Polynomial structures in one-loop amplitudes

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ABSTRACT: A general one-loop scattering amplitude may be expanded in terms of master integrals. The coefficients of the master integrals can be obtained from tree-level input in a two-step process. First, use known formulas to write the coefficients of $(4-2\epsilon)$-dimensional master integrals; these formulas depend on an additional variable, u, which encodes the dimensional shift. Second, convert the u-dependent coefficients of $(4 - 2\epsilon)$-dimensional master integrals to explicit coefficients of dimensionally shifted master integrals. This procedure requires the initial formulas for coefficients to have polynomial dependence on u. Here, we give a proof of this property in the case of massless propagators. The proof is constructive. Thus, as a byproduct, we produce different algebraic expressions for the scalar integral coefficients, in which the polynomial property is apparent. In these formulas, the box and pentagon contributions are separated explicitly.

Contents

1. Introduction

Detailed calculations of multi-particle scattering events are needed in order to analyze new physics at the experiments of the Large Hadron Collider. Computational complexity increases rapidly with the number of legs, even at the amplitude level. New and improved algorithms are being developed to meet these needs. Recent progress at next-to-leading order has been reviewed in [1].

Scattering amplitudes at one-loop level can be understood in terms of an expansion in master integrals [2, 3]. The coefficients of the master integrals may be obtained by direct reduction, or alternatively by solving constraint equations derived from singular structures, most notably unitarity cuts [4 – 30]. In order to obtain complete physical amplitudes from unitarity cuts, we can work in dimensional regularization, where $D = 4 - 2\epsilon$ [31 – 34]. By now, explicit analytic formulas for these coefficients are available [20, 23, 27, 28]. The input quantities are taken from the complete tree-level amplitudes involved in unitarity cuts. There are other promising algorithms for finding the coefficients in 4 or D dimensions [35, 17, 24, 29], or specifically the additional "rational" parts supplementing a pure 4-dimensional expansion [30, 36 – 45].

The formulas of [27], developed in the context of the D-dimensional unitarity analysis of [18, 21], are coefficients of $(4 - 2\epsilon)$-dimensional master integrals; these formulas depend on an additional variable, u, which encodes the dimensional shift. To finish the calculation, we convert the u-dependent coefficients of $(4 - 2\epsilon)$-dimensional master integrals to explicit coefficients of dimensionally shifted master integrals.[1]

We are presently concerned with the adaptation of the formulas of [27] to an efficient numerical algorithm. Two particular issues are addressed in this paper:

- Because the coefficients of the $(4 - 2\epsilon)$-dimensional integrals are polynomials in the variable u, a direct numerical implementation is not obvious.

- The algebraic expression of boxes includes both box and pentagon contributions. The pentagon contribution is signaled by the $(au + b)$ factor in the denominator.

Our aim is to solve these two problems. More concretely, in this paper we accomplish the following:

- The proof of the polynomial property of u: In previous work, some evidence for this assumption was provided. Now, we give a complete proof.

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[1] As an alternative to this last step, complete coefficients of $(4 - 2\epsilon)$-dimensional master integrals could be obtained with the recursion and reduction formulas of [18, 21].

- Simplifying our previous expressions: The algebraic expressions for coefficients given in [27] were the full polynomials in u, i.e. a sum of terms of the form $c_n u^n$. Here, we give expressions for evaluating c_n directly from input quantities.

- Separating the coefficients of boxes and pentagons: We give explicit, separate expressions for coefficients of boxes and pentagons.

For simplicity, the results here are specific to amplitudes with massless propagators. Generalization to the massive case is straightforward for the coefficients of master integrals that have nonvanishing cuts. Based on the present paper, the generalization to the massive case has been presented in [46]. We work within the spinor formalism [47], reviewed in [48].

The paper is organized as follows. In section 2, we organize our input quantities from tree amplitudes, define some key vectors and spinors from the input, and briefly discuss the dimensional shift. Then we proceed to the simplifications of the formulas for coefficients, and the proofs that they are polynomials in u. These are given in sections 3 and 4 for triangles and bubbles, respectively. In section 5, we address box coefficients, and for the first time we present separate formulas for box and pentagon coefficients. Section 6 contains an application of these formulas, within the example of the 5-gluon amplitude. In section 7, we close with a discussion and comparison to a couple of other recent approaches to the problem of one-loop amplitudes. Appendix A contains our definitions of master integrals and dimensional shift identities. Appendix B contains alternate, more explicit expressions for the triangle coefficients which may be better suited for numerical evaluation, since the derivatives have been taken analytically in every case that arises in a renormalizable theory. Appendix C contains many of the details of the polynomial proof for bubble coefficients. Appendix D contains analytic expressions used in cuts of pentagons.

2. Setup and definitions

In this section, we set up some key conventions and definitions used in expressing the coefficients of master integrals, and in our proofs of polynomial dependence.

2.1 Unitarity method

The unitarity cut of a one-loop amplitude is its discontinuity across a branch cut in a kinematic region selecting a particular momentum channel. Specifically, we denote the momentum vector by K. Then, K^2 should be positive, and all other momentum invariants should be negative. The vector K will be a sum of momenta of some of the external legs. The discontinuity is given by

$$\Delta A^{1-\text{loop}} = \int d^D\Phi \ A^{\text{tree}}_{\text{Left}} \ \times \ A^{\text{tree}}_{\text{Right}}, \tag{2.1}$$

where the Lorentz-invariant phase-space (LIPS) of a double cut is defined by inserting two δ-functions representing the cut conditions:[2]

$$d^D\Phi = d^D p \ \delta(p^2)\delta((p-K)^2) \tag{2.2}$$

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[2]The delta functions here should properly be denoted by $\delta^{(+)}$, indicating that they are restricted to the positive light cone. We shall drop the superscript for simplicity.

The "unitarity method" [4, 5] combines the unitarity cuts with the results of reduction to an expansion in master integrals I_i [3]

$$A^{1-\text{loop}} = \sum_i c_i I_i. \tag{2.3}$$

The master integrals in d dimensions with massless propagators are scalar pentagons, scalar boxes, scalar triangles, and scalar bubbles. In the full d-dimensional formalism, there are no cut-free terms.

The n-point scalar integral with massless propagators is

$$-i(4\pi)^{D/2} \int \frac{d^D p}{(2\pi)^D} \frac{1}{p^2 (p-K)^2 \prod_{j=1}^{n-2} (p-P_j)^2}. \tag{2.4}$$

The coefficients c_i in (2.3) are, by construction, cut-free rational functions. In the unitarity method, we do not derive the coefficients of master integrals by performing any reduction. Rather, we take the coefficients as unknowns and proceed to constrain them by performing cuts on both sides of (2.3):

$$\Delta A^{1-\text{loop}} = \sum_i c_i \Delta I_i. \tag{2.5}$$

Any realization of the unitarity method must address the problem of isolating the individual coefficients c_i. The unitarity method succeeds because the cuts of master integrals are logarithms of unique functions of the kinematic invariants.

In [13], it was shown how to obtain scalar box coefficients directly by cutting four propagators rather than two. Similarly explicit analytic formulas for the other coefficients have recently become available [20, 23, 27, 28].

Here, we refer to the formulas given in [27], after setting propagator masses to zero for simplicity. The generalization to the case of massive propagators has now been given in [46].

2.2 Input quantities

Having present the general picture, in this subsection we can start with the following most general expression for a unitarity cut integral:

$$C = \int d^{4-2\epsilon} p \, c(\mu^2) \frac{\prod_{i=1}^m (-2\widetilde{\ell} \cdot P_i)}{\prod_{j=1}^k (p-K_j)^2} \delta^{(+)}(p^2) \delta^{(+)}((p-K)^2). \tag{2.6}$$

We work in the four-dimensional helicity scheme, so that all external momenta K_i are 4-dimensional and only the internal momentum p is $(4-2\epsilon)$-dimensional. We decompose the $(4-2\epsilon)$-dimensional loop momentum as [49, 32]

$$p = \widetilde{\ell} + \vec{\mu}, \tag{2.7}$$

where $\widetilde{\ell}$ is 4-dimensional and $\vec{\mu}$ is (-2ϵ)-dimensional. With the integrand in the form of (2.6), there is a prefactor $c(\mu^2)$ which depends on the external momenta as well as on μ^2. In this discussion we shall be paying careful attention to all dependence on μ^2.

From this starting point, the coefficients of master integrals were listed in [27]. Now, we would like to be able produce the complete 4-dimensional expression, by performing the integral over μ^2 by the recursion and reduction formulas of [18, 21]. To get this complete answer, we need to consider the dependence of the prefactor $c(\mu^2)$ on μ^2, along with the power of μ^2 in the coefficient formulas of [27]. We consider this dependence in terms of the dimensionless parameter u, defined by

$$u = \frac{4\mu^2}{K^2}. \tag{2.8}$$

With this definition, the cut integral (2.6) can then be rewritten as

$$C = \frac{(4\pi)^\epsilon}{\Gamma(-\epsilon)}\left(\frac{K^2}{4}\right)^{-\epsilon}\int_0^1 du\, u^{-1-\epsilon}c(\mu^2)\int\langle\ell d\ell\rangle\,[\ell d\ell]\sqrt{1-u}\frac{(K^2)^{n+1}}{\langle\ell|K|\ell]^{n+2}}\frac{\prod_{j=1}^{n+k}\langle\ell|R_j(u)|\ell]}{\prod_{i=1}^{k}\langle\ell|Q_i(u)|\ell]}, \tag{2.9}$$

The coefficients listed in [27], which are summarized below, are the results of the four-dimensional part of the integral (2.6); they are functions of u. The "four-dimensional cut-constructible" part of the amplitude could be obtained by setting $u \to 0$ in each of these coefficients, inside the expansion of the amplitude in master integrals. The *complete D-dimensional* amplitude requires dealing with this u-dependence. Here it is enough to apply the polynomial reduction identities given in [18, 21]. These identities assume polynomial structure of the coefficients $C(u)$, which is proven in the present paper, and which may also be deduced within other approaches [35]. However, if we desire a result only through $\mathcal{O}(\epsilon^0)$, it may be more efficient to use the dimensionally-shifted basis discussed in [49, 29]. We shall return to this point in the following subsection.

From the initial expression (2.6), we extract all the necessary information, as follows. First, notice the triplet of integers

$$(m,\ k,\ n \equiv m - k) \tag{2.10}$$

which will play an important role. In particular, the value of n constrains the basis of master integrals [4, 5]. If $n \leq -2$, there are contributions only from boxes and pentagons. If $n \geq -1$, contributions from triangles will kick in, and finally if $n \geq 0$, bubble contributions show up as well. This pattern is well known from traditional reduction techniques.

Second, we use the values of K, P_i, and K_j from the expression (2.6) to define the vectors Q_j, R_j, and related important quantities, as follows:[3]

$$q_j \equiv K_j - \frac{K_j \cdot K}{K^2}K \tag{2.11}$$

$$\alpha_j \equiv \frac{K_j^2 - K_j \cdot K}{K^2} \tag{2.12}$$

$$p_j \equiv P_j - \frac{P_j \cdot K}{K^2}K \tag{2.13}$$

$$\beta_j \equiv -\frac{P_j \cdot K}{K^2} \tag{2.14}$$

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[3]These definitions apply specifically to the case with massless propagators. Only a slight modification is necessary for massive propagators [20, 46].

$$Q_j(u) \equiv -(\sqrt{1-u})q_j + \alpha_j K, \tag{2.15}$$

$$= -(\sqrt{1-u})K_j + \left(\frac{K_j^2}{K^2} - (1 - \sqrt{1-u})\frac{K_j \cdot K}{K^2} \right) K \tag{2.16}$$

$$R_j(u) \equiv -(\sqrt{1-u})p_j + \beta_j K \tag{2.17}$$

$$= -(\sqrt{1-u})P_j - (1 - \sqrt{1-u})\frac{P_j \cdot K}{K^2} K \tag{2.18}$$

One important observation is that

$$q_j \cdot K = p_j \cdot K = 0. \tag{2.19}$$

At this point, we wish to make a few more remarks.

- The input quantities are given by K, K_j, P_j. From this we can define $q_j, \alpha_j, p_j, \beta_j$ and $Q_j(u), R_j(u)$. We make reference to the number of these vectors, encoded in the triple of integers (m, k, n).

- To simplify notation when we set $u = 0$, we will write expressions such as $Q_j(u = 0)$, or just Q_j.

- The coefficients of the master integrals are polynomials in u. In this paper, we shall find that the maximum degrees of these polynomials are the following. Pentagon: 0. Box: $[(n+2)/2]$. Triangle: $[(n+1)/2]$. Bubble: $[n/2]$. Here, $[d]$ denotes the greatest integer less than or equal to d.

  For a renormalizable theory we have $n \leq 2$; thus we have the maximum degrees of 2 for boxes, 1 for triangles, and 1 for bubbles. These degrees are consistent with [17, 22] and [29].

- Knowing the maximum value of the degree of the polynomial in u, we can then calculate the coefficient of u^s by the formula

$$c_s = \frac{1}{s!} \frac{d^s C(u)}{du^s} \bigg|_{u \to 0}, \tag{2.20}$$

  so

$$C(u) = \sum_{s=0}^{s_{\max}} \frac{1}{s!} \frac{d^s C(u)}{du^s} \bigg|_{u \to 0} u^s. \tag{2.21}$$

  The expression (2.20) is central in this paper. Since c_s now has an expression where u does not appear (as indicated by the right-hand-side of expression (2.20)), it can be evaluated numerically.[4]

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[4]See [46] for another approach that is possibly more efficient.

Summary of coefficients of 4-dimensional master integrals. For the box coefficient with momenta K, K_r, K_s,

$$C[Q_r, Q_s, K] = \frac{(K^2)^{2+n}}{2} \left(\frac{\prod_{j=1}^{k+n} \langle P_{sr,1}|R_j|P_{sr,2}]}{\langle P_{sr,1}|K|P_{sr,2}]^{n+2} \prod_{t=1,t\neq i,j}^{k} \langle P_{sr,1}|Q_t|P_{sr,2}]} + \{P_{sr,1} \leftrightarrow P_{sr,2}\} \right).$$

For the triangle coefficient with momenta K, K_s,

$$\begin{aligned}
C[Q_s, K] = {} & \frac{(K^2)^{1+n}}{2} \frac{1}{(\sqrt{\Delta_s})^{n+1}} \frac{1}{(n+1)! \langle P_{s,1}\ P_{s,2}\rangle^{n+1}} \\
& \times \frac{d^{n+1}}{d\tau^{n+1}} \left(\frac{\prod_{j=1}^{k+n} \langle P_{s,1} - \tau P_{s,2}|R_j Q_s|P_{s,1} - \tau P_{s,2}\rangle}{\prod_{t=1,t\neq s}^{k} \langle P_{s,1} - \tau P_{s,2}|Q_t Q_s|P_{s,1} - \tau P_{s,2}\rangle} + \{P_{s,1} \leftrightarrow P_{s,2}\} \right)\Bigg|_{\tau=0}.
\end{aligned}$$

For the bubble coefficient with momentum K,

$$C[K] = (K^2)^{1+n} \sum_{q=0}^{n} \frac{(-1)^q}{q!} \frac{d^q}{ds^q} \left(\mathcal{B}_{n,n-q}^{(0)}(s) + \sum_{r=1}^{k} \sum_{a=q}^{n} \left(\mathcal{B}_{n,n-a}^{(r;a-q;1)}(s) - \mathcal{B}_{n,n-a}^{(r;a-q;2)}(s) \right) \right)\Bigg|_{s=0}.$$

where we have made the following definitions:

$$\begin{aligned}
\mathcal{B}_{n,t}^{(0)}(s) \equiv {} & \frac{d^n}{d\tau^n} \Bigg(\frac{1}{n![\eta|\widetilde{\eta}K|\eta]^n} \frac{(2\eta \cdot K)^{t+1}}{(t+1)(K^2)^{t+1}} \\
& \times \frac{\prod_{j=1}^{n+k} \langle \ell|R_j(K+s\eta)|\ell\rangle}{\langle \ell\ \eta\rangle^{n+1} \prod_{p=1}^{k} \langle \ell|Q_p(K+s\eta)|\ell\rangle} |_{|\ell\rangle \to |K-\tau\widetilde{\eta}|\eta]} \Bigg)\Bigg|_{\tau=0}, \\
\mathcal{B}_{n,t}^{(r;b;1)}(s) \equiv {} & \frac{(-1)^{b+1}}{b!\sqrt{\Delta_r}^{b+1} \langle P_{r,1}\ P_{r,2}\rangle^b} \frac{d^b}{d\tau^b} \left(\frac{1}{(t+1)} \frac{\langle P_{r,1} - \tau P_{r,2}|\eta|P_{r,1}]^{t+1}}{\langle P_{r,1} - \tau P_{r,2}|K|P_{r,1}]^{t+1}} \right. \\
& \times \left. \frac{\langle P_{r,1} - \tau P_{r,2}|Q_r\eta|P_{r,1} - \tau P_{r,2}\rangle^b \prod_{j=1}^{n+k} \langle P_{r,1} - \tau P_{r,2}|R_j(K+s\eta)|P_{r,1} - \tau P_{r,2}\rangle}{\langle P_{r,1} - \tau P_{r,2}|\eta K|P_{r,1} - \tau P_{r,2}\rangle^{n+1} \prod_{p=1,p\neq r}^{k} \langle P_{r,1} - \tau P_{r,2}|Q_p(K+s\eta)|P_{r,1} - \tau P_{r,2}\rangle} \right)\Bigg|_{\tau=0}, \\
\mathcal{B}_{n,t}^{(r;b;2)}(s) \equiv {} & \frac{(-1)^{b+1}}{b!\sqrt{\Delta_r}^{b+1} \langle P_{r,1}\ P_{r,2}\rangle^b} \frac{d^b}{d\tau^b} \left(\frac{1}{(t+1)} \frac{\langle P_{r,2} - \tau P_{r,1}|\eta|P_{r,2}]^{t+1}}{\langle P_{r,2} - \tau P_{r,1}|K|P_{r,2}]^{t+1}} \right. \\
& \times \left. \frac{\langle P_{r,2} - \tau P_{r,1}|Q_r\eta|P_{r,2} - \tau P_{r,1}\rangle^b \prod_{j=1}^{n+k} \langle P_{r,2} - \tau P_{r,1}|R_j(K+s\eta)|P_{r,2} - \tau P_{r,1}\rangle}{\langle P_{r,2} - \tau P_{r,1}|\eta K|P_{r,2} - \tau P_{r,1}\rangle^{n+1} \prod_{p=1,p\neq r}^{k} \langle P_{r,2} - \tau P_{r,1}|Q_p(K+s\eta)|P_{r,2} - s\tau P_{r,1}\rangle} \right)\Bigg|_{\tau=0}.
\end{aligned}$$

Note that the prefactor $c(\mu^2)$ has not been included in these formulas for coefficients.

2.3 Some important constructions from input quantities

Given two momenta S, R, we construct two null momenta. If $R^2 = 0$ and $S^2 = 0$, R, S are themselves the two null momenta. If at least one of them is not null, for example $R^2 \neq 0$, then we construct two null momenta as follows.

$$P_{(S,R);i} = S + x_i R, \qquad x_1 = \frac{-2S \cdot R + \sqrt{\Delta(S,R)}}{2R^2}, \quad x_2 = \frac{-2S \cdot R - \sqrt{\Delta(S,R)}}{2R^2}, \quad (2.22)$$

where

$$\Delta(S, R) \equiv (2R \cdot S)^2 - 4R^2 S^2. \tag{2.23}$$

Then, the following quantities necessarily vanish.

$$\begin{aligned}
0 &= \langle P_{(S,R);1}|S|P_{(S,R);2}] = \langle P_{(S,R);2}|S|P_{(S,R);1}] \\
&= \langle P_{(S,R);1}|R|P_{(S,R);2}] = \langle P_{(S,R);2}|R|P_{(S,R);1}] .
\end{aligned} \tag{2.24}$$

We shall use the following identity:

$$\begin{aligned}
\langle P_1|V|P_2] \langle P_2|W|P_1] &= tr\left(\frac{1-\gamma_5}{2} \not{P}_1 \not{V} \not{P}_2 \not{W}\right) \\
&= \frac{1}{2}((2P_1 \cdot V)(2P_2 \cdot W) + (2P_1 \cdot W)(2P_2 \cdot V) \\
&\quad -(2P_1 \cdot P_2)(2V \cdot W) - 4i\epsilon_{\mu\nu\sigma\rho} P_1^\mu V^\nu P_2^\sigma W^\rho).
\end{aligned} \tag{2.25}$$

Any four-dimensional momentum K can be expanded in a basis of four other independent momenta K_i, K_j, K_m, K_n by

$$K = a_m K_m + a_n K_n + a_i K_i + a_j K_j, \tag{2.26}$$

where the coefficients are given by

$$\begin{aligned}
a_m &= \frac{\epsilon(K_i, K, K_j, K_n)}{\epsilon(K_i, K_m, K_j, K_n)}, & a_n &= \frac{\epsilon(K_i, K_m, K_j, K)}{\epsilon(K_i, K_m, K_j, K_n)}, \\
a_i &= \frac{\epsilon(K, K_m, K_j, K_n)}{\epsilon(K_i, K_m, K_j, K_n)}, & a_j &= \frac{\epsilon(K_i, K_m, K, K_n)}{\epsilon(K_i, K_m, K_j, K_n)},
\end{aligned} \tag{2.27}$$

with

$$\epsilon(K_1, K_2, K_3, K_4) \equiv \epsilon_{\mu\nu\rho\xi} K_1^\mu K_2^\nu K_3^\rho K_4^\xi. \tag{2.28}$$

At times, we will write these coefficients in the form $a_m^{(K_i, K_j, K_m, K_n; K)}$ to emphasize the related quantities.

2.4 The dimensionally shifted basis

Since, as we shall demonstrate, our coefficients are polynomials in u, we can translate this information into the dimensionally shifted basis [49]. More explicitly, if we define

$$I_n^D[P^{\alpha_1} \dots P^{\alpha_m}] = -i(4\pi)^{D/2} \int \frac{d^D P}{(2\pi)^D} \frac{P^{\alpha_1} \dots P^{\alpha_m}}{(P^2 - m^2) \dots ((P - \sum_{i=1}^{n-1} k_i)^2 - m^2)}, \tag{2.29}$$

then we have

$$I_n^{(4-2\epsilon)}[(\mu^2)^k] = \frac{\Gamma(k - \epsilon)}{\Gamma(-\epsilon)} I_n^{(4-2\epsilon+2k)}[1]. \tag{2.30}$$

There are two merits of using this basis. First, we can throw away all $\mathcal{O}(\epsilon)$ contributions to make the calculation easier. Second, we improve efficiency. To use the recursion and reduction relations, we first calculated all the contributions by reduction to boxes, triangles and bubbles, and then added them up. With the dimensionally shifted basis, this process of reduction/summation can be done in one step, simplifying calculations. The usefulness of this dimensionally shifted basis has been discussed in [22, 29]. Here, for reference, we discuss this evaluation in appendix A.

3. Triangle coefficients

Now that we have the necessary background information, it is simplest to start with the coefficients of triangles. Some features of this discussion will apply to bubbles as well.

3.1 Simplifying the formula

We write the formula for triangle coefficients from [27] in the notation of the previous section, emphasizing u-dependence.

$$C[Q_s(u), K] = \frac{(K^2)^{1+n}}{2(\sqrt{\Delta(Q_s(u), K)(u)})^{n+1}} \frac{1}{(n+1)! \langle P_{(Q_s(u),K);1}(u) \; P_{(Q_s(u),K);2}(u) \rangle^{n+1}} \tag{3.1}$$

$$\times \frac{d^{n+1}}{d\tau^{n+1}} \left(\frac{\prod_{j=1}^{k+n} \langle P_{(Q_s(u),K);1}(u) - \tau P_{(Q_s(u),K);2}(u) | R_j(u) Q_s(u) | P_{(Q_s(u),K);1}(u) - \tau P_{(Q_s(u),K);2}(u) \rangle}{\prod_{t=1, t \neq s}^{k} \langle P_{(Q_s(u),K);1}(u) - \tau P_{(Q_s(u),K);2}(u) | Q_t(u) Q_s(u) | P_{(Q_s(u),K);1}(u) - \tau P_{(Q_s(u),K);2}(u) \rangle} \right.$$

$$\left. + \{P_{(Q_s(u),K);1}(u) \leftrightarrow P_{(Q_s(u),K);2}(u)\} \right) \Big|_{\tau \to 0},$$

where the $P_{(Q_s(u),K);1,2}(u)$, as depicted in the indices, are constructed in terms of $Q_s(u), K$, as defined in (2.22), and depend on u. In principle we can put (3.1) into (2.20) to take derivatives. However, the u-dependence everywhere might be an obstacle to taking stable derivatives in terms of u in (2.20). In this subsection, we recast this u-dependence in a simpler form.

Using the definition of Q_s from (2.15), and the property (2.19), we find from (2.22), (2.23) that

$$\Delta(Q_s(u), K)(u) = (1-u)(-4q_s^2 K^2),$$
$$x_{1,2}(u) = \frac{-2\alpha_s K^2 \pm \sqrt{\Delta(Q_s(u), K)}}{2K^2}.$$

When we take the square root of $\Delta(Q_s(u), K)$, there is a sign ambiguity. It can be shown that the choice of sign does not affect the final result. To be explicit, we choose the minus sign here, i.e.,

$$\sqrt{\Delta(Q_s(u), K)(u)} = -\sqrt{1-u}\sqrt{-4q_s^2 K^2} \tag{3.2}$$

$$x_{1,2}(u) = -\sqrt{1-u}\left(\frac{\pm\sqrt{-q_s^2 K^2}}{K^2} \right) - \alpha_s \tag{3.3}$$

$$= -(\sqrt{1-u})y_{1,2} - \alpha_s, \tag{3.4}$$

where we have defined new scalar quantities, $y_{1,2}$, as follows:

$$y_{1,2} \equiv \pm \frac{\sqrt{-q_s^2 K^2}}{K^2} = \pm \frac{\sqrt{(K_s \cdot K)^2 - K_s^2 K^2}}{K^2}. \tag{3.5}$$

With these results, we can see that

$$P_{(Q_s(u),K);i}(u) = -(\sqrt{1-u})q_s + \alpha_s K + x_i(u) K$$
$$= -\sqrt{1-u}(q_s + y_i K) = -(\sqrt{1-u})P_{(q_s,K);i}. \tag{3.6}$$

The u-dependence has been factored out; here the null momentum $P_{(q_s,K);i}$ does *not* depend on u, since it is constructed from q_s, K — as indicated in the subscript indices.

Substituting (3.2) and (3.6) back into (3.1), we find that the factor $\sqrt{1-u}$ has cancelled out. Thus we have

$$
C[Q_s, K] = \frac{(K^2)^{1+n}}{2(-\sqrt{1-u})^{n+1}(\sqrt{\Delta(q_s,K)})^{n+1}} \frac{1}{(n+1)! \left\langle P_{(q_s,K);1}\ P_{(q_s,K);2} \right\rangle^{n+1}}
$$
$$
\times \frac{d^{n+1}}{d\tau^{n+1}} \Bigg(\frac{\prod_{j=1}^{k+n} \left\langle P_{(q_s,K);1} - \tau P_{(q_s,K);2} | R_j(u) Q_s(u) | P_{(q_s,K);1} - \tau P_{(q_s,K);2} \right\rangle}{\prod_{t=1,t\neq s}^{k} \left\langle P_{(q_s,K);1} - \tau P_{(q_s,K);2} | Q_t(u) Q_s(u) | P_{(q_s,K);1} - \tau P_{(q_s,K);2} \right\rangle}
$$
$$
+ \{P_{(q_s,K);1} \leftrightarrow P_{(q_s,K);2}\} \Bigg) \Bigg|_{\tau \to 0}.
$$

To simplify further, apply the identity $\langle \ell | QQ | \ell \rangle = 0$ to derive

$$
\langle \ell | Q_t(u) Q_s(u) | \ell \rangle = \left\langle \ell | (Q_t(u) - \frac{\alpha_t}{\alpha_s} Q_s(u)) Q_s(u) | \ell \right\rangle = -\sqrt{1-u} \left\langle \ell \Big| \Big(q_t - \frac{\alpha_t}{\alpha_s} q_s \Big) Q_s(u) \Big| \ell \right\rangle \quad (3.7)
$$
$$
\langle \ell | R_j(u) Q_s(u) | \ell \rangle = \left\langle \ell | (R_j(u) - \frac{\beta_j}{\alpha_s} Q_s(u)) Q_s | \ell \right\rangle = -\sqrt{1-u} \left\langle \ell | \Big(p_j - \frac{\beta_j}{\alpha_s} q_s \Big) Q_s(u) | \ell \right\rangle. \quad (3.8)
$$

If we define two more vectors $\widetilde{q}_t, \widetilde{p}_j$ by

$$
\widetilde{q}_t = (q_t - \frac{\alpha_t}{\alpha_s} q_s), \quad \widetilde{p}_j = (p_j - \frac{\beta_j}{\alpha_s} q_s), \tag{3.9}
$$

then we use the identities (3.7), (3.8) to conclude that

$$
C[Q_s, K] = \frac{(K^2)^{1+n}}{2(\sqrt{\Delta(q_s,K)})^{n+1}} \frac{1}{(n+1)! \left\langle P_{(q_s,K);1}\ P_{(q_s,K);2} \right\rangle^{n+1}}
$$
$$
\times \frac{d^{n+1}}{d\tau^{n+1}} \Bigg(\frac{\prod_{j=1}^{k+n} \left\langle P_{(q_s,K);1} - \tau P_{(q_s,K);2} | \widetilde{p}_j Q_s(u) | P_{(q_s,K);1} - \tau P_{(q_s,K);2} \right\rangle}{\prod_{t=1,t\neq s}^{k} \left\langle P_{(q_s,K);1} - \tau P_{(q_s,K);2} | \widetilde{q}_t Q_s(u) | P_{(q_s,K);1} - \tau P_{(q_s,K);2} \right\rangle}
$$
$$
+ \{P_{(q_s,K);1} \leftrightarrow P_{(q_s,K);2}\} \Bigg) \Bigg|_{\tau \to 0}. \tag{3.10}
$$

Compared to (3.1), the u-dependence in (3.10) is much simpler; all u-dependence here comes *only* from $Q_s(u)$. Thus, (3.10) is well suited for use in (2.20).

How to use the formula (3.10). The degree of this polynomial in u will be seen to be $[(n+1)/2]$. Thus we can get the corresponding coefficients by taking derivatives in u first (from 0 to $[(n+1)/2]$, to get coefficients from each term in the polynomial), and then setting $u = 0$.

For example when $n = -1, 0$ we can set $u = 0$ directly and get

$$C[Q_s, K]_{n \in \{0, -1\}} = \frac{(K^2)^{n+1}}{2(\sqrt{\Delta(q_s, K)})^{n+1}} \frac{1}{\langle P_{(q_s, K);1} \, P_{(q_s, K);2} \rangle^{n+1}}$$

$$\times \frac{d^{n+1}}{d\tau^{n+1}} \left(\frac{\prod_{j=1}^{k+n} \langle P_{(q_s, K);1} - \tau P_{(q_s, K);2} | \widetilde{p}_j Q_s | P_{(q_s, K);1} - \tau P_{(q_s, K);2} \rangle}{\prod_{t=1, t \neq s}^{k} \langle P_{(q_s, K);1} - \tau P_{(q_s, K);2} | \widetilde{q}_t Q_s | P_{(q_s, K);1} - \tau P_{(q_s, K);2} \rangle} \right.$$

$$\left. + \{ P_{(q_s, K);1} \leftrightarrow P_{(q_s, K);2} \} \right) \Bigg|_{\tau \to 0}, \tag{3.11}$$

which is suitable for numerical evaluation. For $n = 1, 2$ the result will take the form of a linear polynomial, $c_0 + c_1 u$. To get c_1 we take one derivative, using

$$\frac{dQ_s(u)}{du} \bigg|_{u=0} = \frac{q_s}{2}. \tag{3.12}$$

In appendix B, we have explicit expressions, free of derivatives, for triangle coefficients when $n \leq 2$.

The formula (3.10) contains u in both numerator and denominator, so it is not so obvious that the total result is simply a polynomial in u. The proof of this property is given in the next subsection.

3.2 Proof that the triangle coefficient is a polynomial in u

We start by considering two quantities that arise in our expressions, in the course of taking derivatives:

$$E_1 \equiv \langle P_{(q_s, K);2} | \widetilde{p}_j Q_s(u) | P_{(q_s, K);1} \rangle + \langle P_{(q_s, K);1} | \widetilde{p}_j Q_s(u) | P_{(q_s, K);2} \rangle \tag{3.13}$$

$$E_2 \equiv \langle P_{(q_s, K);1} | \widetilde{p}_j Q_s(u) | P_{(q_s, K);1} \rangle \langle P_{(q_s, K);2} | \widetilde{p}_j Q_s(u) | P_{(q_s, K);2} \rangle \tag{3.14}$$

By writing $Q_s(u)$ as a linear combination of the $P_{(q_s, K);i}$,

$$Q_s(u) = \left(-\frac{\sqrt{1-u}}{2} + \frac{\alpha_s}{2y_1} \right) P_{(q_s, K);1} - \left(\frac{\sqrt{1-u}}{2} + \frac{\alpha_s}{2y_1} \right) P_{(q_s, K);2}, \tag{3.15}$$

and recalling that $q_s \cdot K = \widetilde{p}_j \cdot K = 0$, we find that

$$E_1 = -\frac{\alpha_s K^2}{\sqrt{-q_s^2 K^2}} (2\widetilde{p}_j \cdot q_s) \langle P_{(q_s, K);1} \, P_{(q_s, K);2} \rangle. \tag{3.16}$$

All u-dependence has dropped out of this expression.

For E_2, similar manipulations show that

$$E_2 = \langle P_{(q_s, K);1} \, P_{(q_s, K);2} \rangle^2 \left(q_s^2 \widetilde{p}_j^2 - (q_s \cdot \widetilde{p}_j)^2 \right) \left(\frac{K^2 \alpha_s^2}{q_s^2} + 1 - u \right), \tag{3.17}$$

which is a polynomial in u.

Now we prove that the full expression (3.10) for the triangle coefficient is a polynomial in u. Throughout this proof, let us abbreviate Q_s by Q and $P_{(q_s, K);i}$ by P_i.

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The triangle coefficient is given in terms of derivatives with respect to τ on an expression where the τ-dependence appears in the factors $\langle P_1 - \tau P_2 | \widetilde{p}_j Q(u) | P_1 - \tau P_2 \rangle$ (in numerator or denominator). After taking the derivatives, we set $\tau = 0$. In this process we will produce the following three combinations: $\langle P_1 | \widetilde{p}_j Q(u) | P_1 \rangle$; E_1; E_2. It is easy to see how the first two combinations arise. The third combination, E_2, appears, for example, in

$$\frac{d^2 \langle P_1 - \tau P_2 | \widetilde{p}_j Q(u) | P_1 - \tau P_2 \rangle}{d\tau^2} = \frac{-2 \langle P_1 | \widetilde{p}_j Q(u) | P_1 \rangle \langle P_2 | \widetilde{p}_j Q(u) | P_2 \rangle}{\langle P_1 | \widetilde{p}_j Q(u) | P_1 \rangle}$$

Consider the τ-dependent factors in the denominator. With each derivative, we effectively add one overall factor of $\langle P_1 - \tau P_2 | X Q(u) | P_1 - \tau P_2 \rangle$ in the denominator and place one new factor, either $(\langle P_1 - \tau P_2 | X Q(u) | P_2 \rangle + \langle P_2 | X Q(u) | P_1 - \tau P_2 \rangle)$ or $(-2 \langle P_2 | X Q(u) | P_2 \rangle \langle P_1 | X Q(u) | P_1 \rangle)$ in the numerator. After taking $n+1$ derivatives, there are $(n+1)$ additional factors $\langle P_1 - \tau P_2 | X Q(u) | P_1 - \tau P_2 \rangle$ in the denominator. Thus, we have exactly $k + n$ factors of $\langle P_1 | X Q(u) | P_1 \rangle$ in both numerator and denominator (after taking the $\tau \to 0$ limit). The u-dependence is exactly cancelled in this part, since we have

$$\frac{\langle P_1 | X Q(u) | P_1 \rangle}{\langle P_1 | X' Q(u) | P_1 \rangle} = \frac{\langle P_1 | X | P_2]}{\langle P_1 | X' | P_2]}. \tag{3.18}$$

The remaining u-dependence comes only through the factor E_2 in the numerator. By our previous calculations (3.16) and (3.17), we see that indeed our final expression is a polynomial in u. Since every sequence of two derivatives in (3.10) will produce one E_2 factor, the degree of the polynomial is $[(n+1)/2]$.

4. Bubble coefficients

Our proof that bubble coefficients are polynomials in u is more complicated than the one for triangle coefficients, so many of the details have been relegated to appendix C. Here we present the simplification of the u-dependence in the formula for bubble coefficients. The idea of the proof is consider the bubble coefficients are polynomials in $\sqrt{1-u}$, and show that the odd powers vanish.

4.1 Simplification

The coefficient of the bubble integral with momentum K is given by [27]

$$C[K] = (K^2)^{1+n} \sum_{q=0}^{n} \frac{(-1)^q}{q!} \frac{d^q}{ds^q} \left(\mathcal{B}_{n,n-q}^{(0)}(s) + \sum_{r=1}^{k} \sum_{a=q}^{n} \left(\mathcal{B}_{n,n-a}^{(r;a-q;1)}(s) - \mathcal{B}_{n,n-a}^{(r;a-q;2)}(s) \right) \right) \Bigg|_{s=0}, \tag{4.1}$$

where

$$\mathcal{B}_{n,t}^{(0)}(s) \equiv \frac{d^n}{d\tau^n} \left(\frac{1}{n! [\eta | \widetilde{\eta} K | \eta]^n} \frac{(2\eta \cdot K)^{t+1}}{(t+1)(K^2)^{t+1}} \right.$$
$$\left. \times \frac{\prod_{j=1}^{n+k} \langle \ell | R_j(u)(K + s\eta) | \ell \rangle}{\langle \ell\, \eta \rangle^{n+1} \prod_{p=1}^{k} \langle \ell | Q_p(u)(K + s\eta) | \ell \rangle} |_{|\ell\rangle \to |K - \tau\widetilde{\eta}|\eta]} \right) \Bigg|_{\tau=0}, \tag{4.2}$$

$$\mathcal{B}_{n,t}^{(r;b;1)}(s) \equiv \frac{(-1)^{b+1}}{b!\sqrt{\Delta(Q_r(u),K)}^{b+1}\left\langle P_{(Q_r(u),K);1}(u)\ P_{(Q_r(u),K);2}(u)\right\rangle^b}$$

$$\frac{d^b}{d\tau^b}\left(\frac{1}{(t+1)}\frac{\left\langle P_{(Q_r(u),K);1}(u)-\tau P_{(Q_r(u),K);2}(u)|\eta|P_{(Q_r(u),K);1}(u)\right]^{t+1}}{\left\langle P_{(Q_r(u),K);1}(u)-\tau P_{(Q_r(u),K);2}(u)|K|P_{(Q_r(u),K);1}(u)\right]^{t+1}}\right.$$

$$\times\frac{\left\langle P_{(Q_r(u),K);1}(u)-\tau P_{(Q_r(u),K);2}(u)|Q_r(u)\eta|P_{(Q_r(u),K);1}(u)-\tau P_{(Q_r(u),K);2}(u)\right\rangle^b}{\left\langle P_{(Q_r(u),K);1}(u)-\tau P_{(Q_r(u),K);2}(u)|\eta K|P_{(Q_r(u),K);1}(u)-\tau P_{(Q_r(u),K);2}(u)\right\rangle^{n+1}}$$

$$\left.\times\frac{\prod_{j=1}^{n+k}\left\langle P_{(Q_r(u),K);1}(u)-\tau P_{(Q_r(u),K);2}(u)|R_j(u)(K+s\eta)|P_{(Q_r(u),K);1}(u)-\tau P_{(Q_r(u),K);2}(u)\right\rangle}{\prod_{p=1,p\neq r}^{k}\left\langle P_{(Q_r(u),K);1}(u)-\tau P_{(Q_r(u),K);2}(u)|Q_p(u)(K+s\eta)|P_{(Q_r(u),K);1}(u)-\tau P_{(Q_r(u),K);2}(u)\right\rangle}\right)\Bigg|_{\tau=0}, \quad (4.3)$$

$$\mathcal{B}_{n,t}^{(r;b;2)}(s) \equiv \frac{(-1)^{b+1}}{b!\sqrt{\Delta(Q_r(u),K)}^{b+1}\left\langle P_{(Q_r(u),K);1}(u)\ P_{(Q_r(u),K);2}(u)\right\rangle^b}$$

$$\frac{d^b}{d\tau^b}\left(\frac{1}{(t+1)}\frac{\left\langle P_{(Q_r(u),K);2}(u)-\tau P_{(Q_r(u),K);1}(u)|\eta|P_{(Q_r(u),K);2}(u)\right]^{t+1}}{\left\langle P_{(Q_r(u),K);2}(u)-\tau P_{(Q_r(u),K);1}(u)|K|P_{(Q_r(u),K);2}(u)\right]^{t+1}}\right.$$

$$\times\frac{\left\langle P_{(Q_r(u),K);2}(u)-\tau P_{(Q_r(u),K);1}(u)|Q_r(u)\eta|P_{(Q_r(u),K);2}(u)-\tau P_{(Q_r(u),K);1}(u)\right\rangle^b}{\left\langle P_{(Q_r(u),K);2}(u)-\tau P_{(Q_r(u),K);1}(u)|\eta K|P_{(Q_r(u),K);2}(u)-\tau P_{(Q_r(u),K);1}(u)\right\rangle^{n+1}}$$

$$\left.\times\frac{\prod_{j=1}^{n+k}\left\langle P_{(Q_r(u),K);2}(u)-\tau P_{(Q_r(u),K);1}(u)|R_j(u)(K+s\eta)|P_{(Q_r(u),K);2}(u)-\tau P_{(Q_r(u),K);1}(u)\right\rangle}{\prod_{p=1,p\neq r}^{k}\left\langle P_{(Q_r(u),K);2}(u)-\tau P_{(Q_r(u),K);1}(u)|Q_p(u)(K+s\eta)|P_{(Q_r(u),K);2}(u)-\tau P_{(Q_r(u),K);1}(u)\right\rangle}\right)\Bigg|_{\tau=0}. \quad (4.4)$$

In this expression, since $P_{(Q_r(u),K);1}(u)$ and $\Delta(Q_r(u),K)$ depend on u, we want to simplify the above expressions as we did in the triangle case. Using (3.2) and (3.6), we see that we can pull out some factors of $\sqrt{1-u}$, giving[5]

$$\mathcal{B}_{n,t}^{(r;b;1)}(s,u) \equiv \frac{1}{b!(\sqrt{1-u})^{b+1}\sqrt{\Delta(q_r,K)}^{b+1}\left\langle P_{(q_r,K);1}\ P_{(q_r,K);2}\right\rangle^b}$$

$$\times\frac{d^b}{d\tau^b}\left(\frac{1}{(t+1)}\frac{\left\langle P_{(q_r,K);1}-\tau P_{(q_r,K);2}|\eta|P_{(q_r,K);1}\right]^{t+1}}{\left\langle P_{(q_r,K);1}-\tau P_{(q_r,K);2}|K|P_{(q_r,K);1}\right]^{t+1}}\right.$$

$$\times\frac{\left\langle P_{(q_r,K);1}-\tau P_{(q_r,K);2}|Q_r(u)\eta|P_{(q_r,K);1}-\tau P_{(q_r,K);2}\right\rangle^b}{\left\langle P_{(q_r,K);1}-\tau P_{(q_r,K);2}|\eta K|P_{(q_r,K);1}-\tau P_{(q_r,K);2}\right\rangle^{n+1}}$$

$$\left.\times\frac{\prod_{j=1}^{n+k}\left\langle P_{(q_r,K);1}-\tau P_{(q_r,K);2}|R_j(u)(K+s\eta)|P_{(q_r,K);1}-\tau P_{(q_r,K);2}\right\rangle}{\prod_{p=1,p\neq r}^{k}\left\langle P_{(q_r,K);1}-\tau P_{(q_r,K);2}|Q_p(u)(K+s\eta)|P_{(q_r,K);1}-\tau P_{(q_r,K);2}\right\rangle}\right)\Bigg|_{\tau=0}, \quad (4.5)$$

Similarly, for the function $\mathcal{B}_{n,t}^{(r;b;2)}(s,u)$,

$$\mathcal{B}_{n,t}^{(r;b;2)}(s,u) \equiv \frac{1}{b!(\sqrt{1-u})^{b+1}\sqrt{\Delta(q_r,K)}^{b+1}\left\langle P_{(q_r,K);1}\ P_{(q_r,K);2}\right\rangle^b}$$

$$\times\frac{d^b}{d\tau^b}\left(\frac{1}{(t+1)}\frac{\left\langle P_{(q_r,K);2}-\tau P_{(q_r,K);1}|\eta|P_{(q_r,K);2}\right]^{t+1}}{\left\langle P_{(q_r,K);2}-\tau P_{(q_r,K);1}|K|P_{(q_r,K);1}\right]^{t+1}}\right.$$

---

[5]One way to see it is to choose $\left|P_{(Q_r(u),K);i}\right\rangle = \left|P_{(q_r,K);i}\right\rangle$ and $\left|P_{(Q_r(u),K);i}\right] = -\sqrt{1-u}|P_{(q_r,K);i}]$; the factor $-\sqrt{1-u}$ cancels out immediately.

$$\times \frac{\left\langle P_{(q_r,K);2} - \tau P_{(q_r,K);1}|Q_r(u)\eta|P_{(q_r,K);2} - \tau P_{(q_r,K);1}\right\rangle^b}{\left\langle P_{(q_r,K);2} - \tau P_{(q_r,K);1}|\eta K|P_{(q_r,K);2} - \tau P_{(q_r,K);1}\right\rangle^{n+1}}$$

$$\times \left. \frac{\prod_{j=1}^{n+k}\left\langle P_{(q_r,K);2} - \tau P_{(q_r,K);1}|R_j(u)(K+s\eta)|P_{(q_r,K);2} - \tau P_{(q_r,K);1}\right\rangle}{\prod_{p=1,p\neq r}^{k}\left\langle P_{(q_r,K);2} - \tau P_{(q_r,K);1}|Q_p(u)(K+s\eta)|P_{(q_r,K);2} - \tau P_{(q_r,K);1}\right\rangle}\right) \right|_{\tau=0}, \quad (4.6)$$

So, the bubble coefficient is now given by (4.1), (4.2), (4.5) and (4.6). Unlike the triangle, since we now have factors of the form $\langle\ell|Q(u)(K+s\eta)|\ell\rangle$ instead of $\langle\ell|Q(u)K|\ell\rangle$, we cannot pull out further factors of $\sqrt{1-u}$. In these expressions, the only u-dependence is coming from $R_j(u)$ and $Q_t(u)$, which is much simpler than the original formula.

The best way to use these formulas is similar to the triangle case. We can see from the formulas (4.2), (4.5), (4.6) that the degree of the polynomial in u is $[n/2]$. Thus we can get the corresponding coefficients by taking derivatives with respect to u and then setting $u = 0$, as in (2.20).

5. The box and pentagon coefficients

Now we consider the box coefficients. This is the most complicated part, although the formula is the simplest! There are two reasons for the complexity. First, the box coefficients contain not only true box coefficients, but also pentagon contributions, indicated by a linear factor $(au + b)$ in the denominator. We should be able to separate the box part from the pentagon part. The second reason is that the null momenta $P_{(Q_j(u),Q_i(u));s}$ depend on u in a very nontrivial way (as $Q_j(u) + x_a Q_i(u)$), unlike the cases of triangles and bubbles.

Given the vectors Q_i, Q_j, K we can construct a vector $q_0^{(q_i,q_j,K)}$ orthogonal to all three:

$$(q_0)_\mu^{(q_i,q_j,K)} \equiv \frac{1}{K^2}\epsilon_{\mu\nu\rho\xi}q_i^\nu q_j^\rho K^\xi \quad (5.1)$$

$$= \frac{1}{K^2}\epsilon_{\mu\nu\rho\xi}K_i^\nu K_j^\rho K^\xi. \quad (5.2)$$

We shall make use of our collection of orthogonality relations:

$$q_i \cdot K = q_j \cdot K = q_0 \cdot K = 0$$
$$q_0 \cdot q_i = q_0 \cdot q_j = q_0 \cdot K = 0 \quad (5.3)$$

Observe the fixed ordering of q_i, q_j in the definition (5.2) of $q_0^{(q_i,q_j,K)}$. Exchanging them leads to a minus sign difference. The ordering is connected with our definition $P_{ji} = Q_j + xQ_i$.

Because new features arise in different cases, we have divided our discussion into the three cases $k = 2$, $k = 3$, and $k \geq 4$.

In the process of simplifying our expression, we also demonstrate that the coefficients are truly polynomials in u. Thus this is a constructive proof.

5.1 The case $k = 2$

In this case, there is exactly one box, whose coefficient is given by

$$\frac{(K^2)^{2+n}}{2} \left(\frac{\prod_{s=1}^{n+2} \left\langle P_{(Q_j(u),Q_i(u));1}(u)|R_s(u)|P_{(Q_j(u),Q_i(u));2}(u) \right]}{\left\langle P_{(Q_j(u),Q_i(u));1}(u)|K|P_{(Q_j(u),Q_i(u));2}(u) \right]^{n+2}} \right.$$

$$\left. + \{ P_{(Q_j(u),Q_i(u));1}(u) \leftrightarrow P_{(Q_j(u),Q_i(u));2}(u) \} \right).$$

Later, we will reduce the other cases to this expression as well. Now we carry out a detailed calculation to show that the u-dependence is polynomial, and we find an expression where the u-dependence is easier to see.

In the numerator, the factors $R_s(u)$ have u-dependence in the form $R_s(u) = -(\sqrt{1-u})p_s + \beta_s K$ (here we do not assume any particular form of β_s), with $p_s \cdot K = 0$. Thus the vector p_s can be expanded in a basis of the three-dimensional vectorspace orthogonal to K, as follows.

$$p_s = a_0^{(q_i,q_j,K;p_s)} q_0^{(q_i,q_j,K)} + a_i^{(q_i,q_j,K;p_s)} q_i + a_j^{(q_i,q_j,K;p_s)} q_j. \tag{5.4}$$

The coefficients in this expansion are:

$$a_i^{(q_i,q_j,K;p_s)} = \frac{(p_s \cdot q_i)q_j^2 - (p_s \cdot q_j)(q_i \cdot q_j)}{q_i^2 q_j^2 - (q_i \cdot q_j)^2} \tag{5.5}$$

$$a_j^{(q_i,q_j,K;p_s)} = \frac{(p_s \cdot q_j)q_i^2 - (p_s \cdot q_i)(q_i \cdot q_j)}{q_i^2 q_j^2 - (q_i \cdot q_j)^2} \tag{5.6}$$

$$a_0^{(q_i,q_j,K;p_s)} = \frac{(p_s \cdot q_0^{(q_i,q_j,K)})}{(q_0^{(q_i,q_j,K)})^2} = \frac{\epsilon(p_s,q_i,q_j,K)}{K^2(q_0^{(q_i,q_j,K)})^2} = \frac{\epsilon(P_s,K_i,K_j,K)}{K^2(q_0^{(q_i,q_j,K)})^2}. \tag{5.7}$$

Using this expansion, we can write

$$R_s(u) = a_0^{(q_i,q_j,K;p_s)} \left(-(\sqrt{1-u})q_0^{(q_i,q_j,K)} \right) + a_i^{(q_i,q_j,K;p_s)} Q_i(u)$$
$$+ a_j^{(q_i,q_j,K;p_s)} Q_j(u) + \beta_s^{(q_i,q_j,K;p_s)} K, \tag{5.8}$$

where we have defined

$$\beta_s^{(q_i,q_j,K;p_s)} \equiv (\beta_s - a_i^{(q_i,q_j,K;p_s)} \alpha_i - a_j^{(q_i,q_j,K;p_s)} \alpha_j). \tag{5.9}$$

Using the result (2.24) that

$$\left\langle P_{(Q_j(u),Q_i(u));1}(u)|Q_{i/j}(u)|P_{(Q_j(u),Q_i(u));2}(u) \right] = 0, \tag{5.10}$$

we have

$$\left\langle P_{(Q_j(u),Q_i(u));1}(u)|R_s(u)|P_{(Q_j(u),Q_i(u));2}(u) \right]$$
$$= -(\sqrt{1-u})a_0^{(q_i,q_j,K;p_s)} \left\langle P_{(Q_j(u),Q_i(u));1}(u)|q_0^{(q_i,q_j,K)}|P_{(Q_j(u),Q_i(u));2}(u) \right]$$
$$+ \beta_s^{(q_i,q_j,K;p_s)} \left\langle P_{(Q_j(u),Q_i(u));1}(u)|K|P_{(Q_j(u),Q_i(u));2}(u) \right]. \tag{5.11}$$

Thus, we can write

$$\frac{\prod_{s=1}^{n+2} \left\langle P_{(Q_j(u),Q_i(u));1}(u)|R_s(u)|P_{(Q_j(u),Q_i(u));2}(u)\right]}{\left\langle P_{(Q_j(u),Q_i(u));1}(u)|K|P_{(Q_j(u),Q_i(u));2}(u)\right]^{n+2}} \tag{5.12}$$

$$= \sum_{h=0}^{n+2} C_h^{(q_i,q_j,K)} \frac{(-\sqrt{1-u})^h \left\langle P_{(Q_j(u),Q_i(u));1}(u)|q_0^{(q_i,q_j,K)}|P_{(Q_j(u),Q_i(u));2}(u)\right]^h}{\left\langle P_{(Q_j(u),Q_i(u));1}(u)|K|P_{(Q_j(u),Q_i(u));2}(u)\right]^h}.$$

Here we have defined

$$C_h^{(q_i,q_j,K)} = \sum_{\substack{S \subseteq \{1,2,\ldots,n+2\} \\ |S|=h}} \prod_{s \in S} a_0^{(q_i,q_j,K;p_s)} \prod_{s \in S^c} \beta_s^{(q_i,q_j,K;p_s)}, \tag{5.13}$$

where S^c denotes the complement of S: $S^c \equiv \{1,2,\ldots,n+2\}\backslash S$.

Now we can show that the box coefficients are indeed polynomials in u, in this case where $k = 2$. By the above expansion, the coefficients are given by sum of the following typical terms. (To simplify the formulas in this proof, we shall now write $P_{ji,a}(u)$ in place of $P_{(Q_j(u),Q_i(u));a}(u)$.)

$$\frac{(-\sqrt{1-u})^h \langle P_{ji,1}(u)|q_0|P_{ji,2}(u)]^h}{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]^h} + \frac{(-\sqrt{1-u})^h \langle P_{ji,2}(u)|q_0|P_{ji,1}(u)]^h}{\langle P_{ji,2}(u)|K|P_{ji,1}(u)]^h} \tag{5.14}$$

$$= (-\sqrt{1-u})^h \frac{\langle P_{ji,1}(u)|q_0|P_{ji,2}(u)]^h \langle P_{ji,2}(u)|K|P_{ji,1}(u)]^h}{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]^h \langle P_{ji,2}(u)|K|P_{ji,1}(u)]^h}$$

$$+ \frac{\langle P_{ji,2}(u)|q_0|P_{ji,1}(u)]^h \langle P_{ji,1}(u)|K|P_{ji,2}(u)]^h}{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]^h \langle P_{ji,2}(u)|K|P_{ji,1}(u)]^h}$$

$$= \frac{(-\sqrt{1-u})^h \left[\left(2i(1-u)\sqrt{\Delta(Q_i(u),Q_j(u))}q_0^2 K^2\right)^h \right.}{\left(K^2(1-u)^2[(2q_i \cdot q_j)^2 - 4q_i^2 q_j^2]\right)^h}$$

$$+ \frac{\left(-2i(1-u)\sqrt{\Delta(Q_i(u),Q_j(u))}q_0^2 K^2\right)^h \right]}{\left(K^2(1-u)^2[(2q_i \cdot q_j)^2 - 4q_i^2 q_j^2]\right)^h}. \tag{5.15}$$

We have used the following results (making repeated use of the identity (2.25)):

$$\langle P_{ji,1}(u)|K|P_{ji,2}(u)]\, \langle P_{ji,2}(u)|K|P_{ji,1}(u)] = \frac{K^2}{Q_i(u)^2}(1-u)^2[(2q_i \cdot q_j)^2 - 4q_i^2 q_j^2]$$

$$\langle P_{ji,1}(u)|q_0|P_{ji,2}(u)]\, \langle P_{ji,2}(u)|K|P_{ji,1}(u)] = 2i(1-u)\frac{\sqrt{\Delta(Q_i(u),Q_j(u))}}{Q_i(u)^2}q_0^2 K^2$$

$$\langle P_{ji,1}(u)|K|P_{ji,2}(u)]\, \langle P_{ji,2}(u)|q_0|P_{ji,1}(u)] = -2i(1-u)\frac{\sqrt{\Delta(Q_i(u),Q_j(u))}}{Q_i(u)^2}q_0^2 K^2$$

and

$$\Delta(Q_i(u),Q_j(u)) = (1-u)\Big\{(1-u)[(2q_i \cdot q_j)^2 - 4q_i^2 q_j^2]$$

$$+ 4K^2[\alpha_i \alpha_j(2q_i \cdot q_j) - \alpha_i^2 q_j^2 - \alpha_j^2 q_i^2]\Big\}. \tag{5.16}$$

Equation (5.15) is our most important result in this subsection. There we can see that when h is odd, we get zero. When h is even, the factor $(1-u)^{2h}$ in the denominator is cancelled by corresponding factors in the numerator. (Notice the overall factor of $(1-u)$ within $\Delta(Q_i(u), Q_j(u))$.) Thus we see that indeed the expression (5.14) is a polynomial in u, specifically,

$$\begin{cases} \frac{2(2i)^h (q_0^2)^h \left\{ (1-u)[(2q_i \cdot q_j)^2 - 4q_i^2 q_j^2] + 4K^2[\alpha_i \alpha_j (2q_i \cdot q_j) - \alpha_i^2 q_j^2 - \alpha_j^2 q_i^2] \right\}^{h/2}}{[(2q_i \cdot q_j)^2 - 4q_i^2 q_j^2]^h} & \text{for } h \text{ even,} \\ 0 & \text{for } h \text{ odd.} \end{cases} \tag{5.17}$$

It is clear that the maximum degree of the polynomial is $[\frac{n+2}{2}]$.

5.1.1 A simpler expression for $k = 2$

The aim of this sub-subsection is to find another expression with the same value as (5.17), but with more transparent u-dependence. We have just seen that all u-dependence has cancelled out, except for the second factor of $(1-u)$ in the first term of $\Delta_{ij}(u)$, as it appears in (5.16). Since (5.17) is now an expression in terms of scalar quantities, we can consider the effect of setting $u = 0$ at the beginning of the calculation. Recovering the expression (5.17) then requires the following single modification:

$$q_0^{(q_i,q_j,K)} \to \alpha^{(q_i,q_j)}(u) q_0^{(q_i,q_j,K)}, \quad \alpha^{(q_i,q_j)}(u) = \frac{\sqrt{1 - u + \frac{4K^2[\alpha_i \alpha_j (2q_i \cdot q_j) - \alpha_i^2 q_j^2 - \alpha_j^2 q_i^2]}{(2q_i \cdot q_j)^2 - 4q_i^2 q_j^2}}}{\sqrt{1 + \frac{4K^2[\alpha_i \alpha_j (2q_i \cdot q_j) - \alpha_i^2 q_j^2 - \alpha_j^2 q_i^2]}{(2q_i \cdot q_j)^2 - 4q_i^2 q_j^2}}}. \tag{5.18}$$

Then,

$$\frac{(-\sqrt{1-u})^h \langle P_{ji,1}(u)|q_0|P_{ji,2}(u)]^h}{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]^h} + \frac{(-\sqrt{1-u})^h \langle P_{ji,2}(u)|q_0|P_{ji,1}(u)]^h}{\langle P_{ji,2}(u)|K|P_{ji,1}(u)]^h}$$

$$= \frac{\langle P_{ji,1}(u=0)|\alpha^{(q_i,q_j)}(u)(-q_0)|P_{ji,2}(u=0)]^h}{\langle P_{ji,1}(u=0)|K|P_{ji,2}(u=0)]^h}$$

$$+ \frac{\langle P_{ji,2}(u=0)|\alpha^{(q_i,q_j)}(u)(-q_0)|P_{ji,1}(u=0)]^h}{\langle P_{ji,2}(u=0)|K|P_{ji,1}(u=0)]^h}. \tag{5.19}$$

Now, all of the u-dependence is concentrated within the $\alpha^{(q_i,q_j)}(u)$. Going back to (5.12), we can perform a similar operation:

$$\frac{\prod_{s=1}^{n+2} \langle P_{ji,1}(u)|R_s(u)|P_{ji,2}(u)]}{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]^{n+2}} + \{P_{ji,1}(u) \leftrightarrow P_{ji,2}(u)\}$$

$$= \frac{\prod_{s=1}^{n+2} \langle P_{ji,1}(u=0)|\widetilde{R}_s(u)|P_{ji,2}(u=0)]}{\langle P_{ji,1}(u=0)|K|P_{ji,2}(u=0)]^{n+2}} + \{P_{ji,1}(u=0) \leftrightarrow P_{ji,2}(u=0)\}. \tag{5.20}$$

where we have defined

$$\widetilde{R}_s(u) \equiv a_0^{(q_i,q_j,K;p_s)} \alpha^{(q_i,q_j)}(u)(-q_0) + \beta_s^{(q_i,q_j,K;p_s)} K. \tag{5.21}$$

With the definition (5.9), we can rewrite $\widetilde{R}_s(u)$ as

$$\widetilde{R}_s = a_0^{(q_i,q_j,K;p_s)}(\alpha^{(q_i,q_j)}(u) - 1)(-q_0) - a_i^{(q_i,q_j,K;p_s)}Q_i(u=0)$$
$$-a_j^{(q_i,q_j,K;p_s)}Q_j(u=0) + R_s(u=0).$$

Now we make use of the properties

$$\langle P_{ji,1}(u=0)|Q_i(u=0)|P_{ji,2}(u=0)] = \langle P_{ji,1}(u=0)|Q_j(u=0)|P_{ji,2}(u=0)] = 0,$$

and the fact that $\widetilde{R}_s(u)$ is defined such that the equation (5.20) is satisfied, we can drop the terms with $Q_{i/j}(u=0)$, so that

$$\widetilde{R}_s(u) \equiv \frac{p_s \cdot q_0^{(q_i,q_j,K)}}{(q_0^{(q_i,q_j,K)})^2}(\alpha^{(q_i,q_j)}(u) - 1)(-q_0^{(q_i,q_j,K)}) + R_s(u=0). \tag{5.22}$$

Equations (5.20) and (5.22) are our final simplest result. All u-dependence has been packaged inside $(\alpha^{(q_i,q_j)}(u) - 1)$, which is zero when $u = 0$. Also, it has now become clear that the degree of the polynomial in u is $[(n+2)/2]$.

Summary. The box coefficient for $k = 2$ is given by

$$C[K_i, K_j]_{k=2} = \frac{(K^2)^{2+n}}{2}\left(\frac{\prod_{s=1}^{n+2}\left\langle P_{(Q_j,Q_i);1}|\widetilde{R}_s(u)|P_{(Q_j,Q_i);2}\right]}{\left\langle P_{(Q_j,Q_i);1}|K|P_{(Q_j,Q_i);2}\right]^{n+2}}\right.$$
$$\left. +\{P_{(Q_j,Q_i);1} \leftrightarrow P_{(Q_j,Q_i);2}\}\right), \tag{5.23}$$

with

$$\widetilde{R}_s(u) = \frac{p_s \cdot q_0^{(q_i,q_j,K)}}{(q_0^{(q_i,q_j,K)})^2}(\alpha^{(q_i,q_j)}(u) - 1)(-q_0^{(q_i,q_j,K)}) + R_s(u=0). \tag{5.24}$$

Let us emphasize again that $P_{(Q_j,Q_i);a}$ is constructed from $Q_j(u=0) + x_a Q_i(u=0)$, so it is *independent* of u.

5.2 The case $k = 3$

In this case, we will see the pentagon show up, and we shall learn how to separate boxes from pentagons. Again, we shall abbreviate the notation of the vector $P_{(Q_j,Q_i);a}$ by $P_{ji,a}$. We evaluate an expression of the form:

$$\frac{\prod_{s=1}^{n+3}\langle P_{ji,1}(u)|R_s(u)|P_{ji,2}(u)]}{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]^{n+2}\langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]} + \{P_{ji,1}(u) \leftrightarrow P_{ji,2}(u)\}. \tag{5.25}$$

Again, we would like to expand $R_s(u)$, or equivalently p_s, in a suitable basis of the vectorspace orthogonal to K. In this case, we do not need to construct the vector $q_0^{(q_i,q_j,K)}$, because we now have three vectors q_i, q_j, q_t available already.

$$p_s = a_t^{(q_i,q_j,q_t;p_s)}q_t + a_i^{(q_i,q_j,q_t;p_s)}q_i + a_j^{(q_i,q_j,q_t;p_s)}q_j. \tag{5.26}$$

Thus,

$$
\begin{aligned}
\langle P_{ji,1}(u)|R_s(u)|P_{ji,2}(u)] = {} & a_t^{(q_i,q_j,q_t;p_s)} \langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)] \\
& + \beta_s^{(q_i,q_j,q_t;p_s)} \langle P_{ji,1}(u)|K|P_{ji,2}(u)] ,
\end{aligned}
\tag{5.27}
$$

where we have defined

$$
\beta_s^{(q_i,q_j,q_t;p_s)} \equiv (\beta_s - \sum_{h=i,j,k} a_h^{(q_i,q_j,q_t;p_s)} \alpha_h).
\tag{5.28}
$$

Now we can expand the rational function within the coefficient formula:

$$
\begin{aligned}
& \frac{\prod_{s=1}^{n+3} \langle P_{ji,1}(u)|R_s(u)|P_{ji,2}(u)]}{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]^{n+2} \langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]} \\
& = \sum_{h=0}^{n+3} C_h^{(q_i,q_j,q_t)} \frac{\langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]^h}{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]^{h-1} \langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]} ,
\end{aligned}
\tag{5.29}
$$

where we have defined

$$
C_h^{(q_i,q_j,q_t)} = \sum_{\substack{S \subseteq \{1,2,\dots,n+3\} \\ |S|=h}} \prod_{s \in S} a_t^{(q_i,q_j,q_t;p_s)} \prod_{s \in S^c} \beta_s^{(q_i,q_j,q_t;p_s)} .
$$

Now, break the sum (5.29) into two parts, by separating the term with $h = 0$ from the rest. In every term with $h > 0$, the factor $\langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]$ from the denominator is cancelled by the numerator. What remains is a term in the form we considered in the previous subsection, the case $k = 2$. That part contributes only to boxes. We shall return to that part in a moment, to find the exact box contribution. Notice that we can observe at this point, from the comparison to the $k = 2$ case, that the degree of the polynomial is again $[(n + 2)/2]$.

The term in (5.29) with $h = 0$ is

$$
\prod_{s=1}^{n+3} \beta_s^{(q_i,q_j,q_t;p_s)} \frac{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]}{\langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]} .
$$

The cut of a pentagon integral has been analyzed in [21]. We clarify its u-dependent behavior in appendix D. It is directly related to the sum of three cut-boxes. The part of the cut-pentagon that is related to the cut-box $C[Q_i, Q_j]$ is

$$
\frac{1}{2K^2} \left(\frac{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]}{\langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]} + \{P_{ji,1}(u) \leftrightarrow P_{ji,2}(u)\} \right) .
\tag{5.30}
$$

Thus, we see that this $h = 0$ term is exactly a pentagon contribution. The coefficient of the pentagon integral must be

$$
C[Q_i, Q_j, Q_t] = (K^2)^{3+n} \prod_{s=1}^{n+3} \beta_s^{(q_i,q_j,q_t;p_s)} ,
\tag{5.31}
$$

which is entirely independent of u.

Now let us return to the box coefficients, using our result (5.23), along with the definition (5.22) applied here to the vector $Q_t(u)$ instead of $R_s(u)$.

$$
\sum_{h=1}^{n+3} C_h^{(q_i,q_j,q_t)} \frac{\langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]^{h-1}}{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]^{h-1}}
$$

$$
\longrightarrow \sum_{h=1}^{n+3} C_h^{(q_i,q_j,q_t)} \frac{\left\langle P_{ji,1}(u=0)|\widetilde{Q}_t(u)|P_{ji,2}(u=0)\right]^{h-1}}{\langle P_{ji,1}(u=0)|K|P_{ji,2}(u=0)]^{h-1}}
$$

$$
= \sum_{h=0}^{n+3} C_h^{(q_i,q_j,q_t)} \frac{\left\langle P_{ji,1}(u=0)|\widetilde{Q}_t(u)|P_{ji,2}(u=0)\right]^{h}}{\langle P_{ji,1}(u=0)|K|P_{ji,2}(u=0)]^{h-1}\left\langle P_{ji,1}(u=0)|\widetilde{Q}_t(u)|P_{ji,2}(u=0)\right]}
$$

$$
- \prod_{s=1}^{n+3} \beta_s^{(q_i,q_j,q_t;p_s)} \frac{\langle P_{ji,1}(u=0)|K|P_{ji,2}(u=0)]}{\left\langle P_{ji,1}(u=0)|\widetilde{Q}_t(u)|P_{ji,2}(u=0)\right]}
$$

$$
= \frac{\prod_{s=1}^{n+3}\left\langle P_{ji,1}(u=0)|\widetilde{\widetilde{R}}_s(u)|P_{ji,2}(u=0)\right]}{\langle P_{ji,1}(u=0)|K|P_{ji,2}(u=0)]^{n+2}\left\langle P_{ji,1}(u=0)|\widetilde{Q}_t(u)|P_{ji,2}(u=0)\right]}
$$

$$
- \prod_{s=1}^{n+3} \beta_s^{(q_i,q_j,q_t;p_s)} \frac{\langle P_{ji,1}(u=0)|K|P_{ji,2}(u=0)]}{\left\langle P_{ji,1}(u=0)|\widetilde{Q}_t(u)|P_{ji,2}(u=0)\right]}
$$

In the last line of this equation, we have defined

$$
\begin{aligned}
\widetilde{\widetilde{R}}_s(u) &\equiv a_t^{(q_i,q_j,q_t;p_s)}\widetilde{Q}_t + \beta_s^{(q_i,q_j,q_t;p_s)}K \\
&= a_t^{(q_i,q_j,q_t;p_s)}a_0^{(q_i,q_j,K;q_t)}(\alpha^{(q_i,q_j)}(u)-1)(-q_0) \\
&\quad + R_s(u=0) - \sum_{\gamma=i,j} a_\gamma^{(q_i,q_j,q_t;p_s)}Q_\gamma(u=0).
\end{aligned} \tag{5.32}
$$

The cumbersome double-tilde notation is a temporary inconvenience, to avoid confusion with $\widetilde{R}_s(u)$, which was defined in (5.21) for the case $k=2$. In fact, we shall discover later that the two quantities are identical.

Using the property $\left\langle P_{ji,1}(u=0)|Q_{i/j}(u=0)|P_{ji,2}(u=0)\right] = 0$, we can redefine this vector as follows:

$$
\widetilde{\widetilde{R}}_s(u) \equiv a_t^{(q_i,q_j,q_t;p_s)}a_0^{(q_i,q_j,K;q_t)}(\alpha^{(q_i,q_j)}(u)-1)(-q_0) + R_s(u=0). \tag{5.33}
$$

Finally, the box coefficient is given by

$$C[Q_i, Q_j]_{k=3} = \frac{(K^2)^{2+n}}{2} \left(\frac{\prod_{j=1}^{n+3} \left\langle P_{(Q_j,Q_i);1} | \widetilde{\widetilde{R}}_j(u) | P_{(Q_j,Q_i);2} \right]}{\left\langle P_{(Q_j,Q_i);1} | K | P_{(Q_j,Q_i);2} \right]^{n+2} \left\langle P_{(Q_j,Q_i);1} | \widetilde{Q}_t(u) | P_{(Q_j,Q_i);2} \right]} \right.$$

$$- \prod_{s=1}^{n+3} \beta_s^{(q_i,q_j,q_t;p_s)} \frac{\left\langle P_{(Q_j,Q_i);1} | K | P_{(Q_j,Q_i);2} \right]}{\left\langle P_{(Q_j,Q_i);1} | \widetilde{Q}_t(u) | P_{(Q_j,Q_i);2} \right]}$$

$$\left. + \{ P_{(Q_j,Q_i);1} \leftrightarrow P_{(Q_j,Q_i);2} \} \right). \tag{5.34}$$

As an alternative to the expansion (5.26) of p_s in the basis q_i, q_j, q_t, we consider another expansion:

$$P_s = \sum_{\alpha=K,K_i,K_j,K_t} a_\alpha^{(K,K_i,K_j,K_t;P_s)} K_\alpha. \tag{5.35}$$

By projecting equation (5.35) onto the vectorspace orthogonal to K, and comparing with (5.26), we see that

$$a_w^{(K,K_i,K_j,K_t;P_s)} = a_w^{(q_i,q_j,q_t;p_s)}, \quad w = i, j, t. \tag{5.36}$$

The advantage of the expansion (5.35) in four vectors is that we can solve for the coefficients explicitly, as in (2.26), and find

$$a_t^{(q_i,q_j,q_t;p_s)} = a_t^{(K,K_i,K_j,K_t;P_s)} = \frac{\epsilon(K_i,K_j,K,P_s)}{\epsilon(K_i,K_j,K,K_t)}. \tag{5.37}$$

Thus, using (5.28), we have

$$\beta_s^{(q_i,q_j,q_t;p_s)} = -\frac{K_i^2 \epsilon(P_s,K_j,K,K_t) + K_j^2 \epsilon(K_i,P_s,K,K_t)}{K^2 \epsilon(K_i,K_j,K,K_t)}$$

$$+ \frac{K^2 \epsilon(K_i,K_j,P_s,K_t) + K_t^2 \epsilon(K_i,K_j,K,P_s)}{K^2 \epsilon(K_i,K_j,K,K_t)}.$$

With the formulas (5.37) and (5.7) for the expansion coefficients written in terms of input vectors, we can simplify the following coefficient in the definition (5.32) of $\widetilde{\widetilde{R}}_s(u)$:

$$a_t^{(q_i,q_j,q_t;p_s)} a_0^{(q_i,q_j,K;q_t)} = -\frac{\epsilon(K_i,K_j,K,P_s)}{\epsilon(K_t,K_i,K_j,K)} \frac{\epsilon(K_t,K_i,K_j,K)}{K^2(q_0^{(q_i,q_j,K)})^2}$$

$$= \frac{\epsilon(P_s,K_i,K_j,K)}{K^2(q_0^{(q_i,q_j,K)})^2} = a_0^{(q_i,q_j,K;p_s)}.$$

We conclude that

$$\widetilde{\widetilde{R}}_s(u) = \widetilde{R}_s(u), \tag{5.38}$$

where the definition of $\widetilde{R}_s(u)$ is taken from (5.24).

5.2.1 Summary of $k = 3$

The pentagon coefficient is given by

$$C[Q_i, Q_j, Q_t] = (K^2)^{3+n} \prod_{s=1}^{n+3} \beta_s^{(q_i, q_j, q_t; p_s)}. \tag{5.39}$$

There are three boxes associated with the triplet of vectors Q_i, Q_j, Q_t. We give the formula for the box involving Q_i and Q_j; the other two may be obtained by exchanging indices.

$$C[Q_i, Q_j]_{k=3} = \frac{(K^2)^{2+n}}{2} \left(\frac{\prod_{r=1}^{n+3} \left\langle P_{(Q_j, Q_i);1} | \widetilde{R}_r(u) | P_{(Q_j, Q_i);2} \right]}{\left\langle P_{(Q_j, Q_i);1} | K | P_{(Q_j, Q_i);2} \right]^{n+2} \left\langle P_{(Q_j, Q_i);1} | \widetilde{Q}_t(u) | P_{(Q_j, Q_i);2} \right]} \right.$$
$$- \prod_{s=1}^{n+3} \beta_s^{(q_i, q_j, q_t; p_s)} \frac{\left\langle P_{(Q_j, Q_i);1} | K | P_{(Q_j, Q_i);2} \right]}{\left\langle P_{(Q_j, Q_i);1} | \widetilde{Q}_t(u) | P_{(Q_j, Q_i);2} \right]}$$
$$\left. + \{ P_{(Q_j, Q_i);1} \leftrightarrow P_{(Q_j, Q_i);2} \} \right), \tag{5.40}$$

where we have made the following definitions:

$$\widetilde{R}_r(u) = \frac{p_r \cdot q_0^{(q_i, q_j, K)}}{(q_0^{(q_i, q_j, K)})^2} (\alpha^{(q_i, q_j)}(u) - 1)(-q_0^{(q_i, q_j, K)}) + R_r(u = 0) \tag{5.41}$$

$$\widetilde{Q}_t(u) = \frac{q_t \cdot q_0^{(q_i, q_j, K)}}{(q_0^{(q_i, q_j, K)})^2} (\alpha^{(q_i, q_j)}(u) - 1)(-q_0^{(q_i, q_j, K)}) + Q_t(u = 0), \tag{5.42}$$

and

$$\beta_s^{(q_i, q_j, q_t; p_s)} = -\frac{K_i^2 \epsilon(P_s, K_j, K, K_t) + K_j^2 \epsilon(K_i, P_s, K, K_t)}{K^2 \epsilon(K_i, K_j, K, K_t)}$$
$$+ \frac{K^2 \epsilon(K_i, K_j, P_s, K_t) + K_t^2 \epsilon(K_i, K_j, K, P_s)}{K^2 \epsilon(K_i, K_j, K, K_t)}. \tag{5.43}$$

5.3 The case $k \geq 4$

If there at least four vectors K_i, then we can use four of them as a basis to expand the momentum vector K:

$$K = \sum_{i=1}^{4} a_i^{(1,2,3,4)} K_i. \tag{5.44}$$

Using the expression (2.16) for $Q_i(u)$, we find

$$\sum_{i=1}^{4} a_i^{(1,2,3,4)} Q_i(u) = \frac{\sum_{i=1}^{4} a_i^{(1,2,3,4)} K_i^2 - K^2}{K^2} K.$$

Use (2.22) to define the two null momenta $P_i(u) = Q_2(u) + x_i Q_1(u)$. Then, we have

$$
\frac{a_4^{(1,2,3,4)}}{\langle P_1(u)|Q_3(u)|P_2(u)]} + \frac{a_3^{(1,2,3,4)}}{\langle P_1(u)|Q_4(u)|P_2(u)]}
$$

$$
= \frac{\left\langle P_1(u)|a_4^{(1,2,3,4)}Q_4(u) + a_3^{(1,2,3,4)}Q_3(u)|P_2(u)\right]}{\langle P_1(u)|Q_3(u)|P_2(u)]\,\langle P_1(u)|Q_4(u)|P_2(u)]}
$$

$$
= \frac{\left\langle P_1(u)|\sum_{i=1}^4 a_i^{(1,2,3,4)}Q_i(u)|P_2(u)\right]}{\langle P_1(u)|Q_3(u)|P_2(u)]\,\langle P_1(u)|Q_4(u)|P_2(u)]}
$$

$$
= \frac{\sum_{i=1}^4 a_i^{(1,2,3,4)}K_i^2 - K^2}{K^2}\frac{\langle P_1(u)|K|P_2(u)]}{\langle P_1(u)|Q_3(u)|P_2(u)]\,\langle P_1(u)|Q_4(u)|P_2(u)]}.
$$

Therefore, we can derive the following identity:

$$
\frac{1}{\langle P_1(u)|Q_3(u)|P_2(u)]\,\langle P_1(u)|Q_4(u)|P_2(u)]} = \tag{5.45}
$$

$$
\frac{K^2}{\sum_{i=1}^4 a_i^{(1,2,3,4)}K_i^2 - K^2}\frac{1}{\langle P_1(u)|K|P_2(u)]}\left(\frac{a_4^{(1,2,3,4)}}{\langle P_1(u)|Q_3(u)|P_2(u)]} + \frac{a_3^{(1,2,3,4)}}{\langle P_1(u)|Q_4(u)|P_2(u)]}\right).
$$

Generalizing to our case with $k \geq 4$, we have

$$
\frac{1}{\prod_{t=1,t\neq i,j}^k \langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]} = \tag{5.46}
$$

$$
\sum_{t=1,t\neq i,j}^k \frac{1}{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]^{k-3}\,\langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]}
$$

$$
\times \prod_{s=1,s\neq i,j,t}^k \left(\frac{a_s^{(i,j,t,s)}K^2}{\sum_{\alpha=i,j,s,t}a_\alpha^{(i,j,t,s)}K_\alpha^2 - K^2}\right).
$$

Thus, we can write

$$
\frac{\prod_{r=1}^{k+n}\langle P_{ji,1}(u)|R_r(u)|P_{ji,2}(u)]}{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]^{n+2}\prod_{t=1,t\neq i,j}^k \langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]} = \tag{5.47}
$$

$$
\sum_{t=1,t\neq i,j}^k \prod_{s=1,s\neq i,j,t}^k \left(\frac{a_s^{(i,j,t,s)}K^2}{\sum_{\alpha=i,j,s,t}a_\alpha^{(i,j,t,s)}K_\alpha^2 - K^2}\right)
$$

$$
\times \frac{\prod_{r=1}^{k+n}\langle P_{ji,1}(u)|R_r(u)|P_{ji,2}(u)]}{\langle P_{ji,1}(u)|K|P_{ji,2}(u)]^{n+k-1}\,\langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]}.
$$

By this formula, we reduce the case with a given n, and $k \geq 4$, to the case with $k_{\text{eff}} = 3$, and $n_{\text{eff}} = n + k - 3$. Using the results of the cases $k = 2$ and $k = 3$, we see explicitly that indeed the coefficients of boxes are polynomials in u.

The coefficients in (5.47) can be given more explicitly using (2.27). We denote the quantity in parentheses by $1/\gamma_s^{(K_i,K_j;K_s,K_t)}$, and

$$
\gamma_s^{(K_i,K_j;K_s,K_t)} \equiv \frac{\sum_{\alpha=i,j,s,t}a_\alpha^{(i,j,t,s)}K_\alpha^2 - K^2}{a_s^{(i,j,t,s)}K^2} \tag{5.48}
$$

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$$= \frac{K_i^2 \epsilon(K, K_j, K_s, K_t) + K_j^2 \epsilon(K_i, K, K_s, K_t) + K_s^2 \epsilon(K_i, K_j, K, K_t)}{K^2 \epsilon(K_i, K_j, K, K_t)}$$
$$+ \frac{K_t^2 \epsilon(K_i, K_j, K_s, K) - K^2 \epsilon(K_i, K_j, K_s, K_t)}{K^2 \epsilon(K_i, K_j, K, K_t)}.$$

The numerator of (5.48) is symmetric in K_i, K_j, K_s, K_t; the denominator singles out K_s, which is why we use the subscript s.

5.3.1 The total box coefficient

We have just shown that when $k \geq 4$, we can use (5.47) to reduce to terms with $k = 3$, read out box coefficients for each of these terms, and eventually add them all up. This approach was useful to prove the polynomial property. For computing amplitudes, we would like to carry out the summation once and for all.

We have used (5.45) and (5.46) to derive (5.47). In each term on the right-hand side of (5.47), there is one pentagon coefficient and one box coefficient. The pentagon coefficients are uniquely associated to different pentagons, with the various Q_t's along with Q_i and Q_j, but the box coefficients all contribute to the same box, with only Q_i and Q_j, so we must add them up.

Upon inspecting the final expression (5.40) for box coefficients in the case $k = 3$, we see that our task is to check that equation (5.45) still holds if we replace $Q_t(u)$ by $\widetilde{Q}_t(u)$ and $P_i(u)$ by $P_i \equiv P_i(u = 0)$. Let us try to copy the derivation.

$$\frac{a_4^{(1,2,3,4)}}{\left\langle P_1 | \widetilde{Q}_3(u) | P_2 \right]} + \frac{a_3^{(1,2,3,4)}}{\left\langle P_1 | \widetilde{Q}_4(u) | P_2 \right]} = \frac{\left\langle P_1 | a_4^{(1,2,3,4)} \widetilde{Q}_4(u) + a_3^{(1,2,3,4)} \widetilde{Q}_3(u) | P_2 \right]}{\left\langle P_1 | \widetilde{Q}_3(u) | P_2 \right] \left\langle P_1 | \widetilde{Q}_4(u) | P_2 \right]}$$
$$= \frac{\left\langle P_1 | \sum_{i=3}^4 a_i^{(1,2,3,4)} Q_i(u=0) + (\alpha^{(q_i,q_j)}(u) - 1)(-q_0) \sum_{i=3}^4 a_i^{(1,2,3,4)} \frac{q_i \cdot q_0}{q_0^2} | P_2 \right]}{\left\langle P_1 | \widetilde{Q}_3(u) | P_2 \right] \left\langle P_1 | \widetilde{Q}_4(u) | P_2 \right]}. \quad (5.49)$$

Then second term in the numerator of (5.49) is zero because $q_i \cdot q_0 = q_j \cdot q_0 = K \cdot q_0 = 0$. Further, we can extend the sum in the numerator of the first term to include $i = 1, 2$, since these terms are individually zero when contracted between spinors for P_1 and P_2.

Because
$$\sum_{i=1}^4 a_i^{(1,2,3,4)} Q_i(u = 0) = \sum_{i=1}^4 a_i^{(1,2,3,4)} \alpha_i K,$$

we have
$$\frac{a_4^{(1,2,3,4)}}{\left\langle P_1 | \widetilde{Q}_3(u) | P_2 \right]} + \frac{a_3^{(1,2,3,4)}}{\left\langle P_1 | \widetilde{Q}_4(u) | P_2 \right]} = \frac{\left\langle P_1 | \sum_{i=1}^4 a_i^{(1,2,3,4)} \alpha_i K | P_2 \right]}{\left\langle P_1 | \widetilde{Q}_3(u) | P_2 \right] \left\langle P_1 | \widetilde{Q}_4(u) | P_2 \right]}.$$

It is now clear that (5.45) and (5.46) will still hold, if we replace $P_{ji}(u) \to P_{ji}(u = 0)$ and $Q_t(u) \to \widetilde{Q}_t(u)$.

Now we perform the summation, using (5.40). There are two terms. The first terms are collected to give

$$\frac{\prod_{r=1}^{k+n} \left\langle P_{ji,1}(u=0)|\widetilde{R}_r(u)|P_{ji,2}(u=0)\right]}{\left\langle P_{ji,1}(u=0)|K|P_{ji,2}(u=0)\right]^{n+2} \prod_{t=1,t\neq i,j}^{k} \left\langle P_{ji,1}(u=0)|\widetilde{Q}_t(u)|P_{ji,2}(u=0)\right]}. \tag{5.50}$$

The total from the second term from (5.40) cannot be simplified further, since each $\beta_s^{(q_i,q_j,q_t;p_s)}$ depends on both P_s and K_t.

5.3.2 Results for $k \geq 4$

The box coefficients are given by

$$C[Q_i, Q_j]_{k\geq 4} = \frac{(K^2)^{2+n}}{2} \left\{ \frac{\prod_{r=1}^{k+n} \left\langle P_{(Q_j,Q_i);1}|\widetilde{R}_r(u)|P_{(Q_j,Q_i);2}\right]}{\left\langle P_{(Q_j,Q_i);1}|K|P_{(Q_j,Q_i);2}\right]^{n+2} \prod_{t=1,t\neq i,j}^{k} \left\langle P_{(Q_j,Q_i);1}|\widetilde{Q}_t(u)|P_{(Q_j,Q_i);2}\right]} \right.$$
$$- \sum_{t=1,t\neq i,j}^{k} \frac{\prod_{s=1}^{n+k} \beta_s^{(q_i,q_j,q_t;p_s)}}{\prod_{w=1,w\neq i,j,t}^{k} \gamma_w^{(K_i,K_j;K_w,K_t)}} \frac{\left\langle P_{(Q_j,Q_i);1}|K|P_{(Q_j,Q_i);2}\right]}{\left\langle P_{(Q_j,Q_i);1}|\widetilde{Q}_t(u)|P_{(Q_j,Q_i);2}\right]} \right\}$$
$$+ \{P_{(Q_j,Q_i);1} \leftrightarrow P_{(Q_j,Q_i);2}\}, \tag{5.51}$$

where $\widetilde{R}_r(u), \widetilde{Q}_t(u), \beta_s^{(q_i,q_j,q_t;p_s)}, \gamma_w^{(K_i,K_j;K_w,K_t)}$ are defined in (5.41), (5.42), (5.43) and (5.48), respectively. All u-dependence is inside $\widetilde{R}(u)$ and $\widetilde{Q}(u)$. This form makes it easier to take the derivative in (2.20).

Pentagon coefficients are given by

$$C[Q_i, Q_j, Q_t] = (K^2)^{3+n} \frac{\prod_{s=1}^{n+k} \beta_s^{(q_i,q_j,q_t;p_s)}}{\prod_{w=1,w\neq i,j,t}^{k} \gamma_w^{(K_i,K_j;K_w,K_t)}}. \tag{5.52}$$

5.4 The degree of the polynomial

In the cases $k = 2$ and $k = 3$, we have seen explicitly that the maximum degree of the polynomial is $[(n+2)/2]$. For $k \geq 4$, the logic discussed after (5.47) implies only that the degree is no greater than $[(n+k-1)/2]$.

However, we can make a stronger claim by performing a different reduction. In the previous subsection, we chose a reduction with a symmetric treatment of the factors $(-2\widetilde{\ell} \cdot P_i)$ in the numerator of (2.6). Alternatively, we could choose not to respect this symmetry in reducing the cases with $k \geq 3$. For example, we can expand P_s in terms of K_i, K_j, K_t, K and use

$$\langle P_{ji,1}(u)|R_s(u)|P_{ji,2}(u)] = a_t^{(q_i,q_j,q_t;p_1)} \langle P_{ji,1}(u)|Q_t(u)|P_{ji,2}(u)]$$
$$+ \beta_s^{(q_i,q_j,q_t;p_s)} \langle P_{ji,1}(u)|K|P_{ji,2}(u)]. \tag{5.53}$$

This reduction translates to the following relation:

$$\text{Box}[m, k, n] \rightarrow \text{Box}[m-1, k-1, n] + \text{Box}[m-1, k, n-1]. \tag{5.54}$$

Upon iteration, we arrive at $k = 2$ for a fixed n. Then, the degree of the polynomial is $[(m-k+2)/2] = [(n+2)/2]$, which is what we wanted to show. (It is clear that the second term in the above reduction will not have a higher degree than the first term.)

6. Gluon example: $A(1^+, 2^+, 3^+, 4^+, 5^+)$

We now present an application to the five-gluon one-loop amplitude in Yang-Mills theory, which was first presented to all orders in ϵ in [32]. By supersymmetry arguments, the computation is equivalent to one with a scalar field circulating in the loop.

This configuration is totally symmetric, so we need only consider any single, representative cut, say C_{12}. The others can be obtained by permuting labels. The cut integrand within (2.6) is the product of two tree amplitudes given in [34], with a factor of 2 for the two internal helicity choices:

$$
\begin{aligned}
I_{12} &= 2A_L(-\ell_2, 1^+, 2^+, -\ell_1)A_R(\ell_1, 3^+, 4^+, 5^+, \ell_2) \\
&= 2\frac{\mu^2[1\,2]}{\langle 1\,2\rangle((\ell_1 - k_2)^2 - \mu^2)}\frac{-\mu^2[5|k_{34}\ell_1|3]}{\langle 3\,4\rangle\langle 4\,5\rangle((\ell_1 + k_3)^2 - \mu^2)((\ell_2 + k_5)^2 - \mu^2)} \\
&= -2\frac{(\mu^2)^2[1\,2]}{\langle 1\,2\rangle\langle 3\,4\rangle\langle 4\,5\rangle}\frac{[5|k_{34}\widetilde{\ell}|3]}{((\widetilde{\ell} - k_2)^2 - \mu^2)((\widetilde{\ell} + k_3)^2 - \mu^2)((\widetilde{\ell} + k_{34})^2 - \mu^2)} \\
&= -2\frac{(\mu^2)^2[1\,2]}{\langle 1\,2\rangle\langle 3\,4\rangle\langle 4\,5\rangle}\frac{(-2\widetilde{\ell}\cdot P_1)}{((\widetilde{\ell} - K_1)^2 - \mu^2)((\widetilde{\ell} - K_2)^2 - \mu^2)((\widetilde{\ell} - K_3)^2 - \mu^2)}.
\end{aligned}
$$

where we have defined

$$
\widetilde{\ell} = \ell_1 = k_{12} - \ell_2, \tag{6.1}
$$

and also that

$$
K = k_{12}, \quad K_1 = k_2, \quad K_2 = -k_3, \quad K_3 = -k_{34}, \quad P_1 = [5\,3]k_3 + [5\,4]\lambda_4\tilde{\lambda}_3.
$$

According to our definitions in (2.6) and (2.10), we have

$$
k = 3, \quad m = 1, \quad n = -2. \tag{6.2}
$$

Since triangles appear only when $n \geq -1$ and bubbles appear only when $n \geq 0$, we are left with only pentagon and box terms in this case. Because $m = 1$, the degree of the polynomial in u is 0. Thus, we can set $u = 0$ in our formula from the beginning.

From our formula (5.39), we find that the pentagon coefficient is

$$
C_{\text{pen}} = -\frac{2(\mu^2)^2[1\,2]s_{12}}{\langle 1\,2\rangle\langle 3\,4\rangle\langle 4\,5\rangle}\beta_1^{(q_1, q_2, q_3; p_1)}. \tag{6.3}
$$

This coefficient is proportional to $(\mu^2)^2$. The integral $I_5^D[(\mu^2)^2]$ is $\mathcal{O}(\epsilon)$, which is what we expect of pentagons.

There are three boxes involved in this cut. Using the formula (5.40), we find that the box coefficient associated with Q_1, Q_2 is

$$
\begin{aligned}
C[Q_1, Q_2] = \frac{-(\mu^2)^2[1\,2]}{\langle 1\,2\rangle\langle 3\,4\rangle\langle 4\,5\rangle}\Bigg\{ &\frac{\langle P_{(Q_2,Q_1);1}|R_1|P_{(Q_2,Q_1);2}]}{\langle P_{(Q_2,Q_1);1}|Q_3|P_{(Q_2,Q_1);2}]} \\
&- \beta_1^{(q_1, q_2, q_3; p_1)}\frac{\langle P_{(Q_2,Q_1);1}|K|P_{(Q_2,Q_1);2}]}{\langle P_{(Q_2,Q_1);1}|Q_3|P_{(Q_2,Q_1);2}]}\Bigg\} + \{P_{(Q_2,Q_1);1} \leftrightarrow P_{(Q_2,Q_1);2}\}
\end{aligned}
$$

$$= \frac{-2(\mu^2)^2[1\ 2]}{\langle 1\ 2\rangle\,\langle 3\ 4\rangle\,\langle 4\ 5\rangle}a_3^{(q_1,q_2,q_3;p_1)}, \tag{6.4}$$

in which we have used (5.27) to simplify the expression.

Similar calculations give

$$C[Q_1,Q_3] = \frac{-2(\mu^2)^2[1\ 2]}{\langle 1\ 2\rangle\,\langle 3\ 4\rangle\,\langle 4\ 5\rangle}a_3^{(q_1,q_3,q_2;p_1)}, \tag{6.5}$$

$$C[Q_2,Q_3] = \frac{-2(\mu^2)^2[1\ 2]}{\langle 1\ 2\rangle\,\langle 3\ 4\rangle\,\langle 4\ 5\rangle}a_3^{(q_2,q_3,q_1;p_1)}. \tag{6.6}$$

Now we check these coefficients against the result in the literature [34, 15], which is (the factor $i/(4\pi)^{2-\epsilon}$ is omitted, and we also changed the result to our convention of the basis definition (2.29))

$$\begin{aligned}
A(1^+,2^+,3^+,4^+,5^+) &= \frac{\epsilon(1-\epsilon)}{\langle 12\rangle\,\langle 23\rangle\,\langle 34\rangle\,\langle 45\rangle\,\langle 51\rangle}\Big(-4i(4-2\epsilon)\epsilon(k_1,k_2,k_3,k_4)I_5^{D+6}[1]+s_{23}s_{34}I_4^{D+4,(1)}[1]\\
&\quad +s_{34}s_{45}I_4^{D+4,(2)}[1]+s_{45}s_{51}I_4^{D+4,(3)}[1]+s_{51}s_{12}I_4^{D+4,(4)}[1]+s_{12}s_{23}I_4^{D+4,(5)}[1]\Big)\\
&= \frac{1}{\langle 1\ 2\rangle\,\langle 2\ 3\rangle\,\langle 3\ 4\rangle\,\langle 4\ 5\rangle\,\langle 5\ 1\rangle}\Big(8i\epsilon(k_1,k_2,k_3,k_4)I_5^{D}[\mu^6]-s_{23}s_{34}I_4^{D,(1)}[\mu^4]\\
&\quad -s_{34}s_{45}I_4^{D,(2)}[\mu^4]-s_{45}s_{51}I_4^{D,(3)}[\mu^4]-s_{51}s_{12}I_4^{D,(4)}[\mu^4]-s_{12}s_{23}I_4^{D,(5)}[\mu^4]\Big). \tag{6.7}
\end{aligned}$$

We have used $I_4^{D}[\mu^4] = -\epsilon(1-\epsilon)I_4^{D+4}[1]$ and $I_5^{D}[\mu^6] = -\epsilon(1-\epsilon)(2-\epsilon)I_5^{D+6}[1]$. In appendix A, we discuss various recursive relations and dimensional shift identities. We now apply the identity (A.9) to get

$$I_5^{D}[\mu^6] = \left(-\frac{1}{\Delta_5}\right)I_5^{D}[\mu^4] + \frac{1}{2}\sum_{i=1}^{5}\left(-\frac{\gamma_{5,i}}{\Delta_5}\right)\,I_4^{D,(i)}[\mu^4]. \tag{6.8}$$

Then we see that we should be able to reproduce the following correspondences. For $C[Q_1,Q_2]$,

$$\begin{aligned}
\frac{2[1\ 2]}{\langle 1\ 2\rangle\,\langle 3\ 4\rangle\,\langle 4\ 5\rangle}a_3^{(q_1,q_2,q_3;p_1)} &= \frac{1}{\langle 1\ 2\rangle\,\langle 2\ 3\rangle\,\langle 3\ 4\rangle\,\langle 4\ 5\rangle\,\langle 5\ 1\rangle}\\
&\quad \times\left(s_{12}s_{23}+4i\epsilon(k_1,k_2,k_3,k_4)\frac{\gamma_{5,5}}{\Delta_5}\right); \tag{6.9}
\end{aligned}$$

for the pentagon,

$$\begin{aligned}
\frac{2[1\ 2]s_{12}}{\langle 1\ 2\rangle\,\langle 3\ 4\rangle\,\langle 4\ 5\rangle}\beta_1^{(q_1,q_2,q_3;p_1)} &= \frac{1}{\langle 1\ 2\rangle\,\langle 2\ 3\rangle\,\langle 3\ 4\rangle\,\langle 4\ 5\rangle\,\langle 5\ 1\rangle}\\
&\quad \times\left(8i\epsilon(k_1,k_2,k_3,k_4)\frac{1}{\Delta_5}\right). \tag{6.10}
\end{aligned}$$

We have checked that these equations (as well as the ones derived from the other two boxes) are consistent with our definitions.

7. Discussion

From the u-dependent formulas for 4-dimensional integral coefficients given in [27], we have now given simpler versions, explicit proofs that they are polynomials, and the formula (2.20) needed for the final evaluation in D dimensions. In this section, we make some remarks comparing our results with two recent papers, [30] and [29].

The authors of [30] discussed the calculation of rational terms. The rational contribution may be split into two parts (eq. (3) of [30]), namely a term depending on $\widetilde{q}^2$ (which is μ^2 in our notation) and the 4-dimensional part. For the former term, the authors of [30] reduce the calculation into effective Feynman diagrams. In our approach, we do not distinguish these two terms; they are treated on the same footing by using dimensionally shifted master integrals. To deal with the 4-dimensional terms independent of $\widetilde{q}^2$, [30] proposed the mass shifted method (eq. (16) of [30]) and following expansion (eqs. (17), (18), (20) of [30]). In our terminology, these are the coefficients of u^a, which we have discussed. The proposal of [30] is to choose different values of $\widetilde{q}^2$, while here we use the derivative. We could also choose to substitute numerical values of u, and then find the coefficient from a linear equation, as detailed recently in [46]. In another recent paper [50], this same numerical approach is implemented in the context of [30].

The authors of [29] treat s_e^2 (which is u in our notation) as an effective dimension. Thus they are able to use a 5-dimensional cut to read off the pentagon coefficient. To get the coefficients, they work in two different dimensions, D_1 and D_2. The paper [29] has thus given a way to deal with the problem of the polarization tensor of a gluon or fermion in arbitrary dimension D. By choosing appropriate loop momenta and solving a linear system of equations, they can separate the coefficients into spurious terms and the terms with various powers of s_e^2. As in our approach, the terms with non-zero powers of s_e^2 will contribute to the coefficients of dimensionally shifted master integrals.

The methods of [29, 30] have been implemented numerically [29, 50 – 52] and have been shown to be stable and efficient.[6] We have not yet attempted a numerical implementation of the procedure given in this paper, and we leave its assessment to future work. Analytically, our algebraic expressions are the most general, since we have not assumed renormalizability, and the power of q in the numerator can be arbitrarily high.

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[6]Note added in revised version: There has recently appeared a numerical implementation of another technique for getting rational parts of one-loop amplitudes [45], based on the generalized-unitarity formalism of [23, 53] combined with an expansion in μ^2.

A. The scalar integrals and dimensional shift identities

The $\mathfrak{D}$-dimensional scalar integral is defined to be

$$I_n^{\mathfrak{D}}[1] \equiv -i(4\pi)^{\mathfrak{D}/2} \int \frac{d^{\mathfrak{D}}p}{(2\pi)^{\mathfrak{D}}} \frac{1}{p^2(p-K_1)^2(p-K_1-K_2)^2\cdots(p+K_n)^2}. \qquad (\text{A.1})$$

We will use $\mathfrak{D}$ to denote the dimensionality, so that we can specifically set

$$D \equiv 4 - 2\epsilon. \qquad (\text{A.2})$$

We also define a very useful symmetric matrix, S, as follows:

$$
\begin{aligned}
S &\equiv -\frac{1}{2}
\begin{pmatrix}
0 & K_1^2 & (K_1+K_2)^2 & \cdots & (K_1+K_2+\cdots K_{n-1})^2 \\
* & 0 & K_2^2 & \cdots & (K_2+K_3+\cdots K_{n-1})^2 \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
* & * & * & 0 & K_{n-1}^2 \\
* & * & * & * & 0
\end{pmatrix} \\
&= -\frac{1}{2}
\begin{pmatrix}
0 & s_1 & s_{12} & \cdots & s_n \\
* & 0 & s_2 & \cdots & s_{n1} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
* & * & * & 0 & s_{n-1} \\
* & * & * & * & 0
\end{pmatrix}.
\end{aligned}
\qquad (\text{A.3})
$$

If there are explicit powers of μ^2 in the numerator, we expand in ϵ as follows,

$$I_n^D[(\mu^2)^k] = \frac{\Gamma(k-\epsilon)}{\Gamma(-\epsilon)} I_n^{D+2k}[1] = -\epsilon \, \Gamma(k) \, I_n^{D+2k}[1] + \mathcal{O}(\epsilon) \qquad (\text{A.4})$$

and deduce that we only need to calculate the coefficient of the $1/\epsilon$ term of $I_n^{D+2k}[1]$, in order to get the rational term. For bubbles and triangles, we need to consider $k \geq 1$; for boxes, we need to consider $k \geq 2$; and for pentagons, we need to consider $k \geq 3$.

We will use two ways to deal with the higher-dimensional scalar integral, mainly following [2].

The first way is by calculating the integral directly, using Feynman parametrization:

$$I_n^{\mathfrak{D}}[1] = (-1)^n \, \Gamma(n - \mathfrak{D}/2) \int_0^1 da_1 \cdots da_n \frac{\delta(1 - \sum_i a_i)}{(a \cdot S \cdot a)^{n-\frac{\mathfrak{D}}{2}}}, \qquad (\text{A.5})$$

where

$$a \cdot S \cdot a = \sum_{i,j=1}^n a_i \, a_j \, S_{ij} .$$

This integral is easy in the cases of bubbles and one-mass or two-mass triangles. However, for three-mass triangles, boxes and pentagons, the integral is complicated.

The second way is by using a recursive relation, which reduces the higher-dimensional scalar integrals to lower-dimensional and lower-point scalar integrals [2]:

$$I_n^{\mathfrak{D}+2}[1] = \frac{1}{(n-1-\mathfrak{D})\,\Delta_n}\left[2\,I_n^{\mathfrak{D}}[1] + \sum_{i=1}^{n}\gamma_{n,i}\,I_{n-1}^{\mathfrak{D},(i)}[1]\right], \tag{A.6}$$

where

$$\gamma_{n,i} = \sum_{j=1}^{n} S_{ij}^{-1}, \qquad \Delta_n = \sum_{i=1}^{n}\gamma_{n,i}. \tag{A.7}$$

If $\mathfrak{D} = D + 2k - 2$, then we have

$$I_n^{D+2k}[1] = \frac{1}{k-\frac{n-3}{2}-\epsilon}\left[\left(-\frac{1}{\Delta_n}\right)I_n^{D+2(k-1)}[1]\right.$$
$$\left. +\frac{1}{2}\sum_{i=1}^{n}\left(-\frac{\gamma_{n,i}}{\Delta_n}\right)I_{n-1}^{D+2(k-1),(i)}[1]\right]. \tag{A.8}$$

Similarly, we can write

$$I_n^D\left[(\mu^2)^k\right] = \frac{k-1-\epsilon}{k-\frac{n-3}{2}-\epsilon}\left[\left(-\frac{1}{\Delta_n}\right)I_n^D\left[(\mu^2)^{k-1}\right]\right.$$
$$\left. +\frac{1}{2}\sum_{i=1}^{n}\left(-\frac{\gamma_{n,i}}{\Delta_n}\right)I_{n-1}^{D,(i)}\left[(\mu^2)^{k-1}\right]\right]. \tag{A.9}$$

The recursive relations are very convenient in dealing with three-mass triangle and higher point cases. For one-mass and two-mass triangles, the matrix S is singular, so these recursive relations are not well defined. However, it is possible to recover the results from massless limits of the three-mass triangle. In practice, then, we can always use these recursive relations, taking a massless limit at the end in special cases (also boxes and pentagons).

In the following, we give compact recursive formulas for bubble, triangle, box and pentagon, for convenient automated evaluation.

A.1 Bubble

For the bubble, the matrix S defined in (A.3) becomes

$$S = -\frac{1}{2}\begin{pmatrix} 0 & K^2 \\ K^2 & 0 \end{pmatrix}, \quad S^{-1} = -2\begin{pmatrix} 0 & \frac{1}{K^2} \\ \frac{1}{K^2} & 0 \end{pmatrix}, \tag{A.10}$$

so

$$\gamma_{2,1} = \gamma_{2,2} = -\frac{2}{K^2}, \quad \Delta_2 = -\frac{4}{K^2}, \tag{A.11}$$

and

$$a \cdot S \cdot a = -a_1 a_2 K^2 . \tag{A.12}$$

Using the recursive relation (A.8), we find

$$I_2^{D+2k}[1] = \frac{1}{k + \frac{1}{2} - \epsilon} \left(-\frac{1}{\Delta_2} \right) I_2^{D+2(k-1)}[1]$$

$$= \frac{1}{(1 + \frac{1}{2})(2 + \frac{1}{2}) \cdots (k + \frac{1}{2})} \left(\frac{K^2}{4} \right)^k I_2^D[1] + \mathcal{O}(\epsilon)$$

$$= \frac{\sqrt{\pi}/2}{\Gamma(k + \frac{3}{2})} \left(\frac{K^2}{4} \right)^k \frac{1}{\epsilon} + \mathcal{O}(\epsilon^0). \tag{A.13}$$

Alternative, we can use the Feynman parametrization to calculate it directly.

$$I_2^{D+2k}[1] = \Gamma(-k + \epsilon) \int_0^1 da_1 da_2 \; \delta(1 - a_1 - a_2) \; (-a_1 a_2 K^2)^{k-\epsilon}$$

$$= \Gamma(-k + \epsilon) \frac{\Gamma(k + 1 - \epsilon)^2}{\Gamma(2k + 2 - 2\epsilon)} (-K^2)^{k-\epsilon}$$

$$= \frac{\Gamma(k + 1)(K^2)^k}{\Gamma(2k + 2)} \frac{1}{\epsilon} + \mathcal{O}(\epsilon^0). \tag{A.14}$$

A.2 Triangle

The matrix S is

$$S = -\frac{1}{2} \begin{pmatrix} 0 & K_1^2 & K_3^2 \\ K_1^2 & 0 & K_2^2 \\ K_3^2 & K_2^2 & 0 \end{pmatrix} = -\frac{1}{2} \begin{pmatrix} 0 & s_1 & s_3 \\ s_1 & 0 & s_2 \\ s_3 & s_2 & 0 \end{pmatrix}. \tag{A.15}$$

Its inverse is

$$S^{-1} = -\frac{1}{s_1 s_2 s_3} \begin{pmatrix} -s_2^2 & s_2 s_3 & s_1 s_2 \\ s_2 s_3 & -s_3^2 & s_3 s_1 \\ s_1 s_2 & s_3 s_1 & -s_1^2 \end{pmatrix}, \tag{A.16}$$

so

$$\gamma_{3,1} = \frac{s_2(s_2 - s_3 - s_1)}{s_3 s_1}, \quad \gamma_{3,2} = \frac{s_3(s_3 - s_1 - s_2)}{s_1 s_2}, \quad \gamma_{3,3} = \frac{s_1(s_1 - s_2 - s_3)}{s_2 s_3},$$

$$\Delta_3 = \frac{s_1^2 + s_2^2 + s_3^2 - 2(s_1 s_2 + s_2 s_3 + s_3 s_1)}{s_1 s_2 s_3}, \tag{A.17}$$

and

$$a \cdot S \cdot a = -(a_1 a_2 K_1^2 + a_2 a_3 K_2^2 + a_3 a_1 K_3^2). \tag{A.18}$$

One-mass and two-mass triangles can be evaluated by Feynman parametrization. If $K_3^2 = 0$, then

$$I_{3;2m}^{D+2k}[1] = -\Gamma(-k + 1 + \epsilon) \int_0^1 da_1 da_2 da_3 \; \delta(1 - a_1 - a_2 - a_3) \; (-a_1 a_2 K_1^2 - a_2 a_3 K_2^2)^{k-1-\epsilon}$$

$$= -\frac{\Gamma(k)}{\Gamma(2k+1)} \frac{(K_1^2)^k - (K_2^2)^k}{K_1^2 - K_2^2} \frac{1}{\epsilon} + \mathcal{O}(\epsilon^0). \tag{A.19}$$

If, in addition, $K_2^2 = 0$, then

$$I_{3;1m}^{D+2k}[1] = -\frac{\Gamma(k)}{\Gamma(2k+1)} (K_1^2)^{k-1} \frac{1}{\epsilon} + \mathcal{O}(\epsilon^0). \tag{A.20}$$

For the three-mass triangle, we use the recursive relation (A.8) repeatedly, and obtain

$$
\begin{aligned}
I_3^{D+2k}[1] &= \frac{1}{k-\epsilon} \left[\left(-\frac{1}{\Delta_3} \right) I_3^{D+2(k-1)}[1] + \frac{1}{2} \sum_{i=1}^{3} \left(-\frac{\gamma_{3,i}}{\Delta_3} \right) I_2^{D+2(k-1),(i)}[1] \right] \\
&= \frac{1}{2} \sum_{\ell=0}^{k-1} \frac{\Gamma(\ell+1)}{\Gamma(k+1)} \left(-\frac{1}{\Delta_3} \right)^{k-\ell} \sum_{i=1}^{3} \gamma_{3,i} \, I_2^{D+2\ell,(i)}[1] + \mathcal{O}(\epsilon^0),
\end{aligned} \tag{A.21}
$$

where we make use of our previously derived bubble result. The first several cases, written explicitly, are

$$I_3^{D+2}[1] = -\frac{1}{2\epsilon} + \mathcal{O}(\epsilon^0)$$

$$I_3^{D+4}[1] = -\frac{1}{24\epsilon}(s_1 + s_2 + s_3) + \mathcal{O}(\epsilon^0)$$

$$I_3^{D+6}[1] = -\frac{1}{360\epsilon}(s_1^2 + s_2^2 + s_3^2 + s_1 s_2 + s_2 s_3 + s_3 s_1) + \mathcal{O}(\epsilon^0)$$

$$I_3^{D+8}[1] = -\frac{1}{6720\epsilon}\left(s_1^3 + s_2^3 + s_3^3 + s_1^2 s_2 + s_1 s_2^2 + s_2^2 s_3 + s_2 s_3^2 + s_3^2 s_1 + s_3 s_1^2 + \frac{4}{3} s_1 s_2 s_3 \right) + \mathcal{O}(\epsilon^0)$$

Note that Δ_3 in (A.21) has cancelled out of the numerator and denominator.

We have verified that the results for one-mass and two-mass triangles are consistent with the massless limit of the three-mass triangle result.

A.3 Box

The matrix S is

$$
\begin{aligned}
S &= -\frac{1}{2} \begin{pmatrix} 0 & K_1^2 & (K_1+K_2)^2 & K_4^2 \\ K_1^2 & 0 & K_2^2 & (K_2+K_3)^2 \\ (K_1+K_2)^2 & K_2^2 & 0 & K_3^2 \\ K_4^2 & (K_2+K_3)^2 & K_3^2 & 0 \end{pmatrix} \\
&= -\frac{1}{2} \begin{pmatrix} 0 & s_1 & s_{12} & s_4 \\ s_1 & 0 & s_2 & s_{23} \\ s_{12} & s_2 & 0 & s_3 \\ s_4 & s_{23} & s_3 & 0 \end{pmatrix}.
\end{aligned} \tag{A.22}
$$

Using the recursive relation (A.8) repeatedly, we find

$$I_4^{D+2k}[1] = \frac{1}{k - \frac{1}{2} - \epsilon} \left[\left(\frac{-1}{\Delta_4} \right) I_4^{D+2(k-1)}[1] + \frac{1}{2} \sum_{i=1}^{4} \left(-\frac{\gamma_{4,i}}{\Delta_4} \right) I_3^{D+2(k-1),(i)}[1] \right]$$

$$= \frac{1}{2} \sum_{\ell=1}^{k-1} \frac{\Gamma(\ell + \frac{1}{2})}{\Gamma(k + \frac{1}{2})} \left(\frac{-1}{\Delta_4}\right)^{k-\ell} \sum_{i=1}^{4} \gamma_{4,i} \; I_3^{D+2\ell,(i)}[1] + \mathcal{O}(\epsilon^0). \tag{A.23}$$

Here we use the identities for triangles. The first few cases, listed explicitly, are

$$I_4^{D+4}[1] = \frac{1}{6\epsilon} + \mathcal{O}(\epsilon^0)$$

$$I_4^{D+6}[1] = \frac{1}{120\epsilon}(s_1 + s_2 + s_3 + s_4 + s_{12} + s_{23}) + \mathcal{O}(\epsilon^0)$$

$$I_4^{D+8}[1] = \frac{1}{2520\epsilon}\left(s_1^2 + s_2^2 + s_3^2 + s_4^2 + s_{12}^2 + s_{23}^2 + s_1 s_2 + s_2 s_3 + s_3 s_4 + s_4 s_1 \right.$$

$$\left. + (s_{12} + s_{23})(s_1 + s_2 + s_3 + s_4) + \frac{1}{2}(s_1 s_3 + s_2 s_4 + s_{12} s_{23})\right) + \mathcal{O}(\epsilon^0)$$

Notice that the factor Δ_4 in (A.23) cancels out.

A.4 Pentagon

The matrix S for the pentagon is

$$S = -\frac{1}{2} \begin{pmatrix} 0 & s_1 & s_{12} & s_{45} & s_5 \\ s_1 & 0 & s_2 & s_{23} & s_{51} \\ s_{12} & s_2 & 0 & s_3 & s_{34} \\ s_{45} & s_{23} & s_3 & 0 & s_4 \\ s_5 & s_{51} & s_{34} & s_4 & 0 \end{pmatrix}. \tag{A.24}$$

Using the recursive relation (A.8) repeatedly, we find

$$I_5^{D+2k}[1] = \frac{1}{k-1-\epsilon} \left[\left(\frac{-1}{\Delta_5}\right) I_5^{D+2(k-1)}[1] + \frac{1}{2} \sum_{i=1}^{5} \left(\frac{-\gamma_{5,i}}{\Delta_5}\right) I_{5-1}^{D+2(k-1),(i)}[1] \right]$$

$$= \frac{1}{2} \sum_{\ell=2}^{k-1} \frac{\Gamma(\ell)}{\Gamma(k)} \left(\frac{-1}{\Delta_5}\right)^{k-\ell} \sum_{i=1}^{5} \gamma_{5,i} \; I_4^{D+2\ell,(i)}[1] + \mathcal{O}(\epsilon^0). \tag{A.25}$$

The first few identities we derive this way are

$$I_5^{D+6}[1] = -\frac{1}{24\epsilon} + \mathcal{O}(\epsilon^0)$$

$$I_5^{D+8}[1] = -\frac{1}{720\epsilon}(s_1 + s_2 + s_3 + s_4 + s_5 + s_{12} + s_{23} + s_{34} + s_{45} + s_{51}) + \mathcal{O}(\epsilon^0)$$

$$I_5^{D+10}[1] = -\frac{1}{20160\epsilon}\left(s_1^2 + s_{12}^2 + s_1 s_2 + s_{12} s_{34} + s_1(s_{12} + s_{23} + s_{45} + s_{51}) \right.$$

$$\left. + \frac{1}{2}(s_1 s_3 + s_1 s_{34} + s_{12} s_{23}) + \text{four cyclic}\right) + \mathcal{O}(\epsilon^0)$$

The factor Δ_5 in (A.25) cancels out.

B. Explicit expressions for triangle coefficients

In this appendix we collect some simplified expressions for triangle coefficients with $n \leq 2$. This is sufficient in renormalizable theories. For general n, we can always go back to the general formula (3.11).

For $n = -1$:

$$C[Q_s, K]_{n=-1} = \frac{1}{2} \left(\frac{\prod_{j=1}^{k-1} \langle P_{(q_s,K);1} | P_j | P_{(q_s,K);2}]}{\prod_{t=1, t \neq s}^{k} \langle P_{(q_s,K);1} | K_t | P_{(q_s,K);2}]} + \{P_{(q_s,K);1} \leftrightarrow P_{(q_s,K);2}\} \right). \text{(B.1)}$$

For $n = 0$:

$$C[Q_s, K]_{n=0} = -\frac{\alpha_s(K^2)^2}{\Delta(q_s, K)} \left\{ \frac{\prod_{j=1}^{k} \langle P_{(q_s,K);1} | P_j | P_{(q_s,K);2}]}{\prod_{t=1, t \neq s}^{k} \langle P_{(q_s,K);1} | K_t | P_{(q_s,K);2}]} \left(-\sum_{j=1}^{k} \frac{2\widetilde{p}_j \cdot q_s}{\langle P_{(q_s,K);1} | P_j | P_{(q_s,K);2}]} \right. \right.$$
$$\left. \left. + \sum_{t=1, t \neq s}^{k} \frac{2\widetilde{q}_t \cdot q_s}{\langle P_{(q_s,K);1} | K_t | P_{(q_s,K);2}]} \right) + \{P_{(q_s,K);1} \leftrightarrow P_{(q_s,K);2}\} \right\}. \text{(B.2)}$$

For $n = 1$, we have linear u-dependence:

$$C[Q_s, K]_{n=1} = \frac{(K^2)^4 \alpha_s^2}{\Delta(q_s, K)^2} \left(\frac{\prod_{j=1}^{k+1} \langle P_{(q_s,K);1} | P_j | P_{(q_s,K);2}]}{\prod_{t=1, t \neq s}^{k} \langle P_{(q_s,K);1} | K_t | P_{(q_s,K);2}]} (\mathcal{F}_1^2 + \mathcal{F}_2) \right.$$
$$\left. + \{P_{(q_s,K);1} \leftrightarrow P_{(q_s,K);2}\} \right), \tag{B.3}$$

where

$$\mathcal{F}_1 = \left(-\sum_{j=1}^{k+1} \frac{(2\widetilde{p}_j \cdot q_s)}{\langle P_{(q_s,K);1} | P_j | P_{(q_s,K);2}]} + \sum_{t=1, t \neq s} \frac{(2\widetilde{q}_t \cdot q_s)}{\langle P_{(q_s,K);1} | K_t | P_{(q_s,K);2}]} \right) \tag{B.4}$$

$$\mathcal{F}_2 = -\sum_{j=1}^{k+1} \left(\frac{(2\widetilde{p}_j \cdot q_s)}{\langle P_{(q_s,K);1} | P_j | P_{(q_s,K);2}]} \right)^2 + \sum_{j=1}^{k+1} \frac{1}{2} \left((1-u) \frac{q_s^2}{\alpha_s^2 K^2} + 1 \right) \frac{\langle P_{(q_s,K);2} | P_j | P_{(q_s,K);1}]}{\langle P_{(q_s,K);1} | P_j | P_{(q_s,K);2}]}$$
$$+ \sum_{t=1, t \neq s}^{k} \left(\frac{(2\widetilde{q}_t \cdot q_s)}{\langle P_{(q_s,K);1} | K_t | P_{(q_s,K);2}]} \right)^2 - \sum_{t=1, t \neq s}^{k} \frac{1}{2} \left((1-u) \frac{q_s^2}{\alpha_s^2 K^2} + 1 \right) \frac{\langle P_{(q_s,K);2} | K_t | P_{(q_s,K);1}]}{\langle P_{(q_s,K);1} | K_t | P_{(q_s,K);2}]}$$
$$\tag{B.5}$$

Finally, for $n = 2$, we again have linear u-dependence:

$$C[Q_s, K]_{n=2} = -\frac{2}{3} \frac{(K^2)^6}{\Delta(q_s, K)^3} \left(\frac{\prod_{j=1}^{k+2} \langle P_{(q_s,K);1} | P_j | P_{(q_s,K);2}]}{\prod_{t=1, t \neq s}^{k} \langle P_{(q_s,K);1} | K_t | P_{(q_s,K);2}]} (\mathcal{F}_1^3 + 3\mathcal{F}_1 \mathcal{F}_2 + \mathcal{F}_3) \right.$$
$$\left. + \{P_{(q_s,K);1} \leftrightarrow P_{(q_s,K);2}\} \right),$$

where

$$\mathcal{F}_1 = \left(-\sum_{j=1}^{k+2} \frac{(2\widetilde{p}_j \cdot q_s)}{\langle P_{(q_s,K);1}|P_j|P_{(q_s,K);2}]} + \sum_{t=1,t\neq s}^{k} \frac{(2\widetilde{q}_t \cdot q_s)}{\langle P_{(q_s,K);1}|K_t|P_{(q_s,K);2}]} \right), \tag{B.6}$$

$$\mathcal{F}_2 = -\sum_{j=1}^{k+2} \left(\frac{(2\widetilde{p}_j \cdot q_s)}{\langle P_{(q_s,K);1}|P_j|P_{(q_s,K);2}]} \right)^2 + \sum_{j=1}^{k+2} \frac{1}{2} \left((1-u)\frac{q_s^2}{\alpha_s^2 K^2} + 1 \right) \frac{\langle P_{(q_s,K);2}|P_j|P_{(q_s,K);1}]}{\langle P_{(q_s,K);1}|P_j|P_{(q_s,K);2}\rangle}$$

$$+ \sum_{t=1,t\neq s}^{k} \left(\frac{(2\widetilde{q}_t \cdot q_s)}{\langle P_{(q_s,K);1}|K_t|P_{(q_s,K);2}]} \right)^2$$

$$- \sum_{t=1,t\neq s}^{k} \frac{1}{2} \left((1-u)\frac{q_s^2}{\alpha_s^2 K^2} + 1 \right) \frac{\langle P_{(q_s,K);2}|K_t|P_{(q_s,K);1}]}{\langle P_{(q_s,K);1}|K_t|P_{(q_s,K);2}]}, \tag{B.7}$$

and

$$\mathcal{F}_3 = \left\{ -\sum_{j=1}^{k+2} 2 \left(\frac{(2\widetilde{p}_j \cdot q_s)}{\langle P_{(q_s,K);1}|P_j|P_{(q_s,K);2}]} \right)^3 + \sum_{t=1,t\neq s}^{k} 2 \left(\frac{(2\widetilde{q}_t \cdot q_s)}{\langle P_{(q_s,K);1}|K_t|P_{(q_s,K);2}]} \right)^3 \right.$$

$$+ \sum_{j=1}^{k+2} \frac{3}{2} \left((1-u)\frac{q_s^2}{\alpha_s^2 K^2} + 1 \right) \frac{\langle P_{(q_s,K);2}|P_j|P_{(q_s,K);1}] (2\widetilde{p}_j \cdot q_s)}{\langle P_{(q_s,K);1}|P_j|P_{(q_s,K);2}]^2}$$

$$\left. - \sum_{t=1,t\neq s}^{k} \frac{3}{2} \left((1-u)\frac{q_s^2}{\alpha_s^2 K^2} + 1 \right) \frac{\langle P_{(q_s,K);2}|K_t|P_{(q_s,K);1}] (2\widetilde{q}_t \cdot q_s)}{\langle P_{(q_s,K);1}|Q_t|P_{(q_s,K);2}]^2} \right\}. \tag{B.8}$$

C. Proof of the polynomial property of bubble coefficients

Here we present a proof that the bubble coefficients are polynomials in u. For this proof, we make use of their derivation from spinor integrals [27], along with certain results of Ossola, Papadopoulos and Pittau (OPP) [17] to analyze the integrand.

Given the cut integral (2.6), bubble coefficients are given by the sum of residues at the poles of the following function (see appendix B of [27]).[7]

$$\sum_{q=0}^{n} \frac{1}{q!} \frac{d^q B_{n,n-q}(s)}{ds^q} \bigg|_{s=0}, \tag{C.1}$$

where the residues of $B_{n,t}(s)$ are taken before the derivative in s, and the function $B_{n,t}(s)$ is defined to be

$$B_{n,t}(s) \equiv \frac{\langle \ell|\eta|\ell]^t}{\langle \ell|K|\ell]^{2+t}} \frac{\prod_{j=1}^{n+k} \langle \ell|R_j(K-s\eta)|\ell\rangle}{\langle \ell|\eta K|\ell\rangle^n \prod_{p=1}^{k} \langle \ell|Q_p(K-s\eta)|\ell\rangle} . \tag{C.2}$$

---

[7]In this discussion, we drop prefactors independent of loop momentum, as well as the possible prefactor $c(\mu^2)$. Also, we have used $(K-s\eta)$ instead of $(K+s\eta)$ in (4.1). This change is compensated by dropping the factor $(-1)^q$.

Bubble contributions in the cut integral (2.6) appear only if $n \geq 0$. In the case that $n = 0$, it is easy to see that we can simply set $s = 0$. Then, $\langle \ell | Q_p K | \ell \rangle = -\sqrt{1-u}\, \langle \ell | q_p K | \ell \rangle$, and $\langle \ell | R_j K | \ell \rangle = -\sqrt{1-u}\, \langle \ell | p_j K | \ell \rangle$, so the u-dependent factor $\sqrt{1-u}$ cancels out of the numerator and denominator.

Our strategy is to decompose $B_{n,t}(s)$ as a power series in $\sqrt{1-u}$. Then we will show that the terms with odd powers of $\sqrt{1-u}$ correspond to spurious terms discussed by OPP. Therefore, they will vanish upon integration, and we will be left with only even powers of $\sqrt{1-u}$, i.e. a polynomial in u.

Note that when we apply the OPP results, we are dealing only with the four-dimensional momentum q (or $\widetilde{\ell}$ in our notation), so we do not need any parts of the OPP formulas involving the extra-dimensional variable $\widetilde{q}^2$. Also, in our case we have $p_0 = 0$, and the mass m_i^2 should be shifted to $m_i^2 + \mu^2$.

We emphasize one point which is crucial for our proof: *the one-to-one correspondence between the form (2.6) and the form (C.1) in $D = 4$ dimensions.* That is, every factor $-2\widetilde{\ell} \cdot P_j$ in (2.6) corresponds to a factor $\left\langle \ell | R_j^{(4D)} (K - s\eta) | \ell \right\rangle$ in (C.1), and vice versa. It is very important that since now we are in pure 4D, the $R_j^{(4D)} = -P_j$, i.e., $R_j^{(4D)} = R_j(u = 0)$. Similarly for the factor $\langle \ell | Q_p(u = 0)(K - s\eta) | \ell \rangle$ in (C.1) and factor $(p - K_j)^2$ in (2.6). In the following proof, we go back and forth freely between these two forms.

C.1 Reducing the number of propagators

The spurious terms of OPP have at most four propagator factors in the denominator. In order to make use of their results, we must begin by reducing our (arbitrary) number of propagators to four or fewer. In our formalism, the corresponding condition on (C.2) is that $k \leq 2$, because we have a unitarity cut.

We perform the reduction in (at most) two steps: first, from $k \geq 4$ to $k \leq 3$, and then from $k = 3$ to $k \leq 2$.

Reducing from $k \geq 4$ to $k \leq 3$. If $k \geq 4$, then there are at least 4 Q_i's in the denominator and at least one R in the numerator of (C.2). Therefore, we can expand the vector R in the basis of the Q_i, as follows.

$$R = \sum_i x_i Q_i \tag{C.3}$$

With this expansion, the original term can be expressed as a sum of four others, in each of which there is a cancellation between numerator and denominator, reducing k to at most 3. Of course, we must be sure that the coefficients x_i are independent of u. To see this, expand Q_i and R as in (2.15) and (2.17) by writing $Q_i = -(\sqrt{1-u})q_i + \alpha_i K$ and $R = -(\sqrt{1-u})p + \beta K$. Then, we find that (C.3) becomes

$$p = \sum_{i=1}^{4} x_i q_i, \qquad \sum_i x_i \alpha_i = \beta \tag{C.4}$$

Here it is clear that the solutions x_i are independent of u. Note that the equation $p = \sum_{i=1}^{4} x_i q_i$ has only three independent components, because the vectors q_i span the 3-dimensional space orthogonal to K. Thus we have four equations giving a unique solution of x_i.

Reducing from $k = 3$ to $k \leq 2$. Now we reduce further, from $k = 3$ to $k \leq 2$. Since $k = 3$ (and we know $n \geq 0$, because we are discussing bubbles) there is more than one R in the numerator. Taking any one of the R, we expand

$$P = y_K K + y_1 K_1 + y_2 K_2 + y_3 K_3.$$

Then,

$$
\begin{aligned}
R &= -\sqrt{1-u}\left(P - \frac{P \cdot K}{K^2} K \right) + \beta K \\
&= \sum_{i=1}^{3} y_i \left\{ -\sqrt{1-u}\left(K_i - \frac{K_i \cdot K}{K^2} K \right) + \alpha_i K \right\} + \left(\beta - \sum_{i=1}^{3} y_i \alpha_i \right) K \\
&= \sum_{i=1}^{3} y_i Q_i + \left(\beta - \sum_{i=1}^{3} y_i \alpha_i \right) K
\end{aligned}
$$

Substituting this expansion into the numerator of (C.2), we obtain

$$
\frac{\langle \ell | R(K - s\eta) | \ell \rangle}{\prod_{i=1}^{3} \langle \ell | Q_i(K - s\eta) | \ell \rangle} = \sum_{t=1}^{3} \frac{y_i}{\prod_{i=1, i \neq t}^{3} \langle \ell | Q_i(K - s\eta) | \ell \rangle} \\
+ \left(\beta - \sum_{i=1}^{3} y_i \alpha_i \right) \frac{s \langle \ell | \eta K | \ell \rangle}{\prod_{i=1}^{3} \langle \ell | Q_i(K - s\eta) | \ell \rangle}
$$

The first three terms fall into the case $k = 2$. The last term, with the factor $s \langle \ell | \eta K | \ell \rangle$ in the numerator, still has $k = 3$, but we see from comparison with (C.2) that we have effectively reduced n by one.[8] Repeating the reduction on the last term, n times, we arrive at a term with $n = 0$. As we discussed in the paragraph following (C.2), such a term is independent of u.

Having accomplished the reduction of our proof to the case $k \leq 2$, we proceed to apply the results of OPP in a case-by-case analysis for $k = 0, 1, 2$.

C.2 Case-by-case analysis

We now analyze each of the cases $k = 0, 1, 2$ in turn, rearranging our integrand (C.2) so that the terms with odd powers of $\sqrt{1-u}$ take the form of the spurious terms of OPP [17], which were proven there to vanish upon integration.

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[8]There is another way to see this point. The presence of a term $\langle \ell | \eta K | \ell \rangle$ implies that there is a factor $(-2\widetilde{\ell} \cdot K)$ in the form (2.6). By the delta-function condition from the 4-dimensional unitarity cut, this factor is equivalent to K^2, so we have reduced n by one.

The case $k = 0$. We apply the OPP result directly and make use of their notation. Recall that we always have $p_0 = 0$. Use (2.18), i.e. $R_j(u) = -\sqrt{1-u}\left(P_j - \frac{P_j \cdot K}{K^2}K\right) + \beta_j K$, and expand P_j as follows (see (2.23) of [17]):

$$P_j = y_1 K + y_n n + y_7 \ell_7 + y_8 \ell_8. \tag{C.5}$$

More concretely,

$$K = \ell_5 + 2\ell_6 \tag{C.6}$$

$$\ell_5 = K - \frac{K^2}{2K \cdot \eta}\eta, \qquad \ell_6 = \frac{K^2}{4K \cdot \eta}\eta \tag{C.7}$$

$$\ell_7 = \lambda_{\ell_5}\widetilde{\lambda}_{\ell_6}, \qquad \ell_8 = \lambda_{\ell_6}\widetilde{\lambda}_{\ell_5}, \qquad n = \ell_5 - 2\ell_6 \tag{C.8}$$

Here η is the same null vector η, chosen arbitrarily, that we used inside $B_{n,t}(s)$. We see immediately that

$$R_j(u) = -(\beta_j - y_n\beta_n - y_{\ell_7}\beta_{\ell_7} - y_{\ell_8}\beta_{\ell_7})R_K + y_n R_n + y_7 R_{\ell_7} + y_8 R_{\ell_8} \tag{C.9}$$

where $R_{\ell_7} = -\sqrt{1-u}\left(\ell_7 - \frac{\ell_7 \cdot K}{K^2}K\right) - \frac{\ell_7 \cdot K}{K^2}K$, and the other three vectors are defined similarly from (2.17). After accounting for orthogonality properties,

$$n \cdot K = \ell_7 \cdot K = \ell_8 \cdot K = 0$$

we can see specifically how the u-dependence enters:

$$R_K = -K, \quad R_n = -(\sqrt{1-u})n, \quad R_{\ell_7} = -(\sqrt{1-u})\ell_7, \quad R_{\ell_8} = -(\sqrt{1-u})\ell_8. \tag{C.10}$$

Now we use the one-to-one correspondence between form (2.6) and form (C.2), that we emphasized at the beginning of this section. In the present analysis of a term of type (C.2) with $k = 0$, and a numerator factor with R_{ℓ_7}, the corresponding term in (2.6) will have the factor $-2\widetilde{\ell} \cdot \ell_7$. If we expand every R_j according to (C.9), then our general term is of the following form:

$$(-2\widetilde{\ell} \cdot K)^{s_K}(-2\widetilde{\ell} \cdot \ell_7)^{s_7}(-2\widetilde{\ell} \cdot \ell_8)^{s_8}(-2\widetilde{\ell} \cdot n)^{s_n}. \tag{C.11}$$

We have introduced integers s_i to denote the powers. The u-dependence of such a term is precisely the factor $\sqrt{1-u}^{s_7 + s_8 + s_n}$.

We need to show that if $s_7 + s_8 + s_n$ is odd, then the term is spurious in the sense of OPP [17]. First of all, the unitarity cut condition means we can replace $(-2\widetilde{\ell} \cdot K) \to K^2$, so the value of n is effectively reduced by one, and we can ignore that factor for the rest of the proof. If either $s_7 = 0$ or $s_8 = 0$, then we see immediately from [17]-(2.29) that the term is spurious. When both s_7, s_8 are nonzero, we use the expression [17]-(2.33) to reduce to the case of [17]-(2.29). If $s_7 \neq s_8$, the conclusion is obvious. But if $s_7 = s_8$, then s_n is odd, and so, after applying [17]-(2.33), $2i + s_n$ is still an odd power, and we can again conclude with [17]-(2.29) that the term is spurious. Finally, we must account for the first two terms in [17]-(2.33). The first is $\sum_{i=0}^{1} \mathcal{O}(D_i)$, which is zero by the unitarity cut condition. The second term is $\mathcal{O}(\widetilde{q}^2)$, which is zero since our present analysis is purely four-dimensional, as we remarked at the beginning of this section.

The case $k = 1$. We continue using the notation of [17], and also its discussion of 3-point like spurious terms. Now we use the following expansion involving the single vector K_i:

$$P_j = y_K K + y_i K_i + y_3 \ell_3 + y_4 \ell_4. \tag{C.12}$$

The vectors ℓ_3, ℓ_4 are defined as $\ell_3 = \lambda_{\ell_1}\widetilde{\lambda}_{\ell_2}$, $\ell_4 = \lambda_{\ell_2}\widetilde{\lambda}_{\ell_1}$, where ℓ_1, ℓ_2 are constructed from K, K_i. Then,

$$\begin{aligned} R_j(u) &= -\sqrt{1-u}\left(P_j - \frac{P_j \cdot K}{K^2}K\right) + \beta_j K \\ &= -(\beta_j - y_i\alpha_i - y_3\beta_{\ell_3} - y_4\beta_{\ell_4})R_K + y_i Q_i + y_3 R_{\ell_3} + y_4 R_{\ell_4} \end{aligned}$$

Now we substitute this expansion into $\langle\ell|R_j(u)(K - s\eta)|\ell\rangle$. The term with Q_i cancels the a factor in the denominator, returning us to the case of $k = 0$, which we have already addressed. The term with R_K reduces n by one, as discussed above. For the remaining two terms, we use $\ell_3 \cdot K = \ell_4 \cdot K = 0$ to write $R_{\ell_3} = -(\sqrt{1-u})\ell_3$ and $R_{\ell_4} = -(\sqrt{1-u})\ell_4$, just as in the case of $k = 0$.

However, unlike the $k = 0$ case, when we put R_{ℓ_3} and R_{ℓ_4} back in (C.2), the power of $\sqrt{1-u}$ is not always given by the power of R_{ℓ_3} and R_{ℓ_4}, so we must be careful. Let us consider the separate cases for each term in the expansion.

- (a) If the term contains neither R_{ℓ_3} nor R_{ℓ_4}, then either Q_i effectively reduces $k = 1$ to $k = 0$, or R_K reduces n to $n = 0$ in n steps. Either way, we know from previous analysis that the odd powers of $\sqrt{1-u}$ drop out.

- (b) If the term contains R_{ℓ_3} or R_{ℓ_4}, but not both, i.e.,

$$\frac{(-2\widetilde{\ell} \cdot \ell_3)^a}{(\widetilde{\ell} - K_i)^2 - \mu^2} \quad or \quad \frac{(-2\widetilde{\ell} \cdot \ell_4)^b}{(\widetilde{\ell} - K_i)^2 - \mu^2}, \quad a, b \neq 0$$

  by [17]-(2.20), the contribution is zero.

- (c) If the term contains both R_{ℓ_3} and R_{ℓ_4}, i.e.,

$$\frac{(-2\widetilde{\ell} \cdot \ell_3)^a(-2\widetilde{\ell} \cdot \ell_4)^b}{(\widetilde{\ell} - K_i)^2 - \mu^2}, \quad a, b \neq 0$$

  then we need to use the first equation of [17]-(2.15) to reduce the pair. There are three terms on the right hand side of the first equation (remembering that the $\mathcal{O}(\widetilde{q}^2)$ does not exist in our case). The first two terms reduce n by two (notice that F depends on μ^2 through the mass), and the third term reduces $k = 1$ to $k = 0$. By this manipulation, we reduce case (c) to either case (a) or case (b).

The case $k = 2$. We use the same expansion of R_j as in the $k = 1$ case, and perform a similar analysis. Factors with R_K factor effectively reduce n by one. Factors with Q_1 reduce $k = 2$ to $k = 1$. For R_{ℓ_3} and R_{ℓ_4}, we need to use equation [17]-(2.15) to simplify further. Similar to the case $k = 1$, we have following three cases:

- (a) If the term contains neither R_{ℓ_3} nor R_{ℓ_4}, then either Q_i reduces $k = 2$ to $k = 1$, or R_K reduces n to $n = 0$ in n steps. Either way, we know from previous analysis that the odd powers of $\sqrt{1-u}$ drop out.

- (b) If the term contains R_{ℓ_3} or R_{ℓ_4}, but not both, i.e.,

$$\frac{(-2\widetilde{\ell}\cdot\ell_3)^a}{((\widetilde{\ell}-K_i)^2-\mu^2)((\widetilde{\ell}-K_j)^2-\mu^2)} \quad \text{or} \quad \frac{(-2\widetilde{\ell}\cdot\ell_4)^b}{((\widetilde{\ell}-K_i)^2-\mu^2)((\widetilde{\ell}-K_j)^2-\mu^2)}, \quad a, b \neq 0$$

then we apply the second equation of [17]-(2.15) repeatedly until we reach the form [17]-(2.18). There are three terms on the right-hand side of [17]-(2.18). The first term will depend on u polynomially through the mass, while the third term will reduce $k = 2$ to $k = 1$. The second term is the spurious term, which gives zero contribution.

- (c) If the term contains both R_{ℓ_3} and R_{ℓ_4}, i.e.,

$$\frac{(-2\widetilde{\ell}\cdot\ell_3)^a(-2\widetilde{\ell}\cdot\ell_4)^b}{((\widetilde{\ell}-K_i)^2-\mu^2)((\widetilde{\ell}-K_j)^2-\mu^2)}, \quad a, b \neq 0$$

then we apply the first equation of [17]-(2.15) to reduce the pair. Then we use the second equation of [17]-(2.15) and finally reach the form of (2.18). The discussion of this case is parallel to case (b).

We conclude that the bubble coefficients, as given in (4.1), are indeed polynomials in u. Knowing this fact, the degree of the polynomial can then be read off from the formulas of section 4; it is seen to be $[n/2]$.

D. Pentagon double cut

The double cut of a pentagon integral, defined according to (2.6) as

$$C[I_5(K; K_1, K_2, K_3)] = \int d^{4-2\epsilon}p \, (\mu^2) \frac{1}{\prod_{j=1}^3 (p - K_j)^2} \delta(p^2)\delta((p - K)^2) \qquad \text{(D.1)}$$

is given by the following expression [21]:

$$C[I_5(K; K_1, K_2, K_3)] = -\int_0^1 du \, u^{-1-\epsilon}\frac{\sqrt{1-u}}{(K^2)^2} \qquad \text{(D.2)}$$

$$\times \left(\frac{S[Q_3, Q_2, Q_1, K]}{4\sqrt{(Q_3\cdot Q_2)^2 - Q_3^2 Q_2^2}} \ln\frac{Q_3\cdot Q_2 - \sqrt{(Q_3\cdot Q_2)^2 - Q_3^2 Q_2^2}}{Q_3\cdot Q_2 + \sqrt{(Q_3\cdot Q_2)^2 - Q_3^2 Q_2^2}}\right. \qquad \text{(D.3)}$$

$$+ \frac{S[Q_3, Q_1, Q_2, K]}{4\sqrt{(Q_3\cdot Q_1)^2 - Q_3^2 Q_1^2}} \ln\frac{Q_3\cdot Q_1 - \sqrt{(Q_3\cdot Q_1)^2 - Q_3^2 Q_1^2}}{Q_3\cdot Q_1 + \sqrt{(Q_3\cdot Q_1)^2 - Q_3^2 Q_1^2}} \qquad \text{(D.4)}$$

$$\left.+ \frac{S[Q_2, Q_1, Q_3, K]}{4\sqrt{(Q_2\cdot Q_1)^2 - Q_2^2 Q_1^2}} \ln\frac{Q_2\cdot Q_1 - \sqrt{(Q_2\cdot Q_1)^2 - Q_2^2 Q_1^2}}{Q_2\cdot Q_1 + \sqrt{(Q_2\cdot Q_1)^2 - Q_2^2 Q_1^2}}\right),$$

where $S[Q_i, Q_j, Q_k, K]$ was defined to be

$$S[Q_i, Q_j, Q_k, K] = \frac{T_1}{T_2}, \tag{D.5}$$

with

$$T_1 = -8 \det \begin{pmatrix} K \cdot Q_k & Q_i \cdot K & Q_j \cdot K \\ Q_i \cdot Q_k & Q_i^2 & Q_i \cdot Q_j \\ Q_j \cdot Q_k & Q_i \cdot Q_j & Q_j^2 \end{pmatrix}; \quad T_2 = -4 \det \begin{pmatrix} Q_k^2 & Q_i \cdot Q_k & Q_j \cdot Q_k \\ Q_i \cdot Q_k & Q_i^2 & Q_i \cdot Q_j \\ Q_j \cdot Q_k & Q_i \cdot Q_j & Q_j^2 \end{pmatrix}. \tag{D.6}$$

Here we rewrite (D.5) so that the u-dependence becomes transparent. We need to define a few auxiliary quantities. In terms of a particular matrix denoted by S,

$$S \equiv \begin{pmatrix} 0 & K^2 & K_1^2 & K_2^2 & K_3^2 \\ K^2 & 0 & (K_1 - K)^2 & (K_2 - K)^2 & (K_3 - K)^2 \\ K_1^2 & (K_1 - K)^2 & 0 & (K_2 - K_1)^2 & (K_3 - K_1)^2 \\ K_2^2 & (K_2 - K)^2 & (K_2 - K_1)^2 & 0 & (K_3 - K_2)^2 \\ K_3^2 & (K_3 - K)^2 & (K_3 - K_1)^2 & (K_3 - K_2)^2 & 0 \end{pmatrix}, \tag{D.7}$$

we define

$$A[K_1; K_2, K_3, K] = -\det \begin{pmatrix} 0 & K_2^2 & K_3^2 & K^2 & K_1^2 \\ K_2^2 & 0 & (K_2 - K_3)^2 & (K_2 - K)^2 & (K_2 - K_1)^2 \\ K_3^2 & (K_3 - K_2)^2 & 0 & (K_3 - K)^2 & (K_3 - K_1)^2 \\ K^2 & (K - K_2)^2 & (K - K_3)^2 & 0 & (K - K_1)^2 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix} \tag{D.8}$$

$$B[K_1, K_2, K_3, K] = \det(S) \sum_{i,j=1}^{5} (S^{-1})_{ij}, \tag{D.9}$$

$$C[K_1, K_2, K_3, K] = 2\det(S). \tag{D.10}$$

Then,

$$S[Q_2, Q_3, Q_1, K] = \frac{4K^2 A[K_1; K_2, K_3, K]}{uK^2 B[K_1, K_2, K_3, K] - C[K_1, K_2, K_3, K]}. \tag{D.11}$$

Now it is evident that the numerator of (D.11) is independent of u, and the denominator is linear in u. Furthermore, $B[K_1, K_2, K_3, K]$ and $C[K_1, K_2, K_3, K]$ are totally symmetric in their arguments, indicating fundamental pentagon nature. The quantity $A[K_1; K_2, K_3, K]$ breaks this symmetry for the first argument, K_1, indicating that the corresponding propagator is the one that is eliminated in order to show up as part of a *box* coefficient.

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