Precision for KKMC Monte Carlo – necessary associated efforts

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To prepare Monte Carlo simulation programs of requested precision (in percent) several associated projects need to be developed in parallel.

(A) Software environments, makefiles configuration scripts, code managers, user interfaces.

(B) Event records. Formats and principles of content, what the things mean. Reference frames, quantum entanglements. History entries.

(C) Phase space with number of particles. Conformal symmetry, non markovian algorithms, crude distributions intermediate resonances, Kinoshita-Lee-Nauenberg (KLN) theorem, iterative solutions, matching phase space boundaries (re-scaling energies to get soft photon boundary

(D) Matrix element: levels of factorization, separation into parts, eikonal QED, full QED remaining EW and QCD parts (hadronization, loop corrections), effective couplings, complex masses and unitarity constraints.

(E) technical separation of amplitudes into parts, real and virtual. Expansion of YFS type, expansion around contact interaction, exact third order (triple bremsstrahlung) amplitudes.

(F) New Physics imprinting. Dark photons, anomalous dipole moments, extending 2-fermion final state generation into 4-fermion final states of processes like $e^+e^- \to ZH \to 4f$.

(G) reliability tests, analytical and semi-analytical benchmarks. Precision is observable dependent. Test environments must be long living.

(H) spin effects, incoming beams polarization, τ leptons spin of final states. Belle 2 as source of better τ-decay hadronic form-factors.

(I) `KKMC` is now-days a good candidate for FCC-ee $e^+e^- \to \tau^+\tau^- n(\gamma)$ MC.

(J) Toward automated β_i terms (after summary)

(*) Let me provide some comments on the above points. This may be of importance for handling long term projects like of Monte Carlo programs.

(A) Software

1. Monte Carlo programs have their development cycle counted in decades.
2. They accumulate lot of physics knowledge as well as knowledge related to tests
3. My experience is that whatever what can not be compiled with ANSI compilers sooner or later bring difficulty.
4. that was the case with software managers. I suffered a lot with `Historian` disappearance
5. That was the case with `root`, when old files became effectively unreadable or old functions became obsolete.
6. That was the case with configuration scripts assuring platform flexibility
7. Also with `makefile`s.
8. Sooner or later you have to deal with ‘simplifications’ with enormous loss of time and frustrations.
9. Usually it hits in inconvenient moments. Your programs are not affected, but benchmarks plots are.

(A) Software

10. Also optimization/improvements of libraries may be unfriendly: random number generator returning values at boundaries that is 0 or 1 may lead to rounding error generated crashes. Integration routine optimization may give integrals which as function of some parameters may have kinks in firs derivatives.
11. long term surviving tests were obtained with ANSI compilable libraries
12. long term surviving projects had human eye decipherable makefile systems
13. Delegating effort to software engineers or collaborators fluent with software, was good but later brought difficulties.

(B) Event records

1. Originally all event records were supposed to represent tree of tracks in the detector: there were incoming beams outgoing stable particles and intermediate resonances.
2. The purpose was to communicate information between theoretical part of simulation and detector response part.
3. The idea was to have vertices and links. Physics information was attributed to links `HEPEVT` or vertices `HepEVT`.
4. Then need of physics appeared and content was somewhat corrupted. History entries appeared, entries before/after hadronization appeared.
5. That was very helpful to optimize reconstruction algorithm.
6. But it brings confusion, every MC had a tendency to write into event record hard process information of slightly different nature.
7. Physically separated event record parts of event tree, such as decays, require careful standard for definition of density matrices.
8. For that in `KKMC` we do not rely of event record. In fact we provide routines

(B) Event records

relating decaying object rest frames with laboratory frame. In this way, two segments of the program, each requiring density matrices of the given object in its rest frame, can have necessary rotation performed in relatively easy, safe and universal way.

9. In many cases we are interested in spin of intermediate object, as source of physics information, not of its decay products. That is more useful for phenomenology purposes.
10. Machine learning approaches change picture a bit, but for purpose of intuition build/systematic studies, optimal variables remain convenient.

(C) Phase space

1. From practical point of view that is central issue.
2. We need to generate number of particles in final state according to some crude distribution as well as provide crude kinematical distribution.
3. Such integrable distribution must follow structure of singularities, collinear, soft as well as e.g. Z boson peak and $1/s$ enhancement of Born cross section for low energies.
4. That is one of the reasons why generation is separated into initial- final- and interference- bremsstrahlung parts.
5. Crude phase-space distribution with the help of event weights need to be modified to get the accurate one. To control singularities, this need to be done together with approximate matrix elements of singularities not very different than the actual ones.
6. Define crude 1-dimensional initial state radiation times simplified Born total cross section. Must be integrable at least numerically. However $\rightarrow$ beamstrahlung $\rightarrow$ 1- to 3-dimensional $\rightarrow$ Thorsten talk.

(C) Phase space

7. The functional generating function of crude distribution is based on poissionian distribution.
8. `KKMC` algorithm is non Markovian and conformal symmetry of QED at eikonal level is used.
9. This enables rigorous order by order improvements.
10. `Photos` algorithm is non Markovian too and start from essentially the same poissionian distribution. Its algorithm does not use conformal symmetry. Phase space boundaries are introduced iteratively for each consecutive particle individually. Advantage is that such particles can be massive, and leading collinear terms are effectively resumed to all orders. Not just soft terms. Disadvantage is that it works for final state emissions only, because KLN theorem is used.
11. both algorithms overcome so called soft-photon boundary issue which is a plague for fixed order Monte Carlos.
12. To get exact parametrization features of matrix elements need to be understood

(C) Phase space

and prepared. Virtual and real corrections.

(D) Matrix element

1. To make such algorithm possible careful study of matrix element is needed.
2. Yennie-Frautchi-Suura work was fundamental for `KKMC`
3. It enables to separate matrix elements into parts : eikonal and then calculable perturbatively $\beta_1, \beta_2, ...$ terms.
4. That means re-ordering of perturbative expansions into more convergent form and with all kinematical configurations and all multi-photon phase space covered already at the zero order of expansion.
5. Rules how to add terms calculated from perturbative corrections require attention.
6. e.g. we need to use appropriate part of single photon emission matrix element for multiple photon configuration, where from the perspective of single photon there is no energy momentum conservation.
7. This need to be done carefully require effort and tests.
8. That is another reason why generation is separated into initial- final- and interference- bremsstrahlung parts.

(D) Matrix element

9. For Bhlumi it is bremsstrahlung from upper and lower fermion lines.
10. in both cases gauge invariance and structure of singularities define details
11. separation of SM results beyond QED is another step of the work.
12. It took years to establish solution to separate out from SM the QED part, genuine weak correction part and
13. line shape corrections: higher order corrections to fermionic loops of Z and γ^* propagators.
14. There is an issue of unitarity for Standard Model. These constraints are known to work for one loop precision level, but what for two-loop electroweak level?

(E) technical separation

1. Formal theory level matrix element separation into parts is not the end of the difficulties.
2. If for example Kleiss-Stirling amplitudes are used, one has to be very careful to avoid mismatches due to rounding errors.
3. That may mean loss of numerical precision of ten orders of magnitude or sometimes 20 orders.
4. Essential is care of numerical aspects of the discussed on previous slide interpolations.
5. It is of no practical help if at least some of such difficulties would disappear if even higher order terms of perturbation expansions would be included.

(F) New Physics

1. Often, new physics requests are made.
2. Then the question is not high precision of New Physics effects, but how to avoid damaging precision of Standard Model.
3. That requires attention and revisit of physics assumption behind main program.
4. Sometimes New Physics may be New Standard Model process.
5. That was the case with $e^+e^- \to \bar{\nu}_e \nu_e n\gamma$. New add-up does not need to be New Physics but additional interaction, ignored previously.
6. It seems that we are on the similar path with processes: $e^+e^- \to Z/H \to \tau^+\tau^- l^+ l^- n\gamma$
7. We have started with dark photons dark scalars for Belle2, Tests with `MadGraph`. For implementation and for approximation in matrix element.
8. Finally careful division of amplitudes into parts will be needed again to assure precision
9. The same will be true for virtual corrections.

(G) reliability

1. It is quite common, at the time of program development to make mistakes or introduce bugs which may come un-noticed at first.
2. To be sure that it does not happen special calculations of benchmark signatures are needed.
3. Usually for such tests semi-analytical or analytical calculations are used.
4. That (usually) assures independence and comparisons are helpful.
5. Simulations with distinct programs can be of the help too. Simpler programs, each providing part of the effects may be used, and their results combined, each used to provide correction due to missing in other programs effect.
6. Such tests are of physical precision or of technical precision.
7. In general evaluation of ambiguities observable dependent. Results can not be attributed to all results of simulations with the particular code.
8. Preparing test distribution, usually requires comparable effort as work on the main code.

(G) reliability

9. There are critical precision thresholds, where old tests require better technical precision.
10. That aspect of the work affects everything, including design of main program.
11. It is essential for reliability to repeat tests whenever precision thresholds are passed.
12. That goes straightforward usually, but sometimes it is up-hill fight.
13. Perk of tests: optimal variables.
14. tests with simplified physics, especially analytical tests. Perk: intuition build-up.

(H) spin effects

1. If in final state short lived particles are present, of decay products living traces in detector then spin state can be used to define interesting observables.
2. That is particularly valuable in case if sensitivity to CP-parity is of interest.
3. Then decays are effectively representing part of the detection, rather than of the process to be measured.
4. That means spin state needs to be available for the people involved in data analysis. The spin and spin response of the particular decay channel: the polarimetic vector in case of τ decays.
5. This does not come for free, not only people involved in data analysis need to be spin savvy.
6. Spin information needs to be available for the user.
7. Reference frames for which spin state is defined need to be clearly defined. In case of `KKMC`, such information is available and boost to lab routines can be used. Then object can be boosted back to rest-frames of τs, this time in conventions of users.

(H) spin effects

8. Quantum entanglement does not simplify the tasks, even if it is of particular interest for CP-sensitivity.
9. But it is useful.

(I) KKMC

1. `KKMC`* head F77 version
2. `KKMC` C++ head version
3. `KKMC`* Belle 2 version
4. `Tauola`* Belle 2 version
5. `Tauola`* default version
6. `Photos`* head F77 version
7. `Photos`* head C++ version
8. `Dizet`* electroweak library
9. For versions marked * I can provide help rather quickly.
10. For other it may take some more time.

(*) Summary

1. One need to keep all these aspects in mind.
2. Each point calls for separate talk.
3. Issues of teams continuity,
4. survival of benchmarks, especially those needed to be re-done when threshold of precision are crossed is often badly documented but essential aspect, danger for project continuity
5. We continue developments for `KKMC` and related Monte Carlo programs, some
6. Personally I am involved in servicing KKMC version of Belle2.
7. I work on basic aspects of algorithm and physics content extension, but some things were out of my imminent duties.
8. But this year is not easy and we can not avoid some difficulties/delays. In particular in service for the users.
9. Man power especially experienced of long term involvement and devotion is big issue.

(*) Summary

10. We plan to do all we can to assure continuity. We miss many people ...
11. The minimum plan is documentation.

Huge nest of activities

Matching things is a challenge too. Technical, social, ...

Examples of recent activities which document work. Usually only part of effort for single point:

- **C.11** Collinearly Enhanced Realizations of the YFS MC Approach to Precision Resummation Theory, **S. Jadach**, B.F.L. Ward, Z.A. Was 2303.14260 Step toward better crude distribution, to improve convergence of pert. exp. beyond CEEX exponentiation with collinear terms as well.
- **I.2** Multi-photon Monte Carlo event generator KKMCee for lepton and quark pair production in lepton colliders, **S. Jadach**, B.F.L. Ward, Z. Was, S.A. Yost, A. Siodmok,Comput.Phys.Commun. 283 (2023), 108556
- **G.8** Adequacy of Effective Born for electroweak effects and TauSpinner algorithms for high energy physics simulated samples, E. Richter-Was, Z. Was

(*) Summary

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- **H.3** TAUOLA update for decay channels with e^+e^- pairs in the final state, S. Antropov, Sw. Banerjee, Z. Was, J. Zaremba Comput.Phys.Commun. 283 (2023), 108592
- **F.7** The tau lepton Monte Carlo Event Generation - imprinting New Physics models with exotic scalar or vector states into simulation samples, Sw. Banerjee, D. Biswas, T. Przedzinski, Z. Was 2112.07330

J details/perspective for D.3

Matrix Element (starting point):

- Directly starting from Feynman rules one can calculate spin amplitude for any QED/QCD process.
- The case of $e^+e^- \to l^+l^-\gamma$ is the backbone of work on matrix elements
- single photon amplitude(momentum k_1 polarization e_1 fermion spinors $u(p)$ and $v(q)$ dropped, other incoming or outgoing fermion pair hidden in J):

$$I = \not{J}\left[\left(\frac{p\cdot e_1}{p\cdot k_1} - \frac{q\cdot e_1}{q\cdot k_1}\right)\right] - \left[\frac{1}{2}\frac{\not{e}_1\not{k}_1}{p\cdot k_1}\right]\not{J} + \not{J}\left[\frac{1}{2}\frac{\not{e}_1\not{k}_1}{q\cdot k_1}\right]$$

three gauge invariant parts. Easy to separate and code separately. First term, eikonal factor, thanks to conformal symmetry can be used in construction of crude distribution.

Other parts can be introduced at rejection step.

Analysis of double bremsstahlung helps to identify parts corresponding to eikonal

J details/perspective for D.3

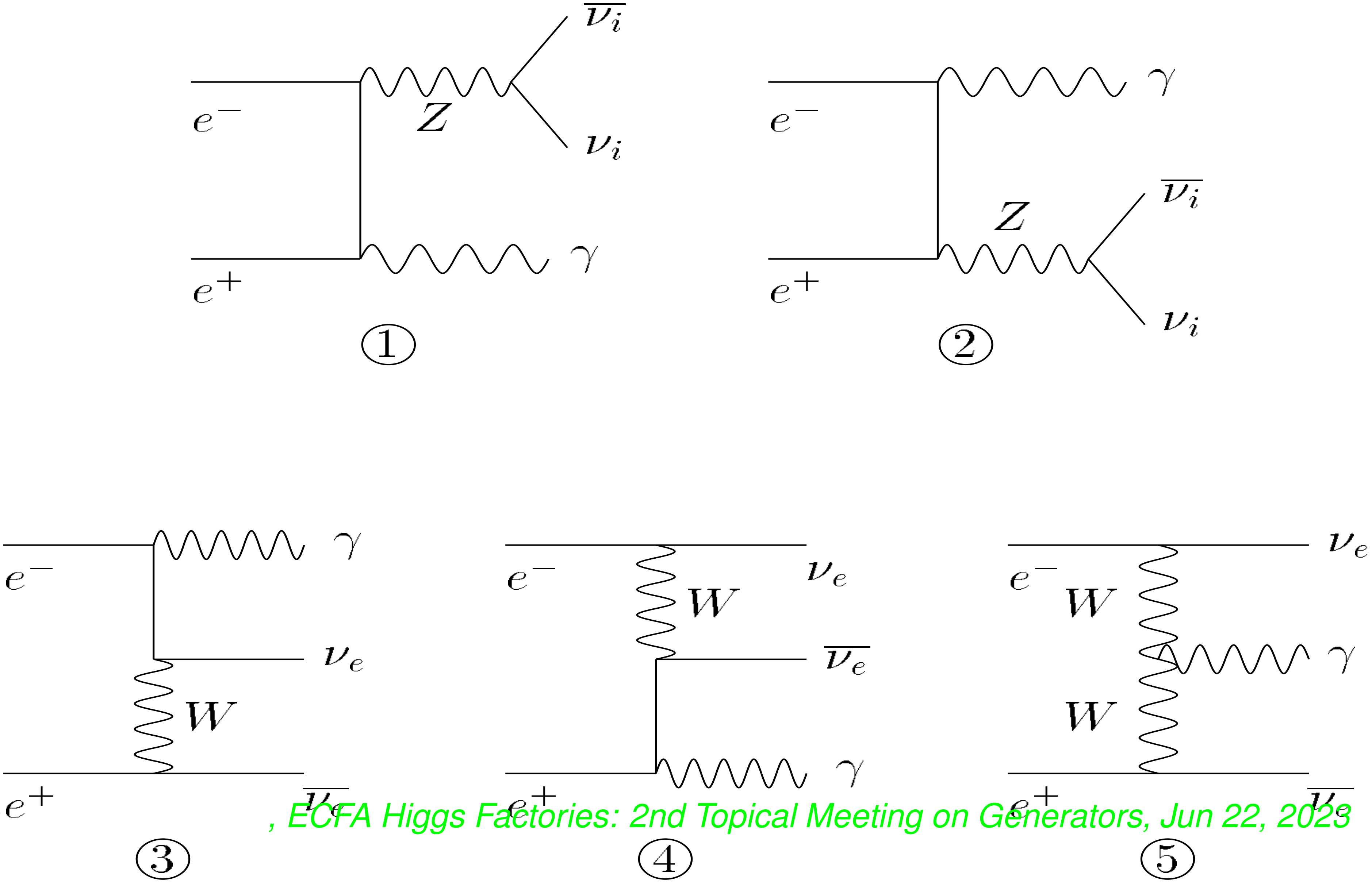
(two) single photon emission parts (beyond eikonal) and remaining genuine double emission part.

Again parts can be treated (summed in) at later steps with the help of some events rejection.

Need to exploit that for configurations where more hard photons are present. Careful treatment of J is needed. That is why it is necessary to generate separately ISR FSR and then IFI interference.

J details/perspective for D.3

Figure 1: *The Feynman diagrams for* $e^+e^- \to \bar{\nu}_e\nu_e\gamma$.



J details/perspective for D.3

$$
\begin{aligned}
&\mathcal{M}_{1\{I\}}\begin{pmatrix} p\, k_1 \\ \lambda\, \sigma_1 \end{pmatrix} = \mathcal{M}^0+\mathcal{M}^1+\mathcal{M}^2+\mathcal{M}^3\\
&\mathcal{M}^0 = eQ_e\ \bar{v}(p_b,\lambda_b)\ \mathbf{M}^{bd}_{\{I\}}\ \frac{\not{p}_a+m-\not{k}_1}{-2k_1p_a}\ \not{\epsilon}^{\star}_{\sigma_1}(k_1)\ u(p_a,\lambda_a)\\
&+eQ_e\ \bar{v}(p_b,\lambda_b)\ \not{\epsilon}^{\star}_{\sigma_1}(k_1)\ \frac{-\not{p}_b+m+\not{k}_1}{-2k_1p_b}\ \mathbf{M}^{ac}_{\{I\}}\ u(p_a,\lambda_a)\\
&\mathcal{M}^1 = \mathcal{M}^{1'}+\mathcal{M}^{1''}\\
&\mathcal{M}^{1'} = +e\ \bar{v}(p_b,\lambda_b)\ \ \mathbf{M}^{bd,ac}_{\{I\}}\ u(p_a,\lambda_a)\epsilon^{\star}_{\sigma_1}(k_1)\cdot(p_c-p_a)\frac{1}{t_a-M_W^2}\,\frac{1}{t_b-M_W^2},\\
&\mathcal{M}^{1''} = +e\ \bar{v}(p_b,\lambda_b)\ \ \mathbf{M}^{bd,ac}_{\{I\}}\ u(p_a,\lambda_a)\epsilon^{\star}_{\sigma_1}(k_1)\cdot(p_b-p_d)\frac{1}{t_a-M_W^2}\,\frac{1}{t_b-M_W^2},\\
&\mathcal{M}^2 = +e\ \bar{v}(p_b,\lambda_b)g^{We\nu}_{\lambda_b,\lambda_d}\ \not{\epsilon}^{\star}_{\sigma_1}(k_1)\ \ v(p_d,\lambda_d)\bar{u}(p_c,\lambda_c)g^{We\nu}_{\lambda_c,\lambda_a}\ \not{k}_1\ \ u(p_a,\lambda_a)\frac{1}{t_a-M_W^2}\,\frac{1}{t_b-M_W^2}\\
&\mathcal{M}^3 = -e\ \bar{v}(p_b,\lambda_b)g^{We\nu}_{\lambda_b,\lambda_d}\ \not{k}_1\ \ v(p_d,\lambda_d)\bar{u}(p_c,\lambda_c)g^{We\nu}_{\lambda_c,\lambda_a}\ \not{\epsilon}^{\star}_{\sigma_1}(k_1)\ \ u(p_a,\lambda_a)\frac{1}{t_a-M_W^2}\,\frac{1}{t_b-M_W^2},
\end{aligned}
\tag{1}
$$

- Once manipulations completed, we separate the complete spin amplitude for the process $e^+e^- \to \bar{\nu}_e\nu_e\gamma$ into *six* individually QED gauge invariant parts. This conclusion is rather straightforward to check, replacing photon polarization vector with its four-momentum. Each of the obtained parts has well defined physical interpretation.
- It is also easy to verify that the gauge invariance of each part can be preserved to the case of the extrapolation, when because of additional photons, condition $p_a+p_b=p_c+p_d+k_1$ is not valid.

J details/perspective for D.3

t-channel and contact interaction expansion This is solution to use ISR/FSR radiation algorithm for processes with t-channel propagators.

It works for 2-photon emissions too.

If W-propagator is frozen with some fixed t-channel transfer amplitudes reduce to the ones of ISR. Dependence can be introduced back at re-weighting β_1 or β_1, β_2 level.

Again some further care was needed.

How to assure pre-conditions for automatization? Some work is needed. It was tough work, but not tough-enough to avoid hand work

Also it was some fun to do it by hand.

Is there a path for automated evaluation of amplitudes ? yes

Is there a path for automated evaluation of their eikonal parts ? yes

Is there a path for automated evaluation of β_i (β_i-like parts ? I hope so

I tried it in several cases like: double bremsstrahlung, pair emissions, scalar QED:

J details/perspective for D.3

τ decays with scalar vector decay products, double gluon emissions in QCD.

It looks promising, but not off shell:

My limited knowledge of mathematics does not help:

1) I do not know enough of differential geometry: *CW-complex is not much more than a name for me*, but it should be introduced into automated calculations to play with infrared singularities. Outcome of accidental chat with mathematician in Lublana, friend of Borut Kersevan

2) I do not know how to play in automated way with sub-groups and induced with them layers of Lorentz group.

Man-power issues, need of efforts for urgent tasks do not help.

So far, it was not of critical importance.

The subject potentially very rewarding, is waiting for less pressing times.

For $e^+e^- \to \nu_e \bar{\nu}_e \gamma\gamma$, pure QED, I was forced to take contribution with virtual charged Higgs in t-channel.

Lesson from Photos development. No conformal symmetry used. It is of no relevance for `KKMC`. One has to be consistent in expansion. If one approximate matrix element (first order only), then the same level of approximation should be done for phase space, which is formally a manifold and matrix element is a function (bi-linear form because $|\mathcal{M}|^{\in}$). Issue is about powers of curvature tensor, appear in interference weight. I have experienced by accident. Expansion has to be consistent for phase-space and $|\mathcal{M}|^{\in}$.