

# Numerical integration of one-loop Feynman diagrams for $N$ -photon amplitudes: implementation notes

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ABSTRACT: We present the main methods used for sampling integration points in the calculation of one-loop Feynman diagrams for  $N$ -photon amplitudes.

KEYWORDS: perturbative QCD, NLO calculation, 1-loop matrix elements.

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## 1 Introduction

These are implementation notes to accompany our paper *Numerical integration of one-loop Feynman diagrams for  $N$ -photon amplitudes*, arXiv:hep-ph/0610028. Specifically, we describe the methods we used for importance sampling in performing the integration by Monte Carlo integration.

We would like to perform an integral of the form

$$I = \int d^4\ell \int_0^1 d\xi^0 \int_0^1 d\xi^1 \cdots \int_0^1 d\xi^N \delta\left(\sum_{i=0}^N \xi^i - 1\right) f(\ell, \xi) . \quad (1.1)$$

In a Monte Carlo integration, we choose  $N_{\text{pts}}$  points  $\{\ell_j, \xi_j\}$  at random with a density  $\rho(\ell, \xi)$  and evaluate the integrand  $f(\xi)$  at these points. Then the integral is

$$I = \lim_{N_{\text{pts}} \rightarrow \infty} \frac{1}{N_{\text{pts}}} \sum_{j=1}^{N_{\text{pts}}} \frac{f(\ell_j, \xi_j)}{\rho(\ell_j, \xi_j)} . \quad (1.2)$$

(We for allow the possibility that some points  $\xi_j$  are outside the integration range of the original integral by setting  $f(\ell, \xi) = 0$  for  $\xi$  outside the integration range.) The integration error with a finite number of points is proportional to  $1/\sqrt{N_{\text{pts}}}$ . The coefficient of  $1/\sqrt{N_{\text{points}}}$  in the error is smallest if

$$\rho(\ell, \xi) \approx \text{const.} \times |f(\ell, \xi)| . \quad (1.3)$$

That is the ideal, but it is not really possible to achieve this ideal to the degree that one has a one part per mill error with one million points. However, one would certainly like to keep  $|f(\ell, \xi)|/\rho(\ell, \xi)$  from being very large. In particular,  $f(\ell, \xi)$  is singular along certain lines (the collinear singularities) and at certain points (the soft singularities). We need to arrange that  $\rho$  is singular at the same places that  $f$  is singular, so that  $f(\ell, \xi)/\rho(\ell, \xi)$  is *not* singular anywhere. Since  $|f(\ell, \xi)|$  can be very large near other lines associated with double parton scattering, we also need to arrange that  $\rho(\ell, \xi)$  is similarly large near these lines.

We construct the desired density in the form

$$\rho(\ell, \xi) = \rho_\ell(\ell) \sum_{J=1}^{N_{\text{alg}}} \alpha_J \rho_J(\xi) . \quad (1.4)$$

Here  $\int d^4\ell \rho_\ell(\ell) = 1$  and there are several density functions  $\rho_J$  with

$$\int d\xi \rho_J(\xi) = 1 . \quad (1.5)$$

We choose probabilities  $\alpha_j$  with

$$\sum_{J=1}^{N_{\text{alg}}} \alpha_J = 1 . \quad (1.6)$$

Each  $\rho_J$  corresponds to a certain algorithm for choosing a point  $\xi$ . For each new integration point, the computer chooses which algorithm to use with probability  $\alpha_J$ .

In the following sections, we describe the more important algorithms used for choosing points  $\xi$ . (The algorithm for choosing points  $\ell$  is quite trivial.) Some methods are more important than others. On the other hand, there is no cost to keeping a method that is of little importance as long as we set its probability  $\alpha_J$  to be small. Thus we have more methods than one would really need, some of them left over from working on a more general problem that includes subtractions for collinear and soft divergences, which are not needed for the  $N$ -photon case. We do not document the not-really-needed algorithms here.

We apologize that the construction of some of the methods for choosing points is quite *ad hoc*. An interested reader of these notes is advised to write his or her own methods. We supply these notes only to document the code and perhaps to suggest a few useful tricks for importance sampling for this kind of problem.

In the following, the variables called  $\xi$  above and in the paper are called  $x$ . This is unfortunate, but we thought it best not to try to change the notation.

## 2 Sampling with a uniform distribution

We would like to perform an integral

$$I = \int_0^1 dx^0 \int_0^1 dx^1 \cdots \int_0^1 dx^N \delta\left(\sum_{i=0}^N x^i - 1\right) f(x) \quad (2.1)$$

using a uniform density of points. We can simply perform the integration over  $x^0$  using the delta function to obtain

$$I = \int_0^1 dx^1 \cdots \int_0^1 dx^N \theta\left(\sum_{i=1}^N x^i < 1\right) f(x) \quad (2.2)$$

with  $x^0 = 1 - \sum_1^n x_i$ .

Define

$$\sum_{i=1}^j x_i = s_j . \quad (2.3)$$

Then the variables  $s_j$  obey  $0 < s_1 < s_2 < \cdots < s_N < 1$  and we have

$$I = \int_0^1 ds^1 \cdots \int_0^1 ds^N \theta(0 < s_1 < s_2 < \cdots < s_n < 1) f(x) . \quad (2.4)$$

We can perform this iteration by choosing variables  $r_i$  in the unit cube and sorting them in order of increasing values. Thus we define  $s_i = r_{\pi(i)}$  such that  $0 < s_1 < s_2 < \cdots < s_N < 1$ . This covers the desired volume  $N!$  times, so

$$I = \frac{1}{N!} \int_0^1 dr^1 \cdots \int_0^1 dr^N f(x) . \quad (2.5)$$

The transformation from  $s_j = r_{\pi(j)}$  to  $x_j$  is

$$x_j = s_j - s_{j-1} \quad (2.6)$$

for  $j \in \{1, \dots, N\}$  with  $s_0 \equiv 0$ .

Thus with this algorithm, each point  $x$  is determined by choosing a point  $r$  in the  $N$ -dimensional unit cube and  $\rho(x)$  for this algorithm is just  $N!$ .

### 3 Sampling for the soft and collinear singularities

The integrand is singular in each of the regions  $x^n \approx 1$ , which corresponds to loop momentum  $n$  in the original graph being soft. There are adjacent collinear singularities corresponding to momenta  $n - 1$  and  $n$  being collinear and to momenta  $n$  and  $n + 1$  being collinear. These are the regions  $x^{n-1} + x^n \approx 1$  and  $x^n + x^{n+1} \approx 1$ . We would like to find an algorithm that produces a density of points  $\rho$  that matches all of these singularities. This density is normalized to  $\int dx \rho(x) = 1$ . Our notation here is that this section describes one algorithm for choosing points and  $\rho(x)$  denotes the density of points thus chosen. This density is *one* of the densities  $\rho_J(x)$  mentioned in the introduction. Thus we could provide an index  $J$ , say  $J = 1$ , to label  $\rho$ , but we omit the extra index. In this algorithm there are sub-algorithms labeled with an index  $n$  that have densities  $\rho_n(x)$ .

We construct the desired density in the form

$$\rho(x) = \sum_{i=1}^N p_n \rho_n(x) \quad (3.1)$$

with the following properties. The  $p_n$  are probabilities with  $\sum p_n = 1$  and the  $\rho_n$  are densities normalized to  $\int dx \rho_n(x) = 1$ . The density  $\rho_n$  reflects the singularity of the integrand in the region  $\mathcal{R}_n$  in which either line  $n$  is soft or lines  $n$  and  $n + 1$  in the loop are collinear or the lines  $n$  and  $n - 1$  in the loop are collinear. We want  $p_n \rho_n$  to have the form

$$p_n \rho_n(x) = \frac{c_n(x)}{[G_n(x)]^{N-1-C}} \cdot \quad (3.2)$$

where  $c_n(x)$  is a slowly varying function of  $n$  and  $x$ ,  $C$  is a positive parameter (perhaps 1), and  $G_n(x)$  is modelled on the behavior of  $\Lambda(x)$  in the region  $\mathcal{R}_n$ . The idea is that the denominator of the integrand contains  $\Lambda^2(x)$  to the power  $N - 1$ . Near one of the singularities, one power of the small parameters will be cancelled, so effectively we have one fewer power of  $\Lambda^2$  in the denominator. We seek to cancel this singularity by means of  $\rho$ .

Recall that when line  $n$  is soft,  $\Lambda^2(\vec{x})$  takes the form

$$\Lambda^2(\vec{x}) \approx \sum_{i \notin \{n-1, n, n+1\}} x^n x^i S_{ni} + x^{n-1} x^{n+1} S_{n-1, n+1} \quad , \quad (3.3)$$

with  $x^n \approx 1$ . Here the range for the index  $i$  includes  $i = 0$  and we have extended the definition of the  $S_{ij}$  to include  $S_{n0} = im_0^2$ . This is also a reasonable approximation in the adjacent collinear regions. We take

$$G_n(x) = \sum_{i \notin \{n-1, n, n+1\}} x^i |S_{ni}|/s + x^{n-1} x^{n+1} |S_{n-1, n+1}|/s \quad . \quad (3.4)$$

For our later use we define a scaled version of  $G_n(x)$ ,

$$g_n(x) = \sum_{i \notin \{n-1, n, n+1\}} a_{ni} x^i + b_n x^{n-1} x^{n+1} \quad , \quad (3.5)$$

where

$$\begin{aligned} a_{ni} &= \lambda_n |S_{ni}|/s_0 \quad , \\ b_n &= \lambda_n |S_{n-1, n+1}|/s_0 \quad . \end{aligned} \quad (3.6)$$

Here  $\lambda_n$  is a parameter available for adjusting the overall normalization and  $s_0$  is a parameter with dimensions of momentum squared that we insert simply to make  $\lambda$  dimensionless. It is convenient to choose  $\lambda_n$  so that

$$\min \left( b_n, \min_{i \notin \{n-1, n, n+1\}} a_{ni} \right) = 1 \quad . \quad (3.7)$$

### 3.1 Choosing points for $\rho_n$

We would like to choose points for an integral

$$I = \left\{ \prod_i \int_0^1 dx^i \right\} \delta \left( \sum_{i=0}^N x^i - 1 \right) \theta(g_n(x) < A_n) f(x) . \quad (3.8)$$

This is the same as the integral in Eq. (2.2) except that we have restricted the integration region by means of a theta function. Here  $A_n$  is a parameter that satisfies

$$0 < A_n < b_n . \quad (3.9)$$

The default choice is  $A_n = 1$ . This gives

$$I = \left\{ \prod_{i \notin \{n\}} \int_0^1 dx^i \right\} \theta(g_n(x) < A_n) \theta(0 < x_n) f(x) . \quad (3.10)$$

Here

$$x^n = 1 - \sum_{i \notin \{n\}} x^i . \quad (3.11)$$

We enforce the condition  $x^n > 0$  by means of a theta function since  $\sum_{i \notin \{n\}} x^i$  could be greater than 1.

Now we change variables from  $\{x^{n-1}, x^{n+1}\}$  to  $\{\bar{x}, \omega\}$  with

$$\begin{aligned} x^{n-1} &= \sqrt{\bar{x}} e^\omega , \\ x^{n+1} &= \sqrt{\bar{x}} e^{-\omega} . \end{aligned} \quad (3.12)$$

Then

$$\bar{x} = x^{n-1} x^{n+1} . \quad (3.13)$$

The condition  $g_n(x) < A_n$  imposes a restriction on  $\bar{x}$ . We have

$$b_n x^{n-1} x^{n+1} = g_n(x) - \sum_{i \notin \{n-1, n, n+1\}} a_{ni} x^i , \quad (3.14)$$

so

$$\bar{x} \leq A_n / b_n . \quad (3.15)$$

Since we choose  $A_n < b_n$ ,  $\bar{x}$  is always less than 1. This gives

$$I = \left\{ \prod_{i \notin \{n-1, n, n+1\}} \int_0^1 dx^i \right\} \int_0^{A_n/b_n} d\bar{x} \int_{-\Omega(\bar{x})}^{\Omega(\bar{x})} d\omega \theta(g_n(x) < A_n) \theta(0 < x_n) f(x) . \quad (3.16)$$

Here the restrictions  $x^{n-1} < 1$  and  $x^{n+1} < 1$  are written

$$|\omega| < \log(1/\sqrt{\bar{x}}) \equiv \Omega(\bar{x}) . \quad (3.17)$$

which is reflected in the integration limit for  $\omega$ .

Next we insert an integral over a variable  $x_s$  that is set equal to  $g_n(x)$ ,

$$\begin{aligned} I = & \int_0^{A_n} dx_s \left\{ \prod_{i \notin \{n-1, n, n+1\}} \int_0^1 dx^i \right\} \int_0^{A_n/b_n} d\bar{x} \int_{-\Omega(\bar{x})}^{\Omega(\bar{x})} d\omega \\ & \times \delta \left( \sum_{i \notin \{n-1, n, n+1\}} a_{ni} x^i + b_n \bar{x} - x_s \right) \theta(0 < x_n) f(x) \end{aligned} \quad (3.18)$$

Next, we introduce scaled variables

$$\begin{aligned} \bar{y} &= (b_n/x_s) \bar{x} , \\ y_i &= (a_{ni}/x_s) x_i . \end{aligned} \quad (3.19)$$

Then

$$\begin{aligned} I = & \frac{1}{b_n} \left[ \prod_{i \notin \{n-1, n, n+1\}} \frac{1}{a_{ni}} \right] \int_0^{A_n} dx_s x_s^{N-2} \left\{ \prod_{i \notin \{n-1, n, n+1\}} \int_0^1 dy_i \right\} \int_0^{A_n/x_s} d\bar{y} \int_{-\Omega(\bar{x})}^{\Omega(\bar{x})} d\omega \\ & \times \delta \left( \sum_{i \notin \{n-1, n, n+1\}} y^i + \bar{y} - 1 \right) \theta(0 < x_n) f(x) \end{aligned} \quad (3.20)$$

We can now use the delta function to perform the  $\bar{y}$  integration. This gives

$$\begin{aligned} I = & \frac{1}{b_n} \left[ \prod_{i \notin \{n-1, n, n+1\}} \frac{1}{a_{ni}} \right] \int_0^{A_n} dx_s x_s^{N-2} \left\{ \prod_{i \notin \{n-1, n, n+1\}} \int_0^1 dy_i \right\} \int_{-\Omega(\bar{x})}^{\Omega(\bar{x})} d\omega \\ & \times \theta \left( \sum_{i \notin \{n-1, n, n+1\}} y^i < 1 \right) \theta(0 < x_n) f(x) . \end{aligned} \quad (3.21)$$

We can perform the integrations over the  $y_i$  by choosing  $N - 2$  points  $r_i$  in the unit cube and then reordering them with a permutation  $\pi$  so that  $r_{\pi(i)} < r_{\pi(i+1)}$ . Then we can set

$$\begin{aligned} y_0 &= r_{\pi(1)} \\ y_{n+i} &= r_{\pi(i)} - r_{\pi(i-1)} \quad i \in \{2, \dots, N - 2\} \end{aligned} \quad (3.22)$$

where we adopt a cyclic notation,  $y_{N+j} = y_j$ . This insures that the sum of the  $y_i$  is less than 1 and gives

$$I = \frac{1}{(N-2)!} \frac{1}{b_n} \left[ \prod_{i \notin \{n-1, n, n+1\}} \frac{1}{a_{ni}} \right] \int_0^{A_n} dx_s x_s^{N-2} \left\{ \prod_{i=1}^{N-2} \int_0^1 dr_i \right\} \int_{-\Omega(\bar{x})}^{\Omega(\bar{x})} d\omega \quad (3.23)$$

$$\times \theta(0 < x_n) f(x) .$$

For the final steps, choose  $x_s$  and  $\omega$  according to the distributions

$$x_s = A_n r_s^{1/C} \quad (3.24)$$

$$\omega = [r_\omega - \frac{1}{2}] 2 \Omega(\bar{x}) ,$$

where  $C$  is a positive parameter and  $r_s$  and  $r_\omega$  are each chosen with a uniform distribution from the interval  $(0, 1)$ . This gives

$$I = \frac{2A_n^C}{C(N-2)!} \frac{1}{b_n} \left[ \prod_{i \notin \{n-1, n, n+1\}} \frac{1}{a_{ni}} \right] \int_0^1 dr_s \int_0^1 dr_\omega \left\{ \prod_{i=1}^{N-2} \int_0^1 dr_i \right\} \quad (3.25)$$

$$\times \Omega(x^{n-1} x^{n+1}) g_n(x)^{N-1-C} \theta(0 < x_n) f(x) .$$

This is

$$I = \int_0^1 dr_s \int_0^1 dr_\omega \left\{ \prod_{i=1}^{N-2} \int_0^1 dr_i \right\} \frac{\theta(0 < x_n) f(x)}{\rho_n(x)} \quad (3.26)$$

with a density of points

$$\rho_n(x) = b_n \left[ \prod_{i \notin \{n-1, n, n+1\}} a_{ni} \right] \frac{C(N-2)!}{2A_n^C} \frac{1}{\Omega(x^{n-1} x^{n+1})} \frac{\theta(g_n(x) < A_n)}{g_n(x)^{N-1-C}} . \quad (3.27)$$

There are some numerical factors and there is a factor  $\Omega(x^{n-1} x^{n+1})$  that is a slowly varying function of its argument when its argument is small. The main factor that is a sensitive function of the  $x_i$  is the power of  $g_n(x)$ . This is the factor that we sought to build into  $\rho_n(x)$ .

Note that with this construction, some of the points  $\{x\}$  will have  $x_n < 0$ . As indicated by the factor  $\theta(0 < x_n)$ , we simply throw these points away (but count the attempt in counting the number of integration points tried).

### 3.2 Choosing the probabilities

We would like to choose points according to the density  $\rho_n(x)$  with probability  $p_n$ , with

$$\sum_{n=1}^N p_n = 1 \quad (3.28)$$

The densities  $\rho_n(x)$  are normalized to  $\int dx \rho(x) = 1$ . By choosing density  $\rho_n$  with probability  $p_n$  we have an effective density  $p_n \rho_n(x)$ . Recall that we would like

$$p_n \rho_n(x) = \frac{c_n(x)}{[G_n(x)]^{N-1-C}} \quad (3.29)$$

where  $c_n(x)$  depends only weakly on  $n$  and  $x$  and  $G_n(x)$  is  $g_n(x)$  with the normalization parameter  $\lambda_n$  set equal to 1. We have

$$\begin{aligned} g_n(x) &= \lambda_n G_n(x) , \\ b_n &= \lambda_n |S_{n-1,n+1}|/s_0 , \\ a_{ni} &= \lambda_n |S_{n,i}|/s_0 , \end{aligned} \quad (3.30)$$

so

$$\rho_n(x) = \lambda_n^C \frac{|S_{n-1,n+1}|}{s} \left[ \prod_{i \notin \{n-1,n,n+1\}} \frac{|S_{ni}|}{s} \right] \frac{C(N-2)!}{2A_n^C} \frac{1}{\Omega(x^{n-1}x^{n+1})} \frac{1}{G_n(x)^{N-1-C}} . \quad (3.31)$$

Here

$$\frac{1}{\lambda_n} = \frac{1}{s_0} \min \left( |S_{n-1,n+1}|, \min_{i \notin \{n-1,n,n+1\}} |S_{ni}| \right) . \quad (3.32)$$

Thus

$$\rho_n(x) = \frac{|S_{n-1,n+1}| \prod_{i \notin \{n-1,n,n+1\}} |S_{ni}| C(N-2)!}{s_0^{N-1} A_n^C \lambda_n^{-C}} \frac{1}{2} \frac{1}{\Omega(x^{n-1}x^{n+1})} \frac{\theta(g_n(x) < A_n)}{G_n(x)^{N-1-C}} . \quad (3.33)$$

We define

$$p_n = \frac{w_n^{(s)}}{\sum_i w_i^{(s)}} \quad (3.34)$$

where

$$w_n^{(s)} = \frac{s_0^{N-1} A_n^C \lambda_n^{-C}}{|S_{n-1,n+1}| \prod_{i \notin \{n-1,n,n+1\}} |S_{ni}|} \quad (3.35)$$

Then

$$p_n \rho_n(x) = \frac{1}{\sum_i w_i^{(s)}} \frac{C(N-2)!}{2} \frac{1}{\Omega(x^{n-1}x^{n+1})} \frac{\theta(g_n(x) < A_n)}{G_n(x)^{N-1-C}} . \quad (3.36)$$

This has the form that we wanted.

## 4 Sampling for double parton scattering singularity

We consider choices of indices  $A$  and  $B$  such that  $S_{A,B+1} > 0$ , and  $S_{A+1,B} > 0$ ,  $S_{A,B} < 0$  and  $S_{A+1,B+1} < 0$ .

We seek to put points near the line

$$\begin{aligned}
x^A &= f_A \bar{x} \ , \\
x^{A+1} &= (1 - f_A) \bar{x} \ , \\
x^B &= f_B (1 - \bar{x}) \ , \\
x^{B+1} &= (1 - f_B) (1 - \bar{x}) \ ,
\end{aligned}
\tag{4.1}$$

where  $\bar{x}$  varies over the range

$$0 < \bar{x} < 1 \ . \tag{4.2}$$

Here  $f_A$  and  $f_B$  are defined by

$$\begin{aligned}
f_A &= \frac{S_{A+1,B} - S_{A+1,B+1}}{\bar{S}} \ , \\
f_B &= \frac{S_{A,B+1} - S_{A+1,B+1}}{\bar{S}} \ .
\end{aligned}
\tag{4.3}$$

where  $\bar{S}$  is give by Eq. (??). The part of  $\Lambda^2$  proportional to two powers of  $x^A, x^{A+1}, x^B, x^{B+1}$  is

$$(x^A, x^{A+1}) \begin{pmatrix} S_{A,B} & S_{A,B+1} \\ S_{A+1,B} & S_{A+1,B+1} \end{pmatrix} \begin{pmatrix} x^B \\ x^{B+1} \end{pmatrix} = 0 \tag{4.4}$$

There is a double parton scattering singularity when

$$\Delta f = \frac{S_{A,B+1} S_{A+1,B} - S_{A,B} S_{A+1,B+1}}{\bar{S}^2} \tag{4.5}$$

vanishes. The idea is to apply this method when  $|\Delta f|$  is small,

$$|\Delta f| < \epsilon_{\text{dps}} \ , \tag{4.6}$$

where  $\epsilon_{\text{dps}}$  is a small parameter that we can adjust. When  $\Delta f = 0$ , the choice (4.1) makes the part of  $\Lambda^2$  proportional to two powers of  $x^A, x^{A+1}, x^B, x^{B+1}$  vanish.

Let  $\mathcal{S}$  be the complement in  $\{0, 1, \dots, N\}$  of  $\{A, A+1, B, B+1\}$ . We write the integration variables  $x^j$  for  $j \in \mathcal{S}$  as

$$x^j = x_s y^j \ , \tag{4.7}$$

where

$$x_s = \sum_{j \in \mathcal{S}} x^j \tag{4.8}$$

so

$$\sum_{j \in \mathcal{S}} y^j = 1 \ . \tag{4.9}$$

Now for the variables  $x^j$  with  $j \notin \mathcal{S}$ , we change variables to  $\bar{x}$ ,  $x_t$  and  $\omega$  and two sign variables  $s_A$  and  $s_B$  that take values  $\pm 1$ . We define

$$\begin{aligned}
x^A &= (1 - x_s)[f_A \bar{x} - s_A \sqrt{x_t} e^\omega]; , \\
x^{A+1} &= (1 - x_s)[(1 - f_A) \bar{x} + s_A \sqrt{x_t} e^\omega] , \\
x^B &= (1 - x_s)[f_B(1 - \bar{x}) - s_B \sqrt{x_t} e^{-\omega}] . \\
x^{B+1} &= (1 - x_s)[(1 - f_B)(1 - \bar{x}) + s_B \sqrt{x_t} e^{-\omega}] ,
\end{aligned} \tag{4.10}$$

Then

$$\sum_{j \in \mathcal{S}} x^j + \sum_{j \notin \mathcal{S}} x^j = 1 , \tag{4.11}$$

as required. Also

$$\begin{aligned}
\bar{x} &= \frac{x^A + x^{A+1}}{1 - x_s} , \\
1 - \bar{x} &= \frac{x^B + x^{B+1}}{1 - x_s} , \\
s_A \sqrt{x_t} e^\omega &= \frac{f_A x^{A+1} - (1 - f_A) x^A}{1 - x_s} , \\
s_B \sqrt{x_t} e^{-\omega} &= \frac{f_B x^{B+1} - (1 - f_B) x^B}{1 - x_s} .
\end{aligned} \tag{4.12}$$

Assuming that  $\Delta f = 0$  so that we have a pinched double parton scattering singularity, the singularity is at  $x_t = x_s = 0$ . In this case  $\Lambda^2$  expanded to first order in  $x_s$  and  $x_t$  is

$$\begin{aligned}
\Lambda^2 &\sim -s_A s_B x_t \bar{S} \\
&+ x_s \sum_{j \in \mathcal{S}} y^j \{ [S_{j,A} f_A + S_{j,A+1} (1 - f_A)] \bar{x} + [S_{j,B} f_B + S_{j,B+1} (1 - f_B)] (1 - \bar{x}) \} .
\end{aligned} \tag{4.13}$$

where  $\bar{S}$  was defined in Eq. (??).

Now let us add imaginary parts to the  $x^i$  for  $i \notin \mathcal{S}$ ,  $x^i \rightarrow x_i + i\eta_i$  with

$$\eta^i = x^i \sum_j S_{ij} x^j / \bar{S} . \tag{4.14}$$

To lowest order in  $x_s$  this amounts to

$$\begin{aligned}
\eta^A &= f_A \bar{x} \frac{S_{A,B+1} - S_{A,B}}{\bar{S}} s_B \sqrt{x_t} e^{-\omega} , \\
\eta^{A+1} &= (1 - f_A) \bar{x} \frac{S_{A+1,B+1} - S_{A+1,B}}{\bar{S}} s_B \sqrt{x_t} e^{-\omega} ,
\end{aligned} \tag{4.15}$$

with a similar result for  $\eta^B$  and  $\eta^{B+1}$ . That is,

$$\begin{aligned}
\eta^A &= f_A(1 - f_A)\bar{x} s_B \sqrt{x_t} e^{-\omega} , \\
\eta^{A+1} &= -f_A(1 - f_A)\bar{x} s_B \sqrt{x_t} e^{-\omega} , \\
\eta^B &= f_B(1 - f_B)(1 - \bar{x}) s_A \sqrt{x_t} e^{\omega} , \\
\eta^{B+1} &= -f_B(1 - f_B)(1 - \bar{x}) s_A \sqrt{x_t} e^{\omega} .
\end{aligned} \tag{4.16}$$

In the case that  $\Delta f \neq 0$ , there are more terms. Assuming  $|\Delta f| \ll 1$  we can retain the term proportional to  $\Delta f$  that is of order zero in  $x_s$  and  $x_t$ . Then, adding these terms and the imaginary terms, we get

$$\begin{aligned}
\Lambda^2 / \bar{S} &\sim s_A s_B x_t \\
&- x_s \sum_{j \in \mathcal{S}} y^j \frac{[S_{j,A} f_A + S_{j,A+1}(1 - f_A)]\bar{x} + [S_{j,B} f_B + S_{j,B+1}(1 - f_B)](1 - \bar{x})}{\bar{S}} \\
&+ i\bar{x} f_A(1 - f_A)x_t e^{-2\omega} + i(1 - \bar{x})f_B(1 - f_B)x_t e^{2\omega} \\
&+ \bar{x}(1 - \bar{x})\Delta f .
\end{aligned} \tag{4.17}$$

This suggests that we should try to choose points so that the density of points is approximately proportional to

$$\frac{1}{[x_t + x_s]^{N-2} + [\bar{x}(1 - \bar{x})|\Delta f|]^{N-2}} . \tag{4.18}$$

(Actually, if we wanted to cancel a factor  $1/[\Lambda^2]^{N-1}$ , we would want a power  $N - 1$  in the density of points. However, we may expect some cancellation to come from the numerator function.)

We have not made use of the imaginary part here. We note that the imaginary part will keep  $\Lambda^2 / \bar{S}$  from being small when  $|\omega|$  is large. However,  $\omega$  is limited to a range

$$\begin{aligned}
\omega_{\max} &= \log \left( \frac{[1 + s_A(2f_A - 1)]\bar{x}}{2\sqrt{x_t}} \right) , \\
\omega_{\min} &= -\log \left( \frac{[1 + s_B(2f_B - 1)](1 - \bar{x})}{2\sqrt{x_t}} \right) ,
\end{aligned} \tag{4.19}$$

in order that  $x^A$ ,  $x^{A+1}$ ,  $x^B$ , and  $x^{B+1}$  lie between 0 and 1. For  $\omega$  in this range, the contour deformation may not help much if  $\bar{x}$  or  $(1 - \bar{x})$  is small. We may note that  $x_t$  needs to be in the range

$$x_t < \bar{x}(1 - \bar{x})[1 + s_A(2f_A - 1)][1 + s_B(2f_B - 1)]/4 . \tag{4.20}$$

Otherwise,  $\omega_{\max} < \omega_{\min}$  and there is no way that  $x^A$ ,  $x^{A+1}$ ,  $x^B$ , and  $x^{B+1}$  can lie between 0 and 1.

To proceed, we begin with an integral

$$I = \int_0^1 dx^0 \int_0^1 dx^1 \cdots \int_0^1 dx^N \delta \left( \sum_{i=0}^N x^i - 1 \right) f(x) . \tag{4.21}$$

We introduce

$$x_s = \sum_{j \in \mathcal{S}} x^j . \quad (4.22)$$

We suppose that  $f(x)$  has support limited to a certain region to be defined. The integration region outside of this region is covered by other methods of choosing points. We write

$$I = \int_0^1 dx_s \prod_{j \in \mathcal{S}} \int_0^1 dx^j \delta\left(\sum_{j \in \mathcal{S}} x^j - x_s\right) \prod_{i \notin \mathcal{S}} \int_0^1 dx^i \delta\left(x_s + \sum_{i \notin \mathcal{S}} x^i - 1\right) f(x) . \quad (4.23)$$

Then

$$I = \int_0^1 dx_s x_s^{N-4} (1-x_s)^3 \prod_{j \in \mathcal{S}} \int_0^1 dy^j \delta\left(\sum_{j \in \mathcal{S}} y^j - 1\right) \prod_{i \notin \mathcal{S}} \int_0^1 dy^i \delta\left(\sum_{i \notin \mathcal{S}} y^i - 1\right) f(x) . \quad (4.24)$$

where  $y^j = x^j/x_s$  for  $j \in \mathcal{S}$  and  $y^j = x^j/(1-x_s)$  for  $j \notin \mathcal{S}$ .

Now for the variables  $y^j$  with  $j \notin \mathcal{S}$ , change variables to  $\bar{x}$ ,  $x_t$  and  $\omega$  and two sign variables  $s_A$  and  $s_B$  that take values  $\pm 1$ . The variables are defined by

$$\begin{aligned} y^A &= f_A \bar{x} - s_A \sqrt{x_t} e^\omega ; , \\ y^{A+1} &= (1-f_A) \bar{x} + s_A \sqrt{x_t} e^\omega , \\ y^B &= f_B (1-\bar{x}) - s_B \sqrt{x_t} e^{-\omega} . \\ y^{B+1} &= (1-f_B)(1-\bar{x}) + s_B \sqrt{x_t} e^{-\omega} , \end{aligned} \quad (4.25)$$

Here  $f_A$  and  $f_B$  are fixed parameters as defined above. Then

$$I = \int_0^1 dx_s x_s^{N-4} (1-x_s)^3 \prod_{j \in \mathcal{S}} \int_0^1 dy^j \delta\left(\sum_{j \in \mathcal{S}} y^j - 1\right) \int_0^1 d\bar{x} \int_0^1 dx_t \int_{\omega_{\min}}^{\omega_{\max}} d\omega \sum_{s_A, s_B} f(x) . \quad (4.26)$$

We will set  $\omega_{\max}$  and  $\omega_{\min}$  below.

Next, change variables from  $\{x_s, x_t\}$  to  $\{x_u, u\}$  defined by

$$\begin{aligned} x_s &= x_u u^{1/(N-3)} , \\ x_t &= x_u (1 - u^{1/(N-3)}) . \end{aligned} \quad (4.27)$$

Note that then  $x_u = x_s + x_t$ . Our intention is to populate the region small  $x_u$ . Therefore we impose an upper bound  $x_u < x_u^{\max}$ , where  $x_u^{\max}$  is adjustable. We assume in this derivation that the support of  $f(x)$  lies in the region  $x_u < x_u^{\max}$ . Now our integral is

$$I = \prod_{j \in \mathcal{S}} \int_0^1 dy^j \delta\left(\sum_{j \in \mathcal{S}} y^j - 1\right) \int_0^1 d\bar{x} \int_0^{x_u^{\max}} dx_u \int_0^1 du \int_{\omega_{\min}}^{\omega_{\max}} d\omega \sum_{s_A, s_B} \frac{(1-x_s)^3}{N-3} x_u^{N-3} f(x) . \quad (4.28)$$

In keeping with our desire to populate the region of small  $x_u$ , we change variables to  $t$  that runs from 0 to 1 and is defined by

$$t = \frac{\log(1 + [x_u/\Delta_u]^{N-2})}{\log(1 + [x_u^{\max}/\Delta_u]^{N-2})} . \quad (4.29)$$

Here  $\Delta_u$  provides a scale such that the density of sampled points grows as  $x_u$  decreases until  $x_u$  is of order  $\Delta_u$ . The inverse relation is

$$x_u = \Delta_u \left[ (1 + [x_u^{\max}/\Delta_u]^{N-2})^t - 1 \right]^{1/(N-2)} . \quad (4.30)$$

We also change variables from  $\omega$  to

$$\tilde{\omega} = \frac{\omega - \omega_{\min}}{\omega_{\max} - \omega_{\min}} . \quad (4.31)$$

This gives

$$\begin{aligned} I = (N-4)! \prod_{j \in \mathcal{S}} \int_0^1 dy^j \delta\left(\sum_{j \in \mathcal{S}} y^j - 1\right) \int_0^1 d\bar{x} \int_0^1 dt \int_0^1 du \int_0^1 d\tilde{\omega} \frac{1}{4} \sum_{s_A, s_B} f(x) \\ \times \frac{4(1-x_s)^3 (\omega_{\max} - \omega_{\min}) \log(1 + [x_u^{\max}/\Delta_u]^{N-2})}{(N-2)!} [x_u^{N-2} + \Delta_u^{N-2}] . \end{aligned} \quad (4.32)$$

Experience with this indicates that one should choose more points where  $\bar{x}(1-\bar{x})$  is small. For this purpose, one can set

$$\begin{aligned} \bar{x} &= \frac{1}{2} (2\bar{r})^{1/(1-a)} & 0 < \bar{r} < 1/2 , \\ 1 - \bar{x} &= \frac{1}{2} (2(1-\bar{r}))^{1/(1-a)} & 1/2 < \bar{r} < 1 . \end{aligned} \quad (4.33)$$

Here  $a$  is an adjustable parameter with  $0 < a < 1$ . The inverse of this is

$$\begin{aligned} \bar{r} &= \frac{1}{2} (2\bar{x})^{1-a} & 0 < \bar{x} < 1/2 , \\ 1 - \bar{r} &= \frac{1}{2} (2(1-\bar{x}))^{1-a} & 1/2 < \bar{x} < 1 . \end{aligned} \quad (4.34)$$

The jacobian is

$$\begin{aligned} \frac{d\bar{r}}{d\bar{x}} &= \frac{1-a}{[2\bar{x}]^a} & 0 < \bar{x} < 1/2 , \\ \frac{d\bar{r}}{d\bar{x}} &= \frac{1-a}{[2(1-\bar{x})]^a} & 1/2 < \bar{x} < 1 . \end{aligned} \quad (4.35)$$

With this change of variables, we have

$$\begin{aligned}
I &= (N-4)! \prod_{j \in \mathcal{S}} \int_0^1 dy^j \delta\left(\sum_{j \in \mathcal{S}} y^j - 1\right) \int_0^1 d\bar{r} \int_0^1 dt \int_0^1 du \int_0^1 d\tilde{\omega} \frac{1}{4} \sum_{s_A, s_B} f(x) \\
&\times \frac{[2 \min(\bar{x}, 1 - \bar{x})]^a 4(1 - x_s)^3 (\omega_{\max} - \omega_{\min}) \log(1 + [x_u^{\max}/\Delta_u]^{N-2})}{(1-a)(N-2)!} [x_u^{N-2} + \Delta_u^{N-2}] .
\end{aligned} \tag{4.36}$$

From this result we can read off the density of points if we choose the  $y^j$  for  $j \in \mathcal{S}$  uniformly on the surface  $\sum y^j = 1$  and choose all the other variables above with a uniform distribution. We find

$$\rho = \frac{(1-a)(N-2)!}{[2 \min(\bar{x}, 1 - \bar{x})]^a 4(1 - x_s)^3 (\omega_{\max} - \omega_{\min}) \log(1 + [x_u^{\max}/\Delta_u]^{N-2})} \frac{\theta(x_u < x_u^{\max})}{x_u^{N-2} + \Delta_u^{N-2}} \tag{4.37}$$

A default choice for  $\Delta_u$  is

$$\Delta_u = c[\Delta_u] \bar{x}(1 - \bar{x}) |\Delta f| , \tag{4.38}$$

where  $c[\Delta_u]$  is an adjustable constant, for instance 0.1. Default choices for  $\omega_{\max}$  and  $\omega_{\min}$  are given in Eq. (4.19). A default choice for  $x_u^{\max}$  based on Eq. (4.20) is

$$x_u^{\max} = c[x_u^{\max}] \bar{x}(1 - \bar{x}) [1 + s_A(2f_A - 1)][1 + s_B(2f_B - 1)]/4 , \tag{4.39}$$

where  $c[x_u^{\max}]$  is an adjustable constant, for instance 4.

## 5 Sampling for collinear singularity

This method is to be applied in the collinear region for partons  $n$  and  $n+1$  under the circumstance that there are two other labels  $A$  and  $B$  (not equal to  $n+2$  or  $n-1$ ) such that the determinant  $S_{n+1,A}S_{n,B} - S_{n+1,B}S_{n,A}$  is suitably small and such that  $S_{n,A}$ ,  $S_{n+1,B}$ ,  $-S_{n+1,A}$ , and  $-S_{n,B}$  all have the same sign. These are the conditions that lead to having almost a ‘‘double’’ pinch in the collinear integration region.

We seek to put points near the point

$$\begin{aligned}
x^n &= f , \\
x^{n+1} &= (1 - f) ,
\end{aligned} \tag{5.1}$$

where  $f$  is defined by

$$f = \frac{S_{n+1,A} - S_{n+1,B}}{S_{n+1,A} - S_{n,A} + S_{n,B} - S_{n+1,B}} . \tag{5.2}$$

Thus  $f$  is a weighted average of

$$\begin{aligned} f_1 &= \frac{S_{n+1,A}}{S_{n+1,A} - S_{n,A}} , \\ f_2 &= \frac{-S_{n+1,B}}{S_{n,B} - S_{n+1,b}} . \end{aligned} \quad (5.3)$$

The difference  $|f_1 - f_2|$  is

$$\Delta f = \left| \frac{S_{n+1,A}S_{n,B} - S_{n+1,B}S_{n,A}}{(S_{n+1,A} - S_{n,A})(S_{n,B} - S_{n+1,B})} \right| . \quad (5.4)$$

The idea is to apply this method when the uncertainty is small,

$$\Delta f < \epsilon_{\text{coll}} , \quad (5.5)$$

where  $\epsilon_{\text{coll}}$  is a small parameter that we can adjust.

To proceed, we begin with an integral

$$I = \int_0^1 dx^0 \int_0^1 dx^1 \cdots \int_0^1 dx^N \delta\left(\sum_{i=0}^N x^i - 1\right) f(x) . \quad (5.6)$$

We introduce

$$x_s = \sum_{j \in \mathcal{S}} x^j , \quad (5.7)$$

where the set  $\mathcal{S}$  is the complement in  $\{0, 1, \dots, N\}$  of  $\{n, n+1, A, B\}$ . We suppose that  $f(x)$  has support limited to a certain region to be defined. The integration region outside of this region is covered by other methods of choosing points. We write

$$I = \int_0^1 dx_s \prod_{j \in \mathcal{S}} \int_0^1 dx^j \delta\left(\sum_{j \in \mathcal{S}} x^j - x_s\right) \prod_{i \notin \mathcal{S}} \int_0^1 dx^i \delta\left(x_s + \sum_{i \notin \mathcal{S}} x^i - 1\right) f(x) . \quad (5.8)$$

Then

$$I = \int_0^1 dx_s x_s^{N-4} (1-x_s)^3 \prod_{j \in \mathcal{S}} \int_0^1 dy^j \delta\left(\sum_{j \in \mathcal{S}} y^j - 1\right) \prod_{i \notin \mathcal{S}} \int_0^1 dy^i \delta\left(\sum_{i \notin \mathcal{S}} y^i - 1\right) f(x) , \quad (5.9)$$

where  $y^j = x^j/x_s$  for  $j \in \mathcal{S}$  and  $y^j = x^j/(1-x_s)$  for  $j \notin \mathcal{S}$ .

We can repeat this with respect to the variables  $\{y^A, y^B\}$ , defining

$$x_t = y^A + y^B . \quad (5.10)$$

We let

$$\begin{aligned}
y^n &= (1 - x_t)[f - \bar{x}] \ , \\
y^{n+1} &= (1 - x_t)[(1 - f) + \bar{x}] \ , \\
y^A &= x_t x_a \ , \\
y^B &= x_t(1 - x_a) \ .
\end{aligned} \tag{5.11}$$

Then

$$\begin{aligned}
I &= \int_0^1 dx_s x_s^{N-4} (1 - x_s)^3 \int_0^1 dx_t x_t (1 - x_t) \int_{-(1-f)}^f d\bar{x} \int_0^1 dx_a \\
&\times \prod_{j \in \mathcal{S}} \int_0^1 dy^j \delta\left(\sum_{j \in \mathcal{S}} y^j - 1\right) f(x) \ .
\end{aligned} \tag{5.12}$$

Now change variables from  $\{x_t, \bar{x}\}$  to  $\{y, r, s\}$ , where  $y$  and  $r$  are continuous variables and  $s$  is a discrete variable taking values  $\pm 1$ . We define these variables by

$$\begin{aligned}
y &= [\bar{x}^2 + (\Delta f)^2] x_t \ , \\
r &= \frac{x_t \lambda_r \Delta f}{\sqrt{\bar{x}^2 + (\Delta f)^2}} \ , \\
s &= \text{sign}(\bar{x}) \ .
\end{aligned} \tag{5.13}$$

(This is because we want this  $y$  to appear in our final density.) Here  $\lambda_r$  is an adjustable parameter. This gives

$$\begin{aligned}
I &= \int_0^1 dx_s x_s^{N-4} (1 - x_s)^3 \int_0^1 dx_a \sum_{s=\pm 1} \int_0^1 dy \int_0^1 dr \frac{1}{3} (1 - x_t) \frac{\sqrt{\bar{x}^2 + (\Delta f)^2}}{|\bar{x}| \lambda_r \Delta f} \\
&\times \prod_{j \in \mathcal{S}} \int_0^1 dy^j \delta\left(\sum_{j \in \mathcal{S}} y^j - 1\right) f(x) \ .
\end{aligned} \tag{5.14}$$

For some values in the indicated range of  $y$  and  $r$ ,  $\{x_t$  and  $\bar{x}\}$  will not be within their proper ranges. We assume that the proper theta functions are included in the definition of  $f(x)$ . Thus bad points contribute zero to the integral.

Now we want to combine  $y$  and  $x_s$ . We define

$$\begin{aligned}
x_s &= x_u u^{1/(N-3)} \ , \\
y &= x_u(1 - u^{1/(N-3)}) \ .
\end{aligned} \tag{5.15}$$

Note that then

$$x_u = y + x_s = [\bar{x}^2 + (\Delta f)^2] x_t + x_s \ . \tag{5.16}$$

Our intention is to populate the region small  $x_u$ . Now our integral is

$$I = \int_0^1 dx_u \int_0^1 dx_a \sum_{s=\pm 1} \int_0^1 du \int_0^1 dr \frac{(1-x_t)(1-x_s)^3}{3(N-3)} \frac{\sqrt{\bar{x}^2 + (\Delta f)^2}}{|\bar{x}| \lambda_r \Delta f} x_u^{N-3} \times \prod_{j \in \mathcal{S}} \int_0^1 dy^j \delta\left(\sum_{j \in \mathcal{S}} y^j - 1\right) f(x) . \quad (5.17)$$

In keeping with our desire to populate the region of small  $x_u$ , we change variables to  $t_u$  that runs from 0 to 1 and is defined by

$$t_u = \frac{x_u(1+a)}{x_u+a} . \quad (5.18)$$

Here  $a$  provides a scale such that the density of sampled points grows as  $x_u$  decreases until  $x_u$  is of order  $a$ . When  $t_u$  runs from 0 to 1,  $x_u$  runs from 0 to 1. Thus we assume that in this derivation  $f(x)$  has support in this region. This gives

$$I = (N-4)! \prod_{j \in \mathcal{S}} \int_0^1 dy^j \delta\left(\sum_{j \in \mathcal{S}} y^j - 1\right) \int_0^1 dt_u \int_0^1 dx_a \frac{1}{2} \sum_{s=\pm 1} \int_0^1 du \int_0^1 dr f(x) \times \frac{2(1-x_t)(1-x_s)^3}{3(N-3)!} \frac{\sqrt{\bar{x}^2 + (\Delta f)^2}}{|\bar{x}| \lambda_r \Delta f} \frac{(x_u+a)^2}{a(1+a)} x_u^{N-3} . \quad (5.19)$$

From this result we can read off the density of points if we choose the  $y^j$  for  $j \in \mathcal{S}$  uniformly on the surface  $\sum y^j = 1$  and choose all the other variables above with a uniform distribution. We find

$$\rho = \frac{3(N-3)!}{2(1-x_t)(1-x_s)^3} \frac{|\bar{x}| \lambda_r \Delta f}{\sqrt{\bar{x}^2 + (\Delta f)^2}} \frac{a(1+a)}{(x_u+a)^2} \frac{\theta(x_u < 1)}{x_u^{N-3}} . \quad (5.20)$$

The most important factor is the factor  $1/x_u^{N-3}$ . The factor  $1/(x_u+a)^2$  essentially restricts  $x_u$  to be of order  $a$ . The factor  $\bar{x} \Delta f / [\bar{x}^2 + (\Delta f)^2]^{1/2}$  is a constant as long as  $\bar{x}^2 \gg (\Delta f)^2$  and suppresses values of  $\bar{x}^2$  much smaller than  $(\Delta f)^2$ .

A default choice for  $a$  is

$$a = \Delta f . \quad (5.21)$$

With this choice,

$$\Delta f \frac{a(1+a)}{(x_u+a)^2} \sim 1 \quad (5.22)$$

for  $x_u \leq a$ . An alternative would be  $a = (\Delta f)^2$ . A default choice for  $\lambda_r$  is  $1/\sqrt{\Delta f}$ .