Introduction to Computer Algebra

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Motivation


Large Hadron Collider

Challenges

The Big Questions

- What is the nature of dark matter?
- What are the properties of the Higgs boson?
- What is the quantum structure of the vacuum?
- . . .

The challenge

- Solve master equation

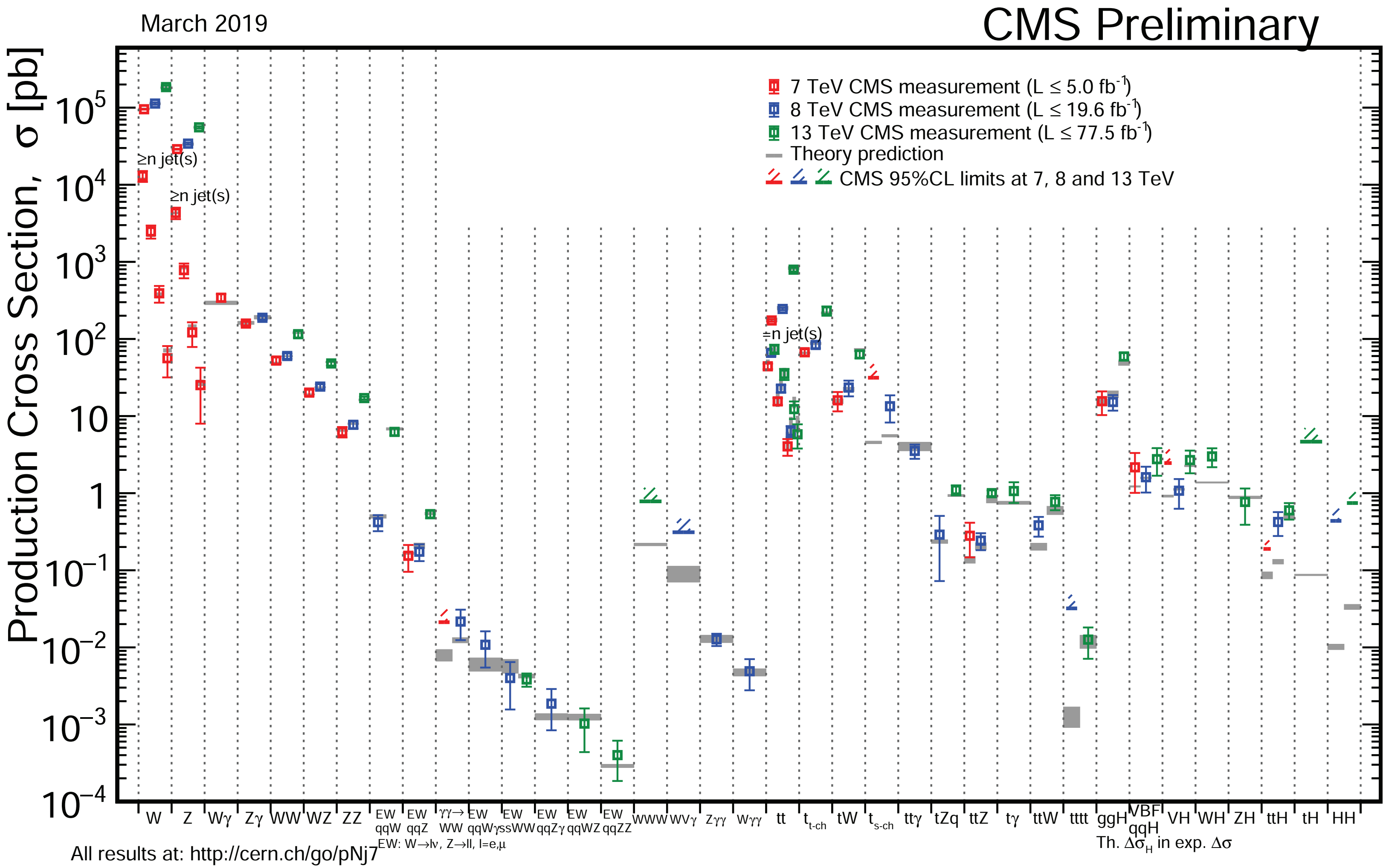
$$\text{new physics} = \text{data} - \text{Standard Model}$$

- LHC experiments deliver high precision measurements
  - searches require understanding of SM background
  - theory has to match or exceed accuracy of LHC data

Standard Model cross sections

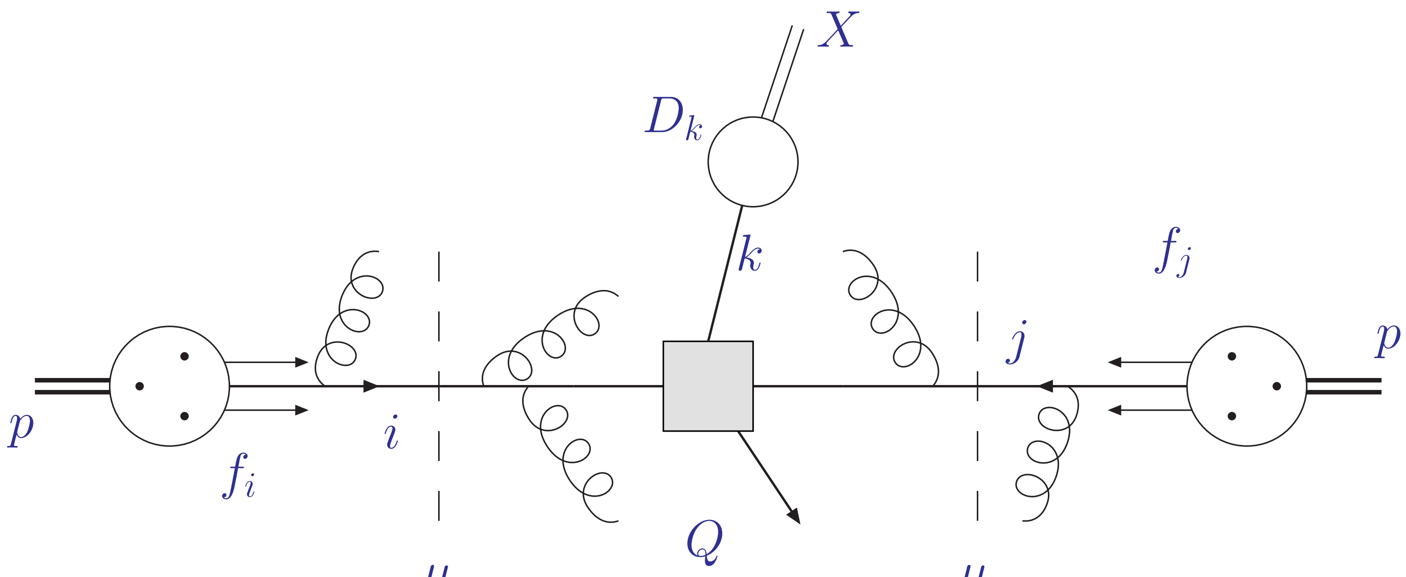
Cross sections for Standard Model processes at the LHC

- Hadroproduction of $\gamma, Z, W^{\pm}$, Higgs, top-quarks, $\ldots$ CMS coll. '18



QCD factorization

QCD factorization



$$\sigma_{pp\to X} = \sum_{ij} f_i(\mu^2) \otimes f_j(\mu^2) \otimes \hat{\sigma}_{ij\to X}\left(\alpha_s(\mu^2), Q^2, \mu^2, m_X^2\right)$$

- Factorization at scale μ
  - separation of sensitivity to dynamics from long and short distances
- Hard parton cross section $\hat{\sigma}_{ij\to X}$ calculable in perturbation theory
  - cross section $\hat{\sigma}_{ij\to k}$ for parton types i, j and hadronic final state X
- Non-perturbative parameters: parton distribution functions f_i, strong coupling α_s, particle masses m_X
  - known from global fits to exp. data, lattice computations, ...

Parton luminosity

- Long distance dynamics due to proton structure

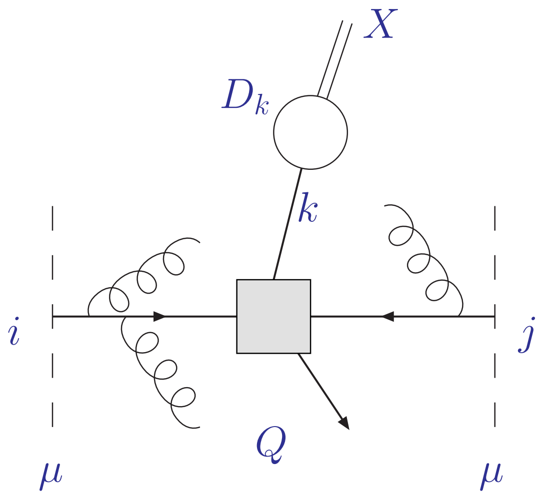
- Cross section depends on parton distributions f_i

$$\sigma_{pp \to X} = \sum_{ij} f_i(\mu^2) \otimes f_j(\mu^2) \otimes \left[\ldots \right]$$

- Parton distributions known from global fits to exp. data
  - available fits accurate to NNLO
  - information on proton structure depends on kinematic coverage

Hard scattering cross section

- Parton cross section $\hat{\sigma}_{ij\to k}$ calculable pertubatively in powers of α_s
  - known to NLO, NNLO, ... ($\mathcal{O}(\text{few}\%)$ theory uncertainty)



- Accuracy of perturbative predictions
  - LO (leading order) ($\mathcal{O}(50-100\%)$ unc.)
  - NLO (next-to-leading order) ($\mathcal{O}(10-30\%)$ unc.)
  - NNLO (next-to-next-to-leading order) ($\lesssim$ $\mathcal{O}(10\%)$ unc.)
  - N^{3}LO (next-to-next-to-next-to-leading order)
  - ...

Perturbation theory at work

QCD Lagrangian

- Classical part of QCD Lagrangian

$$\mathcal{L}_{\rm cl} \quad = \quad -\frac{1}{4} F^a_{\mu\nu} F_a^{\mu\nu} + \sum_{\rm flavors} \bar{\psi}_i \, ({\rm i} \not{D} - m_q)_{ij} \, \psi_j$$

- Matter fields $\psi_i, \bar{\psi}_j$ with $i, j = 1, \dots, 3$ (fundamental rep.)
  - covariant derivative $D_{\mu,ij} = \partial_\mu \delta_{ij} + {\rm i} g_s \, (t_a)_{ij} \, A^a_\mu$
- Field strength tensor $F^a_{\mu\nu}$ with $a = 1, \dots, 8$ (adjoint rep.)
  - covariant derivative $D_{\mu,ab} = \partial_\mu \delta_{ab} - g_s f_{abc} A^c_\mu$
  - $F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu - g_s f_{abc} A^b_\mu A^c_\nu$
- Formal parameters of the theory (no observables)
  - strong coupling $\alpha_s = g_s^2/(4\pi)$
  - quark masses m_q

Quantization

- Gauge fixing (Feynman gauge $\lambda = 1$) $\mathcal{L}_{\rm gauge-fix} \; = \; -\frac{1}{2\lambda} \, \left(\partial^\mu A^a_\mu\right)^2$
- Ghosts (Grassmann fields η) $\mathcal{L}_{\rm ghost} \; = \; \partial_\mu \eta^{a\dagger} \left(D^\mu_{ab} \eta^b\right)$
  (removal of unphysical degrees of freedom for gauge fields) Fadeev, Popov

From Lagrangian to Feynman rules

- Consider action S

$$S = \mathrm{i} \int d^4x \, (\mathcal{L}_{\rm cl} + \mathcal{L}_{\rm gauge-fix} + \mathcal{L}_{\rm ghost}) = S_{\rm free} + S_{\rm int}$$

- Decompose action into free $S_{\rm free}$ and interacting part $S_{\rm int}$
  - $S_{\rm free}$ contains bi-linear terms in fields
  - $S_{\rm int}$ contains interactions
- Derivation of Feynman rules
  - inverse propagators from $S_{\rm free}$
  - interacting parts from $S_{\rm int}$ (in perturbative expansion)

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Examples (I)

- Fermion propagator in QCD from $\bar{\psi}_i \delta_{ij} \, (\mathrm{i}\not{\partial} - m_q) \, \psi_j$
  - substitution $\partial_\mu = -\mathrm{i} p_\mu$ (Fourier transformation)
- Inverse propagator (momentum space) $\Gamma_{ij}^{\bar{\psi}\psi}(p) = -\mathrm{i} \, \delta_{ij} \, (\not{p} - m_q)$
- Check: quark propagator $\Delta_{ij}(p) = +\mathrm{i} \, \delta_{ij} \, \dfrac{1}{\not{p} - m_q + \mathrm{i}0}$
  - causality in Minkowski space: prescription $+\mathrm{i}0$

Examples (II)

- Gluon propagator in QCD from bi-linear terms in $F^a_{\mu\nu} F_a^{\mu\nu}$ and $\mathcal{L}_{\rm gauge-fix}$
  - recall $F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu - g_s f_{abc} A^b_\mu A^c_\nu$
  - recall $\mathcal{L}_{\rm gauge-fix} \; = \; -\frac{1}{2\lambda} \left(\partial^\mu A^a_\mu\right)^2$
- Inverse propagator (momentum space)

$$\Gamma^{AA}_{ab;\mu\nu}(p) \; = \; +{\rm i}\, \delta_{ab} \left[p^2 g_{\mu\nu} - \left(1 - \frac{1}{\lambda}\right) p_\mu p_\nu\right]$$

- Gluon propagator $\Delta^{ab;\mu\nu}(p) \; = \; +{\rm i}\, \delta_{ab} \left[\frac{-g_{\mu\nu}}{p^2} + (1-\lambda) \frac{p_\mu p_\nu}{p^4}\right]$
  - Check: $\Gamma^{AA}_{ac;\mu\rho}(p)\, \Delta^{cb;\rho\nu}(p) \; = \; \delta_a^{\;b}\, g_\mu^{\;\nu}$

Examples (II)

- Gluon propagator in QCD from bi-linear terms in $F^a_{\mu\nu} F_a^{\mu\nu}$ and $\mathcal{L}_{\text{gauge-fix}}$
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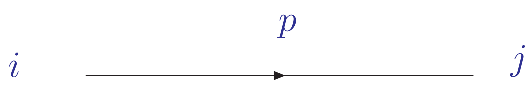
Examples (III)

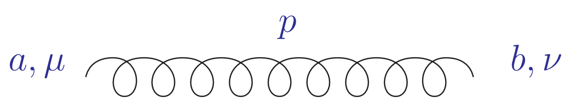
- Interactions derived from S_{int}
  - fermion-gluon interaction from $\bar{\psi}_i \mathrm{i} \not{A}_{ij} \psi_j \longrightarrow -\mathrm{i} t^a_{ij} \gamma_\mu$
- General rule
  - replacement of all ∂_μ by momenta p_μ
    (tedious for 3- and 4-gluon interactions)

Feynman rules (I)

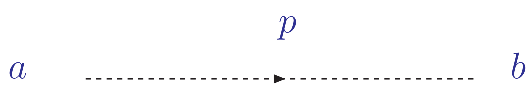
- Propagators
  - fermions, gluons, ghosts
  - covariant gauge



$$\delta^{ij}\,\frac{\mathrm{i}}{\not{p} - m}$$



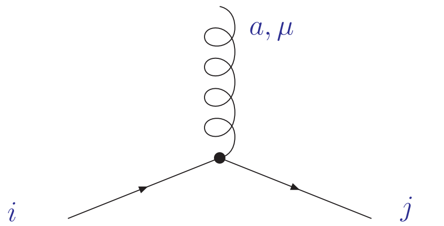
$$\delta^{ab}\,\mathrm{i}\left(\frac{-g^{\mu\nu}}{p^2} + (1-\lambda)\frac{p^\mu p^\nu}{(p^2)^2}\right)$$



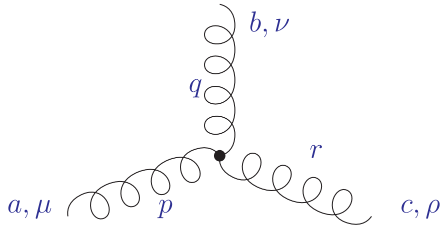
$$\delta^{ab}\,\frac{\mathrm{i}}{p^2}$$

Feynman rules (II)

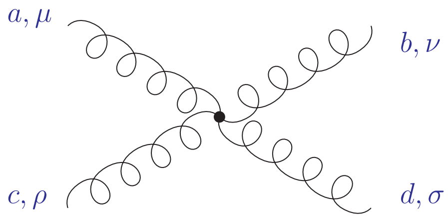
- Vertices



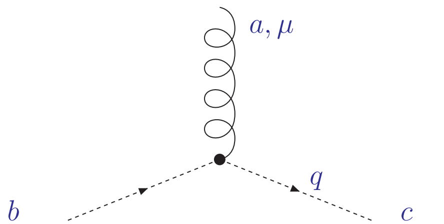
$$-\mathrm{i}\, g\; (t^a)_{ji}\; \gamma^\mu$$



$$-g\, f^{abc}\; \left((p-q)^\rho g^{\mu\nu} + (q-r)^\mu g^{\nu\rho} + (r-p)^\nu g^{\mu\rho}\right)$$



$$-\mathrm{i}\, g^2\, f^{xac} f^{xbd}\; (g^{\mu\nu} g^{\rho\sigma} - g^{\mu\sigma} g^{\nu\rho})$$
$$-\mathrm{i}\, g^2\, f^{xad} f^{xbc}\; (g^{\mu\nu} g^{\rho\sigma} - g^{\mu\rho} g^{\nu\sigma})$$
$$-\mathrm{i}\, g^2\, f^{xab} f^{xcd}\; (g^{\mu\rho} g^{\nu\sigma} - g^{\mu\sigma} g^{\nu\rho})$$



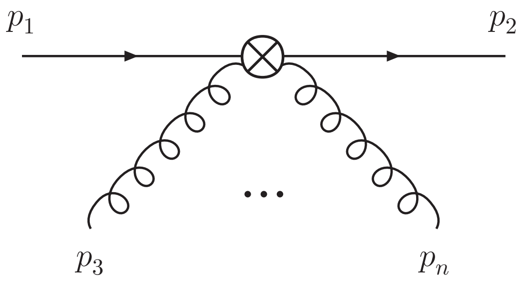
$$g\, f^{abc}\, q^\mu$$

Perturbation theory at work

- Perturbative approach straightforward in principle
  - draw all Feynman diagrams
  - apply Feynman rules and evaluate expressions for matrix elements
  - use standard reduction techniques for loops and phase space integrals
- (Extremely) hard in practice
  - intermediate expressions more complicated than final results
- Known bottlenecks
  - **many diagrams** — many diagrams are related by gauge invariance
  - **many terms in each diagram** — nonabelian gauge boson self-interactions are complicated
  - **many kinematic variables** — allowing the construction of very complicated expressions
- Computer algebra programs are a standard tool

Real life example (I)

Operator matrix elements



- Quark operator of spin-N and twist two
  $O^{\psi}_{\{\mu_1,\ldots,\mu_N\}} = \overline{\psi}\,\gamma_{\{\mu_1} D_{\mu_2} \ldots D_{\mu_N\}}\,\psi$
- N covariant derivatives $D_{\mu,ij} = \partial_\mu \delta_{ij} + \mathrm{i} g_s\,(t_a)_{ij}\,A^a_\mu$
  between quark fields ψ, $\overline{\psi}$
- Feynman rules with new vertices for additional gluons coupling to operator
- Evaluation of operators in matrix elements $A^{\psi\psi}$ with external quark states
- Computation of quantum corrections up to four loops

$$A^{\psi\psi}_{\{\mu_1,\ldots,\mu_N\}} = \langle \psi(p_1) | O^{\psi}_{\{\mu_1,\ldots,\mu_N\}}(-p_1 - p_2) | \overline{\psi}(p_2) \rangle$$

- Zero-momentum transfer through operator reduces problem to computation of propagator-type diagrams

Real life example (II)

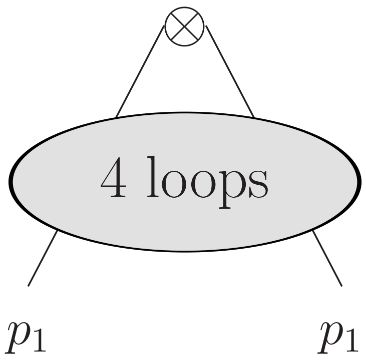
Work flow

- Feynman diagrams for operator matrix elements generated up to four loops with **Qgraf** Nogueira ‘91
- Diagrams of same topology and color factor combined to meta diagrams
  - 1 one-, 7 two-, 53 three- and 650 four-loop meta diagrams for $A^{\psi\psi}$
- Symbolic manipulations with **Form** Vermaseren ‘00; Kuipers, Ueda, Vermaseren, Vollinga ‘12 and multi-threaded version **TForm** Tentyukov, Vermaseren ‘07
- Parametric reduction of four-loop massless propagator diagrams with **Forcer** Ruijl, Ueda, Vermaseren ‘17
- Anomalous dimensions $\gamma(N)$ from ultraviolet divergence of loop corrections to operator in (anti-)quark two-point function

Real life example (III)

Four-loop computation

- Computation of anomalous dimensions $\gamma(N)$ for Mellin moment $N = 18$

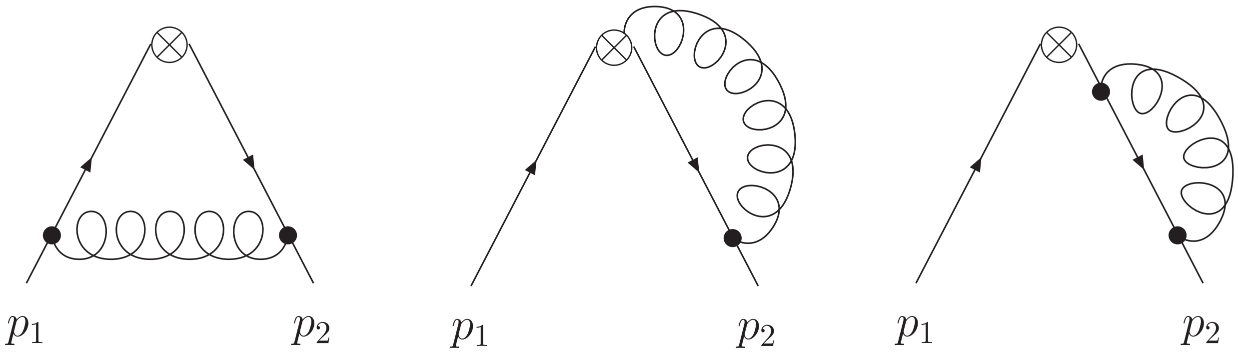


- Hardware
  - multi-core Linux servers with 1 TByte RAM memory and several TByte of disk space
- Run-time
  - CPU time for $N = 18$ added up to 6403 days on a single core (200 days real time with **TForm**)
  - 3.24 TByte of disk space at intermediate stages of computation

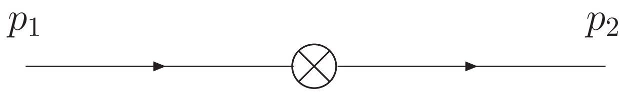
Text book example (I)

One-loop computation

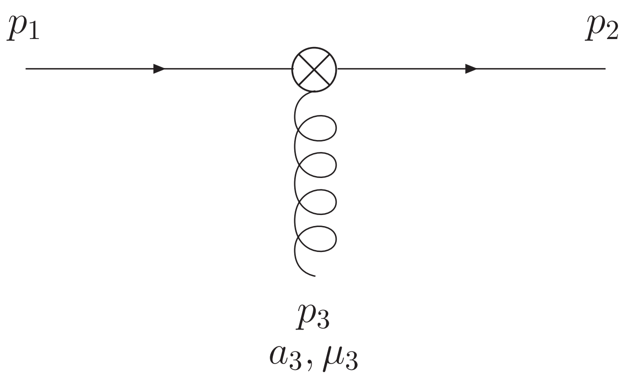
- Feynman diagrams



- New Feynman rules for vertices with light-like vector Δ, $\Delta^2 = 0$



$$\not{\Delta}\,(\Delta \cdot p_2)^{N-1}$$



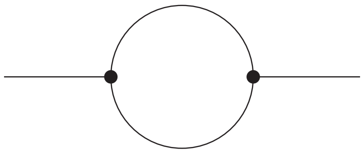
$$-g t^{a_3} \not{\Delta} \Delta^{\mu_3} \sum_{j_1=0}^{N-2} (p_2 \cdot \Delta)^{N-2-j_1} (-p_1 \cdot \Delta)^{j_1}$$

Loop integrals

Loops (I)

- Radiative corrections require integration over loop momenta
  - loop integrals can diverge in ultraviolet $l \to \infty$
  - power counting reveals divergence in ultraviolet
- Example: self-energy in scalar field theory (off-shell momentum $q^2 \neq 0$)

$$\int d^4 l \frac{1}{l^2 (l-q)^2}$$



Dimensional regularization

- Lorentz invariance and $SU(N)$ gauge invariance manifest
- Anlytical continuation in space-time dimension $D = 4 - 2\epsilon$
  - loop integral $\displaystyle\int \frac{d^4 l}{(2\pi)^4} \to \int \frac{d^D l}{(2\pi)^D}$
  - Lorentz index $\mu \in \{0,1,2,3\} \to \{0,1,\dots,D\}$
  - Lorentz vector $p^\mu \in \left(p^0, p^1, p^2, p^3\right) \to \left(p^0, p^1, \dots, p^{D-1}\right)$
  - metric $g^{\mu\nu} g_{\mu\nu} = g^\mu_\mu = D$
  - Dirac algebra $\{\gamma^\mu, \gamma^\nu\} = 2 g^{\mu\nu}$ and $\gamma^\mu \gamma^\nu \gamma_\mu = (2-D)\gamma^\nu$

Loops (II)

- Feynman integral for a given process
- Tensor integrals

$$I^{\mu_1,\mu_2,\cdots}(D;\nu_1,\ldots,\nu_n) = \int d^D p_1 \ldots d^D p_l \frac{p_1^{\mu_1} p_2^{\mu_2} \ldots}{(p_1^2)^{\nu_1} \ldots (p_n^2)^{\nu_n}}$$

  - Lorentz indices $\mu_1, \mu_2, \ldots$
  - l-loops, n-propagators
  - D (complex) space-time dimensions
    (dimensional regularization)
    Bollini, Giambiagi '72; Ashmore '72; Cicuta, Montaldi '72; 't Hooft, Veltman '72

Loops (II)

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- Tensor integrals can be mapped to scalar integrals
  - expand $I^{\mu_1,\mu_2,\cdots}(D;\ldots)$ in tensor structures
  - coefficients of tensor structures are scalar integrals (projectors)
  - scalar products in numerator cancelled via denominators (sometimes, there are irreducible scalar products)

Loops (III)

Upshot

- Scalar integral (l-loops, n-propagators, D dimensions)

$$I(D;\nu_1,\ldots,\nu_n) = \int d^D p_1 \ \ldots \ d^D p_l \ \frac{1}{(p_1^2)^{\nu_1} \ \ldots \ (p_n^2)^{\nu_n}}$$

  - $p_i = f(p_1, ..., p_l)$ (energy-momentum conservation)

Loops (III)

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  - $p_i = f(p_1, ..., p_l)$ (energy-momentum conservation)
- Classification of scalar integrals
  - topology, n-point function (number of loops, legs)
  - scales (number of non-vanishing scalar products of momenta and masses)

Loops (III)

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Task

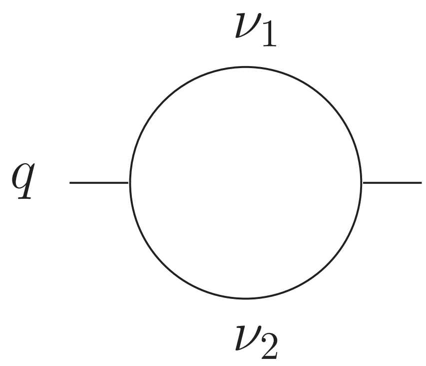
- Calculation of scalar (loop) integrals
- Analytic expressions for $I(D;\nu_1,\ldots,\nu_n)$
  - expansion around integer-valued D space-time dimension (typically four space-time dimensions $D = 4 - 2\epsilon$)

Loops (IV)

Two-point integrals

- Easy example:
  massless one-loop two-point function L1

$$\mathrm{L1} = \int d^D p_1 \, \frac{1}{(p_1^2)^{\nu_1} \, ((p_1 - q)^2)^{\nu_2}}$$



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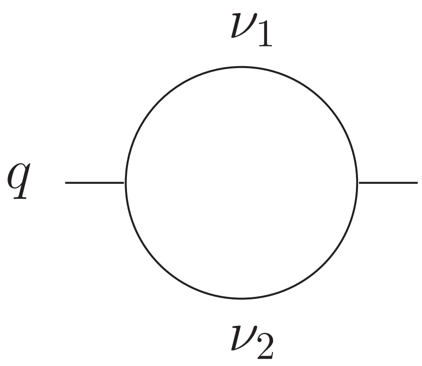

- Results for L1

$$\begin{aligned}\mathrm{L1} \quad &= \quad \mathrm{i}\,(-1)^{\nu_1+\nu_2}\,\pi^{-D/2}\,(-p^2)^{D/2-\nu_1-\nu_2} \;\times \\ &\times \frac{\Gamma(\nu_1+\nu_2-D/2)\Gamma(D/2-\nu_1)\Gamma(D/2-\nu_2)}{\Gamma(\nu_1)\Gamma(\nu_2)\Gamma(D-\nu_1-\nu_2)}\end{aligned}$$

Loops (IV)

Two-point integrals

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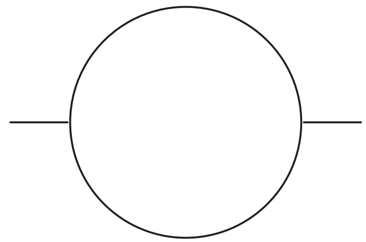

- Results for $\mathrm{L1}$

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- Expansion of Gamma-function in $\epsilon = 2 - \frac{D}{2}$ around positive integers values ($\nu_i \geq 0$)
  - Riemann zeta values $\Gamma(1+\epsilon) = 1 - \epsilon\gamma_E + \frac{\epsilon^2}{2}(\zeta_2 + \gamma_E^2) + \dots$
  - $\overline{\mathrm{MS}}$-scheme puts $\gamma_E = 0$

Text book example (II)

One-loop result

- Computation of loop integral in $D = 4 - 2\epsilon$ dimensions and expansion in ϵ

$$\Delta^{\mu_1} \dots \Delta^{\mu_N} \langle \psi(p_1) | O^{\psi}_{\{\mu_1,\dots,\mu_N\}}(0) | \overline{\psi}(-p_1) \rangle =$$

$$= \quad 1 + \frac{\alpha_s}{4\pi} C_F \frac{1}{\epsilon} \left\{ 4S_1(N) + \frac{2}{N+1} - \frac{2}{N} - 3 \right\} + \mathcal{O}(\alpha_s \epsilon^0) + \mathcal{O}(\alpha_s^2)$$

- Details in chapt. 4.6 of
  The Theory of Quark and Gluon Interactions
  F.J. Yndurain

- One-loop result contains harmonic sum $S_1(N)$

$$S_1(N) = \sum_{i=1}^{N} \frac{1}{i} = 1 + \frac{1}{2} + \frac{1}{3} + \dots \frac{1}{N}$$

$$S_1(N+1) - S_1(N) = \frac{1}{N+1}$$

Symbolic Summation

Symbolic Summation

Polynomial summation

- Examples

$$\sum_{i=0}^{n-1} i = \frac{1}{2}n(n-1)$$

$$\sum_{i=0}^{n-1} i^2 = \frac{1}{6}n(n-1)(2n-1)$$

$$\sum_{i=0}^{n-1} i^3 = \frac{1}{4}n^2(n-1)^2$$

$$\sum_{i=0}^{n-1} i^4 = \frac{1}{30}n(n-1)(2n-1)(3n^2-3n-1)$$

Difference operator

- Introduce operator Δ with $(\Delta f)(n) = f(n+1) - f(n)$
- If $g = (\Delta f)$, then (for $a, b \in \mathbf{N}, a \leq b$)

$$\sum_{i=a}^{b-1} g(i) \qquad = \sum_{i=a}^{b-1} \big(f(i+1) - f(i)\big)$$

Difference operator

- Introduce operator Δ with $(\Delta f)(n) = f(n+1) - f(n)$
- If $g = (\Delta f)$, then (for $a, b \in \mathbf{N}, a \leq b$)

$$\sum_{i=a}^{b-1} g(i) \qquad = \sum_{i=a}^{b-1} \big(f(i+1) - f(i)\big) = \sum_{i=a}^{b-1} f(i+1) - \sum_{i=a}^{b-1} f(i)$$

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$$= \sum_{i=a+1}^{b} f(i) - \sum_{i=a}^{b-1} f(i)$$

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$$= \sum_{i=a+1}^{b} f(i) - \sum_{i=a}^{b-1} f(i) = f(b) - f(a)$$

- Consecutive cancellation of summands: telescoping
- Symbolic summation problem
  $g = (\Delta f)$ with $f = (\sum g)$, operator Δ is left inverse $\Delta(\sum f) = f$
- Cf. symbolic integration (differential operator D)

$$g = Df = \frac{d}{dx} f \quad \longrightarrow \quad \int_a^b dx g(x) = f(b) - f(a)$$

Difference operator (cont'd)

- Differential operator D acts in continuum as $D(x^m) = mx^{m-1}$

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Rising and falling factorials

- Define rising factorials as $f^{\overline{m}} = f(x)f(x+1)\ldots f(x+m-1)$ (also known as Pochhammer symbols $(x)_m$)

Difference operator (cont'd)

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- Action of discrete analog Δ on polynomials?
  - Example: $\Delta(n^3) = 3n^2 + 3n - 1$

Rising and falling factorials

- Define falling factorials as $f^{\underline{m}} = f(x)f(x-1)\dots f(x-m+1)$

Difference operator (cont'd)

- Differential operator D acts in continuum as $D(x^m) = mx^{m-1}$
- Action of discrete analog Δ on polynomials?
  - Example: $\Delta(n^3) = 3n^2 + 3n - 1$

Rising and falling factorials

- Define falling factorials as $f^{\underline{m}} = f(x)f(x-1)\ldots f(x-m+1)$
- Then, with falling factorials

$$\Delta(x^{\underline{m}}) \; = \; mx^{\underline{m-1}} \qquad\qquad \sum_{i=0}^{n-1} i^{\underline{m}} = \frac{1}{m+1} n^{\underline{m+1}}$$

- Conversion of polynomial powers x^m
  (decomposition with Stirling numbers of second kind $\left\{ \begin{matrix} m \\ i \end{matrix} \right\}$)

$$x^m = \sum_{i=0}^{m} \left\{ \begin{matrix} m \\ i \end{matrix} \right\} x^{\underline{i}}$$

  - Stirling numbers of second kind denote # of ways to partition n things in k non-empty sets

Examples

- Polynomials

$$\sum_{i=0}^{n-1} i = \sum_{i=0}^{n-1} i^{\underline{1}} = \frac{1}{2} n^{\underline{2}} = \frac{1}{2} n(n-1)$$

$$\sum_{i=0}^{n-1} i^2 = \sum_{i=0}^{n-1} (i^{\underline{2}} + i^{\underline{1}}) = \frac{1}{3} n^{\underline{3}} + \frac{1}{2} n^{\underline{2}} = \frac{1}{6} n(n+1)(2n+1)$$

$$\sum_{i=0}^{n-1} i^3 = \sum_{i=0}^{n-1} (i^{\underline{3}} + 3i^{\underline{2}} + i^{\underline{1}}) = \frac{1}{4} n^{\underline{4}} + n^{\underline{3}} + \frac{1}{2} n^{\underline{2}} = \frac{1}{4} n^2 (n+1)^2$$

Hypergeometric summation

Definition

- Hypergeometric function ${}_mF_n$

$$ {}_mF_n\left(\begin{matrix} a_1,\ldots,a_m \\ b_1,\ldots,b_n \end{matrix} \middle| z \right) = \sum_{i\geq 0} \frac{a_1^{\overline{i}}\ldots a_m^{\overline{i}}}{b_1^{\overline{i}}\ldots b_n^{\overline{i}}}\,\frac{z^i}{i!} $$

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Examples

$$ {}_0F_0\left(\middle| z \right) = \sum_{i \geq 0} \frac{z^i}{i!} = \exp(z) $$

$$ {}_2F_1\left(\begin{array}{c} a, 1 \\ 1 \end{array} \middle| z \right) = \sum_{i \geq 0} a^{\overline{i}} \frac{z^i}{i!} = \frac{1}{(1-z)^a} $$

$$ {}_2F_1\left(\begin{array}{c} 1, 1 \\ 2 \end{array} \middle| z \right) = z \sum_{i \geq 0} \frac{1^{\overline{i}} 1^{\overline{i}}}{2^{\overline{i}}} \frac{z^i}{i!} = -\ln(1-z) $$

Ratios

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$$r(n) = \frac{g_{n+1}}{g_n}$$

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$$\frac{\begin{pmatrix} m \\ n+1 \end{pmatrix}}{\begin{pmatrix} m \\ n \end{pmatrix}} = \frac{\Gamma(m+1)\Gamma(n+1)\Gamma(m-n+1)}{\Gamma(n+2)\Gamma(m-n)\Gamma(m)} = \frac{-n+m}{n+1}$$

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- Given a hypergeometric term g, is there hypergeometric term f such that $\Delta f = g$?
$$f_{n+1} - f_n = g_n$$

Gospers algorithm

- Gospers algorithm for indefinite hypergeometric summation determines f_n from a given recursion

$$f_n = f_{n-1} + g_{n-1} = f_{n-2} + g_{n-1} + g_{n-2} = \cdots = f_0 + \sum_{k=0}^{n-1} g_k$$

  - Idea: recursive algorithm; telescoping

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- Solve recursion with ansatz $f_n = y(n) g_n$ and (unknown) rational function $y(n)$

$$f_{n+1} - f_n = g_n \qquad \longrightarrow \qquad r(n) y(n+1) - y(n) = 1$$

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- *Upshot*
  - Solve *first-order linear recursion* for $y(n)$

Gospers algorithm (cont'd)

- Given $f_{n+1} - f_n = g_n$ and ansatz $f_n = y(n) g_n$ with rational function $y(n)$, then $r(n) y(n+1) - y(n) = 1$

Gospers algorithm (cont'd)

- Given $f_{n+1} - f_n = g_n$ and ansatz $f_n = y(n)g_n$ with rational function $y(n)$, then $r(n)y(n+1) - y(n) = 1$
- Let $r(n) = \dfrac{a(n)}{b(n)} \dfrac{c(n+1)}{c(n)}$ with polynomials $a(n), b(n), c(n)$ and $\gcd(a(n), b(n+k)) = 1$

Gospers algorithm (cont'd)

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- Let $r(n) = \frac{a(n)}{b(n)} \frac{c(n+1)}{c(n)}$ with polynomials $a(n), b(n), c(n)$ and $\gcd(a(n), b(n+k)) = 1$
- Ansatz for $y(n)$ becomes $y(n) = \frac{b(n-1)}{c(n)} x(n)$ with (unknown) polynomial $x(n)$
- Solve for non-zero $x(n)$

$$a(n)x(n+1) - b(n-1)x(n) = c(n)$$

If non-zero $x(n)$ exists, hypergeometric recursion is summable.

Harmonic summation

- Harmonic sums $S_{m_1,\ldots,m_k}(n)$
  Gonzalez-Arroyo, Lopez, Ynduráin '79; Vermaseren '98; S.M., Uwer, Weinzierl '01
  - recursive definition $S_{\pm m_1,\ldots,m_k}(n) = \sum_{i=1}^{n} \frac{(\pm 1)^i}{i^{m_1}} S_{m_2,\ldots,m_k}(i)$

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  - recursive definition $S_{\pm m_1,\dots,m_k}(n) = \sum_{i=1}^{n} \frac{(\pm 1)^i}{i^{m_1}} S_{m_2,\dots,m_k}(i)$
- Expansion of Gamma-function in $\epsilon = 2 - \frac{D}{2}$ around positive integers values ($n \geq 0$)

$$\frac{\Gamma(n+1+\epsilon)}{\Gamma(1+\epsilon)} \quad = \quad \Gamma(n+1)\, \exp\left(- \sum_{k=1}^{\infty} \epsilon^k \, \frac{(-1)^k}{k} \, S_k(n) \right)$$

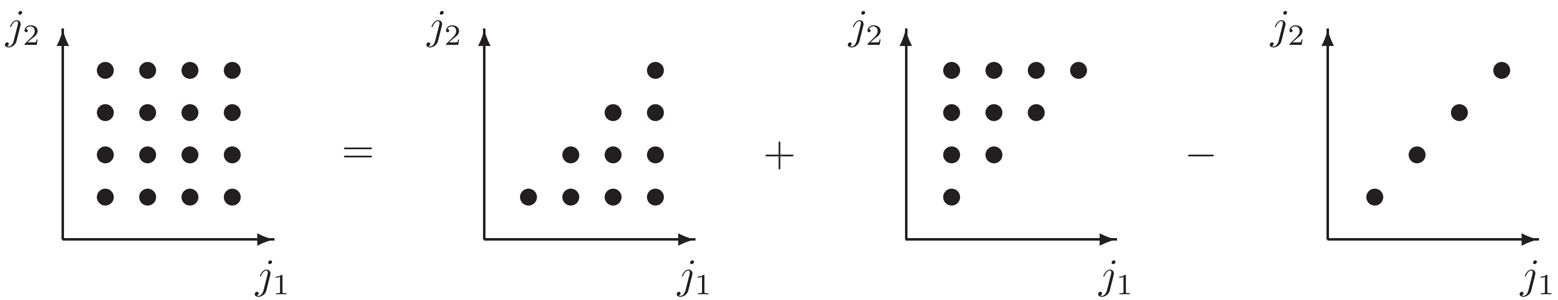
Algorithms for harmonic sums

- Multiplication (Hopf algebra)
  - basic formula (recursion)

$$
\begin{aligned}
S_{m_1,\ldots,m_k}(n) \times S_{m'_1,\ldots,m'_l}(n) \quad = \quad & \sum_{j_1=1}^{n} \frac{1}{j_1^{m_1}} S_{m_2,\ldots,m_k}(j_1) S_{m'_1,\ldots,m'_l}(j_1) \\
& + \sum_{j_2=1}^{n} \frac{1}{j_2^{m'_1}} S_{m_1,\ldots,m_k}(j_2) S_{m'_2,\ldots,m'_l}(j_2) \\
& - \sum_{j=1}^{n} \frac{1}{j^{m_1+m'_1}} S_{m_2,\ldots,m_k}(j) S_{m'_2,\ldots,m'_l}(j)
\end{aligned}
$$

- Proof uses decomposition

$$
\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} \quad = \quad \sum_{i=1}^{n} \sum_{j=1}^{i} a_{ij} + \sum_{j=1}^{n} \sum_{i=1}^{j} a_{ij} - \sum_{i=1}^{n} a_{ii}
$$



Algorithms for harmonic sums (cont'd)

- Convolution (sum over $n-j$ and j)

$$\sum_{j=1}^{n-1} \frac{1}{j^{m_1}} S_{m_2,\dots,m_k}(j) \frac{1}{(n-j)^{n_1}} S_{n_2,\dots,n_l}(n-j)$$

- Conjugation

$$-\sum_{j=1}^{n} \binom{n}{j} (-1)^j \frac{1}{j^{m_1}} S_{m_2,\dots,m_k}(j)$$

- Binomial convolution (sum over binomial, $n-j$ and j)

$$-\sum_{j=1}^{n-1} \binom{n}{j} (-1)^j \frac{1}{j^{m_1}} S_{m_2,\dots,m_k}(j) \frac{1}{(n-j)^{n_1}} S_{n_2,\dots,n_l}(n-j)$$

Multiple scales

- Generalized sums $S(n; m_1, ..., m_k; x_1, ..., x_k)$
  - recursive definition

$$S(n; m_1, ..., m_k; x_1, ..., x_k) = \sum_{i=1}^{n} \frac{x_1^i}{i^{m_1}} S(i; m_2, ..., m_k; x_2, ..., x_k)$$

  - multiple scales $x_1, ..., x_k$
  - depth k, weight $w = m_1 + ... + m_k$

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  - multiple scales $x_1, ..., x_k$
  - depth k, weight $w = m_1 + ... + m_k$
- Special cases

$$S(\infty; m_1, ..., m_k; x_1, ..., x_k) \quad \to \quad \mathrm{Li}_{m_k,...,m_1}(x_k, ..., x_1)$$

multiple polylogarithms

Goncharov '98; Borwein, Bradley, Broadhurst, Lisonek '99

$$S(\infty; m_1, ..., m_k; x, 1, ..., 1) \quad \to \quad H_{m_1,...,m_k}(x)$$

harmonic polylogarithms

Remiddi, Vermaseren '98

$$S(n; m_1, ..., m_k; 1, ..., 1) \quad \to \quad S_{m_1,...,m_k}(n)$$

Euler-Zagier sums

Algorithms for nested sums

- Same structures as for harmonic sums, in particular
  - multiplication

    $$S(n; m_1, ...; x_1, ...) \times S(n; m'_1, ...; x'_1, ...)$$

  - convolution
  - conjugation
  - binomial convolution
- Recursive algorithms analogous to harmonic sums solve multiple nested sums

Higher transcendental functions

- Expansion of higher transcendental functions in small parameter
  - expansion parameter ϵ occurs in the rising factorials (Pochhammer symbols)
- Hypergeometric function

$$ {}_2F_1(a,b;c,x_0) = \sum_{i=0}^{\infty} \frac{a^{\overline{i}} b^{\overline{i}}}{c^{\overline{i}}} \frac{x_0^i}{i!} $$

- First Appell function

$$ F_1(a,b_1,b_2;c;x_1,x_2) = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{a^{\overline{m_1+m_2}} b_1^{\overline{m_1}} b_2^{\overline{m_2}}}{c^{\overline{m_1+m_2}}} \frac{x_1^{m_1}}{m_1!} \frac{x_2^{m_2}}{m_2!} $$

- Second Appell function

$$ F_2(a,b_1,b_2;c_1,c_2;x_1,x_2) = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{a^{\overline{m_1+m_2}} b_1^{\overline{m_1}} b_2^{\overline{m_2}}}{c_1^{\overline{m_1}} c_2^{\overline{m_2}}} \frac{x_1^{m_1}}{m_1!} \frac{x_2^{m_2}}{m_2!} $$

Summary

Perturbation theory at work

- Computer algebra is indispensable tool for computation of perturbative corrections

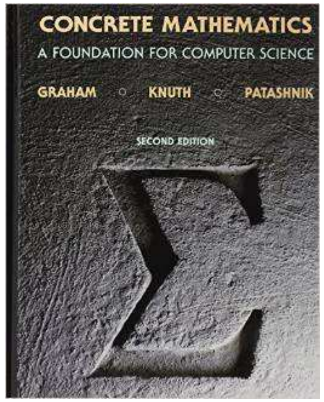
Symbolic sums

- Algorithms for symbolic summation useful to solve Feynman integrals

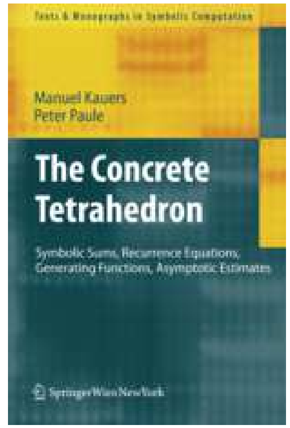
Literature (I)

- Text books
  - *Modern Computer Algebra*
    J. von zur Gathen, J. Gerhard

  - *Concrete Mathematics*
    R. L Graham, D. E. Knuth, O. Pataschnik

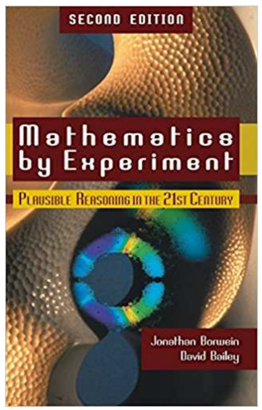


  - *Concrete Tetrahydron*
    M. Kauers, P. Paule



  - *A=B*
    M. Petkovsek, H. S. Wilf, D. Zeilberger   www.math.upenn.edu/~wilf/AeqB.html

  - *Mathematics by Experiment*
    J.M. Borwein, D. Bailey



Literature (II)

- Selected research articles
  - *Harmonic sums, Mellin transforms and integrals*, J. Vermaseren; hep-ph/9806280
  - *Nested sums, expansion of transcendental functions and multi-scale multi-loop integrals*, S.M., P. Uwer, S. Weinzierl; hep-ph/0110083
  - *Gauss hypergeometric function: Reduction, epsilon-expansion for integer/half-integer parameters and Feynman diagrams*, M. Yu. Kalmykov; hep-th/0602028
  - *HypExp 2, Expanding Hypergeometric Functions about Half-Integer Parameters*, T. Huber, D. Maitre; 0708.2443
  - *On the analytic computation of massless propagators in dimensional regularization*, E. Panzer; 1305.2161
  - . . .

Software (I)

Requirements in particle physics

- Symbolic calculations characterized by need for basic operations
  - sorting, gcd, factorization, multiplication
  - symbolic integration/summation
  - solution of systems of equations
  - ...
- Specialized code usually written by the user
  - largely dependent on the physics problem
  - add-on libraries

Software (II)

- Commercial programs: *Mathematica*, *Maple*, . . .
- Freeware/Add-on packages
  - *Mathematica*, *Maple*
    - several packages for hypergeometric summation
      [see for instance `www.math.upenn.edu/~wilf/AeqB.html`]
    - RISC software for symbolic summation and integration
      `www.risc.jku.at/research/combinat/software`
    - expansion of hypergeometric functions *HypExp*, T. Huber, D. Maitre
    - reduction of hypergeometric functions *HyperDire*, V. Bytev
    - hyperlogarithmic integration *HyperInt*, E. Panzer
  - GiNaC `www.ginac.de`
    - *nestedsums*, S. Weinzierl
  - Form `www.nikhef.nl/~form`
    - *Summer6*, J. Vermaseren
    - *XSummer*, S.M., P. Uwer

Exercises 1

Polynomial summmation

- Use *Mathematica* or *Maple* for polynomial summmation.
- Check some of the examples for hypergeometric summation with *Mathematica* or *Maple* like

$$\sum_{i\geq 0} a^{\overline{i}}\,\frac{z^i}{i!} = \frac{1}{(1-z)^a}$$

$$-z\sum_{i\geq 0} \frac{1^{\overline{i}}1^{\overline{i}}}{2^{\overline{i}}}\,\frac{z^i}{i!} = \ln(1-z)$$

- Try to evaluate the sum $\sum_{j_1=1}^{N} \frac{1}{j_1} S_1(j_1)$ in *Mathematica* or *Maple*.

  What happens?

Exercises 2

Harmonic sums

- Use the FORM package SUMMER for manipulation of harmonic sums. Download the package summer.h from http://www.nikhef.nl/~form/maindir/packages/summer/.
  - Evaluate the product of harmonic sums $S_2(N)S_1(N)^2$. Use the procedure basis.prc.
    ```
    #-
    #include summer.h
    .global
    L exampleproduct = S(R(2),N)*S(R(1),N)^2;
    #call basis(S)
    Print;
    .end
    ```
  - Check your result with the following sequence of calls.
    ```
    Multiply, replace_(N,<some_number>);
    #call subesses(S)
    ```

Exercises 3

Harmonic summation (easy)

- Use the FORM package SUMMER for harmonic summmation. Download the package summer.h from
  http://www.nikhef.nl/~form/maindir/packages/summer/.

  - Evaluate the sum $\sum_{j_1=1}^{N} \frac{1}{j_1} S_1(j_1)$ Use the procedure summer.prc.

```
#-
#include summer.h
.global
L examplesum = sum1(j1,1,N)*den(j1)*S(R(1),j1);
#call summer(1)
Print;
.end
```

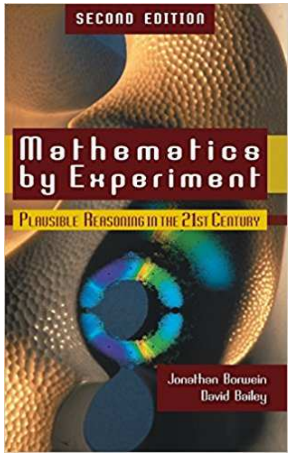
  - Compute examples for the convolution and conjugation of harmonic sums. Use the notation fac(N), invfac(N) and sign(N) with the (obvious) meaning $N!$, $\frac{1}{N!}$ and $(-1)^N$

Exercises 4

Harmonic summation (difficult)

- Use the FORM package XSUMMERfor summmation. Download the package from http://www-zeuthen.desy.de/~moch/xsummer/.
  - Evaluate the sum $\sum_{j_1=1}^{\infty} \frac{1}{(j_1+1)^3} \left(S_{-1}(j_1)\right)^2$

    Borwein, Bailey *Mathematics by Experiment*




```
#-
#define MAXSUM "2"
#define MAXWEIGHT "2"
#include declvars.h
#include declsums.h
L BBexample =
sum1(j1,1,inf)*(-S(R(1),X(-1),j1))^2*den(j1+1)^3;
#call DoSum(1,1)
id acc(x?)  = x;
Print +s;
.end
```

Exercises 5

Hypergeometric functions

- Use the FORM package XSUMMERfor the expansion of the hypergeometric function. Download the package from
  http://www-zeuthen.desy.de/~moch/xsummer/.

$${}_2F_1(1,-\epsilon;1-\epsilon;x_1) \qquad \text{and} \qquad {}_3F_2(-2\epsilon,-2\epsilon,1-\epsilon,1-2\epsilon,1-2\epsilon;x_1)$$

  - Check `ex-hyper.frm` for an implementation

- Alternatively, you can use the *Mathematica* package *HypExp* for this exercise