Bayesian Truncation Errors and Experimental Design for Compton Scattering

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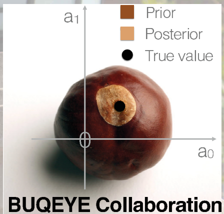


Reliable parameter uncertainties; optimal likelihood of experimental success.

hg/JMcG/DRP *Eur. Phys. J.* **A52** (2016) 139 1511.01952

BAYESIAN UNCERTAINTY QUANTIFICATION: ERRORS IN YOUR EFT:

Jordan Melendez (DNP Thesis Prize 2021), R. Furnstahl, M. Pratola (OSU), D. R. Phillips (Ohio U), J. A. McGovern (U Manchester), hg: 2004.11307
Eur. Phys. J. **A 57** (2021) 81 + **buqeye.github.io**: JUPYTER notebooks

1. Error Bars for Nucleonic Two Photon Response

(a) (Dis)Agreement Significant Only When All Error Sources Explored

Editorial PRA 83 (2011) 040001

PHYSICAL REVIEW A **83**, 040001 (2011)

Editorial: Uncertainty Estimates

The purpose of this Editorial is to discuss the importance of including uncertainty estimates in papers involving theoretical calculations of physical quantities.

It is not unusual for manuscripts on theoretical work to be submitted without uncertainty estimates for numerical results. In contrast, papers presenting the results of laboratory measurements would usually not be considered acceptable for publication The question is to what extent can the same high standards be applied to papers reporting the results of theoretical calculations. It is all too often the case that the numerical results are presented without uncertainty estimates. Authors sometimes say that it is difficult to arrive at error estimates. Should this be considered an adequate reason for omitting them? In order to answer this question, we need to consider the goals and objectives of the theoretical (or computational) work being done. Theoretical papers

accuracy. However, the same is true for the uncertainties in experimental data. The aim is to estimate the uncertainty, not to state the exact amount of the error or provide a rigorous bound.

There are many cases where it is indeed not practical to give a meaningful error estimate for a theoretical calculation; for example, in scattering processes involving complex systems. The comparison with experiment itself provides a test of our theoretical understanding. However, there is a broad class of papers where estimates of theoretical uncertainties can and should be made. Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances:

1. If the authors claim high accuracy, or improvements on the accuracy of previous work.
2. If the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements.
3. If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

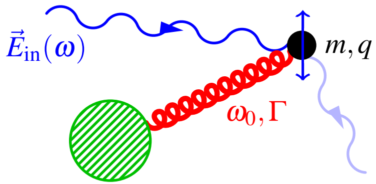
Scientific Method: Quantitative results with corridor of theoretical uncertainties for *falsifiable predictions*.

Need procedure which is established, economical, reproducible: room to argue about "error on the error".

"Double-Blind" Theory Errors: Assess with pretense of no/very limited data.

(b) Polarisabilities: Stiffness of Charged Constituents in El.- Mag. Fields

Example: induced electric dipole radiation from harmonically bound charge, damping Γ Lorentz/Drude 1900/1905



$$\vec{d}_{\rm ind}(\omega) = \underbrace{\frac{q^2}{m}\frac{1}{\omega_0^2-\omega^2-\mathrm{i}\Gamma\omega}}_{=:\,4\pi\,\alpha_{E1}(\omega)}\vec{E}_{\rm in}(\omega)$$

$=: 4\pi\,\alpha_{E1}(\omega)$ "displaced volume" $[10^{-4}\ \mathrm{fm}^3]$

electric scalar dipole polarisability

Energy-dependence dis-entangles *interaction scales, symmetries & mechanisms* with & among constituents.

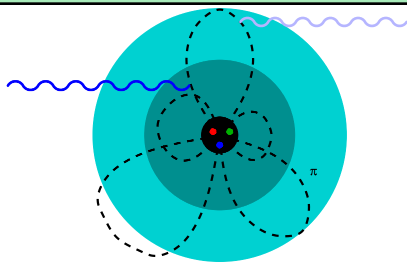
Clean, perturbative probe: χiral symmetry of pion-cloud & its breaking, $\Delta(1232)$, spin-constituents.

Fundamental hadron properties, like charge, mass, mag. moment, $\langle r_N^2\rangle\ldots$ PDG

$$2\pi\left[\underbrace{\alpha_{E1}\,\vec{E}^2+\beta_{M1}\,\vec{B}^2}_{\text{electric, magnetic scalar dipole}}+\underbrace{\gamma_{E1E1}\vec{\sigma}\cdot(\vec{E}\times\dot{\vec{E}})+\gamma_{M1M1}\vec{\sigma}\cdot(\vec{B}\times\dot{\vec{B}})+2\gamma_{M1E2}\sigma^iB^jE_{ij}+2\gamma_{E1M2}\sigma^iE^jB_{ij}}_{\text{spin-dependent dipole response of nucleon-spin constituents}}+\ldots\right]$$

electric, magnetic scalar dipole

spin-dependent dipole response of nucleon-spin constituents

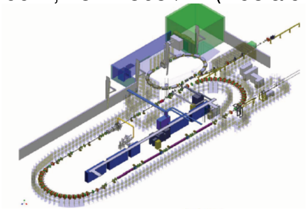


(c) Who Answers The Call?

[Since last US LRP,] substantial progress has been made [. . .], with strong international efforts and synergistic 1094 advancements in experiment and theory. [*The Present and Future of QCD*, US Town Meeting White Paper 2023]

Lattice QCD: relate to fundamental interactions

$\longrightarrow$ *polarQCD* (Alexandru/Lee) 2005-; *NPLQCD* 2006-; *LHPC* (Engelhardt) 2007-; Leinweber/. . . (Adelaide) 2013



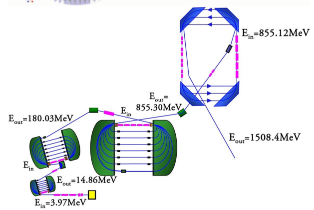
Experiment: Significant investments; data taken/scheduled/approved:

HIγS (TUNL/Duke U. NC, USA; DOE):

> 3000 hrs already committed at $60 - 100$ MeV

proton doubly & beam pol. deuteron unpol & beam pol.

^{3}He unpol & doubly pol. ^{4}He, ^{6}Li unpol.



A2 @ MAMI (Mainz U. Germany; DFG: 5-year SFB):

running, data cooking and planned

proton $100 - 400$ MeV: beam & target pol.

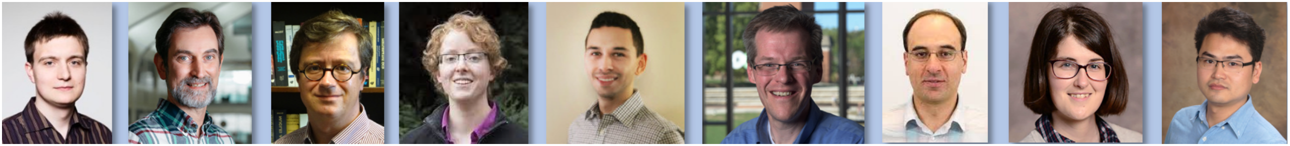
deuteron, ^{3}He, ^{4}He unpol., beam & target pol.

MAXlab (Lund U., Sweden): data cooking continues deuteron $100 - 160$ MeV: unpol.

Chiral EFT: data consistency, binding effects, analysis, extraction

Community Goal: Unified framework with reliable error bars for proton, deuteron, ^{3}He (elastic & inelastic) into $\Delta(1232)$ region.

Goals: Comprehensive picture of Compton scattering and nucleon polarisabilities, with probabilistic interpretation of theory truncation uncertainties.
Guide, support, analyse, predict new generation of experiments, and relate data and lattice QCD.



Joining with **The BUQEYE Collaboration: Bayesian Uncertainty Quantification: Errors in Your EFT**

Jordan Melendez did the work. $\Longrightarrow$ DNP Thesis Prize 2021.
Daniel Phillips and Richard Furnstahl explained it to me.

2. Bayesian Truncation Errors at a Point

(a) The Low-Energy Method: Chiral Effective Field Theory

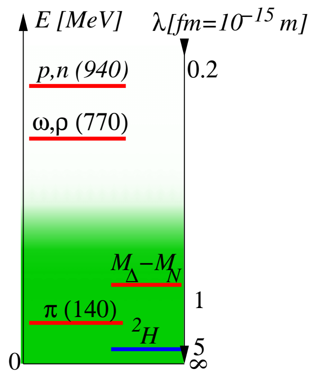
Degrees of freedom $\pi, N, \Delta(1232) +$ **all interactions allowed by symmetries:** Chiral SSB, gauge, iso-spin,...

$\Longrightarrow$ **Chiral Effective Field Theory χEFT $\equiv$ low-energy QCD**

Controlled approximation $\Longrightarrow$ ***Model-independent, error-estimate*.**

Expand in $\frac{\omega}{\Lambda_\chi}$ **and** $\delta = \frac{M_\Delta - M_N}{\Lambda_\chi} \approx \sqrt{\frac{m_\pi}{\Lambda_\chi}} \approx 0.4 \ll 1$ (numerical fact)

Pascalutsa/Phillips 2002

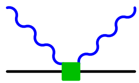
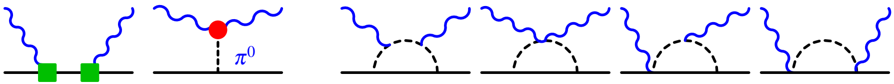
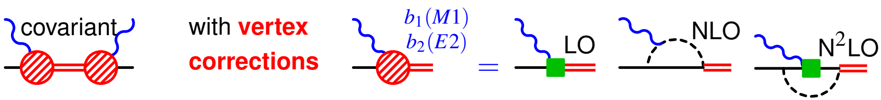
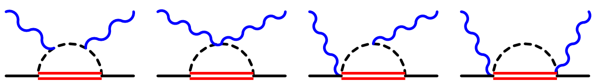
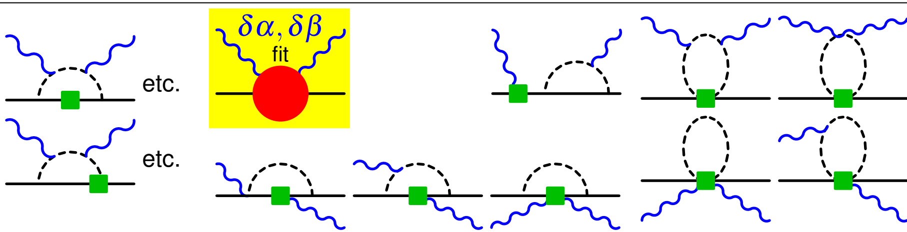


(b) All 1N Contributions to N^{4}LO

Bernard/Kaiser/Meißner 1992-4, Butler/Savage/Springer 1992-3, Hemmert/... 1998
McGovern 2001, hg/Hemmert/Hildebrandt/Pasquini 2003
McGovern/Phillips/hg 2013

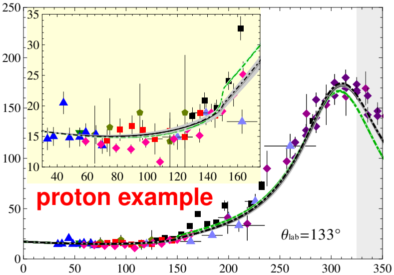
Unified Amplitude: accuracy decreases with ω:

	in low régime	$\omega \lesssim m_\pi$	at least N^{4}LO $(e^2\delta^4)$:	accuracy $\delta^5 \lesssim 2\%$;
or	in high régime	$\omega \sim M_\Delta - M_N$	at least NLO $(e^2\delta^0)$:	accuracy $\delta^2 \lesssim 20\%$.

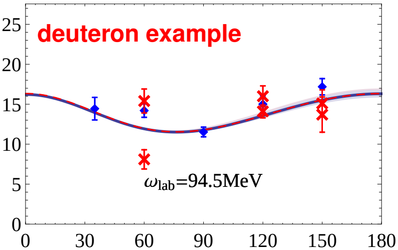
Diagrams	$\omega \lesssim m_\pi$	$\omega \sim M_\Delta - M_N \approx 300$ MeV
 Thomson term: $-\frac{Z^2\alpha_{EM}}{M}$	$e^2\delta^0$ ***LO***	$e^2\delta^0$ ↘NLO
	$e^2\delta^2$ N^{2}LO	$e^2\delta^1$ N^{2}LO
	$e^2\delta^3$ N^{3}LO	$e^2\delta^{-1}$ ↗***LO***
	$e^2\delta^3$ N^{3}LO	$e^2\delta^1$ N^{2}LO
	$e^2\delta^4$ N^{4}LO	$e^2\delta^2$ N^{3}LO

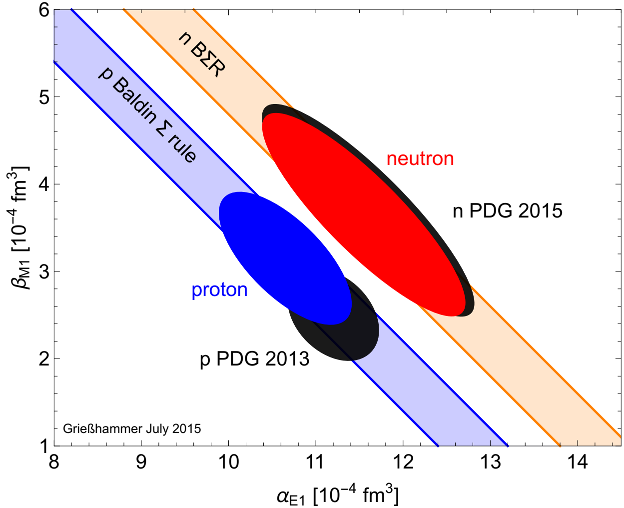
Unknowns: short-distance $\delta\alpha, \delta\beta \Longleftrightarrow$ static α_{E1}, β_{M1} (offset) $\Longrightarrow$ ω-dependence *predicted*.

(c) Scalar Polarisabilities from Consistent p & d Databases

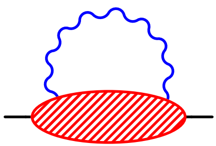


$\Longleftarrow \Delta(1232)$





	α_{E1} $[10^{-4}$ fm$^3]$	β_{M1} $[10^{-4}$ fm$^3]$	χ^2/d.o.f.
proton (Baldin, N^{2}LO) McGovern/Phillips/hg EPJA 2013	$10.65 \pm 0.35_{\text{stat}} \pm 0.2_{\Sigma} \pm 0.3_{\text{theory}}$	$3.15 \mp 0.35_{\text{stat}} \pm 0.2_{\Sigma} \mp 0.3_{\text{theory}}$	113.2/135
neutron (Baldin, NLO) COMPTON@MAX-lab PRL 2014	$11.55 \pm 1.25_{\text{stat}} \pm 0.2_{\Sigma} \pm 0.8_{\text{theory}}$	$3.65 \mp 1.25_{\text{stat}} \pm 0.2_{\Sigma} \mp 0.8_{\text{theory}}$	45.2/44



$\Longrightarrow$ **neutron ≈ proton polarisabilities:** $\alpha_{E1}^{p-n} = -0.9 \pm 1.6_{\text{tot}}$ – **exp. & neutron errors dominate**

$-0.6 \pm 1.2_{\text{tot}}$ PDG 2022

Cottingham ΣR explains $M_\gamma^p - M_\gamma^n$ **with** $\alpha_{E1}^{p-n} = -1.7 \pm 0.4_{\text{tot}}$ **Gasser/Hoferichter/Leutwyler/Rusetzky** 1506.06747

(d) Theorists Have Error Bars: “Truncation” Errors!

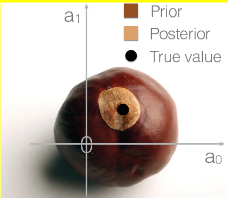
max-criterion: lore since ”time immemorial”
Bayes: e.g. Cacciari/Houdeau 1105.5152
BUQEYE 1506.01343+1511.03618
applied in hg/JMcG/DRP 1511.01952

$$\chi\text{EFT } \alpha_{E1}^{(\mathrm{p})} - \beta_{M1}^{(\mathrm{p})}\ [10^{-4}\ \mathrm{fm}^3]: 7.5 \pm ???_{\text{th}} = 11.2_{\text{LO}} - 3.6_{\text{NLO}} - 0.1_{\text{N}^2\text{LO}} \pm ???_{\text{th}}$$

Observable as series of k terms to N^{k-1}LO: $\mathcal{O}^{(k=2)} = c_0 + c_1\,\delta^1 + c_2\,\delta^2$ +unknown $c_3 \times \delta^3$

Assuming $\delta \simeq 0.4$: $11.2 \quad -9.1\,\delta^1 - 0.6\,\delta^2$ +unknown $\times\,\delta^3$

$\Longrightarrow$ **Estimate next term *“most conservatively”* as** $|$unknown $c_3| \lesssim c_{\max} := \max\{|c_0|;|c_1|;|c_2|\}$.



BUQEYE Collaboration

No infinite sampling pool; data fixed; more data changes confidence.

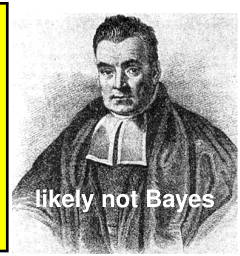
Call upon the Reverend Bayes for probabilistic interpretation!

e.g. **BUQEYE collaboration** Furnstahl/Phillips/… 1506.01343+1511.01952+…

New information increases level of confidence.

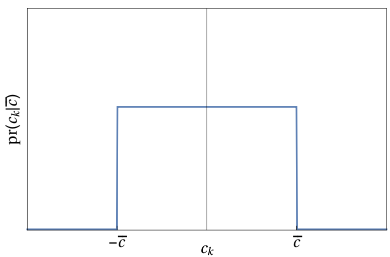
$\Longrightarrow$ **Smaller corrections, more reliable uncertainties.**

Clearly state your premises/assumptions – including *naturalness*.



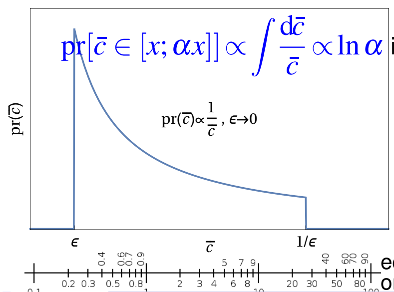
Priors: leading-omitted term dominates ($\delta \ll 1$); putative distributions of *all* c_k's and of largest value $\bar{c}$ in series.

Uniform ~~“least informed/-ative”~~: All values c_k equally likely, given upper bound $\bar{c}$ of series.



“Any upper bound” (*Benford's Law*): $\ln$-uniform prior sets no bias on scale of $\bar{c}$

$$\mathrm{pr}[\bar{c} \in [x;\alpha x]] \propto \int \frac{\mathrm{d}\bar{c}}{\bar{c}} \propto \ln\alpha$$ indep. of x



equi-distributed on $\ln$ scale

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χEFT $\alpha_{E1}^{(p)} - \beta_{M1}^{(p)}$ $[10^{-4}\ \mathrm{fm}^3]$: $7.5 \pm ???_{\text{th}} = \mathbf{11.2}_{\text{LO}} - 3.6_{\text{NLO}} - 0.1_{\text{N}^2\text{LO}} \pm ???_{\text{th}}$

Observable as series of k terms to N^{k-1}LO: $\mathcal{O}^{(k=2)} = c_0 + c_1\,\delta^1 + c_2\,\delta^2$ +unknown $c_3 \times \delta^3$

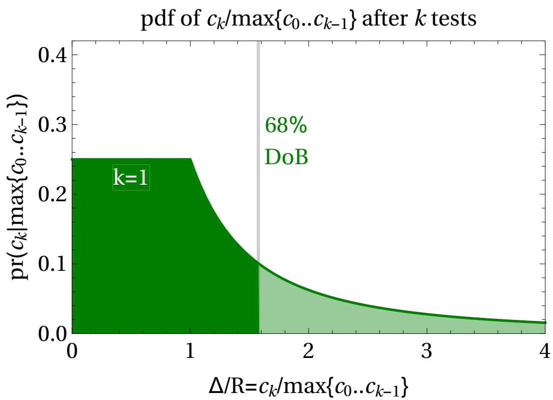
Assuming $\delta \simeq 0.4$: $\mathbf{11.2}\ -9.1\,\delta^1\ -0.6\,\delta^2$ +unknown $\times\,\delta^3$

$\Longrightarrow$ **Estimate next term *“most conservatively”* as** $|$**unknown** $c_3| \lesssim c_{\max} := \max\{|c_0|;|c_1|;|c_2|\}$.

Result: Posterior $\equiv$ *Degree of Belief (DoB)* that next term $c_k\delta^k$ differs from order-k central value by $x\delta^k$.

$$\mathrm{pr}(x|c_{\max},\text{order }k) \propto \int_0^\infty \mathrm{d}\bar{c}\ \mathrm{pr}(\bar{c})\ \mathrm{pr}(x|\bar{c}) \prod_{n=0}^{k-1} \mathrm{pr}(c_n|\bar{c}) \to \frac{k}{k+1}\frac{1}{c_{\max}} \begin{cases} 1 & x \le c_{\max} \\ \frac{1}{x^{k+1}} & x > c_{\max} \end{cases}$$

BUQEYE 1506.01343 eq. (22)



Priors: all c_n “equally likely”, “any upper bound” $\bar{c}$.

order	in $\pm c_{\max}$	$\Delta^{(k)}(68\%)$	$\Delta^{(k)}(95\%)$
LO	$\frac{1}{2} = 50\%$	$1.6\,c_{\max}$	$11 c_{\max} = 7\,\Delta_{68}^{(1)}$
Gauß	68.27%	$1.0\,c_{\max}$	$2.0\,\Delta_{68}^{(k)}$

Laplace’s Law of Succession (flat prior, T/F): Chance that next coefficient $< c_{\max}$ is $\dfrac{k}{k+1}$.

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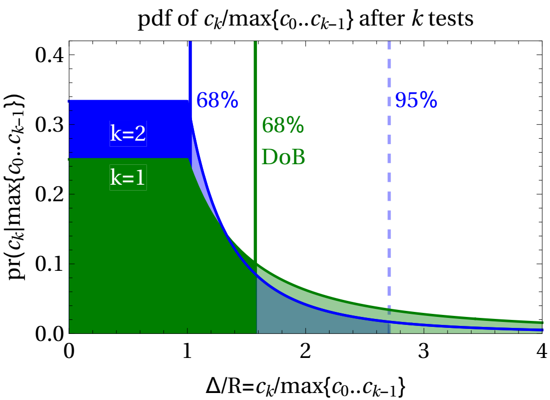

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$\Longrightarrow$ **Estimate next term *"most conservatively"* as** $|$unknown $c_3| \lesssim c_{\max} := \max\{|c_0|;|c_1|;|c_2|\}$.

Result: *Posterior* $\equiv$ *Degree of Belief (DoB)* that next term $c_k\delta^k$ differs from order-k central value by $x\delta^k$.

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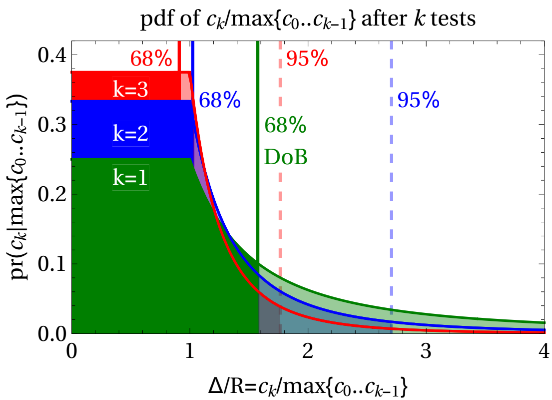

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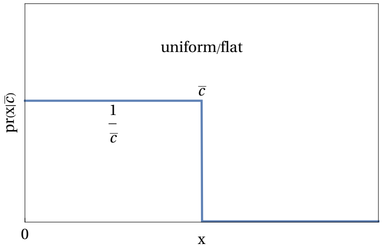
NLO	$\frac{2}{3} = 66.7\%$	$1.0\ c_{\max}$	$2.7 c_{\max} = 2.6\ \Delta_{68}^{(2)}$
N^{2}LO	$\frac{3}{4} = 75\%$	$0.9\ c_{\max}$	$1.8 c_{\max} = 1.9\ \Delta_{68}^{(3)}$
N^{k-1}LO k terms	$\frac{k}{k+1}$	$0.68\frac{k+1}{k} c_{\max}\,(k \ge 2)$	
Gauß	68.27%	$1.0\ c_{\max}$	$2.0\ \Delta_{68}^{(k)}$

$\Longrightarrow$ **Use theory uncertainties with these priors: "$\mathcal{O}^{(k)} \pm \Delta_{68}^{(k)}$": 68% *DoB interval* $[\mathcal{O}^{(k)} - \Delta_{68}^{(k)}; \mathcal{O}^{(k)} + \Delta_{68}]$.**

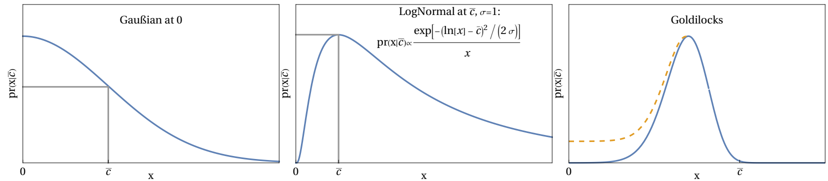
Prior Choice: What is “Natural Size”? (SCOTUS: I Know It When I see It.)

Observable $\mathcal{O} = c_0 + c_1\delta^1 + c_2\delta^2 +$ unknown $\times\ \delta^3$: *assumed* $\delta \approx 0.4$ *& “naturally-sized coefficients”* c_i.



Uniform ~~“Least informative/-ed”~~:

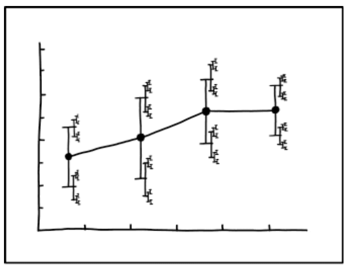
characterised by 1 number: $\bar{c}$.



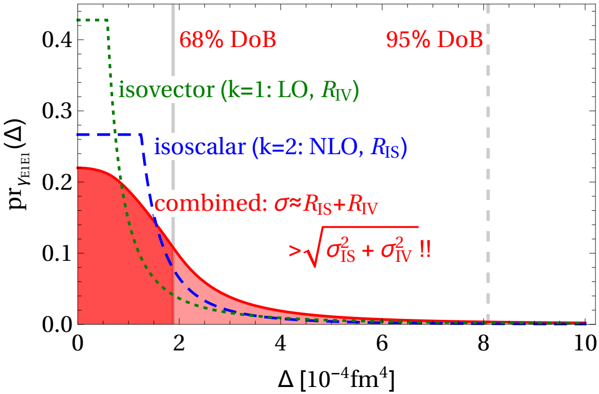
“More informed choices”: more complicated structures, more thought,

more parameters: $\bar{c}$, typ. size, spread,. . .

Buqeye: When $k \geq 2$ orders known, DoBs with
different assumptions about $\bar{c}$, c_n vary by $\lesssim \pm 20\%$ for some “reasonable priors”.



(e) More Bayes Comments



Posterior pdf *not Gauß'ian:*

Plateau & power-law tail.

$\Longrightarrow$ **Do not add in quadrature for convolution**

(more like linear).

Bayes provides well-defined *procedure*!

$\Longrightarrow$ **Quantitative theoretical uncertainties make EFT falsifiable:**

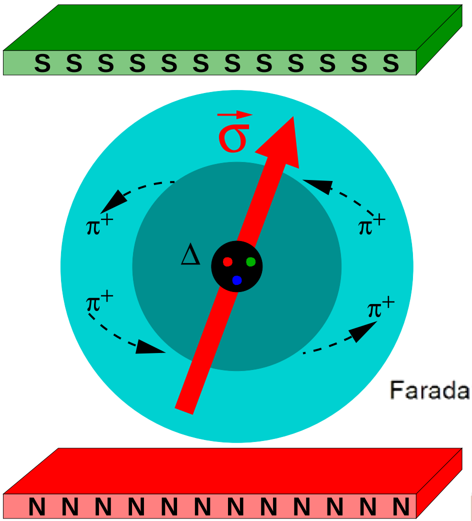
Economical, reproducible procedure: argue about "error on error".

"The aim is to estimate the uncertainty, not to state the exact amount[. . .]"

PRA Editorial 2011

(a) Spin Polarisabilities: Nucleonic Bi-Refringence and Faraday Effect

Optical Activity: Response of spin-degrees of freedom, complements JLab spin programme.



$$\mathcal{L}_{\text{pol}} = 4\pi\, N^\dagger \times \Big\{ \tfrac{1}{2} \Big[\alpha_{E1}\, \vec{E}^2 + \beta_{M1}\, \vec{B}^2 \Big]$$

electric / magnetic scalar dipole

$$+ \tfrac{1}{2} \Big[\gamma_{E1E1}\, \vec{\sigma}\cdot(\vec{E}\times\dot{\vec{E}}) + \gamma_{M1M1}\, \vec{\sigma}\cdot(\vec{B}\times\dot{\vec{B}})$$

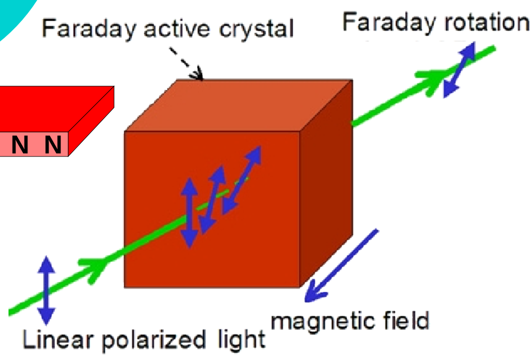
"pure" spin-dependent dipole

$$-2\,\gamma_{M1E2}\, \sigma_i\, B_j\, E_{ij} + 2\,\gamma_{E1M2}\, \sigma_i\, E_j\, B_{ij} \Big] + \dots \Big\} N$$

"mixed" spin-dependent dipole

$+$ quadrupole etc.

$E_{ij} := \frac{1}{2}(\partial_i E_j + \partial_j E_i)$ etc.

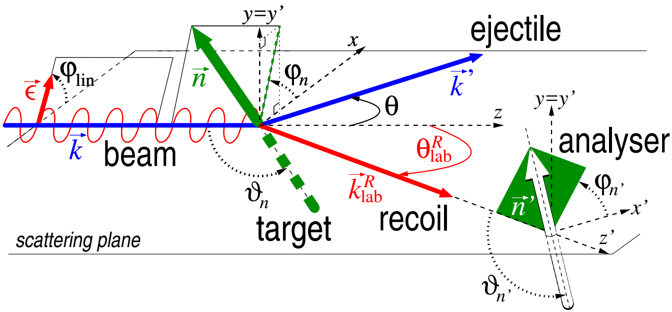


(b) Plethora of Observables for Polarised Beams on Polarised Targets/Recoils

Any Target: 1 **Cross section** — **sets scale for rates**

Proton: $+7$ **Asymmetries:** — 1 **beam,** 1 **target,** 2 **circpol. double,** 3 **linpol. double**

$+5$ **Polarisation Transfers:** — 2 **circpol. beam on pol. recoil,** 3 **linpol. beam on pol. recoil**



$$\frac{1}{2}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\bigg|_{\text{unpol}} \times \Big[\; 1+\xi_3\,\Sigma_3(\omega,\theta) + P n_{y'}\,\Sigma_y(\omega,\theta) + \xi_3\,P n_{y'}\,\Sigma_{3y'}(\omega,\theta) + \xi_1\Big(P n_{x'}\,\Sigma_{1x'}(\omega,\theta) + P n_{z'}\,\Sigma_{1z'}(\omega,\theta)\Big) + \xi_2\Big(P n_{x'}\,\Sigma_{2x'}(\omega,\theta) + P n_{z'}\,\Sigma_{2z'}(\omega,\theta)\Big)\Big]$$

Babusci/Giordano/L'vov/Matone/Nathan 1998, Arenhövel 1991

$\vec{\xi}$: Stokes parameters of photon polarisation

$P\vec{n}$: nucleon polarisation

green: polarisation transfer, setting $P=1$

6 proton polarisabilities $+$ **constraints on** $\alpha_{E1}+\beta_{M1}$, γ_0,**. . . ; experiment: detector settings, feasibilities,. . .**

"At present, single and double polarised data is sorely missing." **Theory letter 1409.1512**

No single measurement to provide definitive answers: multi-parameter extractions, systematics, validation.

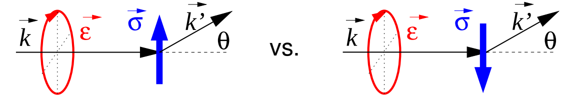
$\Longrightarrow$ **Experiment & Theory must collaborate: validate data/theory, identify *observables with biggest impact.***

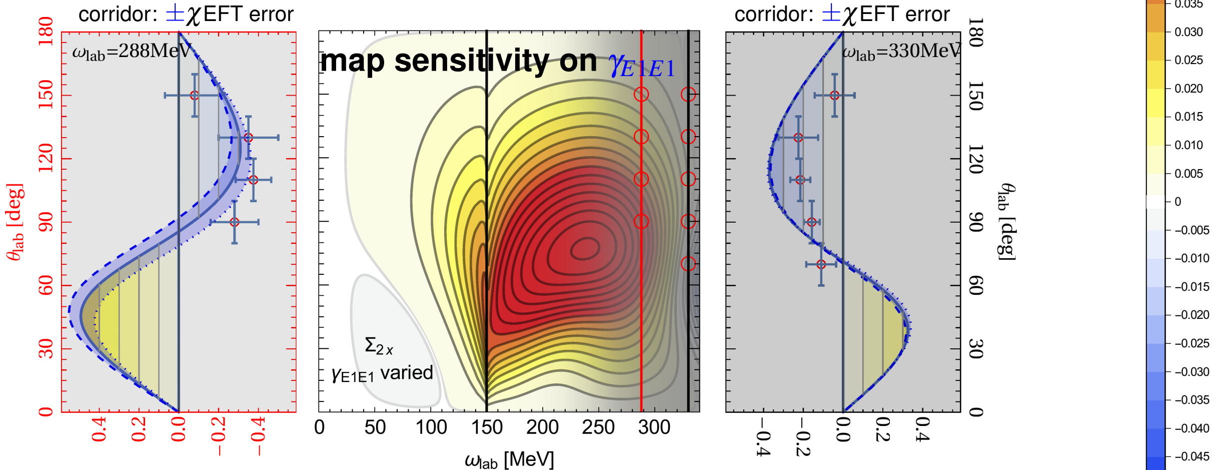
(c) Proton Spin Polarisabilities from Polarised Photons

$\mathcal{O}(e^2\delta^3)$: hg/Hildebrandt/…2003
$\mathcal{O}(e^2\delta^4)$: hg/McG/Ph 1511.0952&1711.11546
exp MAMI: Martel/…PRL 2014; Collicott/…2019

Incoming γ circularly polarised, sum over final states. N-spin in $(\vec{k},\vec{k}')$-plane, perpendicular to $\vec{k}$:

Σ_{2x} :





static $[10^{-4}\ \mathrm{fm}^4]$	γ_{E1E1}	γ_{M1M1}	γ_{E1M2}	γ_{M1E2}
MAMI 2019 proton 1909.02032	-2.8 ± 0.5	2.7 ± 0.4	-0.85 ± 0.7	2.0 ± 0.5
χEFT proton **predicted**	$-1.1\pm1.9_{\text{th}}$	$2.2\pm0.5_{\text{stat}}\pm0.6_{\text{th}}$	$-0.4\pm0.6_{\text{th}}$	$1.9\pm0.5_{\text{th}}$

Theory: most accurate at $\omega\lesssim 230$ MeV $\Longleftrightarrow$ Experiment: high count rates at high ω.

Accounting for theory and experimental limitations: Where is the Sweet-Spot?

(d) How To Spend Your Time & Money Wisely?

Deliberate experimental planning needs to integrate
theory $\oplus$ experimental facts $\oplus$ likeliness of success
to optimise money & time & workforce & reputation in suite of future measurements!
$\Longrightarrow$ **Gain knowledge, test theories, find new effects.**

Challenges: **No Theory Is Perfect: predictions of finite accuracy, better at lower energies.**

Data: noisy, varying degrees of quality & reliability – 1-10% errors, correlations.

Constraints: detector location (walls), difficulty of observables, count rates,. . .

Future with different exp. noise levels: Standard (Ikea) – Doable ($) – Aspirational ($$$)

$\Longrightarrow$ **Need to find "Sweet-Spot" between competing effects, given constraints & tensions.**

High energy: high count rates $\Longrightarrow$ short runs, high statistics —— theory less accurate

Low energy: low count rates $\Longrightarrow$ long runs for adequate statistics —— theory more accurate

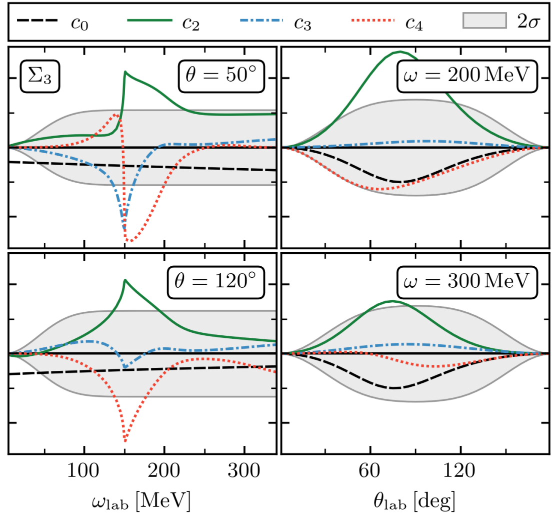
Desired : **"Optimal Impact Machine" (generally accepted/well-defined/reproducible/canned) to identify sequence of experiments with likely high(est) impact & chance of success: strategically placed data with excellent Figures of Merit for more-accurate theory validation, parameter extractions,. . .**

Energy- & angle-dependent Observable

$$\mathcal{O}(\omega,\theta) = c_0(\omega,\theta) + c_2(\omega,\theta)\,\delta^2(p_{\text{typ}}) + c_3(\omega,\theta)\,\delta^3(p_{\text{typ}}) + c_4(\omega,\theta)\,\delta^4(p_{\text{typ}}) + \dots$$

Complications:

- For some $\mathcal{O}$bs, $c_n \equiv 0$ at $\omega = 0$ or $\theta = 0$ or π.
- $\delta(p_{\text{typ}}) \approx \sqrt{\frac{m_\pi+\omega}{2\Lambda_\chi}}$ changes with ω.
- Relative importance of $\Delta(1232)$ changes with ω.
- Structure at pion cusp. $\Longrightarrow$ Skip in $\mathcal{GP}$.



example Σ_3: θ fixed ω fixed

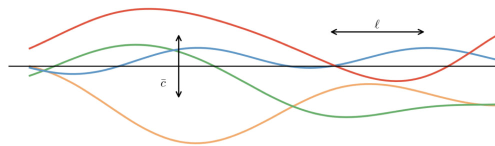
Coefficient functions appear reasonable:

bounded, neither grow nor shrink with order ✓.

Find DoBs per (ω,θ)? ⚡ Close-by strongly / Far-away weakly correlated.

$\Longrightarrow$ **Hypothesis:** $c_n(\omega,\theta)$ as independent draws of **Gaußian Process** $\mathcal{GP}$, i.e. Gaußian at each (ω,θ) with translation-inv. correlation

$$\langle c_n(\omega_1,\theta_1), c_n(\omega_2,\theta_2)\rangle = \bar{c}^2\ \exp - \left[\frac{(\omega_1-\omega_2)^2}{2\ell_\omega^2} + \frac{(\theta_1-\theta_2)^2}{2\ell_\theta^2}\right]$$



mean $\bar{c}$ (prior: $\chi^{-2}(1,1)$) and correlation lengths $(\ell_\omega,\ell_\theta)$ (prior: uniform) same for all orders n, depend on $\mathcal{O}$bs.

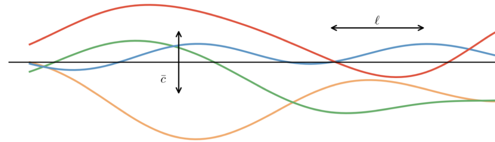
Training: $\bar{c},\ell_\omega,\ell_\theta$ for each $\mathcal{O}$ from known $\{c_n\}$'s. $\Longrightarrow$ typical correlation lengths $\ell_\omega \sim 50$ MeV, $\ell_\theta \sim 45°$

(e) Truncation Errors For Functions: Gaußian Process $\mathcal{GP}$

BUQEYE: PRC 100 (2019) 044001
1904.10581, buqeye.github.io

$\Longrightarrow$ **Hypothesis:** $c_n(\omega,\theta)$ as independent draws of **Gaußian Process** $\mathcal{GP}$, i.e. Gaußian at each (ω,θ) with translation-inv. correlation

$$\langle c_n(\omega_1,\theta_1), c_n(\omega_2,\theta_2)\rangle = \bar{c}^2 \ \exp - \left[\frac{(\omega_1-\omega_2)^2}{2\ell_\omega^2} + \frac{(\theta_1-\theta_2)^2}{2\ell_\theta^2}\right]$$

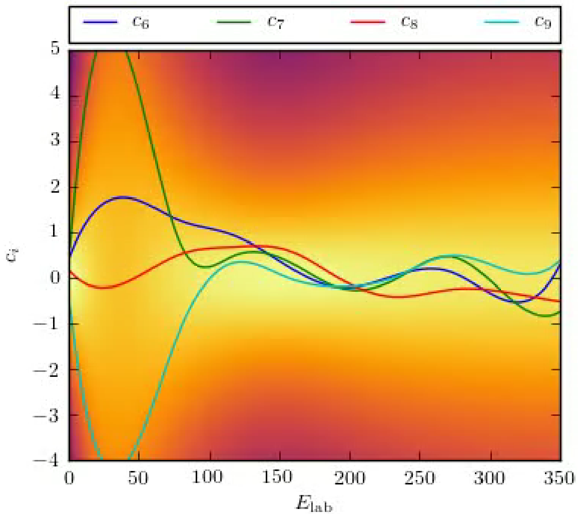


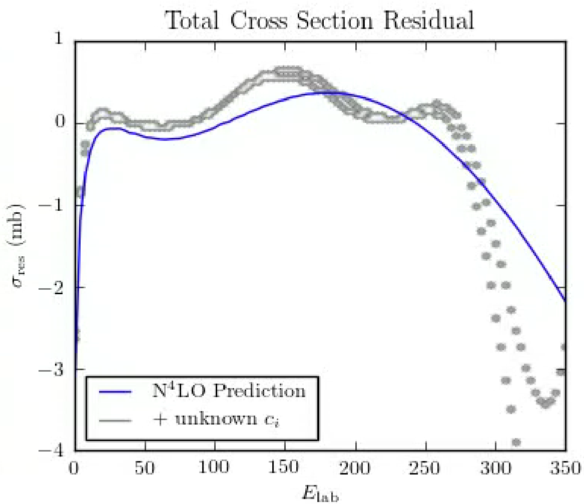
mean $\bar{c}$ (prior: $\chi^{-2}(1,1)$) and correlation lengths $(\ell_\omega,\ell_\theta)$ (prior: uniform) same for all orders n, depend on $\mathcal{O}$bs.

Training: $\bar{c},\ell_\omega,\ell_\theta$ for each $\mathcal{O}$ from known $\{c_n\}$'s. $\Longrightarrow$ typical correlation lengths $\ell_\omega \sim 50$ MeV, $\ell_\theta \sim 45^\circ$

$\Longrightarrow$ **Truncation Error from range of unknown c_n's:** random functions with fixed correlation

buqeye.github.io, see PRC 100 (2019) 044001 1904.10581





OPTIMAL IMPACT MACHINE: Maximise benefits – minimise cost (time, money, workforce, data not taken).

Input: (1) **Present polarisability errors** $\Delta\alpha\beta\gamma$ (th & exp, some correlated) – values $\alpha\beta\gamma$ irrelevant.

(2) χ**EFT Predictions** with truncation errors via $\mathcal{GP}$, increasing as $\omega\nearrow$. posterior predictive distr.

(3) **New Data Position** $\overrightarrow{\omega\theta}$: We took 1 energy with 5 angles (exp. constraints) – values $y(\overrightarrow{\omega\theta})$ irrelevant.

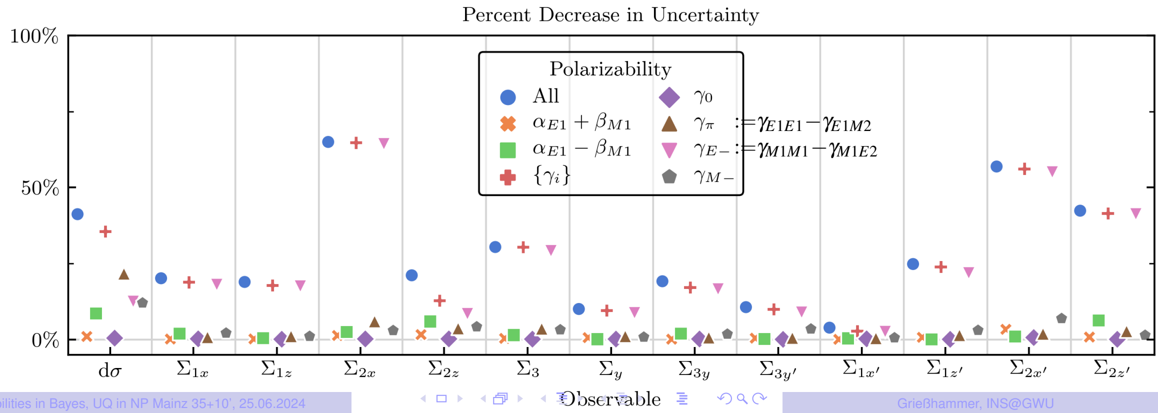
(4) **New Data Quality**: **"Doable ($)"**: cross sections to $\pm 4\%$, asymmetries to ± 0.06 (absolute).

(3+4) $=$ **Expert Elicitation:** Could also add direct penalties for cost, beamtime, event rate,...

here pragmatic: impact of existing data via fits of $\alpha\beta\gamma$; choose uniform exp. constraints.

Utility Gain: What new data at points $\overrightarrow{\omega\theta}$ with results y guessed from theory (with errors) gives likely biggest

$$U_{\rm KL} = \underbrace{\int \mathrm{d}y\ \mathrm{pr}(y|\overrightarrow{\omega\theta}) \int \mathrm{d}(\alpha\beta\gamma)}_{\text{data } y \text{ \& central } \alpha\beta\gamma \text{ marginalised}}\ \underbrace{\mathrm{pr}(\alpha\beta\gamma|y,\overrightarrow{\omega\theta})\ \ln\frac{\mathrm{pr}(\alpha\beta\gamma|y,\overrightarrow{\omega\theta})}{\mathrm{pr}(\alpha\beta\gamma)}}_{\text{Shannon information gain}} \underset{\text{linearisation works very well}}{\overset{\downarrow}{\approx}} \ln\left\langle\frac{\text{error's hypervolume before}}{\text{error's hypervolume after data}}\right\rangle_{\rm avg}$$

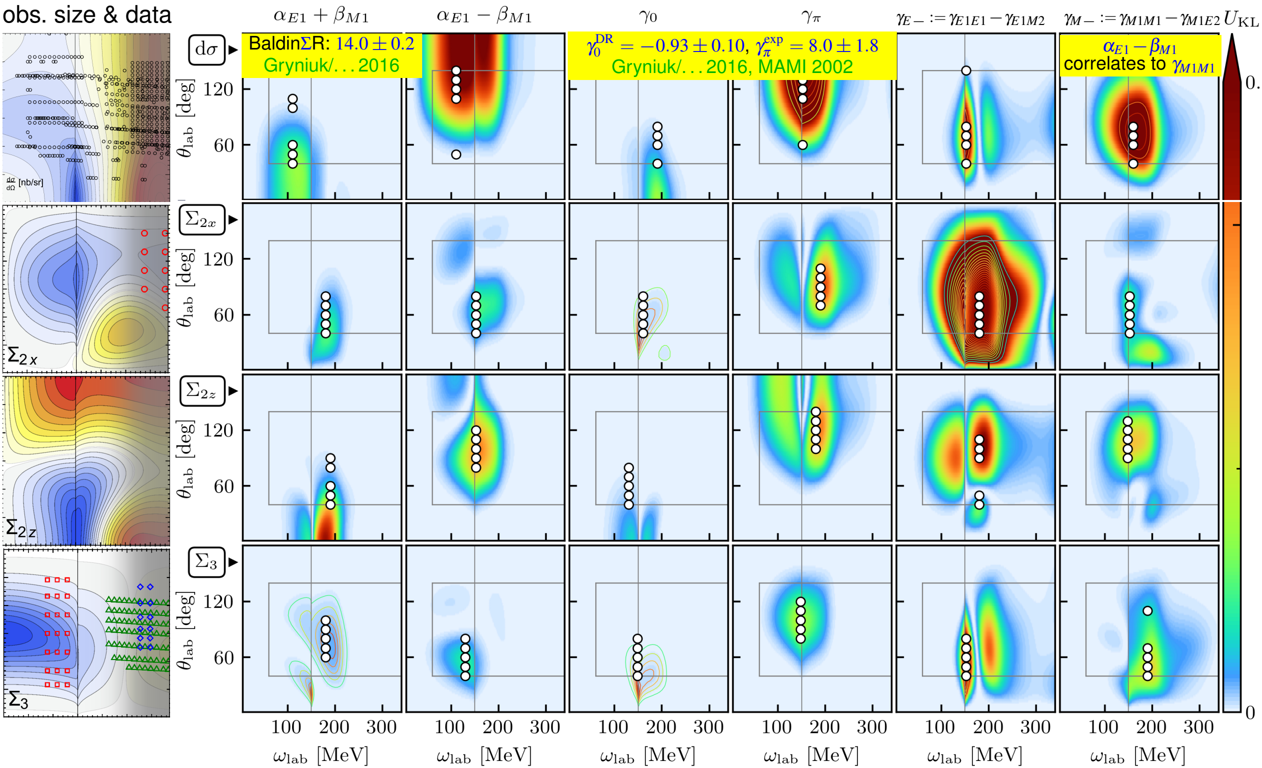


(f) Bayesian Posterior Shrinkage by Intelligent Design

BUQEYE: Melendez/Furnstahl/Pratola/DRP/hgrie/JAMcG/… EPJ**A57** (2021) 81 2004.11307

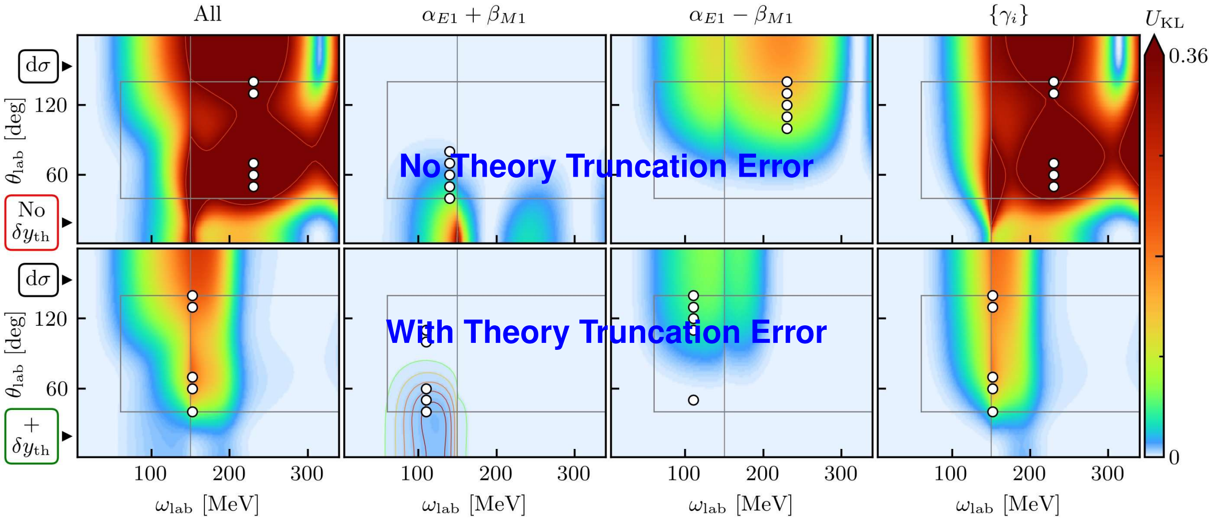
Jupyter notebook at `buqeye.github.io`

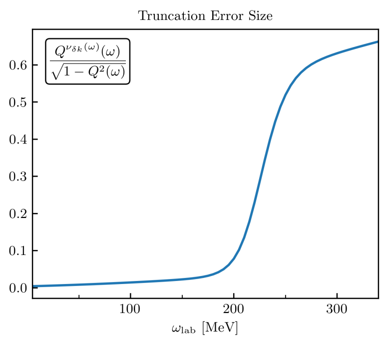
Proton: Which 5 future angles have biggest impact on a particular polarisability?



$\Longrightarrow$ **Focus on** $\mathrm{d}\sigma(100\ \mathrm{MeV})$: $\alpha_{E1}-\beta_{M1}$, $\mathrm{d}\sigma(160\ \mathrm{MeV})$: γ_{M-}; $\Sigma_{2x}(170\ \mathrm{MeV})$: γ_{E-} – ***not*** **beam asym.** Σ_3

(f) Bayesian Posterior Shrinkage by Intelligent Design





$$\mathcal{O} = c_0 + c_2\delta^2 + c_4\delta^3 + c_4\delta^4 + \dots$$

$$\delta = \sqrt{\frac{p_{typ} \sim (\omega \sim m_\pi \nearrow \Delta_M)}{\overline{\Lambda}_\chi}}$$

Forgetting EFT Truncation Error

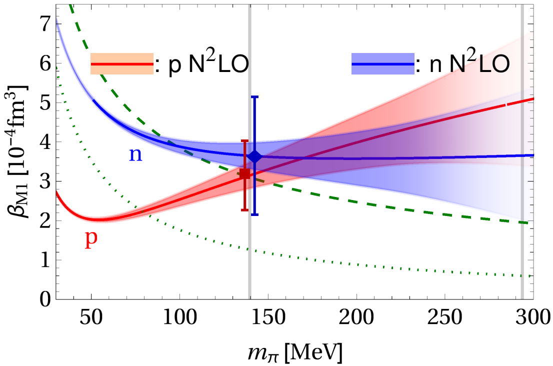
Over-Estimates Signal (scale changed!)

Over-Emphasises Resonance Region!

$\Longrightarrow$ **Wrong data point decision!**

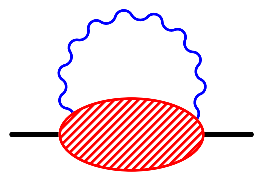
χ**EFT: explicit m_π-dependence** $\mathcal{O} = c_0(m_\pi) + c_1(m_\pi)\delta^1 + c_2(m_\pi)\delta^2 +$ **unknown** $\times\, \delta^3$, **fixed at** m_π^{phys}.

Uncertainties: Bayesian order-by-order at each m_π.



Isospin splitting *statistically* significant for $m_\pi \lesssim 120$ MeV.

$\Longrightarrow$ SPECULATION – NO ERROR BARS



Cottingham Σ Rule: $\beta_{M1}^{\text{p}-\text{n}}$ is *one of several* inputs into the proton-neutron self-energy difference:

$$M_{\text{p}-\text{n}} = M_{\text{p}-\text{n}}^{\text{strong}} + M_{\text{p}-\text{n}}^{\text{em,elastic}} - A\, \beta_{M1}^{\text{p}-\text{n}}$$

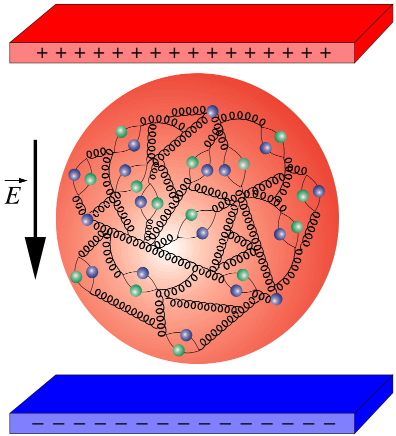
Impact on p-n mass difference?: $-A\beta_{M1}^{\text{p-n}} \approx 0.5$ MeV wants more stable n as $m_q \searrow$, competes with $M_{\text{p-n}}^{\text{strong}}$.

$\rightarrow$ Neutron lifetime $\rightarrow$ Big Bang Nucleosynthesis $\rightarrow$ Anthropic Principle?

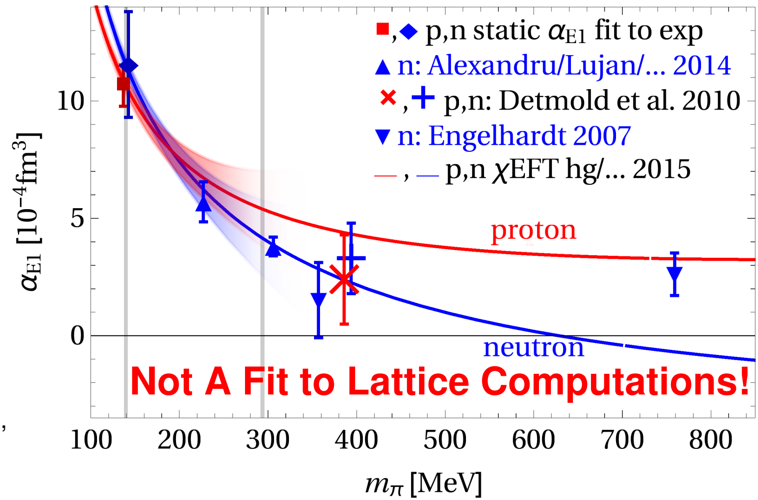
(h) Chiral Extrapolations for Polarisabilities in Lattice QCD

Towards comparable uncertainties in experiment, χEFT and lattice QCD.

χEFT: reliable error estimate for $\frac{m_\pi}{\Lambda_\chi}$ extrapolation. $\Longrightarrow$ ***Fading corridors beyond*** ~ 250 MeV.



Example: static electric polarisability α_{E1}



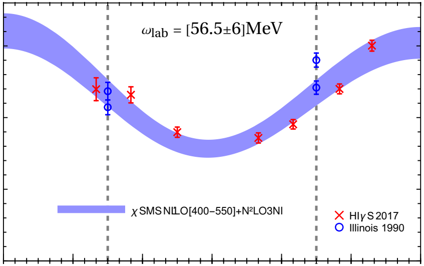
Ongoing: charged sea, $m_\pi \searrow 200$ MeV, larger volumes, more statistics,. . .

Active lattice groups:
Alexandru/Lee/. . . 2005-;
Engelhardt/LHPC 2006-;
EMC/NPLQCD 2006-, 2015-;
Leinweber/Primer/Hall/. . . 2013-

4. Concluding Questions & Comments

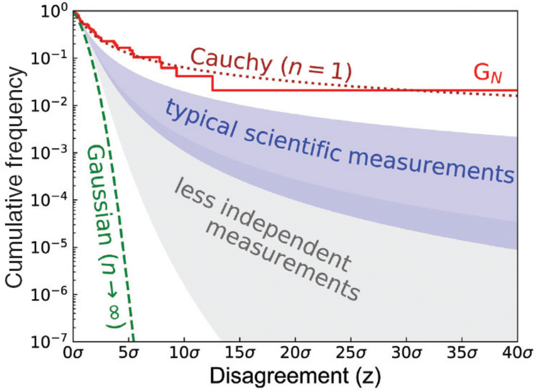
(1) **Are such meetings useful? – YES: Triggered Exp Design collaboration.**

(2) **Outlier Identification:**



How to *reproducibly* prune database with *minimal* theory bias? Overall (sys) errors usually under-estimated? Tension to data cluster in kinematic proximity ("Majority Rules"?), but not when isolated ("Could be Physics")? "Creeping": consistent in one region, inconsistent in another? Traditional: blind to clusters, compares to theory.

(3) **The World Is Not Gaußian!** David Bailey: R. Soc. open sci.4:160600 & Significance Mag. Feb 2018



Cross-disciplinary pre-post study of 50k data for 3k quantities: predicted vs. "actual" probability that datum not statistical fluke:

$z\sigma$ would be probability interval, *if errors Gaußian/Normal.*

$1\sigma \gtrapprox [40;60]\%$ $\quad 3\sigma \approx 10\%$ $\quad 5\sigma \gtrapprox [2;3]\%$

$\Longrightarrow$ **Better quote & use Δ_{68} *and* Δ_{95}, not σ?**

(4) Theory error assessment takes thought & time, frustrating: error bars seem to *increase: step back?!?!*

Reasonable people can reasonably disagree about reasonable assumptions,
but no reasonable discussion without disclosure. arXiv:2111.00930 [nucl-th]
No Excuses: Do what you can; use available tools (BAND, BUQEYE); be honest & pragmatic (no rigor mortis)!

The efficient person gets the job done right. The effective person gets the right job done.