3)^2 = 0 \).
These two simple rules are sufficient for evaluating all contour integrals appearing on the right-hand side of (2.3) in this paper. Finally, scalar integrals appearing on the left-hand side are integrated via the simple rule
\[ \int_{\Gamma_p} d^4p \frac{1}{p^2(p-k_1)^2(p-k_{12})^2(p+k_4)^2} = \frac{1}{(k_1+k_2)^2(k_2+k_3)^2}, \] (2.6)
which is valid as long as at least three of the \( k_i \) satisfy \( k_i^2 = 0 \) (we will not encounter any other cases in the present calculation). We have chosen a simple normalization factor of 1 on the right-hand side of (2.6); this will be adjusted below in (3.3) to match standard conventions for normalizing amplitudes.

**C. Choosing a Sufficient Set of Contours**

In order to proceed systematically we begin by enumerating all planar 3-loop 5-particle topologies which are free of tadpoles, bubbles, and triangles, since such diagrams are unnecessary due to \( \mathcal{N} = 4 \) supersymmetry (see [39] for a thorough discussion). This leaves 17 topologies, of which 5 do not have any associated leading singularities and are therefore of no interest to us. The remaining 12 topologies are shown in fig. 1.

Each topology in fig. 1 has several distinct associated leading singularities, each of which gives rise to an equation via (2.3). The information contained in this collection of equations is highly redundant—the equations obtained from only a small subset of the leading singularities are sufficient to determine all coefficients, while the remaining equations serve as consistency checks. We now present a few details explaining how to extract a set of equations sufficient for determining all coefficients. We have verified a number of the additional equations to check consistency, but have not performed an exhaustive search for all possible leading singularities.

The topologies fall naturally into three different categories according to how we choose to implement the collapse and expand rules. Let us now address each category in turn, giving in each case the details of the simplest topology as an example.
FIG. 1: The planar 3-loop 5-particle topologies associated to leading singularities. Each figure represents a sum over that subset of Feynman diagrams in which all of the indicated propagators are present. We label the external momenta clockwise with $k_1$ at the leg indicated with the arrow.
1. Example 1: Topology $L$

Topology $L$ has several leading singularities, but the simplest ones can be isolated as indicated in the following cartoon:

\begin{align*}
\int dp & \rightarrow \quad \int dq \\
\quad + \mathcal{O}([((q + k_1)^2]^{0}) & \rightarrow \\
\end{align*}

In words: we first integrate the sum of Feynman diagrams over a $p$ contour which collapses the associated massless box, then expand around $(q + k_1)^2 = 0$ keeping only the singular terms indicated. Integrating $q$ over an appropriate contour isolates these singular terms while collapsing the massless box. The final integral over $r$ is again accomplished using the collapse rule.

The leading singularities exposed by these steps are those located at the locus

\begin{align*}
S_L = \{(p, q, r) \in \mathbb{C}^{12} : & \quad p^2 = 0, \quad q^2 = 0, \quad r^2 = 0, \quad (p + k_1)^2 = 0, \quad (r - k_5)^2 = 0, \\
& \quad (r - k_{45})^2 = 0, \quad (r + k_{12})^2 = 0, \quad (q + k_{12})^2 = 0, \quad (p - k_2)^2 = 0, \\
& \quad (q - r)^2 = 0, \quad (p + q + k_1)^2 = 0, \quad (q + k_1)^2 = 0\}.
\end{align*}

For generic external momenta the set $S_L$ consists of 8 distinct points in $\mathbb{C}^{12}$. For each point in $S_L$ there is an associated contour which computes the residue at the point and hence leads to an equation via (2.3).

It remains only to construct an appropriate ansatz for the left-hand side of (2.3). We try a linear combination of the two most natural integrals of topology $L$,

\begin{align*}
L + L_1.
\end{align*}

Here and in what follows we use pictures as shorthand for the corresponding scalar integrands, so for example the first term in (2.9) represents

\begin{align*}
\frac{1}{p^2 q^2 r^2 (p + k_1)^2 (r - k_5)^2 (r - k_{45})^2 (r + k_{12})^2 (q + k_{12})^2 (p - k_2)^2 (q - r)^2 (p + q + k_1)^2}
\end{align*}
while the dotted line in the second picture in (2.9) indicates a factor of \((r + k_1)^2\) in the numerator of the integrand.

Integrating (2.9) over the contours detailed above leads to the expression

\[
\frac{L + L_1(r + k_1)^2}{s_{12}^2 s_{34} s_{45} (r + k_1)^2},
\]

where the denominator factors arise from the Jacobians in (2.6). Equating this to the result of (2.7) and choosing a particular helicity configuration leads to the equation

\[
\frac{L + L_1(r + k_1)^2}{s_{12}^2 s_{34} s_{45} (r + k_1)^2} = A_{\text{tree}}(1^-, 2^-, 3^+, 4^+, 5^+) \delta_{(r,5)}. \tag{2.12}
\]

Of course this must be evaluated on the locus \(S_L\), and it is easy to check that \(S_L\) contains only two different values of \(r\):

\[
r_1 = \lambda_5 \left( \tilde{\lambda}_5 + \frac{\langle 4, 3 \rangle}{\langle 5, 3 \rangle} \lambda_4 \right), \quad r_2 = \left( \lambda_5 + \frac{[4, 3]}{[5, 3]} \lambda_4 \right) \tilde{\lambda}_5, \tag{2.13}
\]

giving us two distinct equations which are sufficient to determine the coefficients \(L\) and \(L_1\) uniquely.

Topologies \(D\), \(G\), and \(N\) proceed in exactly the same manner, except that in these cases more than two integrals appear on the left-hand side. Topologies \(A\), \(C\), \(E\) and \(K\) are also very similar, except that since these three topologies only have 10 exposed propagators (rather than 11) it is necessary to isolate a second hidden singularity by performing a second expansion prior to integrating over \(r\).

2. Example 2: Topology \(M\)

For topology \(M\) it is sufficient to consider even simpler contours. We first collapse and expand the \(p\) box as done above for topology \(L\), arriving at

\[
S_M = \{(p, q, r) \in \mathbb{C}^{12} : p^2 = 0, \ q^2 = 0, \ r^2 = 0, \ (p - k_4)^2 = 0, \ (r + k_1)^2 = 0, \}
\]

At this stage it is convenient to integrate over a symmetric contour of the type considered in [23] where we require that \(\langle q, r \rangle\) and \([q, r]\) separately vanish instead of just \((q + r)^2 = 0\). This leads us to consider the locus

\[
S_M = \{(p, q, r) \in \mathbb{C}^{12} : p^2 = 0, \ q^2 = 0, \ r^2 = 0, \ (p - k_4)^2 = 0, \ (r + k_1)^2 = 0, \}
\]
\[(q + k_{45})^2 = 0, \ (r + k_{12})^2 = 0, \ (p - q - k_{45})^2 = 0, \]
\[(p - k_{45})^2 = 0, \ (q + k_5)^2 = 0, \ \langle q, r \rangle = 0, \ [q, r] = 0 \}. \quad (2.15)\]

For generic external momenta \( S_M \) consists of 4 isolated points, each of which leads to one linear equation for the integral coefficients. Note that the right-hand side of \( (2.3) \) always vanishes for such symmetric contours since the associated product of tree amplitudes must vanish when \( \langle q, r \rangle = 0 = [q, r] \).

For topologies \( B, J \), and \( G \) we proceed along exactly the same lines (we already treated \( G \) in the first example, but additional equations are needed to fix all of the coefficients which appear for this topology). It turns out that for topology \( J \) an interesting and very useful feature emerges: here we model the left-hand side as the linear combination

\[
J + J_1 + \text{several other integrals.} \quad (2.16)
\]

We will not display all of the relevant integrals explicitly, but they all have the property that they either vanish on the locus \( S_J \) (so that they do not enter the associated equations), or they contain the same numerator factor as \( J_1 \) shown here, which we denote by \( \ell^2 \). Now when we perform the \( q \) integral one of the Jacobian factors is \( 1/\ell^2 \), so we obtain the equation

\[
\frac{J}{\ell^2} + J_1 + \text{several other coefficients} = 0. \quad (2.17)
\]

Since \( \ell^2 = 0 \) on the locus \( S_J \), we immediately see that the coefficient \( J \) must vanish in order to avoid a contradiction. Perhaps a safer way to express this is to say that we can consider an equation obtained by multiplying both sides of \( (2.3) \) by \( \ell^2 \) before performing the contour integrals. Having determined that \( J = 0 \), we then see that \( (2.17) \) gives an equation relating \( J_1 \) to the other coefficients. This trick is also useful for other topologies, in particular for \( C \) and \( E \).

3. Example 3: Topology \( R \)

There are five different triple-box 9-propagator topologies, of which topology \( R \) is the only one with associated leading singularities. These are situated on the locus

\[ S_R = \{(p, q, r) \in \mathbb{C}^{12} : p^2 = 0, \ (p + q + k_{15})^2 = 0, \ q^2 = 0, \ (q - k_4)^2 = 0, \ (p - r)^2 = 0, \]
\[(r - k_{23})^2 = 0, \quad r^2 = 0, \quad (r + q + k_{15})^2 = 0, \quad (p + k_1)^2 = 0, \quad (q + k_{15})^2 = 0, \quad (r + k_1)^2 = 0, \quad (r + k_{15})^2 = 0\]. \quad (2.18)

Here the first nine conditions are the visible propagators, while the last three are hidden singularities. In order to see what the right-hand side of (2.3) should be let us begin by integrating out \(q\) to collapse the first box. This leads to

\[\begin{align*}
q & \quad \quad \\
\quad & \quad \quad \\
r & \quad \quad \\
\end{align*}\]

For the first time we find a triangle-triangle diagram rather than a triangle-box or box-box. The Jacobian factor from integrating the corresponding scalar integral is \(1/(q + k_{15})^2(r + k_1)^2\), suggesting that we expand (2.19) to expose either \(1/(q + k_{15})^2\) or the \(1/(r + k_1)^2\) propagator, but it is clearly impossible to expand both simultaneously. Either choice leaves us with a sum over triangle-box Feynman diagrams, which vanishes due to \(\mathcal{N} = 4\) supersymmetry. The right-hand side of (2.3) is therefore zero for the \(R\) topology leading singularities in eq. (2.18).

### III. THE 3-LOOP 5-PARTICLE AMPLITUDE

A basis of integrals which is sufficient for representing all of the leading singularities of the amplitude is shown in fig. 2. By solving the collection of linear equations as explained in the previous section we find their coefficients

\[
A_1 = -s_{12}s_{23}^2 \frac{1 - \gamma_3}{\gamma_3 - \tilde\gamma_3},
\]

\[
B = -s_{12}s_{23}s_{34}s_{45} \frac{\gamma_5}{\gamma_5 - \tilde\gamma_5},
\]

\[
C_1 = -s_{12}s_{51}^2 \frac{\gamma_3}{\gamma_3 - \tilde\gamma_3},
\]

\[
D_1 = s_{12}s_{23}s_{51}^2 \frac{1}{\gamma_3 - \tilde\gamma_3},
\]

\[
D_2 = -s_{23}s_{34}s_{15} \frac{1 - \gamma_4}{\gamma_4 - \tilde\gamma_4},
\]

\[
E = -s_{12}s_{23}s_{51}^2 \frac{1}{\gamma_3 - \tilde\gamma_3},
\]

\[
G_1 = s_{12}s_{23}s_{51}^2 \frac{1}{\gamma_3 - \tilde\gamma_3},
\]

\[
G_{2a} = -s_{23}s_{45}s_{51} \frac{\gamma_2}{\gamma_2 - \tilde\gamma_2},
\]

11
FIG. 2: The 17 independent integrals appearing in the ansatz. Other integrals can be obtained by rotations or reflections. As in fig. 1 we label the external momenta clockwise with \( k_1 \) at the position indicated by the arrow.

\[
G_{2b} = -s_{23}s_{34}s_{45}\frac{1}{\gamma_5 - \tilde{\gamma}_5},
\]

\[
J_1 = -s_{34}s_{45}s_{51}\frac{1}{\gamma_1 - \tilde{\gamma}_1},
\]

\[
K = -s_{12}s_{23}\frac{1}{\gamma_3 - \tilde{\gamma}_3},
\]

\[
L = s_{12}s_{23}s_{51}\frac{1}{\gamma_3 - \tilde{\gamma}_3},
\]

\[
L_1 = -s_{12}s_{34}s_{45}\frac{1}{\gamma_1 - \tilde{\gamma}_1},
\]

\[
M = -s_{12}s_{45}s_{51}\frac{1}{\gamma_2 - \tilde{\gamma}_2},
\]

\[
N = s_{51}s_{12}s_{34}s_{45}\frac{1}{\gamma_1 - \tilde{\gamma}_1},
\]

\[
N_1 = -s_{12}s_{34}s_{45}\frac{1}{\gamma_1 - \tilde{\gamma}_1},
\]

\[
R = s_{23}s_{45}s_{51}\frac{1}{\gamma_1 - \tilde{\gamma}_1}
\]

(3.1)

where we have introduced the quantity

\[
\gamma_i = \left(1 + \frac{\langle i + 2, i + 3 \rangle[i + 3, i]}{\langle i + 2, i + 4 \rangle[i + 4, i]}\right)^{-1},
\]

(3.2)

and \( \tilde{\gamma} \) is given by the parity conjugate of this expression (i.e., \( \langle a, b \rangle \leftrightarrow [a, b] \)). In each case we have suppressed an overall factor of \( A_0^{\text{tree}} \). In order to connect to the standard normalization
conventions used in the study of the BDS ansatz it is necessary to multiply by an overall factor of \((-1/2)^L\). The complete amplitude is therefore assembled via the formula

\[
M_5^{(3)} = A_5^{(3)} / A_5^{\text{tree}} = -\frac{1}{8} \sum_{\text{permutations}} \sum_{\text{integrals}} \frac{1}{S_i} \text{coefficient}_i \times \text{integral}_i. \tag{3.3}
\]

The first sum runs over the 10 cyclic and anti-cyclic orderings of the labels 1, 2, 3, 4, 5 of the external particles and the second sum runs over the 17 integrals in fig. 2. \(S_i\) is a symmetry factor to compensate for possible overcounting: \(S = 2\) for integrals \(B, D_1, D_2, G_{2b}, L, L_1, N,\) and \(R,\) and \(S = 1\) for the others.

The presentation (3.1) makes it simple to read off the parity-even parts of the coefficients, which will be useful in the following section. We find the parity-even parts

\[
A_1 = \frac{1}{2} s_{12}s_{23}, \quad B = -\frac{1}{2} s_{12}s_{23}s_{34}s_{45}, \\
C_1 = \frac{1}{2} s_{12}s_{51}, \quad D_2 = \frac{1}{2} s_{23}s_{34}s_{51}, \\
G_{2a} = \frac{1}{2} s_{23}s_{45}s_{51}, \quad K = \frac{1}{2} s_{12}s_{23}, \\
L_1 = \frac{1}{2} s_{12}s_{34}s_{45}, \quad N_1 = \frac{1}{2} s_{12}s_{34}s_{45}, \\
R = -\frac{1}{2} s_{23}s_{45}s_{51}. \tag{3.4}
\]

with all others vanishing. We note that only the coefficients associated to dual conformal integrals have non-vanishing parity-even parts, as expected based on the pattern of previously studied amplitudes [11, 17, 18, 19, 39].

IV. THE THREE-LOOP BDS ANSATZ

The infrared divergences of higher loop scattering amplitudes in gauge theory are very simply related to those of lower loop amplitudes [40]. In [16, 17], it was conjectured that in \(\mathcal{N} = 4\) SYM this simplicity persists, at least for MHV amplitudes, to the finite terms as well. Although the explicit \(n = 6\) calculation of [11] has now demonstrated, following earlier doubts raised in [20, 21, 22] (see also [41]), that these relations are not true for all \(n,\) it is believed that they should hold for four and five particles at any number of loops since for these cases the amplitudes are determined up to a few constants by dual conformal invariance [9, 20].
The precise form of the BDS ansatz at three loops, in dimensional regularization to $D = 4 - 2\epsilon$, is

$$M_n^{(3)}(\epsilon) = -\frac{1}{3}(M_n^{(1)}(\epsilon))^3 + M_n^{(1)}(\epsilon)M_n^{(2)}(\epsilon) + f^{(3)}(\epsilon)M_n^{(1)}(3\epsilon) + C^{(3)} + O(\epsilon) \quad (4.1)$$

where

$$f^{(3)}(\epsilon) = \frac{11\pi^4}{180} + (5\zeta(2)\zeta(3) + 6\zeta(5))\epsilon + a\epsilon^2, \quad C^{(3)} = b \quad (4.2)$$

in terms of two previously undetermined numerical constants $a$ and $b$. BDS verified by explicit calculation that the 3-loop 4-particle amplitude satisfies (4.1), but the structure of the equation for $n = 4$ is insensitive to the values of $a$ and $b$ as long as they obey the linear relation

$$2a - 9b = -\frac{341}{24}\zeta(6) + 17\zeta(3)^2. \quad (4.3)$$

Here we will use our 3-loop 5-particle amplitude to extract a second linear equation from (4.1) which will finally fix the constants $a$ and $b$.

The calculation of $a$ and $b$ benefits from two simplifications. The first is that we may restrict our attention to the parity-even part of (4.1). If we write each amplitude as a sum of its parity-even and parity-odd parts, $M_5^{(L)} = M_5^{(L)+} + M_5^{(L)-}$, then taking the parity-even part of (4.1) for $n = 5$ gives

$$M_5^{(3)+}(\epsilon) = -\frac{1}{3}(M_5^{(1)+}(\epsilon))^3 + M_5^{(1)+}(\epsilon)M_5^{(2)+}(\epsilon) + f^{(3)}(\epsilon)M_5^{(1)+}(3\epsilon) + C^{(3)} + M_5^{(1)-}(\epsilon)\left(M_5^{(2)-}(\epsilon) - M_5^{(1)+}(\epsilon)M_5^{(1)-}(\epsilon)\right) + O(\epsilon). \quad (4.4)$$

In [19] it was shown that $M_5^{(2)-}(\epsilon) - M_5^{(1)+}(\epsilon)M_5^{(1)-}(\epsilon) = O(\epsilon)$. Since $M_5^{(1)+}(\epsilon)$ itself is also $O(\epsilon)$, we see that the entire last line of (4.4) can be replaced simply by $+O(\epsilon)$. A consequence of the result of [19] is therefore that the parity-even part of the three-loop BDS ansatz can be obtained by making the naive replacement $M_5^{(3)} \rightarrow M_5^{(3)+}$ in (4.1).

The second simplification is to make use of the notion of obstructions introduced in [24] and exploited in the four-loop calculations [25, 38]. We refer the reader to [25] for all of the necessary details, including a detailed algorithm for calculating obstructions. Here we simply remind the reader that for an amplitude $A(x, \epsilon)$ depending on a single kinematic variable $x$, the obstruction $P(\epsilon)$ is defined to be the coefficient of the simple pole at $y = 0$ in the inverse Mellin transform transform, so that

$$A(x, \epsilon) = \int_{-i\infty}^{+i\infty} dy \ x^y \left[(\text{higher order singularities}) + \frac{P(\epsilon)}{y} + (\text{regular at } y = 0)\right]. \quad (4.5)$$
As explained in [25], it is important to understand this relation as holding order by order in \(\epsilon\), rather than at finite \(\epsilon\). The prime advantage of dealing with \(P(\epsilon)\) rather than the full \(A(x, \epsilon)\) is that it is much simpler to compute. Furthermore it is important that obstructions satisfy a product algebra—the obstruction in any product of amplitudes is equal to the product of the individual obstructions.

This concept generalizes straightforwardly to integrals depending on more than one kinematic variable. In the case at hand we have 5-particle integrals depending on five independent variables \(s_{i,i+1}\), and we can extract the obstruction \(P(\epsilon)\) by applying the above procedure five times in succession. Equivalently, we define \(P(\epsilon)\) to be the coefficient of the \(1/(y_1 y_2 y_3 y_4 y_5)\) pole in the 5-fold inverse Mellin transform of \(A(s_{12}, s_{23}, s_{34}, s_{45}, s_{51})\). By applying the algorithm outlined in [25], it is straightforward to find that the obstructions in the one- and two-loop five particle amplitudes are given by

\[
P_5^{(1)}(\epsilon) = -\frac{5}{2} \frac{1}{\epsilon^2} + \frac{5\pi^2}{8} + \frac{179\zeta(3)}{24} \epsilon + \frac{97\pi^4}{1440} \epsilon^2 - \left(\frac{51\pi^2\zeta(3)}{32} - \frac{137\zeta(5)}{8}\right) \epsilon^3
- \left(\frac{763\zeta(3)^2}{72} - \frac{23\pi^6}{3780}\right) \epsilon^4 + \mathcal{O}(\epsilon^5),
\]

\[
P_5^{(2)}(\epsilon) = \frac{25}{8} \frac{1}{\epsilon^4} - \frac{35\pi^2}{24} \frac{1}{\epsilon^2} - \frac{865\zeta(3)}{48} \frac{1}{\epsilon} - \frac{97\pi^4}{1152} + 21.494969\epsilon - 64.357473\epsilon^2 + \mathcal{O}(\epsilon^3).
\] (4.6)

For simplicity we have restricted \(P_5^{(L)}\) here to the parity-even parts of the amplitudes. Note that these expressions satisfy the two-loop ABDK relation

\[
P_5^{(2)}(\epsilon) = \frac{1}{2}(P_5^{(1)}(\epsilon))^2 + (-\zeta(2) - \zeta(3)\epsilon - \zeta(4)\epsilon^2)P_5^{(1)}(\epsilon) - \frac{\pi^4}{72} + \mathcal{O}(\epsilon)
\] (4.7)
as expected.

At three loops, we have found that there are nine independent integrals which contribute to the parity-even part of the 5-particle amplitude. The obstructions for each of these types of integrals, through \(\mathcal{O}(\epsilon^0)\), are

\[
P_{A_1} = \frac{20}{9} \frac{1}{\epsilon^6} + \frac{20\pi^2}{27} \frac{1}{\epsilon^4} - \frac{43\zeta(3)}{2} \frac{1}{\epsilon^3} + \frac{73\pi^4}{432} \frac{1}{\epsilon^2} - \frac{850.242028}{\epsilon} + 34.239832,
\]

\[
P_{B} = \frac{20}{3} \frac{1}{\epsilon^6} - \frac{25\pi^2}{45} \frac{1}{\epsilon^4} - \frac{1495\zeta(3)}{1495} \frac{1}{\epsilon^3} + \frac{135\pi^4}{76} \frac{1}{\epsilon^2} + 1589.962798\frac{1}{\epsilon} + 2824.770745,
\]

\[
P_{C_1} = \frac{20}{9} \frac{1}{\epsilon^6} - \frac{54\pi^2}{36} \frac{1}{\epsilon^4} - \frac{645\zeta(3)}{36} \frac{1}{\epsilon^3} - 12960 \frac{1}{\epsilon^2} + 221.894995\frac{1}{\epsilon} + 1030.164974,
\]

\[
P_{D_2} = \frac{20}{3} \frac{1}{\epsilon^6} - \frac{36\pi^2}{35}\frac{1}{\epsilon^4} - \frac{4\zeta(3)}{4} \frac{1}{\epsilon^3} + 2160 \frac{1}{\epsilon^2} + 231.123687\frac{1}{\epsilon} - 4141.657880,
\]

\[
P_{G_{2a}} = \frac{20}{9} \frac{1}{\epsilon^6} - \frac{155\pi^2}{288} \frac{1}{\epsilon^4} - \frac{563\zeta(3)}{4} \frac{1}{\epsilon^3} - 487\pi^4 \frac{1}{\epsilon^2} + 1294.520402\frac{1}{\epsilon} + 2938.6610 \pm 0.0036,
\]
\[ P_K = \frac{20}{9} \epsilon^6 - \frac{5 \pi^2}{6} \epsilon^4 - \frac{1177 \zeta(3)}{1195} \epsilon^2 + \frac{719 \pi^4}{1} \epsilon^3 + 178.487460 \frac{1}{\epsilon} - 2387.290195, \]
\[ P_{G1} = \frac{9}{35} \epsilon^6 - \frac{18 \pi^2}{85} \epsilon^4 - \frac{1411 \zeta(3)}{1195} \epsilon^2 - \frac{432}{1} \epsilon^3 - \frac{673.319831}{1} \epsilon - 2845.889639, \]
\[ P_{N1} = \frac{15}{3} \epsilon^6 - \frac{455 \pi^2}{36} \epsilon^4 - \frac{136 \zeta(3)}{1} \epsilon^2 + \frac{983 \pi^4}{1} \epsilon^3 + 625.875398 \frac{1}{\epsilon} + 437.509754, \]
\[ P_R = \frac{80 \zeta(3)}{3} \epsilon^3 + \frac{107 \pi^4}{108} \epsilon^2 - 395.562804 \frac{1}{\epsilon} + 923.415196. \] (4.8)

Each expression displays the result obtained after summing over all 10 permutations of the corresponding integral (including in each case the appropriate dual conformal numerator). The estimated error in the numerical results is much smaller than the precision indicated in all cases except for the last term in \( P_{G2a} \), which is the overwhelmingly dominant source of numerical error.

Using the parity-even parts of the coefficients obtained in the previous section, and including the necessary factors of \( \frac{1}{2} \) to avoid overcounting those integrals with flip symmetries, we find the total three-loop obstruction

\[
P^{(3)}_5 = \frac{1}{16} \left( P_{A1} - \frac{1}{2} P_{B} + P_{C1} + \frac{1}{2} P_{D2} + P_{G2a} + P_K + \frac{1}{2} P_{L1} + P_{N1} - \frac{1}{2} P_R \right)
= -\frac{125}{48} \epsilon^6 + \frac{325 \pi^2}{192} \epsilon^4 + \frac{4175 \zeta(3)}{192} \epsilon^3 + \frac{499 \pi^4}{10368} \epsilon^2
- 40.764885 \frac{1}{\epsilon} + 207.1613 \pm 0.0002 + \mathcal{O}(\epsilon) \] (4.9)

Using the results (4.9) and (4.6), we find that the BDS relation (4.1) is satisfied provided that \( a \) and \( b \) satisfy the linear relation

\[ 5a - 18b = 105.482 \pm 0.004. \] (4.10)

Together with (4.3) this implies the solution

\[ a = 85.263 \pm 0.004, \quad b = 17.8241 \pm 0.0009. \] (4.11)

Based on the transcendentality hypothesis, it is expected that each of these numbers should be a linear combination of \( \zeta(6) \) and \( \zeta(3)^2 \) with rational coefficients. However given the limited numerical accuracy of our calculation it seems prudent to avoid speculating on possible exact values for \( a \) and \( b \) at this time.
V. SUMMARY

In this paper we have used the leading singularity method to obtain an ansatz for the four-dimensional cut-constructible part of the 3-loop 5-particle amplitude in $\mathcal{N} = 4$ SYM theory. This means that we have determined the coefficients of the integrals shown in fig. [2] by comparing residues of the ansatz to those of the amplitude on various leading singularities. Although it has not yet been proven that determination of only leading singularities completely determines an amplitude (in principle one might have to add additional integrals that vanish on all leading singularities but that have subleading singularities), the method so far has been found to give the complete answer in all cases where comparison with alternate methods was possible.

Dimensionally regulated amplitudes occasionally contain so-called ‘$\mu$-terms’ which are defined as terms in the integrand which vanish in $D = 4$ but not in $D = 4 - 2\epsilon$ (note that this statement is, in general, completely unrelated to whether or not these terms vanish in $D = 4 - 2\epsilon$ after integration; indeed $\mu$-terms can easily be IR divergent). Since the leading singularity method itself works with strictly four-dimensional loop momenta, it is insensitive to possible $\mu$ terms, although it seems that in principle they could be determined by considering leading singularities in integer dimensions other than 4. However, in all cases that have been studied so far it has been observed that $\mu$-terms separately cancel out of the BDS relation, leaving $C^{(3)}$ unaffected. We can therefore hope that even if the 3-loop 5-particle amplitude contains such terms which we have missed, they would not contribute to the constants $a$ and $b$ computed in section IV.

Finally we emphasize that since our goal in section IV was to streamline the calculation of $a$ and $b$ as much as possible, we have only evaluated the obstructions, not the full amplitude. Consequently we have not checked (even numerically) that the quantity $+C^{(3)}$ appearing in (2.3) is a numerical constant; in principle it could depend on the kinematic variables $s_{i,i+1}$. The method of obstructions is efficient for quickly extracting the ‘constant part’ of $C^{(3)}$ (defined as the coefficient of $1/y$ in the inverse Mellin transform) but is insensitive to any other potential terms in $C^{(3)}$ that depend on the $s_{i,i+1}$. It remains an interesting open problem to verify that there are no such terms.
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