

TALENT COURSE III

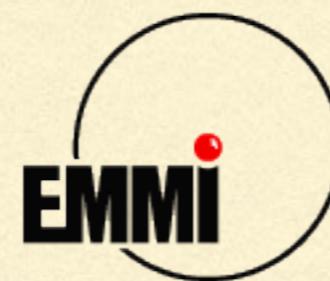
LEARNING FROM DATA: BAYESIAN METHODS AND MACHINE LEARNING

Lecture 19: Dealing with systematic errors

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Ohio University
TU Darmstadt
ExtreMe Matter Institute



OHIO
UNIVERSITY



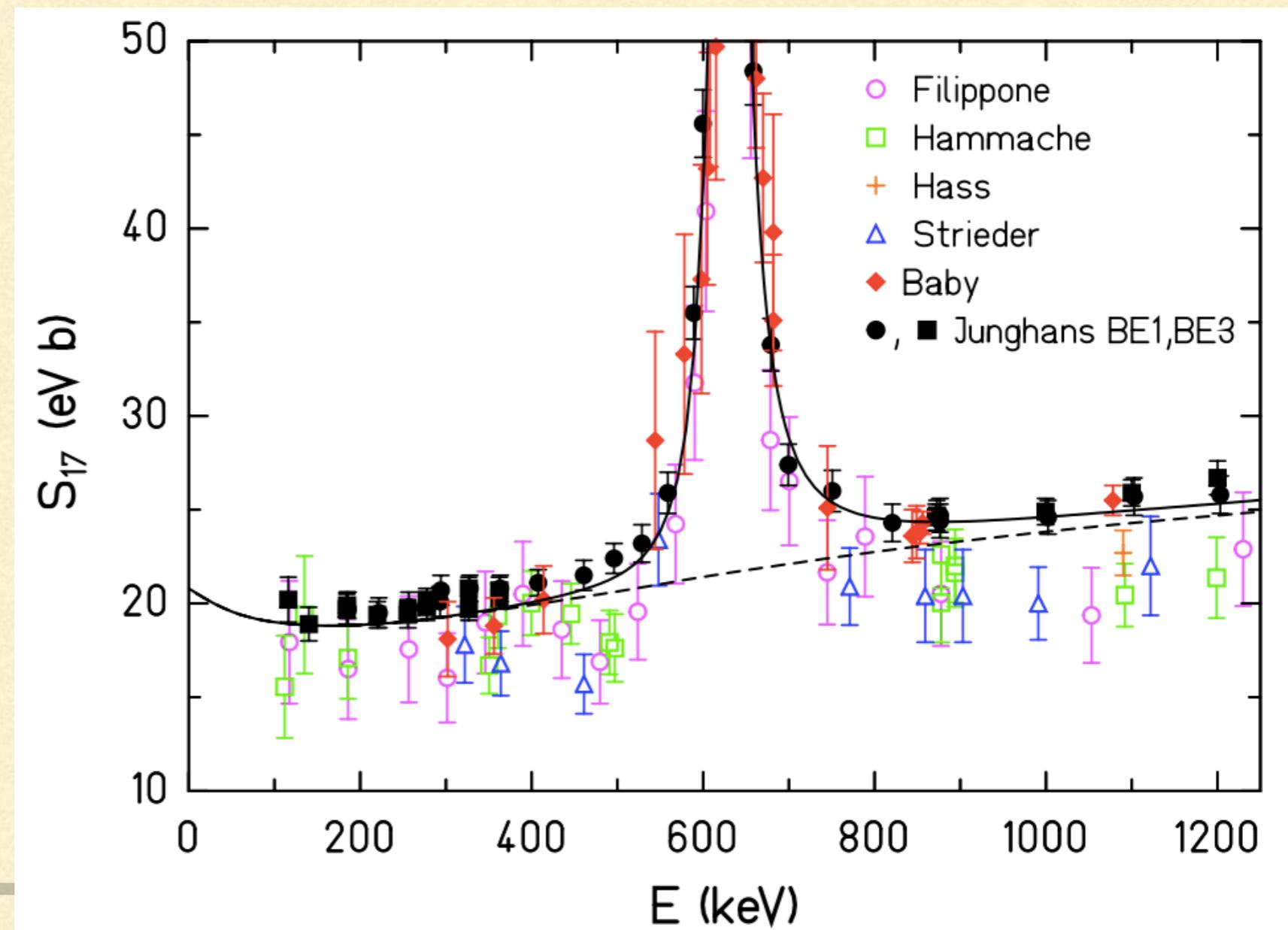
TALENT Course III is possible thanks to funding from the STFC

Systematic errors

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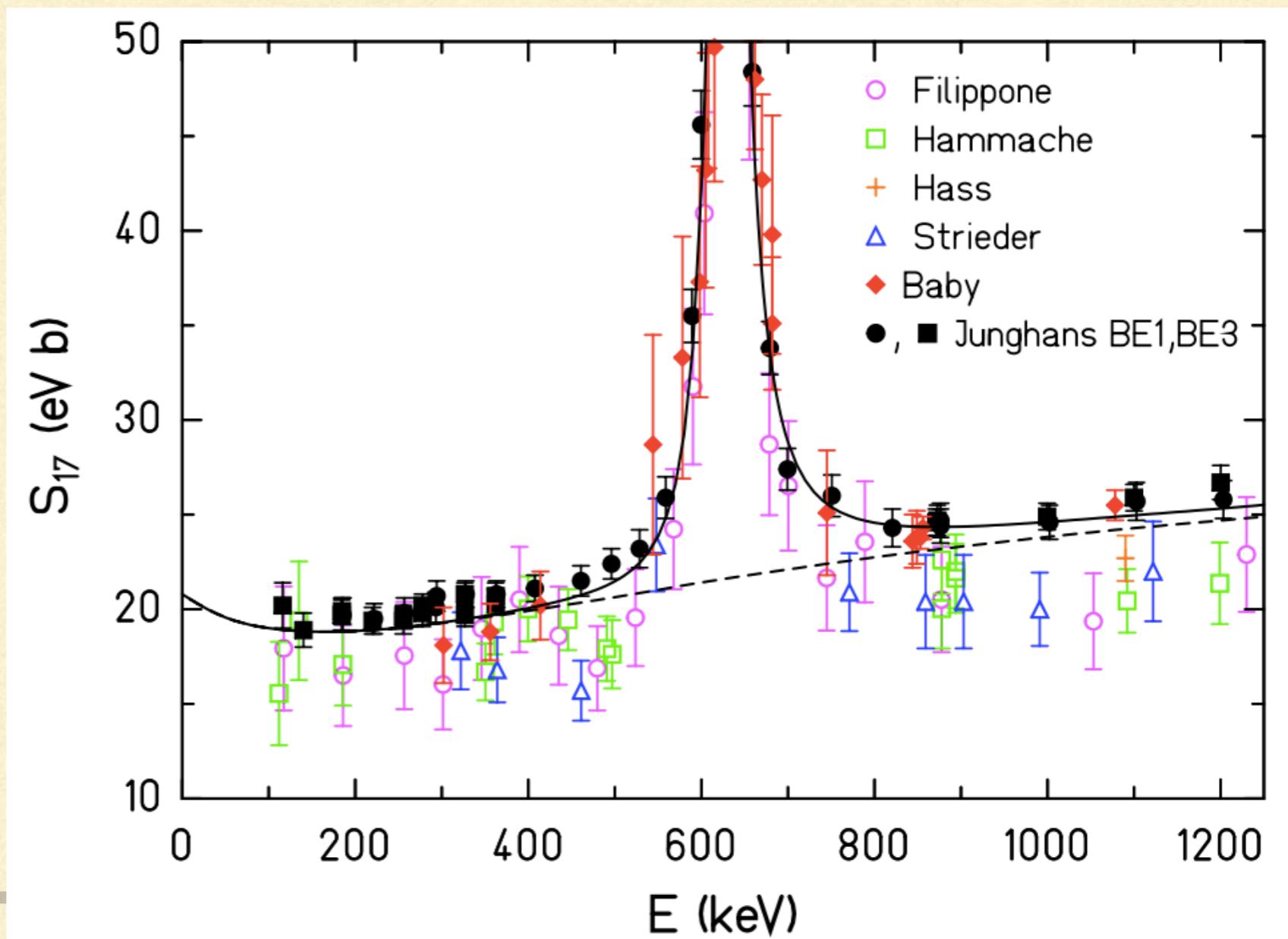
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- Offset
- Normalization errors (CME)
- Theory systematic with known functional dependence
- Energy uncertainty



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d'Agostini NIM A 336, 306 (1994)

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$$Y_1 - Y_2 \sim N(Y_1^{\text{true}} - Y_2^{\text{true}}, \sigma_1^2 + \sigma_2^2)$$

MAP value

- Suppose $Y_1^{\text{true}} = Y_2^{\text{true}} = k$
- Maximizing likelihood gives: $\hat{k} = \frac{Y_1\sigma_1^2 + Y_2\sigma_2^2}{\sigma_1^2 + \sigma_2^2}$

$$\sigma_k^2 = \frac{\sigma_1^2\sigma_2^2}{\sigma_1^2 + \sigma_2^2} + \sigma_c^2$$

Dealing with CMEs

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- d'Agostini bias

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- Minimum occurs at a value that is too small by a factor

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d'Agostini bias & its solution

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- Related to the value of f that minimizes χ^2 , which obeys

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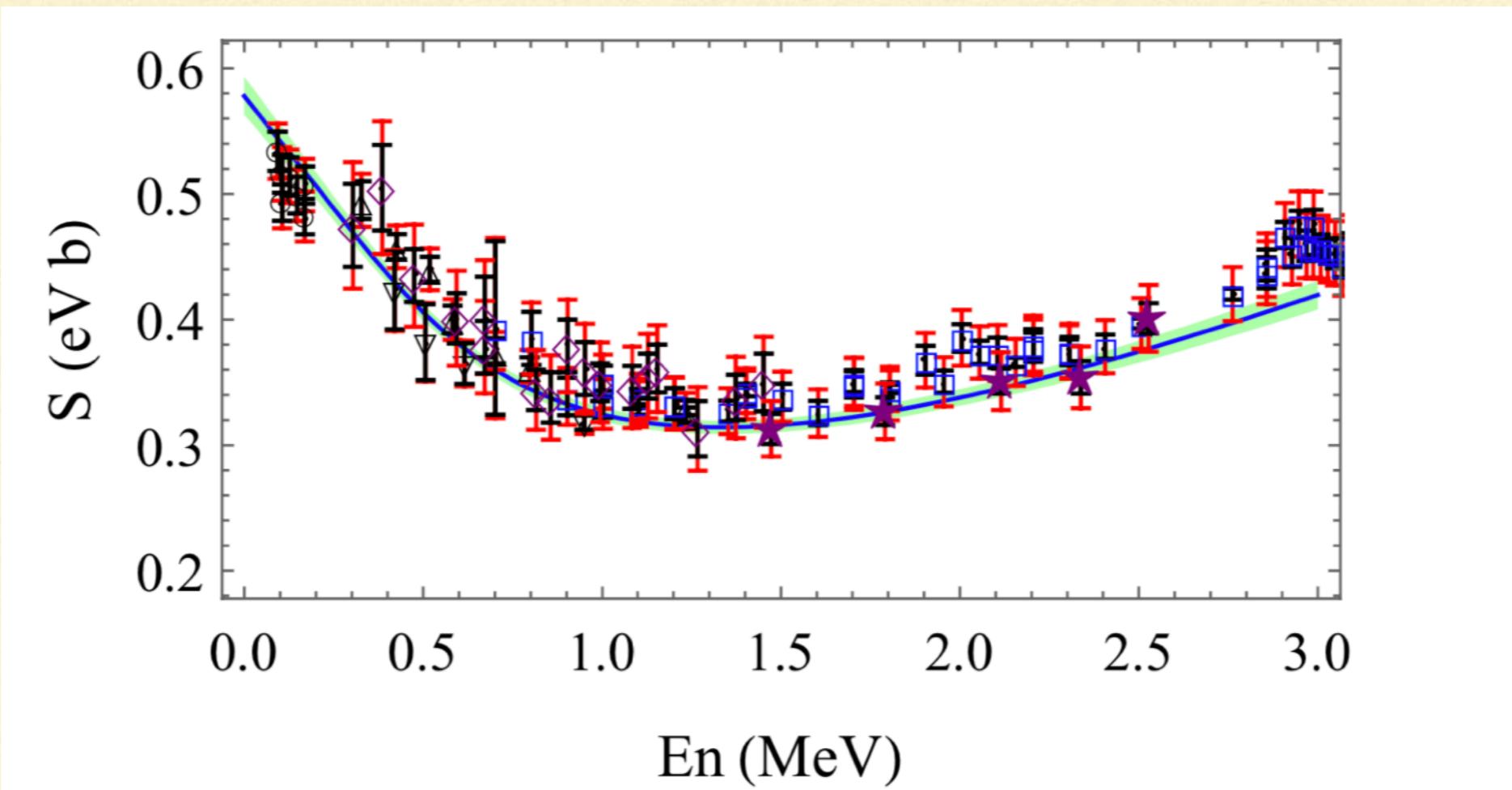
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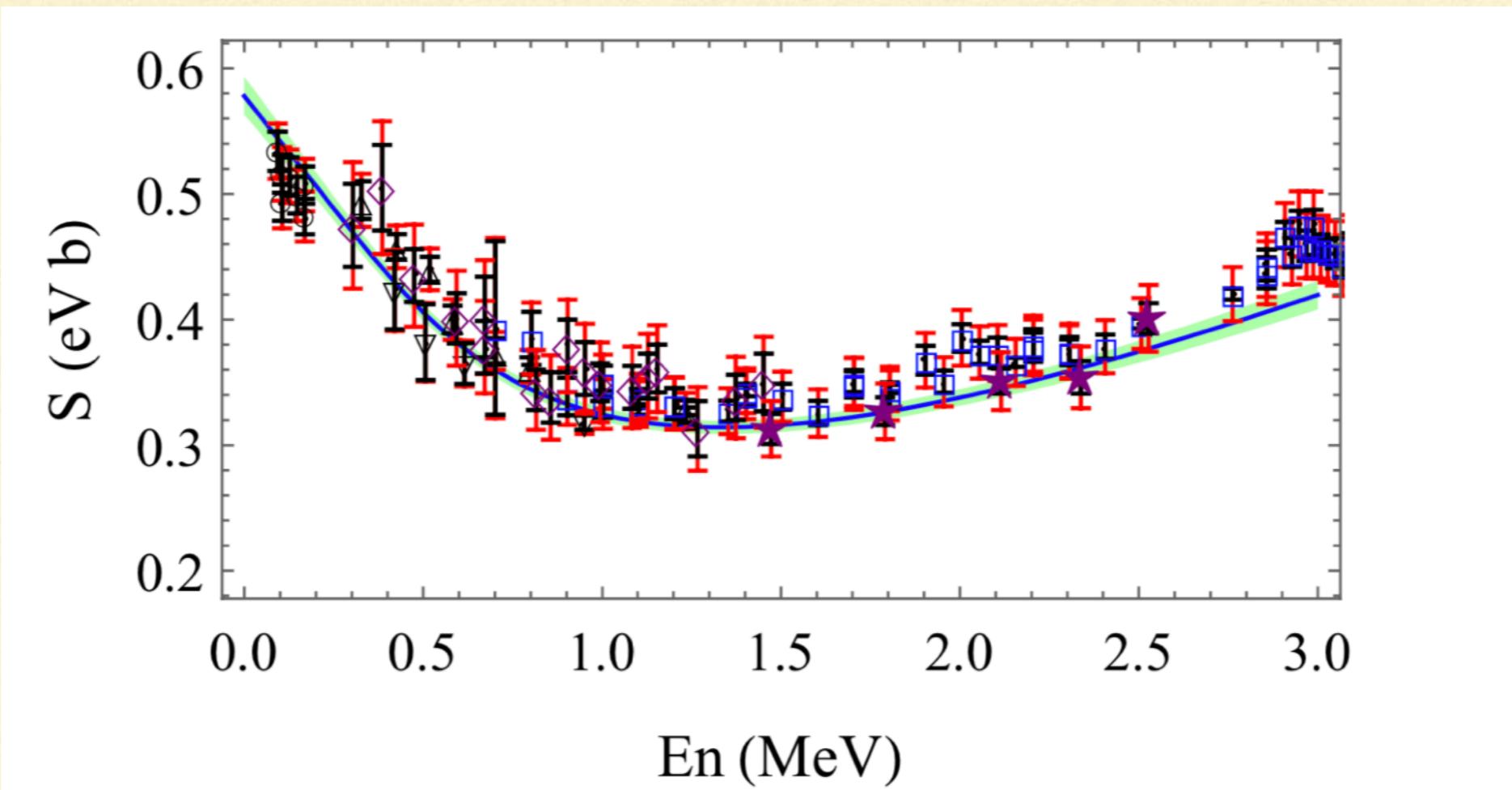
- Or equivalently rescale theory: Bayesian derivation

$$\chi_{\text{MLE}}^2 = \sum_{j=1}^{N_{\text{exp}}} \left\{ \chi_j^2 - \frac{(X'_j)^2}{1 + X''_j f_j^2} \right\}; \quad X'_j = \sum_{i=1}^{N_{\text{data}}^j} \frac{Y_{ji} - Y_{ji}^{\text{true}}}{\sigma_{ji}} \frac{Y_{ji}^{\text{true}}}{\sigma_{ji}}; \quad X''_j = \sum_{i=1}^{N_{\text{data}}^j} \left(\frac{Y_{ji}^{\text{true}}}{\sigma_{ji}} \right)^2$$

Bayesian approach to CMEs

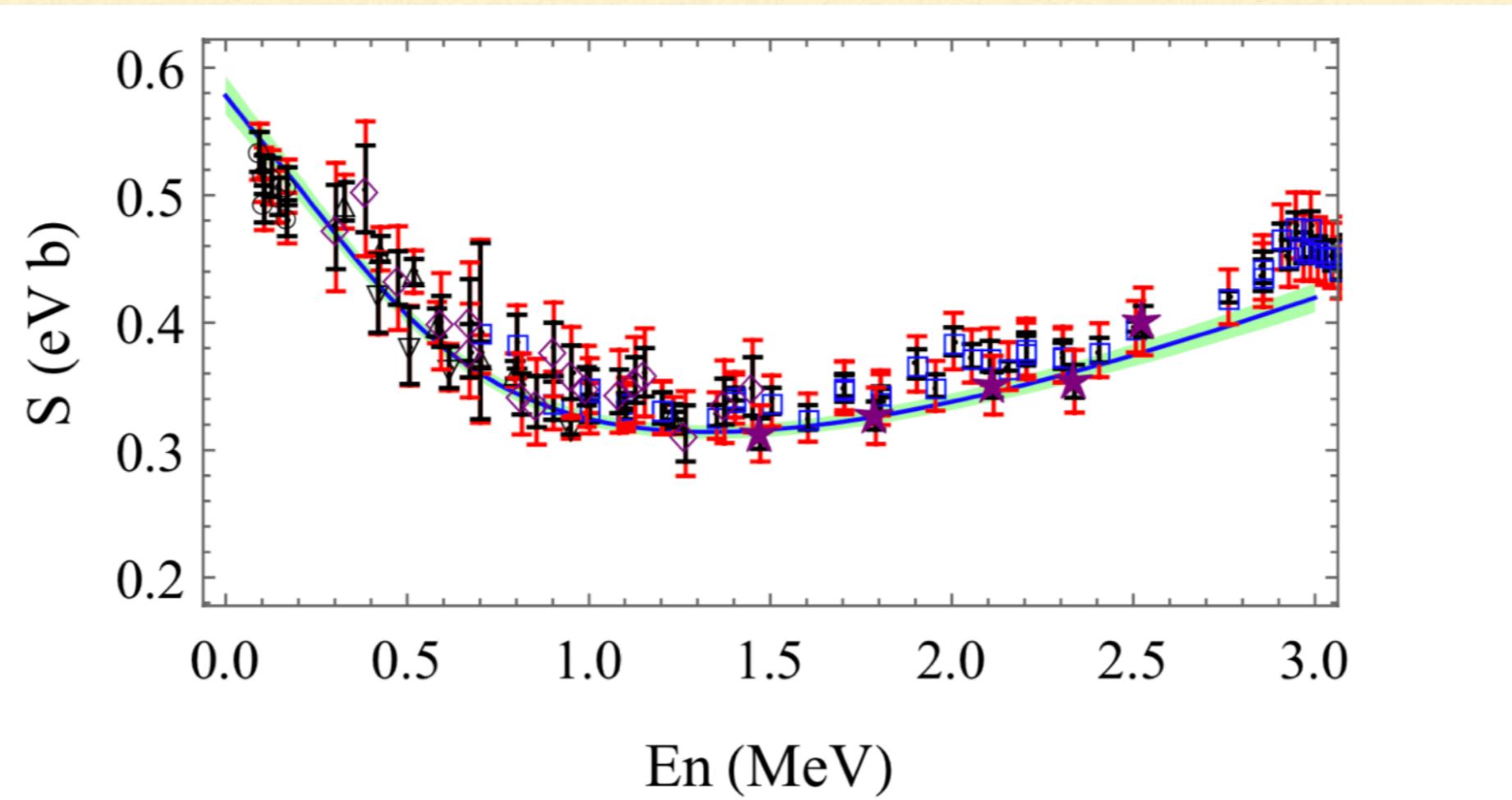


Bayesian approach to CMEs



$$\ln \text{pr}(D | \vec{\theta}, \{\xi_j\}, I) = c - \frac{1}{2} \sum_{j=1}^{N_{\text{expt}}} \sum_{i=1}^{N_{\text{data}}^j} \frac{(d_{ji} - \xi_j S(E_{ji}; \vec{\theta}))^2}{\sigma_{ji}^2}$$

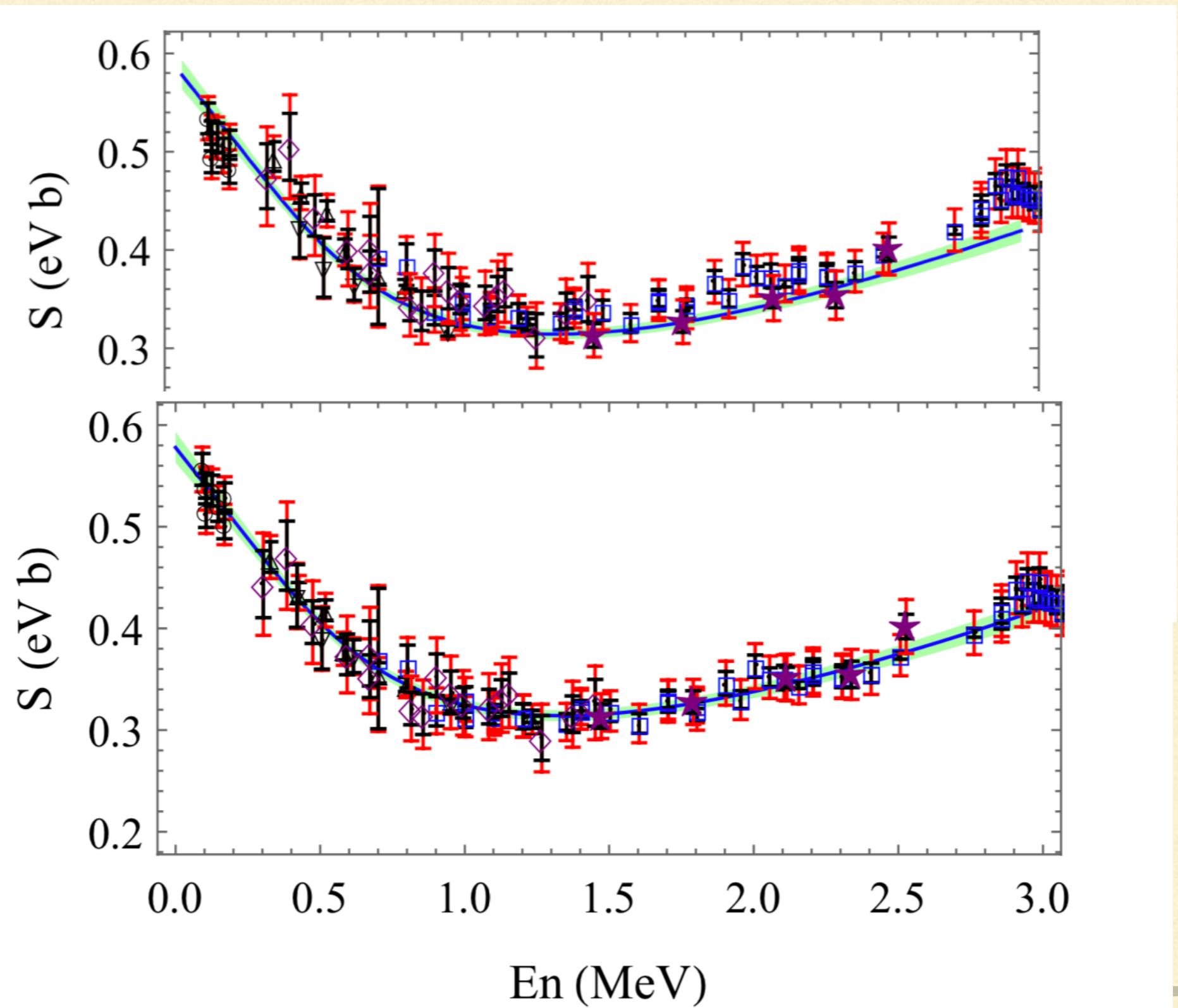
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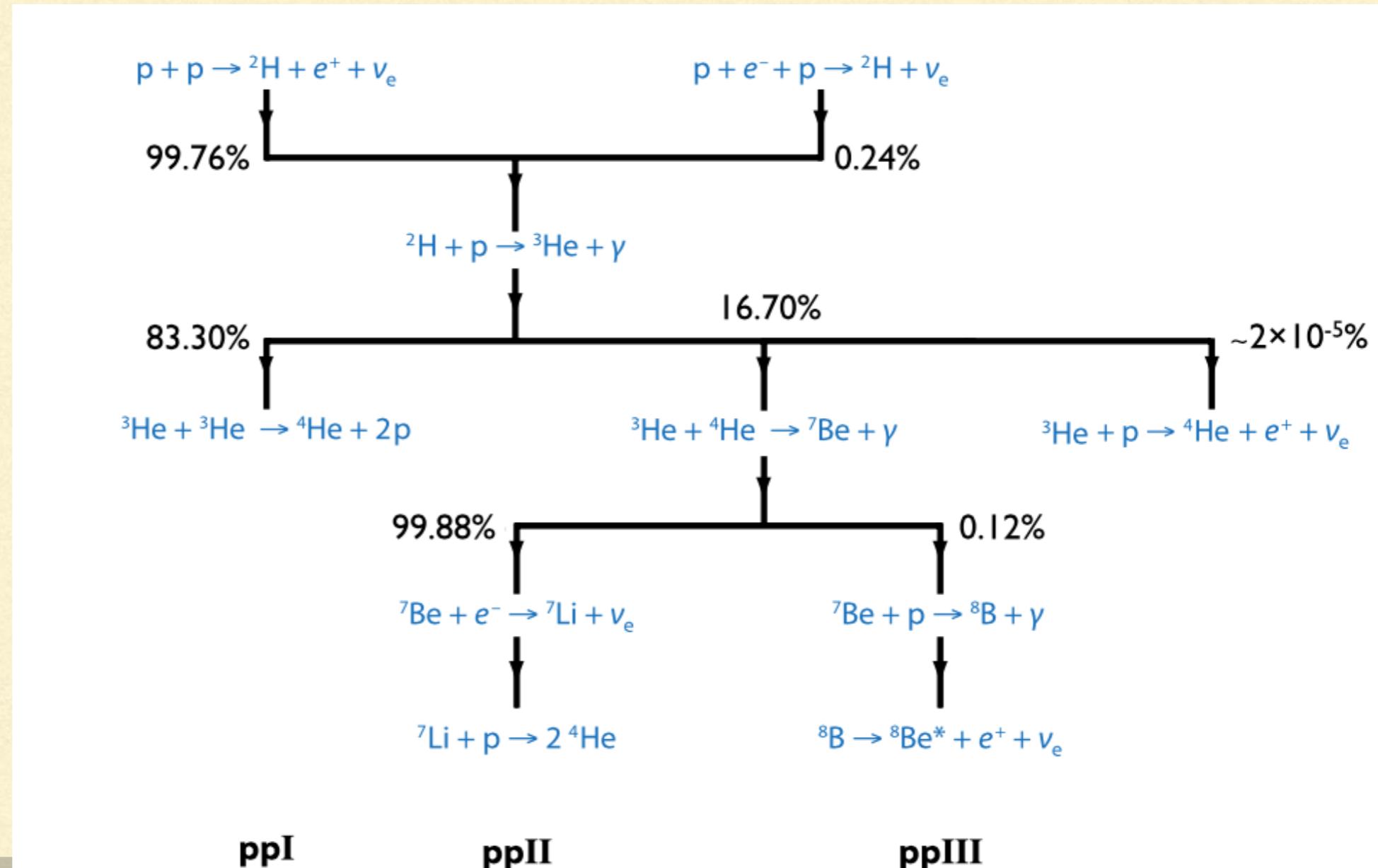
$$\ln \text{pr}(\{\xi_j\} \mid I) = -\frac{1}{2} \sum_{j=1}^{N_{\text{expt}}} \left(\frac{\xi_j - 1}{\epsilon_j} \right)^2$$

Bayesian approach to CMEs



Why is ${}^7\text{Be} + \text{p} \rightarrow {}^8\text{B} + \gamma$ important?

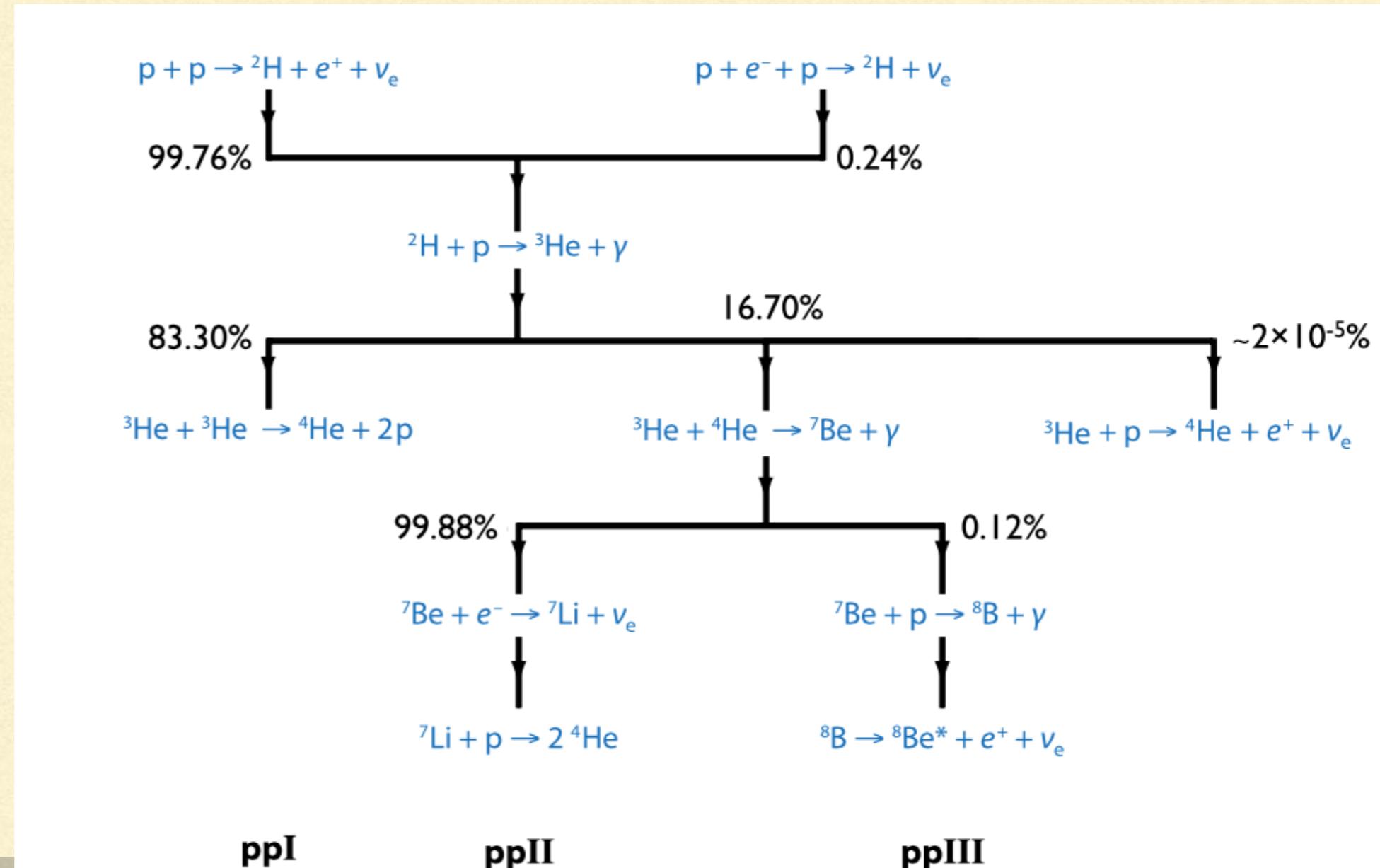
Adelberger et al., Rev. Mod. Phys. 83, 195 (2011)



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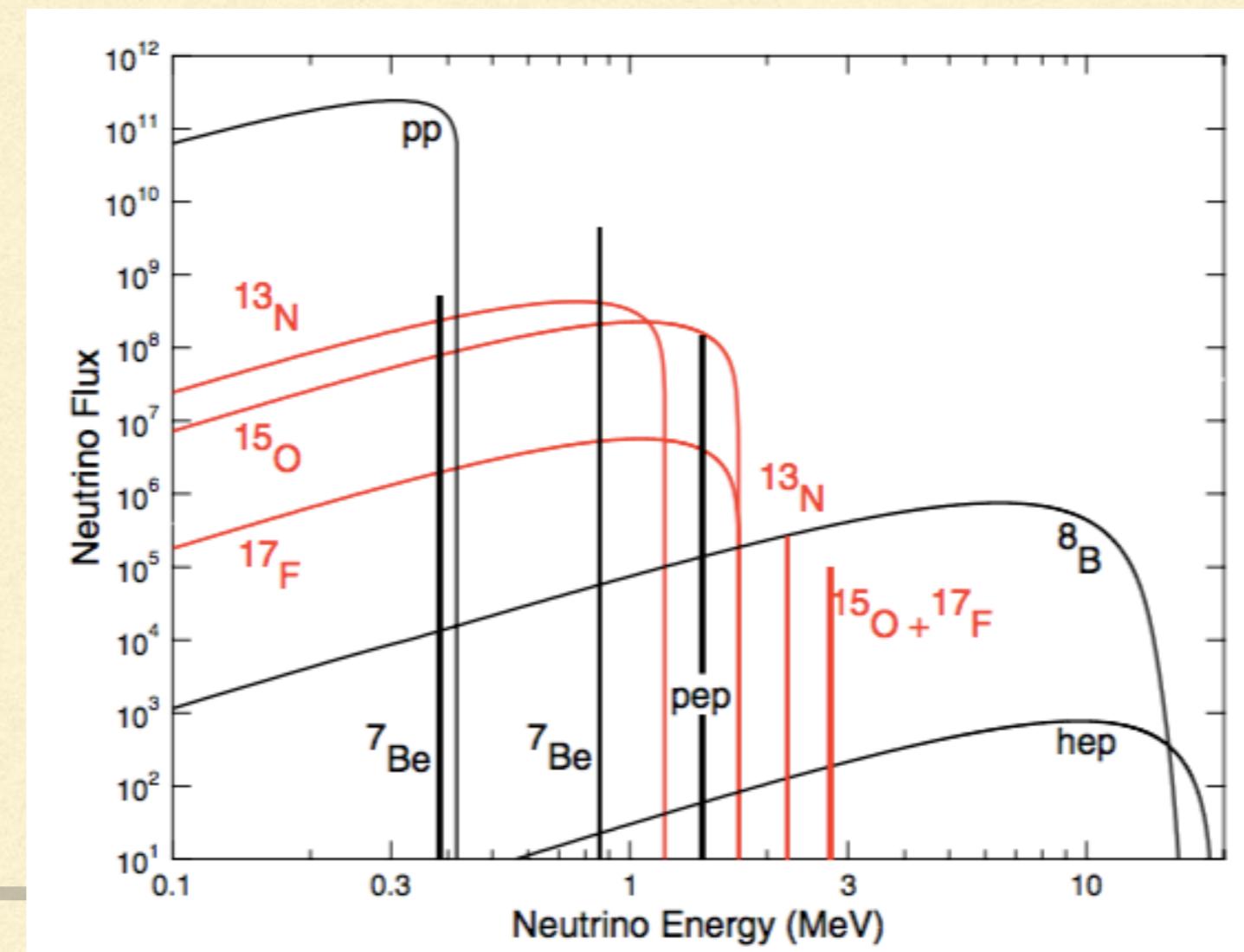
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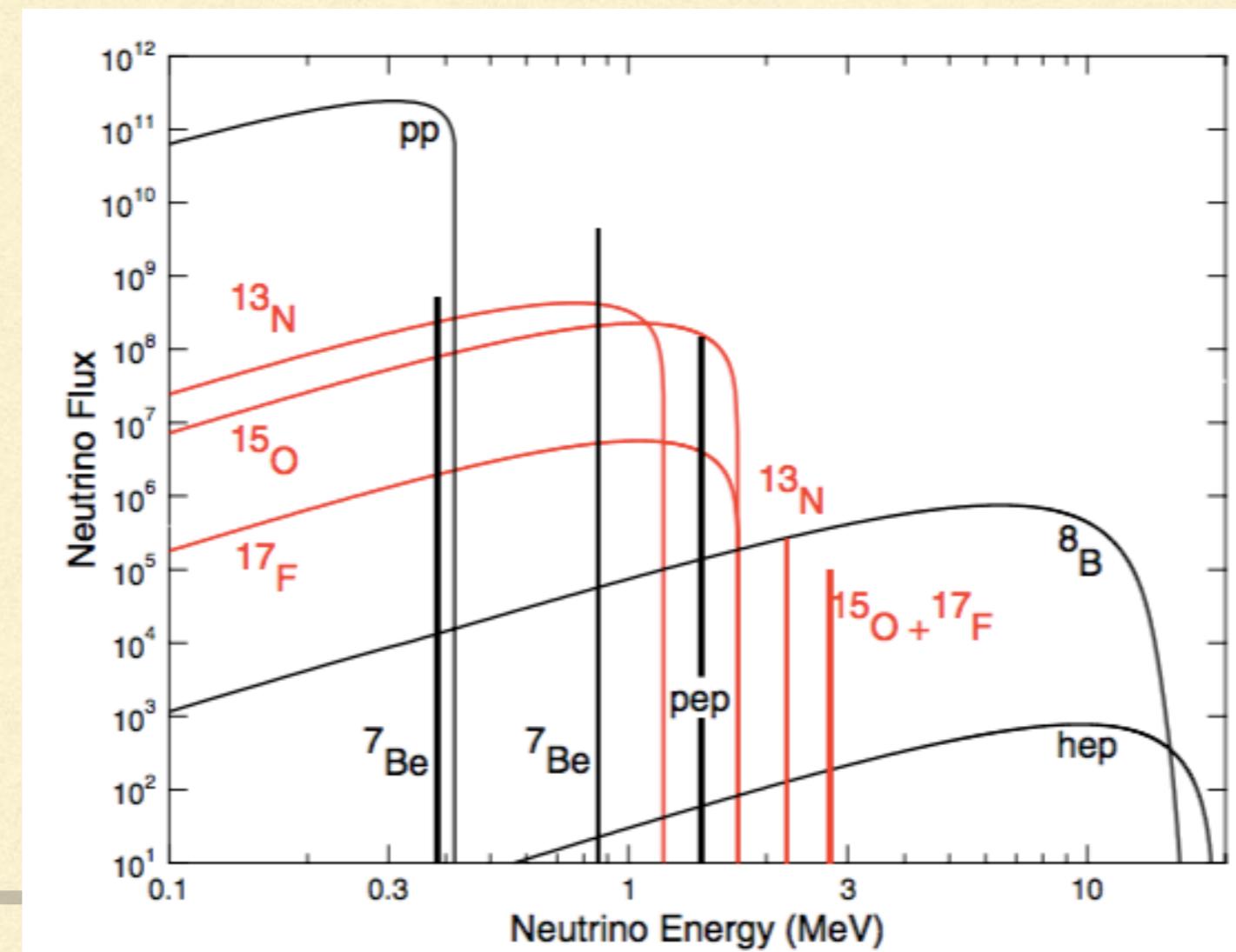
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- Part of pp chain (ppIII)
- Key for predicting flux of solar neutrinos, especially high-energy (${}^8\text{B}$) neutrinos
- Accurate knowledge of ${}^7\text{Be}(\text{p},\gamma)$ needed for inferences from solar-neutrino flux regarding solar composition
→ solar-system formation history



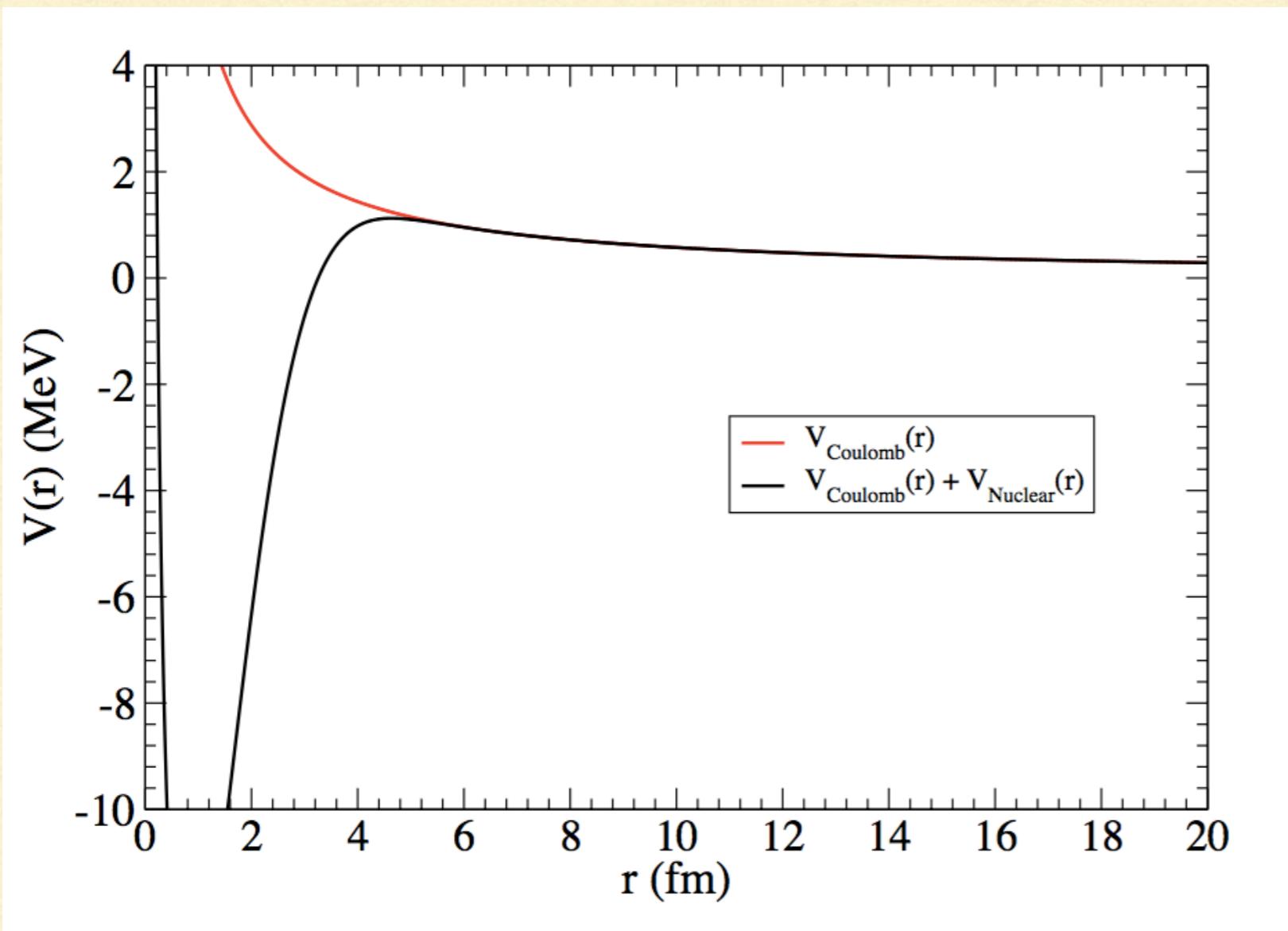
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Thermonuclear reaction rate $\propto \langle v\sigma \rangle \propto \int_0^\infty dE \exp\left(-\frac{E}{k_B T}\right) E \sigma(E)$

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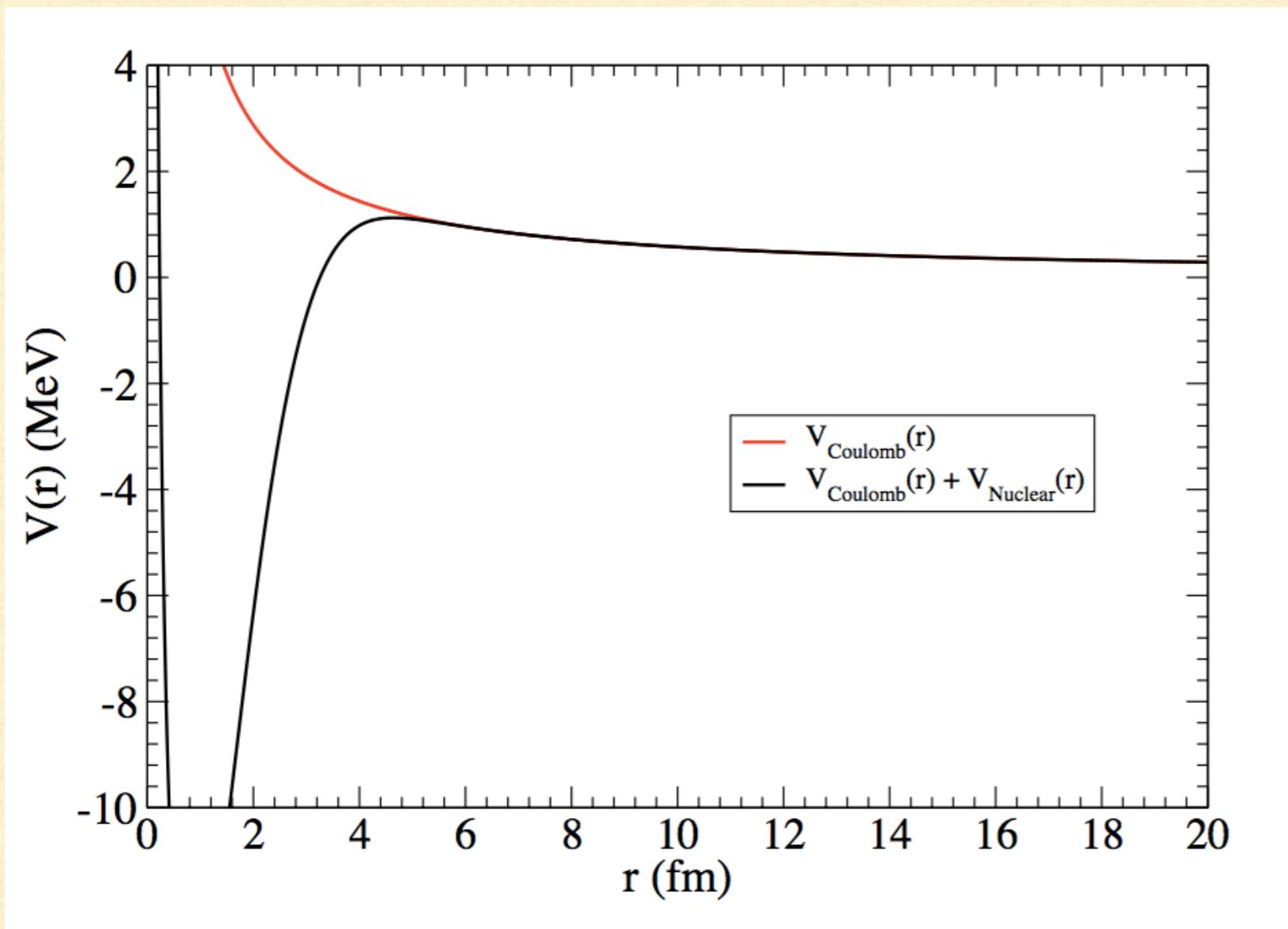
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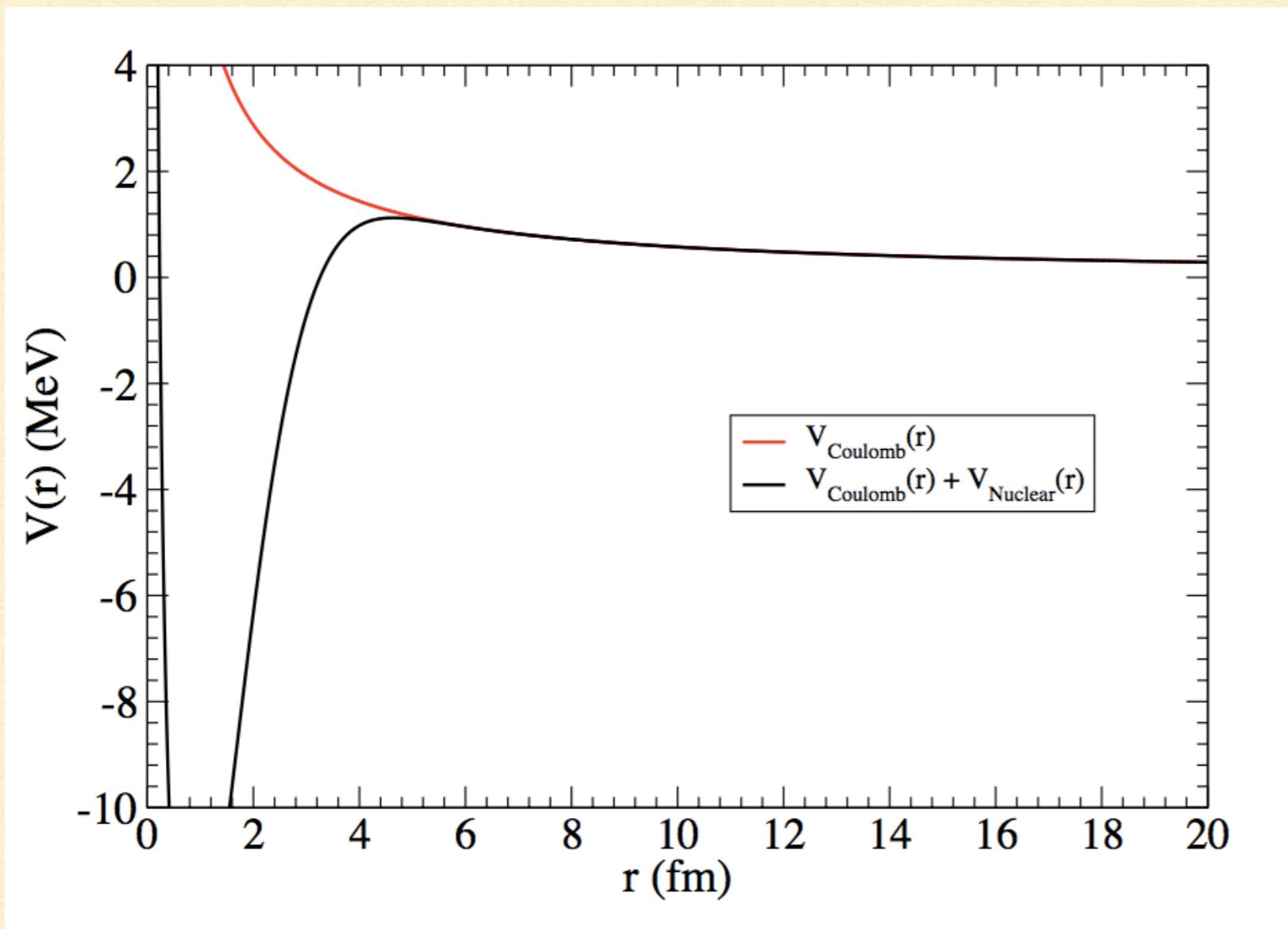
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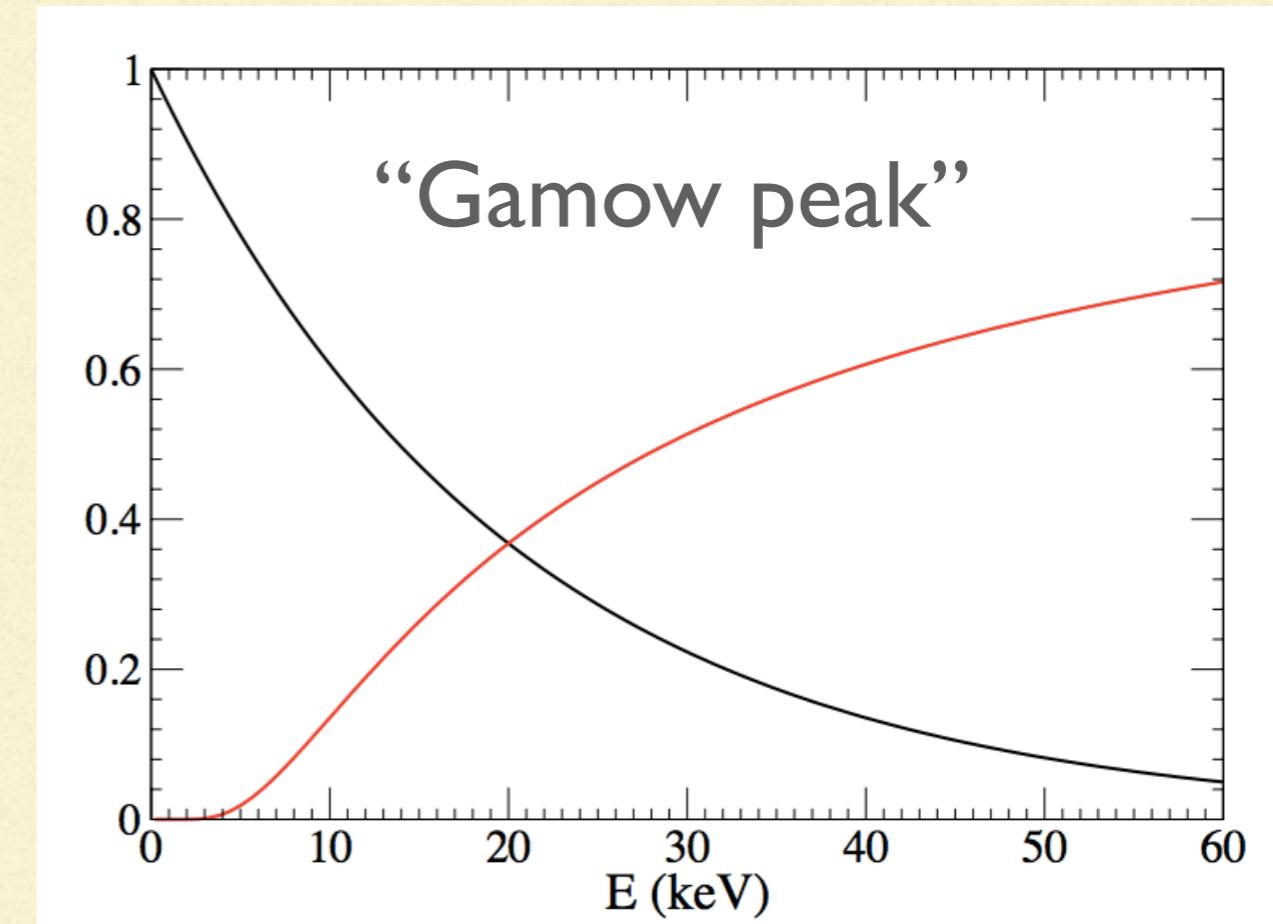
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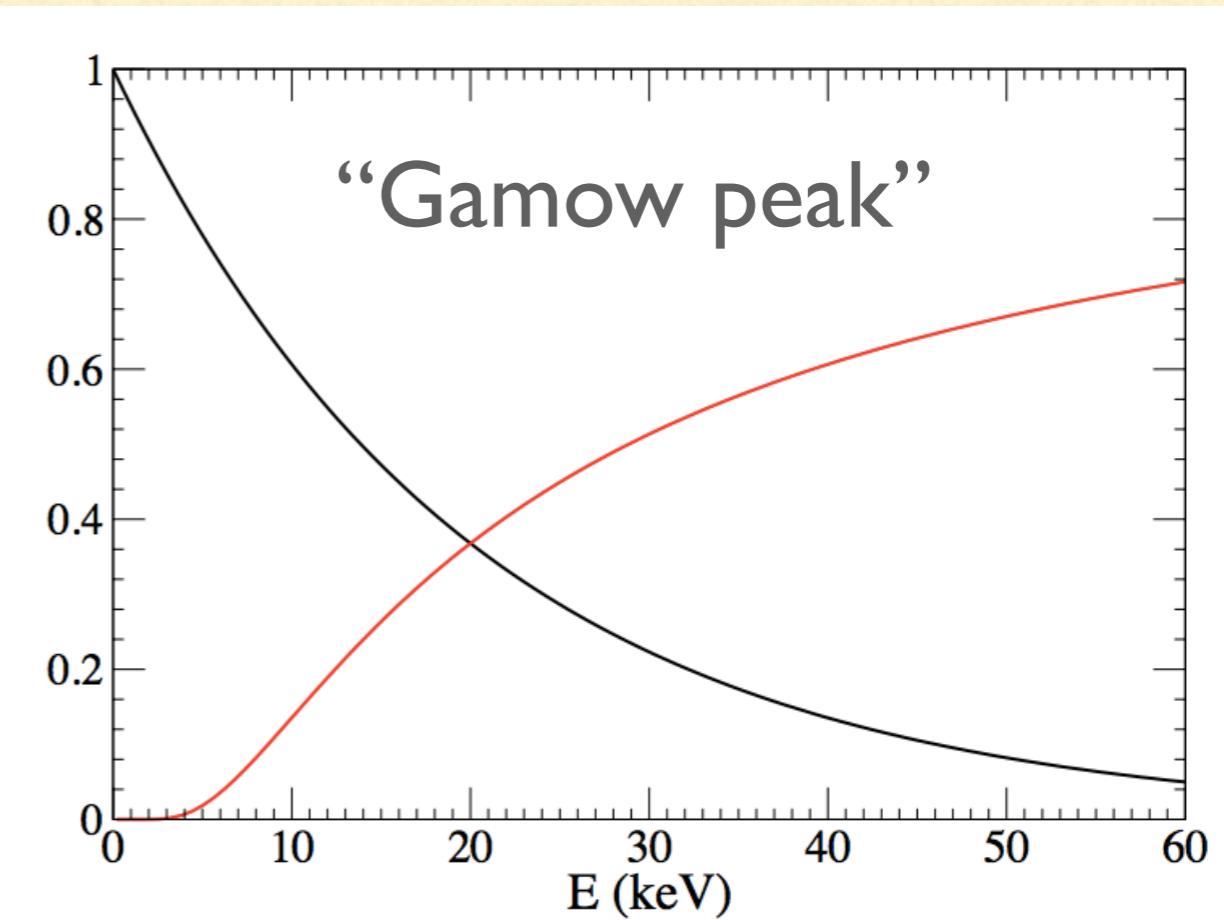
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- EI capture: ${}^7\text{Be} + \text{p} \rightarrow {}^8\text{B} + \gamma$
- Energies of relevance 20 keV



What matters where?

$$\mathcal{M}(E) \propto \int dr A_1 \exp(-\gamma_1 r) \left(1 + \frac{1}{\gamma_1 r}\right) r u_E(r); \quad \gamma_1 = 1/(13 \text{ fm})$$

Dominated by ${}^7\text{Be}$ -p separations \sim 10s of fm

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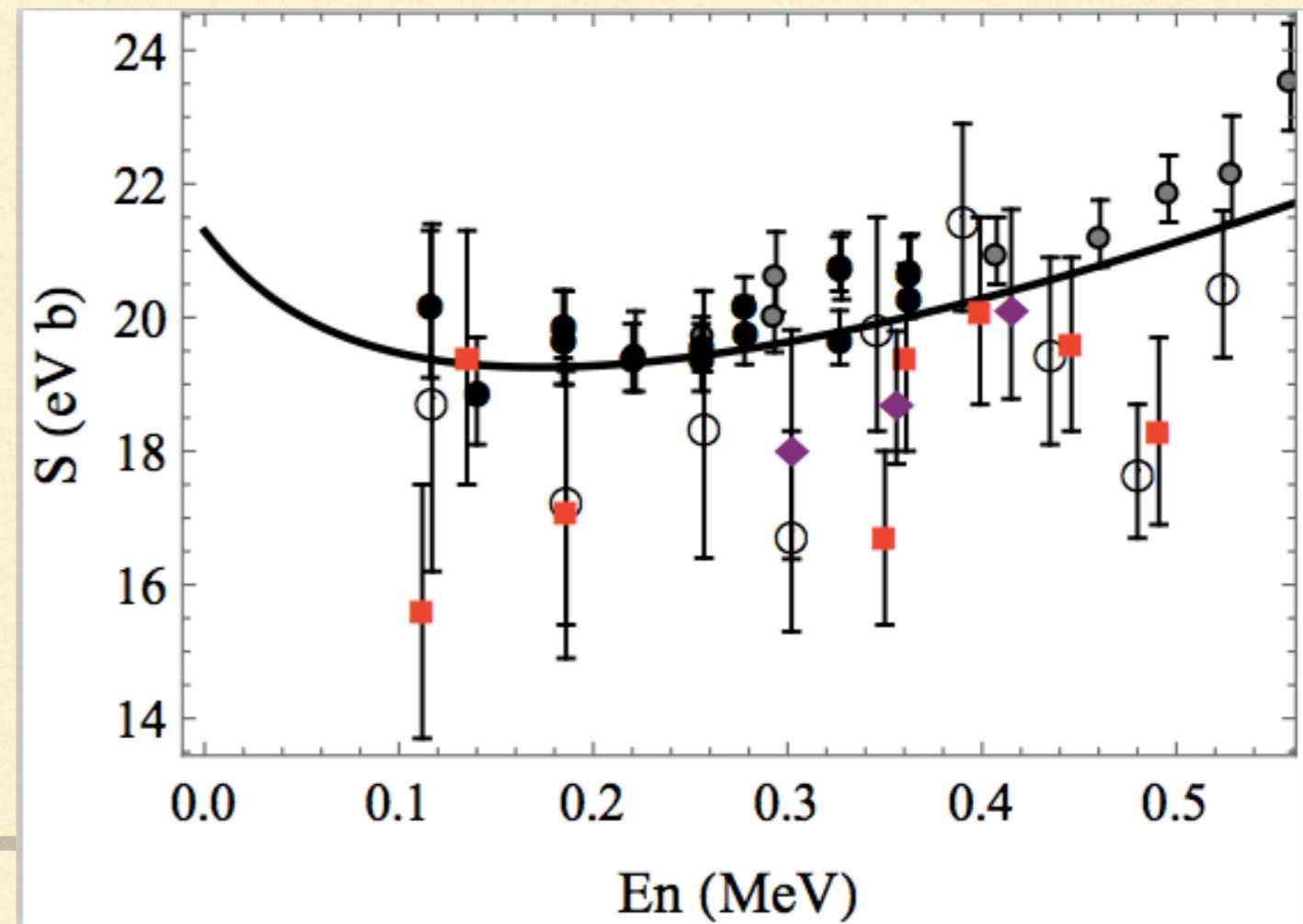
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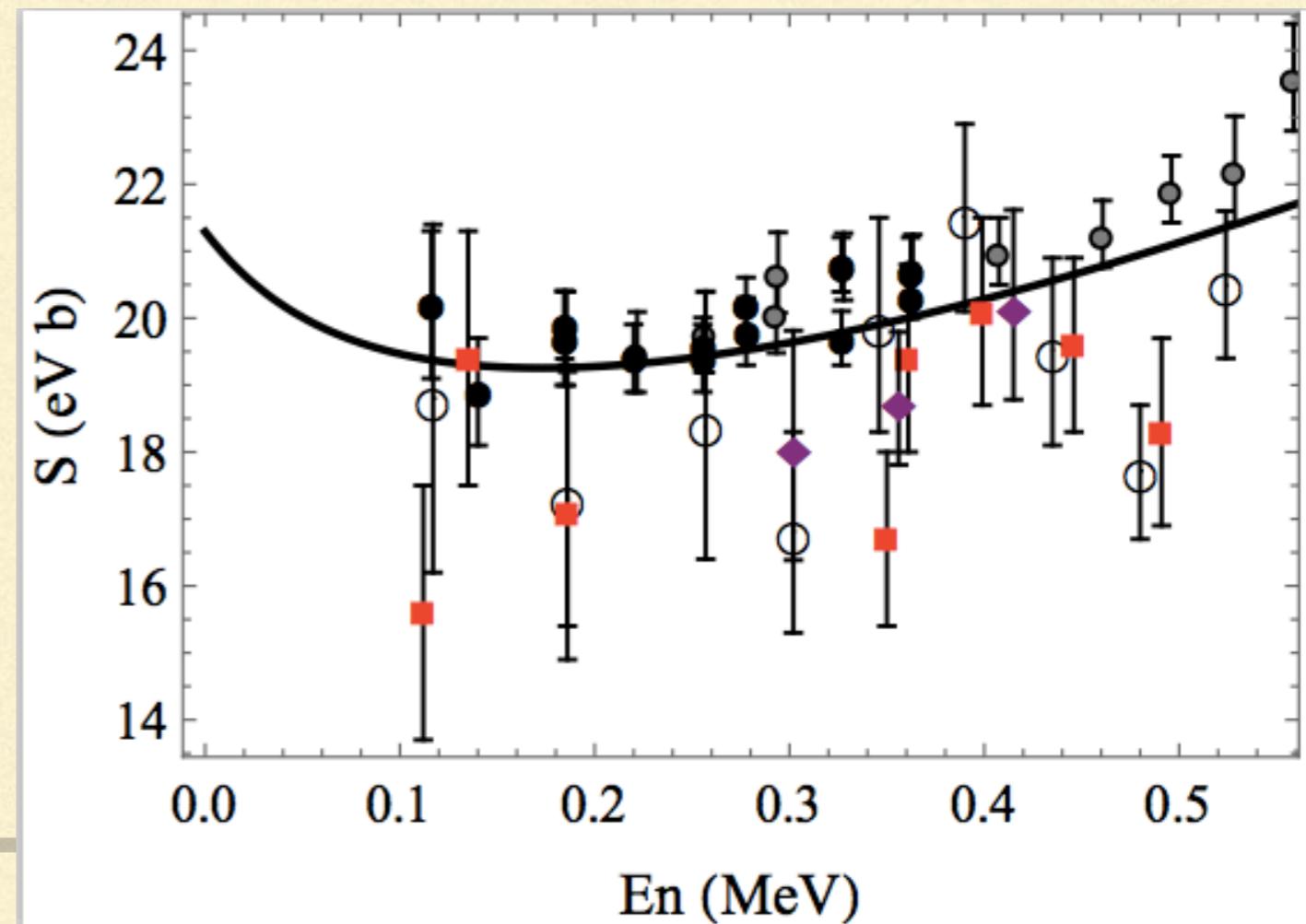
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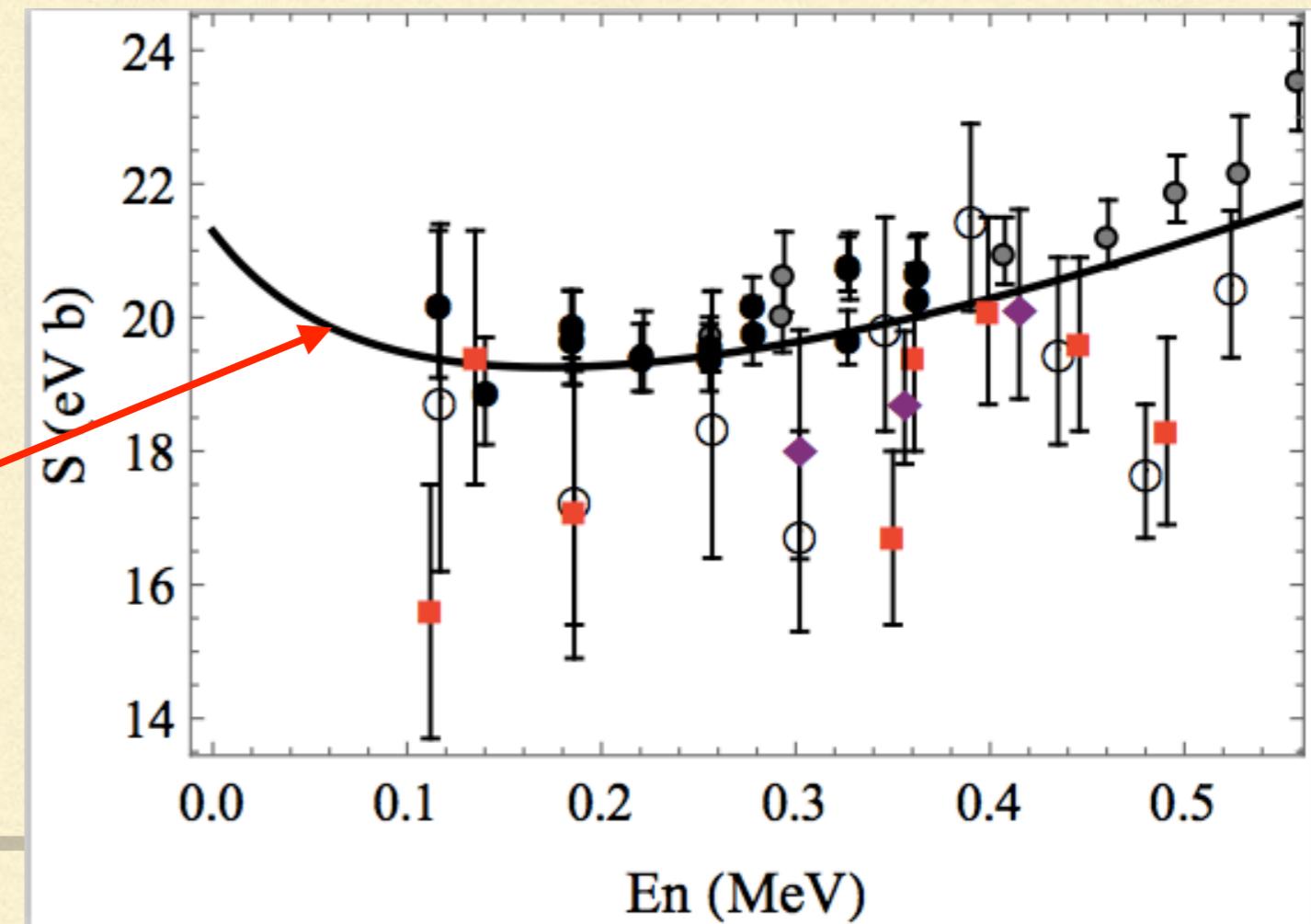
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Bound state (ANC & γ_1)
+ Coulomb



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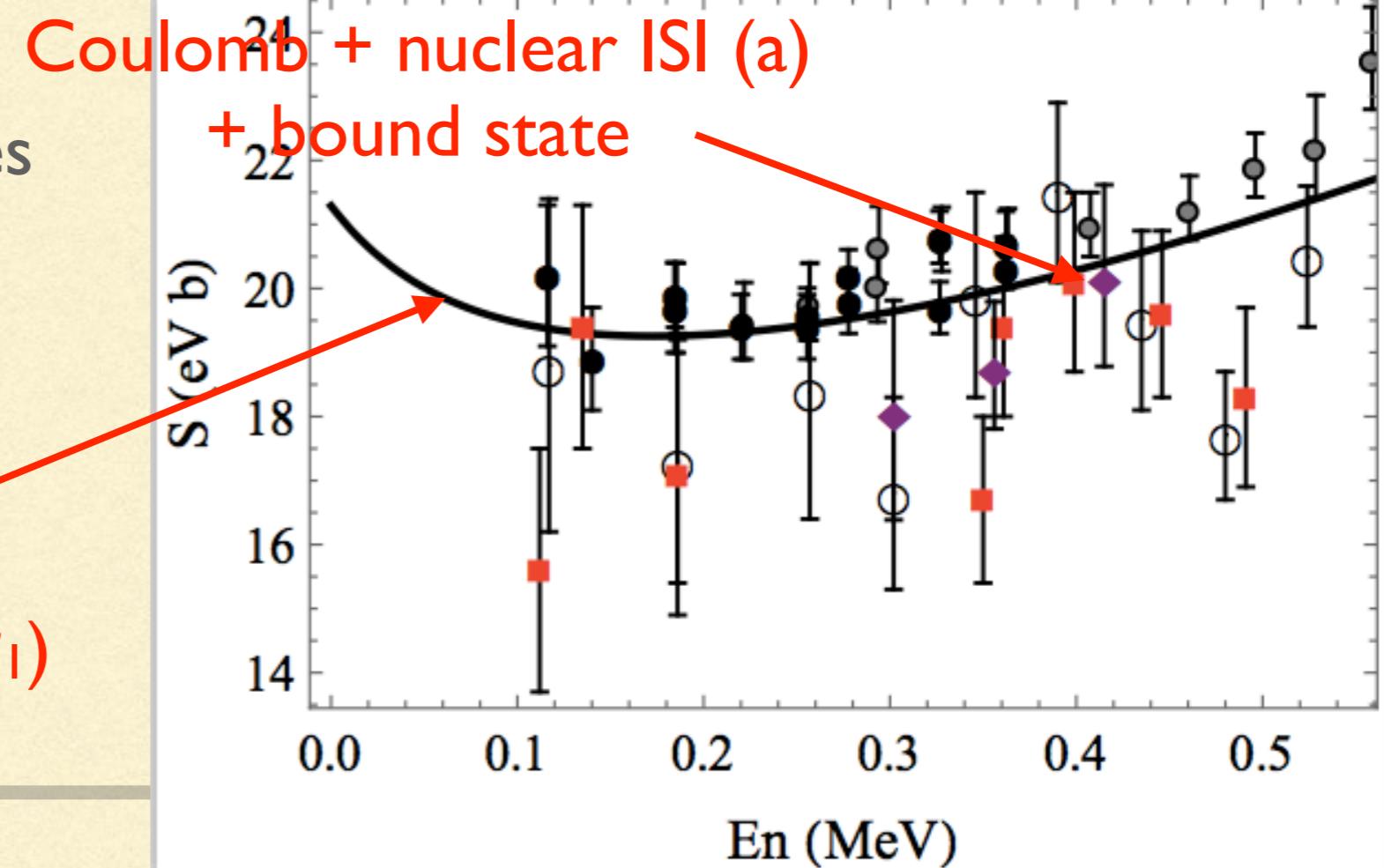
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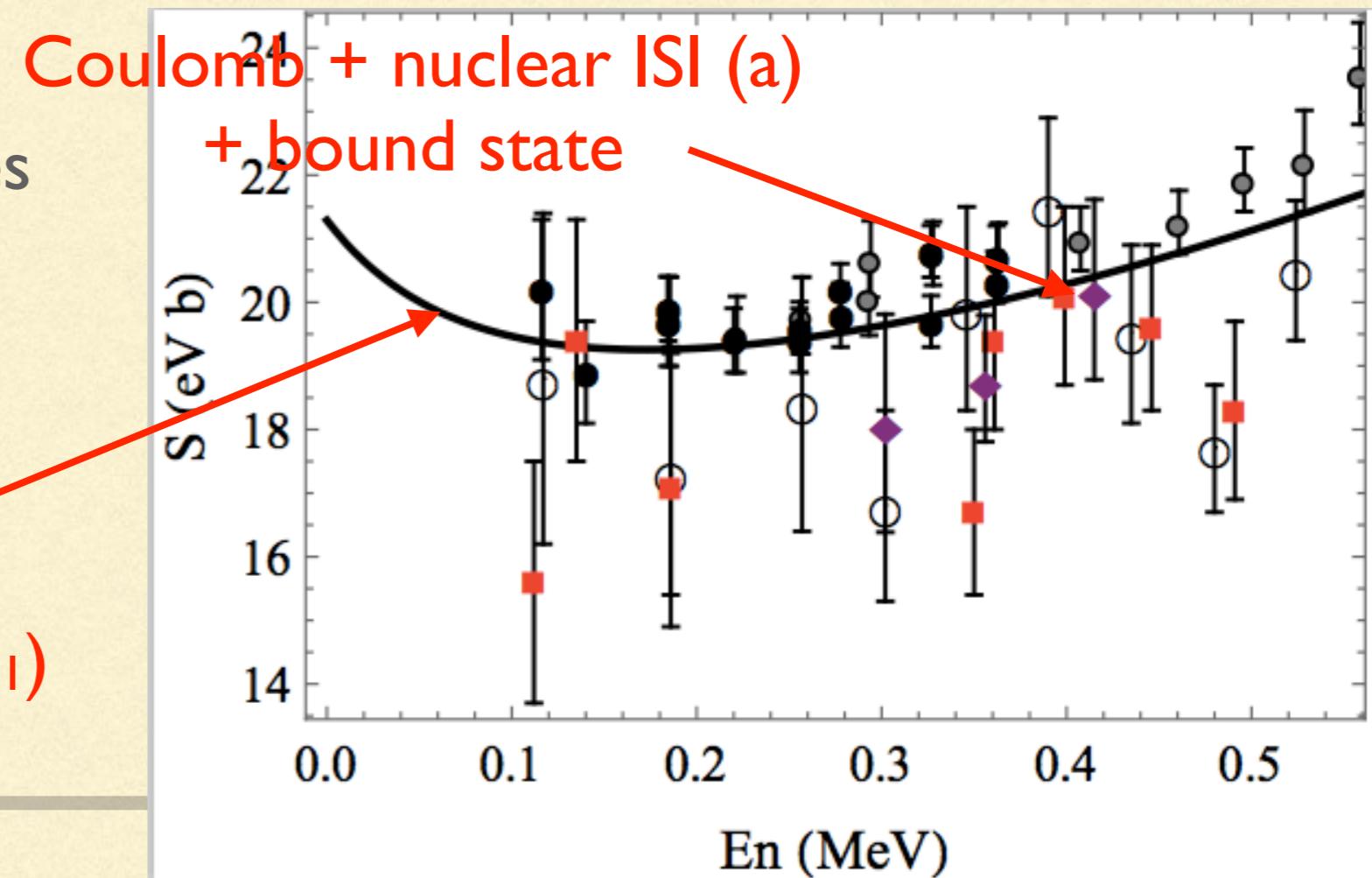
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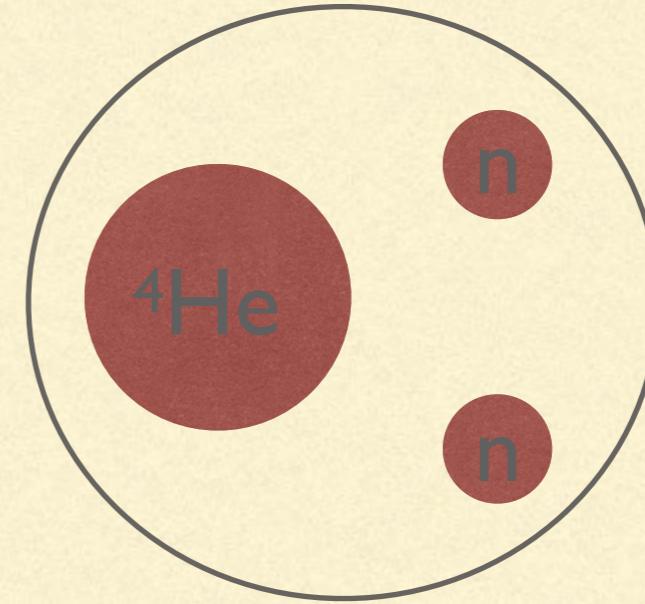
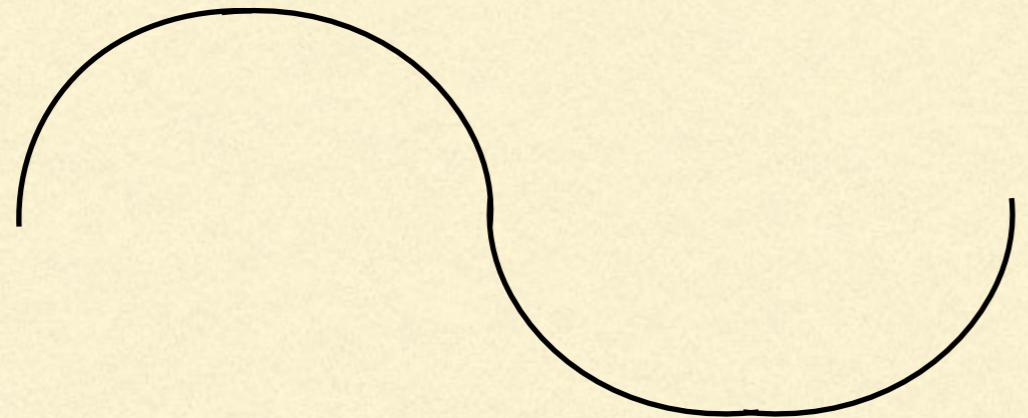
- Extrapolation is not a polynomial: non-analyticities in p/k_C , p/γ_1 , and p/a
- Sub-leading polynomial behavior in E/E_{core}

Bound state (ANC & γ_1) + Coulomb



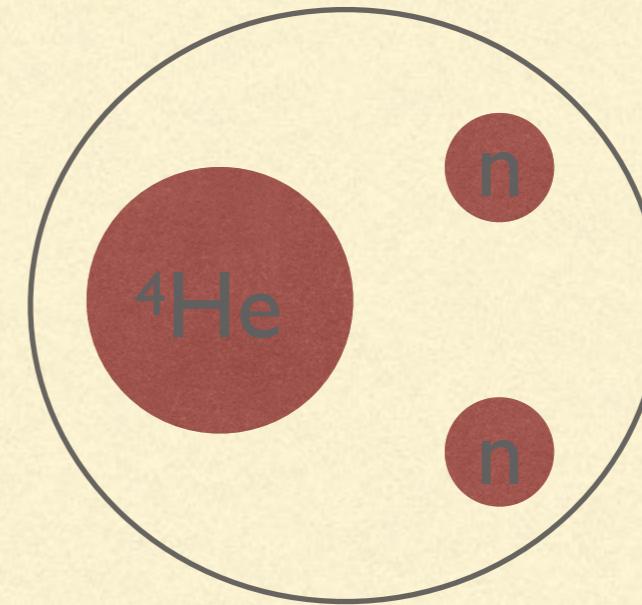
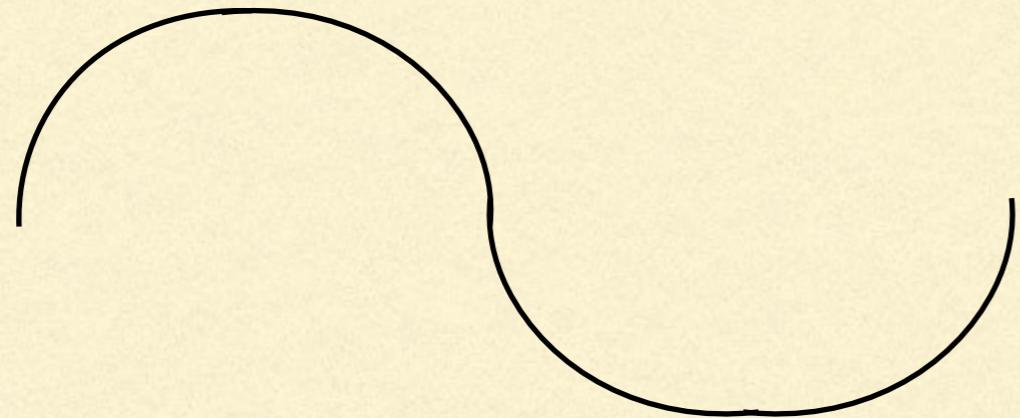
Halo EFT

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



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- Define $R_{\text{halo}} = \langle r^2 \rangle^{1/2}$. Seek EFT expansion in $R_{\text{core}}/R_{\text{halo}}$. Valid for $\lambda \lesssim R_{\text{halo}}$
- Typically $R \equiv R_{\text{core}} \sim 2$ 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

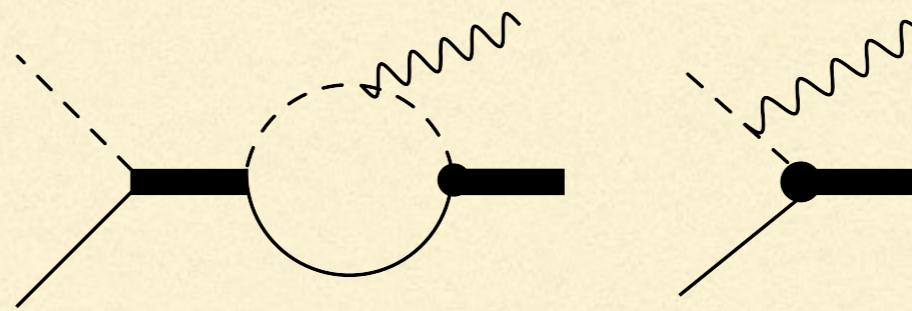
p-wave bound states and capture thereto

Hammer & DP, NPA (2011)

- At LO: p-wave In halo described solely by its ANC and binding energy

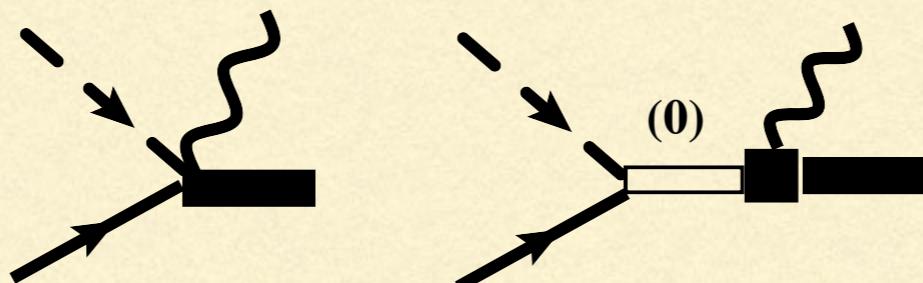
$$u_1(r) = A_1 \exp(-\gamma_1 r) \left(1 + \frac{1}{\gamma_1 r} \right) \quad \gamma_1 = \sqrt{2m_R B}$$

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



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

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



$^7\text{Be} + \text{p} \rightarrow ^8\text{B} + \gamma_{\text{EI}}$ at LO in Halo EFT

Zhang, Nollett, DP, Phys. Rev. C 89, 051602 (2014);
Ryberg, Forssen, Hammer, Platter, EPJA (2014)

- In this system $R_{\text{core}} \sim 3$ fm, $R_{\text{halo}} \sim 15$ fm; scale of Coulomb interactions:
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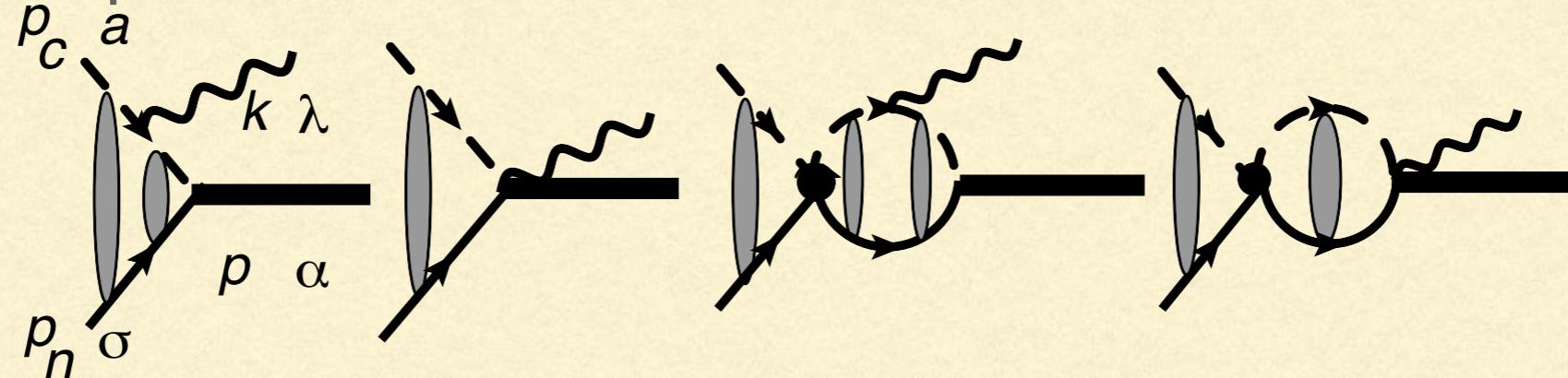
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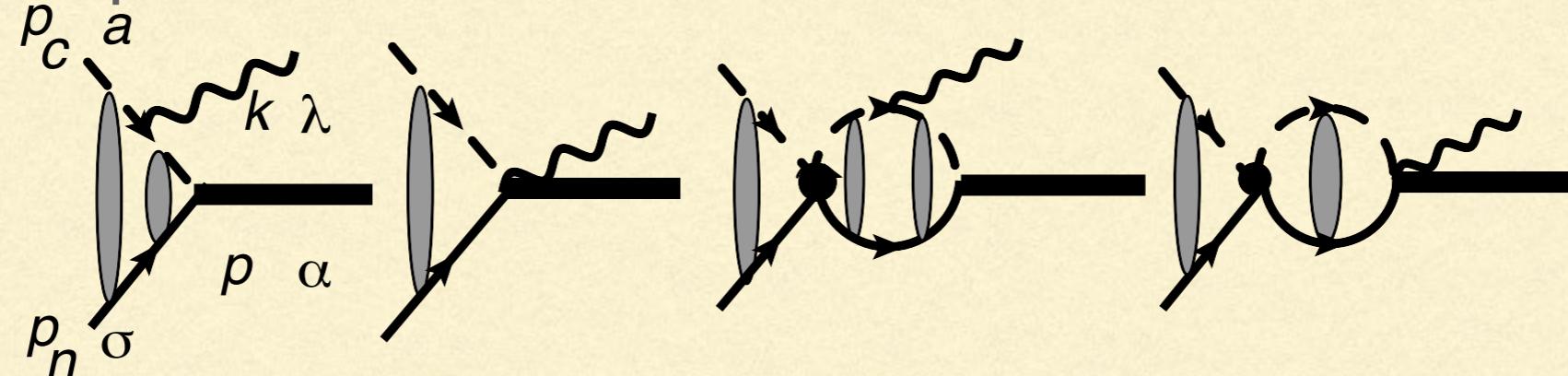
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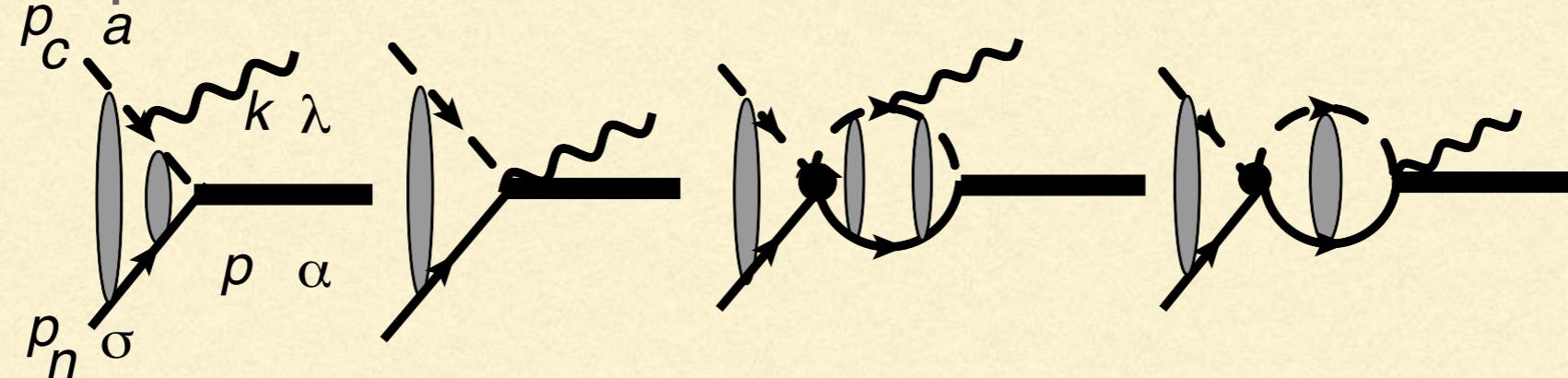


- Scattering wave functions are linear combinations of Coulomb wave functions F_0 and G_0 . Bound state wave function = the appropriate Whittaker function.

${}^7\text{Be} + \text{p} \rightarrow {}^8\text{B} + \gamma_{\text{EI}}$ at LO in Halo EFT

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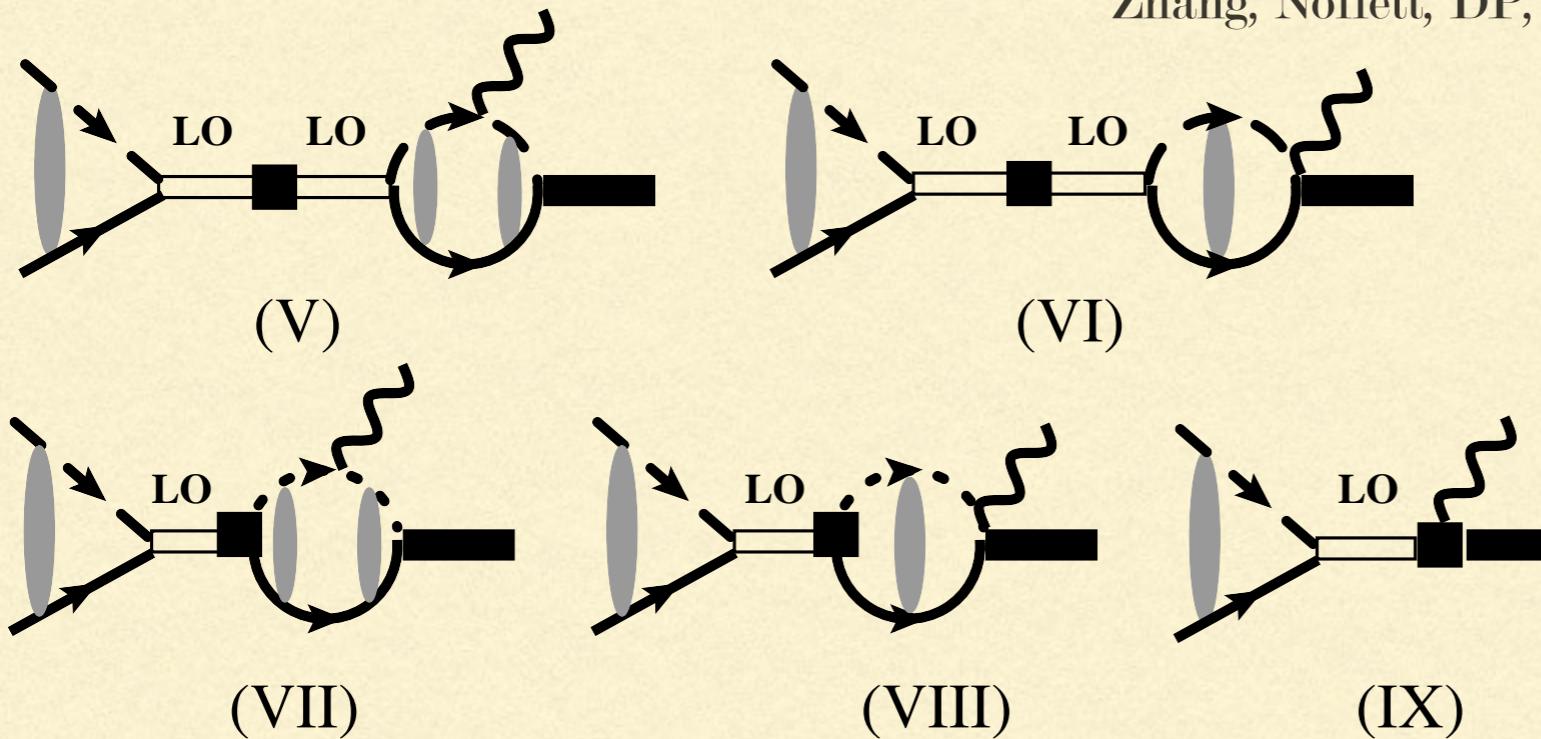
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$$S(E) = f(E) \sum_s C_s^2 \left[|S_{\text{EC}}(E; \delta_s(E))|^2 + |\mathcal{D}(E)|^2 \right]. \text{ Four parameters at leading order}$$

Additional ingredients at NLO

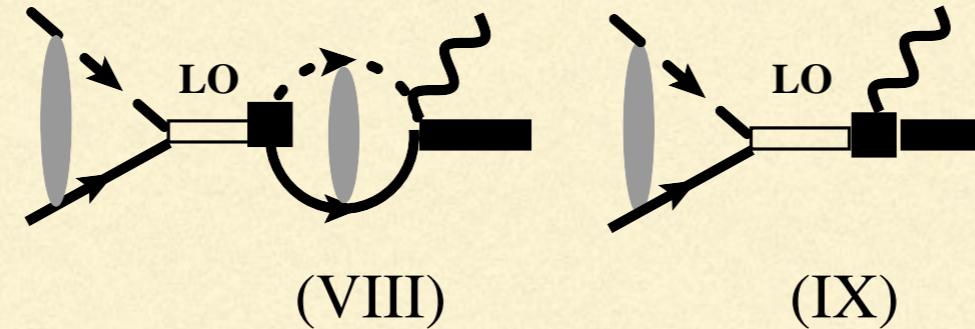
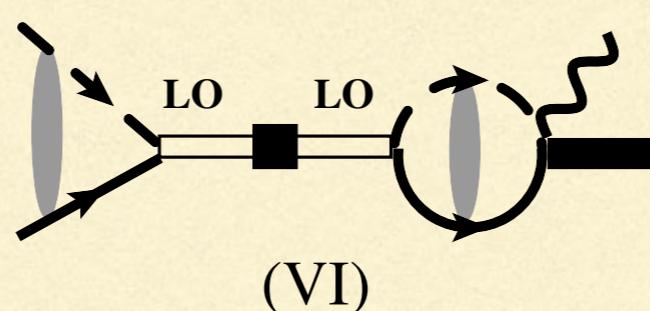
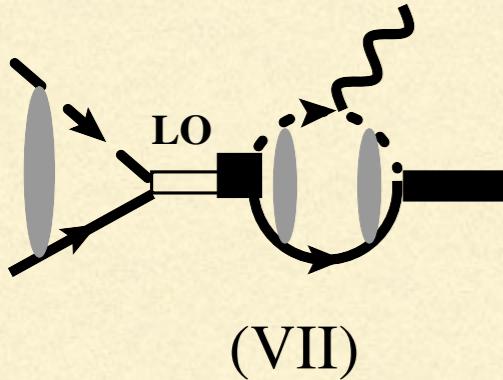
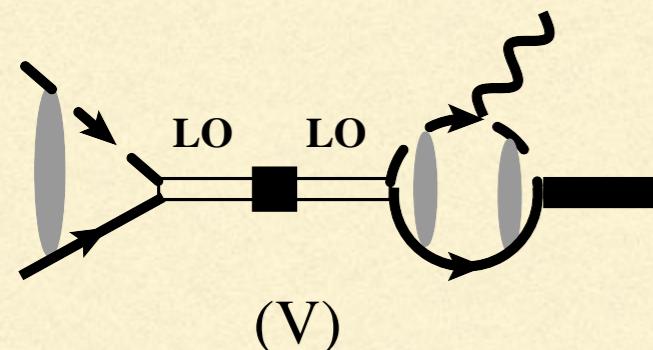


Zhang, Nollett, DP, hys. Lett. B751, 535 (2015), arXiv:1708.04017;
Ryberg, Forssen, Platter, Ann. Phys. (2016)

$$S(E) = f(E) \sum_s C_s^2 \left[|\mathcal{S}_{\text{EC}}(E; \delta_s(E)) + \bar{L}_s \mathcal{S}_{\text{SD}}(E; \delta_s(E)) + \epsilon_s \mathcal{S}_{\text{CX}}(E; \delta_s(E))|^2 + |\mathcal{D}(E)|^2 \right].$$

- Effective ranges in both 5S_2 and 3S_1 : r_2 and r_1
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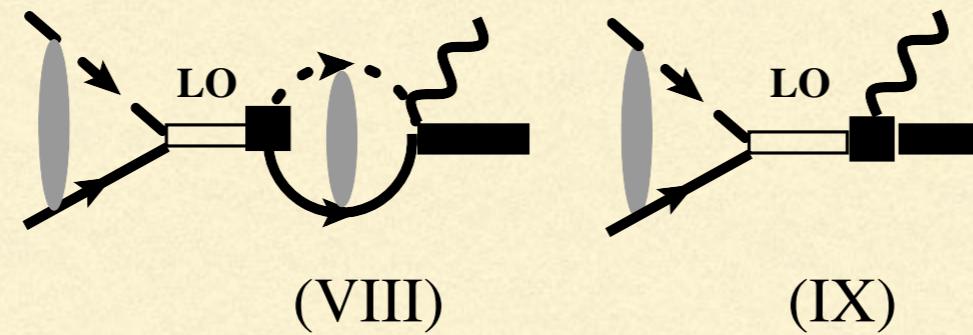
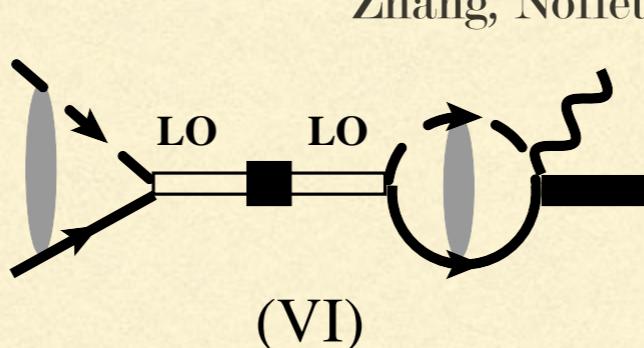
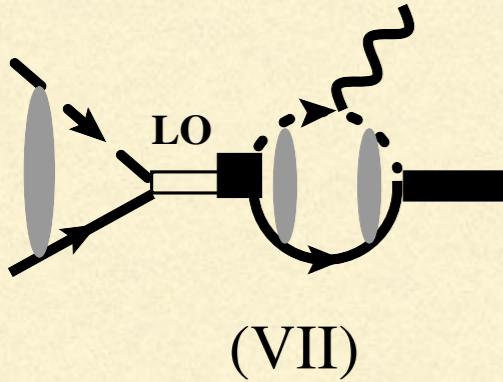
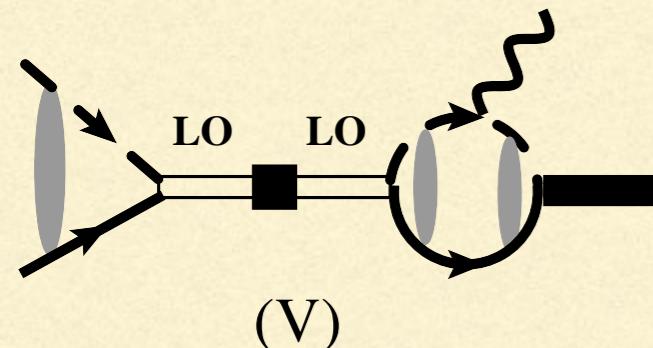
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Five more parameters
at NLO

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Additional ingredients at NLO



(IX)

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Data for ${}^7\text{Be} + \text{p} \rightarrow {}^8\text{B} + \gamma_{\text{EI}}$

- 42 data points for $100 \text{ keV} < E_{\text{c.m.}} < 500 \text{ keV}$
 - Junghans (BEI and BE3)
 - Fillipone
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- Subtract MI resonance: negligible impact at 500 keV and below
- Deal with CMEs by introducing five additional parameters, ξ_i

Building the pdf

$$\text{pr}(\vec{\theta}, \{\xi_j\} | D, I) \propto \text{pr}(D | \vec{\theta}, \{\xi_j\}, I) \text{pr}(\vec{\theta}, \{\xi_j\} | I)$$

$$\ln \text{pr}(D | \vec{\theta}, \{\xi_j\}, I) = c - \frac{1}{2} \sum_{j=1}^{N_{\text{expt}}} \sum_{i=1}^{N_{\text{data}}^j} \frac{(d_{ji} - \xi_j S(E_{ji}; \vec{\theta}))^2}{\sigma_{ji}^2}$$

Building the pdf

- Bayes:

$$\text{pr}(\vec{\theta}, \{\xi_j\} | D, I) \propto \text{pr}(D | \vec{\theta}, \{\xi_j\}, I) \text{pr}(\vec{\theta}, \{\xi_j\} | I)$$

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- Second factor: priors

- Independent gaussian priors for ξ_j , centered at zero and with width=CME
- Gaussian priors for $a_{S=1}$ and $a_{S=2}$, based on Angulo et al. measurement
- Other EFT parameters, $r_{S=1}$, $r_{S=2}$, L_1 , L_2 , ANCs, ϵ_1 , assigned flat priors, corresponding to natural ranges
- No s-wave resonance below 600 keV

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Extrinsic information
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Outputs and lessons

- Posteriors on parameters tell us about physics: which combinations are actually constrained?
 - How do we see when parameters are not well constrained?
 - Extrapolation
 - Does EFT truncation error at NLO affect the answer?
 - Feedback with experiment: systematic errors? Future experiments?
-

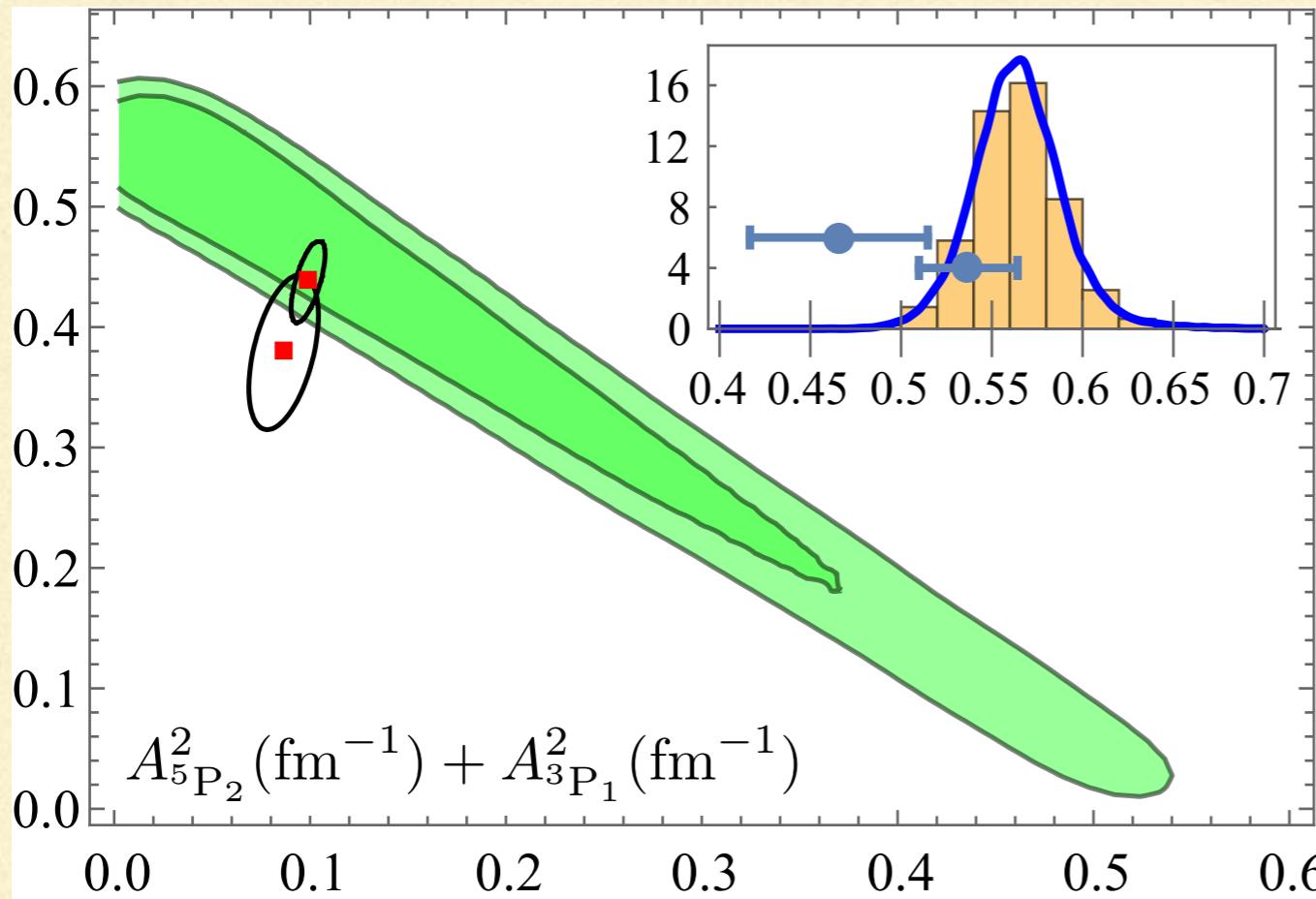
Posterior plots⇒Physics

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$$\text{pr}(g_1, g_2 | D; T; I) = \int \text{pr}(\vec{g}, \{\xi_i\} | D; T; I) \, d\xi_1 \dots d\xi_5 dg_3 \dots dg_9$$

Posterior plots⇒Physics

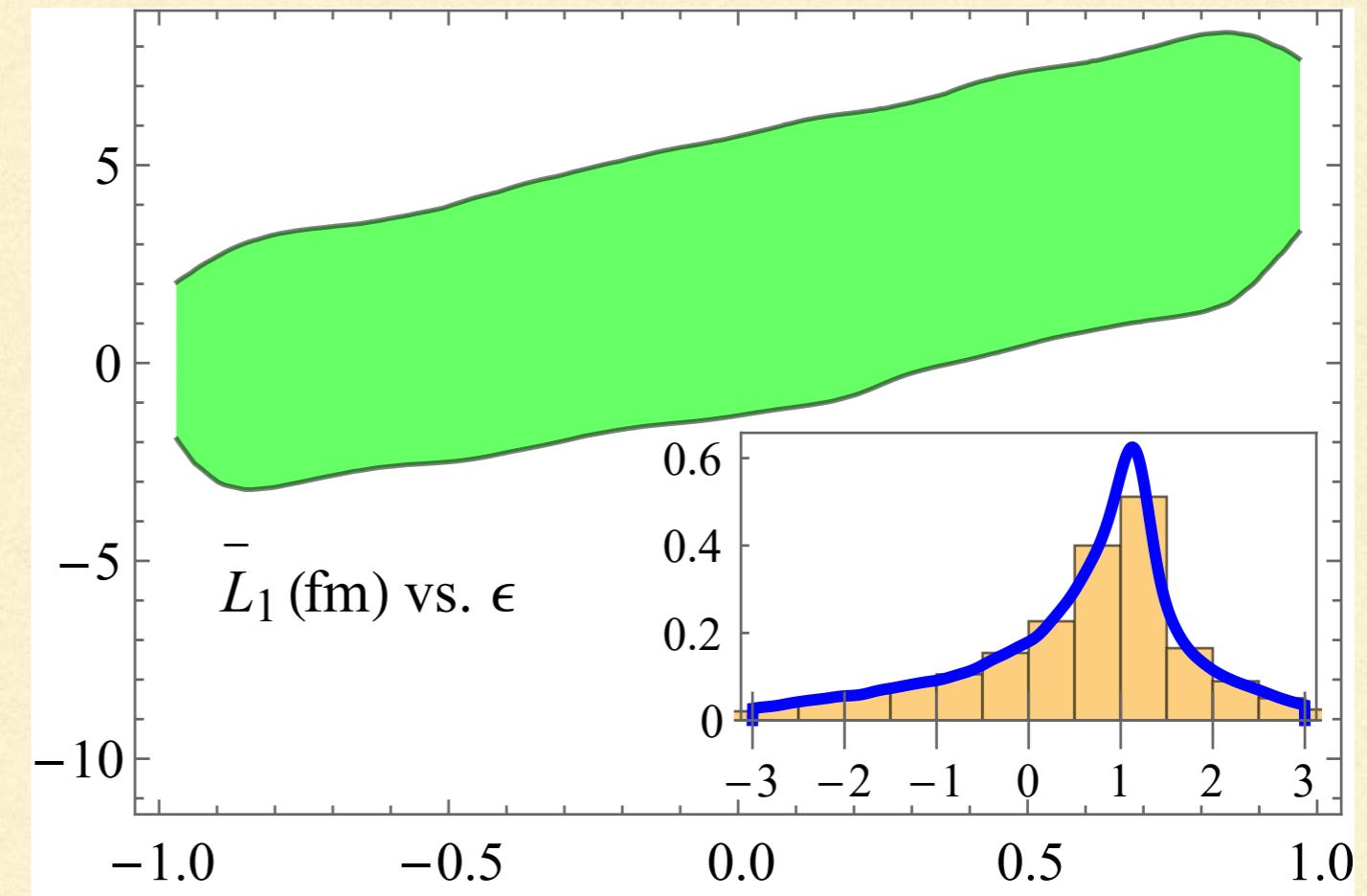
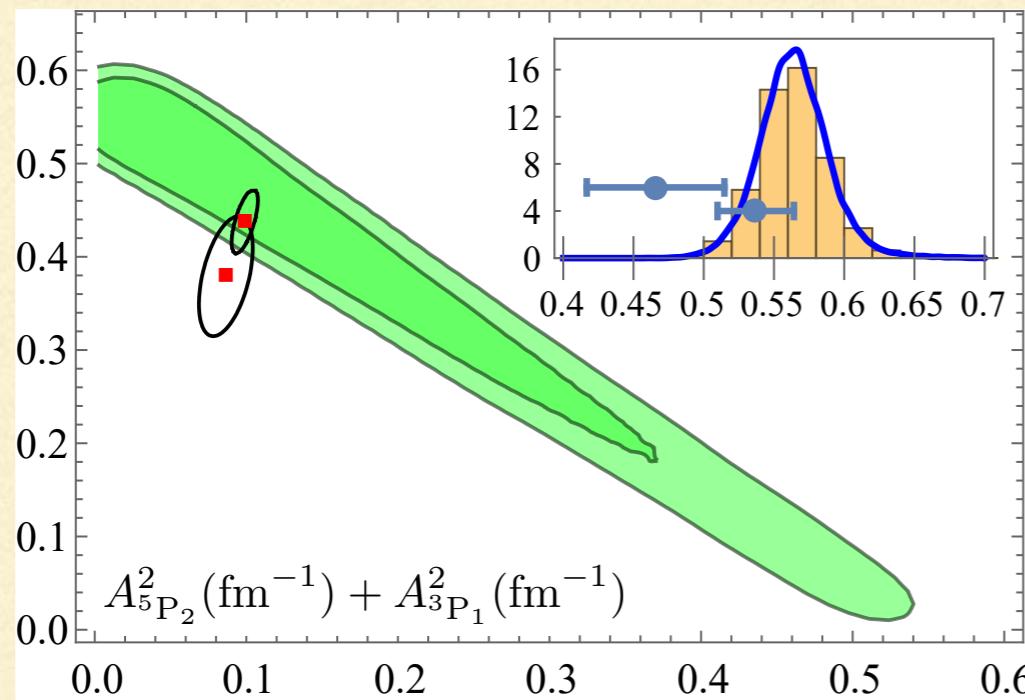
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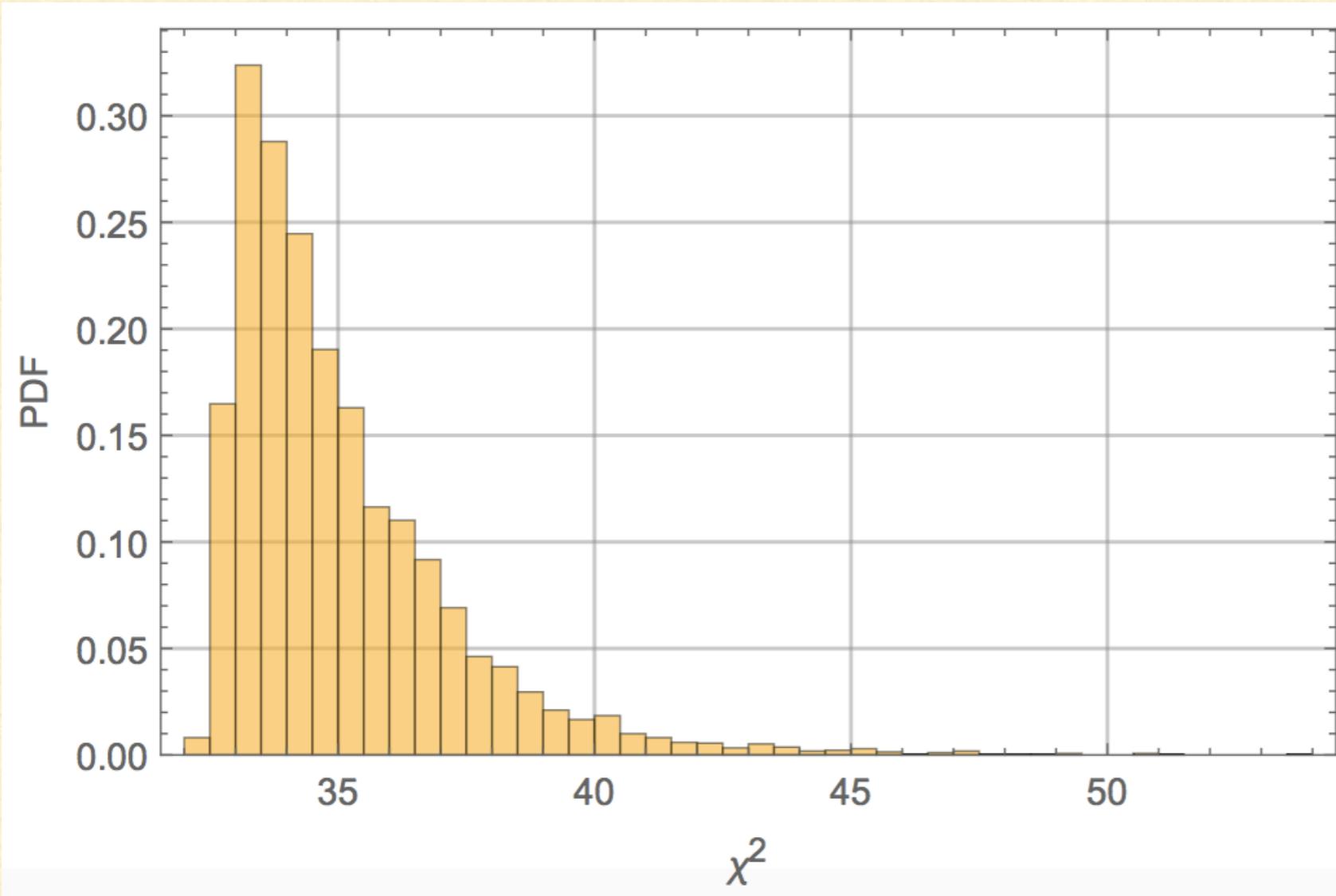
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- ANCs are highly correlated but sum of squares strongly constrained
- One spin-1 short-distance parameter: 0.33 \bar{L}_1 /(fm $^{-1}$) – ϵ_1

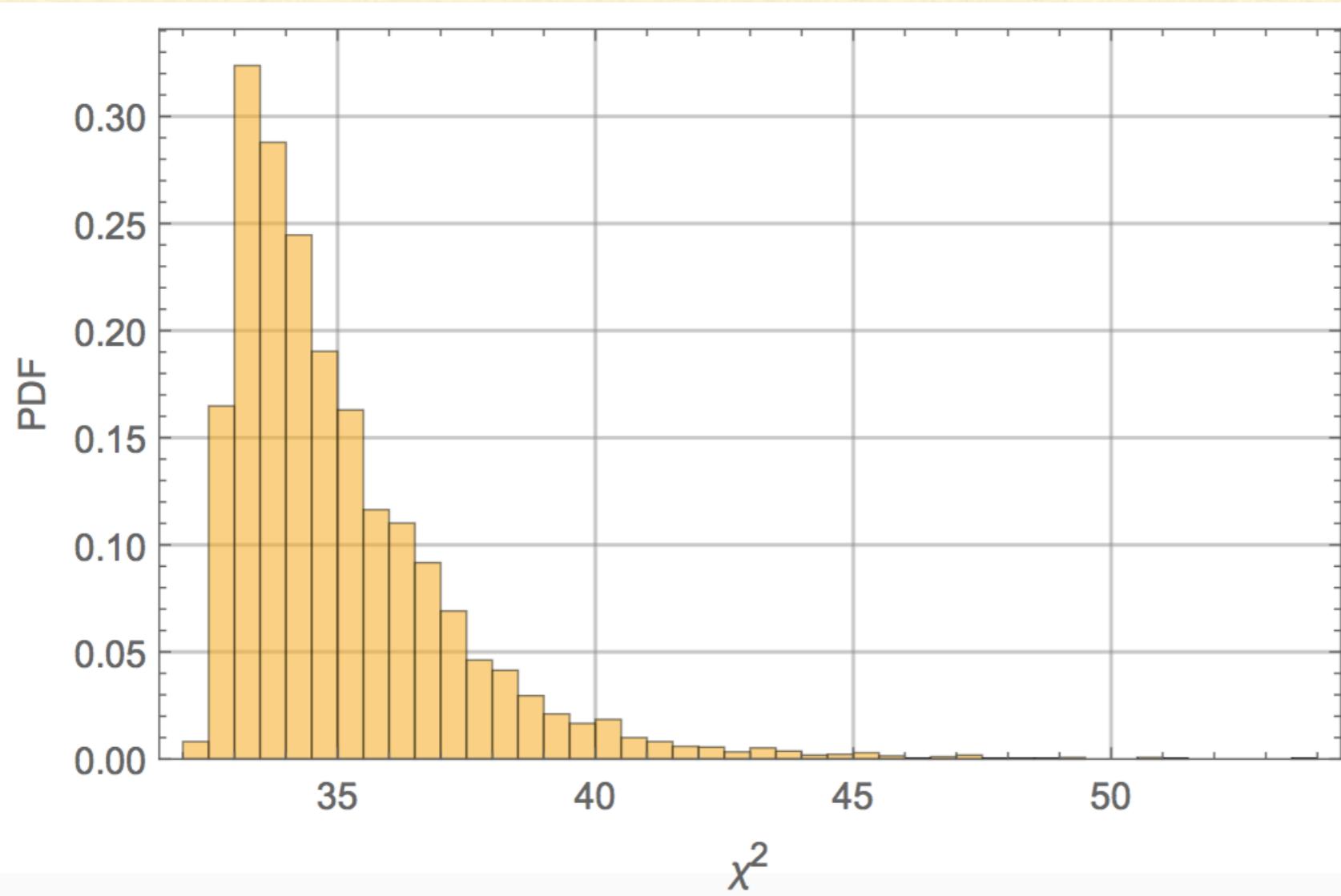
More questions we can answer



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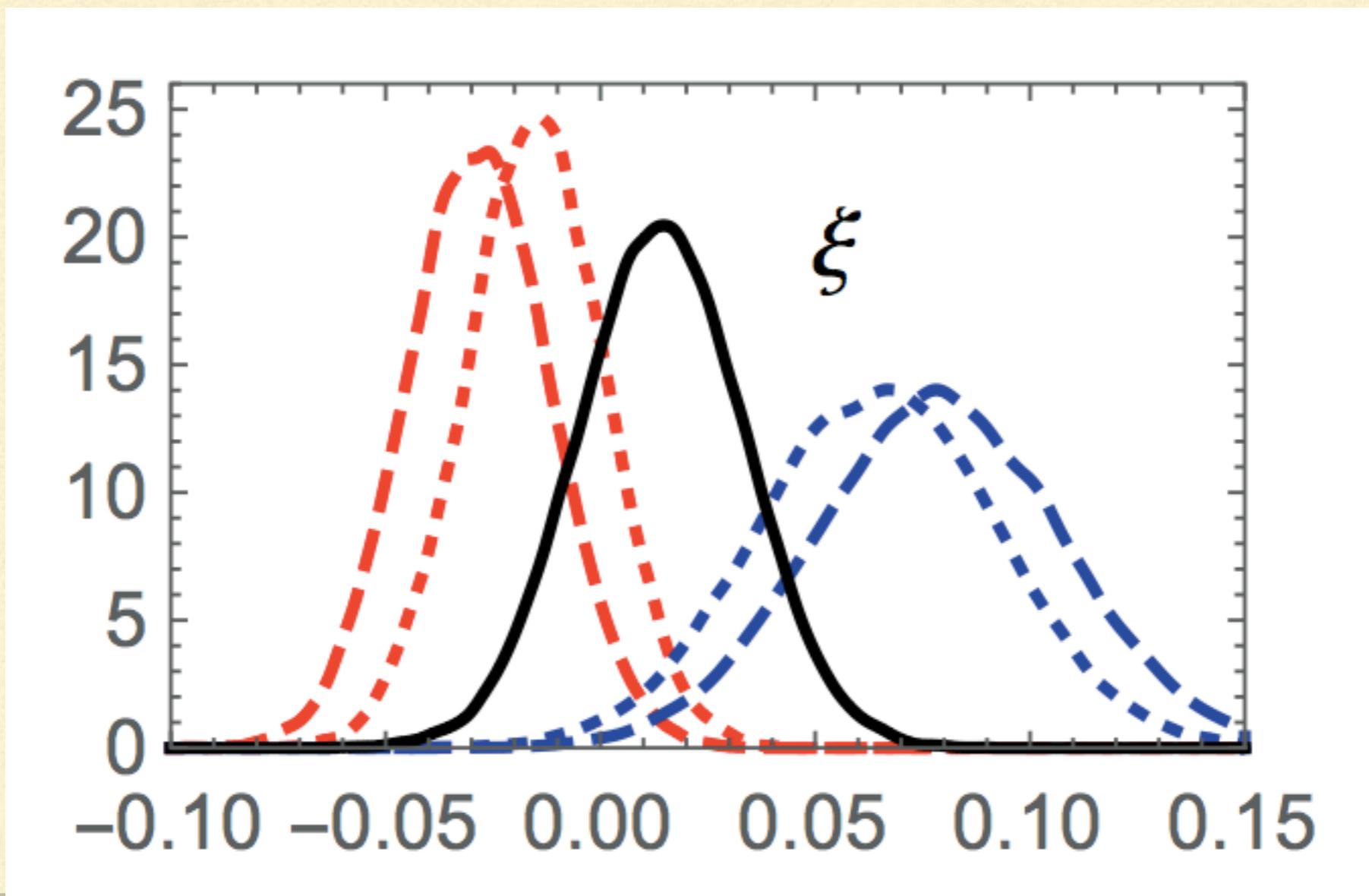
- Is it a “good fit”?



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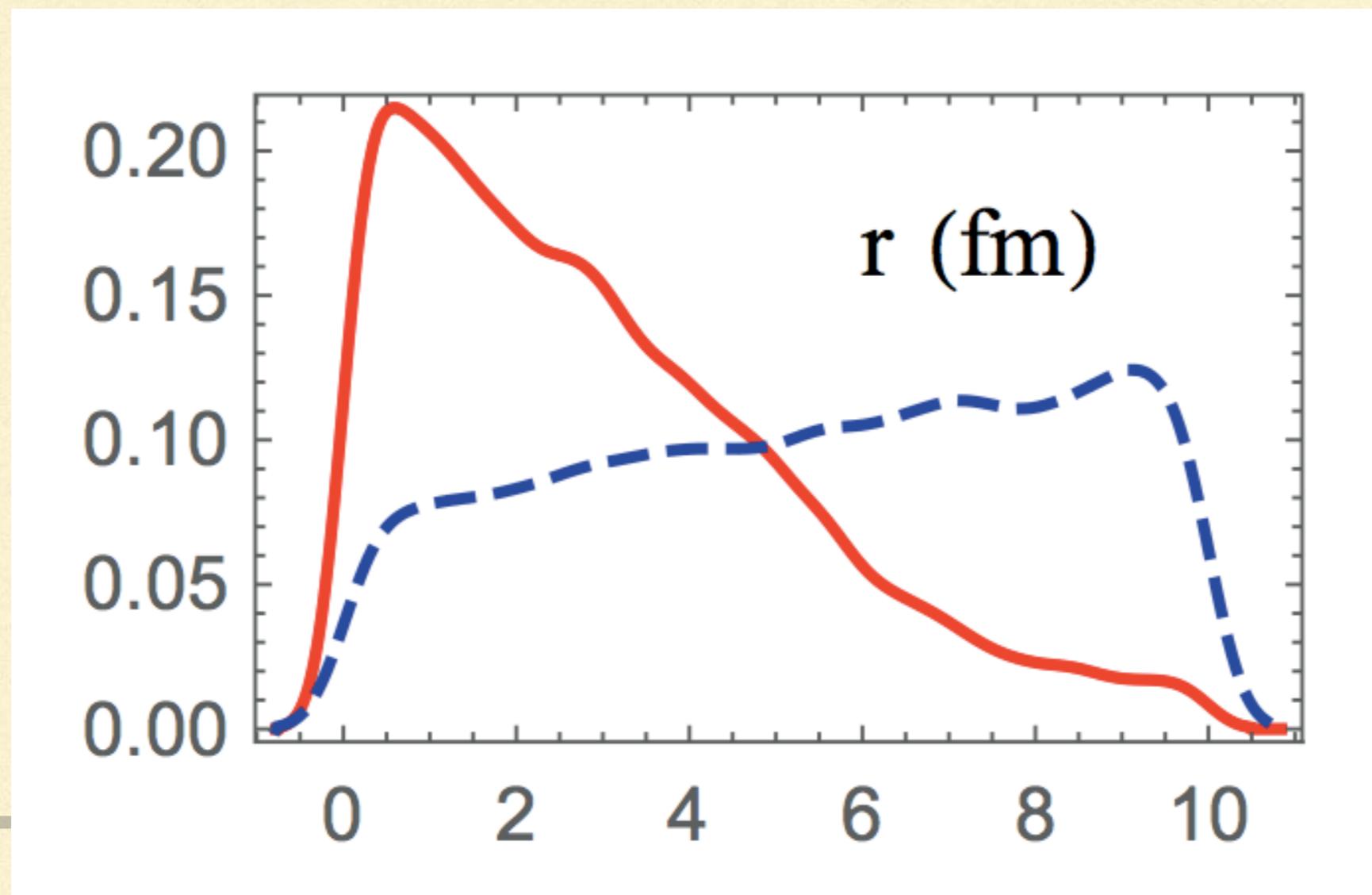
More questions we can answer

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More questions we can answer

- Is it a “good fit”?
- Did the experimentalists understand their systematic errors?
- Are there parameters that are not well constrained by these data?



Final result

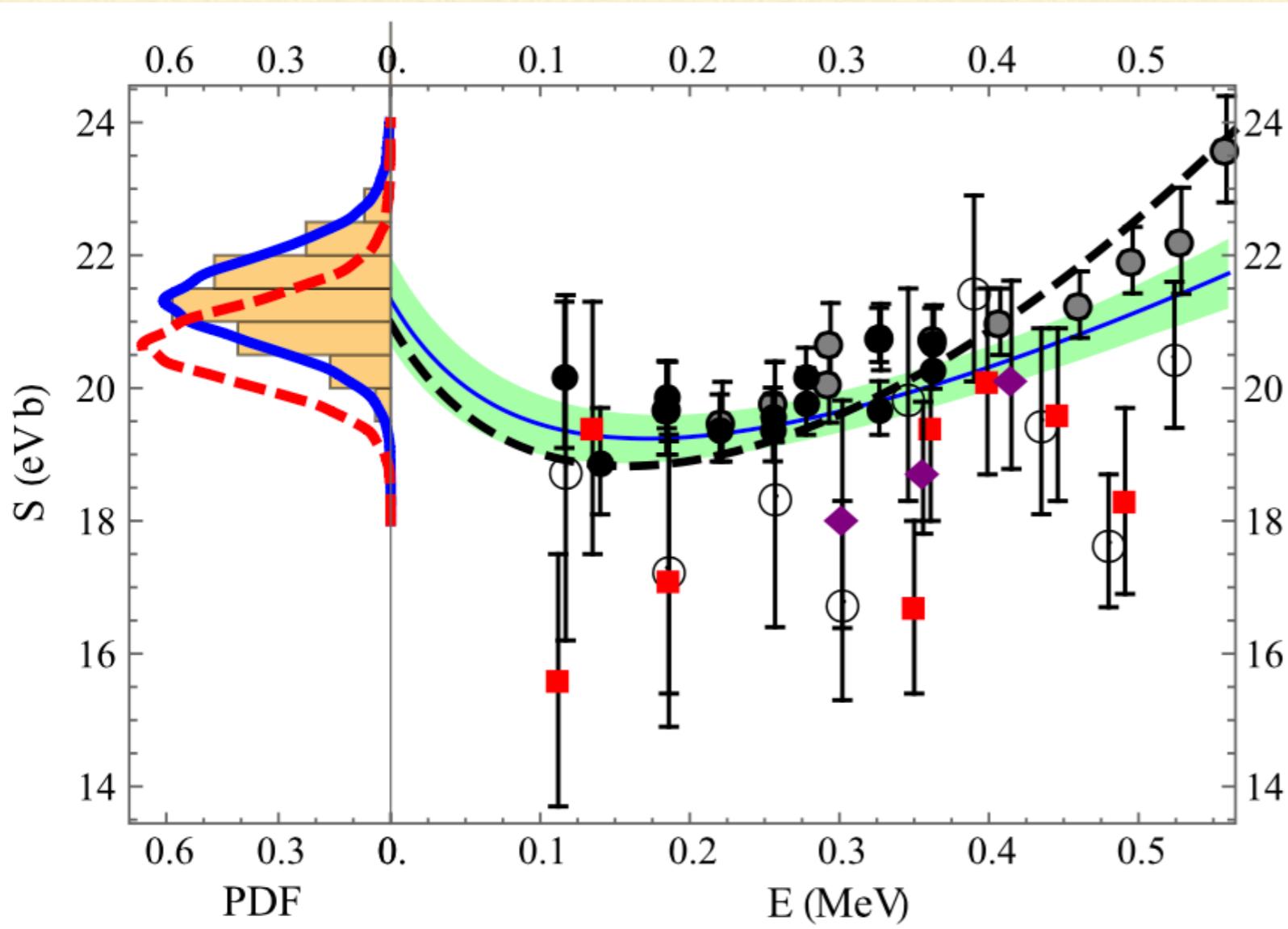
Zhang, Nollett, DP, PLB, 2015

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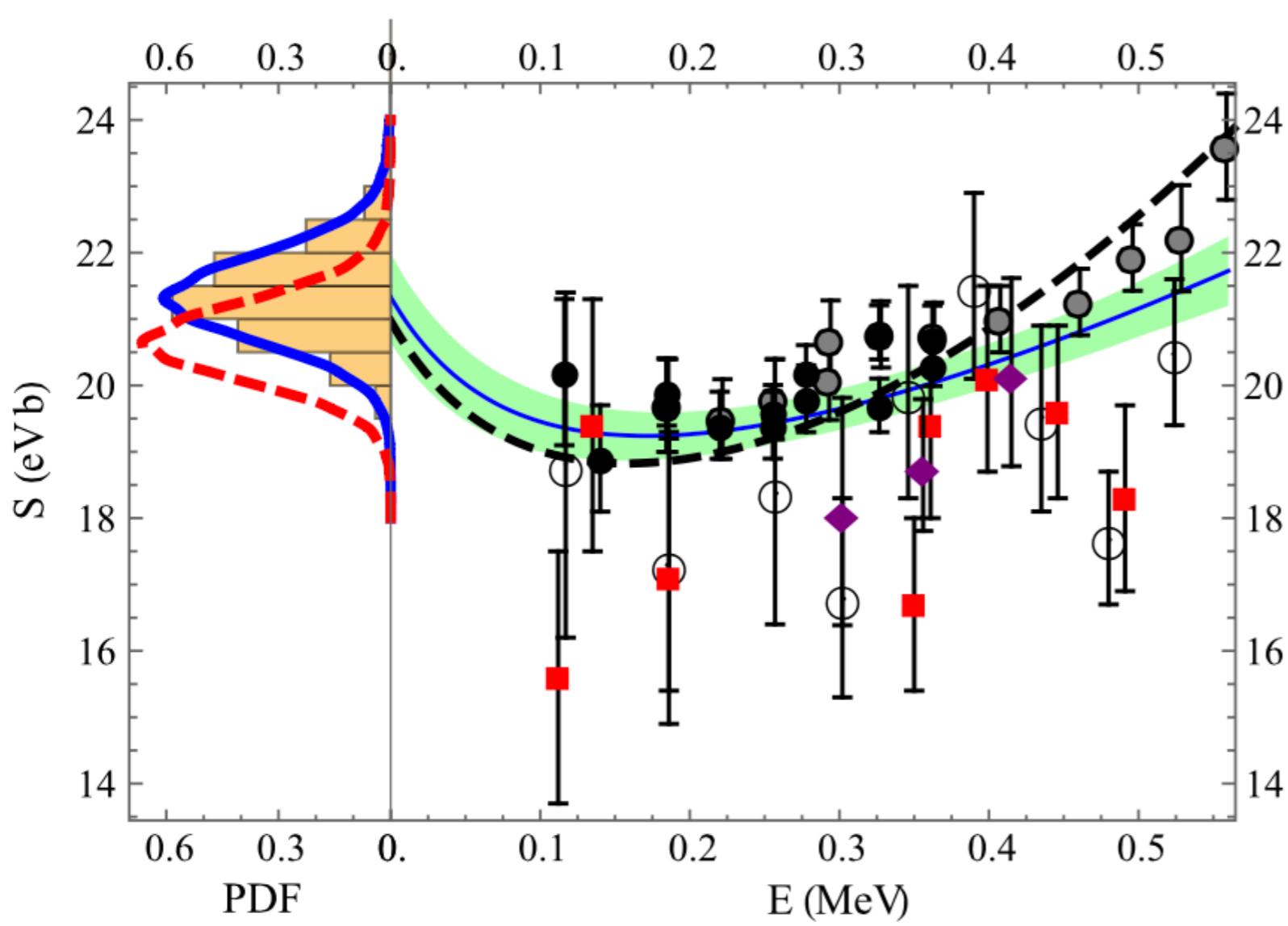
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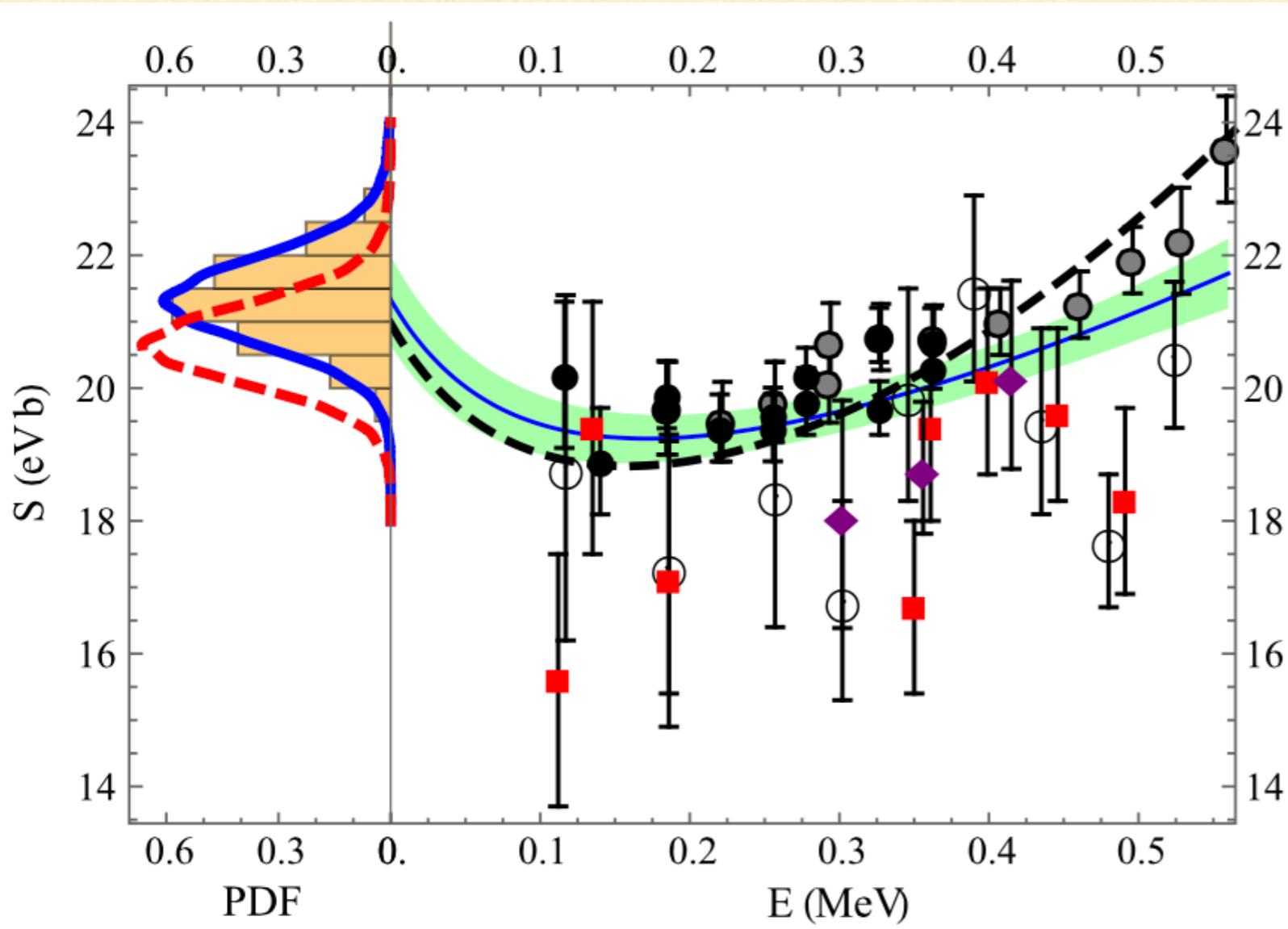


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Uncertainty reduced by
factor of two: model
selection

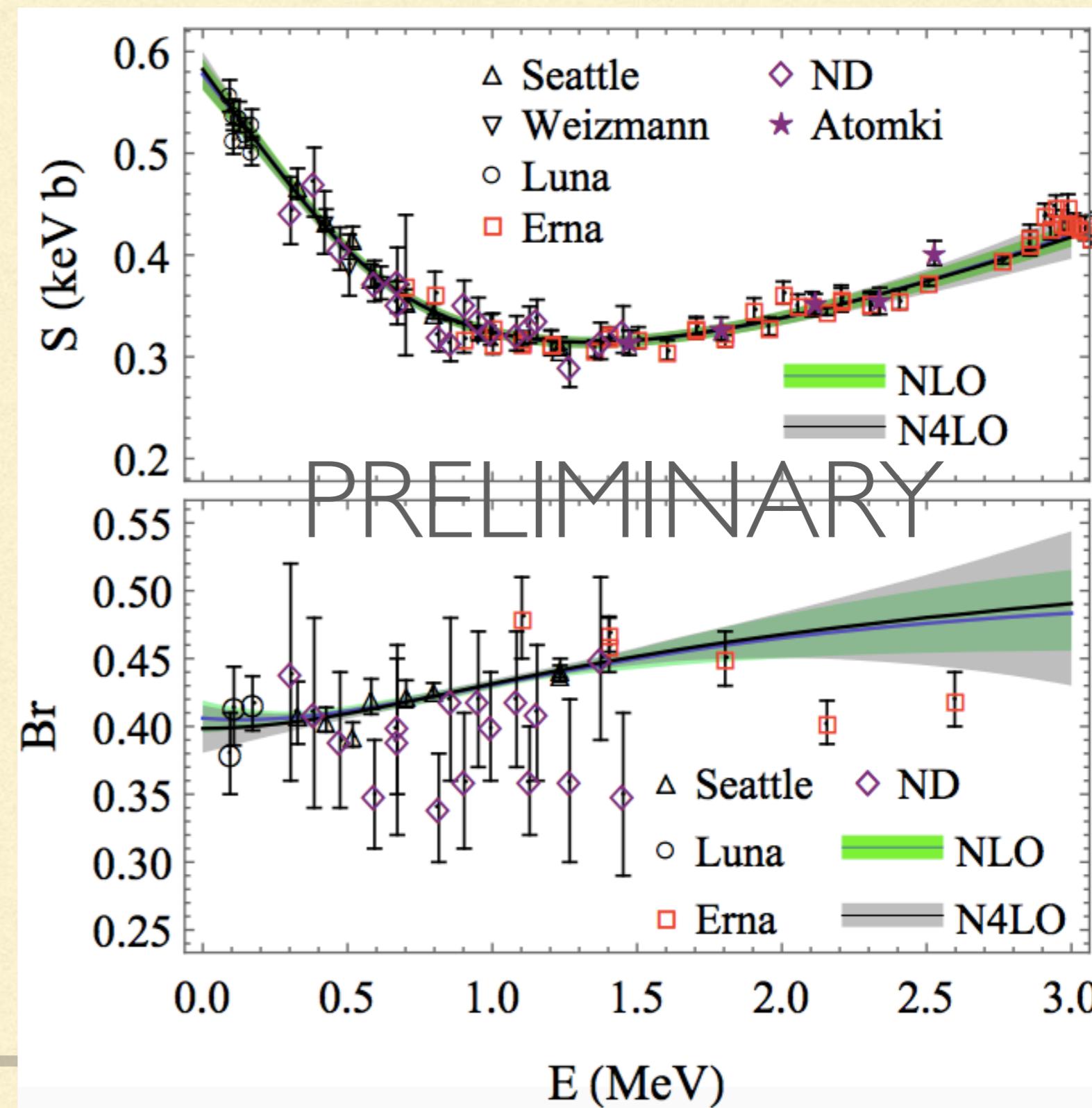
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Zhang, Nollett, DP, in preparation cf. Higa, Rupak, Vaghani, EPJA

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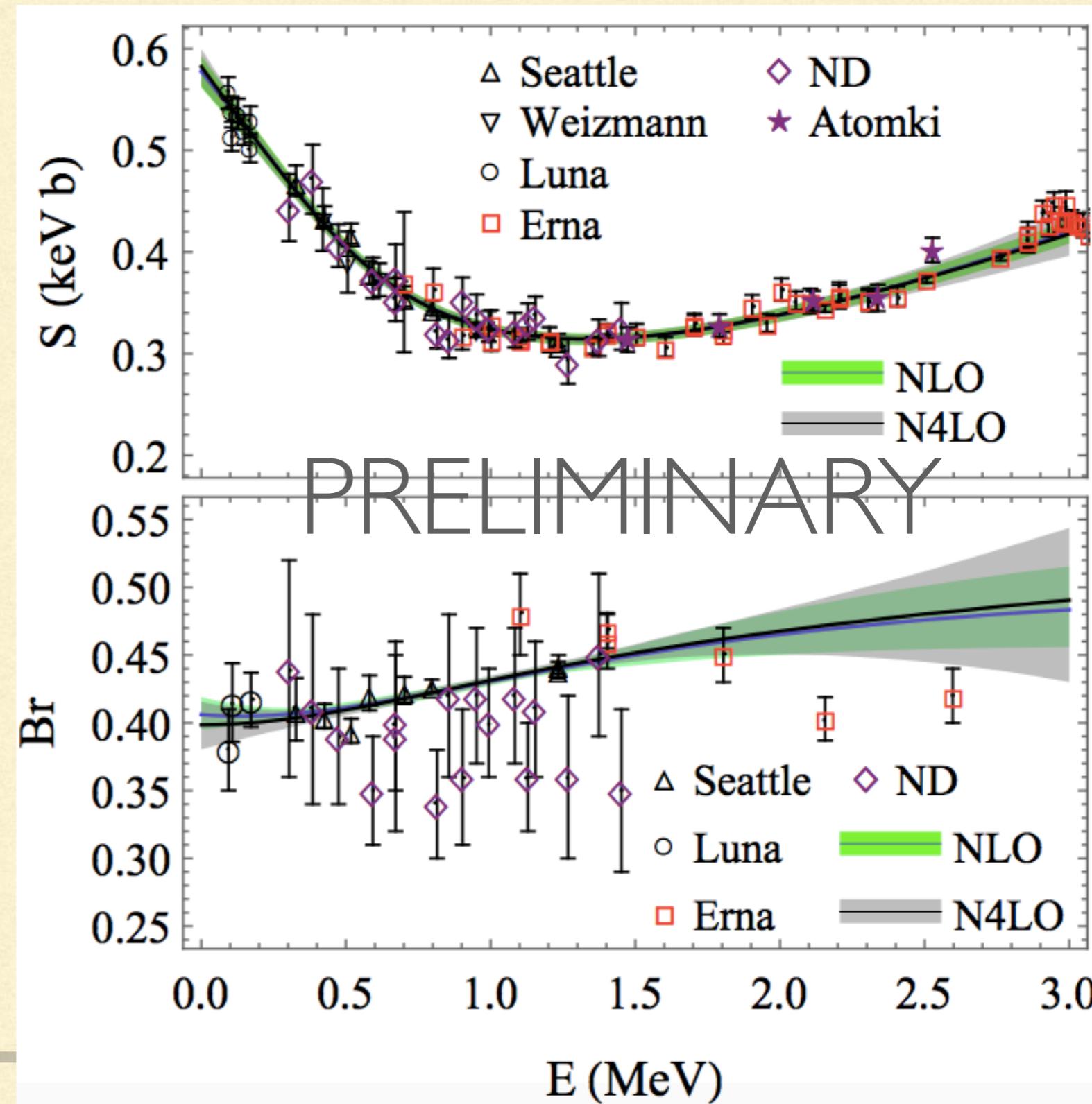
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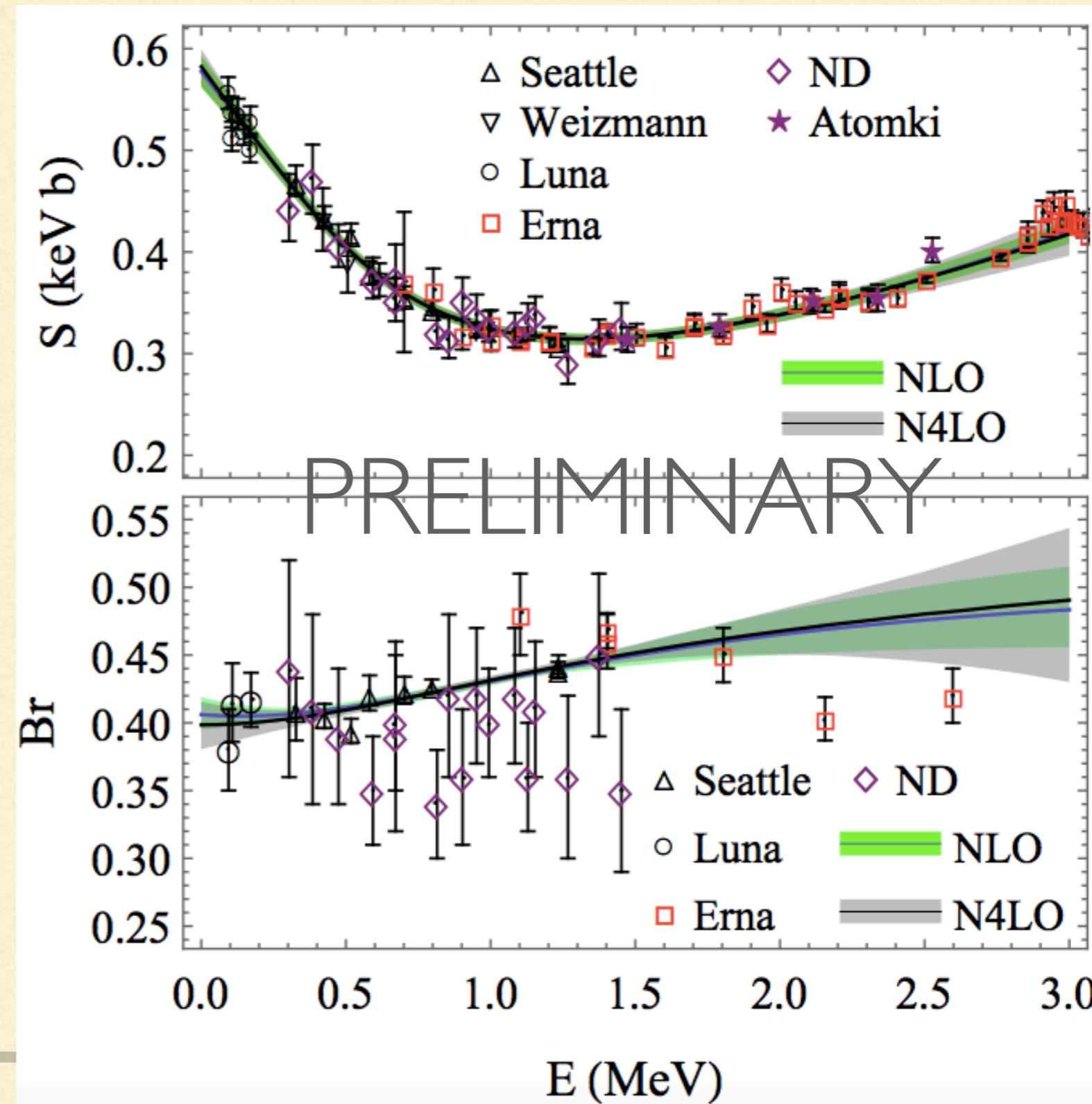
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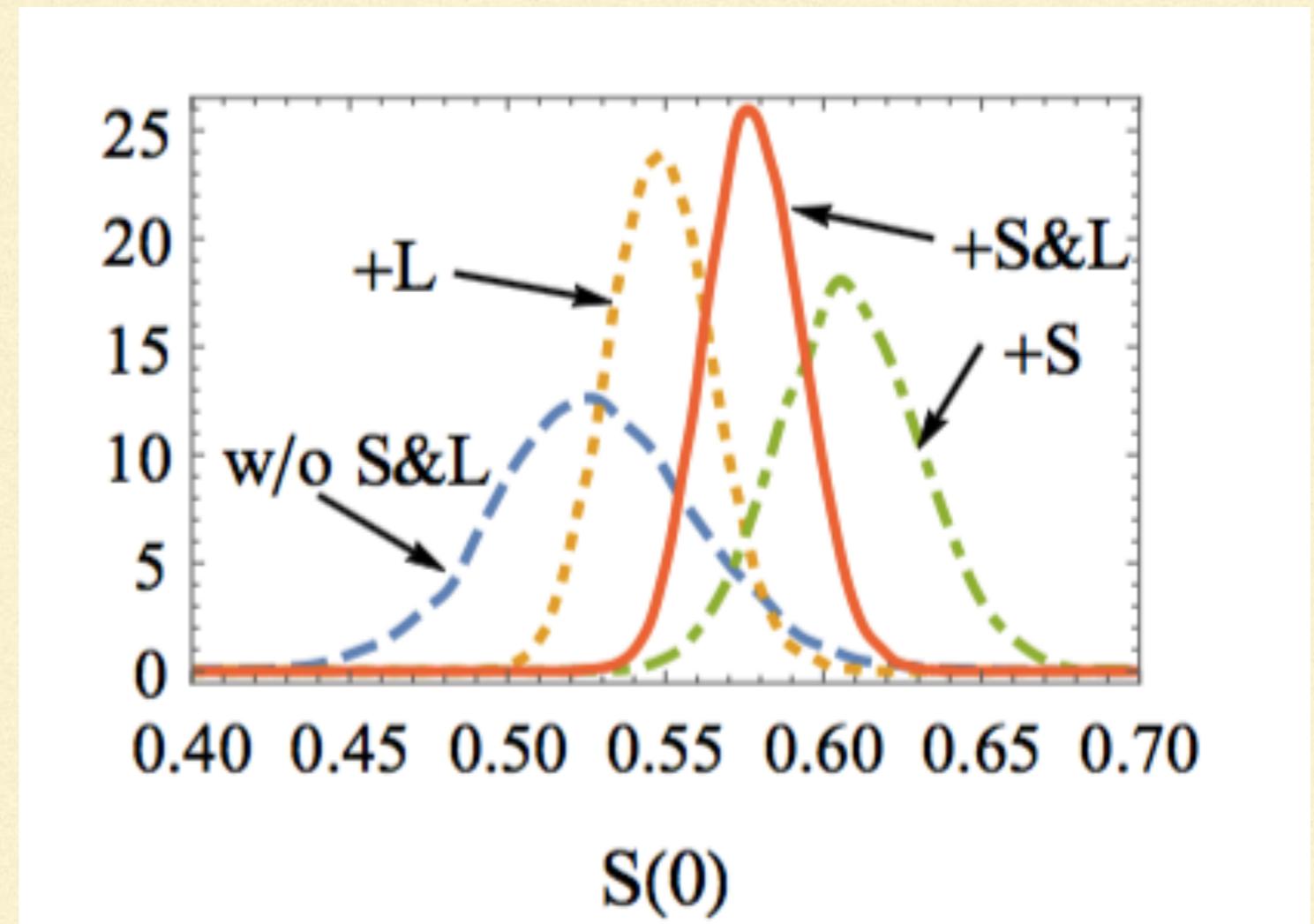
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- Bayesian evidence ratio ≈ 4 for NLO cf. N⁴LO



Impact of different data sets

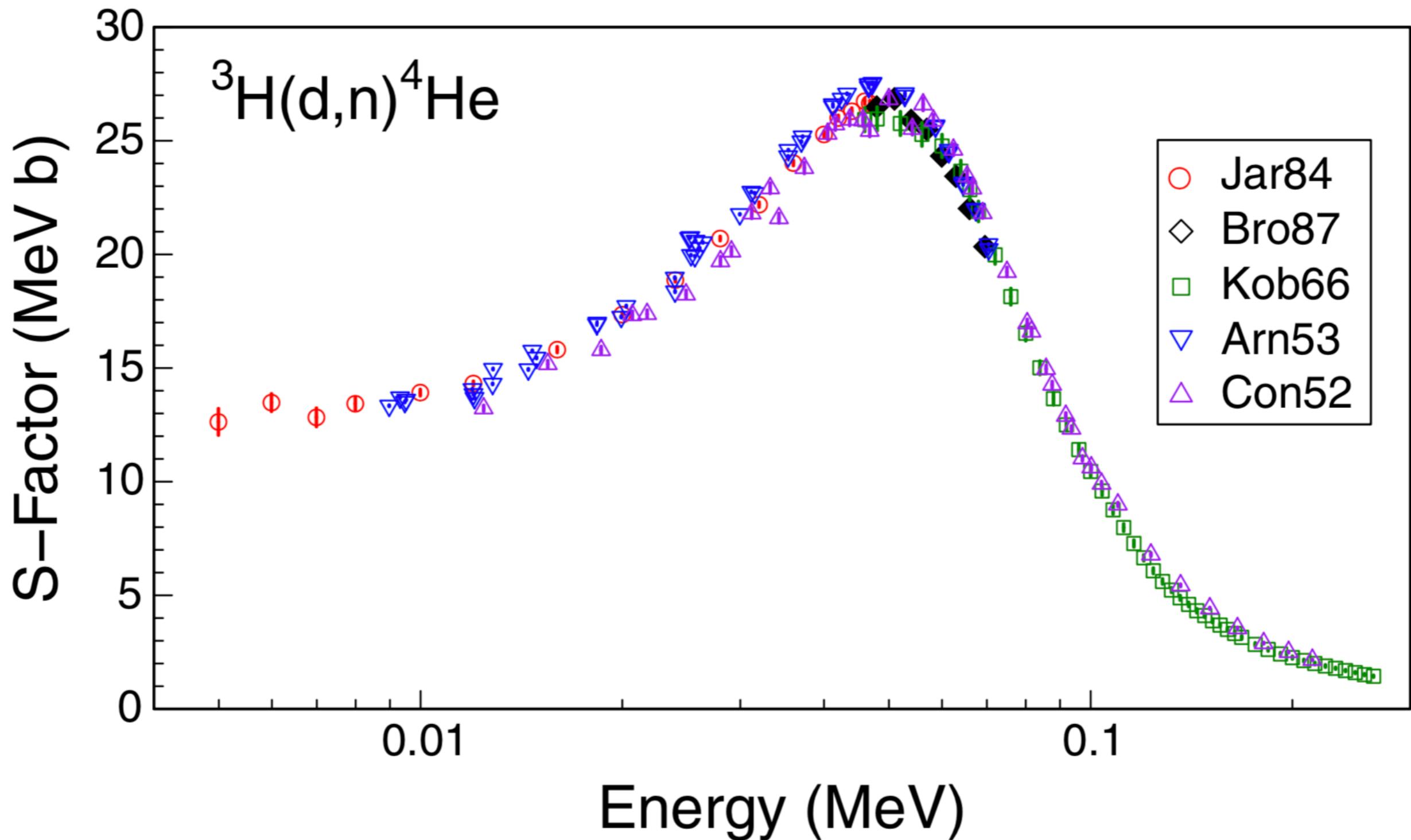
- Floating data within quoted CME crucial for achieving data consistency
- Pdf gets narrower when either of the precise, low-energy data sets are included
- Seattle data push $S(0)$ to higher values, but still possible to find concordance between Seattle, Luna, and older data



PRELIMINARY

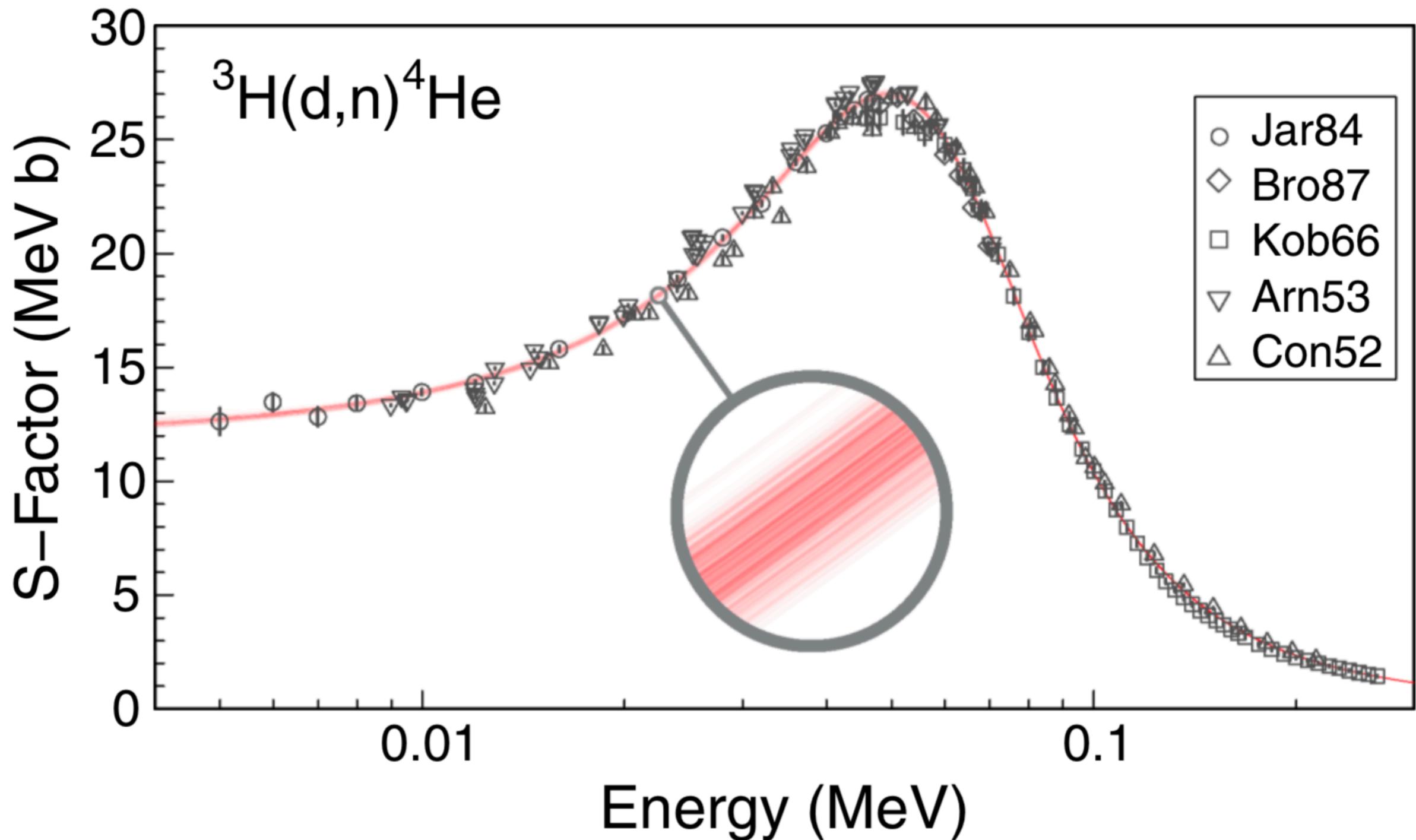
$^3\text{H}(\text{d},\text{n})^4\text{He}$ analysis

de Souza et al., PRC 99, 014619 (2019)



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Analysis

Likelihoods for energy:

$$E'_i \sim N(E_i, \sigma_{E,\text{extr},j}^2), \quad (24)$$

$$E''_{i,j} = f_{E,j} + E'_i, \quad (25)$$

$$E_{i,j}^{\text{exp}} \sim N(E''_{i,j}, \sigma_{E,\text{stat},i}^2). \quad (26)$$

Likelihoods for S -factor:

$$S'_i \sim N(S_i, \sigma_{S,\text{extr},j}^2), \quad (27)$$

$$S''_{i,j} = f_{S,j} \times S'_i, \quad (28)$$

$$S_{i,j}^{\text{exp}} \sim N(S''_{i,j}, \sigma_{S,\text{stat},i}^2). \quad (29)$$

Priors:

$$E_0 \sim U(0.02, 0.08), \quad (30)$$

$$E_B \sim N(0.0, 1.0^2)T(0,), \quad (31)$$

$$(\gamma_d^2, \gamma_n^2) \sim N(0.0, (\gamma_{WL}^2)^2)T(0,), \quad (32)$$

$$(a_d, a_n) \sim U(2.5, 8.0), \quad (33)$$

$$U_e \sim N(0.0, 0.001^2)T(0,), \quad (34)$$

$$E_i \sim U(0.001, 0.3), \quad (35)$$

$$\sigma_{E,\text{extr},j} \sim N(0.0, 0.01^2)T(0,), \quad (36)$$

$$f_{E,j} \sim N(0.0, \xi_j^2), \quad (37)$$

$$\sigma_{S,\text{extr},j} \sim N(0.0, 2.0^2)T(0,), \quad (38)$$

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$$E_B \sim N(0.0, 1.0^2)T(0.,),$$

$$(\gamma_d^2, \gamma_n^2) \sim N(0.0, (\gamma_{WL}^2)^2)T(0.,),$$

$$(a_d, a_n) \sim U(2.5, 8.0),$$

$$U_e \sim N(0.0, 0.001^2)T(0.,)$$

$$E_i \sim U(0.001, 0.3),$$

$$\sigma_{E,\text{extr},j} \sim N(0.0, 0.01^2)T(0.,)$$

$$f_{E,j} \sim N(0.0, \xi_j^2),$$

$$\sigma_{S,\text{extr},j} \sim N(0.0, 2.0^2)T(0.,)$$

$$f_{S,j} \sim LN(0, [\ln(f.u.)_j]^2),$$

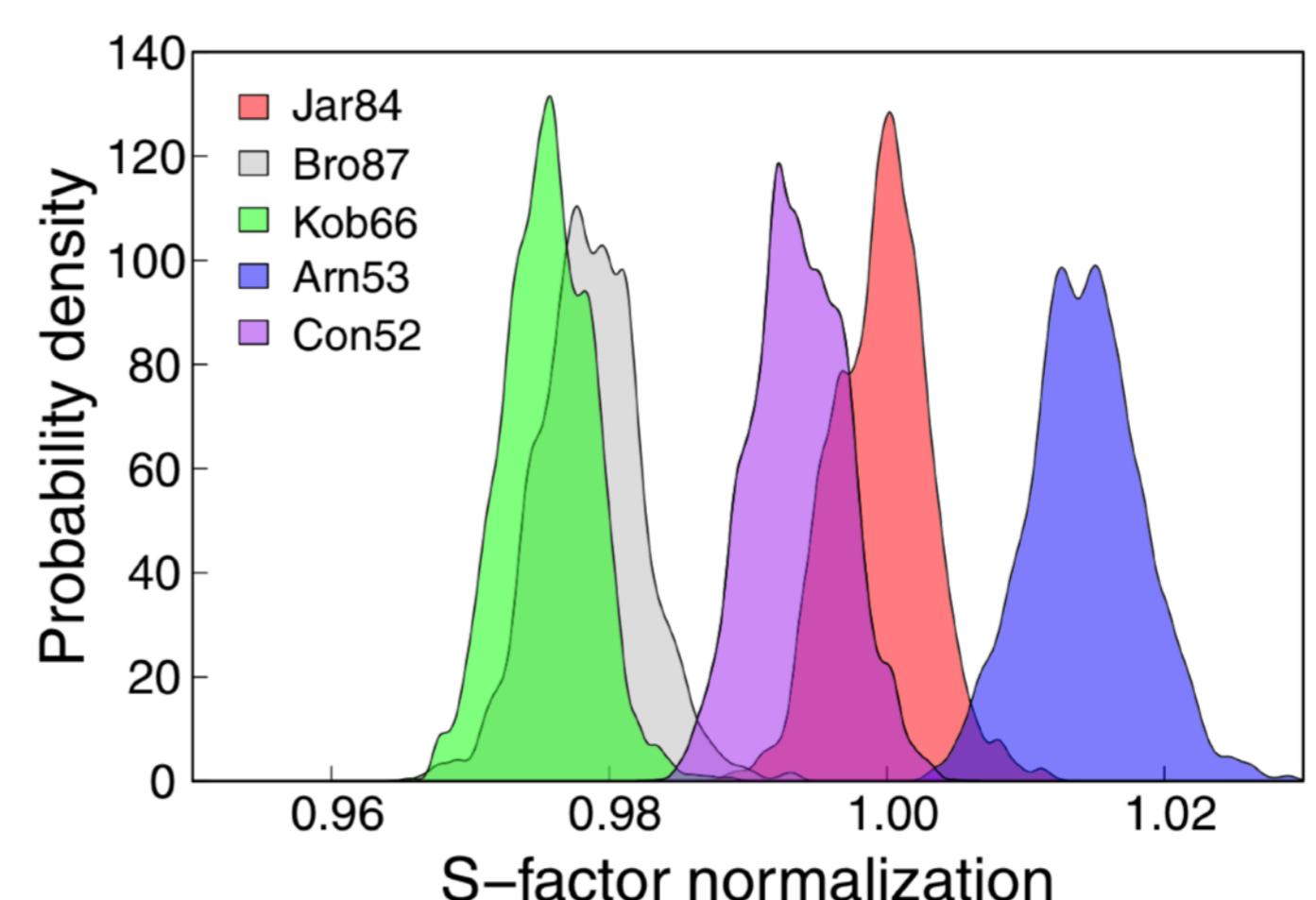


FIG. 7. Marginalized posteriors of the S -factor normalization factors, f_S . The labels refer to the same data sets as shown in Fig. 1. Percentiles of the distributions are listed in Table II.

Systematic error with known functional form

Schindler & DP, Ann. Phys. 324, 682 (2009)

Stump et al., PRD 65, 014012 (2001)

Systematic error with known functional form

Schindler & DP, Ann. Phys. 324, 682 (2009)

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- Return to polynomial fitting example from first mini-project

$$\text{pr}(\vec{a} | D, k_{\max}, \bar{a}) \propto \exp(-\chi^2_{\text{aug}}/2)$$

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$$\text{pr}(\vec{a} | D, k_{\max}, \bar{a}) \propto \exp(-\chi_{\text{aug}}^2/2)$$

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$$\text{pr}(\vec{a}_{\text{res}} | D, k_{\max}, \bar{a}) \propto \exp(-\chi_{\text{marg}}^2/2)$$

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- Equivalent to adding covariance matrices for experimental and EFT error

$$\Sigma = \text{diag}(\sigma_1^2, \dots, \sigma_{N_{\text{expt}}}^2) + \Sigma_{\text{EFT}}$$

Backup Slides

Effective Field Theory

- Simpler theory that reproduces results of full theory at long distances
 - Short-distance details irrelevant for long-distance (low-momentum) physics, e.g., multipole expansion
 - Expansion in ratio of physical scales: $p/\Lambda_b = \lambda_b/r$
 - Symmetries of underlying theory limit possibilities: all possible terms up to a given order present in EFT
 - Short distances: unknown coefficients at a given order in the expansion need to be determined. Symmetry relates their impact on different processes
 - Examples: standard model, chiral EFT, Halo EFT
-

Effective Field Theory

Monet (1881)



Effective Field Theory

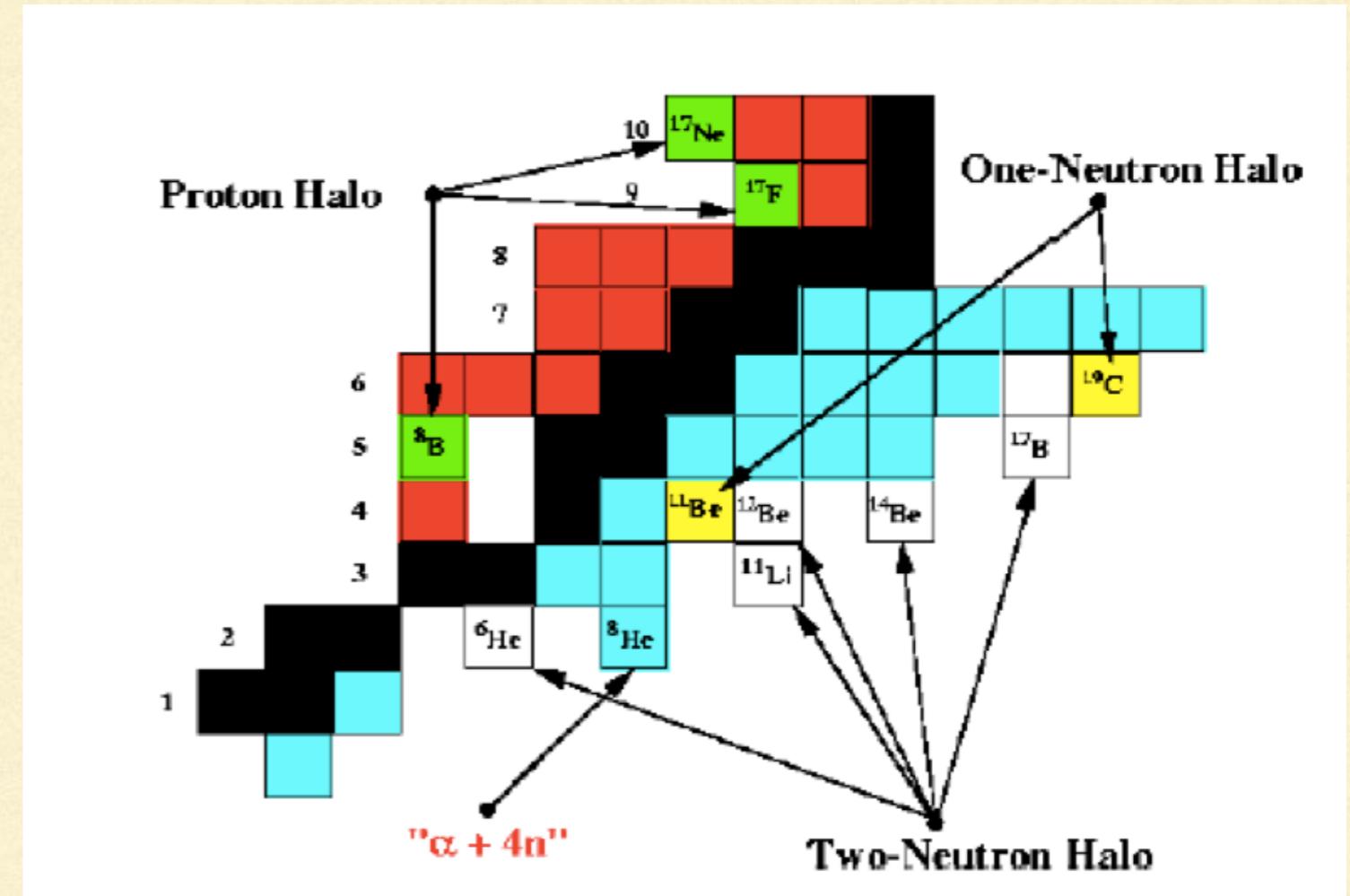
Monet (1881)

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Error grows as first omitted term in expansion

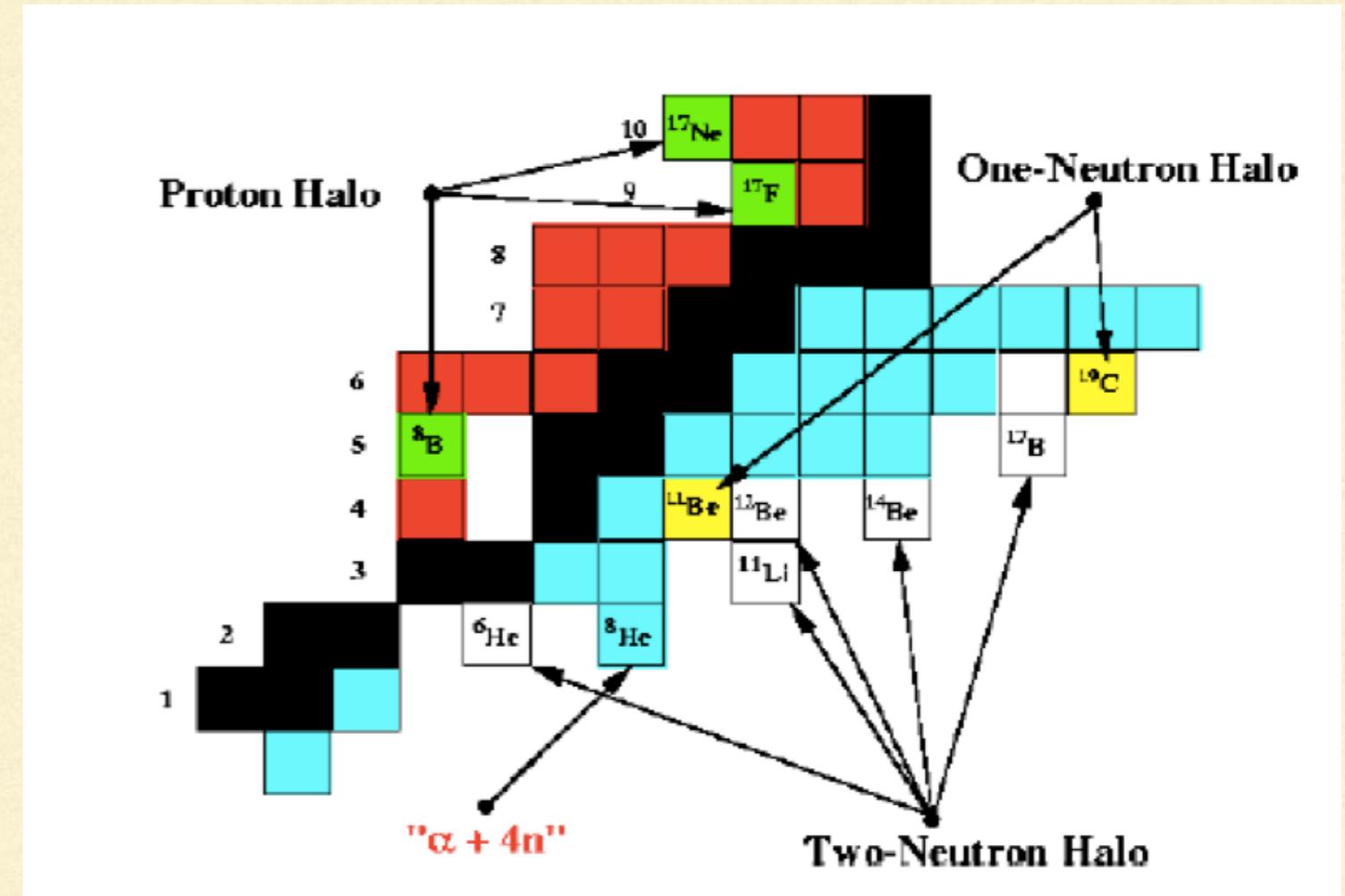
Halo nuclei

<http://nupecc.org>



Halo nuclei

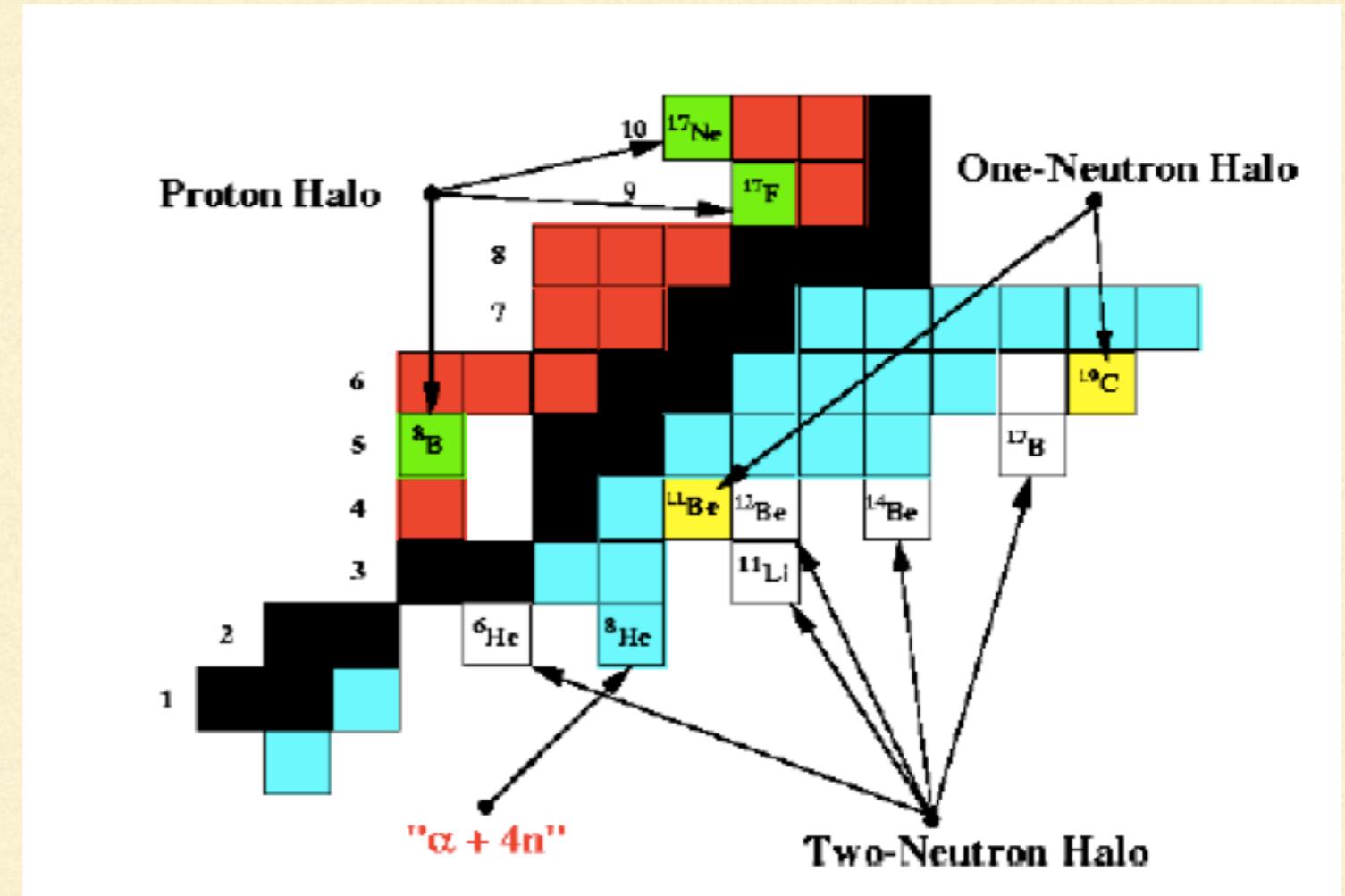
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- A halo nucleus as one in which a few (1, 2, 3, 4, ...) nucleons live at a significant distance from a nuclear core.

Halo nuclei

<http://nupecc.org>

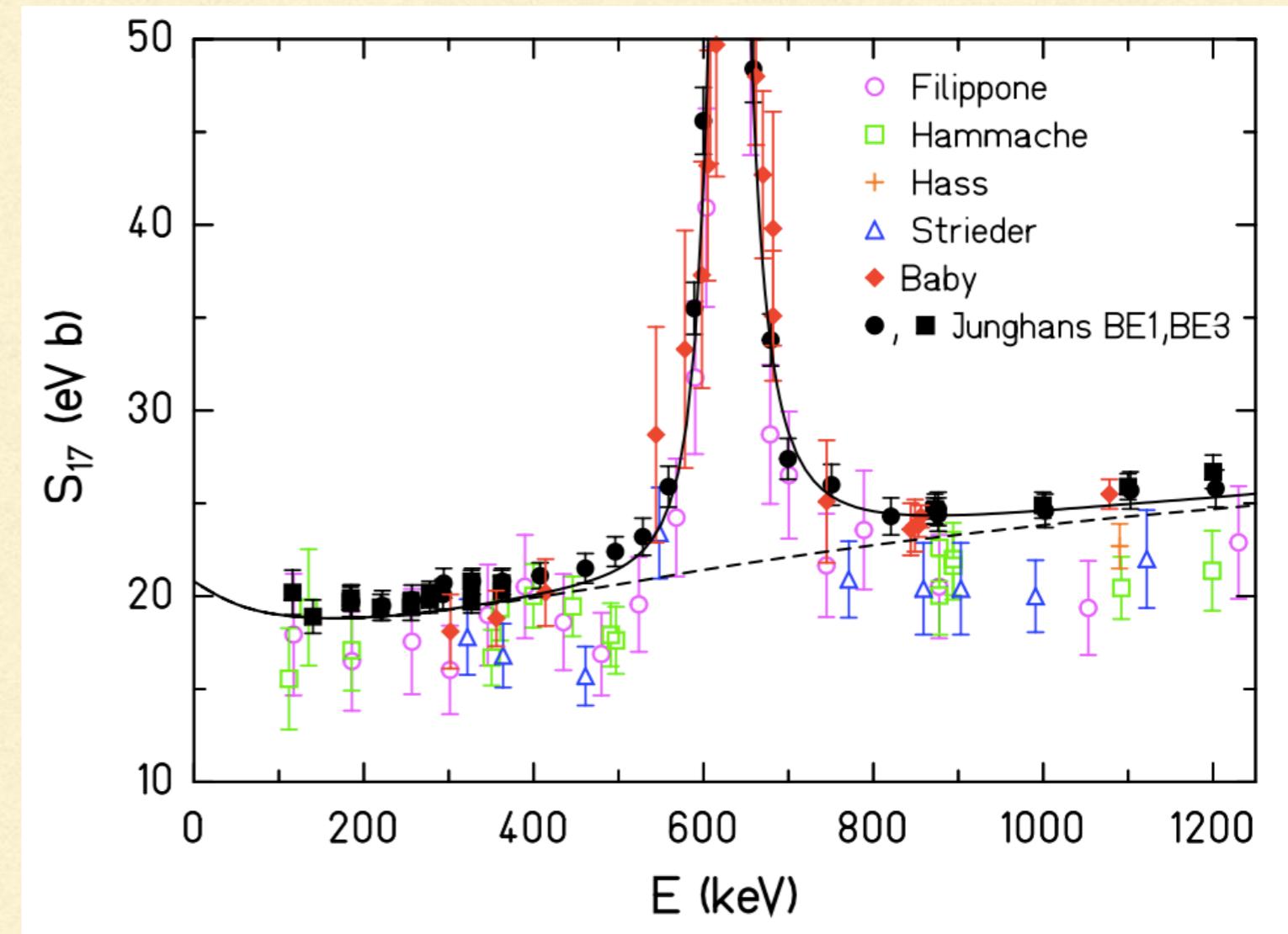


- A halo nucleus as one in which a few (1, 2, 3, 4,...) nucleons live at a significant distance from a nuclear core.
 - Halo nuclei are characterized by small nucleon binding energies, large interaction cross sections, large radii, large E1 transition strengths.

Status as of 2012

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

- Below narrow I^+ resonance proceeds via s- and d-wave direct EI capture
- Energy dependence due to interplay of Coulomb and strong forces
- “Solar fusion II”: community evaluation of cross sections relevant for pp and CNO cycles



■ SF II value: $S(0)=20.8 \pm 0.7 \pm 1.4 \text{ eV b}$

SF I: $S(0)=19^{+4}_{-2} \text{ eV b}$

- Used energy dependence from a “best” calculation. Errors from consideration of energy-dependence in a variety of “reasonable models”