



Section 2

A Modern Computational Technology

- Conversion to nested sums, nested integrals

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Conversion to nested sums, nested integrals

★ Contents

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A goal of (perturbative) calculations: combination of nested sums, nested integrals

$$\sum_{n_1 \geq n_2 \geq \dots \geq n_N \geq 1} f_1(n_1) f_2(n_2) \dots f_N(n_N)$$

$$\int_{x_1 \geq x_2 \geq \dots \geq x_N \geq 0} dx_1 dx_2 \dots dx_N f_1(x_1) f_2(x_2) \dots f_N(x_N)$$

Ex: Harmonic polylogs (HPL), multiple polylogs, multiple zeta values (MZV), etc.

⇒ Reduction to a small set of basis functions/values possible

Here we present a method to convert non-nested sum/integral to nested ones.

$$F(v) = \sum_{n_1=1}^{\infty/f_1(v)} \dots \sum_{n_N=1}^{\infty/f_N(v)} \frac{\lambda_1^{n_1} \dots \lambda_N^{n_N}}{\prod_i (v + c_i + a_{i1}n_1 + \dots + a_{iN}n_N)^{P_i}}$$

implemented in Mathematica package “Wa”

Simple examples:

$$C = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^2} : \text{Catalan const.}$$

$$\sum_{k=1}^{\infty} \sum_{m=1}^{\infty} \frac{1}{(k+m)^2(2m+4k+1)} = 4 - 2C\pi - \frac{\pi^2}{6} - 4 \log 2 + \frac{21}{4} \zeta(3)$$

$$\sum_{k=1}^{\infty} \sum_{m=1}^k \frac{(-1)^{k+m}}{(k+1)^2(2m+1)} = -8 \overset{\text{Z-sum}}{\boxed{\text{Im } Z(\infty; 2, 1; -i, i)}} + 4C \log 2 - \frac{\pi^3}{8} - \frac{\pi^2}{12}$$

$$\text{Im} \sum_{\infty > n_1 > n_2 \geq 1} \frac{(-i)^{n_1} i^{n_2}}{n_1^2 n_2} = -\text{Im} \left[\text{Li}_3 \left(\frac{1+i}{2} \right) \right] - \frac{\pi^3}{128} + \frac{\pi}{32} \log^2 2$$

$$\sum_{k=1}^{\infty} \sum_{m=1}^{\infty} \frac{1}{(1+k+v)^2(1+m+n+v)(m+n+1)}$$

$$= \frac{2}{v} Z(v; 3; 1) + \frac{1}{v} Z(v; 1, 2; 1, 1) - \frac{\pi^2}{6} Z(v; 1; 1) = \frac{2}{v} \sum_{n=1}^v \frac{1}{n^3} + \dots$$

$$f(x) = \int_0^1 dy \log(1-y) \log(1-xy) \log(1+xy) [\log(1-x^2y)]^2 \rightarrow \text{HPLs}$$

Example: Computation of electron $g - 2$

Fine structure const.

$$\alpha^{-1} = 137.035999084(21)$$

determined precisely from anomalous magnetic moment of electron

$$a_e(\text{QED}) = a_e^{(2)} \left(\frac{\alpha}{\pi}\right) + a_e^{(4)} \left(\frac{\alpha}{\pi}\right)^2 + a_e^{(6)} \left(\frac{\alpha}{\pi}\right)^3 + a_e^{(8)} \left(\frac{\alpha}{\pi}\right)^4 + \dots$$

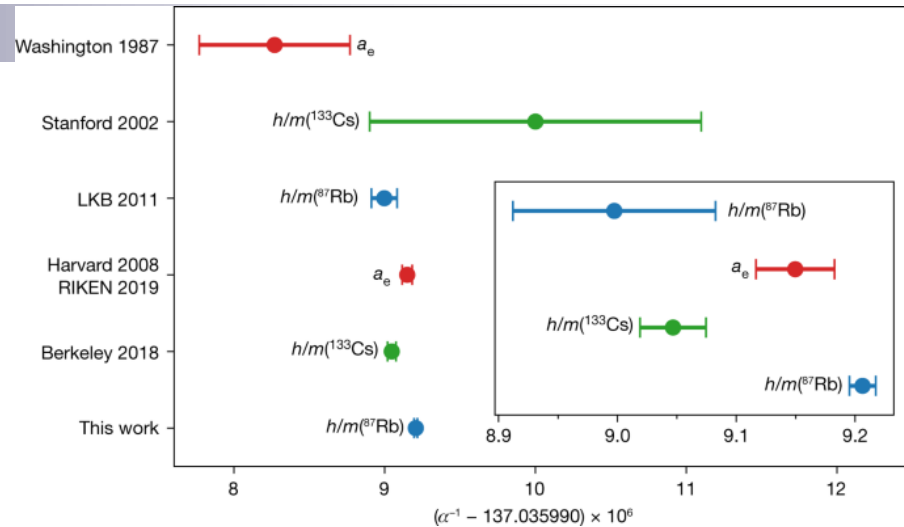
$$a_e^{(2)} = \frac{1}{2}$$

$$a_e^{(4)} = \frac{197}{144} + \frac{\pi^2}{12} + \frac{3}{4}\zeta(3) - \frac{\pi^2}{2} \ln 2 + \sum_{m>n>0} \frac{(-1)^{m+n}}{m^3 n}$$

$$a_e^{(6)} = \frac{83}{72}\pi^2\zeta(3) - \frac{215}{24}\zeta(5) + \frac{100}{3} \left(\text{Li}_4\left(\frac{1}{2}\right) + \frac{1}{24} \ln^4 2 - \frac{1}{24} \pi^2 \ln^2 2 \right) - \frac{239}{2160} \pi^4$$

$$+ \frac{139}{18} \zeta(3) - \frac{298}{9} \pi^2 \ln 2 + \frac{17101}{810} \pi^2 + \frac{28259}{5184}$$

$\mathcal{O}(m_e/m_\mu)$ terms omitted



Application: Computation of NR bound state spectrum

$$\left(-\frac{\Delta}{M} - C_F \frac{\alpha_S}{r}\right) \psi_{nl} = E_n \psi_{nl}$$

$$\Delta E_{nl} = \langle \psi_{nl} | \Delta V | \psi_{nl} \rangle + \langle \psi_{nl} | \Delta V \cdot \bar{G}_{nl} \cdot \Delta V | \psi_{nl} \rangle + \dots$$

$$G(\vec{x}, \vec{y}; E) \equiv \int_{\alpha} \frac{\psi_{\alpha}(\vec{x}) \psi_{\alpha}^*(\vec{y})}{E - E_{\alpha}} = \sum_{l=0}^{\infty} (2l+1) x^l y^l P_l(\cos \theta) G_l(x, y; k)$$

$$x = |\vec{x}|, \quad y = |\vec{y}|, \quad \cos \theta = \frac{\vec{x} \cdot \vec{y}}{x y}, \quad k = \sqrt{-ME}$$

Repr. by Laguerre polynomials:

$$G_l(x, y; k) = \frac{Mk}{2\pi} (2k)^{2l} e^{-k(x+y)} \sum_{m=0}^{\infty} \frac{L_m^{2l+1}(2kx) L_m^{2l+1}(2ky) m!}{(m+l+1-\nu)(m+2l+1)!}$$

Reduced Green fn.:

$$\bar{G}_{nl} = \lim_{E \rightarrow E_n} \left(G - \frac{\psi_{nl} \psi_{nl}^*}{E - E_n} \right)$$

$$\nu = \frac{C_F \alpha_S M}{2k}, \quad \sum_{m=0}^{\infty} L_m^{2l+1}(\rho) t^m = \frac{\exp(-\frac{\rho t}{t+1})}{(1-t)^{2l+2}}$$

$$\Rightarrow \langle \psi_{nl} | \Delta V \cdot \bar{G}_{nl} \cdot \Delta V | \psi_{nl} \rangle \ni \sum_{k=1}^{\infty} \frac{(n-l+k-1)!}{(n+l+k)! k^3} \equiv A(n, l)$$

$$\Rightarrow \langle \psi_{nl} | \Delta V \cdot \bar{G} \cdot \Delta V | \psi_{nl} \rangle \ni \sum_{k=1}^{\infty} \frac{(n-l+k-1)!}{(n+l+k)! k^3} \equiv A(n, l)$$

$$\frac{(n-l+k-1)!}{(n+l+k)!} = \prod_{m=-l}^{+l} \frac{1}{n+k+m} = \sum_{m=-l}^{+l} \frac{R(l, m)}{n+k+m} \quad R(l, m) = \frac{(-1)^{l-m}}{(l+m)!(l-m)!}$$

$$A(n, l) = \sum_{k=1}^{\infty} \sum_{m=-l}^{+l} \frac{R(l, m)}{(k+n+m) k^3}$$

$$\sum_{k=1}^{\infty} \frac{1}{(k+v) k^3} = \frac{\zeta(3)}{v} - \frac{\zeta(2)}{v^2} + \frac{S_1(v)}{v^3},$$

$$S_1(v) = \sum_{k=1}^v \frac{1}{k} : \text{Harmonic sum}$$

$$= \sum_{m=-l}^{+l} R(l, m) \left[\frac{\zeta(3)}{n+m} - \frac{\zeta(2)}{(n+m)^2} + \frac{S_1(n+m)}{(n+m)^3} \right]$$

$$\sum_{m=-l}^{+l} \frac{R(l, m)}{(n+m)^a} = \frac{1}{a!} \left(-\frac{\partial}{\partial k} \right)^a \frac{\Gamma(n-l+k)}{\Gamma(n+l+k+1)} \Big|_{k=0} \quad \text{for } a \geq 0$$

$$= \frac{(n+l)!}{(n-l-1)!} [\zeta(3) - \zeta(2)\{S_1(n+l) - S_1(n-l-1)\}] + \sum_{m=-l}^{+l} \frac{R(l, m)}{(n+m)^3} S_1(n+m)$$

includes only known transcendental numbers and finite sums

How to convert:

$$F(v) = \sum_{n_1=1}^{\infty/f_1(v)} \cdots \sum_{n_N=1}^{\infty/f_N(v)} \frac{\lambda_1^{n_1} \cdots \lambda_N^{n_N}}{\prod_i (v + c_i + a_{i1}n_1 + \cdots + a_{iN}n_N)^{P_i}}$$

Main idea: resum sequence of differences iteratively

$$\begin{aligned} \text{cf. } \Delta f(k) = f(k+1) - f(k) \quad \Rightarrow \quad f(v) &= \sum_{k=1}^{v-1} \Delta f(k) + f(1) \\ &= \sum_{k=1}^{v-1} \left(\sum_{m=1}^{k-1} \Delta^2 f(m) + \Delta f(1) \right) + f(1) \\ &\quad \vdots \end{aligned}$$

Shift invariance of summand:

You can find a set of integers $(\Delta_0, \Delta_1, \dots, \Delta_N)$ s.t. for $\forall i$,

$$v + c_i + a_{i1}n_1 + \cdots + a_{iN}n_N = (v + \Delta_0) + c_i + a_{i1}(n_1 + \Delta_1) + \cdots + a_{iN}(n_N + \Delta_N)$$

Example:

$$S = \sum_{k=1}^{\infty} \sum_{m=1}^{\infty} \frac{(-1)^{k+m}}{(2+m)^2(1+k+m)^2} = \sum_{m=1}^{\infty} \frac{(-1)^m f(m)}{(2+m)^2}$$

$$f(m) = \sum_{k=1}^{\infty} \frac{(-1)^k}{(1+k+m)^2}$$

$$f(m) = [f(m) + f(m-1)] - [f(m-1) + f(m-2)] + \dots$$

$$+ (-1)^m [f(2) + f(1)] - (-1)^m f(1)$$

$$= \sum_{j=2}^m (-1)^{m-j} [f(j) + f(j-1)] - (-1)^m f(1)$$

$$\sum_{k'=0}^{\infty} \frac{(-1)^{k'+1}}{(1+k'+j)^2}$$

$$f(j) + f(j-1) = \sum_{k=1}^{\infty} \frac{(-1)^k}{(1+k+j)^2} + \sum_{k=1}^{\infty} \frac{(-1)^k}{(k+j)^2}$$

$$= \left(\sum_{k=1}^{\infty} - \sum_{k=0}^{\infty} \right) \frac{(-1)^k}{(1+k+j)^2} = -\frac{1}{(1+j)^2}$$

Bulk part cancels
and only surface
term remains.

Example:

$$S = \sum_{k=1}^{\infty} \sum_{m=1}^{\infty} \frac{(-1)^{k+m}}{(2+m)^2(1+k+m)^2} = \sum_{m=1}^{\infty} \frac{(-1)^m f(m)}{(2+m)^2}$$
$$f(m) = \sum_{k=1}^{\infty} \frac{(-1)^k}{(1+k+m)^2}$$

$$\therefore f(m) = (-1)^m \sum_{j=2}^m \frac{(-1)^{1-j}}{(1+j)^2} - (-1)^m \sum_{k=1}^{\infty} \frac{(-1)^k}{(2+k)^2}$$

$-(-1)^m f(1)$

$$\therefore S = \sum_{m=1}^{\infty} \frac{1}{(2+m)^2} \sum_{j=2}^m \frac{(-1)^{1-j}}{(1+j)^2} - \sum_{m=1}^{\infty} \frac{1}{(2+m)^2} \sum_{k=1}^{\infty} \frac{(-1)^k}{(2+k)^2}$$

nested sum

product of single sums