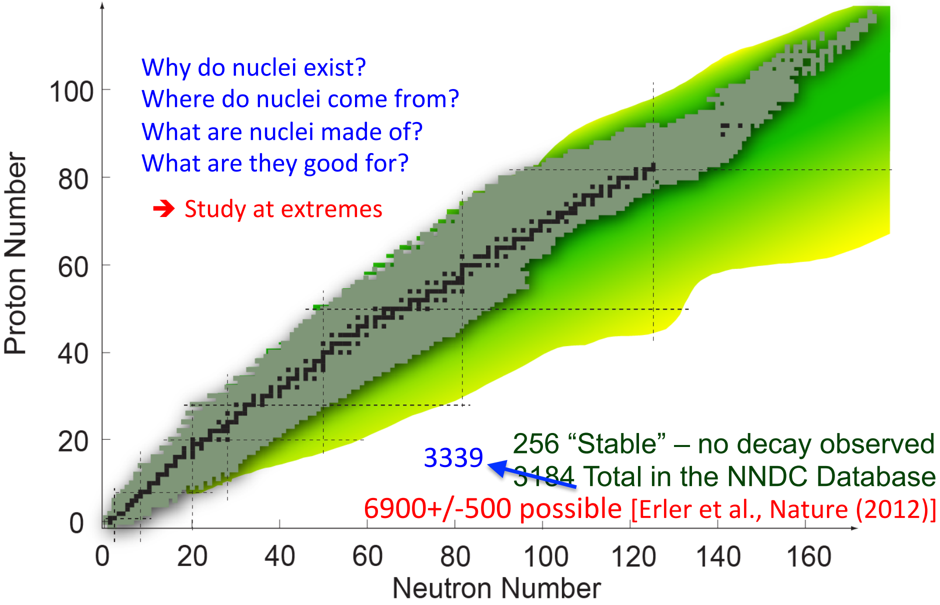
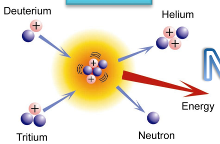
The Nuclear Landscape: What are the physics questions?



NUclear Computational Low-Energy Initiative

fusion



NIF

TJNAF

Validated Nuclear Interactions

LENP facilities

FRIB

Structure and Reactions: Light and Medium Nuclei

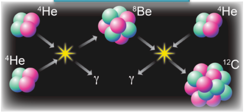
Neutron drops

EOS

Correlations

Structure and Reactions: Heavy Nuclei

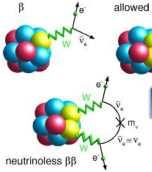
Stellar burning



Ab initio: microscopic inter-nucleon forces connected to QCD

Spectroscopic quality density functional

Neutrinos and Fundamental Symmetries

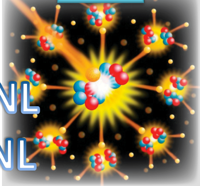


SNS

Majorana

Neutron Stars

Fission

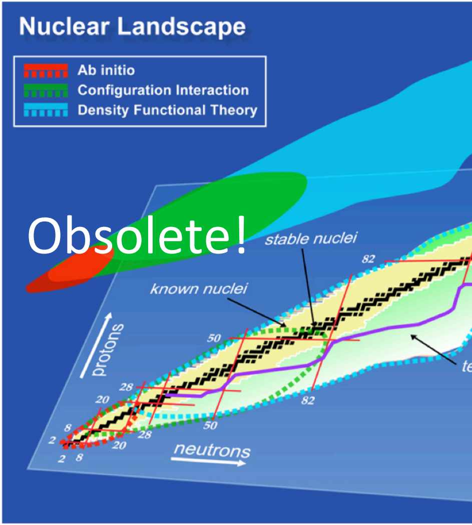


LANL

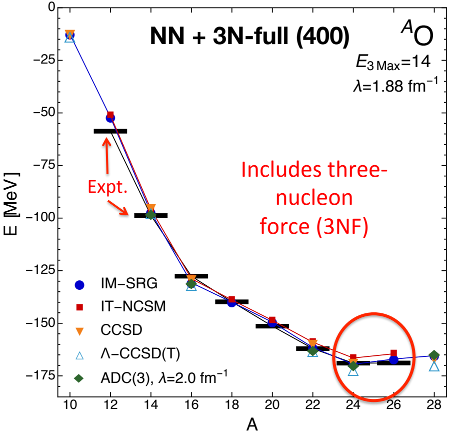
LLNL

Explosion of many-body methods using microscopic input

- Ab initio (new and enhanced methods; microscopic NN+3NF)
  - Stochastic: GFMC/AFDMC (new: with local EFT); lattice EFT
  - Diagonalization: IT-NCSM
  - Non-linear eqs: coupled cluster
  - Flow equations: IM-SRG
  - Self-consistent Green's function
  - Many-body perturbation theory
- Shell model (usual: empirical inputs)
  - Effective SM interactions from coupled cluster, IM-SRG
- Density functional theory
  - Microscopic input, e.g., DME
- Complementary strengths, cross-checks, theory error bars



Oxygen chain with 4 methods [Hergert et al., Cipollone et al. (2013)]



- In-medium SRG, importance-truncated NCSM, coupled cluster, SCGF
- Same Hamiltonian $\Longrightarrow$ test for consistency between *methods*

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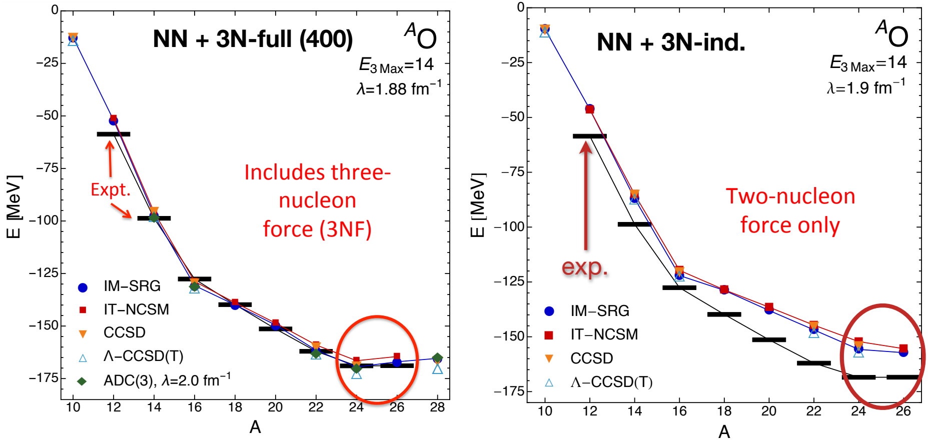


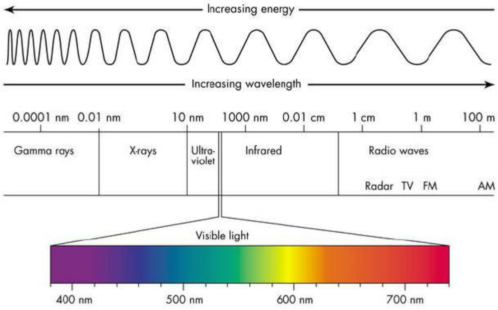
- In-medium SRG, importance-truncated NCSM, coupled cluster, SCGF
- Same Hamiltonian $\Longrightarrow$ test for consistency between *methods*
- Impact of chiral three-nucleon force (3NF) on dripline
- Need precision experiment *and* theory (but where are the error bars?)

Confluence of progress in theory and experiment

- Experimental facilities and technology
  - Precise + accurate mass measurements (e.g., Penning traps)
  - Access to exotic nuclei (isotope chains, halos, etc.)
  - Knock-out reactions (of many varieties)
  - ⋮
- Theory advances, catalyzed by large-scale collaboration
  - Explosion of complementary many-body methods
  - Inputs: effective field theory and renormalization group
  - Computational power and advanced algorithms
- *Precision* comparisons are increasingly possible *if* we can
  - control (and minimize) model dependence
  - quantify theory error bars from all sources
  - treat structure and reactions consistently

EFT common principle: Draw a line between UV and IR

- Separate the short-distance (UV) from long-distance (IR) physics at dividing scale
- Much freedom *how* this is done (e.g., different regulator forms in chiral EFT)
  $\Longrightarrow$ different scales / schemes



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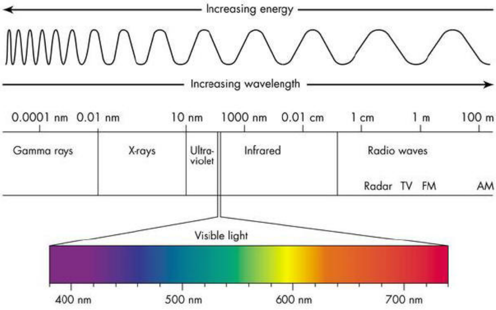

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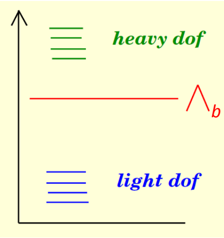
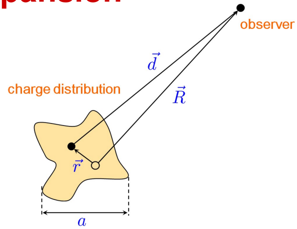


These elements will enable UQ for (chiral) EFT!

Classical analogy to EFT: Multipole expansion

Localized charge distribution $\rho(\mathbf{r})$ in volume characterized by distance *a* has electrostatic potential

$$\phi(\mathbf{R}) \propto \int d^3 r \, \frac{\rho(\mathbf{r})}{|\mathbf{R} - \mathbf{r}|}$$



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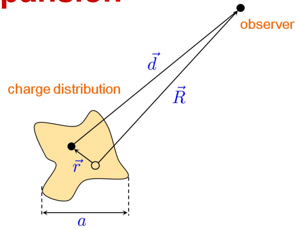

$$\phi(\mathbf{R}) \propto \int d^3r \, \frac{\rho(\mathbf{r})}{|\mathbf{R}-\mathbf{r}|}$$

If we expand $1/|\mathbf{R}-\mathbf{r}|$ for $r \ll R$, we get the multipole expansion

$$\int d^3r \, \frac{\rho(\mathbf{r})}{|\mathbf{R}-\mathbf{r}|} = \frac{q}{R} + \frac{1}{R^3}\sum_i R_i P_i + \frac{1}{6R^5}\sum_{ij}(3R_iR_j - \delta_{ij}R^2)Q_{ij} + \cdots$$

$\Longrightarrow$ *pointlike* total charge q, dipole moment P_i, quadrupole Q_{ij}:

$$q = \int d^3r \, \rho(\mathbf{r}) \qquad P_i = \int d^3r \, \rho(\mathbf{r}) \, r_i \qquad Q_{ij} = \int d^3r \, \rho(\mathbf{r})(3r_ir_j - \delta_{ij}r^2)$$

- Hierarchy of terms from separation of scales $\Longrightarrow$ a/R expansion

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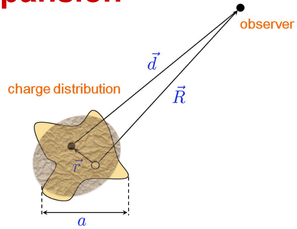

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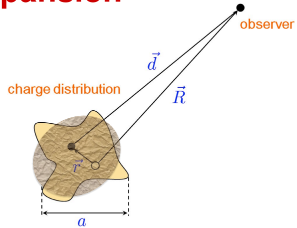

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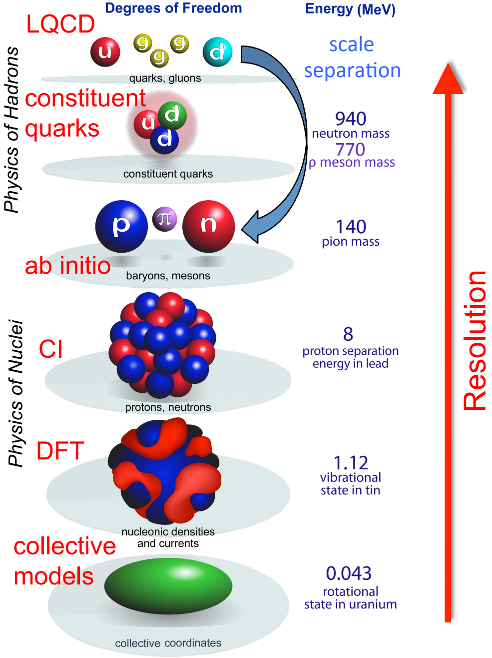
- Hierarchy of terms from separation of scales $\Longrightarrow$ a/R expansion
- Can include *known long-distance* structure $\Longrightarrow$ new expansion
- Can determine coefficients (LECs) by comparing to experimental measurements or matching to actual distribution (if known; cf. LQCD)
- Completeness $\Longrightarrow$ model independent (cf. model of distribution)

Nuclear emergence: using EFT to meet the challenges



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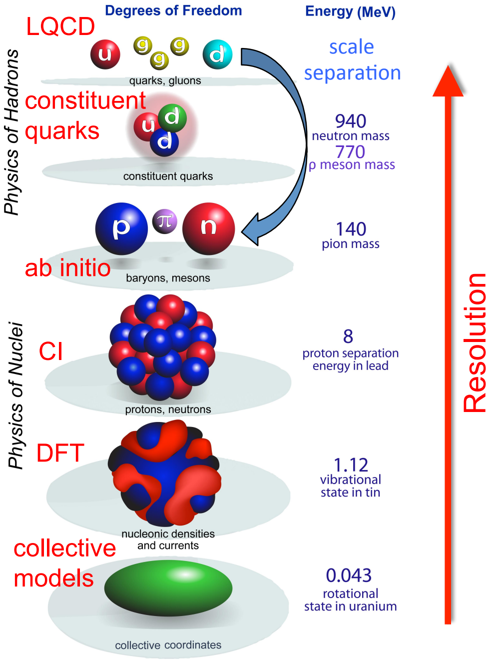
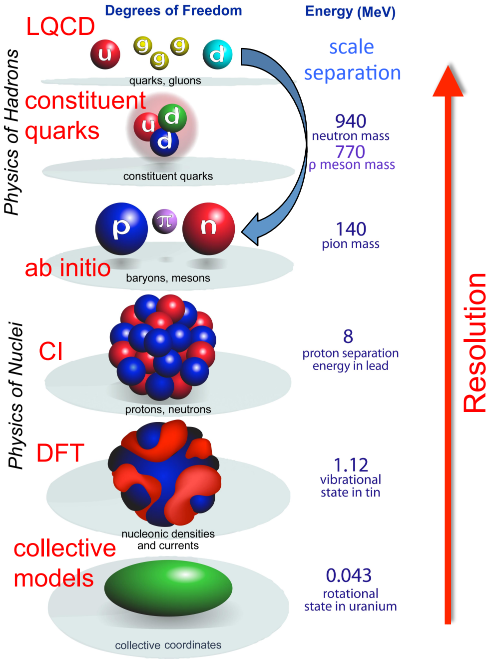


- Emergent degrees of freedom ("more is different")
- Reductionist paradigm: derive from QCD
- EFT takes advantage of scale separation, connects hierarchy via matching (to underlying theory and/or data)

Different EFTs depending on scale/observables of interest



There is not just one EFT!

- Chiral EFT: nucleons, [Δ's,] pions: $\{p, m_\pi\}/\Lambda_\chi \approx m_\rho$
- Pionless EFT: nucleons only (low-energy few-body) or nucleons and clusters (halo)
- EFT for deformed nuclei: systematic collective dofs (see T. Papenbrock talk)
- EFT at Fermi surface (Landau-Migdal theory): quasi-nucleons

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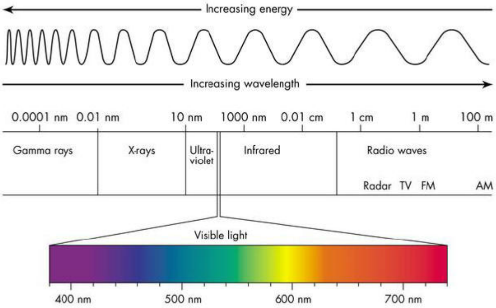

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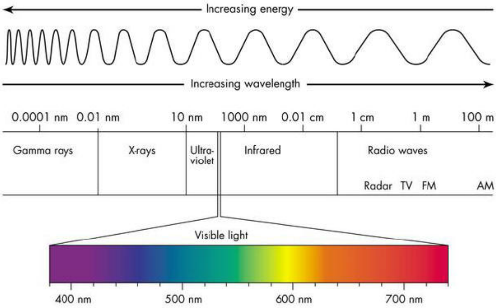

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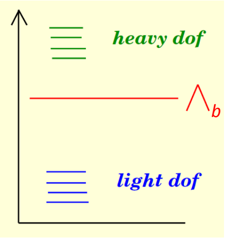

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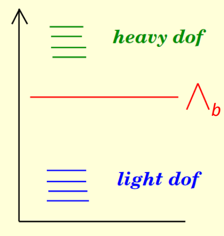
Conceptual basis of chiral effective field theory

- Separate the short-distance (UV) from long-distance (IR) physics (expect $\Lambda_b \approx m_\rho$)
- Regulated contact terms for short-distance physics
- Exploit chiral symmetry $\Longrightarrow$ hierarchical treatment of long-distance pion physics (also regulated)
- As implemented, need regulators in momentum or coordinate space *with cutoffs* $\Lambda \sim 2/R \sim \Lambda_b$



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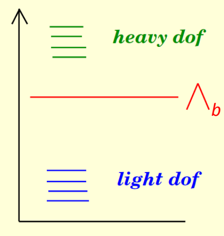
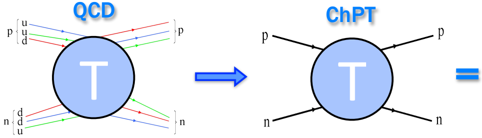
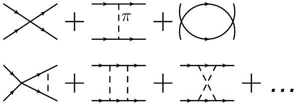






[H. Krebs]

Generate a nonrelativistic potential for many-body methods (not unique!!)

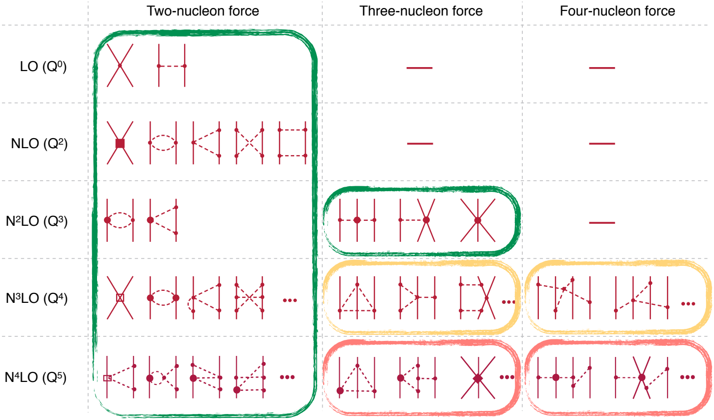
$$\left[\left(\sum_{i=1}^{A} \frac{-\vec{\nabla}_i^2}{2m_N} + \mathcal{O}(m_N^{-3})\right) + \underbrace{V_{2N} + V_{3N} + V_{4N} + \ldots}_{\textit{derived within ChPT}}\right]|\Psi\rangle = E|\Psi\rangle$$

Weinberg '91

Regulators can be local (depends on momentum transfer only) or non-local

Hierarchy of chiral forces with $Q = \{p, m_\pi\}/\Lambda_b$

[figs. from U. Meissner and E. Epelbaum]



worked out and applied   worked out and being applied   calculations in progress

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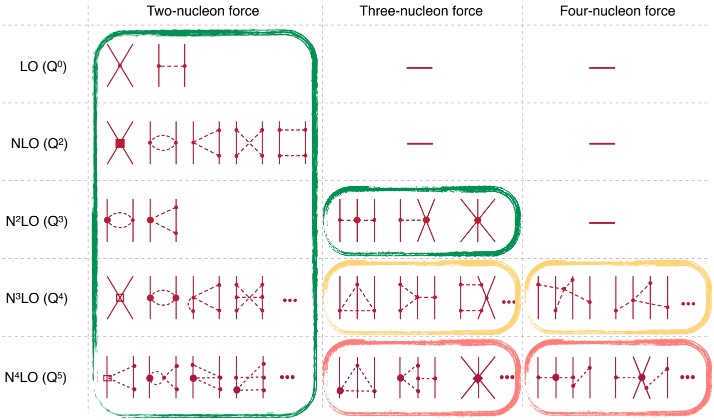

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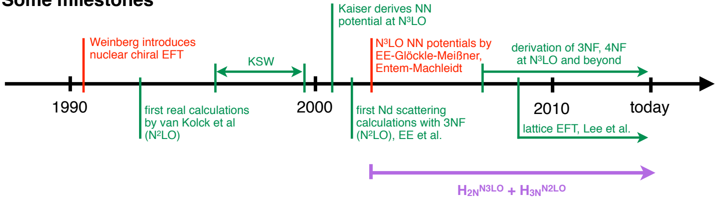
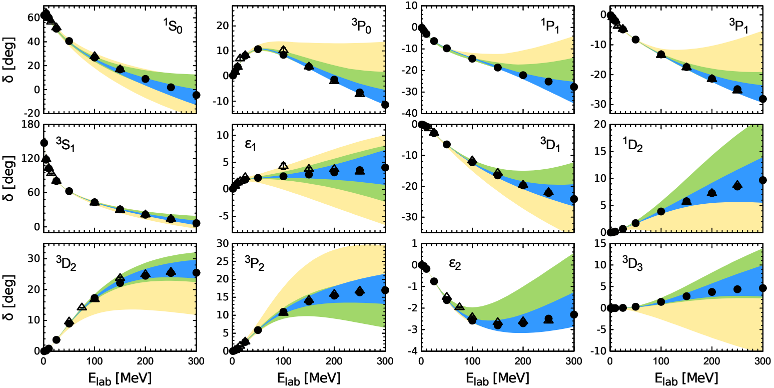
Some milestones



NN phase shifts with uncertainty bands, order-by-order



NLO N²LO N³LO

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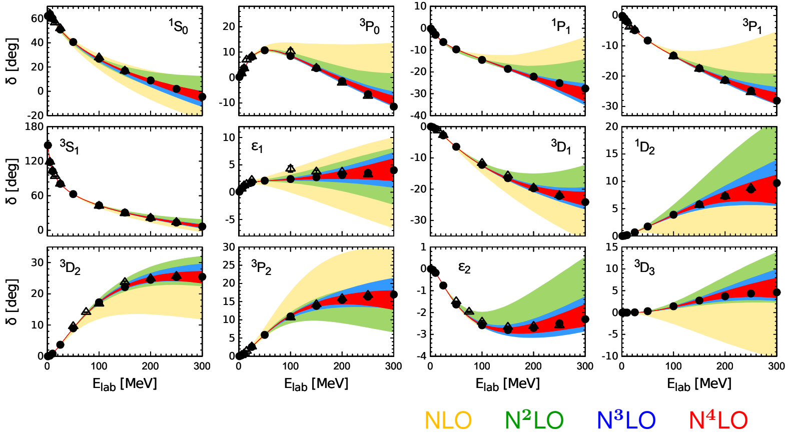
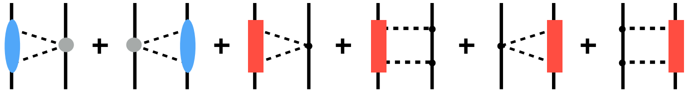




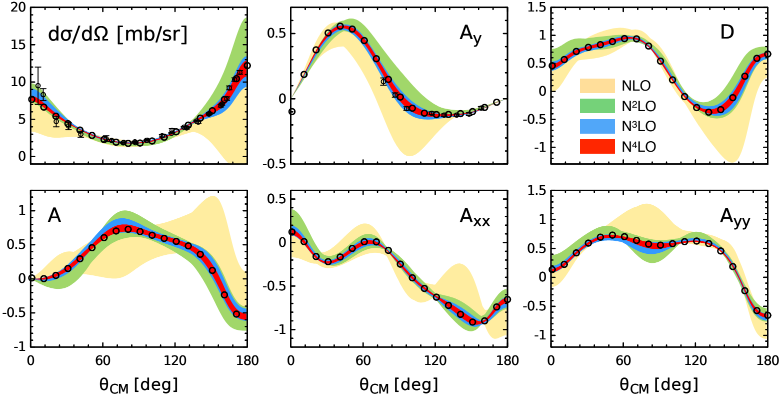
$$\mathcal{L}_{\pi N} = \mathcal{L}^{(1)}_{\pi N} + \mathcal{L}^{(2)}_{\pi N}(c_i) + \mathcal{L}^{(3)}_{\pi N}(d_i) + \mathcal{L}^{(4)}_{\pi N}(e_i)$$

c_i, d_i, e_i
from πN

EKM order-by-order improvement

Model validation: does chiral EFT work as expected? Yes!

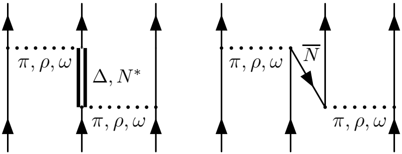
Selected neutron-proton scattering observables at 200 MeV R=0.9fm



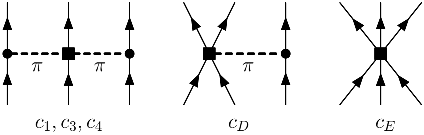
Clear improvement over earlier N^{3}LO potentials (non-local, mom. space)

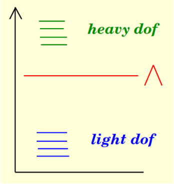
Origin of nuclear three-body forces

- Three-body forces arise from eliminating or decoupling dof's
  - excited states of nucleon
  - relativistic effects
  - high-energy intermediate states
- Possible problem: *N*–Δ mass splitting is only $\sim 300\,\mathrm{MeV}$!
  - Is this long- or short-distance physics?
  - Where should we draw the EFT line?



low ⇓ resolution





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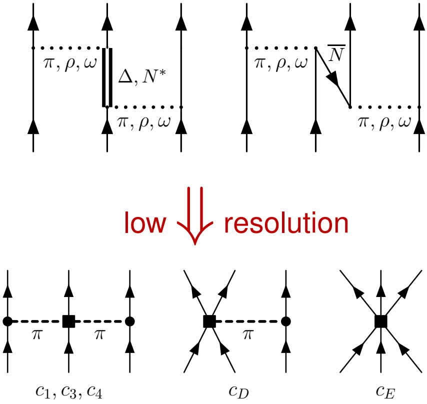
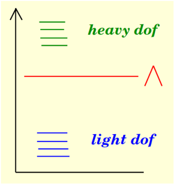
  - Where should we draw the EFT line?
- Scale and scheme dependent!
  - Need consistent NN$\leftrightarrow$NNN
  - What is best Λ for nuclei?

How do we change to $\Lambda < \Lambda_{\text{breakdown}}$ without degrading accuracy? RG!





Challenges for theory (a subset)

- More accurate Hamiltonians and current operators
- Uncertainty quantification (theory error bars)
- *Consistent* structure and reactions
- Implications of scale and scheme dependence

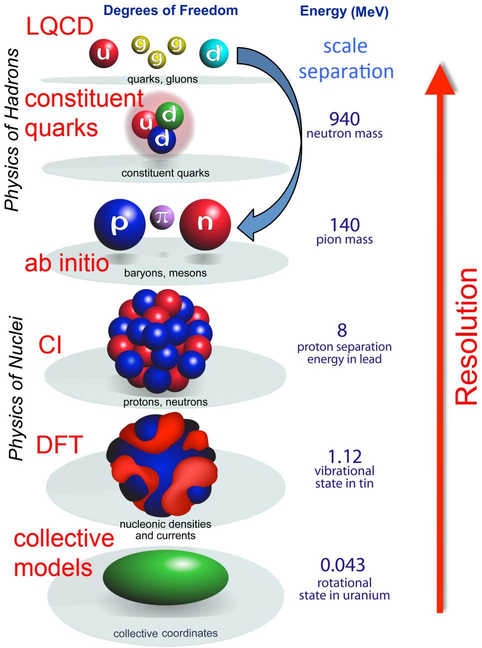
These are all tied together!

Others: computational challenges; chiral EFT with Δ's; connecting to LQCD; induced many-body forces; weak interactions; nuclei, dark matter, and wimps; fitting LECs; ab initio DFT; ...

Summary: Precision nuclear structure and reactions

We're in a golden age for low-energy nuclear physics

- Many complementary methods able to incorporate 3NFs, merge structure and reactions, . . .
- Synergies of analytic theory, computation, and experiment
- Large-scale collaborations facilitate progress
- Fully connected descriptions are within reach
- Many opportunities and challenges for precision physics!



Applying Bayesian methods to LEC estimation

Definitions: (Notation: $\mathrm{pr}(x|I)$ is the pdf of x being true given information I)

$\mathbf{a} \equiv$ vector of LECs $\Longrightarrow$ coefficients of an expansion $(a_0, a_1, \ldots)$

$D \equiv$ measured data (e.g., cross sections)

$I \equiv$ all background information (e.g., data errors, EFT details)

Bayes theorem: How knowledge of $\mathbf{a}$ is updated

$$\underbrace{\mathrm{pr}(\mathbf{a}|D,I)}_{\text{posterior}} = \underbrace{\mathrm{pr}(D|\mathbf{a},I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(\mathbf{a}|I)}_{\text{prior}} \;/\; \underbrace{\mathrm{pr}(D|I)}_{\text{evidence}}$$

The posterior lets us find the most probable values of parameters or the probability they fall in a specified range (“DoB intervals”)

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Bayesian rules of probability as principles of logic [Cox]

1. **Sum rule:** $\int dx\, \mathrm{pr}(x|I) = 1 \quad \longrightarrow \quad \underbrace{\mathrm{pr}(x|I) = \int dy\, \mathrm{pr}(x,y|I)}_{\text{marginalization}}$

2. **Product rule:** $\mathrm{pr}(x,y|I) = \mathrm{pr}(x|y,I)\,\mathrm{pr}(y|I) = \mathrm{pr}(y|x,I)\,\mathrm{pr}(x|I)$

$$\Longrightarrow \quad \mathrm{pr}(x|y,I) = \mathrm{pr}(y|x,I)\,\mathrm{pr}(x|I)/\mathrm{pr}(y|I) \quad (!)$$

Behavior of a χEFT series (particular example)

- Consider χEFT as an expansion in $Q = \{p, m_\pi\}/\Lambda_b$ with $\Lambda_b \approx 600\,\mathrm{MeV}$
- Take the example of an observable, X, whose terms are (with $Q \approx 0.35$):

$$X = 84.8 + 0 - 9.7 + 3.2 = 78.3$$

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- Rewrite as :

$$X = X_{\mathrm{LO}}\left[c_0 + c_1(0.35) + c_2(0.35)^2 + c_3(0.35)^3 + c_4(0.35)^4 + \cdots\right]$$

- We cannot know the result for c_4 before we compute it.
- Two questions:
  - What is the prior expectation for c_4?
  - In fact $\{c_n\} = \{1, 0, -0.92, 0.86\}$. What now is expectation for c_4?

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  - In fact $\{c_n\} = \{1, 0, -0.92, 0.86\}$. What now is expectation for c_4?
- One possibility: $c_4 = \max\{c_0, c_2, c_3\}$

Epelbaum, Krebs, Meißner (2015)
cf. McGovern, Griesshammer, Phillips (2013); many others

Estimating nuclear EFT truncation errors [rjf et al., PRC (2015)]

- Adapt Bayesian technology used in pQCD [Cacciari and Houdeau (2011)]

up to k^{th} order: $$\sigma_{\text{QCD}} \approx \sum_{n=0}^{k} c_n \alpha_s^n \quad \longrightarrow \quad \sigma_{np} \approx \sigma_{\text{ref}} \sum_{n=0}^{k} c_n \left(\frac{p}{\Lambda_b}\right)^n$$

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- Goal: find $\Delta_k \equiv \sum_{n=k+1}^{\infty} c_n z^n$ where $z = \alpha_s$ *or* p/Λ_b (or scaled)
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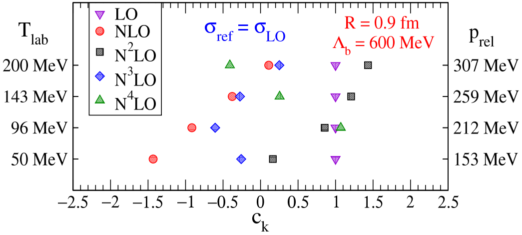
- Check whether c_n's have a bounded distribution for a chiral EFT observable: $\sigma_{np} \approx \sigma_0(c_0 + c_2 z^2 + c_3 z^3 + \cdots)$ with $z = p/600\,\text{MeV}$

- σ_{np} from EKM at $R = 0.9\,\text{fm}$
- Coefficients at four energies
- z from about 1/4 to 1/2
- Natural: $c_n \sim \mathcal{O}(1)$

$\Longrightarrow$ apply as Bayesian priors on c_n, $\bar{c}$



Model for EFT expansion [Schindler/Phillips, (2009)]

"Real world": $g(x) = (1/2 + \tan(\pi x/2))^2$

"Model" $\approx 0.25 + 1.57x + 2.47x^2 + \mathcal{O}(x^3)$
with gaussian noise (5% relative error)

Goal: estimate $\mathbf{a} = \{a_0, a_1, a_2, \cdots\}$

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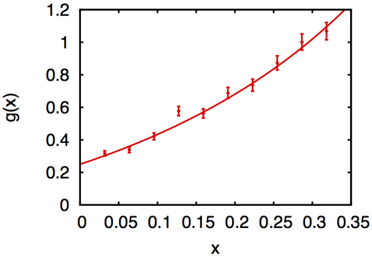

[and many other examples in BUQEYEs arXiv:1511.03618]

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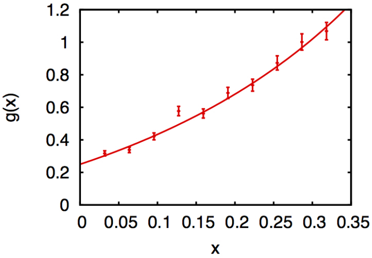

[and many other examples in BUQEYEs arXiv:1511.03618]

Parameter estimation for LECs: given data on g over a range of x, how best to determine the a_i using *all* the data?

- Fit range: manage trade-off between more data (decreased statistical error) and importance of higher orders (increased truncation error)
- Truncated expansion only describes data in limited range
- What order should we use? Too low could underfit (too few terms to describe given data); too high could overfit (too many terms given data).

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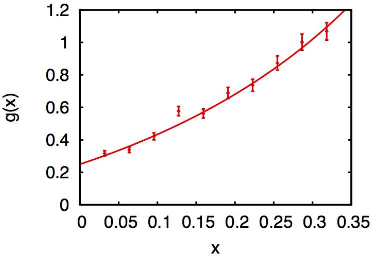

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Compare: $\text{pr}(\mathbf{a}|D, I) \propto \text{pr}(D|\mathbf{a}, I)\,\text{pr}(\mathbf{a}|I)$ with

$a)$ $\text{pr}(\mathbf{a}|I) \propto$ constant

$b)$ $\text{pr}(\mathbf{a}|\bar{a}, I) =$ a prior for natural coefficients (e.g., gaussian)

$\Longrightarrow$ $a)$ $\text{pr}(\mathbf{a}|D, I) \propto e^{-\chi^2/2}$ [uniform prior ($\equiv$ least-squares)]

$\Longrightarrow$ $b)$ $\text{pr}(\mathbf{a}|D, I) \propto e^{-\chi^2/2} \times \left(\prod_{k=0}^{k_{\max}} \frac{1}{\sqrt{2\pi}\bar{a}}\right) \exp\left(-\frac{\mathbf{a}^2}{2\bar{a}^2}\right)$ [naturalness prior]

Comparing results for uniform and naturalness priors

Find the maximum of the posterior distribution and its width to find coefficients and uncertainties as a function of the order ($k_{\max}$)

uniform prior

$k_{\max}$	χ^2/dof	a_0	a_1	a_2
true		0.25	1.57	2.47
1	2.2	0.20 ± 0.01	2.6 ± 0.1	
2	1.6	0.25 ± 0.02	1.6 ± 0.4	3.3 ± 1.3
3	1.9	0.27 ± 0.04	1.0 ± 1	8.1 ± 8.0
4	2.0	0.33 ± 0.07	-1.9 ± 3	45 ± 30
5	1.4	0.57 ± 0.3	-15 ± 7	280 ± 100

- Highly unstable for order $k > 2$
- Errors large and unstable
- But χ^2/dof is ok!

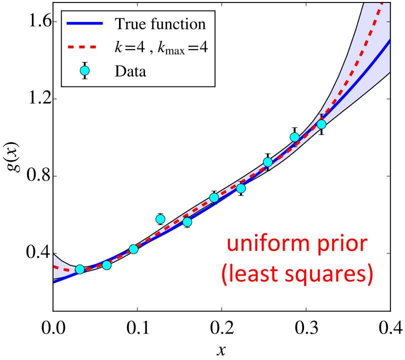
naturalness prior

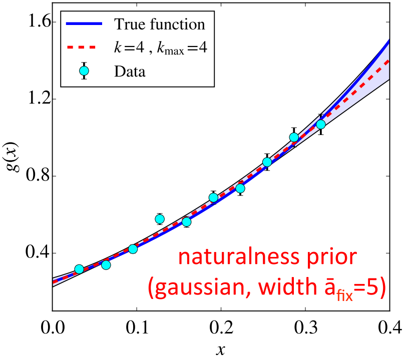
$k_{\max}$	a_0	a_1	a_2
true	0.25	1.57	2.47
1	0.20 ± 0.01	2.6 ± 0.1	
2	0.25 ± 0.02	1.6 ± 0.4	3.1 ± 1
3	0.25 ± 0.02	1.7 ± 0.5	3.0 ± 2
4	0.25 ± 0.02	1.7 ± 0.5	3.0 ± 2
5	0.25 ± 0.02	1.7 ± 0.5	3.0 ± 2

- Stable with order *and* $x_{\max}$!
- Errors are reasonable
- Saturated at $k_{\max} = 2$

Comparing results for uniform and naturalness priors

Find the maximum of the posterior distribution and its width to find coefficients and uncertainties as a function of the order ($k_{\max}$)





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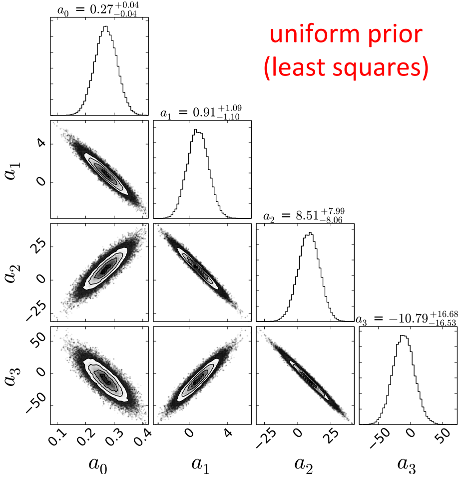
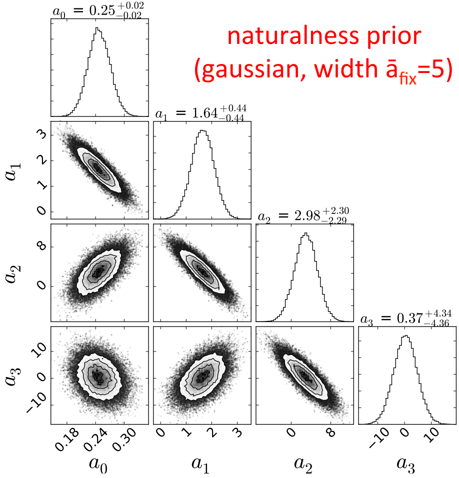


uniform prior (least squares)



naturalness prior (gaussian, width $\bar{a}_{\mathrm{fix}}$=5)

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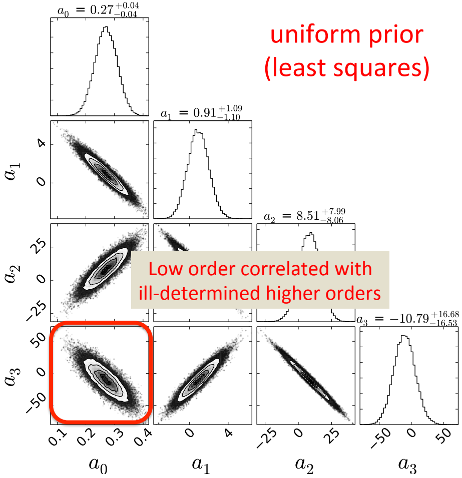

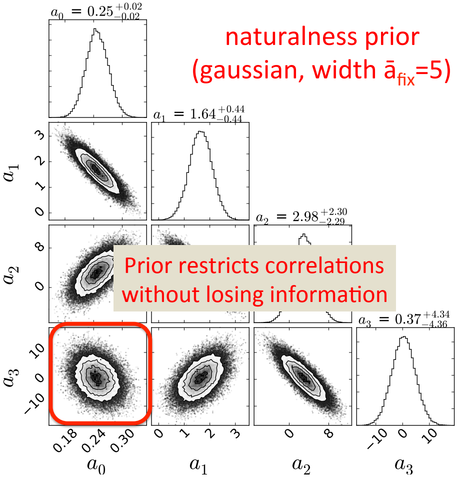

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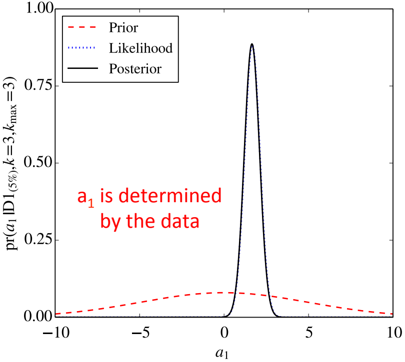
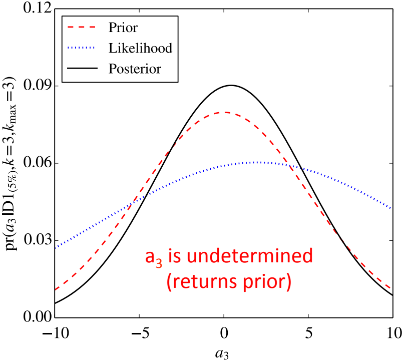


Prior much wider than likelihood.



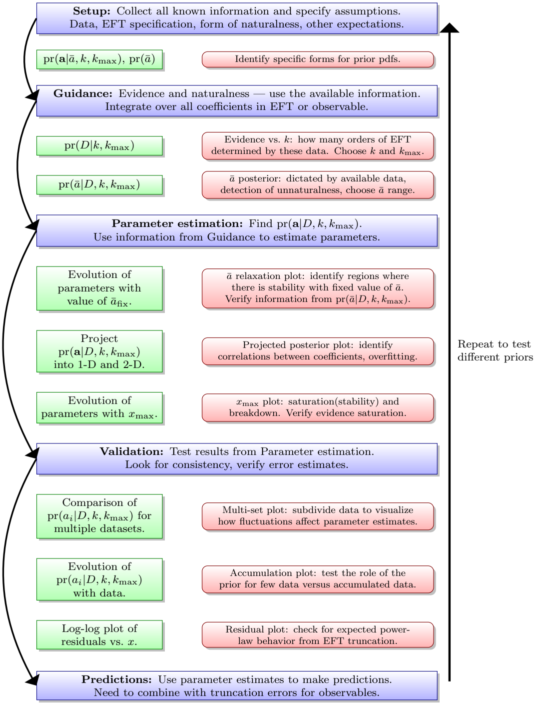
Likelihood much wider than prior.

Questions about the fit

- What $\bar{a}$ should we choose?
- To what order should we fit?
- Does the range of data we choose to fit make a difference?
- Do other functional forms for the prior alter the result?
- How do we know if this result is typical?
- What is the interplay of the prior and the data?
- Is the EFT working "as advertised"?

A diagnostic for each question!

[see arXiv:1511.03618]



Bayesian model selection

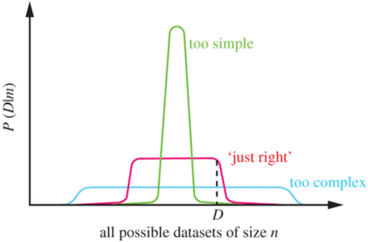
Determine the evidence for different models M_1 and M_2 via marginalization by integrating over possible sets of parameters **a** in different models, same D and information I.

The evidence ratio for two different models:

$$\frac{\mathrm{pr}(M_2|D,I)}{\mathrm{pr}(M_1|D,I)} = \frac{\mathrm{pr}(D|M_2,I)\,\mathrm{pr}(M_2|I)}{\mathrm{pr}(D|M_1,I)\,\mathrm{pr}(M_1|I)}$$

The Bayes Ratio: implements Occam's Razor

$$\frac{\mathrm{pr}(D|M_2,I)}{\mathrm{pr}(D|M_1,I)} = \frac{\int \mathrm{pr}(D|\mathbf{a}_2,M_2,I)\,\mathrm{pr}(\mathbf{a}_2|M_2,I)\,d\mathbf{a}_2}{\int \mathrm{pr}(D|\mathbf{a}_1,M_1,I)\,\mathrm{pr}(\mathbf{a}_1|M_1,I)\,d\mathbf{a}_1}$$



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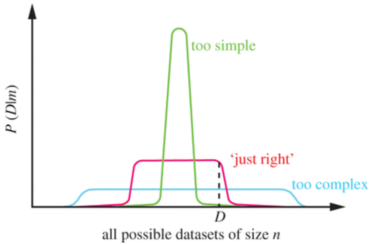
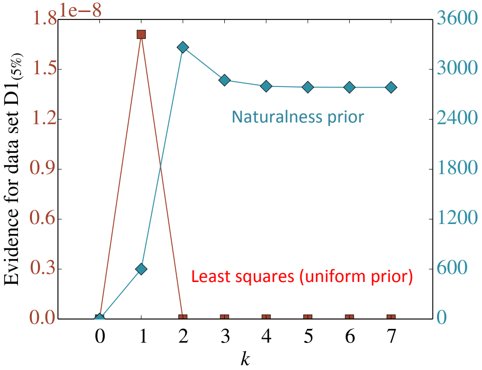


- Note these are integrations over *all* parameters a_n; not comparing fits!
- If the model is too simple, the particular dataset is very unlikely
- If the model is too complex, the model has too much "phase space"

Evidence for an EFT expansion (in z^k)

$$\frac{\int \mathrm{pr}(D|\mathbf{a}_2, M_2, I)\, \mathrm{pr}(\mathbf{a}_2|M_2, I)\, d\mathbf{a}_2}{\int \mathrm{pr}(D|\mathbf{a}_1, M_1, I)\, \mathrm{pr}(\mathbf{a}_1|M_1, I)\, d\mathbf{a}_1}$$

- Suppose M_2 is a higher-order version of M_1 EFT expansion
- Uniform prior exhibits an "Occam Peak" at order $k = 1$
- But naturalness prior shows *saturation* at greater $k = 2$
- See arXiv:1511.03618 for derivation of saturation



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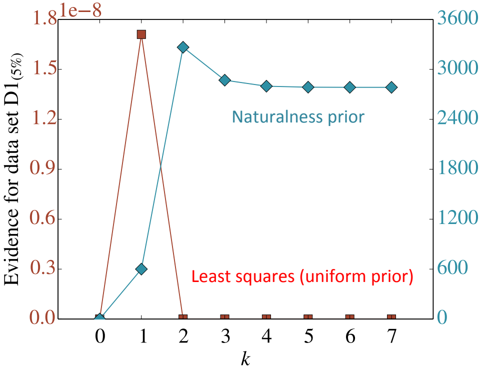

Examples of how we could use this in EFT context:

- Guidance for parameter estimation: How many a_ns from given data?
- Which EFT power counting is more effective? (cf. more parameters)
- Pionless vs. Δ-less χEFT vs. Δ-ful χEFT?