Using Bayesian methods to assess model uncertainty in nuclear physics

Daniel Phillips

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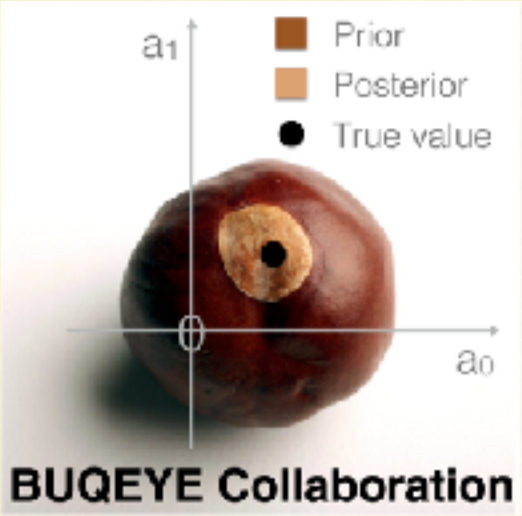


RESEARCH SUPPORTED BY THE DOE OFFICE OF SCIENCE, THE NNSA, AND THE NSF OAC

Nuclear Science model uncertainty

- Neutrinoless double beta decay
- r-process: extrapolation to the dripline and beyond; ties in to other nuclear-structure issues
- Heavy-ion Collisions: energy deposition; pre-hydrodynamic stage; conversion of hydrodynamic output to final-state particles
- Different approaches to reaction dynamics (R-matrix, statistical models, global optical potentials, microscopic optical potentials, …)

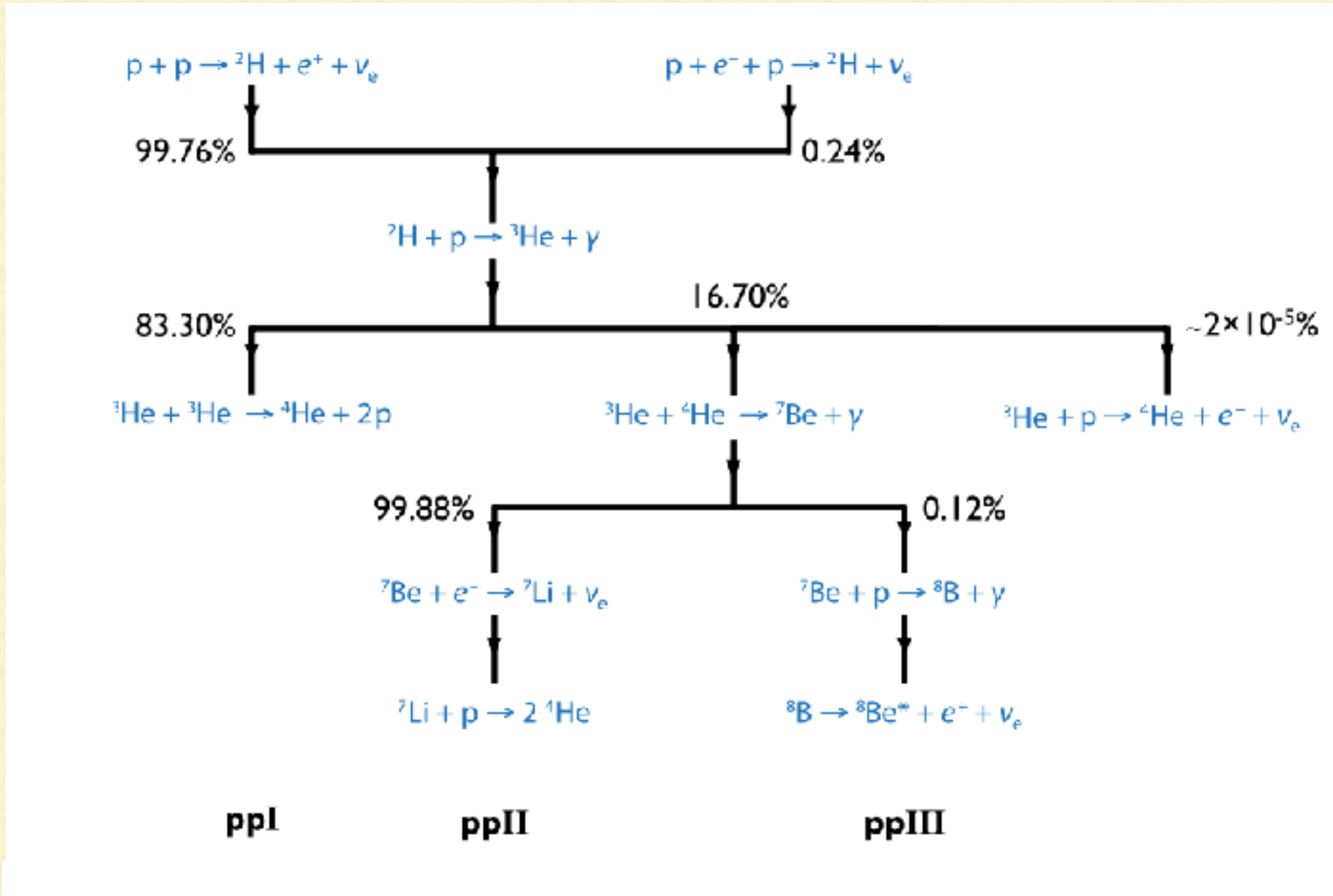
Outline

- $^3He + {}^4He \rightarrow {}^7Be + \gamma$ as an example of how to assess model uncertainty
  - How Halo Effective Field Theory can help
  - From S-factor data to Halo EFT parameters, and back
  - Halo EFT as a "super model"
- Bayesian Model Averaging→Bayesian Model Mixing
  - What is Bayesian Model Averaging?
  - An application: the overall prediction of EDFs for the neutron drip line
  - Toy-model test of BMA
- The BAND Software Framework

Why is ^{3}He(^{4}He,γ) important?

Adelberger et al., Rev. Mod. Phys. 83, 195 (2011)

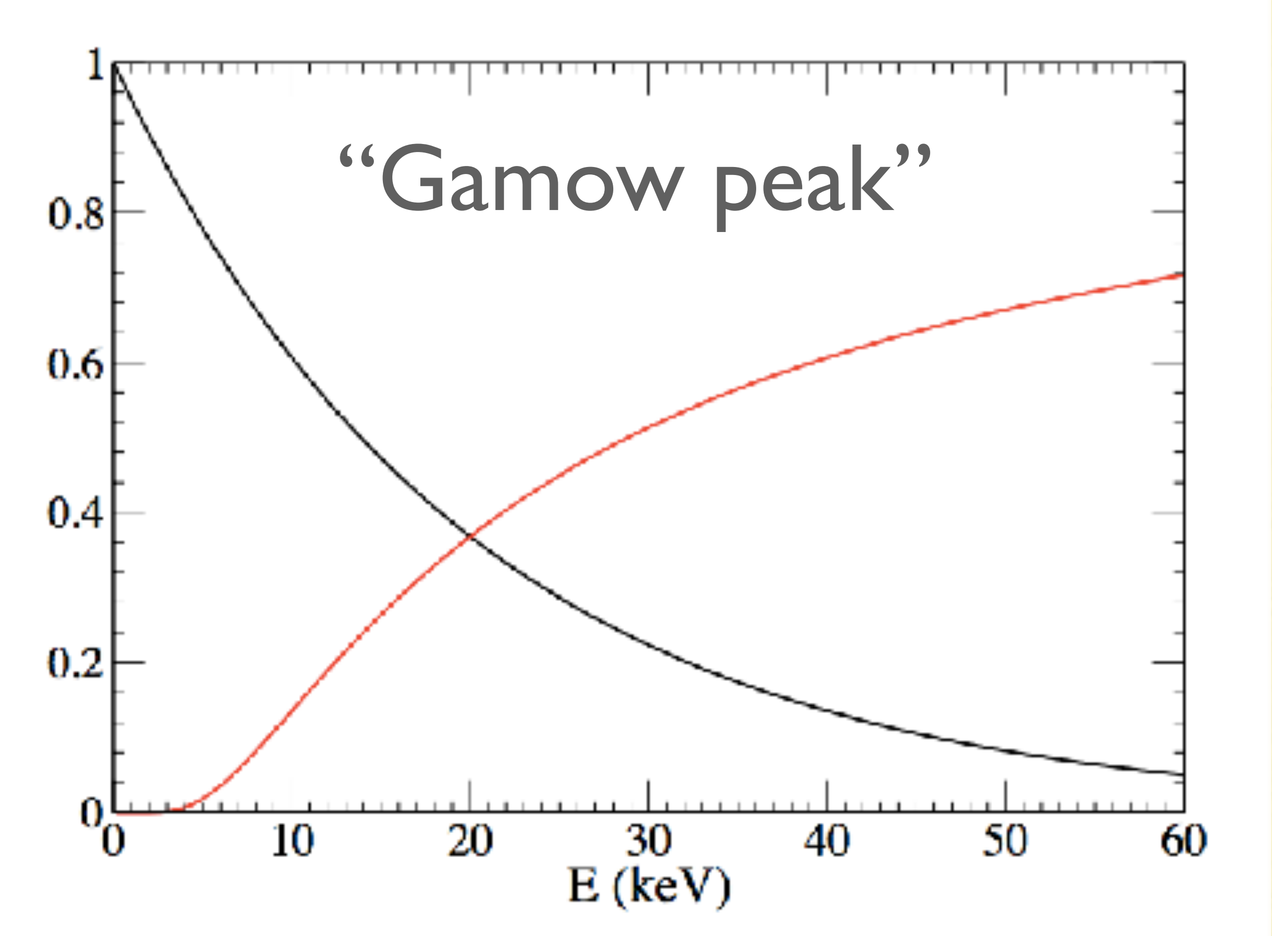
- Accurate knowledge of ^{3}He(^{4}He,γ) needed to reliably predict amount of ^{7}Be in the Sun
- Therefore key for prediction of ^{8}B solar neutrino flux
- BBN implications, but I will not discuss those here



This is an extrapolation problem

Thermonuclear reaction rate $\propto \langle v\sigma \rangle \propto \int_0^\infty dE\, \exp\left(-\frac{E}{k_B T}\right) E\, \sigma(E)$

$$\sigma(E) = \frac{S(E)}{E} \exp\left(-\pi Z_1 Z_2 \alpha_{\rm em} \sqrt{\frac{m_R}{2E}}\right)$$



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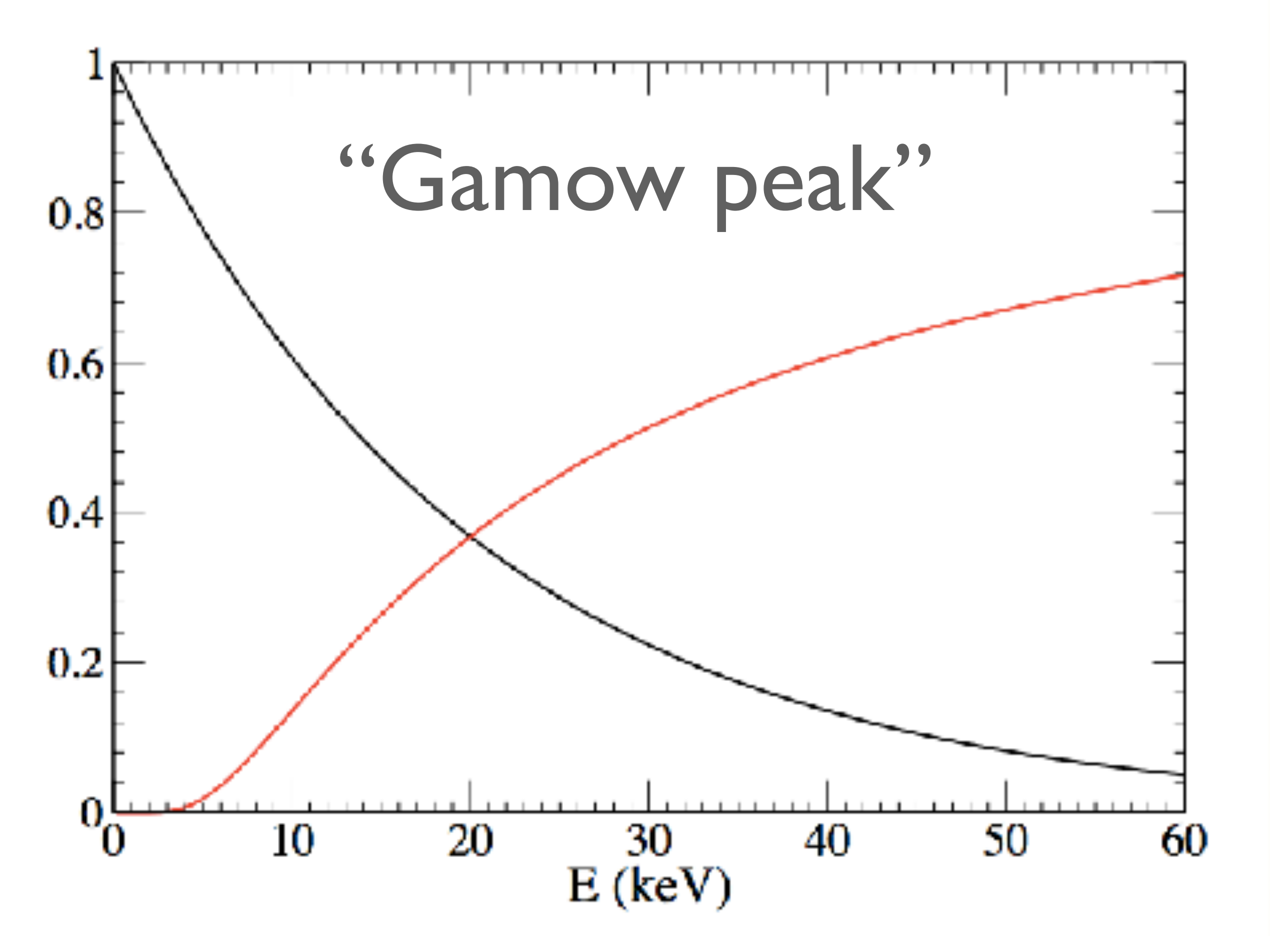
- E1 capture: $^3He + ^4He \rightarrow ^7Be + \gamma$ and $^7Be + p \rightarrow ^8B + \gamma$
- Energies of relevance 20 keV

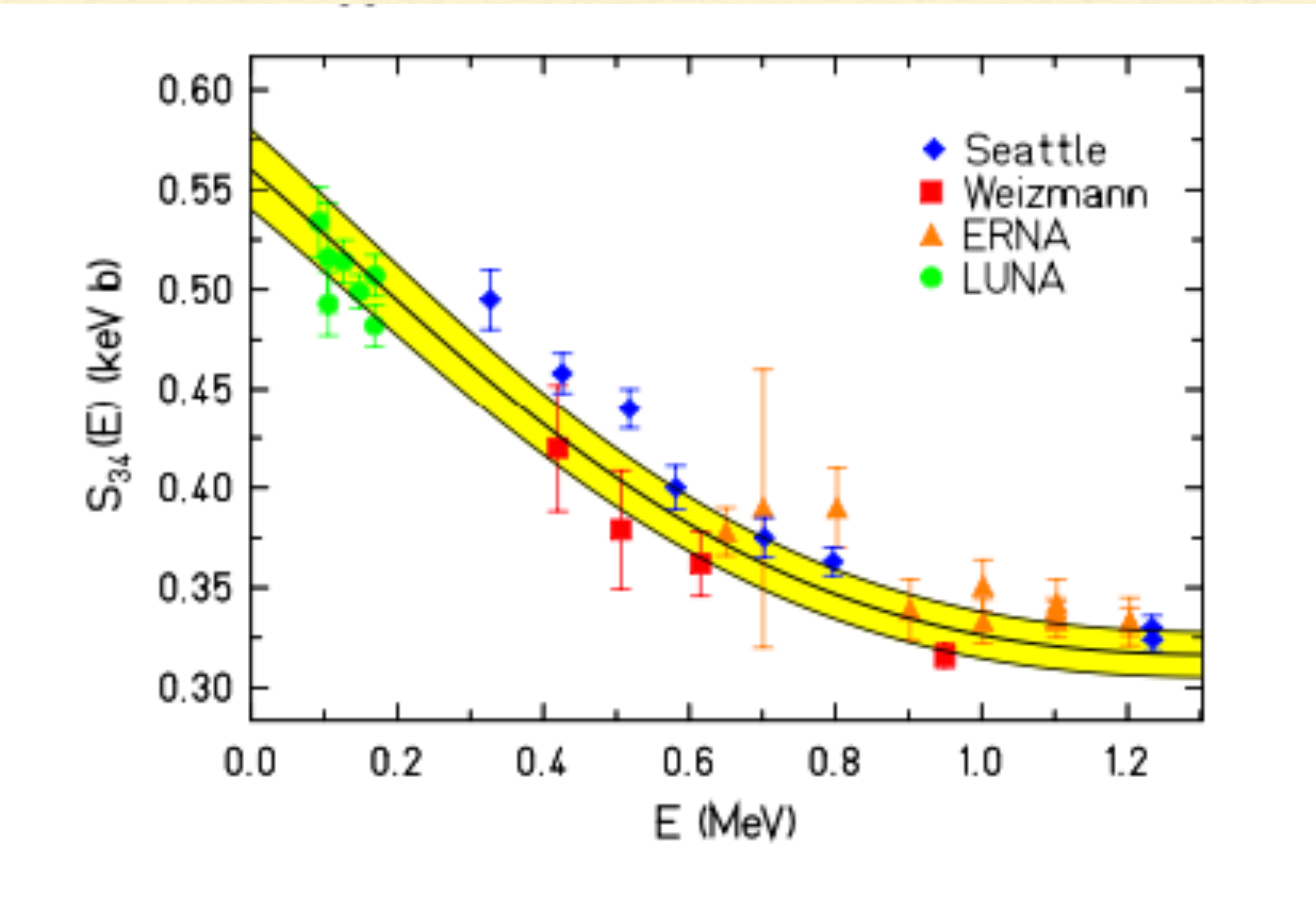


Building a good extrapolant

$\mathscr{M}(E)$ dominated by inter-nucleus separations outside V(r)

$$\mathscr{M}(E) \propto \int dr\, A_1 \exp(-\gamma_1 r)\left(1 + \frac{1}{\gamma_1 r}\right) r(\cot\delta(E)\sin(pr) + \cos(pr))$$

ANC



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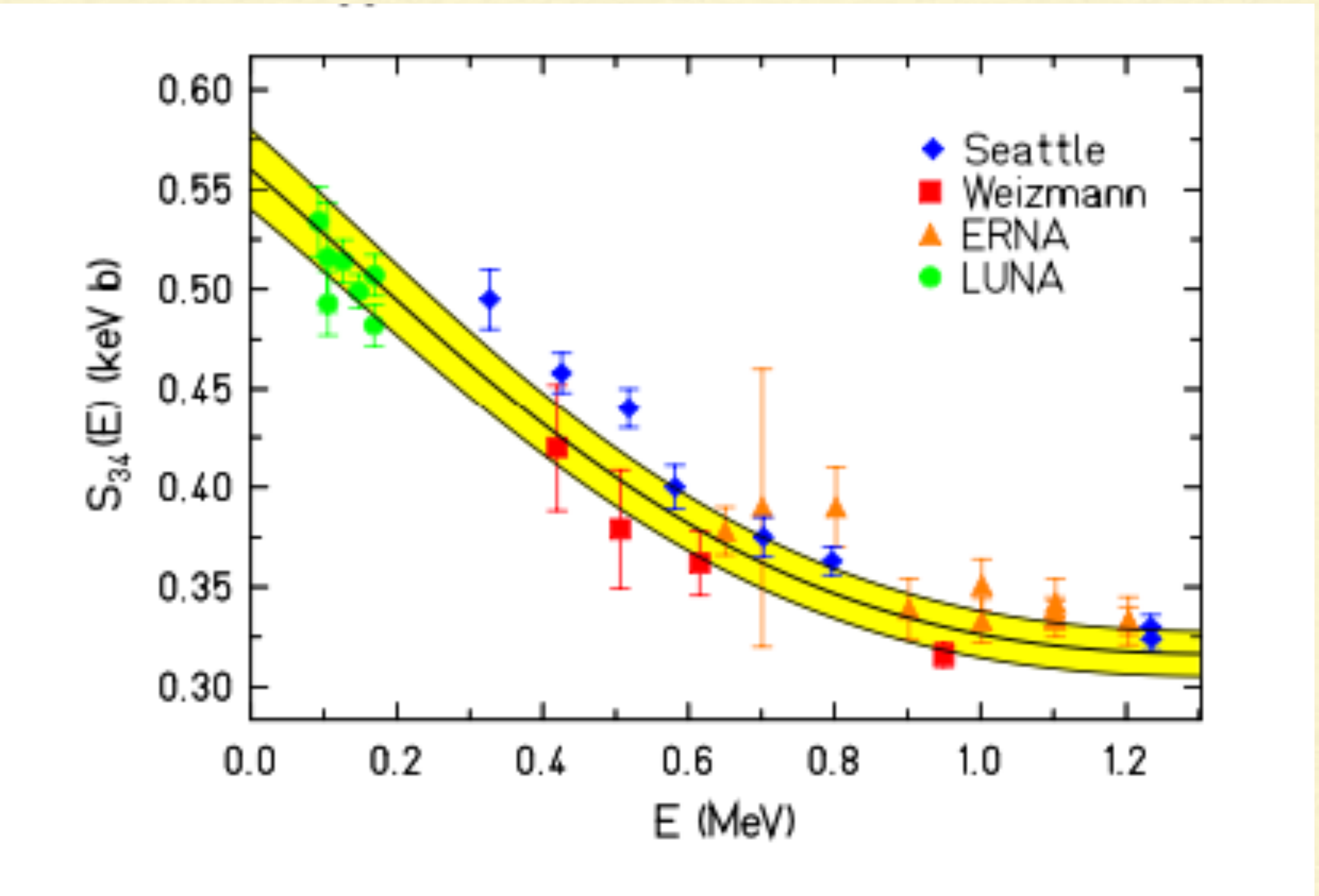

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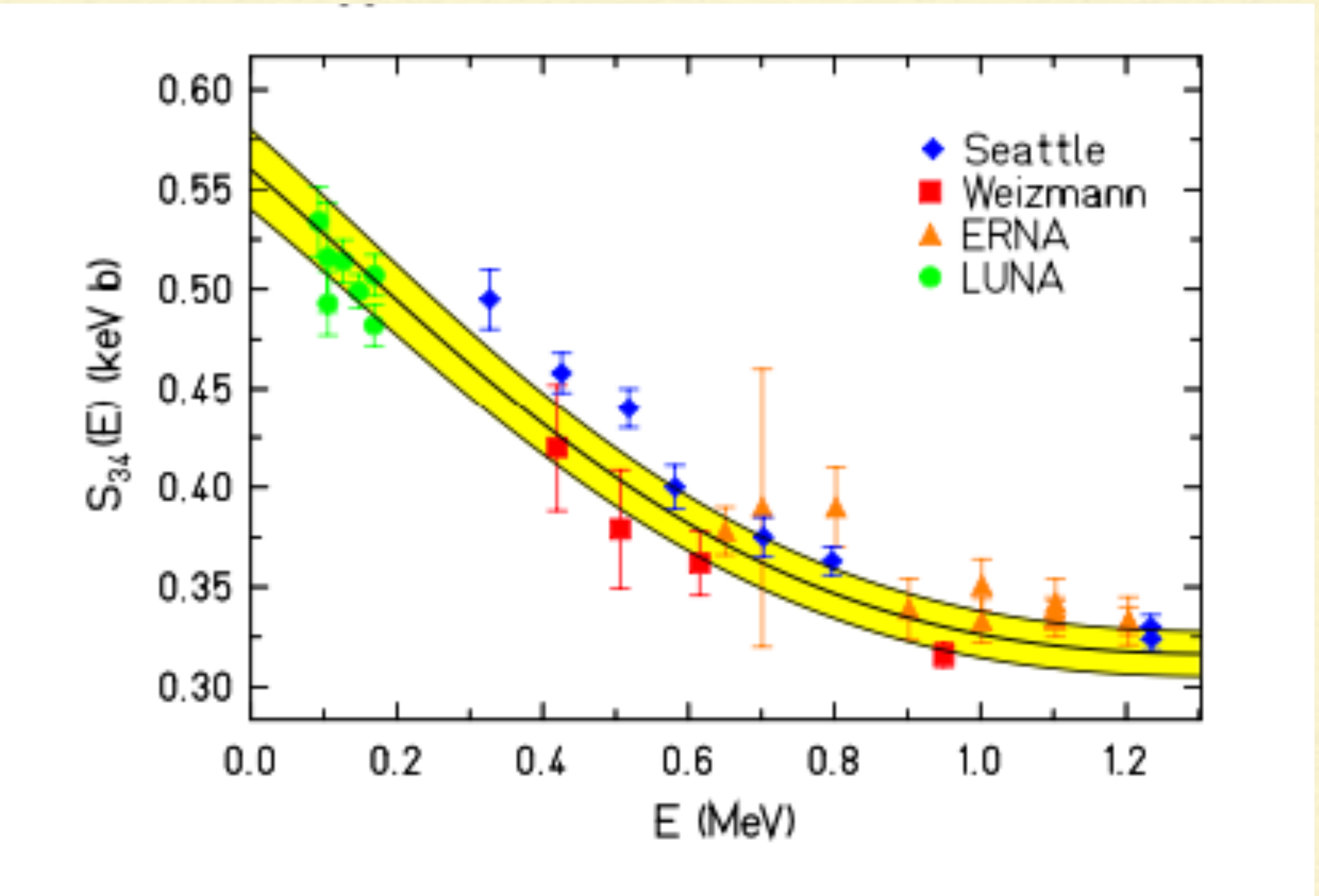

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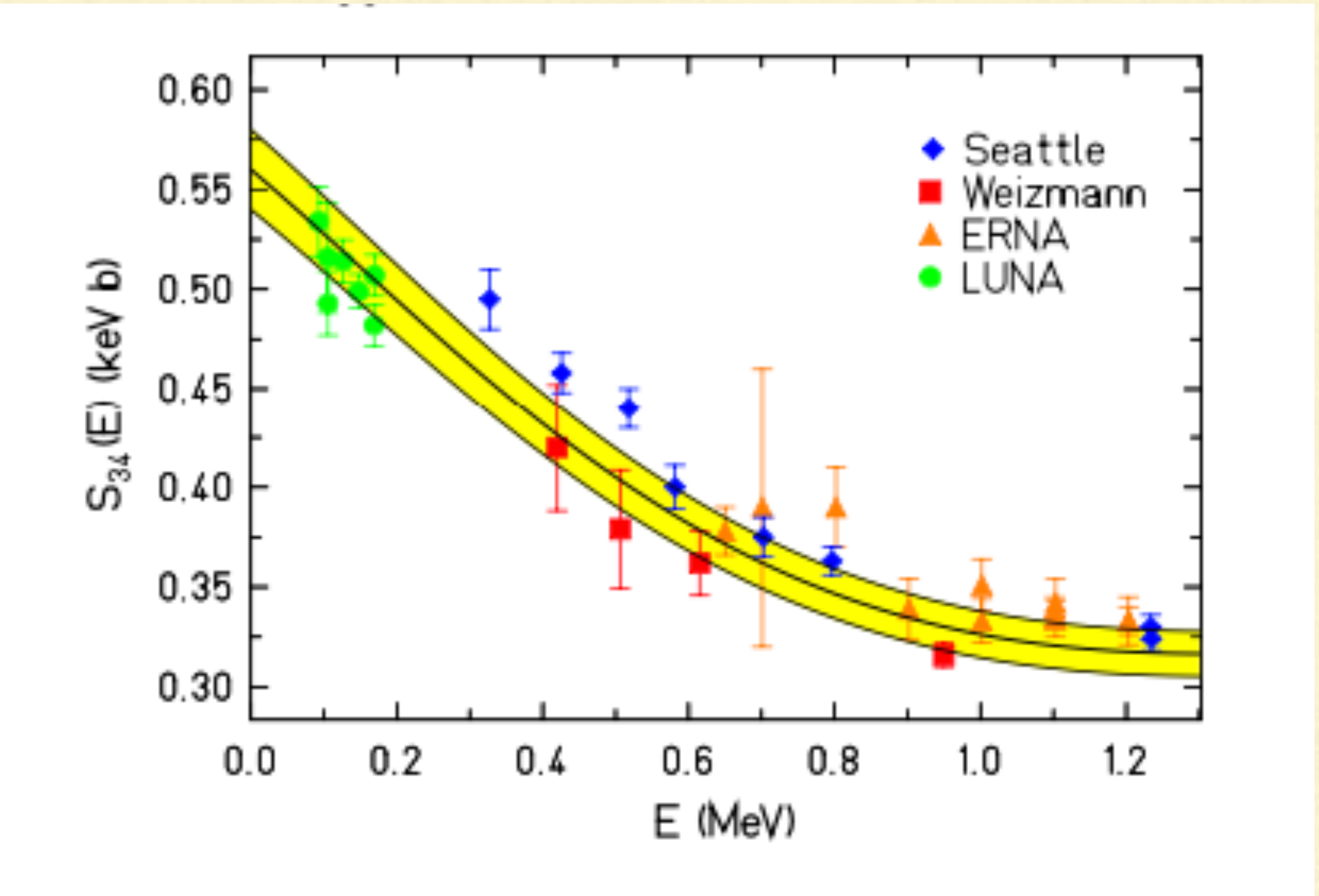

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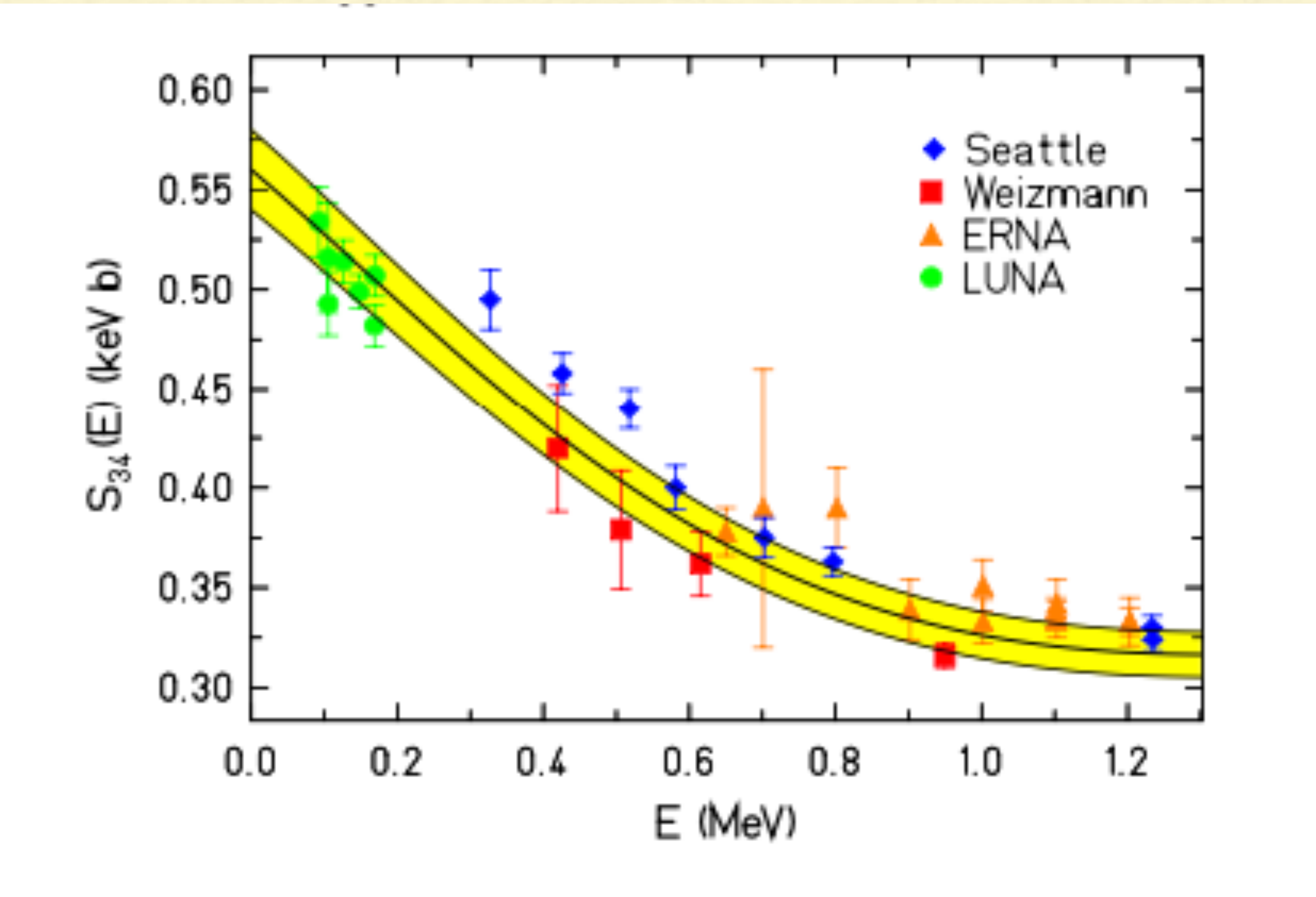
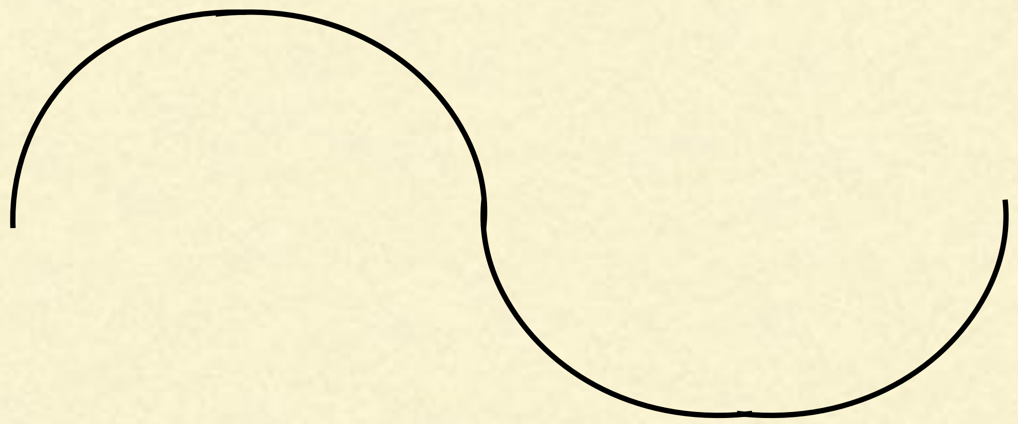
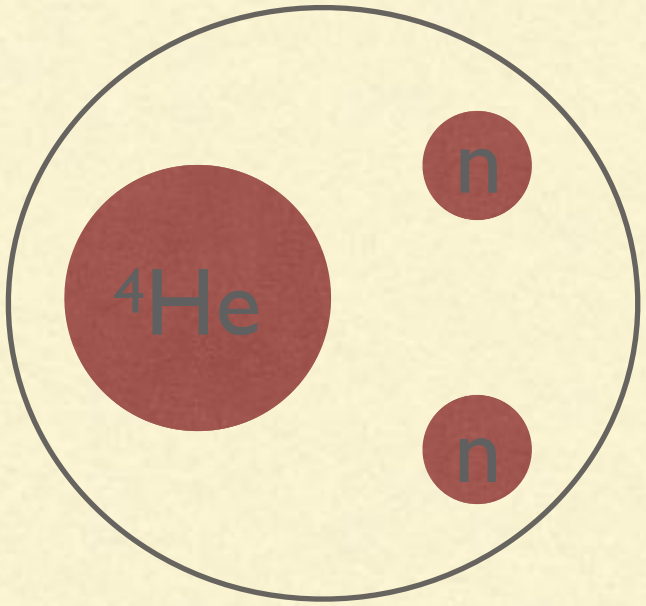
- SFII: energy dependence taken from models, overall size adjusted to data



Halo EFT

$\lambda \gg R_{core}$; $\lambda \lesssim R_{halo}$





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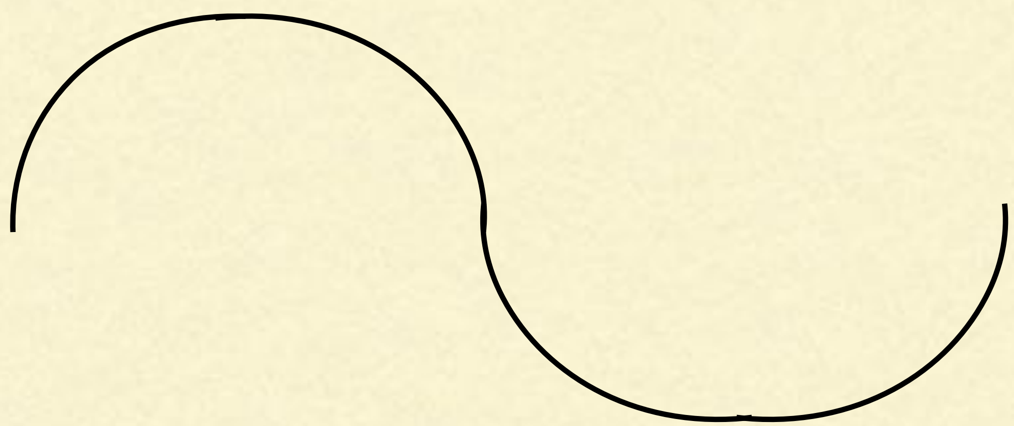
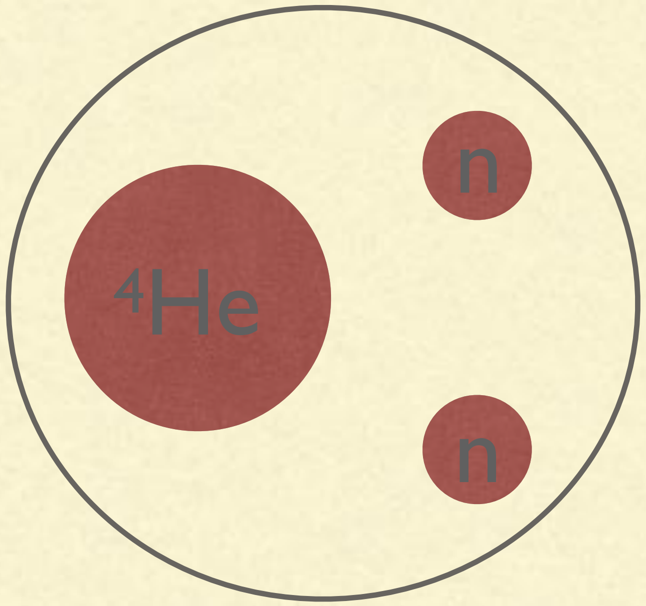




- Define $R_{halo}=\langle r^2\rangle^{1/2}$. Seek EFT expansion in R_{core}/R_{halo}. Valid for $\lambda \lesssim R_{halo}$
- Typically $R \equiv R_{core} \sim 2$ fm. And since $\langle r^2\rangle$ is related to the neutron separation energy we are looking for systems with neutron separation energies less than 1 MeV
- By this definition the deuteron is the lightest halo nucleus, and the pionless EFT for few-nucleon systems is a specific case of halo EFT

Lagrangian: shallow S- and P-states

$$\begin{aligned}\mathcal{L} &= c^\dagger\left(i\partial_t+\frac{\nabla^2}{2M}\right)c+n^\dagger\left(i\partial_t+\frac{\nabla^2}{2m}\right)n \\ &+\sigma^\dagger\left[\eta_0\left(i\partial_t+\frac{\nabla^2}{2M_{nc}}\right)+\Delta_0\right]\sigma+\pi_j^\dagger\left[\eta_1\left(i\partial_t+\frac{\nabla^2}{2M_{nc}}\right)+\Delta_1\right]\pi_j \\ &-g_0\left[\sigma n^\dagger c^\dagger+\sigma^\dagger nc\right]-\frac{g_1}{2}\left[\pi_j^\dagger(n\, i\overleftrightarrow{\nabla}_j\, c)+(c^\dagger\, i\overleftrightarrow{\nabla}_j\, n^\dagger)\pi_j\right] \\ &-\frac{g_1}{2}\frac{M-m}{M_{nc}}\left[\pi_j^\dagger\, i\overrightarrow{\nabla}_j\,(nc)-i\overleftrightarrow{\nabla}_j\,(n^\dagger c^\dagger)\pi_j\right]+\ldots\,,\end{aligned}$$

- c, n: "core", "neutron" fields. c: boson, n: fermion.
- σ, π_j: S-wave and P-wave fields
- Minimal substitution generates leading EM couplings
- Additional EM couplings at sub-leading order

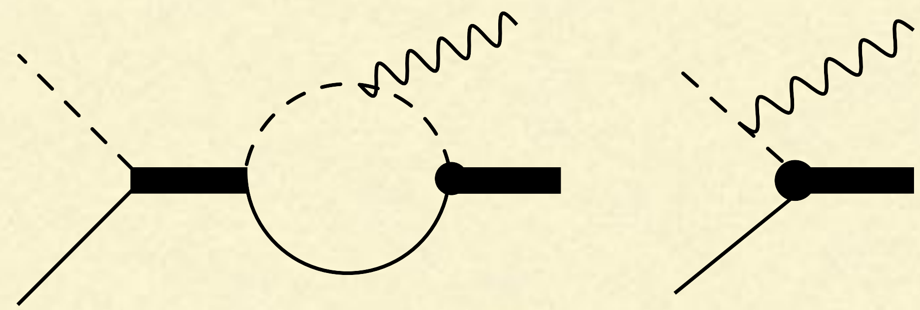
p-wave bound states and capture thereto

Hammer & DP, NPA (2011)

- At LO p-wave 1n halo described solely by its ANC and binding energy

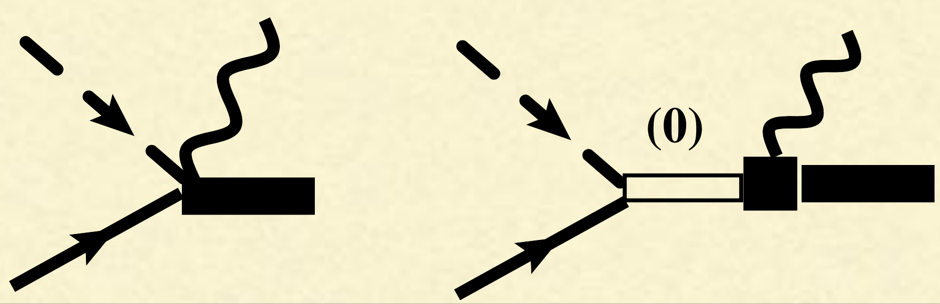
$$u_1(r) = A_1 \exp(-\gamma_1 r)\left(1 + \frac{1}{\gamma_1 r}\right) \qquad \gamma_1 = \sqrt{2m_R B}$$

- Capture to the p-wave state proceeds via the one-body E1 operator: "external direct capture"



$$\mathrm{E1} \propto \int_0^\infty dr\, u_0(r) r u_1(r); \quad u_0(r) = 1 - \frac{r}{a}$$

- NLO: piece of the amplitude representing capture at short distances, represented by a contact operator⇒there is an LEC that must be fit



$^3He + {}^4He \rightarrow {}^7Be + \gamma_{E1}$ at LO in Halo EFT

Zhang, Nollett, DP, J. Phys. G (2020); cf. Rupak, Higa, Vaghani, EPJA (2018)

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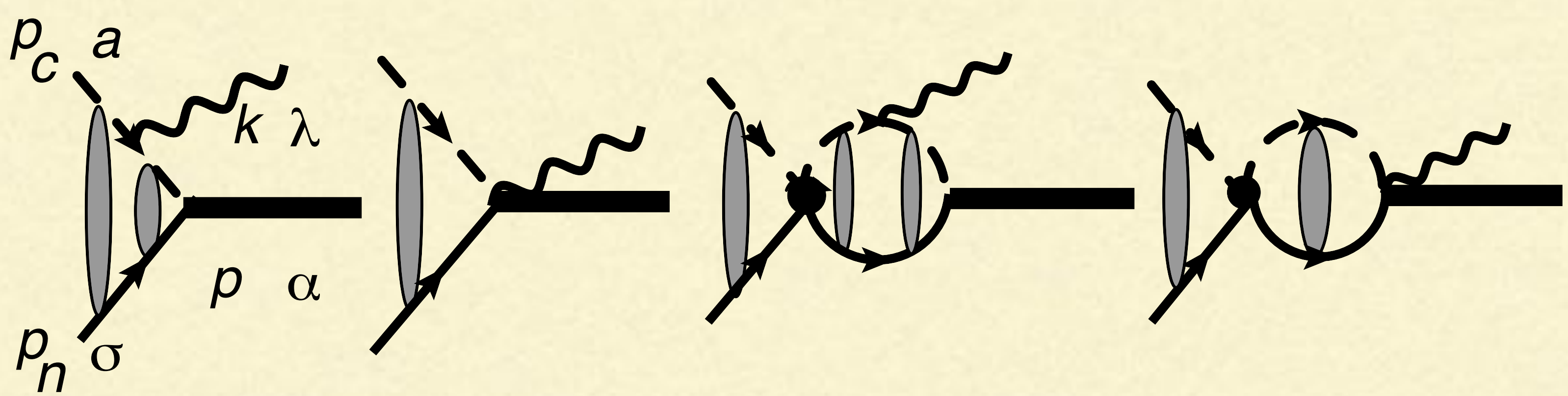

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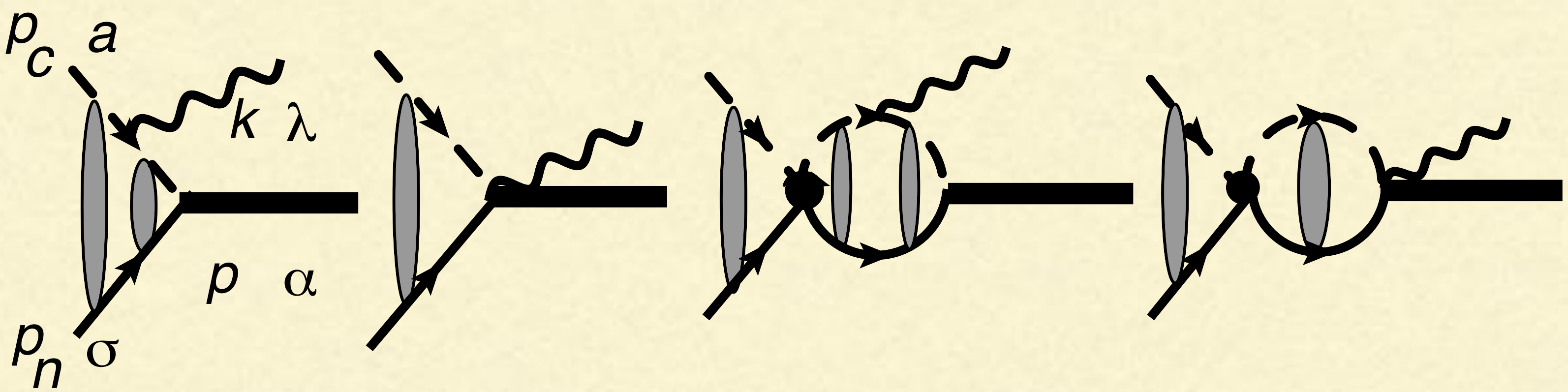

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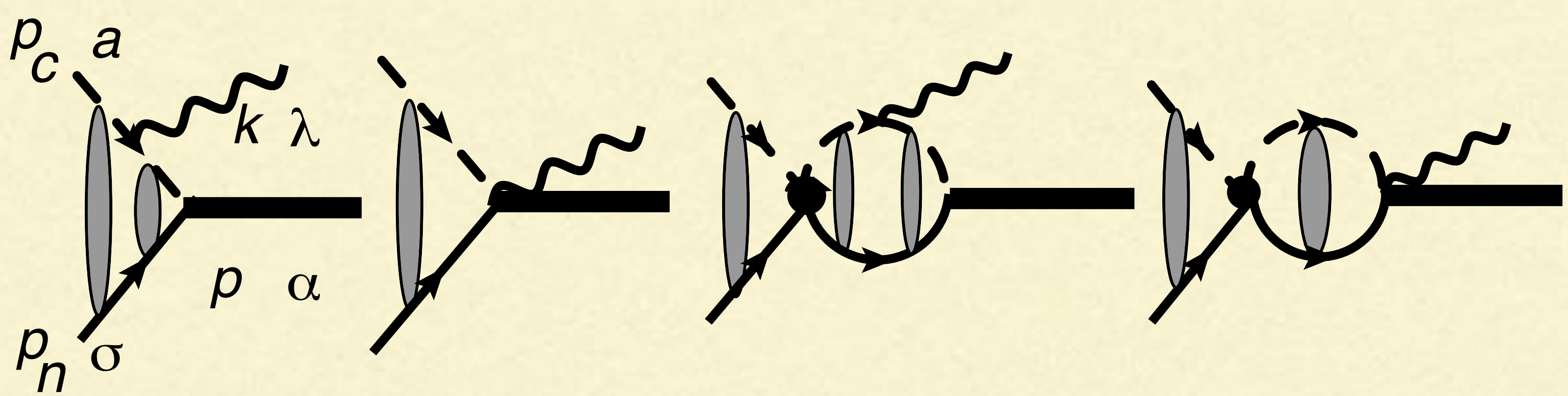

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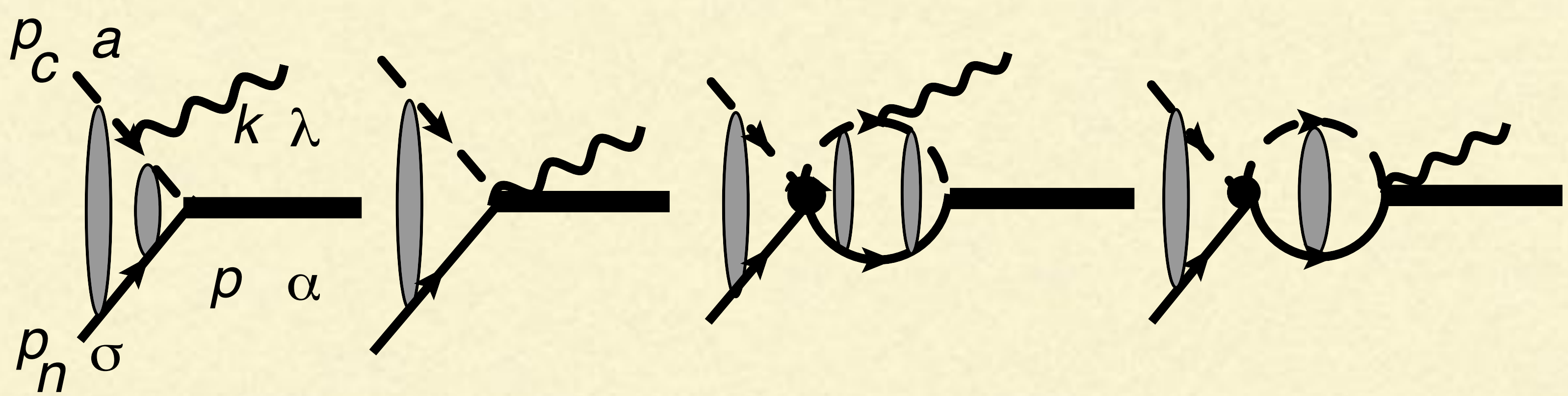

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- Can also predict capture to the excited $1/2^-$ in ^7Be

Three parameters at leading order

Additional ingredients at NLO

Zhang, Nollett, DP, Phys. Lett. B751, 535 (2015), Phys. Rev. C (2018);
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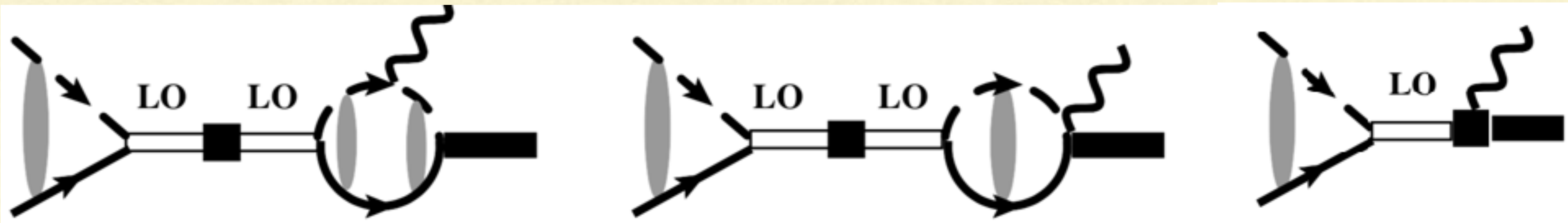

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- Effective range (can add shape parameter which enters at N^{3}LO)
- LECs associated with contact interaction, $\bar{L}$ and $\bar{L}_*$
- Can also consider contact interaction for D-wave capture, $\bar{L}_D$ (enters at N^{4}LO)

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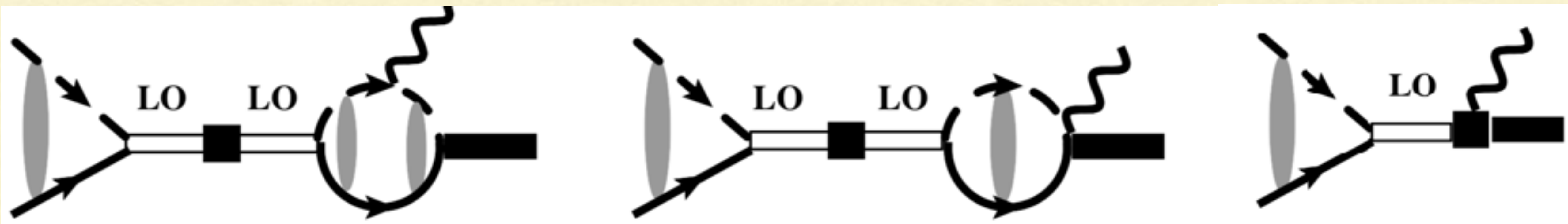

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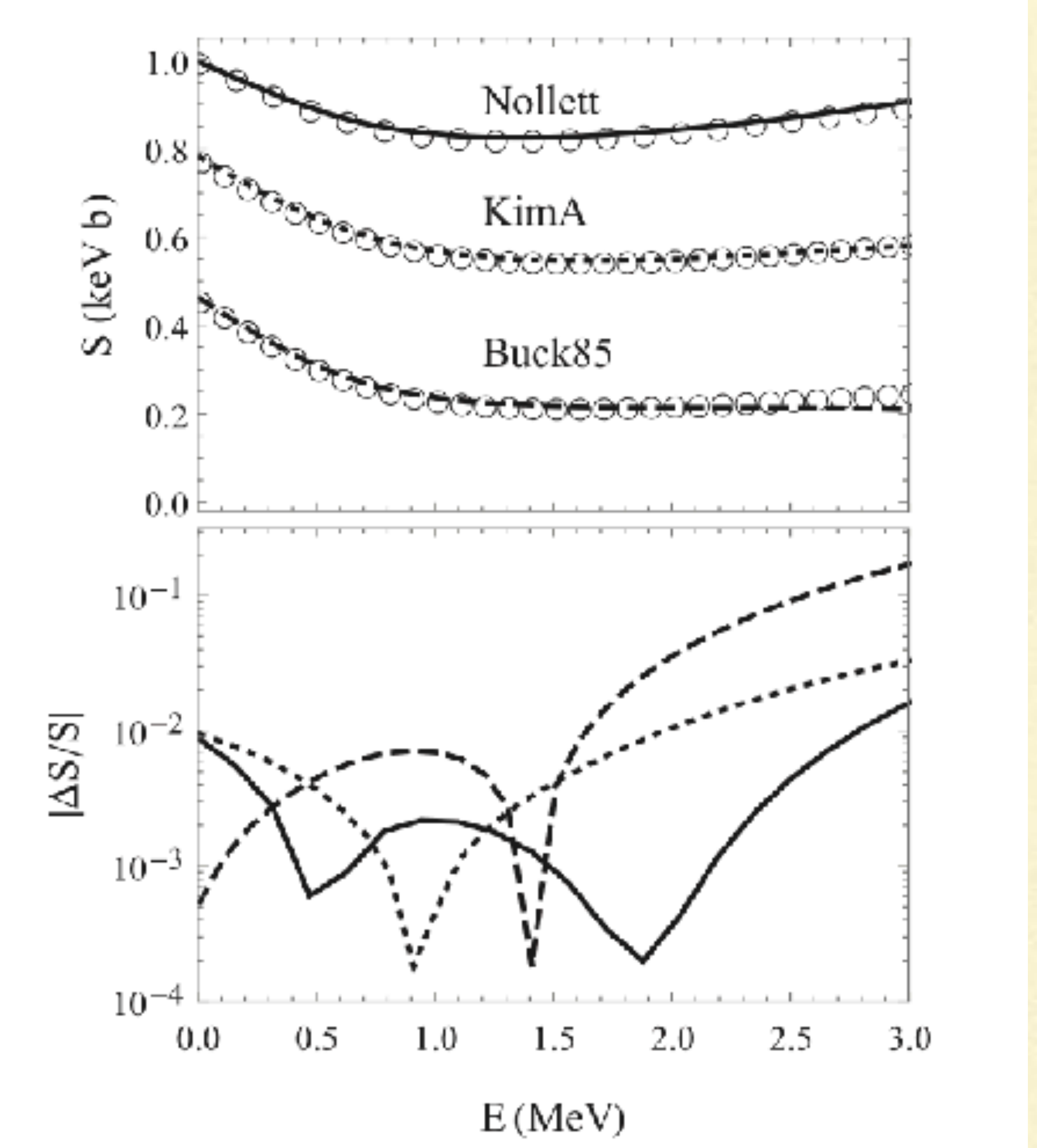

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- Halo EFT is the EFT of all the models used to extrapolate the cross section in "Solar Fusion II": should reproduce them at NLO accuracy in validity region
- Differences are sub-% level between 0 and 1.5 MeV
- Parameters generally obey a~1/R_{halo}, r ~R_{core}, L~R_{core}; some large N4LO parameters

Table 1. EFT parameters obtained from partial-N4LO fits to models from the literature. Quantities are total ANC squared (C^2), the ratio of ES ANC squared to C_T^2, the scattering length, effective range, and shape parameters as well as s-to-p-wave short-distance parameters, $\overline{L}$ and $\overline{L}_*$ and d-to-p-wave short-distance parameters $\overline{L}_D$ and $\overline{L}_{D*}$. The last two rows are the binding energies of ^{7}Be's GS and ES.

	Buck85 [34]	KimA [36]	Nollett [13]
C_T^2 (fm^{-1})	30.33	29.22	21.01
$R_{(P_{1/2})}$	0.4197	0.4192	0.4002
a_0 (fm)	36.97	18.27	29.48
r_0 (fm)	0.9726	0.9979	0.9723
$\mathcal{P}_0$ (fm^3)	−0.3688	−0.086 66	−0.5227
$\overline{L}$	0.9018	0.6434	0.9546
$\overline{L}_*$	0.9079	0.6334	0.9772
$\overline{L}'$	0.091 25	0.5311	0.2240
$\overline{L}_*'$	0.079 64	0.5465	0.2366
$\overline{L}_D$ (fm^4)	−4.541	−1.950	0.5124
$\overline{L}_{D*}$ (fm^4)	−4.844	−3.096	0.3444
B (MeV)	1.608	1.656	1.587
B_* (MeV)	1.163	1.192	1.158

Data for $^3He + ^4He \rightarrow ^7Be + \gamma_{E1}$

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  - Seattle (S)
  - Weizman
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- In general use activation data, to avoid photon emission asymmetry systematic; recoil data from Erna; prompt measurements from Notre Dame
- Deal with CMEs by introducing six additional parameters, ξ_i
- Plus 32 branching-ratio data: CMEs assumed absent there

Bayesian tools

Thomas Bayes (1701?-1761)

http://www.bayesian-inference.com

$$\mathrm{pr}(A|B,I) = \frac{\mathrm{pr}(B|A,I)\mathrm{pr}(A|I)}{\mathrm{pr}(B|I)}$$

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Probability as degree of belief

$$\mathrm{pr}(A|B,I) = \frac{\mathrm{pr}(B|A,I)\,\mathrm{pr}(A|I)}{\mathrm{pr}(B|I)}$$

$$\mathrm{pr}(x|\mathrm{data},I) = \frac{\mathrm{pr}(\mathrm{data}|x,I)\,\mathrm{pr}(x|I)}{\mathrm{pr}(\mathrm{data}|I)}$$

Likelihood: $\mathrm{pr}(\mathrm{data}|x,I)$

Prior: $\mathrm{pr}(x|I)$

Posterior: $\mathrm{pr}(x|\mathrm{data},I)$

Normalization: $\mathrm{pr}(\mathrm{data}|I)$

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Likelihood Prior

$$\mathrm{pr}(x|\mathrm{data},I) = \frac{\mathrm{pr}(\mathrm{data}|x,I)\,\mathrm{pr}(x|I)}{\mathrm{pr}(\mathrm{data}|I)}$$

Posterior Normalization

Marginalization: $\mathrm{pr}(x|\mathrm{data},I) = \int dy\, \mathrm{pr}(x,y|\mathrm{data},I)$

Allows us to integrate out "nuisance" (e.g. higher-order) parameters

Building the pdf

- χ^2 needs to include cross-section and branching-ratio data

$$\chi^2 \equiv \sum_{J}^{N_{\exp}} \left\{ \sum_{j=1}^{N_{s,J}} \frac{\left[(1-\xi_J)S(\overrightarrow{g};E_{Jj}) - D_{Jj}\right]^2}{\sigma_{Jj}^2} + \frac{\xi_J^2}{\sigma_{c,J}^2} \right\} + \sum_{l=1}^{N_{br}} \frac{\left[Br(\overrightarrow{g};E_l) - \tilde{D}_l\right]^2}{\sigma_{br,l}^2}$$

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$$\chi^2 \equiv \sum_{J}^{N_{\exp}} \left\{ \sum_{j=1}^{N_{s,J}} \frac{\left[(1-\xi_J)S(\overrightarrow{g};E_{Jj}) - D_{Jj}\right]^2}{\sigma_{Jj}^2} + \frac{\xi_J^2}{\sigma_{c,J}^2} \right\} + \sum_{l=1}^{N_{br}} \frac{\left[Br(\overrightarrow{g};E_l) - \tilde{D}_l\right]^2}{\sigma_{br,l}^2}$$

- Mild Bayesian priors:
  - Independent gaussian priors for ξ_i, centered at zero and with width=CME
  - Other EFT parameters, a, r, L, and two ANCs assigned flat priors, corresponding to natural ranges
- Probability $e^{-\chi^2/2}$ sampled using Markov Chain Monte Carlo

$^3He(^4He,\gamma)$ results

Zhang, Nollett, DP, JPG (2020)
cf. Higa, Rupak, Vaghani, EPJA (2018)

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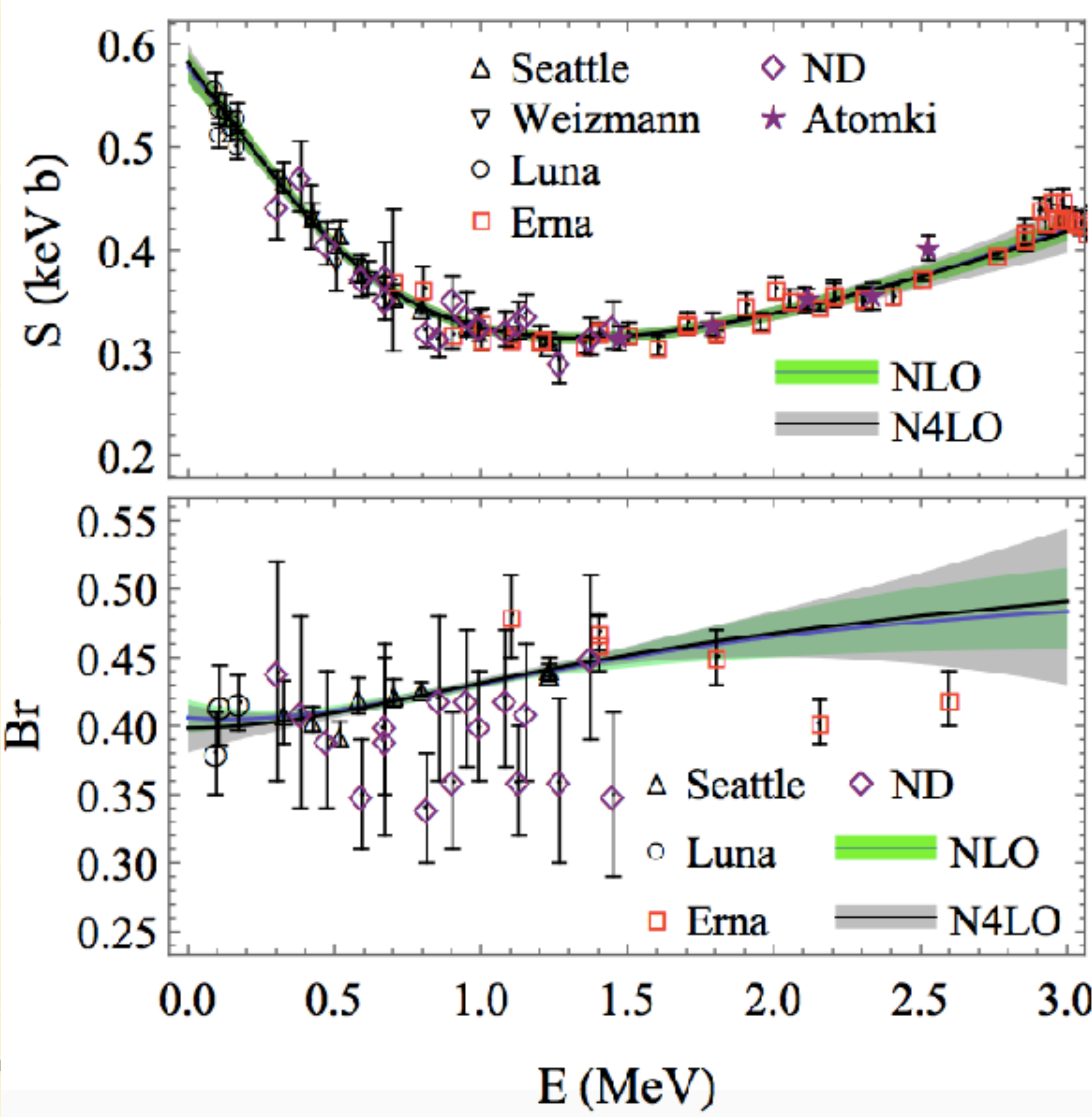

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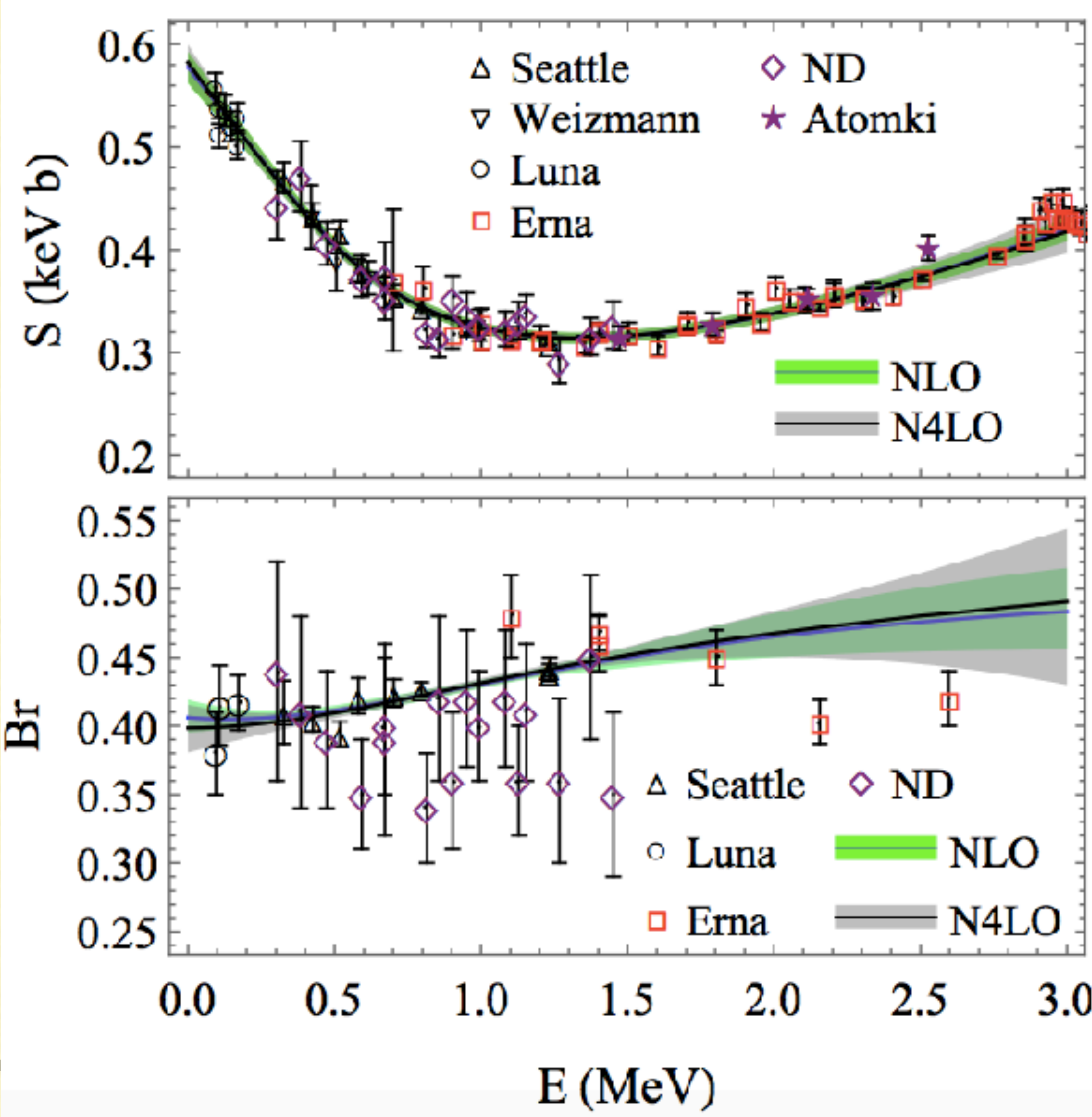

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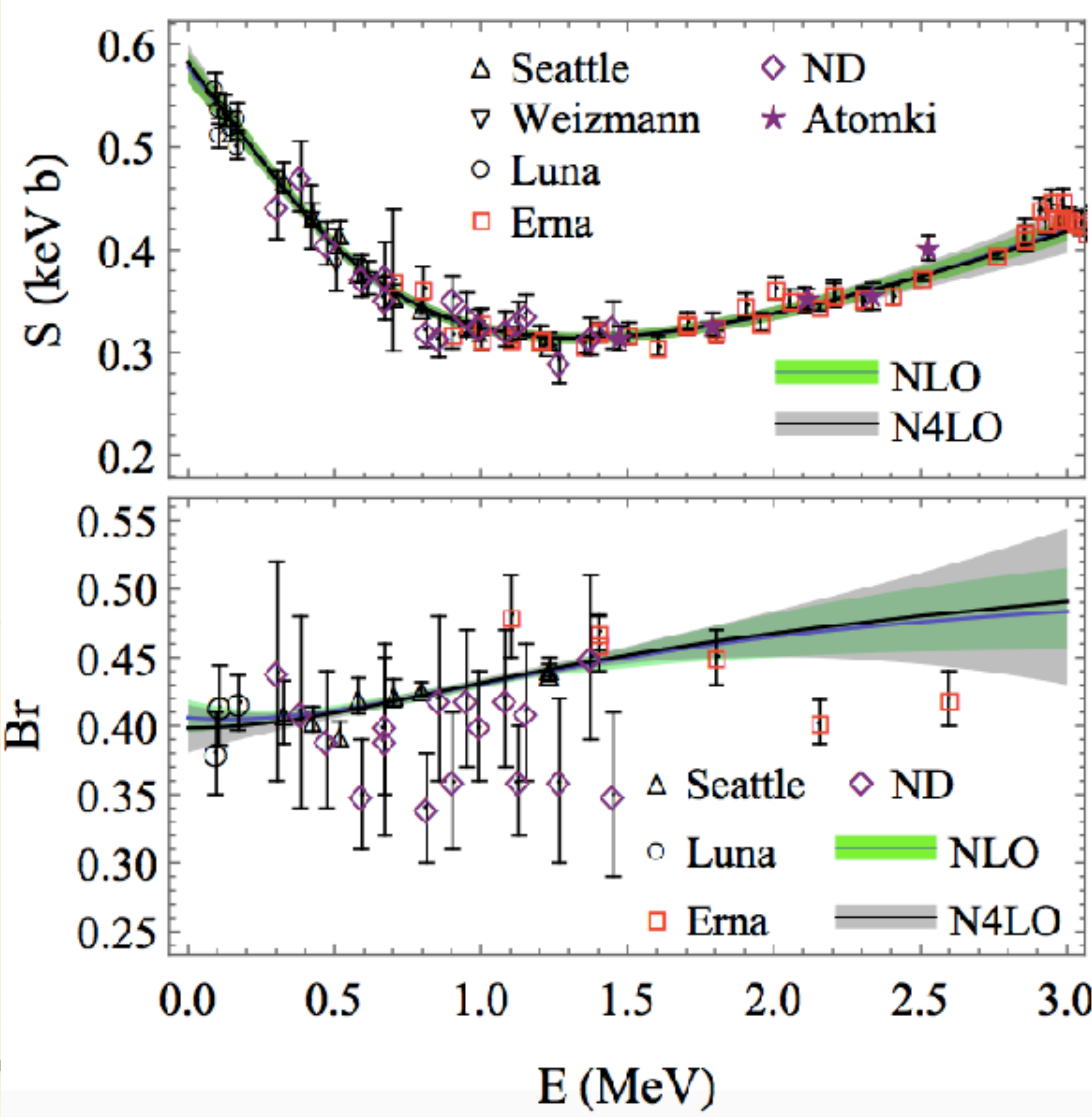
- Bayesian evidence ratio≅6 for NLO cf. N^4LO



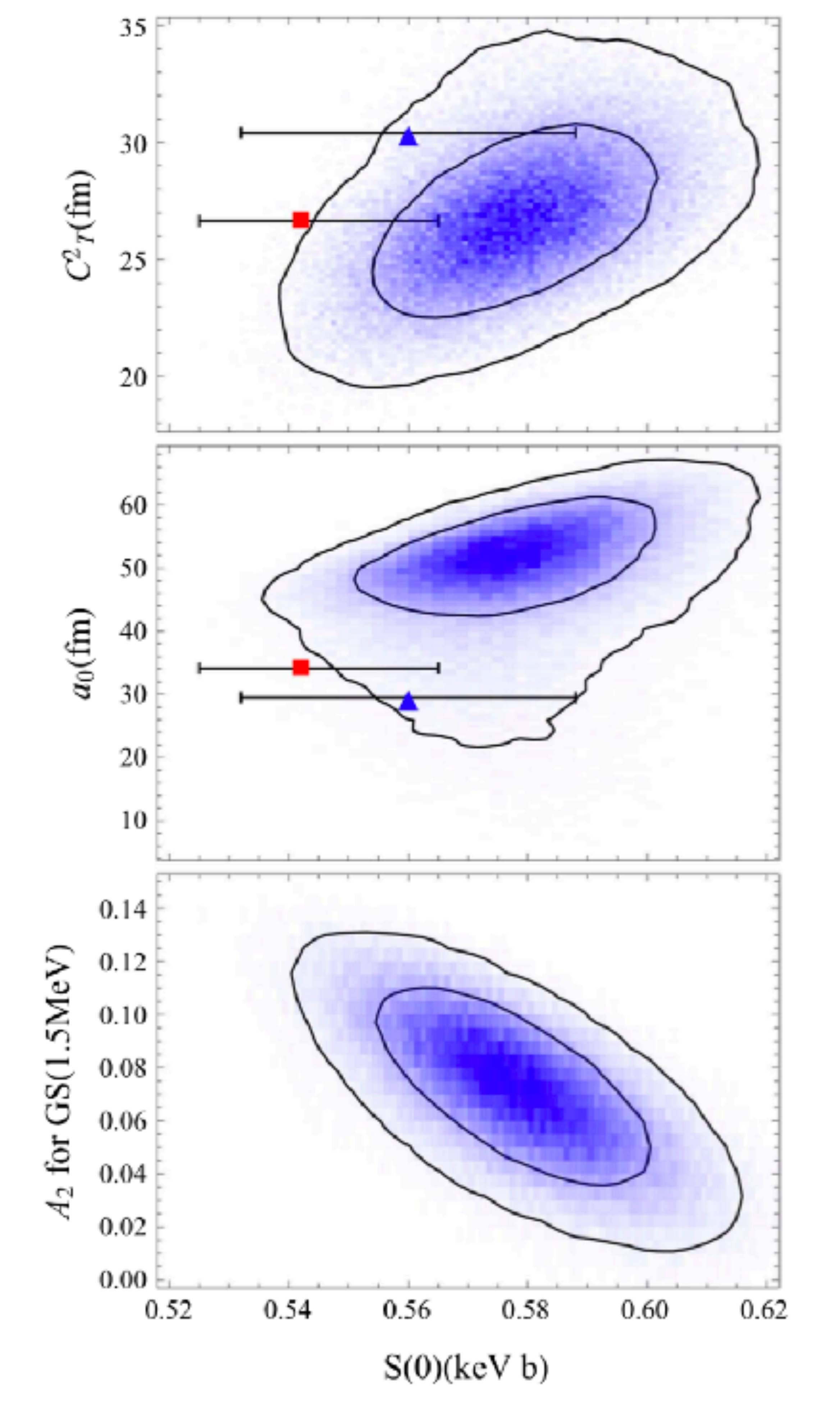
S(0) and its correlants

$$S(0) = 0.578^{+0.015}_{-0.016} \text{ keV b}$$

cf. SFII: $S(0) = 0.56 \pm 0.03 \text{ keV b}$

$$Br(0) = 0.406^{+0.013}_{-0.011}$$

Mostly consistent with other analyses, but 1.5σ higher than that of deBoer et al.



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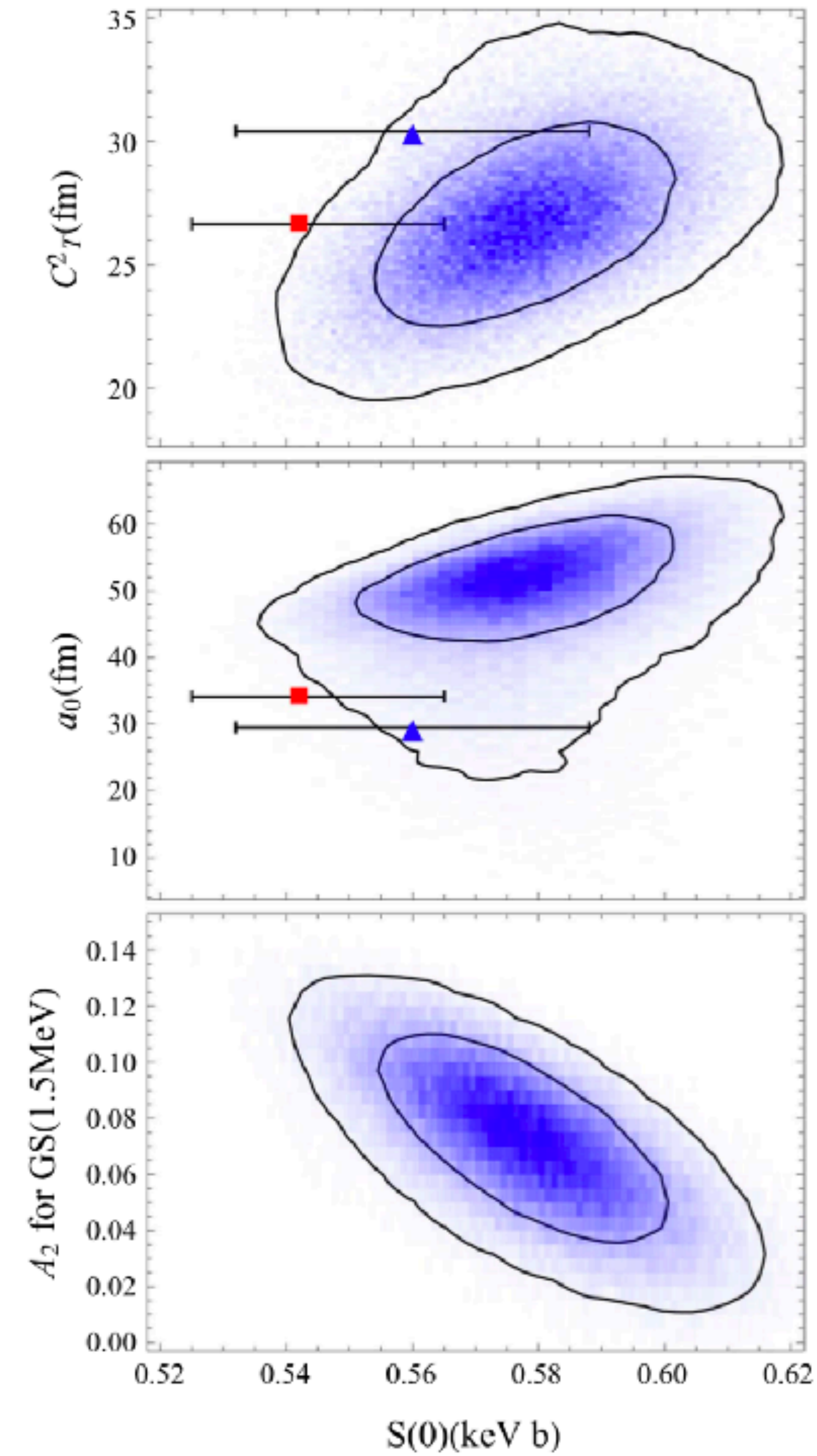

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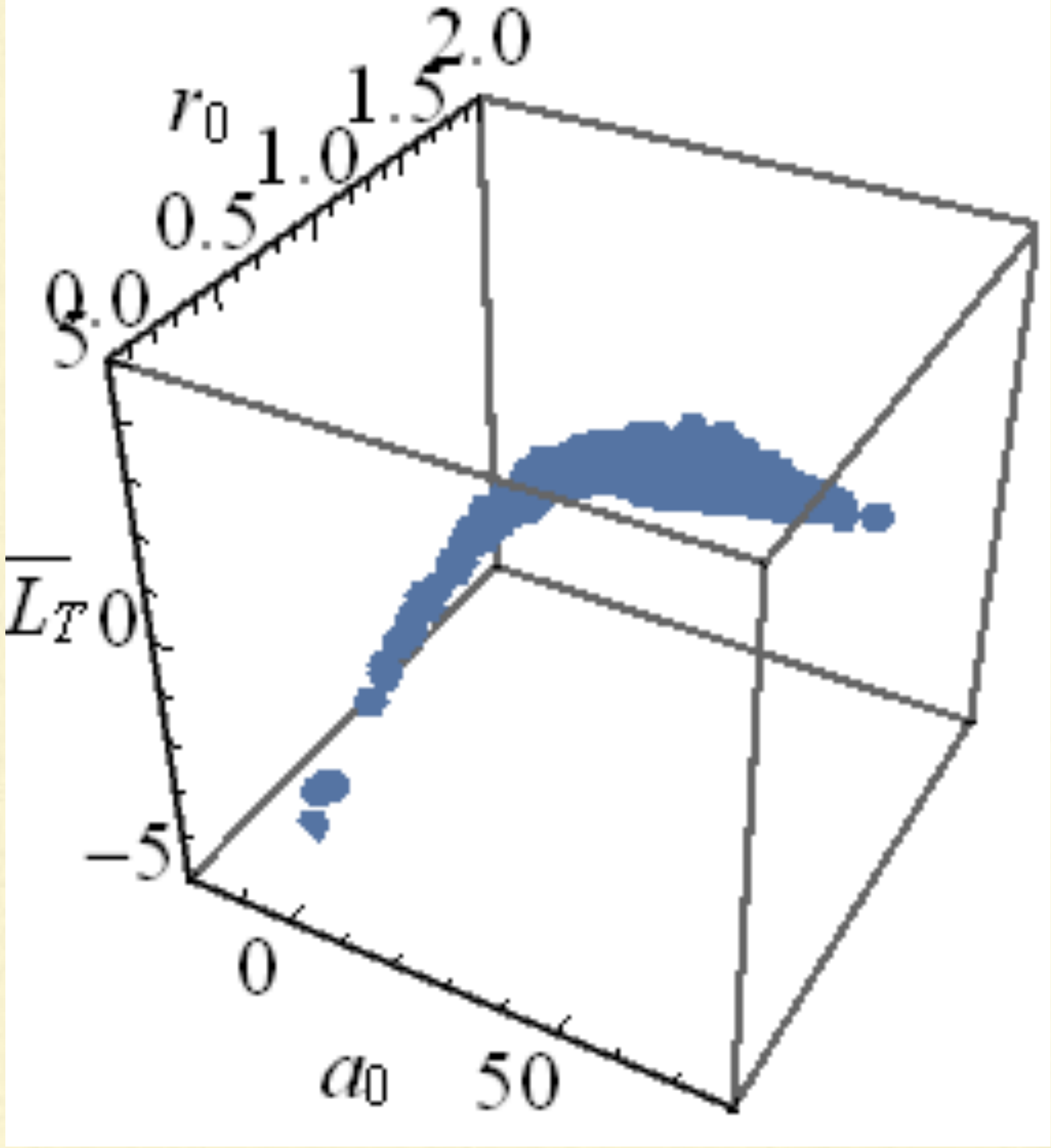


Outline

- $^3He + ^4He \to ^7Be + \gamma$ as an example of how to assess model uncertainty
  - How Halo Effective Field Theory can help √
  - Halo EFT as a "super model" √
  - From S-factor data to Halo EFT parameters, and back √
- Bayesian Model Averaging→Bayesian Model Mixing
  - What is Bayesian Model Averaging?
  - An application: the overall prediction of EDFs for the neutron drip line
  - Toy-model test of BMA
- The BAND Software Framework

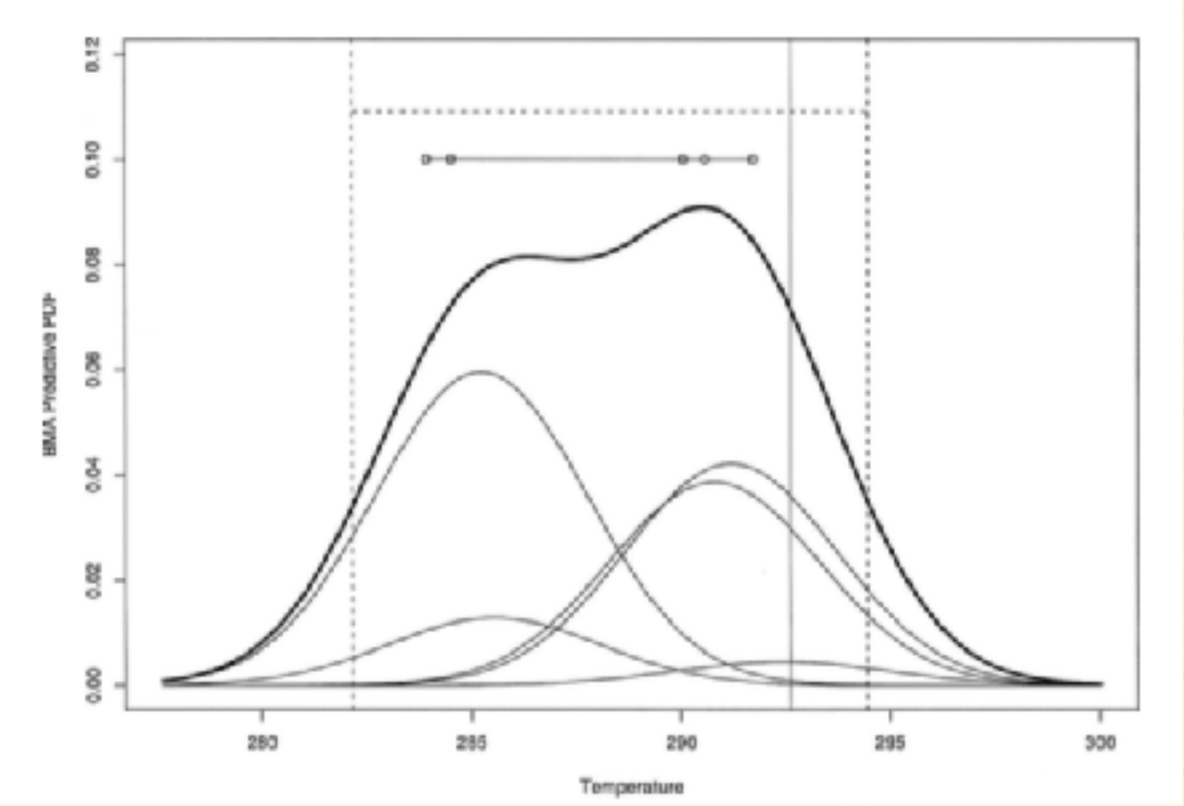
Bayesian Model Averaging

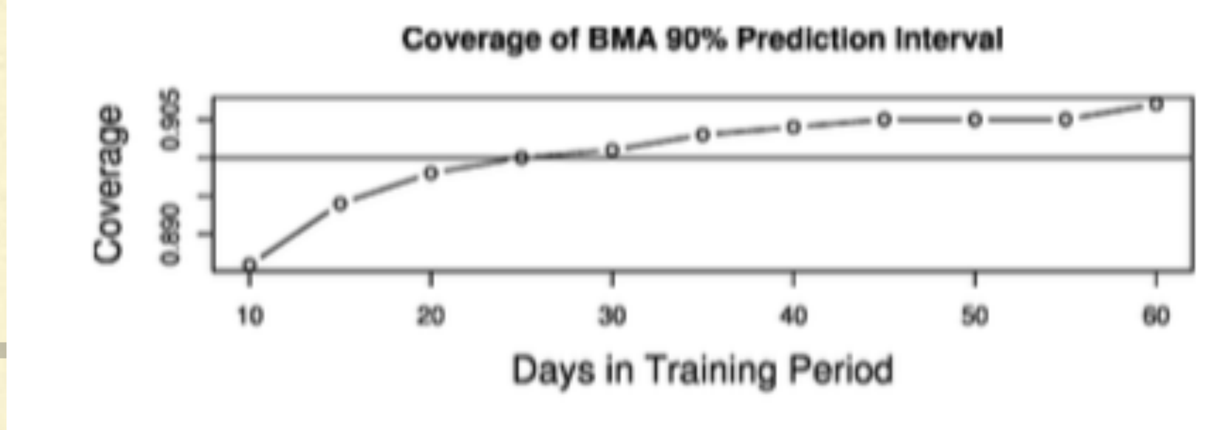
Bayesian Model Averaging: marginalize over a discrete set of models {M}

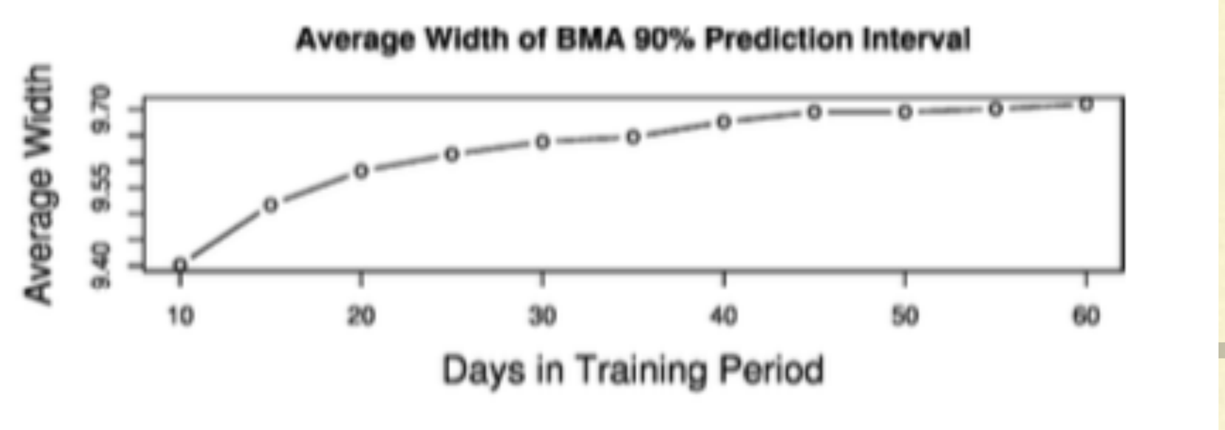
$$\mathrm{pr}(Q\,|\,D,I) = \sum_M \mathrm{pr}(Q\,|\,M,D,I)\,\mathrm{pr}(M\,|\,D,I)$$

- Used in several other fields
- Improves central values and coverage properties in weather forecasting

Raftery et al. (2005)







Bayesian Model Averaging: some details

$$\mathrm{pr}(Q|D,I) = \sum_M \mathrm{pr}(Q|M,D,I)\mathrm{pr}(M|D,I)$$

- Average over models, with weights given by "Bayesian model evidence"

$$\mathrm{pr}(M|D,I) \propto \mathrm{pr}(D|M,I)\mathrm{pr}(M|I)$$

$$\mathrm{pr}(D|M,I) = \int \mathrm{pr}(D|\theta,M,I)\mathrm{pr}(\theta|M,I)d\theta$$

- Requires computation of integral over parameter space: cannot be done using (standard) MCMC

- If set of models {M} includes true model BMA is guaranteed to converge to result from that model as more data acquired: $\mathfrak{M}$ closed

- If set of models {M} does not include true model then BMA will converge to one with smallest KL divergence: $\mathfrak{M}$ open

BMA+EDF: where is the neutron drip line?

Neufcourt et al., PRL (2019); PRC (2020)

- Take 8 Skyrme EDFs: SkM*, SkP,SLy4, SV-min, UNEDF0, UNEDF1, and UNEDF2, as well as Gogny functional DIM and functional BCPM, and FRDM-2012 and Skyrme-HFB model HFB-24

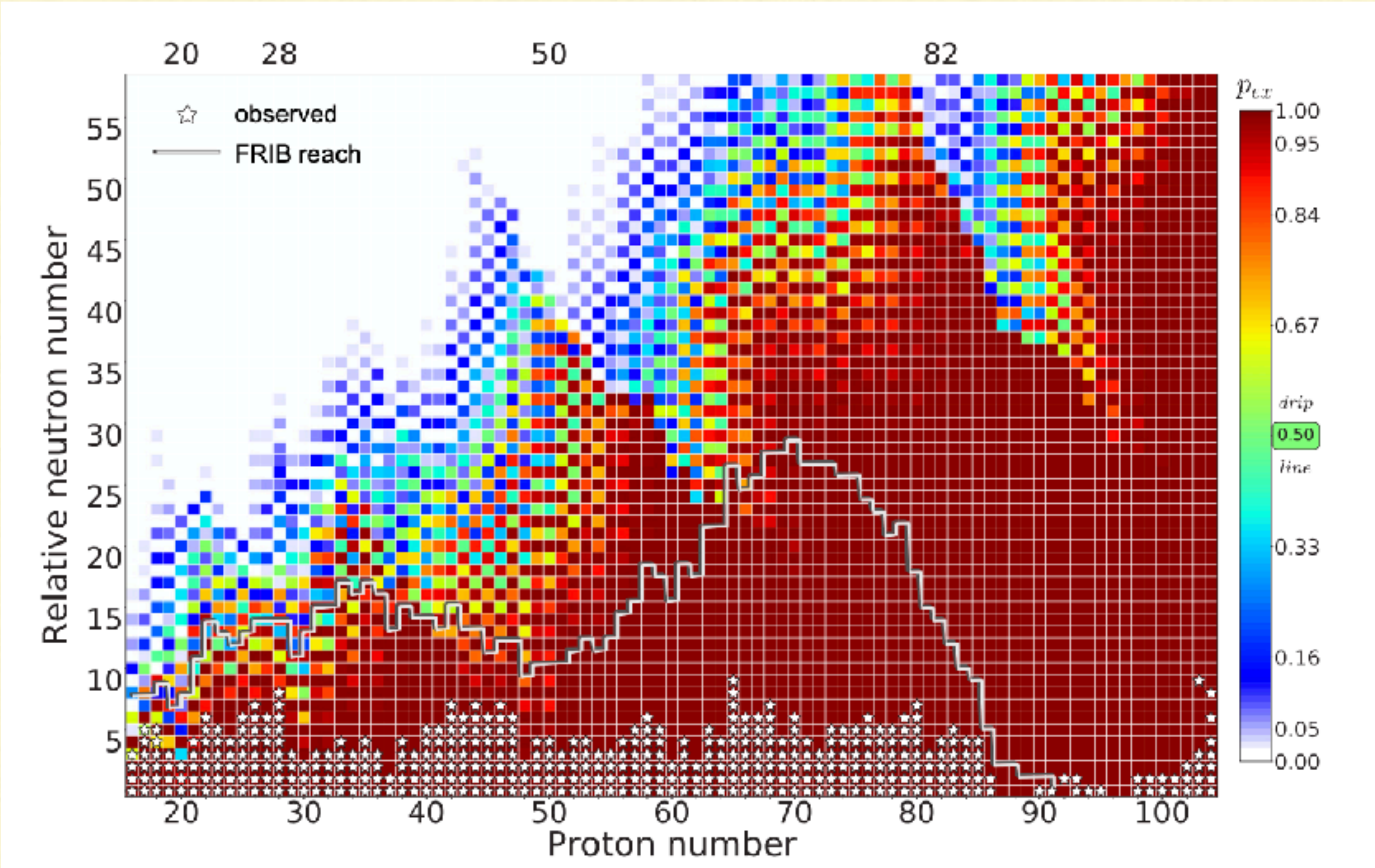
- Each model augmented by Gaussian Process trained to AME2016+ dataset

- Mix models according to weights: $w_k(n) :\propto p[S_{1n/2n}(x) > 0 | \mathscr{M}_k]$ for x one of the 254 neutron-rich nuclei with no neutron-separation energy measured

TABLE I. Model posterior weights obtained in the variants BMA(n) (4) and BMA(p) (5) of our BMA calculations. For compactness, the following abbreviations are used: UNEn = UNEDFn (n = 0,1,2) and FRDM = FRDM-2012.

BMA variant	SkM*	SkP	SLy4	SV-min	UNE0	UNE1	UNE2	BCPM	D1M	FRDM	HFB-24
BMA(n)	0.10	0.10	0.06	0.11	0.12	0.10	0.09	0.06	0.04	0.12	0.09
BMA(p)	0.00	0.03	0.08	0.05	0.04	0.14	0.12	0.04	0.16	0.17	0.17

Results



20
28
50
82
observed
FRIB reach
Relative neutron number
55
50
45
40
35
30
25
20
15
10
5
20
30
40
50
60
70
80
90
100
Proton number
p_{ex}
1.00
0.95
0.84
0.67
drip
0.50
line
0.33
0.16
0.05
0.00

Toy model test for Bayesian methods

Schindler, DP, Ann. Phys., 2009; Wesolowski, Klco, Furnstahl, DP, Thapaliya, JPG, 2016

- Given data $D=\{(d_k,\sigma_k):k=1,...,N\}$ taken at points x_k and a fit function $f(x;\mathbf{a})$ that depends on LECs $\mathbf{a}=\{a_0,a_1,a_2,\ldots\}$, extrapolate to a target point that is either "near" or "far"

- BUT, be careful! f only describes data in a limited domain

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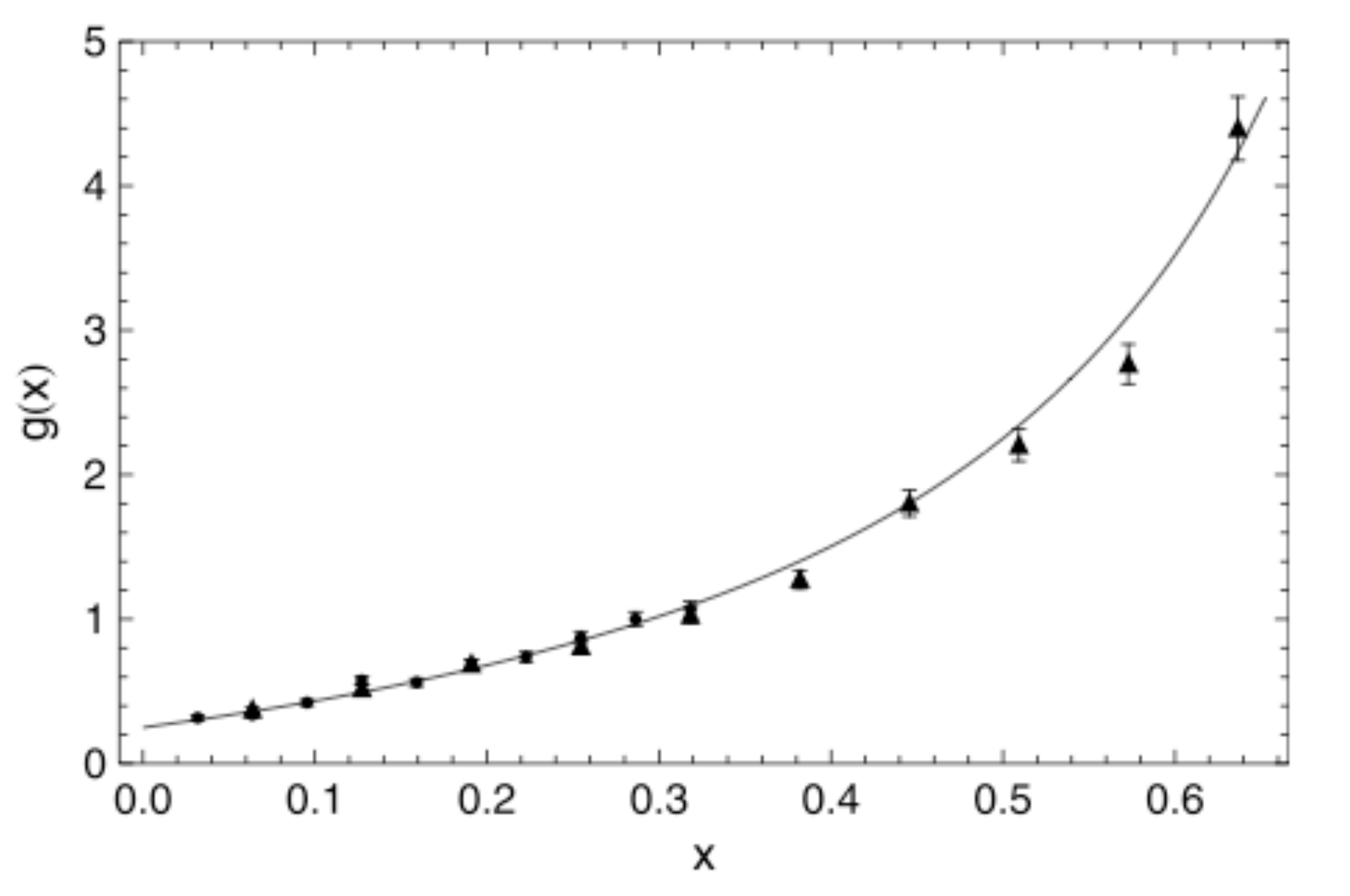

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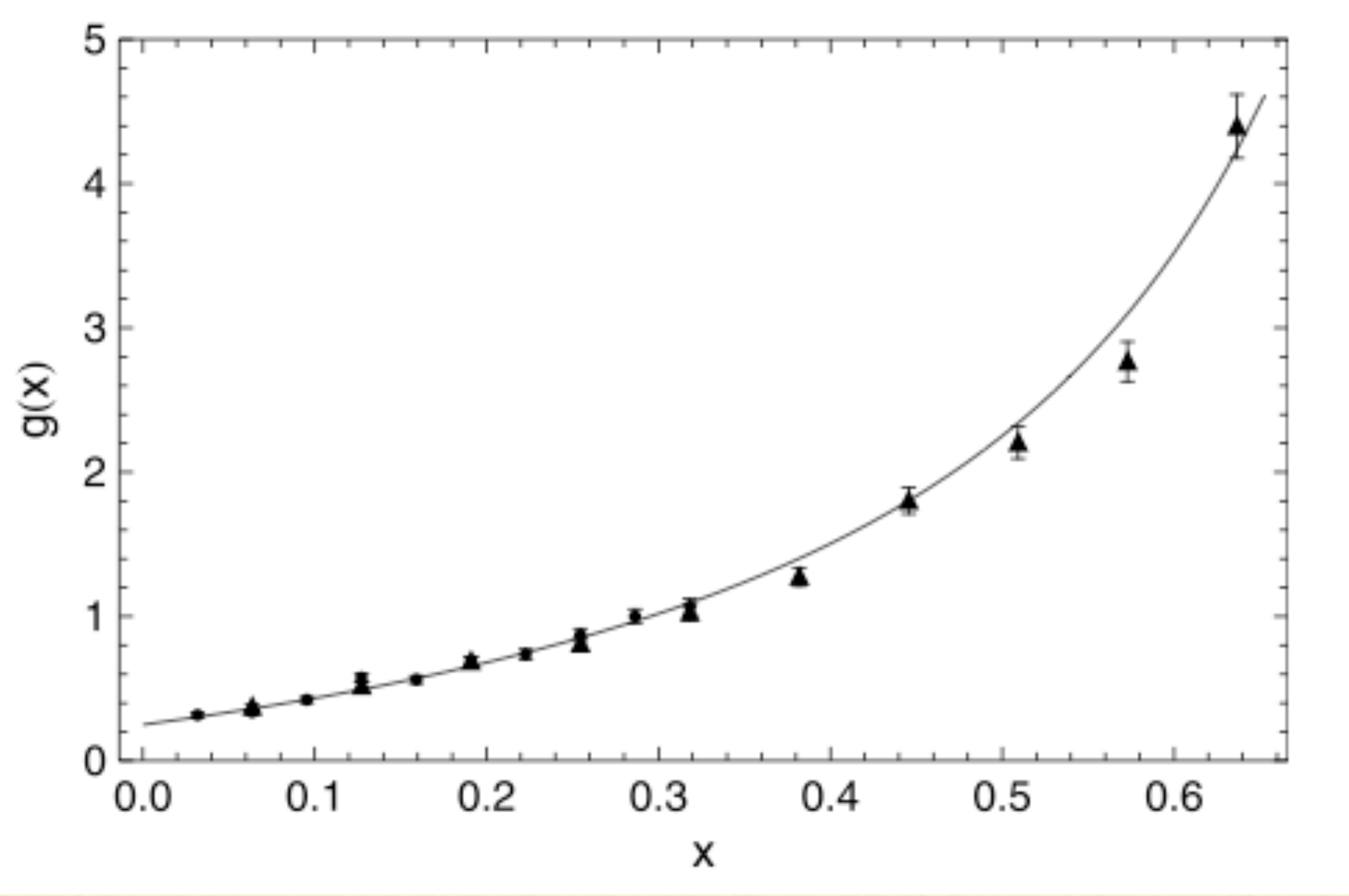

Toy example 1: data from

$$g(x) = (1/2 + \tan(\pi x/2))^2$$

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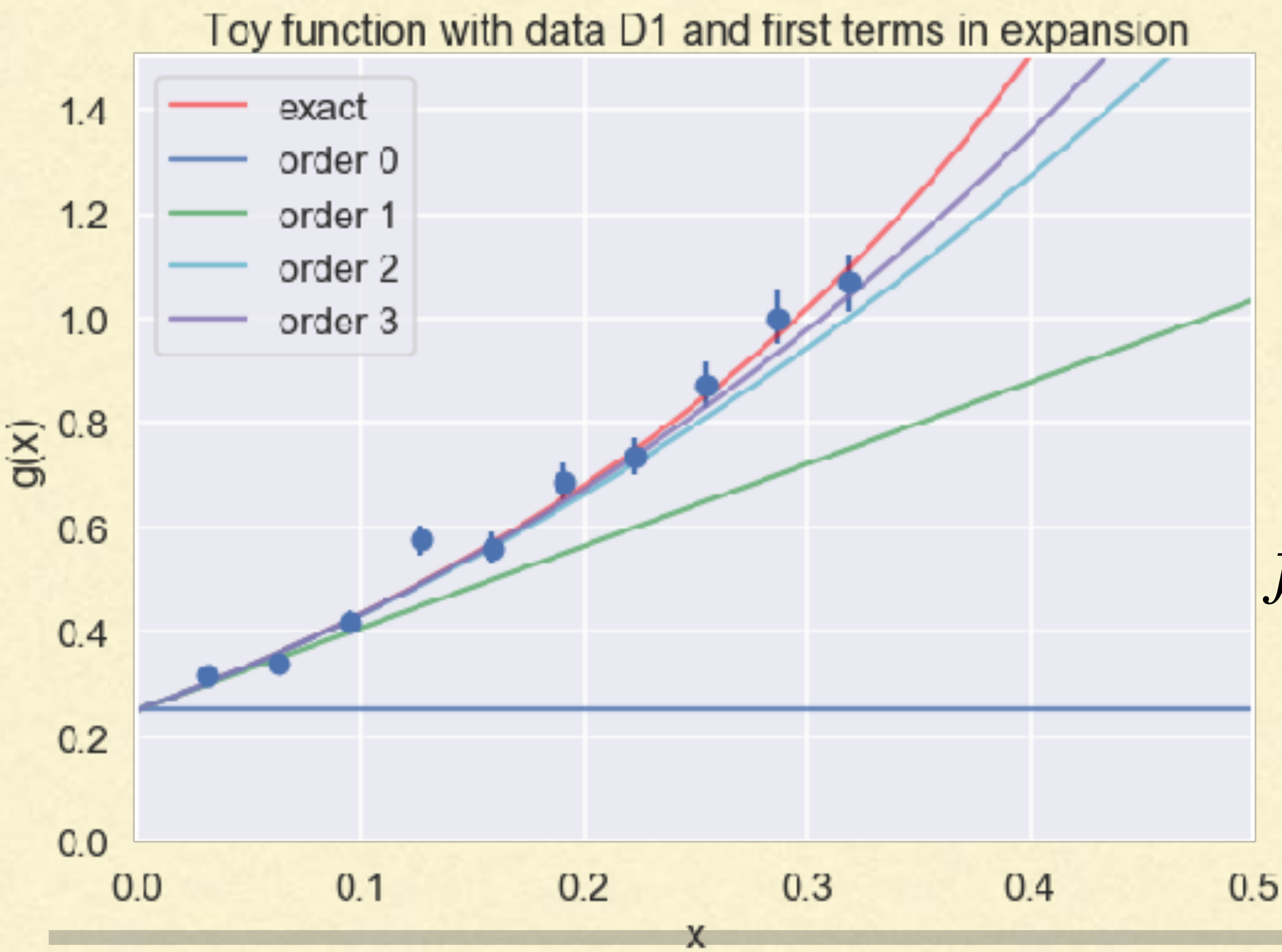

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Fit function:

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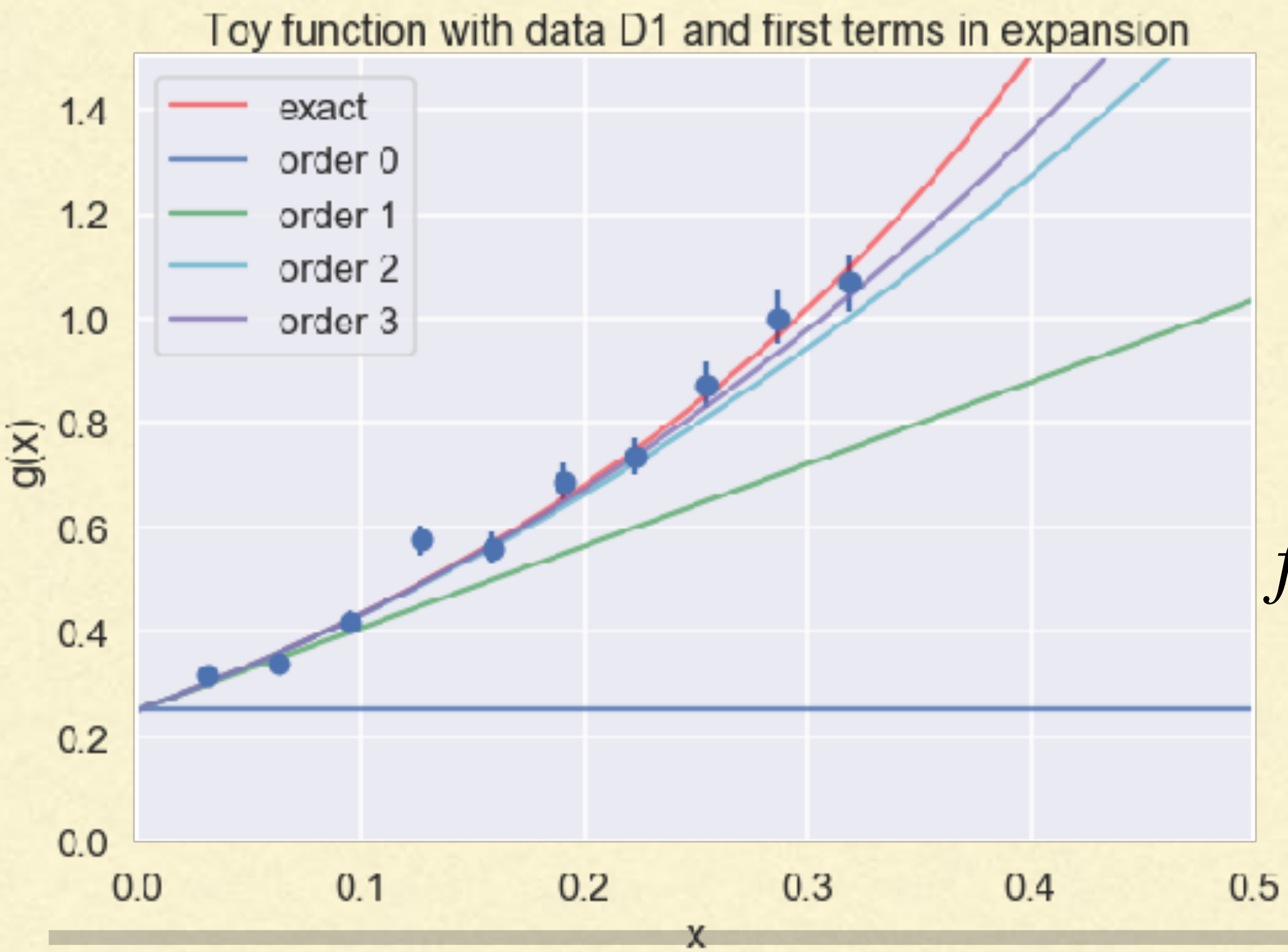

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What order should we take for M?

Coefficient extraction

Wesolowski, Furnstahl, Klco, Phillips, Thapaliya, JPG (2016)

		Uniform prior				Gaussian prior			
k	k_{max}	χ^2/dof	a_0	a_1	a_2	Evidence	a_0	a_1	a_2
0	0	67	0.48±0.01			~ 0	0.48±0.01		
1	1	2.2	0.20±0.01	2.6±0.1		6.0×10^2	0.20±0.01	2.6±0.1	
2	2	1.6	0.25±0.02	1.6±0.4	3.3±1.3	3.3×10^3	0.25±0.02	1.6±0.4	3.1±1
2	3	1.9	0.27±0.04	1.0±1	8.1±8.0	2.9×10^3	0.25±0.02	1.7±0.5	3.0±2
2	4	2.0	0.33±0.07	−1.9±3	45±30	2.8×10^3	0.25±0.02	1.7±0.5	3.0±2
2	5	1.4	0.57±0.1	−15±7	280±100	2.8×10^3	0.25±0.02	1.7±0.5	3.0±2
2	6	1.9	0.59±0.3	−16±20	310±400	2.8×10^3	0.25±0.02	1.7±0.5	3.0±2
True values			0.25	1.57	2.47		0.25	1.57	2.47

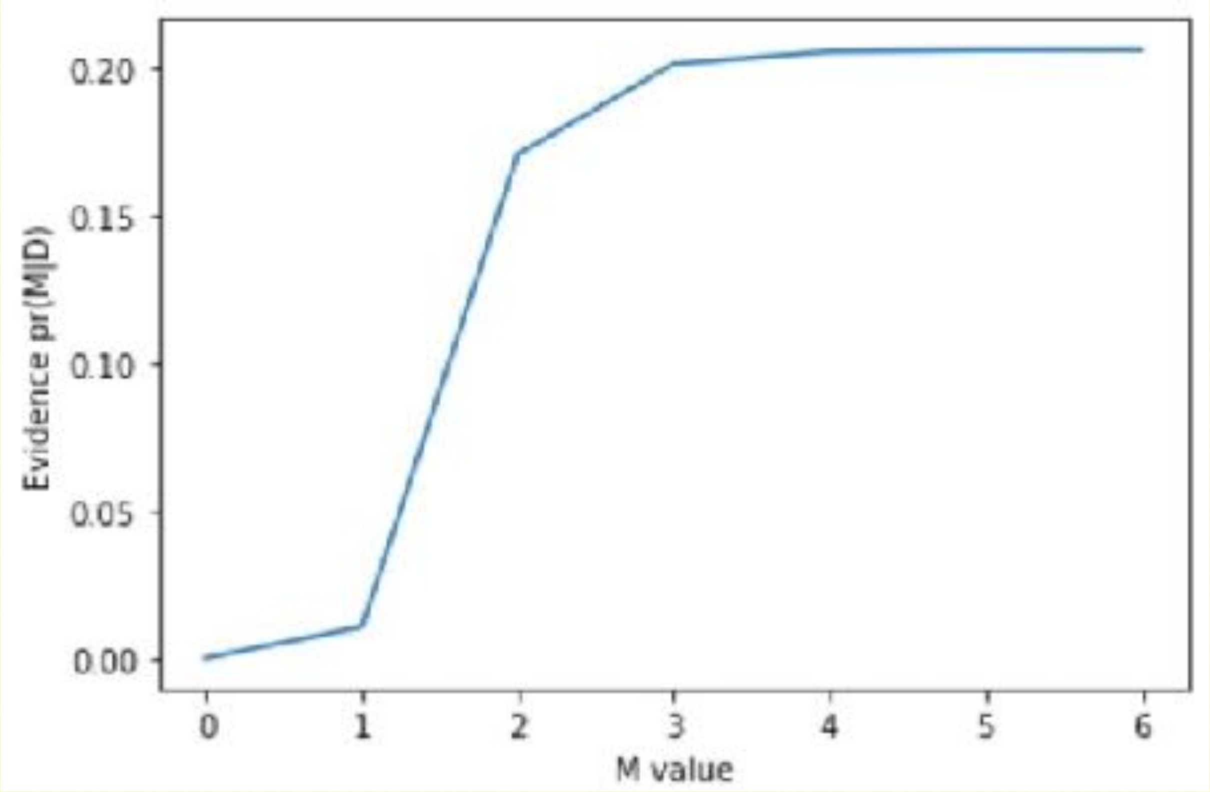
$\bar{a}_{fix}=5$

- Minimizing χ^2 =Least-squares fitting=Uniform prior
- Corresponds to not employing any additional information on the problem, beyond that provided by the data (including errors)
- Similar results up to k=2, not beyond

Model evidence & BMA

Connell, Billig, DP, JPG (2021)

$$\mathrm{pr}(f(x_t)\,|\,D) = \sum_M \mathrm{pr}(f(x_t)\,|\,D, M)pr(M\,|\,D)$$



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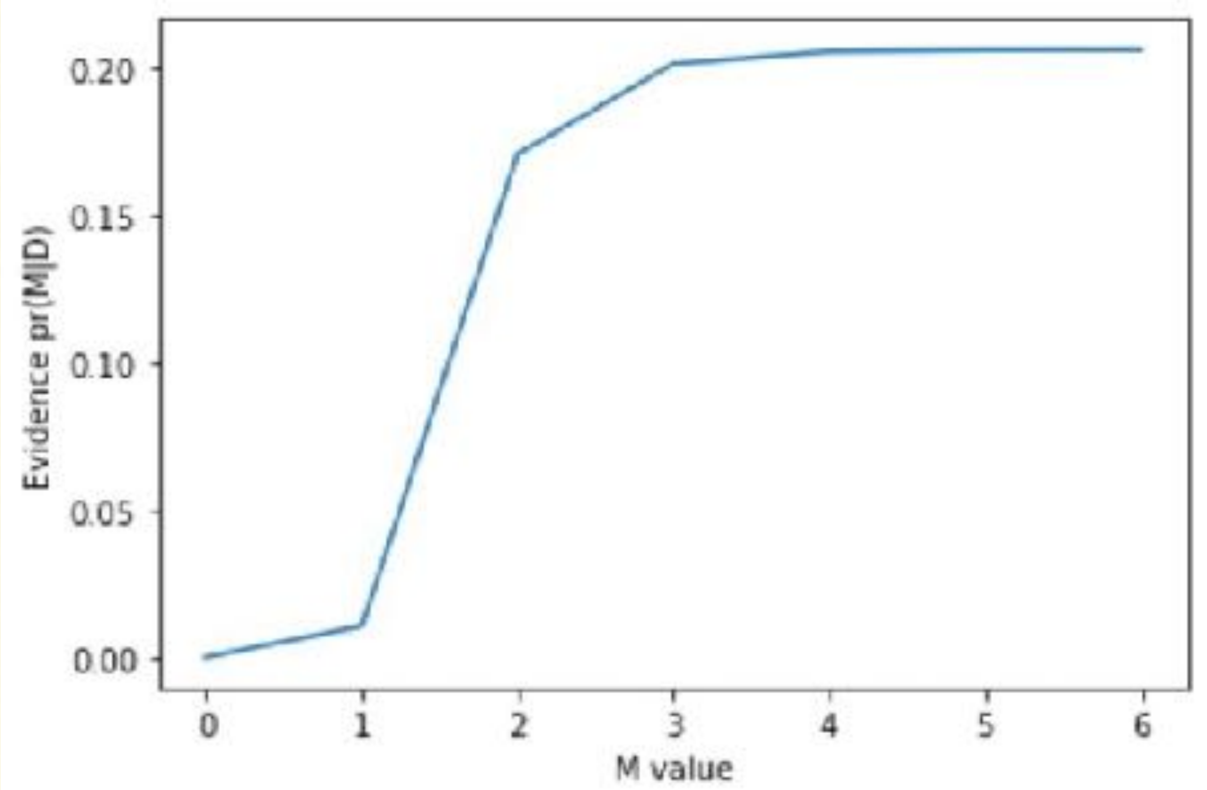

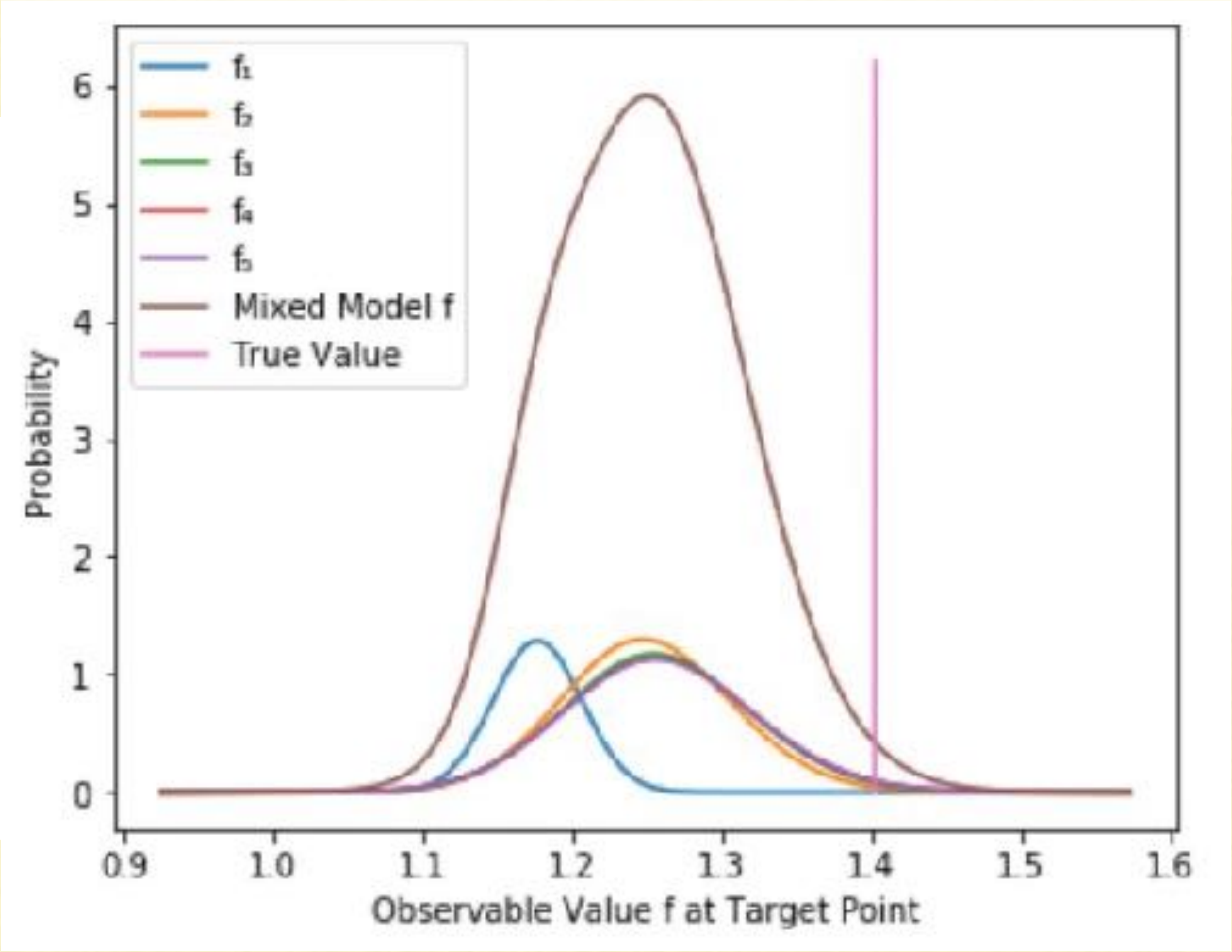

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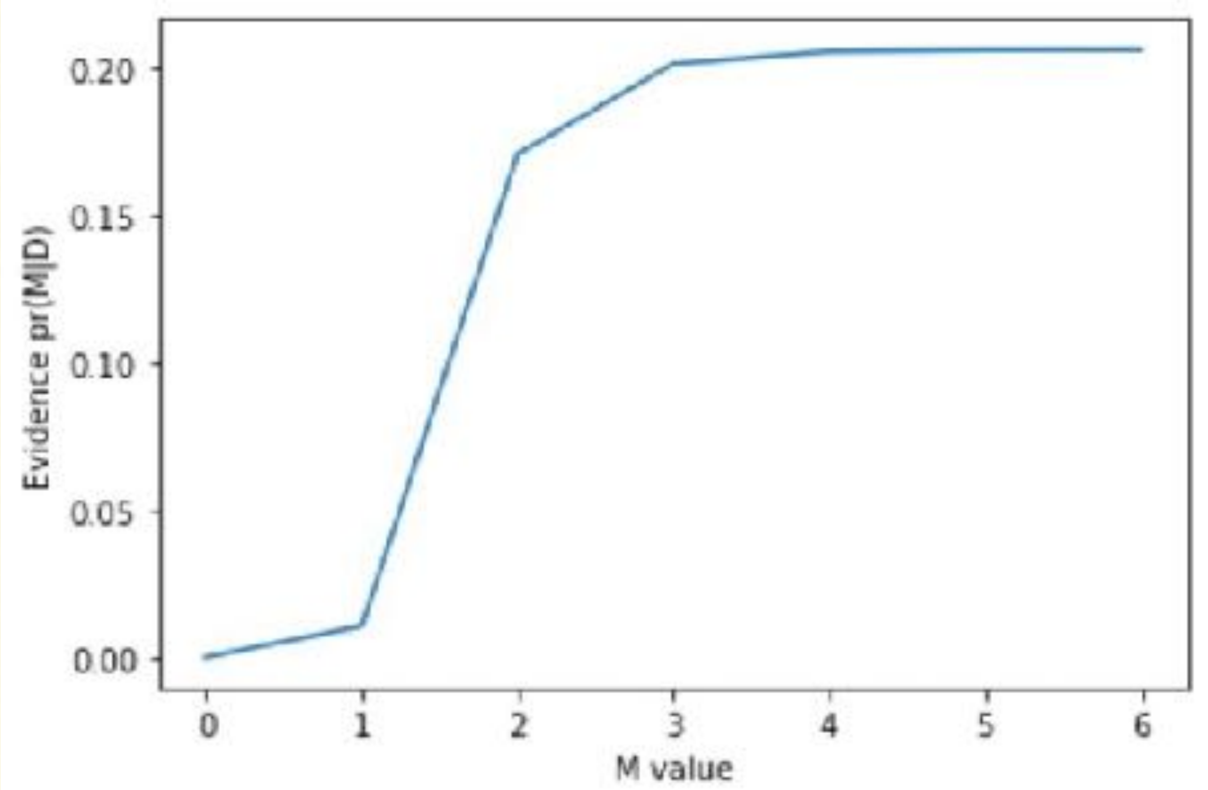

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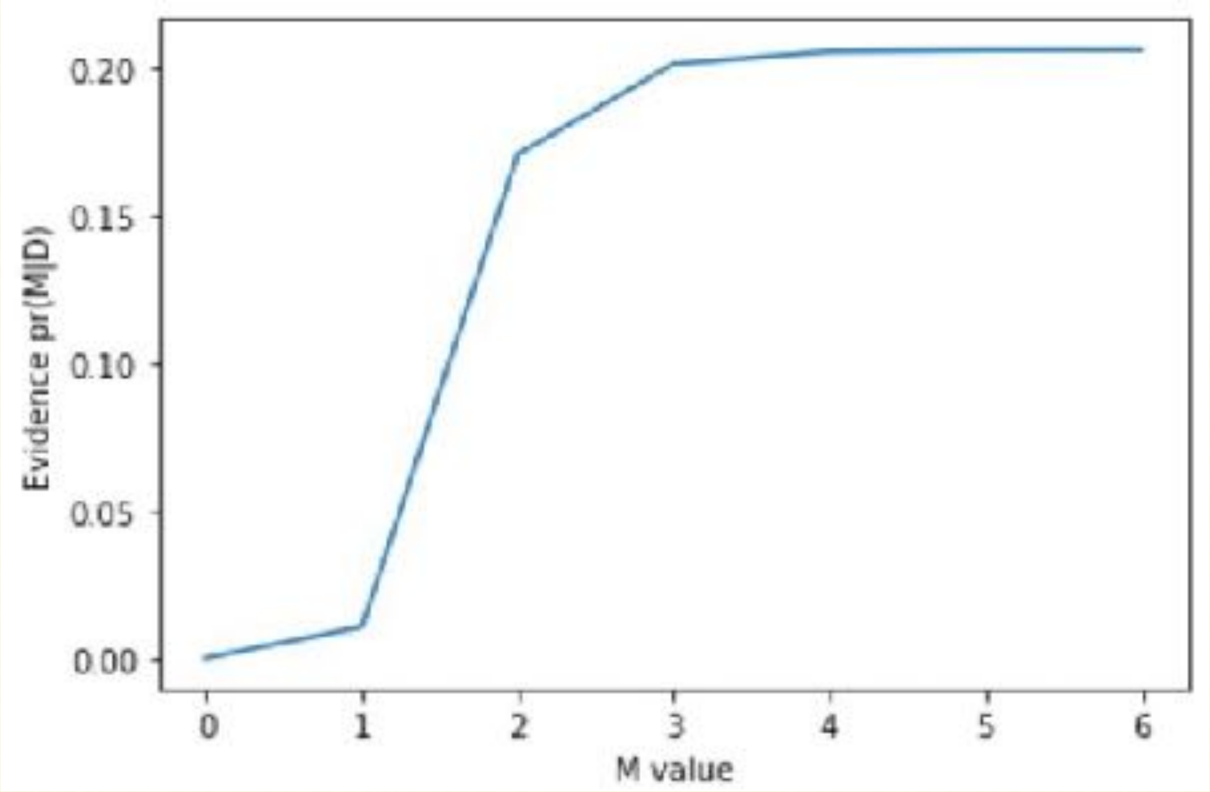

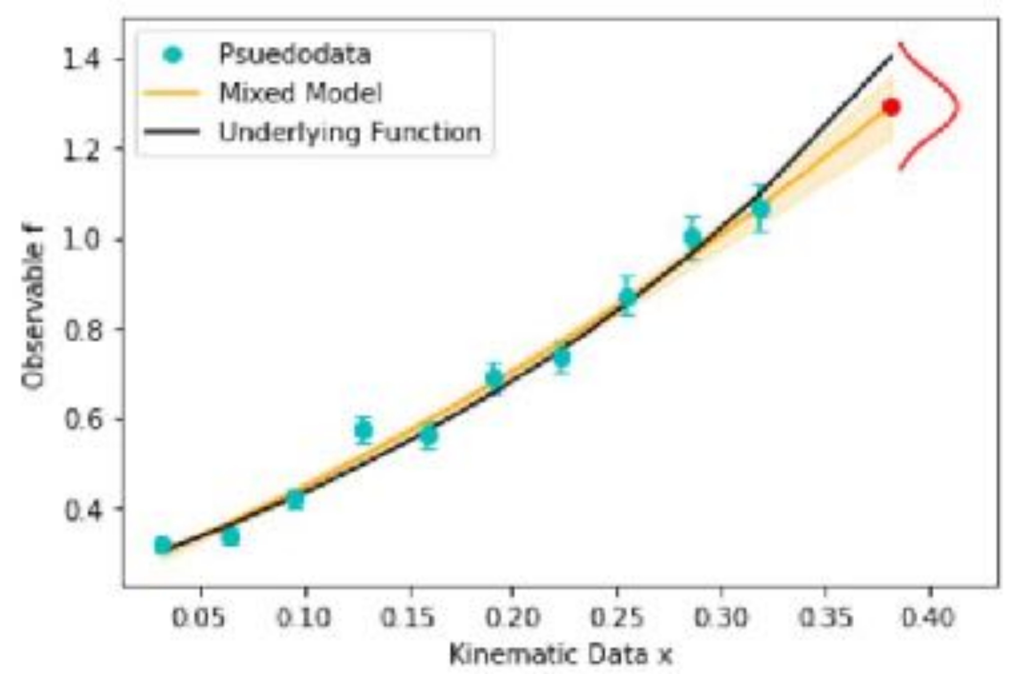

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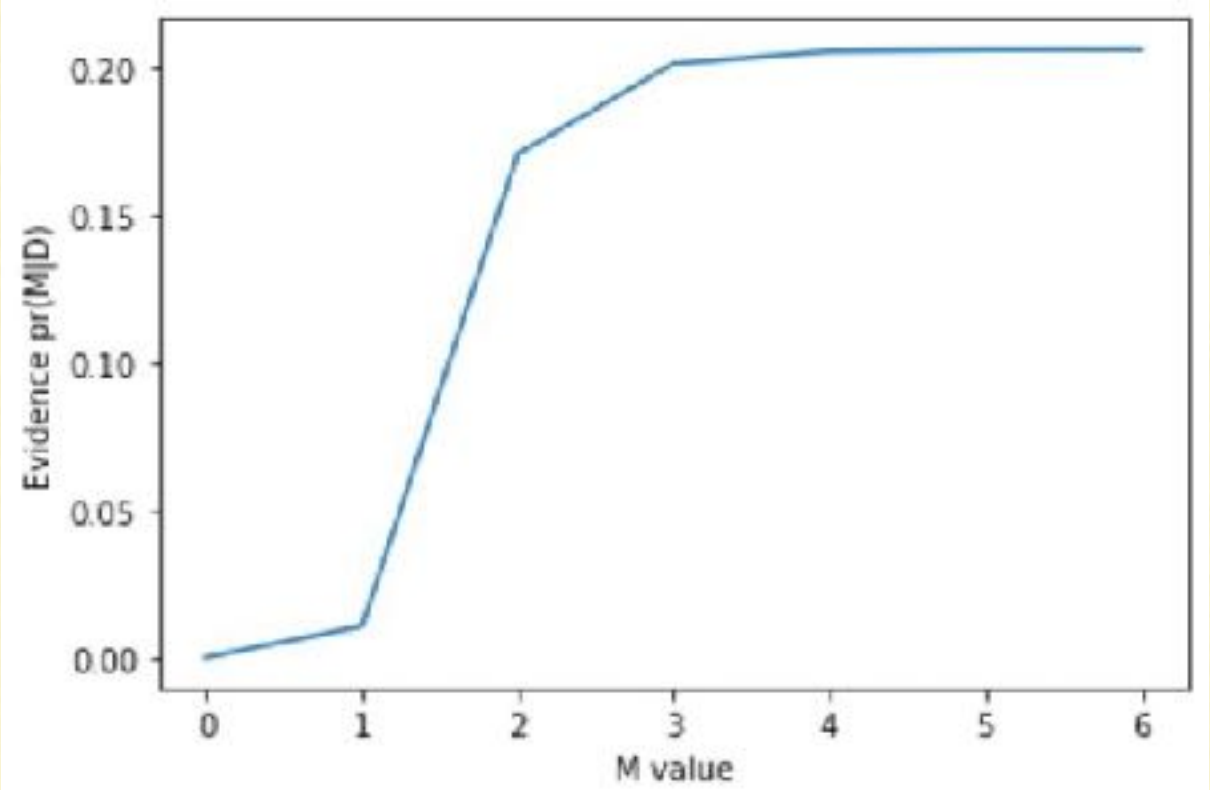
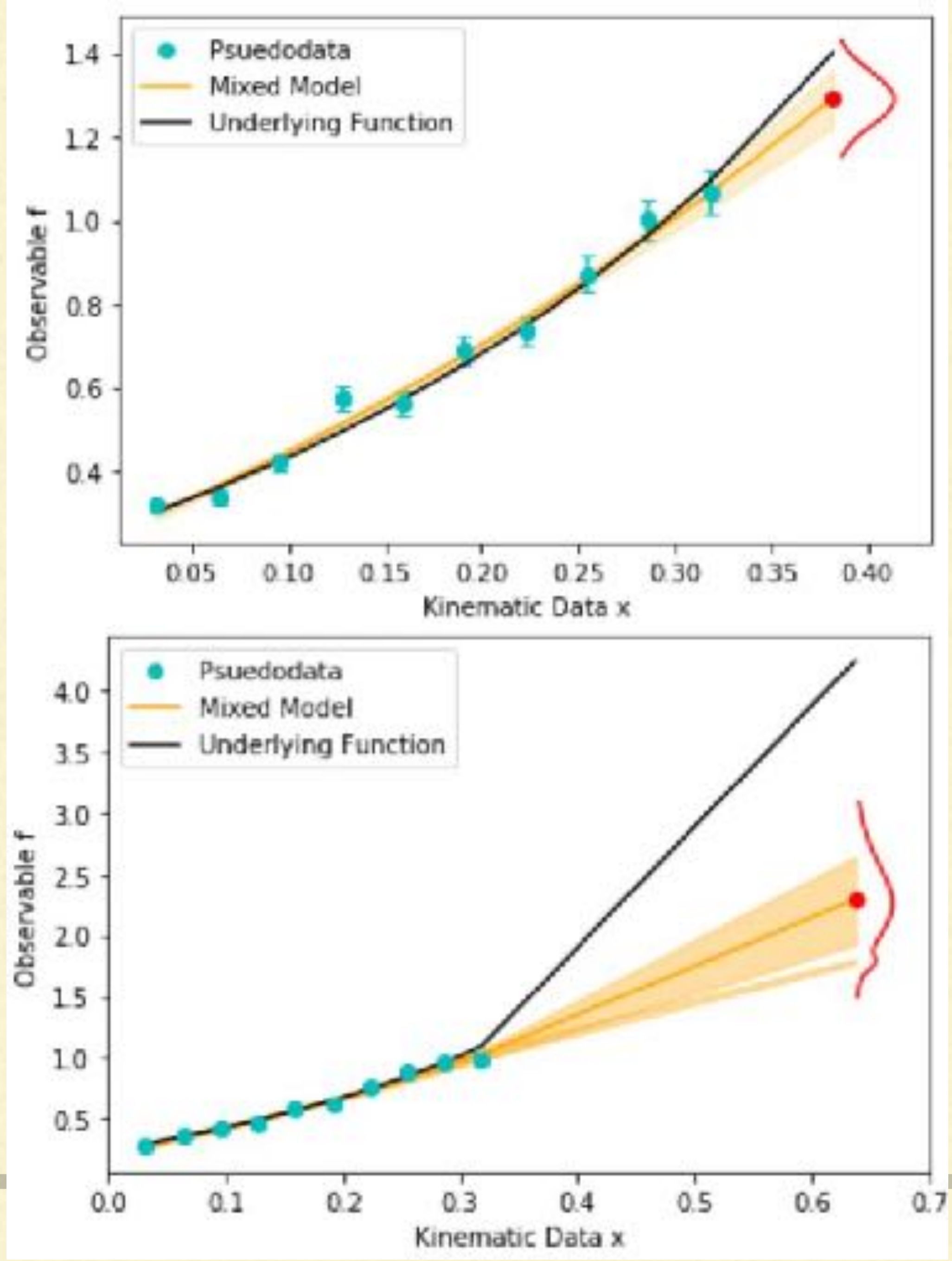
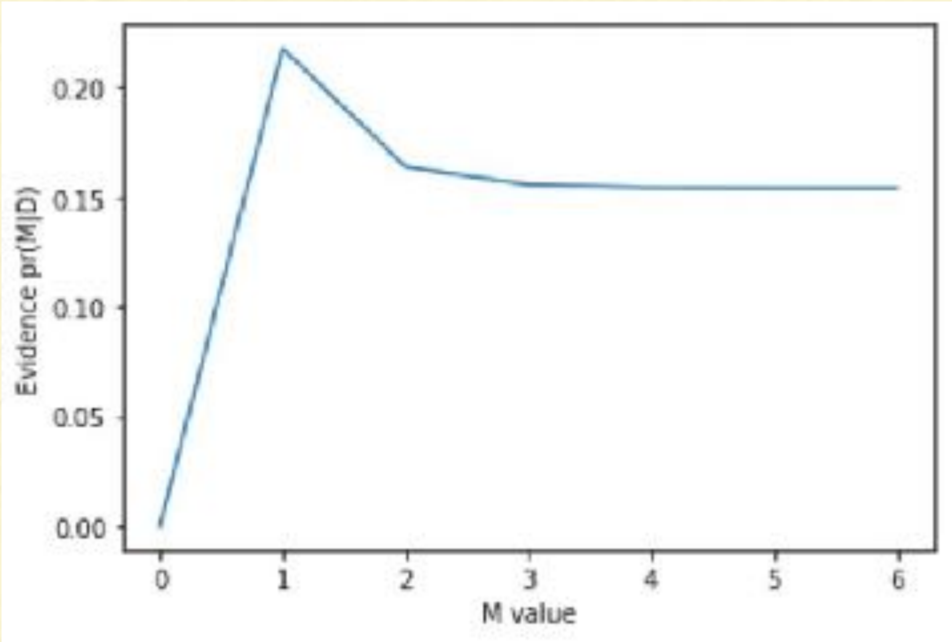
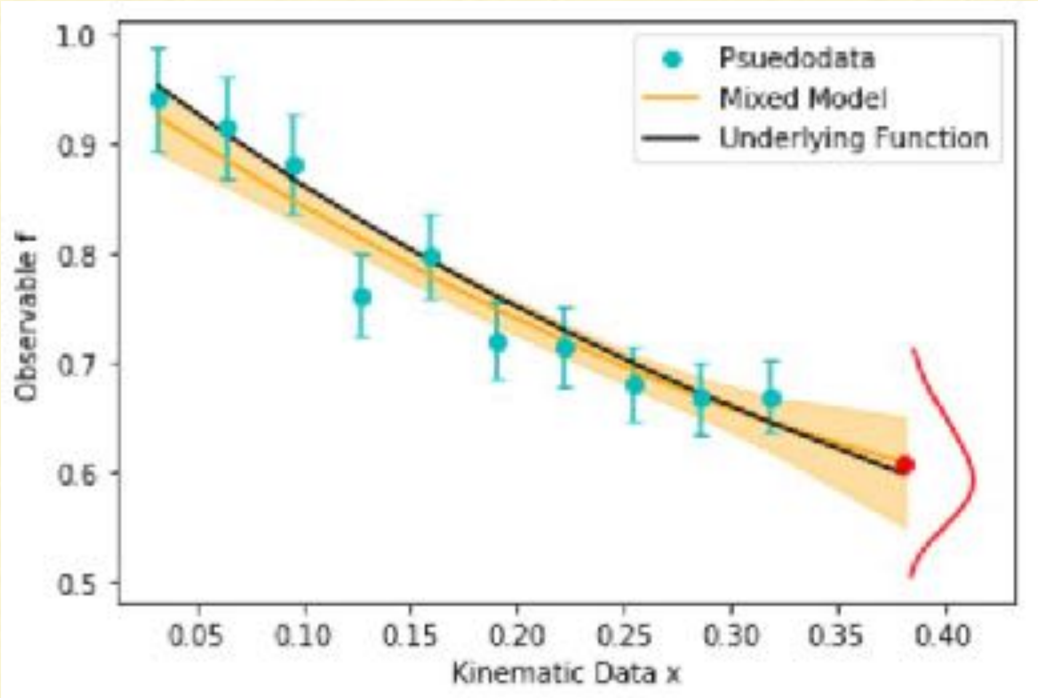


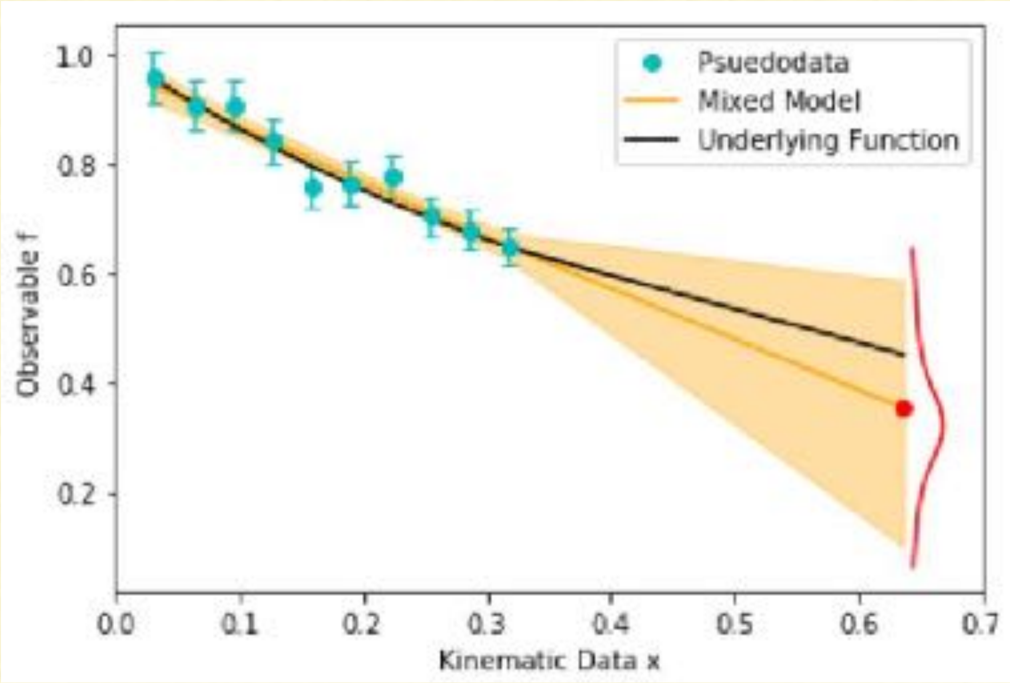


A more docile function

$$g_2(x) = \left(\frac{1.3}{1.3 + x}\right)^2$$







- Performance can be quantified using "Empirical Coverage Probability"

Conclusions from toy model

- In this case both situations are formally "open" but polynomials can describe the second case, so BMA works quite well. BMA extrapolate better than highest-order or highest-evidence model

- BMA not a panacea though: BMA does not help dire situation with $g_1(x)$ as we get close to singularity

- Could choose different weights: stacking uses LOO weights

- But one defect of BMA is that it uses weights based on global model performance. Could also consider locally-defined weights: "Local Bayesian Model Mixing"

- Locally-defined weights can leverage strengths of models in different regions, e.g., mixing expansions in g and 1/g could provide a result (with UQ!) that works well for all g

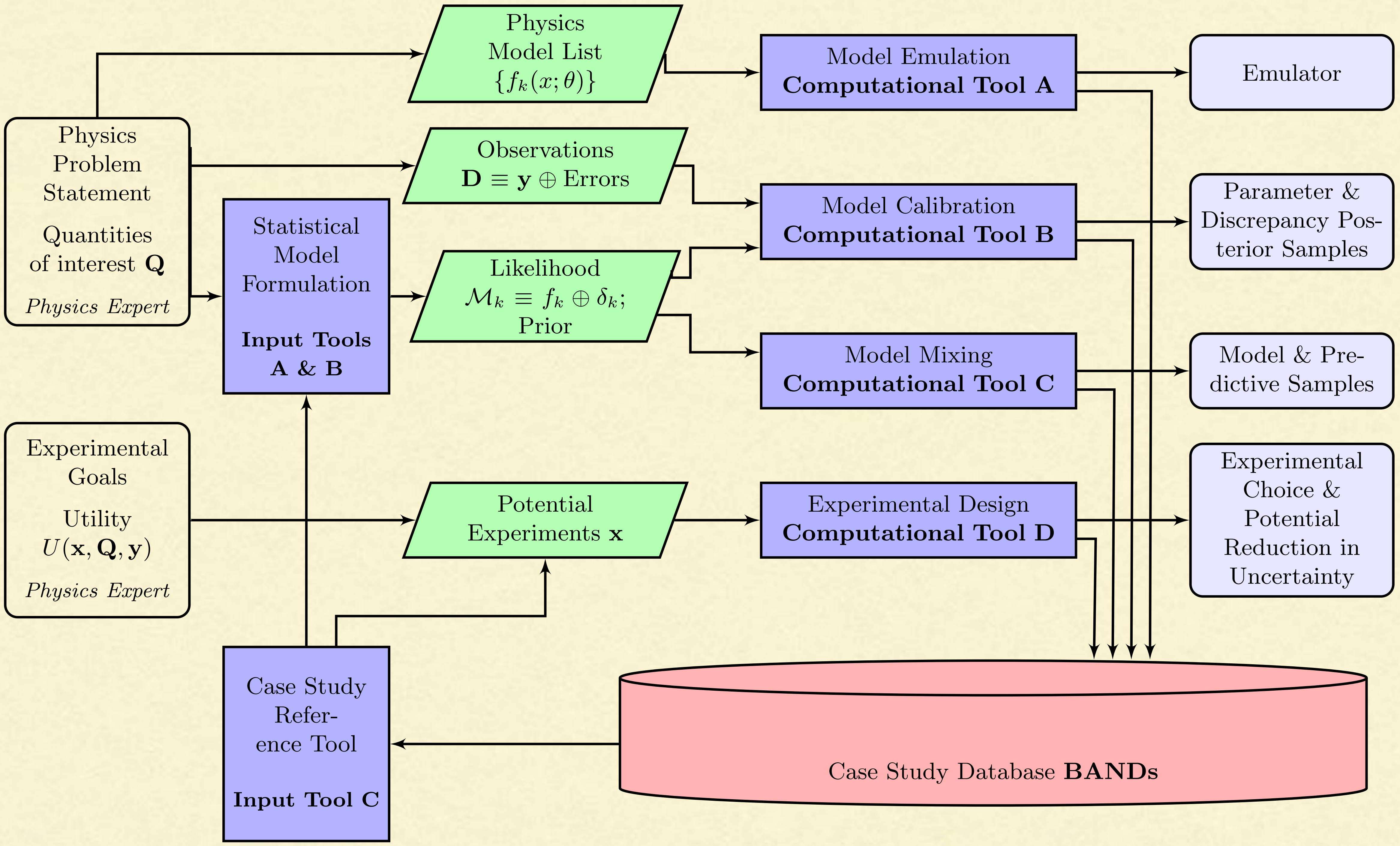
Semposki, Furnstahl, DP (2022)

BAND

Bayesian Analysis of Nuclear Dynamics

- Much progress on Uncertainty Quantification in Nuclear Physics in last few years
- But still some inhibitions regarding use of Bayesian methods:
  - What prior should I choose?
  - Isn't MC sampling too computationally expensive a way to estimate the parameters I care about?
- Difficult to assess model uncertainty
  - Proposal: use "Bayesian Model Mixing" to provide error bars that reflect full error bar for a nuclear-physics prediction, based on best available Nuclear Physics knowledge
- Consistently calibrated and mixed nuclear-physics models can then be used for optimal design of experiments

The Framework



The Team I: Senior Investigators

- Ohio U., Daniel Phillips: Nuclear Physics (PI)
- Michigan State U., Witek Nazarewicz, Filomena Nunes, Scott Pratt: Physics; Taps Maiti, Frederi Viens: Statistics
- Northwestern U., Matthew Plumlee: Statistics, Stefan Wild: Computer Science
- Ohio State U., Dick Furnstahl, Uli Heinz: Physics, Matthew Pratola, Statistics

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Get on the BAND Wagon: A Bayesian Framework for Quantifying Model Uncertainties in Nuclear Dynamics

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15 December 2020

Abstract. We describe the Bayesian Analysis of Nuclear Dynamics (BAND) framework, a cyberinfrastructure that we are developing which will unify the treatment of nuclear models, experimental data, and associated uncertainties. We overview the statistical principles and nuclear-physics contexts underlying the BAND toolset, with an emphasis on Bayesian methodology's ability to leverage insight from multiple models. In order to facilitate understanding of these tools we provide a simple and accessible example of the BAND framework's application. Four case studies are presented to highlight how elements of the framework will enable progress on complex, far-ranging problems in nuclear physics. By collecting notation and terminology, providing illustrative examples, and giving an overview of the associated techniques, this paper aims to open paths through which the nuclear physics and statistics communities can contribute to and build upon the BAND framework.

“BANDifesto”, J. Phys. G **48,** 072001 (2021)

Timeline

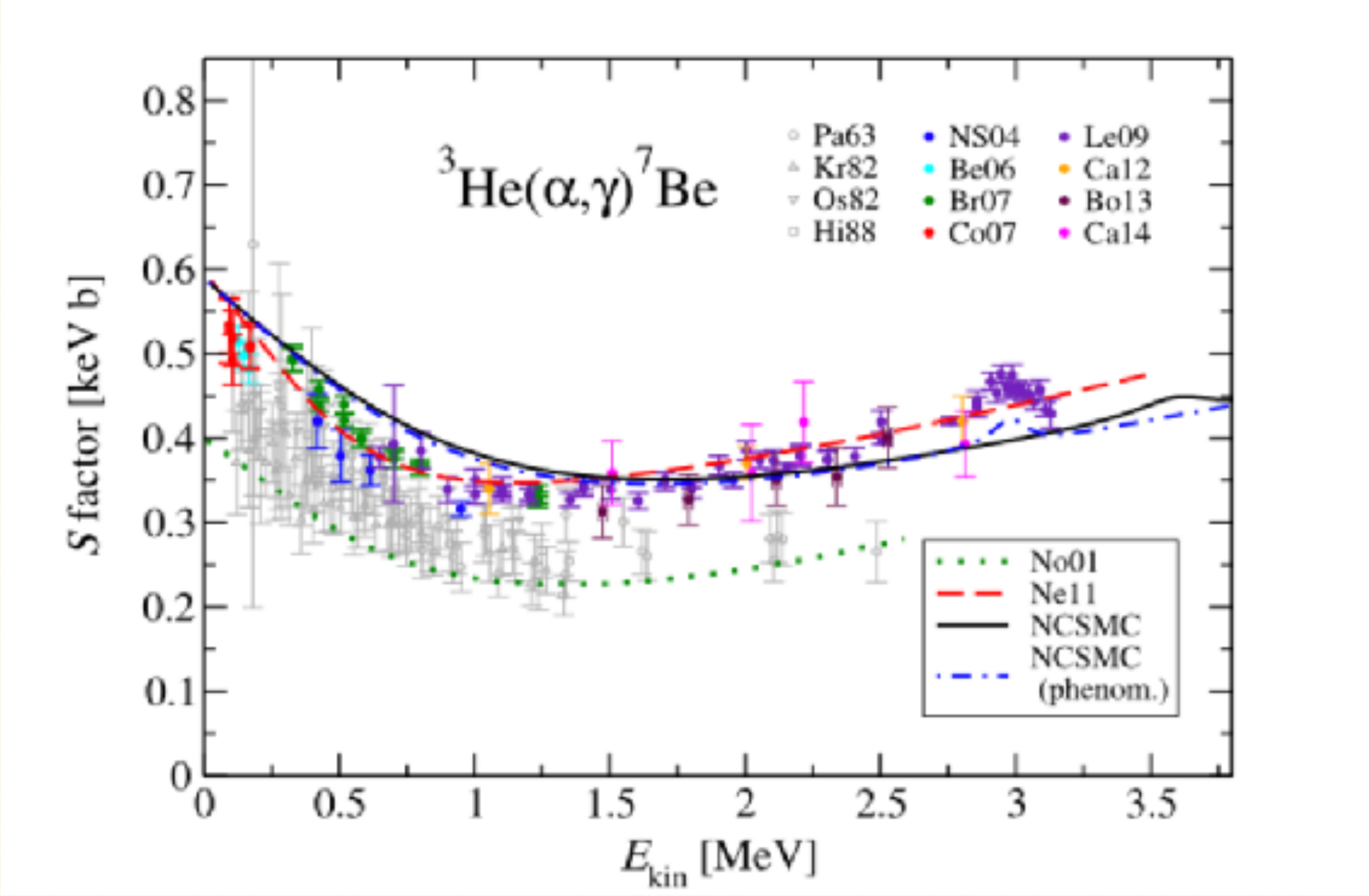
- Year 1: Release of BAND Manifesto; Nuclear-physics codes in repo
- Year 2: Version 1 demo released; POC demos for toy models
- Year 3: Version 2 framework released
- Years 4 & 5: Mature version of BAND Framework released with database; POC demos for experimental planning and forefront nuclear theory; tutorial & bootcamp; workshop for other disciplines
- Throughout: Roundtables with community, BAND camps, tutorials
- Collaboration & input welcomed

https://bandframework.github.io/

Ultimate goal is to build framework that is *generally useful*

Backup slides

Connecting to *ab initio* calculations



Dohet-Eraly et al., PLB (2016)

- ANC extracted from capture data: $C_{P1/2}^2 + C_{P3/2}^2 = 27 \pm 3$ fm^{-1}
- Significant constraints on s-wave scattering parameters already from capture
- Short-distance parameter L_{E1} is smaller for data and for Nollett's ab-initio based calculation than for cluster models. Pauli principle?