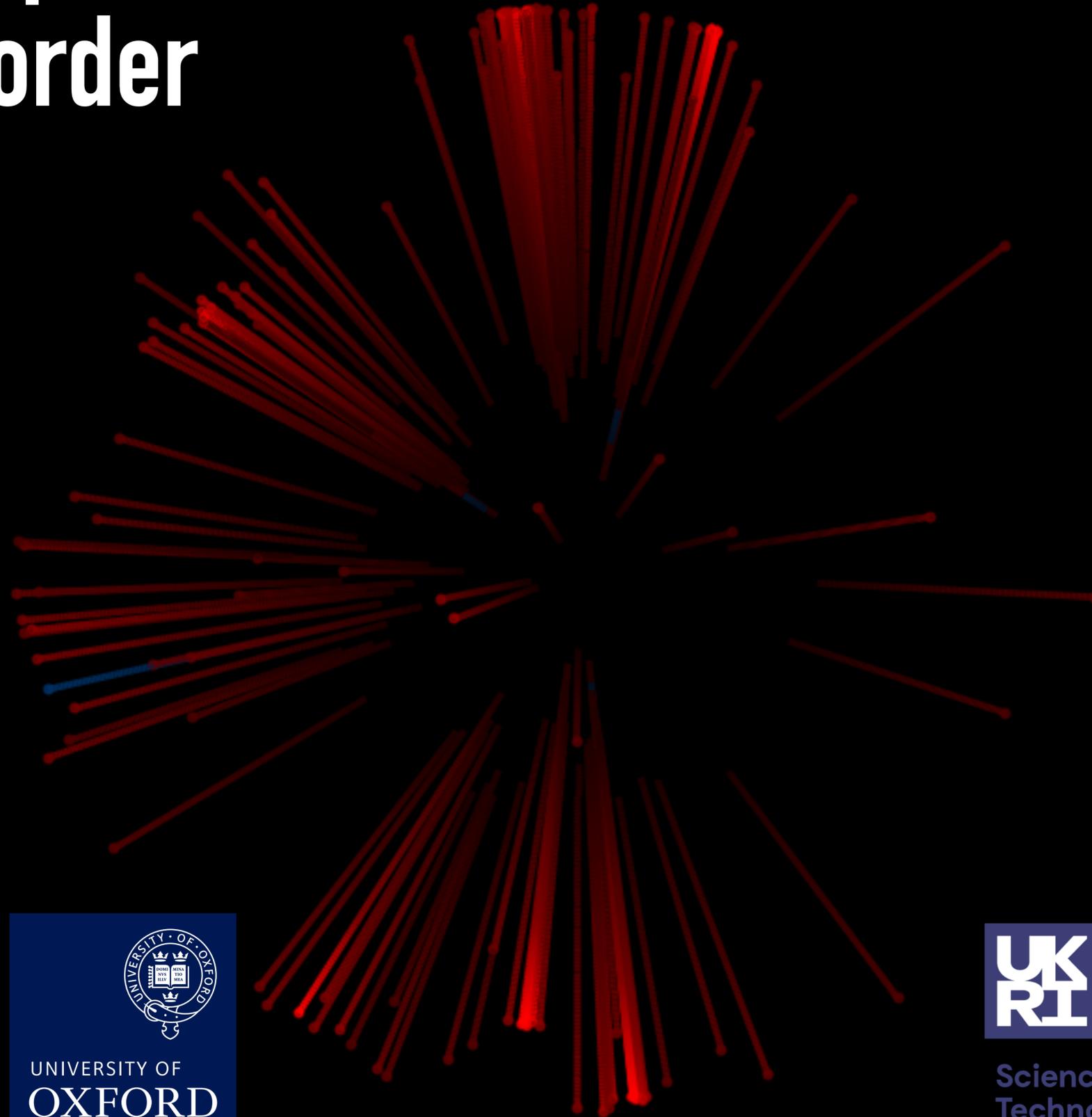
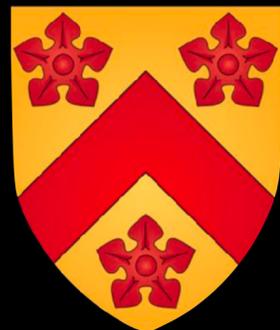


# Positivity in QCD predictions beyond leading order

What is particle Physics?  
KITP, UC Santa Barbara  
March 26, 2025



**Gavin Salam**  
Rudolf Peierls Centre for  
Theoretical Physics  
& All Souls College, Oxford



Science and  
Technology  
Facilities Council





**Melissa van Beekveld**  
NIKEHF



**Mrinal Dasgupta**  
Manchester



**Basem El-Menoufi**  
Monash



**Silvia Ferrario Ravasio**  
CERN



**Keith Hamilton**  
Univ. Coll. London



**Jack Helliwell**  
Monash



**Alexander Karlberg**  
CERN



**Pier Monni**  
CERN



**GPS**  
Oxford



**Nicolas Schalch**  
Oxford



**Ludovic Scyboz**  
Monash



**Alba Soto-Ontoso**  
Granada



**Grégory Soyez**  
IPhT, Saclay



**Silvia Zanoli**  
Oxford

# PanScales

A project to bring logarithmic understanding and accuracy to parton showers



ERC funded  
2018-2024



Frédéric Drever



Rob Verheyen



Rok Medves



Emma Slade

former members

# Logarithmically-accurate and positive-definite NLO shower matching

arXiv:2504.nnnnn



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NIKEHF



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CERN



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# Logarithmically-accurate and **positive-definite NLO** shower matching

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# Why not just plain (N)NLO?

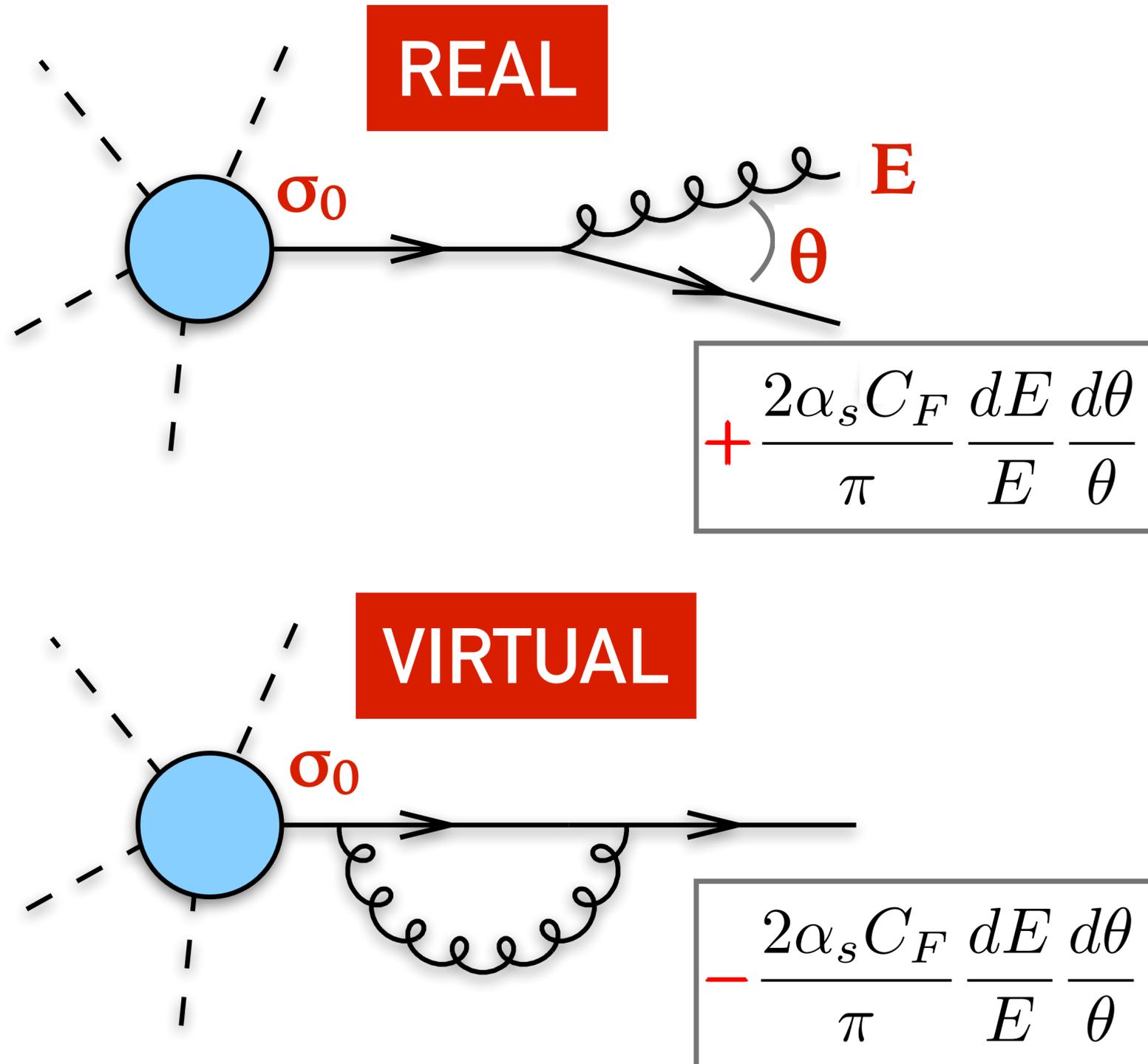
---

incredibly powerful, get scattering cross-sections from first few orders of perturbative expansion in the strong coupling  $\alpha_s$

$$\sigma = \sigma_0 + \alpha_s \sigma_1 + \alpha_s^2 \sigma_2 + \dots$$

LO      NLO      NNLO

# What kind of contributions do we get at NLO?



Divergences are present in both real and virtual diagrams.

They arise when an emission has a small energy ( $E \ll 1$ ) or a small angle ( $\theta \ll 1$ ).

In dim-reg, this brings  $1/\epsilon^2$  for each order in  $\alpha_s$ .

# What a NLO calculation gives you (here, Event2, $e^+e^- \rightarrow q\bar{q}$ )

---

## LO (2-particle) tree-level event

with weight 1.00000

px, py, pz, E = -1.32 -1.38 -49.96 50.00

px, py, pz, E = 1.32 1.38 49.96 50.00

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LO event ( $q\bar{q}$ )

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with weight 1.00000  
px, py, pz, E = -1.32 -1.38 -49.96 50.00  
px, py, pz, E = 1.32 1.38 49.96 50.00

## NLO (3-particle) tree-level event

with **weight 893.22103**, multiplying (alphas/2pi)  
px, py, pz, E = -1.60 -1.75 -49.87 49.93  
px, py, pz, E = 1.31 1.36 49.25 49.29  
px, py, pz, E = 0.30 0.39 0.62 0.79

LO event ( $q\bar{q}$ )

NLO event, with real emission  
~ LO event + extra soft gluon  
and **large positive weight**

# What a NLO calculation gives you (here, Event2, $e^+e^- \rightarrow q\bar{q}$ )

## LO (2-particle) tree-level event

with weight 1.00000  
px, py, pz, E = -1.32 -1.38 -49.96 50.00  
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px, py, pz, E = 1.31 1.36 49.25 49.29  
px, py, pz, E = 0.30 0.39 0.62 0.79

## NLO (2-particle) virtual subtraction event

with **weight -84.49299**, multiplying (alphas/2pi)  
px, py, pz, E = -1.32 -1.38 -49.96 50.00  
px, py, pz, E = 1.32 1.38 49.96 50.00

## NLO (2-particle) virtual subtraction event

with **weight -808.58646**, multiplying (alphas/2pi)  
px, py, pz, E = -1.61 -1.75 -49.94 50.00  
px, py, pz, E = 1.61 1.75 49.94 50.00

## NLO (2-particle) virtual finite event

with weight 2.66667, multiplying (alphas/2pi)  
px, py, pz, E = -1.32 -1.38 -49.96 50.00  
px, py, pz, E = 1.32 1.38 49.96 50.00

LO event ( $q\bar{q}$ )

NLO event, with real emission  
~ LO event + extra soft gluon  
and **large positive weight**

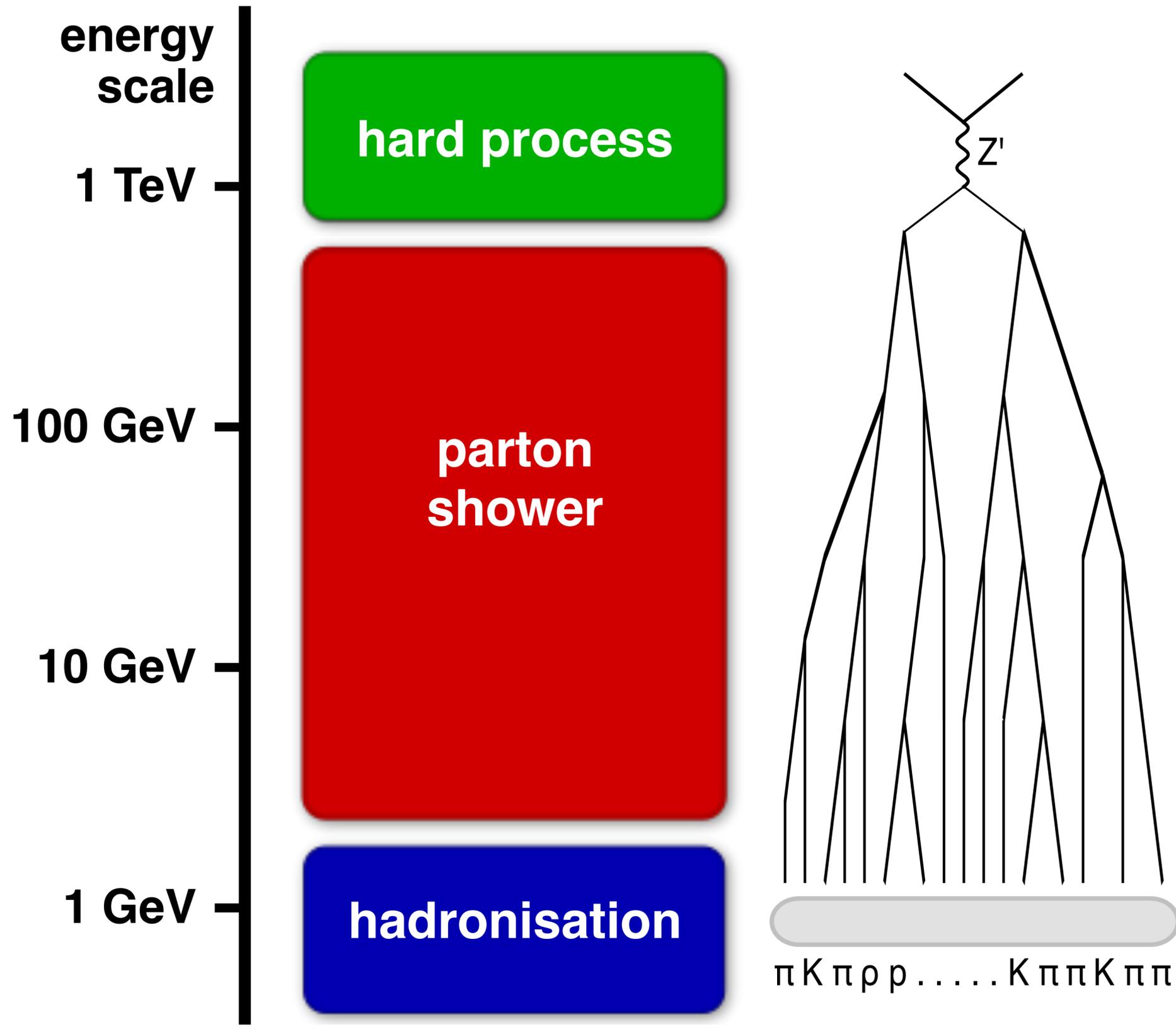
NLO event, “virtual” correction  
~ LO event  
and **large negative weight**

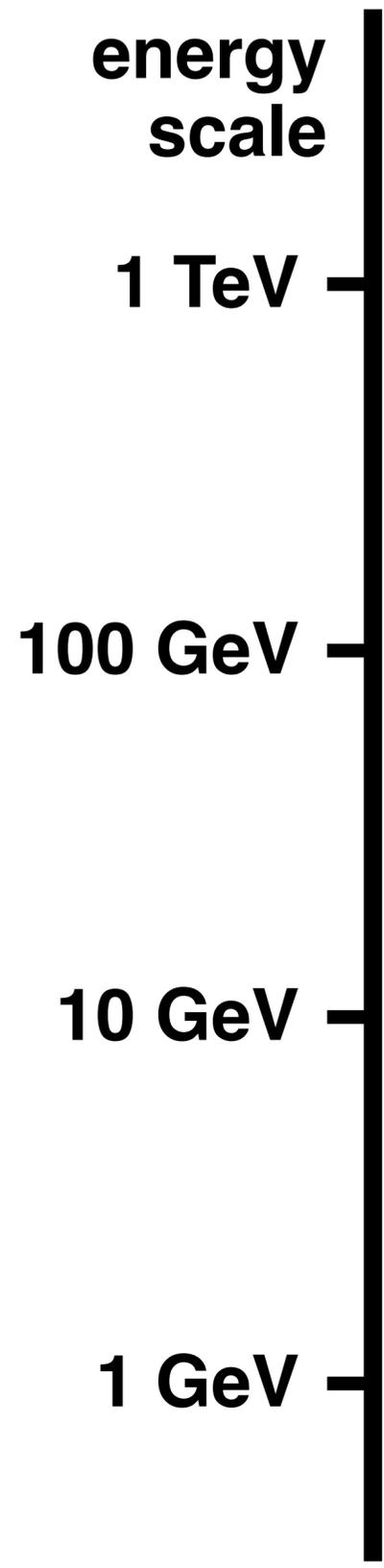
# event weights are $\sim$ probabilities

---

- real life doesn't have negative probabilities
- real life doesn't have (near-)divergent probabilities
- you can evade these problems in perturbation theory if you ask very limited kinds of questions, i.e. nearly always summing real & virtual divergences (infrared safe observable, single momentum scale)\*
- but experiments don't limit themselves to those kinds of questions

\* though there can still be nasty surprises, cf. Chen et al [2102.07607](#), GPS & Slade [2106.08329](#)

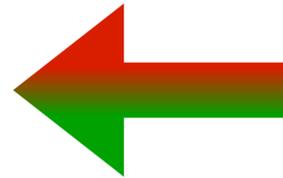
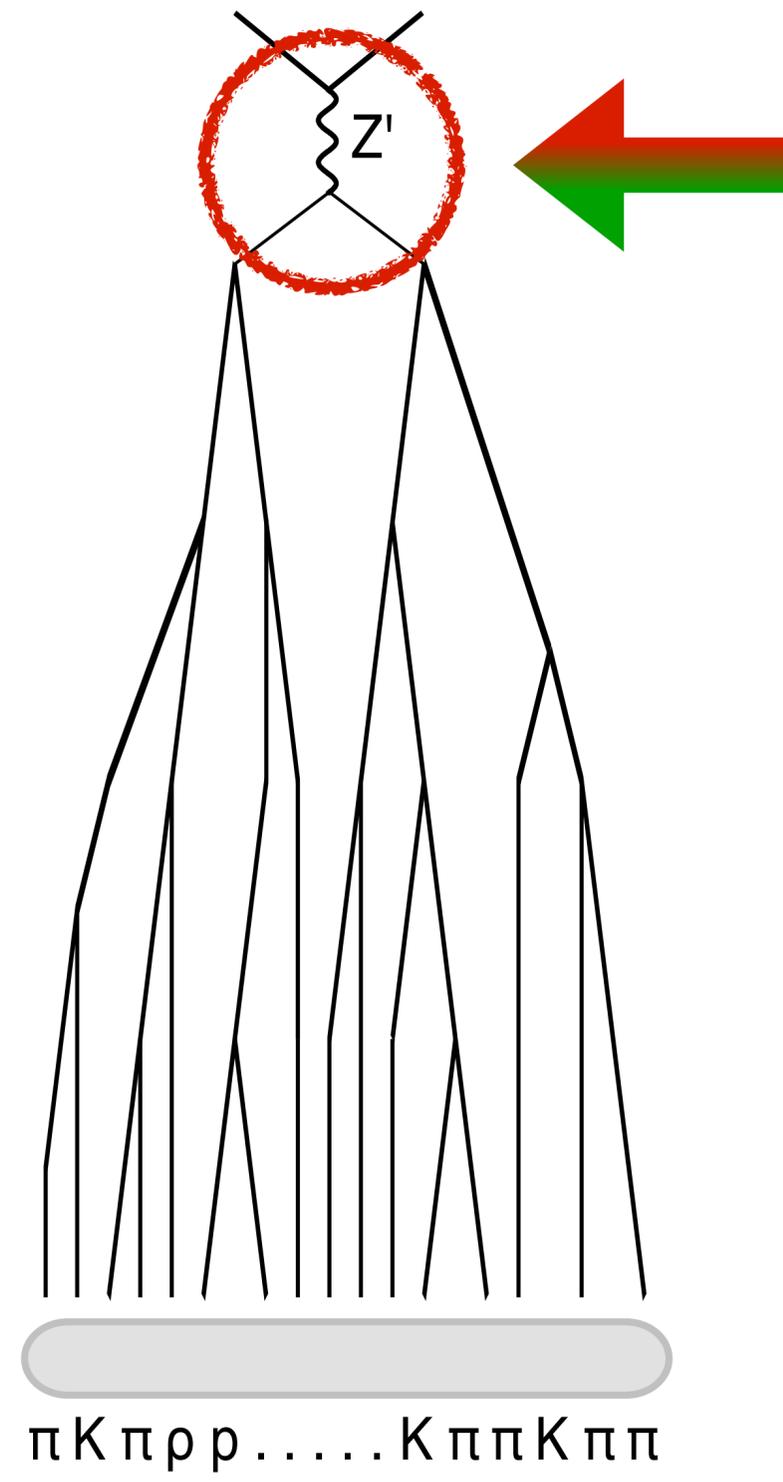




**hard process**

**parton shower**

**hadronisation**



Key innovation of 2002-'04:  
 correct or replace  
 first step so that perturbative  
 expansion of hard process +  
 parton-shower is equivalent to the  
 true NLO.

Frixione & Webber: **MC@NLO**  
[hep-ph/0204244](https://arxiv.org/abs/hep-ph/0204244)

Nason: **POWHEG**  
[hep-ph/0409146](https://arxiv.org/abs/hep-ph/0409146)

[>7500 citations; these methods  
 used also in Sherpa, Herwig]

# Key features of MC@NLO and POWHEG events

---

- MC@NLO and POWHEG methods, supplemented with parton showers + hadronisation models, provide NLO-accurate realistic hadron-level events
- they avoid the problem of (near) divergent event weights
- instead the event weights are just  $\pm 1$

This is a big advantage over “pure” NLO

But the event sample doesn't quite look like a true physical event sample, because there are still some negative weights

# Are negative weights a problem?

---

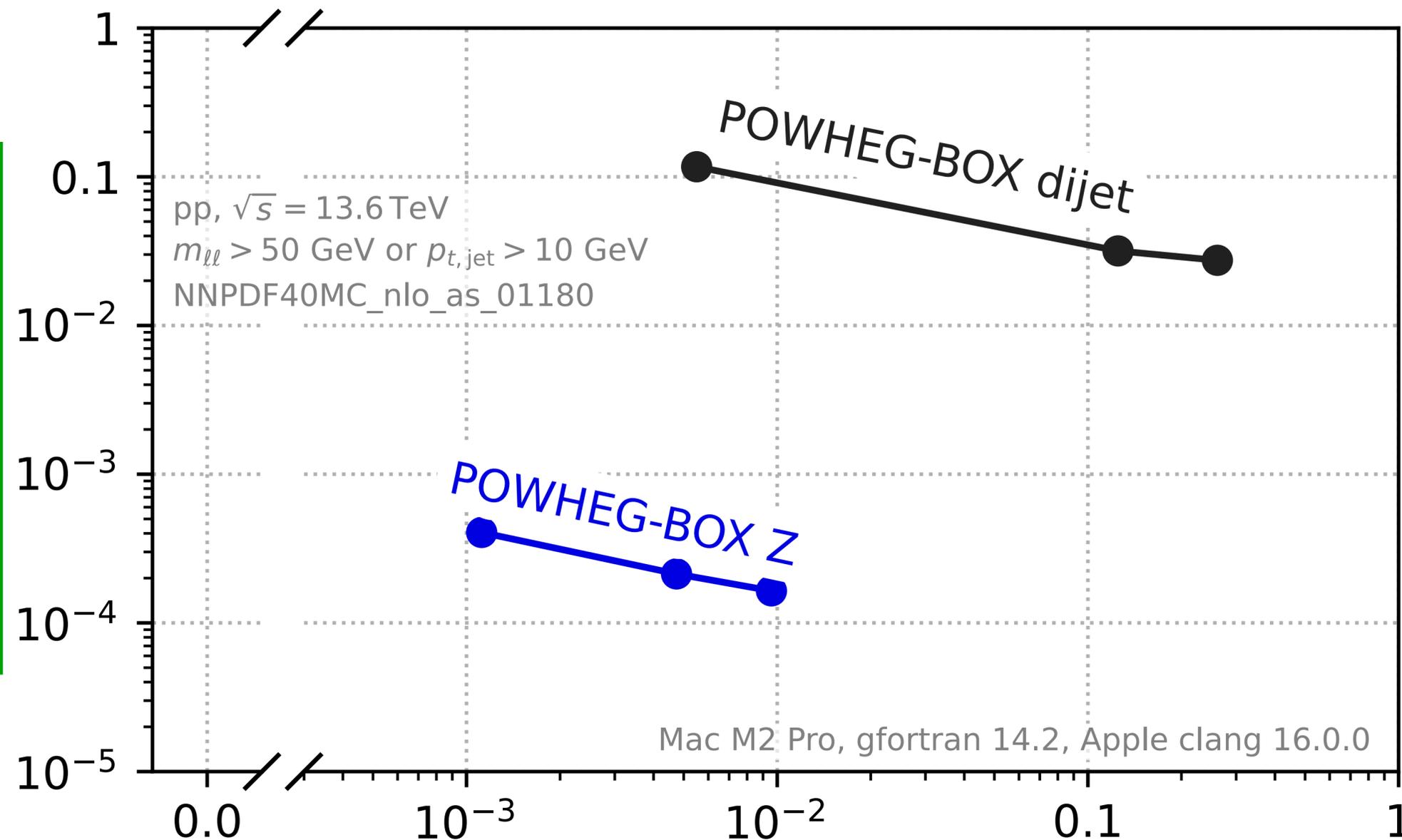
Given fraction  $f$  of negative-weight events, to reach the same statistical error as for  $N$  unit positive-weight events, you need to generate a larger number of events,

$$\frac{N}{(1 - 2f)^2}$$

E.g. for  $f = 15\%$  this doubles the required number of events.

# NLO state of the art [POWHEG]

NLO ev. gen. time vs. negative-weight fraction



time  
per  
event  
(s)

fraction of negative-weight events

More complex processes tend to have higher fractions of negative weights. Mitigation options (e.g. folding, [Nason 0709.2085](#)) often trade off negative weight fraction v. generation time.

Problem usually worse for NNLO event generation

# NLO state of the art [MG5\_aMC — MC@NLO method]

	step-0 (s) (grid setup)	step-1 (s) (integration)	step-2 (s) (generation)	negative S weights
<b><math>pp \rightarrow e^+ e^-</math></b>				
default	1	14	147	7.1%
$2 \times 2 \times 1$ folding	1	33	258	2.1%
$4 \times 4 \times 1$ folding	1	114	781	1.8%
<b>Born spreading</b>	<b>113</b>	<b>30</b>	<b>189</b>	<b>2.0%</b>
<b><math>pp \rightarrow W^+ j</math></b>				
default	10	604	2013	24.2%
$2 \times 2 \times 1$ folding	10	1265	5160	13.2%
$4 \times 4 \times 1$ folding	7	2803	16020	9.0%
<b>Born spreading</b>	<b>355</b>	<b>645</b>	<b>2226</b>	<b>18.8%</b>

*Frederix & Torrielli*  
2310.04160

*wall times for 1  
million events  
on a 12-core i7-8700K  
@ 3.7 GHz desktop  
machine*

# Some LHC experiments' statements on negative weights and machine learning

---

- ATLAS [2211.01136](#): “To avoid the use of negative weights present in the nominal NLO sample in the training of the multivariate discriminant used to separate SM  $t\bar{t}t\bar{t}$  events from background [...], **a sample was produced with similar generator settings, but at LO.**”
- CMS [2411.03023](#): “However, the binary cross-entropy given by Eq. (2), can become negatively unbounded for negative event weights, **making the classification task potentially impossible**”
- ATLAS [2412.15123](#): “Since XGBoost [ML framework] cannot handle negative-weight events, **the absolute value of each event weight is used.**”

# other work trying to reduce negative weight fractions (+ further refs below)

---

K. Danziger, S. Höche and F. Siegert, *Reducing negative weights in Monte Carlo event generation with Sherpa*, [2110.15211](#).

J. R. Andersen and A. Maier, *Unbiased elimination of negative weights in Monte Carlo samples*, *Eur. Phys. J. C* **82** (2022) 433, [[2109.07851](#)].

J. R. Andersen, A. Maier and D. Maître, *Efficient negative-weight elimination in large high-multiplicity Monte Carlo event samples*, *Eur. Phys. J. C* **83** (2023) 835, [[2303.15246](#)].

J. R. Andersen, A. Cueto, S. P. Jones and A. Maier, *A Cell Resampler study of Negative Weights in Multi-jet Merged Samples*, [2411.11651](#).

B. Nachman and J. Thaler, *Neural resampler for Monte Carlo reweighting with preserved uncertainties*, *Phys. Rev. D* **102** (2020) 076004, [[2007.11586](#)].

E.g. “We have demonstrated that the fraction of negative event weights in existing large high-multiplicity samples can be reduced by more than an order of magnitude, whilst preserving predictions for observables within statistical uncertainties.” [[2303.15246](#)]

**are we doing our (perturbative QFT) job properly if we can't deliver guaranteed positive predictions?**

# 3 stages of NLO event generation

---

1. Generate “Born” event, e.g.  $q\bar{q} \rightarrow Z$ , with an overall NLO-correct normalisation
2. Generate real radiation, e.g. extra gluon, with correct real matrix element
3. Let a parton shower generate all remaining perturbative emission

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$$1 + \mathcal{O}(\alpha_s)$$

$$\mathcal{O}(\alpha_s)$$

	NLO event normalisation	Generation of first emission
MC@NLO	can be negative	can be negative
POWHEG*	can be negative	always positive

\* and also the *KrkNLO* [Jadach et al [1503.06849](#)] and *MAcNLOPS* [Nason & GPS, [2111.03553](#)] methods

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	$1 + \mathcal{O}(\alpha_s)$	$\mathcal{O}(\alpha_s)$
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# NLO Born normalisation, inclusive over subsequent branching

$$\begin{array}{ccccccc} \text{Born + NLO norm.} & = & \text{Born} & + & \text{1-loop virtual} & + & \text{real} \\ (LO + NLO) & & (LO) & & (NLO) & & (NLO) \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ \bar{B}(\Phi_B) & = & B_0(\Phi_B) & + & V(\Phi_B) & + & \int R(\Phi_B, \Phi_{\text{rad}}) d\Phi_{\text{rad}}, \\ & & & & \underbrace{\hspace{10em}} & & \\ & & & & \text{relative order } \alpha_s & & \end{array}$$

3 dim. of phase space for one extra emission

## NLO Born normalisation, inclusive over subsequent branching

*Born + NLO norm.* = *Born* + *1-loop virtual* + *real*  
 (LO + NLO) (LO) (NLO) (NLO)

↓ ↓ ↓ ↓ ↓

$\bar{B}(\Phi_B) = B_0(\Phi_B) + \underbrace{V(\Phi_B) + \int R(\Phi_B, \Phi_{\text{rad}}) d\Phi_{\text{rad}}}_{\text{relative order } \alpha_s},$

*3 dim. of phase space for one extra emission*

## Made explicitly finite with counterterms

*counterterm (integrated)* ↓ *counterterm (differential)* ↓

$\bar{B}(\Phi_B) = B_0(\Phi_B) + V(\Phi_B) + C_{\text{int}}(\Phi_B) + \underbrace{\int [R(\Phi) - C(\Phi)] d\Phi_{\text{rad}}}_{\text{relative order } \alpha_s},$

# How does it work in practice?

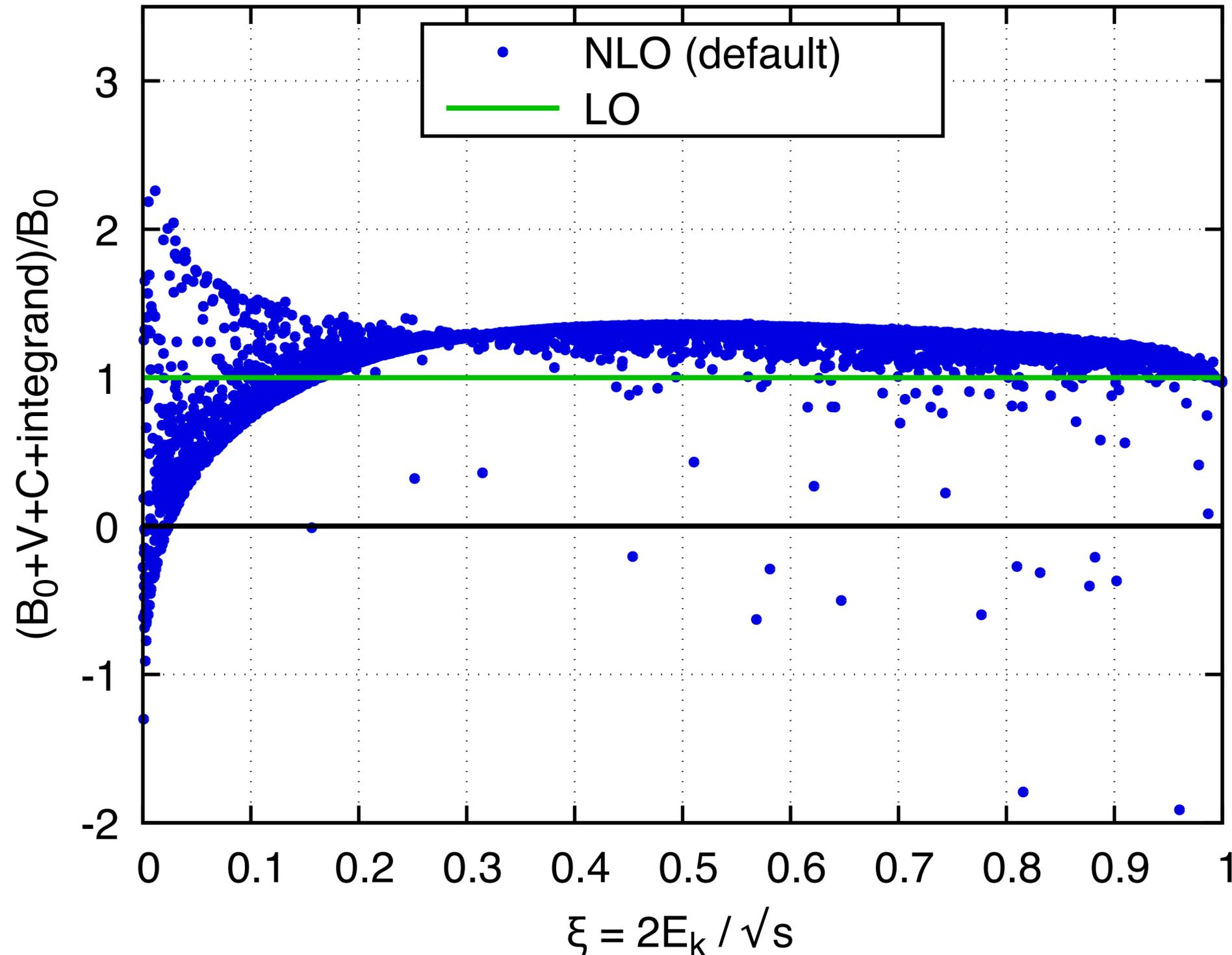
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- Choose a Born phase space point  $\Phi_B$  randomly
- Instead of accurately evaluating the  $d\Phi_{\text{rad}}$  integral, choose a random real phase space point  $\Phi_{\text{rad}}$  and use that to get a “single-point Monte Carlo” estimate for the integral

$$\bar{B}(\Phi_B) = B_0(\Phi_B) + V(\Phi_B) + C_{\text{int}}(\Phi_B) + \underbrace{\int [R(\Phi) - C(\Phi)] d\Phi_{\text{rad}}}_{\text{relative order } \alpha_s},$$

- accept with probability  $|\bar{B}|/\text{max}$ , event weight is sign of  $\bar{B}$

$$\bar{B}(\Phi_B) = B_0(\Phi_B) + V(\Phi_B) + C_{\text{int}}(\Phi_B) + \int [R(\Phi) - C(\Phi)] d\Phi_{\text{rad}},$$



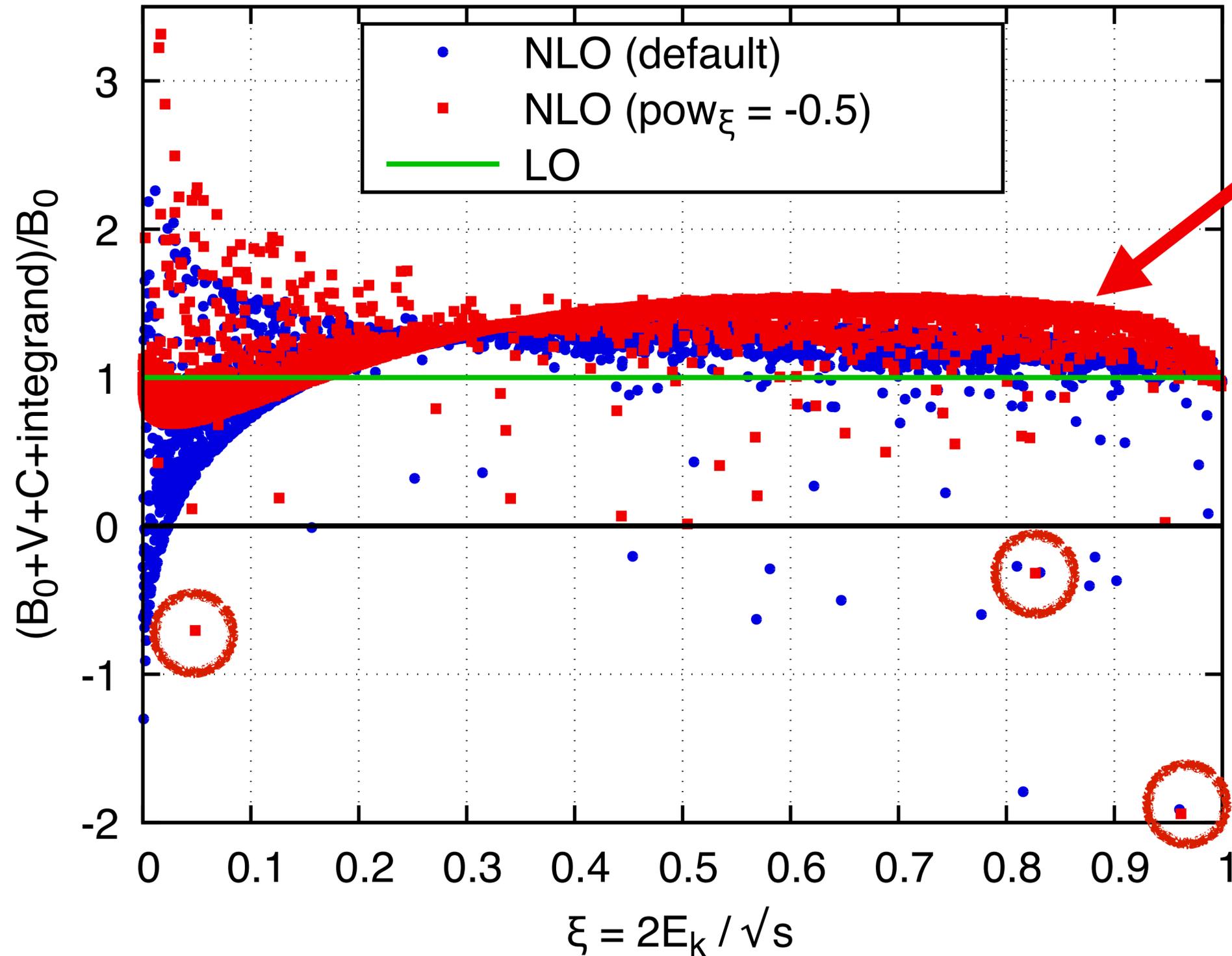
each point  $\equiv$  one Born  
phase space choice and  
one radiation phase space  
choice

Plotted as a function of  
one of the 3 real radiation  
phase space variables

Result should be  
 $1 + \mathcal{O}(\alpha_s)$

But sometimes coefficient  
in front of  $\alpha_s$  is large and  
result is negative

$$\bar{B}(\Phi_B) = B_0(\Phi_B) + V(\Phi_B) + C_{\text{int}}(\Phi_B) + \int [R(\Phi) - C(\Phi)] d\Phi_{\text{rad}},$$



reweighting of integration variables can help\*

But still some negative-weight events and reweighting not always easy or successful

\* recent proposals can be viewed as doing something similar: “Born spreading” [Frederix & Torrielli, [2310.04160](#)] and “ARCANE” [Shyamsunda, [2502.08052](#), [2502.08053](#)]

# Key question

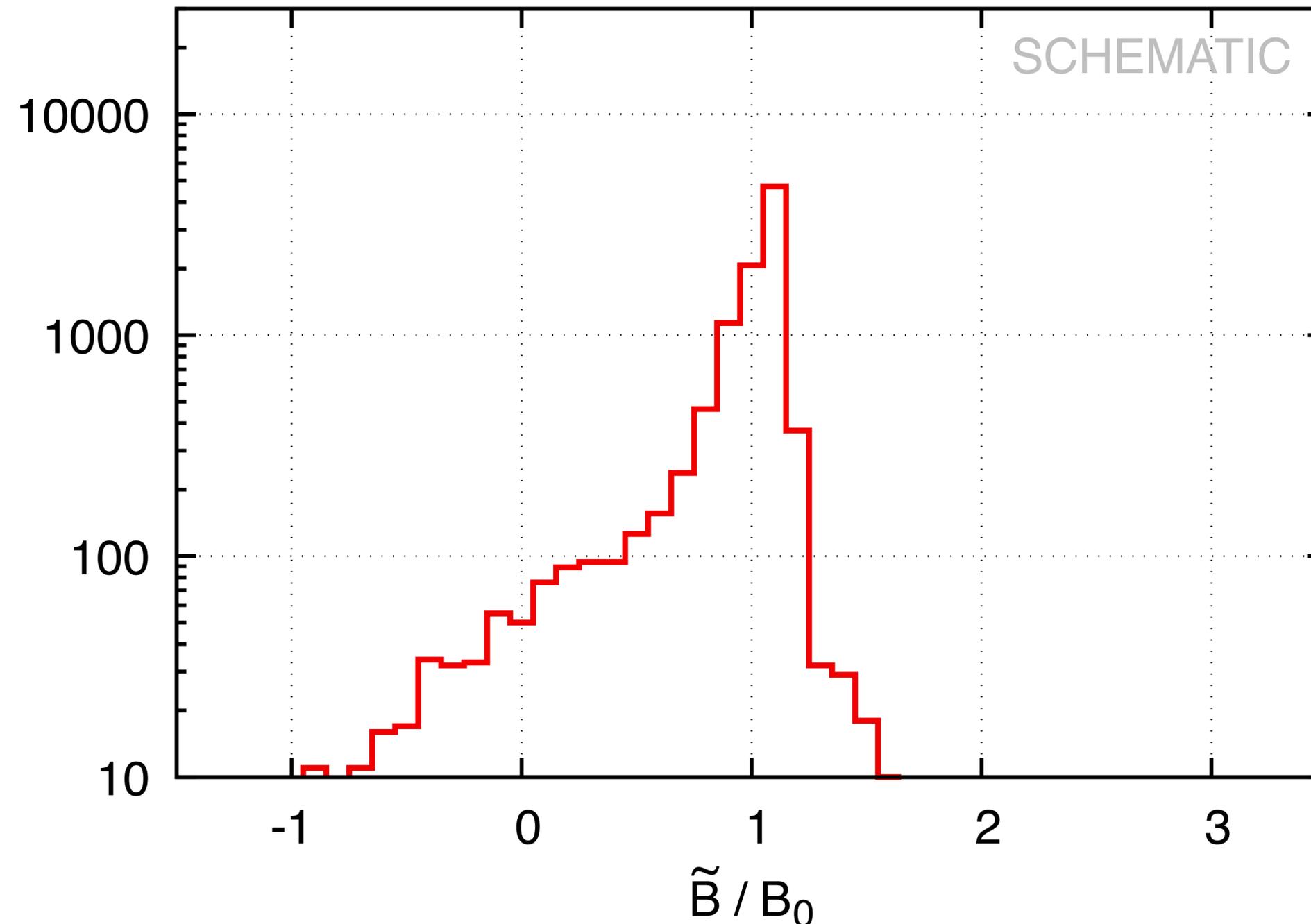
---

- Can you evaluate the following integral fast & reliably, and be both positive and NLO accurate

$$\bar{B}(\Phi_B) = B_0(\Phi_B) + \int [R(\Phi) - C(\Phi)] d\Phi_{\text{rad}},$$

# Could we just discard the negative events?

raw distribution of weights

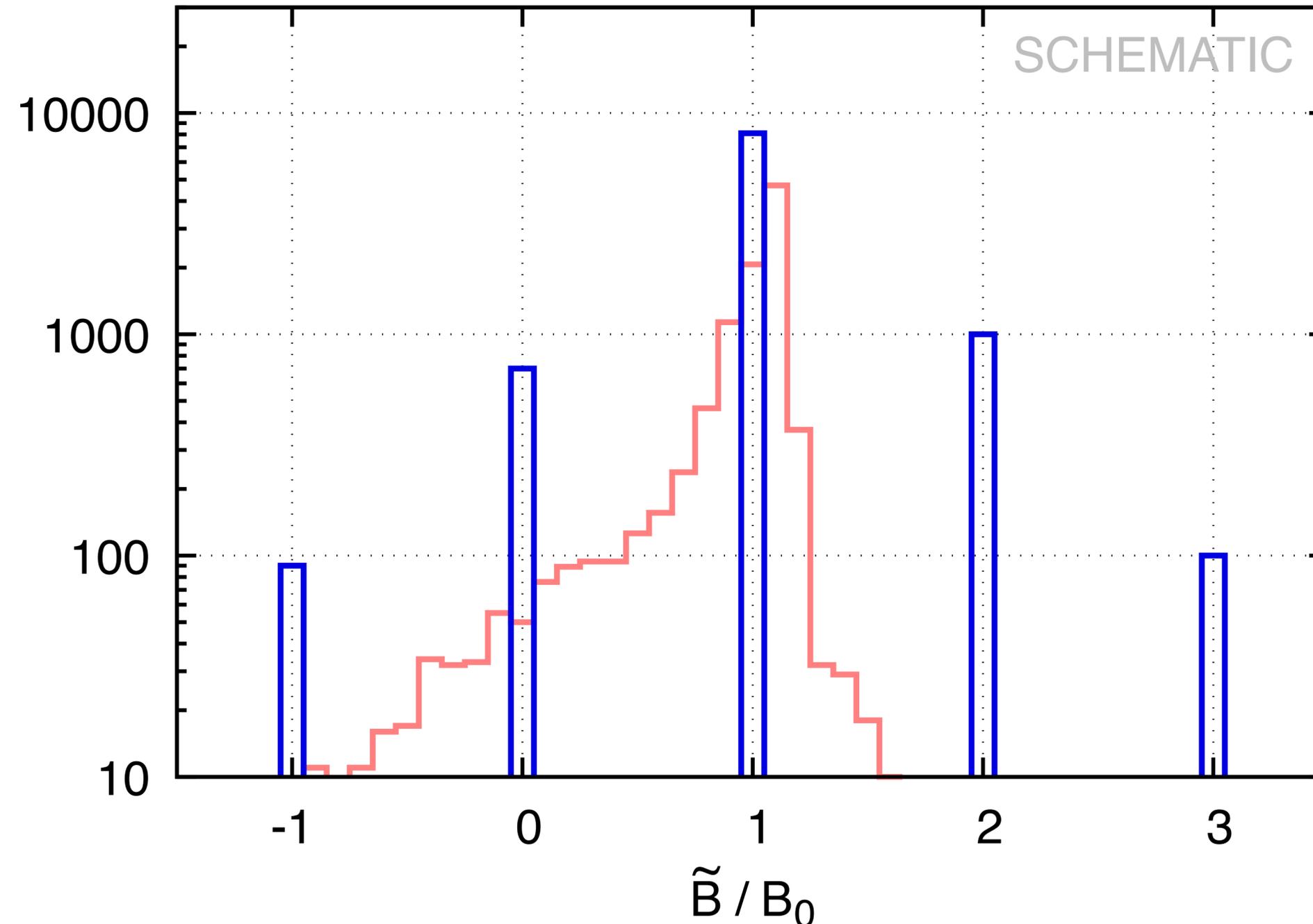


How do you guarantee that what you are discarding is genuinely beyond the NLO order you're trying to control?

E.g. in one toy example discarding negative-weight events would give a spurious  $\alpha_s^{3/2}$  contribution

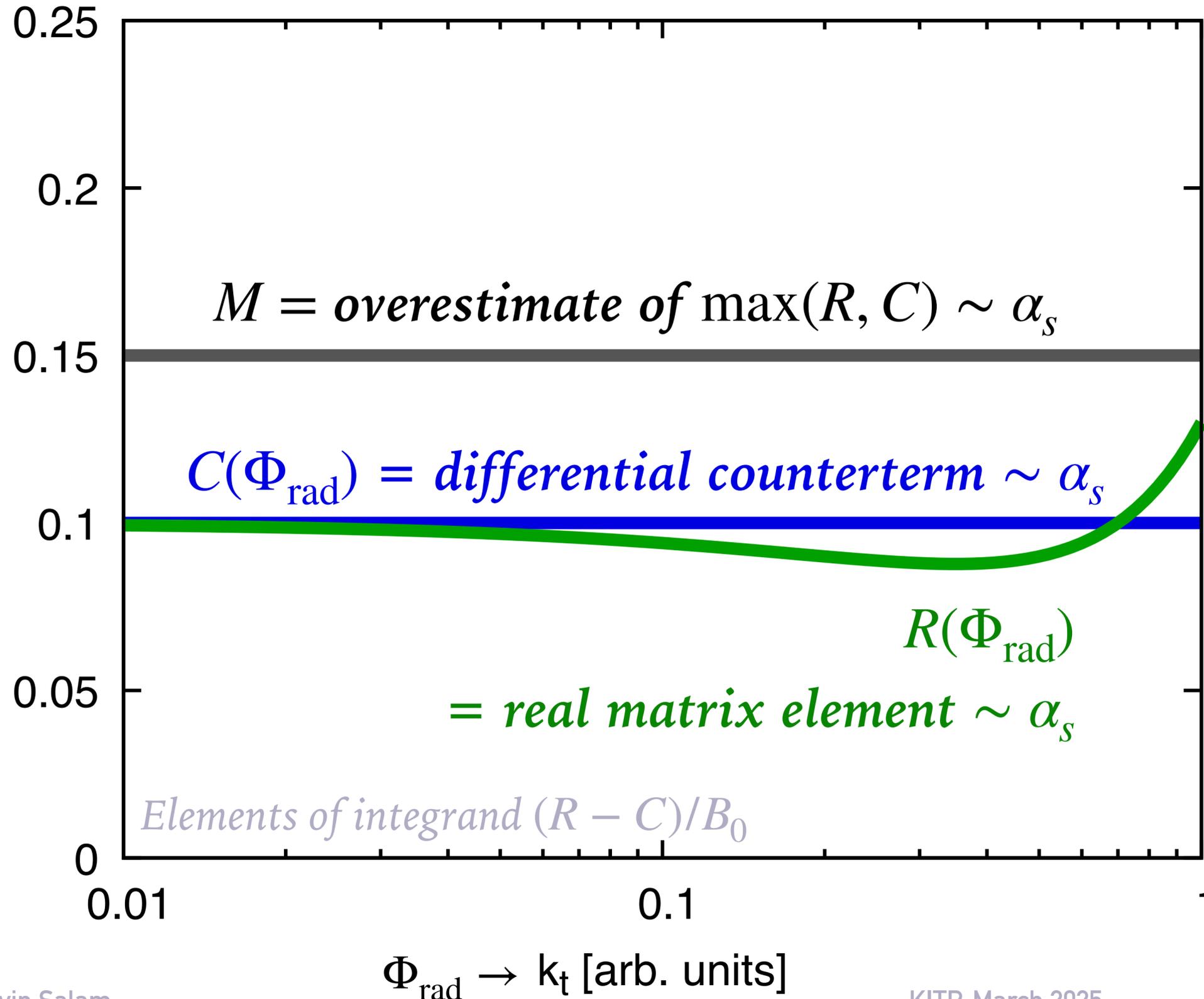
# Core idea: map the integral to an event-by-event integer

discretised distribution of weights



this can be done in a way  
that the sum over the  
distribution gives the  
exact original answer

# illustrate algorithm for one dimension of real phase space ( $k_t$ )



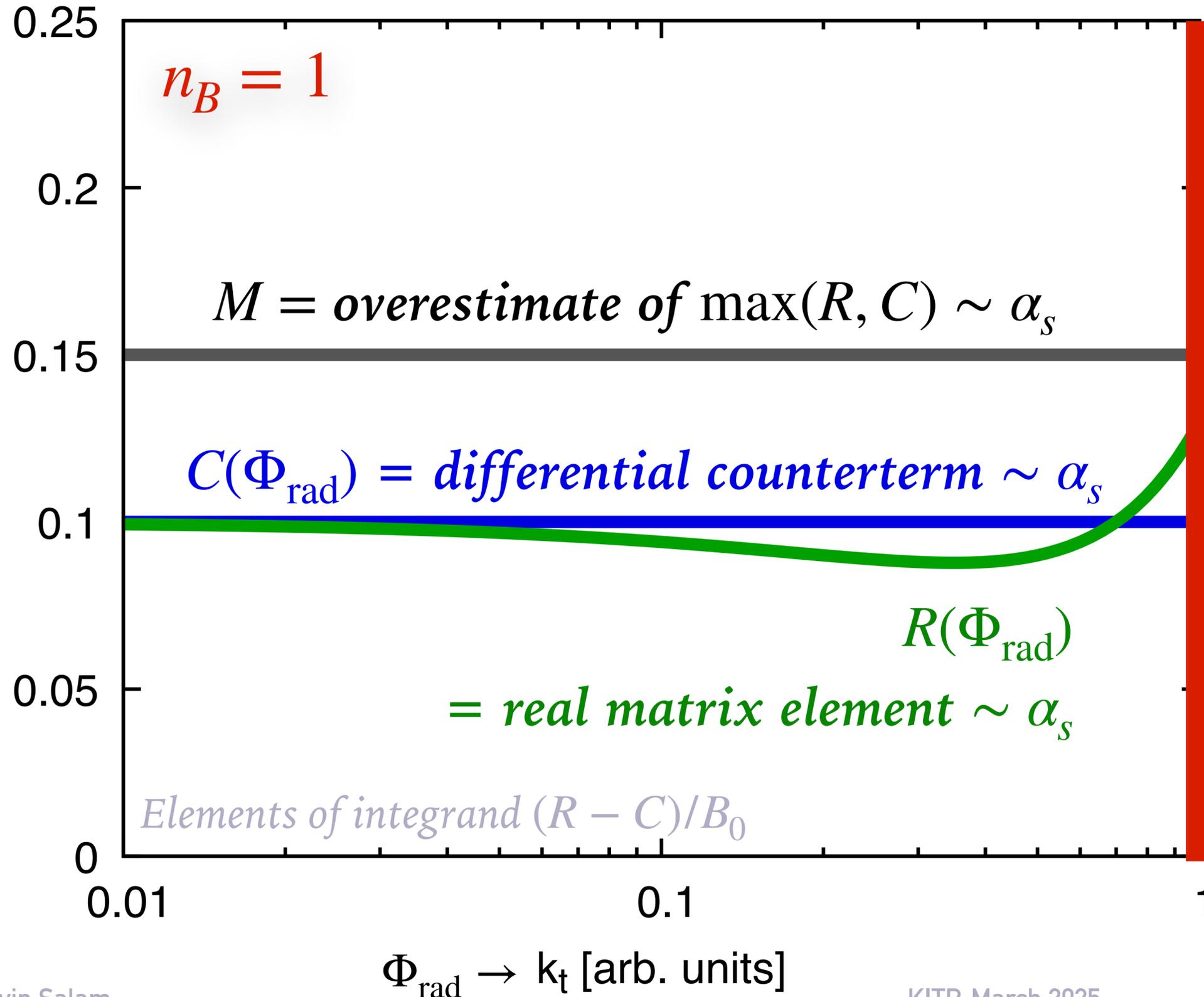
## Start with

- normalisation  $n_B = 1$
- $k_t$  at max allowed value

## Run the following loop:

- From  $\ln k_t$  subtract a random amount sampled from  $e^{-M/B_0 \ln 1/k_t}$
- With probability  $r < \frac{|R - C|}{M}$ 
  - if  $R > C$ :  $n_B \rightarrow n_B + 1$ ,
  - if  $R < C$ :  $n_B \rightarrow n_B - 1$

# illustrate algorithm for one dimension of real phase space ( $k_t$ )



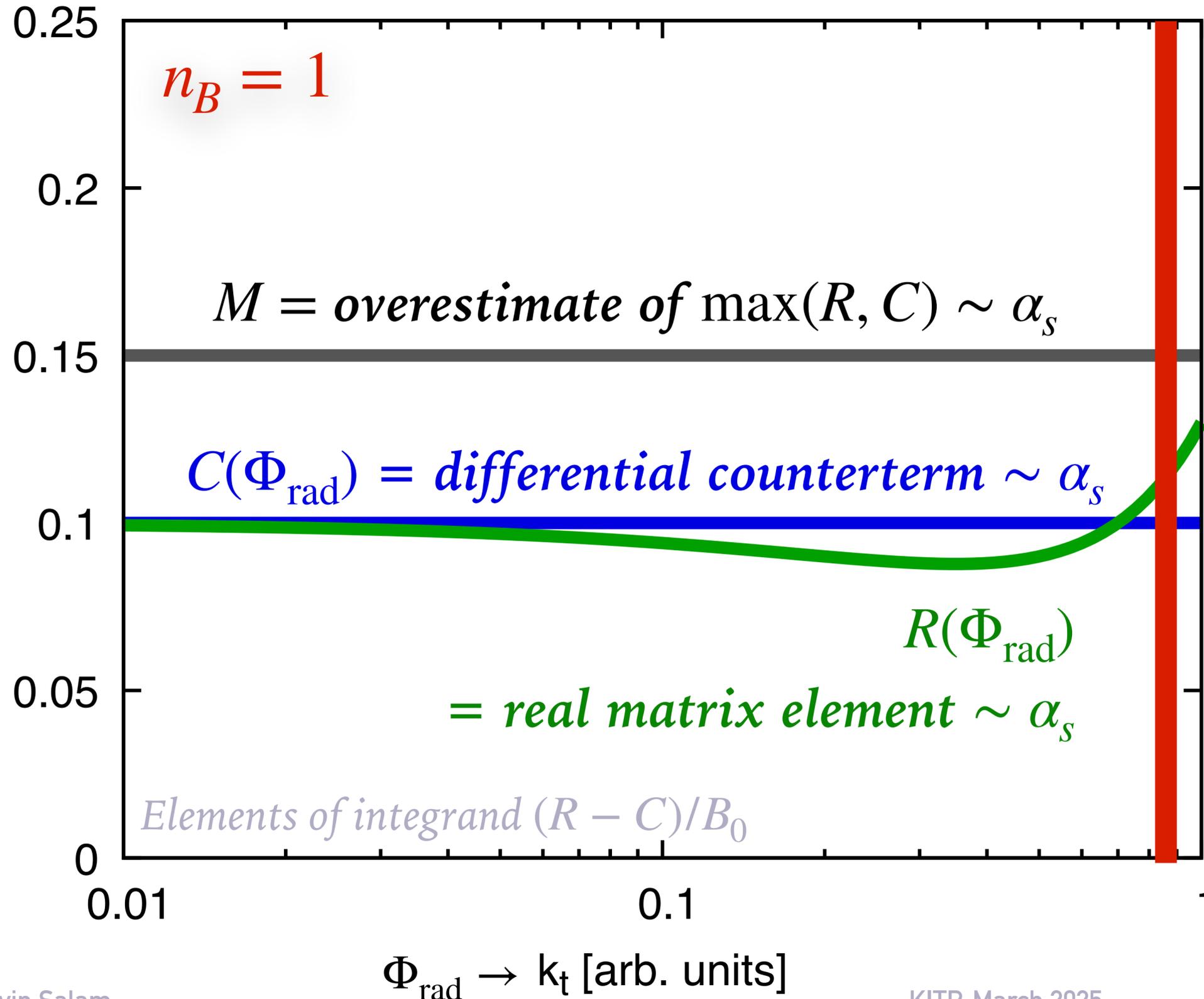
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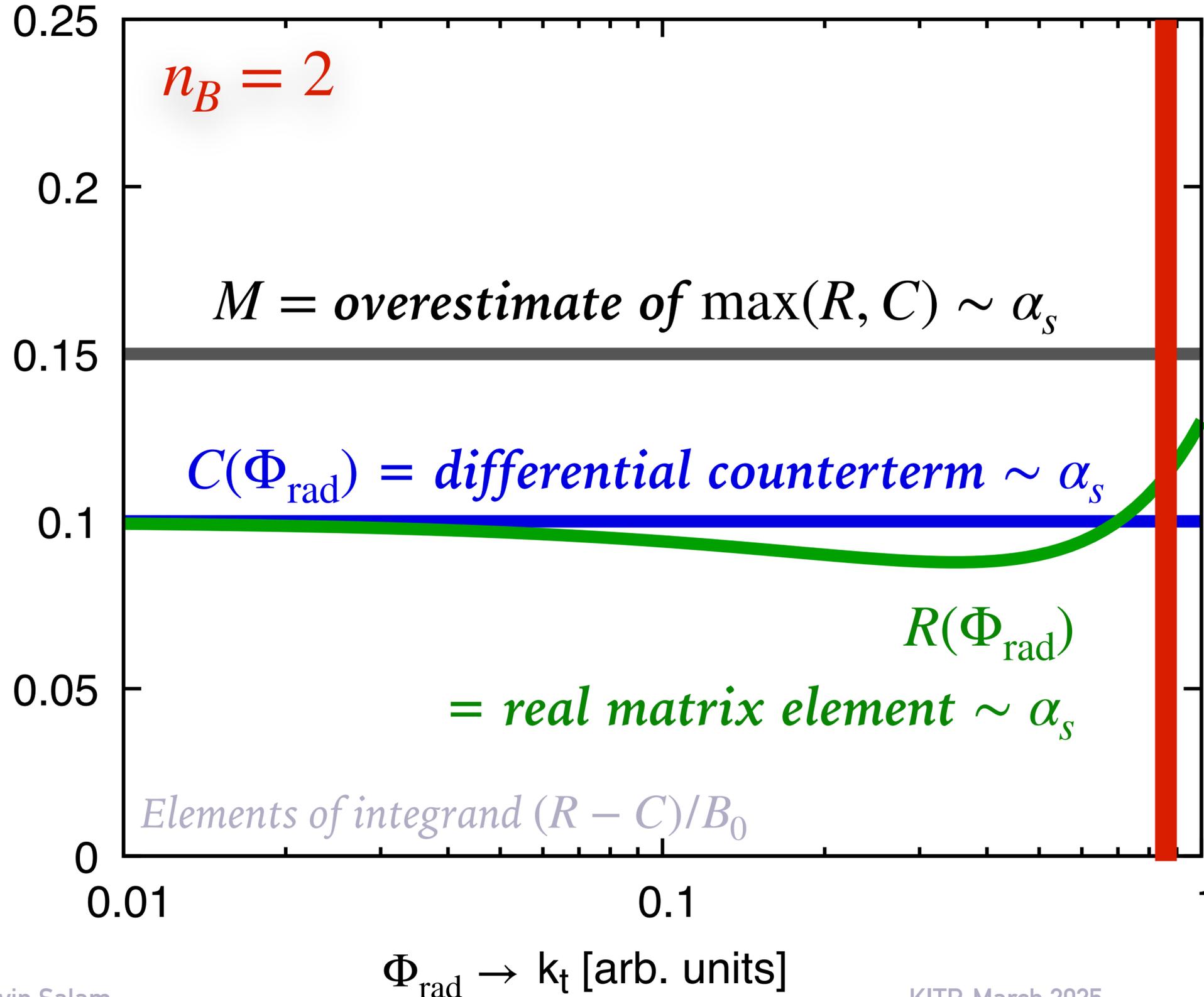
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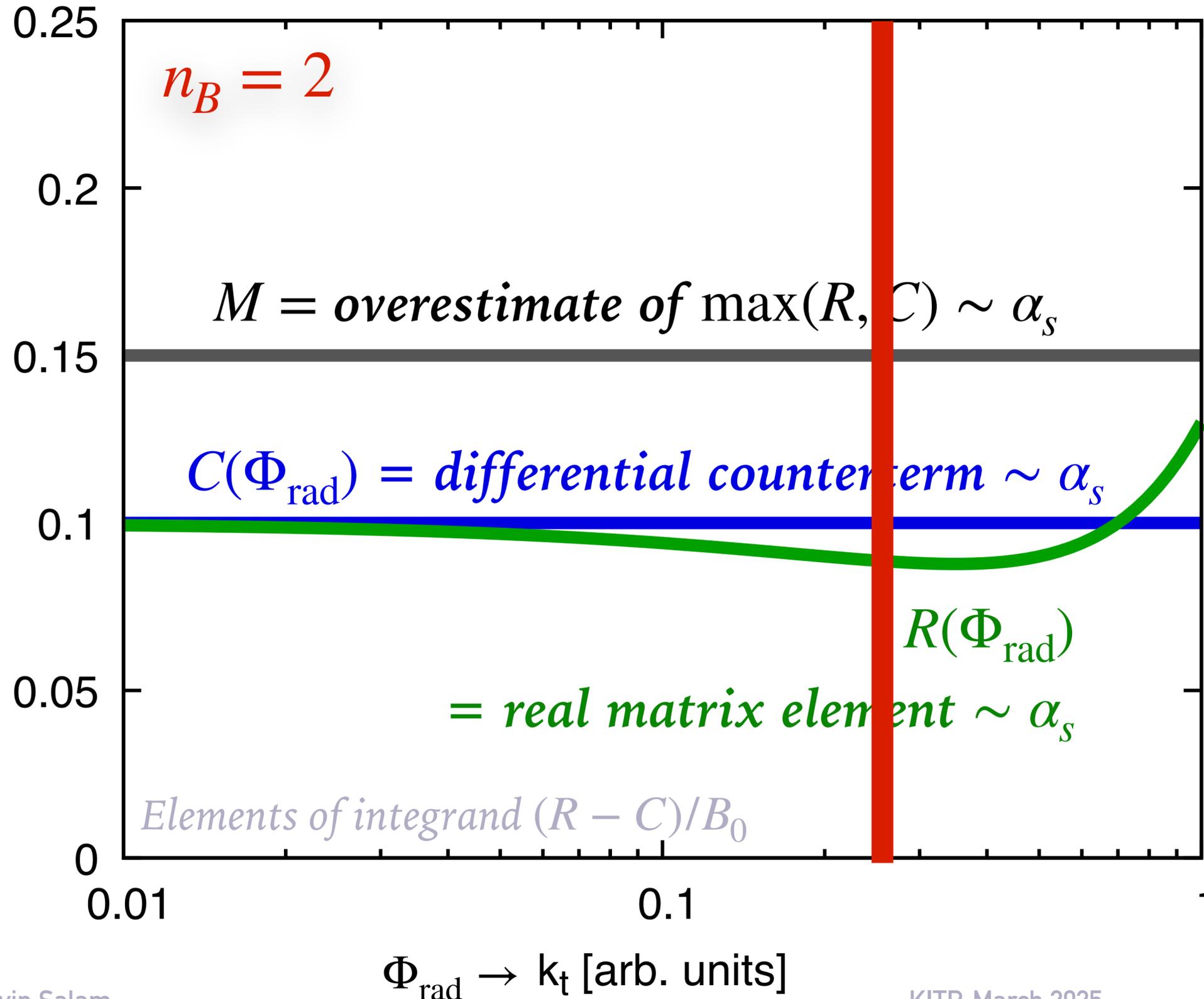
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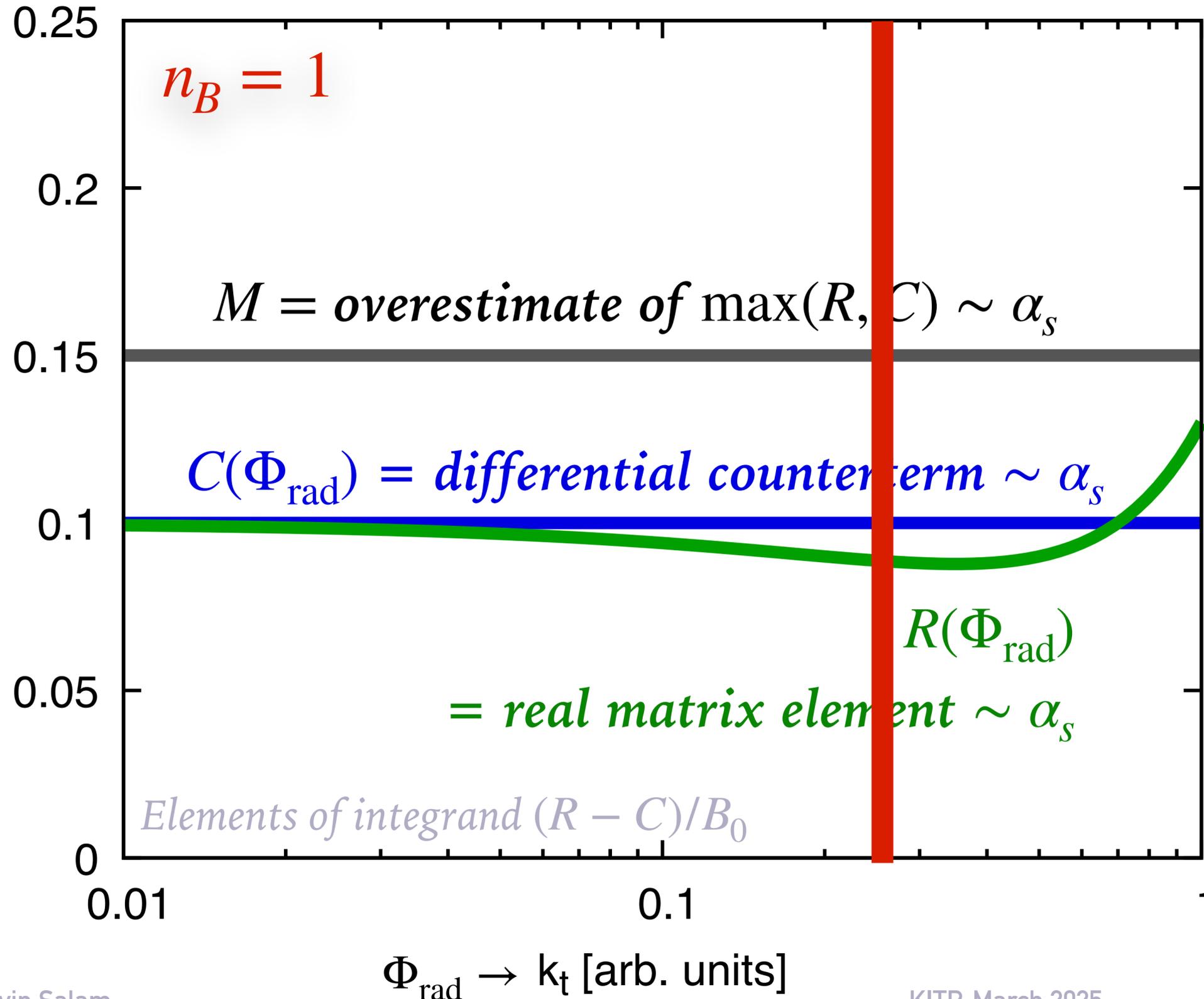
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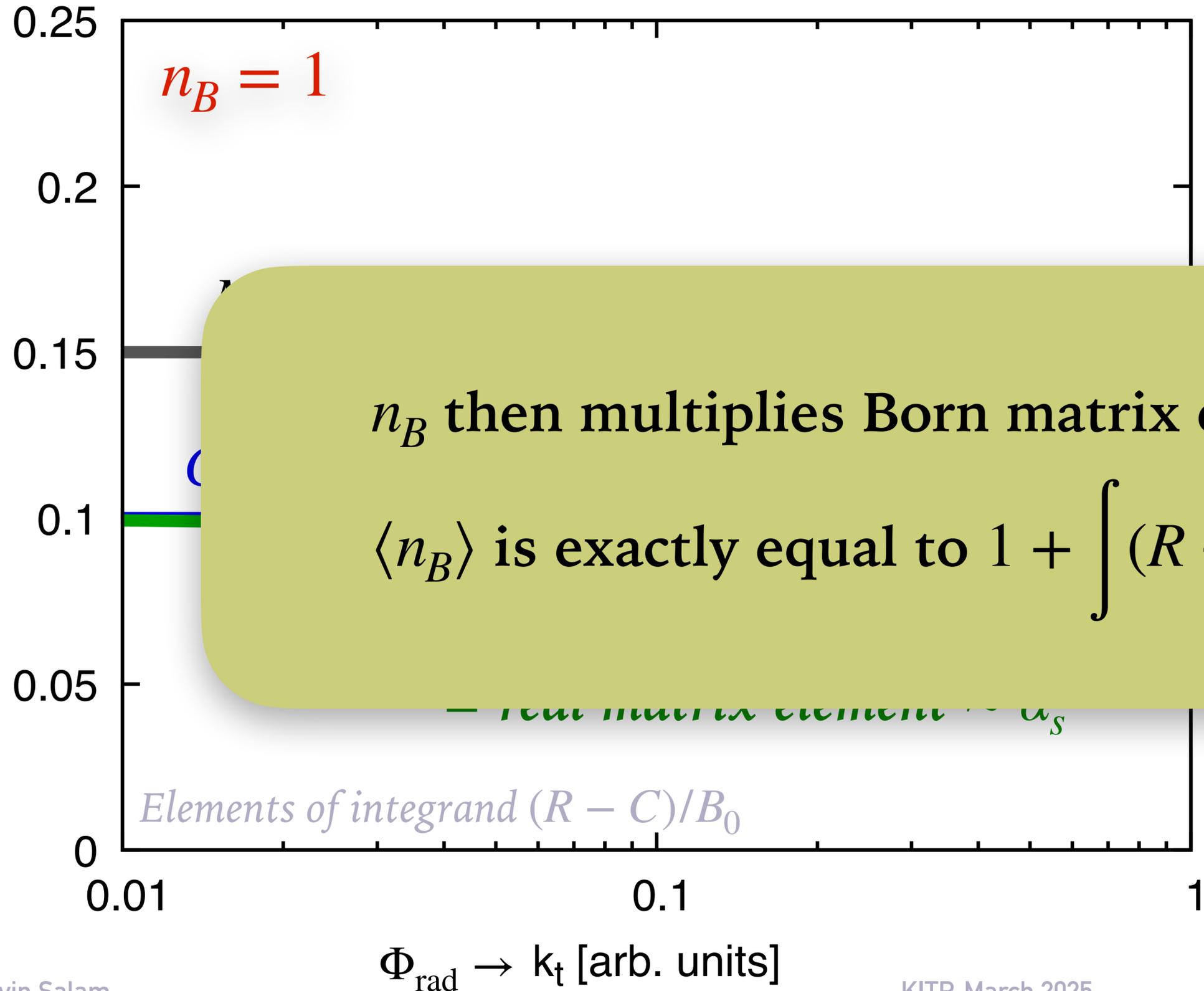
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# illustrate algorithm for one dimension of real phase space ( $k_t$ )



Start with

- ▶ normalisation  $n_B = 1$
- ▶  $k_t$  at max allowed value

$n_B$  then multiplies Born matrix element  $B_0(\Phi_B)$

$$\langle n_B \rangle \text{ is exactly equal to } 1 + \int (R - C)/B_0 d\Phi_{\text{rad}}$$

p:

a random

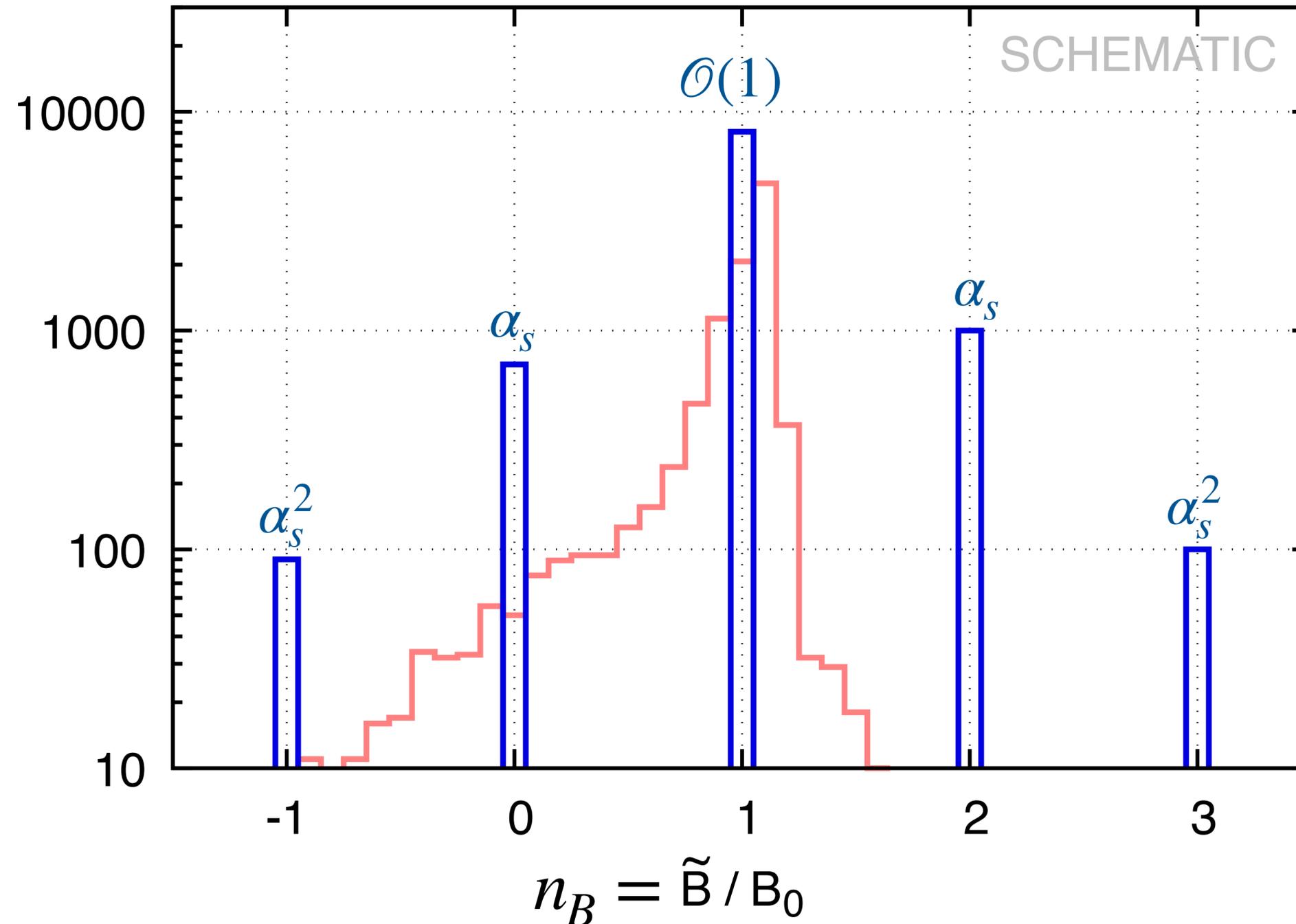
from  $e^{-M/B_0 \ln 1/k_t}$

$$< \frac{|R - C|}{M}$$

- ▶ if  $R > C$ :  $n_B \rightarrow n_B + 1$ ,
- ▶ if  $R < C$ :  $n_B \rightarrow n_B - 1$

# Robust positivity with NLO accuracy (spurious terms from NNLO)

discretised distribution of weights

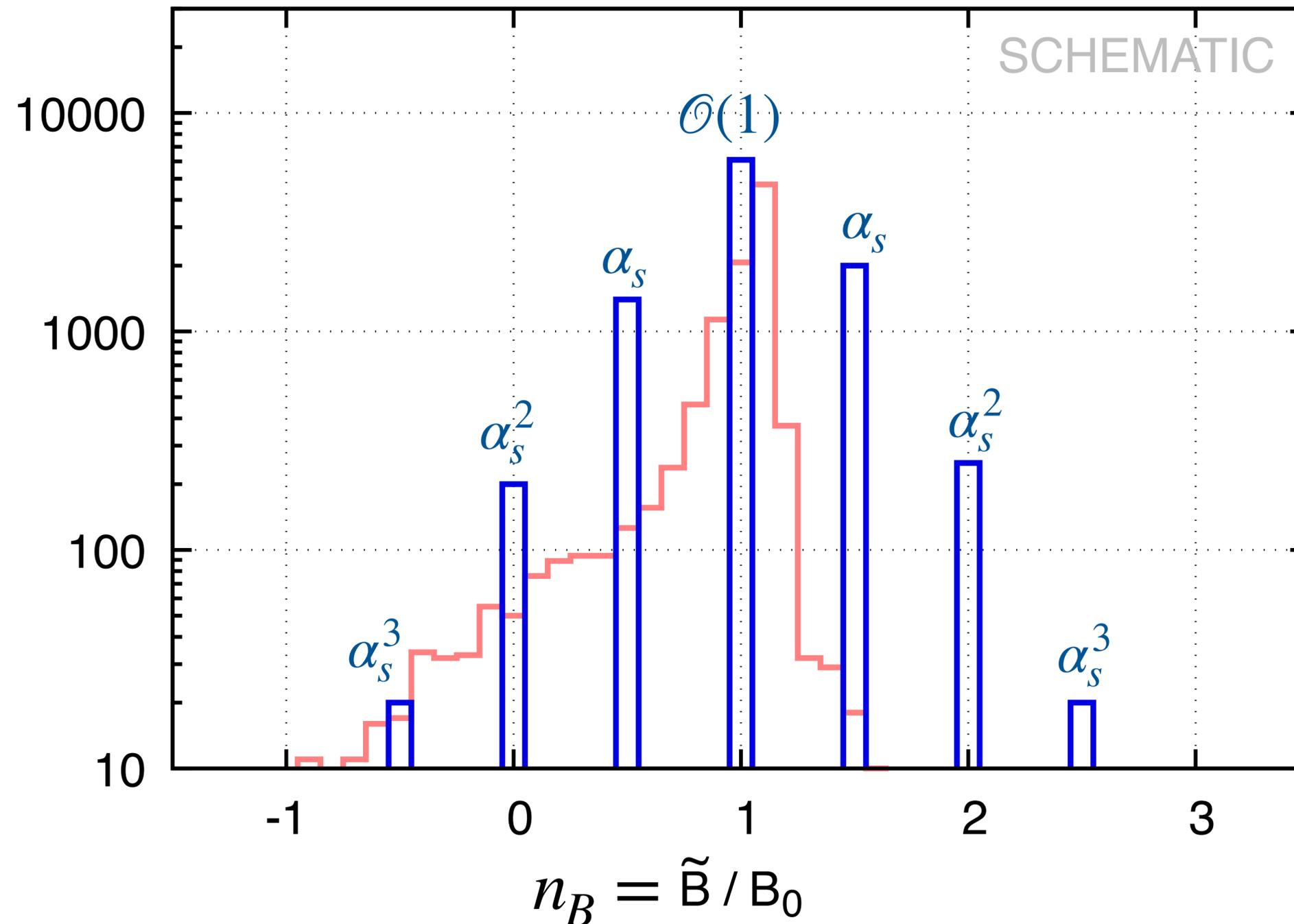


Now if you discard negative-weight events you have a guarantee that you only change the result at NNLO or beyond

Because each decrement of  $n_B$  costs a power of  $\alpha_s$

# Robust positivity with NLO accuracy (spurious terms from N3LO)

discretised distribution of weights



Multiply  $M, R, C$  in the algorithm by factor  $p$  (here  $p = 2$ )

Increment  $n_B$  by  $\pm \frac{1}{p}$

Algorithm gives exactly the same  $\langle n_B \rangle$

Keeping only positive-weight events changes integral by just  $\alpha_s^{p+1}$

# This is a “foundation” algorithm — can be adapted in many ways

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- **ESME**  $\equiv$  Exponentiated Subtraction for Matching Events
- Our implementation actually uses a variant that handles real emissions and NLO normalisation simultaneously (more efficient, only a bit more complex)

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## Algorithm Stream 1 (ESME) Born + NLO rejection

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```
1: Generate Born event according to  $\bar{B}_C$  distribution and set  $v = v_{\max}$ 
2: while  $v > v_{\min}$  do
3:   generate next  $v$  and  $\Phi_2$  according to Sudakov with density  $\rho(v)d \ln v$ , Eq. (3.6)
4:   generate random number  $0 < r < 1$ 
5:   if  $C(\Phi) > R(\Phi)$  then
6:     if  $r > C(\Phi)/M(\Phi)$ : veto emission
7:     else if  $r > R(\Phi)/M(\Phi)$ : return reject event
8:     else: accept emission and return continue shower, accept event
9:   else
10:    if  $r > C(\Phi)/M(\Phi)$ : veto emission
11:    else: accept emission and return continue shower, accept event
12: return accept event
```

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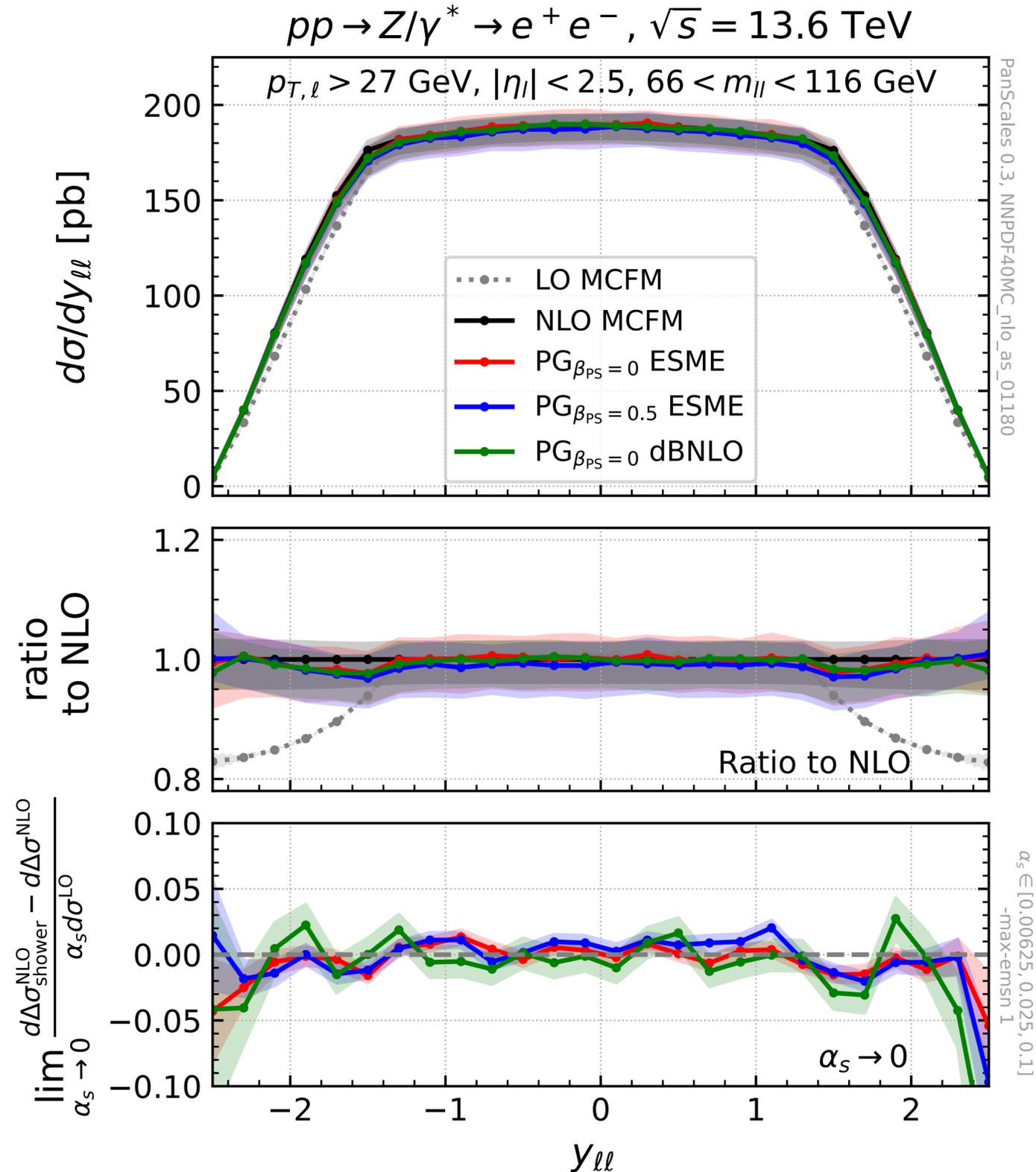
## Algorithm Stream 2 (ESME) NLO addition

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```
1: Generate Born event according to  $\bar{B}_C$  (or  $B_0$ ) distribution and set  $v = v_{\max}$ 
2: while  $v > v_{\min}$  do
3:   generate next  $v$  and  $\Phi_2$  according to Sudakov with density  $\rho(v)d \ln v$ , Eq. (3.6)
4:   generate random number  $0 < r < 1$ 
5:   if  $C(\Phi) > R(\Phi)$  then
6:     if  $r > R(\Phi)/M(\Phi)$ : veto emission
7:     else: return reject event
8:   else
9:     if  $r > R(\Phi)/M(\Phi)$ : veto emission
10:    else if  $r > C(\Phi)/M(\Phi)$ : accept emsn, return continue shower, accept event
11:    else: return reject event
12: return reject event
```

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# Does ESME give the correct answer? → Yes



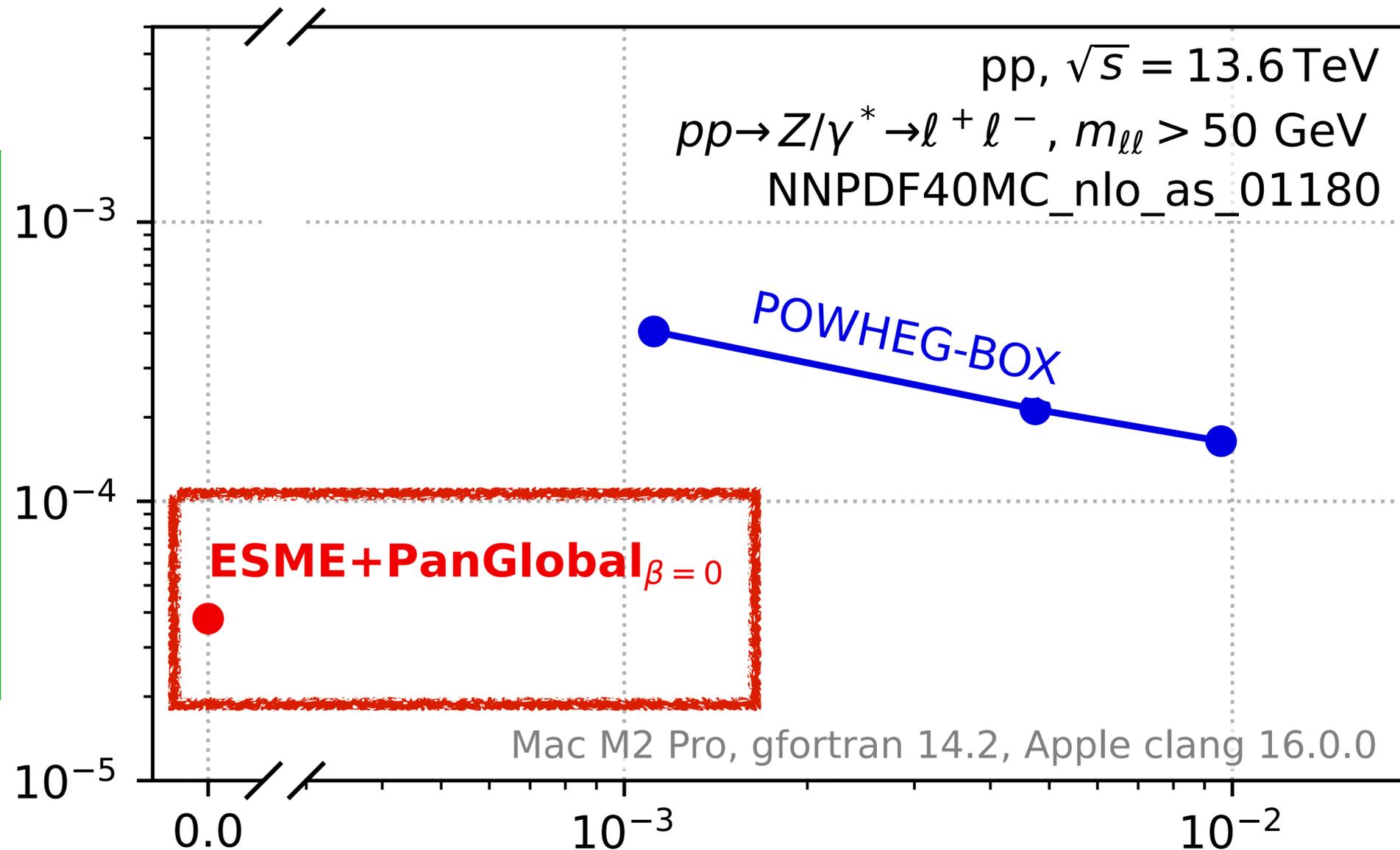
Comparison to exact NLO  
 (and to more standard method, here labelled dBNLO)

Ratio to exact NLO

Check of NLO coefficient

# Is ESME fast enough?

NLO ev. gen. time vs. negative-weight fraction



- ▶ positive definite by construction
- ▶ turns out to be  $\sim 4\times$  faster than fastest of public NLO tools (POWHEG-Boxv2)\*
- ▶ NB: this is a simple process (Drell-Yan) — timing more critical for more complex processes

\* with some effort having gone into optimising it

# Conclusions

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- Positivity *can* be built into NLO calculations
- Price to pay is a change of higher terms beyond NLO
  - these higher order terms appear to be numerically modest
  - higher order terms anyway present for most observables in other NLO matching methods
  - underlying algorithm can be adapted to push them to arbitrary high order, e.g. for NNLO matching
- Underlying algorithms are simple, should be possible for other groups to try them out, also for more complex processes than the ones we studied
- Key step on path to making pQFT predictions simultaneously accurate and physical

# Backup

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## Algorithm 1 General algorithm to convert NLO subtraction integral to integer

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- 1: Set  $n_B = 1$  and  $v = v_{\max}$
  - 2: **while**  $v > v_{\min}$  **do**
  - 3:     generate next  $v$  and  $\Phi_2$  according to Sudakov with density  $\rho(v)d \ln v$ , Eq. (3.6)
  - 4:     generate random number  $0 < r < 1$
  - 5:     **if**  $r < |R(\Phi) - C(\Phi)|/M(\Phi)$  **then**
  - 6:         **if**  $R(\Phi) > C(\Phi)$ :  $n_B \rightarrow n_B + 1$
  - 7:         **else:**                    $n_B \rightarrow n_B - 1$
  - 8: **return**  $n_B$
- 

$n_B$  then multiplies Born matrix element  $B_0(\Phi_B)$

$\langle n_B \rangle$  is exactly equal to  $1 + \underbrace{\int \frac{R - C}{B_0} d\Phi_{\text{rad}}}_{\text{order } \alpha_s}$

$$d\Phi_{\text{rad}} \rightarrow \frac{dv}{v} d\Phi_2$$

$$\Delta(v) = \exp \left[ - \int_v^{v_{\max}} \frac{dv'}{v'} \rho(v') \right]$$

$$\rho(v) = \int d\Phi_2 J \frac{M(\Phi)}{B_0(\Phi_B)}$$

$$M(\Phi) \geq \max[R(\Phi), C(\Phi)]$$

---

## Algorithm 1 General algorithm to convert NLO subtraction integral to integer

---

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- 8: **return**  $n_B$

$\mathcal{O}(\alpha_s)$

$$d\Phi_{\text{rad}} \rightarrow \frac{dv}{v} d\Phi_2$$

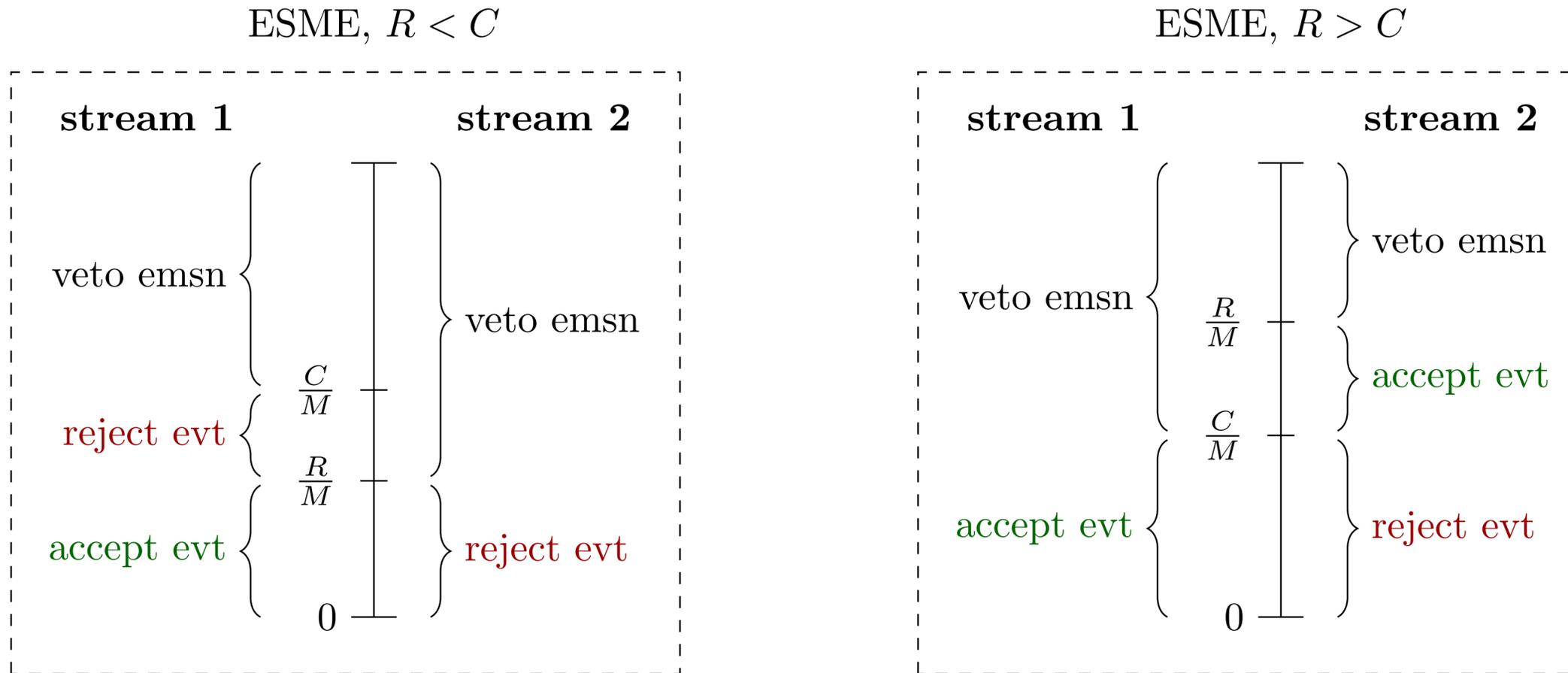
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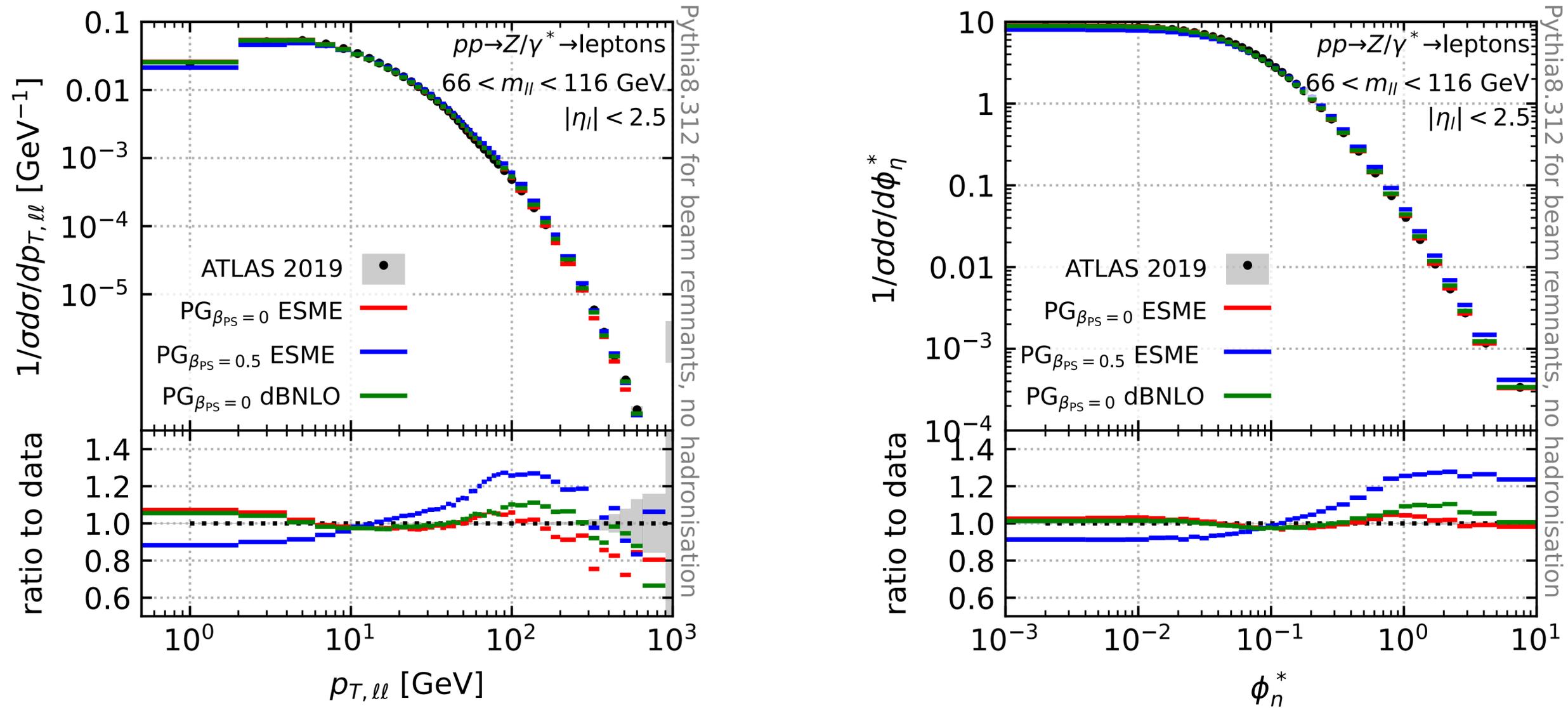
$$M(\Phi) \geq \max[R(\Phi), C(\Phi)]$$

$n_B$  then multiplies Born matrix element  $B_0(\Phi_B)$

$\langle n_B \rangle$  is exactly equal to  $1 + \underbrace{\int \frac{R - C}{B_0} d\Phi_{\text{rad}}}_{\text{order } \alpha_s}$



**Figure 1:** Simple illustration of the different possible actions in the two streams of the ESME algorithm with joint reals and subtractions. The actions are shown separately for the cases  $R(\Phi) < C(\Phi)$  (left) and  $R(\Phi) > C(\Phi)$  (right). In each case, when summing the two streams, one sees that the “accept evt” action occurs with total weight  $R/M$ . One can also verify that the contribution to the total event rate change relative to the  $\bar{B}_C$  normalisation is  $(R - C)/M$ . Recall that the default action in stream 1 (2) is to accept (reject) the event if the shower scale reaches  $v_{\min}$  — only when the action is different from the stream’s default is the total event rate affected.

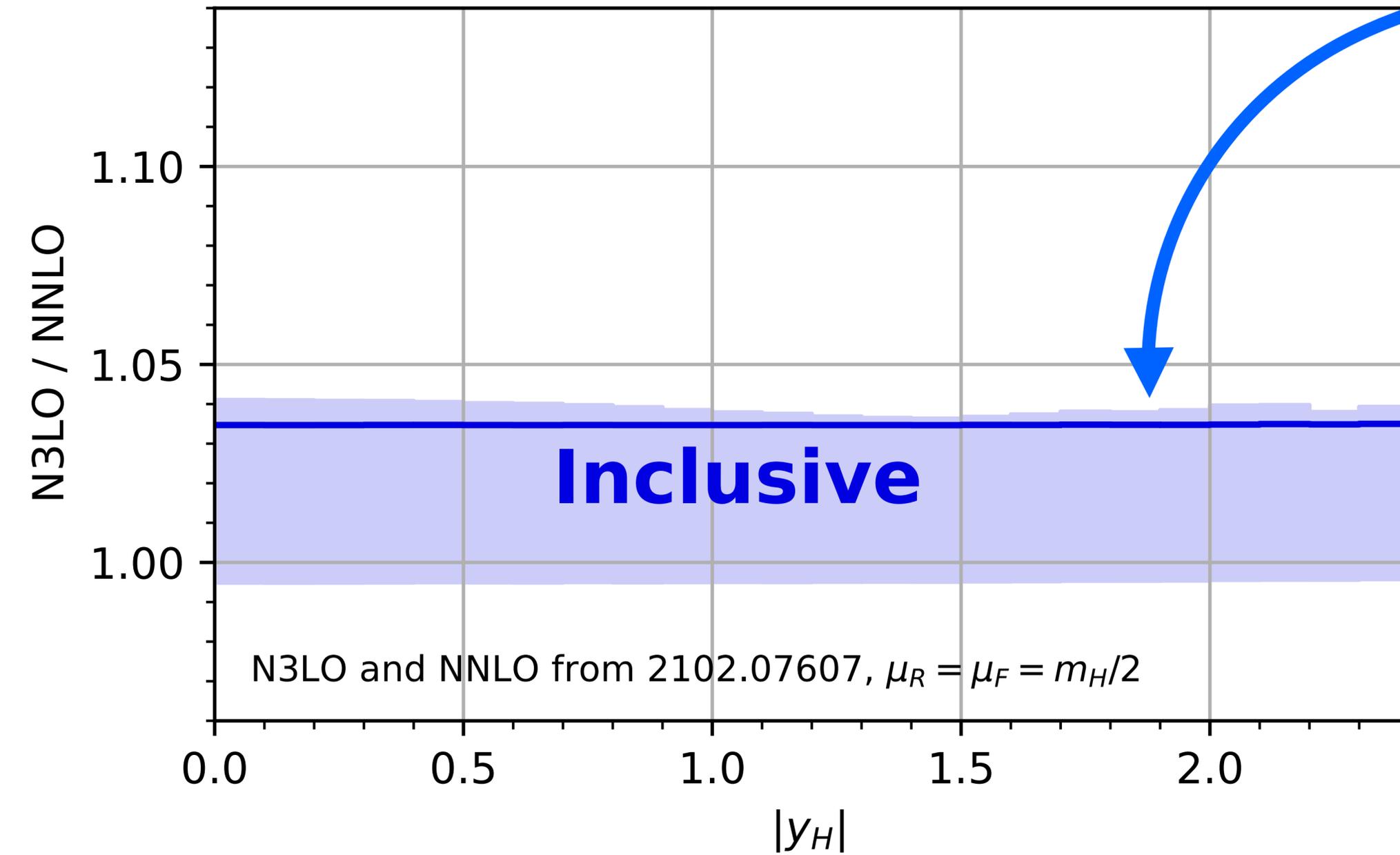


**Figure 11:** PanScales NLL+NLO matched showers, interfaced with Pythia [103], as compared to 13 TeV QED-Born di-lepton data from the ATLAS collaboration [104]. The left-hand plot is for the di-lepton transverse momentum distribution, while the right-hand plot is for the  $\phi_n^*$  variable [105], cf. Eq. (5.1). In the Pythia interface, we include Pythia’s primordial transverse momentum but not hadronisation, QED effects or multi-parton interactions.

Recent surprise:  $H \rightarrow \gamma\gamma$

inclusive N3LO  $\sigma$  uncertainties

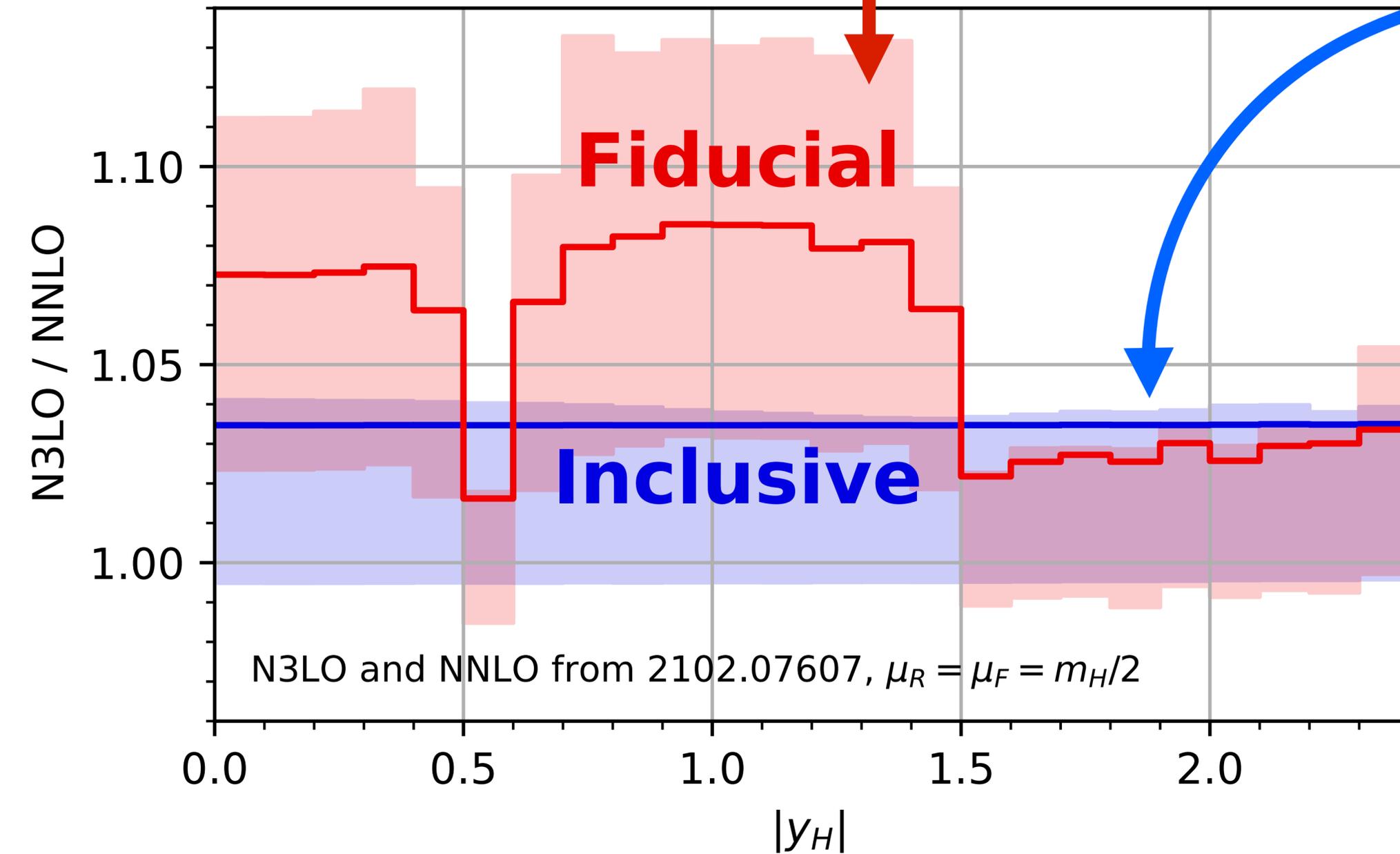
$H \rightarrow \gamma\gamma$ : N3LO K-factor



Chen, Gehrmann, Glover, Huss, Mistlberger & Pelloni, [2102.07607](#)

Recent surprise:  $H \rightarrow \gamma\gamma$  **fiducial N3LO**  $\sigma$  uncertainties  $\sim 2\times$  greater than **inclusive N3LO**  $\sigma$  uncertainties

$H \rightarrow \gamma\gamma$ : N3LO K-factor



“Gold standard” fiducial cross section gives much worse prediction

Why?  
And can this be solved?

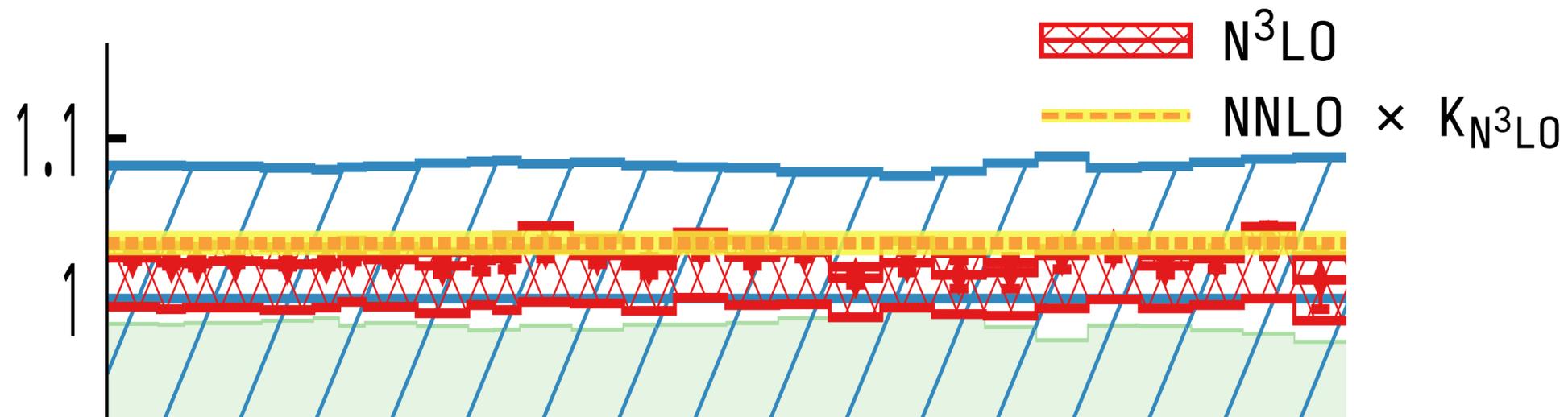
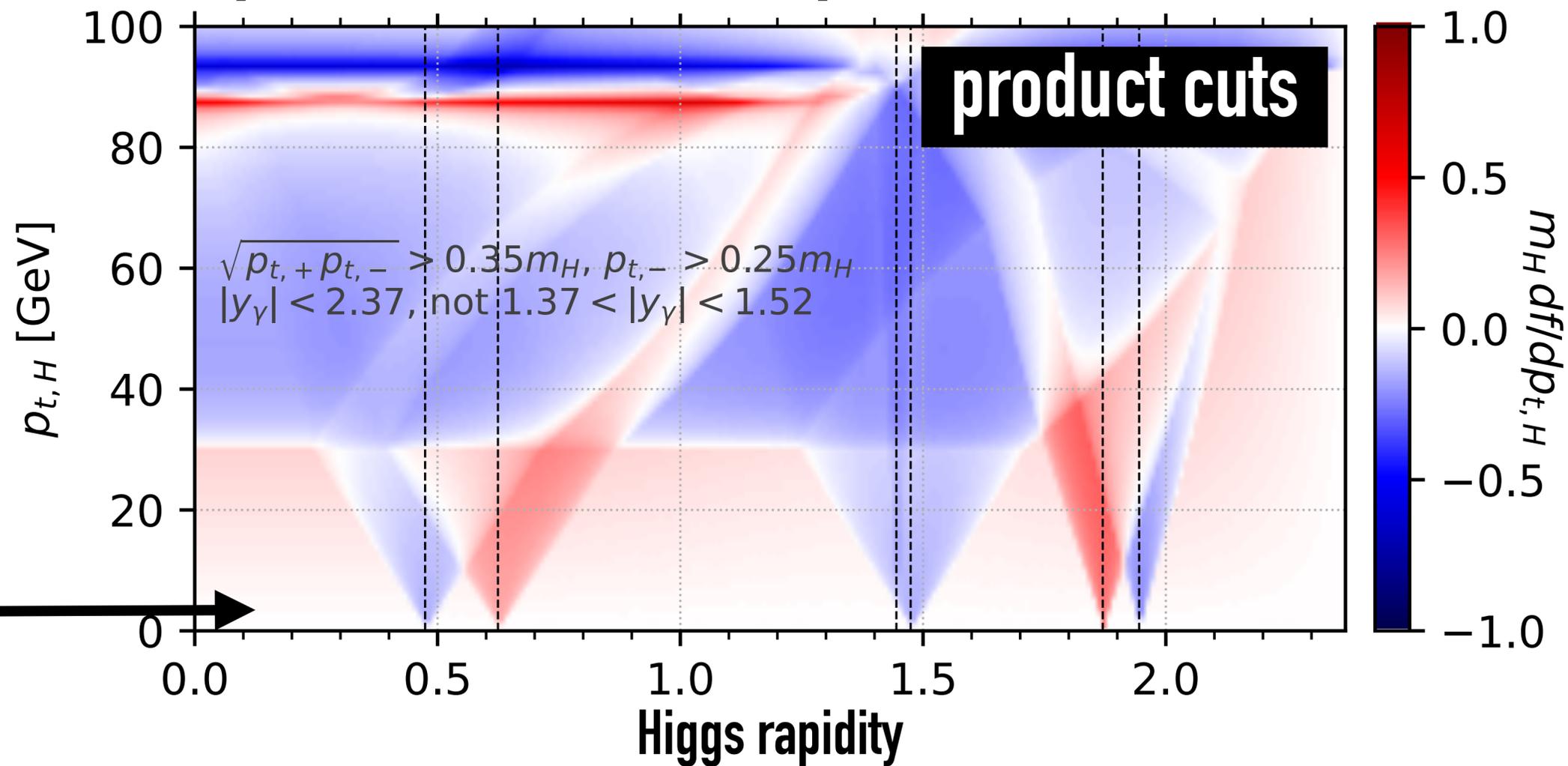
Chen, Gehrmann, Glover, Huss, Mistlberger & Pelloni, [2102.07607](#)

interplay with  $\eta_\gamma$  cuts

$f(p_{t,H}, y_H)$  has **zero** linear  $p_{t,H}$  derivative at  $p_{t,H} = 0$

fixed-order perturbation theory will be fine

$p_{t,H}$  derivative of acceptance: white = 0



Huss et al preliminary @ Higgs 2021