Numerical Evaluation of Feynman Loop Integrals by Reduction to Tree Graphs

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ABSTRACT

We present a new method for the numerical evaluation of loop integrals which is based on the Feynman Tree Theorem. The loop integrals are replaced by phase-space integration over fictitious extra on-shell particles. This integration can be performed alongside with the Monte-Carlo integration of ordinary phase space, avoiding the time-consuming nesting of loop evaluation inside the integrand, and directly leading to NLO event generation. We systematically construct subtractions, necessary to cancel both ultraviolet divergences and the extra threshold singularities in phase-space which arise in the numerical evaluation. Infrared singularities can be dealt with by standard methods. As a proof of concept, we apply the method to NLO Bhabha scattering in QED and construct the corresponding NLO Monte Carlo event generator.

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1 Introduction

The advent of the LHC has initiated a strong activity in the development of new methods and tools aiming at an efficient computation of processes at next-to-leading order (NLO) in perturbation theory. Automated programs exist which simulate events at leading order (LO) with many (typically, up to six or eight) final-state partons without factorizing them into production and decay [1–6]. These can be interfaced and properly matched to parton-shower algorithms and thus provide a powerful tool for the simulation of events with complex final states at particle colliders. For specific applications, this program has already been extended to NLO processes.

Especially at hadron colliders, the LO predictions are highly scale-dependent and lack important contributions, so it becomes increasingly important to simulate proper events at the NLO level.

The cancellation of IR divergences and the inclusion of subtraction terms in NLO calculations are well understood in principle, and their implementation in universal event generators is in progress. A crucial problem of NLO event generation originates from the loop contributions to multi-parton matrix elements. The number of individual Feynman graphs rises dramatically with the number of external legs, and tensor reduction methods increase the number of terms even more. This poor scaling behavior, and the associated instabilities due to large numerical cancellations in matrix elements, make it worthwhile to investigate different and alternative approaches to the problem of automatic NLO computation and simulation.

A particular alternative approach to evaluating amplitudes at the loop level is to exploit their analytic properties. Observing that any amplitude can be decomposed into cut contributions and a simple rational part, one can construct the coefficients of a set of basic integrals by cutting lines of the loop graph in a particular way and evaluating the resulting tree-level amplitudes. In the recent past, some $2 \rightarrow 4$ processes for the LHC have been computed using either of these two main techniques [7–15], and there are several groups aiming at a full automatization of NLO processes.

In this paper, we propose a new method for the evaluation of loop integrals, which allows for direct numerical computation without reduction to a set of basic integrals. The matrix element is re-expressed using an improved version of the Feynman Tree Theorem (FTT) [16–18]. Roughly speaking, this theorem relates loop graphs to tree graphs, and it is nothing but the relation of relativistic Feynman-graph perturbation theory to “old-fashioned” non-relativistic perturbation theory. It holds in any local relativistic field theory. The loop integrals are transformed into phase space integrals and are evaluated numerically along with the phase space integral over of the external partons of the process under consideration. So, there is only one step of numerical integration involved in the computation of any particular integrated cross section or distribution. We therefore can make use of powerful existing technologies for numerical phase-space integration by tree-level event generators to evaluate processes at the one-loop level.

There has recently been increased interest in the Feynman tree theorem. In [19] it was used to prove the covariance of non-MHV amplitudes at one-loop level obtained from MHV diagrams, as well as for the calculation of MHV scattering amplitudes in $\mathcal{N} = 4$ super Yang-Mills theory. In [20], single cuts were used to simplify one-loop scattering amplitudes in massless gauge theories.

An algorithm for the direct numerical integration of NLO processes by the FTT method was developed first for massless amplitudes by Soper et al. [21,22]. There, internal on-shell or
threshold singularities were found to be a serious obstacle to numerical phase-space integration. To avoid these singularities, contour deformation of the integration into the complex plane was used, either in three-momentum space or in Feynman-parameter space.

In the present work we allow for massive particles. Threshold singularities are handled by a specially tailored subtraction procedure that allows us to stay in the space of real integration parameters. This enables us to directly implement the integrands in an ordinary Monte Carlo event generator, and it also gives a handle on the treatment of overlapping singularities in the integration region, which can occur in integrals from six external legs on.

In a project independent of the present one, Catani et al. [23] exploited the relation between loop integrals and phase space integrals to express loop amplitudes as sum of tree amplitudes arising solely from single cuts. Contributions from multiple cuts which are present in the Feynman Tree Theorem, are compensated by a non-trivial $i\epsilon$-prescription in the propagators.

The paper is structured as follows. In a first technical part, we develop the method. In section 2.1 we review the derivation of the Feynman Tree Theorem and provide an improved version where the initial $i\epsilon$ prescription disappears, allowing for a direct numerical integration. In the following sections 2.2 to 2.4 we propose renormalization and regularization schemes and discuss the treatment of infrared divergences. We then discuss the types of internal singularities that can arise in the numerical evaluation and present the construction of appropriate subtraction function in Sec. 2.5. In the next part, section 3 we discuss the implementation of this method in a Monte Carlo cross section integration and event generation for Bhabha scattering in QED. We thereafter conclude and give an outlook.

# 2 The Method

## 2.1 Feynman Tree Theorem

The starting point of our approach is a theorem by R. Feynman [16–18], which was formally stated in order to invest the renormalizability of a quantum theory of gravitation. The idea is to decompose loop propagators into advanced Green functions and a delta function. When integrating over the zero component of the loop momentum, the delta functions will set the internal momentum of the associated propagator on-shell. This has the effect of opening or cutting the loop. The Feynman Tree Theorem states, that a loop integral can be expressed as the sum of all possible cuts of its propagators. Terms with one cut propagator can be interpreted as tree-level processes with an additional outgoing and an additional incoming particle with identical momentum. The original integration over the loop momentum becomes a phase space integration for the additional particle. This extra integration is peculiar since its phase space is not restricted by the available process energy.

Operating on every loop diagram, a full one-loop $m \rightarrow n$ matrix element can be rewritten as the coherent sum of all possible $m \rightarrow n + p + \bar{p}$ tree level processes with an additional integration over the phase space of the particle $p$ and its corresponding antiparticle $\bar{p}$ obtained by crossing from the initial state.

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1Preliminary studies for the present project can be found in [24]. Additional details of the techniques involved are presented in [25].
2.1.1 Derivation

In the following, we will briefly review the derivation of the Feynman Tree Theorem, closely following [17] (see also [19]). In the next section, we give a modified version of the Tree Theorem which is better suited for numerical integration.

The integrand $I(k)$ of a loop integral can be written as a product of Feynman Green functions $F$ of the Klein-Gordon operator times a regular function $N(k)$ in the numerator. The latter may depend on the integration momentum $k$ and have Lorentz and Dirac indices but is not of interest in the following. Suppressing the possible indices, we have

$$I(k) = N(k) \prod_i F(k + p_i, m_i),$$

where we used the letter $F$ to indicate the use of the Feynman prescription. The $p_i$ are linear combinations of external momenta, the $m_i$ the masses of the physical particle the propagator corresponds to. We define

$$F_i \equiv F(k + p_i, m_i) = \frac{i}{(k + p_i)^2 - m_i^2 + i\epsilon}.$$  

(2)

Note that we only consider cases where the $k$-dependence in the denominator of a propagator is of the form (2). Here and in the following, we use ‘t Hooft-Feynman gauge, where gauge boson propagators take on this simple structure in the denominator.

In the following, we want to replace the Feynman Green functions $F_i$ by advanced Green functions $A_i$, where both poles lie in the upper $k^0$-half complex plane. We define

$$E_i = \sqrt{(\vec{k} + \vec{p}_i)^2 + m_i^2}.$$  

(3)

Performing a partial-fraction decomposition in (2), and similar for $A_i$, we get

$$F_i = \frac{i}{2(E_i - i\epsilon)} \left( \frac{1}{k^0 - (-p_i^0 + E_i) + i\epsilon} - \frac{1}{k^0 - (-p_i^0 - E_i) - i\epsilon} \right),$$  

(4)

$$A_i = \frac{i}{2E_i} \left( \frac{1}{k^0 - (-p_i^0 + E_i) - i\epsilon} - \frac{1}{k^0 - (-p_i^0 - E_i) + i\epsilon} \right).$$  

(5)

Using a representation of the delta function

$$2\pi i\delta(u) = \lim_{\epsilon \to +0} \left( \frac{1}{u - i\epsilon} - \frac{1}{u + i\epsilon} \right),$$  

(6)

the difference of the Feynman and advanced Green function $F_i - A_i$ is given by:

$$\Delta_l^i = \frac{2\pi}{2E_i} \delta(k^0 - (-p_i^0 + E_i)).$$  

(7)

Here, we ignored the imaginary part in the prefactor of the Feynman Green function (4). Being independent of $k^0$, it is not relevant in the following. The superscript $l$ indicates that this delta function picks out the propagator pole, which originally was situated in the lower half plane, setting the momentum $k + p_i$ on its mass shell with a positive energy component. The $k^0$ integration over a product of advanced Green functions $A_i$ vanishes, since for two or more
Green functions the integrand falls of sufficiently fast for large $k^0$. Thus, one can close the contour of integration in the lower half plane where no poles are situated:

$$0 = \int N(k) \prod_i A_i. \quad (8)$$

Replacing $A_i$ with $F_i - \Delta^i$, we get:

$$0 = \int N(k) \left[ F \cdots F - \sum \Delta^i F \cdots + \sum \Delta^i \Delta^i F \cdots - \ldots + (-1)^n \sum \Delta^i \cdots \Delta^i \right], \quad (9)$$

where we skipped indices in the terms in the brackets.

Equation (9) is the Feynman Tree Theorem \[16,17\]. Since the delta functions cancel the integration, it states that a loop integral can be expressed as a sum of tree amplitudes. The first sum runs over all permutations where one propagator is replaced by a delta function, the second sum runs over all terms including two delta functions, and so on. The first term on the right-hand side, which contains only Feynman Green functions, is the original integrand (1). In the following the term cutting a propagator of a loop will refer to one of the terms in (9), where a propagator was replaced by a delta function.

In [23], equation (9) was the starting point for constructing a method that re-expresses loop amplitudes as a sum of tree amplitudes that involve single cuts only. The cost of this simplification lies in an exchange of the Feynman propagators (4) by propagators that acquire a rather complicated $i\epsilon$ prescription.

To make use of the FTT in a numerical evaluation of loop integrals involving only real numbers, at some point we have to set the $i\epsilon$ terms in the denominators to zero. Clearly, this can not be done in a naïve way, since terms including the delta functions $\Delta^i$ were derived precisely from a configuration of Feynman and advanced Green functions with a unique description of the poles in the complex $k^0$-plane.

2.1.2 Improved Version

We can re-express the Feynman Green functions $F_i$ by use of the identity:

$$\frac{1}{x - a \pm i\epsilon} = \mathcal{P} \frac{1}{x - a} \mp i\pi \delta(x - a), \quad (10)$$

where $\mathcal{P}$ is Cauchy’s Principal Value, which is obtained by evenly approaching the singular point from both sides such that the diverging pieces cancel each other. Applying this identity to the Feynman Green function (4) and again skipping the $i\epsilon$ term in the factor in front of the brackets we get:

$$F_i = \frac{i}{2E_i} \left( \mathcal{P} \frac{1}{k^0 - (-p^0_i + E_i)} - \frac{1}{k^0 - (-p^0_i - E_i)} - i\pi \delta(k^0 - (-p^0_i + E_i)) \right)$$

$$\equiv \mathcal{P} + \frac{1}{2} \Delta^i + \frac{1}{2} \Delta^u_i, \quad (11)$$

where we defined $\Delta^u_i$ as the delta function that sets the zero component of the negative momentum of the associated propagator $i$:

$$\Delta^u_i = \frac{2\pi}{2E_i} \delta(k^0 - (-p^0_i - E_i)). \quad (12)$$
$P_i$ stands for the propagator with no $i\epsilon$-prescription in the denominator:

$$P_i = \frac{i}{(k+p_i)^2 - m_i^2}. \quad (13)$$

In numerical evaluations of tree amplitudes, propagators of this form, without $i\epsilon$-terms, are used. Inserting (11) in (9), we therefore get after some combinatorics a version of the Tree Theorem (9) which is better suited for numerical evaluations:

$$\int I(k) = \int N(k) \left[ \Delta^1 P_2 \cdot \cdot \cdot P_n + P_1 \Delta^1 P_3 \cdot \cdot \cdot P_n + \ldots + P_1 \cdot \cdot \cdot P_{n-1} \Delta^1 \right]$$

$$+ \int N(k) \sum_{\text{perm.}} C_{LU P} \Delta^L \Delta^U P^P,$$  \quad (14)

$$C_{LU P} = \frac{1}{2L+U} \left( 1 - (-1)^L \right). \quad (15)$$

Since the structure of (14) is still very similar to (9), we will from now on refer to (14) as the Feynman Tree Theorem.

The sum runs over all possible permutations, where the functions $(\Delta^1, \Delta^u, P)$ appear $(L,U,P)$ times, with the additional constraint $L+U+P = n$. The coefficient $C_{LU P}$ stands in front of every term. Note that terms with an even number of $\Delta^1$ functions vanish. This is a generalization of the observation that a loop integral does not get an imaginary part at a momentum constellation where two poles in the lower $k^0$-half plane coincide. This is in contrast to a pinch singularity, where the contour of integration is trapped between poles in the lower and upper half plane. We will discuss these contributions in more detail in section 2.5.

We explicitly wrote out the terms containing one $\Delta^1$ function in the first line of (14). Here, in each term, one of the propagators of the original loop is replaced by a delta function. After $k^0$ integration, all of these terms can be interpreted as tree graphs with one additional incoming and outgoing particle and an additional phase space integral over this particles momentum,

$$\int \frac{d^3k}{(2\pi)^3 2E_i}. \quad (16)$$

Note however, that the momentum which is put on-shell is $k+p_i$ and the integration is performed over $k$. In general, one must not shift the integration momentum in a single term only, since the integrand consists of several terms which are coherently summed up. Some of these terms may have peaks or may even be UV divergent, since we will not use dimensional regularization. Only in the sum of the individual tree graphs, these singularities will then be cancelled.

When a propagator is replaced by $\Delta^1_i$, setting $k+p_i$ on the mass shell, the remaining numerator can be read as the product of one additional incoming and outgoing external on-shell particle,

$$(k + p_i + m) = \sum_{\lambda} u_{\lambda}(k + p_i) \bar{u}_{\lambda}(k + p_i); \quad (17)$$

$$(k + p_i - m) = \sum_{\lambda} v_{\lambda}(k + p_i) \bar{v}_{\lambda}(k + p_i); \quad (18)$$

$$-g_{\mu \nu} = \sum_{\sigma} \epsilon_{\mu}^{\lambda}(k + p_i; \sigma) \epsilon_{\nu}(k + p_i; \sigma), \quad (19)$$
where the sum runs over all physical and unphysical internal states. For a cut fermion propagator, we will obtain the particle if the momentum flow of the loop is in the same direction as the fermion number flow, and the antiparticle otherwise.

2.1.3 Construction of graphs

Thus, any loop graph can be re-expressed as a sum of tree graphs. Turning this around, one can create the complete set of tree graphs with an inclusive incoming and outgoing particle, and sew these loose ends together to obtain loop diagrams again. One thus finds all one-loop corrections to a given $2 \rightarrow n$ process by considering all possible tree graphs with two additional particles, writing schematically

$$\mathcal{M}^{1\text{-loop}}(2 \rightarrow n) \iff \sum_X \mathcal{M}^{\text{Tree}}(2 \rightarrow n + X + \bar{X}) + \ldots$$ (20)

Here, the sum runs over the particle content of the theory, and we flipped the initial state particle to the corresponding antiparticle in the final state, using crossing symmetry.

In principle, this expression includes also tadpole diagrams and self-energy corrections to external on-shell legs. These may be set to zero by appropriate renormalization conditions; in that case, they can be ignored in the right-hand side of (20).

The creation of all relevant Feynman graphs contributing to a process in a given order is therefore reduced to the task of creating tree-level graphs with the corresponding additional particles. For this task, powerful tools exist. However, we cannot always shift momentum in the individual tree graphs freely, since as stated above, some graphs may have ultraviolet divergences which only in the coherent sum of the tree graphs cancel. Therefore, we cannot fully exploit the reduction mechanisms implemented in these tools.

2.1.4 Monte-Carlo integration

The remaining three-dimensional integral over the loop momentum can now be pulled out of the individual graphs and put in front of the amplitude, together with the phase space integrals over the external particles which is present in a cross-section calculation. Since the extra integration is also of the form of a phase-space integral, techniques developed for the integration, in particular multi-channel sampling, can immediately be adopted. Furthermore, this integration can be performed simultaneously with the external phase space integration.

Using a suitable Monte Carlo integration routine, going from Born-level processes to loop level merely amounts to an increase of the integration dimension. If integration mappings and multi-channel weights can be successfully adapted to this situation, this results just in a minor increase in the number of sampling points, if one wants to achieve a NLO precision at the same level as the LO calculation.\footnote{Of course, the calculation now involves amplitudes with an increased number of external legs, so it is essential to use a matrix-element generator with optimal scaling behavior.}

From the viewpoint of Monte-Carlo event generation, each sampling point corresponds to a particular configuration of external and internal momenta in the original loop amplitude, and the accumulation of sampling points resolves both loop and phase-space integration at the same time. This is in contrast to traditional analytical methods, where for each individual configuration of external momenta the analytical result of the loop integration has to be numerically evaluated. This task normally includes a time-costly calculation of a large number of
polylogarithms, and it is subject to numerical instabilities associated to Gram determinants, as an artifact of tensor reduction techniques.

The modified phase-space integrals inherit both the UV divergences and the IR singularities of the original loop amplitudes. Dimensional regularization and renormalization cannot be used without modifying phase space, which impedes a straightforward interpretation of physical events, so we do not consider it. In the next two sections we will instead introduce subtraction graphs as counterterms for the elimination of UV divergences and discuss the treatment of infrared poles.

2.1.5 The role of multiple cuts

The first line of (14) can also be interpreted as the result of the $k_0$ integration of the original loop, when the contour is closed in the lower half plane and only single, simple poles are picked up. Setting $i\epsilon$ to zero afterwards leads to wrong results if poles fall together and form double or multiple poles. In (14), there are additional subleading contributions which are collected in the sum in the second line, indicated by the dots in (20). These terms give a non-vanishing contribution, if the momenta of the propagators they were replaced with, go on-shell simultaneously. Since after the $k_0$ integration there are still $\delta$-functions left, these terms will get support for two dimensional surfaces, lines or points in the three-dimensional phase space volume, depending on the initial number of $\Delta_i$ functions. Since each $\Delta_i$ effectively lowers the dimension of the integration by one, the contribution of these terms can be calculated rather easily.

Replacing a propagator by a delta function reduces the number of factors $i$ by one. Terms in (14) with an even number of $\Delta_i$ will therefore give an imaginary contribution to the final result, terms with an odd number a real contribution.

Whether these terms give a non-vanishing contribution, can already be inferred from the integrand of the terms in the first line of (14). When replacing the original integral by a sum over tree graphs with one additional on-shell particle, the remaining propagators can become singular, or in other words, internal lines can get on-shell at certain values of the momentum $\vec{k}$. This leads to a peak structure which is resembled by the sub-leading terms in (14). In section 2.5 we will give the construction of smoothing functions which cancel these peaks.

2.2 Renormalization and Regularization

Going from Born-level to loop-level calculations, the initial relation between the bare parameters in the Lagrangian and the physical ones is destroyed. To restore this relation, renormalization constants are introduced, which also absorb ultraviolet divergences arising in loop calculations. These additional free parameters of the theory have to be fixed by imposing renormalization conditions.

As long as we are dealing with massive theories, a convenient set of conditions is the on-shell renormalization scheme,

$$\text{Re } i\Gamma^{(2)}_{\alpha\beta}(-p, p)\Phi^\beta(p)\bigg|_{p^2=m^2} = 0$$

$$\text{Res } (-\Gamma^{(2)}(p))^{-1}\bigg|_{p^2=m^2} = 1$$

$$\Gamma^{(3)}(p_1, \lambda)\bigg|_{p^2=m^2} = \lambda^3_0$$

$$\Gamma^{(4)}(p_1, \lambda)\bigg|_{p^2=m^2} = \lambda^4_0,$$ (21)

This requires the pole of the real part of propagators to coincide with the corresponding particle mass, with residue 1. Vertex functions are set equal to the tree level vertex functions for on-shell
external legs.

In massless QCD, there is no on-shell scheme, and it is important to satisfy Ward (or Slavnov-Taylor) identities order by order. However, we can nevertheless impose physical renormalization conditions for observable quantities and use them for defining appropriate subtractions, and it is well known that Ward identities can be satisfied, in any subtraction scheme, by introducing a complete set of counterterms with fixed coefficients. Since our proof-of-concept example is in the context of massive QED, we postpone the construction of QCD (and Standard-Model) counterterms to future work.

In multiplicative renormalization, the conditions (21) are used to relate and fix all of the renormalization constants $\delta Z_i$. By eliminating all redundancies from the renormalization conditions, one ends up with only a handful of constants with rather simple analytic expressions. These are sufficient to renormalize any diagrams in perturbation theory.

In the majority of one-loop calculations, ultraviolet divergent loop integrals are evaluated in dimensional regularization or variations of that scheme. Divergent pieces are extracted as analytic poles in the regulator $\epsilon$ and cancelled against the poles in the counterterms. Using the Feynman Tree Theorem to get a numerically integrable expression for the loop integral, we do not consider an extension of the dimension of integration and an algebraic reduction to finally extract the ultraviolet divergent pieces. In contrast to this procedure, we make use of a variation of the BPHZ procedure [26–28], which results in loop graphs acting as counterterms, which can be evaluated under the same phase space integral over the loop momentum.

Consider a 1PI one-loop graph $\Gamma^n(p_1, \ldots, p_n)$ with superficial degree of divergence $\omega(\Gamma)$. We define the T operator as a Taylor expansion around on-shell momenta $\bar{p}_i$, with $\bar{p}_i^2 = m_i^2$:

$$T \circ \Gamma^n(p_1, \ldots, p_n) = \Gamma^n(\bar{p}_1, \ldots, \bar{p}_n) + \sum_{i}^{n-1} (p_i - \bar{p}_i)^\mu \frac{\partial \Gamma^n}{\partial p_i^\mu} \bigg|_{p_1 = \bar{p}_1, \ldots, p_n = \bar{p}_n} +$$

$$\ldots + \frac{1}{d!} \sum_{i_1, \ldots, i_d}^{n-1} (p_{i_1} - \bar{p}_{i_1})^{\mu_1} \ldots (p_{i_d} - \bar{p}_{i_d})^{\mu_d} \frac{\partial^d \Gamma^n}{\partial p_{i_1}^{\mu_1} \ldots \partial p_{i_d}^{\mu_d}} \bigg|_{p_1 = \bar{p}_1, \ldots, p_n = \bar{p}_n},$$

up to $d = \omega(\Gamma)$. With this T operator, the renormalized 1PI n-point functions

$$\hat{\Gamma}^n(p_1, \ldots, p_n) = \Gamma^n(p_1, \ldots, p_n) - T \circ \Gamma^n(p_1, \ldots, p_n)$$

fulfill the renormalization conditions (21). Note, that we consider the external four-vectors in Minkowski space and not Euclidean space, which is commonly used in schemes derived from the BPHZ prescription. In our formulation, the subtraction terms arising from (22) can be complex valued. However, only the real part is needed for renormalization. For two-loop calculations, it therefore might be necessary to further restrict the subtraction terms to be the real parts of the considered graphs.

The expressions resulting from (22) can also be interpreted as loop graphs and are easily derived from the original Feynman graph.

The hard scattering part of the virtual cross section in a NLO computation of a $2 \to n$ process can therefore be written as

$$\sigma_v^{(1)} \propto \int d\Pi_n 2 \Re(\mathcal{M}^{\text{Born}}(\mathcal{M}_n^{\text{loop}} + \mathcal{M}_n^{\text{CT}})^*),$$

(24)
where we left out any parton distribution function, fragmentation or cut functions. We can now use the Feynman Tree Theorem again to cut the loop graphs and collect the individual loop integrals in a common phase-space integral:

\[
\sigma_v^{(1)} \propto \int d\Pi_n \int \frac{d^3k}{(2\pi)^3} 2\text{Re}(\mathcal{M}_n^{\text{Born}}(\mathcal{M}_{n+1}^{\text{Tree}} + \mathcal{M}_{n+1,\text{CT}}^*)^*).
\]

The resulting integrals are ultraviolet finite by construction. There are still ambiguities in (22) for the choice of the on-shell momenta \(\vec{p}_i\). To assure local cancellation of infrared divergences between the virtual matrix elements and the real emission graphs, these have to be chosen in a specific way, which will be described in section 2.4.

2.3 IR cancellations

Physically, an initial or final particle state cannot be distinguished from a state with an additional number of soft photons. It was pointed out by Kinoshita [29], Lee and Nauenberg [30] that the sum over all degenerate states is infrared safe in each order of perturbation theory. In the case of QED corrections this means that if the Born cross section of the real emission process \(\sigma_{\text{re}}^{(1)}\) with \(n\) particles and an additional photon in the final state is added to the virtual cross section \(\sigma_v^{(1)}\) the resulting total cross section is finite [31]. Assuming that the detector cannot resolve photons of energy less than \(\Delta E_s\), one can split up the real emission cross section, which is of the same order in perturbation theory than the virtual cross section, into a soft and a hard part,

\[
\sigma_{\text{re}}^{(1)} = \sigma_{\text{soft}}^{(1)}(\Delta E_s) + \sigma_{\text{hard}}^{(1)}(\Delta E_s)
\]

\[
\sigma_{\text{soft}}^{(1)}(\Delta E_s) \propto \int d\Pi_n \int \frac{d^3k}{(2\pi)^3} 2E_k |\mathcal{M}_{n+1}^{\text{Born}}|^2
\]

\[
\sigma_{\text{hard}}^{(1)}(\Delta E_s) \propto \int d\Pi_{n+1} |\mathcal{M}_{n+1,\text{CT}}^*|^2
\]

and add the soft part to \(\sigma_v^{(1)}\). The form of the two phase space integrals in (27) and (25) look very similar, they only differ by an implicit delta function conserving overall momentum of the virtual and the real emission process. We can therefore find a simple approximation of the real emission processes for momenta \(k < \Delta E_s\), such that the soft infrared poles in the virtual graphs are cancelled locally on the integrand level, allowing a numerical evaluation of (25).

Using the Tree Theorem to cut a loop graph, the infrared divergent part of the resulting integrand arises solely from the cut of massless propagators connecting two external on-shell particles. As an example, consider the photon exchange of two charged incoming fermions, as shown in figure 1. Before cutting any propagator the relevant part of the integrand reads:

\[
\frac{d^4k}{(2\pi)^4} \frac{\ldots (k + \vec{p}_1 + m_1)\gamma^\mu u_\lambda(p_1)}{k^2 + 2kp_1} \frac{-ig_{\mu\nu} \ldots (k + \vec{p}_2 + m_2)\gamma^\nu u_\sigma(p_2)}{k^2 - 2kp_2},
\]

where for better readability we chose the integration momentum such that it is equivalent to the momentum flowing through the photon line. Cutting this line, we get

\[
\frac{d^3k}{(2\pi)^3 2|k|} \sum_{\sigma} \frac{\ldots (k + \vec{p}_1 + m_1)\gamma^\mu u_\lambda(p_1)}{2kp_1} \ldots (k + \vec{p}_2 + m_2)\gamma^\nu u_\sigma(p_2) \bigg|_{k_0 = |\vec{k}|},
\]

\[
(-2kp_2) \sum_{\sigma} \frac{\ldots (k + \vec{p}_1 + m_1)\gamma^\mu u_\lambda(p_1)}{2kp_1} \ldots (k + \vec{p}_2 + m_2)\gamma^\nu u_\sigma(p_2) \bigg|_{k_0 = |\vec{k}|},
\]

\[
\frac{d^3k}{(2\pi)^3 2|k|} \sum_{\sigma} \frac{\ldots (k + \vec{p}_1 + m_1)\gamma^\mu u_\lambda(p_1)}{2kp_1} \ldots (k + \vec{p}_2 + m_2)\gamma^\nu u_\sigma(p_2) \bigg|_{k_0 = |\vec{k}|},
\]

\[
\frac{d^3k}{(2\pi)^3 2|k|} \sum_{\sigma} \frac{\ldots (k + \vec{p}_1 + m_1)\gamma^\mu u_\lambda(p_1)}{2kp_1} \ldots (k + \vec{p}_2 + m_2)\gamma^\nu u_\sigma(p_2) \bigg|_{k_0 = |\vec{k}|},
\]

\[
\frac{d^3k}{(2\pi)^3 2|k|} \sum_{\sigma} \frac{\ldots (k + \vec{p}_1 + m_1)\gamma^\mu u_\lambda(p_1)}{2kp_1} \ldots (k + \vec{p}_2 + m_2)\gamma^\nu u_\sigma(p_2) \bigg|_{k_0 = |\vec{k}|},
\]
which is logarithmically divergent in the limit $|\vec{k}| \to 0$. This loop amplitude is multiplied with a Born amplitude $M_{\text{Born}}$. Neglecting the term $\frac{1}{k}$ in the numerator we can shift the incoming photon line on the leg of particle 1 to the Born matrix element, whose relevant part is just the Dirac wave function $\bar{u}_\lambda$ of this particle connected to a Dirac matrix $\gamma^\rho$:

$$\frac{\ldots (\not{p}_1 + m_1)\gamma^\mu u_\lambda(p_1)\bar{u}_\lambda(p_1)\gamma^\rho \ldots}{2kp_1} \epsilon_{\mu}(k, \sigma) \to \frac{\ldots u_\lambda(p_1)\bar{u}_\lambda(p_1)\gamma^\rho (\not{p}_1 + m_1)\gamma^\rho \ldots}{2kp_1} \epsilon_{\mu}(k, \sigma).$$  \hspace{1cm} (31)

Taking the hermitian conjugate of the right part and adding another $\frac{1}{k}$ term in the numerator, we get

$$\frac{\ldots \bar{u}_\lambda(p_1)\gamma^\mu (\not{p}_1 + m_1)\gamma^\rho \ldots}{2kp_1} \epsilon_{\mu}(k, \sigma) \to \frac{\ldots \gamma^\rho (\not{k} + \not{p}_1 + m_1)\gamma^\mu u_\lambda(p_1)}{2kp_1} \epsilon^*_{\mu}(k, \sigma).$$  \hspace{1cm} (32)

This corresponds to the Born diagram with an additional outgoing on-shell photon attached to one external line times an overall factor $-1$, which would usually arise from the propagator adjacent to the emitted photon,

$$(k - p_1)^2 - m^2 = -2kp_1.$$  \hspace{1cm} (33)

After the above transformations, which involved manipulations of the numerator of $O(|\vec{k}|)$, the original loop becomes also a Born graph with a photon emitted from particle 2. Thus, in the limit $|\vec{k}| \to 0$ the divergent piece of the one-loop contribution is exactly cancelled by the product of two real emission diagrams.

If we obtain the two real emission diagrams from the loop diagram in the way shown above, momentum conservation is violated in both graphs at some vertex. This happens, because the initial delta function conserving the momenta of the external particles in the initial loop diagram is still present in the real emission diagrams. The additional particle violates momentum conservation. Although the integration measure is the same in both cases, the true real emission diagrams are accompanied by a delta function $\delta(P - \sum q_f - q_\gamma)$ conserving overall momentum.

Momentum conservation at some vertices is also violated in the soft photon approximation, e.g. cf. [22,33]. Here, following the same reasoning as above, the contribution of real emission diagrams in the soft limit is approximated by the Born amplitude times a prefactor. This factor can be evaluated analytically, e.g., when regulated by a photon mass. Adding this expression to the analytic results of loop graphs, the divergent terms, logarithms of the photon mass, cancel.
If we want to evaluate the soft real emission diagrams and the loop corrections under the same integral, we need a method of implementing the projection of the, e.g. $2 \rightarrow n + \gamma$ real emission graphs onto the $2 \rightarrow n$ virtual graphs. Reversing the above approximation, we could add the product of two real emission diagrams with momentum violation at the first vertex after the emission of the massless particle. However, adding the product of the two diagrams will only cancel the infrared divergence in the product of the loop graph with the corresponding Born graph. We intend to apply the Feynman Tree Theorem on the amplitude level and compute the interference with the Born terms after summation of all contributing loop graphs. Applying the Tree Theorem to products of loop and Born graphs would lead to a drastic increase of the number of terms, if a process with several Born terms is considered.

We therefore need a prescription of incorporating the effect of real emission diagrams in single infrared divergent loop graphs. In the following, we set the term with the cut propagator associated with the massless particles to zero for $|\vec{k}| < \Delta E_s$. This simple prescription is sufficient for the QED process considered in the present paper, as demonstrated by the numerical results. For a generic solution one would have to adapt a method such as phase-space slicing or dipole subtraction to the present situation.

2.4 UV subtractions and IR divergences

There is a one-to-one correspondence between the interference terms of Born graphs with loop diagrams with a cut massless particle and the product of two real emission diagrams of this particle, regarding the infrared behavior. This means that for any virtual infrared divergence in an unrenormalized loop, there is a product of two real emission diagrams with emission of this particle from external legs, cancelling this divergence.

However, there are still infrared divergent terms left. On the one hand those which correspond to the square of one real emission diagram and therefore would arise from self-energy corrections to an external particle, which are set to zero by the on-shell renormalization scheme. On the other hand, further infrared divergent contributions arise from subtraction diagrams used as counterterms to cancel ultraviolet divergent virtual contributions. In this section we will argue that by a certain choice of the subtraction diagrams these additional infrared divergences cancel and the final result is infrared finite.

The following considerations apply to the case of QED, but the generalization to QCD and the SM, given a suitable renormalization scheme, is straightforward.

In QED, there are three primitively ultraviolet divergent graphs $\Gamma$. These are the photon and electron self-energy and the vertex correction. The renormalized one-loop photon self-energy is infrared finite. In the following we will argue that the infrared divergent terms of the square of real emission diagrams and of the electron self-energy will be compensated by the subtraction diagrams of the vertex corrections.

Consider an amplitude $M_0$ with an incoming on-shell electron with momentum $p$ and mass $m$. The electron line is attached to a vertex $\mathcal{V}$. If we radiate off a real photon from this line and square the amplitude, the infrared divergent term can be obtained from soft photon approximation and reads:

$$I_{re} = -e^2 |M_0|^2 \cdot \int \frac{d^3 k}{(2\pi)^3 |\vec{k}|} \frac{m^2}{(pk)^2}. \quad (34)$$

The radiative correction to the vertex $\mathcal{V}$ is infrared divergent if the outgoing fermion line is on-shell. As shown in section 2.3 this divergence is cancelled by the product of two real emission
diagrams with the photon attached to the incoming and outgoing fermion line, respectively. As argued in section 2.2, to relate experimental results with theoretical calculations we subtract the vertex correction at the Thomson limit where the momentum of the photon attached to the vertex \( V \) is zero and the fermion going through the vertex is on-shell. If we split the subtraction term in two pieces, where in one term the on-shell fermion line through the vertex \( V \) has momentum of the incoming electron and in the second term it has the momentum of the outgoing fermion, the loop contribution of one of these terms is

\[
\frac{1}{2} (-ie)^2 \int \frac{d^4k}{(2\pi)^4} \cdots \frac{\gamma_k (\not{p} + \not{k} + m) (-ie\gamma_\mu) (\not{p} + \not{k} + m) \gamma^\alpha}{k^2 (k^2 + 2pk)^2} \cdots ,
\]

(35)

where we explicitly pulled out the couplings \((-ie)\) from the \(\gamma_\alpha\) and the factors \((i, -i)\) coming from the propagators. As can be seen from (35), the ultraviolet contribution of the subtraction terms are independent from the external momenta of the vertex correction. Thus, the subtraction graph can be split in parts with different momentum assignments without affecting the cancellation of the UV divergence.

Cutting the photon line of the loop with momentum \( k \) and neglecting terms proportional to \( k \) in the numerator we get:

\[
-\frac{e^2}{2} \int \frac{d^3k}{(2\pi)^3 |k|} \cdots \frac{4m(-iep_\mu)}{(2pk)^2} \cdots .
\]

(36)

If we straighten the fermion line such that throughout the graph it has the on-shell momentum \( p \), with no momentum flowing in or out at any vertex, this fermion line can be written as a chain of products of Dirac wave functions and \(\gamma\)-matrices:

\[
\cdots \bar{u}(p)\gamma_\kappa u(p)\bar{u}(p)\gamma_\lambda u(p)\bar{u}(p)p_\mu u(p)\bar{u}(p)\cdots ,
\]

(37)

where at the place of the former vertex correction only a factor proportional to \( p_\mu \) remains. Making use of the Gordon identity

\[
\bar{u}(p)p_\mu u(p) = m\bar{u}(p)\gamma_\mu u(p),
\]

(38)

the infrared divergent term can be factored out of the amplitude.

\[
-\frac{e^2}{2} \int \frac{d^3k}{(2\pi)^3 |k|} \frac{4m^2}{(2pk)^2} \cdot \mathcal{M}'_0.
\]

(39)

Here, \( \mathcal{M}'_0 \) is the matrix element \( \mathcal{M}_0 \) with all lines attached to the fermion line bearing zero momentum. Since we factored out the infrared divergent part, we can divide by \( \mathcal{M}'_0 \) and multiply by \( \mathcal{M}_0 \), to compensate for the projection onto the straight fermion line. In explicit calculations we therefore subtract the graph with the vertex correction, where we keep the momentum of the fermion fixed throughout the graph and neglect the denominator of the rest of the matrix element which does not belong to the loop. We then divide by the same matrix element without vertex correction and multiply by the basic amplitude \( \mathcal{M}_0 \). Doing so, we apply the correct subtraction terms to the unrenormalized loop graph in the sense that in the limit, where the momentum of the photon attached to \( V \) vanishes, the one-loop graph and the subtraction graphs cancel each other. This leaves the Born graph, which just contains the electric charge at the vertex, \((-ie\gamma_\mu)\), as required by the renormalization conditions. Since the
uv-ir subtraction terms: the vertex correction is renormalized by the subtraction of two graphs with zero incoming photon momentum. when the photon propagator of the loops is cut, the arising infrared divergences in the interference term are compensated by the product of real emission diagrams depicted on the right hand side.

ultraviolet contributions of the subtraction graphs are independent of the external momenta ab initio, this procedure does not invalidate the uv cancellation.

The resulting infrared divergent term of the interference with the amplitude \( M_0 \), which comes with a factor 2 in the final cross section, becomes:

\[
I_{v1} = -e^2 |M_0|^2 \int \frac{d^3k}{(2\pi)^3} \frac{m^2}{|k| (pk)^2},
\]

which exactly cancels the above infrared divergent term (34) of the soft real emission when subtracted from the unrenormalized vertex correction. the second half of the subtraction term, \( I_{v2} \), is equivalent to \( I_{v1} \) with \( p \) replaced by the on-shell momentum \( \bar{q} \) of the outgoing fermion. if this is an external particle, the infrared divergence is cancelled by the corresponding real emission diagrams and we are finished. this case is summarized in figure 2. on the left hand side we depicted the renormalized vertex correction. the coefficients are given by \( c_i = M_0 M_0^{-1}(p_i) \). when the photon lines of the loops are cut, the infrared divergences arising in the interference term are cancelled by the real emission diagrams shown on the right hand side.

If the outgoing fermion belongs to an internal line, we will show in the following that the infrared divergent part is cancelled by the subtraction terms to the self-energy correction to this internal line.

As was shown in section 2.2, in the case of an self-energy correction to an internal charged fermion line, we need two subtraction terms to cancel the uv divergence. we subtract the same graph at an on-shell momentum \( \bar{q} \) aligned to the original momentum \( q \) and the derivative of the self-energy with respect to \( q \) at \( \bar{q} \). the relevant part of this diagram is given by the electron self-energy

\[
- e^2 \int \frac{d^4k}{(2\pi)^4} \frac{\gamma_\alpha(\not{q} + \not{k} + m)\gamma^\alpha}{k^2((k+q)^2 - m^2)} \dot{\gamma}_\mu((\not{k} + \not{q} - m)^\mu). \tag{41}
\]

Replacing \( q \) by \( \bar{q} \) will not lead to an infrared singular term, since the singularity in the denominator is cancelled by the integration measure. making use of the identity

\[
\frac{\partial}{\partial q^\mu} (\not{k} + \not{q} - m) = \frac{i}{(\not{k} + \not{q} - m)} (\gamma^\mu (\not{k} + \not{q} - m)), \tag{42}
\]

the second subtraction term can simply be obtained by straightening the fermion line through the self-energy part, insertion of a dirac gamma matrix \( \gamma_\mu \) in the fermion line and multiplying by \( (q - \bar{q})^\mu \):

\[
- ie^2 \int \frac{d^4k}{(2\pi)^4} \frac{\gamma_\alpha(\not{q} + \not{k} + m)(\not{q} - \not{\bar{q}})(\not{q} + \not{k} + m)\gamma^\alpha}{k^2((k+q)^2 - m^2)^2} \dot{\gamma}_\mu((\not{k} + \not{q} - m)^\mu). \tag{43}
\]
Cutting the photon line and simplifying the numerator, the divergent part is
\[-e^2 \cdot \int \frac{d^3k}{(2\pi)^3|k|} \frac{i(q - \bar{q})\bar{\gamma}_\mu q_\mu}{(\bar{q}k)^2} \cdot \cdots (-\bar{q} + 2m) \cdots . \tag{44}\]

We can again interpret the fermion line as a chain of Dirac wave functions. Thus, the factor 
\((-\bar{q} + 2m)\) simplifies to \(m\) and with the use of the Gordon identity \([\text{38}]\) we write
\[i(q - \bar{q})\bar{\gamma}_\mu q_\mu = m \cdot i(q - \bar{q})\gamma_\mu = m \cdot i(\bar{q} - m).\]  

This is \(m\) times \(M_0'\), the matrix element with an insertion of \(i(\bar{q} - m)\) at the place of the original self-energy correction. Like in the case of the vertex correction we then have a Lorentz scalar factored out of the amplitude \(M_0'\) with a straight fermion line. To project this counterterm on the onto the matrix element with the original kinematics, \(q\) instead of \(\bar{q}\), we multiply by \(M_0'^{-1}\) and the Born matrix element with the additional insertion \(i(\bar{q} - m)\) at the place of the original self-energy correction. With the two propagators connecting to this 2-point vertex we have:
\[\cdots \frac{i(\bar{q} + m)}{q^2 - m^2} i(q - m) \frac{i(\bar{q} + m)}{q^2 - m^2} \cdots \cdots \frac{-i(\bar{q} + m)}{q^2 - m^2} \cdots ,\]  

which is proportional to the Born matrix element \(M_0\). Multiplying again with \(2M_0\) to calculate the interference term contributing to the cross section, the infrared divergent part of the subtraction terms to the electron self-energy reads:
\[I_\Sigma = 2e^2 |M_0|^2 \cdot \int \frac{d^3k}{(2\pi)^3|k|} \frac{m^2}{(\bar{q}k)^2}. \tag{47}\]

When subtracted from the unrenormalized self-energy correction, half of the infrared divergent term cancels the contribution coming from the subtraction graph of the vertex correction \(I_{v2}\), obtained from \([\text{10}]\) by replacing \(p\) with \(\bar{q}\). Following the fermion line further we again come to a vertex and its correction terms will cancel the second half of the infrared divergent term of the subtraction graphs of electron self-energy. This goes on until the last vertex, where the second infrared contribution of its subtraction graphs will then be compensated by the squared amplitude of the real emission of a photon of the external line following this vertex.

This completes our renormalization prescription, which trivially extends to processes with multiple Born graphs. We constructed subtraction graphs which cancel all possible ultraviolet divergences and give further infrared divergent contributions such that in the sum of all graphs contributing to a given process the infrared divergences cancel. Furthermore the renormalized vertex functions obey the renormalization conditions \([\text{21}]\) such that the experimentally measured observables can directly be related to the theoretical predictions without any further analytic correction.

We showed that in QED we have a complete prescription to incorporate the on-shell renormalization scheme and cancel all infrared and ultraviolet divergences. Although not rigorously proven, this method should also be applicable to the electroweak standard model. Subtraction graphs to only ultraviolet divergent vertices can be found by the introduced BPHZ mechanism. In case of a photonic correction, where infrared divergences are expected, the proposed method of this section should also lead to finite results.
2.5 Threshold singularities

When the momentum integration is performed in the first line of (14), the integrand might get peaks in parts of the phase space where momenta of un-cut propagators are on-shell. These regions are open or closed two-dimensional surfaces in the three-dimensional integrand. Intersections of these surfaces correspond to kinematic situations where two or more momenta of internal lines become on-shell at the same time. The occurrence of such peaks, although analytically integrable, leads to problems in the numerical evaluation of the integrand. Subtraction terms with zero real value but with the same peak structure will smooth the integrand and allow for a better convergence in the numerical evaluation. In this section we will give the conditions under which peaks of the integrand arise and calculate the corresponding fixing functions.

Cutting a propagator $P_i$ in a loop leads to a delta function $\Delta^i_l$, given in (7), which effectively sets the four-vector $k + p_i$ on its mass-shell at $(k + p_i)^2 = m_i^2$ with positive zero component. There are two possible situations under which another propagator $P_j$ can get singular. Its original $k_0$-poles lie either in the lower or upper half plane, which corresponds to the positive and negative zero components $\pm E_j$. After the $k_0$ integration the relevant term of the integrand in the Tree Theorem (14) reads:

$$\Delta^i_l P_j R(k) = \frac{1}{2E_i} \frac{i}{[(p_j^0 - p_i^0) + (E_i - E_j)][(p_j^0 - p_i^0) + (E_i + E_j)]} R(-p_j^0 + E_i, \vec{k}),$$

where $R(k)$ is the analytic remainder of the term, containing the numerator and denominators of further propagators which for now are assumed to be non-singular in the integration volume. If the first factor in the denominator vanishes for some $\vec{k}$, both momenta of the two propagators $P_i$ and $P_j$ get on-shell with a positive zero component. In other words, at this constellation of the integration momentum $\vec{k}$, the two poles in the lower $k_0$ half plane of the original loop momentum coincide. Therefore, we will also encounter this singularity when propagator $P_j$ is cut:

$$\Delta^j_l P_i R(k) = \frac{1}{2E_j} \frac{i}{[(p_i^0 - p_j^0) + (E_j - E_i)][(p_i^0 - p_j^0) + (E_j + E_i)]} R(-p_i^0 + E_j, \vec{k}).$$

In the limit of the first factor becoming zero, the residue of the combined contribution vanishes:

$$\lim_{(p_i^0 - p_j^0) + (E_i - E_j) \to 0} \left( (p_j^0 - p_i^0) + (E_i - E_j) \right) \left( \Delta^i_l P_j R(k) + \Delta^j_l P_i R(k) \right)$$

$$= \frac{i}{2E_i 2E_j} \left( R(-p_i^0 + E_i, \vec{k}) - R(-p_j^0 + E_i, \vec{k}) \right) = 0.$$

Thus, if the two terms are added, the peaks will compensate each other and the integrand can safely be evaluated numerically in this case.

Whenever a propagator $P_j$ gets singular in the integration region, one of the corresponding delta functions, $\Delta^i_l$ or $\Delta^j_u$ get support at these regions in phase space. Therefore, the final result for the loop integral gets further contributions from the higher order terms in the Feynman Tree Theorem (14), if these threshold peaks in the integration region are encountered during the integration of the leading order terms in (14).

The situation described above would correspond to a coincidence of two poles in the lower $k^0$ half plane. However, in the sum of the tree graphs, there are two peaks arising from two
different tree graphs, which cancel in the sum. Accordingly, we also did not get a term in (14) with only two $\Delta_l$. Therefore, just like there is no peak in the sum of the tree level contribution there is also no imaginary contribution to the final result in this case.

In the case where the second factor in (18) becomes singular, we will get a peak which remains in the sum of the tree graphs. This happens, if one pole of the lower $k_0$-half plane coincides with a pole in the upper half plane. In this case, there is a term with one $\Delta_l$ and one $\Delta_u$ which get support simultaneously and lead to the imaginary part of the loop graph.

2.5.1 Conditions for Internal Singularities

We can look for general conditions under which a loop propagator $P_j$ becomes singular if we cut a propagator $P_i$, and give equations for the corresponding surfaces. Cutting propagator $P_i$, we have:

$$0 \equiv (k + p_j)^2 - m_j^2 |_{k_0 = -p_i^0 + \sqrt{(k + p_i)^2 + m_i^2}},$$

$$\equiv ((k + p_i) + (p_j - p_i))^2 - m_j^2 |_{k_0 = -p_i^0 + \sqrt{(k + p_i)^2 + m_i^2}},$$

$$\equiv m_i^2 - m_j^2 + 2(k + p_i)(p_j - p_i) + (p_j - p_i)^2 |_{k_0 = -p_i^0 + \sqrt{(k + p_i)^2 + m_i^2}}. \quad (51)$$

The occurrence and the shape of the peaks depend on the value of $p_{ji}^2 \equiv (p_j - p_i)^2$. We can distinguish 4 kinematic regions, separated by $p_{ji}^2 = 0$ and the two nodes $\lambda(p_{ji}^2, m_i^2, m_j^2) = 0$ of the kinematical function $\lambda$, defined by

$$\lambda(x, y, z) = x^2 + y^2 + z^2 - 2xy - 2xz - 2yz. \quad (52)$$

The different regimes are depicted in figure 3.

We switch to Lorentz frames where the calculation of solutions to (51) is particularly simple. We first discuss the case of negative $p_{ji}^2$.

- $p_{ji}^2 < 0$, Region I
Here, we cannot find a rest frame of \( p_j - p_i \), however, we can define a Lorentz transformation projecting \( p_j - p_i \) onto the z-axis:

\[
\Lambda^{\mu\nu}(p_j - p_i)_{\nu} = (0, 0, 0, p_{ji}^z),
\]

(53)

\[
-p_{ji}^z = (p_j - p_i)^2,
\]

(54)

\[
k^{\mu\nu} \equiv \Lambda^{\mu\nu} k_{\nu}.
\]

(55)

Using this transformation we get for (51):

\[
0 \overset{1}{=} m_i^2 - m_j^2 + 2(k + p_i)(p_j - p_i) + (p_j - p_i)^2,
\]

\[
\overset{L.T.}{=} m_i^2 - m_j^2 + 2k(p_j - p_i) + p_j^2 - p_i^2,
\]

\[
\Rightarrow k^2_\alpha = \frac{(p_j^2 - m_j^2) - (p_i^2 - m_i^2)}{2p_{ji}^z}.
\]

(56)

There are no further conditions for this singularity to appear. Thus, we will always encounter it in the case of \((p_j - p_i)^2 < 0\). However, if we cut propagator \( P_j \), propagator \( P_i \) will exactly have the same singularity with opposite sign. This can be seen from the derivation of (56) by interchanging indices \( i \) and \( j \), but applying the same Lorentz transformation as before. As a result we have the situation described in the beginning of this section and the two peaks will cancel each other in the sum of the tree graphs.

• \( p_{ji}^2 > 0 \), Regions II - IV

Here, we apply a Lorentz transformation to get into the rest frame of \( p_j - p_i \):

\[
(p_j - p_i)^\mu \rightarrow p_{ji}^{\mu} = \Lambda^{\mu\nu}(p_j - p_i)_{\nu} = (p_{ji}^0, 0),
\]

(57)

\[
p_{ji}^{02} = (p_j - p_i)^2.
\]

(58)

We indicate \( k' \) as the Lorentz transformed on-shell momentum:

\[
k^\mu = (\sqrt{k'^2 + m_i^2}, \vec{k}') = \Lambda^{\mu\nu}(k + p_i)_{\nu}.
\]

(59)

With this parameterization of \( k^{\mu\nu} \) the Lorentz transformation has to be of proper orthochronous type, which implies that \( p_{ji}^0 \) may be both positive or negative. We thus get from (51):

\[
m_i^2 - m_j^2 + 2p_{ji}^0 \sqrt{k'^2 + m_i^2 + p_{ji}^{02}} = 0,
\]

(60)

\[
\sqrt{k'^2 + m_i^2} = \frac{m_j^2 - m_i^2 - p_{ji}^{02}}{2p_{ji}^0}.
\]

(61)

\[
\Rightarrow k'^2 = \frac{1}{4p_{ji}^02}(m_i^4 + m_j^4 + p_{ji}^{04} - 2m_i^2p_{ji}^{02} - 2m_j^2p_{ji}^{02} - 2m_i^2m_j^2).
\]

(62)

Therefore, the integrand gets singular at

\[
k_s = \frac{\lambda^\pm(p_{ji}^{02}, m_i^2, m_j^2)}{2|p_{ji}^0|},
\]

(63)

\(^3\text{Bold letters indicate absolute values of spatial vectors}\)
the surface of a sphere with radius $k_s$. The kinematical function $\lambda$ is defined in (52). To get to equation (63), two conditions have to be met to satisfy equations (61) and (62):

\begin{equation}
\frac{m_i^2 - m_j^2 - p_{ji}^0}{2p_{ji}^0} > 0, \tag{64}
\end{equation}

\begin{equation}
\lambda(p_{ji}^0, m_i^2, m_j^2) > 0. \tag{65}
\end{equation}

The function $\lambda(p_{ji}^0, m_i^2, m_j^2)$ is positive for $p_{ji}^0 < (m_i - m_j)^2$ and $p_{ji}^0 > (m_i + m_j)^2$. Condition (65) therefore defines the three kinematic ranges for $p_{ji}^0 > 0$, depicted in figure 3. If the kinematical function $\lambda$ is positive we have to check if condition (64) is fulfilled. We also check the similar condition of propagator $P_i$ getting singular if propagator $P_j$ is cut. This condition reads

\begin{equation}
\frac{m_i^2 - m_j^2 - p_{ji}^0}{2p_{ji}^0} < 0. \tag{66}
\end{equation}

**II:** $0 < p_{ji}^0 < (m_i - m_j)^2$

Suppose $m_i > m_j$. Then condition (64) simplifies to $p_{ji}^0 < 0$. The numerator of (66) is:

\begin{equation}
m_i^2 - m_j^2 - p_{ji}^0 > m_i^2 - m_j^2 - (m_i^2 - 2m_i m_j + m_j^2) = 2m_j(m_i - m_j) > 0. \tag{67}
\end{equation}

Thus, condition (66) is now $p_{ji}^0 < 0$, the same as (64). Therefore, if these conditions are fulfilled, we will get a singularity in both terms, when propagator $P_i$ is cut and propagator $P_j$ gets singular and vice versa. Again, this is the situation described in the introduction to this section, when both zero components of the on-shell momenta are positive. This can be seen in the following. If propagator $P_i$ is cut, the denominator of propagator $P_j$ can be written as:

\begin{equation}
\left[ \sqrt{k^2 + m_i^2 + p_{ji}^0} - \sqrt{k^2 + m_j^2} \right] \cdot \left[ \sqrt{k^2 + m_i^2 + p_{ji}^0} + \sqrt{k^2 + m_j^2} \right]. \tag{68}
\end{equation}

The first factor corresponds to the pole in the lower $k_0$ half plane. Its vanishing indicates the coincidence of the original poles of the two propagators. We have

\begin{equation}
\sqrt{k^2 + m_i^2 + p_{ji}^0} = \frac{m_i^2 - m_j^2 + p_{ji}^0}{2p_{ji}^0} > \frac{m_j^2 - 2m_i m_j + m_i^2}{2p_{ji}^0} = \frac{2m_j(m_j - m_i)}{2p_{ji}^0} > 0. \tag{69}
\end{equation}

Therefore, the second factor is strictly positive and the singularity can only arise from the first factor. Thus, the two poles of the lower half plane fall together and the corresponding peaks cancel each other as shown above. The analysis for $m_j > m_i$ is analogous and leads to the same result.

**III:** $(m_i - m_j)^2 < p_{ji}^0 < (m_i + m_j)^2$

In this region condition (65) is not fulfilled. Therefore the integrand does not get a singular contribution from propagator $j$.

**IV:** $(m_i + m_j)^2 < p_{ji}^0$

In this case the numerator of condition (64) as well of condition (66) is strictly negative. Thus, exactly one of the two condition is fulfilled. Note also that if condition (64) is
fulfilled, meaning \( p_{ji}^0 < 0 \), the second factor of (68) vanishes. Thus, while one propagator gets on-shell with a positive zero component, the other has a negative zero component. Here, the singularity is not compensated by another term in the Tree Theorem, and we will add a fixing function to cancel this singularity, as will be shown in section 2.5.2. In this kinematic range, the final result also gets a contribution from the double delta terms in equation (14). This adds to the imaginary part of the integral. Here, we have exactly the situation of the optical theorem, where to calculate the imaginary part of a forward scattering amplitude two propagators are set on-shell simultaneously.

- \( \lambda = 0 \)

There are two more cases which we have not discussed yet: \( p_{ji}^2 = (m_i - m_j)^2 \) and \( p_{ji}^2 = (m_i + m_j)^2 \). In case the two points fall together, we either have \( m_i = 0 \) or \( m_j = 0 \) or both at the same time. These are mass singularities, where the integrand is not just singular but divergent. These divergences are compensated by the addition of real emission graphs, as discussed in section 2.4.

If the kinematical function \( \lambda \) gets zero at two different values of \( p_{ji}^2 \), which happens if both masses are non-zero, the argumentation of the case \( p_{ji}^2 < (m_i - m_j)^2 \) does not change in the limit \( p_{ji}^2 = (m_i - m_j)^2 \) and we do not encounter any peaks in the integrand. However, if \( p_{ji}^2 = (m_i + m_j)^2 \), we are at the threshold where the two real particles with masses \( m_i \) and \( m_j \) can be produced at the same time. These are Coulomb singularities, where higher order corrections in perturbation theory can become equally important. To get meaningful results, resummation methods can be applied, e.g. cf. [34]. In general, these peaks are pointlike and integrable, setting the origin of the integration variables to this point and using spherical coordinates will smooth these peaks.

### 2.5.2 Fixing Functions

We are now going to construct subtraction terms (which we denote as fixing functions) which will compensate the singularities of the integrand without adding a real part to the result.

Suppose we have replaced propagator \( P_i \) with \( \Delta_i^l \) and propagator \( P_j \) gets singular on a surface in the integration volume, thus conditions (64) and (65) are fulfilled. The integral is then

\[
\int \frac{d^3k}{2\sqrt{(k + p_i)^2 + m_i^2}} \frac{R(k)}{(k + p_i + p_j - p_i)^2 - m_j^2},
\]

where \( R(k) \) is the analytic rest of the integrand and \( k + p_i \) is taken on-shell. We now change the integration momentum to the three-momentum of \( k^{\mu} = \Lambda^{\mu\nu}(k + p_i)_\nu \) in the rest frame of \( p_j - p_i \) and switch to spherical coordinates with radial coordinate \( k' \)

\[
\int \frac{k'^2dk'd\Omega}{2\sqrt{k'^2 + m_i^2} m_j^2 - m_i^2 + 2p_{ji}^0 \sqrt{k'^2 + m_i^2 + p_{ji}^0}}.
\]

Here we used the Lorentz invariance of the integration measure \( d^3k/2E_i \). In this system the peak lies on a surface of a sphere with radius \( k_s \) given by (63). Expanding the denominator

---

4The idea of adding a zero to the integrand which smooths the peaks is taken from [24]. In this section we will give an construction of single fixing functions and also derive fixing functions in case of overlapping peaks.
around $k_s$ yields

$$
\int \frac{k'^2 dk' d\Omega}{2\sqrt{k'^2 + m_i^2}} \frac{R(\Lambda^{-1}k' - p_i)}{\sqrt{k'^2 + m_i^2}(k' - k_s) + \mathcal{O}((k' - k_s)^2)}.
$$

Taking the limit $k' \to k_s$ the residue of the integrand is

$$
\text{Res}(k'_s) = \frac{k_s}{4p_{ji}'} R(\Lambda^{-1}k'_s - p_i).
$$

Here, $k'_s$ is a four-vector with the spatial part fixed onto the surface with radius $k_s$:

$$
k'_s = (\sqrt{k_s^2 + m_i^2}, k_s \frac{k'}{|k'|}).
$$

If we subtract

$$
\frac{\text{Res}(k'_s)}{k' - k_s}
$$

from the integrand, this additional term does not add to the principal value of the integral if it is integrated over a region with symmetrical borders around the singular point $k_s$. The peak of the original integrand vanishes.

Thus, we can define a fixing function, which in the rest frame of $p_j - p_i$ reads

$$
\text{Fix}(k', k'_s) \equiv \frac{k_s R(\Lambda^{-1}k'_s - p_i)}{4p_{ji}'} \left( \frac{1}{k' - k_s} - \frac{2k' - k_s}{c^2} + \frac{(k' - k_s)^3}{c^4} \right) \theta(k' - (k_s + c)) \theta((k_s + c) - k'),
$$

with $\theta(x)$ being the step function. Here, we also added a linear and cubic term in $(k' - k_s)$, to make the joined integrand continuous and differentiable at the artificial borders introduced by the theta functions. Since the integration over the radial coordinate $k'$ runs from zero to infinity, the width $c$ of this subtraction term can maximally be taken to be the radius $k_s$. In the numerical evaluation stable results were obtained, when we took the width of support of the subtraction term equal to the infrared cutoff, $c = \Delta E_s$.

Transforming back to the original momentum of integration, we get

$$
\int d\k' d\Omega \text{Fix}(k', k'_s) = \int \frac{d^3k'}{k'^2} \text{Fix}(k', k'_s) = \int \frac{||\Lambda|| d^3k'}{\Lambda(k + p)^2} \text{Fix}(||\Lambda(k + p)||, k'_s(\Lambda(k + p))),
$$

where $\Lambda(k + p)$ is the spatial part of the transformed four-vector and $||\Lambda||$ the corresponding Jacobian. In (77), we also indicated the dependence of the fixed four-vector $k'_s$ on the spatial integration momentum $k'$ in the second argument of the fixing function.

When added to the integrand, the subtraction term (77) cancels the peak which arises when a pole in the lower $k^0$ half plane and a pole in the upper half plane fall together in the original loop integrand. Note that the double delta term in (14) including $\Delta_1^i$ and $\Delta_2^j$ is supported at $k' = k_s$ and adds an imaginary part to the result.

### 2.5.3 Overlapping Peaks

If propagator $P_i$ is cut, there might also exist a further propagator $P_k$ fulfilling the conditions (64) and (65) in addition to propagator $P_i^\parallel$. If this is the case, another fixing function has to

---

5 The kinematical function $\lambda(p^2, m_i^2, m_i^2)$ of two adjacent loop propagators can only be positive if the momentum $p^2$ of the external particle is off-shell. For loop graphs with only on-shell external legs, the above possibility...
be added to the same integrand smoothing the second peak. In a general inertial frame the peaks have the form of rotational ellipsoids. In principle, these two peaks may overlap, leading to a line in the integration volume where both propagators $P_j$ and $P_k$ can get singular at the same time. This is equivalent to a non-vanishing contribution of a term including the three delta functions $\Delta^l_i \Delta^u_j \Delta^v_k$ in (14). In this case we have to add a further fixing function.

The conditions for the occurrence of the two peaks, (64) and (65), as well as the condition for an intersection of these peaks can be checked numerically. When cutting propagator $P_i$ in the rest frame of $p_j - p_i$, the radius of the sphere where propagator $P_j$ gets singular is given by (63). With this we can construct the on shell four-vector (74). We now transform into the rest frame of $p_k - p_i$:

$$k_\mu' = \Lambda^{\mu\nu} k_{s\nu}, \quad k_s = (\sqrt{k_i^2 + m_i^2}, k_s, \frac{k_s}{|k_s|}).$$  \hspace{1cm} (78)

Similar to (61), propagator $P_k$ gets singular if

$$m_i^2 - m_k^2 + 2\sqrt{p_{ki}^2 p_{ki}^{0}} \sqrt{k_i^2 + m_i^2 + p_{ki}^2} = 0,$$  \hspace{1cm} (79)

where $k_s'$ is the absolute value of the spatial part of the four-vector $k_s'$ in (78) and $p_{ki}^0$ is the non-transformed zero component of $p_{ki} = p_k - p_i$. Using

$$\Lambda(\beta) k = \gamma^2 (k_0 - \beta k)^2 - m^2,$$ with $\beta = \frac{p^0}{\sqrt{p^2}}, \quad \gamma = \frac{|p^0|}{\sqrt{p^2}}.$$

we get

$$m_i^2 - m_k^2 + 2\sqrt{p_{ki}^2 p_{ki}^{0}} \gamma (k_i^0 - \beta k_s^0) + p_{ki}^2 = 0.$$  \hspace{1cm} (80)

Using $\gamma = \frac{|p^0|}{\sqrt{p_{ki}^2}}$ and equation (61) to replace $k_0^0$ we obtain:

$$\beta k_s = \frac{m_i^2 - m_k^2 + p_{ki}^0}{2p_{ki}^0} + \frac{m_j^2 - m_i^2 + p_{ji}^0}{2p_{ji}^0}. \hspace{1cm} (81)$$

This condition is fulfilled if the righthand side is between the bounds $+|\beta k_s|$ and $-|\beta k_s|$. If this is the case, we have to add a third fixing function in the region where the two singularities overlap. This will be shown in the following.

For better readability, we are now changing to a more symbolic notation. Suppose the integrand has the form:

$$f(r, \theta, \phi) \frac{(r - a)(r'(r, \theta, \phi) - b)},$$

where $r, \theta, \phi$ are spherical coordinates in the integration system and $r'$ a function of these coordinates which is the radial coordinate in another coordinate frame. The function $f(r, \theta, \phi)$ represents the non-singular rest of the integrand. The fixing function which cancels the first peak can be written as:

$$\text{Fix}_1 = \frac{f(a, \theta, \phi)}{(r - a)(r'(a, \theta, \phi) - b)}.$$  \hspace{1cm} (82)

of two additional propagators getting singular at the same time is therefore given from six-point functions on. For $n_{\text{off}}$ off-shell external legs, this situation can only occur for loops with at least $6 - n_{\text{off}}$ propagators.
Here, the non-singular part is fixed at $r = a$. The line over the factor in the denominator indicates that the fixing function is to be subtracted from the original integrand in a region symmetric around the corresponding singularity. One could imagine adding a second fixing function to cancel the second peak similarly. In the region where the two singularities overlap, one would naturally add a third function which fixes the numerator to points on the intersection line and projects each singular factor onto the singular surfaces of the other factor:

$$\text{Fix}_3 = \left. \frac{f(a, \theta, \phi)}{(r - a)} - \frac{1}{(r'(a, \theta, \phi) - b)} \right|_{r' = b}.$$  \hspace{1cm} (85)

However, unless the two peaks are orthogonal to each other, this third fixing function does not cancel the remaining peaks but gives rise to new singularities. These occur at points where the opening angle of the two normals to the singular surfaces is small. Here, the two factors in the denominator will become very small if projected onto the surfaces. Being of second order in that small distance, these peaks will not be cancelled by the fixing functions (84), where only one of the two factors will be small at this point. Therefore, this naive approach cannot be used.

We therefore have to find an alternative way to cancel the peaks. If only the second singularity, $(r' - b)^{-1}$ in (83) was present, the expression for the fixed integrand would read:

$$\frac{f(r, \theta, \phi) - f(r, \theta, \phi)}{(r'(r, \theta, \phi) - b)}
\bigg|_{r' = b}. \hspace{1cm} (86)$$

In the limit $r' \to b$, this is equivalent to the derivative of $f$ with respect to $r'$ at $r' = b$ and we can interpret (86) as a result of an operation on $f$ similar to differentiation without taking the limit $r' \to b$. If we assume $f$ to be differentiable, no singularities are introduced. Using the construction of the fixing function introduced in the beginning of this section, expression (86) is continuous and differentiable. We can therefore again operate on (86) to get the difference equation with respect to $r$:

$$\frac{f(r, \theta, \phi)}{(r - a)(r'(r, \theta, \phi) - b)} - \left. \frac{f(r, \theta, \phi)}{(r - a)(r'(r, \theta, \phi) - b)} \right|_{r' = b}
+ \frac{f(a, \theta, \phi)}{(r - a)(r'(a, \theta, \phi) - b)} - \left. \frac{f(a, \theta, \phi)}{(r - a)(r'(a, \theta, \phi) - b)} \right|_{r' = b}. \hspace{1cm} (87)$$

This expression is again continuous and does not have any peaks. The last three terms can therefore be interpreted as fixing functions to the original integrand. However, the second and forth term are not zero anymore. The factor $(r - a)$ is not fixed to a constant $r'$ and gives asymmetric contributions if the fixing function is subtracted in a region symmetric around $r' = b$. To get reliable results, the region where these fixing functions are used should therefore be small. Our (arbitrary) choice of using the energy resolution $\Delta E$ as the width of support of the fixing functions restricts the corresponding error to the same magnitude as power corrections induced by the standard treatment of IR cancellations.

The above analysis extends to any number of propagators which get singular simultaneously. We can always start with a non-singular function $f$ and apply the difference equation (86), transform into another frame and again using (86) with respect to another variable and so on. However, an accurate estimation of the inflicted error by adding these fixing function is still missing.
2.5.4 Higher-Order Fixing Functions

The subtraction terms added by the renormalization scheme to cancel the UV divergent terms sometimes contain squared propagators. Performing the $k^0$ integration, one has to take the derivative of the analytic rest of the integrand with respect to $k^0$ before replacing it according to the delta function obtained from the cut propagator. It can happen that another propagator gets singular and the resulting peak would be of second order. In this case one can construct a further fixing function. The relevant term of the integrand in the rest frame, similar to (71), is

$$I_2 = \frac{k^2}{2\sqrt{k^2 + m_i^2}} \frac{R(\Lambda^{-1}k' - p_i)}{m_i^2 - m_j^2 + 2p_{ji}^0 \sqrt{k^2 + m_i^2} + p_{ji}^0}.$$

(88)

Expanding numerator and denominator separately around $k' - k_s$ we get

$$I_2 = \frac{\sqrt{k_s^2 + m_i^2} k_s R(k_s) + (2R(k_s) + k_s R'(k_s))(k' - k_s) + \mathcal{O}((k' - k_s)^2)}{k_s + (k' - k_s) + \mathcal{O}((k' - k_s)^2)}.$$

(89)

where we wrote $R(k_s)$ for $R(\Lambda^{-1}k_s - p_i)$. Multiplying by $(k' - k_s)^2$ we get the coefficients of the poles in the Laurent series by taking the limit $k' \to k_s$ or taking the derivative with respect to $k'$ and then taking the limit:

$$I_2 = \frac{r_{-2}}{(k' - k_s)^2} + \frac{r_{-1}}{(k' - k_s)} + \ldots,$$

(90)

$$r_{-2} = \frac{\sqrt{k_s^2 + m_i^2}}{8p_{ji}^0} R(k_s),$$

(91)

$$r_{-1} = \frac{\sqrt{k_s^2 + m_i^2}}{8p_{ji}^0} R(k_s) + \frac{k_s R'(k_s)}{k_s}.$$

(92)

For the first order peak we can construct a fixing function equivalent to (76) with the new residue $r_{-1}$. For the second order pole we define the fixing function as:

$$\text{Fix}_2(k', k_s') \equiv r_{-2} \left( \frac{1}{(k' - k_s)^2} + \frac{2}{c^2} - \frac{3(k' - k_s)^2}{c^4} \right) \Theta(k' - (k_s - c)) \Theta((k_s + c) - k').$$

(93)

Here, the expression in the brackets results from taking the derivative of the corresponding expression of an already fixed first order function with respect to $k$. Since we defined the first order fixing function in (76) such that after addition to the singular function the resulting expression is differentiable, also the derivative does not develop a singularity. Transforming the two fixing functions back to the original momentum frame and subtracting them from the integrand removes the peaks. Note that applying the difference equation (86) twice at the same point in the same coordinate frame would have lead to the same result.
3 Proof of Concept - Bhabha Scattering

As a first application, we evaluate the one-loop cross section of Bhabha scattering in massive QED. This $e^+e^- \rightarrow e^+e^-$ scattering process is of great importance in electron-positron colliders for the precise measurement of the luminosity at the interaction point. For small angles, this process is dominated by the kinematic singularity of the photon exchanged in the t-channel. The differential cross section in this limit is proportional to the scattering angle $\theta^{-4}$, and therefore gives a high event rate and allows for a precise determination of the luminosity. The experimental accuracy aimed for the luminosity measurement at the planned ILC is below 1%\footnote{To get an overview of the present status of Bhaba scattering calculations, cf. \cite{40,42} and references therein.}, cf. \cite{35}. To match this experimental precision, theoretical predictions of the Bhabha scattering cross section should have at least the same accuracy. Therefore, higher-order corrections have to be included in the calculations and implemented in the Monte Carlo event generators. The QED $\mathcal{O}(\alpha)$ corrections were calculated long ago \cite{36,38}, followed by the one-loop electroweak corrections \cite{39}.\footnote{To get an overview of the present status of Bhaba scattering calculations, cf. \cite{40,42} and references therein.}

The Bhabha scattering process is ideally suited to demonstrate the evaluation of processes at NLO by the Feynman Tree Theorem. The one-loop result for the cross section is well known and can easily be produced using automated loop-graph evaluation tools. Real radiation is well under control and can also be calculated and simulated using automated tools. On the FTT side, Bhabha scattering is a process where most complications inherent in the method – UV subtractions, IR cancellations, and threshold singularities – are present simultaneously. There are ten graphs in the one-loop corrections, which after rewriting them as tree graphs lead to a rich structure in the integrand. This has to be treated by multichannel integration methods. Furthermore, the smallness of the electron mass compared to the energy of 500 GeV where we evaluate the process provides a stringent test of the stability of the numerical integration.

The results shown in the following include the virtual corrections as well as the soft real emission parts. Addition of the hard emission part would not change our results qualitatively and could be obtained straightforwardly in a multi purpose event generator. Nevertheless, the stated numerical results for NLO cross sections should be interpreted bearing in mind the missing hard real emission part.

3.1 Implementation

We created analytical expressions for the loop graphs in computer-readable form using the Mathematica- and FORM-based packages \texttt{FeynArts} and \texttt{FormCalc}\cite{43,44}. Here, we blocked the reduction to tensor integrals, such that we obtained squared matrix elements with the loop momentum still present in scalar products. These matrix elements were then handed over to a specially crafted Mathematica program that creates subtraction graphs, cuts the loops and, where needed, calculates the fixing functions. For each tree graph, the program creates parameterizations (integration channels) which map the resulting phase space onto the unit hypercube, taking into account the peak structure. The resulting expressions for the matrix elements and the channels are then written out in Fortran code.

As an integration routine, we choose the multi-channel algorithm \texttt{VAMP}\cite{45}. We compare the final results for the cross section and angular distribution to an independent calculation that proceeds along the usual way of integration via tensor reduction, dimensional regularization, $\overline{\text{MS}}$ subtraction, and numerical evaluation of the analytical result, using \texttt{FeynArts} and \texttt{FormCalc}.\footnote{To get an overview of the present status of Bhaba scattering calculations, cf. \cite{40,42} and references therein.}
In case of the photon self-energies, we only consider the electron loops. These corrections are infrared finite and have a transverse Lorentz structure. Here, the final loop contribution is just a correction factor to the Born matrix elements, and we use a compact expression in terms of scalar integrals, which is then evaluated using the Feynman Tree Theorem.

### 3.2 Integration Results

In figure 4, we show the differential cross section resulting of a single vertex correction in the s-channel. For this and the following plots of the differential cross section, we insert a center of mass energy of $\sqrt{s} = 500\text{GeV}$ and an infrared soft energy cutoff of $E_{\text{soft}} = 5\text{GeV}$. The results are in complete agreement with *FeynArts*. This single graph already involves a fixing function that cancels the threshold peak which corresponds to the two leptons in the s-channel becoming on-shell. Furthermore, this plot confirms the correct implementation of the ultraviolet subtraction scheme proposed in sections 2.2 and 2.4. Since, the leptons are back to back, there is essentially only one collinear peak in the integrand. Nevertheless we can deduce from the plot that the adaption of the grids in the multi-channel approach to this peak works quite efficient. With 10000 sampling points, the error estimate on the numerical integration as returned by the Monte-Carlo integrator is less than 1%.

In figure 5, we separately show the differential cross section for the complete s-channel contribution and the full correction, since the s-channel is small compared to the t-channel contribution in almost all of the phase space. In both cases, there are residual collinear peaks left in the integrand. As before, the results from the multi-channel integrator have an error of $O(1\%)$.

Figure 6 shows the total cross section as function of the squared beam energy $s$. Results are again in complete agreement with *FeynArts*.

### 3.3 Event Generation

So far, we have used multichannel integration for the purpose of obtaining a numerically stable cross section and angular distribution. As mentioned in section 2.1, we aim at using the Feynman Tree Theorem to produce individual events at NLO level in a general purpose Monte Carlo
package. Here, we demonstrate the applicability by constructing a partonic event generator for the Bhabha scattering process.

The core of a Monte Carlo event generator is the hard partonic sub-process. This is a $2 \rightarrow n$ scattering matrix element with $(3n - 4)$ independent kinematic variables $x_i$. Any random choice of these variables defines an event. For the actual sampling, we make use of the multi-channel integration routine VAMP, which distributes the number of sampling points between different integration channels based on their relative contributions to the variance, and simultaneously adapts a discrete binning of each integration dimension for each channel in order to internally minimize this variance contribution. We assign a weight $w_i$ to each sampled event, which is the value of the integrand containing the original matrix element multiplied by Jacobians arising from transformations between integration channels and from grid adaption. These weighted events can be transformed into a sequence of unweighted events, i.e., physics simulation, by a simple rejection algorithm. A particular event is accepted if a randomly chosen number $r \in [0, 1]$ is lower than the ratio of the weight $w_i$ of this event and a maximal weight $w_{\text{max}}$. The maximal event usually cannot be calculated but has to be inferred from previous preparatory runs.

The resulting partonic events are subject to further refinements: convolution of the initial state by structure functions, parton shower and photon radiation, hadronization, and finally detector simulation. These parts are not considered here.

Using the integrand obtained from the Feynman Tree Theorem, we will generate unweighted events on the level of a hard partonic sub-process, whose phase space includes the on-shell momentum of a loop particle. This loop particle is obviously unobservable, and its momentum has to be integrated over when considering physical observables. However, this unphysical degrees of freedom opens the possibility of negative event weights. Each physical phase space point corresponds to three extra dimensions of unphysical loop momenta, and the events at this point will come both with positive and negative weights. In the average, the event weight at this point is positive definite, but fluctuations are possible.

This source of negative event weights is distinct from the usual problem of negative event weights near an IR/collinear singularity. In that case, the problem can in principle be solved by a suitable resummation prescription, although this is often not done or technically impossible.

Figure 5: Differential cross section of $\mathcal{O}(\alpha)$-correction to s-channel Bhabha scattering (left) and the full $\mathcal{O}(\alpha)$-correction (right).
The physical event weight has to be positive (precisely, unity), for each event, at any phase-space point. The negative event weights in our case, by contrast, are inherent in the approach and cancel out in the average over most part of phase space. In the vicinity of IR singularities, our approach suffers from the usual source of negative weights as well, since we have not applied any resummation. When unweighting our events, we make use of the usual approach of unweighting events with positive and negative weight separately, so we have an event sequence with weight of either $+1$ or $-1$.

As explained above, in addition to the phase-space variables $x_i$ of the $n$ final state particles we now simultaneously sample the three variables $k_i$ of the original loop momentum. Thus, the number of dimension of the integration is given by $(3n-1)$ for a $2 \to n$ process. Since the error inflicted by the acceptance-rejection method is a purely statistical one, the addition of the phase space variables of the inclusive (loop) particles does not influence the error. However, the reweighting efficiency, which is given by the number of kept events divided by the total amount sampled, will generally decrease. In any new variable the grids of the integration methods have to adapt to the shape of the integrand. It is therefore helpful to use as much information about the peak structure as possible to create the corresponding channels, which allow for an efficient adaption of the integration grids.

We accept an event if
\begin{equation}
    r \leq \frac{|w_i|}{w_{\pm}^{\text{max}}},
\end{equation}

with random number $r \in [0,1]$ and $w_{\pm}^{\text{max}} = \max(|w_{\text{max}}|,|w_{\text{min}}|)$ being the absolute maximal weight encountered in the grid adaption and integration steps. Each event was assigned an additional flag $\pm 1$ according to the sign of $w_i$. The inclusion of events with negative weights increases the error as well as reduces the efficiency, since the number of kept events is bigger than the effective number of events, which is the difference of positive and negative events.

In figure 7 we show results for Bhabha scattering separately for the s-channel contribution, and for the complete result in the forward scattering region. We emphasize that these results take only into account the LO and NLO partonic QED cross section without any extras, while a generator of practical use should include all effects from beamstrahlung and resummed ISR, resummed FSR, and NLO electroweak contributions as well as NNLO QED contributions. Nevertheless, for our numerical simulation we have adapted the parameter settings taken for typical processes at a planned linear collider [35,46].
To demonstrate the handling of negative events, we used a small infrared cutoff of 0.5% of the center of mass energy $\sqrt{s} = 500\text{GeV}$ in the s-channel contribution. This leads to a differential cross section which is negative in parts of the phase space. The total Born and NLO cross sections are obtained from Monte Carlo integration of the grids set up for event generation:

$$
\sigma_{\text{tot}}^{\text{Born}} = 0.34745(29)\text{pb}; \quad \sigma_{\text{tot}}^{\text{NLO}} = 0.0338(58)\text{pb}.
$$

Using only the Born level result, we generated 100000 unweighted events which corresponds to an integrated luminosity of about $L = 290\text{fb}^{-1}$. Since the Born result is strictly positive, we did not encounter any negative weights. Here, the efficiency is

$$
\text{eff}_{\text{Born}} = \frac{n_{\text{evts}}}{n_{\text{calls}}} = 61\%,
$$

where we adapted the grid in 6 iterations using 1000 samples each, discarded the integral and performed an integration with a total number of 15000 samples in three iterations. Comparing the NLO with the Born cross section, we want to generate 9736 unweighted events. If we allow for events with a negative weight, it follows that we have to generate events until the difference of positive and negative events equals 9736. Since in this case the integrand is rather equally distributed among positive and negative values, we had to generate a total amount of about 360000 events (186644 positive and 176908 negative). The efficiency for generating all events is $\text{eff}_{\text{NLO}}^{\text{tot}} = 4.1\%$, however, the efficiency of generating events which finally show up in the histogram after the negative events are subtracted from the positive ones in each bin, namely 11655 events, is at the per mil level: $\text{eff}_{\text{hist}}^{\text{NLO}} = 0.2\%$. Clearly, this is a rather extreme case where a huge scale ratio ($\sqrt{s}$ vs. electron mass / energy resolution) enters the game, and the differential cross section is small and even (without resummation) negative in some regions of the phase space. Therefore, it is natural that the integrand is spread among positive and negative values which hampers an efficient event generation.

Here, further manipulation of the integrand like dipole subtraction, or mapping the negative onto the positive parts might improve the behavior. Nevertheless, even without such additional improvements, the results are reliable and stable.
The right-hand plot of figure 7 shows events in the forward scattering region. The covered region corresponds to $\theta_{\text{min}} = 26\text{mrad}$ and $\theta_{\text{max}} = 154\text{mrad}$ [46]. The integrated cross sections for the Born and the NLO process are:

$$
\sigma_{\text{Born}}^{\text{tot}} = 5981.9(2.3)\text{pb}; \quad \sigma_{\text{NLO}}^{\text{tot}} = 2736(82)\text{pb}.
$$

We generated 50000 events for the Born process with an efficiency of $\text{eff}_{\text{Born}} = 72\%$, requiring about 23000 events for the NLO process. These were accepted with an efficiency of $\text{eff}_{\text{NLO}}^{p+n} = 11\%$, dropping down to $\text{eff}_{\text{NLO}}^{p-n} = 1.8\%$, accounting for the effect of negative events.

4 Conclusions

We have developed a new method for computing NLO corrections to scattering cross sections. The method is based on the Feynman tree theorem and bears some similarities to other methods which draw on cuts and analyticity properties of Feynman integrals. However, our approach differs in the fact that all integrals are transformed into ordinary phase-space integrals (albeit with unusual boundaries) that can be handled by an ordinary numerical multi-channel phase-space integrator. To this hand, we had not just to implement subtractions for UV and IR singularities, but furthermore subtraction functions (fixing functions) for threshold singularities which do not cause problems in the usual semi-analytic methods.

By computing the complete result for a well-known process and constructing an unweighted NLO event generator, we could show that the method actually works, even in kinematically difficult regions of parameter space. The resulting code could be added to a standard tree-level event generator, and it is straightforward in principle to extend the method to other processes, or even handle them automatically.

Extending the method to the full Standard Model and multi-particle processes, it promises three important advantages over more conventional semi-analytic algorithms: (i) While the evaluation of a simple process such as Bhabha scattering is clearly more complicated than by standard methods, the computational complexity does not increase dramatically with the number of legs in loop diagrams. Evaluating a NLO $n$-particle process should require similar CPU resources as a LO $n+1$-particle process, summed inclusively over all particle species. This is handled regularly by standard universal event generators. (ii) The presence of masses in loop graphs does not worsen the performance. Instead, it improves the numerical stability. Therefore, we expect the method to be most useful for models with many mass scales (such as the MSSM), once a proper definition of subtractions and renormalization conditions has been set up. (iii) Combining loop integration and phase-space sampling in a single step, we avoid a whole layer in the calculation. In particular, all terms are evaluated only up to the level of precision that is required by the actual simulation.

However, there is still a long way before this method can actually improve the simulation of physics processes in the Standard Model or its extensions. On the one hand, we have to handle the more complicated IR behavior of QCD and state suitable renormalization conditions for the non-abelian theory. On the other hand, the method has to be augmented by a consistent treatment of unstable states such as $W$ and $Z$ bosons, which appear in loops and, in our case, would become artificial external particles in event samples. Nevertheless, the method, if it can be applied to the complete Standard Model has distinct advantages that warrant its further development towards realistic complete LHC and ILC applications.
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