The Precision Monte Carlo Event Generator \mathcal{KK} For Two-Fermion Final States In e^+e^- Collisions[†]

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Abstract

We present the Monte Carlo event generator $\mathcal{K}\mathcal{K}$ version 4.13 for precision predictions of the Electroweak Standard Model for the process $e^+e^- \rightarrow f\bar{f} + n\gamma$, $f = \mu, \tau, d, u, s, c, b$, at centre-of-mass energies from τ lepton threshold to 1 TeV, that is for LEP, SLC, future Linear Colliders, b, c, τ -factories, etc. Effects due to photon emission from initial beams and outgoing fermions are calculated in QED up to second order, including all interference effects, within Coherent Exclusive Exponentiation (CEEX), which is based on Yennie–Frautschi–Suura exponentiation. Electroweak corrections are included in first order, with higher-order extensions, using the DIZET 6.21 library. Final-state quarks hadronize according to the parton shower model using JETSET. Beams can be polarized longitudinally and transversely. Decay of the τ leptons is simulated using the TAUOLA library, taking into account spin polarization effects as well. In particular the complete spin correlations density matrix of the initial-state beams and final state τ 's is incorporated in an exact manner. Effects due to be amstrahlung are simulated in a realistic way. The main improvements with respect to KORALZ are: (a) inclusion of the initial-final state QED interference, (b) inclusion of the exact matrix element for two photons, and (c) inclusion of the transverse spin correlations in τ decays (as in KORALB).

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PROGRAM SUMMARY

Title of the program: $\mathcal{K}\mathcal{K}$ version 4.13.

Computer:

any computer with the FORTRAN 77 compiler and the UNIX operating system Operating system:

UNIX, program was tested under AIX 4.x, HP-UX 10.x and Linux

Programming language used: FORTRAN 77 with popular extensions such as long names, etc.

High-speed storage required: < 10 MB

No. of cards in combined program and test deck: about 21,800, without JETSET, TAUOLA and PHOTOS.

Keywords: Quantum electrodynamics (QED), Standard Model, electroweak interactions, heavy boson Z, spin polarization, spin correlations, radiative corrections, initial-state radiation (ISR), final-state radiation (FSR), QED interference, Monte Carlo (MC) simulation and generation, coherent exclusive exponentiation (CEEX), Yennie–Frautschi–Suura (YFS) exponentiation, LEP2, linear collider, TESLA.

Nature of the physical problem: The fermion pair production is and will be used as an important data point for precise tests of the standard electroweak theory at LEP and future linear colliders at higher energies. QED corrections to fermion pair production (especially τ leptons) at *c*-quark and *b*-quark factories has to be known to second order, including spin polarization effects. The Standard Model predictions at the per mille precision level, taking into account multiple emission of photons for realistic experimental acceptance, can *only* be obtained using a Monte Carlo event generator.

Method of solution: The Monte Carlo methods are used to simulate most of the twofermion final-state processes in e^+e^- collisions in the presence of multiphoton initial-state radiation. The latter is described in the framework of exclusive coherent exponentiation (CEEX) based on Yennie–Frautschi–Suura exclusive exponentiation (YFS/EEX). CEEX treats correctly to infinite order not only infrared cancellations but also QED interferences and narrow resonances. The matrix element according to standard YFS exponentiation is also provided for tests. For quarks and τ leptons, the appropriate simulation of hadronization or decay is included. Beam polarization and spin effects, both longitudinal and transverse, in tau decays are properly taken into account.

Restrictions on the complexity of the problem: In the present version, electron (Bhabha), neutrino and top quark final states are not included (they will be in a future version). Additional fermion pair production is not included. Third-order QED corrections in leading-logarithmic approximation are included only in the auxiliary YFS/EEX matrix element (which can be activated with the help of input parameters). Electroweak corrections should not be trusted above the *t*-quark threshold. The total cross section for light quarks for $\sqrt{s} < 10$ GeV requires an improvement using experimental data.

Typical running time: On the IBM PowerPC M43P240 installation (266 MHz, 65 CERN units) 4 sec per constant-weight event are needed. This result is for a *default/recommended* setting of the input parameters, with *all* hadronization/decay libraries switched ON.

1 Introduction

Monte Carlo (MC) event generators have the double purpose to compensate for detector inefficiencies and to provide theoretical predictions for distributions and integrated cross sections. The second task is more important and difficult. Precision predictions of the Standard Model, with a total error below 0.5%, for the process of production of the fermion pair in electron-positron scattering $(e^-e^+ \rightarrow \mu^-\mu^+)$ were first obtained for energies close to the Z resonance with the MC event generator KORALZ [1] (see also the latest version [2]). The prototype of the modern MC event generator for this process was constructed earlier [3], but it could not deliver sub-per cent precision, because it did not include electroweak corrections and second order QED corrections (it later became a part of the KORALZ package). KORALZ was originally developed for a simulation of the τ -pair production and decay, and later on was extended to muon, quark and neutrino pairs, $e^-e^+ \to f\bar{f}$, with $f = \mu, \tau, d, u, s, c, b, \nu$. The Bhabha scattering $e^-e^+ \to e^-e^+$ was never included in KORALZ and a dedicated precision MC event generator BHLUMI [4,5] was developed for this process. BHLUMI, at the expense of specializing to small scattering angles, could deliver at LEP1 energies the integrated cross section with the record total precision of 0.06% [6]. It should be stressed, however, that the high-precision level of KORALZ and BHLUMI was achieved thanks to exclusive exponentiation [7] (EEX) based on the classical work of Yennie–Frautschi–Suura (YFS) [8], in which the multiple soft and hard real photons are treated in a completely realistic way, i.e. four-momenta are generated, and the infrared (IR) cancellations between real and virtual soft photons occur exactly to infinite order.

At the end of LEP2 operation the total cross section for the process $e^-e^+ \rightarrow f\bar{f}$ will have to be calculated with a precision of 0.2%–1%, depending on the event selection [9]. The arbitrary differential distributions also have to be calculated with the corresponding precision. In future linear colliders (LCs) the precision requirement can be substantially stronger, especially for the high luminosity option, as in the TESLA case. The above new requirements necessitate the development of a new calculational framework for the QED corrections and the construction of new dedicated MC programs. The present work is an important step in this direction.

The main limiting factor that prevents us from getting more precise theoretical predictions for the $e^-e^+ \rightarrow f\bar{f}$ process is higher-order QED radiative corrections (the QED part of electroweak Standard Model). In order to achieve the 0.2% precision tag, the virtual corrections have to be calculated up to 2–3 loops and the multiple bremsstrahlung up to 2–3 hard photons, integrating exactly the multiphoton phase space for the arbitrary event selection (phase-space limits).

The MC event generators KORALZ and BHLUMI, although representing the state of the art of MC evaluation of QED radiative corrections for $e^-e^+ \rightarrow f\bar{f}$ at the beginning of the LEP2 run, are strongly limited in their development towards higher precision. The main limitation is rooted in the use of the spin-summed differential cross sections in the otherwise so successful YFS/EEX – instead of using spin amplitudes directly¹. For this

¹ This was a sensible choice; for instance, it has saved precious CPU time, which was a big problem

reason, certain interferences such as the one between initial-state radiation (ISR) and final-state radiation (FSR) had to be neglected, especially in the calculations beyond first order. Also, in any processes with more Feynman diagrams, such as the Bhabha process, EEX suffers from the proliferation of the interference terms, especially beyond first order. EEX neglects ISR-FSR interferences. However, they were often unimportant – at the Z peak much below 1% of the integrated cross section. The analogous QED interferences among photons emitted from electron and positron in small-angle Bhabha were also small, of order 0.01%, at the small-angle range of the luminosity measurement. Further improvement on the precision for off-Z-peak (LEP2) and for large-angle Bhabha scattering definitely requires reintroduction of these interferences. This is achieved in a natural way by reformulating the exponentiation entirely in terms of spin amplitudes. This turns out to be quite a non-trivial task, and it was done only recently, see refs. [10,11]. The resulting new "reincarnation" of the YFS exponentiation, called the *coherent exclusive* exponentiation (CEEX), was born. The CEEX scheme is implemented in the present $\mathcal{K}\mathcal{K}$ MC program for the first time. In fact we have described in ref. [10] only the first $\mathcal{O}(\alpha^1)_{\text{CEEX}}$ version, with the pure QED matrix element, while in the present program we have already implemented the bulk of the QED $\mathcal{O}(\alpha^2)_{\text{CEEX}}$ matrix element, and also $\mathcal{O}(\alpha)$ electroweak (EW) corrections. This new, $\mathcal{O}(\alpha^2)_{\text{CEEX}}$, important development of CEEX, together with the wealth of numerical results, will be published separately [12].

in the MC calculations, a decade ago.

1.1 Ultimate MC event generator for two-fermion final states

Having briefly introduced the reader to the history and the main characteristics of the subject of the MC event generators for the $e^-e^+ \rightarrow f\bar{f}$ process, let us come to the important question: What is the most complete list of requirements that the precision MC event generator for the $e^-e^+ \rightarrow f\bar{f}$ process should fulfil in order to satisfy the needs of the experiments in the present and future e^-e^+ colliders, that is for the entire centre-of-mass energy range from the τ production threshold up to 1 TeV? This would cover experiments at LEP, SLC, *b*-factories, *c*-factories, τ -factories, future linear colliders such as TESLA, JLC and NLC, and also high-luminosity experiments at the Z resonance, the so-called Z-factories.

In the following we try to answer the above question, and complete the list of the desired features of the ultimate MC event generator for two-fermion final states:

- The total precision of the integrated cross section has to be at least 0.2%. From the above, it automatically follows that we need for the QED part and electroweak corrections the entire first-order $\mathcal{O}(\alpha)$ and the QED second-order $\mathcal{O}(\alpha^2)$, at least in the leading-log (LL) approximation with the exponentiation, e.g. with the $\mathcal{O}(\alpha^2 L^2)$ contributions, especially for ISR. In fact the QED second-order subleading $\mathcal{O}(\alpha^2 L^1)$ and third-order leading $\mathcal{O}(\alpha^3 L^3)$ are also mandatory, at least for the discussion of the theoretical error, but preferably present in the actual MC matrix element. The inclusion of $f \bar{f} f' \bar{f}'$ four-fermion final states will often be necessary, especially the production of the additional soft fermion pair of light fermions. The Z-factory option with 10⁹ statistics would be the most demanding experiment, asking for precision better than 0.02%! Note that here we do not attempt to define individual precision requirements for all kinds of distributions and averages, such as charge and spin asymmetries. We assume that their precision should correspond to a precision of 0.2%-0.02% for the integrated cross sections.
- The other role of MC event generators is to provide a *realistic picture of the process* for the detector studies. It means that it is highly *undesirable* to integrate out certain final-state topologies. For instance we know that contributions from collinear real photons and from virtual photons combine in such a way that the net effect in the integrated cross section is zero or negligible. Nevertheless, for experiments it is of vital importance to have all real photons manifestly in the MC event, even very soft and very collinear ones: it helps enormously to understand correctly the operation of a detector, and hence to reduce the experimental systematic errors. The same is true for the emission of additional light-fermion pairs. The above *maximal exclusivity* requirement leads directly to *exponentiation* in the MC event generator, that is to a procedure in which the perturbative expansion is reorganized in such a way that contributions from IR real and virtual singularities cancel to infinite order. The remaining non-IR corrections are included in $\mathcal{O}(\alpha^2)$.
- For the initial beams and outgoing unstable τ leptons and t-quarks spin polariza-

tions, including all spin correlations, have to be fully taken into account, also in the presence of the real bremsstrahlung photons. For beams the longitudinal polarization of both beams is the minimum requirement. For decaying final fermions, longitudinal polarizations are often not sufficient – transverse polarizations are necessary, both for τ leptons and for t-quarks. In fact not only polarizations are required, but also the effects of exact spin correlation between spin polarization vectors of two outgoing fermions. This again makes it mandatory to the use spin amplitudes and/or spin density matrices for the fermion production and decay processes.

- Non-QED electroweak corrections to the $e^-e^+ \to f\bar{f}$ process are usually calculated separately and combined later on with QED corrections in an manner that is, beyond $\mathcal{O}(\alpha)$, an "ad hoc" recipe. It is not done at the level of the spin amplitudes, but rather in terms of the inclusive distributions, having integrated some photon phase space e.g. transverse momenta beforehand. Typically such an ad hoc procedure is based on the second- or third-order "structure functions" for the incoming electron, adding subleading first- and second-order corrections. It can be questioned whether such an approach is really justified at the precision level of 0.2%, because it is too far from the solid environment of the Lagrangian, Feynman diagrams and the exact phase space. The Monte Carlo based on the spin amplitudes offers a natural realization of such an environment. It is therefore the only viable solution for the problem of combining QED and non-QED corrections beyond first order, without any unnecessary ambiguities. Such a Monte Carlo can then be used to cross-check (calibrate) the popular semi-analytical approaches, which employ all kinds of ad hoc recipes. This important role should not be underestimated, as the semi-analytical programs have many advantages of their own and will always be around.
- Effects due to beamstrahlung will be present at future linear colliders and thus should be implemented in the MC event generator. The beamstrahlung structure functions should be a "user function", supplied (or replaced) easily by the user, without any loss of the efficiency of the MC program. Note that the "luminosity energy spectrum" will be known from machine simulation only to a certain extent; the true distribution will have to be determined from the inspection of the e⁻e⁺ → ff process, most probably for f = e, at small (~ 1°) or intermediate (~ 10°) angles. In such a case, reliable MC predictions of the Standard Model (SM) integrated cross sections and distributions in the presence of beamstrahlung, with the non-trivial event selection criteria, are of vital importance. In this context, the Z radiative return, i.e. the e⁻e⁺ → γZ subprocess, may also play an important role.
- The MC event generator should be maximally upgradable to other processes. Although, in this specification, we concentrate on the precision SM prediction for the two-fermion final states, the MC program should be constructed in such a way that inclusion of the other similar standard processes such as $e^-e^+ \rightarrow W^+W^-$ or nonstandard processes (supersymmetric) should be relatively easy. Also the change of electron beam to muon beam should be possible. This requires in practice that the

MC program be constructed right from the beginning in a *highly modular* way. The Object-Oriented Programming (OOP) approach would help.

- For quark final states, the photon emission should be well combined with the *quark-gluon parton shower*, properly taking QED and QCD corrections at the NLL level.
- Last but not least the program should also have the option to run in a *maximally inclusive* mode in which the type of the final state (fermion) is chosen randomly, event per event, exactly according to its integrated cross section. This requirement is not as trivial as it may seem, since the integrated cross section, in the MC, is typically known at the end of the run (from the average MC weights).

Let us note that the above specification goes far beyond the very ambitious (at the time) specification of the "ultimate MC" formulated at the end of the 1989 LEP1 Workshop. How far are we with \mathcal{KK} MC on the road to this ultimate goal?

Feature	KORALB	KORALZ	$\mathcal{K}\mathcal{K}$ now	<i>KK</i> 2000
QED type	$\mathcal{O}(\alpha)$	EEX	CEEX, EEX	CEEX, EEX
CEEX(ISR+FSR)	none	none	$\{\alpha, \alpha L; \alpha^2 L^2, \alpha^2 L^1\}$	$\{\ldots\alpha^2 L^1; \boldsymbol{\alpha^3 L^3}\}$
EEX(ISR*FSR)	none	$\{\alpha, \alpha L, \alpha^2 L^2\}$	$\{\alpha, \alpha L, \alpha^2 L^2, \alpha^3 L^3\}$	$\{\ldots \alpha^2 L^2, \alpha^3 L^3\}$
ISR-FSR int.	$\mathcal{O}(lpha)$	$\mathcal{O}(lpha)$	$\{\alpha, \alpha L\}_{CEEX}$	$\{\alpha, \alpha L\}_{CEEX}$
Exact bremss.	1γ	1, 2 coll. γ	1, 2, 3coll. γ	up to 3 γ
Electroweak	No Z-res.	DIZET 6.x	DIZET 6.x	New version?
Beam polar.	long+trans.	longit.	long+trans.	long+trans.
τ polar.	long+trans.	longit.	long+trans.	long+trans.
Hadronization		JETSET	JETSET	PYTHIA
au decay	TAUOLA	TAUOLA	TAUOLA	TAUOLA
Inclusive mode		No	Yes	Yes
Beamstrahlung		No	Yes	Yes
Beam spread		No	Yes	Yes
$\nu\nu$ channel		Yes	No	Yes
ee channel		No	No	Yes
tt channel		No	No	yes?
WW channel		No	No	yes?

Table 1: List of features of the present \mathcal{KK} MC, compared to older MCs for fermion pair production, and future plans.

1.2 How far are we on the road to the Ultimate MC?

The present specification of the \mathcal{KK} MC is summarized in Table 1, where we have also given those of KORALZ and KORALB for comparison.

As we see, the present \mathcal{KK} MC has already all the functionality of KORALB. The \mathcal{KK} MC fulfils completely our ultimate specification for the spin treatment. Up to now, the first and the only MC event generator fulfilling the above specification was KORALB [13, 14]. However, KORALB is limited to $\sqrt{s} < 30$ GeV, because of the lack of the Z-resonance and it does not include more than one photon emission – it is based on the pure first-order QED calculation, without exponentiation. In KORALZ, longitudinal polarization effects are implemented at the level of the differential distribution for initial beams and for outgoing fermions (including longitudinal spin correlations). Effects due to transverse spin polarizations are omitted. In the present \mathcal{KK} program these limitations are removed – the complete longitudinal and transverse polarizations are implemented for beams and outgoing fermions, including all spin correlations exactly, as in KORALB, also in the presence of multiple real photons.

As compared to KORALB, there is still one improvement to be done in the \mathcal{KK} MC: the CEEX matrix element does not generally rely on the assumption $m_{\tau} \ll \sqrt{s}$, but certain parts of the actually implemented virtual corrections may still rely on this approximation, notably the spin amplitudes for the γ - γ box. This approximation is not really necessary and will be corrected in the future version.

As compared to KORALZ, the \mathcal{KK} MC covers all its functionality, except for the presence of the neutrino channels. We plan to implement the neutrino channel in the next version. The most important new features in the present \mathcal{KK} with respect to KORALZ is the inclusion of ISR–FSR interference, which at LEP2 modifies the total cross section and charge asymmetry by about 2%, the inclusion of the second-order subleading corrections and the inclusion of the exact matrix element for two hard photons.

The $\mathcal{K}\mathcal{K}$ MC is the first full-scale event generator to include the bulk of second order NLL corrections, and it may easily incorporate second-order NNLL corrections. In fact the exact double bremsstrahlung and exact two-loop virtual corrections are already included, but for the moment there is no need to complete the missing NNLL corrections since they are $\sim 10^{-5}$.

2 Physics content

The present version of $\mathcal{K}\mathcal{K}$ MC includes first-order $\mathcal{O}(\alpha)$ QED and electroweak corrections and almost complete $\mathcal{O}(\alpha^2)$ QED corrections due to the emission of photons from the initial- and final-state fermions. It does not include the emission of an additional fermion pair.

2.1 Two types of QED matrix element

The QED part of the calculation is based on the new $\mathcal{O}(\alpha^2)$ calculation with coherent exclusive exponentiation (CEEX) at the amplitude level. The older QED matrix element based on exclusive exponentiation (EEX) at the differential distribution level (amplitudes squared and spin summed) of the BHLUMI type is still present and is used as a backup solution, for various tests. In particular the EEX matrix element includes $\mathcal{O}(\alpha^3 L^3)$ corrections, which are still absent in our CEEX; it therefore provides a useful estimate of these corrections.

2.1.1 CEEX spin amplitudes

Defining the Lorentz-invariant phase space as

$$\int d\text{LIPS}_n(P; p_1, p_2, ..., p_n) = \int (2\pi)^4 \delta^{(4)} \left(P - \sum_{i=1}^n p_i \right) \prod_{i=1}^n \frac{dp^3}{(2\pi)^3 2p_i^0},\tag{1}$$

we write the $\mathcal{O}(\alpha^r)$ CEEX total cross section for the process

$$e^{-}(p_a) + e^{+}(p_b) \to f(p_c) + \bar{f}(p_d) + \gamma(k_1) + \gamma(k_2) + \dots + \gamma(k_n), n = 0, 1, 2, \dots, n,$$
 (2)

with polarized beams and decays of unstable final fermions sensitive to fermion spin polarizations, following refs. [10, 12], as follows:

$$\sigma^{(r)} = \frac{1}{\text{flux}(s)} \sum_{n=0}^{\infty} \int d\text{LIPS}_{n+2}(p_a + p_b; p_c, p_d, k_1, \dots, k_n) \ \rho_{\text{CEEX}}^{(r)}(p_a, p_b, p_c, p_d, k_1, \dots, k_n),$$
(3)

where

$$\rho_{\text{CEEX}}^{(r)}(p_a, p_b, p_c, p_d, k_1, k_2, \dots, k_n) = \frac{1}{n!} e^{Y(\Omega; p_a, \dots, p_d)} \bar{\Theta}(\Omega) \sum_{\sigma_1, \dots, \sigma_n = \mp 1} \sum_{\lambda_A, \bar{\lambda}_A = \mp 1} \sum_{\substack{\lambda_A, \bar{\lambda}_A = \mp 1\\ j_{i,j,l,m=0}}} \hat{\varepsilon}_1^i \hat{\varepsilon}_2^j \sigma_{\lambda_a \bar{\lambda}_a}^i \sigma_{\lambda_b \bar{\lambda}_b}^j \mathfrak{M}_n^{(r)} \left(\begin{smallmatrix} p_{k_1 k_2} \dots & k_n\\ \lambda \sigma_1 \sigma_2} \dots & \sigma_n \end{smallmatrix} \right) \left[\mathfrak{M}_n^{(r)} \left(\begin{smallmatrix} p_{k_1 k_2} \dots & k_n\\ \bar{\lambda} \sigma_1 \sigma_2} \dots & \sigma_n \end{smallmatrix} \right) \right]^* \sigma_{\bar{\lambda}_c \lambda_c}^l \sigma_{\bar{\lambda}_d \lambda_d}^m \hat{h}_3^l \hat{h}_4^m,$$

$$(4)$$

where, in order to shorten this and other formulas, we use a compact collective notations

$$\binom{p}{\lambda} = \binom{p_a \, p_b \, p_c \, p_d}{\lambda_a \, \lambda_b \, \lambda_c \, \lambda_d}$$

for fermion four-momenta p_A and helicities $\lambda_A, A = a, b, c, d$,

For k = 1, 2, 3, σ^k are Pauli matrices and $\sigma^0_{\lambda,\mu} = \delta_{\lambda,\mu}$ is the unit matrix. The components $\hat{\varepsilon}_1^j, \hat{\varepsilon}_2^k, j, k = 1, 2, 3$, are the components of the conventional spin polarization vectors of e^- and e^+ respectively, defined in the so-called GPS fermion rest frames (see ref. [11] for the exact definition of these frames). We define $\hat{\varepsilon}_A^0 = 1$ in a non-standard way (i.e. $p_A \cdot \hat{\varepsilon}_A = m_e, A = a, b$). The *polarimeter* vectors \hat{h}_C are similarly defined in the appropriate GPS rest frames of the final unstable fermions $(p_C \cdot \hat{h}_C = m_f, C = c, d)$. Note that, in general, \hat{h}_C may depend in a non-trivial way on the momenta of all decay products, see refs. [11, 15–17] for details. We did not introduce polarimeter vectors for bremsstrahlung photons, i.e. we take advantage of the fact that all high-energy experiments are completely blind to photon spin polarizations. See next subsection for more on spin effects.

WE define the complete set of spin amplitudes for emission of n photons in $\mathcal{O}(\alpha^r)_{\text{CEEX}}$, r = 0, 1, 2 as follows:

$$\mathfrak{M}_{n}^{(0)}\left(\begin{smallmatrix}pk_{1}\\\lambda\sigma_{1}\\\cdots\sigma_{n}\end{smallmatrix}\right) = \sum_{\{\wp\}} \prod_{i=1}^{n} \mathfrak{s}_{[i]}^{\{\wp_{i}\}} \beta_{0}^{(0)}\left(\begin{smallmatrix}p\\\lambda\\\vdots\\X_{\wp}\end{smallmatrix}\right),$$
(5)

$$\mathfrak{M}_{n}^{(1)}\begin{pmatrix}pk_{1}\\\lambda\sigma_{1}\end{pmatrix} = \sum_{\{\wp\}} \prod_{i=1}^{n} \mathfrak{s}_{[i]}^{\{\wp_{i}\}} \left\{ \beta_{0}^{(1)}\begin{pmatrix}p\\\lambda;X_{\wp}\end{pmatrix} + \sum_{j=1}^{n} \frac{\beta_{1\{\wp_{j}\}}^{(1)}\begin{pmatrix}pk_{j}\\\lambda\sigma_{j};X_{\wp}\end{pmatrix}}{\mathfrak{s}_{[j]}^{\{\wp_{j}\}}} \right\},\tag{6}$$

$$\mathfrak{M}_{n}^{(2)}\left(\begin{smallmatrix} p_{\lambda}\sigma_{1} \dots \sigma_{n} \\ \lambda\sigma_{1} \dots \sigma_{n} \end{smallmatrix}\right) = \\ = \sum_{\{\wp\}} \prod_{i=1}^{n} \mathfrak{s}_{[i]}^{\{\wp_{i}\}} \left\{ \beta_{0}^{(2)}\left(\begin{smallmatrix} p \\ \lambda; X_{\wp} \end{smallmatrix}\right) + \sum_{j=1}^{n} \frac{\beta_{1\{\wp_{j}\}}^{(2)}\left(\begin{smallmatrix} pk_{j} \\ \lambda\sigma_{j} \end{smallmatrix}; X_{\wp} \right)}{\mathfrak{s}_{[j]}^{\{\wp_{j}\}}} + \sum_{1 \le j < l \le n} \frac{\beta_{2\{\wp_{j}\wp_{l}\}}^{(2)}\left(\begin{smallmatrix} pk_{j}k_{l} \\ \lambda\sigma_{j}\sigma_{l} \end{smallmatrix}; X_{\wp} \right)}{\mathfrak{s}_{[j]}^{\{\wp_{j}\}}\mathfrak{s}_{[l]}^{\{\wp_{l}\}}} \right\}.$$

$$(7)$$

The *coherent* sum is taken over set $\{\wp\}$ of all 2^n partitions – the partition \wp is defined as a vector $(\wp_1, \wp_2, \ldots, \wp_n)$; $\wp_i = 1$ for an ISR and $\wp_i = 0$ for an FSR photon; see the analogous construction in refs. [18,19]. The set of all partitions is explicitly the following:

$$\{\wp\} = \{(0,0,0,\ldots,0), (1,0,0,\ldots,0), (0,1,0,\ldots,0), (1,1,0,\ldots,0), \ldots, (1,1,1,\ldots,1)\}.$$

The s-channel four-momentum in the (possibly) resonant s-channel propagator is $X_{\wp} = p_a + p_b - \sum_{i=1}^{n} \wp_i k_i$.

At $\mathcal{O}(\alpha^r)$ we have to provide functions $\beta_k^{(r)}, k = 0, 1, ..., r$, from Feynman diagrams, which are infrared-finite by construction [8]. Their actual precise definitions can be found in refs. [10,12]. Here we shall define only the most essential ingredients. The lowest-order $\beta_0^{(0)}$ are just Born spin amplitudes times a certain kinematical factor

$$\beta_0^{(0)}\left(^p_{\lambda};X\right) = \mathfrak{B}\left(^p_{\lambda};X\right) \quad \frac{X^2}{(p_c + p_d)^2}.$$
(8)

The Born spin amplitudes $\mathfrak{B}\left(_{\lambda}^{p}; X\right)$ and other spin amplitudes are calculated using the spinor technique of Kleiss and Stirling (KS) [20,21] reformulated in ref. [11] (GPS). Soft factors $\mathfrak{s}_{[i]}^{(\omega)}, \omega = 0, 1$, are complex numbers, see ref. [11] for exact definitions; here we only need to know their absolute values

$$\left|\mathfrak{s}_{[i]}^{(1)}\right|^{2} = -\frac{e^{2}Q_{e}^{2}}{2} \left(\frac{p_{a}}{k_{i}p_{a}} - \frac{p_{b}}{k_{i}p_{b}}\right)^{2}, \quad \left|\mathfrak{s}_{[i]}^{(0)}\right|^{2} = -\frac{e^{2}Q_{f}^{2}}{2} \left(\frac{p_{c}}{k_{i}p_{c}} - \frac{p_{d}}{k_{i}p_{d}}\right)^{2}.$$
(9)

The factor $\overline{\Theta}(\Omega)$ defines the infrared (IR) integration limits for real photons. More precisely for a single photon, complementary domain Ω includes the IR divergence point k = 0, which is *excluded* from the MC phase space, we define a characteristic function $\Theta(\Omega, k) = 1$ for $k \in \Omega$ and $\Theta(\Omega, k) = 0$ for $k \notin \Omega$. The characteristic function for the phase space included in the integration is $\overline{\Theta}(\Omega, k) = 1 - \Theta(\Omega, k)$. The characteristic function for *all* photons in the MC phase space is

$$\bar{\Theta}(\Omega) = \prod_{i=1}^{n} \bar{\Theta}(\Omega, k_i).$$
(10)

In the present program we opt for an Ω traditionally defined by the photon energy cut condition $k^0 < E_{\min}$. Consequently, the YFS form factor [8] reads

$$Y(\Omega; p_a, ..., p_d) = Q_e^2 Y_\Omega(p_a, p_b) + Q_f^2 Y_\Omega(p_c, p_d) + Q_e Q_f Y_\Omega(p_a, p_c) + Q_e Q_f Y_\Omega(p_b, p_d) - Q_e Q_f Y_\Omega(p_a, p_d) - Q_e Q_f Y_\Omega(p_b, p_c),$$
(11)

where

$$Y_{\Omega}(p_{1}, p_{2}) \equiv 2\alpha \tilde{B}(\Omega, p_{1}, p_{2}) + 2\alpha \Re B(p_{1}, p_{2})$$

$$\equiv -2\alpha \frac{1}{8\pi^{2}} \int \frac{d^{3}k}{k^{0}} \Theta(\Omega; k) \left(\frac{p_{1}}{kp_{1}} - \frac{p_{2}}{kp_{2}}\right)^{2} + 2\alpha \Re \int \frac{d^{4}k}{k^{2}} \frac{i}{(2\pi)^{3}} \left(\frac{2p_{1}+k}{2kp_{1}+k^{2}} - \frac{2p_{2}-k}{2kp_{2}-k^{2}}\right)^{2}$$
(12)

is given analytically in terms of logarithms and Spence functions [12]. As we see, the above YFS form factor includes terms due to the initial-final state interference (IFI). In the MC with exponentiation it would be possible to do without Ω (declare it empty) and rely uniquely on the IR regularization with small photon mass m_{γ} only [10]. In that case formulas (12) for the YFS form factor would include only the second virtual photon integral.

2.1.2 EEX differential distributions

In the case of exclusive exponentiation (EEX), we deal with a spin-summed differential distribution. We neglect the IFI and each photon is therefore attributed either to the initial or to the final state fermion pair. The initial state photon momenta are denoted

by $k_i, i = 1, 2, ..., n$, and final state momenta as $k'_i, i = 1, 2, ..., n'$. We shall consider the process $e^-(p_1) + e^+(p_2) \rightarrow f(q_1) + \bar{f}(q_2) + n(\gamma(k_j)) + n'(\gamma(k_l))$.

In the present description of the EEX matrix element and in the following sections on the Monte Carlo algorithm, we use an *alternative notation for the fermion momenta*:

$$p_1 \equiv p_a, \qquad q_1 \equiv p_c p_2 \equiv p_b, \qquad q_2 \equiv p_d.$$
(13)

This is because such a notation has already been used for a long time in low-level MC programs and in the EEX distributions; we have therefore decided to keep it also in the relevant parts of the paper. We hope that it will help the user to understand the code more easily. On the other hand the notation with p_A , A = a, b, c, d, and $k_i, i = 1, ..., n$, is very handy in building up a very compact tensor notation, with letters for fermion indices and numerals for photon indices, in the tensor notation for the multiple photon spin amplitudes; see ref. [12], the previous section, and the relevant parts of the program.

Denoting the Lorentz invariant phase space²,

$$d\tau_n(P; p_1, p_2, ..., p_n) = \prod_{j=1}^n \frac{d^3 p_j}{2p_j^0} \,\delta^{(4)} \left(P - \sum_{j=1}^n p_j\right),\tag{14}$$

the $\mathcal{O}(\alpha^r)$ EEX total cross-section

$$\sigma_{EEX}^{(r)} = \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \frac{1}{n!} \frac{1}{n'!} \int d\tau_{n+n'+2} (p_1 + p_2; q_1, q_2, k_1, \dots, k_n, k_1', \dots, k_n') \rho_{EEX}^{(r)}, \quad r = 0, 1, 2, 3,$$
(15)

is expressed in terms of the fully differential multiphoton distribution

$$\rho_{EEX}^{(r)}(p_1, p_2, q_1, q_2, k_1, ..., k_n, k'_1, ..., k'_n) = e^{Q_e^2 Y_{\Omega_I}(p_1, p_2) + Q_f^2 Y_{\Omega_F}(q_1, q_2)} \\
\prod_{j=1}^n 2\tilde{S}_I(k_j) \,\bar{\Theta}(\Omega_I; k_j) \prod_{l=1}^{n'} 2\tilde{S}_F(k'_l) \,\bar{\Theta}(\Omega_F; k'_l) \Biggl\{ \bar{\beta}_0^{(r)}(X, p_1, p_2, q_1, q_2) \\
+ \sum_{j=1}^n \frac{\bar{\beta}_{1I}^{(2)}(X, p_1, p_2, q_1, q_2, k_j)}{\tilde{S}_I(k_j)} + \sum_{l=1}^{n'} \frac{\bar{\beta}_{1F}^{(2)}(X, p_1, p_2, q_1, q_2, k_l)}{\tilde{S}_F(k_l)} \\
+ \sum_{n\geq j>k\geq 1} \frac{\bar{\beta}_{2II}^{(2)}(X, p_1, p_2, q_1, q_2, k_j, k_k)}{\tilde{S}_I(k_j)\tilde{S}_I(k_k)} + \sum_{n'\geq l>m\geq 1} \frac{\bar{\beta}_{2FF}^{(2)}(X, p_1, p_2, q_1, q_2, k_l, k_m)}{\tilde{S}_F(k_l)\tilde{S}_F(k_m)} \\
+ \sum_{j=1}^n \sum_{l=1}^{n'} \frac{\bar{\beta}_{2IF}^{(2)}(X, p_1, p_2, q_1, q_2, k_j, k_l)}{\tilde{S}_I(k_j)\tilde{S}_F(k_l)} + \sum_{n\geq j>k\geq l\geq 1} \frac{\bar{\beta}_{3III}^{(3)}(X, p_1, p_2, q_1, q_2, k_j, k_k, k_l)}{\tilde{S}_I(k_j)\tilde{S}_I(k_k)}\Biggr\}.$$
(16)

²This phase space has a slightly different normalization from that of the previous section.

The YFS soft factors for real photons emitted from the initial- and final-state fermions read

$$\tilde{S}_{I}(k_{j}) = -Q_{e}^{2} \frac{\alpha}{4\pi^{2}} \left(\frac{p_{1}}{k_{j}p_{1}} - \frac{p_{2}}{k_{j}p_{2}} \right)^{2}, \qquad \tilde{S}_{F}(k_{l}) = -Q_{f}^{2} \frac{\alpha}{4\pi^{2}} \left(\frac{q_{1}}{k_{l}q_{1}} - \frac{q_{2}}{k_{l}q_{2}} \right)^{2}.$$
(17)

The IR domains Ω_I and Ω_F are different for ISR and for FSR – this is easier to implement in the MC. We define Ω_I with the condition $k^0 < E_{\min} \ll \sqrt{s}$ in the rest frame of $P = p_1 + p_2$ called the CMS frame, and Ω_F with $k'^0 < E'_{\min} \ll 2m_f$ in the rest frame of $Q = q_1 + q_2$ referred to as QMS. The rest frame of $X = P - \sum_{j=1,n} k_j$ will be referred to as the XMS frame. In EEX we generally use small mass approximation $m_e, m_f, \ll \sqrt{s}$ (in the following sections we shall however use finite m_f wherever necessary). In this case the YFS form factors of eqs. (12) for the above Ω 's are very simple:

$$Y_{e}(\Omega_{I}; p_{1}, p_{2}) = \gamma_{e} \ln \frac{2E_{min}}{\sqrt{(p_{1} + p_{2})^{2}}} + \frac{1}{4}\gamma_{e} + Q_{e}^{2}\frac{\alpha}{\pi}\left(-\frac{1}{2} + \frac{\pi^{2}}{3}\right),$$

$$Y_{f}(\Omega_{F}; q_{1}, q_{2}) = \gamma_{f} \ln \frac{2E_{min}}{\sqrt{(q_{1} + q_{2})^{2}}} + \frac{1}{4}\gamma_{f} + Q_{f}^{2}\frac{\alpha}{\pi}\left(-\frac{1}{2} + \frac{\pi^{2}}{3}\right),$$

$$\gamma = \gamma_{e} = 2Q_{e}^{2}\frac{\alpha}{\pi}\left(\ln \frac{2p_{1}p_{2}}{m_{e}^{2}} - 1\right), \quad \gamma_{f} = 2Q_{f}^{2}\frac{\alpha}{\pi}\left(\ln \frac{2q_{1}q_{2}}{m_{f}^{2}} - 1\right).$$
(18)

Again the IR-finite functions $\bar{\beta}_k^{(r)}, k = 0, 1, ..., r$ (defined at the level of squared spinsummed spin amplitudes) are calculated, in principle, from the Feynman diagrams and they are defined completely in ref. [12]³.

Here, let us only give the explicit definition of lowest order

$$\bar{\beta}_{0}^{(0)}(X, p_{1}, p_{2}, q_{1}, q_{2}) = \frac{1}{4} \sum_{k,l=1,2} \frac{d\sigma^{\text{Born}}}{d\Omega} (X^{2}, \vartheta_{kl})$$
(19)

where

$$\vartheta_{11} = \angle (\vec{p}_1, \vec{q}_1), \quad \vartheta_{12} = \angle (\vec{p}_1, -\vec{q}_2), \quad \vartheta_{21} = \angle (-\vec{p}_2, \vec{q}_1), \quad \vartheta_{22} = \angle (-\vec{p}_2, -\vec{q}_2), \tag{20}$$

and where all three-vectors are taken in the rest frame of the four-momentum $X = p_1 + p_2 - \sum_{j=1}^n k_j$, called the XMS. The above $\bar{\beta}_0^{(0)}$ function is proportional to the Born differential cross section $d\sigma^{\text{Born}}(s,\vartheta)/d\Omega$, for $e^+e^- \to f\bar{f}$.

2.2 Spin effects

Spin effects are treated in the most general way. For initial beams we use as an input the full spin polarization vectors and for the outgoing τ we contract the τ -production spin

 $^{^{3}}$ In reality they are constructed there by combining in a clever way first-order results and results of the triple convolution of the Altarelli–Parisi kernels. This solution has several practical advantages.

amplitudes with the polarimeter vectors of the two decaying τ 's defined in exactly the same rest frames of the τ 's where the spin quantization axes of the τ 's were defined in the first place. To find out exactly these frames was a little bit of an exercise, because for the calculation of the spin amplitudes [10] for the $e^-e^+ \to f\bar{f}n(\gamma)$ process we use the Kleiss-Stirling technique, for which these spin quantization frames have been found in ref. [11]. We call them the GPS frames of the fermions (beam e^{\pm} and τ^{\pm}). At the practical level, we have written a subprogram that performs the Lorentz transformations from the four GPS frames to the CMS frame. This subprogram is used to transform all τ decay products from the GPS τ rest frames to CMS frame. The polarization vectors of the incoming e^{\pm} have also to be provided in the GPS frames of e^{\pm} . It is simple to obtain by consecutive Lorentz transformation from the experimentally defined frames of e^{\pm} to CMS frame and later to GPS frames. It amounts to making the three-dimensional Wigner-Wick rotation of the beam polarization vectors from the experimentally defined frame to the GPS frame (in practice it is a rotation around the beams, due to the smallness of the electron mass). All of the above technique is an extension of the methodology used in KORALB [13]. For more details, see refs. [10, 11].

Let us finally touch briefly upon another very serious problem relevant to implementation of spin effects and its solution. In eq. (3) the single spin amplitude $\mathfrak{M}_n^{(1)}$ already contains $2^{n}(n+1)$ terms (due to 2^{n} ISR-FSR partitions). The grand sum over spins in eq. (3) counts $2^{n}4^{4}4^{4} = 2^{n+16}$ terms! Altogether we expect up to $N \sim n2^{2n+16}$ operations in the CPU time expensive complex (16 bytes) arithmetics. Typically in $e^-e^+ \rightarrow \mu^-\mu^+$ the average photon multiplicity with $k^0 > 1$ MeV is about 3, corresponding to $N \sim 10^7$ terms. In a sample of 10^4 MC events there will be a couple of events with n = 10and $N = 10^{12}$ terms, clearly something that would "choke" completely any modern, fast workstation. There are several simple tricks that help to ease the problem; for instance, objects such as $\sum_{a} \hat{\varepsilon}^{a}_{i} \sigma^{a}_{\lambda \bar{\lambda}}$ and the \mathfrak{s} -factors are evaluated only once and stored for multiple use. However, this is not sufficient. What really helps to substantially speed up the numerical calculation in the Monte Carlo program is the following trick of *photon spin* randomization. Instead of evaluating the sum over photon spins σ_i , i = 1, ..., n, in eq. (3), we generate randomly one spin sequence of $(\sigma_1, ..., \sigma_n)$ per MC event and the MC weight is calculated only for this particular spin sequence! In this way we save one hefty 2^n factor in the calculation time⁴. Mathematically this method is correct, i.e. the resulting cross section and all MC distributions will be the same as if we had used in the MC weight the original eq. (3) (see a formal proof of the above statement in Section 4 of ref. [22]). Let us stress again that it is possible to apply this photon spin randomization trick because (a) the typical high-energy experiment is blind to photon spin polarization, so that we did not need to introduce the polarimeter vectors for photons in eq. (3), and (b) for our (circular) choice of photon spin polarizations the cross section is rather weakly sensitive to them, so the method does not lead to any significant loss in the MC efficiency.

⁴The other 2^n factor due to coherent summation over partitions cannot be eliminated, unless we give up on narrow resonances.

2.3 Electroweak corrections

Electroweak (EW) corrections are implemented using the DIZET library [23], more precisely using its most recent version, 6.21, the same as is used in the ZFITTER [24] semi-analytical program⁵. The method we use to implement EW corrections is rather simillar to that in KORALZ [1]: they enter through modified coupling constants in the Born cross section, and in order to save CPU time, correction factors are stored in the look-up tables; see the relevant section later.

In the absence of EW corrections, coupling of two neutral bosons γ and Z are defined in a conventional way:

$$\begin{aligned} G_{\lambda}^{Z,f} &= g_{V}^{Z,f} - \lambda g_{A}^{Z,f}, \quad G_{\lambda}^{\gamma,f} = g_{V}^{Z,f}, \; \lambda = +, - = R, L, \\ g_{V}^{\gamma,e} &= Q_{e} = 1, \; g_{V}^{\gamma,f} = Q_{f}, \; g_{A}^{\gamma,e} = 0, \; g_{A}^{\gamma,f} = 0, \\ g_{V}^{Z,e} &= \frac{2T_{e}^{3} - 4Q_{e}\sin^{2}\theta_{W}}{4\sin\theta_{W}\cos\theta_{W}}, \; g_{V}^{Z,f} = \frac{2T_{f}^{3} - 4Q_{f}\sin^{2}\theta_{W}}{4\sin\theta_{W}\cos\theta_{W}}, \\ g_{A}^{Z,e} &= \frac{2T_{e}^{3}}{4\sin\theta_{W}\cos\theta_{W}}, \; g_{A}^{Z,f} = \frac{2T_{f}^{3}}{4\sin\theta_{W}\cos\theta_{W}}, \end{aligned}$$
(21)

where T_f^3 is the isospin of the left-handed component of the fermion $(T_d^3 = -1/2, T_e^3 = -1/2)$.

As in KORALZ [1], we implement the EW corrections as follows: the γ and Z propagators are multiplied by the corresponding two functions (scalar formfactors due to vacuum polarizations):

$$H_{\gamma} = \frac{1}{2 - \Pi_{\gamma}}, \quad H_Z = 16 \sin^2 \theta_W \cos^2 \theta_W \frac{G_{\mu} M_Z^2}{\alpha_{\text{qeD}} 8\pi \sqrt{2}} \rho_{\text{EW}}.$$
 (22)

In addition the vector couplings of Z get multiplied by extra form factors. First of all we replace

$$g_V^{Z,e} = \frac{2T_e^3 - 4Q_e \sin^2 \theta_W}{4 \sin \theta_W \cos \theta_W} \quad \text{by} \quad \frac{2T_e^3 - 4Q_e \sin^2 \theta_W F_{EW}^e(s)}{4 \sin \theta_W \cos \theta_W}$$

$$g_V^{Z,f} = \frac{2T_f^3 - 4Q_f \sin^2 \theta_W}{4 \sin \theta_W \cos \theta_W} \quad \text{by} \quad \frac{2T_f^3 - 4Q_f \sin^2 \theta_W F_{EW}^f(s)}{4 \sin \theta_W \cos \theta_W}$$
(23)

where $F_{EW}^e(s)$ and $F_{EW}^f(s)$ are electroweak form factors provided by the DIZET program and they correspond to electroweak vertex corrections.

The electroweak box diagrams require a more complicated treatment. In the Born spin amplitudes we have essentially two products of the coupling constants:

$$G_{\lambda}^{Z,e}G_{-\lambda}^{Z,f} = (g_{V}^{Z,e} - \lambda g_{A}^{Z,e})(g_{V}^{Z,f} + \lambda g_{A}^{Z,f}) = g_{V}^{Z,e}g_{V}^{Z,f} - \lambda g_{A}^{Z,e}g_{V}^{Z,f} + \lambda g_{V}^{Z,e}g_{A}^{Z,f} - g_{A}^{Z,e}g_{A}^{Z,f},$$

$$G_{\lambda}^{Z,e}G_{\lambda}^{Z,e} = (g_{V}^{Z,e} - \lambda g_{A}^{Z,e})(g_{V}^{Z,f} - \lambda g_{A}^{Z,f}) = g_{V}^{Z,e}g_{V}^{Z,f} - \lambda g_{A}^{Z,e}g_{V}^{Z,f} - \lambda g_{V}^{Z,e}g_{A}^{Z,f} + g_{A}^{Z,e}g_{A}^{Z,f}.$$

$$(24)$$

⁵We would like to thank the authors of DIZET for help in implementing DIZET in the \mathcal{KK} MC.

In the above, the following replacement is done for the doubly-vector component

$$g_V^{Z,e} g_V^{Z,f} \Longrightarrow \frac{4T_e^3 T_f^3 - 8T_e^3 Q_f F_{EW}^f(s) - 8T_f^3 Q_e F_{EW}^e(s) + 16Q_f Q_f F_{EW}^{ef}(s,t)}{16\sin^2 \theta_W \cos^2 \theta_W}, \qquad (25)$$

where the new form factor $F_{EW}^{ef}(s,t)$ corresponds to electroweak boxes and is angle dependent.

In CEEX the Born spin amplitudes modified in the above way enter everywhere as building block, also in the spin amplitudes for the single and multiple real photons. In EEX the Born spin amplitudes with the modified couplings enter into the Born differential cross section, which is the basic building block in all EEX differential distributions. In both cases it thus constitute an improvement with respect to KORALZ, electroweak corrections are calculated for every occurrence of Born-like building block of the amplitude and not only once per event. Note also that we do not need to discuss final-state mass terms at this point.

2.4 Beamstrahlung

Beamstrahlung is the effect of loss of the beam energy due to the electron–bunch interaction. It is essentially the emission of two effective photons strictly collinear with the beams, as an additional strictly collinear ISR.

In the MC program, we require that the 2-dimensional beamstrahlung structure function be the "user function", supplied or easily replaced by the user, without any loss of efficiency of the MC program.

The most general form of the modification of the differential distributions due to beamstrahlung in $e^{-}(p_a) + e^{+}(p_b) \rightarrow X$ reads as follows:

$$d\sigma^{bst}(p_a, p_b; X) = \int dz_1 dz_2 \mathcal{D}(z_1, z_2, \sqrt{s}) d\sigma(z_1 p_a, z_2 p_b; X), \qquad (26)$$

where $\mathcal{D}(z_1, z_2)$ is the double differential beamstrahlung "luminosity spectrum" for simultaneous beamstrahlung from both beams. The luminosity spectrum is assumed to be in the most general form

$$\mathcal{D}(z_1, z_2) = \delta(1 - z_1)\delta(1 - z_2)\rho_0 + \delta(1 - z_1)\rho_1(z_2) + \delta(1 - z_2)\rho_1(z_1) + \rho_2(z_1, z_2), \quad (27)$$

where ρ_0 is a constant and $\rho_1(z)$ and $\rho_2(z_1, z_2)$ are analytical functions for $z \in [0, 1)$. More precisely we allow for power-like integrable singularities at $z_i = 1$:

$$\rho_1(1-\epsilon) \sim \epsilon^{\alpha}, \quad \rho_2(1-\epsilon, z_2) \sim \epsilon^{\beta}, \quad \rho_2(z_1, 1-\epsilon) \sim \epsilon^{\beta}.$$
(28)

The functions ρ_i are regarded as completely arbitrary and we require that the \mathcal{KK} MC be able to cope efficiently with any beamstrahlung luminosity spectrum of the above most general type.

In the present version of the program, we include the beamstrahlung spectra as implemented in the CIRCE package of T. Ohl [25]. The CIRCE package is based on the results from the machine simulation program GuineaPig for linear colliders [26]. Generation of the z_i variables is done at the very beginning of the generation, together with the emission of the QED ISR total photon energy. The technical problem to be solved is hence the following: How to generate up to three variables, the two variables z_1, z_2 for beamstrahlung and one z = 1 - v for ISR, according to an arbitrary, highly singular probability density distribution? Not only are the beamstrahlung spectrum and ISR photon distribution strongly singular, but in addition the MC algorithm has to deal efficiently with singularities due to resonances and thresholds in the reduced CMS energy variable $s'' = sz_1z_2z$.

Furthermore, owing to the presence of the δ 's in the general beamstrahlung distribution of eq. (28), four branches in the MC generation are present: one 1-dimensional, two 2dimensional and one 3-dimensional, corresponding to each term in eq. (28). In each branch the corresponding subset of the z_1, z_2 and z variables is generated, using the special general-purpose MC generation program Foam [27], developed recently for exactly this type of problem. In the present version, we also include another solution for the above task based on the classical Vegas program [28], customized to our needs. This second solution based on Vegas is, however, much less efficient than the principal one (Vegas will probably be removed in the future version). Vegas is extremely efficient in calculating the value of an integral using the MC method, but our problem is different: the variables z_1, z_2 and z are generated at the beginning of the whole \mathcal{KK} MC algorithm; consequently they have to be generated with the weight equal 1 (otherwise we would waste CPU time for calculating for instance the complicated QED matrix element for "unworthy" weighted events). To this task, Vegas is not very well suited (see a more detailed discussion in ref. [27]). The new MC tool Foam is specialized for exactly this difficult task of generating unweighted events efficiently, according to an arbitrary multidimensional probability distribution.

Even if we use powerful MC tool such as Foam, it is worthwhile to improve the efficiency of the MC generation by the appropriate change of integration variables (mapping). Let us take the most complicated case with $\int dz_1 dz_2 dz$ where z = s'/s, and s' is "after ISR". By the trial and error method, we have found that the best mapping for $\sqrt{s} < 1$ TeV is:

$$x_1 = 1 - z_1, \ x_2 = 1 - z_2, \ v = 1 - z x_1 = r_1^{1/\alpha}, \ x_2 = r_2^{1/\alpha}, \ v = r_3^{1/\gamma} v_{\text{max}},$$
 (29)

where $0 < r_i < 1$ are used by Foam, α is from CIRCE and, for the ISR, we have $\gamma \sim 2(\alpha_{QED}/\pi) \ln(s/m_e^2)$. The integral gets transformed into:

$$\int dz_1 dz_2 dz F(z_1, z_2, sz_1 z_2 z) \Theta(1 - z_1 z_2 z - v_{\max})$$

$$= \int_0^1 dr_1 dr_2 dr_3 \frac{v v_{\max}}{r_3 \gamma} \frac{x_1}{r_1 \alpha} \frac{x_2}{r_2 \alpha} \Theta(1 - z_1 z_2 z - v_{\max}) F(z_1, z_2, sz_1 z_2 z) \quad (30)$$

$$= \int_0^1 dr_1 dr_2 dr_3 \frac{v_{\max} \Theta(1 - z_1 z_2 z - v_{\max})}{(\alpha x_1^{\alpha - 1})(\alpha x_2^{\alpha - 1})(\gamma v^{\gamma - 1})} F(z_1, z_2, sz_1 z_2 z)$$

Note that this mapping only takes care⁶ of singularities at $z_i = 1$; for the Z resonance

⁶ Surprisingly, a more sophisticated mapping gives worse efficiency for both Foam and Vegas!

peak and the phase-space limit $1 - z_1 z_2 z < v_{\text{max}}$, the importance sampling is done by Foam (or Vegas).

For energies up to 1 TeV the efficiency of the MC is better by a factor of more than 10 with Foam than with Vegas.

3 Monte Carlo algorithm

In this section we describe in detail the numerical Monte Carlo algorithm used to generate final-state four-momenta, i.e. points within the Lorentz invariant phase space, according to eq. (3) for CEEX and eq. (16) for EEX. We shall not only describe the actual algorithm implemented in the present MC but also try to explain why we opted for certain solutions, and not for others.

We start with a brief discussion of some important general issues. First of all, we would like to stress that we treat the MC technique as a means of integrating *exactly* over the phase space, without any approximation⁷. Generally, our approach is that of the textbooks on quantum mechanics: the differential cross section is the phase-space times the scattering amplitudes from Feynman diagrams, squared, spin-summed. The MC technique is basically the numerical method of integration over the phase space. Our MC is in fact more than the phase-space integration, because we require that events (lists of four-momenta) be generated with weight equal 1, i.e. we directly *simulate* the scattering process. It is quite a strong restriction on the MC algorithm, see below, and it means that our MC program is not merely a *phase-space integrator*, but the full-scale MC event generator (MCEG).

Concerning the Monte Carlo techniques, let us remind the reader that there are only a handful of elementary techniques such as weighting-rejection, mapping and multibranching⁸ – the whole art being to combine them into one bigger algorithm, see ref. [22] for more detailed discussion. We shall also generally follow the notation and terminology of ref. [22]. There also exists a special group of *self-adapting* MC techniques/programs, such as the very popular MC integrator Vegas [28], which work, in principle, for arbitrary integrand distributions (just like a standard Gaussian integration program integrates any external function). We use in \mathcal{KK} , for this role, the newly developed Foam [27] selfadapting program and the old Vesko1 (part of YFS2 [30]) as building blocks of our MC, along with other elementary techniques.

In general, we tried to minimize the use of the multibranching technique and rely as much as possible on the method of reweighting, constructing several layers of weights – the total weight being their product. Nevertheless, we have three multibranchings, one for the types of the final fermions $f = e, \mu, \tau, d, u, s, c, b$, another one for the photon partitions (for *n* photons there are 2^n ways of attributing photons to ISR or FSR), and finally for helicities of the bremsstrahlung photons (for *n* photons there are 2^n helicity assignments). Each of these three multibranchings is well justified and unavoidable see below.

In the development of the present MC algorithm there are certain *critical issues*, in other words, there are some problems that had to be solved, otherwise it would have been practically impossible to realize the entire MC. Typically, we have seen two possible solutions of an important problem, and we have opted for one of them. In the following

⁷ It is necessary to stress it because in the MC event generators for QCD this may not be the case. In particular, the four-momentum conservation may be imposed at the end of the generation by certain ad hoc adjustments, which introduce an uncontrolled correction to phase-space normalization.

⁸ The multibranching technique is referred to in other papers [29] as a multichannel technique.

we list these critical issues, explaining how the solution was found and/or the critical option chosen.

- Problem of the sum over partitions in the weight due to IFI. It was realized already in ref. [31] that the effect of the quantum-mechanical interference between photon emissions from initial- and final-state charges (IFI) can be introduced by means of the weight $w^{\text{IFI}} = \rho(q_c, q_d, k_1, \dots, k_n) / \rho'(q_c, q_d, k_1, \dots, k_n)$, where ρ includes IFI and ρ' neglects it. In MC events are generated according to ρ' in the first place. Both ρ and ρ' include the sum over 2^n ways of attributing photons to initial and final states, the so-called photon partitions. The natural way of generating ρ' is to use multi-branching and generate an event for a single partition at a time. Generation of ρ' involves the introduction of the additional "kinematical" weight of its own. The possible complication to be avoided is the sum over these kinematical weights over all 2^n partitions. Fortunately, this can be done: it is sufficient to multiply w^{IFI} by the kinematical weight for a single partition, the one that is actually generated. The formal proof of this can be found in ref. [22]. The acceptance rate for n photons due to w^{IFI} is 2^{-n} . It is a severe problem and only the partial, brute-force solution is applied at present. A better solution, taking into account that IFI is destructive for backward scattering and constructive for forward scattering, is needed in the future.
- Photon helicity generation. The sum over partitions in w^{IFI} already costs a lot of CPU time. Another sum over 2ⁿ photon helicities would render the project impractical, even with the present CPU processors. The solution is to introduce multibranching for 2ⁿ photon helicities and generate photon helicities event by event⁹. It is justified, because high-energy experiment detectors are insensitive to photon polarizations; consequently the various photon helicity configurations (branches) contribute equally. Invoking the principles of ref. [22], we can calculate weights like w^{IFI} for just one helicity configuration, the actual one. The sum over 2ⁿ photon helicities is avoided.
- Fermion-type generation versus photon-energy generation. In the MC we generate flavours according to cross sections that take ISR into account in an approximate way¹⁰, and the MC weight corrects it to the true value later. The approximate cross section involves a numerical integral over the ISR total energy, which has to be done before the MC generation starts. The integral can be done (i) for each flavour separately, (ii) or just once, for the flavour-summed cross section. In the MC generation the above corresponds to two options: (i) the fermion type is generated first, and the total energy loss due to ISR, just for this fermion, is generated next;

 $^{^{9}}$ Such a "randomization" of photon helicities was already used in ref. [21].

¹⁰ Fermion-type (flavour) could be generated more simply, according to a crude cross-section equal to the Born cross-section, and the MC would correct the flavour rate in a way depending on the radiative correction, differently for each type of a fermion. Such a solution is unacceptable because, in the presence of the Z, ISR corrections are huge, a factor ~ 3 , and the method would be rather inefficient.

(ii) the total energy loss due to ISR is generated first, for all fermions, and the type of the fermion using the Born cross section for the reduced centre-of-mass energy is generated next. We have chosen the second option.

- Comoving frame for the generation of FSR photons. Generating FSR photons is much more difficult than ISR photons because momenta of the final fermions "move", i.e. they are themselves variables in the phase-space integral, contrary to beams in ISR, which are fixed (except for beamstrahlung). Moreover, FSR emission distributions are also the simplest in the rest frame of the final fermions. For the construction of the FSR algorithm, it was critical to reparametrize the phase space in such a way that photon integrals are formulated in the reference frame attached to outgoing fermions. This comoving frame was used for FSR generation in the earliest version of the YFS3 MC which was incorporated in the KORALZ program since the version distributed at the time of the 1989 LEP1 workshop. The detailed derivation of the above phase space re-parametrization introducing the comoving frame can be found in ref. [32].
- Common IR boundary for ISR and FSR. Since ISR photons are generated in CMS. and FSR photons in the rest frame of the final fermions (QMS), the easiest is therefore to introduce the IR cut for real photons in terms of minimum energy in these two frames. This defines the IR boundary, and IR domains inside them, which are different for ISR and FSR real photons (the Lorentz-boosted sphere is ellipsoidal). This is not a problem, as long as the IFI is neglected. For the CEEX, however, the IFI is present and the IR boundary has to be common (for the basic MC in which IFI is neglected). The problem may look very difficult; however, an inspection of the proof of the independence of the total cross section on the IR boundary for the non-IFI case tells us that we may simply take the common IR domain, which contains both ISR and FSR domains, and, for each event, we may "remove from the record" all photons that are inside the new common IR domain. The above is true, however, only for events weight 1, not for the weighted events, that are present internally in the MC. For weighted events, such a procedure of "photon-removal" can still be done, provided it is accompanied by the additional weight, calculable analytically. The above procedure of the "photon-removal with the weight" was already implemented in the earliest version of YFS3 in KORALZ (although it was not really necessary for the EEX matrix element there); however, it was never documented¹¹.
- Small photon mass as IR regulator in the MC. There exists all the time an interesting option in the MC implementation of the YFS exponentiation, which was never exploited that is to use the photon mass as an IR regulator in the MC. The back-of-the-envelope estimate shows that its disadvantages are a slightly more complicated algorithm for the generation of the photon momenta and higher photon multiplicity.

¹¹ The analogous procedure was introduced in BHLUMI, where it was documented [4], and later on exploited for the construction of BHWIDE [33]).

A clear advantage is that such a cut-off is Lorentz-invariant: this would therefore make it automatically the same for ISR and FSR, so that we would not need to do any gymnastics with the IR boundaries, as described in the previous point.

The user who is familiar with our programs KORALZ and BHLUMI may be puzzled by the fact that we often we point out to some parts of the basic MC algorithm for QED bremsstrahlung, which have existed for a decade but are still unpublished or undocumented; let us comment briefly on this point. On the one hand, the full-scale ISR and FSR multiphoton generator YFS3 with the EEX matrix element was never published as a stand-alone program, for instance because of the lack of EW corrections, and it was absorbed into KORALZ. Its ISR algorithm was rather well documented in ref. [30], but its FSR algorithm was never in fact documented in detail. In the following sections we do this for the first time. Another reason for this time-lag is that the role of the MC programs at LEP1 for fermion pairs, perhaps with the exceptions of Bhabha scattering and τ pair production, was limited to removing detector acceptance, and was not really a primary source of the SM predictions. The simple two-particle final state could be described fairly well with simple semi-analytical calculations such as ZFITTER. In LEP2 the role of the MC as a source of SM predictions seems to be more important, mainly because of the rise of the IFI corrections, and because of the very strong phenomenon of the Z radiative return¹².

In the following we shall describe the algorithm of the Monte Carlo generation of the events according to CEEX and/or EEX differential distributions. The algorithm is built using elementary methods of weighting and multibranching with occasional use of the mapping (change of integration variables) wherever it is possible and/or profitable. The weights are usually products of several component weights ordered in a "chain". Their role is to counter another "chain" of simplifications that were introduced in order to turn very difficult original differential distributions into simpler ones, in which we can integrate manually over certain integration variables (that is to generate them with the help of mapping), one by one. The remaining small subset of variables for which we are not able to perform the manual/analytical integration/mapping is treated with the help of the self-adapting Monte Carlo tool – in our case it is Foam and/or Vesko1 (optionally Vegas). The above "bottom-to-top" procedure of simplifications countered by weights, multibranchings, and integrations/mappings will be described in the following subsections, starting with removing IFI (countered by w^{IFI}), then simplifying the SM/QED matrix element, reorganizing phase space (mapping), integrating simplified ISR and FSR emission distributions (mapping), summing over photon multiplicities, etc., such that in the end we are left with only the integral over photon energy loss due to ISR and optionally due to beamstrahlung, which is fed into Vesko1 or Foam. In the MC program the order of action is "top-to-bottom", i.e. the photon energy loss due to ISR is generated first (together with beamstrahlung, if present), then the type of the fermion, the ISR photon multiplicity and momenta, the FSR photon multiplicity and momenta, and the series of weights brings us back to the desired EEX or CEEX differential distributions. The order

¹² It is even more true for the W^-W^+ channel because of the 4-body final-state kinematics.

of the multibranching and weighting elementary methods can be interchanged, with some care, and the rules for doing it are given in ref. [22]. We shall exploit this possibility, as already indicated.

3.1 Weights and distributions in general

Let us describe the whole organization of the weights and distributions in our MC. We have four principal distributions, pure phase space, model, crude and primary. Their ratios are the principal weights in the MC.

• The pure Lorentz-invariant phase space (LIPS) distribution of eq. (14), which includes four-momentum conservation δ 's. It will not be generated directly in our MC¹³. It is our basic reference differential distribution in the sense that all other differential distributions of interest to us can be expressed in its terms:

$$d\sigma(r_1, ..., r_n) = \rho(r_1, ..., r_n) \ d\tau_n(P; r_1, ..., r_n)$$
(31)

where the *density distributions* (we shall use this terminology)

$$\rho(r_1, ..., r_n) = d\sigma(r_1, ..., r_n) / d\tau_n(P; r_1, ..., r_n),$$
(32)

are analytical¹⁴, except for some simple discontinuities, with no δ 's.

• The model distribution is a density distribution corresponding to a physical model

$$\rho^{\text{Mod}}(r_1, r_2, \dots, r_n) = d\sigma^{\text{Mod}}(r_1, r_2, \dots, r_n) / d\tau_{n+2}(P; r_1, r_2, \dots, r_n), \qquad (33)$$

and it is our ultimate aim to generate MC events according to this differential distribution. Usually, we have to deal with several variants (perturbative orders) of the model distribution, with similar properties, that is to say, peaks.

• The crude distribution is a density distribution

$$\rho^{\mathrm{Cru}}(r_1, r_2, \dots, k_n) = d\sigma^{\mathrm{Cru}}(r_1, r_2, k_1, \dots, k_n) / d\tau_n(P; r_1, r_2, k_1, \dots, k_n),$$
(34)

which is rather close to the *physical model distribution*, in fact it is close to all model distributions of a certain class, and it should be *maximally simple*. It should be Lorentz-invariant, with no unnecessary traces of the internal technicalities of the MC, just a maximally simple function of dot-products of the four-momenta. It should have the same pattern of peaks as all model distributions of a certain class. Here and later, r_1, r_2 will correspond to the momenta of the outgoing fermions, whereas k_i will denote the momenta of the photons. In such cases we will write the phase-space dimension explicitly as n + 2.

¹³ It is integrable, but not analytically, except for n = 2, 3.

¹⁴We limit ourselves to the fermion pair production process. The τ decays and quark–gluon parton showers are not included in the discussion.

• The primary distribution is a density distribution,

$$d\rho^{\Pr}(\xi_1,\xi_2,\ldots,\xi_n),\tag{35}$$

defined primarily in the space Σ of variables ξ_i with the following properties:

- The integral $\int d\rho^{\text{Pri}}(\xi_1, \ldots, \xi_n)$ is known independently; in most cases from analytical integration, or an independent numerical integration of the Gauss type, or from a special independent MC run.
- A well-defined mapping $r \to \xi$ exists. The image of this mapping Σ_{LIPS} does not necessarily cover the entire Σ . For $\xi \in \Sigma_{\text{LIPS}}$ the inverse maping $\xi \to r$ exists.

We may therefore define

$$\rho^{\mathrm{Pri}}(r_1, r_2, \dots, k_n) = d\sigma^{\mathrm{Pri}}(\xi_1, \xi_2, \dots, \xi_n) / d\tau_{n+2}(P; r_1, r_2, \dots, k_n),$$
(36)

restricted to $\xi \in \Sigma_{\text{LIPS}}$ and which is the distribution actually generated at the lowest level of the Monte Carlo. A 0 weight will be assigned to MC points $\xi \notin \Sigma_{\text{LIPS}}$. The ρ^{Pri} corresponds to events generated according to $d\rho^{\text{Pri}}$, with all weights ignored (set to 1); it is "inelegant", with traces of many technicalities, not necessarily Lorentzcovariant, roughly similar to the physical model distribution. Its unique, great property is that it *can* actually be generated and integrated. Its integral $\int \sigma^{\text{Pri}}$ sets the whole normalization of the MC.

The main rationale for introducing the intermediate *crude distribution*, which obviously stands between the primary and model distributions, is a very strong practical need of modularity of the MC program. For instance we want to use the same low-level MC event generator for both EEX and CEEX models. (As the example of BHLUMI shows, on top of the low-level with exponentiation one may even impose a model distribution without exponentiation.) We definitely want the MC event generator to have a well defined low-level MC part, which generates weighted events according to the *crude distribution*, that is with the weight

$$W^{\operatorname{Cru}}(r_1, r_2, \dots, r_n) = \frac{d\sigma^{\operatorname{Cru}}(r_i(\xi_j))}{d\sigma^{\operatorname{Pri}}(r_i)} = \frac{\rho^{\operatorname{Cru}}(r_i)}{\rho^{\operatorname{Pri}}(r_i)}, \quad \xi \in \Sigma_{\operatorname{LIPS}},$$

$$W^{\operatorname{Cru}}(r_1, r_2, \dots, r_n) = 0, \quad \xi \notin \Sigma_{\operatorname{LIPS}},$$
(37)

with the importance sampling corresponding to the entire group of physical models. The above weight is provided by the low-level MC to the outside world *numerically*, without any further details on how the event (r_1, r_2, \ldots, r_n) was actually produced – just as a black box.

The *model weight* for the *m*-th model is the ratio

$$W_m^{\text{Mod}}(r_1, ..., r_n) = \frac{d\sigma_m^{\text{Mod}}(r_1, ..., r_n)}{d\sigma^{\text{Cru}}(r_1, ..., r_n)} = \frac{\rho_m^{\text{Mod}}(r_1, ..., r_n)}{\rho^{\text{Cru}}(r_1, ..., r_n)},$$
(38)

calculated in a separate module, and in this module the crude distribution ρ^{Cru} needs to be known *functionally* i.e., it is calculated locally, using a certain analytical expression in terms of the four-momenta of the event, and without any access to information from the lower-level MC (we even assume that such an information is already trashed). Of course, the total weight is the product of the two:

$$W_m^{\text{Tot}} = W^{\text{Cru}} W_m^{\text{Mod}}, \tag{39}$$

and the total cross section is given by

$$\sigma_m^{\text{Tot}} = \langle W_m^{\text{Tot}} \rangle \ \sigma^{\text{Pri}} \tag{40}$$

This organization is definitely fully modular.

Note also that although we did not require that the crude distribution be analytically integrable, such a property is strongly welcomed for the purpose of the technical tests.

3.2 Crude differential distribution for EEX

We define the crude differential distribution with respect to the standard Lorentz invariant phase space as follows:

$$\rho_{[\dot{n},n']}^{\text{Cru}}(q_1, q_2; \dot{k}_1, \dots, \dot{k}_{\dot{n}}; k'_1, \dots, k'_{n'}) \equiv \frac{d\sigma_{Cru}}{d\tau_{n+n'+2}(P; q_1, q_2, \dot{k}_1, \dots, \dot{k}_{\dot{n}}, k'_1, \dots, k'_{n'})} \\
= \frac{1}{\dot{n}!} \frac{1}{n'!} \frac{\sigma_{\text{Born}}(s_X)}{4\pi} \frac{s_X}{s_Q} \frac{2}{\beta_f} \prod_{j=1}^{\dot{n}} 2\tilde{S}_e(\dot{k}_j) \bar{\Theta}_e(\dot{k}_j) \ e^{\gamma_e \ln \varepsilon_e} \prod_{l=1}^{n'} 2\tilde{S}_f(k'_l) \bar{\Theta}_f(k'_l) \ e^{\gamma_f \ln \varepsilon_f} , \tag{41}$$

where $\varepsilon_e = 2E_{\min}/\sqrt{2p_1p_2}$, $\varepsilon_f = 2E'_{\min}/\sqrt{2q_1q_2}$ $\beta_f = (1 - 4m_f^2/s_Q)^{1/2}$, $s_Q = 2q_1q_2 + 2m_f^2$, and we "dotted" the ISR photons in order to avoid a notation clash for CEEX in the next section. The above distribution features a maximum resemblance to the actual QED matrix element from the point of view of peaks and singularities, and is very simple. The infrared and collinear singularities are in \tilde{S} soft factors. The $\sigma_{\text{Born}}(s_X)$ has a resonance peak in s_X . The flux-like s_Q/s_X factor is already present at $\mathcal{O}(\alpha^1)$ in the QED matrix element, and it can also be obtained from the leading-log approximation at any order. It is also necessary to include it in the primary distribution, in order to get reasonable MC weights at $\mathcal{O}(\alpha^1)$ and higher orders.

How did we get the above distribution? It was rather simple. We have taken the $\mathcal{O}(\alpha^0)$ version of eq. (15), with only the $\bar{\beta}_0^{(0)}$ term of eq. (19) in which we "averaged" over the angles in $d\sigma^{\text{Born}}$ and we have taken YFS form factors with the first term only, so that the IR finiteness is preserved. The kinematical factor s_X/s_Q was adjusted to $\mathcal{O}(\alpha^1)$ and LL. The factor $2/\beta_f$ is a pure convention.

The above crude distribution is for EEX only; in CEEX it would only fit one single partition.

3.3 Crude for CEEX and multibranching over partitions

In the EEX model we neglect IFI; we can therefore consider each bremsstrahlung photon to be attributed to the initial or final state; this is also true for the crude distribution for EEX. In CEEX the crude distribution of eq. (41) is no longer usable, because it does not include the sum over partitions. To see it better, think about constructing the model weight as in eq. (38), with the CEEX distribution in the numerator and the EEX crude distribution of eq. (41) in the denominator. The resulting weight would be wildly fluctuating. Let us therefore approach the problem in a more systematic way and construct a realistic crude distribution for CEEX by simplifying the density distribution in eq. (3), much as we did for EEX. Neglecting all spin effects (unpolarized case) and taking the $\mathcal{O}(\alpha^0)$ version of eq. (3) we get

$$\rho(p_c, p_d, k_1, \dots, k_n) = \frac{d\sigma^{(0)}}{d\mathrm{LIPS}_{n+2}(P; p_c, p_d, k_1, \dots, k_n)} \\
= \frac{1}{n!} \frac{e^{Y(\Omega; p_a, \dots, p_d)} \bar{\Theta}(\Omega)}{\mathrm{flux}(s)} \frac{1}{4} \sum_{\sigma_i = \mp 1} \sum_{\lambda_i = \mp 1} \mathfrak{M}_n^{(0)} \left(\begin{smallmatrix} p_{k_1 k_2} \dots k_n \\ \lambda \sigma_1 \sigma_2 \dots \sigma_n \end{smallmatrix} \right) \left[\mathfrak{M}_n^{(0)} \left(\begin{smallmatrix} p_{k_1 k_2} \dots k_n \\ \lambda \sigma_1 \sigma_2 \dots \sigma_n \end{smallmatrix} \right) \right]^* \\
= \frac{e^Y \bar{\Theta}}{4s} \frac{1}{n!} \sum_{\sigma_i, \lambda_i} \sum_{\{\wp\}} \sum_{\{\wp'\}} \left(\prod_{i=1}^n \mathfrak{s}_{[i]}^{\wp_i} \mathfrak{B} \left(\begin{smallmatrix} p \\ \lambda \end{smallmatrix}; X_{\wp_i} \right) \frac{X_{\wp_i}^2}{s''} \right) \left(\prod_{j=1}^n \mathfrak{s}_{[j]}^{\wp'_j} \mathfrak{B} \left(\begin{smallmatrix} p \\ \lambda \end{smallmatrix}; X_{\wp'_j} \right) \frac{X_{\wp'_j}^2}{s''} \right)^*,$$
(42)

where $s'' = (p_c + p_d)^2$. In the crude distribution we, of course, want to neglect the IFI. Neglecting it in the above formula means dropping non-diagonal terms $\wp' \neq \wp$. In addition, in order to preserve IR cancellation we simplify the YFS form factor as well:

$$Y(\Omega; p_a, ..., p_d) \to \gamma_e \ln \varepsilon_e + \gamma_f \ln \varepsilon_f.$$

As a result we obtain

$$\rho(p_c, p_d, k_1, \dots, k_n) = \frac{1}{n!} \frac{e^{\gamma_e \ln \varepsilon_e + \gamma_f \ln \varepsilon_f}}{4s} \sum_{\{\wp\}} \prod_{i=1}^n \bar{\Theta}(k_i) \sum_{\sigma_i} \left| \mathfrak{s}_{[i]}^{\wp_i} \right|^2 \sum_{\lambda_i} \left| \mathfrak{B}\left(\lambda_i^p; X_{\wp_i} \right) \right|^2 \frac{X_{\wp_i}^4}{(s'')^2}.$$
(43)

We can easily identify

$$\sum_{\sigma_i} \left| \mathfrak{s}_{[i]}^{\omega_i} \right|^2 = -8\pi^3 \tilde{S}_{\omega}(k_i), \quad \tilde{S}_1(k_i) \equiv \tilde{S}_I(k_i), \quad \tilde{S}_0(k_i) \equiv \tilde{S}_F(k_i)$$

and also the Born-like expression

$$\sum_{\lambda_i} |\mathfrak{B}(^p_{\lambda}; X_{\wp_i})|^2 \frac{X^2_{\wp_i}}{s''} \sim \frac{d\sigma^{\mathrm{Born}}}{d\Omega} (s, s'', t, u, t', u', X^2_{\wp_i}),$$

which is weakly dependent on the dot-products $s = 2p_a p_b$, $s'' = 2p_c p_c$, $t = -2p_a p_c$, $t' = -2p_b p_d$, $u = -2p_a p_d$, $u' = -2p_b p_c$; it strongly depends on the $X^2_{\wp_i}$ in the Z resonance

propagator. We do not enter into the details of defining the above because we replace it by an "angular average" anyway:

$$\sum_{\lambda_i} |\mathfrak{B} \left(^p_{\lambda}; X_{\wp_i}\right)|^2 \frac{X_{\wp_i}^2}{s''} \to \frac{\sigma^{\mathrm{Born}}(X_{\wp_i}^2)}{4\pi}.$$

Finally, the crude distribution for CEEX we define as follows

$$\rho_{[n]}^{\text{Cru}}(p_c, p_d, k_1, \dots, k_n) = \frac{d\sigma_{\text{CEEX}}^{\text{Cru}}}{d\tau_{n+2}(P; p_c, p_d, k_1, \dots, k_n)} = \frac{1}{n!} \sum_{\{\wp\}} \frac{1}{s} e^{\gamma_e \ln \varepsilon_e + \gamma_f \ln \varepsilon_f} \frac{\sigma^{\text{Born}}(X_{\wp_i}^2)}{4\pi} \frac{X_{\wp_i}^2}{s''} \frac{2}{\beta_f} \prod_{i=1}^n \bar{\Theta}(k_i) \tilde{S}_{\wp_i}(k_i).$$
(44)

(The overall factor like $2/\beta_f$, is just a convention.) It is almost obvious that the above distribution is the crude distribution for EEX of eq. (41) summed over partitions – it is important to check it, at least to get statistical factors right. (We shall come to the question of the common IR boundary Ω later on.) For example for n = 2, omitting final fermion momenta, we have

$$\rho_{[2]}^{Cru}(k_1, k_2) = \frac{1}{2!} \left(2! \rho_{[2,0]}^{Cru}(k_1, k_2;) + 1! 1! \rho_{[1,1]}^{Cru}(k_1; k_2) + 1! 1! \rho_{[1,1]}^{Cru}(k_2; k_1) + 2! \rho_{[0,2]}^{Cru}(; k_1, k_2) \right)$$

$$\tag{45}$$

and putting together [1,0] and [0,1] we have

$$\rho_{[2]}^{Cru}(k_1, k_2) = \rho_{[2,0]}^{Cru}(k_1, k_2;) + \rho_{[1,1]}^{Cru}(k_1; k_2) + \rho_{[0,2]}^{Cru}(; k_1, k_2).$$
(46)

As we now see, for arbitrary photon multiplicity we have the following relations between crude distributions for CEEX and EEX

$$\rho_{[n]}^{\text{Cru}}(k_1, ..., k_n) = \sum_{\dot{n}+n'=n} \rho_{[\dot{n},n']}^{Cru}(k_1, ..., k_{\dot{n}}; k_1, ..., k_{n'})$$
(47)

where again we have "folded in" together all

$$\binom{n}{n'} = \frac{n!}{\dot{n}! \, n'!}$$

contributions with the same ISR and/or FSR multiplicity.

In the Monte Carlo we generate for a given n one of the $\rho_{[n,n']}^{Cru}$ distributions and we implicitly understand that in order to get all 2^n partitions we have to undo the above "folding in", that is we have to perform the proper Bose symmetrization of the photon momenta; in other words, we must permute the momenta of all photons randomly, so that no trace is left of the primary ISR/FSR origin of a given photon. The above is always understood when we say that, we generate in the MC, all 2^n partitions using multibranching methods.

The above rule is important to remember, because the MC code itself may be misleading for two reasons: first of all we exploit the equivalence principle of ref. [22], in order to reorganize our weights, and the model weight for CEEX is multiplied by the crude weight for one of the partitions only, and not by the sum of crude weights over all partitions (branches) – so one may easily get the wrong impression that the multi-branching over partitions is absent. Secondly, in the low-level MC, when generating the *primary* primitive distribution, we do not generate first n and later n', with $\dot{n} = n - n'$, but rather n'and \dot{n} independently of each other, taking advantage of the particular properties of the Poisson distributions that govern them and allow us to do it.

The bottom line is the following: the crude distributions for CEEX and EEX can be, and are provided by the same low-level Monte Carlo, because of the identity (47), and because the multibranching over partitions is practically equivalent to Bose symmetrization. Understandably, this has great practical importance.

3.4 Model weight and total weight

The model weight for the $\mathcal{O}(\alpha^{(r)})$ EEX is the following

$$W_{\text{EEX}}^{(r)}(q_1, q_2; \dot{k}_1, \dots, \dot{k}_{\dot{n}}; k'_1, \dots, k'_{n'}) = \frac{\rho_{EEX}^{(r)}(p_1, p_2, q_1, q_2, \dot{k}_1, \dots, \dot{k}_{\dot{n}}, k'_1, \dots, k'_{n'})}{\rho_{[\dot{n}, n']}^{\text{Cru}}(q_1, q_2; \dot{k}_1, \dots, \dot{k}_{\dot{n}}; k'_1, \dots, k'_{n'})},$$
(48)

where the model distribution in the numerator is from eq. (16), and the crude distribution in the denominator is from eq. (41).

The model weight for the $\mathcal{O}(\alpha^{(r)})$ CEEX is the following

$$W_{\text{CEEX}}^{(r)}(p_a, p_b, p_c, p_d, k_1, k_2, \dots, k_n) = \frac{\rho_{\text{CEEX}}^{(r)}(p_a, p_b, p_c, p_d, k_1, k_2, \dots, k_n)}{\rho_{[n]}^{\text{Cru}}(p_c, p_d, k_1, k_2, \dots, k_n)(2\pi)^{3(n+2)-4}},$$
(49)

 $\langle \rangle$

where the model distribution in the numerator is from eq. (4), and the crude distribution in the denominator is from eq. (44). The factor $(2\pi)^{3(n+2)-4}$ is due to the difference in the normalization of $dLIPS_n$ and $d\tau_n$.

As explained in the previous section the corresponding total weight is

$$W_{\text{CEEX}}^{(r)\text{1ot}}(p_a, p_b, p_c, p_d, k_1, k_2, \dots, k_n) = W_{\text{CEEX}}^{(r)}(p_a, p_b, p_c, p_d, k_1, k_2, \dots, k_n) W^{\text{Cru}}(p_a, p_b, p_c, p_d, k_1, k_2, \dots, k_n)$$
(50)

and

$$W_{\text{EEX}}^{(r)\text{Tot}}(q_1, q_2; \dot{k}_1, \dots, \dot{k}_{\dot{n}}; k'_1, \dots, k'_{n'}) = W_{\text{EEX}}^{(r)}(q_1, q_2; \dot{k}_1, \dots, \dot{k}_{\dot{n}}; k'_1, \dots, k'_{n'}) W^{\text{Cru}}(q_1, q_2; \dot{k}_1, \dots, \dot{k}_{\dot{n}}; k'_1, \dots, k'_{n'}),$$
(51)

where W^{Cru} is exactly the same, provided we do for CEEX the proper Bose–Einstein symmetrization. However, even this is strictly speaking unnecessary because the CEEX matrix element is Bose-symmetric anyway, by construction.

Only one of many model weights is the *principal weight* used for a rejection of the events. Of course we choose the best one, that is the $\mathcal{O}(\alpha^{(2)})$ CEEX-type. The other ones are available, and we use them for tests.

3.5 Phase-space reorganization

Our starting point is the phase-space integral of eq. (41) for the crude total cross section, which can be rewritten as follows

$$\sigma^{\rm Cru} = \int ds_X \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \int d\tau_{n+1}(P; k_1, \dots, k_n, X) \frac{1}{n!} \prod_{j=1}^n \tilde{S}_e(k_j) \bar{\Theta}_e(k_j) \\\int d\tau_{n'+2}(X; k_1', \dots, k_{n'}' q_1, q_2) \frac{1}{n'!} \prod_{l=1}^{n'} \tilde{S}_f(k_l') \bar{\Theta}_f(k_l') \frac{\sigma_{\rm Born}(s_X)}{4\pi} \frac{s_X}{s_Q} \frac{2}{\beta_f} e^{\gamma_e \ln \varepsilon_e} e^{\gamma_f \ln \varepsilon_f}$$
(52)

where $P = p_1 + p_2$.

The integral above is Lorentz-invariant and, in principle, can be evaluated in any reference frame, not necessarily in the laboratory frame where $\vec{P} = 0$ and $p_1 = (p^0, 0, 0, p^3)$, which we call PMS. The implicit assumption is also that all momenta in the phase space are in the same reference frame at the time of the evaluation. The reality of the MC world is more complicated. Although the final product, the list of all four-momenta (MC event), is given to the user in one universal frame, the laboratory frame, in the intermediate stages the integral is split into Lorentz-invariant parts and each part is worked out separately, in the *local* Lorentz frame, which is the most convenient for generating subgroup of four-momenta in this subintegral. Then, momenta of this subgroup/subintegral are Lorentz-transformed to the laboratory. The MC generator is not fully documented if the relevant *local* frames and the Lorentz transformation connecting them to one another and to the laboratory system are not unambiguously defined. In this section we shall make an effort to do it.

In the case of the above integral we take advantage of the Lorentz invariance of $d\tau_{n'+2}(X; , k'_1, \ldots, k'_n q_1, q_2)$ and we transform all its variables to the frame where $X = \hat{X} = (\sqrt{s_X}, 0, 0, 0)$, the XMS frame, and put bars on top of them to mark this:

$$\sigma^{\rm Cru} = \int ds_X \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \int d\tau_{n+1}(P; k_1, \dots, k_n, X) \frac{1}{n!} \prod_{j=1}^n \tilde{S}_e(k_j) \bar{\Theta}_e(k_j) \\\int d\tau_{n'+2}(\bar{X}; , \bar{k}'_1, \dots, \bar{k}'_n \bar{q}_1, \bar{q}_2) \frac{1}{n'!} \prod_{l=1}^{n'} \tilde{S}_f(\bar{k}'_l) \bar{\Theta}_f(\bar{k}'_l) \frac{\sigma_{\rm Born}(s_X)}{4\pi} \frac{s_X}{s_Q} \frac{2}{\beta_f} e^{\gamma_e \ln \varepsilon_e} e^{\gamma_f \ln \varepsilon_f},$$
(53)

This operation is still not defined unambiguously, unless we specify the direction of two space-like axes in the new frame or, equivalently, write down explicitly the Lorentz transformation L_X from XMS to CMS and back.

Before we do this, let us note that there are at least three main ways of fixing the z-axis in the XMS frame. Two possibilities are to use as a direction for the z-axis threemomenta of beams, $\vec{p_1}$ or $-\vec{p_2}$ (they are not the same if $s \neq s_X$). We call them XMS1 and XMS2 correspondingly. Note that these frames were introduced in refs. [31,34]. The other choice is to use as z-axis in the XMS frame the direction of the \vec{P} , that is the direction of the boost connecting PMS and XMS (that is the direction opposite to the total four-momentum of the ISR photons). This choice we shall call simply XMS, as it was used in ref. [14]. A third choice is to do a so-called parallel boost B_X along the direction of the \vec{X} in PMS. The corresponding transformation matrix is

$$B_X = \begin{bmatrix} \frac{X^0}{M_X}, & \frac{\vec{X}^T}{M_X} \\ \\ \frac{\vec{X}}{M_X}, & I + \frac{\vec{X} \otimes \vec{X}}{M_X(M_X + X^0)} \end{bmatrix}, \quad X^2 = M_X^2, \quad (54)$$

where T marks the matrix transposition and \otimes marks the tensor product. This is our choice in the present version of the program (the same as in the YFS3 MC). Note that, in general, in the XMS frame defined with the above transformation, the z-axis is not parallel to $\vec{p_1}$ or $-\vec{p_2}$. The transformation from our XMS to CMS is

$$k'_{i}|_{CMS} = L_X \bar{k}'_i, \quad q_i|_{CMS} = L_X \bar{q}_i, \quad L_X = B_X.$$
 (55)

The transformations for other types of XMS are given explicitly in ref. [32].

Now comes an important point. As already indicated, the emission of the FSR photons is done in the comoving frame attached to the momenta q_i of outgoing fermions, that is in the frame where $\vec{Q} = q_1 + q_2 = 0$ and $q_1 = (q_1^0, 0, 0, |q_1^3|)$. We shall call it QMS. So why do we not transform immediately from XMS to QMS, and generate photons there? The problem is that $Q = X - \sum k'_i$, and in order to get from XMS to QMS we have to know k'_i in the first place. We are stuck. The solution is to reparametrize the FSR integral with the help of the integration over the Lorentz group; the details are given in ref. [32]. Here we just apply the result of this work and obtain the new formula:

$$\sigma^{\operatorname{Cru}} = \int ds_X \sum_{n=0}^{\infty} \frac{1}{n!} \prod_{j=1}^n \frac{d^3 k_j}{2k_j^0} 2\tilde{S}_e(k_j) \bar{\Theta}_e(k_j) \,\delta\left(s_X - (P - \sum_{j=0}^n k_j)^2\right) e^{\gamma_e \ln \varepsilon_e}$$
$$\int d\psi d \cos \omega \frac{\sigma_{\operatorname{Born}}(s_X)}{4\pi}$$
$$\sum_{n'=0}^{\infty} \frac{1}{n'!} \int ds_Q \prod_{l=1}^{n'} \frac{d^3 \tilde{k}'_l}{2\tilde{k}'_l^0} 2\tilde{S}_f(\tilde{k}'_l) \bar{\Theta}_f(\tilde{k}'_l) \,\delta\left(s_X - (\hat{Q} + \sum_{j=0}^{n'} \tilde{k}'_j)^2\right) e^{\gamma_f \ln \varepsilon_f},$$
$$\tilde{K} \equiv \sum \tilde{k}'_j, \ \hat{Q} \equiv (\sqrt{s_Q}, 0, 0, 0), \ \hat{q}_1 \equiv \frac{\sqrt{s_Q}}{2} (1, 0, 0, \beta_f), \ \hat{q}_2 \equiv \frac{\sqrt{s_Q}}{2} (1, 0, 0, -\beta_f),$$
(56)

in which those variables with a tilde are defined in the QMS. Note that the Jacobian due to the reparametrization of the FSR integral cancels exactly the factor $(s_X/s_Q)(2/\beta_f)$. The explicit transformation from QMS to XMS defines the meaning of the new ψ, ω integration variables:

$$k_{i} = L_{A}k_{i}, \quad \bar{q}_{i} = L_{A}\hat{q}_{i},$$

$$L_{A} = R_{3}(\psi)R_{2}(\omega)B_{\hat{X}}^{-1}, \quad \hat{X} = \hat{Q} - \sum \tilde{k}_{j}'.$$
(57)

The most important fact is that the explicit integration over q_1 and q_2 has disappeared completely! The angles ψ, ω parametrize the three-dimensional orientation of the momenta set $(\bar{k}'_1, \ldots, \bar{k}'_n, \bar{q}_1, \bar{q}_2)$ as a whole in XMS.

The above treatment of the FSR phase space is the simplest one – this is why we adopted it. Note that the angles ψ, ω have no direct geometric meaning of polar angles of a certain momentum in a certain frame – they are just parameters in the Lorentz transformation. In particular, momenta \vec{q}_1 and $-\vec{q}_1$ do not coincide with the z-axis in XMS. Such an arrangement is, however, possible. It corresponds to a different transformation L_A and the integral (56) would look slightly different. Such an alternative solution is described in detail in ref. [32].

The crude integral of eqs. (41) and (56) can be rewritten as follows:

$$\sigma^{\mathrm{Cru}} = \sum_{f=\mu,\tau,d,u,s,c,b} \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \int d\tau_{n+n'+2}(P;q_1,q_2,k_1,\dots,k_n,k'_1,\dots,k'_{n'}) \\ \times \rho^{\mathrm{Cru}}_{[n,n']}(q_1,q_2;k_1,\dots,k_n;k'_1,\dots,k'_{n'}) \\ = \sum_{f=\mu,\tau,d,u,s,c,b} \int ds_X \ \sigma^f_{\mathrm{Born}}(s_X) \ \int \frac{d\psi d\cos\omega}{4\pi} \\ \sum_{n=0}^{\infty} \frac{1}{n!} \prod_{j=1}^n \frac{d^3k_j}{k_j^0} \tilde{S}_e(k_j) \bar{\Theta}_e(k_j) \ \delta \left(s_X - (P - \sum_{j=0}^n k_j)^2\right) e^{\gamma_e \ln \varepsilon_e} \\ \sum_{n'=0}^{\infty} \frac{1}{n'!} \int ds_Q \ \prod_{l=1}^{n'} \frac{d^3\tilde{k}'_l}{\tilde{k}'_l^0} \tilde{S}_f(\tilde{k}'_l) \bar{\Theta}_f(\tilde{k}'_l) \ \delta \left(s_X - (\hat{Q} + \sum_{j=0}^{n'} \tilde{k}'_j)^2\right) e^{\gamma_f \ln \varepsilon_f}.$$
(58)

This clearly factorizes into independent ISR and FSR parts, with the integration over the effective mass s_X pulled out as a principal integration variable. The above integral is ready for the MC generation.

Let us stress again that in all the above reorganization of the phase space for the σ^{Cru} , from eq. (41) through eq. (52) to eq. (58), we only changed variables with *no* approximations, with full control of the Jacobians of all mappings. For completeness we write the total transformation from QMS down to CMS:

$$k'_{i}|_{CMS} = B_{X}L_{A}k'_{i}, \quad q_{i}|_{CMS} = B_{X}L_{A}\hat{q}_{i},$$

$$L_{A} = R_{3}(\psi)R_{2}(\omega)B_{\hat{X}}^{-1}, \quad X = X|_{CMS}, \quad \hat{X} = \hat{Q} - \sum_{j}\tilde{k}'_{j}$$
(59)

and \hat{X} is defined in the rest frame of the outgoing fermions.

In the following sections we shall introduce variables that are used directly in the MC generation, separately for ISR and FSR, and we shall define *primary* differential distributions generated at the lowest level of the MC algorithm. We start with the FSR – in this case the corresponding *primary* differential distribution sums up to unity, and next we elaborate on the case of ISR. The case of FSR will be described in detail, while the case of ISR will only be summarized, since it was already discussed in ref. [30].

3.6 FSR momenta

In the following we shall describe the MC algorithm for the generation of the FSR photon momenta. Although it was used for almost a decade [1,35], it is the first time that it is described in full detail. Let us consider the FSR part of the crude integral of eq. (58):

$$\mathfrak{F}_{n'} = \frac{1}{n'!} \int_{4m_f^2}^{s_X} ds_Q \prod_{j=1}^{n'} \int \frac{d^3 \tilde{k}'_j}{\tilde{k}'_j} \,\tilde{S}_f(\tilde{k}'_j) \Theta(\tilde{k}'_j - E'_{\min}) \,\delta\left(s_X - \left(\hat{Q} + \sum_{l=0}^{n'} \tilde{k}'_l\right)^2\right) e^{\gamma_f \ln \varepsilon_f},$$

$$\gamma_f = Q_f^2 \,\frac{\alpha}{\pi} \,\frac{1 + \beta_f^2}{\beta_f} \,\left(\ln\frac{1 + \beta_f}{1 - \beta_f} - 1\right) = Q_f^2 \,\frac{\alpha}{\pi} \,\frac{1 + \beta_f^2}{\beta_f} \,\left(\ln\frac{(1 + \beta_f)^2}{\mu_f^2} - 1\right),$$

$$\beta_f = (1 - \mu_f^2)^{1/2}, \ \mu_f^2 = \frac{4m_f^2}{s_Q}, \ \varepsilon_f = \frac{2E'_{\min}}{\sqrt{s_Q}}, \ \hat{Q} = (\sqrt{s_Q}, 0, 0, 0),$$
(60)

where we restored finite m_f , photon momenta \tilde{k}'_l are defined in the QMS rest frame of the outgoing fermions – the natural reference frame to describe the emission of the FSR photons – and E'_{\min} is the real photon minimum energy in this frame. Let us now express the photon momenta in units of $\frac{1}{2}\sqrt{s_Q}$, as well as introduce polar parametrization and other auxiliary notation:

$$\tilde{k}'_{j} \equiv \frac{\sqrt{s_{Q}}}{2} \bar{k}_{j} \equiv \frac{\sqrt{s_{Q}}}{2} x_{j} (1, \sin \theta_{j} \cos \phi_{j}, \sin \theta_{j} \sin \phi_{j}, \cos \theta_{j}),$$

$$\tilde{K}' = \sum_{l=0}^{n'} \tilde{k}'_{l} \equiv \frac{\sqrt{s_{Q}}}{2} \bar{K}.$$
(61)

With the help of the above we are able to eliminate the δ -function:

$$\int_{4m_f^2}^{s_X} ds_Q \,\delta\left(s_X - \left(\hat{Q} + \sum_{l=0}^{n'} \tilde{k}_l'\right)^2\right) = \int_{4m_f^2}^{s_X} ds_Q \,\delta\left(s_X - s_Q\left(1 + \bar{K}^0 + \frac{1}{4}\bar{K}^2\right)\right) \\ = \frac{\Theta\left(s_Q(\bar{k}_1, \dots, \bar{k}_{n'}) - 4m_f^2\right)}{1 + \bar{K}^0 + \frac{1}{4}\bar{K}^2},$$
(62)

and from now on

$$s_Q = s_Q(\bar{k}_1, \dots, \bar{k}_{n'}) \equiv \frac{s_X}{1 + \bar{K}^0 + \frac{1}{4}\bar{K}^2}.$$
(63)

Also the single-photon distribution gets transformed:

$$\frac{d^{3}\tilde{k}'_{j}}{\tilde{k}'_{j}^{0}}\tilde{S}_{f}(\tilde{k}'_{j}) = \frac{dx_{j}}{x_{j}}\frac{d\phi_{j}}{2\pi}\,d\cos\theta_{j}\,\frac{\alpha}{\pi}\,f\left(\theta_{j},\frac{m_{f}^{2}}{s_{Q}}\right),$$

$$f\left(\theta_{j},\frac{m_{f}^{2}}{s_{Q}}\right) = \frac{1+\beta_{f}^{2}}{\delta_{1j}\delta_{2j}} - \frac{\mu_{f}^{2}}{2}\,\frac{1}{\delta_{1j}^{2}} - \frac{\mu_{f}^{2}}{2}\,\frac{1}{\delta_{2j}^{2}}, \quad \delta_{1j} = 1 - \beta_{f}\cos\theta_{j}, \quad \delta_{2j} = 1 + \beta_{f}\cos\theta_{j},$$
(64)

and the whole integral is transformed into the semi-factorized form:

$$\mathfrak{F}_{n'} = \frac{1}{n'!} \prod_{j=1}^{n'} \int_{\varepsilon_f}^{\infty} \frac{dx_j}{x_j} \int_{0}^{2\pi} \frac{d\phi_j}{2\pi} \int_{-1}^{1} d\cos\theta_j \frac{\alpha}{\pi} f\left(\theta_j, \frac{m_f^2}{s_Q}\right) \frac{\Theta(s_Q - 4m_f^2)}{1 + \bar{K}^0 + \frac{1}{4}\bar{K}^2} e^{\gamma_f \ln\varepsilon_f}.$$
 (65)

The reader should not, however, be misled by the apparent simplicity of the above integral – it does not factorize yet into a product of independent integrals, one per photon, because the collective dependence on all photon momenta \bar{k}_j is entering everywhere through the variable s_Q , see eq. (63).

Another complication due to the use of $\frac{1}{2}\sqrt{s_Q}$ as an energy scale is that, in the case of the hard FSR photon, the upper limit of x_j extends to large values, not really to infinity because of the $\Theta(s_Q - 4m_f^2)$; nevertheless, this is not very convenient for the MC integration. This is cured with the following change of variables:

$$y_{i} = \frac{x_{i}}{1 + \sum x_{j}}, \quad x_{i} = \frac{y_{i}}{1 - \sum y_{j}},$$

$$1 + \sum_{j} x_{j} = \frac{1}{1 - \sum_{j} y_{j}} = 1 + \bar{K}^{0} = 1 + \frac{2K' \cdot Q}{s_{Q}} = \frac{s_{X}}{s_{Q}} \left(1 - \frac{{K'}^{2}}{s_{X}}\right),$$
(66)

which leads to

$$\mathfrak{F}_{n'} = \frac{1}{n'!} \prod_{j=1}^{n'} \int_{\varepsilon_f/(1+\bar{K}^0)}^{1} \frac{dy_j}{y_j} \int_{0}^{2\pi} \frac{d\phi_j}{2\pi} \int_{-1}^{1} d\cos\theta_j \frac{\alpha}{\pi} f\left(\theta_j, \frac{m_f^2}{s_Q}\right) \frac{1+\bar{K}^0}{1+\bar{K}^0 + \frac{1}{4}\bar{K}^2} \Theta(s_Q - 4m_f^2) e^{\gamma_f \ln\varepsilon_f}.$$
(67)

With the new variables the condition $s_Q > 4m_f^2$ (easily implementable in the MC) translates approximately into $\sum_j y_j < 1$. Furthermore, we have

$$\frac{1+\bar{K}^0}{1+\bar{K}^0+\frac{1}{4}\bar{K}^2} \le 1,$$

which is ideal for the MC ¹⁵. The new IR limit $y_j > \varepsilon_f/(1 + \bar{K}^0)$ is however inconvenient for the MC. The solution is to substitute

$$\varepsilon_f = \delta_f \ (1 + \bar{K}^0) \tag{68}$$

where $\delta_f \ll 1$ is from now on the new IR regulator for FSR real photons. Note that this sets

$$E_{\min}'' = \delta_f \frac{1}{2} \sqrt{s_Q} (1 + \bar{K}^0) = \delta_f \frac{1}{2} \sqrt{s_Q} \left(1 + \frac{2K' \cdot \hat{Q}}{s_Q} \right)$$
(69)

¹⁵ In the case of ISR a similar factor is causing a lot of trouble because it has a negative coefficient in front of \bar{K}^2 and the corresponding contribution to the MC weight is not well bounded from above.

as a lower limit for the photon energy in the QMS, which is *higher* than the previous one $E'_{\min} = \frac{1}{2}\sqrt{s_Q}\delta_f$ (for $\varepsilon = \delta_f$). Consequently, we have to keep the value of δ_f very low, in fact we need¹⁶ $\delta_f \ll m_f^2/s_X$, which can be a problem for f = e.

3.6.1 Simplifications and MC generation

Up to this point, the FSR integral of eq. (60) was transformed without any approximations and the integral was conveniently parametrized for the MC generation:

$$\mathfrak{F}_{n'} = \frac{1}{n'!} \prod_{j=1}^{n'} \int_{\delta_f}^{1} \frac{dy_j}{y_j} \int_{0}^{2\pi} \frac{d\phi_j}{2\pi} \int_{-1}^{1} d\cos\theta_j \,\frac{\alpha}{\pi} \, f\left(\theta_j, \frac{m_f^2}{s_Q}\right) \\ \frac{1 + \bar{K}^0}{1 + \bar{K}^0 + \frac{1}{4}\bar{K}^2} \,\Theta(s_Q - 4m_f^2) \,e^{\gamma_f \ln(\delta_f(1 + \bar{K}^0))}.$$
(70)

There is also a one-to-one correspondence between the points in the Lorentz-invariant phase space and the points in space of our new variables:

$$\{n', (\tilde{k}'_1, \dots, \tilde{k}'_{n'})\} \leftrightarrow \{n', (y_j, \theta_j, \phi_j), j = 1, \dots, n'\}.$$
(71)

We can also write explicitly the differential distributions in the two *equivalent* parametrizations

$$\frac{d\mathfrak{F}_{n'}}{ds_Q\delta\left(s_X - \left(\hat{Q} + \sum_{l=0}^{n'} \tilde{k}_l'\right)^2\right)\prod_{j=1}^{n'} \frac{d^3\tilde{k}_j'}{2\tilde{k}_j'^0}} = \frac{\Theta(s_Q - 4m_f^2)}{n'!} e^{\gamma_f \ln\left(\frac{2E''_{\min}}{\sqrt{s_X}}\right)} \prod_{j=1}^{n'} 2\tilde{S}_f(\tilde{k}_j')\Theta(\tilde{k}_j' - E''_{\min}),$$

$$\frac{d\mathfrak{F}_{n'}}{\prod_{j=1}^{n'} dy_j \ d\cos\theta_j \ d\phi_j} = \frac{\Theta(s_Q - 4m_f^2)}{n'!} e^{\gamma_f \ln(\delta_f(1 + \bar{K}^0))} \left(\frac{\alpha}{2\pi^2}\right)^{n'} \prod_{j=1}^{n'} \frac{\Theta(y_j - \delta_f)}{y_j} f\left(\theta_j, \frac{m_f^2}{s_Q}\right).$$
(72)

We are now ready to introduce the *simplifications* leading us to a *primary* distribution, which can be integrated analytically and generated using standard uniform random numbers. The simplifications are¹⁷

$$f\left(\theta_{j}, \frac{m_{f}^{2}}{s_{Q}}\right) \to \bar{f}\left(\theta_{j}, \frac{m_{f}^{2}}{s_{X}}\right) = \frac{1 + \bar{\beta}_{f}^{2}}{\bar{\beta}_{f}} \frac{1}{1 - \bar{\beta}_{f}^{2} \cos^{2} \theta_{j}},$$

$$\frac{1 + \bar{K}^{0}}{1 + \bar{K}^{0} + \frac{1}{4}\bar{K}^{2}} \Theta(s_{Q} - 4m_{f}^{2}) \to 1,$$

$$e^{\gamma_{f} \ln(\delta_{f}(1 + \bar{K}^{0}))} \to e^{\bar{\gamma}_{f} \ln(\delta_{f})},$$
(73)

¹⁶ This should be listed as a disadvantage of the actual method of the MC treatment of the FSR.

¹⁷ We drop the mass term from $f(\theta_i)$ for the same reasons as in the case of ISR; see next subsection.

where

$$\bar{\beta}_f = (1 - (m_f^2/s_X)^2)^{1/2}, \quad \bar{\gamma}_f = Q_f^2 \frac{\alpha}{\pi} \frac{1 + \bar{\beta}_f^2}{\bar{\beta}_f} \ln \frac{1 + \bar{\beta}_f}{1 - \bar{\beta}_f}.$$
(74)

The main purpose of the above is to remove any complicated dependence on the momenta of all photons through s_Q – it is achieved trivially by replacing s_Q by s_X . With this hard FSR photons, get stronger collinear peaks at $\cos \theta_j = \pm 1$ in the primary differential distribution. The resulting FSR *primary* differential distribution is:

$$\frac{d\mathfrak{F}_{n'}^{\mathrm{Pri}}}{\prod_{j=1}^{n'} dy_j \ d\cos\theta_j \ d\phi_j} = e^{\bar{\gamma}_f \ln(\delta_f)} \left(\frac{\alpha}{2\pi^2}\right)^{n'} \prod_{j=1}^{n'} \frac{\Theta(y_j - \delta_f)}{y_j} \bar{f}\left(\theta_j, \frac{m_f^2}{s_X}\right),\tag{75}$$

1

and the compensating weight transforming the primary distribution into the crude distribution is

$$w_{\rm FSR}^{\rm Cru} = \frac{d\mathfrak{F}_{n'}}{d\mathfrak{F}_{n'}^{\rm Pri}} = \frac{1 + \bar{K}^0}{1 + \bar{K}^0 + \frac{1}{4}\bar{K}^2} \,\Theta(s_Q - 4m_f^2) \,e^{\gamma_f \ln(\delta_f(1 + \bar{K}^0)) - \bar{\gamma}_f \ln(\delta_f)} \prod_{j=1}^{n'} \,\frac{f\left(\theta_j, \frac{m_f^2}{s_Q}\right)}{\bar{f}\left(\theta_j, \frac{m_f^2}{s_X}\right)}.$$
(76)

Events $\{n', (y_j, \cos \theta_j, \phi_j), j = 1, ..., n'\}$ generated according to $d\mathfrak{F}_{n'}^{Prim}$, defined in eq. (77) below with the weight $w_{\text{FSR}}^{\text{Cru}}$, will be distributed (if rejection is applied) according to the differential distribution, that is the integrand in eq. (72), as desired. There is only one thing to be remembered: removing $\Theta(s_Q - 4m_f^2)$ in the primary distribution means that we cannot map every event generated according to $d\mathfrak{F}_{n'}^{\mathrm{Pri}}$ into a Lorentz-invariant phase-space point, the unambiguous mapping exists in a strict sense in only one direction:

$$\{n', (\tilde{k}'_1, \dots, \tilde{k}'_{n'})\} \to \{n', (y_j, \theta_j, \phi_j), j = 1, \dots, n'\}.$$

This is, however, not really a serious problem because it occurs only for the events with $w_{\rm FSR}^{\rm Cru} = 0$, while for events with $w_{\rm FSR}^{\rm Cru} \neq 0$ we are able to map

$$\{n', (\tilde{k}'_1, \dots, \tilde{k}'_{n'})\} \leftarrow \{n', (y_j, \theta_j, \phi_j), j = 1, \dots, n'\}.$$

Nevertheless, one should keep in mind that some 0-weighted events generated by the FSR algorithm do not have four-momenta assigned to them.

Finally we may check that, as advertised, the integral over the FSR primary distribution can be evaluated analytically:

$$\sum_{n'=0}^{\infty} \mathfrak{F}_{n'}^{\mathrm{Pri}} = \sum_{n'=0}^{\infty} \frac{1}{n'!} \prod_{j=1}^{n'} \int_{\delta_f}^{1} \frac{dy_j}{y_j} \int_{0}^{2\pi} \frac{d\phi_j}{2\pi} \int_{-1}^{1} d\cos\theta_j \,\frac{\alpha}{\pi} \,\bar{f}\left(\theta_j, \frac{m_f^2}{s_X}\right) e^{\bar{\gamma}_f \ln(\delta_f)} = \sum_{n'=0}^{\infty} e^{-\bar{\gamma}_f \ln\frac{1}{\delta_f}} \frac{1}{n'!} \left(\bar{\gamma}_f \ln\frac{1}{\delta_f}\right)^{n'} = \sum_{n'=0}^{\infty} e^{-\langle n' \rangle} \,\frac{\langle n' \rangle^{n'}}{n'!} = 1.$$
(77)

The photon multiplicity for the primary distribution is the standard Poisson distribution, with the average

$$\langle n' \rangle = \bar{\gamma}_f \ln \frac{1}{\delta_f},\tag{78}$$

and the overall normalization is trivially equal to 1, which is a natural choice for the FSR anyway.

The MC generation of the distribution (75) is rather easy. It is fully factorized – variables $\cos \theta_j$, ϕ_j and y_j can be generated independently. The distribution of ϕ_j is just flat and the distribution of y_j is trivial to generate:

$$\phi_j = 2\pi r_{1j}, \quad y_j = \delta_f^{r_{2j}},$$
(79)

where r_{ij} are the standard uniform random numbers $0 < r_{ij} < 1$. The distribution of $\cos \theta_j$ requires applying the branching method: it is split into two components

$$\frac{2}{1-\bar{\beta}_f \cos^2 \theta_j} = \frac{1}{1-\bar{\beta}_f \cos \theta_j} + \frac{1}{1+\bar{\beta}_f \cos \theta_j},\tag{80}$$

and $\cos \theta_j$ is generated according to one component, chosen with the equal probability between the two. For example, if the first component $1/(1 - \bar{\beta}_f \cos \theta_j)$ is chosen then

$$\cos\theta_j = \frac{1}{\bar{\beta}_f} \left\{ (1 - (1 + \bar{\beta}_f) \left(\frac{1 - \bar{\beta}_f}{1 + \bar{\beta}_f}\right)^{r_{3j}} \right\},\tag{81}$$

where r_{3j} is another uniform random number.

3.7 ISR momenta

In the following we shall describe the MC algorithm of the generation of the ISR photon momenta. The algorithm was already described¹⁸ in ref. [30], and for the sake of completeness we shall describe it here, but without going into the fine details. Let us consider the ISR part of the crude integral of eq. (58) for one final fermion type f:

$$\Im_{n} = \frac{1}{n!} \int ds_{X} \ \sigma_{\text{Born}}^{f}(s_{X}) \quad \prod_{j=1}^{n} \int \frac{d^{3}k_{j}}{k_{j}^{0}} \tilde{S}_{e}(k_{j}) \Theta(k_{j}^{0} - E_{\min}) \ \delta\left(s_{X} - \left(P - \sum_{j=0}^{n} k_{j}\right)^{2}\right) e^{\gamma e \ln \varepsilon_{e}}$$

$$\tag{82}$$

where $E_{\min} = \varepsilon_e \frac{1}{2} \sqrt{s}$ is the minimum energy of the real ISR photon in the laboratory CMS. In the first step we introduce the variable $v = 1 - s_X/s$ and order energies of the photons

$$\Im_{n} = \int_{0}^{v_{\max}} dv \ \sigma_{\text{Born}}^{f}(s(1-v)) \prod_{j=1}^{n} \int \frac{d^{3}k_{j}}{k_{j}^{0}} \tilde{S}_{e}(k_{j})$$

$$\Theta(k_{1}^{0}-k_{2}^{0}) \Theta(k_{2}^{0}-k_{3}^{0}) \dots \Theta(k_{n}^{0}-E_{\min}) \ \delta\left(v - \frac{2KP - K^{2}}{s}\right) e^{\gamma_{e} \ln \varepsilon_{e}},$$
(83)

¹⁸ The essential part of the algorithm was given in ref. [36].

where $K = \sum_{j=0}^{n} k_j$ and $v_{\text{max}} = 1 - 4m_f^2/s$. Now we rescale all momenta and introduce a polar parametrization

$$k_i = \eta \bar{k}_i = \eta x_i (1, \sin \theta_i \sin \phi_i, \sin \theta_i \cos \phi_i, \cos \theta_i);$$
(84)

we fix the scaling factor η such that $\bar{k}_1^0 = x_1 = v$:

$$\begin{aligned} \mathfrak{I}_{n} &= \int d\eta \,\delta(\eta - k_{1}^{0}/v) \,\int_{0}^{v_{\max}} dv \,\sigma_{\mathrm{Born}}^{f}(s(1-v)) \,\prod_{j=1}^{n} \int \frac{d^{3}k_{j}}{k_{j}^{0}} \tilde{S}_{e}(k_{j}) \\ &\Theta(k_{1}^{0} - k_{2}^{0}) \,\Theta(k_{2}^{0} - k_{3}^{0}) \dots \Theta(k_{n}^{0} - E_{\min}) \,\delta\left(v - \frac{2KP}{s} + \frac{K^{2}}{s}\right) e^{\gamma e \ln \varepsilon_{e}} \\ &= \int_{0}^{v_{\max}} dv \,\sigma_{\mathrm{Born}}^{f}(s(1-v)) \,\prod_{j=1}^{n} \int_{0}^{1} \frac{dx_{j}}{x_{j}} \int_{0}^{2\pi} \frac{d\phi_{j}}{2\pi} \int_{-1}^{1} d\cos\theta_{j} \,\frac{\alpha}{\pi} f(\cos\theta_{j}) \\ &\delta(v - x_{1}) \,\Theta(x_{1} - x_{2}) \,\Theta(x_{2} - x_{3}) \dots \Theta(\lambda_{0}x_{n} - \varepsilon) \,e^{\gamma e \ln \varepsilon_{e}} \,\mathcal{J}(\bar{K}, v), \end{aligned}$$

$$\end{aligned}$$

where η_0 is the solution¹⁹ of the equation $v - \frac{2\bar{K}P}{s}\eta + \frac{\bar{K}^2}{s}\eta^2 = 0$ and $\mathcal{J}(\bar{K}, v)$ is an overall Jacobian factor:

$$\mathcal{J}(\bar{K},v) = \frac{v}{\eta_0} \frac{1}{\frac{2\bar{K}P}{s} - \frac{\bar{K}^2}{s} 2\eta_0} = \frac{1}{2} \left(1 + \frac{1}{\sqrt{1 - Av}} \right),$$

$$\eta_0 = \frac{\sqrt{s}}{2} \frac{v}{\bar{K}^0} \frac{2}{1 + \sqrt{1 - Av}} \equiv \frac{\sqrt{s}}{2} \lambda_0, \quad A = \frac{\bar{K}^2 P^2}{(\bar{K}P)^2} = \frac{\bar{K}^2}{(\bar{K}^0)^2} \le 1, \quad 0 \le \lambda_0 \le 1,$$
(86)

and the photon angular distribution is governed by

$$f(\cos\theta_j) = \frac{2}{(1-\beta\cos\theta_j)(1+\beta\cos\theta_j)} - \frac{2m_e^2}{s} \frac{1}{(1-\beta\cos\theta_j)^2} - \frac{2m_e^2}{s} \frac{1}{(1+\beta\cos\theta_j)^2}.$$
 (87)

3.7.1 Simplifications and MC generation

Up to this point the ISR integral of eq. (82) was transformed without any approximation and we maintain, modulo ordering of the photon energies, the one-to-one correspondence of the points in the Lorentz-invariant phase space and in the space of the new variables:

$$\{n, (\tilde{k}_1, \dots, \tilde{k}_n)\} \leftrightarrow \{n, (x_j, \theta_j, \phi_j), j = 1, \dots, n\}.$$
(88)

Before we define the *primary* differential distribution to be generated in the MC, let us write once again explicitly the two *equivalent* (modulo energy ordering) parametrizations

¹⁹Note that for a single photon A = 0 and $\eta_0 = s^{1/2}/2$.

of the ISR crude differential distribution:

$$\frac{d\mathfrak{I}_{n}}{ds_{X}\prod_{j=1}^{n}\frac{d^{3}k_{j}}{2k_{j}^{0}}} = \frac{1}{n!}\sigma_{\mathrm{Born}}^{f}(s_{X})\prod_{j=1}^{n}2\tilde{S}_{e}(k_{j})\Theta(k_{j}^{0}-E_{\mathrm{min}})e^{\gamma_{e}\ln\varepsilon_{e}}, n > 0,$$

$$\frac{d\mathfrak{I}_{n}}{dv\prod_{j=1}^{n}dx_{j}d\cos\theta_{j}d\phi_{j}} = \sigma_{\mathrm{Born}}^{f}(s(1-v))\left(\frac{\alpha}{2\pi^{2}}\right)^{n}\delta(v-x_{1})\frac{\Theta(\lambda_{0}x_{n}-\varepsilon)}{x_{n}}$$

$$\prod_{j=1}^{n-1}\frac{\Theta(x_{j}-x_{j-1})}{x_{j}}\prod_{j=1}^{n}f(\cos\theta_{j})e^{\gamma_{e}\ln\varepsilon_{e}}\mathcal{J}(\bar{K},v), n > 0,$$

$$\frac{d\mathfrak{I}_{0}}{ds_{X}} = \sigma_{\mathrm{Born}}^{f}(s)\delta(s_{X}), \quad \frac{d\mathfrak{I}_{0}}{dv} = \sigma_{\mathrm{Born}}^{f}(s)\delta(v), n = 0.$$
(89)

The *simplifications* leading to the ISR *primary* differential distribution are the following:

$$f(\cos\theta_j) \to \bar{f}(\cos\theta_j) = \frac{2}{(1 - \beta\cos\theta_j)(1 + \beta\cos\theta_j)},$$

$$\mathcal{J}(\bar{K}, v) \to \mathcal{J}_0(v) = \frac{1}{2} \left(1 + \frac{1}{\sqrt{1 - v}} \right),$$

$$\Theta(\lambda_0 x_n - \varepsilon) \to \Theta(x_n - \varepsilon),$$

(90)

where

$$\bar{\gamma}_e = 2(\alpha/\pi)\ln(s/m_e^2). \tag{91}$$

The resulting ISR *primary* differential distribution is

$$\frac{d\mathfrak{I}_{n}^{\mathrm{Pri}}}{dv\prod_{j=1}^{n}dx_{j}d\cos\theta_{j}d\phi_{j}} = \sigma_{\mathrm{Born}}^{f}(s(1-v))\left(\frac{\alpha}{2\pi^{2}}\right)^{n}\delta(v-x_{1})\frac{\Theta(x_{n}-\varepsilon)}{x_{n}}$$
$$\prod_{j=1}^{n-1}\frac{\Theta(x_{j}-x_{j-1})}{x_{j}}\prod_{j=1}^{n}\bar{f}(\cos\theta_{j})\ e^{\gamma_{e}\ln\varepsilon_{e}}\ \mathcal{J}_{0}(v),\ n>0,\qquad(92)$$
$$\frac{d\mathfrak{I}_{0}^{\mathrm{Pri}}}{dv} = \sigma_{\mathrm{Born}}^{f}(s)\ \delta(v),\ n=0.$$

and the corresponding weight is

$$w_{\rm ISR}^{\rm Cru} = \frac{d\mathfrak{I}_n}{d\mathfrak{I}_n^{\rm Pri}} = \Theta(\lambda_0 x_n - \varepsilon) \, \frac{\mathcal{J}(\bar{K}, v)}{\mathcal{J}_0(v)} \, \prod_{j=1}^n \frac{f(\cos\theta_j)}{\bar{f}(\cos\theta_j)} \,. \tag{93}$$

Let us explain and justify the simplifications of eqs. (90). The replacement $f(\cos \theta) \rightarrow \overline{f}(\cos \theta)$ is not really necessary in the present context of building an efficient MC algorithm for ISR. We could do without it, because the $f(\cos \theta)$ distribution is rather simple. The problem is really in the model weight at $\mathcal{O}(\alpha^1)$ and higher orders. As is well known in the

soft limit, the helicity-non-conserving spin-amplitude contribution vanish, on the other hand, a perfect helicity conservation contradicts the angular-momentum conservation for a photon emitted exactly parallel to the respective emitting fermion, and this is reflected in the photon distribution

$$f(\cos\theta_j) = \frac{2\sin^2\theta_j}{[(1 - \beta\cos\theta_j)(1 + \beta\cos\theta_j)]^2},\tag{94}$$

which has explicit zeros at $\cos \theta_j = \pm 1$. When we admit the exact $\mathcal{O}(\alpha^1)$ hard photon emission matrix element, then for hard photons these regions close to $\cos \theta_j = \pm 1$ will be filled in by the helicity-non-conserving contributions, and the model weight based on $f(\cos \theta)$ would fluctuate wildly when we approach in division by $f(\cos \theta)$, division by 0. The solution is not to have these zeros at all, at the level of the primary distribution, and this is why we opted for $\bar{f}(\cos \theta)$. In such a case the product of the model and crude weight will be regular at $\mathcal{O}(\alpha^1)$ and beyond.

The other two simplifications are introduced for purely technical reasons. The simplification $\mathcal{J} \to \mathcal{J}_0$ is especially costly in terms of the MC efficiency because, for $v \to 1$, it introduces the "spurious" singularity $(1-v)^{-1/2}$. Together with the usual $(1-v)^{-1}$ from $\sigma_{\text{Born}}^f(s(1-v))$, it builds up strong singularity $(1-v)^{-3/2}$ in the primary differential distribution, and huge primary integrated cross section $\int^{1-4m_f^2/s} dv(1-v)^{-3/2} \sim s^{1/2}/m_f$. It is almost completely compensated by the very high rejection rate of events close to v = 1 due to the ratio $\mathcal{J}(\bar{K}, v)/\mathcal{J}_0(v)$ in $w_{\text{ISR}}^{\text{Cru}}$. The rejection rate is $\sim (m_f/s^{1/2}) \ln(4m_f^2/s)$. For muons 99% of events are rejected. However, in most of the applications, this effect can be easily eliminated by setting $v_{\text{max}} = 0.999$ or lower.

The above problem is unfortunately unavoidable in the actual MC algorithm for the ISR. It can be traced back to the fact that the present MC algorithm is not very well suited for the emission of the two photons of large effective mass, such as the simultaneous emission of two hard photons along two beams. The present algorithm "folds in" together the energies of photons emitted from both beams. A more sophisticated algorithm, in which photons emitted from two beams are generated independently, is needed in order to eliminate this problem.

The $\Theta(\lambda_0 x_n - \varepsilon)$ contribution to the weight has interesting consequences. As discussed in refs. [30, 36] it leads directly²⁰ to a characteristic factor $F(\gamma_e) = e^{-C\gamma_e}/\Gamma(1 + \gamma_e)$ in the $d\sigma/dv$ and in the total cross section.

²⁰ As shown in refs. [30] this is not completely straightforward. In fact $F(\gamma_e)$ is not present for $v < \varepsilon$; it is nevertheless present in the integrated cross section, since the corresponding negative contribution is located just above $v = \varepsilon$.

Finally, let us integrate analytically the ISR *primary* differential distribution

$$\mathfrak{I}^{\mathrm{Pri}} = \sum_{n=0}^{\infty} \mathfrak{I}_{n}^{\mathrm{Pri}} = \sum_{n=0}^{\infty} \int_{0}^{v_{\mathrm{max}}} dv \, \sigma_{\mathrm{Born}}^{f}(s(1-v)) \prod_{j=1}^{n} \int_{0}^{1} \frac{dx_{j}}{x_{j}} \int_{0}^{2\pi} \frac{d\phi_{j}}{2\pi} \int_{-1}^{1} d\cos\theta_{j} \, \frac{\alpha}{\pi} \bar{f}(\cos\theta_{j}) \\ \delta(v-x_{1}) \, \Theta(x_{1}-x_{2}) \, \Theta(x_{2}-x_{3}) \dots \Theta(x_{n}-\varepsilon) \, e^{\gamma_{e}\ln\varepsilon_{e}} \, \mathcal{J}_{0}(v) \\ = \int_{0}^{v_{\mathrm{max}}} dv \, \sigma_{\mathrm{Born}}^{f}(s(1-v)) \, \mathcal{J}_{0}(v) \, e^{\gamma_{e}\ln\varepsilon_{e}} \left(\delta(v) + \Theta(v-\varepsilon)\frac{1}{v}\sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left(\bar{\gamma}_{e}\ln\frac{v}{\varepsilon}\right)^{n-1}\right) \\ = \int_{0}^{\varepsilon} dv \, \gamma_{e}v^{\gamma_{e}-1}\sigma_{\mathrm{Born}}^{f}(s) + \int_{\varepsilon}^{v_{\mathrm{max}}} dv \, \sigma_{\mathrm{Born}}^{f}(s(1-v)) \, \mathcal{J}_{0}(v) \, \bar{\gamma}_{e}v^{\bar{\gamma}_{e}-1}\varepsilon^{\gamma_{e}-\bar{\gamma}_{e}}.$$
(95)

How do we generate the primary differential distribution $d\Im^{\text{Pri}}$? We start with the generation of v according to

$$\frac{d\mathfrak{I}^{\mathrm{Pri}}}{dv} = \sigma_{\mathrm{Born}}^f(s(1-v)) \ \mathcal{J}_0(v) \ \bar{\gamma}_e v^{\bar{\gamma}_e - 1} \varepsilon^{\gamma_e - \bar{\gamma}_e}.$$
(96)

This is done by using a general-purpose MC tool such as Vesko1 or Foam; care is taken of any possible resonance or threshold in the $\sigma_{\text{Born}}^f(s(1-v))$. In the next step, photon multiplicity n is generated. For $v < \varepsilon$ we have simply n = 0, and for $v > \varepsilon$ the photon multiplicity distribution is:

$$\mathfrak{I}_{n}^{\mathrm{Pri}} = \mathrm{const} \times \frac{1}{(n-1)!} \left(\bar{\gamma}_{e} \ln \frac{v}{\varepsilon} \right)^{n-1}, \tag{97}$$

which is just the shifted-by-one Poisson distribution P_{n-1} , with the average $\langle n-1 \rangle = \bar{\gamma}_e \ln(v/\varepsilon)$. The angles $\cos \theta_j$ and ϕ_j are generated in the same way as in the previously discussed case of FSR.

3.8 Getting common IR boundary for FSR and ISR

Let us consider the case of EEX:

$$\sigma_{\rm EEX}^{(r)} = \int W_{\rm EEX}^{(r)} \, d\sigma^{\rm Cru} \,, \tag{98}$$

where the model weight $W_{\text{EEX}}^{(r)}$ is defined in eq. (48) in terms of the $\mathcal{O}(\alpha^r)$ EEX differential distribution of eq. (16). Using eq. (52) with the later substitution

$$\varepsilon_f = \delta_f \left(1 + \frac{2QK'}{s_Q} \right), \quad K' = \sum_{i=0}^{n'} k'_i, \tag{99}$$

which was introduced in order to facilitate the MC generation, we obtain

$$\sigma_{\text{EEX}}^{(r)}\{A\} = \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \int d\sigma_{[n,n']}^{\text{Cru}}(\Omega_{I}, \Omega_{F}) \quad A(n, k_{1}, \dots, k_{n}; n', k'_{1}, \dots, k'_{n'}; p_{i}, q_{i}) \\
\times W_{\text{EEX}}^{(r)}(n, k_{1}, \dots, k_{n}; n', k'_{1}, \dots, k'_{n'}; p_{i}, q_{i}) \\
d\sigma_{[n,n']}^{\text{Cru}}(\Omega_{I}, \Omega_{F}) \equiv ds_{X} \quad \frac{\sigma_{\text{Born}}(s_{X})}{4\pi} d\tau_{n+1}(P; k_{1}, \dots, k_{n}, X) \ e^{\gamma_{e} \ln \varepsilon_{e}} \frac{1}{n!} \prod_{j=1}^{n} 2\tilde{S}_{e}(k_{j})\bar{\Theta}(\Omega_{I}, k_{j}) \\
\times d\tau_{n'+2}(X; k'_{1}, \dots, k'_{n'}, q_{1}, q_{2}) \quad \frac{s_{X}}{s_{Q}} \quad \frac{2}{\beta_{f}} \ e^{\gamma_{f} \ln \left(\delta_{f} \frac{s_{Q}+2K'Q}{s_{Q}}\right)} \frac{1}{n'!} \prod_{l=1}^{n'} 2\tilde{S}_{f}(k'_{l})\bar{\Theta}(\Omega_{F}, k'_{l}) ,$$
(100)

where for the sake of the discussion of the IR cancellations we have introduced a general acceptance function A. Every physical, i.e. IR-safe, observable corresponds uniquely to one or more such acceptance functions. Just to give an example: the total cross section corresponds to $A \equiv 1$, the forward-backward asymmetry is related to A expressed in terms of final fermion momenta like $A = \Theta(q_1^3)$, the cross section for the production of exactly two photons above $E_0 = 1$ GeV corresponds to $A = \sum_{i,j} \Theta(k_i^0 - E_0)\Theta(k_j^0 - E_0)$, and so on. The acceptance function corresponding to a physically meaningful, IR-safe, observable has to obey one important rule

$$\lim_{k_i \to 0} A(n, k_1, \dots, k_{i-1}, k_i, k_{i+1}, \dots, k_n) = A(n-1, k_1, \dots, k_{i-1}, k_{i+1}, \dots, k_n),$$
(101)

and a similar rule should hold for FSR photons (in EEX we can make a distinction between ISR and FSR photons because we neglect ISR–FSR interference).

So far we kept the IR domains different for ISR and FSR, for ISR Ω_I was defined by: $k_j^0 < \varepsilon_e \frac{1}{2}\sqrt{s}$ in the laboratory CMS system where $\vec{p_1} + \vec{p_2} = 0$, while for FSR Ω_F was defined by $k'_j^0 < \delta_f((s_Q + 2K'Q)/s_Q)\frac{1}{2}\sqrt{s_Q}$ in the QMS system where $\vec{q_1} + \vec{q_2} = 0$. Our task is now to bring the two IR domains together.

We know that the total cross section and any IR-safe observable are completely independent of Ω_F and Ω_I . The self-suggesting solution is, loosely speaking, to set δ_f so small that we always have $\Omega_F \subset \Omega_I$, and simply neglect all FSR photons $k'_i \in \delta\Omega = \Omega_I \setminus \Omega_F$, that is just remove them from the list of the generated momenta in the MC. Note that because $(s_Q + 2K'Q)/s_Q \sim s_X/s_Q \ll s_X/(4m_f^2)$ we may need $\delta_f/\varepsilon \ll s/(4m_f^2)$.

Let us work out the details of the above method, providing a formal proof of its validity. The above prescription definitely leads to a certain new crude distribution

$$d\sigma^{\operatorname{Cru}^*}_{[n,n']}(\Omega_I,\Omega_I)$$

in which the IR-domain $\Omega = \Omega_I$ is common for ISR and FSR photons. The question is: What is the above new crude distribution?

It turns out to be calculable analytically. (In the calculation we follow closely the algebra of the formal proof of the independence of the physical observables on the IR

domain Ω as given in ref. [12].) Let us consider the internal FSR subintegral in eq. (100), that is all ISR photon momenta are fixed;

$$\Im\{A\} = \sum_{n'=0}^{\infty} \int d\tau_{n'+2}(X; k'_1, \dots, k'_{n'}, q_1, q_2) \frac{1}{n'!} \prod_{l=1}^{n'} 2\tilde{S}_f(k'_l) \bar{\Theta}(\Omega_F, k'_l) b(k'_1, \dots, k'_{n'}; p_i, q_i)$$

$$b(k'_1, \dots, k'_{n'}; p_i, q_i) \equiv e^{\gamma_f \ln\left(\delta_f \frac{s_Q + 2K'Q}{s_Q}\right)} \frac{s_X}{s_Q} \frac{2}{\beta_f}$$

$$\times W_{\text{EEX}}^{(r)}(n, k_1, \dots, k_n; n', k'_1, \dots, k'_{n'}; p_i, q_i) A(n, k_1, \dots, k_n; n', k'_1, \dots, k'_{n'}; p_i, q_i).$$
(102)

Following $\Omega_I = \Omega_F \bigcup \delta \Omega$ we split every photon integral into two parts and reorganize the sum factorizing out the integral over $\delta \Omega$:

$$\Im\{A\} = \sum_{n'=0}^{\infty} \frac{1}{n'!} \prod_{l=1}^{n'} \left\{ \int \frac{d^3k'_l}{k'_l^0} \Theta(\delta\Omega, k'_l) \, \tilde{S}_f(k'_l) + \int \frac{d^3k'_l}{k'_l^0} \, \bar{\Theta}(\Omega_I, k'_l) \, \tilde{S}_f(k'_l) \right\} \\ \int d\tau_{n'+2}(X, k'_i; q_1, q_2) \, b(k'_1, \dots, k'_{n'}; p_i, q_i) \\ = \sum_{n'=0}^{\infty} \frac{1}{n'!} \sum_{s=0}^{n'} \binom{n'}{s} \left\{ \int \frac{d^3k}{2k^0} \, \Theta(\delta\Omega, k') \, \tilde{S}_f(k') \right\}^s \\ \int d\tau_{n'+2-s}(X - \sum_{1}^{s}; k'_1, \dots, k'_{n'-s}, q_1, q_2) \, \prod_{l=1}^{n'-s} \bar{\Theta}(\Omega_I, k'_l) \, \tilde{S}_f(k'_l) \, b(k'_1, \dots, k'_{n'-s}; p_i, q_i)$$
(103)

where $\Theta(\delta\Omega, k') = 1$ for $k' \in \delta\Omega$ and = 0 otherwise. The most important ingredient in the above algebraic transformation was that the model weight $W_{\text{EEX}}^{(r)}$, due to the particular expansion of $\rho_{\text{EEX}}^{(r)}$ into $\bar{\beta}$ -components, see eq. (16), also fulfils the "IR-safeness" condition

$$\lim_{k'_{i} \to 0} W_{\text{EEX}}^{(r)}(n', k'_{1}, \dots, k'_{i-1}, k'_{i}, k'_{i+1}, \dots, k'_{n'}) = W_{\text{EEX}}^{(r)}(n'-1, k'_{1}, \dots, k'_{i-1}, k'_{i+1}, \dots, k'_{n'}),$$
(104)

and consequently the function $b(k'_1, \ldots, k'_{n'}; p_i, q_i)$ as well. The resulting integral

$$\Im\{A\} = \sum_{n'=0}^{\infty} \int d\tau_{n'+2}(X; k'_1, \dots, k'_{n'}, q_1, q_2) \frac{1}{n'!} \prod_{l=1}^{n'} 2\tilde{S}_f(k'_l) \bar{\Theta}(\Omega_I, k'_l) \\ \exp\left(\int \frac{d^3k}{2k^0} \Theta(\delta\Omega, k) 2\tilde{S}_f(k)\right) b(k'_1, \dots, k'_{n'}; p_i, q_i)$$
(105)

gets an additional exponential factor, which is easy to interpret. It can be expressed in terms of the function

$$\tilde{B}(\Omega, q_1, q_2) = -\frac{1}{8\pi^2} \int \frac{d^3k}{k^0} \Theta(\Omega; k) \left(\frac{q_1}{kq_1} - \frac{q_2}{kq_2}\right)^2$$

as follows

$$\exp\left(\int \frac{d^3k}{2k^0}\,\Theta(\delta\Omega,k)\,2\tilde{S}_f(k)\right) = \exp\left(2Q_f^2\alpha\tilde{B}(\Omega_I,q_1,q_2) - 2Q_f^2\alpha\tilde{B}(\Omega_F,q_1,q_2)\right).$$

We have therefore found out by explicit calculation that in the proposed method, in which for Ω_F much smaller than Ω_I we skip photons that fall into $\delta\Omega = \Omega_I \setminus \Omega_F$, the distribution of the remaining photons is the following

$$d\sigma_{[n,n']}^{\text{Cru}^{*}}(\Omega_{I},\Omega_{I}) = ds_{X} \frac{\sigma_{\text{Born}}(s_{X})}{4\pi} d\tau_{n+1}(P;k_{1},\dots,k_{n},X) e^{\gamma_{e}\ln\varepsilon_{e}} \frac{1}{n!} \prod_{j=1}^{n} 2\tilde{S}_{e}(k_{j})\bar{\Theta}(\Omega_{I},k_{j}) \\ \times d\tau_{n'+2}(X;k_{1}',\dots,k_{n'}',q_{1},q_{2}) \frac{s_{X}}{s_{Q}} \frac{2}{\beta_{f}} e^{R_{F}(\Omega_{I})} \frac{1}{n'!} \prod_{l=1}^{n'} 2\tilde{S}_{f}(k_{l}')\bar{\Theta}(\Omega_{I},k_{l}') \\ R_{F} = \gamma_{f} \ln\left(\delta_{f} \frac{s_{Q}+2K'Q}{s_{Q}}\right) + 2Q_{f}^{2}\alpha\tilde{B}(\Omega_{I},q_{1},q_{2}) - 2Q_{f}^{2}\alpha\tilde{B}(\Omega_{F},q_{1},q_{2}).$$
(106)

Also note that, by construction, the integral value is preserved

$$\sum_{n,n'} \int d\sigma_{[n,n']}^{\operatorname{Cru}^*}(\Omega_I,\Omega_I) = \sum_{n,n'} \int d\sigma_{[n,n']}^{\operatorname{Cru}}(\Omega_I,\Omega_F).$$

Now, since the IR boundary in the above new distribution has changed for FSR photons, we cannot continue to use the $\rho_{EEX}^{(r)}$ of eq. (16). We have to use another $\rho_{EEX}^{*(r)}$ in which we replace $\tilde{B}(\Omega_F)$ by $\tilde{B}(\Omega_I)$ in the YFS form factor, see eq. (11):

$$\rho_{\text{EEX}}^{*(r)} = \rho_{\text{EEX}}^{(r)} e^{2Q_f^2 \alpha(\tilde{B}(\Omega_I, q_1, q_2) - \tilde{B}(\Omega_F, q_1, q_2))},$$

and consequently, since the model weight is the ratio of the model and crude distributions, the new exponential factors cancel out, and the new model weight is functionally exactly the same

$$W_{\text{EEX}}^{*(r)} = W_{\text{EEX}}^{(r)}.$$

In the new MC calculation

$$\sigma_{\text{EEX}}^{(r)} = \int W_{\text{EEX}}^{*(r)} \, d\sigma^{\text{Cru}^*} = \int W_{\text{EEX}}^{(r)} \, d\sigma^{\text{Cru}^*} \tag{107}$$

both the product of the weights and the normalization is the same. The above result is so trivial that, in fact, in the MC program for the EEX model we change almost nothing – we are only omitting hidden photons in the calculation of the model weight. This simplicity reflects the basic fact that very soft photons are unimportant for all IR-safe integrand functions.

The term $\gamma_f \ln(\ldots)$ in R_F is cancelled by $\tilde{B}(\Omega_F)$ and there is in fact no dependence on Ω_F nor δ_f in $d\sigma_{[n,n']}^{\text{Cru}*}(\Omega_I, \Omega_I)$ any more. The IR cancellation is now assured by the term

$$2\frac{\alpha}{\pi} \left(\ln \frac{2q_1q_2}{m_f^2} - 1 \right) \ln \varepsilon,$$

which is implicitly present in $\tilde{B}(\Omega_I, q_1, q_2)$.

The situation is, however, not as good as we described above. There is one important complication due to the use of the weighted events, at the level of the crude distribution. Let us go back again to the case of EEX

$$\sigma_{\rm EEX}^{(r)} = \int W_{\rm EEX}^{(r)} W_{\rm FSR}^{\rm Cru} W_{\rm ISR}^{\rm Cru} \, d\sigma^{\rm Pri}.$$
 (108)

Now the problem is that photons in $\delta\Omega$ cannot be "hidden", because $W_{\rm FSR}^{\rm Cru}$ does not obey the "IR-safeness" condition

$$\lim_{k'_{i} \to 0} W_{\text{FSR}}^{\text{Cru}}(n', k'_{1}, \dots, k'_{i}, \dots, k'_{n'}) = W_{\text{FSR}}^{\text{Cru}}(n'-1, k'_{1}, \dots, k'_{i-1}, k'_{i+1}, \dots, k'_{n'}) \frac{f\left(\theta_{i}, \frac{m_{f}^{2}}{s_{Q}}\right)}{\bar{f}\left(\theta_{i}, \frac{m_{f}^{2}}{s_{Q}}\right)}.$$

Even the softest photons contribute the finite ratio (f/\bar{f}) , and this contribution is essential for the IR-cancellations and for the overall normalization.

There is, however, a way of saving our method of replacing Ω_F with Ω_I . Let us repeat again the calculation of eq. (103) assuming that photons "hidden" inside $\delta\Omega$ do not contribute the factor (f/\bar{f}) to the overall weight. We are able to carry out the calculation as before, obtaining the modified exponential factor

$$\Im'\{A\} = \sum_{n'=0}^{\infty} \int d\tau_{n'+2}(X; k'_1, \dots, k'_{n'}, q_1, q_2) \frac{1}{n'!} \prod_{l=1}^{n'} 2\tilde{S}_f(k'_l) \bar{\Theta}(\Omega_I, k'_l) \\ \exp\left(\int_{\delta\Omega} \frac{d^3k}{k^0} \tilde{S}_f(k) \frac{\bar{f}(\theta, m_f^2/s)}{f(\theta, m_f^2/s_Q)}\right) b(k'_1, \dots, k'_{n'}; p_i, q_i),$$
(109)

It is very important that the effect due to the omission of (f/\bar{f}) in the overall weight can be evaluated analytically, and therefore *corrected for* analytically. In other words we shall be able to compensate analytically for the missing average contribution to $W_{\rm FSR}^{\rm Cru}$ from the hidden photons. The evaluation of the integral over $\delta\Omega$ is based on the observation that

$$\tilde{S}_{f}^{*}(k) = \tilde{S}_{f}(k) \frac{\bar{f}(\theta, m_{f}^{2}/s)}{f(\theta, m_{f}^{2}/s_{Q})} = -Q_{f}^{2} \frac{\alpha}{4\pi^{2}} \left(\frac{q_{1}^{*}}{kq_{1}^{*}} - \frac{q_{2}^{*}}{kq_{2}^{*}}\right)^{2},$$

where q_i^* , i = 1, 2, are defined such that $(q_i^*)^2 = m_f^2(s_Q/s)$. Furthermore, in the QMS, they have the same directions as the original $\vec{q_i}$ and the same total energy, $q_1^{*0} + q_2^{*0} = \sqrt{s_Q}$. With the help of the above we get

$$I_{\delta\Omega} = \int_{\delta\Omega} \frac{d^3k}{k^0} \, \tilde{S}_f(k) \frac{\bar{f}(\theta, m_f^2/s)}{f(\theta, m_f^2/s_Q)} = 2\alpha Q_f[\tilde{B}(\Omega_I, q_1^*, q_2^*) - \tilde{B}(\Omega_F, q_1^*, q_2^*)].$$

We have at our disposal an analytical representation of the function $B(\Omega, q_1, q_2)$, for spherical Ω and regularized with m_{γ} , in terms of logarithmss and dilogarithms, for arbitrary q_i , not necessarily antiparallel. Although $I_{\delta\Omega}$ is IR-finite by definition, it is useful to keep m_{γ} and evaluate separately $\tilde{B}(\Omega_I)$ in the CMS and $\tilde{B}(\Omega_F)$ in QMS, where the corresponding IR-boundaries are spherical, and subtract the results afterwards. We may calculate \tilde{B} 's in any frame, because they are (when regularized with m_{γ}) essentially Lorentz-invariant – we only need to transform IR-boundaries Ω correctly from one frame to another.

Summarizing: in the realistic case of the weighted events (with non-IR-safe weights) the method in which we hide photons in $\delta\Omega = \Omega_I \setminus \Omega_F$ leads to a new crude distribution similar to that in eq. (106) with the new

$$R_F = \gamma_f \ln\left(\delta_f \frac{s_Q + 2K'Q}{s_Q}\right) + 2Q_f^2 \alpha \tilde{B}(\Omega_I, q_1^*, q_2^*) - 2Q_f^2 \alpha \tilde{B}(\Omega_F, q_1^*, q_2^*).$$
(110)

As a consequence, the above exponential factor does not cancel out exactly in the model weight with the correction to the YFS form factor as before, and we have the following additional correcting factor in the model weight:

$$W_{\text{hide}} = e^{-2\alpha Q_f[\tilde{B}(\Omega_I, q_1^*, q_2^*) - \tilde{B}(\Omega_F, q_1^*, q_2^*)] + 2\alpha Q_f[\tilde{B}(\Omega_I, q_1, q_2) - \tilde{B}(\Omega_F, q_1, q_2)]}.$$
(111)

It should be really present in the model weight, but in the program, for historical reasons and for convenience, it is included in the crude weight.

The important profit from the above method is that with the above fix we can now make our calculation for the CEEX model with the ISR-FSR interference (IFI) switched on.

Note that the above treatment is more elaborate than the analogous one in BHLUMI because it is valid for finite m_f , while in BHLUMI we use the approximation $m_f \ll \sqrt{s}$. The correcting weight in BHLUMI is a simple one-line expression while here it expressed by a long series of logarithms and dilogarithms.

Let us finally add a side remark: another valid method of realizing a hypothetical Monte Carlo with common Ω for ISR and FSR is to generate photons using small Ω_F and to apply a brute-force rejection of all events with one or more photons falling into Ω_I . This was used in the early version of BHLUMI. We do not like this method because it may lead to an excessive number of events with zero weight, lowering substantially the efficiency of the MC.

3.9 Photon multiplicity enrichment

Let us finally describe yet another complication of the *primary* distribution, which is introduced for technical reasons, i.e. in order to get better total weight distribution, and a smaller rejection rate in the process of turning weighted events into unweighted events. This modification is not necessary for weighted events. (It can be switched off by adjusting input data).

The problem is essentially due to the introduction of the ISR-FSR interference, which we have already called IFI. As already known from the $\mathcal{O}(\alpha^1)$ case, the weight that introduces IFI is sharply peaked around 1 and has a strict upper bound $W_{\text{IFI}} \leq 2$. The destructive interference with the weights $W_{\text{IFI}} \sim 0$ occurs in the backward scattering (in the fermion scattering angle) and there is a little constructive interference $W_{\text{IFI}} \sim 2$, mostly in the forward direction. The maximum weight = 2 or a factor of 2 in the *primary* primary cross section solves the problem, at the expense of the factor of 2 rejection rate [14,31].

In the case of *n* photons, however, the same leads to: the maximum weight = 2^n or equivalently the increase of the *primary* cross section by a factor of 2^n , and consequently increase of the generated photon multiplicity by a factor of 2. Of course, almost all of this increase is artificial, and it is compensated by W_{IFI} , leaving only some small net effect due to IFI in the MC events. A more sophisticated method would be to increase the *primary* primary cross section (and photon multiplicity) more selectively, that is in a way dependent on the fermion scattering angle. For the moment we do not do it. It may be done in the future. What we do is the following: we increase the *primary* cross section by a factor of 2^{λ} , where λ is not equal to 2, but is adjusted empirically so that the tail of the total MC weight is acceptable. We have found that the value $\lambda \sim 1.25$ is the optimal one.

The introduction of the above λ factor affects all formulas for the *primary* cross section and for W^{Cru} in a rather trivial way, so we do not write it explicitly. The only non-trivial modification is in the compensating factor for the *hidden* photons in the previous section. This can be understood and implemented as a modification of the electric charge of the final fermion $Q_f \to \lambda Q_f$ in the *primary* cross section.

3.10 Entire MC algorithm top-to-bottom

Specializing to the CEEX model, we can summarize the results of the three previous sections as follows

$$\sigma_{\text{CEEX}}^{(r)}\{A\} = \sum_{f=\mu,\tau,d,u,s,c,b} \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \int A W_{\text{CEEX}}^{(r)} W_{\text{FSR}}^{\text{Cru}} W_{\text{ISR}}^{\text{Cru}} W_{\text{hide}} \, d\sigma_{[n,n']}^{\text{Pri}*}(\Omega_I).$$
(112)

Here $d\sigma_{[n,n']}^{\text{Pri}^*}(\Omega_I)$ is obtained from the product of the ISR and FSR primary differential distributions

$$d\sigma_{[n,n']}^{\mathrm{Pri}}(\Omega_I,\Omega_F) = d\mathfrak{I}_n^{\mathrm{Pri}}(\Omega_I) \ d\mathfrak{F}_{n'}^{\mathrm{Pri}}(\Omega_F), \tag{113}$$

see eqs. (75) and (92), by means of hiding/ignoring FSR photons in $\delta\Omega$. Consequently, in the evaluation of $W_{\text{CEEX}}^{(r)}$ and of all other weights, only momenta outside the common IR-domain Ω_I enter.

The value of the integrated cross section with the acceptance function A is obtained in the MC run in a standard way

$$\sigma_{\text{CEEX}}^{(r)}\{A\} = \langle A W_{\text{CEEX}}^{(r)} W_{\text{FSR}}^{\text{Cru}} W_{\text{ISR}}^{\text{Cru}} W_{\text{hide}} \rangle \sigma^{\text{Pri}^*}.$$
 (114)

The acceptance function A may for instance define the entire cross section $(A \equiv 1)$, or just a single bin in the histogram of $\cos \theta$ for the outgoing fermion, or any other IR-safe observable. The overall normalization is based on

$$\sigma^{\operatorname{Pri}^{*}} = \sum_{f=\mu,\dots,b} \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \int d\sigma_{[n,n']}^{\operatorname{Pri}^{*}}(\Omega_{I}) = \sum_{n=0}^{\infty} \int d\mathfrak{I}_{n}^{\operatorname{Pri}}(\Omega_{I}) \sum_{n'=0}^{\infty} \int d\mathfrak{F}_{n'}^{\operatorname{Pri}}(\Omega_{F})$$
$$= \sum_{f=\mu,\dots,b} \sum_{n=0}^{\infty} \int d\mathfrak{I}_{n}^{\operatorname{Pri}}(\Omega_{I}) = \sum_{f=\mu,\dots,b} \int_{0}^{1} dv \ \sigma_{\operatorname{Born}}^{f}(s(1-v)) \ \mathcal{J}_{0}(v) \ \bar{\gamma}_{e} v^{\bar{\gamma}_{e}-1} \varepsilon^{\gamma_{e}-\bar{\gamma}_{e}},$$
(115)

where we have exploited the property $\int \sum d\mathfrak{F}^{\text{Pri}}(\Omega_F) \equiv 1$ of eq. (77), and the ISR part is taken from eq. (95). Note that we have put $v_{\text{max}} = 1$, understanding that $\sigma_{\text{Born}}^f(s) = 0$ below the threshold, $s < 4m_f^2$.

We shall now describe the entire generation of the MC event according to $d\sigma_{[n,n']}^{\operatorname{Pri}*}(\Omega_I)$ from the top to the bottom, as is done in the program, starting from the generation of vdescribing the total energy loss due to ISR, the type of final fermion f and the photon multiplicities n and n'. Generation of photon energies and angles comes later, using methods already described in detail in the previous section.

3.11 ISR spectrum and fermion type

First comes the important practical question: Shall we (a) generate first the fermion type f and later v or (b) vice versa? Both options are technically realizable. In case (a) we would calculate numerically

$$\sigma_f^{\mathrm{Pri}^*} = \int_0^1 dv \ \sigma_{\mathrm{Born}}^f(s(1-v)) \ \mathcal{J}_0(v) \ \bar{\gamma}_e v^{\bar{\gamma}_e - 1} \varepsilon^{\gamma_e - \bar{\gamma}_e},\tag{116}$$

for $f = \mu, \tau, d, u, s, c, b$, and generate fermion type f first; and later on, for a given f, we would generate the variable v according to

$$\frac{d\sigma_f^{\operatorname{Pri}^*}}{dv} = \sigma_{\operatorname{Born}}^f(s(1-v)) \ \mathcal{J}_0(v) \ \bar{\gamma}_e v^{\bar{\gamma}_e - 1} \varepsilon^{\gamma_e - \bar{\gamma}_e}.$$
(117)

This looks as a natural solution; however, the generation and integration of the ISR spectrum $d\sigma_f^{\text{Pri}*}/dv$ is done numerically in a MC module that creates a look-up matrix, which memorizes very precisely the shape of the distribution during the initialization phase of the MC run (before MC event generation). In this method we would need several initializations, creating several tables of this kind. This is feasible, but not very convenient. The situation is much worse, when beamstrahlung is switched on because in this case the 1-dimensional problem of the generation of v is replaced with the 3-dimensional problem of generating v, z_1, z_2 , and consequently we would need to manage several sets of 3-dimensional look-up matrices. This would make the initialization phase rather long in CPU time, and the tables would occupy a lot of processor memory.

We think that the above scenario is still technically realizable, even in the presence of beamstrahlung. Nevertheless, we decided for option (b), which is in our opinion more economical. In this case, we generate first the v variable (the case of beamstrahlung is described below) according to a distribution summed up over final-state flavour:

$$\frac{d\sigma^{\operatorname{Pri}^*}}{dv} = \sum_{f=\mu,\dots,b} \sigma^f_{\operatorname{Born}}(s(1-v)) \ \mathcal{J}_0(v) \ \bar{\gamma}_e v^{\bar{\gamma}_e - 1} \varepsilon^{\gamma_e - \bar{\gamma}_e};$$
(118)

next, for a given v, we generate the final-state flavour f according to a probability

$$P_f = \frac{\sigma_{\text{Born}}^f(s(1-v))}{\sum_{g=\mu,\dots,b} \sigma_{\text{Born}}^g(s(1-v))}.$$
(119)

3.12 Inclusion of beamstrahlung

In the presence of beamstrahlung, the flavour-summed three-dimensional distribution to be generated in the very beginning of the MC algorithm is

$$\frac{d\sigma^{\operatorname{Pri}^*}}{dvdz_1dz_2} = \sum_{f=\mu,\dots,b} \sigma^f_{\operatorname{Born}}(s(1-v)z_1z_2) \mathcal{J}_0(v) \,\bar{\gamma}_e v^{\bar{\gamma}_e-1} \varepsilon^{\gamma_e-\bar{\gamma}_e} \mathcal{D}(z_1,z_2,\sqrt{s});$$
(120)

see also eq. (26). The above 3-dimensional distribution is explored and memorized in the look-up matrices in the initialization phase of the MC run. This allows us to generate v, z_1, z_2 in a very efficient way for arbitrary σ_{Born} and arbitrary beamstrahlung structure function $\mathcal{D}(z_1, z_2, \sqrt{s})$. As discussed previously, we admit in $\mathcal{D}(z_1, z_2, \sqrt{s})$ δ -like singularities in z_i and, as a result, the MC integration of $d\sigma^{\text{Pri}^*}/dvdz_1dz_2$ is split into three branches with three separate look-up matrices. The above organization assures that the beamstrahlung structure function can be a completely arbitrary "user function".

Next, for a given set (v, z_1, z_2) , the final fermion flavour f is generated with the probability

$$P_f = \frac{\sigma_{\text{Born}}^f(s(1-v)z_1z_2)}{\sum_{g=\mu,\dots,b} \sigma_{\text{Born}}^g(s(1-v)z_1z_2)}.$$
(121)

3.13 Photon multiplicities and momenta

Having defined the total ISR loss variable v or vz_1z_2 , the ISR photon momenta are generated first, and the FSR photon momenta are generated second. For $v < \varepsilon$ the ISR photon multiplicity is zero and for $v > \varepsilon$ it is generated according to the shifted Poisson distribution P_{n-1} with $\langle n \rangle = \bar{\gamma}_e \ln(v/\varepsilon)$, see eq. (97), where, in the presence of beamstrahlung, the modified $s' = sz_1z_2$ enters instead of s into the definition of $\bar{\gamma}_e$, see eq. (91). Next, all ISR photons are generated according to the distribution $d\mathfrak{I}_n^{\text{Pri}}$ of eq. (92), with the methods already described. The crude weight of eq. (93) is calculated.

Having generated ISR photons (and optionally beamstrahlung) we now know the total four-momentum of the final fermions plus FSR momenta

$$X = p_a z_1 + p_b z_2 - \sum_{j=1}^n k_j,$$
(122)

but to start generation of the FSR momenta we need to know only $s_X = X^2$. First, the FSR photon multiplicity n' is generated according to a Poisson distribution with the average defined in eq. (78). Then, FSR momenta are generated in the rest frame of $Q = q_1 + q_2$ (QMS). More precisely, their dimensionless energy parameters and angles are generated, according to the corresponding FSR primary distribution of eq. (75), such that the $s_Q = Q^2$ needs not be known. The s_Q is determined as a fraction of s_X with the help of eq. (63), such that photon four-momenta can be constructed in absolute (GeV) units in QMS.

At this point we need to generate angles ψ and ω in the transformation form QMS down to CMS defined in eq. (59). Knowing the momentum $\hat{X} = \hat{Q} - \sum_{j} \tilde{k}'_{j}$ in the QMS we may apply this transformation and calculate final fermion momenta in the CMS where $\vec{p}_{1} + \vec{p}_{2} = \vec{p}_{a} + \vec{p}_{b} = 0$. In the case of beamstrahlung this transformation bring us to a frame where $\vec{p}_{1}z_{1} + \vec{p}_{2}z_{2} = 0$, and we need an additional boost along beams to brings generated momenta to the laboratory system. The same boost is done for ISR photons.

Removal (hiding) of the FSR photons in $\delta\Omega$ is done at the end of the generation of the FSR photons. All remaining photons have the common IR-domain Ω_I defined in the CMS where $\vec{p_1} + \vec{p_2} = \vec{p_a} + \vec{p_b} = 0$ or in the presence of beamstrahlung in the frame where $\vec{p_1}z_1 + \vec{p_2}z_2 = 0$.

4 Structure of the program

In the following we shall describe the topography of the distribution directory, then the programming rules which we follow, and finally we shall briefly describe the functionality of the principal modules of the program.

4.1 Topography of the distribution

The program source code is organized into *modules*, also called *pseudo-classes*, which are located in several Unix-type subdirectories of the distribution directory KK-all. The distribution directory also contains one additional subdirectory, ffbench, with demonstration (template) programs and one subdirectory, dok, with the documentation. The essential part of the source code of the \mathcal{KK} Monte Carlo event generator is located in the two subdirectories KK2f and bornv. The tool box of various utilities is located in the subdirectory glibk, the electroweak library is located in dizet, the MC library of the τ lepton decays TAUOLA is in the subdirectory tauola, PHOTOS in the subdirectory photos and the hadronization package JETSET is in the subdirectory jetset.

KK2f	-all	
	KK2f	Event generator: KK2f, KarLud, KarFin, GPS, QED3, HepEvt, PseuMar, TauPair
	bornv	Event generator: BornV, MBrA, MBrB, Vesk1, BStra, FoamA, FoamB, FoamC, VegasA,B,C
	glibk	Library of utilities: GLK, MathLib
	dizet	Library electroweak corrections: DZface , DIZET 6.21 sub-directory: tabtest
	tauola	Tau-lepton decays: TAUOLA 2.6
	photos	Radiative corrections in decays: PHOTOS 2.02
	jetset	Hadronization of quarks: JETSET 7.2
	dok	Documentation in postscript: KKcpc.ps.gz
	ffbench	Demo programs, example input data, benchmark outputs sub-directories: demo, Inclusive, Mu, Tau, Down, Up, Botom, Beast

 $Figure \ 1:$ Topography of the distribution directory

4.2 Programming rules

The program is written in Fortran77 with popular extensions such as long variable names, long source lines, etc., which are available on all platforms. In the *Makefile* in the main directory KK-all, there is a collection, of f77 compilation flags, for Linux, AIX, HPUX and ALPHA compilers, which should be used to activate these extensions. The program is written in such a way that its translation to an object-oriented language such as C++ should not be very difficult. In fact the program is divided into modules, which have the structure of the C++ classes, as far as it is possible to do it within f77. Below we characterize the rules according to which the program was written.

Each pseudo-class with the name Module consists of a separate source file Module.f and the header file Module.h. Each module obeys the following rules:

- There is only one common block /c_Module/ which contains all class member variables, which is placed in the header file Module.h. Each subroutine in the Module.f source file includes an INCLUDE 'Module.h' statement. The outside programs should never include directly /c_Module/. All input/output communication is done with the help of dedicated, easy to use, subroutines.
- Variables in /c_Module/ are *class members* and all have the special prefix "m_" in their name, for example m_Iterat is the number of iterations.
- The user has access to some class members through "getters" and "setters"; see below.
- Strong typing is imposed with the help of IMPLICIT NONE.
- Initializator with the name Module_Initialize performs initialization. Typically it initializes variables in /c_Module/.
- Finalizer with the name Module_Finalize, summarizes the whole run, sets output values in /c_Module/, prints output, etc.
- Maker with the name Module_MakeSomething, or a similar one, does the essential part of the job, for instance a maker Module_MakeEvent generates a single MC event.
- Setter with the name Module_SetVariable is called from the outside world to set m_Variable in /c_Module/. For example CALL BornV_SetCMSene(100d0) sets the variable m_CMSene=100d0. Only certain privileged variables have a right to be served by their own setter, the other ones are in principle "private".
- Getter with the name Module_GetVariable is called from the outside world to get the m_Variable from /c_Module/. It is a preferred way of sending output information to the outside world. For example, with the help of CALL KK2f_GetXsecMC(xSecPb, xErrPb) one gets the MC cross section xSecPb and its error xErrPb in the user program.

In the following we shall describe all pseudo-classes and their role.

4.3 KK2f: Top-level class

The main purpose of this top-level pseudo-class is to provide the user interface, see section 6 on the usage of the program. Let us list and explain the main entries in this class:

- KK2f_ReaDataX('data_file',iReset,imax,xpar) reads the input data file. It should be called twice, once with INTEGER iReset=1, for the default data file .KK2f_defaults, which is placed in the main directory KK-all. The user has to provide a link to this file, or absolute path in the name of the file. (Copying it to the local directory is not recommended.) It should be called for the second time for the user data ./user_data with INTEGER iReset=0, in order to modify some entries in the input of the program. The variable INTEGER imax is the dimension of the DOUBLE PRECISION xpar(imax). For the moment imax≤ 3000 is required, but we reserve imax= 10000 for future use. The flag INTEGER iReset=0 is for reading data with resetting all undefined values to zero, while with iReset=1 only entries listed in the data file are modified.
- KK2f_Initialize(xpar) initializes the whole MC generator. This initializer calls initializers of other classes like BornV_Initialize, KarLud_Initialize, KarFin_Initialize, QED3_Initialize, GPS_Initialize, TauPair_Initialize. It initializes also the database for the branching over final fermion flavours in the class MBrA. Note that BornV_Initialize reads from the disk look-up tables for the electroweak corrections and KarLud_Initialize manages initialization of the ISR energy spectrum either with the help of Vesk1 class or, in the presence of the beamstrahlung, with the help of the Bstra class, which in turn initializes three copies of the Foam package, FoamA, FoamB, FoamC (or of Vegas package, VegasA, VegasB, VegasC).
- KK2f_Make generates a single event. It calls KarLud_Make to make ISR photons, KarFin_Make to make FSR photons and KK2f_Merge to merge all photons in a single list. It invokes KK2f_MakePhelRand to generate the photon helicities randomly, calculates the EEX model weight using CALL QED3_Make and/or the CEEX model weight using CALL GPS_Make. Optional rejection is performed to produce weight-1 events and the weight book-keeping is done separately for each final fermion type using MBrA_Fill. Finally, quarks are hadronized using HepEvt_Hadronize (interface to JETSET), or τ decays are simulated with all spin effects (including all spin correlations). This is done using subprograms of the TauPair class (interface to TAUOLA).
- KK2f_GetPhotAll(Nphot,PhoAll) provides the user with the momenta of all photons: DOUBLE PRECISION PhoAll(100,4) and photon multiplicity INTEGER Nphot. Alternatively, Nphot is provided by KK2f_GetNphot(Nphot) and the *i*-th photon momentum by KK2f_GetPhoton1(iPhot,Phot), with DOUBLE PRECISION Phot(4).
- $KK2f_GetFermions(q1,q2)$ provides the user with the momenta of the final fermions DOUBLE PRECISION q1(4),q2(4).

- KK2f_GetBeams(p1,p2) provides the user with the momenta of the beams DOUBLE PRECISION p1(4),p2(4).
- KK2f_GetWtAll(WtMain,WtCrud,WtSet) can be used to get access to the main MC weight WtMain and the list of all alternative weights WtSet(1000). The weight for the crude differential cross section WtCrud is also provided. All of them are DOUBLE PRECISION type. Alternatively, the getter KK2f_GetWt(WtMain,WtCrud) may be more convenient.
- KK2f_Finalize may be called at the end of the MC run, in order to perform the final book-keeping and printing.
- KK2f_GetXSecMC(XSecPb,XErrPb) should be called after calling KK2f_Finalize in order to get the total cross section (in picobarns) and its absolute error: DOUBLE PRECISION XSecPb, XErrPb.
- KK2f_GetVersion(Version) and KK2f_GetDate(Date) provide the user with the version number DOUBLE PRECISION Version and the release data CHARACTER*14 Date information. This should help to keep track of the development of the program.
- KK2f_Print(ie1,ie2) can be used to print the actual MC events, limiting their serial number to stay between INTEGER ie1 and INTEGER ie2.

There are several other getters in the **KK2f** class, which are mainly for internal use.

Let us briefly list other subroutines in the $\mathbf{KK2f}$ class, which are not called by the user of the program:

- KK2f_WignerIni(KFbeam,CMSene,PolBeam1,PolBeam2, Polar1,Polar2) does Wigner rotation for spin polarization vectors of beams. Beam polarization vectors (in input data) are defined in the beam particle rest frames, which are reached from the CMS by a simple z-boost without any rotation. (The first beam is parallel to the z-axis.)
- KK2f_ZBoostAll(exe) performs a z-boost on all momenta of the event. This z-boost corresponds to beamstrahlung or beam spread and is done at the very end of generation, after the calculation of the matrix element.
- KK2f_DsigOverDtau(mout,Rho) is only for documentation and testing purposes. It calculates the distribution $d\sigma/d\tau$ corresponding to WtCrud, normalized with respect to $d\tau$ = Lorentz invariant phase space.
- KK2f_Merge merges lists of ISR and FSR photon momenta. The resulting merged photons are ordered according to their energy.
- KK2f_MakePhelRand generates the photon helicities randomly.

4.4 HepEvt: HEP event record class

The pseudo-class **HepEvt** has the double purpose of (a) being another user interface, alternative to getters in **KK2f**, and (b) managing also the hadronization of quarks. The user may also traditionally put the common block of the **HepEvt** class directly into its code. It is a **DOUBLE PRECISION** version of the standard PDG /HEPEVT/ common block, for a maximum of 2000 particles.

```
! maximum number of particles
 INTEGER nmxhep
PARAMETER (nmxhep=2000)
DOUBLE PRECISION
                  phep, vhep
INTEGER nevhep, nhep, isthep, idhep, jmohep, jdahep
COMMON /d_HepEvt/
$
     nevhep,
                      ! serial number
$
                      ! number of particles
     nhep,
$
     isthep(nmxhep),
                      ! status code
$
     idhep(nmxhep),
                      ! particle ident KF
$
     jmohep(2,nmxhep), ! parent particles
$
     jdahep(2,nmxhep), ! childreen particles
$
     phep(5,nmxhep), ! four-momentum, mass [GeV]
$
     vhep(4,nmxhep)
                      ! vertex [mm]
SAVE /d_hepevt/
                  _____
```

Let us now list and explain the subprograms in the **HepEvt** class.

- HepEvt_Fill fills in all of common block /d_HepEvt/ using the subprogram Hep-Evt_Fil1. Momenta are provided by getters from KarLud and KarFin.
- HepEvt_Fil1 writes a single particle record into the common block /d_HepEvt/.
- HepEvt_Hadronize(HadMin) arranges jets with the help of LuJoin and LuShow, and hadronizes quarks using LuExec.
- CALL HepEvt_GetBeams(p1,p2) provides four-momenta of the two beams DOUBLE PRECISION p1(4),p2(4).
- CALL HepEvt_GetFfins(q1,q2) provides four-momenta of the two final fermions DOU-BLE PRECISION q1(4),q2(4).
- CALL HepEvt_GetPhotAll(NphAll,PhoAll) provides the photon multiplicity INTEGER NphAll and the photon four-momenta DOUBLE PRECISION PhoAll(100,4).
- HepEvt_GetPhotBst(nPhot,Phot) provides the multiplicity INTEGER nPhot (=0,1,2) and four-momenta DOUBLE PRECISION Phot(100,4) of the beamstrahlung photons.
- HepEvt_LuHepc This is the double-precision version of LUHEPC of JETSET. It translates DOUBLE PRECISION /c_HepEvt/ into the old style REAL*4 Lund commons.

4.5 KarLud: Crude level MC for ISR

The simulation of ISR together with the beamstrahlung and generation of the type of final-fermion flavour is implemented in the **KarLud** pseudo-class. Let us now list and explain all subprograms in the **KarLud** class:

- KarLud_Initialize(xpar_input,XCrude) is the initializer of the class. It initializes the generation of v with the help of Vesk1_Initialize or of v, z_1, z_2 with the help of BStra_Initialize. It defines the primary integrated cross section on which the entire normalization is based.
- KarLud_SmearBeams implements beam spread. This is correct only for a small spread < 2 GeV. It should not be used together with beamstrahlung, since this has not been tested yet. The distribution is Gaussian $\rho(X) = N \exp((X \text{CMSene}/2)^2/(2\text{DelEne}^22))$ (DelEne is the dispersion of the beam energy Ebeam, not of CMSene).
- KarLud_Make(PX,wt_ISR) generates ISR photons with the help of other subprograms; PX(4) is the four-momentum left after photon emission, wt_ISR is the ISR component of the "crude weight". The other subroutines called here are: KarLud_SmearBeams (see below), BornV_SetCMSene(XXXene), which resets the CMS four-momentum in BornV in the case of beam smearing, Vesk1_Make, which generates the variable v, in the absence of beamstrahlung (alternatively it is done with VegasA_Generate for KeyFix=2), or BStra_Make, which generates v, z₁, z₂ in case of beamstrahlung. The ISR photons are generated with the help of KarLud_YFSini, see below, and the type of final-state fermion KF is generated with the help of MBrA_GenKF. Finally, if FSR is off, then final momenta are produced locally with the help of KinLib_phspc2
- KarLud_Finalize(Mode, XKarlud, KError) calculates the crude cross section XKarlud and its error KError, and prints out final statistics. The crude cross section is coming from the Vesk1_Finalize (alternatively from VegasA_GetIntCrude) or, in case of beamstrahlung, from BStra_GetXCrude,
- KarLud_YFSini(XXXene,vv, PX,Wtlni) is generating the ISR photon momenta. Its input is the total energy available XXXene, and vv= v. Wtlni is the ISR component of the "crude weight" and PX(4) is the four-momentum left after photon emission. KarLud_YFSini calls BornV_GetAvMult to get the average ISR multiplicity, KarLud_PoissGen and KarLud_AngBre, see below.
- KarLud_PoissGen generates photon multiplicity.
- KarLud_AngBre generates photon angle.
- KarLud_ZBoostAll performs *z*-boosts of all photons.
- KarLud_GetPhotons(nphot,sphot) provides all ISR photons.
- KarLud_GetPhoton1(iphot,phot) provides single ISR photons.

- KarLud_GetPX(PX) provides four-momentum PX, see above.
- KarLud_GetBeams(p1,p2) provides the beam momenta. In the case of beamstrahlung p1,p2) are beams *after* beamstrahlung.
- KarLud_GetBeasts(p1,p2) provides the collinear photons of the beamstrahlung.

4.6 KarFin: Crude level MC for FSR

The FSR is implemented in the **KarFIN** class. This package was already used in the KORALZ [1] program for some time. Thanks to recent improvements it now works properly without any approximations close to τ threshold. The $m_f \ll \sqrt{s}$ approximation is not used anymore.

Let us now list and explain all subprograms in the **KarFin** class:

- KarFin_Initialize initializes some internal variables (weight book-keeping).
- KarFin_Make(PX,amfi1,amfi2,CharSq,WtFin) generates FSR photons with the help of other subprograms, see below. PX is the four-momentum of the entire FSR system (fermions + photons), amfi1,amfi2 are masses of the final charged pair (not necessarily equal), CharSq is the final-state fermion charge squared and WtFin is the FSR part of the crude weight.
- KarFin_YFSfin(PX,amfi1,amfi2,CharSq,WtFin) generates momenta of the FSR photons. PX, amfi1, amfi2, CharSq, WtFin are as defined above. It calls KarFin_PoissGen and KarFin_AngBre to generate photon multiplicity and angles, then KarFin_Kinf1 and and KarFin_Piatek see below.
- KarFin_Kinf1(PX,...,phsu) transforms from the rest frame of Q=q1+q2 QMS down to the laboratory through the intermediate rest frame of PX=q1+q2+phsu.
- KarFin_Piatek(Mas1,Mas2,CharSq,WtMlist, Wt3)²¹ optionally removes photons below E_{min} from the list of photons, appropriately modifying the crude weight. Mas1,2 = fermion masses, WtMlist = list of mass weights (f/f) for all photons. Wt3 = product of (f/f) for the alive (not hidden) photons. The correcting weight is calculated with the help of BVR_Btildc, calculating B̃ for q_i^{*} and BVR_Btilda for q_i.
- KarFin_PoissGen generates the photon multiplicity randomly.
- KarFin_AngBre generates the photon angles randomly.
- KarFin_Kinf1 transforms the final fermions and all photons from QMS through the Z-frame to CMS. Random rotation with angles ψ, ω is applied in the intermediate rest frame of PX (Z boson) using KarFin_BostEul.

²¹ Written in CERN, Piatek≡Friday, 22.IX.1989 (S.J.)

- KarFin_BostEul performs Lorentz transformations consisting of: (1) parallel boost from the final fermions rest frame to fermions + photons rest frame (Z frame); (2) two rotations with angles ψ, ω ; (3) parallel boost to the laboratory system CMS.
- KarFin_ZBoostAll(exe) does an additional z-boost of all particles in case of beamstrahlung.
- KarFin_Finalize prints final statistics.
- KarFin_GetNphot(nphot) provides the FSR photon multiplicity.
- KarFin_GetPhoton1(iphot, phot) provides the four-momentum of a single FSR photon.
- KarFin_GetPhotons(nphot,sphot) provides the four-momenta of all FSR photons.
- KarFin_GetFermions(qf1,qf2) provides the four-momenta of the final fermions.
- KarFin_WtMass(WtMass) provides the product of (f/\bar{f}) for the alive (not hidden) photons.

4.7 BornV class: particle data base and ISR spectrum

Class **BornV** is serving as a data-base for fermion properties such as mass, charge, isospin, colour and other fermion-type dependent parameters relevant to MC generation, like the maximum weight for rejection. It also reads from the disk and keeps the EW form factors produced by the interface to DIZET 6.21.

All other classes use the data-base of the **BornV** class through its getters, see below. The data-base is located in the class common block c_BornV, which is initialized by BornV_Initialize from the default input data file KK-all/.KK2f_defaults passed by arguments from KK2f_Initialize. Optionally, only after user modifications, see section 6 on the usage of the program.

For this particular class it is instructive to look into the list of the *class member* variables in the class common block/c_BornV/. Below we quote part of the BornV.h source code:

```
COMMON /c_BornV/
* Tables of EW formfactors
    $ m_cyy(m_poin1+1,7,16),
                                       ! formfactor, table
    $ m_czz(m_poin2+1,7,16),
                                        ! formfactor, table
    $ m_ctt(m_poin3+1,m_poinT+1,7,16), ! formfactor, table
    $ m_clc(m_poin4+1,m_poinT+1,7,16), ! formfactor, table
    $ m_syy(m_poin1+1,16),
                                       ! QCD correction, table
                                        ! QCD correction, table
    $ m_szz(m_poin2+1,16),
    $ m_stt(m_poin3+1,m_poinT+1,16),
                                        ! QCD correction, table
    $ m_slc(m_poin3+1,m_poinT+1,16),
                                       ! QCD correction, table
    $ m_GSW(100), ! form-factors,
                                        at the actual energy/angle
```

\$ m_QCDcor, ! QCD correction, at the actual energy/angle *----- EVENT -----\$ m_CMSene, ! Initial value of CMS energy \$ m_CMSene, ! Initial value of CMS energy \$ m_XXXene, ! CMS energy after beamstrahlung or beam spread \$ m_x1, ! 1-z1 = x1 for first beam(strahlung) \$ m_x2, ! 1-z2 = x2 for second beam(strahlung) \$ m_vv, ! v = 1-sprim/s \$ m_AvMult, ! Average photon multiplicity CRude at given v \$ m_YFSkon, ! YFS formfactor finite part \$ m_YFS_IR, ! YFS formfactor IR part _____ \$ m_vvmin, ! minimum v, infrared cut \$ m_vvmax, ! maximum v \$ m_HadMin, ! minimum hadronization mass [GeV] * Basic QED------\$ m_alfinv, ! 1/alphaQED, Thomson limit \$ m_alfpi, ! alphaQED/pi \$ m_Xenph, ! Enhancement factor for Crude photon multipl. \$ m_Xenph, * EW parameters ! Z mass \$ m_MZ, \$ m_amh, ! Higgs mass \$ m_amtop, ! Top mass \$ m_swsq, ! sin(thetaW)**2 \$ m_gammz, ! Z width \$ m_amw, ! W mass ! W width ! Fermi constant (from muon decay) \$ m_gammw, \$ m_Gmu, * Table of fermion parameters, quarks (1->6) and leptons (11->16) \$ m_KFferm(20), ! fermion KFcode (1->6) and (11->16) \$ m_NCf(20), ! number of colours \$ m_Qf(20), ! electric charge \$ m_T3f(20), ! isospin, L-hand component \$ m_helic(20), ! helicity or polarization \$ m_amferm(20), ! fermion mass \$ m_auxpar(20), ! auxiliary parameter \$ m_IsGenerated(20), ! Generation flag, only for SemiAn.! * Normalisation \$ m_gnanob, ! GeV⁽⁻²⁾ to nanobarns * Initial/final fermion types \$ m_KFini, ! KF code of beam * Test switches \$ m_KeyINT, ! ISR/FSR intereference switch \$ m_KeyElw, ! Type of Electroweak Library \$ m_KeyZet, ! Z-boson on/off \$ m_KeyWtm, ! Photon emission without mass terms \$ m_out ! output unit for printouts \$

*-----

Let us now list and explain all subprograms in the **BornV** class:

- BornV_Initialize(xpar) initializes data members in /c_BornV/.
- BornV_StartEW(xpar) initializes electroweak formfactors in /c_BornV/. There are two versions of this routine: one in KK-all/bornv/BornV_StartEW.f which reads electroweak formfactors from the disk file and another one in KK-all/dizet/BornV_StartEW.f which calculates it using DIZET library. See section 4.13 for more details.
- BornV_ReadAll reads from the disk-file pretabulated EW form factors for μ and τ leptons, and for d, u, b quarks. For s, c quarks the form factors of d, u are used.
- BornV_ReadFile(DiskFile,KFfin) reads from the disk a single file for a single final fermion.
- BornV_StartDZ(xpar) Initialized DIZET library using current input data in xpar.
- BornV_ReBin1, BornV_ReBin1a, BornV_ReBin2, BornV_ReBin2a subroutines map the variable $r \in (0, 1)$ (random number) into $v \in (0, v_{\text{max}})$. Various methods are used to do it, with various kinds of the mapping function.
- DOUBLE PRECISION FUNCTION BornV_RhoFoamC(xarg) is the integrand for FoamC in the 3-dimensional mode for beamstrahlung. Remember that BornV_Crude and BornV_MakeRho use the hidden input m_XXXene. BornV_Crude is in the R-units (point-like cross-section at √s=m_XXXene). It defines m_vv, which is later on exported to KarLud.
- DOUBLE PRECISION FUNCTION BornV_RhoFoamB(xarg) is the integrand for FoamB in the two-dimensional mode for beamstrahlung (it defines m_vv).
- DOUBLE PRECISION FUNCTION BornV_RhoFoamA(xarg) is the integrand for FoamA in the one-dimensional mode for beamstrahlung off and on (it defines m_vv).
- DOUBLE PRECISION FUNCTION BornV_RhoVesko1(R) is the integrand of Vesko1. (The comment about hidden input m_XXXene applies.) In the case of beamstrahlung the additional normalization factor Circee(1d0,1d0) is added inside BStra_Initialize (it defines m_vv).
- BornV_MakeGami(CMSene,gamiCR,gami) calculates GamiCR= $\bar{\gamma}_e$ and gami= γ_e as functions of CMSene.
- BornV_MakelSR(Rho) This procedure is tightly related to ISR photon generation in KarLud. It provides Rho(m_vv, m_XXXene), the primary distribution of v. It also calculates m_AvMult, which is later used in KarLud_YFSini; m_YFSkon ,m_YFS_IR, which are later used in GPS_Make and QED3_Make.

- DOUBLE PRECISION FUNCTION BornV_Crude(vv) calculates the crude total Born cross section summed over fermion types. It exploits the fact that the Born differential distribution reads $a + b \cos \theta + d \cos^2 \theta$. (Hidden input is m_XXXene). It is used in BornV_RhoVesko1, BornV_RhoFoamA, etc.
- DOUBLE PRECISION FUNCTION BornV_Differential(Mode,KFf,svar,CosThe,...) is the Born differential distribution. For Mode=0 it is a crude version of pure Born, no spin, no EW corrections. For Mode=1 it is the full result with EW corrections spin, etc. In this mode it is used in QED3, and for all kinds of tests. For Mode=3 it is used in the tests of pretabulation. In this case GSW(s,theta) has to be provided from the outside, with the help of BornV_SetGSW²².
- DOUBLE PRECISION FUNCTION BornV_Simple(KFi,KFf,svar,costhe) provides for BornV_Differential an unsophisticated Born differential distribution without EW corrections, with the Z and γ s-channel exchange.
- DOUBLE PRECISION FUNCTION BornV_Integrated(KFfin,svar) is used only in semianalytical programs. It calculates the total Born cross section. For KFfin = 0 it sums over all allowed flavours; otherwise, for KFfin.NE.0, it calculates the cross section for the actual value of m_KFfin.
- DOUBLE PRECISION FUNCTION BornV_Dizet(Mode,KFi,KFf,svar,CosThe,...) provides for BornV_Differential the differential Born cross section with/without EW corrections. For Mode=0 it provides pure Born and for Mode=1 electroweak corrections are added. KFi,KFf can also be negative for an antiparticle; in this case it is important to produce tables with the correct input KFini, KFfin.
- BornV_InterpoGSW(KFf,svar,CosThe) calculates EW form factors from look-up tables, using linear interpolation.
- BornV_givizo(idferm,ihelic,sizo3,charge,kolor) provides electric charge, weak isospin and colour of the fermion, where idferm =1,2,3,4 denotes: neutrino, lepton, up, down quark; negative idferm=-1,-2,-3,-4, denotes the corresponding antiparticle; ihelic = +1, -1 denotes right- and left-handedness (chirality) sizo3 is the third projection of weak isospin (±1/2), charge is the electric charge (in units of magnitude of the electron charge), kolor is the QCD colour, 1 for lepton, 3 for quarks.
- DOUBLE PRECISION FUNCTION BornV_SigOnb(CMSene) provides the point-like muon cross section in nanobarns for the normalization purpose.

Communication subprograms (setters and getters) used by all other classes are the following:

²² Note that in the test mode KeyEwl=0 and Mode=1 we use BornV_Simple, which will perhaps have to be changed in the future, because of the lack of spin effects. At this stage, however, we are bound to use it because the KeyZet etc. are implemented only in BornV_Simple and not in BornV_Dizet.

- BornV_GetParticle(KFferm, mass, Qf, T3f, NCf); for the fermion type INTEGER KFferm provides its QCD colour INTEGER NCf, mass, electric charge and weak isospin DOUBLE PRECISION mass, Qf, T3f.
- DOUBLE PRECISION FUNCTION BornV_GetMass(KFferm); for the fermion type IN-TEGER KFferm provides its mass.
- DOUBLE PRECISION FUNCTION BornV_GetCharge(KFferm); for the fermion type INTEGER KFferm provides its electric charge.
- INTEGER FUNCTION BornV_GetColor(KFferm); for the fermion type INTEGER KFferm provides its QCD colour.
- DOUBLE PRECISION FUNCTION BornV_GetAuxPar(KFferm); for the fermion type INTEGER KFferm it provides its auxiliary parameter.
- BornV_SetKeyElw(KeyElw) sets the EW switch KeyElw.
- BornV_GetKeyElw(KeyElw) gets the EW switch KeyElw.
- BornV_GetKeyZet(KeyZet) sets the Z boson switch KeyZet.
- BornV_SetKeyZet(KeyZet) gets the Z boson switch KeyZet.
- BornV_SetCMSene(CMSene) sets the CMS total energy CMSene.
- BornV_SetMZ(MZ) sets the Z boson mass.
- BornV_GetMZ(MZ) gets the Z boson mass.
- BornV_GetGammZ(GammZ) gets the Z boson width.
- BornV_GetGmu(Gmu) gets the G_{Fermi} .
- BornV_GetSwsq(Swsq) gets the electroweak mixing angle.
- BornV_GetAlfInv(AlfInv) gets the α_{QED}/π .
- BornV_GetAvMult(AvMult) provides the average ISR multiplicity.
- BornV_GetYFSkon(YFSkon) provides the finite part of the YFS form factor. Used in QED3.
- BornV_GetYFS_IR(YFS_IR) provides IR (cut-off-dependent) part of the ISR YFS form factor. Used in QED3.
- BornV_GetQCDcor(QCDcor) provides the QCD correction factor, defined by DIZET.
- BornV_GetVV(vv) provides v = vv.

- BornV_GetVXX(vv,x1,x2) provides v = vv, $x_i = 1 z_i = x1,x2$.
- BornV_GetGSW(GSW) provides the EW form factors GSW(k) k=1,...,7. It is used in GPS and in BornV_Dizet. Note that BornV_InterpoGSW has to be called before, in order to interpolate properly.
- BornV_SetGSW(GSW). For special tests of pretabulation the values of EW form factors GSW(k) k=1,...,7 can be set with this subprogram from outside.

4.8 Bstra, IRC and MBrB classes for beamstrahlung

As was already described, the MC integral for beamstrahlung and ISR has three components: $\int dv dz_1 dz_2$, $\int dv dz_1$ and $\int dv$ ($\int dv dz_2$ is obtained by symmetrization). The corresponding three-fold branching method is managed by the class **MBrB**. The class **Bstra** contains mainly the interface to the Foam and Vegas packages, which generate in each branch the corresponding subset of the variables v, z_1, z_2 .

Since Foam makes look-up tables for the distribution to be generated, we need three copies of the Foam, which are FoamA, FoamB, FoamC. Similarly for Vegas. There are only five subprograms in the Bstra class:

- BStra_Initialize(KeyGrid,Xcrude) initializes FoamA, FoamB, FoamC (or VegasA, VegasB, VegasC) and the MBrB for book-keeping in the three-fold branching. It also provides the primary integrated cross section used to establish the overall normalization in Karlud and KK2f.
- $BStra_Make(vv, x1, x2, MCwt)$ randomly chooses one of the branches with the help of MBrB_GenKF.
- BStra_Finalize(Integ,Errel) is calculating the total cross section using the average provided by MBrB_MgetAve. This is for control only.
- BStra_GetXCrude(XCrude) provides the primary integrated cross section that enters the overall normalization.
- BStra_GetIntegMC(IntegMC,ErReIMC) provides the value of the primary integrated cross section from the entire MC run. This is for control only.

The CIRCE library of the beamsstrahlung structure functions [25] is placed in the IRC module. The only changes are: adding prefix IRC_ to names of all subprograms and the common block /circom/ is renamed as /c_IRC/. It is exploited in the BStra class.

4.9 BVR class: virtual corrections

The class **BVR** is a collection of the complex functions used in the calculation of the virtual corrections. It provides also the \tilde{B} function necessary to calculate the compensating weight in the procedure of the removal of the FSR photons, see subsection 3.8. It has its own library of complex logarithms and dilogarithms.

4.10 QED3 class: EEX distributions

The EEX differential distributions is implemented in the **QED3** module. This module is rather monolithic. It contains the initializer **QED3_Initialize**, the maker **QED3_Make** and several small functions for calculating virtual corrections and up to third-order leading-logarighmic structure functions. The basic ingredient in the EEX differential distributions is the Born differential distribution that comes from the **BornV** class.

4.11 GPS class: CEEX Matrix element

The CEEX matrix element is programmed in the **GPS** class. It calculates spin amplitudes for the $e^-e^+ \rightarrow f\bar{f}n\gamma$ process. It has grown to a very large module (almost 5000 lines of code) and will therefore be split in the next version into a low-level library of GPS tools and the module **CEEX**, which calculates solely the CEEX spin amplitudes.

The main subprogram in the **GPS** class is GPS_Make, which calculates $\mathcal{O}(\alpha^r) r = 0, 1, 2$ CEEX spin amplitudes m_AmpExpo0(4,4,4,4), m_AmpExpo1(4,4,4,4), m_AmpExpo2(4,4,4,4) of the DOUBLE COMPLEX type. Photon helicities are generated randomly in the upper class **KK2f** and provided with the getter KK2f_GetPhel. Virtual corrections are provided by subprograms from the **BVIR** class. Masses, charges, isospin of the particles are provided by the getters of the **BornV** class and the electroweak form factor come from DIZET 6.21 through the interface subprogram BornV_GetGSW. The three model weights $\mathcal{O}(\alpha^r), r = 0, 1, 2, \text{ are calculated in GPS_Make using GPS_MakeRho for polarized beams and unpolarized final fermions. Subprogram GPS_MakeRho2 is calculating model weights for polarized beams and polarized final fermions. It is used by Taupair_ImprintSpin to implement spin effects in <math>\tau$ decays.

Let us now list and explain three groups of subprograms in the **GPS** class, (a) the main subprograms calculating the spin amplitudes, (b) the library of basic tools and (c) the communication subprograms (setters and getters). The first group includes:

- GPS_Initialize initializes of the class. It sets some coupling constants, Pauli matrices, the axial gauge vector β .
- GPS_Make is the main routine that calculates spin amplitudes m_AmpExpo0, m_AmpExpo1 and m_AmpExpo2. Spin amplitudes are calculated in such a way that they are first set to zero and then, in the sum over partitions, they are incremented by β₀^(r) with the help of GPS_BornPlus, by β₁^(r) with the help of GPS_HinPlus and GPS_HfinPlus, and by β₂^(r) with help of GPS_HiiPlus, GPS_HffPlus and GPS_HffPlus. Three model weights are calculated using GPS_MakeRho and set to m_WtSet(i), i=1,2,3 (or to m_WtSet(i),i=51, 52, 53 if ISR-FSR interference is switched off). The best weight is set as m_WtBest = m_WtSet(3) (or m_WtSet(53)). Weights are available through getter GPS_GetWtSet, see below.
- GPS_MakeRho(ExpoNorm) calculates differential distributions (normalized to Lorentzinvariant phase space) from spin amplitudes m_AmpExpoi, i = 1, 2, 3, for polarized

beams and *unpolarized* final fermions. Beam polarizations are set from outside with the help of GPS_SetPolBeams.

- GPS_MakeRho2(wt0,wt1,wt2) is used in Taupair_ImprintSpin and it calculates the differential distributions (normalized to Lorentz-invariant phase space) from spin amplitudes m_AmpExpoi, i = 0, 1, 2, for polarized beams and *polarized* final fermions. Final-state polarimeter vectors are set from outside with the help of GPS_SetHvectors.
- GPS_BornPlus calculates the spin amplitudes of $\beta_0^{(r)}$. It is optimized for summation over partitions. Virtual corrections (boxes and vertices) are included.
- GPS_Born provides the Born spin amplitudes used in the construction of the hard non-IR parts: in GPS_HiniPlus, GPS_HfinPlus and other subprograms. It is essentially a simplified clone of GPS_BornPlus.
- GPS_EWFFact creates form factors for electro-weak corrections. They are in vector couplings (multiplied by the correcting factors). Because of the $\cos \theta$ dependence of WW boxes, we had to introduce CosThetD parameter.
- GPS_HiniPlus calculates the IR-finite part of 1-photon amplitudes for ISR $\beta_{1\{1\}}^{(r)}$. (It is equivalent to a testing subprogram GPS_Hini).
- GPS_HfinPlus calculates the IR-finite part of 1-photon amplitudes for FSR $\beta_{1\{0\}}^{(r)}$. (It is equivalent to a testing subprogram GPS_Hfin).
- GPS_HffPlus calculates the IR-finite part of 2-photon amplitudes for FSR $\beta_{1\{00\}}^{(r)}$.
- GPS_HiiPlus calculates the IR-finite part of 2-photon amplitudes for ISR $\beta_{1\{11\}}^{(r)}$.
- GPS_HifPlus calculates the IR-finite part of 2-photon amplitudes $\beta_{1\{10\}}^{(r)}$ for one ISR and one FSR photon.

Let us now list and explain the subprograms that play a role of the library of basic tools. (In the future version to be isolated as a separate class, or even several classes). This group includes:

- GPS_PartitionStart(nphot,last) initializes the first partition in the sum over partitions.
- $\mathsf{GPS}_\mathsf{PartitionPlus}$ updates the partition vector m_isr , checks if it is the last partition.
- GPS_BornZero(AmpBorn) sets AmpBorn to zero.
- GPS_BornCopy(AmpBorn, AmpBorn2) copies AmpBorn into AmpBorn2.
- GPS_BornSumSq(AmpBorn,Sum) sums up AmpBorn amplitudes squared.
- GPS_TralorPrepare prepares transformation for Tralor, according to GPS rules. The resulting Lorentz transformation matrix is stored for multiple use.

- GPS_GPS(xi,eta,Rot) defines the basis vectors e_1, e_2, e_3 from ξ and η according to GPS rules. Columns in the matrix Rot are e_1, e_2, e_3 . This subprogram is called in GPS_TralorPrepare.
- GPS_TralorDolt(id,pp,q) transforms the four-vector pp from rest frame of fermion id to LAB, q is the result. It uses a Lorentz transformation, prepared and memorized in the subprogram GPS_TralorPrepare, which has to be called first. This organization saves CPU time in the case of multiple calls for several τ decay products.
- GPS_TralorUnDo(id,pp,q) is the inverse of GPS_TralorDolt. It transforms pp from the laboratory to the rest frame of the final fermion, q is the result. It uses a Lorentz transformation, prepared and memorized in the subprogram GPS_TralorPrepare, which has to be called first.
- GPS_TraJacobWick(Mode,QQ,pp,rr) is for tests only. It is a Tralor-type transformation for the classical Jacob–Wick quantization axes. Not optimized.
- GPS_RmatMake is for tests only. It translates Born spin amplitudes into a doublespin density matrix m_AmpBorn $\rightarrow R_{ab}$
- GPS_MakeU(ph,sigma,p1,m1,p2,m2,U) builds the transition matrix U, $(\bar{u} \notin u)$.
- GPS_MakeV(ph,sigma,p1,m1,p2,m2,V) builds the transition matrix V, $(\bar{v} \notin v)$.
- GPS_MakeUb(ph,sigma,p1,m1,p2,m2,U) builds the transition matrix U, $(\bar{u} \notin u)$.
- GPS_MakeVb(ph,sigma,p1,m1,p2,m2,V) builds the transition matrix V, $(\bar{v} \notin v)$.
- GPS_MatrU(Cfact,ph,sigma,p1,m1,p2,m2,U) builds the transition matrix U, $(\bar{u} \notin u)$.
- GPS_MatrV(Cfact,ph,sigma,p1,m1,p2,m2,V) builds the transition matrix V, $(\bar{v} \notin v)$.
- GPS_MatrUb(Cfact,ph,sigma,p1,m1,p2,m2,U) builds the transition matrix U, $(\bar{u} \notin u)$.
- GPS_MatrVb(Cfact,ph,sigma,p1,m1,p2,m2,V) builds the transition matrix V, $(\bar{v} \notin v)$.
- DOUBLE COMPLEX FUNCTION GPS_Sof1(sigma,ph,pf) calculates the single soft photon contribution to the \mathfrak{s} -factor.
- DOUBLE COMPLEX FUNCTION GPS_Sof1b(sigma,ph,pf,mf) calculates the single soft photon contribution to the \mathfrak{s} -factor.
- DOUBLE COMPLEX FUNCTION GPS_soft(sigma,ph,p1,p2) calculates the two-fermion s-factor.
- DOUBLE COMPLEX FUNCTION GPS_bfact(sigma, phot, pferm) calculates the diagonal element of the *U*-matrix for the massive fermion (the numerator in the s-factor).

- DOUBLE COMPLEX FUNCTION GPS_softb(sigma,ph,p1,m1,p2,m2) calculates the s-factor.
- DOUBLE COMPLEX FUNCTION GPS_bfacb(sigma,phot,pferm,mass) calculates the diagonal element of the U-matrix for massive fermion (the numerator in the s-factor).
- DOUBLE COMPLEX FUNCTION GPS_iProd1(L,p,q) calculates the basic inner product of spinors s_λ(p,q) = ū_λ(p)u_{-λ}(q). We exploit the identity s₋(p,q) = −[s₊(p,q)]^{*}.
- DOUBLE COMPLEX FUNCTION GPS_iProd2(Lamp,p,mp,Lamq,q,mq) calculates the general spinor product s_{λ1,λ2}(p,q) for massive spinors u and/or v; mp and mq are the masses of four-vectors p and q. Negative mass means an antiparticle.
- DOUBLE PRECISION FUNCTION GPS_XiProd(p,q) is the auxiliary function called in GPS_iProd2.

The last group includes communication subprograms (setters and getters) and some miscellaneous routines for debugging:

- GPS_BPrint(nout,word,AmpBorn) prints 16 spin amplitudes of AmpBorn in a nice format on output unit nout.
- GPS_GetXi(xi,eta) provides ξ , the basic light-like vector in the laboratory frame, entering the definition of all spinors (called k_0 in Kleiss–Stirling papers).
- GPS_SetKeyArb(KeyArb) GPS_GetKeyArb(KeyArb) sets KeyArb, which is switching on/off the use of m_b, KeyArb=0 means $\beta \rightarrow \xi$.
- GPS_Setb1 GPS_Setb2 switches the axial gauge vector $\beta = b$ to another predefined value. This is for testing the gauge invariance of the spin amplitudes.
- GPS_GetWtSet(WtBest,WtSet) provides a complete list of weights.
- GPS_SetKeyINT(KeyINT) sets the IFI switch KeyINT
- GPS_SetPolBeams(PolBeam1,PolBeam2) sets the beam polarization vectors. One should not forget the Wigner rotation to the GPS frame!
- GPS_SetHvectors(HvecFer1,HvecFer2) sets the final-fermion polarimeter vectors.

4.12 TAUOLA and PHOTOS

TAUOLA and PHOTOS are placed in KK-all/tauola and KK-all/photos. They communicate with the rest of the program through an interface class **Taupair** located in KKall/KK2f. The initialization is performed in the **Tauface** class as well. The other, very important role of **Taupair** is to implement spin effects in the decays of both τ 's, including all spin correlations with the rejection method according to the special spin weight; as in KORALB [14]. The spin weight is:

$$W_{\rm spin} = \frac{\sum_{\sigma_r,\lambda_A,\bar{\lambda}_A} \sum_{i,j,l,m} \hat{\varepsilon}_1^i \hat{\varepsilon}_2^j \sigma_{\lambda_a \bar{\lambda}_a}^i \sigma_{\lambda_b \bar{\lambda}_b}^j \mathfrak{M}_n^{(r)} \begin{pmatrix} p_{k_1 k_2} \dots k_n \\ \lambda \sigma_1 \sigma_2 \dots \sigma_n \end{pmatrix} \left[\mathfrak{M}_n^{(r)} \begin{pmatrix} p_{k_1} \dots k_n \\ \bar{\lambda} \sigma_1 \dots \sigma_n \end{pmatrix} \right]^{\star} \sigma_{\bar{\lambda}_c \lambda_c}^l \sigma_{\bar{\lambda}_d \lambda_d}^m \hat{h}_3^l \hat{h}_4^m}{\sum_{\sigma_r,\lambda_A} \sum_{i,j} \left| \mathfrak{M}_n^{(r)} \begin{pmatrix} p_{k_1 k_2} \dots k_n \\ \lambda \sigma_1 \sigma_2 \dots \sigma_n \end{pmatrix} \right|^2}$$
(123)

Note that in the present version of the program we include at this step not only the finalstate spin effects but also beam-polarization effects. This is not a very economical solution, especially for strongly polarized beams, when we may get large rejection rates (roughly equal to the ratio of polarized to unpolarized Born cross section). The radical solution of this problem is to introduce longitudinal polarizations in the Born cross section as used in the *crude* and *primary* integrated cross section. At the moment they are completely unpolarized.

In order to save CPU time a special method of "recycling" the τ decay events is devised (see below). The interface supplies also the subroutine TRALO4, which is required by TAUOLA in order to transform τ decay products to the laboratory frame.

Some additional subroutines, necessary for the proper functioning of TAUOLA and PHOTOS, are placed in KK-all/KK2f/Tauface.f.

- Taupair_Initialize(xpar) initializes TAUOLA and PHOTOS packages with the help of INIMAS, INITDK, INIPHY and DEKAY. It initializes the book-keeping for the spin weight, that is the weight used to introduce all spin effects in τ decays.
- Taupair_Finalize prints the average spin weight.
- Taupair_Make1 generates in the first step the unpolarized τ decays using DEKAY. The polarimeter vectors m_HvecTau1 and m_HvecTau2 are determined.
- Taupair_ImprintSpin introduces spin effects with the help of rejection using spin weight. The polarimeter vectors are sent to GPS with the help of GPS_SetHvectors and the spin weight is calculated with the help of GPS_MakeRho2; the event is then rejected or accepted. For the rejected event the τ -pair event is "recycled", that is each τ decay product is Euler-rotated and reused in the rejection method. The procedure is repeated until the event is accepted. The whole procedure is correct because we know exactly the average of the spin weight.
- Taupair_Make2 transforms accepted τ decay products to the CMS by calling DEKAY(11) and DEKAY(12). The transformation is defined according to the GPS rules, for each τ by GPS_tralorPrepare, and is performed with the help of GPS_TralorDolt hidden inside the TRALO4 routine.
- Taupair_Clone performs the "recycling" of a τ -pair by means of the Euler rotation in the rest frame of each τ .

- Tralo4(Kto,P,Q,AM), see above.
- FILHEP(N,IST,ID,JMO1,JMO2,JDA1,JDA2,P4,PINV,PHFLAG) writes single particles in τ-decay into HepEvt class. For historical reasons HepEvt_Fil1 is not used directly.
- Taupair_SetKeyClone(KeyClone) sets KeyClone. KeyClone switches between two operational modes of Taupair_Clone. Both of the modes implement a valid solution.
- Taupair_GetIsInitialized(IsInitialized) gets to know the outside world if TAUOLA is active (IsInitialized=1).
- Taupair_GetHvectors(HvecFer1,HvecFer2) provides the polarimetric *h*-vectors.

4.13 Electroweak library

The library of electroweak (EW) corrections is placed in the KK-all/dizet subdirectory. In the initialization phase the EW form factors dependent on s', fermion type and some of them (electroweak boxes) also on the scattering angles, are placed in the look-up tables. During the event generation they are interpolated in s' and $\cos\theta$ and provided to the **GPS** module, where the CEEX spin amplitudes are calculated, or used in the BornV_Dizet being used (through BornV_Differential) in the **QED3**, where the EEX distributions are calculated. The main aim of the above organization it to speed up the MC by using the EW form factor from look-up tables instead of calculating them, in fact many times, for each MC event. This reason may be even more important in the future version of the EW corrections which will be slower, owing to the inclusion of more genuine two-loop corrections.

There are two modes of the initialization of the EW look-up tables. In the default mode they are calculated and stored in several disk files, each for one fermion type, and in the initialization of the \mathcal{KK} MC run these tables are read by the **BornV** module. This mode is more conservative (safer), because the Fortran77 program providing electroweak corrections does not need to be linked and executed together with the proper MC event generator. We do not therefore need to worry about the clashes of the names of the procedures and common blocks, and the possible problems with re-initialization of the EW library for different types of the fermions is avoided²³. In the actual implementation the EW library DIZET is run separately, under a special main program KK-all/dizet/TabMain.f, together with an interface module **DZface**, which acts as an interface to the **Dizet** library, properly setting the input data to **Dizet** and writing the EW form factors in the disk file.

One important disadvantage of the above method is that the input parameters of the EW corrections, such as the Higgs mass, cannot be changed easily (for fitting), because it requires re-producing new look-up tables of the EW corrections. This is why we also

²³ This reason seems to be now less important than in the early stages of the development of the \mathcal{KK} MC, because most of the \mathcal{KK} MC code now fulfils the rules of programming in sections 4.2.

implemented the second interface to EW library DIZET in which the look-up tables are calculated in the initialization phase of the MC run (in this case the EW library is linked with the entire MC program).

How are the EW tables produced in the default method? This is done by invoking in the KK-all/dizet/ one of the commands:

make tables	#	it makes	all tables	
make table.mu	#	it makes	./table.mu	using ./input.mu
make table.tau	#	it makes	./table.tau	using ./input.tau
make table.down	#	it makes	./table.down	using ./input.down
make table.up	#	it makes	./table.up	using ./input.up
make table.botom	#	it makes	./table.botom	using ./input.botom

The input data should be used the same as in the MC run. In fact, the **BornV** module is checking if the important EW input data used to generate tables match the actual data provided by the user for the MC run. If not then the program stops.

How does one avoid producing EW tables on the disk (and apply the second method)? For the instructions see KK-all/ffbench/Makefile.

The interface **DZface** to **DIZET** of the Dubna–Zeuthen EWRC group version 6.21 is based on the analogous interface in KORALZ 4.x. Let us now list and explain the subprograms in the interface module **DZface**

- DZface_Initialize(KFfin, xpar) is the class initializer. Initialization of DIZET is done with CALL DIZET(NPAR,...). NPAR and other input parameters are defined in the xpar vector, see Table 4.
- DZface_ReaDataX(DiskFile, iReset, imax, xpar) is functionally the same as KK2f_ReaDataX.
- DZface_Tabluj fills in the EW form factors into look-up tables in /c_BornV/. The factors are provided by DZface_MakeGSW (see below). Tabulation is done in the three ranges of \sqrt{s} with different numbers of points. The energy ranges and numbers of points are defined in BornV.h.
- DZface_WriteFile(DiskFile) writes tables of the EW form factors into a disk file.
- DZface_Clone(KFfin) copies tables calculated for the actual m_KFfin into tables for KFfin. It is used to create tables for c and s quarks using tables of u and d quarks (saving a little bit of CPU time).
- DZface_MakeGSW(Mode,ww,cosi,GSW,QCDcorN) gets the EW form-factors GSW and QCD corrections QCDcorN out of DIZET, at $\sqrt{s} =$ ww and cos $\theta =$ cosi. EW form-factors are obtained with the CALL rokanc(...), while QCD corrections come from DZface_QCDtab (see below).
- DZface_QCDtab(Mode,ww,QCDcorN) makes QCD corrections with the CALL qcdcof(...). It is done in an iterative way in order to find out the QCD corrections at a given \sqrt{s} .

Note that the QED coupling constant the alfinv is separate from the alfinv used in the bremsstrahlung part of \mathcal{KK} and the fermion masses in Dizet are isolated from those in \mathcal{KK} .

4.14 Random number generators

The \mathcal{KK} program in the present version uses exclusively the RANMAR random number generator [37, 38]. It is reprogrammed as the pseudo-class **PseuMar**. Its singleprecision generator is accessible with the help of the double-precision interface routine **PseuMar_MakeVec**. In this way we avoid possible interference with libraries of JETSET, PHOTOS and TAUOLA, which have their own independent random-number generators, and typically also have their own version of the RANMAR generator.

4.15 Other modules

Every MC program of this size has to have its own tools for book-keeping of the MC weights and for making histograms of the weight distribution. In the \mathcal{KK} MC the built-in histogramming package **GLK** plays this role. Histogramming entries are similar to those of the CERN library HBOOK. Apart from histogramming, it also has the capability of "measuring" several properties of the MC weight. This weight monitoring is done with the entries GLK_Mbook, GLK_Mfill, GLK_MgetAll, GLK_MgetNtot, GLK_MgetAve and GLK_Mprint. The **GLK** module features also simple, though versatile, graphical capabilities – it can plot histograms by exploiting the LATEX environment picture.

The other auxiliary package is **MathLib.f**, which includes subprograms for Gaussian integration and some transcendental functions. The \mathcal{KK} MC does not need any external mathematical library.

5 Semianalytical "normalization anchor"

In the complicated MC program aspiring to a precission of order 10^{-4} , it is critical to master the overall normalization at this precision level. This can be done by comparing the program results with another MC program or with a semi-analytical calculation, that is the calculation in which as many integrations as possible are carried out analytically and the remaining ones are done with the Gaussian method²⁴. Such a test of MC normalization is of critical importance – this is why we call it a *normalization anchor*.

It is not trivial to analytically integrate the multiphoton phase space; nevertheless, for simple or simplified exponentiated distributions such as EEX and simple or absent kinematical cuts, such an integration is possible, see refs. [12, 39].

Here, since our aim is essentially limited to the very precise numerical test of the MC phase-space integration, we have chosen the $\mathcal{O}(\alpha^0)$ EEX model, that is the Born differential cross section multiplied by the soft factors, see eqs. (15) and (16).

 $^{^{24}\}mathrm{This}$ is the way the Zfitter phase space integration is done.

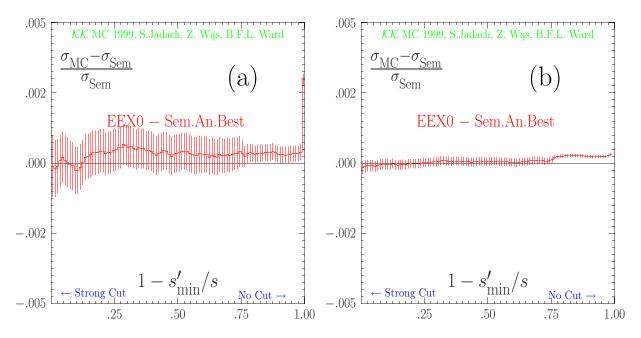


Figure 2: Test of the normalization of the low-level part of the Monte Carlo, for simplified QED multiphoton distribution. The difference of the MC result and semianalytical result divided by semi-analytical is plotted as a function of $v_{\text{max}} = 1 - s'_{\text{min}}/s$. Test is done for $\mu^+\mu^-$ final state at $\sqrt{s} = 189$ GeV. In case (a) $v_{\text{max}} = 1 - 4m_{\mu}^2/s$ is taken; the last bin represent the entire phase phase space. In case (b) $v_{\text{max}} = 0.999$.

In this case it is relatively easy to obtain by analytical integration the $\mathcal{O}(\alpha^0)$ EEX cross section, keeping terms $L^0\alpha^1, L^1\alpha^1, L^2\alpha^2$, where L is the big logarithm, for both ISR and FSR. For the ISR, however, due to the Z resonance, and γ^* peak at s' = 0, in order to reach the necessary precision of order 10^{-4} , it is necessary to analytically calculate two additional terms of orders $L^1\alpha^2$ and $L^3\alpha^3$. This was done in ref. [12], and the relevant semianalytical formula looks as follows:

$$\sigma_{\rm SAN}^{f} = \int_{0}^{v_{\rm max}} dv \, \sigma_{\rm Born}^{f} \left(s(1-u)(1-v) \right) \, D_{ISR}(v) \, D_{FSR}(u),$$

$$D_{ISR}(v) = e^{\frac{-C\gamma_{e}}{\Gamma(1+\gamma_{e})}} \, e^{\frac{1}{4}\gamma_{e} + \frac{\alpha}{\pi} \left(\frac{1}{2} + \frac{\pi^{2}}{3}\right)} \, \gamma_{e} v^{\gamma_{e}-1} \left(1 - \frac{1}{4}\gamma_{e} \ln(1-v) - \frac{1}{2}\frac{\alpha}{\pi} \ln^{2}(1-v) + 0 \, \gamma_{e}^{2} \right),$$

$$D_{FSR}(u) = e^{\frac{-C\gamma_{f}}{\Gamma(1+\gamma_{f})}} \, e^{\frac{1}{4}\gamma_{f} - \frac{1}{2}\gamma_{f} \ln(1-u) + \frac{\alpha}{\pi} \left(\frac{1}{2} + \frac{\pi^{2}}{3}\right)} \, \gamma_{f} u^{\gamma_{f}-1} \left(1 - \frac{1}{4}\gamma_{f} \ln(1-u) \right),$$

$$(124)$$

Note that the coefficient in front of the $\mathcal{O}(L^3\alpha^3)$ term is zero, as marked explicitly. We have checked numerically that the ISR term of $\mathcal{O}(L^1\alpha^2)$ is worth several per cent for the cross section located close to v = 1.

In fig. 2 we present the comparison of the \mathcal{KK} MC with the above semianalytical formula. The difference between the MC result and the semianalytical result is divided by

the semianalytical result. The comparison is done for the $\mu^+\mu^-$ final state at $\sqrt{s} = 189$ GeV, as a function of $v_{\rm max}$. In the last point (bin) the entire phase space is covered, $v_{\rm max} = 1 - 4m_{\mu}^2/s$. We conclude that we control the phase-space integration at the level of 2×10^{-4} for $v_{\rm max} < 0.999$, including the Z radiative return, and at the level of 3×10^{-3} for no cuts at all.

Parameter	Position and meaning
CMSene	xpar(1) (=100): \sqrt{s} , centre-of-mass (CMS) energy [GeV]
DelEne	xpar(2) (=0d0): Beam energy spread [GeV]
Ninp	<pre>xpar(3) (=5): Input unit number (unused)</pre>
Nout	xpar(4) (=16): Output unit number
LevPri	xpar(5) (=0): PrintOut Level $0,1,2$
Ie1Pri	xpar(6) (=1): PrintOut Start point
Ie2Pri	xpar(7) (=1): PrintOut End point
IdYFS*	xpar(8) (=600): Pointer for internal histograms
\texttt{WtMax}^*	xpar(9) (=1): Maximum weight for rejection
KeyWgt	xpar(10) (=0): Switch between constant =0 and variable =1 weight events
${\tt IdeWgt}^*$	xpar(11) (=74): Ident of the EEX principal weight
KeyELW	xpar(12) (=1) : Type of electroweak corrections, =0 only for tests, =1 default
	for DIZET
$vvmin^*$	xpar(16) (=1D-5): Minimum real photon energy in units of beam energy
vvmax	xpar(17) (=1d0): Maximum value of $v = 1 - s'/s$ -variable, where s' is mass
	squared of $f\bar{f}$ system including FSR photons! See more comments in the text.
$DelFac^*$	xpar(18) (=1d-3): FSR cut eps=vvmin*DelFac
${\tt NphMax}^{**}$	xpar(19) (=100): Hard-wired maximum photon multiplicity
KeyISR	xpar(20) (=1): Test switch, KeyISR=0 switches off the ISR
KeyFSR	xpar(21) (=1): Test switch, KeyFSR=0 switches off the FSR
KeyPia ^{**}	<pre>xpar(22) (=1): Removal of FSR photons below Emin=Ene*Delta in CMS,</pre>
	for KeyPia=0,1 removal is OFF,ON
mltISR**	<pre>xpar(23) (=0): Special tests: fixed ISR multiplicity for mltISR>0</pre>
mltFSR**	<pre>xpar(24) (=0): Special tests: fixed FSR multiplicity for mltFSR>0</pre>
KeyFix	xpar(25) (=0): Type of ISR, for KeyFix=0,1 QED without beamstrahlung,
	for KeyFix=2 beamstrahlung is ON, see also KeyGrid
KeyWtm**	xpar(26) (=0): Special tests only: mass terms in "crude" MC photon distrib.
KeyINT	xpar(27) (=2): Switch of ISR-FSR Interference (IFI), for KeyINT=0 it is
v ana	OFF, for KeyINT=2 it is ON, KeyINT=1 is only for special tests
KeyGPS	xpar(28) (=1): Level of new exponentiation CEEX, note vmaxGPS overrules
IZ 0 CD	KeyGPS for each type of final fermion
KeyQSR	xpar(29) (=1): Photon emission from the final quarks is ON,OFF for KerOSP 0.1
	KeyQSR=0,1

Table 2: List of input parameters of the \mathcal{KK} generator. General and related to QED radiation input parameters. Default values in brackets. User may change, with precautions, the starred items, while the doubly starred ones should never be changed.

Parameter	Position and meaning
AlfInv*	xpar(30) (=137.0359895D0): Inverse of α_{QED}
\texttt{GNanoB}^*	xpar(31) (=389.37966D3): $\text{GeV}^{-2} \rightarrow [\text{nb}]$ conversion factor
${\tt Gfermi}^*$	xpar(32) (= 1.16639d-5): Fermi coupling $[GeV^{-2}]$
	Technical cuts for non-IR real photon corrections etc.
Xenph**	xpar(40) (=1.25d0): Enhancement factor for "crude" photon multiplicity
$vcut1^*$	xpar(41) (=1.d-9): Techn. cut for single non-IR bremss. correction
$vcut2^*$	xpar(42) (=5.d-2): Techn. cut for double non-IR bremss. correction
vcut3*	xpar(43) (=0.1d0): Techn. cut for triple non-IR bremss. correction
	QCD flags/data
KeyHad	<pre>xpar(50) (=1): Hadronization/showering flag, for KeyHad=0,1 hadronization</pre>
	is OFF,ON.
HadMin*	xpar(51) (=0.200d0): Minimum mass [GeV] for hadronization/showering
alfQCD*	xpar(52) (=0.118d0): $\alpha_{\rm QCD}$
	Non zero beam polarization may require adjustment of WtMax
spin1x	xpar(61) (=0d0): polarization vector beam 1, x-component
spin1y	xpar(62) (=0d0): polarization vector beam 1, y -component
spin1z	xpar(63) (=0d0) : polarization vector beam 1, z-component
spin1x	xpar(64) (=0d0): polarization vector beam 2, x -component
spin1y	xpar(65) (=0d0): polarization vector beam 2, y-component
spin1z	xpar(66) (=0d0): polarization vector beam 2, z-component
	Beamstrahlung parameters for Thorsten Ohl's package CIRCE
IRCroots	xpar(71) (=350d0): \sqrt{s} [GeV] discrete values 350,500,800GeV
IRCacc	<pre>xpar(72) (=3d0): accelerator type</pre>
IRCver	<pre>xpar(73) (=5d0): version number</pre>
IRCdat	xpar(74) (=19980505d0): date
IRCxchat	<pre>xpar(75) (=1): printout level</pre>
${\tt KeyGrid}^*$	<pre>xpar(76) (=2): Activated by setting KeyFix=2 KeyGrid=2 invokes Foam,</pre>
	KeyGrid= $0, -1, +1$ invokes Vegas: KeyGrid= 0 creates and writes Vegas grid
	on the disk, $KeyGrid = -1$ creates and dumps grid on the disk, $=+1$ reads only

Table 3: List of input parameters of the \mathcal{KK} generator in xpar vector. General parameters and QED radiation. Default values in brackets. User may change, with precautions, the starred items, while the doubly starred ones should never be changed.

6 Use of the program

In this section we will familiarize the reader with the input and output parameters, and the use of the present version of the \mathcal{KK} Monte Carlo. We will present two simple demonstration main programs. Their double role is to serve as a useful template for the user to create his/her own main program and to help the user to check quickly that the newly installed \mathcal{KK} generator runs correctly. We shall describe in detail all the input parameters of \mathcal{KK} .

Parameter	Position and meaning
KFini*	xpar(400) (= 11): Beam flavour code
	<i>j</i> -th fermion is included in MC generation if its $Mask(j)=1$
Mask(1)	xpar(401) (=1): Mask variable for d quark
Mask(2)	xpar(402) (=1): Mask variable for u quark
Mask(3)	xpar(403) (=1): Mask variable for s quark
Mask(4)	xpar(404) (=1): Mask variable for c quark
Mask(5)	xpar(405) (=1): Mask variable for b quark
Mask(13)	xpar(413) (=1): Mask variable for muon lepton
Mask(15)	xpar415() (=1): Mask variable for tau lepton
	Basic electroweak input data
MZ	xpar(502) (=91.187D0): Mass of Z-boson [GeV] (PDG 1996)
SwSq	xpar(503) (=.22276773D0): $\sin^2(\theta_W)$ where θ_W is EW mixing angle
GammZ	xpar(504) (= 2.50072032D0): Z width (from Dizet)
${\tt MasPhot}^*$	xpar(510) (= 1D-60): Photon mass used as IR regulator
	The data base record below is for d quark, $j = 1$
KFferm(j)*	<pre>xpar(501+10*j) (= 1): Flavour code</pre>
NCf(j)*	<pre>xpar(502+10*j) (= 3): Number of colours</pre>
Qf(j)*	xpar(503+10*j) (=-1): 3×charge
T3f(j)*	xpar(504+10*j) (=-1): $2 \times T3L = 2 \times Isospin$ for left component
Helic(j)*	xpar(505+10*j) (= 1): $2 \times$ helicity, not used
Mferm(j)*	xpar(506+10*j) (= 0.010d0): Mass [GeV] (PDG)
MfCon(j)*	<pre>xpar(506+10*j) (= 0.100d0): Constituent mass, not used</pre>
WtMax(j)*	<pre>xpar(507+10*j) (= 5.0d0): Maximum weight for rejection</pre>
AuxPar(j)*	<pre>xpar(508+10*j) (= 0.99d0): below vmaxGPS CEEX, above EEX</pre>
	More electroweak input data
Ibox	<pre>xpar(801) (= 1): EW box flag, input for Dizet</pre>
MH	<pre>xpar(805) (= 100D0): Higgs mass, input for Dizet</pre>
Mtop	xpar(806) (= 175D0): Top mass, input for Dizet
NPAR(j)	xpar(900+j), $j = 1, 21$: Input flags for Dizet 6.21

Table 4: List of input parameters of the \mathcal{KK} generator. Initial/final fermion properties and EW parameters. Default values in brackets. User may change, with precautions, the starred items, while the doubly starred ones should never be changed.

6.1 Principal entries of \mathcal{KK}

The principal entries of the \mathcal{KK} package, which the user will call in his/her application in order to generate a series of MC events, were already listed and described briefly in Section 4. Here we shall add more information on their functionality. The calling sequence constituting a typical Monte Carlo run will look as follows:

```
CALL KK2f_ReaDataX('./.KK2f\_defaults',1,10000,xpar)! reading default input
CALL KK2f_ReaDataX('./user.input', ,0,10000,xpar)! reading user's input
CALL KK2f_Initialize(xpar) ! initialize generator
DO loop=1,10000 ! loop over MC events
```

Parameter	Position and meaning
Jak1	xpar(2001) (=0): First τ decay mask
Jak2	xpar(2002) (=0): Second τ decay mask
idff**	xpar(2003) (=15): PDG ident of the first τ
itdkRC	xpar(2004) (=1): QED rad. switch in leptonic decays
xk0dec*	xpar(2005) (=0.001d0): IR-cut for QED rad. in leptonic decays
KeyA1	xpar(2006) (=1d0): Type of a_1 current
$Cabib^{**}$	xpar(2007) (=0.975d0): Cosine of Cabibbo angle
GV^*	xpar(2008) (= 1d0): Vector coupling g_V in τ decay
GA^*	xpar(2009) (=-1d0): Axial coupling g_A in τ decay
BRA1	xpar(2010) (= 0.5d0): In 3-pion decay BR of $\pi^+\pi^-\pi^-$ (vs $\pi^-\pi^0\pi^0$)
BRKS	xpar(2011) (=0.6667d0): In K^* decay BR of $K^+\pi^0$ (vs π^+K^0)
BRKO	xpar(2012) (=0.5d0) : Probability of K^0 to be K_S
BRKOB	xpar(2013) (=0.5d0) : Probability of K_B^0 to be K_S
	Branching ratios
BRAE	xpar(2101) (=17.810d-2): Branching ratio $\tau^- \rightarrow e^-$. IMPORTANT! Entry
	$2101~{\rm set}$ smaller than -1d0 will activate internal defaults of Tauola. In such a
	case all input from 2008-2122 will be IGNORED
BRAMU	xpar(2102) (=17.370d-2): Branching ratio $\tau^- \rightarrow \mu^-$
BRAPI	xpar(2103) (=11.080d-2): Branching ratio $\tau^- \rightarrow \pi^-$
BRA2PI	xpar(2104) (=25.320d-2): Branching ratio $\tau^- \rightarrow \pi^-, \pi^0$
BRA3PI	xpar(2105) (=18.380d-2): Branching ratio $\tau^- \rightarrow a_1^-$
	Other branching ratios are in xpar(2106-2122), see .KK2f_defaults

Table 5: Input parameters for the TAUOLA package. For a complete description, see the Manual of TAUOLA [16]. Default values in brackets. User may change, with precautions, the starred items, while the doubly starred ones should never be changed.

CALL KK2f_Make	! generate single event
ENDDO	
CALL KK2f_Finalize	! final book-keeping
CALL KK2f_GetXSecMC(XSecPb,XErrPb)	! get total cross section

In the first call of KK2f_ReaDataX, default data are read into the array REAL*8 xpar(10000). The $\mathcal{K}\mathcal{K}$ itself has almost no data hidden in the source code. (This is not true for TAUOLA and JETSET). The file .KK2f_defaults is read first into array xpar. This file of defaults is provided in the main distribution directory. The user should *never modify it*. It can be copied to a local directory or, better, a symbolic link should be created to the original file. The .KK2f_defaults is rather large and the user is usually interested only in changing some subset of these data. In the second call on KK2f_ReaDataX the user can overwrite the default data with his/her own smaller set of input data, which are placed in the user.input file. See next subsection for more details on the input data.

The KK2f_Initialize is invoked to initialize the generator. It reads input data from array xpar, prints them and sends them down to various modules and auxiliary libraries. The program entries have to be called in strictly the same order as in the above example.

At this point we are ready to generate a series of the MC events. The generation of a single event is done with the help of KK2f_Make. After the generation loop is completed, we may invoke KK2f_Finalize, which does final book-keeping, prints various pieces of information on the MC run, and calculates the total MC integrated cross section and its statistical error in units of picobarn. In order to access the total cross section the user should call the routine KK2f_GetXSecMC(XSecMC,XErrMC).

6.2 Input data

As we stated previously, in the second call on KK2f_ReaDataX the users can overwrite the default with their own preferred values. Note that the user should never modify certain data items (without consulting authors of the program) and that the other ones can be changed by the user, see below. For example the simplest input data, which define only the CMS energy, look as follows:

BeginX
*<ia><----data----><----comments---->
1 190d0 CmsEne =CMS total energy [GeV]
EndX

As we see, data cards start with the keyword BeginX and end with the keyword EndX. The comment lines are allowed – they start with * in the first column. In the comments we specify the meaning of the data, their range, and whether the user is allowed to modify them. The data themselves are in a fixed format, with the address *i* in xpar(i) followed by the data value and trailing comment. The four examples of input data sets for the two demonstration programs ffbench/demo.f and ffbench/ProdMC.f in the subdirectories ffbench/Mu, ffbench/Inclusive and the other ones, provide useful templates for the typical user data. The complete set of all user data in KK2f_defaults is described in detail in Tables 2–5. Understandably, the user will manipulate, in most cases, only a small subset of the data and, in most cases, will stick to the default values.

6.3 MC events and other output

The principal output of \mathcal{KK} is the Monte Carlo *event*, which is just a list of final-state four-momenta in [GeV] units and flavours, encoded in the standard /d_HepEvt/ common block, see section 4.4.

All beam, photon and parton momenta before hadronization are available alternatively through "getter" subroutines from class **KK2f**, see section 4.3 or **HepEvt**:

```
DOUBLE PRECISION p1(4),p2(4),p3(4),p4(4),PhoAll(100,4)

INTEGER NphAll

....

CALL HepEvt_GetBeams(p1,p2) ! get beam momenta

CALL HepEvt_GetFfins(p3,p4) ! get momenta of two final fermions

CALL HepEvt_GetPhotAll(NphAll,PhoAll) ! get photon multiplicity and momenta
```

where NphAll is the total photon multiplicity (see also the ffbench/ProdMC.f example). Note that beamstrahlung photons are added to the record as two zero-angle ISR photons, so that total energy is conserved. Alternatively, beamstrahlung photon momenta are also available through a dedicated getter:

DOUBLE PRECISION PhoBst(100,4) CALL HepEvt_GetPhotBst(NphBst,PhoBst)

Parameter	Position and meaning
WtSet(71)	EEX $\mathcal{O}(\alpha^0)$
WtSet(72)	EEX $\mathcal{O}(\alpha^1)$
WtSet(73)	EEX $\mathcal{O}(\alpha^2)$
WtSet(74)	EEX $\mathcal{O}(\alpha^3)$
WtSet(201)	CEEX $\mathcal{O}(\alpha^0)$
WtSet(202)	CEEX $\mathcal{O}(\alpha^1)$
WtSet(203)	CEEX $\mathcal{O}(\alpha^2)$
WtSet(251)	CEEX $\mathcal{O}(\alpha^0)$ without ISR-FSR interference
WtSet(252)	CEEX $\mathcal{O}(\alpha^1)$ without ISR-FSR interference
WtSet(253)	CEEX $\mathcal{O}(\alpha^2)$ without ISR-FSR interference

Table 6: The meaning of the weights in the WtSet.

6.4 Weighted events, alternative weights

Normally, the user will run the program in the mode with the weight equal to 1. Running in the mode with weighted events may be useful for various tests. It can be useful, for example as a cross check, in the situation when one selects output events strongly, that is imposes cuts that eliminate all but say 1 event in a 1000. If at the same time it is seen from the output of KK2f_finalize that the cross section corresponding to $w > w_{\text{max}}$ is at the similar level of 10^{-3} , it is then necessary to cross check if the accepted events do not coincide, by bad luck, with the "overweighted" events. If it were true, then the cross section and the distribution of the accepted events could be affected by factor of 2 or more. In that sense the weighted events are "safer".

It should be kept in mind that, although we have set the maximum weights for the rejection rather high, the user may try an untested configuration of the input data for which the cross section corresponding to $w > w_{\text{max}}$ is too high. We recommend that the user always check, at the end of the run, the output from KK2f_finalize, the table in which the percentage of the "spill over" cross section corresponding to $w > w_{\text{max}}$ is given.

The other advantage of the weighted events is that in most cases one needs less CPU time to get the same statistical error in the cross sections and in the histogram. It can be profitable if one needs to perform many runs with various input parameters.

In the run with weighted events the user may access the principal weight WtMain and the auxiliary weights WtSet through another getter:

DOUBLE PRECISION WtSet(1000), WtMain, WtCrud CALL KK2f_GetWtAll(WtMain,WtCrud,WtSet)

see also the ffbench/ProdMC.f example. The actual auxiliary weight should be defined as WtCrud*WtSet(i). Note that events with WtCrud=OdO may have undefined four-momenta, so the user should protect his program against crashing upon an attempt of working out the kinematics of such an event.

The weights WtCrud and WtSet are also defined in the run with WtMain=1d0. They can be recorded and used in the subsequent run in order to estimate the effects that are included or excluded in the auxiliary weight WtSet(i). The meaning of the most important weights in WtSet is described in table 6.

How to get cross sections and distributions corresponding to WtSet(i) using an event generated with WtMain =1 and recorded on the tape?

- The user should *record on the tape* the vector WtSet for each event, together with WtCrud and WtMain.
- In the subsequent run, to weight events from the tape, each event should be weighted with the ratio²⁵ WtSet(i)/ WtSet(203), because in the standard case WtMain=WtCrud*WtSet(203).

A typical application of the above method could be to find out, for a given arbitrary distribution or cross section, the estimate of *physical precision* due to higher orders. We recommend that the user take half of the difference $\mathcal{O}(\alpha^2) - \mathcal{O}(\alpha^1)$ as an estimate of the physical precision. This can be calculated by applying the above method with the following weight: (WtSet(203)-WtSet(202))*WtCrud/Wtmain.

The above method cannot be used for varying the input parameters of the SM, such as the Higgs mass, because this would require recalculating WtSet. We may provide such a capability in the next versions.

6.5 Frequently asked questions on program use

Some additional information, useful for practical use of the program is collected as answers to "frequently asked questions":

- *How does one properly normalize total cross section?* Look into two demonstration programs in ffbench subdirectory.
- How does one update tables of electroweak corrections?

```
cd KK-all/dizet
make all (or make table.tau etc.)
```

²⁵ This will not work for muons with v > 0.999 and quarks with v > 0.99 where, for technical reasons we use WtMain=WtCrud*WtSet(74). This restriction is not important for most of practical purposes.

For more details see section 4.13.

- How does one switch on beamstrahlung? Include KeyFix=2 and KeyGrid=2 in the user input data. An example program is included in ffbench subdirectory.
- How does one switch off radiation for quarks? Include KeyQSR=0 in the user input data.
- How does one switch from CEEX to EEX for quarks? Include vmaxGPS=0 for all quarks in the user input data.
- How does one update compilation flags everywhere? Compilation flags are set for AIX. Examples of f77 flags for HPUX, Linux, ALPHA are in ./ffbench/Makefile. In order to update centraly makefiles in all subdirectories do the following:

cd ./ffbench
make makflag

This causes the mapping makefile.template - > makefile in all subdirectories, updating compilation flags everywhere with the ones from ./ffbench/Makefile.

- How does one calculate the QED physical error for a given observable? Calculate the difference between $\mathcal{O}(\alpha^2)_{\text{CEEX}}$ and $\mathcal{O}(\alpha^1)_{\text{CEEX}}$ and the difference between $\mathcal{O}(\alpha^2)_{\text{CEEX}}$ and $\mathcal{O}(\alpha^3)_{\text{EEX}}$. This can be done by running the MC with weighted events and taking the difference of the weights or with unweighted events, following instructions in the previous section.
- *How can one be sure about the technical precision?* The problem may arise for strong selection cuts. In this case we advise the user to rerun the program with weighted events and check whether the results are the same.

7 Outlook and conclusions

As is summarized in Table 1, the present version of the \mathcal{KK} MC has almost the full functionality of the older KORALZ and KORALB event generators. The most important new features in the present \mathcal{KK} are the ISR-FSR interference, the second-order subleading corrections, and the exact matrix element for two hard photons. This makes \mathcal{KK} already a unique source of SM predictions for the LEP2 physics program. The inclusion of the beamstrahlung makes it useful for the LC studies. Note that for these the electroweak correction library has to be reexamined. The most important omission in the present version is the lack of neutrino and electron channels. Let us stress that the present program is an excellent starting platform for the construction of the second-order Bhabha MC generator based on CEEX exponentiation. We hope to be able to include the Bhabha and neutrino channels soon, possibly in the next version. The other important directions for the development are the inclusion of the exact matrix element for three hard photons, together with virtual corrections up to $\mathcal{O}(\alpha^3 L^3)$ and the emission of the light fermion pairs. The inclusion of the W^+W^- and $t\bar{t}$ final states is still in a farther perspective.

Acknowledgements

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Appendix: Output of the demonstration program

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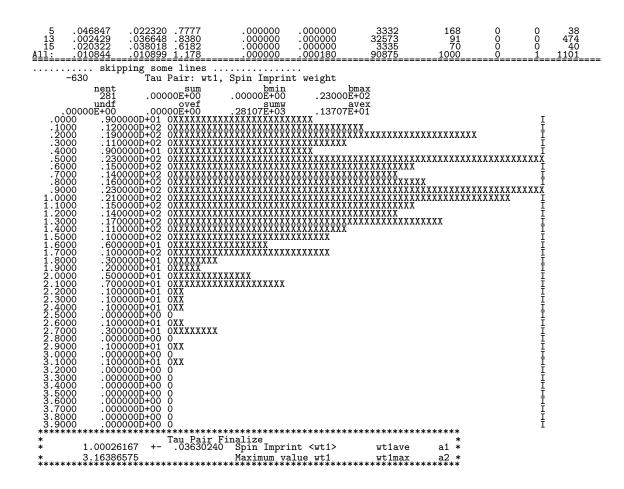
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<pre>* 2.0825838 ***********************************</pre>	<pre>W width W width W</pre>	**************************************	**************************************
<pre>* 2.0825838 ***********************************</pre>	<pre>W width W width C ms energy average Beam energy spread ISR on/off switch Type of ISR Elect_weak switch Fixed nphot mult. Max. photon mult. W width W widt</pre>	**************************************	**************************************
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*	9.4892226	of fin:	al fermion		x-crude	[nb]		Xcrunb	**	*
*		1	II ICIMIO			nal ferm		KFfin	**	*
* *	.10000000				mass of Xborn [R	final fe	rm.	amferm Xborn	** **	*
*	5.0000000					mpling p	ar.	WtMax	**	*
*	.99000000	_			vmax for	CEEX	,	vmaxGPS	**	*
*	.10000000	2			KF of fi	nal ferm final fe	ion	KFfin amferm	** **	*
*	2.1445691				Xborn [R			Xborn	**	*
*	5.0000000					mpling p		WtMax	**	*
* *	.99000000	3			vmax for	CEEX nal ferm	ion	vmaxGPS	** **	*
*	.20000000	5			mass of	final fe	rm.	KFfin amferm	**	*
*	1.3410294				Xborn [R	.]		Xborn	**	*
*	5.0000000					mpling p		WtMax	**	*
* *	.99000000	4			vmax for KF of fi	nal ferm		vmaxGPS KFfin	** **	*
*	1.3000000	-			mass of	final fe	rm.	amferm	**	*
* *	2.1445691				Xborn LR		~ ~	Xborn	** **	*
*	5.0000000				vmax for	mpling p		WtMax vmaxGPS	**	* *
*	.99000000	5				nal ferm		KFfin	**	*
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*	1.3410294 5.0000000				Xborn LR		or	Xborn WtMax	** **	*
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*		13			KF of fi	nal ferm	ion	KFfin	**	*
* *	.10565830				mass of Xborn [R	final fe	rm.	amferm Xborn	** **	*
*	8.0000000					.] mpling p	ar.	Xborn WtMax	**	*
*	.99900000				vmax for	CEEX	,	vmaxGPS	**	*
* *	1.7770000	15			KF of fi	nal ferm	ion	KFfin	** **	*
*	1.2225177				Xborn [R	final fe	1	amferm Xborn	**	*
*	8.0000000					mpling p	ar.	WtMax	**	*
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* * * * * * * * * * * * * * * * * * *	Parame .10000000F ********** TAUDLA In: Adopted to .10565830 *********** ****************	eters pa 0 0 1 15 2-02 ******** itialization constant skipped ************************************	assed from ************************************	n KK d d c P P R I I I I I I I I I I I I I I I I I	to Tauco ec. type ec. type urrent t DG id 1 .c. swit R-cut fo ********* NE INIMA AMEL AMMU ********* NE INIMA AMEL AMMU ********* IA LIBRA ER, M. J: LISHED IS RN-TH-61 RN TH-61 RN TH-61 RN TH-61 RN TH-61 RN TH-61 RN TH-61 RN TH-61 SCOUTINE DECAY MO ********* sting (s P_X .000 .000	la: 1-st ta 2-nd ta ype a1 d st tau cch lept r lept r ********* S: (tau-mas electroo muon-ma ********* 1995* CH, Z.WA EZABEK, WASM AT N COMP: 56 SEPTE 93 NOVEM C: INITIA DE TAU- ********* ummary) P-y .000 .000	u ec. dec. .c. ********************************	Jak2 KeyA1 idff itdkRC xkOdec ************************************	t02 t03 t05 t05 t05 ****** ***** ***** ***** ****** ******	•• W **********************************
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* 90875 * 4370.16701351	total no of events	nevtot	== *			
* 4363.65383283 +289664	ISRcru [R] 39 ISRbest [R],ISRerr	ISRcru ISRbest	== *			
* 4370.1670 * .0000000E+00	XKarlud [R] KError [R]	XKarlud KError	== *			
***************************************	***************	*******	****** ******			
* Report on w * 90875	t_ISR of KarLud	nowtot	* == *			
* 0	total no of events wt<0 events	nevtot nevneg	== *			
* .01551546 +006668 * 67.80514951 +452155		wt_ISR xskarl	== *			
***************************************	*********	*******				
* .99850963 +000066	38 Average WT of Vesk1		== *			
	07 xs_est gauss [R] 38 xcve/xcgs-1	xcgaus	== *			
******	***********************					
**************************************	**************************************	*********	****** *			
* 180070 * .99710113 +000179	generated events	nevgen wt1	a2 * a5 *			
* .99980533 +000026		wt2	a6 *			
* .99929387 +000612	37 photon ang. dist. MASS WEIGHTS	wt3	a7 * *			
* .95525378 +000521	08 removal wgt wtrem		b1 *			
* 89774 * 0	no. of raw events wt6=0 events		b2 * b3 *			
* .99957099 +000519 * 0	44 control wgt wctrl marked photons	MarTot	b4 * a5 *			
* .1000000E-02	emin	hariot	b6 *			
* .1000000E-07 * .15689398	delta raw ph. multipl.		b7 * b8 *			
* 6.0000000	Highest phot. mult.		b9 *			
**************************************	Finalize END	*****	*******			
* Ка	rFin Finalize		*			
* 180070 * .99634044 +000640	generated events 27 general weight	nevgen wt	a2 * a1 *			
* .15643916 *******************************	aver. ph. multi.	avmlt	a3 *			
-640 KK2f: Photon		****	* * * * * * *			
nent sum 1000 .00000E+00	bmin k .00000E+00 .33000E	max +03				
undf ovef	SIIMW	vex				
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