Automated computation meets hot QCD

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We give a short review on recent progress in the field of automated calculations in finite-temperature field theory, where integration-by-parts techniques have proven (almost) as useful as in the zero-temperature case. Furthermore, we provide one concrete example of an evaluation of a new three-loop master sum-integral that exhibits maximal divergence.
1. Introduction

In ordinary zero-temperature perturbative field theory, this conference series has witnessed a rapid development of automated computer-algebra aided approaches over the past decade or so. Triggered perhaps by the integration-by-parts (IBP) method [1, 2] that received an enormous boost from its algorithmic description by Laporta [3], the problem of reducing the large variety of Feynman integrals that occur in a given perturbative computation to a small number of master integrals can nowadays be regarded as solved, in the sense that there exist independent public computer-algebraic implementations [4–6] which, given sufficient hardware resources, perform this step in an automated way. Concerning the subsequent evaluation of master integrals, the degree of automation is less developed – after all, integration is still an art. However, besides a much better understanding of the analytic structure of the numbers and functions that are contained in the perturbative series [7–10], there has been progress in developing powerful approaches to obtain analytic results [3, 11] as well as stable and fast numerical tools [12, 13] that promise to be applicable to large classes of Feynman integrals.

In this note, we will discuss the corresponding situation for finite-temperature perturbation theory. The present state of affairs is that, while many of the methods and algorithmic tools developed for zero-temperature field theory (such as generation and classification of Feynman graphs, efficient color and Lorentz algebra as well as IBP reduction methods) can be – and have been – applied with only minor adjustments to finite-temperature systems, only very few master sum-integrals that remain after the IBP reduction step are known (see, e.g. Refs. [14–18] or the review [19]). It seems difficult to profit from the comparably mature zero-temperature techniques for this step, due to the very different analytical structure that the sums bring about. Here, we will therefore give only a brief discussion on thermal IBP methods, to concentrate then on sum-integral evaluation, producing a new result for a phenomenologically relevant case.

2. Sum-integral reduction via IBP

The basic principle of the IBP method [1, 2] applies to any integral, and can hence also be applied to the sum-integrals that occur in finite-temperature field theories. The Matsubara sums are simply left untouched, while their summands are interpreted as massive loop integrals in a reduced space-time dimension and with masses provided by the Matsubara frequencies, with the IBP relations acting upon these massive loop integrals. A more detailed review of these techniques is given e.g. in Ref. [20]. Similar to the zero-temperature case, the linear relations among sum-integrals – as generated by IBP on the Matsubara summands – can be systematically used for a sum-integral reduction step, employing a variant of the Laporta algorithm [3]. This approach has been successfully used for a number of higher-order calculations in finite-temperature QCD (for examples, see e.g. [20–22]), to enable basis transforms among master sum-integrals (see below), or even to aid in managing the infrared (IR) behavior of Matsubara summands when evaluating master integrals [23]. To show two concrete examples, IBP has revealed that a non-trivial 2-loop sunset-sum-integral [24] and a non-trivial 3-loop mercedes-sum-integral vanish identically:

\[
\sum \int \frac{1}{P^2 Q^2 (P - Q)^2} \overset{\text{IBP}}{=} 0, \quad J_{111111}^{000} \overset{\text{IBP}}{=} 0, \quad (2.1)
\]
where we have used a generic notation for massless bosonic 3-loop vacuum sum-integrals

\[ J_{abcddef}^{ab\gamma} \equiv \int_{\mathbb{R}^{8d}} \frac{(P_0)^\alpha (Q_0)^\beta}{[P^2]^\alpha [Q^2]^\beta [(P - Q)^2]^\gamma [P - R]^2]^\delta [Q - R]^2]^\epsilon . \]  

(2.2)

In our notation, bosonic (Euclidean) four-momenta are denoted by \( P = (P_0, P) = (2\pi nT, \mathbf{p}) \), with \( T \) being temperature of the thermal system, inverse propagators are \( P^2 = P_0^2 + \mathbf{p}^2 \), and the sum-integral symbol stands for

\[ \int_{\mathbb{R}^{8d}} T \sum_{n \in \mathbb{Z}} \int \frac{d^d \mathbf{p}}{(2\pi)^d} \, , \quad \text{with} \quad d = 3 - 2\epsilon . \]  

(2.3)

A class of 1-loop bosonic tadpoles that we will need below can be evaluated analytically as

\[ I_k = \int_{\mathbb{R}^{8d}} \frac{1}{16 \pi^2} = \frac{2T \zeta(2s - d)}{(2\pi T)^{s-\frac{d}{2}}} \frac{\Gamma(s - \frac{d}{2})}{(4\pi)^{d/2} \Gamma(s)} . \]  

(2.4)

In Ref. [22], it has been shown that the computation of NNLO corrections to the spatial string tension of pure Yang-Mills theory (mapped to Taylor coefficients of background-gauge-field self-energies [21]) can be reduced to 3-loop basketball-type master sum-integrals \( K_i \) (and products of simpler 1-loop ones \( I_i \), giving the gauge-invariant expression

\[ \Pi_{T3}^{1}(0) = C_A^3 \left( \sum_{i=1}^{9} \beta_i (d) K_i + \beta_{10}(d) \Gamma_0 I_1 + \beta_{11}(d) \Gamma_1 I_1 + \beta_{12}(d) \Gamma_2 I_2 \right) \]  

(2.5)

\[ \{K_1, \ldots, K_9\} = \{ J_{220011}^{000}, J_{320001}^{000}, J_{222100}^{000}, J_{541001}^{000}, J_{540101}^{000}, J_{740101}^{000}, J_{730111}^{000}, J_{721001}^{000}, J_{820101}^{000} \} , \]  

(2.6)

where the coefficients \( \beta_i \) are rational functions that contain simple and double poles in \( 1/(d - 3) \), and where all massless bosonic 3-loop vacuum sum-integrals \( K_i \) have been represented in terms of the notation introduced in Eq. (2.2). After an extensive reverse search in our IBP database, it proves possible to transform the above expression into the equivalent representation

\[ \Pi_{T3}^{1}(0) = C_A^3 \left( \sum_{i=1}^{6} r_i (d) V_i + r_7 (d) \Gamma_0 \Gamma_0 I_1 + r_8 (d) \Gamma_1 \Gamma_2 I_1 + r_9 (d) \Gamma_2 \Gamma_2 I_2 \right) \]  

(2.7)

\[ \{V_1, \ldots, V_6\} = \{ J_{220011}^{000}, J_{320001}^{000}, J_{222100}^{000}, J_{541001}^{000}, J_{540101}^{000}, J_{740101}^{000} \} , \]  

(2.8)

which, much in the spirit of the epsilon-finite basis advocated in Ref. [25], does not contain divergences in the coefficients \( r_i(d) \) as \( d \rightarrow 3 \) (note that \( V_6 = K_2 \) was already contained in the old basis listed in Eq. (2.6), and was kept since it has already been evaluated in Ref. [18]). Eq. (2.7) can now serve as a convenient starting point for determining the spatial string tension, once the five unknown master sum-integrals \( \{V_1, \ldots, V_5\} \) have been evaluated up to their constant parts. For \( V_1 \), see the next section.

3. A 3-loop master sum-integral of dimension zero

Let us now turn to a concrete example of 3-loop sum-integrals, to demonstrate the main techniques that are used in the master integral evaluation step. Here, we work in \( d = 3 - 2\epsilon \) spatial dimensions, and wish to evaluate the \( \epsilon \)-expansion of \( V_1 \) given in Eq. (2.8) up to the constant term.
V1 is a sum-integral of spectacles-type, for which a generic evaluation procedure has been discussed in Ref. [26]. Subtracting subdivergences, the sum-integral is split into its finite part (which can typically be computed only numerically in configuration space), and its divergent part (which can be expressed analytically in terms of Zeta and Gamma functions), treating the P0 = 0 mode separately (softening the IR via IBP relations if needed). We thus decompose V1 as

\[ V_1 \equiv \int_{12110}^{000} \frac{1}{P^2} \Pi_{21}(P) \Pi_{11}(P) \]

\[ = \int_{P'} \frac{1}{P^2} \left\{ (\Pi_{21} - \Pi_{11}^E) + (\Pi_{11} + \Pi_{11}^E) + (\Pi_{21} - \Pi_{21}^E) \right\} + \]

\[ + \int_{P'} \frac{1}{P^2} \left\{ \Pi_{21}^E + \Pi_{11}^E + \Pi_{21}^E \right\} + \int_{P'} \delta_{P_0} \left( \Pi_{21}^E + \Pi_{11}^E \right) , \]

where the first line collects the finite pieces (the primed sum excludes the P0 = 0 term), the second line the divergent pieces as well as the zero-mode, and we have used the 1-loop 2-point structures

\[ \Pi_{ab}(P) \equiv \int_Q \frac{1}{|Q^2 + [(P - Q)^2]|^2} , \]

\[ \Pi_{ab}^E \equiv \int_Q \frac{1}{|Q^2 + [(P - Q)^2]|^2} , \]

where \( G(s_1, s_2, d) = \frac{\Gamma(\frac{s_1}{2} - 1) \Gamma(\frac{s_2}{2} - d)}{(4\pi)^{d/2} \Gamma(s_1) \Gamma(s_2) \Gamma(d - s_1 - s_2)} , \)

\[ \Pi_{ab}^F \equiv \int_Q \frac{1}{2\pi T} , \]

\[ \Pi_{ab}^E \equiv \int_Q \frac{1}{|Q^2 + [(P - Q)^2]|^2} . \]

We will in the following evaluate the various contributions to V1 of Eq. (3.2) in turn.

### 3.1 Finite pieces

Using inverse 3d Fourier transforms of the 2-point functions, the first term of Eq. (3.2) reads

\[ \int_{P'} \frac{1}{P^2} \times (\Pi_{21} - \Pi_{11}^E) \times (\Pi_{11} - \Pi_{11}^E) \]

\[ = T \sum_{\delta} \int \frac{1}{(2\pi)^3} \frac{1}{P^2} \times T \int \frac{1}{(2\pi)^3} d^3 \epsilon \frac{e^{i\epsilon \cdot \bar{r}}}{|\epsilon|} \sum_{Q_0} \frac{e^{-|Q_0| - |Q_0 + \bar{r}|}}{|Q_0|} \times \frac{T^3}{4} \int d^3 s \left( \coth \frac{s}{2} \right) e^{-|\bar{r}|} + O(\epsilon) \]

\[ = 2 \times \sum_{n,m} \int_{0}^{\infty} dx \int_{0}^{\infty} dy \left( \coth y - \frac{1}{y} \right) \frac{e^{-|n|m + |n|m + m|y|}}{|n|m} \left( e^{-|n|x - |y|} - e^{-|n|(x+y)} \right) + O(\epsilon) \]

\[ = \frac{1}{2} \sum_{n,m} \int_{0}^{\infty} \frac{dy}{y} \left( \coth y - \frac{1}{y} \right) \left[ 6y [\ln(1 - e^{-2y}) + y]^2 - \pi^2 [\ln(1 - e^{-2y}) + 4y] - 14y^3 + \right. \]

\[ + 6 \ln(1 - e^{-2y}) \text{Li}_2(e^{-2y}) + 12y \left[ \text{Li}_2(1/(1-e^{-2y})) - i\pi \ln(1 - e^{-2y}) \right] - 6 \text{Li}_3(1 - e^{-2y}) \bigg] + O(\epsilon) \]

\[ = \frac{c_1}{(4\pi)^6} + O(\epsilon) , \quad c_1 \approx 0.6864720593640618954(1) , \]

where we have used dimensionless variables such as \( \bar{r} = 2\pi T |x| \) and \( \bar{Q}_0 = Q_0/(2\pi T) = m \); performed the momentum integration as well as the angular integration in configuration space in the third line; integrated over \( x \) and performed both sums in the fourth line; and performed the last step simply via Mathematica’s numerical integration routine.
In full analogy\(^1\), we get for the second term of Eq. (3.2)

\[
\sum_{p_F} \frac{1}{(2\pi)^3} \times (\Pi^F_{01} - \Pi^B_{11}) \\
= T \sum_{p_0} \int \frac{d^3p}{(2\pi)^3} \frac{1}{P^2} \times \left( - \frac{T}{4\pi} |p_0| \right) \times \frac{T^3}{4} \int d^3r \frac{e^{p_0r}}{r^2} \left( \coth \frac{r}{\bar{T}} - 1 \right) e^{-|p_0|r} + \mathcal{O}(\varepsilon)
\]

where \(G \approx 1.28243\) is the Glaisher constant. Similarly, the third term of Eq. (3.2) evaluates as

\[
\sum_{p_F} \frac{1}{(2\pi)^3} \times (\Pi^F_{21} - \Pi^B_{21}) \times (\Pi^F_{11} - \Pi^B_{11}) \\
= T \sum_{p_0} \int \frac{d^3p}{(2\pi)^3} \frac{1}{P^2} \times \left( - \frac{T}{2\pi^2} \right) \int d^3r \frac{e^{p_0r}}{r^2} \left[ f_{210}(r, |p_0|) \right] \times \left( - \ln \frac{p_F^2}{16\pi^2} \right) + \mathcal{O}(\varepsilon)
\]

with

\[
f_{210}(x, n) \equiv e^{2nx}B(e^{-2x}, n+1, 0) + H_n - \ln(1 - e^{-2x}) + e^{2nx}\text{Ei}(-2nx) + \ln \frac{2x}{n} - \frac{\gamma - x}{6}\n\]

where we have used the incomplete Beta function \(B(z, n+1, 0) = \int_0^z \frac{t^n}{1 - t} dt = - \ln(1 - z) - \sum_{m=1}^n \frac{z^m}{m}\), harmonic numbers \(H_n = \sum_{m=1}^n 1/m\) and exponential integral \(\text{Ei}(z) = \int z e^t/t dt\). After integrating over \(p\) the angular \(r\) integration was trivial, leaving Eq. (3.8) where the summation converges somewhat slowly and the evaluation of the integrand itself is costly since it contains special functions; for the numerical precision given above, we have truncated the sum at \(n_{\text{max}} = 7000\) and estimated the remainder by fitting to a power-law \(a/n^b\) in the interval \(n \in [7000, 19000]\) (obtaining \(b \approx 1.9\)) and summing this fit to infinity.

### 3.2 Divergent pieces

Introducing the following 2-loop vacuum sum-integrals (see e.g. Appendix A and B of Ref. [26])

\[
A(s_1, s_2; s_3; s_4; d) \equiv \frac{f_{tQ}}{[Q^2]^{s_1}[P^2]^{s_2}[(P - Q)^2]^{s_3}} \\
= \frac{2T^2 \zeta(2s_{123} - 2d - s_4)}{(4\pi)^d} \frac{\Gamma(s_{123} - 4d)\Gamma(s_{12} - 2d - s_1)\Gamma(d/2)\Gamma(s_{123} - d)}{(\Gamma(s_{12})\Gamma(s_3)\Gamma(s_1)(d/2)\Gamma(s_{123} - d)})^s_4
\]

\[
L(s_1, s_2; s_3; s_4; s_5; d) \equiv \frac{f_{tQ}}{[P^2]^{s_1}[Q^2]^{s_2}[(P + Q)^2]^{s_3}} \\
\approx \frac{1}{(d - 5)(d - 2)} I_1 I_2
\]

\(^1\)Here, we use \(\Pi^{\text{IBP}}_{11} \approx \frac{1}{d - 3} \sum_{3} \frac{2\gamma - 2}{(p^2 - m^2)^{d-3}} \Pi^{B}_{11} \approx \frac{1}{d - 3} \sum_{3} \frac{2\gamma - 2}{(p^2 - m^2)^{d-3}} \Pi^{B}_{11} \approx \frac{1}{d - 3} \sum_{3} \frac{2\gamma - 2}{(p^2 - m^2)^{d-3}} \Pi^{B}_{11}\), where we have treated \(|p_0|\) as a mass in the 3d 1-loop self-energy integrals \(\Pi^{B}_{00}\), and noticed that \(\Pi^{F}_{11}\) is finite at \(d = 3\), and that the tadpole \(\Pi^{F}_{00}\) is known analytically.
and noting from Eqs. (3.3),(3.5) that $\Pi^D \sim 1/[p^2]^x$ are simple powers, the fourth, fifth and sixth terms of Eq. (3.2) are effectively 2-loop structures and can be evaluated analytically as

$$\begin{align*}
\int \frac{1}{p^2} \Pi_2 (\Pi_2 - \Pi_2^b) \Pi_1^b = & G(1,1,d+1) \left[ L(211;00;d) - A(121;0;d) - A(211;0;d) \right], \\
\int \frac{1}{p^2} \Pi_2 (\Pi_2 - \Pi_1^b) = & G(1,1,d+1) \left[ G(2,1,d+1) \hat{I}_{5-d} + L_2 \hat{I}_{7-d} + l_1 \hat{I}_{9-d} \right], \\
\int \frac{1}{p^2} \Pi_2 \Pi_1^b = & G(1,1,d+1) A(2,(5-d)/2,1;0;d),
\end{align*}$$

(3.13) (3.14) (3.15)

where we have used the abbreviation $\hat{I}_s \equiv (2\pi T)^{d-3} I_{s+(d-3)/2}$. All three expressions contain poles as $d \rightarrow 3$; the first two contribute starting from $1/\varepsilon^3$, the last one merely from $1/\varepsilon$.

### 3.3 Zero mode

The seventh term of Eq. (3.2) can be decomposed into finite (first line) and divergent parts as

$$\begin{align*}
\int \frac{1}{p^2} \delta_0 \frac{1}{p^2} \Pi_2 \Pi_1 = & \int \frac{1}{p^2} \delta_0 \frac{1}{p^2} \left( \Pi_2 - \Pi_2^b \right) \left( \Pi_1 - \Pi_1^b \right) + \\
& + \int \frac{1}{p^2} \left\{ \Pi_2^b \Pi_1 + \Pi_2 \left( \Pi_1 + \Pi_1^b \right) - \Pi_2^b \left( \Pi_1 + \Pi_1^b \right) \right\},
\end{align*}$$

(3.16)

In full analogy to Sec. 3.1, the first (finite) term is treated in 3d coordinate space, as

$$\begin{align*}
\int \frac{1}{p^2} \delta_0 \frac{1}{p^2} \times \left( \Pi_2 - \Pi_2^b \right) \times \left( \Pi_1 - \Pi_1^b \right) = & T \int \frac{d^3p}{(2\pi)^3} \frac{1}{p^2} \times \frac{T}{2(4\pi)^2} \int d^3r e^{ipr} \left[ -2 \ln (1 - e^{-2r}) \right] \times \frac{T^3}{4} \int d^3s e^{ips} \left( \coth \frac{s}{\varepsilon} - \frac{1}{s} - 1 \right) + O(\varepsilon) \\
= & - \frac{T}{(4\pi)^6} \int_0^\infty dx \int_0^\infty dy \int_0^\infty dz \ln (1 - e^{-2r}) \left( \coth y - \frac{1}{y} - 1 \right) + O(\varepsilon) \\
= & \frac{1}{(4\pi)^6} \int_0^\infty dy \left( \coth y - \frac{1}{y} - 1 \right) \left[ 4y^3 - 2\pi y^2 + 3 \left[ L_3 (e^{2y}) + 2\pi i y^2 \right] - 3\zeta(3) \right] + O(\varepsilon) \\
= & \frac{c_3}{(4\pi)^6} + O(\varepsilon), \quad c_3 \approx 10.33244698246374834(1).
\end{align*}$$

(3.17)

In full analogy to Sec. 3.2, the second (divergent) part of Eq. (3.16) contains 1- and 2-loop structures $G$ and $A$ only and is hence known fully analytically in terms of Gamma and Zeta functions:

$$\begin{align*}
\int \frac{1}{p^2} \delta_0 \frac{1}{p^2} \left\{ \Pi_2^b \Pi_1 + \Pi_2 \left( \Pi_1 + \Pi_1^b \right) - \Pi_2^b \left( \Pi_1 + \Pi_1^b \right) \right\} = & T G(2,1,d) A(4 - d/2,1;1;0;d) + T G(1,1,d) A(3 - d/2,2,1;0;d) + \\
& + G(1,1,d+1) A((5 - d)/2,2,1;0;d) - 0_{\text{scalefree}}.
\end{align*}$$

(3.18)

### 3.4 Result

Collecting from Eqs. (3.6), (3.7), (3.9), (3.13), (3.14), (3.15), (3.17), (3.18) and expanding around $d = 3 - 2\varepsilon$, we finally obtain

$$V_1 = \frac{1}{6(4\pi)^6} \left( \frac{e^{\beta T}}{4\pi T^2} \right)^3 \left[ \frac{1}{e^{\beta T}} + \frac{3}{\beta^2} + \frac{1}{e^{\beta T} - 6\gamma e^\beta - \frac{3\pi^2}{4} - 12\gamma - 3\zeta(3)} \right] +$$

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\[
\begin{align*}
&+ \left[ 51 - 42 \gamma_E^2 + 4 \pi^2 \left( \frac{19}{16} \ln(2\pi) - 12 \ln G \right) + 2 \ln(2) \left( 12 - 12 \gamma_E^2 - 24 \gamma_1 - \zeta(3) \right) + \\
&+ 6 \gamma_E \left( 3 \zeta(3) - 4 - 4 \gamma_1 \right) - 84 \gamma_1 - 36 \gamma_1^2 + \frac{25}{2} \zeta(3) - 16 \zeta'(3) + 6 (c_1 + c_2 + c_3) \right] + O(\varepsilon) \\
\approx \frac{1}{6(4\pi)^6} \left( \frac{1}{T^2} \right)^{3\varepsilon} \left( 1 - \frac{2.86143}{\varepsilon^3} + \frac{15.2646}{\varepsilon} + 47.77(1) + O(\varepsilon) \right),
\end{align*}
\]

with \( (c_1 + c_2 + c_3) \approx 7.817(1) \), where the numerical error is dominated by Eq. (3.9). The analytic part of the result contains the Glaisher constant \( G \), for which \( 12 \ln(G) = 1 + \zeta'(-1)/\zeta(-1) \), zeta values as well as the Stieltjes constants \( \gamma_i \), defined by \( \zeta(1+\varepsilon) = 1/\varepsilon + \gamma_E - \gamma_1 \varepsilon + \gamma_2 \varepsilon^2/2 + O(\varepsilon^3) \).

Note that our 3-loop sum-integral \( V_1 \) does contain a \( 1/\varepsilon^3 \) divergence, as would be naturally expected from the fact that the 1-loop tadpoles of Eq. (2.4) diverge as \( 1/\varepsilon \) at most (recall that \( d = 3 - 2\varepsilon \) in our notation). This is in fact the first example where we observe such behavior – all previously known non-trivial 3-loop cases in fact started at order \( 1/\varepsilon^2 \).

4. Conclusions

While automated methods for Feynman integral reduction work well when applied to the sum-integrals that arise in finite temperature perturbation theory, the step of evaluating the resulting master sum-integrals is in a much less mature state. Only a small number of non-trivial higher-loop sum-integrals are known so far, their evaluation resting on a case-by-case analysis with intricate subdivergence subtraction techniques, such as demonstrated here on the example of a new bosonic 3-loop tadpole that enters in a NNLO determination of the spatial string tension. Typical results are partly analytic and partly numeric, since often the constant terms of the Laurent series cannot be obtained in closed form, but mapped onto simple finite low-dimensional representations.

Future progress in the field of classification and evaluation of sum-integrals would certainly give a boost to the field of finite temperature field theory. It will be interesting to see whether this progress originates again from a fruitful application of zero-temperature methods (such as e.g. Mellin-Barnes representations, classes of multiple nested sums and integrals such as harmonic polylogarithms, or systematic numerical methods based on sector decomposition), or whether completely new ideas and structures are needed.

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