It is described how the method of sector decomposition can serve to disentangle overlapping infrared singularities, in particular those occurring in the calculation of the real emission part of $e^+e^-\rightarrow 2$ jets and $e^+e^-\rightarrow 3$ jets at NNLO.

2. SECTOR DECOMPOSITION

The method of sector decomposition acts on parameter integrals and serves to factorize singularities which have an overlapping structure, as in the following simple example:

$I = \int_0^1 dx_1 \int_0^{x_1} dx_2 \frac{x_1^{-1-\epsilon}}{x_1 + x_2} [x_1 + x_2]^{-1}$

Decomposing the parameter space into two sectors where the integration variables are ordered and remapping the integration range to the unit square factorizes the singularity:

$I = \int_0^1 dx_1 \int_0^{x_1} dx_2 \frac{x_1^{-1-\epsilon}}{x_1 + x_2} [\Theta(x_1 - x_2) + \Theta(x_2 - x_1)]$

(1) \hspace{1cm} (2)
The substitution $x_2 = x_1 t_2$ in sector (1) and $x_1 = x_2 t_1$ in sector (2) leads to

$$I = \int_0^1 dx_1 x_1^{-1-\epsilon} \int_0^1 dt_2 (1 + t_2)^{-1}$$

$$+ \int_0^1 dx_2 x_2^{-1-\epsilon} \int_0^1 dt_1 t_1^{-1-\epsilon} (1 + t_1)^{-1}.$$

For more complicated functions, this procedure may have to be iterated, but the principle is simple and easily automated. This is particularly true for multi-loop integrals because they have, after Feynman parametrization and integration over the loop momenta, the following universal form ($L$ is the number of loops, $N$ the number of propagators and $D$ the space-time dimension)

$$G = (-1)^N \Gamma(N - LD/2) \int \prod dx_j \delta(1 - \sum_{i=1}^N x_i) \frac{U(x)^{N-(L+1)D/2}}{\Phi(x, \{s, m^2\})^{N-LD/2}},$$

where $U$ and $\Phi$ are polynomials in the Feynman parameters and $\Phi$ also contains kinematic invariants. Applying the sector decomposition algorithm [14] to loop integrals in the form [10] isolates the dimensionally regulated poles in terms of factorizing Feynman parameters. Then subtractions of the singularities are carried out, using identities like

$$\int_0^1 dx_1 x_1^{-1+\kappa} \Phi(x_1, \hat{x})$$

$$= \frac{1}{\kappa} \int_0^1 dx_1 \Phi(x_1, \hat{x}) \delta(x_1) +$$

$$\int_0^1 dx_1 x_1^{-1+\kappa} [\Phi(x_1, \hat{x}) - \Phi(0, \hat{x})],$$

where $\hat{x} = x_2, \ldots, x_N$ and $\lim_{x_1 \to 0} \Phi(x_1, \hat{x})$ is finite by construction, such that the second term in [2] is a plus distribution:

$$\int_0^1 dx_1 x_1^{-1+\kappa} [\Phi(x_1, \hat{x}) - \Phi(0, \hat{x})]$$

$$= \sum_{n=0}^{\infty} (\kappa \epsilon)^n \int_0^1 dx_1 \left[ \ln^n(x_1) \right] \frac{\Phi(x_1, \hat{x})}{x_1}.$$

Doing these subtractions for all $x_i$ results in a Laurent series

$$I = \sum_{k=-2L}^{b} \epsilon^k C_k + O(\epsilon^{b+1}),$$

where the order $b$ of expansion in $\epsilon$ is in principle only limited by CPU time. However, the pole coefficients $C_k$ being sums of complicated parameter integrals, their analytical evaluation is in general impossible. Therefore they are integrated numerically. For multi-loop integrals involving more than one kinematic invariant, Euclidean points have to be chosen in order to have stable numerics. In this way, results have been obtained [18] for example for massless 2-loop 4-point functions with 2 off-shell legs, where no analytical results exist yet, all 4-point master integrals needed for the calculation of 2-loop Bhabha scattering with massive fermions (analytical results exist for two of them [19][20][21]), two-point functions with 4 and 5 loops, and for the planar massless 3-loop 4-point function with on-shell legs calculated analytically by V.A. Smirnov [22].

3. PHASE SPACE INTEGRALS

The phase space integration for the production of $N$ massless particles $q \to p_1, \ldots, p_N$ can be written as

$$\int d\Phi_{1 \to N} = (2\pi)^{N-D(N-1)}$$

$$\prod_{j=1}^{N} d^D p_j \delta^+(p_j^2) \delta(q - \sum_{i=1}^{N} p_i)$$

$$= (2\pi)^{N-D(N-1)} 2^{1-N}$$

$$\prod_{j=1}^{N-1} d^{D-1} p_j \frac{\Theta(E_j)}{E_j} \delta^+([q - \sum_{i=1}^{N-1} p_i]^2).$$

At this point one could pick a particular frame and integrate over energies $E_j$ and angles $\theta_j$, but for our purposes it is more convenient to integrate over the scaled invariants $s_{ij}/q^2$, $s_{ij} = (p_i + p_j)^2$, because in this way the singularities are located at the origin of parameter space and no particular axis is preferred. The transformation to the
introduction of a Jacobian which is proportional to
the square root of the determinant of the Gram
matrix $G_{ij} = 2p_i p_j$. The phase space then takes the form

$$\int d\Phi_{1\to N} = C^{(N)}_Γ (q^2)^{(N-1)D/2-N} \int \prod_{j=1}^{n_s} dx_j \delta(1 - \sum_{i=1}^{n_s} x_i) \left[ \frac{N(N-1)}{D(N+1)} \right] \frac{D(N+1)}{2} \Theta(\Delta N)$$ (3)

$$\begin{align*}
n_s &= N(N-1)/2 \\
\Delta N &= | \det G[q^2]^{-N} \\
C^{(N)}_Γ &= (2\pi)^{N-D(N-1)/2} 2^{-N} \Gamma(D/2) \times V(D-1) \ldots V(D-N+1) \\
V(D) &= 2\pi^{D/2} / \Gamma(D/2).
\end{align*}$$

3.1. 1 → 4 phase space

As an example, let us consider the integration of some squared matrix element $|M_4|^2$ over the 1 → 4 partonic phase space, relevant for the calculation of $e^+ e^- \rightarrow 2$ jets at NNLO:

$$\begin{align*}
\int d\Phi_{1\to 4} &= C^{(4)}_Γ (q^2)^{3D/2-5} \\
\int \prod_{j=1}^{6} dx_j \delta(1 - \sum_{i=1}^{6} x_i) |M_4|^2 \\
[-\lambda(x_1 x_6, x_2 x_5, x_3 x_4)]^{-1/2-\epsilon} \Theta(\lambda)
\end{align*}$$ (4)

$$\lambda(x, y, z) = x^2 + y^2 + z^2 - 2(xy + xz + yz).$$

The matrix element is of the form

$$|M_4|^2 \sim \frac{P_1(\bar{x}, \epsilon)}{(x_2 + x_4 + x_6)(x_3 + x_5 + x_6)x_4} + \frac{P_2(\bar{x}, \epsilon)}{x_2(x_2 + x_4 + x_6)^2} + \ldots,$$

where the $P_k(\bar{x}, \epsilon)$ are some polynomials in the variables $x_i$. We again see the sums of Feynman parameters in the denominator, corresponding to triple invariants $s_{ijk}$, giving rise to an overlapping structure. Therefore, the form of the integral (4) is very similar to the one in eq. (1) for loop integrals and the overlapping singularities can be disentangled by the same principle. However, there are also very important differences to loop integrals. The most important one consists in the fact that in phase space integrals, non-polynomial structures (square roots) appear. For example, solving the constraint $-\lambda > 0$ in (4) for $x_6$ leads to $x_6^- < x_6 < x_6^+$ with $x_6^\pm = (\sqrt{x_4 x_6} \pm \sqrt{x_3 x_4})^2 / x_1$. The substitution $x_6 \rightarrow (x_6^+ - x_6^-) y_6 + x_6^- \text{ remaps the integration range of } x_6 \text{ to an integral from } 0 \text{ to } 1 \text{ again and factorizes the } \lambda\text{-term:}$

$$\begin{align*}
[-\lambda]^{-1/2-\epsilon} &= [x_1^2 (x_6^+ - x_6)(x_6 - x_6^-)]^{-1/2-\epsilon} \\
&\rightarrow [y_6 (1 - y_6)]^{-1/2-\epsilon} [x_1(x_6^+ - x_6^-)]^{-1/2-\epsilon}.
\end{align*}$$

However, it is possible to eliminate the square roots by quadratic transformations, except in factors like $(1 - y_6^2)^{-1/2-\epsilon}$, which do not lead to singularities in $\epsilon$ and therefore are not subject to further sector decomposition. This nice feature will be spoiled in the 1 → 5 case.

The implementation of sector decomposition for the 1 → 4 phase space served for the calculation of all master phase space integrals which are needed for any 1 → 4 process in massless QCD. These master integrals have been derived and calculated analytically as well as numerically in [12].

Moreover, the method also can deal with the full matrix element without reduction to master integrals. This has been demonstrated in [10]. To split the calculation into smaller pieces, one can write the squared matrix element as a sum over different topologies. As the calculation is naturally parallelized by this subdivision into topologies, the overall runtime is given by the most difficult topology, which took about 9 hours for a precision of 0.1% and less than two hours for a precision of 1% on a Pentium IV 2.2 GHz PC.

3.2. 1 → 5 phase space

The 1 → 5 partonic phase space, relevant for the calculation of $e^+ e^- \rightarrow 3$ jets at NNLO, in-
volves the integration over 9 independent invariants:
\[
\int d\Phi_{1\rightarrow5} = C_5^{(5)} \int \prod_{j=1}^{10} dx_j \delta(1 - \sum_{i=1}^{10} x_i) \left| \Delta_5(\vec{x}) \right|^{(D-6)/2} \Theta(\Delta_5).
\]
Note that \( C_5^{(5)} \sim V(D - 4) = 2\pi^{-\epsilon}/\Gamma(-\epsilon) \) is of order \( \epsilon \), therefore the integral \( \int d\Phi_{1\rightarrow5} \) contains a fake singularity in \( \left| \Delta_5(\vec{x}) \right|^{(D-6)/2} = \left| \Delta_5(\vec{x}) \right|^{-1-\epsilon} \), but this presents no problem for sector decomposition as the algorithm will extract the singular factor and the \( \epsilon \)-expansion subroutine will take the prefactor of order \( \epsilon \) into account, such that the fake singularity will be eliminated automatically. What is more of a problem are the non-polynomial structures which occur here, because denominators of the form \( g(x, y) = a + x + y - \sqrt{a^2 + x + y} \), where \( a \) is a constant, can produce a singularity for \( x, y \rightarrow 0 \) without having the right scaling behaviour amenable to sector decomposition. The task is to transform such terms away without increasing the complexity of the integrand too much. It should be noted that the size of the expressions in the 1 \( \rightarrow \) 5 case is considerably larger than in the 1 \( \rightarrow \) 4 case, such that it becomes much more important to produce as few subsectors as possible.

The simplest example to calculate is the 5-particle phase space volume without any matrix element. In \( \int d\Phi_{1\rightarrow5} \) a general analytic expression for the 1 \( \rightarrow \) \( N \) phase space volume is given, such that the numerical result can be easily checked. By sector decomposition, one obtains
\[
\int d\Phi_{1\rightarrow5} = \frac{(4\pi)^{4\epsilon-7}}{\Gamma(1-2\epsilon)\Gamma(2-2\epsilon)} \left[ 0.00347 + 0.05469\epsilon + 0.44336\epsilon^2 + 2.47424\epsilon^3 + 10.7283\epsilon^4 + \mathcal{O}(\epsilon^5) \right]
\]
which agrees with the analytical result to an accuracy of 0.5% after a runtime of about 10 minutes.

3.3. One loop plus single real emission

Apart from the double real emission and the two-loop virtual contributions to the cross section of \( e^+e^- \rightarrow \) jets at NNLO, there is also a contribution where one-loop virtual corrections are combined with single real emission. In this class, the most complicated diagram which can occur in the calculation of \( e^+e^- \rightarrow 2 \) jets is a box graph with one off-shell leg. This type of diagram can easily be calculated by sector decomposition: The one-loop box can be expressed by Hypergeometric functions \( _2F_1(1, -\epsilon, 1-\epsilon; x_i/x_j) \). Then the parameter representation of the Hypergeometric functions can be used and the resulting one-dimensional parameter integrals can be combined with the ones for the 3-particle phase space to end up with a 4-dimensional parameter integral which can be directly fed into the sector decomposition routine.

For \( e^+e^- \rightarrow 3 \) jets, the most complicated one-loop diagrams are pentagons with one off-shell leg. These could be reduced to boxes by standard reduction techniques \cite{23,24}, but as the reduction introduces inverse determinants of kinematic matrices which may lead to numerical instabilities, it is more convenient to apply the sector decomposition routine for loop integrals directly to the pentagon which is of the form
\[
I_5 = -\Gamma(3+\epsilon) \int \prod_{i=1}^{5} dz_i \delta(1 - \sum_{i=1}^{5} z_i) \mathcal{F}^{3+\epsilon}
\]
\[
-\mathcal{F} = s_{12} z_1 z_5 + s_{23} z_1 (z_4 + z_1 + z_5) + s_{13} z_5 (z_1 + z_2) + s_{14} z_5 (z_1 + z_2 + z_3) + s_{24} z_1 (z_4 + z_5) + s_{34} (z_1 + z_2) (z_4 + z_5).
\]
After sector decomposition in the variables \( z_i \), one obtains an expression where the poles of the virtual integral already have been extracted:
\[
I_5 = \sum_{\alpha=0}^{2} P_\alpha/e^\alpha,
\]
\[
P_\alpha = \int_0^1 4^{-\alpha} \prod_{i=1}^{1} dt_i G(t_i, s_{12}, \ldots, s_{34}),
\]
\[
\lim_{t_i \rightarrow 0} G \neq 0.
\]
This expression can then be inserted into the 4-particle phase space and one can proceed with decomposition in the scaled invariants \( x_1, \ldots, x_6 \). Note that no problems with thresholds will occur here as the kinematics is such that all invariants \( s_{ij} \) are non-negative.
4. SUMMARY AND OUTLOOK

The automated sector decomposition algorithm is a powerful method to isolate overlapping infrared poles and to calculate numerically not only multi-loop integrals, but also phase space integrals where some of the particles can become theoretically unresolved, leading to infrared singularities. In particular, the method allows the calculation of the one-loop plus single real emission and the double real emission contribution to $e^+e^- \rightarrow 2$ or 3 jets at NNLO without having to establish a subtraction scheme and to integrate analytically over complicated subtraction terms. The inclusion of a measurement function also does not present a problem, as has been demonstrated already in [17], such that a fully differential Monte Carlo program can be constructed based on this method. The only drawback of the method is the fact that it generates a large number of functions, but it has been shown already that in the case of $e^+e^- \rightarrow 2$ jets at NNLO, this does not lead to unacceptable integration times. Further, the functions are numerically well-behaved by construction. How the NNLO calculation of the process $e^+e^- \rightarrow 3$ jets with this method performs numerically will turn out in the near future.

The generalization to other processes than $e^+e^-$ annihilation is feasible, but cases where some of the kinematic invariants take negative values cannot be treated without further development of the method.

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