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Higher-order radiative corrections for the $e^-e^+ \rightarrow b\bar{b}$
massive process

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NYILATKOZAT

(A DE TTK hallgatóinak diplomadolgozatához/szakdolgozatához)

AlulírottFekésházy Levente..... (Neptun kód: ...XFN4ZE.....) jelen nyilatkozat aláírásával kijelentem, hogy a

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Kijelentem továbbá, hogy a dolgozat készítése során az önálló munka tekintetében a témavezetőt nem tévesztettem meg. Meg nem engedett segítséget nem vettem igénybe, a dolgozatot más oktatási intézményben szakdolgozatként vagy diplomamunkaként korábban nem nyújtottam be.

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¹ 1999. évi LXXVI. tv. 34. § (1) A mű részletét – az átvető mű jellege és célja által indokolt terjedelemben és az eredetihez híven – a forrás, valamint az ott megjelölt szerző megnevezésével bárki idézheti.

36. § (1) Nyilvánosan tartott előadások és más hasonló művek részletei, valamint politikai beszédek tájékoztatás céljára – a cél által indokolt terjedelemben – szabadon felhasználhatók. Ilyen felhasználás esetén a forrást – a szerző nevével együtt – fel kell tüntetni, hacsak ez lehetetlennek nem bizonyul.

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1 Introduction

1.1 Motivation: $e^-e^+ \rightarrow b\bar{b}$ forward-backward asymmetry

In my master thesis I have calculated the double real contribution to the Next-to-Next-to-Leading-Order (NNLO) QED+QCD corrections to the massive $e^-e^+ \rightarrow b\bar{b}$ process; this process is particularly interesting due to the forward-backward asymmetry. This asymmetry can be qualitatively defined by the ratio of the difference over the sum of the forward (N_f) and backward (N_b) events; where forward means that the final state b -quark is produced in the hemisphere defined by the direction of the electron beam.

$$A_{fb}^b = \frac{N_f - N_b}{N_f + N_b}, \quad (1.1)$$

where

$$N_f = \int_0^1 \frac{d\sigma}{d\Omega} d\Omega, \quad N_b = \int_{-1}^0 \frac{d\sigma}{d\Omega} d\Omega. \quad (1.2)$$

From all of the $e^-e^+ \rightarrow Z \rightarrow f\bar{f}$ asymmetries this can be measured with the highest precision; as b -jets can be easily distinguished due to their secondary vertex. The measurements were done at LEP at $\sqrt{s} \approx m_Z$ energies, which gave an average of $(A_{fb}^b)_{exp} = 0.0992 \pm 0.0016$ [1].

This asymmetric phenomenon can be explained in the framework of the Standard Model. Fermions are grouped into two distinct groups; left-handed weak-isospin doublets and right-handed weak-isospin singlets. The weak neutral boson, the Z boson, couples to these groups differently. Thus when it decays, it favors one kind; this causes asymmetries in the $e^-e^+ \rightarrow f\bar{f}$ cross sections. These asymmetries are ultimately driven by the charge of the fermion (Q_f) and the weak mixing angle ($\sin^2(\Theta)_W$).

$$\frac{d\sigma}{d\cos(\Theta)} = \frac{3}{8} \sigma_{f\bar{f}}^{\text{tot}} ((1 + \cos^2(\Theta)) + 2\mathcal{A}_f \cos(\Theta)), \quad (1.3)$$

where

$$\mathcal{A}_f = 2 \frac{1 - 4|Q_f| \sin^2(\Theta)_{eff}^f}{1 + (1 - 4|Q_f| \sin^2(\Theta)_{eff}^f)^2}, \quad (1.4)$$

and $\sin^2(\Theta)_{eff}^f$ is the effective fermion mixing angle, which includes electroweak corrections. Today the most precise prediction is the purely QCD NNLO calcula-

tion with value $(A_{fb}^b)_{th} = 0.1030 \pm 0.0002$. [2]

As one can see the measured and the theoretical value deviates with 2.1σ . The anticipated new e^-e^+ colliders in the TeV region, like the FCC-ee [3] or CLIC [4], promise to have far better precision than LEP. Thus there is an increased interest of more precise theoretical calculation of the $e^-e^+ \rightarrow b\bar{b}$ process.

In this work I have done the first steps for a more accurate theoretical calculation, which might enable us to get closer to the solution of this puzzle.

1.2 Short historical review

In physics we try to quantify the processes we observe in the universe; from the simple pendulum, through the formation of galactic clusters, to the collision of elementary particles. For this purpose we do experiments, from which we gather data. In this data we recognize patterns; these patterns are put into shape with the help of mathematical equations and symbols. These equations and symbols alone do not contain physics, the physics is in the physical dimensions associated with the symbols.

If these patterns can be derived by some axioms, which themselves are mathematical equations, then the set of these axioms are called a physical model. Naturally all physical models have an interval of validity, which is determined by the axioms.

Historically the earliest successful model which described our world was Newton's classical mechanics, then came thermodynamics and electromagnetism. With these models physicist and mathematicians could explain every experimental data till the XIX. century; experiments like the photoelectric effect or Planck's radiation law were unexplainable with classical theorems.

These puzzles were unsolved until 1926, the invention of quantum mechanics. This new model triumphantly explained such complex and mysterious things like the electron structure of an atom, specific heat of bodies at low temperature, or conductors.

Unfortunately this model had shortcomings. One of the main axioms, the Schrödinger equations had a very narrow validity. It was a non-relativistic¹ equation which described spinless particles. Another drawback arose when physicist wanted to treat quantum mechanical many-body systems. They got N coupled differential equations, where N is the number of particles. This ponderosity was not unknown, the same happened in classical physics; though this time it was

¹The marking of the non-relativistic quality as a shortcoming is debatable. As Schrödinger first came up with a relativistic equation (the now called Klein-Gordon equation), but as it was incapable to describe the electron structure of the atom, he had to abandon it.

different. The differential equations were first order and most importantly, two particles in the same quantum state were indistinguishable.

With the latter in mind physicist described many-body systems by calculating the number of particles in each state rather than the state of each particle. This outstanding move was named second quantization, as in this way the Hamiltonian looked like a sum of expectation values. The model was named quantum field theory, as the fundamental objects of the model were fields not particles; particles were mere excitations of said fields.

Below we give a brief account how quantum field theory arises from second quantization and then discuss how it is used to build models for particle physics. We point the reader to the textbooks [5–7] for a complete introduction to these topics.

1.3 Quantum field theory

1.3.1 Second quantization and field operators

Let us examine a system build up from N particles with pair interaction. We have N coupled first order differential equations:

$$\partial_t |\psi_1(t)\rangle = H_1 |\psi_1(t)\rangle \quad (1.5)$$

$$\partial_t |\psi_2(t)\rangle = H_2 |\psi_2(t)\rangle \quad (1.6)$$

$$\dots \quad (1.7)$$

$$\partial_t |\psi_N(t)\rangle = H_N |\psi_N(t)\rangle, \quad (1.8)$$

where $|\psi_i\rangle$ is the state vector of the i -th particle and $H_i = \frac{p_i^2}{2m} - \sum_{j=1}^N V_{ij}$ is the i -th particle's Hamiltonian. We can write it in a shorter form:

$$\partial_t |\Psi(x_1, x_2, \dots, x_N, t)\rangle = H |\Psi(x_1, x_2, \dots, x_N, t)\rangle, \quad (1.9)$$

where x_i denotes the i -th particle and $H = \sum_{i=1}^N T - \frac{1}{2} \sum_{i,j=1}^N V_{ij}$ is the Hamiltonian. It is convenient to expand the state vector in a set of stationary plane waves:

$$|\Psi(x_1, x_2, \dots, x_N)\rangle = \sum_{E_i} C(E_1, E_2, \dots, E_N, t) |\psi(x_1)\rangle_{E_1} \dots |\psi(x_N)\rangle_{E_N}, \quad (1.10)$$

where E_i represent the complete set of single-particle quantum numbers belonging to x_i . As one can see all the time dependency is in the constant C . By the

orthonormality of the state functions:

$$\sum_{E_i} |C(E_1, E_2, \dots, E_N, t)|^2 = 1. \quad (1.11)$$

We can rewrite this sum according to the fact that in quantum mechanics particles cannot be distinguished.

$$\sum_{E_i} 1 \sum_{n_i} |C(n_1, n_2, \dots, n_N, t)|^2 = 1, \quad (1.12)$$

where n_i represents the number of particles with the set of quantum numbers E_i . The first sum can be computed if we think of it as a combinatoric problem: putting N objects into boxes with n_1 objects in the first box, n_2 objects in the second and so on. Thus:

$$\sum_{E_i} 1 = \frac{N!}{n_1! n_2! \dots n_N!}. \quad (1.13)$$

By defining

$$f(n_1, n_2, \dots, n_N, t) \equiv \left(\frac{N!}{n_1! n_2! \dots n_N!} \right)^{1/2} C(n_1, n_2, \dots, n_N, t) \quad (1.14)$$

we get

$$\sum_{n_i} |f(n_1, n_2, \dots, n_N, t)|^2 = 1, \quad (1.15)$$

thus

$$\begin{aligned} |\Psi(x_1, x_2, \dots, x_N)\rangle &= \sum_{E_i} f(n_1, n_2, \dots, n_N, t) \\ &\quad \sum_{E_i} \left(\frac{n_1! n_2! \dots n_N!}{N!} \right)^{1/2} |\psi(x_1)\rangle_{E_1} \dots |\psi(x_N)\rangle_{E_N}. \end{aligned} \quad (1.16)$$

Let us introduce the time-independent state vectors

$$|n_1 n_2 \dots n_\infty\rangle, \quad (1.17)$$

which satisfy the orthogonality and completeness relations

$$\begin{aligned} \langle n'_1 n'_2 \dots n'_\infty | n_1 n_2 \dots n_\infty \rangle &= \delta_{n_1 n'_1} \delta_{n_2 n'_2} \dots \delta_{n_\infty n'_\infty}, \\ \sum_{n_i} |n_1 n_2 \dots n_\infty \rangle \langle n_1 n_2 \dots n_\infty| &= 1. \end{aligned} \quad (1.18)$$

In this basis, a system, which contains infinitely many quantum states can be written as

$$|\Psi(t)\rangle = \sum_{n_i} f(n_1, n_2, \dots, n_\infty, t) |n_1 n_2 \dots n_\infty\rangle. \quad (1.19)$$

Of course as this new state vector depends only on the number of particles in a given state we need to rewrite the operators so they directly influence the number of particles in a state. These are the so-called stepping operators. For bosons:

$$\begin{aligned} [a_k, a_{k'}^\dagger] &= \delta_{kk'}, \\ [a_k, a_{k'}] &= [a_k^\dagger, a_{k'}^\dagger] = 0, \\ a_k^\dagger a_k |n_k\rangle &= n_k |n_k\rangle, \\ a_k |n_k\rangle &= n_k^{1/2} |n_k - 1\rangle, \\ a_k^\dagger |n_k\rangle &= (1 + n_k)^{1/2} |n_k + 1\rangle. \end{aligned} \quad (1.20)$$

For fermions:

$$\begin{aligned} \{a_k, a_{k'}^\dagger\} &= \delta_{kk'}, \\ \{a_k, a_{k'}\} &= \{a_k^\dagger, a_{k'}^\dagger\} = 0, \\ a_k^\dagger a_k |n_k\rangle &= n_k |n_k\rangle, \\ a_k |n_k\rangle &= n_k^{1/2} |n_k - 1\rangle, \\ a_k^\dagger |n_k\rangle &= (1 + n_k)^{1/2} |n_k + 1\rangle. \end{aligned} \quad (1.21)$$

With stepping operators, or most commonly called creation and annihilation operators, the Hamiltonian takes the form

$$H = \sum_{ij} b_i^\dagger \langle i | T | j \rangle b_j + \frac{1}{2} \sum_{ijkl} b_i^\dagger b_j^\dagger \langle ij | V | kl \rangle b_l b_k, \quad (1.22)$$

where the $|i\rangle$ refers to the state vector in the quantum state i . For convince let us

introduce the linear combination of creation and destruction operators:

$$\phi(x) \equiv \sum_k \psi_k(x) a_k, \quad (1.23)$$

$$\phi(x)^\dagger \equiv \sum_k \psi_k(x) a_k^\dagger, \quad (1.24)$$

these are called field operators. Here the single-particle wave functions are the coefficients and the sum is over the complete set of quantum numbers. They can bare other indexes, for example spin or spinor indexes. As they are made up from stepping operators, one can easily derive the following commutation (anti-commutation) relations:

$$[\phi_\alpha(x), \phi(x')^\dagger_\beta] = \sum_k \psi_k(x)^\dagger_\alpha \psi(x')^\dagger_\beta = \delta_{\alpha\beta} \delta(x - x') \quad (1.25)$$

$$[\phi_\alpha(x), \phi(x')_\beta] = [\phi_\alpha(x)^\dagger, \phi(x')^\dagger_\beta] = 0 \quad (1.26)$$

With the help of the field operators the Hamiltonian can be written as

$$H = \int d^3x \phi(x)^\dagger T(x) \phi(x) + \frac{1}{2} \int \int d^3x d^3x' \phi(x)^\dagger \phi(x')^\dagger V(x, x') \phi(x') \phi(x). \quad (1.27)$$

This is where the name second quantization came from. In first quantization we take an observable from classical mechanics and treat it as an operator. The new quantum mechanical observable is an expectation value of the form $\int d^3x \psi(x) Q \psi(x)^\dagger$, where Q is the operator and $\psi(x)$ is the wave vector. The form of the Hamiltonian above suggests that it is the sum of two expectation values, which would be an observable. But we treat it as an operator, just as we treated the classical mechanical measurable quantity Q as an operator in first quantization. However ϕ here denotes the field operators not the wave functions, thus there are no expectation values! From here we extend this train of thought to any operator and get

$$J = \sum_{ij} \langle i | J | j \rangle a_i^\dagger a_j = \int d^3x \phi(x)^\dagger J(x) \phi(x) \quad (1.28)$$

as the general form of any second quantized operator.

1.3.2 Quantum mechanical pictures and orderings

There are different ways of viewing quantum mechanics. Namely

Schrödinger picture: in this picture the states are time dependent but not the

operators. The equation which describes the time evolution of said states is the Schrödinger equation (throughout we use units in which $\hbar = c = 1$):

$$i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle. \quad (1.29)$$

It can be easily shown that any state at time t can be written as a function of the state at t_0 in the form:

$$|\psi(t)\rangle = \exp(-iH(t - t_0))|\psi(t_0)\rangle. \quad (1.30)$$

Heisenberg picture In this picture the operators are time dependent rather than the states as in the previous one. The equation of time evolution reads:

$$i\partial_t A_H = [A_H, H]. \quad (1.31)$$

There is a connection between the Schrödinger and Heisenberg pictures

$$|\psi_H\rangle = \exp(iHt)|\psi_S\rangle, \quad (1.32)$$

$$A_H = \exp(iHt)A_S \exp(-iHt). \quad (1.33)$$

One can easily see that at time $t = t_0$ the states and operators are the same in both pictures. Furthermore one can show that the expectation values remain the same regardless which picture we use.

Interaction picture: In this picture both the states and the operators are time dependent. The Hamiltonian is separated into two parts ($H = H_0 + H_I$), one part is the well known kinetic part (H_0), the other is the interaction part (H_I). The connection between the interaction and Schrödinger picture is given by the

$$|\psi_I\rangle = \exp(iH_0t)|\psi_S\rangle, \quad (1.34)$$

$$A_I = \exp(iH_0t)A_S \exp(-iH_0t), \quad (1.35)$$

equations. The equations of time evolution are:

$$\partial_t|\psi_I\rangle = H_I|\psi_I\rangle, \quad (1.36)$$

$$i\partial_t A_I = [A_I, H_I]. \quad (1.37)$$

Naturally the expectation values are the same as in the Schrödinger or in

the Heisenberg picture. Furthermore all pictures are the same at $t = t_0$. It can be shown that the time evolution of states can be expressed by a single operator, most commonly referred to as the S matrix,

$$|\psi_I(t)\rangle = S(t, t_0)|\psi_I(t_0)\rangle. \quad (1.38)$$

This operator has the following properties,

$$\begin{aligned} S(t, t) &= 1, \\ S(t_3, t_2)S(t_2, t_1) &= S(t_3, t_1), \\ S(t_1, t_2)S(t_2, t_1) &= 1 \rightarrow S(t_2, t_1) = S(t_1, t_2)^{-1}, \\ S(t_2, t_1) &= S(t_2, t_1)^\dagger \text{ unitarity,} \\ S(t_2, t_1) &= S(t_2)S(t_1). \end{aligned} \quad (1.39)$$

We can also say something of the explicit expression of S if we put it into the state evolution equation.

$$\partial_t S(t, t_0) = H_I S(t, t_0), \quad (1.40)$$

Converting it to an integral equation,

$$S(t, t_0) = 1 - i \int_{t_0}^t H_I(t') S(t', t_0) dt'. \quad (1.41)$$

This is a so-called Volterra equation due to having the independent variable t in the upper limit of the integral. In some special cases with the right assumptions it can be solved by iteration; we assume we can do this.

$$S(t, t_0) = \sum_{n=0}^{\infty} \frac{-i^n}{n!} \int_{t_0}^{t_1} \dots \int_{t_0}^t dt_n T[H_I(t_1) \dots H_I(t_n)] \quad (1.42)$$

where the operator T is the time ordering operator, which ensures casualty.

$$T(H(t_4)H(t_1)H(t_2)H(t_3)) = H(t_1)H(t_2)H(t_3)H(t_4), \quad (1.43)$$

if $t_1 < t_2 < t_3 < t_4$.

Furthermore it can be shown with an adiabatic interaction Hamiltonian, that the interacting system's state vector at t can be calculated as:

$$|\psi_I(t)\rangle = S(t, -\infty)|\psi_0\rangle, \quad (1.44)$$

where $|\psi_0\rangle$ is the ground state of the non-interacting system. Adiabatic means at infinite distances the interaction is turned off; as they approach each other at time $-T$ the interaction is turned on; after the scattering process as they go to infinity and at time T the interaction is turned off. Thus

$$|\psi_I(\infty)\rangle = S(\infty, -\infty)|\psi_0\rangle. \quad (1.45)$$

1.4 Particle physics and quantum field theory

In the previous section we have seen that one can redefine the quantum mechanical many body problem with a procedure called second quantization. Furthermore one can write the state vector in the interaction picture at any time as a function of the non-interacting state vector. The two states are connected by the S matrix, which can be written as a series of the Hamiltonian.

So far we have spoken generally and have not paid any attention to the interactions' nature. In this subsection we will see how can one describe particle physics with the help of field theory. This is nothing else but constructing the right Lagrangian.

1.4.1 Field equation

Field theory got its name from the fact that we use field operators. These can be interpreted as collections of infinitely many harmonic oscillators, one (or possibly several) at every space time point, and with the creation and annihilation operators we excite some of them. Even in this picture we do not abandon the law of minimal action. With the standard derivation one finds the Euler-Lagrange equations and the Hamiltonian for fields to be:

$$\frac{\partial \mathcal{L}}{\partial \phi_i} - \frac{\partial}{\partial x^\alpha} \left(\frac{\partial \mathcal{L}}{\partial \phi_{i,\alpha}} \right) = 0, \quad i = 1, 2, \dots, N \quad (1.46)$$

$$\mathcal{H} = \frac{\partial \mathcal{L}}{\partial \phi_{i,0}} \phi_{i,0} - \mathcal{L}, \quad (1.47)$$

where we used four vectors $x^\alpha = (x^0, x^1, x^2, x^3)$ and $\partial \phi_{i,\alpha} = \partial \phi_i / \partial x^\alpha$. Furthermore $\mathcal{L}$ and $\mathcal{H}$ are called Lagrangian and Hamiltonian density

$$L = \int_V d^4x \mathcal{L} \quad (1.48)$$

$$H = \int_V d^4x \mathcal{H}, \quad (1.49)$$

however in the English literature they often call it simply Lagrangian and Hamiltonian.

1.4.2 Symmetries

Through observing our surrounding we can deduce the fact that symmetries exist in nature. For example in classical mechanics we have time reversal, translational and rotational symmetries.

Symmetries can be discrete or continuous, for example parity transformation is discrete, while translational symmetry is continuous; the latter can be global or local. Local means we can choose the parameters of the transformation independently at any space-time point.

Global symmetries lead to conserved quantities, as Noether's theorem states:

if the Lie group G is a symmetry of the system, then there is a conserved physical quantity belonging to each generator of G .

Local symmetries lead to interactions for example:

- $U(1) \rightarrow$ electromagnetic force,
- $SU(3) \rightarrow$ strong force.

1.5 Fundamental fields

To describe an interacting field, first we must describe a non-interacting one, thus we need the equation of motion of the field. This equation can be derived from symmetries though they were first derived from other principles or just simply guessed.

For relativistic neutral scalar fields, for example π^0 s, we need the Klein-Gordon equation:

$$(\partial_\mu \partial^\mu + m^2)\phi = 0; \tag{1.50}$$

its corresponding Lagrangian is:

$$\mathcal{L} = \frac{1}{2} \partial_\mu \phi \partial^\mu \phi - \frac{1}{2} m^2 \phi^2. \tag{1.51}$$

For relativistic non-scalar particles, for instance electron and protons, we have the Dirac equation:

$$(i\gamma^\mu \partial_\mu - m)\phi = 0, \tag{1.52}$$

where γ^μ are the Dirac matrices, they are the only four 4x4 linearly independent matrices. Its corresponding Lagrangian is:

$$\mathcal{L} = \bar{\phi}(i\gamma^\mu\partial_\mu - m)\phi, \quad (1.53)$$

where $\bar{\phi} = \phi^\dagger\gamma^0$ is the adjoint of ϕ .

These all describe particles moving in space-time interacting with nothing.

1.5.1 Quantum electrodynamics

As stated earlier the local U(1) symmetry causes the electromagnetic interaction. It is due to the fact that, if we want a field equation to be invariant under the same symmetry both globally and locally we need the derivative of the field to transform as the field itself. To achieve this we need to introduce a new vector field.

So for example the Dirac equation is invariant under the global U(1) symmetry

$$\phi \rightarrow \phi' = \phi \exp(-i\alpha), \quad (1.54)$$

$$\bar{\phi} \rightarrow \bar{\phi}' = \bar{\phi} \exp(i\alpha), \quad (1.55)$$

where α is just a constant. We get the conserved current and charge:

$$j^\mu = q\bar{\phi}(x)\gamma^\mu\phi(x), \quad (1.56)$$

$$q = \int d^3x \phi^\dagger(x)\phi(x). \quad (1.57)$$

Furthermore if we want more and require invariance under local U(1) transformation:

$$\phi \rightarrow \phi' = \phi \exp(-iqf(x)), \quad (1.58)$$

$$\bar{\phi} \rightarrow \bar{\phi}' = \bar{\phi} \exp(iqf(x)), \quad (1.59)$$

we find that the Lagrangian will be invariant only if we introduce the covariant derivative:

$$D_\mu\phi = (\partial_\mu + iqA_\mu(x))\phi(x). \quad (1.60)$$

The Lagrangian will take the form:

$$\begin{aligned}\mathcal{L} &= \bar{\phi}(x)(i\gamma^\mu D_\mu - m)\phi = \\ &= \bar{\phi}(x)(i\gamma^\mu \partial_\mu - m)\phi - q\bar{\phi}\gamma^\mu \phi A_\mu(x).\end{aligned}\tag{1.61}$$

We can interpret the terms as the first one is the non-interacting while the second one is the interaction Lagrangian. Of course the new field should have its own kinetic term in the Lagrangian, thus the full QED Lagrangian is:

$$\mathcal{L} = \bar{\phi}(i\gamma^\mu \partial_\mu - m)\phi + ej^\mu A_\mu - \frac{1}{4}F^{\mu\nu}F_{\mu\nu},\tag{1.62}$$

where the last term is the aforementioned kinetic term of the vector field, and $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$.

1.5.2 Quantum chromodynamics

To explain the inner structure of the proton physicist introduced the quark model, though it was not fully satisfactory and had some contradictions with experiment. To resolve these they added an additional charge, called colour to the theory.

To summarize, we have six quarks u, d, c, s, t, b and three colours, red, blue and green. All quarks carry colour charges, but only particles that do not have an overall colour charge (i.e., carry all three colour charges at once or carry a colour charge as well as the corresponding anti-colour charge) can be directly observed. In this case the aforementioned object's colour is white.

White objects can be made up from a quark-antiquark pair or from three quarks.

The corresponding symmetry is SU(3). It is a non-Abelian symmetry because its generators are not commuting:

$$[F_i, F_j] = if_{ijk}F_k,\tag{1.63}$$

where f_{ijk} is the structure constant. The free quark Lagrangian is just the Dirac Lagrangian with colours:

$$\mathcal{L} = \bar{\phi}_r^f(i\gamma^\mu \partial_\mu - m)\phi_r^f + \bar{\phi}_g^f(i\gamma^\mu \partial_\mu - m)\phi_g^f + \bar{\phi}_b^f(i\gamma^\mu \partial_\mu - m)\phi_b^f,\tag{1.64}$$

where the lower index is the colour and the upper is the flavour ($f = u, d, c, s, t, b$).

This is invariant under the transformation:

$$\phi^f \rightarrow \phi^{f'} = \exp\left(\frac{i}{2}\alpha_i\lambda_i\right)\alpha_i\lambda_i\phi^f, \quad (1.65)$$

$$\bar{\phi}^f \rightarrow \bar{\phi}^{f'} = \bar{\phi}^f \exp\left(-\frac{i}{2}\alpha_i\lambda_i\right)\alpha_i\lambda_i, \quad (1.66)$$

where $i = (1, \dots, 8)$, α_i is an arbitrary real number and λ_i represents the eight linearly independent 3×3 matrices. The conserved current and charge are:

$$s_i^\mu = \frac{1}{2}\bar{\phi}^f(x)\gamma^\mu\phi^f(x), \quad (1.67)$$

$$F_i = \frac{1}{2}\int d^3x \bar{\phi}^{f\dagger}(x)\phi^f(x) \quad (1.68)$$

It is important to note, that only F_3 and F_8 commute and there are three colour singlet states which are eigenvalues for both operators. The other ones change the colour of the state which they are acting upon.

Demanding the Lagrangian to be invariant under the local SU(3) symmetry means that it should not change under the following transformation of fields:

$$\phi^f \rightarrow \phi^{f'} = \exp\left(\frac{i}{2}\alpha_i\lambda_i\omega_j(x)\right)\alpha_i\lambda_i\omega_j(x)\phi^f, \quad (1.69)$$

$$\bar{\phi}^f \rightarrow \bar{\phi}^{f'} = \bar{\phi}^f\alpha_i\lambda_i\omega_j(x), \quad (1.70)$$

where $\omega_j(x)$ is an arbitrary function. This criterion can be achieved by the introduction of the covariant derivative in the form of

$$D^\mu\phi^f(x) = \left(\partial^\mu + \frac{i}{2}g_s\lambda_iA_i^\mu\right)g_s\lambda_iA_i^\mu\phi^f. \quad (1.71)$$

Of course these A_i vector fields need their own free Lagrangian, thus the whole QCD Lagrangian is:

$$\begin{aligned} \mathcal{L} = & \bar{\phi}_r^f(i\gamma^\mu\partial_\mu - m)\phi_r^f + \bar{\phi}_g^f(i\gamma^\mu\partial_\mu - m)\phi_g^f + \bar{\phi}_b^f(i\gamma^\mu\partial_\mu - m)\phi_b^f \\ & - \frac{1}{2}g_s s_i^\mu A_{i\mu}(x) - \frac{1}{4}G_{i\mu\nu}(x)G_i^{\mu\nu}(x), \end{aligned} \quad (1.72)$$

where $G_i^{\mu\nu}(x) = F_i^{\mu\nu} + g_s f_{ijk}A_j^\mu A_k^\nu$.

1.6 CoLoRFulNNLO

As it was stated above, if we have the proper Lagrangian we can compute an approximation of the interacting system, which can be refined order by order. Though difficulties arose along the way. For example expanding the S matrix, we got a complicated and long expression, from which we have to gather the terms corresponding to physical processes. Additionally the model also has shortcomings, which result in divergent integrals.

These problems were solved by different mathematical tools, developed in the second half of the XX. century. Nowadays to get the amplitudes we use Feynman diagrams. This pictorial method enables us to first sketch a graphical representation of the physical processes then translate those to mathematical expressions.

When we integrate our expressions to all energies, including very high and very low frequencies, divergences surface; these are labeled Ultra Violent (UV) and Infra Red (IR) respectively. These are managed by mathematical methods called regularization and renormalization. First, regularization is used to give a precise meaning to infinite quantities so they can be manipulated consistently in intermediate stages of the calculation. There are numerous regularization schemes, in this work I use dimensional regularization. This means we calculate everything in $d = 4 - 2\varepsilon$ dimensions, then at the very end, take the limit $\varepsilon \rightarrow 0$. After this, renormalization takes care of the UV singularities, which appear due to the fact that in our equations we use the bare particles' properties (e.g. mass or charge) and not the actual physical ones. Finally, IR singularities cancel between the so-called real emission and virtual corrections for properly defined, so-called IR and collinear-safe, physical quantities. However, these singularities must still be handled in a consistent way before actual computations can be performed. One option is to 'reshuffle' the infinities between real emission and virtual corrections in a way that we get a finite result for both. This approach is called subtraction, because divergences are subtracted from real emission contributions and then added back to virtual ones in an integrated form.

In recent years, physicist have used different subtraction schemes to overcome the difficulties related to IR divergences. For this work I have used CoLoR-FulNNLO, this scheme was described in full detail in [8–10]. Here I just present the necessary parts, which are essential to understand my work.

1.6.1 Notation

Let us consider a generic cross section, which produces m jets. Due to asymptotic freedom at 'high' energies the strong coupling constant becomes small enough to

do a power expansion.

$$\sigma_m = \alpha_S^p(\mu)(\sigma_m^{LO} + \alpha_S(\mu)\sigma_m^{NLO} + \alpha_S^2(\mu)\sigma_m^{NNLO}) \quad (1.73)$$

We can write the differential cross section as:

$$d\sigma_n = d\phi_n(p_1, \dots, p_n; Q) |\mathcal{M}(p_1, \dots, p_n)|^2, \quad (1.74)$$

where $d\phi_n$ is the space phase measure

$$d\phi_n(p_1, \dots, p_n; Q) = \prod_{i=1}^n \frac{d^d p_i}{(2\pi)^d - 1} \delta_+(p_i^2) (2\pi)^d \delta^{(d)}\left(\sum_{i=1}^n p_i - Q\right), \quad (1.75)$$

Q is the energy of the collision and $|\mathcal{M}(p_1, \dots, p_n)|^2$ is the squared matrix element.

We can write the NNLO cross section as:

$$\sigma_m^{NNLO} = \int_{m+2} d\sigma_{m+2}^{RR} J_{m+2} + \int_{m+1} d\sigma_{m+1}^{RV} J_{m+1} + \int_m d\sigma_m^{RR} J_m, \quad (1.76)$$

where J_n denotes the jet function that defines the observable we are interested in.

My work focused on the QCD+QED doubly-real emission's infra red part for the process $e^+e^- \rightarrow b\bar{b}$. This means I treated those cases when there are two additional particles in the final state, namely an extra photon and an extra gluon in addition to the bottom quark-antiquark pair. Singularities arose because these new particles can be soft, collinear or both at the same time.

Soft means, it has such a low energy we cannot detect it in measurements. But it is still there, thus we must account for it. Collinear means, it becomes collinear with a detected particle. Again, in our data we see no new particle, due to the finite angular resolution of the detectors, but it might be still there.

1.6.2 Factorization formulae

The structure of these unresolved emissions are the same in QCD for every process. This means, to get the squared NNLO matrix elements in the appropriate limits, we just need to multiply the NLO matrix element with a function, which depends on the kinematics. These splitting functions are known for NNLO accuracy [11]. For me two had significance:

the Altarelli-Parisi splitting kernel:

$$\langle s | \hat{P}_{qg}^{(0)}(z_i, z_r, k_\perp) | s' \rangle = C_F \left(\frac{1+z_i^2}{1-z_i} - \varepsilon(1-z_i) \right) \delta_{ss'}. \quad (1.77)$$

Where I used the Sudakov parametrization:

$$p_i^\mu = z_i p^\mu + k_\perp^\mu - \frac{k_\perp^2 n^\mu}{z_i(2np)}, \quad (1.78)$$

$$p_r^\mu = (1 - z_i) p^\mu - k_\perp^\mu - \frac{k_\perp^2 n^\mu}{(1 - z_i)(2np)}, \quad (1.79)$$

with $p^2 = n^2 = 0$ and $pk_\perp = nk_\perp = 0$. The limit manifests itself by substituting $k_\perp = \lambda k_\perp$ and taking the limit $\lambda \rightarrow 0$.

We can write the matrix element in collinear limit as

$$\mathbf{C}_{ir} |\mathcal{M}_{n+1}^{(0)}(p_i, p_r, \dots)|^2 = 8\pi\alpha_S \mu^{2\varepsilon} \frac{1}{s_{ir}} \hat{P}_{qg}^{(0)}(z_i, z_r, k_\perp) \otimes |\mathcal{M}_n^{(0)}(p_{(ir)}, \dots)|^2, \quad (1.80)$$

where $s_{ik} \equiv 2p_i p_k$.

the Eikonal function:

$$\mathcal{S}_{ik}(r) = \frac{2s_{ik}}{s_{ir}s_{kr}}, \quad (1.81)$$

where $s_{ik} \equiv 2p_i p_k$, the same as before.

We can write the matrix element in soft limit as

$$\mathbf{S}_r |\mathcal{M}_{n+1}^{(0)}(p_i, p_r, \dots)|^2 = -8\pi\alpha_S \mu^{2\varepsilon} \sum_i \sum_{k \neq i} \frac{1}{2} \mathcal{S}_{ik}(r) \otimes |\mathcal{M}_{n,(i,k)}^{(0)}(\cancel{p_r}, \dots)|^2, \quad (1.82)$$

1.6.3 Subtraction terms

We have multiple possibilities of one or more particle going unresolved.

A1: There is a chance that only one particle becomes undetectable. In our case:

- i) the gluon or the photon is soft,
- ii) the photon is collinear with the electron or positron,

But there is an overlap between the cases. There is a non zero probability of the photon being collinear with the positron or electron while it is also soft. We need to subtract it, otherwise we would count this instance twice. Thus we can write:

$$\mathbf{A}_1 |\mathcal{M}_{m+2}^{(0)}|^2 = (\mathbf{C}_{16} + \mathbf{C}_{26}\mathbf{S}_5 + \mathbf{C}_6 - \mathbf{C}_{16}\mathbf{S}_6 - \mathbf{C}_{26}\mathbf{S}_6) |\mathcal{M}_{m+2}^{(0)}|^2. \quad (1.83)$$

Note that because the bottom quark and antiquark is treated as massive in our calculation, collinear gluon emission does not lead to a singularity.

A2 Of course we have the case when both the gluon and photon becomes unresolved:

- i) the photon is collinear with the electron or positron while the gluon is soft,
- ii) both the photon and gluon is soft.

So we have:

$$\mathbf{A}_2 |\mathcal{M}_{m+2}^{(0)}|^2 = (\mathbf{C}_{16}\mathbf{S}_5 + \mathbf{C}_{26}\mathbf{S}_5 + \mathbf{S}_{56} - \mathbf{C}_{16}\mathbf{S}_5\mathbf{S}_{56} - \mathbf{C}_{26}\mathbf{S}_5\mathbf{S}_{56}) |\mathcal{M}_{m+2}^{(0)}|^2, \quad (1.84)$$

where the last two terms are the overlap terms.

A12 But there is overlap (**A12**) between the **A1** and **A2** singularities as well, which we have to subtract. We can get this multiplying the **A2** operator with the **A1**. We will get quite a few terms, from which we have to root out the non-physical ones. For example those, where the photon would be collinear with both the electron and positron. After these computations, we get:

$$\begin{aligned} \mathbf{A}_{12} |\mathcal{M}_{m+2}^{(0)}|^2 = & \left((\mathbf{C}_{16})\mathbf{C}_{16}\mathbf{S}_5 + (\mathbf{C}_{16})\mathbf{S}_{56} + (-\mathbf{C}_{16}\mathbf{S}_6)\mathbf{S}_{56} + \right. \\ & (\mathbf{C}_{16})(-\mathbf{C}_{16}\mathbf{S}_5\mathbf{S}_{56}) + (-\mathbf{C}_{16}\mathbf{S}_6)\mathbf{C}_{16}\mathbf{S}_5 + \\ & (-\mathbf{C}_{16}\mathbf{S}_6)(-\mathbf{C}_{16}\mathbf{S}_5\mathbf{S}_{56}) + \\ & (\mathbf{C}_{26})\mathbf{C}_{26}\mathbf{S}_5 + (\mathbf{C}_{26})\mathbf{S}_{56} + (-\mathbf{C}_{26}\mathbf{S}_6)\mathbf{S}_{56} + \\ & (\mathbf{C}_{26})(-\mathbf{C}_{26}\mathbf{S}_5\mathbf{S}_{56}) + (-\mathbf{C}_{26}\mathbf{S}_6)\mathbf{C}_{26}\mathbf{S}_5 + \\ & (-\mathbf{C}_{26}\mathbf{S}_6)(-\mathbf{C}_{26}\mathbf{S}_5\mathbf{S}_{56}) + \\ & (\mathbf{S}_5)\mathbf{C}_{16}\mathbf{S}_5 + (\mathbf{S}_5)(-\mathbf{C}_{16}\mathbf{S}_5\mathbf{S}_{56}) + (\mathbf{S}_5)\mathbf{S}_{56} + \\ & (\mathbf{S}_5)\mathbf{C}_{26}\mathbf{S}_5 + (\mathbf{S}_5)(-\mathbf{C}_{26}\mathbf{S}_5\mathbf{S}_{56}) + \\ & (\mathbf{S}_6)\mathbf{C}_{16}\mathbf{S}_5 + (\mathbf{S}_6)(-\mathbf{C}_{16}\mathbf{S}_5\mathbf{S}_{56}) + (\mathbf{S}_6)\mathbf{S}_{56} + \\ & \left. (\mathbf{S}_6)\mathbf{C}_{26}\mathbf{S}_5 + (\mathbf{S}_6)(-\mathbf{C}_{26}\mathbf{S}_5\mathbf{S}_{56}) \right) |\mathcal{M}_{m+2}^{(0)}|^2. \end{aligned} \quad (1.85)$$

Hence the whole subtraction in shorthand notation reads:

$$\mathbf{A} |\mathcal{M}_{m+2}^{(0)}|^2 = (\mathbf{A}_1 + \mathbf{A}_2 - \mathbf{A}_{12}) |\mathcal{M}_{m+2}^{(0)}|^2. \quad (1.86)$$

1.7 Momentum mapping

Though these formulas give us the the right matrix elements and subtraction terms, the matrix elements on the right and left hand side of these equations depend on different kinematic variables. Thus we need to map the left hand side variables to the right hand side in such a delicate way, that we do not violate momentum conservation, and the mass-shell conditions.

I present two kind of mappings; the ones, which take us from a configuration with 5 momenta to one with only 4 momenta ($5 \rightarrow 4$), and the other one which takes us from a configuration with 6 momenta to one with only 5 momenta ($6 \rightarrow 5$). We get the $6 \rightarrow 4$ mapping by applying the $6 \rightarrow 5$ and then the $5 \rightarrow 4$ mapping consecutively. These mappings were also used in [12].

1.7.1 Soft mapping NLO

In this case we want to map the momenta $(p_1, p_2, p_3, p_4, p_5)$ to $(\hat{p}_1, \hat{p}_2, \hat{p}_3, \hat{p}_4)$. We can do this with the mapping:

$$\hat{p}_3 = \Lambda_\nu^\mu(\hat{K}, K) \frac{1}{\Delta} (p_3^\mu - \gamma_1 p_5^\mu) \quad (1.87)$$

$$\hat{p}_4 = \Lambda_\nu^\mu(\hat{K}, K) \frac{1}{\Delta} (p_4^\mu - \gamma_2 p_5^\mu), \quad (1.88)$$

where

$$\Delta = \sqrt{1 - \frac{s_{35}s_{45}s_{5Q}}{Q^2 s_{35}s_{45} - m_b^2 s_{5Q}^2}}, \quad (1.89)$$

and

$$\gamma_1 = \frac{m_b^2 s_{45}s_{5Q}}{Q^2 s_{35}s_{45} - m_b^2 s_{5Q}^2}; \quad \gamma_2 = \frac{m_b^2 s_{45}s_{5Q}}{Q^2 s_{35}s_{45} - m_b^2 s_{5Q}^2}. \quad (1.90)$$

One can make sure that with these definitions we have $\hat{p}_1^2 = \hat{p}_2^2 = m_b^2$ and $\hat{K}^2 = K^2$, where

$$K^\mu = Q^\mu, \quad \hat{K}^\mu = \frac{1}{\Delta} (p_1^\mu + p_2^\mu - (\gamma_1 + \gamma_2) p_3^\mu). \quad (1.91)$$

Furthermore we have the proper Lorentz transformation:

$$\Lambda_\nu^\mu(K, \hat{K}) = g_\nu^\mu - \frac{2(K + \hat{K})^\mu (K + \hat{K})_\nu}{(K + \hat{K})^2} + \frac{2\hat{K}^\mu K_\nu}{K^2}. \quad (1.92)$$

1.7.2 Soft mapping NNLO

Now let us examine the NNLO case, we want to map the momentums $(p_1, p_2, p_3, p_4, p_5, p_6)$ to $(\hat{p}_1, \hat{p}_2, \hat{p}_4, \hat{p}_5, \hat{p}_{56})$, such that $\hat{p}_1^2 = \hat{p}_2^2 = m_b^2$ and $\hat{p}_{56}^2 = 0$.

$$\hat{p}_{56} = \frac{1}{\beta}(p_5^\mu + p_6^\mu - \alpha Q^\mu), \quad (1.93)$$

$$\hat{p}_n = \Lambda_\nu^\mu(K, \hat{K})p_n^\nu, \quad n = 1, 2, \quad (1.94)$$

where

$$\alpha = \frac{1}{2} \left[y_{(56)Q} - \sqrt{y_{(56)Q}^2 - 4y_{56}} \right], \quad \beta = \frac{\sqrt{y_{(56)Q}^2 - 4y_{56}} \sqrt{y_{(56)Q}^2 - 4y_{56}}}{y_{(56)Q} - y_{56}}, \quad (1.95)$$

and $y_{(56)Q} = y_{5Q} + y_{6Q}$, additional to $y_{ar} = \frac{2p_a p_r}{Q^2}$. Λ has the same definition as before, but now with:

$$K^\mu = Q^\mu - p_5^\mu - p_6^\mu, \quad \hat{K}^\mu = Q^\mu - \hat{p}_{56}^\mu. \quad (1.96)$$

1.7.3 Initial-final collinear mapping NNLO

For this mapping it is convenient to leave the momentum of the observing initial state parton's momentum unchanged, furthermore for further convince let us define the momentum of the new parton ($\hat{p}_{ar}$) to be parallel with the original momentum (p_a^μ). Thus

$$\hat{p}_{ar}^\mu = x_a p_a^\mu, \quad \hat{p}_n^\mu \Lambda(K, \hat{K})_\nu^\mu p_n^\nu, \quad n \neq a, b, r, \quad (1.97)$$

where Λ has the same definition as before with

$$K = Q - p_r, \quad \hat{K} = Q - (1 - x_a)p_a. \quad (1.98)$$

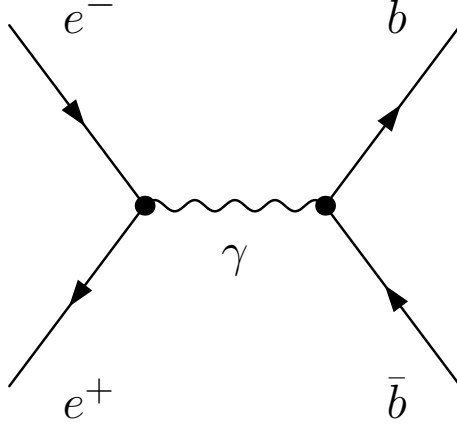
This transformation is a Lorentz transformation only, when $K^2 = \hat{K}^2$. Using this condition we can compute x_a ,

$$x_a = 1 - \frac{p_r Q}{p_a Q}. \quad (1.99)$$

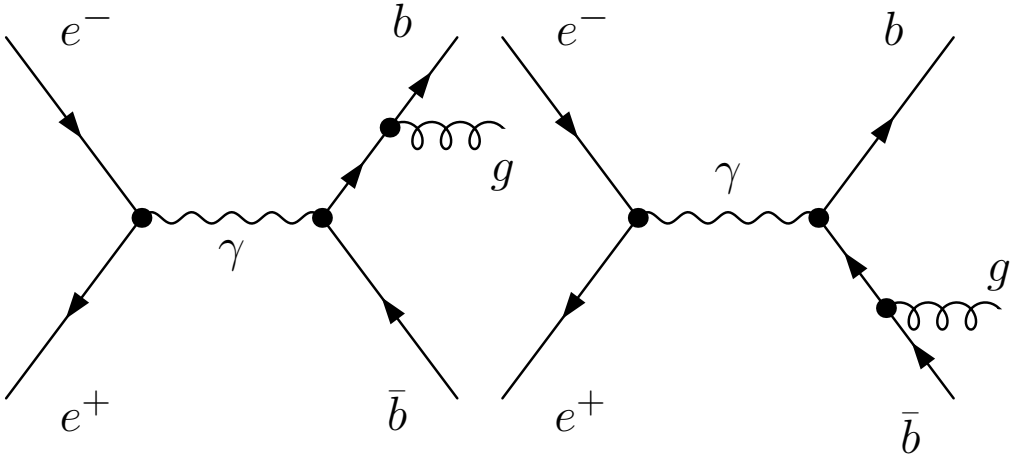
2 Calculations

2.1 Matrix elements

For NNLO cross sections the calculation of the matrix elements require great computational effort, since there can be dozens of Feynman diagrams. In my case there were ten, as one can see on Figures 1, 2, 3. That means I needed to calculate 2×100 traces, for convenience I automatized the process. I have used the Wolfram Mathematica language and the pre-made package Tracer for handling the Dirac algebra. Of course there exist packages even for Mathematica, which do the exact same thing; though my goal was rather educational than scientific. Nevertheless, I managed to make a significantly faster program than FeynCalc [13–15].



(a) Feynman diagram for the $e^-e^+ \rightarrow b\bar{b}$ process.



(b) Feynman diagrams for the $e^-e^+ \rightarrow b\bar{b}g$ process.

Figure 1

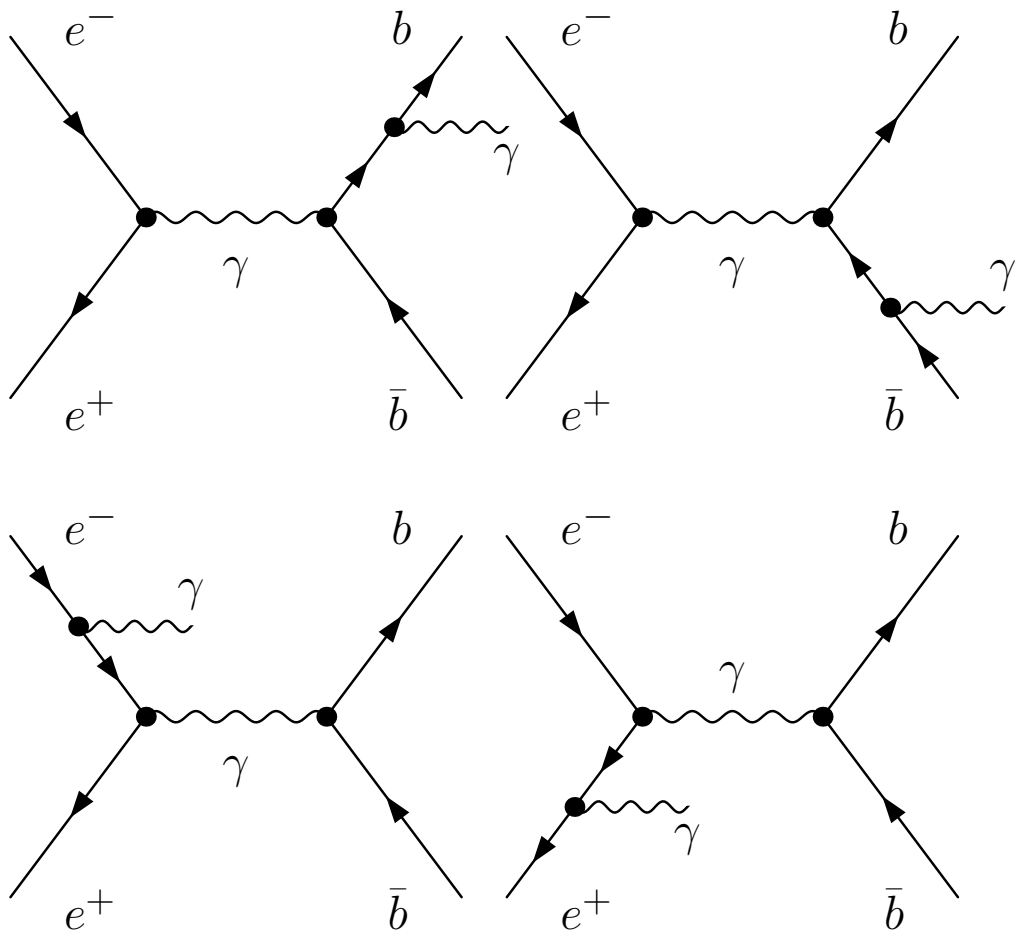
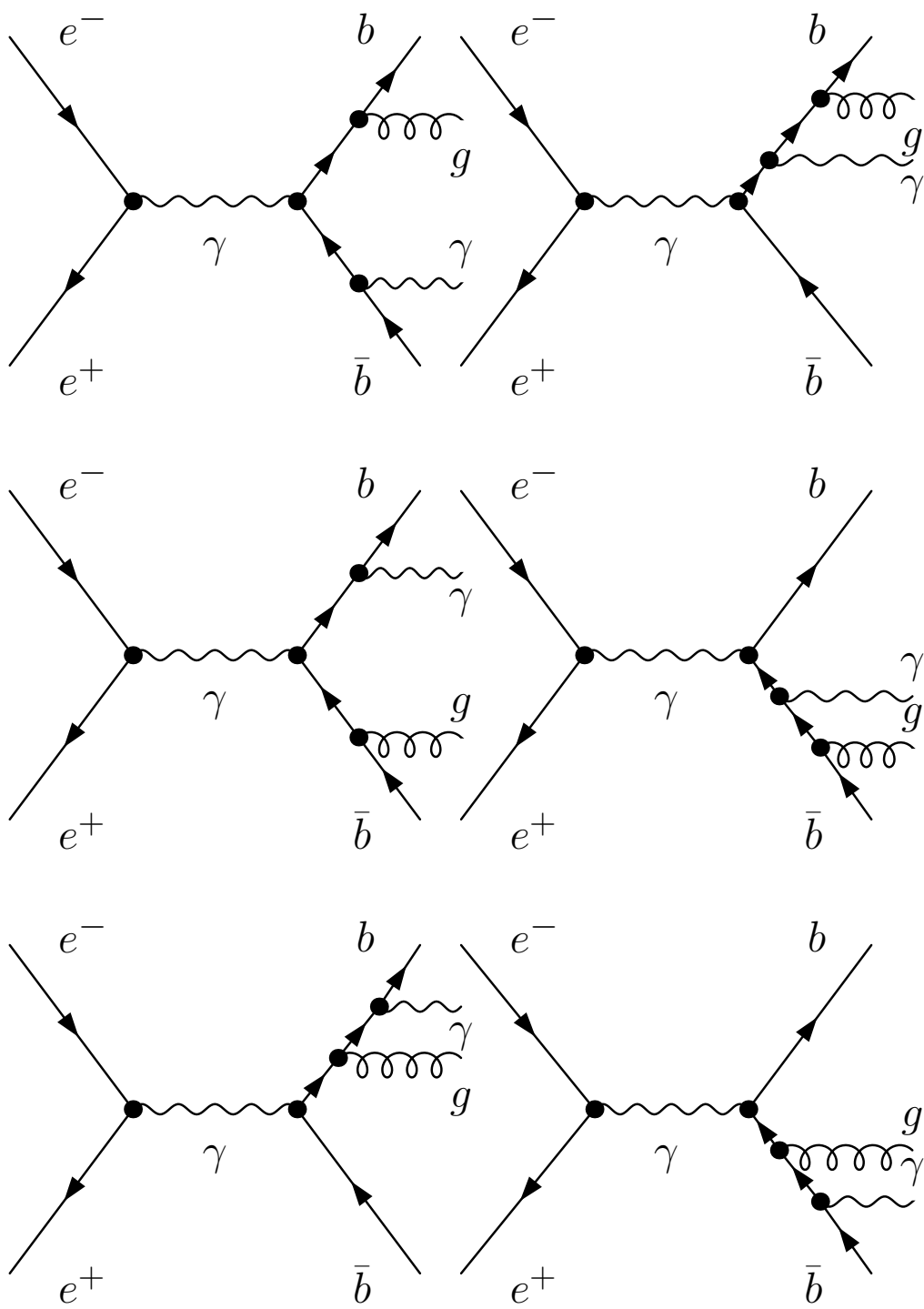


Figure 2: Feynman diagrams for the $e^- e^+ \rightarrow b \bar{b} \gamma$ process.



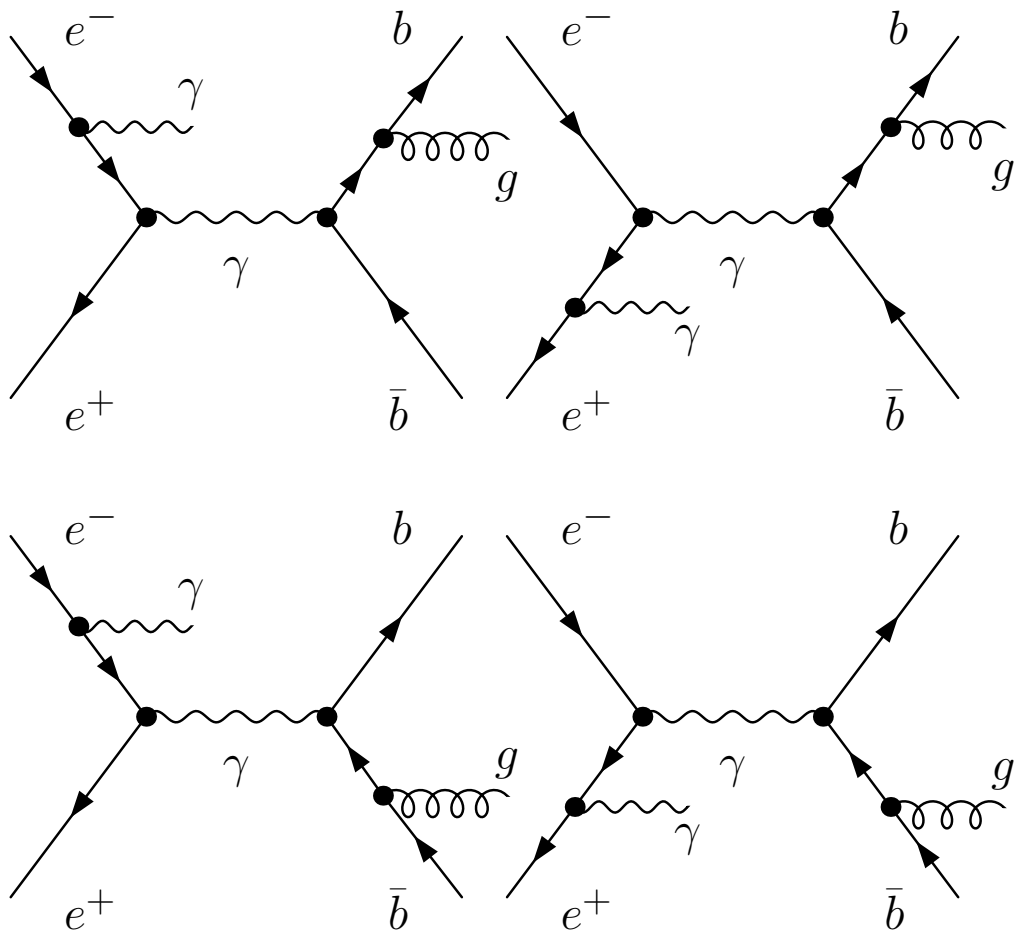


Figure 3: Feynman diagrams for the $e^- e^+ \rightarrow b \bar{b} \gamma g$ process.

2.1.1 Own program

My program only needs minimal user input and can be extended easily. In my following explanation I will take the $e^-e^+ \rightarrow b\bar{b}g$ calculation as an example.

The program's main objects are lists. First the user has to create an appropriate list for the objects. There are two types of objects:

1. particles;

```
{type, mass, wave function, spin index, momentum}
```

2. not particles; eg. vertex factors

```
{type, index, vertex factor}
```

or propagators

```
{type, factor}
```

The only exception is the photon propagator as it is a list formed by the denominator of the photon propagators from different diagrams;

```
{denominator of the photon propagator from diagram no.1,  
denominator of the photon propagator from diagram no.2, ...}
```

The user has to declare the particle and non-particle objects, eg.:

```
Particles={e, q}  
NotParticles={g, p}
```

The user also has to put the particles on shell and introduce the Mandelstam variables. It is all done by the command *OnShell* from the Tracer package.

After all these, one has to 'sketch' the Feynman-diagrams, for example in the case of a single tree diagram:

```
Amplitudes1 =  
{outgoing particle no.3, vertex no.2, outgoingparticle no.4,  
incoming particle no.2, vertex no.1, incoming particle no.1}.
```

Any other things are taken care of by the program. So to sum up, the user needs to

1. declare the particles one-by-one,
2. declare the particle and non-particle types,
3. ‘sketch’ the Feynman-diagrams.

2.1.2 Example

First I declare the particles:

```
r1 = {e, me, bu, r, p1};
r2 = {e, -me, bv, r, p2};
r3 = {q, mq, u, s, p3};
r4 = {q, -mq, v, s, p4};
```

Then I define the quark propagators, along with the list of the photon propagators’ denominators:

```
FotonProps = {s12, s12};
QuarkProp1 = {p, (p3 + p5 + mq U)/s35};
QuarkProp2 = {p, (-p4 - p5 + mq U)/s45};
```

After this the vertices and object types:

```
v1 = {g, alpha, e};
v2 = {g, alpha, eq};
v3 = {g, delta, gs};
v4e = {g, mu, e};(*Photon from electron.*)
v4q = {g, mu, eq};(*Photon from quark.*)

(* Storing of particle and notparticle types. *)
Particles = {e, q};
NotParticles = {g, p};
```

We need the Mandelstam variables as well:

```
(* Restrictions. *)
OnShell[on, {p1, 0}, {p2, 0}, {p3, mq^2}, {p4, mq^2}, {p5, 0}, {p1,
p2, s12/2}, {p1, p3, s13/2}, {p1, p4, s14/2}, {p1, p5, s15/2}, {p2,
p3, s23/2}, {p2, p4, s24/2}, {p2, p5, s25/2}, {p3, p4,
s34/2}, {p3, p5, s35/2}, {p4, p5, s45/2}];
```

Next I sketch the Feynman diagrams and calculate their amplitudes:

```
(* Calculation of the amplitudes. *)
NumberOfDiagrams = 2;
sol = {};
alltraces = {};

(* Defining the amplitudes, read from the feynman diagrams.*)
Amplitude1 = {r3, v3, QuarkProp1, v2, r4, r2, v1, r1};
Amplitude2 = {r3, v2, QuarkProp2, v3, r4, r2, v1, r1};

(* Calculation of the conjugate amplitudes*)
ConjugateAmplitude1 = Reverse[Amplitude1] //. alpha -> nu;
ConjugateAmplitude2 = Reverse[Amplitude2] //. alpha -> nu;

(* Making a list from these for calculating the squaredamplitudes.*)
Amplitudes = {Amplitude1, Amplitude2};
ConjugateAmplitudes = {ConjugateAmplitude1, ConjugateAmplitude2};
```

This is all the input which was needed. We can run the program, which will give us the amplitude. The only drawback of my program is that, it does not really care about the constant factors. Thus one is forced to manually add the colour factors and minus signs coming from the real emissions' spin sums.

2.1.3 FeynCalc

For verifying purposes, I have also calculated all of the matrix elements with FeynCalc. Here I briefly summarize the verbatim on the same example.

First we need to draw the diagrams with FeynArts:

```
DiagramEEtoBBGluon =
InsertFields[
CreateTopologies[0,
2 -> 3], {F[2, {1}], -F[2, {1}]} -> {F[4, {3}], -F[4, {3}], V[5]},
InsertionLevel -> {Classes}, Model -> "SMQCD",
ExcludeParticles -> {S[_], V[2]}];
```

Then FeynCalc applies the Feynman rules. A quick note, for some reason FeynCalc writes the propagators' denominator with final state momenta, which causes

the final expressions to be longer than necessary, as the program cannot simplify. Thus we need to manually change them with the help of energy conservation.

```
AmpEEtoBBGluon =
FC_FACConvert[CreateFeynAmp[DiagramEEtoBBGluon],
IncomingMomenta -> {p1, p2}, OutgoingMomenta -> {p3, p4, p5},
UndoChiralSplittings -> True, ChangeDimension -> D, List -> False,
SMP -> True, Contract -> True, DropSumOver -> True,
FinalSubstitutions -> {SMP["m_b"] -> SMP["m_q"]}];

AmpEEtoBBGluon = AmpEEtoBBGluon /. {
Plus[p3, p4, p5] -> Plus[p1, p2],
SMP["m_e"] -> 0}
```

We need to change to the Mandelstam variables. Unfortunately, the original FeynCalc function, which would do this, has a bug. So I wrote my own:

```
ToMandelstam[momentas_, masses_] :=
Block[
{},
ToMandelstam::error =
"The two given lists are not the same size. Momentas: '1', Masses: \
'2'.";

If[ Length[momentas] != Length[masses],
Message[ToMandelstam::error, Length[momentas] , Length[masses]]];

Table[
Table [
If[i == j,

ScalarProduct[momentas[[i]], momentas[[j]]] = masses[[i]]^2
,

ScalarProduct[momentas[[i]], momentas[[j]]] =
1/2 ToExpression["s" \langle > ToString[i] \langle > ToString[j]]
]
, {j, i, Length[momentas]}
```

```

]
, {i, 1, Length[momentas]}
];
]

```

After this, we can easily calculate the amplitudes:

```

FCClearScalarProducts[];
ToMandelstam[{p1, p2, p3, p4, p5}, {0, 0, SMP["m_q"], SMP["m_q"], 0}]

SquaredAmpEEtoBBGluon =
Simplify[DiracSimplify[(DoPolarizationSums[#1, p5,
0] &)[(FermionSpinSum[#1,
ExtraFactor -> 1/2^2] &)[(SUNSimplify[#1, Explicit -> True,
SUNNTtoCAC_F -> True] &)[
FeynAmpDenominatorExplicit[
AmpEEtoBBGluon*ComplexConjugate[AmpEEtoBBGluon]]]]]]];

```

Before we could use the results, we need to convert it to input form, as FeynCalc uses TraditionalForm.

```

SquaredAmpEEtoBBGluon;
% /. {SMP["e"] -> e, SMP["m_q"] -> mb, D -> 4 - 2 \[Epsilon],
CA -> Nc, SMP["g_s"] -> gs, \!\(TraditionalForm\`C_F\) -> C_F};
% // StandardForm // ToString // ToExpression;
FeynCalcEEtoBBGluonSaved = %;

```

I verified both numerically and analytically that the expressions I derived are in full agreement with those computed by FeynCalc for all of the processes discussed.

2.2 Subtraction terms

After I had compared my results analytically and numerically with the output I got from FeynCalc, I have calculated the splitting functions and eikonal functions. Both by hand and by taking the appropriate limit of the NNLO amplitude, then divided it with the proper NLO or LO amplitude. After I had calculated these ‘fundamental’ limits, I also calculated the overlap parts as well by taking the limits of the fundamental formulas. These are my results:

	$\mathbf{A}_1$
$\mathbf{S}_5$	$-\frac{2m_b^2}{s_{35}^2} - \frac{2m_b^2}{s_{45}^2} + \frac{2s_{34}}{s_{35}s_{45}}$
$\mathbf{S}_6$	$-\frac{2m_b^2}{9s_{36}^2} - \frac{2m_b^2}{9s_{46}^2} + \frac{2s_{12}}{s_{16}s_{26}} + \frac{2s_{13}}{3s_{16}s_{36}}$ $-\frac{2s_{14}}{3s_{16}s_{46}} - \frac{2s_{23}}{3s_{26}s_{36}} + \frac{2s_{24}}{3s_{26}s_{46}} + \frac{2s_{34}}{9s_{36}s_{46}}$
$\mathbf{C}_{16}$	$-2\left(\frac{1+x^2}{s_{16}(-1+x)x} - \frac{(-1+x)\varepsilon}{s_{16}x}\right)$
$\mathbf{C}_{26}$	$-\left(\frac{1+x^2}{s_{26}(-1+x)x} - \frac{(-1+x)\varepsilon}{s_{26}x}\right)$
$\mathbf{C}_{16}\mathbf{S}_6$	$\frac{4}{s_{16}(x-1)}$
$\mathbf{C}_{26}\mathbf{S}_6$	$\frac{4}{s_{26}(x-1)}$

	$\mathbf{A}_2$
$\mathbf{S}_{56}$	$\left(-\frac{2m_b^2}{s_{36}^2}-\frac{2m_b^2}{s_{46}^2}+\frac{2s_{34}}{s_{36}s_{46}}\right)\times$ $\left(-\frac{2m_b^2}{9s_{36}^2}-\frac{2m_b^2}{9s_{46}^2}+\frac{2s_{12}}{s_{16}s_{26}}+\frac{2s_{13}}{3s_{16}s_{36}}\right.$ $\left.-\frac{2s_{14}}{3s_{16}s_{46}}-\frac{2s_{23}}{3s_{26}s_{36}}+\frac{2s_{24}}{3s_{26}s_{46}}+\frac{2s_{34}}{9s_{36}s_{46}}\right)$
$\mathbf{C}_{16}\mathbf{S}_5$	$-\left(\frac{1+x^2}{s_{16}(-1+x)x}-\frac{(-1+x)\varepsilon}{s_{16}x}\right)\left(-\frac{2m_b^2}{s_{36}^2}-\frac{2m_b^2}{s_{46}^2}+\frac{2s_{34}}{s_{36}s_{46}}\right)$
$\mathbf{C}_{26}\mathbf{S}_5$	$-\left(\frac{1+x^2}{s_{25}(-1+x)x}-\frac{(-1+x)\varepsilon}{s_{25}x}\right)\left(-\frac{2m_b^2}{s_{36}^2}-\frac{2m_b^2}{s_{46}^2}+\frac{2s_{34}}{s_{36}s_{46}}\right)$
$\mathbf{C}_{16}\mathbf{S}_5\mathbf{S}_{56}$	$-\frac{16C_F m_b^2}{s_{16}s_{35}^2(-1+x)}-\frac{16C_F m_b^2}{s_{16}s_{45}^2(-1+x)}+\frac{16C_F s_{34}}{s_{16}s_{35}s_{45}(-1+x)}$
$\mathbf{C}_{26}\mathbf{S}_5\mathbf{S}_{56}$	$-\frac{16C_F m_b^2}{s_{26}s_{35}^2(-1+x)}-\frac{16C_F m_b^2}{s_{26}s_{45}^2(-1+x)}+\frac{16C_F s_{34}}{s_{26}s_{35}s_{45}(-1+x)}$

	$\mathbf{A}_{12}$
$(\mathbf{C}_{16})\mathbf{C}_{16}\mathbf{S}_5$	$-4C_F \left(-\frac{2mb^2}{s_{35}^2} - \frac{2mb^2}{s_{45}^2} + \frac{2s_{34}}{s_{35}s_{45}} \right) \times \frac{(-1 - x^2 + \epsilon - 2x\epsilon + x^2\epsilon)}{s_{16}(-1+x)x}$
$(\mathbf{C}_{16})\mathbf{S}_{56}$	$-\frac{16C_F m_b^2}{s_{26}s_{35}^2(-1+x)} - \frac{16C_F m_b^2}{s_{26}s_{45}^2(-1+x)} + \frac{16C_F s_{34}}{s_{26}s_{35}s_{45}(-1+x)}$
$(\mathbf{C}_{16}\mathbf{S}_6)\mathbf{S}_{56}$	$-\frac{16C_F m_b^2}{s_{26}s_{35}^2(-1+x)} - \frac{16C_F m_b^2}{s_{26}s_{45}^2(-1+x)} + \frac{16C_F s_{34}}{s_{26}s_{35}s_{45}(-1+x)}$
$(\mathbf{C}_{16})\mathbf{C}_{16}\mathbf{S}_5\mathbf{S}_{56}$	$\frac{16C_F m_b^2}{s_{26}s_{35}^2(-1+x)} + \frac{16C_F m_b^2}{s_{26}s_{45}^2(-1+x)} - \frac{16C_F s_{34}}{s_{26}s_{35}s_{45}(-1+x)}$
$(\mathbf{C}_{26})\mathbf{C}_{26}\mathbf{S}_5$	$-4C_F \left(-\frac{2mb^2}{s_{35}^2} - \frac{2mb^2}{s_{45}^2} + \frac{2s_{34}}{s_{35}s_{45}} \right) \times \frac{(-1 - x^2 + \epsilon - 2x\epsilon + x^2\epsilon)}{s_{26}(-1+x)x}$
$\mathbf{C}_{26}\mathbf{S}_{56}$	$-\frac{16C_F m_b^2}{s_{26}s_{35}^2(-1+x)} - \frac{16C_F m_b^2}{s_{26}s_{45}^2(-1+x)} + \frac{16C_F s_{34}}{s_{26}s_{35}s_{45}(-1+x)}$
$(\mathbf{C}_{26}\mathbf{S}_6)\mathbf{S}_{56}$	$-\frac{16C_F m_b^2}{s_{26}s_{35}^2(-1+x)} - \frac{16C_F m_b^2}{s_{26}s_{45}^2(-1+x)} + \frac{16C_F s_{34}}{s_{26}s_{35}s_{45}(-1+x)}$
$(\mathbf{C}_{26})\mathbf{C}_{26}\mathbf{S}_5\mathbf{S}_{56}$	$\frac{16C_F m_b^2}{s_{26}s_{35}^2(-1+x)} + \frac{16C_F m_b^2}{s_{26}s_{45}^2(-1+x)} - \frac{16C_F s_{34}}{s_{26}s_{35}s_{45}(-1+x)}$
$(\mathbf{C}_{26}\mathbf{S}_6)\mathbf{C}_{26}\mathbf{S}_5$	0
$(\mathbf{C}_{26}\mathbf{S}_6)\mathbf{C}_{26}\mathbf{S}_5\mathbf{S}_{56}$	0

	$\mathbf{A}_{12}$
$(\mathbf{S}_5)\mathbf{C}_{16}\mathbf{S}_5$	$-4C_F\left(-\frac{2mb^2}{s_{35}^2}-\frac{2mb^2}{s_{45}^2}+\frac{2s_{34}}{s_{35}s_{45}}\right)\times$ $\frac{(-1-x^2+\epsilon-2x\epsilon+x^2\epsilon)}{s_{16}(-1+x)x}$
$(\mathbf{S}_5)\mathbf{C}_{26}\mathbf{S}_5$	$-4C_F\left(-\frac{2mb^2}{s_{35}^2}-\frac{2mb^2}{s_{45}^2}+\frac{2s_{34}}{s_{35}s_{45}}\right)\times$ $\frac{(-1-x^2+\epsilon-2x\epsilon+x^2\epsilon)}{s_{16}(-1+x)x}$
$(\mathbf{S}_5)\mathbf{S}_{56}$	$\left(-\frac{2m_b^2}{s_{36}^2}-\frac{2m_b^2}{s_{46}^2}+\frac{2s_{34}}{s_{36}s_{46}}\right)\times$ $\left(-\frac{2m_b^2}{9s_{36}^2}-\frac{2m_b^2}{9s_{46}^2}+\frac{2s_{12}}{s_{16}s_{26}}+\frac{2s_{13}}{3s_{16}s_{36}}\right.$ $\left.-\frac{2s_{14}}{3s_{16}s_{46}}-\frac{2s_{23}}{3s_{26}s_{36}}+\frac{2s_{24}}{3s_{26}s_{46}}+\frac{2s_{34}}{9s_{36}s_{46}}\right)$
$(\mathbf{S}_5)\mathbf{C}_{16}\mathbf{S}_5\mathbf{S}_{56}$	$-\frac{16C_Fm_b^2}{s_{26}s_{35}^2(-1+x)}-\frac{16C_Fm_b^2}{s_{26}s_{45}^2(-1+x)}+\frac{16C_Fs_{34}}{s_{26}s_{35}s_{45}(-1+x)}$
$(\mathbf{S}_5)\mathbf{C}_{26}\mathbf{S}_5\mathbf{S}_{56}$	$-\frac{16C_Fm_b^2}{s_{26}s_{35}^2(-1+x)}-\frac{16C_Fm_b^2}{s_{26}s_{45}^2(-1+x)}+\frac{16C_Fs_{34}}{s_{26}s_{35}s_{45}(-1+x)}$
$(\mathbf{S}_6)\mathbf{C}_{26}\mathbf{S}_5$	0
$(\mathbf{S}_6)\mathbf{C}_{16}\mathbf{S}_5$	0
$(\mathbf{S}_6)\mathbf{S}_{56}$	$\left(-\frac{2m_b^2}{s_{36}^2}-\frac{2m_b^2}{s_{46}^2}+\frac{2s_{34}}{s_{36}s_{46}}\right)\times$ $\left(-\frac{2m_b^2}{9s_{36}^2}-\frac{2m_b^2}{9s_{46}^2}+\frac{2s_{12}}{s_{16}s_{26}}+\frac{2s_{13}}{3s_{16}s_{36}}\right.$ $\left.-\frac{2s_{14}}{3s_{16}s_{46}}-\frac{2s_{23}}{3s_{26}s_{36}}+\frac{2s_{24}}{3s_{26}s_{46}}+\frac{2s_{34}}{9s_{36}s_{46}}\right)$
$(\mathbf{S}_6)\mathbf{C}_{26}\mathbf{S}_5$	0
$(\mathbf{S}_6)\mathbf{C}_{26}\mathbf{S}_5\mathbf{S}_{56}$	0

2.3 Test of the subtraction terms

We must check numerically if we have got the right subtraction terms. The steps are the following:

1. step: generating a random phase space point;
2. step: generating a new particle with the appropriate momentum;
3. step: mapping the momenta;
4. step: calculating the factorization formulas with the mapped momentum;
5. step: comparison of the generated phase space point and the factorized matrix element convergence,
6. step: subtracting all of the counter-terms from the NNLO matrix element.

For generating random phase space points and splitting the particles I used an already written code by dr. Gábor Somogyi. I will not give a detailed description of the code as it is beyond the scope of this thesis. Though I will explain the main commands and give some example output.

2.3.1 Random phase space point

The author of the code implemented the RAMBO (Random Momenta Beautifully Organized) [16] phase space generator in Mathematica. In the inspected process there are massive particles thus we need the RAMBOM command. This gives a random phase space point with massive outgoing particles. (Incoming particles always assumed to be massless.)

```
RAMBOM[energy,  
  fraction of energy of initial particle no.1,  
  fraction of energy of initial particle no.2,  
  no. of particles,  
  {mass of final particle no.1,  
   mass of final particle no.2, ...}  
]
```

Let us take for example a case when we have a colliding energy of 100 GeV, with the initial particles both having the same amount of energy; we have three final particles, from which two are massive with mass 5 GeV.

```
PSini=RAMB0m[100, 1, 1, 3, {5, 5, 0}]
```

Incoming momenta:

```
=====
x,          y,          z,          E,          m^2
-----
{0,0,50.,50.}      0
{0,0,-50.,50.}     0
Sum
{0,0,0,100.}      10000.
```

Outgoing momenta:

```
=====
x,          y,          z,          E,          m^2
-----
{27.6157,29.2182,-8.88301,41.4758}      25.
{3.71175,-21.7793,12.9134,26.0744}      25.
{-31.3275,-7.43886,-4.03042,32.4499}     0
Sum
{0,0,0,100.}      10000.
```

2.3.2 Generating a new particle

At the next step we need to generate a new particle with appropriate momentum. We can do this with the function SinGen; this implements the inverse of the Nagy-Soper momentum mapping [17] with free parameters controlling the collinearity and softness of the new particle(s). For initial state splitting:

```
SinGen[initial phase space,
  mass of split particle,
  mass of new particle,
  no. of particle to split,
  collinearity,
  softness
]
```

The collinearity and softness parameter can be changed in the interval (0,1) with zero corresponding to the most collinear or soft configuration allowed.. So

for example if we take the pervious configuration and split one of the incoming momenta, we find:

```
PSfin=SinGen[PSini, 0, 0, 1, 1/10, 3/10]
```

```

    Incoming momenta:
=====
x,          y,          z,          E,          m^2
-----
{0,0,59.7614,59.7614}      0
{0,0,-59.7614,59.7614}    0
Sum
{0,0,0,119.523}          14285.7
Outgoing momenta:
=====
x,          y,          z,          E,          m^2
-----
{30.8996,26.2178,-14.9331,43.4759}    25.
{5.87525,-23.7561,9.00231,26.5502}    25.
{-28.8335,-9.71765,-8.41194,31.5684}   0
{-7.94137,7.25596,14.3427,17.9284}    0
Sum
{0,0,0,119.523}          14285.7

```

2.3.3 Split random phase space point convergence

We need to make sure the randomly generated and then split point converges to the right phase space limit. To check this we need to make the new momentum soft or collinear with another momentum. For this we need to generate split phase points with, for example, more and more collinear momenta.

```
PSfin = SinGen[PSini, 0, 0, 1, 1/10^itno, 3/10]
```

where $itno = 1, 2, \dots, 10$. We can see as $itno$ grows s_{16} logarithmically converges to 0.

Convergence of generated phase space point term $\mathcal{C}_{16}$

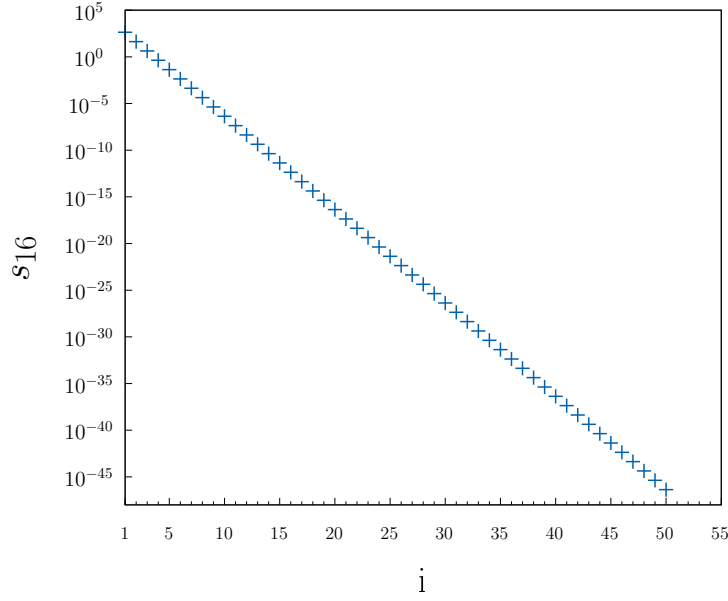


Figure 4: Convergence of a randomly generated $p_1||p_6$ collinear configuration.

By writing out the matrix $A_{ij} = s_{ij}$, we can see that only s_{16} is small.

$$\begin{pmatrix} 0. & 1. & 0.12827 & 0.577948 & 0.293781 & 3 \times 10^{-11} \\ 1. & 0. & 0.0884643 & 0.287733 & 0.323803 & 0.3 \\ 0.12827 & 0.0884643 & 0.0035 & 0.167049 & 0.00770531 & 0.0384805 \\ 0.577948 & 0.287733 & 0.167049 & 0.0035 & 0.521746 & 0.173387 \\ 0.293781 & 0.323803 & 0.00770531 & 0.521746 & 0. & 0.0881328 \\ 3 \times 10^{-11} & 0.3 & 0.0384805 & 0.173387 & 0.0881328 & 0. \end{pmatrix}$$

Furthermore writing out all the cosines of angles, we can point out that, the cosine of the angle between the 6th's and 1st's particles' momentum is 1; thus the 6th particle's momentum became collinear with the 1st.

$$\begin{pmatrix} 0. & 1. & 0.12827 & 0.577948 & 0.293781 & 3 \times 10^{-11} \\ 1. & 0. & 0.0884643 & 0.287733 & 0.323803 & 0.3 \\ 0.12827 & 0.0884643 & 0.0035 & 0.167049 & 0.00770531 & 0.0384805 \\ 0.577948 & 0.287733 & 0.167049 & 0.0035 & 0.521746 & 0.173387 \\ 0.293781 & 0.323803 & 0.00770531 & 0.521746 & 0. & 0.0881328 \\ 3 \times 10^{-11} & 0.3 & 0.0384805 & 0.173387 & 0.0881328 & 0. \end{pmatrix}$$

2.3.4 Mapping the momenta

As was mentioned before, on the two sides of Eq. 1.86 we have different momenta, thus we need to map the left hand side's set of momenta to the right hand side's set. I implemented the mappings presented in the previous section in Mathematica.

```
(* Note a is supposed to be initial state, so a = 1 or 2, r is final
state, so r > 2*)
CarMapBoosted[aa_, bb_, rr_, p_] :=
Module[
{pavec, pbvec, prvec, Q, yrQ, x, pmapped},
pavec = p[[aa]];
pbvec = p[[bb]];
prvec = p[[rr]];
Q = pavec + pbvec;
yrQ = (2 dot[prvec, Q])/dot[Q, Q];
x = 1 - yrQ;

pmapped = Delete[p, {{aa}, {bb}, {rr}}];
pmapped =
Table[
LTR[Q - prvec, Q - (1 - x) pavec, pmapped[[i]]],
{i, 1, Length[pmapped]}];
If[aa \!langle bb,
{pmapped = Insert[pmapped, x pavec, aa];
pmapped = Insert[pmapped, pbvec, bb]},
{pmapped = Insert[pmapped, pbvec, bb];
pmapped = Insert[pmapped, x pavec, aa]}
];

pmapped
];
```

```

SrMapBoostedNL0[rr_, p_] :=
Module[
{mq2, P, s1r, s2r, srP, \[Gamma]1, \[Gamma]2, \[CapitalDelta],
pmapped},

mq2 = dot[p[[3]], p[[3]]];
P = p[[1]] + p[[2]];
s1r = 2 dot[p[[3]], p[[rr]]];
s2r = 2 dot[p[[4]], p[[rr]]];
srP = 2 dot[p[[rr]], P];
\[Gamma]1 = (mq2 s2r srP)/(dot[P, P] s1r s2r - mq2 srP^2);
\[Gamma]2 = (mq2 s1r srP)/(dot[P, P] s1r s2r - mq2 srP^2);
\[CapitalDelta] = Sqrt[
1 - (s1r s2r srP)/(dot[P, P] s1r s2r - mq2 srP^2)];

pmapped = p;
pmapped[[3]] =
LTR[1/\[CapitalDelta] (p[[3]] +
p[[4]] - (\[Gamma]1 + \[Gamma]2) p[[rr]]), P,
1/\[CapitalDelta] (p[[3]] - \[Gamma]1 p[[rr]])];
pmapped[[4]] =
LTR[1/\[CapitalDelta] (p[[3]] +
p[[4]] - (\[Gamma]1 + \[Gamma]2) p[[rr]]), P,
1/\[CapitalDelta] (p[[4]] - \[Gamma]2 p[[rr]])];
pmapped = Delete[pmapped, rr];

pmapped
];

```

```

SrMapBoostedNNLO[aa_, rr_, p_] :=
Module[
{P, y56, y56P, \[Alpha], \[Beta], p56, pmapped},

P = p[[1]] + p[[2]];
y56 = (2 dot[p[[5]], p[[6]])/dot[P, P];
y56P = (2 dot[p[[5]], P])/dot[P, P] + (2 dot[p[[6]], P])/dot[P, P];
\[Alpha] = 1/2 (y56P - Sqrt[y56P^2 - 4 y56]);
\[Beta] = Sqrt[y56P^2 - 4 y56]/(y56P - y56);
p56 = 1/\[Beta] (p[[5]] + p[[6]] - \[Alpha] P);

pmapped = p;
pmapped[[3]] =
LTR[P - p[[5]] - p[[6]], P - p56, p[[3]]];
pmapped[[4]] =
LTR[P - p[[5]] - p[[6]], P - p56, p[[4]]];
pmapped[[rr]] = p56;
pmapped = Delete[pmapped, aa];

pmapped
];

```

2.3.5 Calculation of subtraction terms with the generated momenta

We need to plug in these randomly generated momenta to the formulas to check them numerically. But we should be careful how we build up the subtraction terms,

- i) when we treat the A_1 limit, we just need to use the appropriate mapping from the previous subsection. If it is build up from more than one limit, we simply take the innermost one.
- ii) when we treat the A_2 terms, we take appropriate $6 \rightarrow 5$, then the $5 \rightarrow 4$ limit. When it is build up from more than two limits, we again take the innermost one.

- iii) when we treat the A_{12} terms, we take the innermost limit of the A_1 term then the innermost A_2 limit. We also have to substitute the momenta from the proper set to the subtraction formulae. We need to identify which part comes from the A_1 and which comes from the A_2 limits. We substitute the original momenta to the A_1 term and the once mapped momenta to the A_2 term.

For example:

```
CpelCpelSgBoosted[aa_, bb_, rr_, p_] :=
Module[
{pH, pHH, Mb2,
Sar, S34, S35, S45, X,
pavec, prvec, p3vec, p4vec, p5vec, nvec,
CpelCpelSg},

(* Mapped momenta that enter the factorized matrix element *)
pH = CarMapBoosted[aa, bb, rr, p];
pHH = SrMapBoostedNLO[5, pH];

(* Definition of objects appearing in factorization formula *)
pavec = p[[aa]];
prvec = p[[rr]];
p3vec = pH[[3]];
p4vec = pH[[4]];
p5vec = pH[[5]];
nvec = p[[1]] + p[[2]];

S34 = 2 dot[p3vec, p4vec];
S35 = 2 dot[p3vec, p5vec];
S45 = 2 dot[p4vec, p5vec];
Sar = 2 dot[pavec, prvec];
X = dot[pavec - prvec, nvec]/dot[pavec, nvec];
Mb2 = dot[p3vec, p3vec]; (*mass squared*)
```

```
(* Factorization formula *)
CpelCpelSg = (
4 CF (-((2 Mb2)/S35^2) - (2 Mb2)/S45^2 + (2 S34)/(S35 S45)) (-1 -
X^2 + \[Epsilon] - 2 X \[Epsilon] + X^2 \[Epsilon]))/(
Sar (-1 + X) X)*epembb[pHH];

CpelCpelSg = CpelCpelSg // Expand;
CpelCpelSg
];
```

where the factor containing the X variable comes from the A_1 collinear part, so I used the original momenta, while the renaming term comes from the A_2 term, so I used the boosted momenta. Another is:

```
CpelSpSgpSubBoosted[aa_, rr_, p_] :=
Module[
{pH, pHH, Mb2,
Sar, S34, S35, S45, X,
pavec, prvec, p3vec, p4vec, p5vec, nvec,
CpelSpSgpSub},

(* Mapped momenta that enter the factorized matrix element *)
pH = SrMapBoostedNNLO[5, 6, p];
pHH = SrMapBoostedNLO[5, pH];

(* Definition of objects appearing in factorization formula *)
pavec = p[[aa]];
prvec = p[[rr]];
p3vec = pH[[3]];
p4vec = pH[[4]];
p5vec = pH[[5]];
nvec = p[[1]] + p[[2]];

S34 = 2 dot[p3vec, p4vec];
S35 = 2 dot[p3vec, p5vec];
S45 = 2 dot[p4vec, p5vec];
Sar = 2 dot[pavec, prvec];
X = dot[pavec - prvec, nvec]/dot[pavec, nvec];
```

```

Mb2 = dot[p3vec, p3vec]; (*mass squared*)

(* Factorization formula *)
Cp1SpSgpSub = -8 CF (-((2 Mb2)/S35^2) - (2 Mb2)/S45^2 + (2 S34)/(
S35 S45))*1/(Sar (-1 + X))
*epembb[pHH];

Cp1SpSgpSub = Cp1SpSgpSub // Expand;
Cp1SpSgpSub
];

```

where, though the A_1 limit has a collinear term we only take the innermost soft mapping, then take the most right soft mapping from A_2 . The second factor ($1/(\text{Sar } (-1 + X))$ in the code above) corresponds to the A_1 limit thus we evaluate it with the original momenta but we substitute the once mapped momenta to the first factor ($-\left(\frac{2 \text{ Mb2}}{S35^2} - \frac{2 \text{ Mb2}}{S45^2} + \frac{2 \text{ S34}}{S35 S45}\right)$ above).

To summarize the above discussion in a more precise way, I present the following table, which contains, which mapping should one take and which momenta one ought to use to evaluate the subtraction terms.

	$\mathbf{A}_1$
$\mathcal{S}_5$	$-\frac{2m_b^2}{s_{35}^2} - \frac{2m_b^2}{s_{45}^2} + \frac{2s_{34}}{s_{35}s_{45}}$ $\{p\}_6 \xrightarrow{Soft\ NLO} \{\hat{p}\}_5$
$\mathcal{S}_6$	$-\frac{2m_b^2}{9s_{36}^2} - \frac{2m_b^2}{9s_{46}^2} + \frac{2s_{12}}{s_{16}s_{26}} + \frac{2s_{13}}{3s_{16}s_{36}}$ $-\frac{2s_{14}}{3s_{16}s_{46}} - \frac{2s_{23}}{3s_{26}s_{36}} + \frac{2s_{24}}{3s_{26}s_{46}} + \frac{2s_{34}}{9s_{36}s_{46}}$ $\{p\}_6 \xrightarrow{Soft\ NLO} \{\hat{p}\}_5$
$\mathcal{C}_{16}$	$-2\left(\frac{1+x^2}{s_{16}(-1+x)x} - \frac{(-1+x)\varepsilon}{s_{16}x}\right)$ $\{p\}_6 \xrightarrow{Collinear} \{\hat{p}\}_5$
$\mathcal{C}_{26}$	$-2\left(\frac{1+x^2}{s_{26}(-1+x)x} - \frac{(-1+x)\varepsilon}{s_{26}x}\right)$ $\{p\}_6 \xrightarrow{Collinear} \{\hat{p}\}_5$
$\mathcal{C}_{16}\mathcal{S}_6$	$\frac{4}{s_{16}(x-1)}$ $\{p\}_6 \xrightarrow{Soft\ NLO} \{\hat{p}\}_5$
$\mathcal{C}_{26}\mathcal{S}_6$	$\frac{4}{s_{26}(x-1)}$ $\{p\}_6 \xrightarrow{Soft\ NLO} \{\hat{p}\}_5$

	$\mathbf{A_2}$
$\mathcal{S}_{56}$	$\left(-\frac{2m_b^2}{s_{36}^2} - \frac{2m_b^2}{s_{46}^2} + \frac{2s_{34}}{s_{36}s_{46}} \right) \times$ $\left(-\frac{2m_b^2}{9s_{36}^2} - \frac{2m_b^2}{9s_{46}^2} + \frac{2s_{12}}{s_{16}s_{26}} + \frac{2s_{13}}{3s_{16}s_{36}} \right.$ $\left. - \frac{2s_{14}}{3s_{16}s_{46}} - \frac{2s_{23}}{3s_{26}s_{36}} + \frac{2s_{24}}{3s_{26}s_{46}} + \frac{2s_{34}}{9s_{36}s_{46}} \right)$ $\{p\}_6 \xrightarrow{Soft \ NNLO} \{p'\}_5 \xrightarrow{Soft \ NLO} \{\hat{p}\}_4$
$\mathcal{C}_{16}\mathcal{S}_5$	$-\left(\frac{1+x^2}{s_{16}(-1+x)x} - \frac{(-1+x)\varepsilon}{s_{16}x} \right) \left(-\frac{2m_b^2}{s_{36}^2} - \frac{2m_b^2}{s_{46}^2} + \frac{2s_{34}}{s_{36}s_{46}} \right)$ $\{p\}_6 \xrightarrow{Soft \ NNLO} \{p'\}_5 \xrightarrow{Collinear} \{\hat{p}\}_4$
$\mathcal{C}_{26}\mathcal{S}_5$	$-\left(\frac{1+x^2}{s_{25}(-1+x)x} - \frac{(-1+x)\varepsilon}{s_{25}x} \right) \left(-\frac{2m_b^2}{s_{36}^2} - \frac{2m_b^2}{s_{46}^2} + \frac{2s_{34}}{s_{36}s_{46}} \right)$ $\{p\}_6 \xrightarrow{Soft \ NNLO} \{p'\}_5 \xrightarrow{Collinear} \{\hat{p}\}_4$
$\mathcal{C}_{16}\mathcal{S}_5\mathcal{S}_{56}$	$-\frac{16C_F m_b^2}{s_{16}s_{35}^2(-1+x)} - \frac{16C_F m_b^2}{s_{16}s_{45}^2(-1+x)} + \frac{16C_F s_{34}}{s_{16}s_{35}s_{45}(-1+x)}$ $\{p\}_6 \xrightarrow{Soft \ NNLO} \{p'\}_5 \xrightarrow{Soft \ NLO} \{\hat{p}\}_4$
$\mathcal{C}_{26}\mathcal{S}_5\mathcal{S}_{56}$	$-\frac{16C_F m_b^2}{s_{26}s_{35}^2(-1+x)} - \frac{16C_F m_b^2}{s_{26}s_{45}^2(-1+x)} + \frac{16C_F s_{34}}{s_{26}s_{35}s_{45}(-1+x)}$ $\{p\}_6 \xrightarrow{Soft \ NNLO} \{p'\}_5 \xrightarrow{Soft \ NLO} \{\hat{p}\}_4$

	$\mathbf{A}_{12}$
$(\mathcal{C}_{16})\mathcal{C}_{16}\mathcal{S}_5$	$-4C_F\left(-\frac{2m_b^2}{s_{35}'^2}-\frac{2m_b^2}{s_{45}'^2}+\frac{2s_{34}'}{s_{35}'s_{45}'}\right)\times$ $\frac{(-1-x^2+\epsilon-2x\epsilon+x^2\epsilon)}{s_{16}(-1+x)x}$ $\{p\}_6 \xrightarrow{Collinear} \{p'\}_5 \xrightarrow{Soft\ NLO} \{\hat{p}\}_4$
$(\mathcal{C}_{16})\mathcal{S}_{56}$	$16C_F\left(-\frac{m_b^2}{s_{35}'^2}-\frac{m_b^2}{s_{45}'^2}+\frac{s_{34}'}{s_{35}'s_{45}'}\right)\frac{1}{s_{16}(-1+x)}$ $\{p\}_6 \xrightarrow{Collinear} \{p'\}_5 \xrightarrow{Soft\ NLO} \{\hat{p}\}_4$
$(\mathcal{C}_{16}\mathcal{S}_6)\mathcal{S}_{56}$	$16C_F\left(-\frac{m_b^2}{s_{35}'^2}-\frac{m_b^2}{s_{45}'^2}+\frac{s_{34}'}{s_{35}'s_{45}'}\right)\frac{1}{s_{16}(-1+x)}$ $\{p\}_6 \xrightarrow{Soft\ NNLO} \{p'\}_5 \xrightarrow{Soft\ NLO} \{\hat{p}\}_4$
$(\mathcal{C}_{16})\mathcal{C}_{16}\mathcal{S}_5\mathcal{S}_{56}$	$16C_F\left(-\frac{m_b^2}{s_{35}'^2}-\frac{m_b^2}{s_{45}'^2}+\frac{s_{34}'}{s_{35}'s_{45}'}\right)\frac{1}{s_{16}(-1+x)}$ $\{p\}_6 \xrightarrow{Collinear} \{p'\}_5 \xrightarrow{Soft\ NLO} \{\hat{p}\}_4$
$(\mathcal{C}_{26})\mathcal{C}_{26}\mathcal{S}_5$	$-4C_F\left(-\frac{2m_b^2}{s_{35}'^2}-\frac{2m_b^2}{s_{45}'^2}+\frac{2s_{34}'}{s_{35}'s_{45}'}\right)\times$ $\frac{(-1-x^2+\epsilon-2x\epsilon+x^2\epsilon)}{s_{26}(-1+x)x}$ $\{p\}_6 \xrightarrow{Collinear} \{p'\}_5 \xrightarrow{Soft\ NLO} \{\hat{p}\}_4$
$(\mathcal{C}_{26})\mathcal{S}_{56}$	$16C_F\left(-\frac{m_b^2}{s_{35}'^2}-\frac{m_b^2}{s_{45}'^2}+\frac{s_{34}'}{s_{35}'s_{45}'}\right)\frac{1}{s_{26}(-1+x)}$ $\{p\}_6 \xrightarrow{Collinear} \{p'\}_5 \xrightarrow{Soft\ NLO} \{\hat{p}\}_4$
$(\mathcal{C}_{26}\mathcal{S}_6)\mathcal{S}_{56}$	$16C_F\left(-\frac{m_b^2}{s_{35}'^2}-\frac{m_b^2}{s_{45}'^2}+\frac{s_{34}'}{s_{35}'s_{45}'}\right)\frac{1}{s_{26}(-1+x)}$ $\{p\}_6 \xrightarrow{Soft\ NNLO} \{p'\}_5 \xrightarrow{Soft\ NLO} \{\hat{p}\}_4$

	$\mathbf{A}_{12}$
$(\mathcal{C}_{26})\mathcal{C}_{26}\mathcal{S}_5\mathcal{S}_{56}$	$\frac{16C_F\left(-\frac{m_b^2}{s_{35}'^2}-\frac{m_b^2}{s_{45}'^2}+\frac{s_{34}'}{s_{35}'s_{45}'}\right)\frac{1}{s_{26}(-1+x)}}{\{p\}_6 \xrightarrow{\text{Collinear}} \{p'\}_5 \xrightarrow{\text{Soft NLO}} \{\hat{p}\}_4}$
$(\mathcal{S}_5)\mathcal{C}_{16}\mathcal{S}_5$	$\frac{-4C_F\left(-\frac{2mb^2}{s_{35}^2}-\frac{2mb^2}{s_{45}^2}+\frac{2s_{34}}{s_{35}s_{45}}\right)\times\frac{(-1-x'^2+\epsilon-2x'\epsilon+x'^2\epsilon)}{s_{16}(-1+x')x'}}{\{p\}_6 \xrightarrow{\text{Soft NNLO}} \{p'\}_5 \xrightarrow{\text{Soft NLO}} \{\hat{p}\}_4}$
$(\mathcal{S}_5)\mathcal{C}_{26}\mathcal{S}_5$	$\frac{-4C_F\left(-\frac{2mb^2}{s_{35}^2}-\frac{2mb^2}{s_{45}^2}+\frac{2s_{34}}{s_{35}s_{45}}\right)\times\frac{(-1-x'^2+\epsilon-2x'\epsilon+x'^2\epsilon)}{s_{26}(-1+x')x'}}{\{p\}_6 \xrightarrow{\text{Soft NNLO}} \{p'\}_5 \xrightarrow{\text{Soft NLO}} \{\hat{p}\}_4}$
$(\mathcal{S}_5)\mathcal{S}_{56}$	$\frac{\left(-\frac{2m_b^2}{s_{36}^2}-\frac{2m_b^2}{s_{46}^2}+\frac{2s_{34}}{s_{36}s_{46}}\right)\times\left(-\frac{2m_b^2}{9s_{36}'^2}-\frac{2m_b^2}{9s_{46}'^2}+\frac{2s_{12}'}{s_{16}'s_{26}'}+\frac{2s_{13}'}{3s_{16}'s_{36}'}-\frac{2s_{14}'}{3s_{16}'s_{46}'}-\frac{2s_{23}'}{3s_{26}'s_{36}'}+\frac{2s_{24}'}{3s_{26}'s_{46}'}+\frac{2s_{34}'}{9s_{36}'s_{46}'}\right)}{\{p\}_6 \xrightarrow{\text{Soft NNLO}} \{p'\}_5 \xrightarrow{\text{Soft NLO}} \{\hat{p}\}_4}$

	$\mathbf{A}_{12}$
$(\mathcal{S}_5)\mathcal{C}_{16}\mathcal{S}_5\mathcal{S}_{56}$	$16C_F\left(-\frac{m_b^2}{s_{35}^2}-\frac{m_b^2}{s_{45}^2}+\frac{s_{34}}{s_{35}s_{45}}\right)\frac{1}{s'_{16}(-1+x')}$ $\{p\}_6 \xrightarrow{Soft\ NNLO} \{p'\}_5 \xrightarrow{Soft\ NLO} \{\hat{p}\}_4$
$(\mathcal{S}_5)\mathcal{C}_{26}\mathcal{S}_5\mathcal{S}_{56}$	$16C_F\left(-\frac{m_b^2}{s_{35}^2}-\frac{m_b^2}{s_{45}^2}+\frac{s_{34}}{s_{35}s_{45}}\right)\frac{1}{s'_{26}(-1+x')}$ $\{p\}_6 \xrightarrow{Soft\ NNLO} \{p'\}_5 \xrightarrow{Soft\ NLO} \{\hat{p}\}_4$
$(\mathcal{S}_6)\mathcal{S}_{56}$	$\left(-\frac{2m_b^2}{s_{36}'^2}-\frac{2m_b^2}{s_{46}'^2}+\frac{2s_{34}'}{s_{36}'s_{46}'}\right)\times$ $\left(-\frac{2m_b^2}{9s_{36}^2}-\frac{2m_b^2}{9s_{46}^2}+\frac{2s_{12}}{s_{16}s_{26}}+\frac{2s_{13}}{3s_{16}s_{36}}\right.$ $\left.-\frac{2s_{14}}{3s_{16}s_{46}}-\frac{2s_{23}}{3s_{26}s_{36}}+\frac{2s_{24}}{3s_{26}s_{46}}+\frac{2s_{34}}{9s_{36}s_{46}}\right)$ $\{p\}_6 \xrightarrow{Soft\ NNLO} \{p'\}_5 \xrightarrow{Soft\ NLO} \{\hat{p}\}_4$

2.3.6 Comparison of convergences

Lastly, I made sure I had got the right subtraction terms. First I verified that in the appropriate limit each subtraction term cancels the NNLO matrix element. For example for the limit $\mathcal{C}_{16}$ I have done this by the following code:

```
NumRand = 50;
PSfin = {};
results = {};
rnd1 = RandomReal[{1, 9}, {NumRand, 2}, WorkingPrecision -> 400]/10;
rnd2 = RandomReal[{1, 9}, {NumRand, 2}, WorkingPrecision -> 400]/10;
AbsoluteTiming[
results =
ParallelTable[
PrintTemporary["i: ", i];

PSini = N[RAMB0m[rsnum, 1, 1, 3, {mqnum, mqnum, 0}], 400];

PSfin = SinGen[PSini, 0, 0, 1, #1/10^(i), #2/10^( 1)] & @@@ rnd1;

smallinv =
2 dot#[#[[1]], #[[6]]]/dot#[#[[1]] + #[[2]], #[[1]] + #[[2]]] & /@
PSfin;

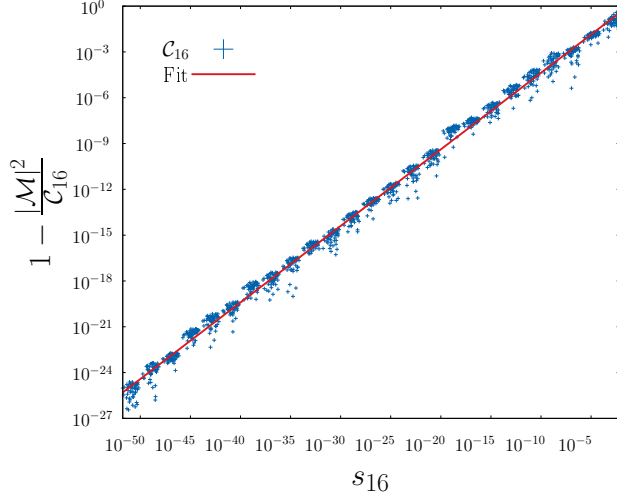
ME = epembbgga[#] & /@ PSfin;
SUB = CleptonphotonSubBoosted[1, 2, 6, #] & /@ PSfin;

Transpose[{smallinv, Abs[1 - ME/SUB] /. {\[Epsilon] -> 0}},
{i, 1, 50, 2}
];
]
```

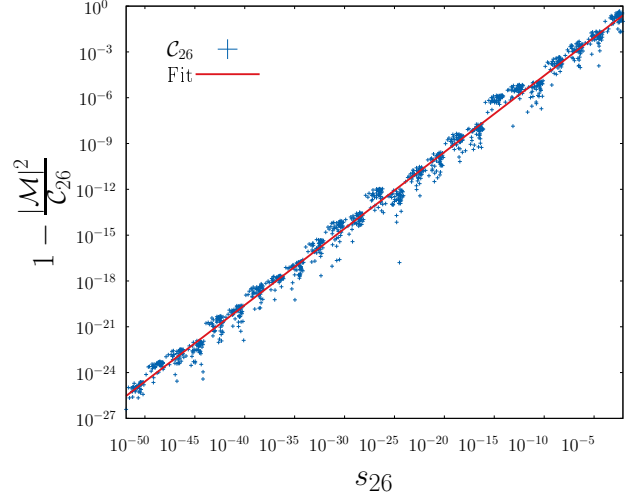
Furthermore, I made sure the complete subtraction holds in all limits, in the whole phase space. To do this, I have generated 10'000 random phase space points of the same magnitude in the proper limit, then calculated both the matrix element and $\mathbf{A}|\mathcal{M}_{m+2}^{(0)}|^2$.

As one can see on Figure 5 the subtraction terms individually cancel the matrix element in the proper limits, while on 6 we can see the whole subtraction expression converges to the matrix element in all limits.

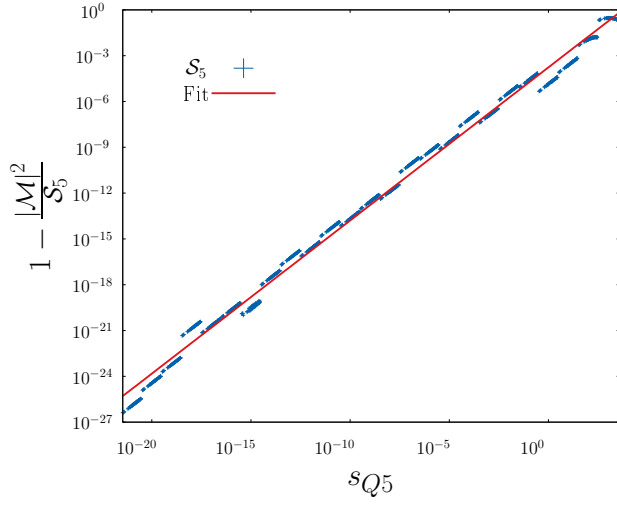
Convergence of subtraction term $\mathcal{C}_{16}$



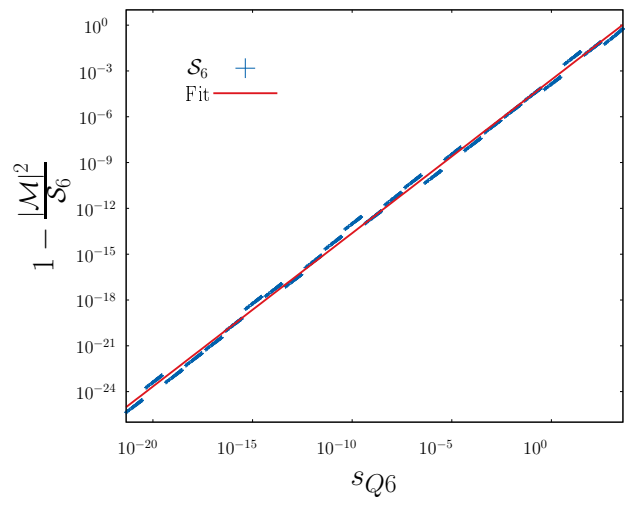
Convergence of subtraction term $\mathcal{C}_{26}$



Convergence of subtraction term $\mathcal{S}_5$



Convergence of subtraction term $\mathcal{S}_6$



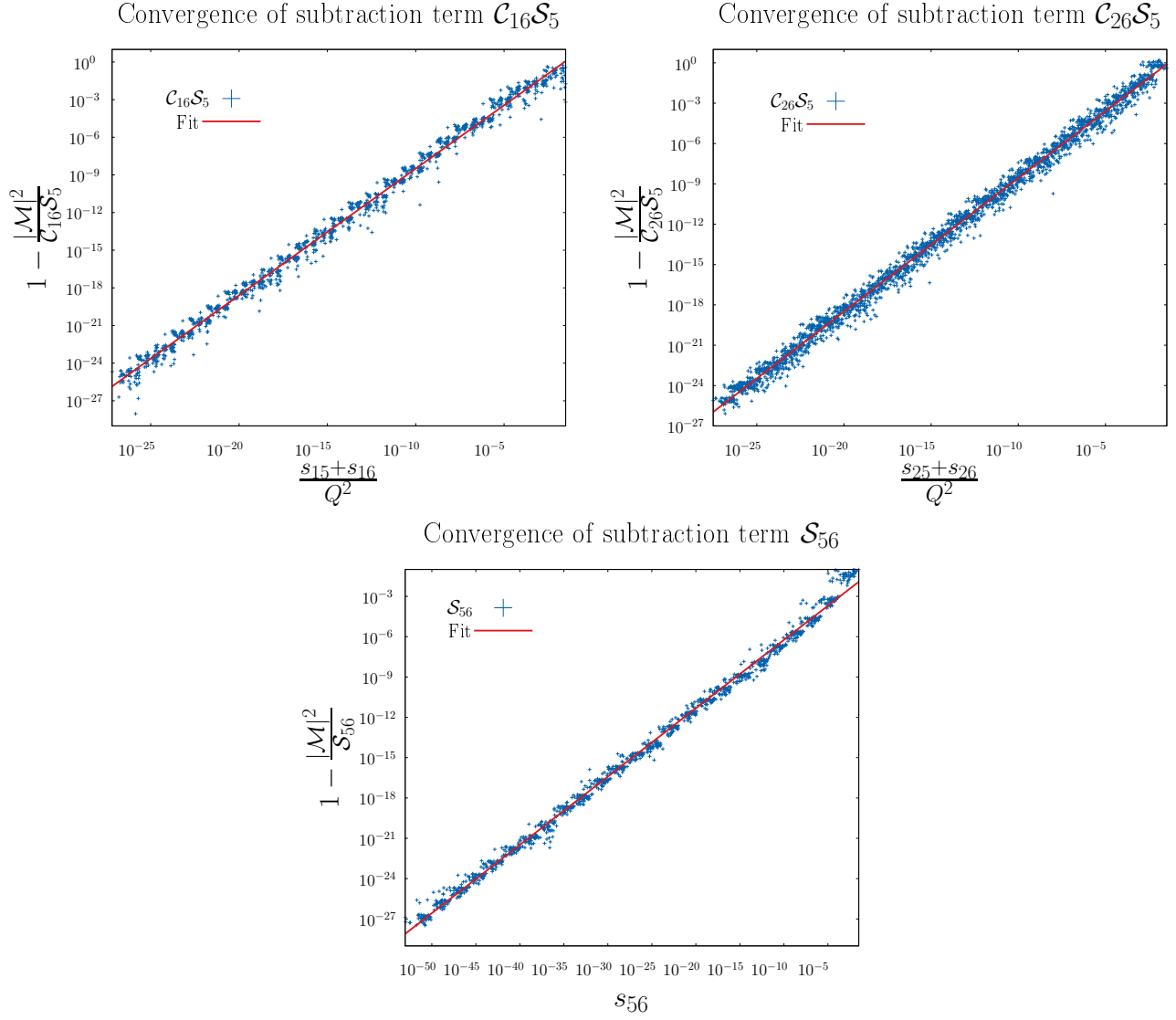
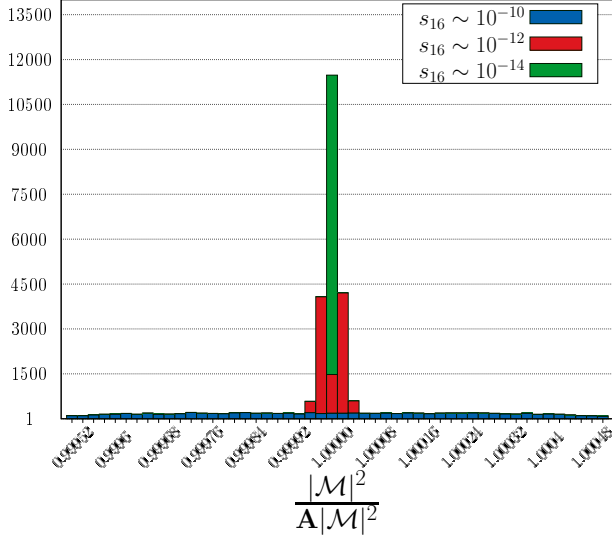
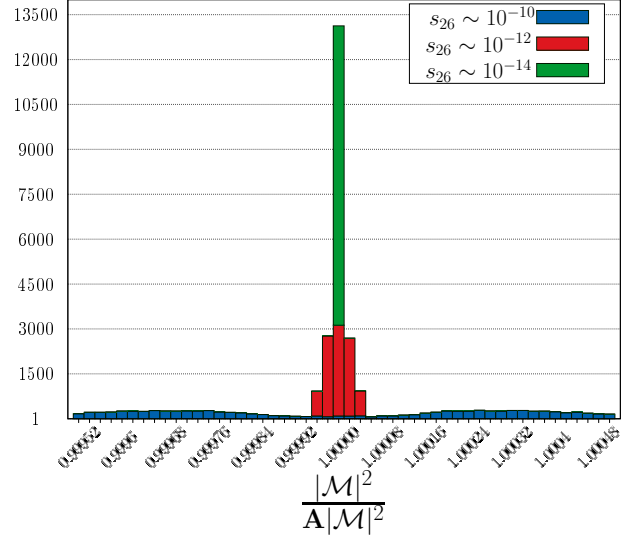


Figure 5: Convergence of individual subtraction terms.

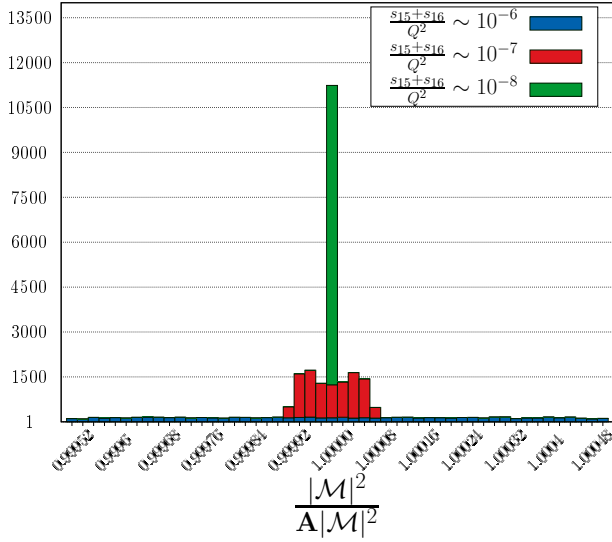
Complete subtraction term in the limit $\mathcal{C}_{16}$



Complete subtraction term in the limit $\mathcal{C}_{26}$



Complete subtraction term in the limit $\mathcal{C}_{16}\mathcal{S}_5$



Complete subtraction term in the limit $\mathcal{C}_{16}\mathcal{S}_5$

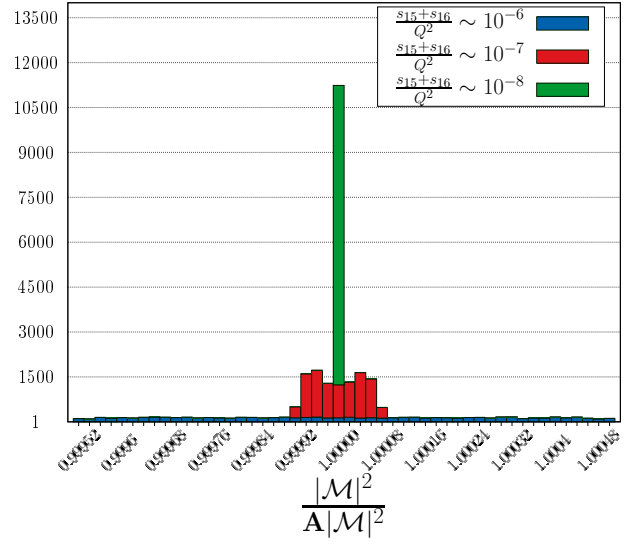


Figure 6: Convergence of the complete subtraction.

3 Conclusions

In this master thesis I have calculated the QED+QCD NNLO doubly-real emission part of the $e^-e^+ \rightarrow b\bar{b}$ process. This process is particularly interesting due to the 2.1σ deviation between theory prediction and LEP measurements of the bottom quark forward-backward asymmetry.

During this work I have made a program which automatically calculates Feynman diagrams with minimal user input, calculated the proper matrix elements and cross-checked them with FeynCalc, furthermore I have also calculated the CoLoRFulNNLO subtraction terms for this process and checked their validity.

In order to complete the calculation of the NNLO QED+QCD corrections to the bottom quark forward-backward asymmetry, the subtraction terms derived in this thesis must be integrated over the momenta of the unresolved emissions so that they can be combined with the virtual corrections. Furthermore, the real-virtual contributions to this process must be evaluated. With these additional elements in place, we will be able to present the most precise theoretical prediction for this asymmetry to date.

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