Numerical evaluation of multi-loop integrals without contour deformation

Roberto Pittau

CERN & U. of Granada

DESY-HU Theory-Seminar

CERN, November 25^{th} 2021

Evaluating multi-loop integrals

Very active field!

- See Gudrun Heinrich's [2009.00516] for a recent review

- Here, I'll report on the numerical approach of R.P. and Bryan Webber [2110.12885]

Outline

1. *How to avoid contour Deformation* **(CD)** *for threshold singularities*

   $\Rightarrow$ **MC** evaluation of loop integrals:

2. *Integrating over loop energy components*
3. *"Gluing" together lower-loop substructures*
4. *UV*
5. *IR*

The LO past to understand the multi-loop present

Why high-multiplicity $(n_p \sim 10)$ **LO** perturbative calculations are nowadays the bread and butter of high-energy particle physics simulations?

i) 4 dimensions
ii) No UV/IR divergences
iii) No contour deformation to compute integrals

Take, for instance,

$$\sigma^{\rm cut}_{n_p=10} := \int_{\rm cut} d\Phi_{10}\, |M|^2$$

- Nobody would ever try to compute $\sigma^{\rm cut}_{n_p=10}$ analytically
- Due to i), ii), iii), **MC** methods can be used to find a numerical approximation of $\sigma^{\rm cut}_{n_p=10}$

The LO past to understand the multi-loop present

Why high-multiplicity $(n_p \sim 10)$ **LO** perturbative calculations are nowadays the bread and butter of high-energy particle physics simulations?

i) 4 dimensions
ii) No UV/IR divergences $\Downarrow$ **Major bottleneck**
iii) No **contour deformation** to compute integrals

Take, for instance,

$$\sigma^{\text{cut}}_{n_p=10} := \int_{\text{cut}} d\Phi_{10}\, |M|^2$$

- Nobody would ever try to compute $\sigma^{\text{cut}}_{n_p=10}$ analytically
- Due to i), ii), iii), **MC** methods can be used to find a numerical approximation of $\sigma^{\text{cut}}_{n_p=10}$

The basic 1-dim threshold singularity

- The core of the procedure is a change of variable such that the $\frac{1}{x+i\epsilon}$ behaviour of the integral $I := \lim_{\epsilon\to 0}\int_{-1}^{1} dx \frac{1}{x+i\epsilon}$ is flattened with $x \in \mathbb{R}$: $x + i\epsilon = e^{i\pi(1-z)}$ $\Rightarrow$ $I = -i\pi \fint_0^1 dz$
- We impose $x \in \mathbb{R}$ by parametrizing $z = \alpha + i\beta$ with

$$\alpha, \beta \in \mathbb{R} \text{ and } \frac{\epsilon}{\pi} \leq \alpha \leq 1 - \frac{\epsilon}{\pi} \Rightarrow$$

$$\pi\beta = \ln \frac{\epsilon}{\sin[\pi(1-\alpha)]}, \quad x = x_\alpha := \frac{\epsilon}{\tan[\pi(1-\alpha)]}$$

- Thus, $dz = d\alpha \left(1 + i\frac{d\beta}{d\alpha}\right)$ or $dz = d\beta \left(\frac{d\alpha}{d\beta} + i\right)$ $\Rightarrow$

$$\fint_0^1 dz = \lim_{\epsilon\to 0} \frac{1}{g_\epsilon} \int_{\epsilon/\pi}^{1-\epsilon/\pi} d\alpha \left(1 + i\frac{x_\alpha}{\epsilon}\right), \quad g_\epsilon := 1 - \frac{2\epsilon}{\pi}$$

Adding a numerator $f(x) := \phi(x)/(x+i\epsilon)$

- $I_f := \int_{-1}^{1} dx\, f(x) := \int_0^1 dy\, [f(-y)+f(y)]$ ⇒

$$I_f = -\frac{i\pi}{g_\epsilon}\int_{\epsilon/\pi}^{1/2} d\alpha \left[\left(1 - i\frac{y_\alpha}{\epsilon}\right)\phi(-y_\alpha) + \left(1 + i\frac{y_\alpha}{\epsilon}\right)\phi(y_\alpha)\right]$$

$$I_f = -\frac{i\pi}{g_\epsilon}\int_{\beta_-}^{\beta_+} d\beta \left[\left(\frac{\epsilon}{-y_\beta} + i\right)\phi(-y_\beta) - \left(\frac{\epsilon}{y_\beta} + i\right)\phi(y_\beta)\right]$$

where

$$\begin{aligned} y_\alpha &:= |x_\alpha| = \epsilon/\tan(\alpha\pi), \\ y_\beta &:= e^{\pi\beta}\sqrt{1-\left(\frac{\epsilon}{e^{\pi\beta}}\right)^2}, \quad \beta_- = \frac{1}{\pi}\ln\frac{\epsilon}{\sin\epsilon}, \quad \beta_+ = \frac{\ln\epsilon}{\pi} \end{aligned}$$

Translating to a MC language

- $I_f = \int_0^1 d\rho \, \frac{f(-y)+f(y)}{g_i(y)}$ with $i = 1 \div 2$

$$
\begin{aligned}
g_1(y) &= \frac{2\epsilon}{\pi(y^2+\epsilon^2)}, \;\; y = \frac{\epsilon}{\tan(\alpha\pi)}, \;\; \alpha = \frac{\epsilon}{\pi} + \frac{\rho g_\epsilon}{2} \\
g_2(y) &= -\frac{g_\epsilon}{\ln(\sin\epsilon)} \frac{y}{(y^2+\epsilon^2)}, \;\; y = e^{\pi\beta}\sqrt{1-\left(\frac{\epsilon}{e^{\pi\beta}}\right)^2},
\end{aligned}
$$

$$
\beta = \frac{\ln(\epsilon) - \rho\ln(\sin\epsilon)}{\pi}
$$

- Alternative derivation of $g_{1,2}(y)$ in [2110.12885]
- Multichanneling: $I_f = \int_0^1 d\rho \, \frac{f(-y)+f(y)}{g_{\rm tot}(y)}$, $d\rho = g_{\rm tot}(y)dy$

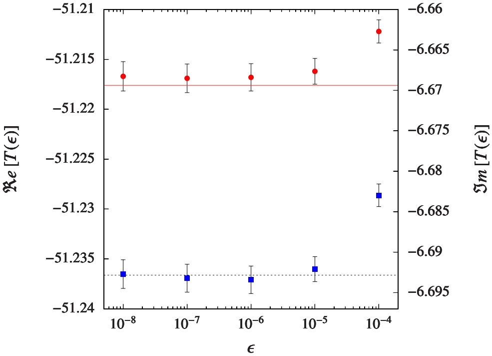
$$
g_{\rm tot}(y) = \alpha_1 g_1(y) + \alpha_2 g_2(y) + \sum_{i=3}^{N_{\rm ch}} \alpha_i (g_i(-y) + g_i(y))
$$

- Extension to n-fold integrals straightforward

Choosing ϵ via a test function

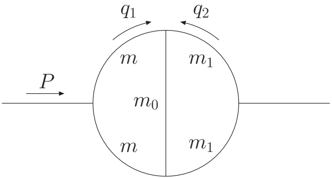
- $T(\epsilon) = \int_{-1}^{1} \prod_{j=1}^{3} \left(\frac{dx_j}{x_j + i\epsilon} \right) \sum_{j_1,j_2,j_3=0}^{1} x_1^{j_1} x_2^{j_2} x_3^{j_3}$

$$= (8 - 6\pi^2) + i\pi(\pi^2 - 12)$$



- With $10^{-8} \le \epsilon \le 10^{-6}$ **MC** estimates accurate at the level of two parts in 10^5

Integrating over loop energy components



$= S_2(m, m_0, m_1)$

- When $P/m = (\sqrt{\tau}, \vec{0})$ and $m_1 = m$, $\omega_i := q_i/m = (t_i, \vec{\rho}_i)$

$$S_2(m, m_0, m) = \frac{1}{m^2} \int d^4\omega_1 d^4\omega_2 \prod_{j=1}^{5} \frac{1}{\sigma_j + i\epsilon}$$

$$\sigma_1 = \omega_1^2 - 1,\ \sigma_2 = \omega_2^2 - 1,$$

$$\sigma_3 = \sigma_1 + \tau - 2\sqrt{\tau}\, t_1,\ \sigma_4 = \sigma_2 + \tau + 2\sqrt{\tau}\, t_2,$$

$$\sigma_5 = (t_1 + t_2)^2 - \rho_1^2 - \rho_2^2 - 2\rho_1\rho_2 c_\theta - \mu_0$$

with $\mu_0 := m_0^2/m^2$

- The integration over $t_{1,2}$ and angular variables gives

$$S_2(m, m_0, m) = \frac{2\pi^4}{m^2\tau} \sum_{\lambda_{1,2}=\pm} \int_{-\infty}^{\infty} dr_1 \int_{-\infty}^{\infty} dr_2 \, \frac{F(r_1, r_2, \lambda_1, \lambda_2)}{(r_1 - i\epsilon)(r_2 - i\epsilon)}$$

where $(A_i := r_i + \lambda_i \sqrt{\tau}/2)$

$$F(r_1, r_2, \lambda_1, \lambda_2) = \lambda_1 \lambda_2 \, \theta(A_1 - 1)\theta(A_2 - 1) \times \ln \frac{r_1 + r_2 + \sqrt{(\sqrt{A_1^2 - 1} + \sqrt{A_2^2 - 1})^2 + \mu_0} - i\epsilon}{r_1 + r_2 + \sqrt{(\sqrt{A_1^2 - 1} - \sqrt{A_2^2 - 1})^2 + \mu_0} - i\epsilon}$$

- Threshold singularities at $r_{1,2} = i\epsilon$ are present when $\lambda_{1,2} = +1$ if $\sqrt{\tau} > 2$

$-m^2\tau/\pi^4 S_2(m,0,m)$

$\rho := 4/\tau$	**MC** result	Analytic result*
.1	8.49(1) $-i$ 1.94(2)	8.495 $-i$ 1.927
.3	9.34(1) $-i$ 5.47(2)	9.340 $-i$ 5.460
.5	9.19(1) $-i$ 9.71(1)	9.195 $-i$ 9.716
.7	7.39(1) $-i$ 15.79(1)	7.396 $-i$ 15.783
.9	-1.03(2) $-i$ 27.591(8)	-1.061 $-i$ 27.581
1.1	-15.538(2) $-i$ 1.8314(4)$\times 10^{-5}$	-15.540 $+i$ 0
1.3	-7.9915(8) $-i$ 5.1218(7)$\times 10^{-6}$	-7.9921 $+i$ 0
1.5	-5.5608(6) $-i$ 2.9000(4)$\times 10^{-6}$	-5.5614 $+i$ 0
1.7	-4.2990(5) $-i$ 2.0139(3)$\times 10^{-6}$	-4.2996 $+i$ 0
1.9	-3.5153(5) $-i$ 1.5412(2)$\times 10^{-6}$	-3.5157 $+i$ 0

- 10^9 (10^{10}) **MC** shots when $\rho > 1$ $(\rho < 1)$

$*$ D. J. Broadhurst, Z.Phys.C 47 (1990) 115

- $-\frac{m^2\tau}{\pi^4} S_2(m,m,m) = 8.582(6) - i\,2.706(4)$, $\rho = .1$ with 10^9 shots

Gluing lower-loop structures

- $P := p_1 + p_2 \to p_3 + p_4$ and $\omega := \frac{q}{m} = (t, \rho c_\theta, \rho s_\theta s_\phi, \rho s_\theta c_\phi)$
- Rescaled propagators belonging to q:

$$\sigma_0 := q^2/m^2 - \mu_0, \qquad \sigma_1 := (q-P)^2/m^2 - \mu_1,$$
$$\sigma_2 := (q-p_2)^2/m^2 - \mu_2, \quad \sigma_3 := (q-p_3)^2/m^2 - \mu_3$$

- $\sigma_{0,1}$ are used as integration variables by multiplying the integrand by $1 = \int d\sigma_0 \int d\sigma_1 \, \Delta(\sigma_0, \sigma_1, \rho, t)$, where

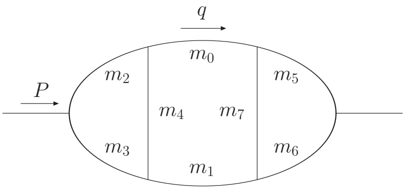
$$\Delta(\sigma_0, \sigma_1, \rho, t) := \delta(\sigma_0 + \mu_0 + \rho^2 - t^2)\delta(\sigma_1 - \sigma_0 + \mu_1 - \mu_0 - \tau + 2\sqrt{\tau} t)$$

- The functionals appear

$$\Phi_1^{(\mu_0,\mu_1)}[J_1] := \int d^4\omega \, J_1 \, \Delta(\sigma_0, \sigma_1, \rho, t),$$
$$\Phi_j^{(\mu_0,\mu_1,\mu_j)}[J_j] := \int d^4\omega \, \frac{J_j}{\sigma_j + i\epsilon} \Delta(\sigma_0, \sigma_1, \rho, t), \quad j = 2, 3$$

- Assuming J_1 independent of any angular variable and J_2 (J_3) of θ (ϕ) allows one to compute them once for all

$S_3(\{\mu_k\})$



$= S_3(\{\mu_k\})$

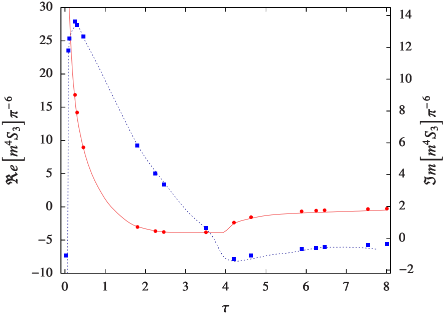
- $m^4 S_3(\{\mu_k\}) = \fint \prod_{j=0}^{1} \left(\frac{d\sigma_j}{\sigma_j + i\epsilon}\right) \Phi_1^{(\mu_0,\mu_1)}[C_L C_R]$ with

$$
\begin{aligned}
C_L &:= C(\tau, \sigma_1 + \mu_1, \sigma_0 + \mu_0, \mu_2, \mu_3, \mu_4), \\
C_R &:= C(\tau, \sigma_1 + \mu_1, \sigma_0 + \mu_0, \mu_5, \mu_6, \mu_7)
\end{aligned}
$$

computed with `OneLOop` by A. van Hameren [1007.4716]

$m^4 S_3(1,1,0,0,0,0,0,0)$

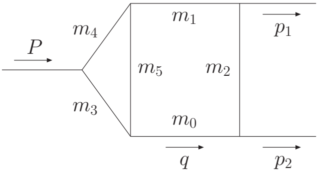
- Red bullets (blue squares) refer to the real (imaginary) part computed with 10^9 **MC** shots per point
- Lines obtained from A. Ghinculov [hep-ph/9604333]



- Masses are not a problem: with 10^9 **MC** shots and $\tau = 10$

$$\frac{m^4}{\pi^6} S_3(1,1,2,3,4,5,6,7) = 1.1453(8) \times 10^{-1} - i\,4.11(1) \times 10^{-2}$$

Planar two-loop vertex

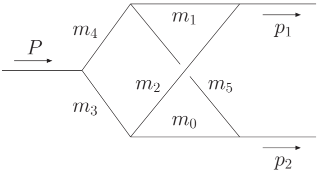


$$= V_2(\{\mu_k\}) \quad \left(\tau_i := \frac{p_i^2}{m^2}\right)$$

- $m^4 V_2(\{\mu_k\}) = \oint \prod_{j=0}^{1} \left(\frac{d\sigma_j}{\sigma_j + i\epsilon}\right) \Phi_2^{(\mu_0,\mu_1,\mu_2)}[C_L]$
- $m^4 V_2(\{\mu_k\}) = \oint \prod_{j=3}^{4} \left(\frac{d\sigma_j}{\sigma_j + i\epsilon}\right) \int_{-1}^{1} \frac{dc_\theta}{2} \Phi_1^{(\mu_3,\mu_4)}[D_R]$

τ	τ_1	τ_2	$\{\mu_k\}$	**MC** result (10^9 shots)
10	2	3	$\{1,2,3,4,5,6\}$	-2.751(7) $-i$ 6.729(7)
-100	-4	7	$\{0,1,12,7,8,9\}$	-1.025(1)$\times 10^{-1}$ $+i$ 1.5(7)$\times 10^{-4}$
50	30	30	$\{6,23,2,9,9,9\}$	9.307(4)$\times 10^{-1}$ $-i$ 1.347(4)$\times 10^{-1}$
-40	1	1	$\{0,0,0,0,0,0\}$	5.918(6) $-i$ 9.51(3)
1000	0	0	$\{1,1,1,1,1,1\}$	-3.558(4)$\times 10^{-3}$ $+i$ 2.3557(8)$\times 10^{-2}$

Non-planar two-loop vertex

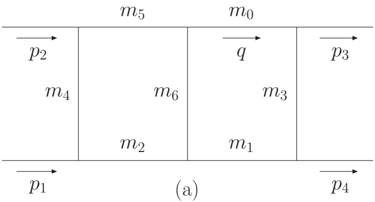


$= V_2^{np}(\{\mu_k\})$

- $m^4 V_2^{np}(\{\mu_k\}) = \oint \prod_{j=3}^{4} \left(\frac{d\sigma_j}{\sigma_j + i\epsilon}\right) \int_{-1}^{1} \frac{dc_\theta}{2} \Phi_1^{(\mu_3,\mu_4)}[D^{np}]$
- $\{\mu_k\} = \{1,1,1,1,1,1\}$ and $\tau_1 = \tau_2 = 0$

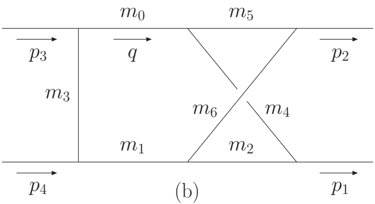
τ	**MC** result (10^9 shots)
2.1	-1.538(8)$\times 10^1$ $-i$ 6(6)$\times 10^{-2}$
10	8.7(1)$\times 10^{-1}$ $-i$ 2.5415(9)$\times 10^1$
100	1.8848(6) $+i$ 7.469(6)$\times 10^{-1}$
1000	2.660(2)$\times 10^{-2}$ $+i$ 7.788(2)$\times 10^{-2}$

Planar and non-planar double box



(a)

$$= B_2(\{\mu_k\})$$

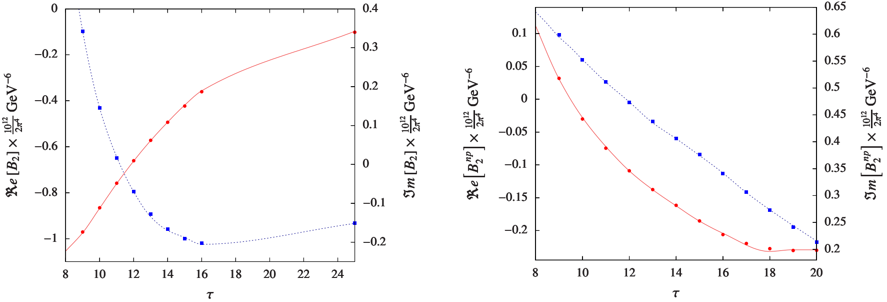


(b)

$$= B_2^{np}(\{\mu_k\})$$

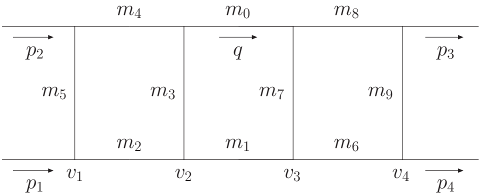
- $m^6 B_2(\{\mu_k\}) = \displaystyle\fint \prod_{j=0}^{1} \left(\frac{d\sigma_j}{\sigma_j + i\epsilon}\right) \Phi_3^{(\mu_0,\mu_1,\mu_3)}[D_L]$
- $m^6 B_2^{np}(\{\mu_k\}) = \displaystyle\fint \prod_{j=0}^{1} \left(\frac{d\sigma_j}{\sigma_j + i\epsilon}\right) \Phi_3^{(\mu_0,\mu_1,\mu_3)}[D_R]$

A comparison



- $\mu_k = \{1, 1, 1, 3.24, 3.24, 1, 3.24\}$
  $\tau_i = 1,\ \chi := (p_2 - p_3)^2/m^2 = -4,\ m = 50\ \text{GeV},\ 10^9\ \text{shots}$
- Lines from F. Yuasa *et al.* [1112.0637]

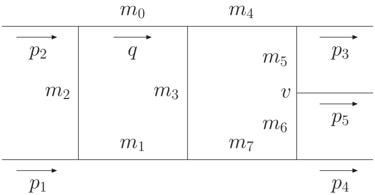
Triple box



$$= B_3(\{\mu_k\})$$

- $m^8 B_3(\{\mu_k\}) =$
$$\oint \prod_{j=0}^{1} \left(\frac{d\sigma_j}{\sigma_j + i\epsilon} \right) \int_{-1}^{1} \frac{dc_\theta}{2} \int_0^{2\pi} \frac{d\phi}{2\pi} \Phi_1^{(\mu_0,\mu_1)} \left[D_L(c_\theta) D_R(c_\theta, s_\phi) \right]$$
- $\tau = 50,\ \chi = -4,\ \tau_i = \mu_0 = \mu_1 = 1,\ \mu_{2\div 9} = 0,\ 10^9$ shots $\Rightarrow$
$$m^8 B_3 = -9.393(9) - i\, 0.374(9)$$
- Non planar cases can be treated likewise

Two-loop pentabox



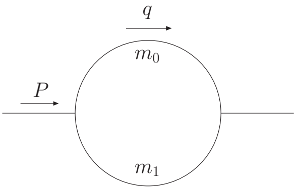
$= E_2(\{\mu_k\})$

- $m^8 E_2 = \int \prod_{j=0}^{1} \left(\frac{d\sigma_j}{\sigma_j + i\epsilon}\right) \int_{-1}^{1} \frac{dc_\theta}{2} \int_0^{2\pi} \frac{d\phi}{2\pi}\, \Phi_1^{(\mu_0,\mu_1)} \left[\frac{E(\omega)}{\sigma_2 + i\epsilon}\right]$
- With the input of [2110.12885] one obtains

$$m^8 E_2 = 0.1125(1) - i\, 0.0041(1)$$

- Non-planar case attained by replacing the pentagon $E(\omega)$

UV divergences



$= B_{\rm FDR}$

$(\bar{q}^2 := q^2 - \mu^2 + i\epsilon)$

$(M_1^2(q) := m_1^2 + 2(q \cdot P) - P^2)$

- $B_{\rm FDR} = \int [d^4 q] \frac{1}{\bar{D}_0 \bar{D}_1}, \ \bar{D}_0 := \bar{q}^2 - m_0^2, \quad \bar{D}_1 := \bar{q}^2 - M_1^2(q)$

$$\frac{1}{\bar{D}_0 \bar{D}_1} = \left[\frac{1}{\bar{q}^4}\right] + \frac{m_0^2}{\bar{q}^2 \bar{D}_0 \bar{D}_1} + \frac{M_1^2(q)}{\bar{q}^4 \bar{D}_1}$$

$$B_{\rm FDR} := \lim_{\mu \to 0} \int d^4 q \left(\frac{m_0^2}{\bar{q}^2 \bar{D}_0 \bar{D}_1} + \frac{M_1^2(q)}{\bar{q}^4 \bar{D}_1} \right) \Bigg|_{\mu = \mu_R}$$

$$B_{\rm FDR} = \int d^4 q \left\{ \frac{1}{D_0 D_1} - \frac{1}{(q^2 - \mu_R^2 + i\epsilon)^2} \right\}$$

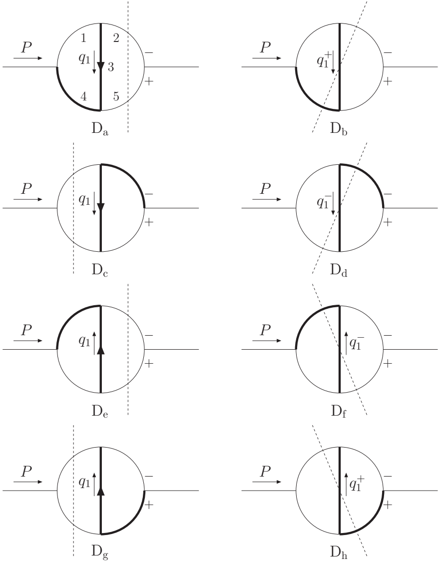
Integrating over q_0 $(m = m_0 = m_1 = 2\mu_R)$

- $B_{\rm FDR} = 2i\pi^2 \fint dr \frac{F(r)}{r - i\epsilon}$ with $F(r)$ given in [2110.12885]
- Threshold singularity when $\sqrt{\tau} > 2$

$\sqrt{\tau}$	Numerical result (10^8 shots)	Analytic result
0.2	$2(2)\times10^{-6}$ $-i$ $1.3614(3)\times10^1$	0 $-i$ 1.3616×10^1
0.4	$2(2)\times10^{-6}$ $-i$ $1.3411(3)\times10^1$	0 $-i$ 1.3415×10^1
0.6	$2(2)\times10^{-6}$ $-i$ $1.3065(3)\times10^1$	0 $-i$ 1.3068×10^1
1.5	$2(2)\times10^{-6}$ $-i$ 8.705(1)	0 $-i$ 8.7063
1.9	$4(4)\times10^{-7}$ $-i$ 2.0737(3)	0 $-i$ 2.0739
2.1	-9.455(1) $+i$ 4.162(1)	-9.4541 $+i$ 4.1616
4	$-2.6854(3)\times10^1$ $-i$ $1.6453(5)\times10^1$	-2.6852×10^1 $-i$ 1.6456×10^1
10	$-3.0377(5)\times10^1$ $-i$ $3.828(2)\times10^1$	-3.0380×10^1 $-i$ 3.8280×10^1
50	$-3.0990(6)\times10^1$ $-i$ $7.112(5)\times10^1$	-3.0981×10^1 $-i$ 7.1094×10^1
100	$-3.1009(6)\times10^1$ $-i$ $8.473(7)\times10^1$	-3.1000×10^1 $-i$ 8.4825×10^1

- The gluing approach can also be adapted to the UV case

IR divergences, $\varphi^* \to \varphi\varphi(\varphi)$ in $g\,\phi^3$



- $\sum_{j=a,b,c,d} \mathrm{D_j} = 0$
- $\frac{s}{g^4} \sum_{j=a,c} \mathrm{D_j^u} = 254.83814\cdots$
- One must have

$$\frac{s}{g^4}\left(\mathrm{D_a^s} + \mathrm{D_c^s} + \mathrm{D_b} + \mathrm{D_d}\right) =$$

$$-254.83814\cdots$$

A MC estimate

$\frac{\mu^2}{s}$	$\frac{s}{g^4}(\mathrm{D}_\mathrm{a}^\mathrm{s} + \mathrm{D}_\mathrm{c}^\mathrm{s} + \mathrm{D}_\mathrm{b} + \mathrm{D}_\mathrm{d})$
10^{-10}	-254.81(1)
10^{-11}	-254.83(1)
10^{-12}	-254.84(1)

- The correct result is precisely approached and the **MC** error does not grow when decreasing μ^2/s, which is an indication that the local cancellation works as expected

Thanks!

Backup slides

From $[-\infty, +\infty]$ to $[-1, 1]$

- This is achieved by changing variable: $\sigma = \frac{x}{1-x^2}$

$$\int d\sigma \frac{\phi(\sigma)}{\sigma + i\epsilon} = \int_{-1}^{1} dx \, \frac{1+x^2}{1-x^2} \phi\Big(\frac{x}{1-x^2}\Big) \frac{1}{x + i\epsilon}$$

- Improper integrals defined via the Cauchy principal value are easily computed given the symmetric treatment around $\sigma = 0$