Solving Master Integrals Via Numerical Differential Equations

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圈积分及相空间积分计算系列讲座

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Outline

I. **Introduction**

II. **Numerical differential equations**

III. **Application – auxiliary mass flow**

IV. **Summary and outlook**

Era of precision physics

➢ Physics at Large Hadron Collider

- improving requirements on theoretical predictions
- new NNLO and N3LO cross sections
- bottleneck problems: integrals reduction, master integrals calculation

➢ Integrals reduction

- prohibitive algebraic complexity
  - non-planar contribution of $pp \to \gamma\gamma\gamma$ missed [Chawdhry, et al, 20']
- "basis" of special functions not fully known
  - elliptic sectors in H+jet production in QCD [Bonciani, et al, 16'] [Bonciani, et al, 20] [Frellesvig, et al, 20']

Methods

➢ Integrals reduction

- integration-by-parts [Chetyrkin, Tkachov, 81'] [Laporta, 00']
- syzygy equation [Gluza, Kajda, Kosower, 11'] [Schabinger, 12'] [Larsen, Zhang, 16']
- finite field interpolation [Manteuffel, Schabinger, 15'] [Peraro, 16']
- intersection numbers [Mastrolia, Mizera, 19'] [Frellesvig, et al, 19']
- matching [Liu, Ma, 19'] [Wang, Li, Basat, 19'] [Guan, Liu, Ma, 20'] [Basat, Li, Wang, 21']

➢ Master integrals calculation

- differential equation and its canonical form [Kotikov, 91'] [Henn, 13']
- Mellin-Barnes representation [Smirnov, 99']
- sector decomposition [Binoth, Heinrich, 00']
- difference equation [Tarasov, 96'] [Laporta, 00'] [Lee, 09']
- numerical differential equation [Caffo, et al, 08'] [Czakon, 08'] [Lee, et al, 17']
- auxiliary mass flow [Liu, Ma, Wang, 18']

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Overview

➢ Dimensional regulated integral family

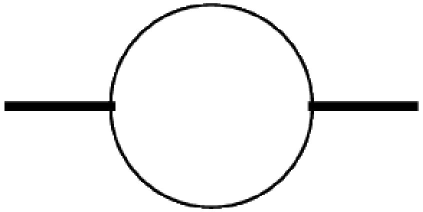
$$I(\epsilon,\vec{s}) \equiv \int \prod_{i=1}^{L} \frac{\mathrm{d}^{4-2\epsilon}\ell_i}{\mathrm{i}\pi^{2-\epsilon}} \frac{1}{\mathcal{D}_1^{\nu_1}\cdots\mathcal{D}_N^{\nu_N}}$$

- $\{D_1,\cdots,D_N\}$ with $N=\frac{L(L+1)}{2}+L\,E$
- $\vec{s}=\{p_i^2, p_i\cdot p_j, m_i^2\}$
- integration-by-parts identities → master integrals $\vec{I}$
- derivatives + IBP identities → differential equation

$$\frac{\partial}{\partial s_i}\vec{I}=A_i\vec{I}$$

- general solution + boundary condition → final solution

➢ One-loop two-point



$$\mathcal{D}_1 = \ell^2 - m^2, \quad \mathcal{D}_2 = (\ell + p)^2 - m^2$$

$$\vec{I} = \{I(1,0),\ I(1,1)\}$$

- $s := p^2 = 1,\ m^2 = x$

$$\frac{\partial}{\partial x}\vec{I} = \begin{pmatrix} -\frac{\epsilon-1}{x} & 0 \\ \frac{2(\epsilon-1)}{x(4x-1)} & -\frac{2(2\epsilon-1)}{4x-1} \end{pmatrix} \vec{I}$$

- basic features:
  - block-triangular
  - rational functions with only first-order poles: $x = 0, x = 1/4$

Simple Examples

$$\frac{\partial}{\partial x}\vec{I} = \begin{pmatrix} -\frac{\epsilon-1}{x} & 0 \\ \frac{2(\epsilon-1)}{x(4x-1)} & -\frac{2(2\epsilon-1)}{4x-1} \end{pmatrix} \vec{I}$$

- general solution for $I_1 \to c_1\, x^{1-\epsilon}$
- general solution for $I_2 \to c_2(x)(1-4x)^{1/2-\epsilon}$, with

$$c_2'(x) = -2c_1(\epsilon-1)(1-4x)^{\epsilon-\frac{3}{2}}x^{-\epsilon}$$

$$I_2 = c_2(1-4x)^{\frac{1}{2}-\epsilon} + 2c_1 x^{1-\epsilon}\,{}_2F_1\left(\frac{1}{2}(3-2\epsilon), 1-\epsilon; 2-\epsilon; 4x\right)(1-4x)^{\frac{1}{2}-\epsilon}$$

- Hypergeometric functions encountered

Simple Examples

$$\frac{\partial}{\partial x}\vec{I} = \begin{pmatrix} -\frac{\epsilon-1}{x} & 0 \\ \frac{2(\epsilon-1)}{x(4x-1)} & -\frac{2(2\epsilon-1)}{4x-1} \end{pmatrix}\vec{I}$$

- numerical solution: power series expansion of I_2 near $x = x_0$
- x_0 regular: $I_2 = \sum_{n=0}^{\infty} f_n (x - x_0)^n$
  - all $f_n (n \geq 1)$ can be reduced to f_0 by differential equation
- $x_0 = 0$: $I_2 = \sum_{n=0}^{\infty} f_n x^n + x^{1-\epsilon} \sum_{n=0}^{\infty} g_n x^n$
  - left part: homogeneous, right part: non-homogeneous
- $x_0 = 1/4$: $I_2 = (1/4 - x)^{1/2-\epsilon} \sum_{n=0}^{\infty} f_n (1/4 - x)^n + \sum_{n=0}^{\infty} g_n (1/4 - x)^n$
  - left part: homogeneous, right part: non-homogeneous

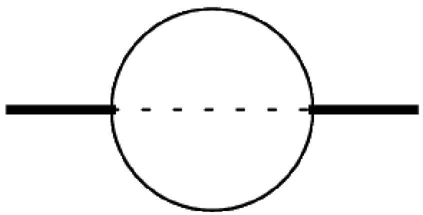
Simple Examples

$$\frac{\partial}{\partial x}\vec{I} = \begin{pmatrix} -\frac{\epsilon-1}{x} & 0 \\ \frac{2(\epsilon-1)}{x(4x-1)} & -\frac{2(2\epsilon-1)}{4x-1} \end{pmatrix} \vec{I}$$

- example of calculation: the analytic part near $x = 1/4$
- $I_1 = \sum_{n=0}^{\infty} h_n (1/4 - x)^n$, h_n known to us
- How to calculate the expansion of $2(\epsilon - 1) I_1 / \left(x(4x-1)\right)$?
  - first expand the coefficients to $\sum_{n=-1}^{\infty} a_n (1/4 - x)^n$, then perform series multiplication? $\sim O(N^2)$
  - $2(\epsilon - 1) I_1 = \left(x(4x-1)\right) \sum_{n=-1}^{\infty} b_n (1/4 - x)^n$, then solve via matching. $\sim O(N)$
  - in general, $\frac{P(x)}{Q(x)} \times I(x) \sim [\deg(P) + \deg(Q)] N$

Simple Examples

➢ Two-loop two-point



$$\mathcal{D}_1 = \ell_1^2 - m^2, \mathcal{D}_2 = \ell_2^2 - m^2, \mathcal{D}_3 = (\ell_1 + \ell_2 + p)^2,$$

$$\mathcal{D}_4 = (\ell_1 + p)^2, \mathcal{D}_5 = (\ell_2 + p)^2$$

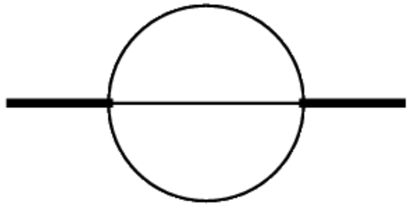
$$\vec{I} = \{I(1,1,0,0,0), I(1,1,1,0,0), I(1,1,1,0,-1)\}$$

- $s := p^2 = 1,\ m^2 = x$

$$\frac{\partial}{\partial x}\vec{I} = \begin{pmatrix} -\frac{2(\epsilon-1)}{x} & 0 & 0 \\ -\frac{2(\epsilon-1)}{x(4x-1)} & -\frac{2(5\epsilon x-4x+\epsilon-1)}{x(4x-1)} & \frac{6(\epsilon-1)}{x(4x-1)} \\ -\frac{2(\epsilon-1)}{4x-1} & \frac{2\epsilon x^2-\epsilon x-\epsilon+1}{x(4x-1)} & -\frac{3(2x-1)(\epsilon-1)}{x(4x-1)} \end{pmatrix}\vec{I}$$

- asymptotic behavior: the eigenvalues of residue matrix near $x = 0$
  - for the block of I_2 and I_3, the behaviors are $0, 1-\epsilon$ (homogeneous) and $2-2\epsilon$ (non-homogeneous)

➢ Example with second order poles



$$\mathcal{D}_1=\ell_1^2-m^2, \mathcal{D}_2=\ell_2^2-m^2, \mathcal{D}_3=(\ell_1+\ell_2+p)^2-m^2,$$

$$\mathcal{D}_4=(\ell_1+p)^2, \mathcal{D}_5=(\ell_2+p)^2$$

$$\vec{I}=\{I(1,1,0,0,0), I(1,1,1,0,0), I(2,1,1,0,0)\}$$

- $s := p^2 = 1,\ m^2 = x$

$$\frac{\partial}{\partial x}\vec{I}=\begin{pmatrix} -\frac{2(\epsilon-1)}{x} & 0 & 0 \\ 0 & 0 & 3 \\ \boxed{\frac{2(\epsilon-1)^2}{(x-1)x^2(9x-1)}} & -\frac{(3x-1)(2\epsilon-1)(3\epsilon-2)}{(x-1)x(9x-1)} & -\frac{45\epsilon x^2-18x^2-30\epsilon x+10x+\epsilon}{(x-1)x(9x-1)} \end{pmatrix}\vec{I}$$

- second-order pole: removable through a basis transformation
  - $\vec{I} = diag\{1,1,x^{-1}\}.\vec{J}$
  - for more general cases, see [Lee, 14']

The algorithm

➢ Power expansion near a point $x = x_0$

- determine the asymptotic behaviors from the normalized differential equation : homogenous + nonhomogeneous

$$I_i = \sum_{\mu\in S}(x-x_0)^{\mu}\sum_{k=0}^{k_\mu}\log(x-x_0)^k\sum_{n=0}^{\infty}c_{i,\mu,k,n}(x-x_0)^n$$

  - regular: $S = \{0\}, k_0 = 0$
  - singular: $S = \{-2\epsilon, 1+\epsilon, \cdots\}, k_\mu \geq 0$
- reduce the higher-order coefficients in the expansion to lowest one via the differential equation
- determine the lowest order coefficient by the boundary condition (input)

The algorithm

➢ Error estimation

- consider a Taylor expansion $f(x) = \sum_{n=0}^{\infty} f_n x^n$

$$
\begin{aligned}
f(x) &= \sum_{n=0}^{N} f_n x^n + \sum_{n=N+1}^{\infty} f_n x^n \\
&= \sum_{n=0}^{N} \tilde{f}_n x^n + \sum_{n=0}^{N} \delta_n x^n + \sum_{n=N+1}^{\infty} f_n x^n \\
&\equiv \tilde{f}(x) + E_1(x) + E_2(x)
\end{aligned}
$$

- note: $\delta_n \sim \delta_0 / r^n$, $f_n \sim f_0 / r^n$, with r the convergence radius
- $E_1(x) \sim \delta_0 (1 - (x/r)^{N+1})/(1 - x/r)$
- $E_2(x) \sim f_0 (x/r)^{N+1}/(1 - x/r)$
- a reasonable choice: $x/r = 1/2$, then $e \coloneqq (E_1 + E_2)/f_0 \sim \delta_0/f_0 + 2^{-N}$
- precision $p \sim N \sim t$, totally in proportion to the time consumption

Boundary condition

- singular point: $I(x) \sim c_1(x-x_0)^{\mu_1} + c_2(x-x_0)^{\mu_2} + \cdots$
  - method of region [Beneke, Smirnov, 98'] [Smirnov, 99']
  - parametric representation

- regular point: $I(x_0)$
  - sector decomposition
  - auxiliary mass flow (recommended!) (can also be used to calculate integrals point-by-point, see [Yang, Zhang, et al, 20'] [Hansen, Wang, 20'] [Hansen, Wang, 21'])

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➢ Dimensional regulated integral family

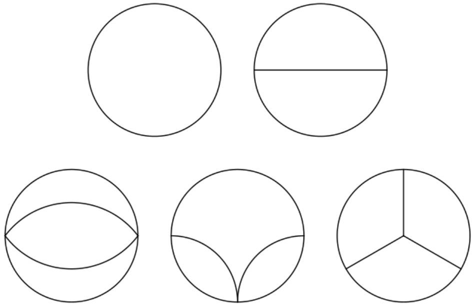
$$I(\epsilon,\vec{s},\eta)\equiv\int\prod_{i=1}^{L}\frac{\mathrm{d}^{4-2\epsilon}\ell_i}{\mathrm{i}\pi^{2-\epsilon}}\prod_{\alpha=1}^{N}\frac{1}{(\mathcal{D}_\alpha+\eta)^{\nu_\alpha}}$$

- η: the auxiliary mass parameter

$$I_{\text{phy}}(\epsilon,\vec{s})\equiv\lim_{\eta\to \mathrm{i}0^+}I(\epsilon,\vec{s},\eta)$$

- near $\eta=\infty$: $\frac{1}{(\ell+p)^2-m^2+\eta}=\frac{1}{\ell^2+\eta}+\cdots$

- vacuum integrals:



[Davydychev, Tausk, 93']
[Broadhurst, 99']
[Kniehl, Pikelner, Veretin, 17']
[Pikelner, 18']

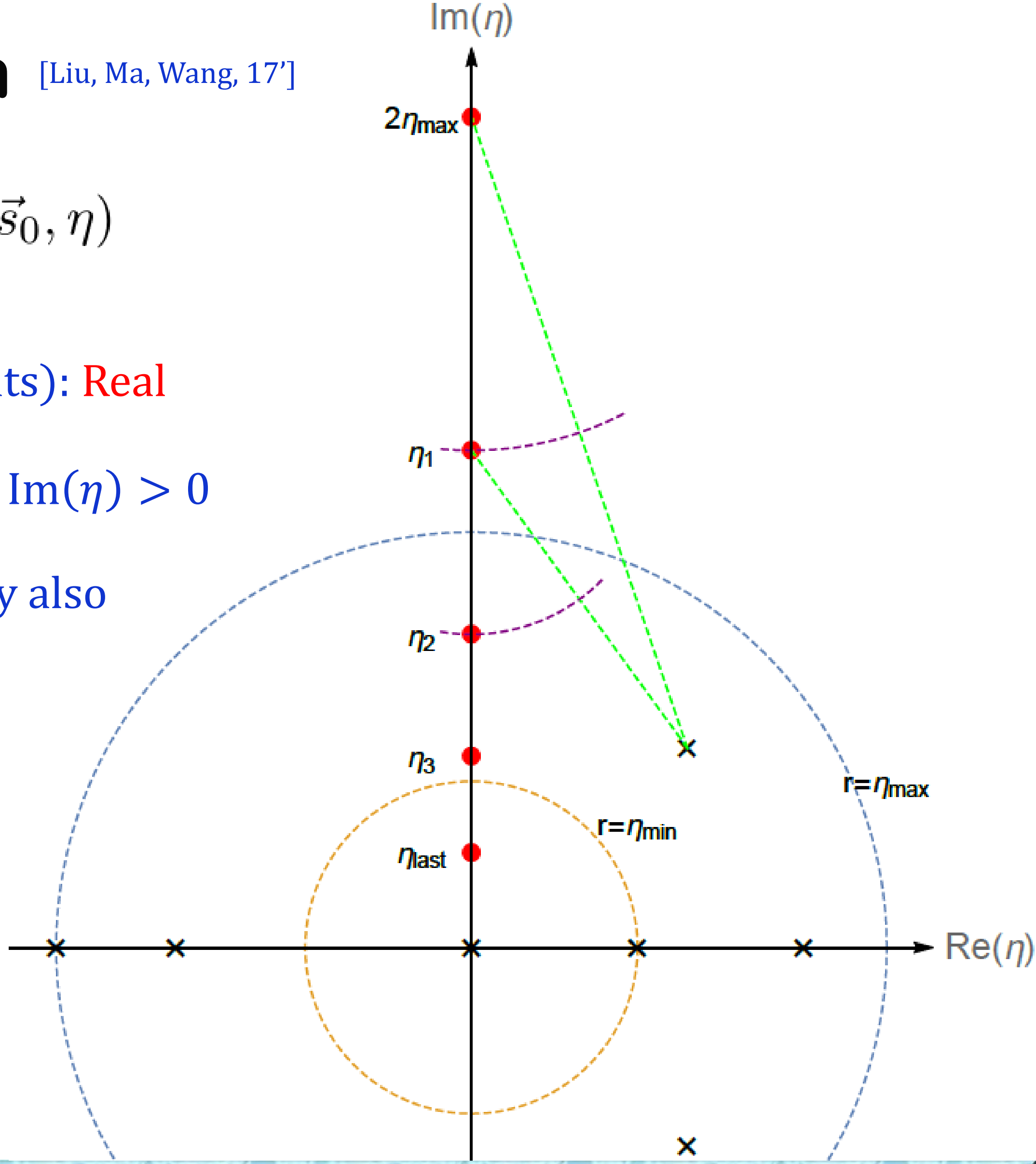
* auxiliary mass expansion: $I(\epsilon,\vec{s},\eta)=\eta^{(2-\epsilon)L-\sum\nu_\alpha}\sum_{n=0}^{\infty}M_n(\epsilon,\vec{s})\eta^{-n}$

[Liu, Ma, 19']
[Wang, Li, Basat, 19']
[Basat, Li, Wang, 21']

➢ Differential equation [Liu, Ma, Wang, 17']

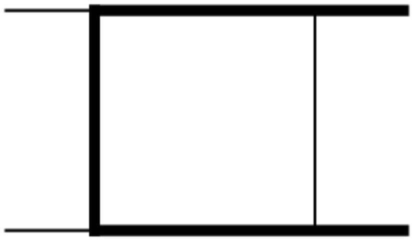
$$\frac{\partial}{\partial \eta}\vec{I}(\epsilon,\vec{s}_0,\eta) = A(\epsilon,\eta)\vec{I}(\epsilon,\vec{s}_0,\eta)$$

- physical singularities (branch points): Real
- $\frac{1}{(\ell+p)^2-m^2+\text{Re}(\eta)+i\,\text{Im}(\eta)}$ off-shell for $\text{Im}(\eta)>0$
- singularities far from real axis: may also affect the convergence of solution
- evaluate at η_{next}: $(\eta_{\text{next}}-\eta_0)\sim\frac{r}{2}$



Infrared Divergences

➢ Example: one-loop four-point integral



$s = 10, t = -3, m^2 = 1$

- eta-reg: $-0.1309\,\mathrm{i}\sqrt{\eta} + (0.0665971 - 0.101394\,\mathrm{i})\log(\eta) - (0.29347 - 0.0201092\,\mathrm{i})$
- dim-reg: $\eta^{-\epsilon} f_1(\epsilon) + f_2(\epsilon) + \eta^{\frac{1}{2}-\epsilon} f_3(\epsilon)$
  - $f_1(\epsilon) = (-0.0665971 + 0.101394\,\mathrm{i})\epsilon^{-1} + (-0.280099 - 0.267748\,\mathrm{i})$
  - $f_2(\epsilon) = (0.0665971 - 0.101394\,\mathrm{i})\epsilon^{-1} + (-0.0133705 + 0.287857\,\mathrm{i})$
  - $f_3(\epsilon) = -0.1309\,\mathrm{i}$
  - take $\eta \to 0$, only $f_2(\epsilon)$ survives

Discussion

➢ Advantages

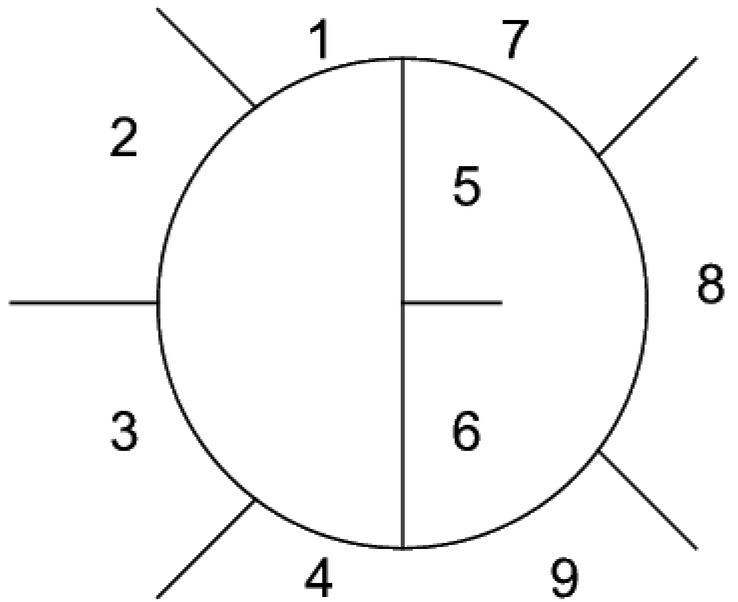
- systematic: in principle can be applied to any process
- efficient: $p \sim t$
- not sensitive to the choice of $\vec{s}_0$

➢ Problems

- effect of the extra mass scale: many more master integrals, hard to set up differential equation for complicated problems
  - develop much more powerful integral reduction method
  - reduce the effect of extra mass scale

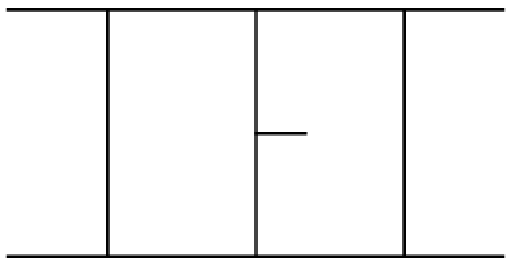
Strategy to introduce η

➢ Structure of Feynman diagrams



- loop: {1,2,3,4,5,6}, {1,2,3,4,7,8,9}, {5,6,7,8,9}
- branch: {1,2,3,4}, {5,6}, {7,8,9}
- possible mode: “all”, “loop”, “branch”, “propagator”

➢ Example: two-loop double-pentagon

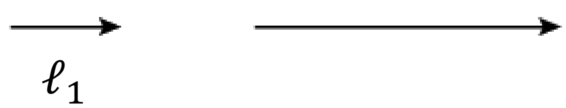


- before introducing η : 108
- all: 476
- loop: 305, 319
- branch: 233, 234
- propagator: 176, 178, 220
- propagator mode seems to be the cheapest

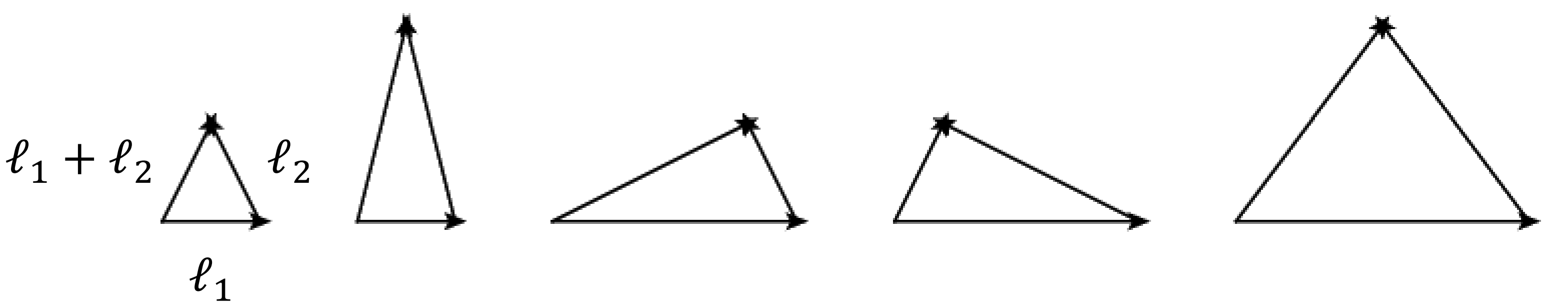
Integration regions

➢ General integration region

- loop momentum of each branch can be either $O(1)$ or $O(\sqrt{\eta})$
- momentum conservation



- regions for one-loop: (S), (L)



- regions for two-loop: (S,S,S), (S,L,L), (L,S,L), (L,L,S), (L,L,L)
- $R_1 = 2, R_2 = 5, R_3 = 15, \ldots$

Expansion

➢ Expansion in each region

- all large: single-mass vacuum integrals

$$\frac{1}{(\ell+p)^2-m^2+\eta} \sim \frac{1}{\ell^2+\eta}$$

- mixed: factorized integrals with a factor being vacuum integrals

$$\frac{1}{(\ell_{\rm S}+\ell_{\rm L}+p)^2-m^2+\eta} \sim \frac{1}{\ell_{\rm L}^2+\eta}$$

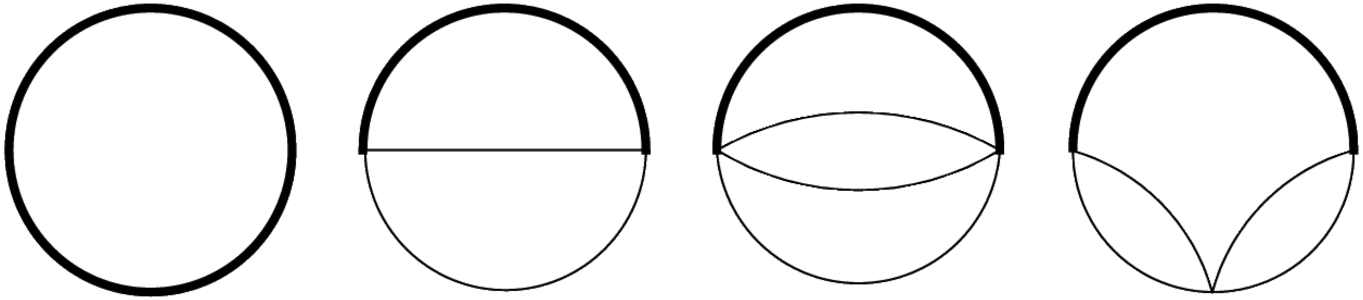
- all small: integrals with fewer propagators

$$\frac{1}{(\ell+p)^2-m^2+\eta} \sim \frac{1}{\eta}$$

Recursively set up

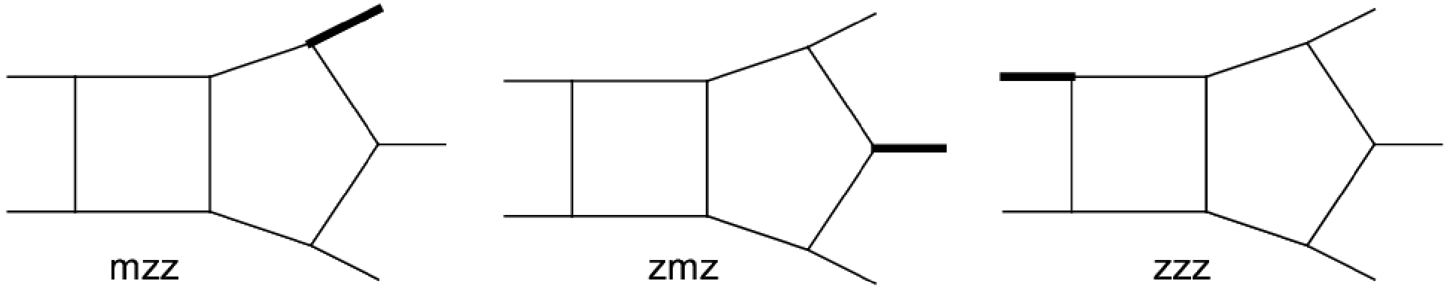
➢ Algorithm (propagator mode)

1. Introduce auxiliary mass to a propagator for target family
2. Reduce boundary integrals to boundary master integrals
3. If boundary master integrals are known to us, stop; else, set family which contains unknown integrals to be target and return to step 1



Examples

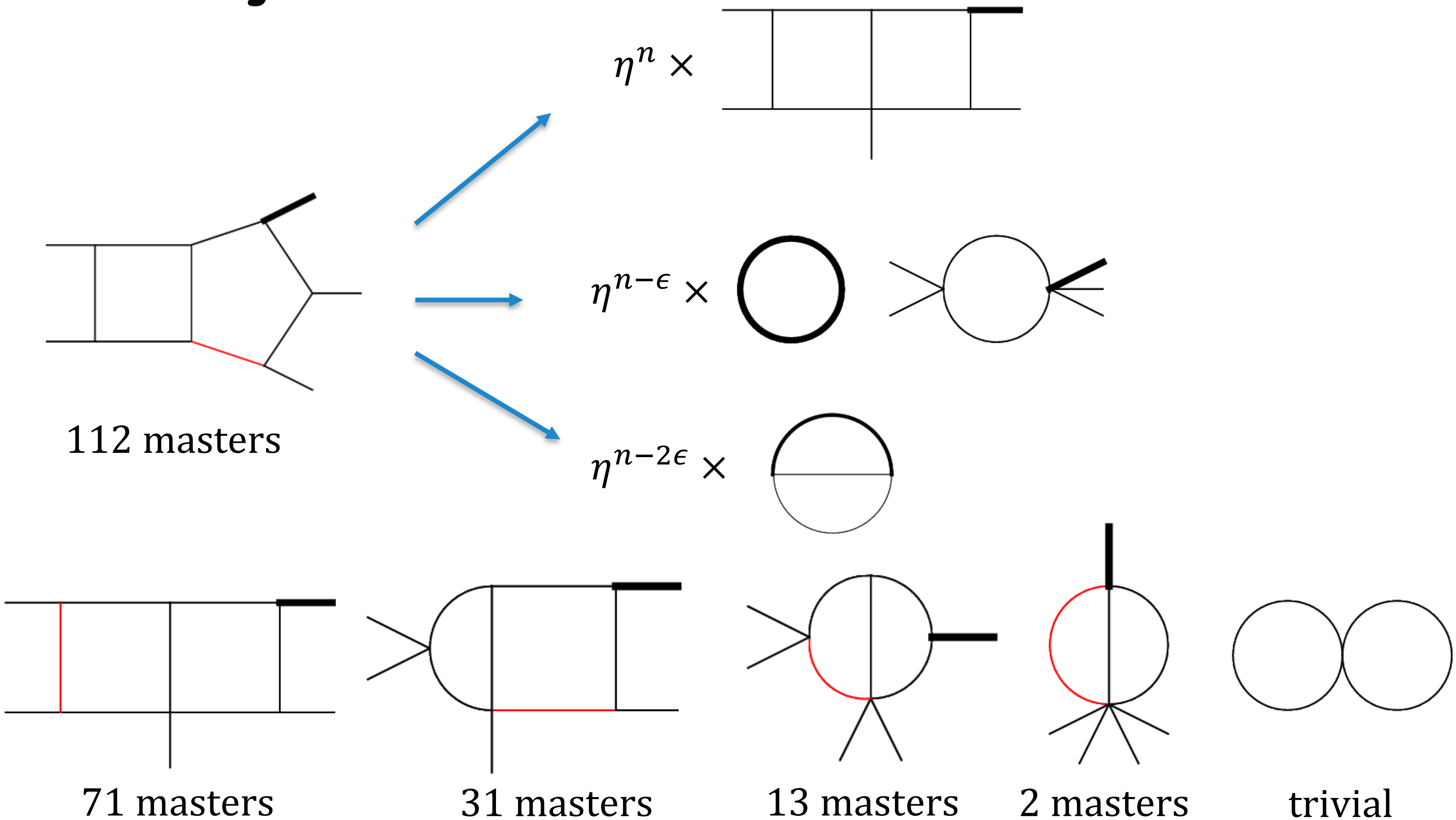
➢ **Example: two-loop five-point one-mass** [Abreu, Ita, Moriello et al, 20']
[Canko, et al, 20']



- $\vec{s} = \{m^2, s_{12}, s_{23}, s_{34}, s_{45}, s_{15}\}$
- master integrals: 74, 75, 86

Examples

- **The family "mzz"**



Examples

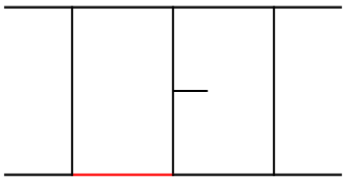
- $\vec{s}_0 = \{\frac{137}{50}, -\frac{22}{5}, \frac{241}{25}, -\frac{377}{100}, \frac{13}{50}, \frac{249}{50}\}$
- solve systems to get 16 correct digits: 10 h + 4 h
- $I_{\mathrm{phy}}[1,1,1,1,1,1,1,1,0,0,\text{-}1]$:

$$\frac{1.419205041065608 + 0.\times 10^{-36}\, i}{\mathrm{eps}^4} + \frac{2.712069420001789 + 9.486868391456017\, i}{\mathrm{eps}^3} - \frac{23.64601796152245 - 17.39902613661114\, i}{\mathrm{eps}^2} - \frac{38.52314440274530 + 23.56371708766445\, i}{\mathrm{eps}} - (5.79127129445584 + 16.41879693197834\, i) - (217.3029986433433 + 26.8459329371091\, i)\, \mathrm{eps} + O(\mathrm{eps}^2)$$

Examples

➢ Example: two-loop double-pentagon

[Chicherin, Gehrmann, Henn et al. 18’]
[Chicherin, Sotnikov, 20’]

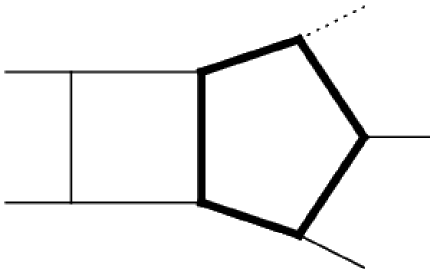


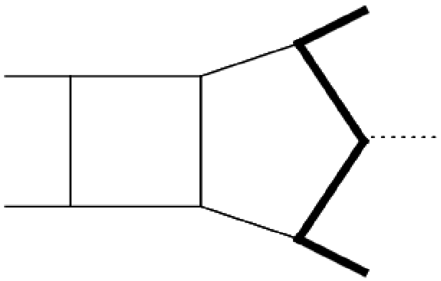
- $\vec{s} = \{s_{12}, s_{23}, s_{34}, s_{45}, s_{15}\} \to \{4, -\frac{113}{47}, \frac{281}{149}, \frac{349}{257}, -\frac{863}{541}\}$
- master integrals: $108 \to 176$
- time consumption: 40 h + 9 h
- $I_{\text{phy}}[1,1,1,1,1,1,1,1,0,0,0]$:

$$-\frac{0.06943562517263776 + 0. \times 10^{-36}\, i}{\text{eps}^4} + \frac{1.162256636711287 + 1.416359853446717\, i}{\text{eps}^3} + \frac{37.82474332116938 + 15.91912443581739\, i}{\text{eps}^2} + \frac{86.2861798369034 + 166.8971535711277\, i}{\text{eps}} - (4.1435965578662 - 333.0996040071305\, i) - (531.834114822928 - 1583.724672502141\, i)\, \text{eps} + O(\text{eps}^2)$$

Examples

➢ Example: massive two-loop five-point integrals





- $\vec{s} = \{s_{12}, s_{13}, s_{14}, s_{23}, s_{24}, m_h^2, m_t^2\}$
- mass mode: 173 → 173
- 110 h + 3.5 h

- $\vec{s} = \{s_{12}, s_{13}, s_{14}, s_{23}, s_{24}, m_h^2, m_t^2\}$
- 112 → 153
- 15 h + 5.5 h

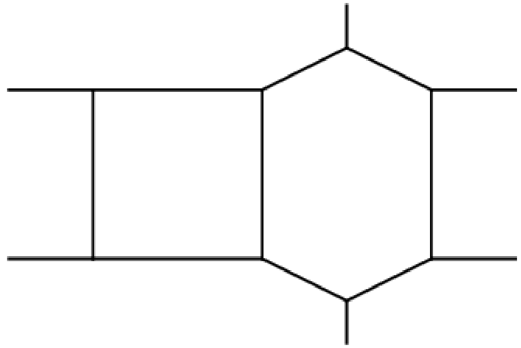
- $\vec{s}_0 = \{-(11/29), -(83/111), 9/14, 5/54, 11/23, 13/25, 1\}$
- $I^{\mathrm{L}}_{\mathrm{phy}}[1,1,1,1,1,1,1,1,0,0,0]$:

$$\frac{0.2423817728289377 + 0.\times 10^{-17}\, i}{\mathrm{eps}^2} + \frac{0.4053317523924661 + 0.\times 10^{-17}\, i}{\mathrm{eps}} + (0.2495153176904204 + 0.\times 10^{-17}\, i) - (0.3871860805812495 + 0.\times 10^{-17}\, i)\,\mathrm{eps} + O(\mathrm{eps}^2)$$

- $I^{\mathrm{R}}_{\mathrm{phy}}[1,1,1,1,1,1,1,1,0,0,0]$:

$$-\frac{1.733862437148516 + 0.\times 10^{-35}\, i}{\mathrm{eps}^4} - \frac{1.253769351252980 + 2.991960008727288\, i}{\mathrm{eps}^3} - \frac{0.536738276646420 + 10.343102095089467\, i}{\mathrm{eps}^2} + \frac{43.0506232784289 5 - 44.17661124884178\, i}{\mathrm{eps}} + (307.6203997981029 - 189.8119294459303\, i) + (1213.425315637774 - 812.997107316634\, i)\,\mathrm{eps} + O(\mathrm{eps}^2)$$

➢ Example: two-loop six-point integrals



- $\vec{s} = \{s_{12}, s_{13}, s_{14}, s_{15}, s_{23}, s_{24}, s_{25}, s_{34}, s_{35}\}$ with D-dim external legs
- $211 \rightarrow 289$
- $400\ \text{h} + 23\ \text{h}$

- $\vec{s}_0$={1, 19/25, -11/10, -11/25, 71/26, 66/31, -13/24, -76/29, -85/28}
- $I_{\text{phy}}[1,1,1,1,1,1,1,1,1,0,0,0,0]$:

$$-\frac{0.05548129894682673 + 0.\times 10^{-36}\, i}{\text{eps}^4} - \frac{0.572584535428102 + 3.105682821655971\, i}{\text{eps}^3} + \frac{9.33557823385437 - 13.03316413285356\, i}{\text{eps}^2} + \frac{32.39125016729625 - 16.23642338083992\, i}{\text{eps}} + (59.40191683114858 - 28.11177133669424\, i) + (143.4862936844010 - 28.3073224401266\, i)\,\text{eps} + O(\text{eps}^2)$$

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III. Application – auxiliary mass flow

IV. Summary and outlook

Summary and outlook

- Numerical differential equation is a powerful tool to solve master integrals.
- As an application, the auxiliary mass flow method, can be to calculate master integrals systematically and efficiently.
- In future, we believe these methods could be applied to cutting-edge problems: $t\bar{t}H, t\bar{t}j, \ldots$

Thank you!