#### Master integrals and generalized polylogarithms: focus on fast and efficient evaluation

Damiano Tommasini (N.C.S.R. Demokritos)

In collaboration with Costas Papadopoulos, Hjalte Frellesvig and Chris Wever

Funded by: APISTEIA-1283 HOCTools



UCLARadcor-Loopfest 2015

18 June 2015

## Outline

- Introduction: looking forward for 2-loop calculations
- Evaluation of Master Integrals expressed as Goncharov Multiple polylogarithms (GPs) and Li functions
   See also Papadopoulos, Wever, Tancredi's... talks
- Looking forward for new algorithms from  $\text{Li}_n(x)$  to  $\text{Li}_{22}(x,y)$

## Introduction

• Amplitude reduction @ 1-loop (OPP method) lead to so called NLO revolution

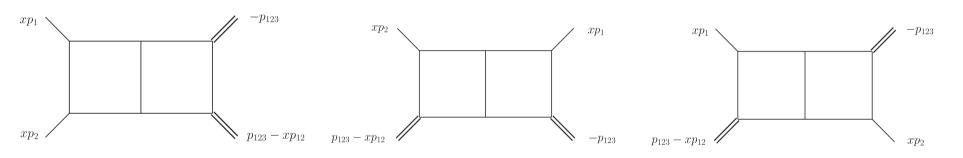
$$= \sum d_{i_1 i_2 i_3 i_4} + \sum c_{i_1 i_2 i_3} + \sum b_{i_1 i_2} + \sum a_{i_1} + \sum c_{i_1 i_2 i_3} + R$$

- Highly desirable: reduction @ 2-loops
  - Need to compute Master Integrals
  - Understand how to do amplitude reduction
     Both steps are done in several cases, but still a lot has to be done.

 $S = (q_1 + q_2)^2 = (q_3 + q_4)^2, \quad T = (q_1 - q_3)^2 = (q_2 - q_4)^2$  $U = (q_1 - q_4)^2 = (q_2 - q_3)^2, \quad q_3^2 = M_3^2, q_4^2 = M_4^2$ 

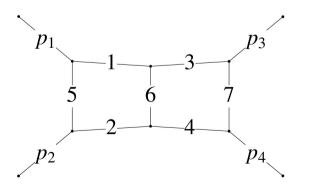
• x-parametrization

[ **PTW**: C. G. **P**apadopoulos, D**T**, C. **W**ever '14]



• xyz-parameterization

[ HMS: J. M. Henn, K. Melnikov, V. A. Smirnov '14; GMT: T. Gehrmann, A. von Manteuffel, L. Tancredi '15]

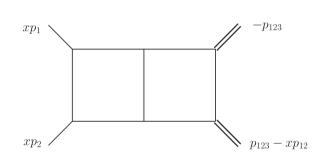


 $S = (q_1 + q_2)^2 = (q_3 + q_4)^2, \quad T = (q_1 - q_3)^2 = (q_2 - q_4)^2$  $U = (q_1 - q_4)^2 = (q_2 - q_3)^2, \quad q_3^2 = M_3^2, q_4^2 = M_4^2$ 

x-parametrization

[ **PTW**: C. G. **P**apadopoulos, D**T**, C. **W**ever '14]

5



$$q_{1} = xp_{1}, \quad q_{2} = xp_{2}, \quad q_{3} = p_{123} - xp_{12}, \quad q_{4} = p_{123}$$
$$p_{i}^{2} = 0, \quad s_{12} := p_{12}^{2}, \quad s_{23} := p_{23}^{2}, \quad q := p_{123}^{2},$$
$$S = s_{12}x^{2}, \quad T = q - (s_{12} + s_{23})x,$$
$$M_{3}^{2} = (1 - x)(q - s_{12}x), \quad M_{4}^{2} = q$$

• XYZ-parameterization [HMS: J. M. Henn, K. Melnikov, V. A. Smirnov '14; GMT: T. Gehrmann, A. von Manteuffel, L. Tancredi '15]

$$\begin{array}{c} \begin{array}{c} \begin{array}{c} p_{1} \\ p_{1} \\ \hline \\ & 5 \\ & 6 \\ & 7 \\ \hline \\ & & \\ \end{array} \end{array} \begin{array}{c} p_{3} \\ \hline \\ & p_{4} \end{array} \begin{array}{c} p_{12} : p_{1} = -q_{3}, p_{2} = -q_{4}, p_{3} = q_{1}, p_{4} = q_{2} \\ p_{13} : p_{1} = -q_{3}, p_{2} = q_{1}, p_{3} = -q_{4}, p_{4} = q_{2} \\ p_{23} : p_{1} = q_{2}, p_{2} = -q_{4}, p_{3} = -q_{3}, p_{4} = q_{1} \\ \hline \\ & s = \bar{m}^{2}(1 + \bar{x})^{2}, \\ & t = -\bar{m}^{2}\bar{x}((1 + \bar{y})(1 + \bar{x}\bar{y}) - 2\bar{z}\bar{y}(1 + \bar{x})) p_{4}^{2} = \bar{m}^{2}(1 - \bar{x}^{2}\bar{y}^{2}) \end{array}$$

$$s = m^2(1+x)(1+xy), \ t = -m^2xz, \ p_3^2 = m^2, \ p_4^2 = m^2x^2y$$

- The parameterizations are different, but they describe the same physics
- Example: mapping valid for PTW to HMS q < s12

$$\bar{x} = -1 + (s12x)/q$$
$$\bar{y} = (q - qx)/(q - s12x)$$
$$\bar{z} = (q - qx + s23x)/(q - s12x)$$
P23:
$$\bar{x} = -1 + (s12x)/q$$
$$\bar{y} = (q - qx)/(q - s12x)$$
$$\bar{z} = (q - (s12 + s23)x)/(q - s12x)$$

- Different parameterizations, different solution strategies
   analytic results looks differently (clearly they are equivalent)
- Sample of results for P12, as function of GPs

$$G[1, x] \left( G\left[\frac{s_{12+s_{23}}}{s_{12}}, x\right] \left( -\frac{G\left[0, \frac{q}{s_{12}}, x\right]}{s_{12^2}} + \frac{G\left[0, \frac{q}{q-s_{23}}, x\right]}{s_{12^2}} \right) + G\left[0, 1 - \frac{s_{23}}{q}\right] + G\left[0, \frac{1 - \frac{s_{23}}{q}}{q}\right] + \frac{G\left[0, \frac{q}{q-s_{23}}, x\right]}{s_{12^2}} + \frac{G\left[0, \frac{q}{q-s_{23}}, \frac{g}{q-s_{23}}, \frac{g}{s_{12^2}} + \frac{G\left[0, \frac{q}{q-s_{23}}, \frac{g}{s_{12}}, \frac{g}{s_{12}} + \frac{G\left[0, \frac{q}{q-s_{23}}, \frac{g}{s_{12}} + \frac{G\left[0, \frac{g}{q-s_{23}}, \frac{g}{s_{1$$

G[-1, x] ( $i\pi - G[0, y] + 2G[0, z]$ ) +  $i\pi G\left[-\frac{1}{y}, x\right]$  -

xyz-parametrization

$$i \pi G\left[-\frac{1}{z}, x\right] + G\left[0, z\right] \left(2 G\left[-\frac{1}{y}, x\right] - G\left[-\frac{1}{z}, x\right] - G\left[-\frac{z}{y}, x\right]\right) - G\left[-\frac{z}{y}, x\right] - G\left[-\frac{z}{y$$

- We can evaluate the Master Integrals by Mathematica interfaced with GiNac (just for timing comparison).
- We test some "random" phase space poins: {S,T,  $p_3^2$ ,  $p_4^2$ }  $phys1a = \{5.687, -0.243333, 0.017, 5.\}$ phys1b = {8., -2., 3., 1.}  $phys1c = \{130.05, -20.85, 66.7, 5.5\}$ phys2a = {5.64667, -1.52222, 0.213333, 3.}  $phys2b = \{3., -0.6666667, 0.5, 1.\}$ phys2c = {226.875, -25.1667, 175.125, 2.33333}

• Speed comparison for different solutions in different points (all times are expressed in seconds)

P12-29 G	5111111100		
point	HMS	PTW	GMT trad
phys1a	0,3	1600	18
phys1b	8,3	260	1,1
phys1c	11	200	8,4
phys2a	0,63	470	14
phys2b	3,1	630	8,7
phys2c	11	210	14

• PTW is in general much slower than other solutions

 There are large and almost random differences in computational times between different libraries but also in different points. Those difference are partially related to computing MI in edges of phase space, but also on explicit expressions as letters inside GPs

#### INSERT: GPs evaluation in GiNaC

• Definition 
$$G(z_1,...,z_k;y) = \int_0^y \frac{dt_1}{t_1-z_1} \int_0^{t_1} \frac{dt_2}{t_2-z_2} \dots \int_0^{t_{k-1}} \frac{dt_k}{t_k-z_k}$$

• Evaluation: algorithm dependent on the input values

$$- |y| \le |z_j| \text{ for all } j \quad y/z_1 \ne 1$$

$$G(z_1, ..., z_k; y) = \sum_{j_1=1}^{\infty} \dots \sum_{j_k=1}^{\infty} \frac{1}{j_1 + ... + j_k} \left(\frac{y}{z_1}\right)^{j_1} \frac{1}{j_2 + ... + j_k} \left(\frac{y}{z_2}\right)^{j_2} \dots \frac{1}{j_k} \left(\frac{y}{z_k}\right)^{j_k}$$

- if |y| > |z|  $G(z, y) = G(y, z) G(0, z) + I\pi G(0, y)$ in general if  $|y| > |z_i|$   $G(\dots z_i \dots, y) = \sum (\dots) G(\dots)$  Analytic continuation
- slow convergence if  $|y/z| \sim 1$  (Holder convolution or other strategies)  $G(z_1, ..., z_w; 1) = \sum_{j=0}^{w} (-1)^j G\left(1 - z_j, 1 - z_{j-1}, ..., 1 - z_1; 1 - \frac{1}{p}\right) G\left(z_{j+1}, ..., z_w; \frac{1}{p}\right)$

 $\text{"Fast" } G(1,2,3;0.001) \to 5 \cdot 10^{-4} \text{sec.} \quad \text{"Slow" } G(1,2,3;1.999) \to 4 \cdot 10^{-2} \text{sec.}$ 

#### P12-29 G111111100 (scalar)

point	HMS	PTW	PWT + fibBas	GMT trad
phys1a	0,3	1600	24	18
phys1b	8,3	260	1,4	1,1
phys1c	11	200	0,84	8,4
phys2a	0,63	470	3,0	14
phys2b	3,1	630	5,8	8,7
phys2c	11	210	0,86	14

• PTW solution is native in Euclidean region of phase space. We are testing the library in physical space analytic continuation is needed

GPs up to weigth 4

• Speed comparison or different solutions i Log, Lin and Ling points (all times are expressed in seconds)

P12-29 G11111100 (scalar)					
point	HMS	PTW	PWT + fibBas	GMT trad	GMT opt
phys1a	0,3	1600	24	18	0,27
phys1b	8,3	260	1,4	1,1	0,16
phys1c	11	200	0,84	8,4	0,14
phys2a	0,63	470	3,0	14	0,17
phys2b	3,1	630	5,8	8,7	0,17
phys2c	11	210	0,86	14	0,19

In GMT optimized solution is typically faster than other solutions

GPs up to weigth 4

• Speed comparison or different solutions i Log, Lin and Ling points (all times are expressed in seconds)

#### P12-29 G11111100 (scalar)

-20 C1111111m0

point	HMS	PTW	PWT + fibBas	GMT trad	GMT opt
phys1a	0,44	1600	25	63	1,1
phys1b	12	300	1,5	4,2	0,41
phys1c	17	230	0,86	31	0,58
phys2a	0,72	520	3,2	47	0,55
phys2b	4,8	670	6,1	35	0,66
phys2c	17	240	0,88	52	0,69

• In GMT optimized solution is typically faster than other solutions, but not always: Holder convolution is mapping back  $Li_n$  and  $Li_{22}$  to GP up to weight 4!!!

 $Li_{22}(x,y) = G(0, 1/x, 0, 1/(xy); 1) = G(1 - 1/(xy), 1, 1 - 1/x, 1; 1/p) + \dots$ 

### Main message

- Once we have analytic solution for some MI we prefer to simplify it in order to achieve a fast evaluation
- It is NOT obvious what is the best expression, not always expression made of few GPs is the fastest expression to be evaluated.
- MAYBE: according to different regions and limits in the phase space, there could be differently optimized expressions
- Another possibility: Log,  $Li_n$  and  $Li_{22}$  basis of functions seems promising, but computational algorithm needs improvements in order to avoid mapping back to GPs

# Fast $\operatorname{Li}_{n}(z)$ evaluation: Crandal algorithm

Given any complex number z, we can evaluate  $\text{Li}_n(z)$  by four cases:

- If z=1, we just plug special value
- If  $|z| < \frac{1}{2}$  evaluate by definition

$$\mathrm{Li}_n(1) = \zeta(n)$$

$$\operatorname{Li}_n(z) = \sum_{k=1}^\infty z^k / k^n$$

• If |z| > 2 use inversion relation

$$\operatorname{Li}_{n}(1/z) = (-1)^{n} \left( -\operatorname{Li}_{n}(z) + \frac{(2\pi i)^{n}}{n!} B_{n}\left(\frac{\log z}{2\pi i}\right) + 2\pi i\Theta(z)\frac{\log^{n-1} z}{(n-1)!} \right)$$

where  $B_n$  is the standard Bernoulli polynomial  $\Theta(z) := 1$ , if  $\Im(z) < 0$  or  $z \in [1, \infty]$ , else  $\Theta = 0$ 

# Fast $\operatorname{Li}_{n}(z)$ evaluation: Crandal algorithm

Given any complex number z, we can evaluate  $\text{Li}_n(z)$  by four cases:

- If z=1, we just plug special value
- If  $|z| < \frac{1}{2}$  evaluate by definition

$$\operatorname{Li}_n(1) = \zeta(n)$$

Li<sub>n</sub>(z) = 
$$\sum_{k=1}^{\infty} z^k / k^n$$

• If 
$$|z| > 2$$
 use inversion relation  
 $\operatorname{Li}_n(1/z) = (-1)^n \left( -\operatorname{Li}_n(z) + \frac{(2\pi i)^n}{n!} B_n\left(\frac{\log z}{2\pi i}\right) + 2\pi i\Theta(z) \frac{\log^{n-1} z}{(n-1)!} \right)$   
• Else ( $|z| \sim 1$ ) use log expansion:

$$\operatorname{Li}_{n}(z) = \sum_{m=0}^{\infty} \frac{\zeta(n-m)}{m!} \log^{m} z + \frac{\log^{n-1} z}{(n-1)!} \left(H_{n-1} - \log(-\log z)\right)$$

Log expansion of  $Li_n(z)$  around one nicely captures its singular structure. <sup>16</sup> Furthermore it is efficient formula for numerical evaluation

# Fast $\operatorname{Li}_{22}(x,y)$ evaluation: Crandal-style algorithm

Given any complex numbers (x,y), we can evaluate  $Li_{22}(x,y)$  by four cases:

- If x=y=1, we just plug special value  $\text{Li}_{22}(1,1) = \pi^4/120$
- If |x| and |xy| are "small" evaluate by definition  $\operatorname{Li}_{2,2}(x,y) = \sum_{j_1=1}^{\infty} \sum_{j_2=1}^{\infty} \frac{x^{j_1}}{(j_1+j_2)^2} \frac{(xy)^{j_2}}{j_2^2}$
- If |x| and |xy| are "large" use inversion relations, for example:

$$\operatorname{Li}_{22}(1/x, 1/y) = \operatorname{Li}_{22}(y, x) + \frac{31\pi^4}{360} + 3\operatorname{Li}_4(y) - 3\operatorname{Li}_4(x) + \dots$$

The actual numerical values for "small" and "large" will be defined empirically after numerical implementation in order to minimize the computational cost. Approximatively ½ and 2.

# Fast $\operatorname{Li}_{22}(x,y)$ evaluation: Crandal-style algorithm

Given any complex numbers (x,y), we can evaluate  $Li_{22}(x,y)$  by four cases:

- If x=y=1, we just plug special value  $\text{Li}_{22}(1,1) = \pi^4/120$
- If |x| and |xy| are "small" evaluate by definition  $\operatorname{Li}_{2,2}(x,y) = \sum_{j_1=1}^{\infty} \sum_{j_2=1}^{\infty} \frac{x^{j_1}}{(j_1+j_2)^2} \frac{(xy)^{j_2}}{j_2^2}$
- If |x| and |xy| are "large" use inversion relations, for example:

$$\operatorname{Li}_{22}(1/x, 1/y) = \operatorname{Li}_{22}(y, x) + \frac{31\pi^4}{360} + 3\operatorname{Li}_4(y) - 3\operatorname{Li}_4(x) + \dots$$

• Else ( $|x| \sim 1$ ) use generalization of log expansion (Li<sub>2</sub> function is needed): Li<sub>22</sub>(x, y)  $\simeq$  Polynomia ( $\{x, y, \log(\{x, y\}), \text{Li}_2(\{x, y\})\}$ )

### Work in progress: we have analytic expressions, but further <sup>18</sup> simplifications has to be done.

## Summary

- Not all the needed two-loop Master Integrals are known yet, but it is already time to start thinking how to make a library of them
- In particular it is important trying to understand how to simplify them, but first of all we must understand what does it mean: "simplified"
- Large set of MI can be expressed in Log,  $Li_n$  and  $Li_{22}$  basis (not all, some require Elliptic functions): faster algorithms are welcome!
- There is room to improve the computational algorithms, soon news concerning  $Li_{22}$  will come!