Multiloop computation in perturbative QCD : technological advancement and automation

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DESY-RISC collaboration
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Success of a theory lies in absolute predictions of the experiments.

The Standard Model is the most successful theory in describing the elementary particles and their fundamental interactions, due to combined effort from both the magnificent experiments like Tevatron, HERA, LHC etc. and precise theory predictions, namely perturbative calculations.

Tevatron	LHC	FCC/ILC
the top quark	the Higgs boson	BSM physics?!
fundamental laws $\sim 10\%$	fundamental laws $\sim 5\%$	more precision!
agreement with NLO theory predictions	agreement with NNLO theory predictions	More precise theory predictions needed!

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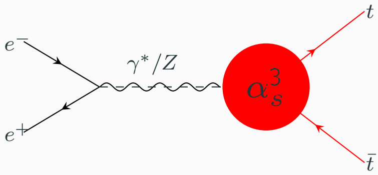

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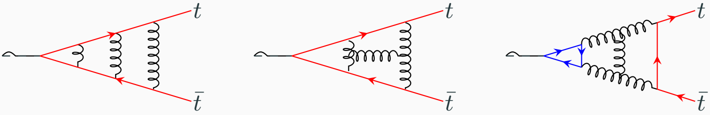
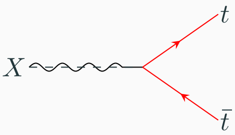


+ many more

Notation

The process

We consider the decay of a color neutral massive particle to a pair of heavy quark of mass m.



Notation

$$X(q) \to t(q_1) + \bar{t}(q_2)$$

$$X = V, A, S, P$$

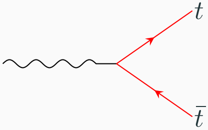
$$s = \frac{q^2}{m^2} = -\frac{(1-x)^2}{x}$$

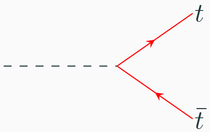
The general structure

Vector and Axial Vector

V: $-i\delta_{ij}v_Q\left(\gamma^\mu\, F_{V,1} + \frac{i}{2m}\sigma^{\mu\nu}q_\nu\, F_{V,2}\right)$

A: $-i\delta_{ij}a_Q\left(\gamma^\mu\gamma_5\, F_{A,1} + \frac{1}{2m}q^\mu\gamma_5\, F_{A,2}\right)$





Scalar and Pseudo Scalar

$-\frac{m}{v}\delta_{ij}\left[s_Q F_S + i p_Q \gamma_5 F_P\right]$

Computational details

The generic procedure

$d = 4 - 2\epsilon$

- Draw the Feynman diagrams -> QGRAF [Nogueira]

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- Now the general form

$$\int \frac{d^d l_1}{(2\pi)^{d/2}} \frac{d^d l_2}{(2\pi)^{d/2}} \frac{d^d l_3}{(2\pi)^{d/2}} \frac{\text{const} \times \text{Poly}(s) \times \text{DotProduct}(l_1, l_2, l_3, q_1, q_2)}{l_1^2 l_2^2 l_3^2 \cdots (l_2 - p_1)^2 \cdots}$$

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- Decomposition of the dot products to obtain scalar integrals

$$\frac{2l.p}{l^2(l-p)^2} = \frac{l^2 - (l-p)^2 + p^2}{l^2(l-p)^2} = \frac{1}{(l-p)^2} - \frac{1}{l^2} + \frac{p^2}{l^2(l-p)^2}$$

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- Numerous identity relations (IBPs) among scalar integrals : reduce number of integrals drastically $\Rightarrow$ compute the remaining integrals

Integration by parts identities (IBPs)

- *IBPs* : reduce the number of integrals to compute [Tkachov, Chetyrkin]

Generalization of Gauss's theorem in d dimension

Within dimensional regularization, all integrals in d dimension are well-defined and convergent $\Rightarrow$ integrand must be zero at boundary

$$\int \prod_{i=1}^{l} \mathcal{D}^d l_i \frac{\partial}{\partial l_j^\mu} \left(\frac{v^\mu}{D_1^{n_1} \dots D_m^{n_m}} \right) = 0 \quad \Big|_{v \equiv l,p}$$

Example : Consider

$$\mathcal{I}(n) = \int \frac{d^d l}{(2\pi)^{d/2}} \frac{1}{l^2 (l-p_1)^2 ((l-p_1-p_2)^2)^n}$$

The identity for $v \equiv l$ gives a recursion relation

$$\mathcal{I}(n+1) = (-1)^n \frac{(d-(n+3)) \cdots (d-4)(d-3)}{n! s^n} \mathcal{I}(1)$$

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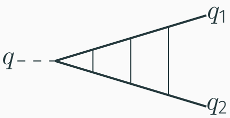
- $\sim 10^6$ identities for our process
- So the problem boils down to solve an algebraic linear system of equations relating the integrals - several programs (AIR, FIRE, Kira, LiteRed ...) available - we use CRUSHER [Marquard, Seidel]

Computing the master integrals

A scalar integral can be expressed as

$$J(\nu_1, \dots, \nu_n) = \left((4\pi)^{2-\epsilon} e^{\epsilon\gamma_E}\right)^3 \int \frac{d^d l_1}{(2\pi)^d} \frac{d^d l_2}{(2\pi)^d} \frac{d^d l_3}{(2\pi)^d} \frac{1}{D_1^{\nu_1} \dots D_n^{\nu_n}}$$

For example



$$\begin{aligned} &l_1^2 - m^2, (l_1 - q)^2 - m^2, (l_1 - l_2)^2, \\ &l_2^2 - m^2, (l_2 - q)^2 - m^2, (l_2 - l_3)^2, \\ &l_3^2 - m^2, (l_3 - q)^2 - m^2, (l_1 - q_1)^2 \end{aligned}$$

To evaluate the integral $\rightarrow$ Feynman parametrization, Mellin-Barnes ...
We use the method of differential equations!

Using differential equations

$$\frac{q^2}{m^2} = -\frac{(1-x)^2}{x}$$

The integral is a function of d, q^2 and m^2.

$$J(1,1,1,1,1,1,1,1,1) \equiv f(d,\, q^2,\, m^2) \equiv f(d,\, x)$$

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$$\frac{d}{dx} J_i = \text{some combinations of integrals}$$

$$\Downarrow \text{ IBP identities}$$

$$= \sum_j c_{ij} J_j$$

c_{ij}'s are rational function of d and x.

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$$d_x \begin{pmatrix} J_1 \\ J_2 \\ J_3 \\ J_4 \\ \vdots \\ J_n \end{pmatrix} = \begin{bmatrix} \bullet & \bullet & \bullet & \bullet & \cdots & \bullet \\ \bullet & \bullet & \bullet & \bullet & \cdots & \bullet \\ \bullet & \bullet & \bullet & \bullet & \cdots & \bullet \\ \bullet & \bullet & \bullet & \bullet & \cdots & \bullet \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \bullet & \bullet & \bullet & \bullet & \cdots & \bullet \end{bmatrix} \begin{pmatrix} J_1 \\ J_2 \\ J_3 \\ J_4 \\ \vdots \\ J_n \end{pmatrix}$$

$$d_x \mathbb{J} = \mathbb{A}(d, x)\mathbb{J}$$

Canonical Basis

The choice of MIs is not unique!
The idea is to find a basis such that the deqs decouple as $\epsilon \to 0$

[Kotikov; Henn]

$$d_x \tilde{\mathbb{J}} = \epsilon \tilde{\mathbb{A}}(x) \tilde{\mathbb{J}}$$

Now one can perform Laurent series expansion in ϵ and trivially solve the deqs as at each order the homogeneous solutions are constants.

Algorithm to find such basis by [Lee]
and implementation in `Epsilon, Canonica` ...

Drawback : Finding such a basis is not always possible.

Generic Basis

$$d_x \begin{pmatrix} J_1 \\ J_2 \\ J_3 \\ J_4 \\ \vdots \\ J_n \end{pmatrix} = \begin{bmatrix} \bullet & \bullet & \bullet & \bullet & \cdots & \bullet \\ \bullet & \bullet & \bullet & \bullet & \cdots & \bullet \\ \bullet & \bullet & \bullet & \bullet & \cdots & \bullet \\ \bullet & \bullet & \bullet & \bullet & \cdots & \bullet \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \bullet & \bullet & \bullet & \bullet & \cdots & \bullet \end{bmatrix} \begin{pmatrix} J_1 \\ J_2 \\ J_3 \\ J_4 \\ \vdots \\ J_n \end{pmatrix}$$

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To solve such a system, it would be best to organize it in such a way that it diagonalizes, or at least it takes a block-triangular form.

$$d_x \begin{pmatrix} J_1 \\ J_2 \\ J_3 \\ J_4 \\ \vdots \\ J_n \end{pmatrix} = \begin{bmatrix} \bullet & \bullet & \bullet & \bullet & \cdots & \bullet \\ 0 & \bullet & \bullet & \bullet & \cdots & \bullet \\ 0 & \bullet & \bullet & \bullet & \cdots & \bullet \\ 0 & 0 & 0 & \bullet & \cdots & \bullet \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \bullet \end{bmatrix} \begin{pmatrix} J_1 \\ J_2 \\ J_3 \\ J_4 \\ \vdots \\ J_n \end{pmatrix}$$

Let's consider the 12^{th} blob from below

$$\frac{d}{dx}\begin{pmatrix} J_1 \\ J_2 \\ J_3 \end{pmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} \\ c_{21} & c_{22} & c_{23} \\ c_{31} & c_{32} & c_{33} \end{bmatrix}\begin{pmatrix} J_1 \\ J_2 \\ J_3 \end{pmatrix} + \begin{pmatrix} R_1(\epsilon, x) \\ R_2(\epsilon, x) \\ R_3(\epsilon, x) \end{pmatrix},$$

$$c_{11} = \frac{(7 + 6x + 7x^2 - 2d(1 + x + x^2))}{x(1 + x)^2},$$

$$c_{12} = \frac{(-4 + d)(-10 + 3d)}{2(-3 + d)^2(1 + x)^2},$$

$$c_{13} = \frac{(d^2(15 + 8x + 15x^2) + 8(20 + 9x + 20x^2) - 2d(49 + 24x + 49x^2))}{4(-3 + d)^2 x(1 + x)^2}, \ldots$$

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Each order in ϵ-expansion gives a much simpler form

$$\frac{d}{dx}\begin{pmatrix} J_1^{-3} \\ J_2^{-3} \\ J_3^{-3} \end{pmatrix} = \begin{bmatrix} \frac{1}{x} + \frac{2}{1-x} & 0 & \frac{1}{1+x} - \frac{2}{x} - \frac{3}{1-x} \\ -\frac{1}{x} + \frac{2}{1+x} & \frac{1}{1+x} - \frac{1}{x} - \frac{1}{1-x} & \frac{1}{x} - \frac{2}{1+x} \\ \frac{1}{x} + \frac{2}{1-x} & 0 & \frac{1}{1+x} - \frac{2}{x} - \frac{3}{1-x} \end{bmatrix}\begin{pmatrix} J_1^{-3} \\ J_2^{-3} \\ J_3^{-3} \end{pmatrix} + \begin{pmatrix} R_1^{-3}(x) \\ R_2^{-3}(x) \\ R_3^{-3}(x) \end{pmatrix},$$

Algorithm

- A natural first step is to reduce the system to a higher order equation in a single unknown.
  `Note that, the inverse operation is trivial!`
- The classical/naive method to achieve this uncoupling is the cyclic vector algorithm. But, it gives a complicated decoupled equation.
- Use smarter uncoupling algorithms, e.g. `Zürcher` algorithm.
- The homogeneous solutions and uncoupling procedure are similar for each order.
- Now, what remains is to integrate the nonhomogeneous parts.

`Sigma` [Schneider], `OreSys` [Gerhold, Schneider]
and `HarmonicSums` [Ablinger, Blümlein, Schneider]

Iterated integrals and Harmonic polylogarithms (HPLs)

The nonhomogeneous parts have the following structure

$$\int dx\ K_{m_n}(x)\ f(x, \ln(x), \mathrm{Li}_n(x), \ldots)$$

$$K_m(x) = \left\{\frac{1}{x}, \frac{1}{1-x}, \frac{1}{1+x}, \frac{1}{1-x+x^2}, \frac{x}{1-x+x^2}\right\} \equiv \left\{0, 1, -1, \{6,0\}, \{6,1\}\right\}$$

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On the other hand, given a set of integration kernels $K_i(t)$, one can define

$$\mathcal{I}(m_n, \ldots m_1, x) = \int_{x_0}^{x} K_{m_n}(t)\mathcal{I}(m_{n-1}, \ldots m_1, t) dt$$

For example,

$$\mathrm{Li}_n(x) = \int_0^x \frac{dt}{t}\; \mathrm{Li}_{n-1}(t)$$

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Hence, one defines a new set of functions, called the HPLs

[Remiddi, Vermaseren, Gehrmann, Goncharov]

$$H(m_n, \ldots, m_1, x) = \int_0^x K_{m_n}(t) H(m_{n-1}, \ldots, m_1, t) dt$$

Some important properties :

Shuffle algebra, Scaling invariance and integration-by-parts identities

There exists a basis $\Rightarrow$ Fast numerical evaluation

Results

Results & Checks

- Computational : Automation to solve a single scale and first order factorizable system of differential equations.
- Phenomenological : We have performed UV renormalization and obtained all the form factors which are necessary to obtain N^3LO QCD corrections to top pair productions at electron-positron colliders.

$$F_{V,1}^{(3)}, F_{V,2}^{(3)}, F_{A,1}^{(3)}, F_{A,2}^{(3)}, F_{S}^{(3)}, F_{P}^{(3)}$$

✓ We agree with the results from Lee $et\, al.$ obtained using different method

✓ The results reproduce the universal infrared structure

✓ Chiral Ward identity is satisfied between $F_{A,i}^{(3)}$ and $F_{P}^{(3)}$

Remarks

- For non-planar contributions, large differential equations $\sim$ 50 MBs!
- Also first-order non-factorizable differential equations appear!
  $\Rightarrow$ Solutions are Elliptic polylogarithms
- A proper generalization for iterative integrals over elliptic polylogarithms is needed!

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We are at a crossroad!

New mathematical structures are emerging in loop calculations! An entirely new branch of research is opening, putting together computer scientists, mathematicians, particle physicists and string theorists. Maybe what we need now, is a fresh look at the problem with fresh ideas!

One-loop and beyond

$F_{V,i}^{(1)}, F_{A,i}^{(1)}$ [Arbuzov, Bardin, Leike '92; Djouadi, Lampe, Zerwas '95]

$F_S^{(1)}, F_P^{(1)}$ [Braaten, Leveille '80; Sakai '80; Drees, Hikasa '90]

$F_{V,i}^{(2)}, F_{A,i}^{(2)}$ [Altarelli, Lampe '93; Ravindran, van Neerven '98; Catani, Seymour '99]

$F_S^{(2)}, F_P^{(2)}$ [Gorishnii *et. al.* '91; Chetyrkin, Kwiatkowski '95; Harlander, Steinhauser '97]

Two-loop

$F_I^{(2)}$ [Bernreuther, Bonciani, Gehrmann, Heinesch, Leineweber, Mastrolia, Remiddi '04,'05]

$F_{V,i}^{(2)}(\mathcal{O}(\epsilon))$ [Gluza, Mitov, Moch, Riemann '09]

$F_I^{(2)}(\mathcal{O}(\epsilon^2))$ [Ablinger, Behring, Blümlein, Falcioni, Freitas, Marquard, Rana, Schneider '17]

Three-loop

$F_{V,i}^{(3)}|_{\mathrm{large\,N}}$ [Henn, Smirnov, Smirnov, Steinhauser '16]

$F_{V,i}^{(3)}, F_{A,i}^{(3)}, F_S^{(3)}, F_P^{(3)}|_{\mathrm{large\,N+full}\,n_l}$ [Lee, Smirnov, Smirnov, Steinhauser '18]

$F_{V,i}^{(3)}, F_{A,i}^{(3)}, F_S^{(3)}, F_P^{(3)}|_{\mathrm{large\,N+full}\,n_l}$ [Ablinger, Blümlein, Marquard, Rana, Schneider '18]

Thank you for your attention!