#### Simulation of New Physics signatures and interfering SM backgrounds Z. Was\*,

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(A) Exp. Data and New Physics: Define observables, later: detetector acceptance, higher order matrix elements, structure functions, evolution kernels, algebraic programs.

(B) Full control of phase-space parametrization and approximations is essential for many of MC techniques, weighted events, correlated samples, Machine Learning.

(C) New Physics effects are expected small. SM bacground is large need precision.

(D) Efforts to preserve KKMC as main simulation tool for  $e^+e^- \rightarrow \tau^+\tau^- n(\gamma)$  at Belle 2:

- 1. Flexible  $\tau$  decay channels, for SM and NP. Hope: Belle 2 hadronic currents public?
- 2. Imprint into KKMC events: anomalous magnetic/electric moments using weights.
- 3. Imprint into KKMC events: additional NP particles: dark photons or new light scalars.
- 4. tauola and photos MC's for  $\tau$  decays and radiative corrections in decays: new exotic resonances decaying to  $l^+l^-$  added.

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• (E) My talk focus on Belle 2, but useful for FCC and LHC too.

#### **Phase space and Monte Carlo**

• (1) For the precision predictions and integration over acceptance regions for realistic observables, Monte Carlo techniques are indispensable.

- (2) It is convenient to use explicit and exact phase space parametrization,
- (3) and all approximations localized in matrix elements.
- (4) I mean approximate matrix elements, but of explicit and fully controlled approximations..
- (5) I know how into such programs New Physics effects can be injected.

 (6) Approximations on New Physics effects a acceptable, but for SM often interfering background no precision compromise!

• I will use KKMC Monte Carlo for  $e^+e^- \rightarrow \tau^+\tau^-(n\gamma)$  process (with  $\tau$  decays).

• KKMC has well established precision tag and is installed in Belle 2 collaboration software. Changes for NP, bring minor changes to the code only:

• S. Banerjee, D. Biswas, T. Przedzinski and Z. Was, "The tau lepton Monte Carlo Event Generation - imprinting New Physics models with exotic scalar or vector states into simulation samples," [arXiv:2112.07330 [hep-ph]].

• S. Banerjee, A.Yu. Korchin and Z. Was "Anomalous magnetic and electric dipole moments and spin correlations in production of  $\tau$ -lepton pairs, IFJ-PAN-IV-2022-12, Sept. 2022.

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# (A) New physics signatures

Start: new physics model builders identify potentially dtetctable signatures.

First step luminosity, NP cross section, idealized asymmety ...

Difficulties: orders of magnitude larger background need to be taken into account.

Imperfection in background evaluation or New Physics

Precision background estimation and flexibility for tools modifications/extensions is fundamental for final evaluations.

#### (B) precision of SM must be preserved.

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#### **Phase space and Monte Carlo**

(1) For the precision predictions and integration over acceptance regions for realistic observables, Monte Carlo techniques are indispensable.

- (2) It is convenient to use explicit and exact phase space parametrization,
- (3) and have all approximations localized in matrix elements.
- (4) I mean approximate but explicit matrix elements.
- (5) New Physics effects can be injected into such programs in unambiguous way.

(6) Approximations for New Physics effects are OK. For SM, often interfering background **no precision compromise!** 

#### • I will use KKMC Monte Carlo for $e^+e^- \rightarrow \tau^+\tau^-(n\gamma)$ process (with $\tau$ decays).

• KKMC has well established (and improving) precision tag. It is installed in Belle 2 collaboration software. Changes for NP, bring minor changes to the code only:

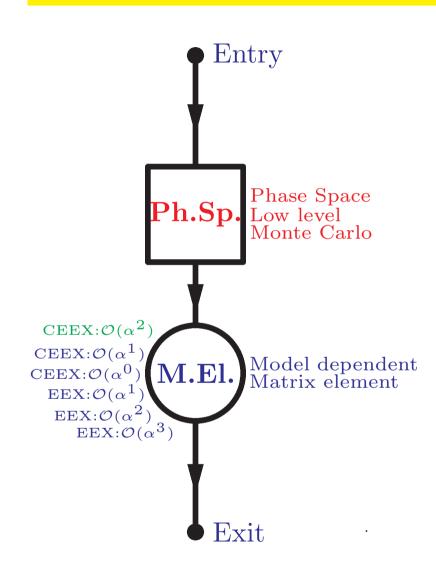
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### (B) precision of SM must be preserved.

#### KKMC follow textbook principle "matrix element $\times$ full phase space"



- Phase-space Monte Carlo simulator is a module producing "raw events" (including importance sampling for possible intermediate resonances/singularities)
- Library of Matrix Elements; input for "model weight"; independent module
- This was used extensively for LEP precision Monte Carlos. It is true for KKMC as used in Belle collaboration for τ lepton pair production with decays and multiphoton radiation.
- Correlated samples techniques. Lots of technicalities collected in Phys. Rev. D41 (1990) 1425.
- Solutions useful for New Physics event weights!

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#### To start: $M^{SM}$ and $M^{SM+NP}$ are needed.

- OK, for **anomalous magnetic/electric dipole** moments implementation in  $e^+e^- \rightarrow \tau^+\tau^-(n\gamma)$  process ( $\tau$  decays included).
- Seem trivial, but one has to keep in mind practical details.
- I will say little about reliability proofs, even though they are essential.
- Important is to preserve SM (interfering-) bulk of the process!
- Check if factorization properties for NP match with what is in SM. Precision requirements for New Physics implementation are not high. Use of interpolated Born configurations in presence of hard bremsstrahlung photons is OK.
- Next slide: condition of work with KKMC Monte Carlo.

Formalism for  $\tau^+\tau^-$ : phase space  $\times$  M.E. squared

• Because narrow  $\tau$  width ( $\tau$  propagator works as Dirac  $\delta$ ), cross-section for  $f\bar{f} \rightarrow \tau^+ \tau^- Y$ ;  $\tau^+ \rightarrow X^+ \bar{\nu}$ ;  $\tau^- \rightarrow \nu \nu$  reads (norm. const. dropped):

$$d\sigma = \sum_{spin} |\mathcal{M}|^2 d\Omega = \sum_{spin} |\mathcal{M}|^2 d\Omega_{prod} \ d\Omega_{\tau^+} \ d\Omega_{\tau^-}$$

$$\mathcal{M} = \sum_{\lambda_1 \lambda_2 = 1}^{2} \mathcal{M}_{\lambda_1 \lambda_2}^{prod} \ \mathcal{M}_{\lambda_1}^{\tau^+} \mathcal{M}_{\lambda_2}^{\tau^-}$$

- Pauli matrices orthogonality  $\delta_{\lambda}^{\lambda'} \delta_{\bar{\lambda}}^{\bar{\lambda}'} = \sum_{\mu} \sigma_{\lambda \bar{\lambda}}^{\mu} \sigma_{\mu}^{\lambda' \bar{\lambda}'}$  completes condition for production/decay separation with  $\tau$  spin states.
- core formula of spin algorithms, wt is product of density matrices of production and decays, 0 < wt < 4, < wt >= 1 useful properties.

$$d\sigma = \left(\sum_{spin} |\mathcal{M}^{prod}|^2\right) \left(\sum_{spin} |\mathcal{M}^{\tau^+}|^2\right) \left(\sum_{spin} |\mathcal{M}^{\tau^-}|^2\right) wt \ d\Omega_{prod} \ d\Omega_{\tau^+} \ d\Omega_{\tau^-}$$

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Simplified kinematic for NP implementation. Cross section:

$$wt_{ME} = \left(\sum_{spin} |\mathcal{M}^{prod \ SM + NP}|^2\right) / \left(\sum_{spin} |\mathcal{M}^{prod \ SM}|^2\right)$$

Complicated is spin weight

$$wt_{spin} = \left(\sum_{ij} R_{ij}^{SM+NP} h_+^i h_-^j\right) / \left(\sum_{ij} R_{ij}^{SM} h_+^i h_-^j\right)$$

The  $R_{ij}$  depend on kinematic of au-pair production,  $h^i_{\pm}$  on  $au^{\pm}$  decays.

Spin quantization frames orientation need care. It must be the same for production and decay.

We use KKMC routines to transfer  $h^i_{\pm}$  to lab frame and another routines to transfer back to  $\tau^{\pm}$  but oriented as in New Physics calculation.

In this way reference frames are OK and impact of photons on phase space parametrisations is under control.

Solution works for all au decays!

*a*- magnetic dipole moment, *b*- electric dipole moment couplings.

$$R_{11} = \frac{e^4}{4\gamma^2} \left( 4\gamma^2 \operatorname{Re}(a) + \gamma^2 + 1 \right) \sin^2(\theta),$$

$$R_{12} = -R_{21} = \frac{e^4}{2} \beta \sin^2(\theta) \operatorname{Re}(b),$$

$$R_{13} = R_{31} = \frac{e^4}{4\gamma} \left[ (\gamma^2 + 1) \operatorname{Re}(a) + 1 \right] \sin(2\theta),$$

$$R_{22} = -\frac{e^4}{4} \beta^2 \sin^2(\theta),$$

$$R_{23} = -R_{32} = -\frac{e^4}{4} \beta \gamma \sin(2\theta) \operatorname{Re}(b),$$

$$R_{33} = \frac{e^4}{4\gamma^2} \left[ \left( 4\gamma^2 \operatorname{Re}(a) + \gamma^2 + 1 \right) \cos^2(\theta) + \beta^2 \gamma^2 \right],$$

$$R_{14} = -R_{41} = \frac{e^4}{4} \beta \gamma \sin(2\theta) \operatorname{Im}(b),$$

$$R_{24} = R_{42} = \frac{e^4}{4} \beta^2 \gamma \sin(2\theta) \operatorname{Im}(a),$$

$$R_{34} = -R_{43} = -\frac{e^4}{2} \beta \sin^2(\theta) \operatorname{Im}(b),$$

$$R_{44} = \frac{e^4}{4\gamma^2} \left[ 4\gamma^2 \operatorname{Re}(a) + \beta^2 \gamma^2 \cos^2(\theta) + \gamma^2 + 1 \right].$$
(1)

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#### Tests and example results

1) Check that formula/algorithm for spin effects can be used instead of the native KKMC one.

2) Same as -1) but for configurations when hard photons are requested to be present. Test of interpolation to bremsstrahlung configurations.

3) Both  $\tau^{\pm}$  decay to  $\pi^{\pm}\pi^{0}\nu$ . Test distribution: acoplanarity of the visible decay products oriented half- planes. All momenta in the visible decay products system rest frame.

$$y_1 = \frac{E_{\pi^-} - E_{\pi^0}}{E_{\pi^-} + E_{\pi^0}}, \qquad y_2 = \frac{E_{\pi^+} - E_{\pi^0}}{E_{\pi^+} + E_{\pi^0}}$$
(2)

4) Observable does not rely on decay vertex position.

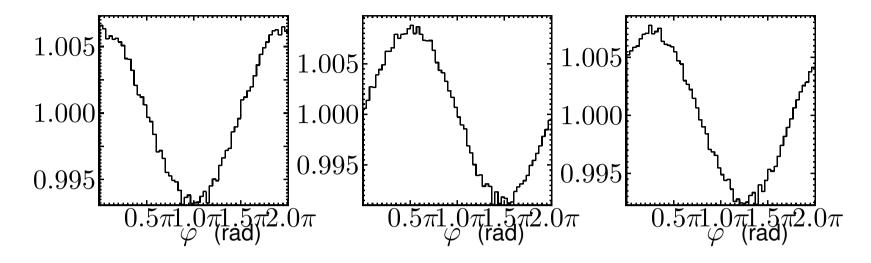


Figure 1: Distribution over acoplanarity angle  $\varphi$  of the ratio  $wt_{spin}^{anomalous}$  for  $\sqrt{s} = 10.5$  GeV. Constraint  $y_1y_2 > 0$  is imposed. Left:  $\operatorname{Re}(a_{NP}) = 0.04$  and other couplings are zero, Center:  $\operatorname{Re}(b_{NP}) = 0.04$  and other couplings are zero, Right:  $\operatorname{Re}(a_{NP}) = 0.04 \cos(\pi/4)$ ,  $\operatorname{Re}(b_{NP}) = 0.04 \sin(\pi/4)$  and other couplings are zero. This is idealized (test of the principle) observable. In practice Machine Learning approach, helpful to combine impact from all  $\tau$  decay channels will be more appropriate.

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#### (D) Event record, phase space extra particles injection 12

• PHOTOS (by E.Barberio, B. van Eijk, Z. W., P. Golonka) is used since 1989 to simulate the effects of radiative corrections in decays.

Full events of complicated mother-daughter tree structure of consecutive decays are generated earlier. PHOTOS eventually modify decay (tree branching).

- Web pages of TAUOLA, PHOTOS and MC-TESTER projects:
- Phase-space is again exact and parametrization under full control
- Matrix element: from factorization and with simplifications. Required lots of work.
- For lepton pair emission algorithm works similarly.
- It can be used not only for QED but for New Physics too. Dark photon, extra scalar/pseudo-scalar imprinting into final state. New Physics particles with consecutive decays to lepton pairs.

#### (D) Event record, phase space extra particles injection 13

Phase Space Formula of Photos

$$dLips_{n+1}(P \to k_1...k_n, k_{n+1}) = dLips_n^{+1 \ tangent} \times W_n^{n+1},$$

$$dLips_n^{+1\ tangent} = dk_{\gamma}d\cos\theta d\phi \times dLips_n(P \to \bar{k}_1...\bar{k}_n),$$
  
$$\{k_1, \dots, k_{n+1}\} = \mathbf{T}(k_{\gamma}, \theta, \phi, \{\bar{k}_1, \dots, \bar{k}_n\}).$$
 (3)

- 1. One can verify that if  $dLips_n(P)$  was exact, then this formula lead to exact parametrization of  $dLips_{n+1}(P)$
- 2. Practical implementation: Take the configurations from n-body phase space.
- 3. Turn it back into some coordinate variables.
- 4. construct new kinematical configuration from all variables.
- 5. Forget about temporary  $k_{\gamma} \theta \phi$ . From now on, only weight and four vectors count.
- A lot depend on T. Options depend on matrix element: must tangent at singularities. Simultaneous use of several T is possible and necessary/convenient if more than one charge is present in final state.

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#### (D) Event record, phase space extra particles injection 14

#### Phase Space: (main formula)

If we choose

$$G_n : M_{2...n}^2, \theta_1, \phi_1, M_{3...n}^2, \theta_2, \phi_2, \dots, \theta_{n-1}, \phi_{n-1} \to \bar{k}_1 \dots \bar{k}_n$$
 (4)

and

$$G_{n+1} : k_{\gamma}, \theta, \phi, M_{2...n}^2, \theta_1, \phi_1, M_{3...n}^2, \theta_2, \phi_2, \dots, \theta_{n-1}, \phi_{n-1} \to k_1 \dots k_n, k_{n+1}$$
(5)

then

$$\mathbf{T} = G_{n+1}(k_{\gamma}, \theta, \phi, G_n^{-1}(\bar{k}_1, \dots, \bar{k}_n)).$$
(6)

The ratio of the Jacobians form the phase space weight  $W_n^{n+1}$  for the transformation. Such solution is universal and valid for any choice of *G*'s. However,  $G_{n+1}$  and  $G_n$  has to match matrix element, otherwise algorithm will be inefficient (factor  $10^{10}$  ...).

In case of PHOTOS  $G_n$ 's

$$W_n^{n+1} = k_\gamma \frac{1}{2(2\pi)^3} \times \frac{\lambda^{1/2} (1, m_1^2 / M_{1...n}^2, M_{2...n}^2 / M_{1...n}^2)}{\lambda^{1/2} (1, m_1^2 / M^2, M_{2...n}^2 / M^2)},$$
(7)

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#### (D) Add extra particles

once phase-space adjusted, again  $M^{SM} \rightarrow M^{SM+NP}$  is enough.

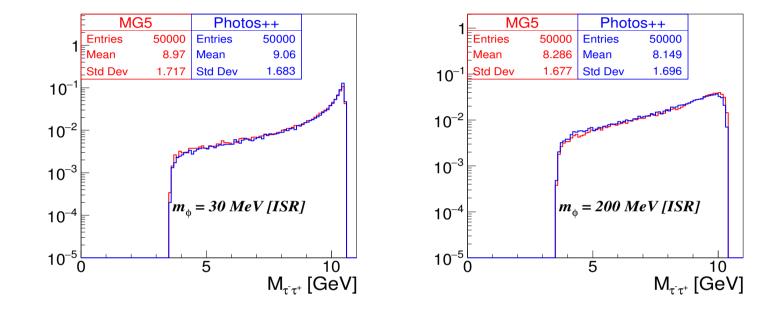


Figure 2: Belle 2 center of mass energies  $e^-e^+ \rightarrow \tau^-\tau^+\phi_{\text{Dark Scalar}}(\rightarrow e^-e^+)$  Case of dark scalar of 30 and 200 MeV. Simulation of KKMC+Photos is compared with the one based on MadGraph. Emission kernel was inspired from that comparison. At start, QED pair emission kernel was used. Spin correlations of  $\tau$ -s modified by rotation of  $\tau^-$  decay products.

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# (E) Outlook software side

- Motivation 2021 2022 requests from Belle 2 collaboration.
- Numerical results I have presented are for illustration.
- Small New Physics effects of large SM background
- Weights and correlated event samples: good for systematic and evaluation of ambiguities.
- Challenge: all to be ported to experiments software environment.
- Time consuming if new program or even new program versions are needed.
  - 1. For electric/magnetic dipole moment KKMC internal functions for boost from  $\tau$  rest-frame to lab frame and internal variables  $h^i_{\pm}$  were used. No need to libraries recompilation, event sample not modified at all.
  - 2. Forf dark photon emission, it was a bit more complicated. Events kinematic is then modified, but change could be introduced at fully constructed event and with the new program photospp. No need to change and test new version of the main code.
- It is important that some of the internal functions or data of main simulation program are not private but can be accessed by the user. Keep that in mind for C++ programs.

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### (E) Outlook: physics input

- Symmetries helped spin amplitudes separation into parts valid all over the phase space.
- Alternatively comparisons with MadGraph simulation was used.
- It forms input for Monte Carlo design. This aspect of the work was not covered in my talk.
- It is also helpful for New Physics imprinting into precision Monte Carlo programs.
- I concentrated on applications for Belle 2: cases of Anomalous Magnetic/Electric dipole moment and later dark scalar/pseudoscalar/photon imprinting into SM event sample.
- My strategy for work on spin amplitudes was as follows:
  - 1. Calculate spin amplitudes by hand, using algebraic manipulation program to check for misprints.
  - 2. Identify most singular (or most peculiar terms).
  - 3. Localize terms which combine them into symmetry invariant set.
  - 4. Continue work on remaining terms.
  - 5. Return to point 2, until nothing is left.

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# (E) Outlook: physics input

- The way how amplitudes are calculated was important.
- Kleiss-Stirling techniques, numerical stability. How to use amplitudes when energy-momentum conservation is corrupted by further photons.
- For New Physics instead of formal work, approximations obtained from educative guess and validated by comparison with MadGraph simulations only, were used.
- For dipole moments interpolation to Born kinematic was used.
- It is possible to extend presented applications for other processes and other experiments like LHC, FCC, ... applications.
- Implementation of New Physics processes into kinematic configurations with bremsstrahlung photons requires checks if (approximately) basic spin amplitudes structures remain, once New Physics effects are introduced.
- Statement *minor modification of the code* seem unimportant. But it is not. One has to introduce New Physics modification in such a way that interfaces to detector simulation and experimental validation remain valid.

# (E) Skipped but critically important aspects

- Symmetries help separation of spin amplitudes into parts....
- ... useful for fully differential and valid all over the phase space predictions.
- That is important for Monte Carlo and calculations of multidimensional distributions.
- separate dominant SM predictions of sub-theories like QED (eikonal QED), QCD.
- Those are parts which need to be taken to higher orders.
- Calculation of small higher order terms present in full SM may be then avoided.
- Similarities between amplitudes (often identical dominant parts) of distinct processes, useful. Nothing new. Basis of of YFS exponentiation, factorization theorems. Also fake supersymmetric-like relations can be seen.
- All this is useful for technicalities of Monte Carlo constructions.
- Disadvantage: pressure on automated methods and higher orders validity proofs.
- Anyway: at LEP separation was indispensable, at LHC too.
- What future will decide? Keep these methods in tool-box.
- Message: Do not drop the topic out. It bring sometimes pain, but fun too.

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# (E) On work strategies

- My strategy was as follows:
  - 1. Calculate spin amplitudes by hand, using algebraic manipulation program to check for misprints.
  - 2. Identify most singular (or most peculiar terms).
  - 3. Localize terms which combine them into symmetry invariant set.
  - 4. Continue work on remaining terms.
  - 5. Return to point 2, until nothing is left..
- Of course starting point, choice of the way how amplitudes are calculated is important.
- But more often than not, I could identify required pattern.
- In fact pattern was usually of more details than what was needed.
- This talk as invitation for common efforts?
- Thank you.

### (E) On work strategies

I was talking about new applications supporting usefulness of long living projects developed in Cracow like KKMC Tauola, photos, TauSpinner thanks to acumulated to experience they remain competitive for more than 3 decades now.

How to convice community of future users.

Attempt to get new people into projects development: challenge.

Work with new people fine for some time, but may be challenging for long term perspective like that of FCC.

Educated/trained people choose other careers; often outside physics, outside Poland/Europe.