Structural Aspects of Numerical Loop Calculus

Do we need it?
What is it about?
Can we handle it?

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A Paradigm: FD & HTF

When possible diagrams are written in terms of multiple

Nielsen - Goncharov polylogarithms

$$\mathrm{Li}_{m_1,\cdots,m_n}(z_1,\cdots,z_n) = \sum_{\infty>i_1>\cdots>i_n>0} \prod_{l=1}^{n} \frac{z_l^{i_l}}{i_l^{m_l}}.$$

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Induce an expansion in terms of Bernoulli numbers (miracolous acceleration of convergence), e.g.

$$S_{2,p}(z) \; = \; \mathrm{Li}_{3,\{1\}_{p-1}}(z,\{1\}_{p-1}) = \frac{1}{p!}\sum_{l=0}^{\infty} \frac{B_l}{(l+p)\, l!}\,\zeta^{l+p}, \quad \zeta = -\ln(1-z),$$

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$$S_{1,2}(z) \;=\; \mathrm{Li}_{2,1}\left(z,1\right) = \sum_{n=2}^{\infty} \sum_{p=1}^{n-1} \frac{z^n}{n^2} \frac{1}{p},$$

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Use

$$\sum_{p=1}^{n-1} \frac{1}{p} = \psi(n) - \psi(1) = \int_0^1 dx\, \frac{1-x^{n-1}}{1-x},$$

Obtain

$$S_{1,2}(z) = \int_0^1 \frac{dx}{1-x} \sum_{n=2}^{\infty} [\frac{z^n}{n^2} - \frac{1}{x}\,\frac{(x\,z)^n}{n^2}] = \int_0^1 \frac{dx}{1-x}\,[\mathrm{Li}_2\,(z) - \frac{1}{x}\,\mathrm{Li}_2\,(z\,x)]$$

$$= \;-\,\mathrm{Li}_3\,(z) - \int_0^1 \frac{dx}{x-1}\,[\mathrm{Li}_2\,(z\,x) - \mathrm{Li}_2\,(z)].$$

continued...

For multiple polylogarithms we can derive similar results by using the Lerch Φ function:

$$\sum_{l=1}^{n-1} \frac{z^{l-1}}{l^p} = \Phi(z,p,1) - z^{n-1}\,\Phi(z,p,n), \qquad \Phi(z,p,n) = \frac{(-1)^{p-1}}{\Gamma(p)} \int_0^1 dx\, \frac{x^{n-1}}{1-x\,z}\, \ln^{p-1} x,$$

giving

$$\sum_{l=1}^{n-1} \frac{z^l}{l^p} = (-1)^{p-1} \frac{z}{\Gamma(p)} \int_0^1 dx\, \ln^{p-1} x\, \frac{1-(x\,z)^{n-1}}{1-x\,z}.$$

For instance we have

$$\mathrm{Li}_{n_1,n_2}(z_1,z_2) = \frac{(-1)^{n_2}}{(n_2-1)!} \Big\{ I_{n_1,n_2-1}(z_1\,z_2) - z_2 \int_0^1 dx\, \frac{\ln^{n_2-1} x}{1-x\,z_2} \left[\mathrm{Li}_{n_1}(z_1) - \mathrm{Li}_{n_1}(x\,z_1\,z_2)\right] \Big\},$$

$$I_{n_1,n_2}(z_1\,z_2) = \int_0^1 \frac{dx}{x}\, \ln^{n_2} x\, \mathrm{Li}_{n_1}(x\,z_1\,z_2),$$

$$I_{n_1,n_2} = (-1)^{n_1-1} \frac{n_2!}{(n_1+n_2-1)!}\, I_{1,n_1+n_2-1}(\zeta) = (-1)^{n_2}\, n_2!\, \mathrm{Li}_{n_1+n_2+1}(\zeta).$$

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The simple, fully massive, two-loop Sunset becomes a combination of Lauricella functions, leading to hugly multiple sums with multiple binomial coefficients and argument $\neq 1$.

$$F_C(a, b; c_1, \cdots, c_n; z_1, \cdots, z_n) \;=\; \prod_{i=1}^{n} \sum_{m_i=0}^{\infty} \frac{(a)_M\,(b)_M}{\Pi_{i=1}^{n}\,(c_i)_{m_i}} \prod_{i=1}^{n} z_i^{m_i},$$

$$M \;=\; m_1 + \cdots + m_n, \qquad \sum_{i=1}^{n} \mid x_i^{1/2} \mid < 1 \;\equiv\; |p^2| < (m_1 + m_2 + m_3)^2.$$

can be analytically continued in the region $|p^2| > (m_1 + m_2 + m_3)^2$ but around-threshold behavior is not available.

Actually we know that the Sunset has an integral representation in terms of products of Bessel functions (analytical cont. $J \to I$ and $K \to H$).

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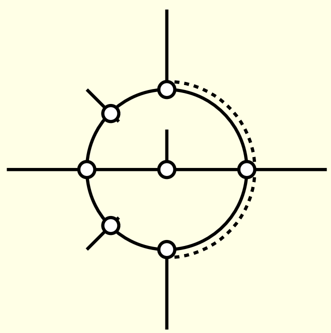
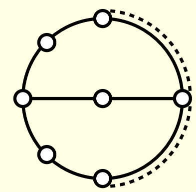
$$\textbf{Sunset}(p,m_1,m_2,m_3) \propto \int_0^{\infty} dx\, x^{1-2\nu}\, J_{\nu}(qx)\prod_{i=1}^{3} K_{\nu}(m_i x), \qquad \nu = \frac{n}{2}-1, \quad q^2 = -p^2.$$

Arbitrary FD are Generalized Sunsets

Combining q_1, q_2 and $q_1 - q_2$ propagators in any two-loop diagram (left) we obtain the integral of a Sunset (right),



$$= \quad \int_0^1 dx_1 \cdots$$



But **GSunset** $(\alpha_1, \cdots, \alpha_3) \;\propto\; (1 - \frac{p^2}{M^2})^{2\,(n+1)-\alpha}, \qquad \alpha = \sum_i \alpha_i, \quad M^2 = \sum_i m_i^2,$

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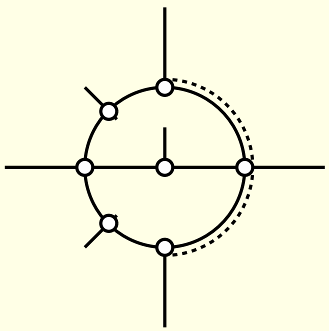

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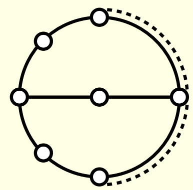

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So that integration over external Feynman parameters has severe stability problems since the $\{x\}$-dependent normal threshold is always $\in$ integration region.

For all one is worth $\cdots$ although it's fun

With some effort we can cast the Sunset S_{112} into a combinations of integrals

$$\int_0^X \frac{dx}{y}\,\{\mathrm{Li}_2\left(\frac{1}{x}\right)\;;\;\ln(1-\frac{1}{x})\},$$
$$\int_0^X \frac{dx}{(x-x_0)\,y}\,\{\mathrm{Li}_2\left(\frac{1}{x}\right)\;;\;\ln(1-\frac{1}{x})\},$$

where $y^2 = a_0\,x^4 + 4\,a_1\,x^3 + 6\,a_2\,x^2 + 4\,a_3\,x + a_4$**,**

and where $X\,,\,x_0\,,\,a_0\,,\cdots a_4$ **are functions of** p^2 **and of internal masses.**

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But is it useful to introduce a new class of functions $\otimes$ new diagram?

General approach for numerical evaluation of arbitrary FD

$$G = \sum \left[\frac{1}{B_G} \int_S dx \, \mathcal{G}(x) \right],$$

Smoothness requires that the kernel in and its first N derivatives should be continuous functions with N as large as possible. However, in most cases we will be satisfied with absolute convergence, e.g. logarithmic singularities of the kernel. This is particularly true around the zeros of B_G where the large number of terms obtained by requiring continuous derivatives of higher order leads to large numerical cancellations.

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B_G is a function of masses and external momenta whose zeros correspond to true singularities of G, if any.

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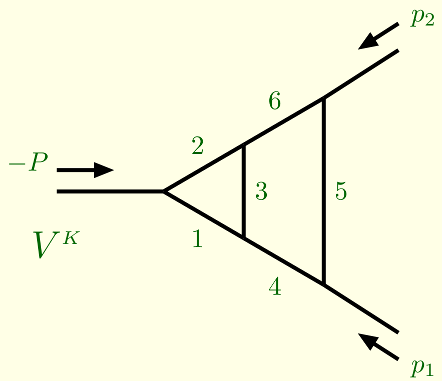
Algorithms of smoothness, example

The irreducible two-loop vertex diagrams V^K. External momenta are flowing inwards.



$$V_0^K = \int_0^1 dx \int_0^x dy \; \boxed{\textbf{linear combination of}} \; \{x\,, y\} - \boxed{\textbf{dependent}} \; C_0.$$

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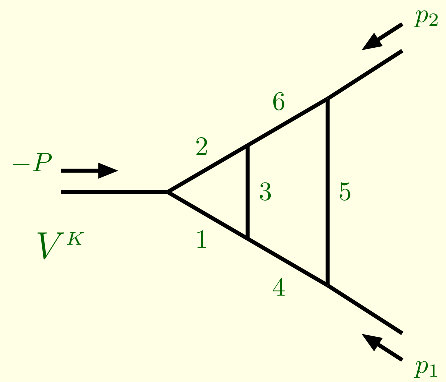

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$$\approx \quad \int d\{x\}\, \frac{1}{P(\{x\})}\, \ln(1 + \frac{P(\{x\})}{Q(\{x\})})$$

Parameter dependent C_0 functions

$$C_0(\lambda\,;\, a\dots f) \;=\; \int_0^1 dx \int_0^x dy\, V^{-1-\lambda\,\epsilon}(x,y), \qquad V(x,y) = ax^2 + by^2 + cxy + dx + ey + f - i\,\delta.$$

The total result (no problem for ho in ϵ) reads as follows:

$$C_0 \;=\; C_{00} - \frac{1}{2}\,\lambda\,\epsilon\,C_{01} + \mathcal{O}\left(\epsilon^2\right),$$

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Step 1 **Define** α **to be a solution of** $b\,\alpha^2 + c\,\alpha + a = 0,$

introduce (TV trick) $A(y) = (c + 2\,\alpha b)\,y + d + e\,\alpha, \quad B(y) = b\,y^2 + e\,y + f.$

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continued...

Next

Transform $y \to y + \alpha\, x, \to V(x,y) = A(y)\, x + B(y),$

split $\int_0^1 dx \int_0^x dy \longrightarrow \int_0^1 dx \int_{-\alpha x}^{\overline{\alpha} x} dy = \int_0^{\overline{\alpha}} dy \int_{y/\overline{\alpha}}^1 dx - \int_0^{-\alpha} dy \int_{-y/\alpha}^1 dx, \quad \overline{\alpha} = 1 - \alpha,$

transform again $: y = \overline{\alpha}\, y'$ **or** $y = -\alpha\, y',$

use $-\frac{1}{\lambda\, A \epsilon}\partial_x\, (A\, x + B)^{-\lambda\epsilon} = (A\, x + B)^{-1-\lambda\epsilon},$ **and integrate by parts**.

Introduce $A_1(y) = A(\overline{\alpha}\, y), \quad A_2(y) = A(-\alpha\, y), \quad B_1(y) = B(\overline{\alpha}\, y), \quad B_2(y) = B(-\alpha\, y),$

and also $Q_{1,2}(y) = A_{1,2}(y) + B_{1,2}(y),\ Q_{3,4}(y) = A_{1,2}(y)\, y + B_{1,2}(y),\ Q_{5,6}(x,y) = A_{1,2}(y)\, x + B_{1,2}$

The result is

$$C_{0,n} = \int_0^1 dy\, \mathcal{C}_{0,n}(y),$$

with Subtracted logarithms $\ln^n \mathcal{Q}_{1,2}(y) = \ln^n Q_{1,2}(y) - \ln^n B_{1,2}(y)$

$$\mathcal{C}_{0,n} = \frac{\overline{\alpha}}{A_1}\left[\ln^{n+1} \mathcal{Q}_1 - \ln^{n+1} \mathcal{Q}_3\right] + \frac{\alpha}{A_2}\left[\ln^{n+1} \mathcal{Q}_2 - \ln^{n+1} \mathcal{Q}_4\right].$$

Recovering the anomalous threshold

Suppose that we are considering a one-loop C_0-function with $p_1^2 = p_2^2 = -m^2$ and $m_1 = m_3 = m, m_2 = M$. Consider now one of the terms in the result, say $\ln \mathcal{Q}_1/A_1$; we have a singularity when the zero of A_1, i.e.

$$\overline{\alpha}\, y \;=\; -\frac{d + e\,\alpha}{c + 2\,b\,\alpha},$$

is also a zero of B_1, which may occur only if $s\,(s - 4\,m^2 + M^2) = 0$, the anomalous threshold for this configuration.

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Integrable singularities and sector decomposition

One of the main problems in numerical multidimensional integration is to handle integrable singularities lying in arbitrary regions of the integration volume;

Extensions of standard techniques are to be preferred to procedures that automatically adapt themselves to the rate of variation of the integrand at each point (Quasi - Semi - Analytical approach).

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however a source of numerical instabilities is connected to the region where $x \approx y \approx 0$, since N/D are vanishing small in the argument of the logarithm.

continued...

A nice solution is to adopt a sector decomposition to factorize their common zero. We obtain

$$I \;=\; \int_0^1 dx \int_0^1 dy \,[\ln\,(1+\frac{1}{a+y}) + \frac{1}{x}\,\ln\,(1+\frac{x}{a\,x+1})].$$

continued...

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one can gain several orders of magnitude improvement in the returned error.

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A more realistic example:

$$H \;=\; \int_0^1 dx \int_0^1 dy\, \frac{1}{x}\, \ln[1 + \frac{x}{a\,x+\chi(y)}], \qquad \chi(y) = h\,(y-y_-)\,(y-y_+) - i\,\delta, \qquad \delta \to 0_+.$$

continued...

Suspect that $0 < y_- < y_+ < 1,$

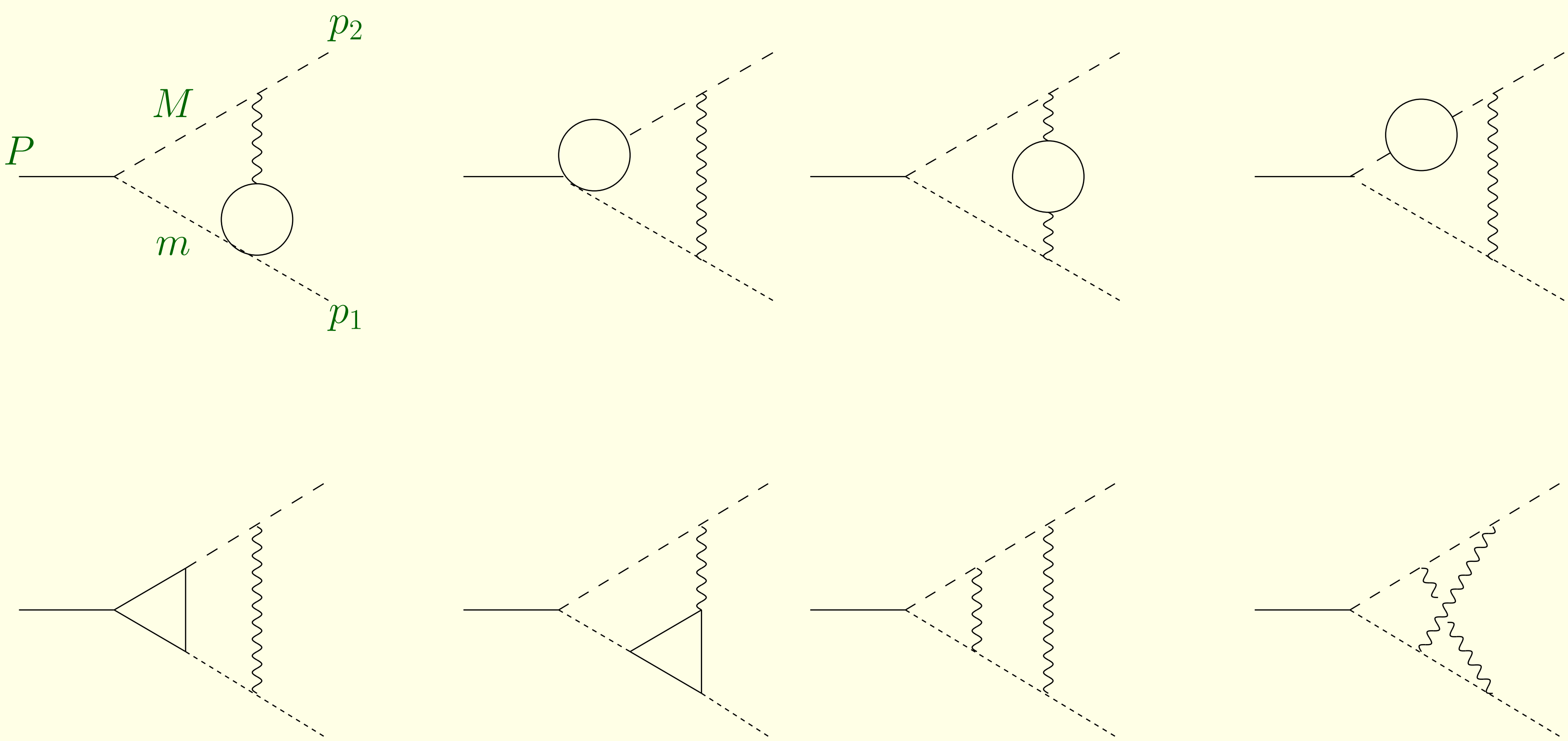
Split $[0\,,\,1] \quad \to \quad [0\,,\,y_-] \quad \oplus \quad [y_-\,,\,y_+] \quad \oplus \quad [y_+\,,\,1],$

Transform $y = y_-\,y', \quad y = (y_+ - y_-)\,y' + y_-, \quad y = (1 - y_+)\,y' + y_+,$

In this way all the zeros of N/D are located at the corners of $[0,1]^2$ and we can apply a sector decomposition to obtain 7 sectors giving the following result:

$$
\begin{aligned}
H &= \int_0^1 dx \int_0^1 dy\,[\mathcal{H}_1 + \frac{1}{x}\,\mathcal{H}_2],\\
\mathcal{H}_1 &= y_-\,\ln[1 + \frac{1}{a - h\,y_+\,y_-\,(y_-\,(1-xy) - y_+)}] + \Delta y\,\ln[1 + \frac{1}{a - h\,(\Delta y)^2\,(1-xy)y}]\\
&+ \Delta y\,\ln[1 + \frac{1}{a - h\,(\Delta y)^2\,y}] + (1-y_+)\,\ln[1 + \frac{1}{a + h\,(1-y_+)^2\,x\,y^2 + h\,\Delta y\,(1-y_+)y}],\\
\mathcal{H}_2 &= y_-(1-y)\,\ln[1 + \frac{x}{a\,x - h\,y_-\,(y_-\,y - y_+)}] + \Delta y\,\ln[1 + \frac{x}{a\,x - h\,(\Delta y)^2}]\\
&+ (1-y_+)\,\ln[1 + \frac{x}{a\,x + h\,(1-y_+)\,((1-y_+)\,y + \Delta y)}], \qquad \Delta y = y_+ - y_- > 0.
\end{aligned}
$$

Something difficult: IR configurations



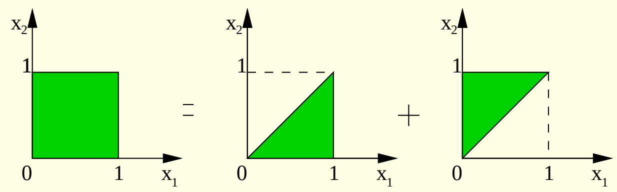
Sector decomposition for pedestrians

In multi-loop diagrams the IR singularities are often overlapping. Procedure:

- **Place the singular points at the hedge of the parameters space and remap variables to the unit cube. Example:**

$$I \;=\; \int_0^1 dx\,dy\,P^{-2-\epsilon}(x,y), \qquad P(x,y) = a\,(1-y)\,x^2 + b\,y$$

- **Decompose the integration domain**



$$\int_0^1 dx \int_0^1 dy \;=\; \int_0^1 dx \int_0^x dy + \int_0^1 dy \int_0^y dx$$

continued...

- **Remap the variables to the unit cube**

$$I \;=\; \int_0^1 dx\,dy\,x\,P^{-2-\epsilon}(x,xy) + \int_0^1 dx\,dy\,y\,P^{-2-\epsilon}(xy,y),$$

Factorize $$I \;=\; \int_0^1 dx\,dy\left[x^{-1-\epsilon}\,P_1^{-2-\epsilon}(x,y) + y^{-1-\epsilon}\,P_2^{-2-\epsilon}(x,y)\right],$$

$$P_1 \;=\; a\,(1-x\,y)\,x + b\,y, \qquad P_2 = a\,(1-y)\,x^2 + b$$

- **Iterate the procedure until all polynomials are free from zeros.**
- **Perform a Taylor expansion in the factorized variables and integrate to extract the IR poles:**

$$I_2 \;=\; -\frac{1}{\epsilon}\int_0^1 dx\,P_2^{-2-\epsilon}(x,0) + \int_0^1 dx\int_0^1 dy\,\frac{P_2^{-2}(x,y) - P_2^{-2}(x,0)}{y}.$$

If $\mathbf{a, b > 0}$ we can integrate numerically, but this doesn't work

continued...

- **Remap the variables to the unit cube**

$$I = \int_0^1 dx\, dy\, x\, P^{-2-\epsilon}(x, xy) + \int_0^1 dx\, dy\, y\, P^{-2-\epsilon}(xy, y),$$

Factorize

$$I = \int_0^1 dx\, dy \left[x^{-1-\epsilon}\, P_1^{-2-\epsilon}(x, y) + y^{-1-\epsilon}\, P_2^{-2-\epsilon}(x, y)\right],$$

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Infrared singularities and hypergeometric functions

In most of the two-loop cases sector decomposition has drawbacks:

with the consequence that one cannot find any adeguate smoothness algorithm to handle the final integration.

A second procedure

The polynomial V of the IR C_0 can be rewritten as

This transformation is designed to make V linear in x and a for all IR diagrams we seek for a transformation that make the Feynman integrand linear in some variable.

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$$V(x,y) \;=\; m^2\,x^2 + m^2\,y^2 + (s - 2\,m^2)\,x\,y - 2\,m^2\,x - (s - 2\,m^2)\,y + m^2;$$

transformation $\quad y = y' + \alpha\,x \quad$ **with** $\quad m^2\,\alpha^2 + (s - 2\,m^2)\,\alpha + m^2 = 0.$

This transformation is designed to make V linear in x and a for all IR diagrams we seek for a transformation that make the Feynman integrand linear in some variable.

continued...

$$C_0 \; = \; C_0^1 + C_0^2$$

$$C_0^1 \; = \; -\,(1-\alpha)\,\int_0^1 dy\,\int_0^y dx\,V_1^{-1-\epsilon/2}(x,y), \qquad C_0^2 = \alpha\,\int_0^1 dy\,\int_0^y dx\,V_2^{-1-\epsilon/2}(x,y),$$

with polynomials

$$V_1 \; = \; [s\,(1+\alpha)\,y - s + 2\,(1-\alpha)\,m^2]\,x - \alpha\,s\,y^2 - 2\,(1-\alpha)\,m^2\,y + m^2,$$
$$V_2 \; = \; \{[\alpha\,s + 2\,(1-\alpha)\,m^2]\,x - [\alpha\,s + (2\,\alpha-1)\,m^2]\}\,y.$$

The x-integration has the general form

$$I_i(y) \; = \; \int_0^y dx[B_i(y) - A_i(y)\,x]^{-1-\epsilon/2}, \qquad i=1,2, \quad = y\,B_i^{-1-\epsilon/2}\,{}_2F_1(1+\epsilon/2\,,\,1\,;\,2\,;\,\frac{A_i}{B_i}\,y).$$

Using well-known properties

$${}_2F_1(1+\frac{\epsilon}{2}\,,\,1\,;\,2\,;\,z) \; = \; \frac{2}{\epsilon}\,[-\,{}_2F_1(1\,,\,1+\frac{\epsilon}{2}\,;\,1+\frac{\epsilon}{2}\,;\,1-z) + (1-z)^{-\epsilon/2}\,{}_2F_1(1\,,\,1-\frac{\epsilon}{2}\,;\,1-\frac{\epsilon}{2}\,;\,1-z)],$$

continued...

we derive $$I_i(y) = -\frac{2}{A_i\,\epsilon}\,B_i^{-\epsilon/2}\,[1-(1-\frac{A_i}{B_i}\,y)^{-\epsilon/2}].$$

For $i=1$ we can simply expand around $\epsilon=0$ obtaining

$$C_0^1 = \int_0^1 dy\,\frac{1}{A_1(y)}\,\ln[1-\frac{A_1(y)}{B_1(y)}\,y],$$

for $i=2$ we find

$$\begin{aligned} A_2(y) &= a(s,m^2)\,y, \qquad B_2(y) = b(s,m^2)\,y^2, \\ a(s,m^2) &= \alpha\,s + 2\,(1-\alpha)\,m^2, \qquad b(s,m^2) = -\,\alpha\,s + (2\,\alpha-1)\,m^2. \end{aligned}$$

It follows that

$$\begin{aligned} C_0^2 &= a^{-1}(s,m^2)\,b^{-\frac{\epsilon}{2}}(s,m^2)\,\int_0^1 dy\,y^{-1+\epsilon}\,\ln[1-\frac{a(s,m^2)}{b(s,m^2)}]\,\{1-\frac{\epsilon}{4}\,\ln[1-\frac{a(s,m^2)}{b(s,m^2)}]\} \\ &= a^{-1}(s,m^2)\,\ln[1-\frac{a(s,m^2)}{b(s,m^2)}]\,\{\frac{1}{\epsilon}-\frac{1}{4}\,\ln[1-\frac{a(s,m^2)}{b(s,m^2)}]-\frac{1}{2}\,\ln\,b(s,m^2)\}. \end{aligned}$$

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where, for $m \ll |p^2|$ there are instabilities around $y = 0$

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- ♢ Now that Basics are ready next talk will be on Physical Observables.