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Top quark pairs at two loops and Reduze 2

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We report on progress for the analytical calculation of the two–loop corrections to top quark pair production at hadron colliders. For the light fermionic corrections in the gluon channel, we discuss the analytical solution for the master integrals of a non-planar double box with a massive propagator. The result in terms of Goncharov's multiple polylogarithms is handled using systematic reductions based on the symbol map and the coproduct. We discuss new features of the computer program Reduze 2. It provides a fully distributed variant of Laporta's algorithm to reduce loop integrals. New graph matroid based algorithms allow to calculate shift relations between Feynman integrals in a fully automated way.

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1. Top quark pair production at NNLO

Top quark pair production has been studied in detail both at the Tevatron and the LHC. In order to match the experimental precision, theoretical predictions beyond the next-to-leading order (NLO) are necessary [1]. Several precision predictions for the total cross section and some distributions are available [2, 3, 4, 5, 6], taking into account different approximations to the next-to-next-to-leading-order (NNLO) corrections and resummations of logarithmic terms. For the quark initiated channels, an exact NNLO prediction for the total cross section was presented [7, 8, 9] employing semi-numerical methods.

For both, the quark and the gluon initiated channels, different building blocks of the NNLO prediction are known also analytically. For the two–loop corrections, this includes the high-energy limit [10, 11] and the infrared poles with full mass dependence [12]. In [13, 14, 15], the fermionic and leading colour contributions in the $q\bar{q}$ channel and the leading colour contributions in the gg channel were given. The one-loop squared contributions are known [16, 17, 18, 19] for some time. Subtraction terms needed to combine the results with the contributions for one or two additional partons in the final state were presented in [20, 21, 22, 23, 24, 25].

Our setup for computing the analytical two-loop corrections to top quark pair production is as follows. We generate diagrams with `QGRAF` [26], reduce the loop integrals and compute the interference terms with `Reduze 2` [27, 28]. For the master integrals, we employ the method of differential equations [29]. Integration constants are fixed by evaluating Mellin-Barnes representations in different kinematical limits. For planar topologies we use `AMBRE` [30] for the generation of Mellin-Barnes representations and `MB.m` [31] for their expansions.

2. Light fermionic two–loop corrections to $gg \to t\bar{t}$

For the two–loop corrections to $gg \to t\bar{t}$ which involve a closed light fermion loop [32], we computed 11 new master integrals in terms of Goncharov's multiple polylogarithms (GPLs) [33] via the method of differential equations. The most involved topology is a non–planar double box with one massive propagator, see figure 1. A major source of complexity originates from the fact that this non-planar topology has cuts in the Mandelstam variables s, t and u at the same time. We find three master integrals for this topology. For the kinematic variables $x = (\beta-1)/(\beta+1)$ and $y = -t/m^2$ and a suitable choice of master integrals, the differential equations decouple after expansion in $\varepsilon = (4-d)/2$ and can be integrated. Here, $\beta = \sqrt{1-4m^2/s}$, m is the top mass and d the number of space-time dimensions. We fix the integration constants from symmetry conditions as well as regularity constraints and asymptotic expressions obtained from an explicit Mellin-Barnes calculation. The Mellin-Barnes representation was obtained (for a different choice of master integrals) by direct integration of Feynman parameters similar to the massless case [34]. Our Mellin-Barnes setup was successfully cross-checked against numerical samples obtained with `SecDec 1` [35, 36, 37] for the leading poles. For the result we employ GPLs defined recursively by $G(\{w_1,w_2,\dots,w_n\},z) = \int_0^z G(\{w_2,\dots,w_n\},z')\mathrm{d}z'/(z'-w_1)$ with the special rules $G(\{\},z) = 1$ and $G(\{w_1,\dots,w_n\},z) = \ln^n z/n!$ for $w_1 = \dots = w_n = 0$, see also [38, 39]. Our result for the master integrals up to the finite pieces involves $\mathscr{O}(10^3)$ GPLs with maximal weight 4. These functions are

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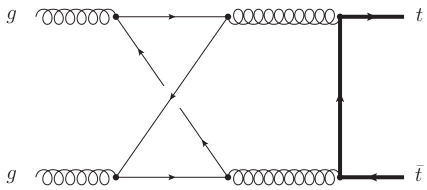

Figure 1: A non–planar double box diagram with a massive propagator (thick line) contributing to the light fermionic corrections to top quark pair production in the gluon channel.

$G(\{w_1,\ldots,w_{n\leq 4}\},y)$ for $w_i \in \{0,-1,-x,-1/x,-1/x-x,-1/x-x+1\}$ and $G(\{w_1,\ldots,w_{n\leq 4}\},x)$ for $w_i \in \{0,\pm 1,\pm i,(1\pm i\sqrt{3})/2\}$.

The complexity of these multiple polylogarithms makes it difficult to handle them with traditional methods. A fast and reliable numerical evaluation via real valued functions, expansions for asymptotic kinematics and establishing special features such as symmetries requires a systematic approach to functional identities between multiple polylogarithms. The *symbol map* associates to each multiple polylogarithm a linear combination of tensors which fulfil a "generalised logarithm law" in form of simple algebraic rules. It was demonstrated [40] in the context of $N=4$ Super-Yang-Mills theory that the symbol captures essential information about the multiple polylogarithms in a form suitable to allow for drastic simplifications of amplitudes, see also [41]. We successfully applied symbol map techniques to our results in the context of QCD with a mass and were able to considerably simplify expressions for poles in ε. For example, the $1/\varepsilon$ pole of the corner integral for the non–planar topology discussed above contained 39 GPLs with weight 3, while the simplified expression contains only one weight 3 classical polylogarithm: $\mathrm{Li}_3(y_1 z_1/(y_1+z_1))$ with $y_1 = y+1$, $z_1 = z+1$ and $z = -u/m^2$. Recently, algorithmic approaches have been proposed in [42] for the symbol calculus.

A breakthrough for the domain of applicability of these methods has been achieved by extending [43] the symbol calculus employing the *coproduct* [44]. In this way, also subleading degree terms can be treated algebraically except for pure constants, which may be addressed by numerically assisted methods. This was demonstrated in [43] for multi–scale two–loop QCD corrections. We successfully apply these methods to algorithmically reduce our results for top quark pair production to a set of independent functions. Our results show that also for the finite terms of the ε expansion significant simplifications can be achieved, although not necessarily as dramatic as for the $1/\varepsilon$ contribution described above. In contrast to the QCD application in [43], our results contain genuine multiple polylogarithms, which can't be expressed in terms of classical polylogarithms alone but require functions such as e.g. $\mathrm{Li}_{22}(u,v)$.

It will be interesting to see to what extend symbol calculus based methods can be used directly for *solving* master integrals in the multivariate case, see for example [45, 46].

3. Reduze 2

Reduze is a computer program written in C++ to reduce Feynman integrals. It represents a central tool for our calculations of two–loop corrections to top quark pair production. Version 2 [28] provides a major rewrite and extension of its predecessor Reduze 1 [27]. New features include

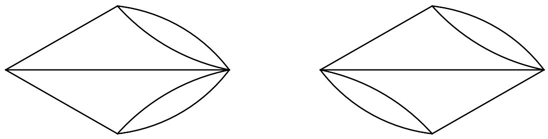

Figure 2: Two vacuum graphs which are not isomorphic but have equivalent scalar propagators nevertheless. The graphs are related by a twist and their matroids are isomorphic.

the distributed reduction of *single topologies* on multiple computers or processor cores via a distributed variant of Laporta's algorithm [47, 48, 49]. The parallel reduction of *different topologies* is supported via a modular, load balancing job system. We observe significant speed-ups for using up to $\mathscr{O}(100)$ cores in applications for $t\bar{t}$ production.

Reduze 2 also provides fast graph and matroid based algorithms, which allow for the identification of equivalent topologies and integrals. These algorithms automatically detect and explicitly construct shifts of loop momenta such that one set of propagators is transformed into another set of propagators. Where applicable, this transformation may be supplemented by a crossing of external legs. These *shift relations* can be used to automatically eliminate ambiguities between loop integrals in the reductions or to map graphs generated by other programs such as QGRAF to integral families (complete sets of propagators). Reduze 2 provides support for multiple integral families and can therefore essentially work out reductions for full amplitudes in terms of unique master integrals in a fully automated fashion. There may be shift symmetries which map a sector (selection of propagators from an integral family) but not every integral of it onto itself. We wish to point out, that in some cases these symmetries provide additional reductions which are not found by typical finite sets of integration-by-parts relations.

We propose a new shift finding algorithm to find a possible shift relation between the *propagators* of two graphs via a *matroid isomorphism* test. The latter is reduced to graph isomorphism tests for twisted graphs.

Note that a shift relation may exist even if two graphs are not isomorphic, see figure 2 for an example. A more appropriate object to consider is the matroid rather the graph itself. In this context, matroids generalise the concept of a graph by taking into account only the linear dependencies of the graph edges without reference to the vertices. For simplicity, let us first restrict to biconnected vacuum graphs, where all propagators have the same mass. The relevant information of such a graph is encoded in the first Symanzik polynomial ($\mathscr{U}$ polynomial). It was observed in [50] that two such $\mathscr{U}$ polynomials are isomorphic exactly if their matroids are isomorphic. In turn, the two graph matroids are isomorphic exactly if the two graphs are isomorphic after a series of twists. A twist breaks a graph into pieces by disconnecting edges at two vertices and reconnecting the subgraphs with flipped orientation.

Generalising the idea to cases with external momenta and different internal masses we end up with the following algorithm to find a possible shift between two sets of propagators:

1. Generate graphs for each of the two sets of propagators.

2. Colour the edges according to the masses (prolong lines by introducing two–point vertices).

3. For each graph, connect the external legs with a new vertex.

4. Decompose each graph into triconnected components to find all possible twists.

5. Minimise each graph by performing twists (remove auxiliary vertices from twisted graph and map to canonical label accounting for graph isomorphisms).

6. Check for graph isomorphism between minimised graphs.

In our tests, this method outperforms a direct combinatorial matching of propagators by orders of magnitude and is thus applicable to higher loop orders.

4. Conclusion

Considerable progress was made towards the complete NNLO prediction for top quark pair production at hadron colliders. We discussed new ingredients such as an analytical result for the light fermionic two–loop corrections in the gluon channel. The techniques and tools employed to obtain them are useful also for other processes. The symbol and coproduct calculus for Goncharov's multiple polylogarithms represents a significant step forward in the accessibility and automated calculation of analytical results for multi-scale amplitudes beyond the one-loop approximation. With Reduze 2 an open source program is available for the fully distributed reduction of loop integrals. Moreover, the package provides new graph and matroid based algorithms to calculate shift relations for Feynman integrals.

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