Computer algebra tools for quarkonium NLO computations

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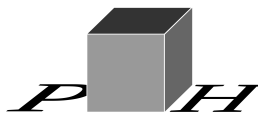
Quarkonia as Tools 2023
in
Centre Paul Langevin, Aussois, France
9th of January 2023



Outline

Motivation

- Perturbative quantum field theory (QFT) calculations often mean evaluation of Feynman diagrams
- Higher order perturbative calculations are challenging but also necessary
- Increasing experimental precision (high luminosity LHC, . . .) calls for better theory input
- The challenges are often of technical rather than conceptual nature
- New advances require better algorithms and a lot of computer power
- Software tools are indispensable

A typical Feynman diagram calculation may involve many different building blocks ...

Diagrams
- Feynman rules
- Diagram generation
- Filtering
- Topologies

Amplitudes
- Expansions
- Dirac algebra
- Color algebra
- Tensor reduction
- Projectors

Loop integrals
- Partial fractioning
- IBP reduction
- Mappings between integrals
- Master integral evaluation

Miscellaneous
- Renormalization
- Phase space
- Matching
- Phenomenology
- ...

... many of which can be automatized completely or to some extent!

- Symbolic manipulations are usually automatized using **FORM** [Vermaseren, 2000; Kuipers et al., 2013] and **Mathematica**
- Other frameworks (e. g. **Maple**, **GiNaC** [Bauer et al., 2002], **Reduce** etc.) can be useful for different tasks
- Writing big codes from scratch can be time-consuming and error-prone
- More pragmatic approach: employ tools available on the market, combine them in a smart way
- Many calculations up to 1-loop are automatizable either fully or to some extent
- In the field of heavy quarkonia we have **HELAC-ONIA** [Shao, 2016], **MadGraph** /**MadOnia** [Alwall et al., 2014; Artoisenet et al., 2008], **FDC** [Wang, 2004], **HepLib** [Feng et al., 2023], **FeynCalc** [VS et al., 2020] + **FeynOnium** [Brambilla, Chung, VS, Vairo, 2020]
- However, often quarkonium calculations (especially beyond tree-level) are done by chaining different tools together using private codes.

Diagram generation

- Two main tools on the market: **FeynArts** [Hahn, 2001] and **QGRAF** [Nogueira, 1993]
- **FeynArts** is an all-in-one solution: diagram generation, visualization, Feynman rules insertion
  - Easy to use, works with **Mathematica**, new models can be added via **FeynRules** [Christensen & Duhr, 2009; Alloul et al., 2014]
  - Can become slow when generating and filtering large (> 100) numbers of diagrams
  - Often preferred in tree-level and 1-loop calculations
- **QGRAF** only generates the amplitudes but does not visualize them or insert Feynman rules
  - New models are easy to write, only need to specify vertices and types of fields (bosonic/fermionic)
  - Output can be formatted to be readable by any CAS
  - Visualizing diagrams requires additional tools (e. g. **GraphViz**)
  - Need additional codes for inserting Feynman rules
  - Extremely fast, even when producing millions of diagrams, preferred tool in the multi-loop community

Dirac and color algebra

- Theories with fermions ⇒ Dirac matrices in the amplitudes
- Dimensional regularization (loop integrals) implies that the algebra must be done in D dimensions
- Need to simplify chains with common indices/momenta and calculate traces in D dimensions

$$\gamma^\mu\gamma^{\nu_1}\dots\gamma^{\nu_n}\gamma_\mu = (d-4)(-1)^n\gamma^{\nu_1}\dots\gamma^{\nu_n} + 2(-1)^n\gamma^{\nu_3}\gamma^{\nu_2}\gamma^{\nu_1}\gamma^{\nu_4}\dots\gamma^{\nu_n} + 2\sum_{j=4}^{m}(-1)^{n-j}\gamma^{\nu_j}\gamma^{\nu_1}\dots\gamma^{\nu_{j-1}}\gamma^{\nu_{j+1}}\dots\gamma^{\nu_n},$$

$$\not{p}\gamma^{\nu_1}\dots\gamma^{\nu_n}\not{p} = (-1)^n p^2\gamma^{\nu_1}\dots\gamma^{\nu_n} + 2\sum_{i=1}^{n}(-1)^{i+1}\gamma^{\nu_1}\dots\gamma^{\nu_{i-1}}\gamma^{\nu_{i+1}}\dots\gamma^{\nu_n}\not{p}p^{\nu_i}$$

- Issues with γ^5: cannot simultaneously preserve $\{\gamma^\mu,\gamma^5\}=0$ and the cyclicity of the trace in D dimensions
- Different schemes for treating γ^5: NDR [Chanowitz et al., 1979], BMHV [Breitenlohner & Maison, 1977; 't Hooft & Veltman, 1972], Larin [Larin, 1993], ...
- See [Gnendiger et al., 2017] for a good overview
- Ready-to-use tools: **Tracer** [Jamin & Lautenbacher, 1993], **FormTracer** [Cyrol et al., 2017], **FeynCalc**, **Package-X** [Patel, 2015, 2017], **HepMath** [Wiebusch, 2015]

- QCD is a nonabelian SU(3) gauge theory ⇒ Feynman rules involve color algebra
- Calculations are usually done for a generic N, helps to understand the structure of the results
- Standard rules to eliminate common indices and do the traces

$$
\begin{aligned}
(AT^aBT^aC) &= \frac{1}{2}(AC)\,\mathrm{Tr}(B) - \frac{1}{2N}ABC \\
(AT^aB)\,\mathrm{Tr}(CT^aD) &= \frac{1}{2}(ADCB) - \frac{1}{2N}(AB)\,\mathrm{Tr}(CD) \\
\mathrm{Tr}(AT^aB)\,\mathrm{Tr}(CT^aD) &= \frac{1}{2}\,\mathrm{Tr}(ADCB) - \frac{1}{2N}\,\mathrm{Tr}(AB)\,\mathrm{Tr}(CD) \\
T^aT^b &= \frac{1}{2N}\delta^{ab} + \frac{1}{2}d^{abc}T^c + \frac{1}{2}if^{abc}T^c \\
if^{abc} &= 2\,\mathrm{Tr}(T^a[T^b,T^c]) \\
d^{abc} &= 2\,\mathrm{Tr}(\{T^a,T^b\}T^c)
\end{aligned}
$$

- Automatizable using e. g. **ColorMath** [Sjödahl, 2013], **FormTracer**, **FeynCalc**, **color.h** [van Ritbergen et al., 1999]

Loop integrals

- Upon simplifying Dirac and color algebra we get

$$i\mathcal{M} \to \sum_i c_i^{\mu_{j_1}\cdots\mu_{j_n}} I_{\mu_{j_1}\cdots\mu_{j_n}}$$

  - $c_i^{\mu_{j_1}}$ mostly made of Dirac matrices, polarization vectors and Levi-Civita tensors
  - $I_{\mu_{j_1}\cdots\mu_{j_n}}$ are tensor loop integrals
  - Naive (text book) approach: calculate each integral separately
  - Better: try to reduce them to a smaller set of *master* integrals
- But first we need to get rid of tensor indices!
- Two popular methods: projectors or tensor reduction
  - Projectors: work out projection operators P_i in Dirac and color space for all possible contributions

$$\mathcal{M} = \sum_k a_k I_k \Rightarrow I_k = \mathrm{Tr}(P_i \mathcal{M})$$

  - Tensor reduction: for each integral write down the ansatz with all possible tensor structures, then contract and solve a system of linear equations

$$I_{\mu_{j_1}\cdots\mu_{j_n}} = \sum_j r_j^{\mu_{j_1}\cdots\mu_{j_n}} I_j$$

- I_j are scalar integrals with scalar products in numerators and propagators raised to integer powers
- These scalar integrals are still not all independent!

- Common technique at 1-loop: Passarino-Veltman [Passarino & Veltman, 1979]
  - PaVe-workflow: tensor reduction $\rightarrow$ PaVe coefficients functions B_{11}, C_{001} etc.
    $\overset{\text{PaVe reduction}}{\rightarrow}$ PaVe scalar functions $A_0, B_0, C_0, D_0, ...$
  - Bottom line: Every 1-loop I_j (quadratic propagators!) mapped to a linear combination of $A_0, B_0, C_0, D_0, ...$
  - PaVe functions are well understood, can be evaluated analytically (**Package-X**) or numerically (**LoopTools** [Hahn & Perez-Victoria, 1999], ...)
- Multi-loop: no x-loop PaVe functions, proceed on a case-by-case basis
  - Main idea: reduce each x-loop scalar integral I_j to a smaller set of *master integrals* (MI)
  - Main technique: reduction via integration-by-parts identities (IBPs) [Chetyrkin & Tkachov, 1981; Tkachov, 1981]
  - IBP-reduction done via publicly available tools **FIRE**, [Smirnov & Chuharev, 2020], **Kira** [Klappert et al., 2021], **LiteRed** [Lee, 2014]
  - Profit: Calculate only the MI, instead of every I_j

- To set up the IBP-reduction we need to map each I_j to an integral family (also called topology)
- A topology is a set of propagators that form a basis (complete and linearly independent set)
- Example: 1-loop Box
  - The topology is made of 4 propagators that form a complete basis

$$\{q^2 - m_0^2, \quad (q+p_1)^2 - m_1^2, \quad (q+p_2) - m_2^2, \quad (q+p_3)^2 - m_3^2\}$$

  - Compact notation for integrals from this topology

$$G_{\text{box11}}(1,1,1,1), \quad G_{\text{box11}}(1,1,0,2), \quad G_{\text{box11}}(1,0,0,0), \quad G_{\text{box11}}(1,2,0,-1)$$

  - `box11` is the identifier of this topology, can be a number or any other string
  - The indices denote powers of the corresponding propagators

$$G_{\text{box11}}(1,2,0,-1) \equiv \int_q \frac{1}{[q^2 - m_0^2]} \frac{1}{[(q+p_1)^2 - m_1^2]^2} [(q+p_3)^2 - m_3^2]$$

- The reduction is done topology-wise: G's with more/higher indices $\Rightarrow$ G's with less/lower indices
- In principle, one *could* reduce each single integral separately, but this is *extremely* inefficient

- What if the corresponding propagators do not form a basis?
- For linear/quadratic propagators there can be two reasons:
  1) The basis is overdetermined due to linearly dependent propagators
  2) The basis is incomplete due to missing propagators
- Missing propagators: Just add some suitable scalar products to have the complete basis
- Heavy quarkonium calculations: linearly dependent propagators when switching to the center of mass kinematics
- Example: Integral with linearly dependent propagators

$$\int_l \frac{1}{[l^2]} \frac{1}{[(k_1+l-P/2)^2-m^2]} \frac{1}{[(l-P/2)^2-m^2]} \frac{1}{[(l+P/2)^2-m^2]}$$

Splits into two pieces when applying partial fraction decomposition

$$\frac{1}{2}\left(\int_l \frac{1}{[l^2]^2} \frac{1}{[(k_1+l-P/2)^2-m^2]} \frac{1}{[(l-P/2)^2-m^2]} + \int_l \frac{1}{[l^2]^2} \frac{1}{[(k_1+l-P/2)^2-m^2]} \frac{1}{[(l+P/2)^2-m^2]}\right)$$

- Tools for finding such relations: **MultivariateApart** [Heller & von Manteuffel, 2022], **$APART** [Feng, 2012], **FeynCalc**

- Starting point: amplitudes with many propagators and numerators. Need to
  - Identify present topologies and rewrite integrals as $G_{\text{topo}}(1,\dots) \Rightarrow$ easy
  - Minimize the number of topologies via suitable mappings $\Rightarrow$ not that easy
- Example: I_1 and I_2 fit into the same topology (actually, they are identical)
  - Unfortunately, this is not obvious in the propagator representation

$$I_1 = \int_q \frac{1}{[q^2 - m_1^2]} \frac{1}{[(q-p_1)^2 - m_2^2]} \frac{1}{[(q-p_2)^2 - m_3^2]}$$

$$I_2 = \int_q \frac{1}{[(q+p_1+p_2)^2 - m_1^2]} \frac{1}{[(q+p_2)^2 - m_2^2]} \frac{1}{[(q+p_3)^2 - m_3^2]}$$

  - There exists a suitable loop-momentum shift

$$I_1 \overset{q \to q + p_1 + p_2}{=\!=} I_2$$

- Finding such shifts in a *systematic* way is challenging.
- Enumerating all possible shifts by brute force is rather *hopeless*, especially beyond 1 loop ...

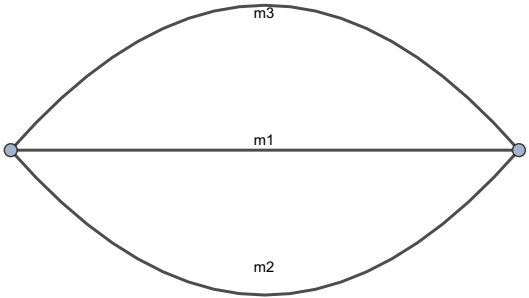
- More efficient: represent loop integrals through Feynman-parametric integrals or graphs
- Feynman parametric representation of an L-loop scalar Minkowskian integral [Nakanishi 1971, Zavialov 1979, Smirnov 2006]

$$\left(\frac{e^{\varepsilon\gamma_E}}{i\pi^{d/2}}\right)^L \int \frac{\left(\prod_{i=1}^L d^d k_i\right)}{P_1^{m_1}\dots P_N^{m_N}} = \frac{(-1)^{N_m}\Gamma(N_m - \frac{Ld}{2})}{\prod_{j=1}^N \Gamma(m_j)} \int_0^\infty \prod_{j=1}^N dx_j x_j^{m_j-1}\, \delta\left(1 - \sum_{i=1}^N x_i\right) \frac{\mathcal{U}^{N_m - \frac{(L+1)d}{2}}}{\mathcal{F}_M^{N_m - \frac{Ld}{2}}}$$

with N quadratic/eikonal propagators P_i and $N_m = \sum_{i=1}^N m_i$ with $m_i \geq 0$

- Euclidean case: remove $(-1)_m^N$, replace $\mathcal{F}_M$ with $\mathcal{F}_E$
- **Symanzik polynomials $\mathcal{U}$ and $\mathcal{F}$** encode most of the integral properties (nice summary in [Bogner & Weinzierl, 2010])
- Main advantage: ambiguity under shifts of loop momenta eliminated!
  - Employ a function of $(\mathcal{U}, \mathcal{F})$ and m_i to characterize the given loop integral (topology)?
  - Find mappings between different topologies?
  - In principle, yes! But things are not so simple ...

- Introduce the characteristic polynomial P
- Popular choices: $P = \mathcal{U} \times \mathcal{F}$ or $P = \mathcal{U} + \mathcal{F}$
- P depends on the Feynman parameters x_i and is not unique!
- Ambiguity under shifts of loop momenta $\Rightarrow$ ambiguity under permutations of x_i
- A new P' from P by permuting x_i (e. g. $x_1 \leftrightarrow x_2$) still describes the same loop integral
- Need to find some *canonical ordering* of the Feynman parameters x_i in the given P
- Possible solution: Algorithm invented by Alexey Pak [Pak, 2012]
- Rough idea: Write P as a matrix, find the canonical form by swapping/sorting rows and columns

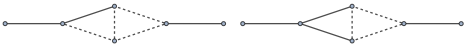


$$= -\Gamma(3-d) \int_{x_i} \underbrace{(x_1x_2 + x_1x_3 + x_2x_3)}_{\mathcal{U}}^{3-\frac{3d}{2}}$$
$$\underbrace{(x_1x_2 + x_1x_3 + x_2x_3)(m_1^2x_1 + m_2^2x_2 + m_3^2x_3)}_{\mathcal{F}}^{d-3}$$

- Pak algorithm: canonical ordering of x_i + symmetries between the corresponding lines.
- Very detailed description in the PhD thesis of Jens Hoff [J. S. Hoff, 2015]
- Technical implementation in **Mathematica** straightforward
  - Automatic calculation of $\mathcal{U}$ + $\mathcal{F}$ in **UF.m** (now part of **FIESTA** [Smirnov et al., 2022] and **FIRE**)
  - Many of Pak's ideas implemented in **TopoID** [J. Hoff, 2016], `https://github.com/thejensemann/TopoID`
- Pak algorithm + UF-parametrization pave way to
  - Topology identification
  - Mappings between master integrals
  - Derivation of Feynman-parametric representations for analytic calculations
  - Analytic regularization [Panzer, 2015a, 2014, 2015b]
  - And many more!
- Corresponding routines available in **FeynCalc**, **tapir** [Gerlach et al., 2023], **pySecDec** [Borowka et al., 2018], **LiteRed**

- Suppose that you are done with the IBP-reduction [Chetyrkin & Tkachov, 1981; Tkachov, 1981] of your loop integrals, what are the next steps?
  - Find mappings between master integrals from different integral families
  - Visualize your unique master integrals
  - Calculate them analytically/numerically?

- With Pak algorithm at our disposal finding mappings between master integrals is straightforward
- Example (using **FeynCalc**): 2-loop self-energies with one or two massive lines



```
In[1]:= topos = {FCTopology[prop2Lv1, {FAD[p1], FAD[{p1 + q1, m}], FAD[p2], FAD[p2 + q1], FAD[p1 - p2]}, {p1, p2}, {q1}, {}, {}],
          FCTopology[prop2Lv2, {FAD[p1], FAD[{p2, m}], FAD[{p2 + q1, m}], FAD[p1 + q1], FAD[-p1 + p2]}, {p1, p2}, {q1}, {}, {}]};
```

- We have a list of master integrals that are not all unique

```
In[2]:= glis = {GLI[prop2Lv1, {0, 1, 1, 1, 1}], GLI[prop2Lv2, {0, 1, 1, 1, 1}], GLI[prop2Lv2, {1, 0, 1, 1, 1}],
          GLI[prop2Lv2, {1, 1, 0, 1, 1}], GLI[prop2Lv2, {1, 1, 1, 0, 1}]}
```

- **FeynCalc** identifies three mappings between our masters

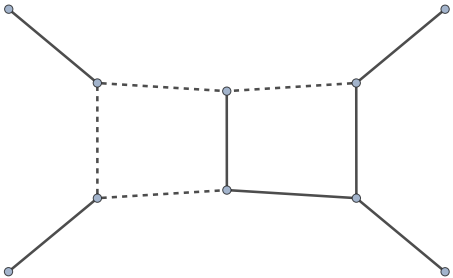
```
In[3]:= FCLoopFindIntegralMappings[glis, topos][[1]]
```

$$\text{Out[3]=}\ \{G^{\text{prop2Lv2}}(1,0,1,1,1)\to G^{\text{prop2Lv1}}(0,1,1,1,1),G^{\text{prop2Lv2}}(1,1,0,1,1)\to G^{\text{prop2Lv1}}(0,1,1,1,1),G^{\text{prop2Lv2}}(1,1,1,0,1)\to G^{\text{prop2Lv2}}(0,1,1,1,1)\}$$

- Working principle based on `FindRules` from **FIRE**
- Could also use **LiteRed**'s `FindSymmetries`

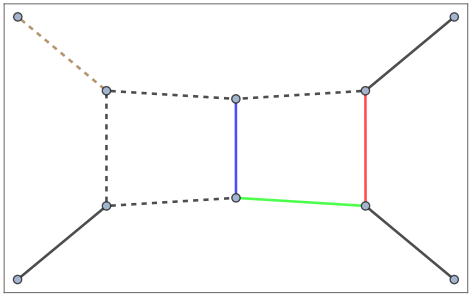
- Given a propagator representation of a loop integral, how to obtain its graph representation?
- Can be done using **AZURITE** [Georgoudis et al., 2017], **PlanarityTest**, [Bielas et al., 2013], **LiteRed** and also **FeynCalc**
- Two-step approach: `FCLoopIntegralToGraph` reconstructs the graph, `FCLoopGraphPlot` plots it.

```
In[4]:= FCLoopIntegralToGraph[FAD[{p1, m1}, {p2, m2}, {Q1 + p1, m3}, Q2 - p1, Q1 + p1 + p2, Q2 - p1 - p2, Q2 + Q3 - p1 - p2], {p1, p2}];
        FCLoopGraphPlot[%]
```



- The plot can be styled to make it more visually appealing

```
In[5]:= FCLoopIntegralToGraph[FAD[{p1, m1}, {p2, m2}, {Q1 + p1, m3}, Q2 - p1, Q1 + p1 + p2, Q2 - p1 - p2, Q2 + Q3 - p1 - p2], {p1, p2}];
        FCLoopGraphPlot[%, GraphPlot -> {MultiedgeStyle -> 0.35, Frame -> True}, Style -> {
        {"InternalLine", _, _, mm_ /; ! FreeQ[mm, m1]} -> {Red, Thick},
        {"InternalLine", _, _, mm_ /; ! FreeQ[mm, m2]} -> {Blue, Thick},
        {"InternalLine", _, _, mm_ /; ! FreeQ[mm, m3]} -> {Green, Thick},
        {"ExternalLine", Q1} -> {Brown, Thick, Dashed}}]
```



- At NLO we have plenty of options for the evaluation of 1-loop master integrals (quadratic propagators)
  - Analytically via **Package-X**
  - Numerically using **LoopTools**, **Collier** [Denner et al., 2017], **OneLOop** [van Hameren, 2011], **QCDLoop** [Carrazza et al., 2016], ...
- Beyond 1-loop things are not that simple
  - Numerical evaluation using **FIESTA** and **pySecDec**
  - Analytic results can be difficult to get, unless already available in the literature.
    - Plethora of different methods, impossible to discuss in one talk
    - Probably the most promising technique are differential equations [Kotikov, 1991a, 1991b, 1991c; Bern et al., 1994; Remiddi, 1997; Gehrmann & Remiddi, 2000; Henn, 2013]

Summary and Outlook

Summary

- Loop calculations is a vibrant field with new ideas being developed on a monthly basis
- Useful for heavy quarkonia, where often at least 1-loop accuracy is needed to match the experimental precision
- As far as 1-loop virtual corrections are concerned, all necessary tools for analytic results are publicly available
- It only takes dedication and willingness to learn how to use those programs