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PRECISION CALCULATIONS OF HEAVY BOSON PRODUCTION - YFS MONTE CARLO APPROACH

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In this talk I present the current status of the family of Monte Carlo programs for four-fermion physics based on the Yennie-Frautschie-Suura resummation of soft real and virtual photons. I focus on their applications to LEP2.

1 Introduction

The role of Monte Carlo (MC) codes at LEP2 is more important than at LEP1. This is primarily because the physics is more complicated: we deal with a multitude of four-fermion final states, their topology is complicated and not that many semi-analytical results exist. As a consequence, for example, the W-mass fits are performed at LEP2 with the help of MC. At the time of the LEP2 Workshop in 1995 a list of wishes concerning the features of the "ultimate Monte Carlo" was constructed, and the goal of 0.5% precision tag for the total cross-section for WW-physics was set [1]. As the experiment is already well advanced it is time to confront these expectations with reality. I will do it for the family of four-fermion MC codes based on the YFS technique: KoralW, YFSWW and YFSZZ developed by our group. Let me begin with a small technical introduction.

2 YFS Monte Carlo Approach to Four-Fermion Calculations

In their classical paper [2], Yennie, Frautschie and Suura (YFS) reorganized the perturbative series of QED photonic corections for an arbitrary process in a manifestly infrared (IR) finite way. The key step was in the extraction of the universal real ($\tilde{S}$) and virtual (S) functions containing IR singularities. After properly integrating and resumming them to *all orders* the remaining new perturbative series in $\bar{\beta}_n$ functions became IR-finite. As compared to the fixed-order approach this layout is especially convenient for MC algorithms. One is not faced here with problems of IR cut-off, negative distributions or large real–virtual cancellations. Moreover, one can generate a *multiple* photonic bremsstrahlung instead of just one or two photons at most. This approach has been pioneered by two of us (SJ and BFLW) in refs. [3,4,5]. In mathematical terms, the master formula of YFS series, adapted to the MC needs, is the following [3,4,5]:

$$\sigma = \sum_{n=0}^{\infty} \frac{1}{n!} \int \prod_{i=1}^{4} \frac{d^3q_i}{q_i^0} \left(\prod_{i=1}^{n} \frac{d^3k_i}{k_i^0} \tilde{S}(p_1,p_2,k_i) \right) \delta^{(4)} \left(p_1 + p_2 - \sum_{i=1}^{4} q_i - \sum_{i=1}^{n} k_i \right)$$
$$\exp\left(2\alpha \Re B + \int \frac{d^3k}{k^0} \tilde{S}(p_1,p_2,k)(1-\theta_\epsilon) \right) \left[\bar{\beta}_0^{(3)}(p_r^{\mathcal{R}}, q_s^{\mathcal{R}}) + \sum_{i=1}^{n} \frac{\bar{\beta}_1^{(3)}(p_r^{\mathcal{R}}, q_s^{\mathcal{R}}, k_i)}{\tilde{S}(k_i)} \right.$$
$$\left. + \sum_{i>j}^{n} \frac{\bar{\beta}_2^{(3)}(p_r^{\mathcal{R}}, q_s^{\mathcal{R}}, k_i, k_j)}{\tilde{S}(k_i)\tilde{S}(k_j)} + \sum_{i>j>l}^{n} \frac{\bar{\beta}_3^{(3)}(p_r^{\mathcal{R}}, q_s^{\mathcal{R}}, k_i, k_j, k_l)}{\tilde{S}(k_i)\tilde{S}(k_j)\tilde{S}(k_l)} \right] \Theta_\epsilon^{cm}.$$

To explain it very briefly, the $\exp(\dots)$ function is the place where IR virtual ($\Re B$) and real ($\int \tilde{S}$) singularities cancel; $\prod d^3k_i \tilde{S}$ describe the multiple photonic emission and $\sum \bar{\beta}_i$ is the perturbative expansion of a non-IR part of the matrix element (truncated to the third order). To lowest order, $\bar{\beta}_0$ is just the Born matrix element. This formula is the basis of the MC codes that we developed for four-fermion physics.

3 The "Four-Fermion MC Toolbox"

For the moment we provide three complementary MC codes: KoralW, YFSWW and YFSZZ. I will refer to them together as "Four-Fermion MC Toolbox".

• **KoralW**

The main features of KoralW [6,7,8] are: (1) it generates all four-fermion final states with the complete massive Born-level matrix elements and two pre-samplers for complete, massive, four-fermion phase space. The matrix element comes from the automated package GRACE v. 2.0. (2) Anomalous

WWV couplings are included in CC03 graphs. (3) Multiple initial-state photons with finite p_T are generated by the YFS technique and a QED $\mathcal{O}(\alpha^3)$ leading-log matrix element is included. (4) Coulomb effect," Naive QCD" correction and non-diagonal CKM matrix are included. (5) JETSET, PHOTOS and TAUOLA are interfaced. (6) Semi-analytical routine KorWan for CC03 graphs is included. (7) Analysis of Bose-Einstein effect is done as a stand-alone application (in C++) [9].

As compared with the previous version (1.33) the main novelties of v. 1.41 are the following: (1) we have added a second, independent presampler for the four-fermion phase space, which becomes a very powerful test of the code; (2) we have added the third-order leading-log correction to the QED ISR matrix element; (3) the anomalous couplings can now be parametrized in three different ways; (4) any combination of final states can now be specified by the user; (5) CKM matrix and colour reconnection probability are now input parameters.

The most difficult part of the code is the phase-space generator. The origin of the difficulty is in the multitude and complexity of the available final states. Naively counting one has to deal with 9×9 decay channels of WW (CC processes) and 11×11 of ZZ (NC processes), 202 in total. Each channel can contribute up to 100 Feynman graphs, so the total number of "objects" to integrate exceeds 10 000. The solution lies in a *multi-branch MC algorithm*. This approach can already be found in TAUOLA [10,11] and FERMISV [12] MC codes. The general formula is the following:

$$\sigma = \int d\mathrm{Phsp}\, |M|^2 = \left\langle \frac{|M|^2}{\tilde{f}_{CR}} \right\rangle_{d\tilde{\rho}} \int d\tilde{\rho},$$

$$d\tilde{\rho} = d\mathrm{Phsp}\, \tilde{f}_{CR} = \sum_{i}^{Branch} ds_1^i ds_2^i \prod_{j=1}^{3} d\cos\theta_j^i \; d\phi_j^i \; \lambda_j^i \; p_i \; \tilde{f}_{CR}^i.$$

Skipping details (see [8]), let me only say that the process specific information is hidden in the $\tilde{f}_{CR}^i$ functions. These functions must contain all mass and angular singularities of the Feynman diagrams: $1/s, 1/[(s-M^2)^2+M^2\Gamma^2], 1/t, 1/u$ and so on. All the above simple functions are used in $\tilde{f}_{CR}^i$ in the form of subsequent sub-branches with their own splitting probabilities. It is a non-trivial task to fine-tune all these coefficients to get the efficient modelling of all the matrix elements.

• **YFSWW**

Starting from the same master formula, the YFSWW code [13,14,15] features the $\mathcal{O}(\alpha)$ corrections to W-pair production: (1) CC03 (signal) graphs are included in the matrix element; (2) first-order corrrections for WW production

process are included in the exact form of refs. [16,17] as well as in an improved Born approximation of ref. [18]; (3) YFS-type bremsstrahlung is generated from both initial and intermediate (WW) states; (4) anomalous couplings are included in the Born matrix element; (5) JETSET, PHOTOS and TAUOLA are interfaced.

On the technical side, YFSWW presents a number of new ideas. First of all the YFS scheme originally derived for fermions had to be extended to bosons. In a nutshell this is possible since soft photons are "blind" to spin. Both the fermionic and bosonic vertices look the same in the IR limit:

$$\lim_{k\to 0}\left[\cdots\frac{i(-iQ_e e\gamma^\mu)}{\not p' - m_e + i\epsilon}u(p)\right] = \cdots\frac{(Q_e e)(2p^\mu - k^\mu)}{k^2 - 2kp + i\epsilon}u(p), \qquad \text{[fermions]}$$

$$\lim_{k\to 0}\Bigg[\cdots\frac{(-i)(g^{\alpha''\alpha'} - p'^{\alpha''}p'^{\alpha'}/M_W^2)}{p'^2 - M_W^2 + i\epsilon}(iQ_W e)[g_{\alpha'\beta}(2p-k)^\mu + g^\mu_{\alpha'}(-p+2k)_\beta + g^\mu_\beta(-p'-2k)_{\alpha'}]\epsilon_-^\beta(p)\Bigg] = \cdots\frac{(Q_W e)(2p^\mu - k^\mu)}{k^2 - 2kp + i\epsilon}\epsilon_-^{\alpha''}(p). \qquad \text{[vect. bosons]}$$

The second important extension of the original YFS paper [2] was in deriving the YFS form factors in the case of heavy massive particles, contrary to the original small mass approximation of ref. [2]. These functions can be found in [13]. Next, since photons are radiated from the W-bosons with a finite width, one must do it in a way that respects gauge invariance. We did it by adding compensating loop corrections that restore gauge invariance in a similar way as in refs [19,20]. Finally, we had to avoid double counting of Coulomb effect in the matrix element and in YFS virtual B-function, both arising from the same type of loop corrections. We have done that by a proper redefinition of the B-function.

With the help of the YFSWW code we can evaluate the size of $\mathcal{O}(\alpha)$ corrections, see the table below (on the example of the $c\bar{s}e\bar{\nu}_e$ final state).

E_{CM} [GeV]	σ_0 [pb]	$(\sigma_1^{ex} - \sigma_1^{LL})/\sigma_0$	$(\sigma_1^{ex} - \sigma_1^{ap})/\sigma_0$
161	0.1768	-0.83%	$+0.22\%$
175	0.5891	-1.32%	-0.006%
190	0.6792	-1.71%	-0.22%
205	0.6850	-2.22%	-0.61%
500	0.2710	-4.72%	-3.09%

The main novelty of this result is that the corrections are calculated within the realistic full four-fermion MC framework, allowing for any experimental cuts. The numbers show that the $\mathcal{O}(\alpha)$ correction, of about 2%, is similar

in size to the $e^+e^- \to W^+W^-$ case analysed in the literature, see [1] and refs. therein. Therefore it must be included in the MC in order to reach the targeted 0.5% precision level. The approximate Born cross-section barely fits within the 0.5% limit, depending on the actual highest energy available at LEP2.

The last question to be addressed here is how to combine various physical corrections of KoralW and YFSWW? This almost trivial question requires some attention [21] since certain effects, if they are put together improperly, can lead to severe effects, such as the case of running W-width in background graphs [20]. The natural way out is to use a "Multiparameter Linear Interpolation", that is just a series expansion around the "minimal" CC03 cross-section: $\sigma_{MLI} = \sigma_{CC03} + (\sigma_{CCall} - \sigma_{CC03}) + (\sigma_{\mathcal{O}(\alpha)} - \sigma_{CC03}) + \ldots (\Gamma(s), \text{ACC, NQCD}, \ldots)$. As the above expression has quite a few terms it becomes impractical in actual usage. We have shown in ref. [21] an example of the total cross section (with some cuts) that one can equivalently use a "Common Sense Interpolation" by switching on all available corrections in the same MC run, provided one does some minimal cross-checks for each type of observables. This way the above expresion would be reduced to two corrections only (from KoralW and YFSWW), and one day, if also $\mathcal{O}(\alpha)$ corrections are included in KoralW, to just one MC run.

• **YFSZZ**

YFSZZ [22] is a dedicated code for the production and decay of Z-pairs in the process $e^+e^- \to ZZ \to f_1\bar{f}_1 f_2\bar{f}_2$. It features: (1) signal NC02 (ZZ doubly resonant) matrix element; (2) anomalous ZZV couplings; (3) multiple YFS-based bremsstrahlung with an $\mathcal{O}(\alpha^2)$ leading-log QED matrix element. This code is yet to be explored and developed as the physics of Z-pairs progresses.

4 Precision of "Four-Fermion Toolbox"

We can now turn to the basic question: What is the overall precision of the (KoralW+YFSWW) "Toolbox" for the WW physics at LEP2? As stated earlier, we focus on the total cross-section with an eye on a 0.5% precision level.

• **KoralW**

(1) *Technical precision* is estimated at 0.2% based on: (a) internal comparisons of two presamplers, (b) comparisons with other codes [1,21], (c) comparisons with semi-analytical results of the KorWan code (for CC03 matrix element).

(2) *Physical precision* is estimated at 2% based on the size of the $\mathcal{O}(\alpha)$ correction calculated by the YFSWW code.

• **YFSWW**

(1) *Technical precision* is estimated at 0.2% by comparing results of two technically different implementations of the code: YFSWW-2 and YFSWW-3

as well as comparison with KoralW.

(2) *Physical precision* is still under study. Preliminary estimate of 0.5% uses in particular the fact that the so-called "non-factorizable" corrections are negligible. This was first pointed out by Fadin, Khoze and Martin [23,24,25] and then worked out in detail by other groups [26,27,28,29,30].

• **Total**

Collecting the above uncertainties, we can give the *preliminary* estimate of the precision of the (KoralW + YFSWW) "Toolbox" for the total cross-sections of the WW-physics at LEP2 to be **0.5%** (preliminary).

5 Under the carpet

From previous sections one may get the impression that our "Four-Fermion MC Toolbox" is almost finished. Unfortunately this is not true, especially for the NC processes. I will present some of the outstanding problems. They are of a universal type and can be even several times bigger than the 0.5% precision tag, see ref. [8] for more comments.

• **Numerical instabilities**

The ratio m_e^2/s is at LEP2 of the order of 10^{-12}. Together with delicate gauge and unitarity cancellations it leads to numerical instability problems in the matrix element calculations. Let me give an explicit example with an event generated by KoralW in the $e^-\bar{\nu}_e\nu_e e^+$ channel:

```
 pdg            p_x                  p_y                  p_z                   E
  11 -.000000341278492 -.000001614768132  92.983165682216736 92.983165683620868
 -12 -.633000329710363  .109862863634447 -11.985324403772751 12.002531455067720
  12  .771573326908979  .358415826559387 -70.475962939695890 70.481097753801436
 -11 -.138572655920124 -.468277075425702 -10.521878338748095 10.533205107509984
                    four-fermion weight = 913570469940928.500
```

The outgoing electron is highly collinear, the corresponding transfer small, and the four-fermion weight (i.e. matrix element) is huge. Now, let us modify by hand the last two digits of the p_z components of four-momenta and rerun the event:

```
 pdg            p_x                  p_y                  p_z                   E
  11 -.000000341278492 -.000001614768132  92.983165682216722 92.983165683620868
 -12 -.633000329710363  .109862863634447 -11.985324403772731 12.002531455067720
  12  .771573326908979  .358415826559387 -70.475962939695876 70.481097753801436
 -11 -.138572655920124 -.468277075425702 -10.521878338748115 10.533205107509984
                    four-fermion weight = 25094.3831593953582
```

The four-fermion weight (matrix element) has changed by 11 orders of magnitude! What can we do about this? We can use a quadruple precision. Our experience shows that it cures the problems. However it requires a complex quadruple precision that is not available on all platforms. Also the speed of the calculation is much lower. For that and other reasons, specified later on, we prefer another solution – impose additional *post-generation* cut-offs on these

dangerous corners of the phase space:

(1) In the case of the CC-type processes it is only a tiny angular cone around the beams, of the size of 10^{-6} rad. It influences the total cross-section below 0.2% and can be hidden in the technical precision for the time being.

(2) In the case of NC-type processes the situation is much worse. There are two regions (for final states with the e^+e^- pair) that we had to cut out: when invariant mass of produced pairs is smaller than $\sqrt{8}$ GeV or when the *sum* of transverse momenta squared of visible particles is smaller than 600 GeV^2. Note that this latter cut allows an e^+e^- pair to go to the beam pipe.

• Limitations of ISR

The ISR-based description of bremsstrahlung breaks down for final states with at least one electron (positron) collinear to the beam. For such processes the t-channel photon exchange is dominant. In other words the bremsstrahlung is governed by $\log|t|/m_e^2$ instead of $\log s/m_e^2$. As a result of the missing $\log|t|/s$, too much radiation is generated, especially in the high-p_T region. Depending on the actual cuts this can significantly affect the cross-section. How can it be cured? First of all by adding all the radiation (interferences) missing in the soft limit. This means that the YFS program should be applied to *all six* external particles. Although radiation in the two s- and t-channels separately is already implemented in MC codes (YFS3 and BHLUMI, respectively), it is nonetheless not easy technically to merge them into one coherent algorithm in the case of four-fermion final states. (In the case of two fermions, this has already been done in BHWIDE MC code [31] by some of us.)

However, even if we have the radiation corrected in the soft limit we would still be missing part of the hard photonic corrections. Can these be dangerous? Consider the following event in the LAB frame ($e^+e^-d\bar{d}$ from KoralW) with a hard transverse photon (note that this event passes the cuts defined in the previous section):

```
                ================ LAB frame ===================
 pdg              p_x                p_y                p_z                 E
 PHO  5.91545655722838  47.82076396799343   2.67297019944074 48.25932927890828
 PHO  -.00000027637796   -.00000037152652   -.14955853849146   .14955853849218
 PHO   .01336462801524    .00882331258921    .02409193017994   .02892896864438
 PHO   .00000005382246    .00000005171260    .00563331053129   .00563331053178
   1  -.24118785025702  -1.90677419291787  -2.58051680257066  3.21762744428852
  -1  -.01773699286484   -.01532459077309    .98308780906072   .98341806182419
  11  -.11234211241339    .42661722421839  60.88292736560235 60.88452568487788
 -11 -5.55755400715285 -46.33410540129616 -61.83863527375292 77.47097871243272
                  angles of decay products with resp to beams:
      d quark          d~ quark            e-                 e+
-.80199753074017   .99971586568334   .99997374838494   -.79821678134001
```

The problem appears when we transform it to the "effective frame". In order to calculate the matrix element that is defined just for four-fermions, the momentum carried out by photons has to be compensated for and some

"effective" on-shell electron "beams" have to be constructed. After the transformation the event becomes:

```
                    ============ effective CMS frame =============
 pdg              p_x               p_y                p_z                  E
   1 -.008731476493231  .021808545200827  -2.679767691308820  2.679889313144880
  -1 -.016063888417215 -.021968761695611   1.057202898562928  1.057600417800303
  11  .000815509213020 -.001379443999798  66.011587576947306 66.011587598375669
 -11  .023979855697426  .001539660494582 -64.389022784201416 64.389027269943767
                     angles of decay products with resp to beams:
      d quark           d~ quark              e-                 e+
-.99996157863668    .99966881915163     .99999999970535   -.99999993036524
```

As we see, we have created a "monster" – a very "small angle" configuration out of a quite transversal event. This leads to a physically unjustified enhancement in the matrix element calculation, i.e. to high weights or even numerically unstable ones. What is the solution? Surely, one needs the complete $\mathcal{O}(\alpha)$ or even higher order photonic corrections. This is a very difficult task for the future. For now we use temporary fix-up by cutting out the high p_T photons with $\sum p_T^2 \geq 300$ GeV^2. Unfortunately, it is not a completely effective cut and on an occasion numerical instabilities survive.

6 Summary

In this talk I presented the "Four-Fermion MC Toolbox". It consists of three MC programs: (1) KoralW with all four-fermion processes, YFS-based ISR and anomalous WWV couplings; (2) YFSWW with CC03 matrix element, $\mathcal{O}(\alpha)$ electroweak corrections to W-pair production, (Initial+WW)-state YFS-based bremsstrahlung and anomalous WWV couplings; (3) YFSZZ with NC02 matrix element, anomalous ZZV couplings and YFS-based ISR. The current precision of the codes for the WW physics at LEP2 is 2% for KoralW and 0.5% (preliminary) for YFSWW for the total cross section. Based on this we expect the corresponding total precision of the Toolbox to reach the gold-plated 0.5% level soon. The important limitations that need to be resolved in the future concern the final states with electrons (positrons) at small angles, that is mostly the NC-type processes. They include: (1) numerical instabilities in matrix element (under control by applying cuts or by the use of a quadruple precision); (2) lack of "t-channel" bremsstrahlung; (3) lack of hard-photon matrix element. We are on the way to resolving these problems, and we are looking forward to it with excitement.

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