

# Systematics in Flavour Physics Analyses (rare decays)

### Systematic Effects and Nuisance Parar BIRS, Banff, Canada, April 27, 2023 Slavomira Stefkova (KIT)

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## Flavour experiments in nutshell

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## **Collider Flavour Physics: Belle II and LHCb**

- Two active collider flavour physics experiments specialising in *B*-physics: LHCb and Belle II
- The **main differences** with respect to other ATLAS and CMS experiments:
  - Generally more sensitive to lower deposits: mass of *B*-meson ~ 5.2 GeV (*B*-hadron at LHCb)
  - The innermost detector has excellent vertex resolution close to IP 0



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## **B-decays measurements (and others)**

### • *B*-decay can be **abundant** or **rare**:

- Precision measurements of CP violation (rare and abundant)
- Indirect searches for NP in rare *B*-decays (rare)
- Indirect searches for NP in semileptonic *B*-decays (abundant)
- Spectroscopy of *B*-decays (abundant)

- Belle II and LHCb also well suited
  - for measurements of decays involving *c* and  $\tau$
  - for direct searches for NP, e.g DM, mediators connected to DM, leptoquarks, Z', .....

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## **B-decays measurements (and others)**

- *B*-decay can be **abundant** or **rare**: 0
  - Precision measurements of CP violation (rare and abundant)
  - Indirect searches for NP in rare *B*-decays (rare)
  - Indirect searches for NP in semileptonic *B*-decays (**abundant**)
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  - for direct searches for NP, e.g leptoquarks, Z', .....







### Direct



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 $\boldsymbol{s}$ 



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Heisenberg's uncertainty principle:  $\Delta E \Delta t >$ Mass of the particle can be very high  $W^+$  $\boldsymbol{s}$ b u, c, t







## What do we measure in rare *B*-decays?



### Theoretically cleaner



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**Parameter of interests:** 

#### 1. $\mathscr{B} \rightarrow 1$ parameter of interest

Signal strength of the process (1  $\mu$  = SM expectation) 2. Angular observables  $\rightarrow$  several parameters of interest: e.g: angular observables of  $B \rightarrow K^{*0}\mu^+\mu^- P_5'$ ,  $F_L$ ,  $A_{FB}$ 3. Ratios  $\rightarrow$  2 parameters of interests:

e.g: signal strengths of two processes  $R(K) = \frac{\mathscr{B}(B^+ \to K^+ \mu^+ \mu^-)}{\mathscr{B}(B^+ \to K^+ e^+ e^-)} = \frac{\varepsilon(B^+ \to K^+ e^+ e^-)}{\varepsilon(B^+ \to K^+ \mu^+ \mu^-)} \times \frac{N(B^+ \to K^+ \mu^+ \mu^-)}{N(B^+ \to K^+ e^+ e^-)}$ 

### How often does *B*-decay into the decay products? rare $\rightarrow \mathscr{B}(\text{process}) < 1 \times 10^{-5}$







## LHCb and Belle II: measurement style

For measuring *B* of rare *B*-decays **LHCb uses mostly relative** and **Belle II absolute approach**:

$$\overset{\circ}{\mathscr{B}}(B^{+} \to \mu^{+}\mu^{-}\mu^{+}\nu) = \mathscr{B}(B^{+} \to J/\psi(\to \mu^{+}\mu^{-})K^{+}) \times \frac{\varepsilon(B^{+} \to J/\psi(\to \mu^{+}\mu^{-})K^{+})}{\varepsilon(B^{+} \to \mu^{+}\mu^{-}\mu^{+}\nu)} \times \frac{N(B^{+} \to \mu^{+}\mu^{-}\mu^{-}\mu^{-})K^{+}}{N(B^{+} \to J/\psi(\to \mu^{+}\mu^{-})K^{+})} \times \frac{N(B^{+} \to \mu^{+}\mu^{-}\mu^{-})K^{+}}{N(B^{+} \to J/\psi(\to \mu^{+}\mu^{-})K^{+})} \times \frac{N(B^{+} \to \mu^{+}\mu^{-})K^{+}}{N(B^{+} \to J/\psi(\to \mu^{+})K^{+})} \times \frac{N(B^{+} \to \mu^{+}\mu^{-})K^{+}}{N(B^{+} \to K^{+})} \times \frac{N(B^{+} \to \mu^{+}\mu^{-})K^{+}}{N(B^{+} \to K^{+})} \times \frac{N(B^{+} \to \mu^{+})K^{+}}{N(B^{+} \to K^{+})} \times \frac{N(B^{+}$$

- - Relative measurements have advantage in cancelling uncertainties due to accelerator



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• Systematic uncertainties need to be derived on the efficiencies in Belle II or on relative efficiencies in LHCb:









# Model-building

**Model Description** 

**Encode systematic uncertainties** 

Parametrised functions: (Crystal Balls,

- exponential, Gauss, ...)
- Density Estimates (KDE)

ametrised  
stograms 
$$f(n, a \mid \eta, \chi) = \prod_{c \in \text{channels } b \in \text{bins}_c} Pois(n_{cb} \mid \nu_{cb}(\eta, \chi))$$
  
Simultaneous measurement  
of multiple channels for "auxiliary measurement









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# **Types of systematic uncertainties**

#### Accelerator





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#### **External Measurement**







 $+ \sigma_{tot}$  $+ \sigma_{par}$ 

 $\mu = 4128 \pm 150$  $\sigma = 566 \pm 62$ 

## How do we get systematic variations?

#### → Systematic uncertainties can affect shape, normalisation or both

What samples do we use?

- 1. Alternative models (simulation)
- Calibration samples (mixture of simulation and data) 2.
- 3. Signal embedding samples (mixture of simulation and data)
- 4. (Orthogonal) data samples (data)

What methods do we use? [<u>T.Blake (Phystat 2021)</u>]:

- Generate a large number of pseudo-experiments from a varied model and 0 determine observables using the nominal model...(bootstrap method)
- Repeat the determination of the observables in data using a different set of assumptions...(alternative method)





**Practical examples of systematics\*** \*mixture of good, bad and ugly









## Systematic uncertainties: Accelerator

Accelerator	$\mathscr{B}(B^+ \to K^+ \nu \bar{\nu})$ <b>(Belle II)</b>
Delivered Luminosity	Integrated Luminosity (Calibration)
<b>B-dataset</b>	Number of <i>BB</i> (Calibration)

#### $\mathscr{B}(B^+ \to K^+ \nu \bar{\nu}) = 5 \times 10^{-6}$ [Phys. Rev. Lett. 127, 181802 (2021)]

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$$\mathscr{B}(B^+ \to \mu^+ \mu^- \mu^+ \nu) = 1 \times 10^{-9}$$
  
[Eur. Phys. J. C 79 (2019) 675]







## Systematic uncertainties: Detector

Detector	$\mathscr{B}(B^+ \to K^+ \nu \bar{\nu})$ <b>(Belle II)</b>	$\mathscr{B}(B^+ \to \mu^+ \mu^- \mu^+ \nu)$ (LHCb)
Tracking of charged particles	Tracking efficiency (Calibration)	Tracking efficiency (Calibration)
Measurement of energy deposit (photons)	Uncertainty on the absolute energy for photons (Calibration)	100- Event: 6
Measurement of energy deposit (others)	Uncertainty on the absolute energy for other clusters (Calibration)	50-
Particle Identification	Uncertainty on the PID corrections (Calibration)	
		-100-
		-100 -50 0 50 100 x (cm)

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Theory	$\mathscr{B}(B^+ \to K^+ \nu \bar{\nu})$ (Belle II)	$\mathscr{B}(B^+ \to \mu^+ \mu^- \mu^+ \nu)$ (LHCb)
Signal shape	Form Factor Uncertainty (theory model)	
Signal model		Signal Model (Alternative simulation model)







## Systematic uncertainties: Simulation

Simulation	$\mathscr{B}(B^+ \to K^+ \nu \bar{\nu})$ (Belle II)	$\mathscr{B}(B^+ \to \mu^+ \mu^- \mu^+ \nu)$ (LHCb)
<b>B-production kinematics</b>		Kinematic reweighting (Calibration)
Uncertainty on background BF	Uncertainty on the BF of leading <i>B</i> -background (alternative models)	
Background normalisation	Continuum background (Orthogonal data sample)	
Missing background template		Modelling of $B^+ \rightarrow (D \rightarrow (\eta \rightarrow \mu \mu) \mu \nu)$ (alternative fitting model)



## **Systematic uncertainties: Further Analysis**

Further Analysis	$\mathscr{B}(B^+ \to K^+ \nu \bar{\nu})$ (Belle II)	$\mathscr{B}(B^+ \to \mu^+ \mu^- \mu^+ \nu)$ (LHCb)
Background shape		Background shape modelling (Alternative fitting model)
Fitting bias		Fitting bias (Alternative simulation models)







## Methods: capturing correlations, assessing data-model compatibility

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## Few words about correlations...

Search for  $B^+ \to K^+ \nu \bar{\nu}$  decays: binned fit



## **Correlated systematics (I)** Bootstrap

Method explained in [S.Glazov (Phystat 2021)]

- PID (statistical error= $\sigma$ ): Ο
  - Non-trivial correlations PID corrections computed in bins of  $(p_T, \theta)$ 0

  - Construct covariance matrix 0

$$\mathscr{B}(B^+ \to K^+ \nu \bar{\nu})$$

Full covariance



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• Produce alternative simulations with bootstrap method: central values varied with lognormal  $(0, \sigma)$ 

• Translation to nuisance parameters: SVD decomposition + leading eigenvectors as the nuisances









### **Correlated systematics (II) MVA-Gaussian**

Data-driven estimate of a particular background:

- Using multivariate gaussian constraints to input or preserve the correlation of this systematics



• Fit to "sideband" data and then propagate the result of the fit together with the correlation to the main fit









# **Data-model compatibility**

Using toy-based method:

0

- The toys are generated using observed data counts based on Poisson statistics 0
- In order to avoid double counting of the fluctuations, the observed counts are subtracted from each 0 toy and the expectation is added instead
- 0



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This way the toys are centered around the Asimov dataset which by construction has no fluctuations









# **Statistical modelling challenges in rare** decays

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# **Rare-decay searches/measurements**

#### The main goal is to suppress the background as much as possible

Low-statistics samples  $\rightarrow$  trade-off between smoothness and fit stability 0

#### **Control samples are not always so easy to get by!**

- 0
- 0

#### Rare signal decays can have as background decays that are also rare:

- 0
- 0 strength to be unconstrained if you know it exists?

#### Calibration samples may not be necessarily very large

Some of the analyses of rare decays are MC statistical error becomes prominent 0

Sometimes it is quite challenging to find a control sample (this is especially true for LHCb) Inflates the nuisances (if it does not make the nuisance parameters basically unconstrained)

Signal rare decays may have backgrounds that have never been measured and are not modelled Incorporating such decays in your model is always very challenging? Is signal "background"



## Conclusion

#### In this presentation I have summarised the

- Statistical modelling of rare B-decay searches/measurements
- Shown examples of systematic uncertainties that are treated as nuisances 0
- Show examples of how correlated systematic are computed and propagated into the model 0
- Highlighted few problems with statistical modelling and propagation of nuisances relevant for rare decay searches

## Thank you!















#### Another pitfall of very low statistics samples:

- If signal resolution very narrow (near delta like), dance of fitting to single events
- Asymptotic approximation may not hold



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## Aside: DM searches







# HistFactory Template



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# HistFactory Template

Modifiers and Constraints

Description	Modification	Constraint Term $c_\chi$	Input	Factor	"Data"
Uncorrelated Shape	$\kappa_{scb}(\gamma_b)=\gamma_b$	$\prod_{b} \operatorname{Pois} \left( r_{b} = \sigma_{b}^{-2} \big    ho_{b} = \sigma_{b}^{-2} \gamma_{b}  ight)$	$\sigma_b$	<b>Bin-wise</b>	Per-bin
Correlated Shape	$\Delta_{scb}(lpha)=f_{p}\left(lphaert\Delta_{scb,lpha=-1},\Delta_{scb,lpha=1} ight)$	$\mathrm{Gaus}(a=0 \alpha,\sigma=1)$	$\Delta_{scb,lpha=\pm 1}$	Global	Per-bin
Normalisation Unc.	$\kappa_{scb}(lpha)=g_{p}\left(lphaert \kappa_{scb,lpha=-1},\kappa_{scb,lpha=1} ight)$	$\mathrm{Gaus}(a=0 \alpha,\sigma=1)$	$\kappa_{scb,lpha=\pm 1}$	Global	Per-sample
MC Stat. Uncertainty	$\kappa_{scb}(\gamma_b)=\gamma_b$	$\prod_b \mathrm{Gaus}\left(a_{\gamma_b}=1 \gamma_b,\delta_b ight)$	$\delta_b^2 = \sum_s \delta_{sb}^2$	<b>Bin-wise</b>	Per-bin
Luminosity	$\kappa_{scb}(\lambda)=\lambda$	$\mathrm{Gaus}(l=\lambda_0 \lambda,\sigma_\lambda)$	$\lambda_0, \sigma_\lambda$	Global	Nothing
Normalisation	$\kappa_{scb}(\mu_b)=\mu_b$			Global	Nothing
Data-driven Shape	$\kappa_{scb}(\gamma_b)=\gamma_b$			<b>Bin-wise</b>	Nothing

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- Correlated Shape: same source of uncertainty wh (e.g PID, tracking inefficiency, ...)
- MC Stat. uncertainty: uncertainty due to the finite sample size of the datasets
- Luminosity especially useful if cross-section is to be measured

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• Correlated Shape: same source of uncertainty which has a different effect on the various sample shapes

e sample size of the datasets be measured



Reconstruction	B+ -> K+ nu \bar{nu} (Belle II)	B+ ->mu+ mu- mu+ nu (LHCb)	
		Trigger efficiency	
	Tracking efficiency	Tracking effciency	

## Systematic Uncertainties



Further Analysis	B+ -> K+ nu \bar{nu} (Belle II)	B+ ->mu+ mu- mu+ nu (LHCb)	
		Trigger efficiency	
	Tracking efficiency	Tracking effciency	

## Systematic Uncertainties



# When do we integrate systematics?

• When we know something in our analysis chain is maybe incorrect impacting on the measurement: 1. Wrong  $\rightarrow$  we apply corrections (known as calibrations)

- 2. Uncertain  $\rightarrow$  we do cross-checks:
  - 1. If passed with no major impact on the measurement  $\rightarrow$  no action
  - 2. If major impact on the measurement  $\rightarrow$  analysis is not robust
  - 3. If minor impact → **systematics and nuisance parameters**















# **SuperKEKB**

SuperKEKB operates nominally at  $\sqrt{s} = 10.58$  GeV

- $\Upsilon(4S) \rightarrow B\bar{B}$  in 96 %
- Currently 363 fb<sup>-1</sup> ~ 390 mil. *B*-meson pairs
  ~1/2 Belle, ~ BaBar
- Record-breaking  $\mathscr{L}_{inst} = 4.7 \times 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$



Slavomira Stefkova, 23.03.2023, Dresden



- Now in long shutdown (LS1) until this autumn
- Final aim: operate at  $30 \times \text{higher } \mathscr{L}_{\text{inst}}$  than KEKB at a cost of  $\mathcal{O}(10) \times \text{higher}$  backgrounds
- Final luminosity goal:  $\mathscr{L}_{int} = 50 \text{ ab}^{-1}$







### Four types of backgrounds at *e*<sup>+</sup>*e*<sup>-</sup> colliders:

• Continuum Backgrounds  $e^+e^- \rightarrow q\bar{q}$ , where

$$q \in (s, c, d, u)$$
 and  $e^+e^- \rightarrow \tau \overline{\tau}$ 

- *B*-backgrounds
  - misidentified
  - mis-reconstructed
  - combinatorial

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## Backgrounds at *e*<sup>+</sup>*e*<sup>-</sup> Collider

#### Continuum backgrounds







### Four types of backgrounds at $e^+e^-$ colliders:

• Continuum Backgrounds  $e^+e^- \rightarrow q\bar{q}$ , where

$$q \in (s, c, d, u)$$
 and  $e^+e^- \rightarrow \tau \overline{\tau}$ 

- *B*-backgrounds
  - misidentified
  - mis-reconstructed
  - combinatorial
- Beam-backgrounds: 0

 $\mathscr{L}_{inst}$ 

with

crease

- Touschek scattering, Coulomb scattering, synchrotron radiation, injection background, ...
- Luminosity Backgrounds:

 $\circ e^+e^- \rightarrow e^+e^-\gamma\gamma \rightarrow e^+e^-e^+e^-$ 

## Backgrounds at e<sup>+</sup>e<sup>-</sup> Collider

#### Continuum backgrounds



## **Belle II Detector**





## **Belle II Detector**



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### **New PXD** arrived safely to KEK!

B

**Belle II Deutschland** @belle2germany · Mar 18

Auch Detektoren haben weite Wege hinter sich! Unser neuer Pixeldetektor PXD2 hat sich am Mittwoch morgen auf den Weg vom @desy in Hamburg nach Japan gemacht. Damit nichts kaputt geht, bekam der empfindliche Detektor einen eigenen Sitzplatz. Mehr dazu: belle2.de/detail/belle-i...

K<sub>L</sub> and muon detector (KLM) **Muon ID efficiency ~ 90 %** 

**Charged PID detectors (TOP + ARICH) Pion mis-ID efficiency ~ 5** % Kaon ID-efficiency ~ 90 %









### Belle II is best-suited to measure *B*-decays with significant missing energy



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## $B \rightarrow K^{(*)} \nu \bar{\nu} Event in Belle II$



Typical  $B \rightarrow K^{(*)} \nu \bar{\nu}$  event benefits from

- Detector with nearly full  $4\pi$  coverage with excellent sensitivity to low deposits
- Cleaner environment compared to LHCb
- Constraints from well-known initial state kinematics





### Belle II is best-suited to measure *B*-decays with significant missing energy



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# $B \rightarrow K^{(*)} \nu \bar{\nu} \bar{\nu} Event in Belle II$



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Typical  $B \to K^{(*)} \nu \bar{\nu}$  event benefits from

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- Cleaner environment compared to LHCb
- Constraints from well-known initial state kinematics

#### **Challenges of rare** *B***-decays**

• High reconstruction efficiency for visible particles • Excellent MC modelling 

**Challenges of channels with neutrinos** • Excellent understanding of the neutral objects  $(\pi^0, K_L^0, K_S^0, n, \gamma, ...)$ 









• Quarks, leptons and interactions within the SM are the main protagonists of flavour physics

- *B*-decays are especially good probes since
  - *B*-hadrons are light enough to be produced abundantly and heavy enough to have many decays
  - Predictions for SM observables are well-known
- With *B*-decays we perform
  - Precision measurements of CP violation

• (In-)direct searches for NP in rare decays

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# Beam-backgrounds

Single-beam backgrounds:

- $\triangleright$  Touschek scattering  $\rightarrow$  scattering of particles within a bunch  $\rightarrow$ Touschek rate  $\propto N_{particles} \times \rho \rightarrow I \times \frac{1}{\sigma_{v} n_{b}}$
- **beam-gas scattering**  $\rightarrow$  Coulomb scattering and Bremsstrahlung (scattering off gas molecules)  $\rightarrow$  **Beam-gas rate**  $\propto N_{gas molecules} \times$  $N_{\text{particles}} \rightarrow \mathbf{P} \times \mathbf{I} \times \mathbf{Z}_{\text{eff}}^2$
- $\triangleright$  synchrotron radiation background  $\rightarrow$  consequence of a radial acceleration of the beam's particles achieved in bending magnets and quadrupoles
- $\triangleright$  injection background  $\rightarrow$  continuous injection of charge into beam bunch modifying the beam bunch

Luminosity backgrounds:

backgrounds above cannot be reduced!

**DESY.** 

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Single-beam backgrounds can be mitigated with beam-steering, collimators, and vacuum-scrubbing

▷ two-photon background → leading luminosity background ( $e^+e^- \rightarrow e^+e^-\gamma\gamma \rightarrow e^+e^-e^+e^-$ ), unlike any of the



## Belle II vs LHCb

#### LHCb

#### single-arm detector longitudinal momentum of B not known









# SuperKEKB vs KEKB



	KEKB		SuperKEKB (Juni 2022)		SuperKEKB	
	LER	HER	LER	HER	LER	ł
Energie [GeV]	3.5	8	4	7	4	
#Bunches	1584		2249		1800	
β⁺ <sub>x</sub> /β⁺ <sub>y</sub> [mm]	1200/5.9	1200/5.9	80/1.0	60/1.0	32/0.27	25
I [A]	1.64	1.19	1.46	1.15	2.8	
Luminosität [10 <sup>34</sup> cm <sup>-2</sup> s <sup>-1</sup> ]	2.1		4.65 (Rekord!)		60	
Int. Luminosität [ab <sup>-1</sup> ]	1		0.43		50	











## Statistical model

#### Set-up binned fit using HistFactory statistical model

- - Signal and background templates from MC
  - Separate templates for all backgrounds: mixed *B*, charged *B*,  $c\bar{c}$ ,  $u\bar{u}$ ,  $s\bar{s}$ ,  $d\bar{d}$ ,  $\tau^{-}\tau^{+}$ 0
  - All systematics included via nuisance parameters:
    - background normalisation uncertainty 0
    - tracking inefficiency 0
    - neutral energy mis-calibration for photons 0
    - neutral energy mis-calibration for unmatched photons 0
    - uncertainty on PID correction due to limited statistics 0
    - uncertainty on branching fractions of leading background processes 0
    - uncertainty on SM form factor 0
  - **Total number of fit parameters:** 0
    - 175 nuisance parameters  $\phi$
    - 1 parameter of interest (signal strength= $\mu$ )
    - $1 \mu = SM \mathscr{B}(B^+ \to K^+ \nu \bar{\nu}) = (4.6 \pm 0.5) \times 10^{-6}$

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[PRL 127, 181802 (2021)]

• Likelihood based on <u>HistFactory</u> formalism implemented with <u>pyhf</u> + cross-check with sghf: simplified Gaussian model





• Systematic uncertainties (normalisations of Systematic Effects and Nuisance Parameters in Particle Physics Data Analy bkg S yields, BR of the leading B-decays, **49** 









## Fit validation

Entries

#### **Perform Fit Bias Check**

- Used because of high  $\mathscr{B}$  and clean signature
- Generate toys with signal strength  $\mu = 1, 5, 20$ 0 and check pulls =  $\frac{\mu_{fit} - \mu_{inj}}{\mu_{fit}}$
- Results: o bias, expected  $\mu$  recovered, very good agreement between pyhf and sghf



[PRL 127, 181802 (2021)]



#### **Check Data-Model Compatibility**

- Generate toys and check fit quality
- Results: *p*-value shows good data model compatibility for both pyhf and sghf









## What we learnt from fit? [PRL 127, 181802 (2021)]

1.  $c\bar{c}$ ,  $s\bar{s}$  continuum backgrounds are pulled up by 40%

- Inclusive tag approach shows the best performance 2.
  - 1. 3.5 better than HAD tag
  - 2. 20% better than SL Belle tag
  - 3. 10% better than HAD and SL tag
- BSM  $B^+ \rightarrow K^+ \nu \bar{\nu}$  already with 1 ab<sup>-1</sup> 3.



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## **Re-(interpretations)**

### Partial reinterpretation can be done as Belle II publishes $\epsilon_{sig}$ as a function of $q^2$ :

- Reminder: default signal model  $\rightarrow$  PHSP model with SM form factor reweighting [arXiv:1409.4557]
- At low  $q^2$  maximum signal efficiency of 13%
- No sensitivity for  $q^2 > 16 \text{ GeV}^2/c^2$
- All public plots at **HEPData**

#### For full re-(interpretation):

• Provide full likelihood



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