Ab initio nuclear physics with chiral EFT

Andreas Ekström (UT/ORNL)

Progress in Ab Initio Techniques in Nuclear Physics
February 23-26, 2016, TRIUMF, Vancouver, BC, Canada

Overview

- *Simultaneous optimization*
- *UQ applied to proton-proton fusion*
- *Chiral EFT tailored to the HO-basis*
- *Optimizing the 3NF at N3LO*

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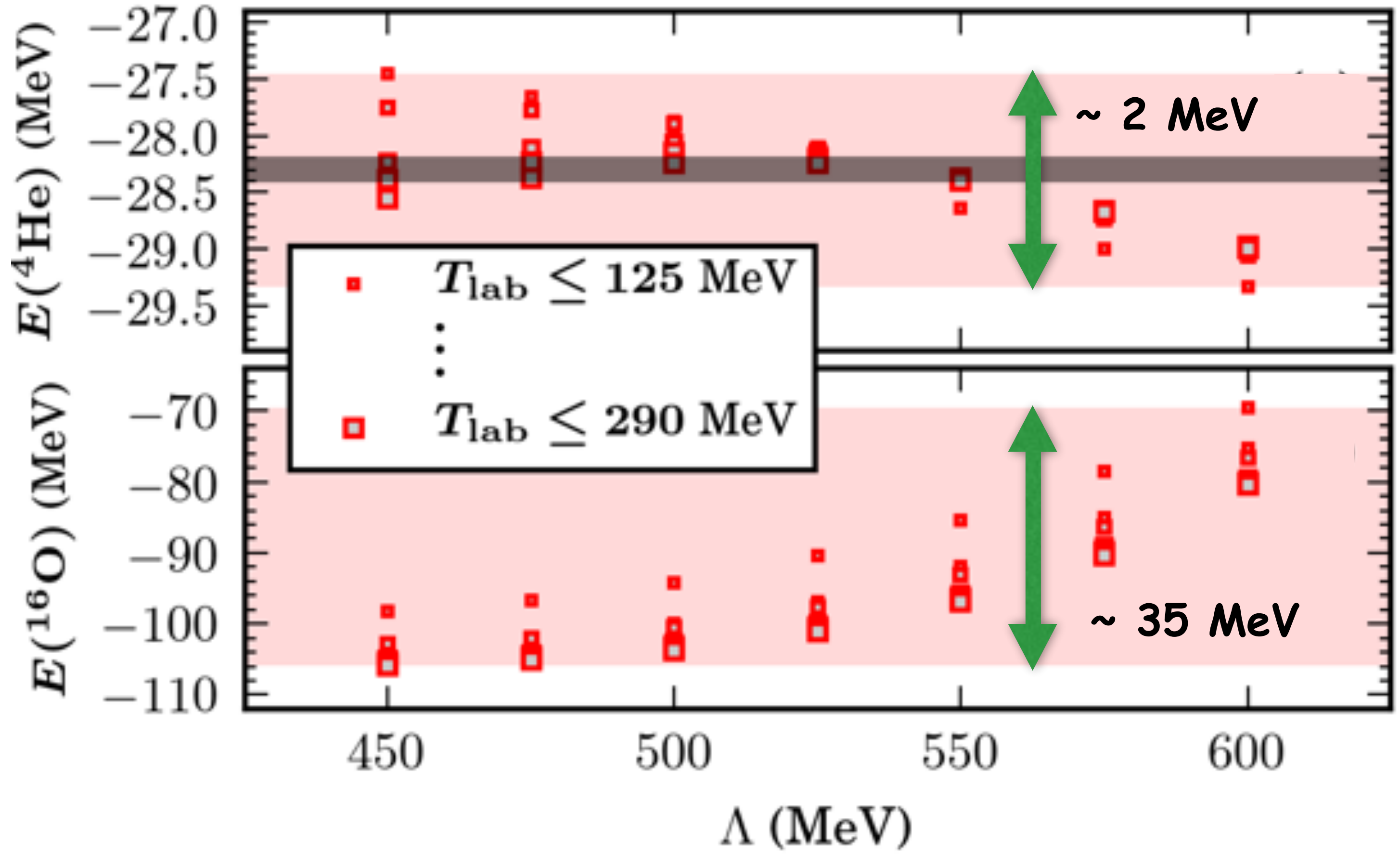

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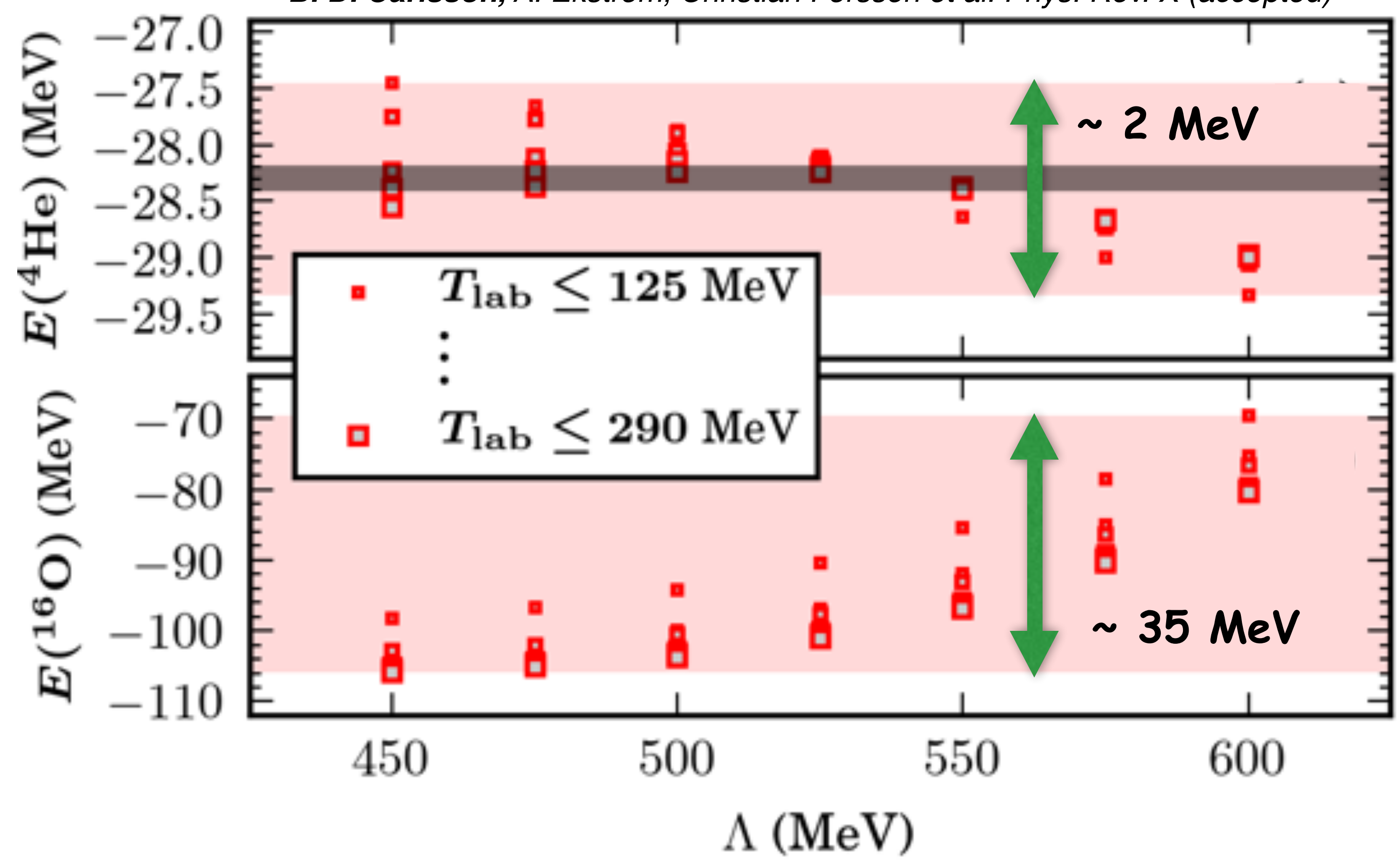

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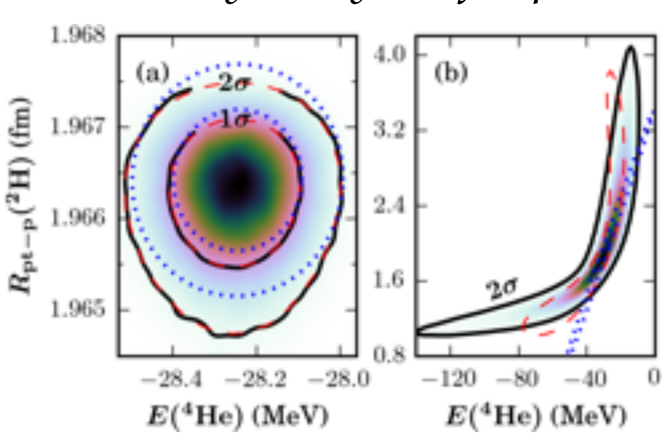

Robust parameter estimation
Three-nucleon scattering data.
The information content of heavy nuclei.
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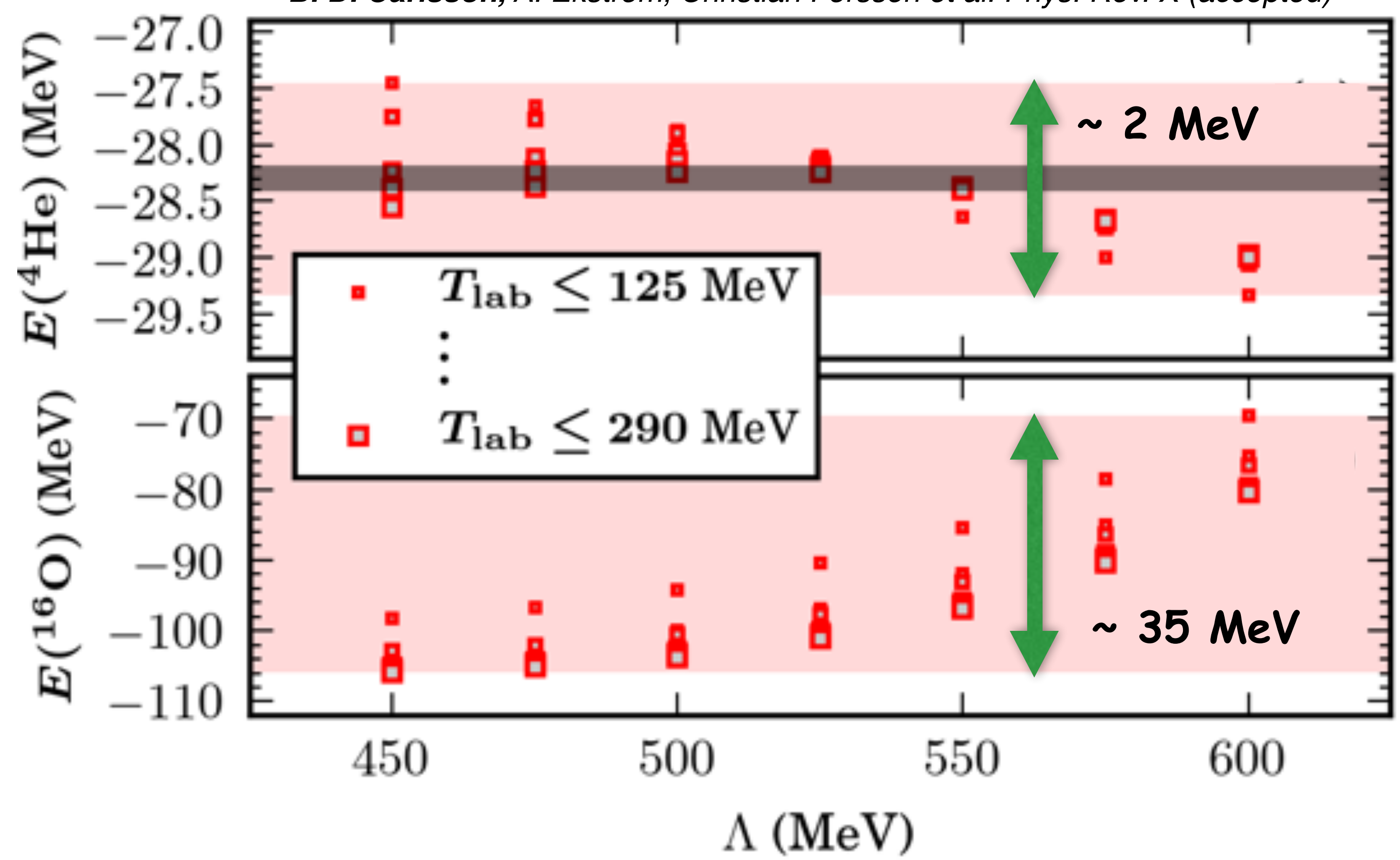

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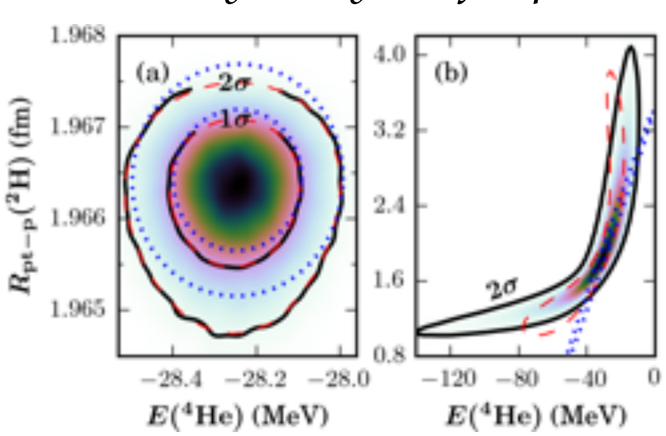

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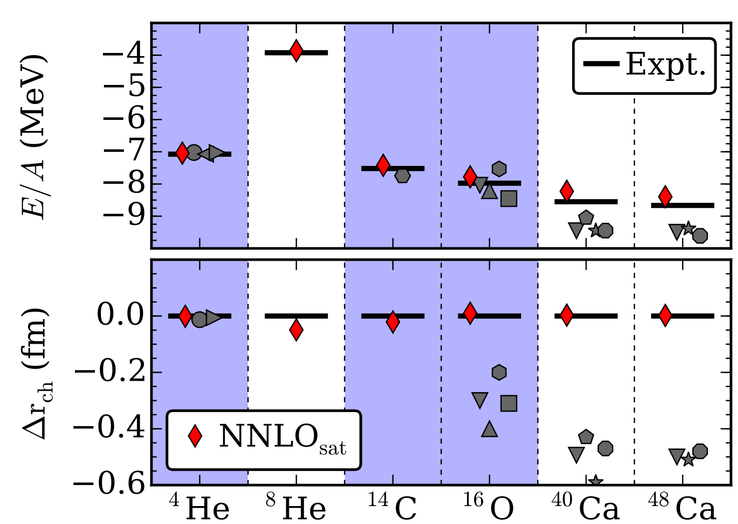

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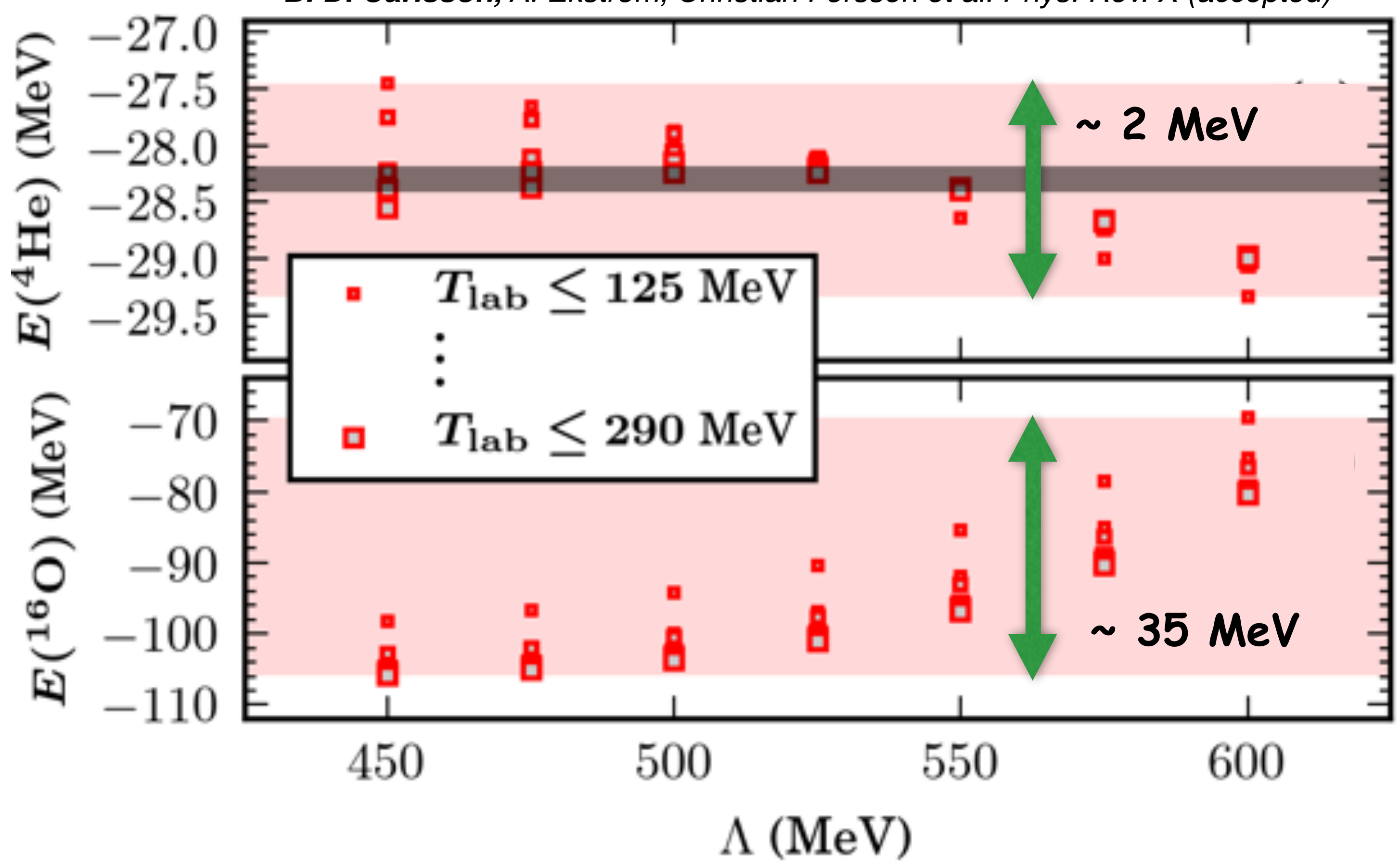

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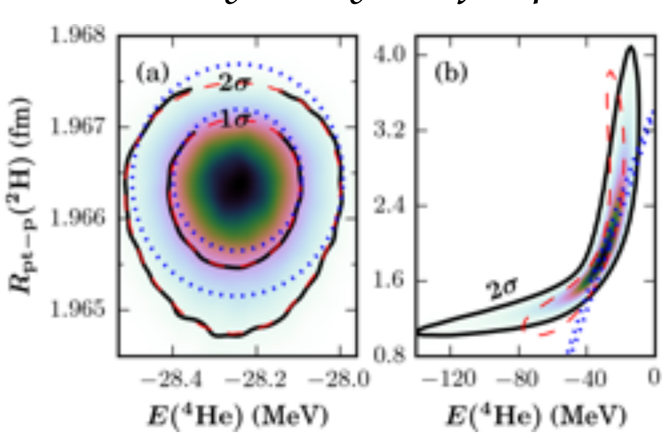

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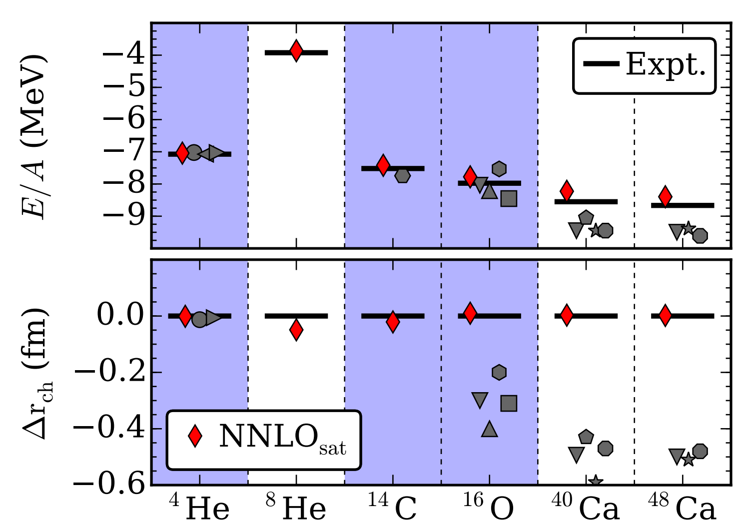
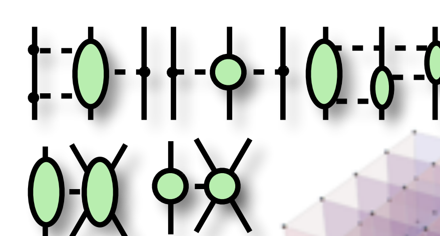
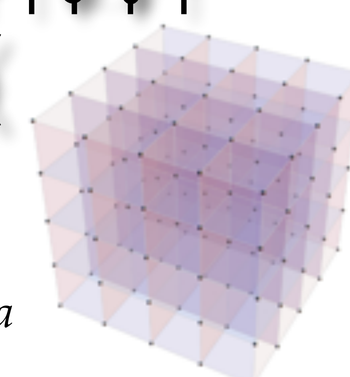


3. *Continue efforts towards higher orders of the chiral expansion, and possibly revisit the power counting.*

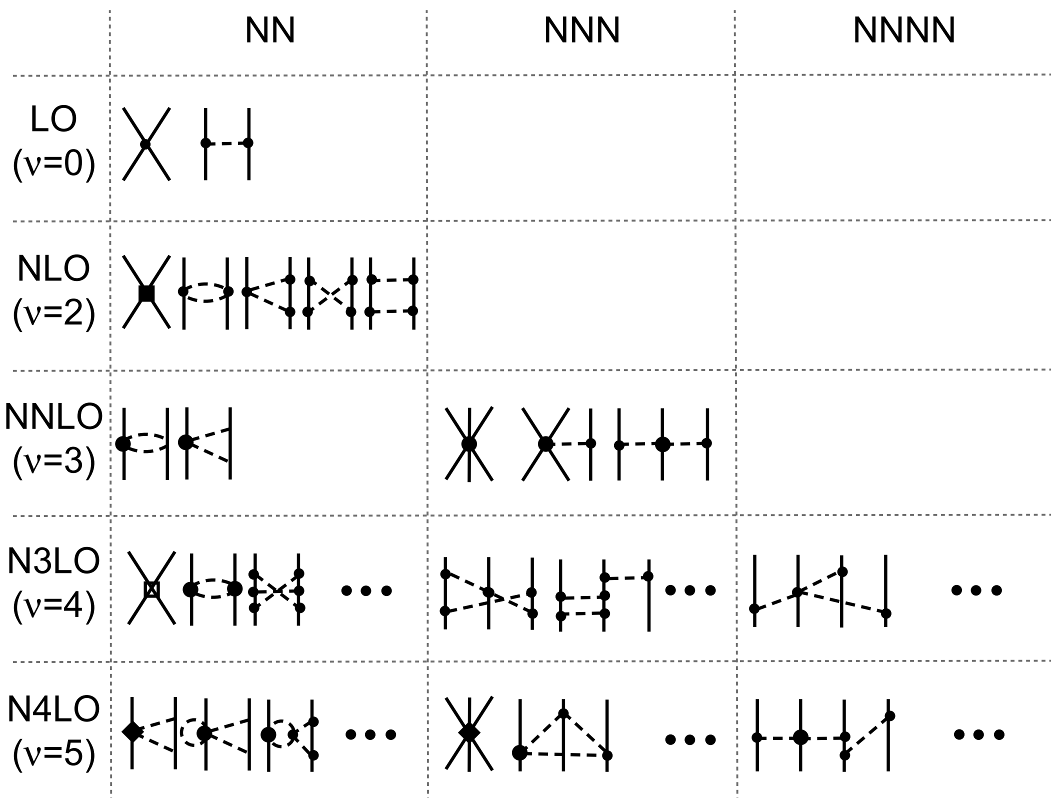




Delta resonances
Other regulators
Lattice QCD data
Modified PC
…

Simultaneous optimization

chiral EFT is our tool to analyze the nuclear interaction



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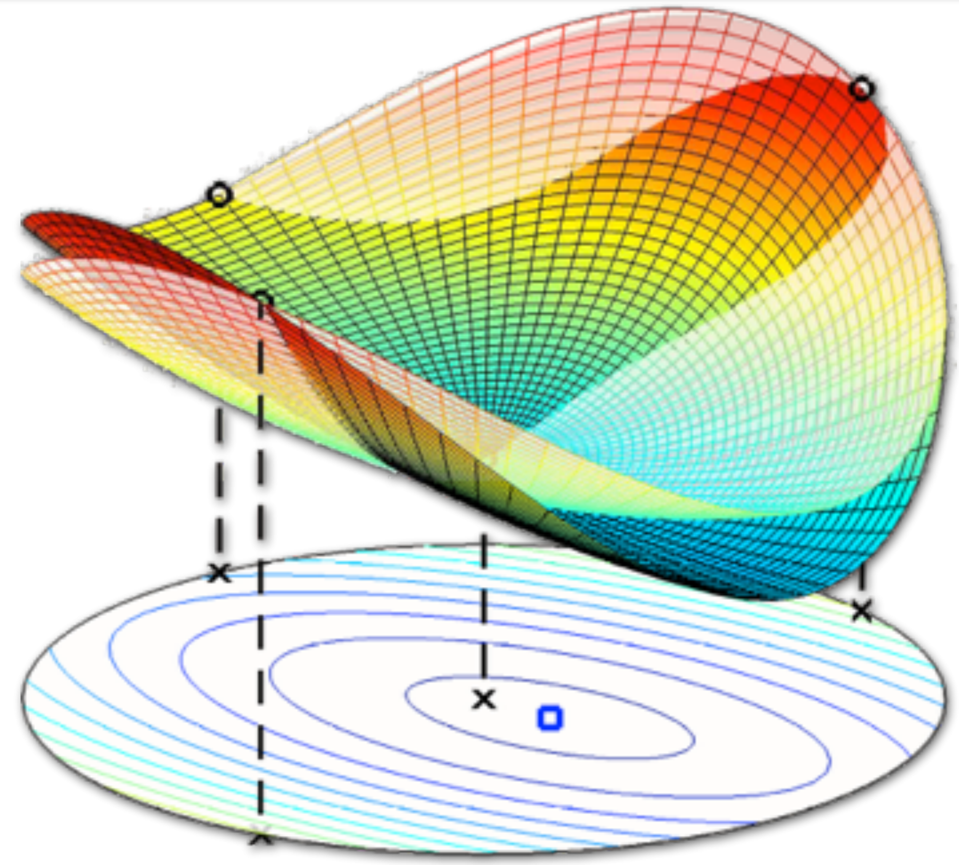

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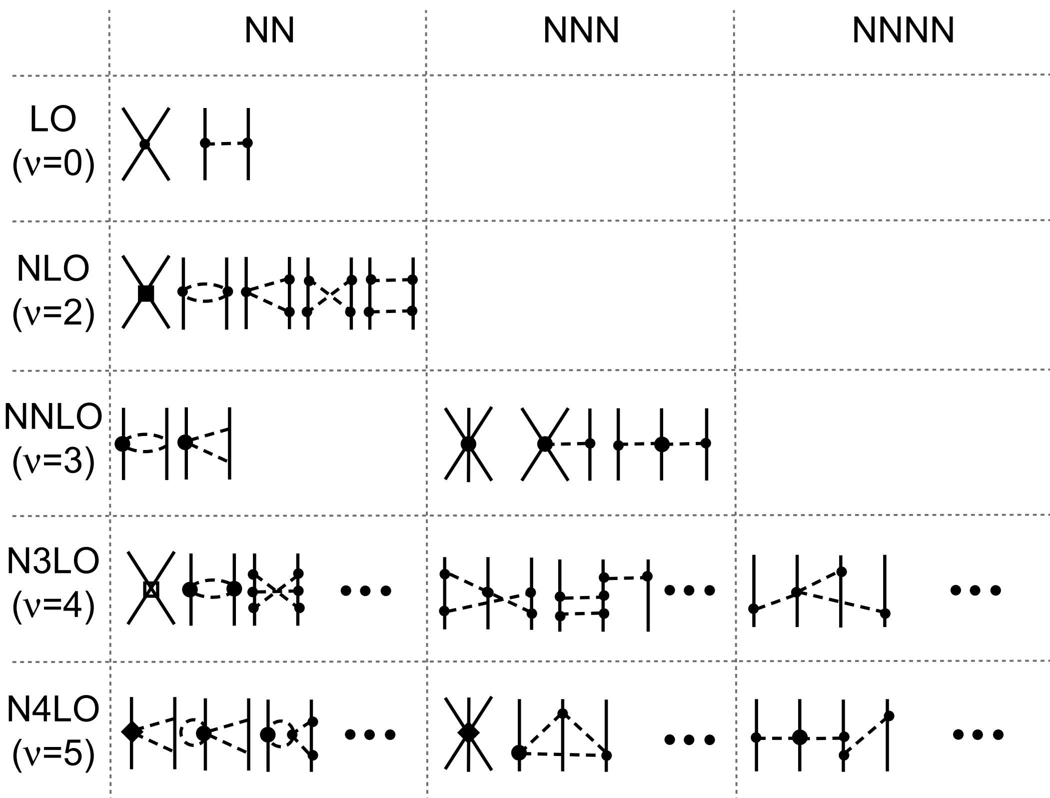

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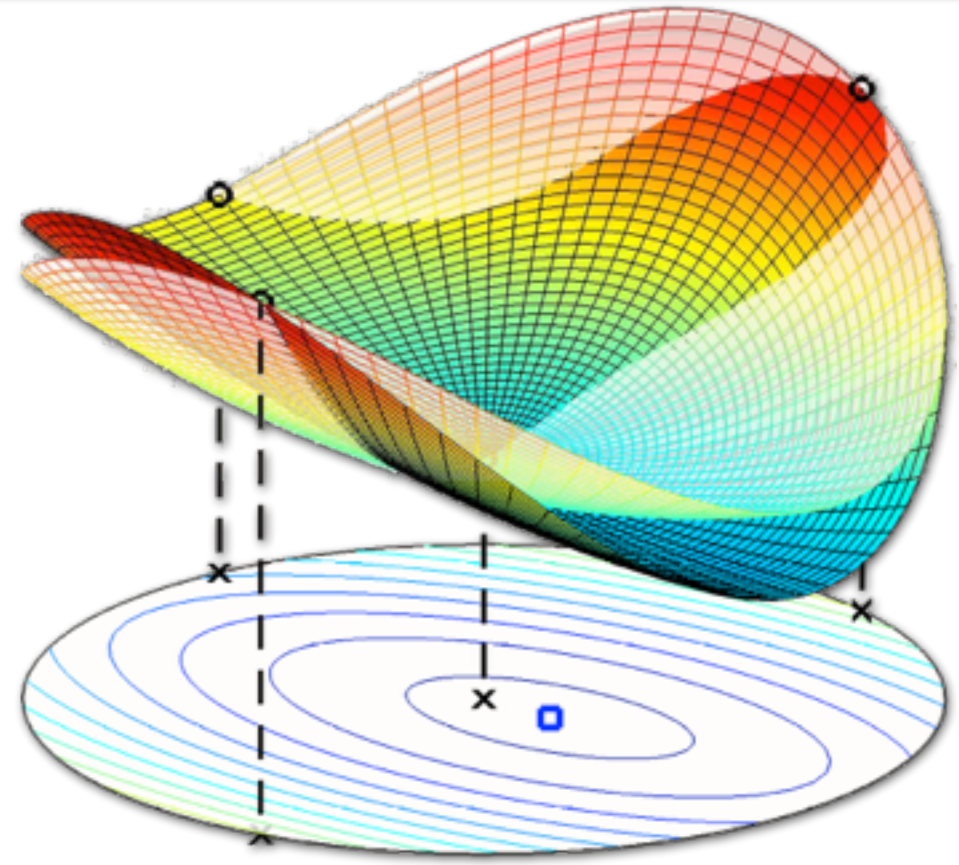

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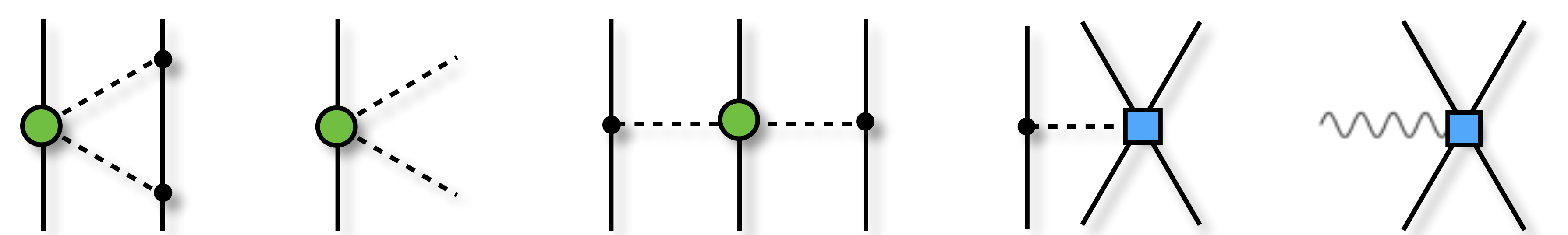

two-nucleon interaction | pion-nucleon scattering | three-nucleon interaction | three-nucleon interaction | external probe current

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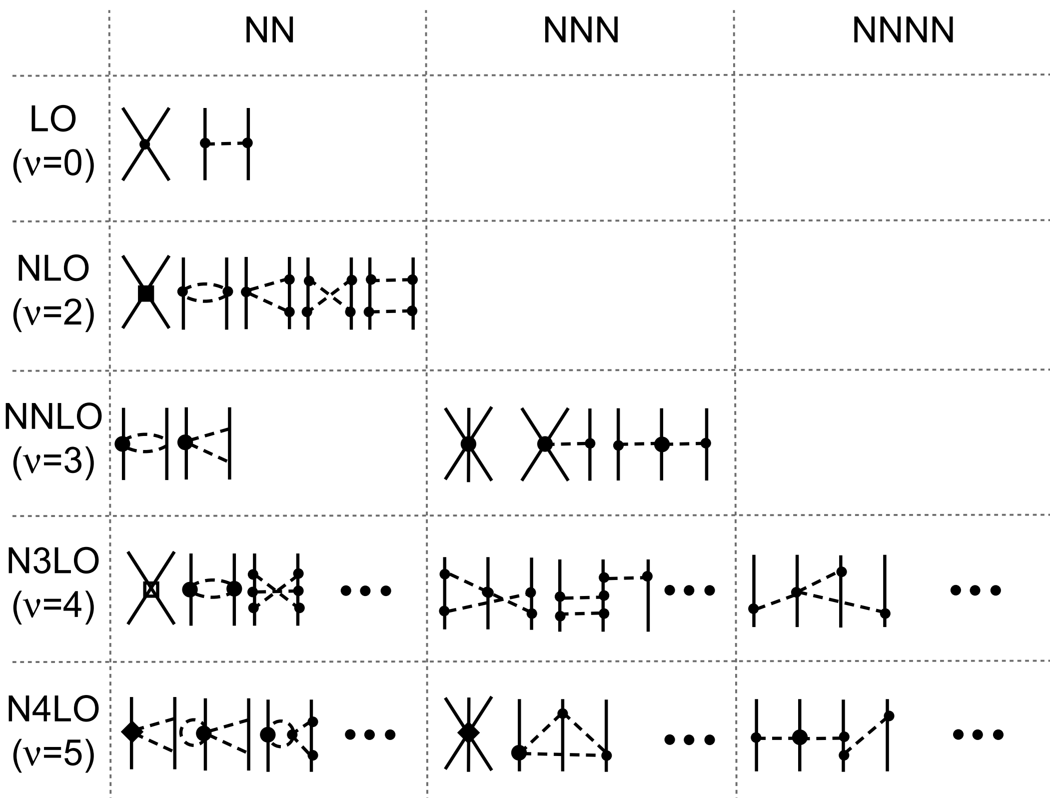

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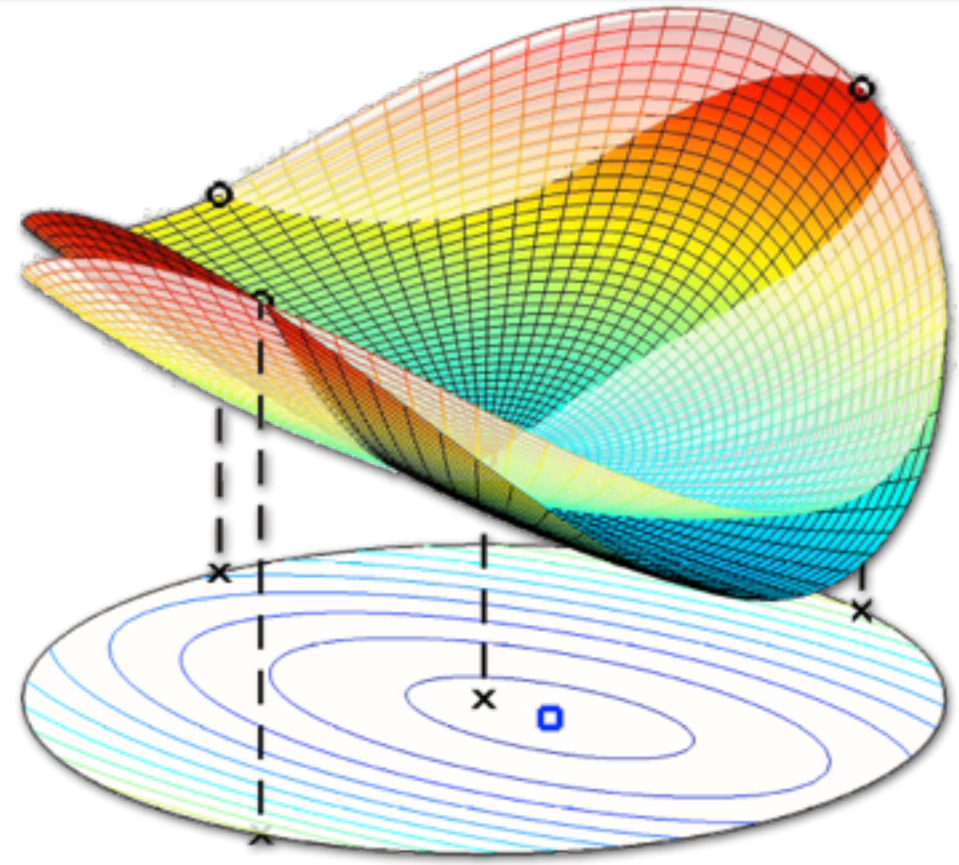

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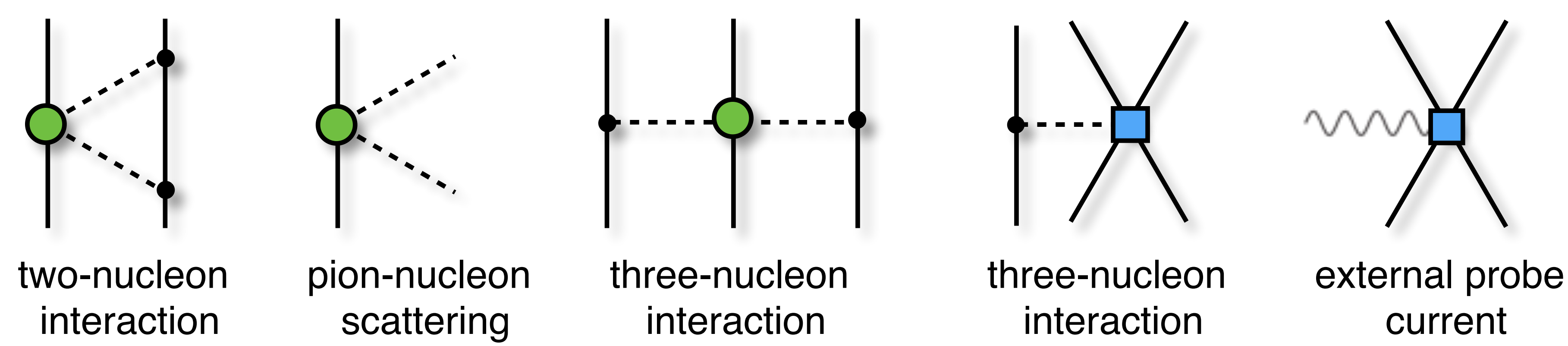

$$\chi^2(\mathbf{p}) \equiv \sum_{i\in\mathbb{M}} R_i^2(\mathbf{p}) = \sum_{k\in\pi\mathrm{N}} R_k^2(\mathbf{p}) + \sum_{j\in\mathrm{NN}} R_j^2(\mathbf{p}) + \sum_{l\in\mathrm{NNN}} R_l^2(\mathbf{p})$$

UQ with $N2LO_{sim}$

Simultaneous optimization is critical in order to

- find the optimal set of LECs.
- capture all relevant correlations between them.
- reduce the statistical uncertainty.
- attain order-by-order convergence.

Within such an approach we find that statistical errors are, in general, small, and that the total error budget is dominated by systematic errors.

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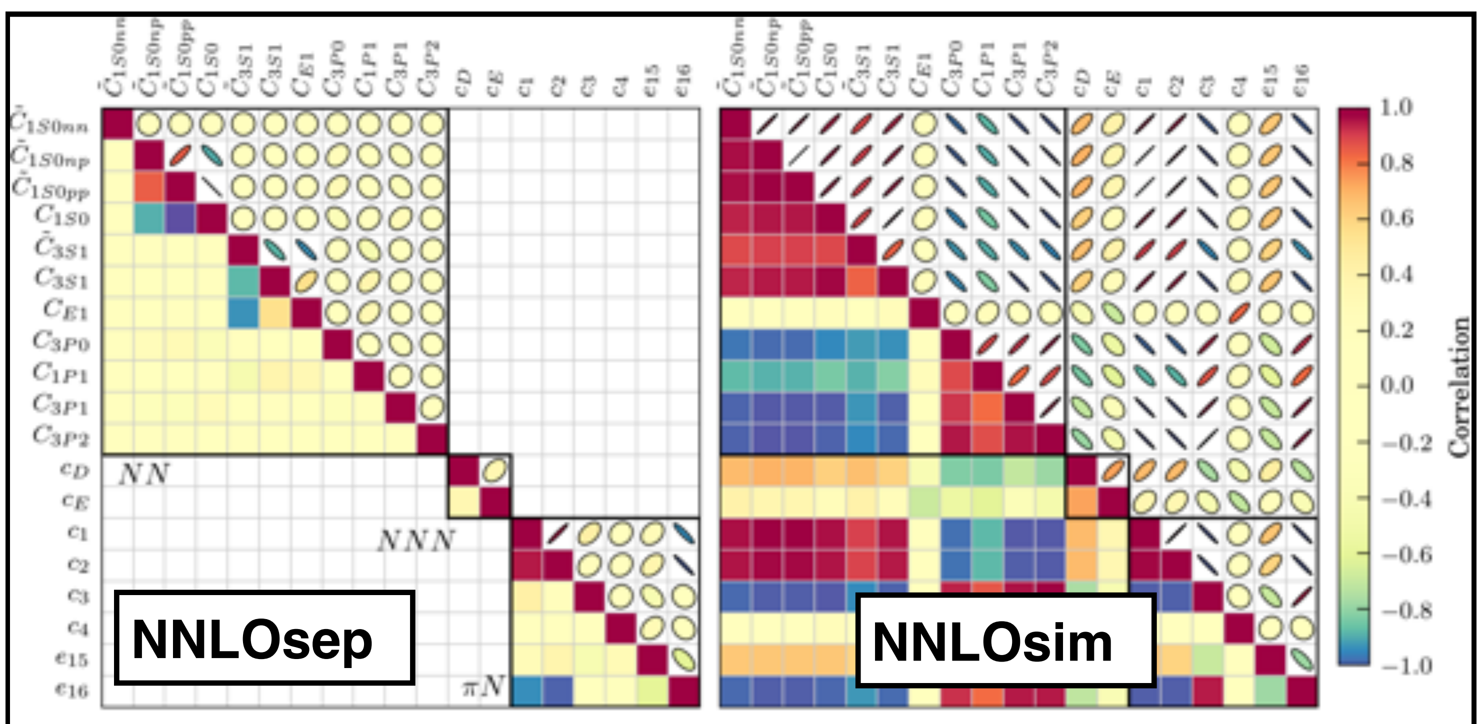

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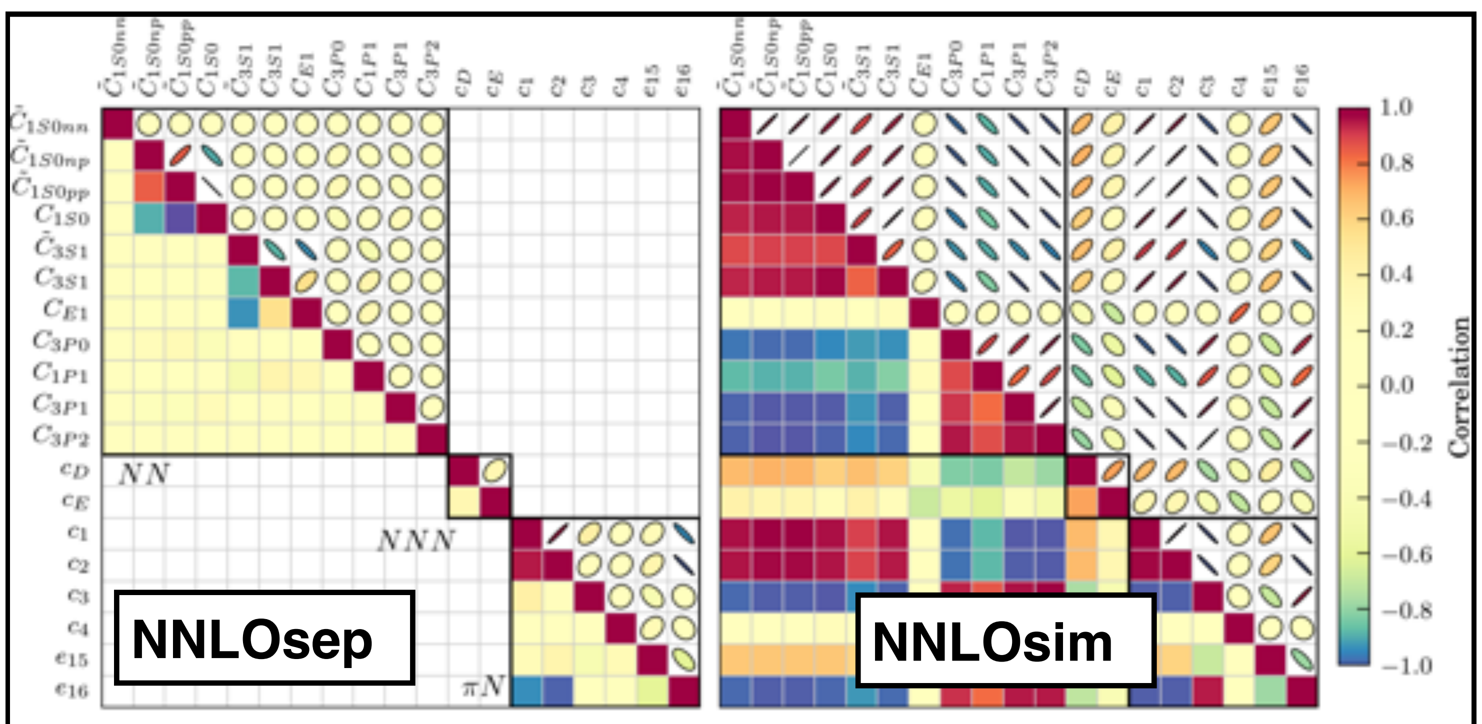

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All 42 different sim/sep potentials, as well as the respective covariance matrices are available as supplemental material.

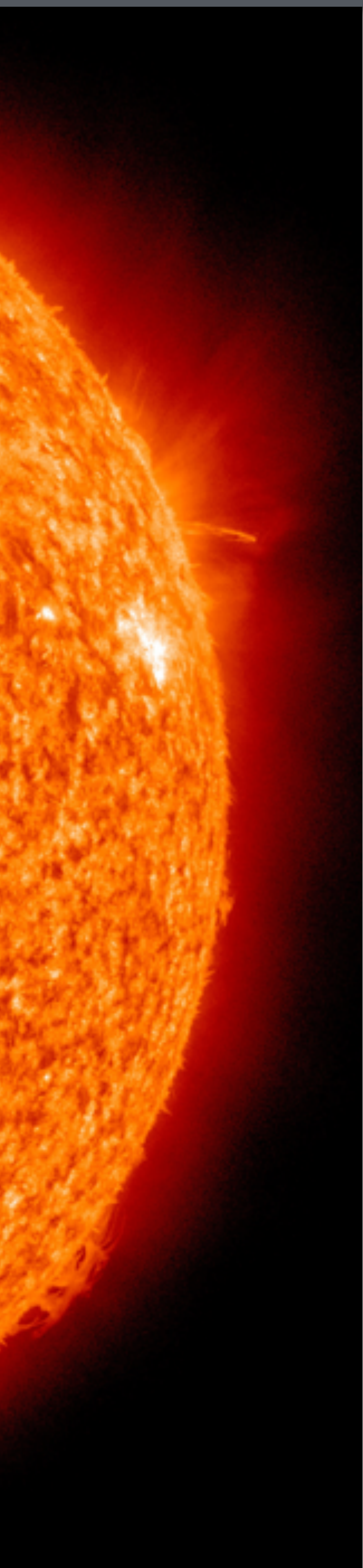
LO-NLO-NNLO
7 different cutoffs: 450,475,..,600 MeV
6 different NN-scattering datasets

$$\begin{aligned}\mathrm{Cov}(\mathrm{A},\mathrm{B}) &\equiv \mathbb{E}[(\mathcal{O}_\mathrm{A}(\mathbf{p})-\mathbb{E}[\mathcal{O}_\mathrm{A}(\mathbf{p})])(\mathcal{O}_\mathrm{B}(\mathbf{p})-\mathbb{E}[\mathcal{O}_\mathrm{B}(\mathbf{p})])]\\ &\approx \mathbb{E}[(\tilde{J}_{A,i}x_i + \frac{1}{2}\tilde{H}_{A,ij}x_ix_j - \frac{1}{2}\tilde{H}_{A,ii}\sigma_i^2)\\ &\times(\tilde{J}_{B,k}x_k + \frac{1}{2}\tilde{H}_{B,kl}x_kx_l - \frac{1}{2}\tilde{H}_{B,kk}\sigma_k^2)]\\ &= \tilde{\mathbf{J}}_A^T\mathbf{\Sigma}\tilde{\mathbf{J}}_B + \frac{1}{2}(\boldsymbol{\sigma}^2)^T(\tilde{\mathbf{H}}_A\circ\tilde{\mathbf{H}}_B)\boldsymbol{\sigma}^2,\end{aligned}$$

compute the derivatives of your own observables wrt LECs, then explore:

- ***cutoff variations***
- ***order-by-order evolution***
- ***LEC UQ/correlations***

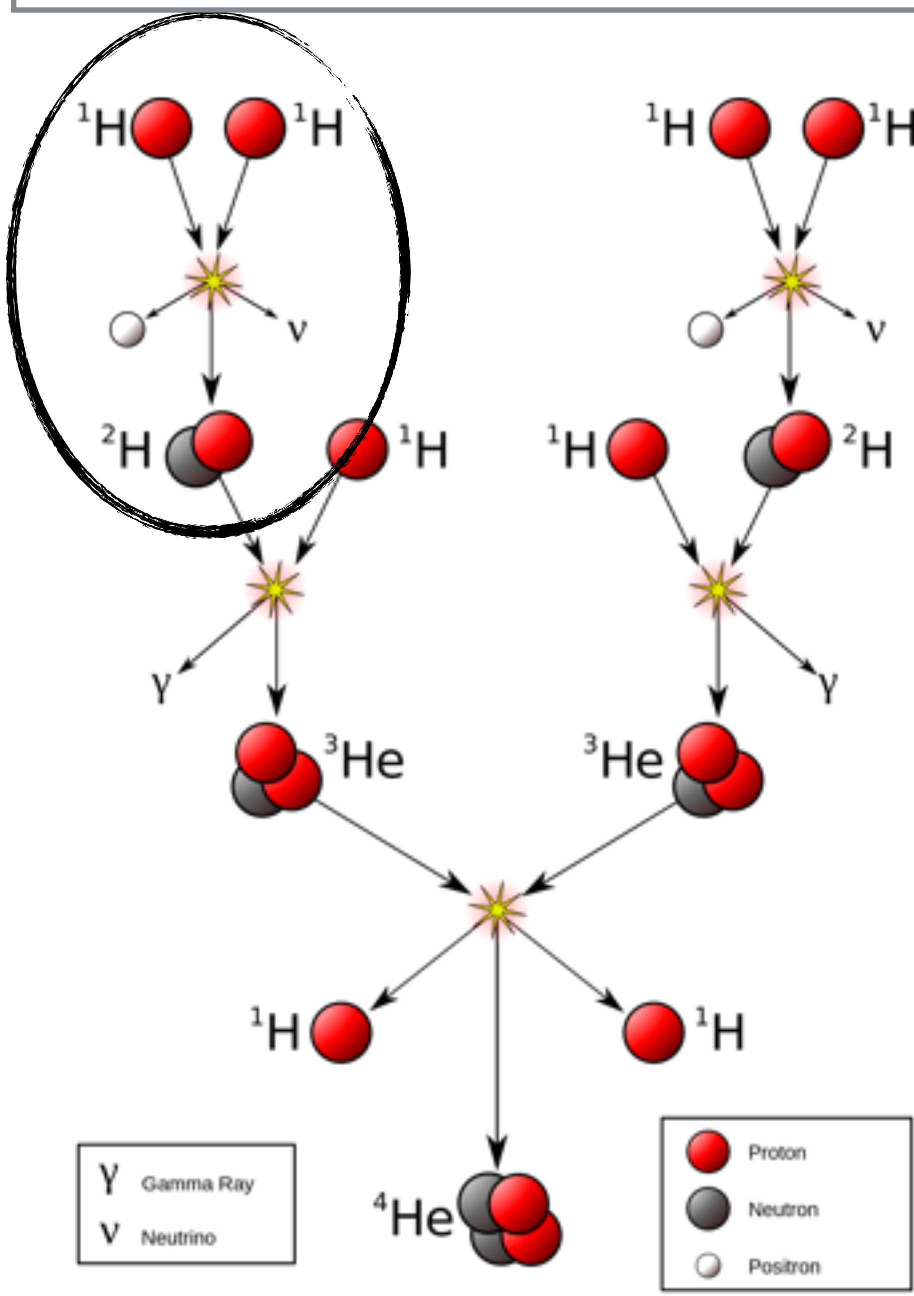
UQ applied to proton-proton fusion



In the core of the Sun, energy is released through sequences of nuclear reactions that convert hydrogen into helium. The primary reaction is thought to be the fusion of two protons with the emission of a low-energy neutrino and a positron.

$$p + p \rightarrow d + e^{+} + \nu_e$$
$$S(E) = \sigma(E) E e^{2\pi\eta}$$

$$\sigma(E) = \int \frac{d^3 p_e}{(2\pi)^3} \frac{d^3 p_\nu}{(2\pi)^3} \frac{1}{2E_e} \frac{1}{2E_\nu} \times$$
$$2\pi\delta\left(E + 2m_p - m_d - \frac{q^2}{2m_d} - E_e - E_\nu\right)$$
$$\frac{1}{v_{rel}} F(Z, E_e) \frac{1}{4} \sum |\langle f | \hat{H}_W | i \rangle|^2$$



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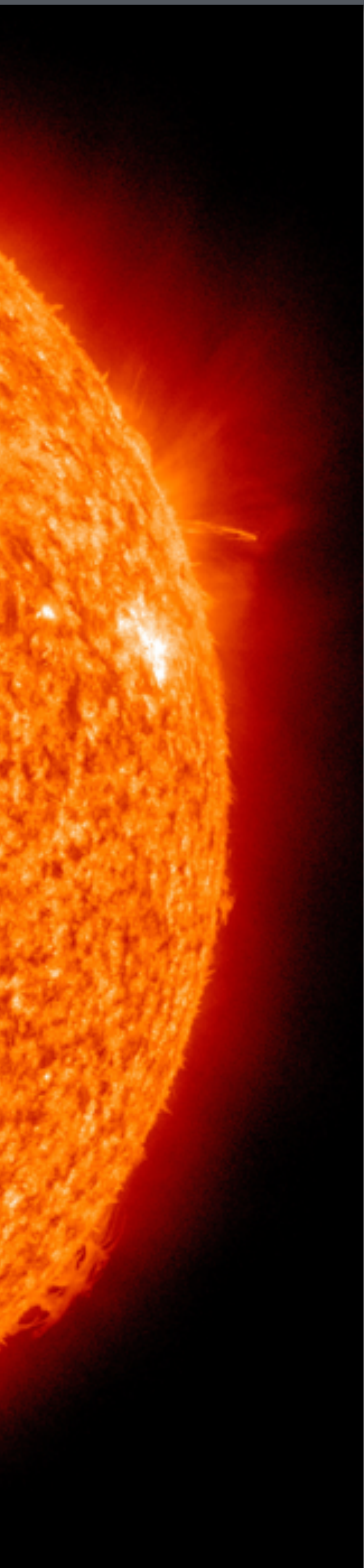

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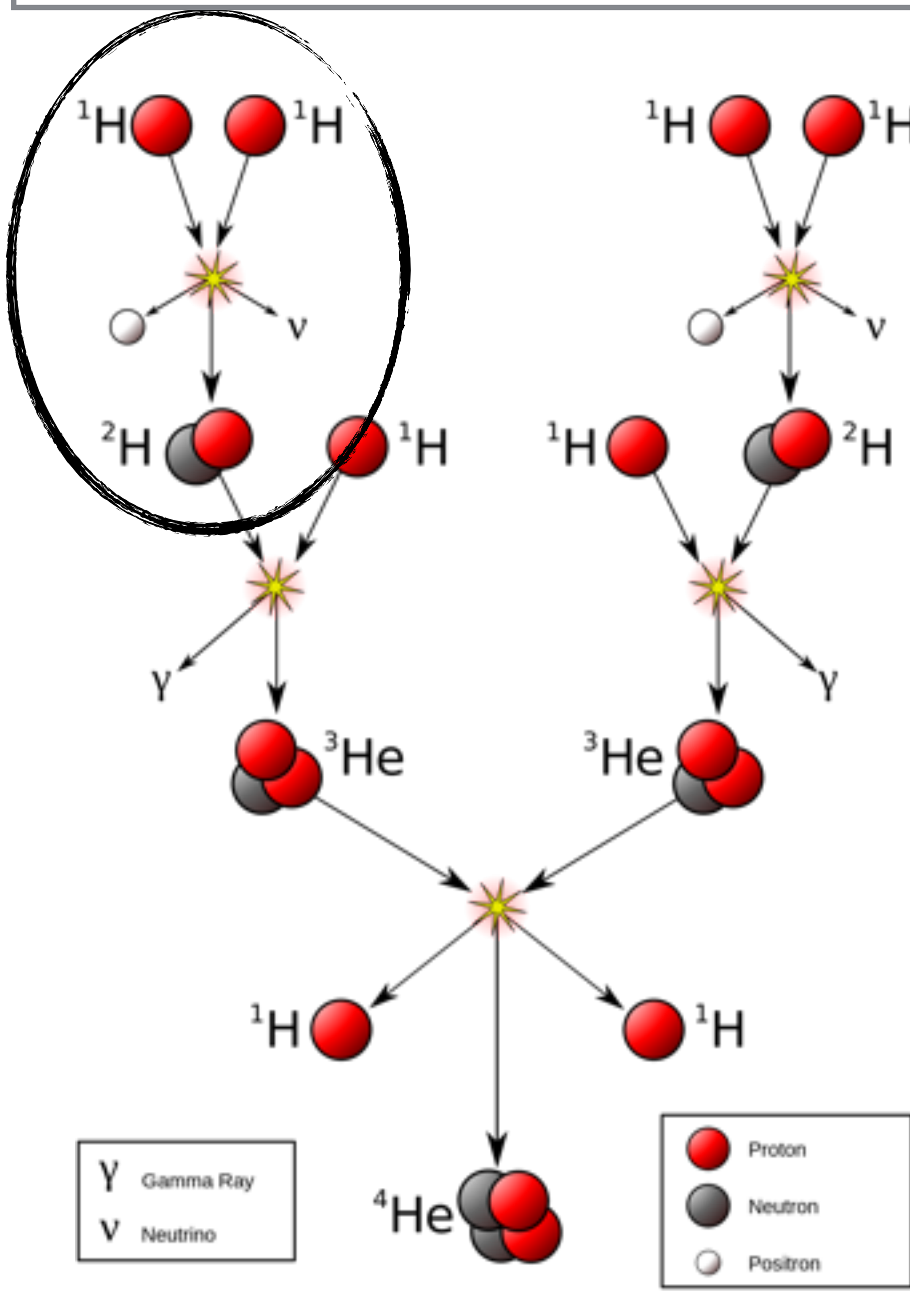

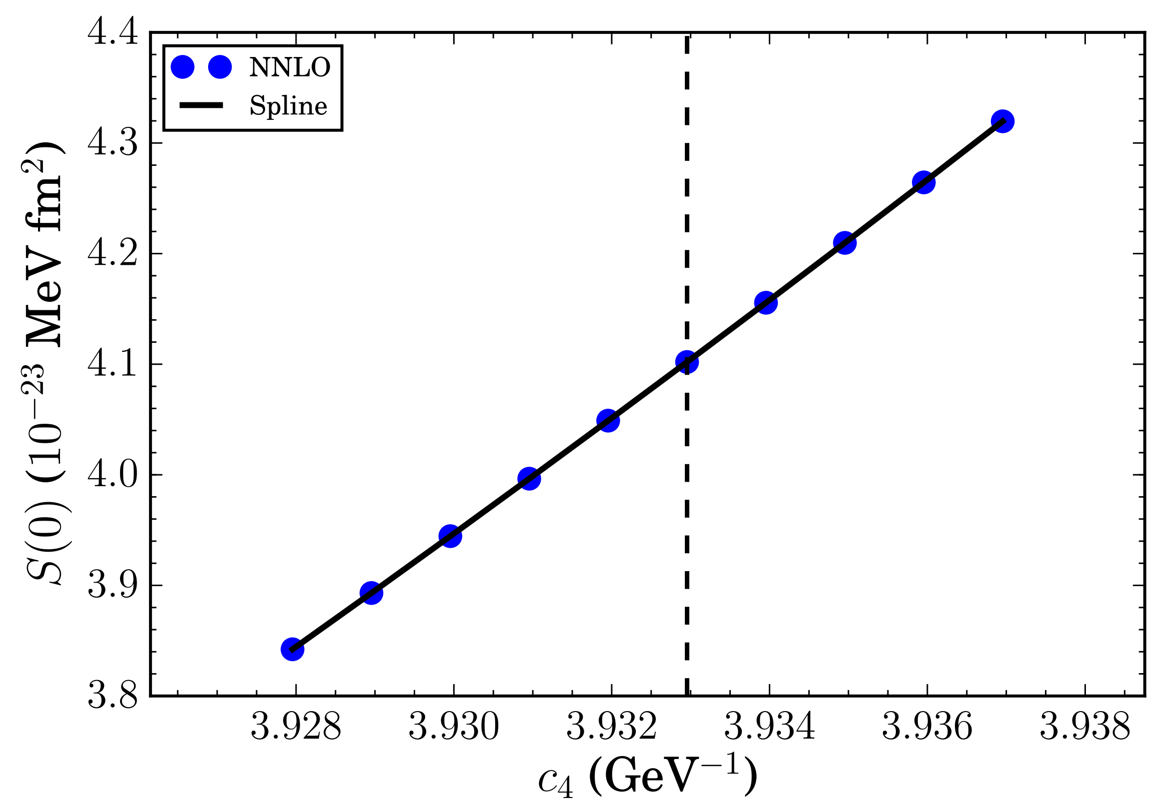

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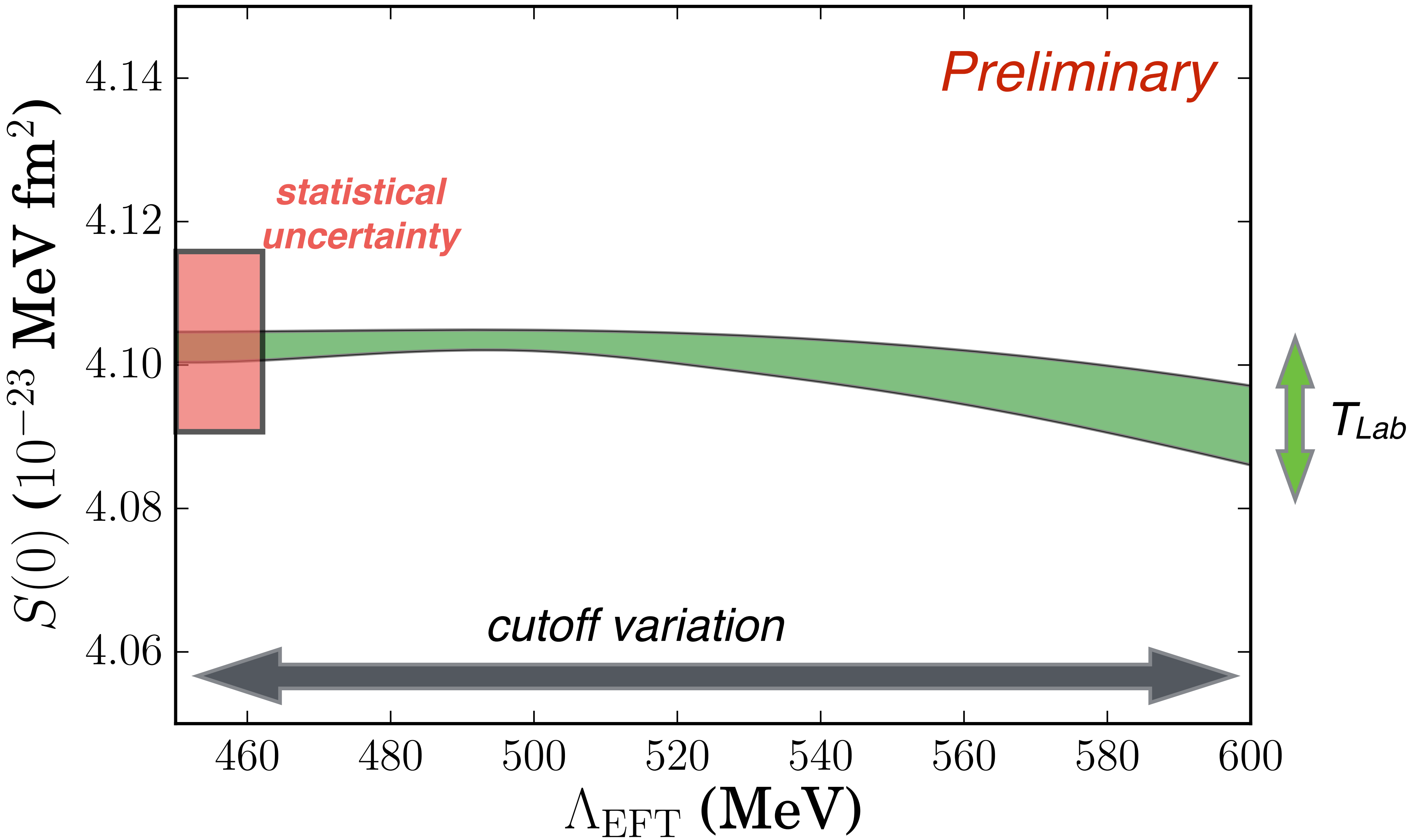

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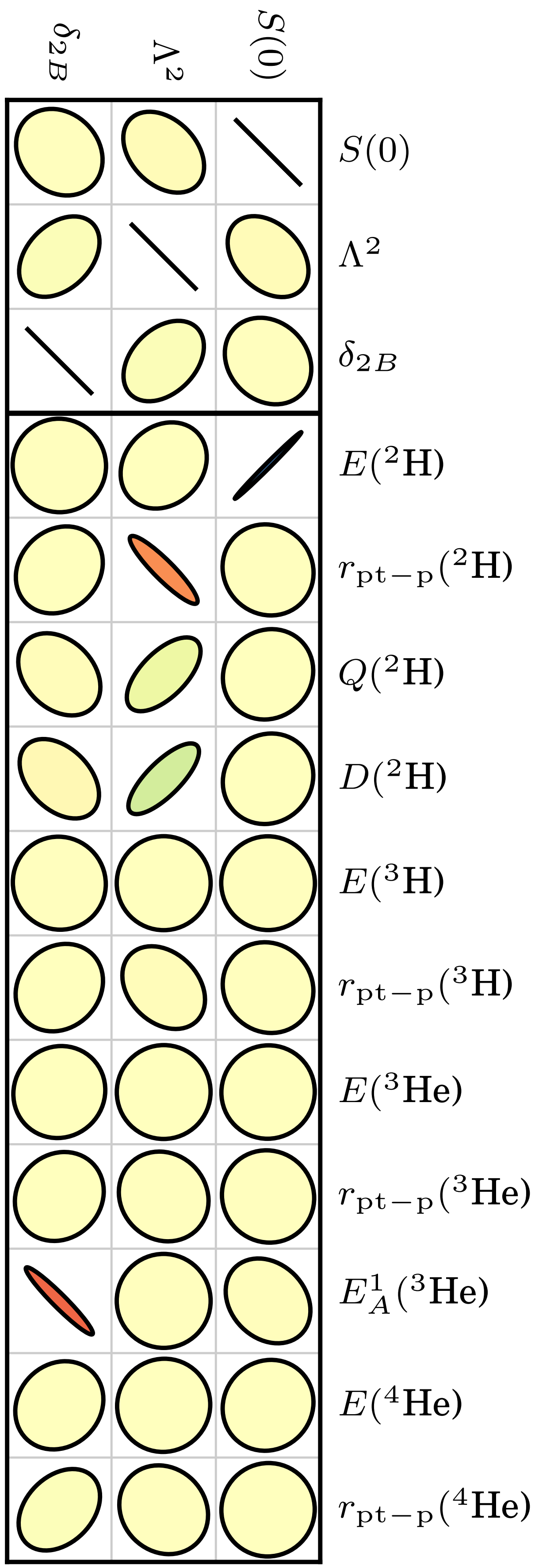

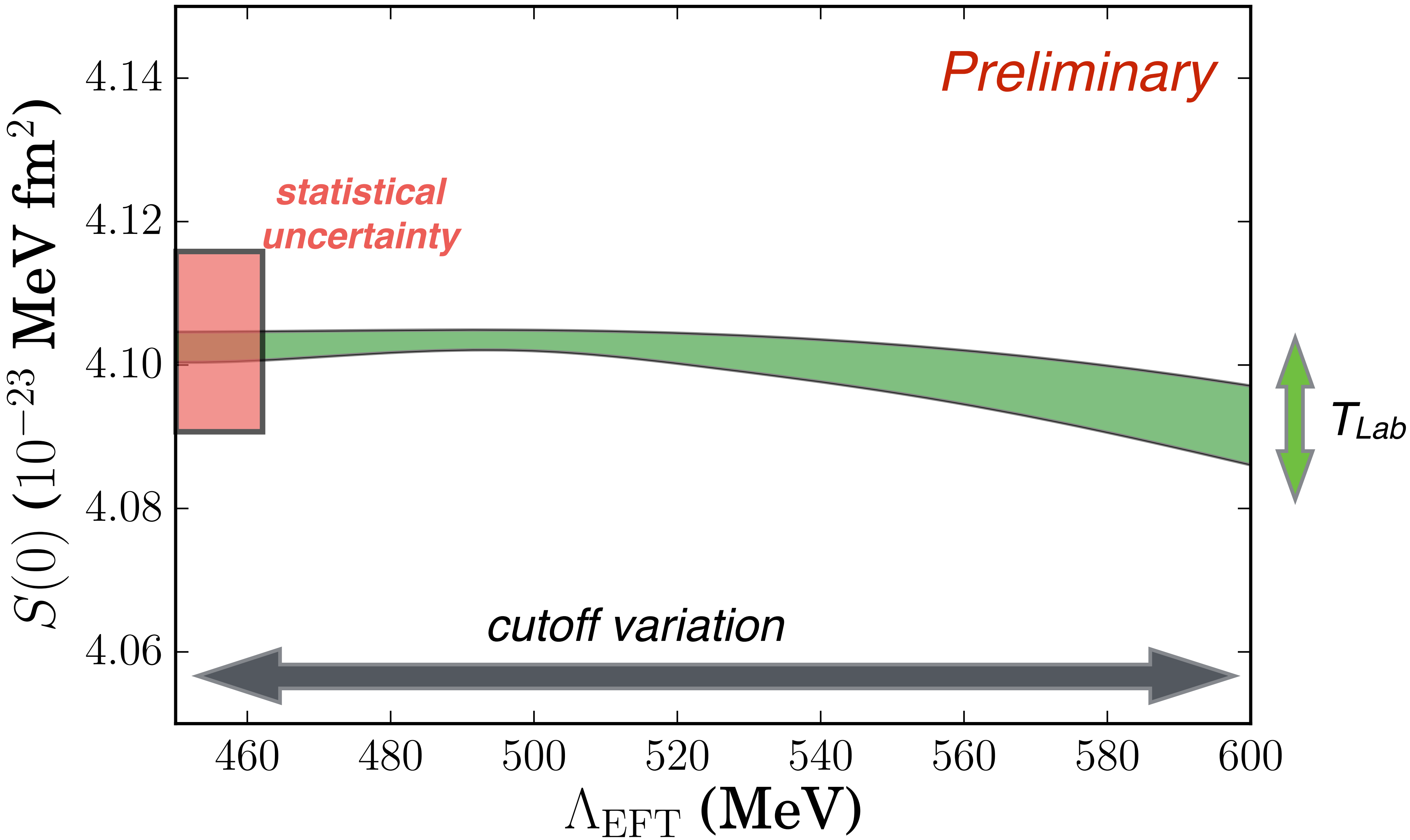

correlation analysis:

S(0) - E(^{2}H): *phase space*
Λ^2-r(^{2}H): *radial overlap*
Λ^2-rQ(^{2}H): *radial overlap*
δ_{2B}-E1A: *2B-current operator*

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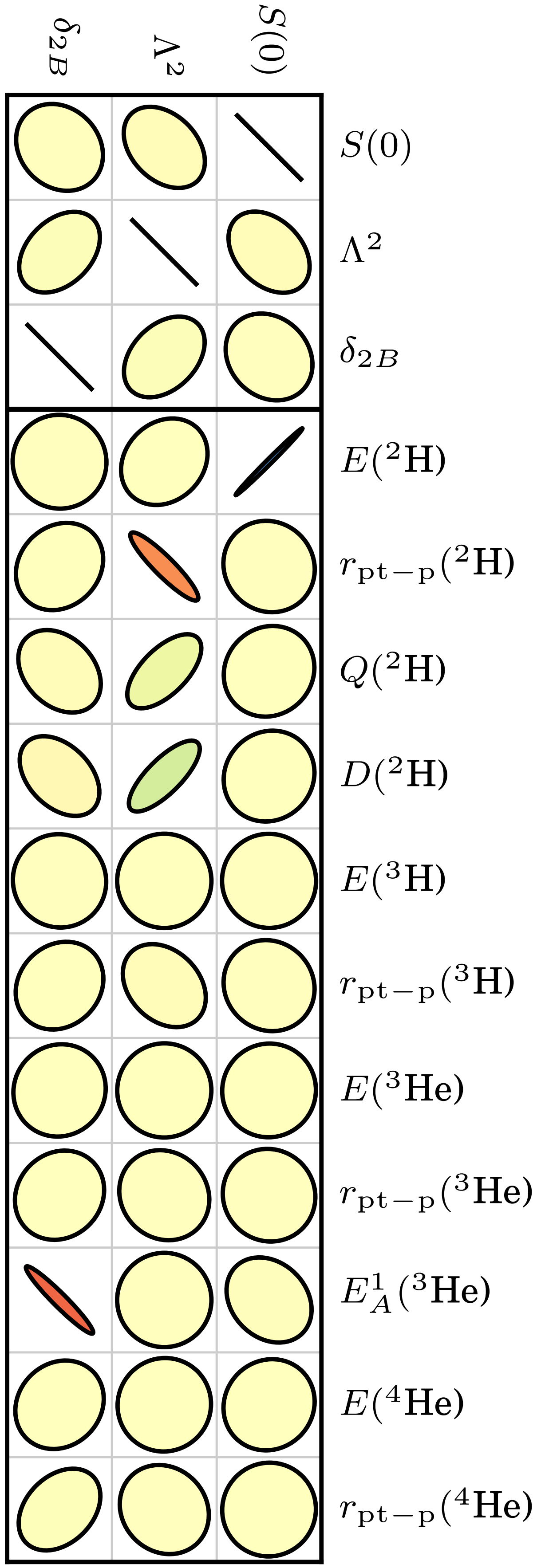

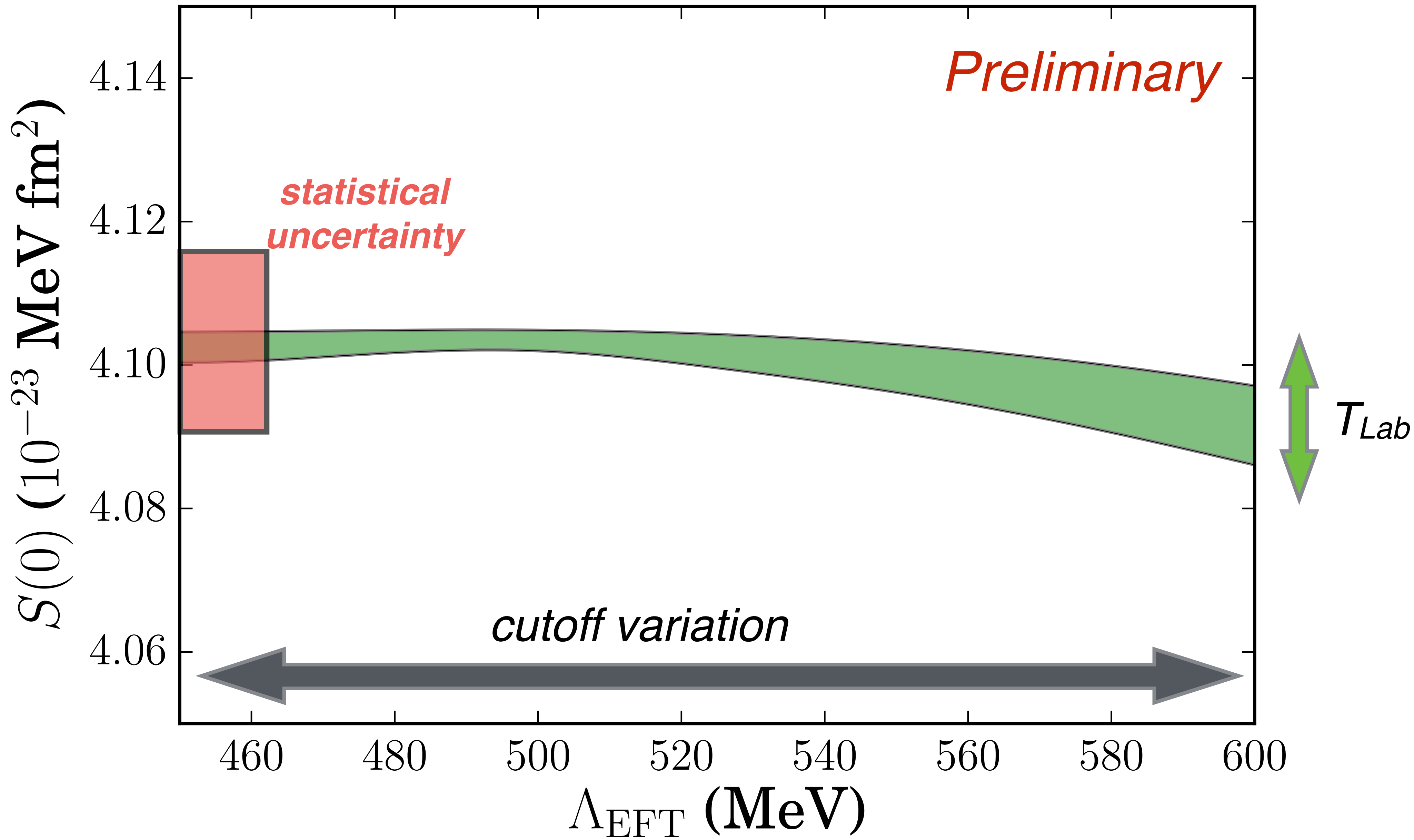

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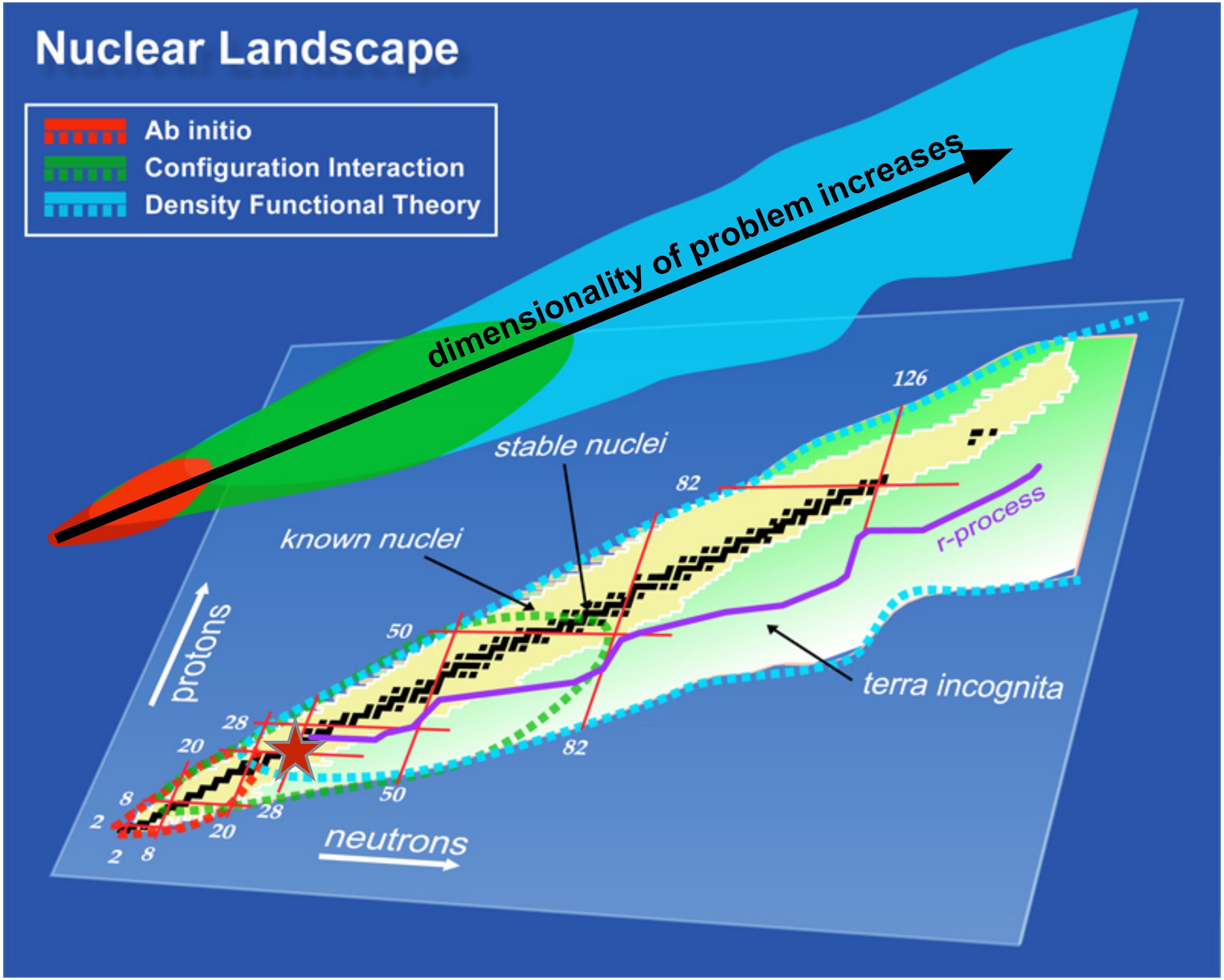
- *Insofar most consistent xEFT-study of this reaction*
- *Correlation study indicates sound statistical analysis*
- *Cutoff variation not large source of error*
- *Statistical error in S(0) is 3 times larger than what was previously thought*
- *Central value is most likely also larger due to previously neglected systematic uncertainties.*

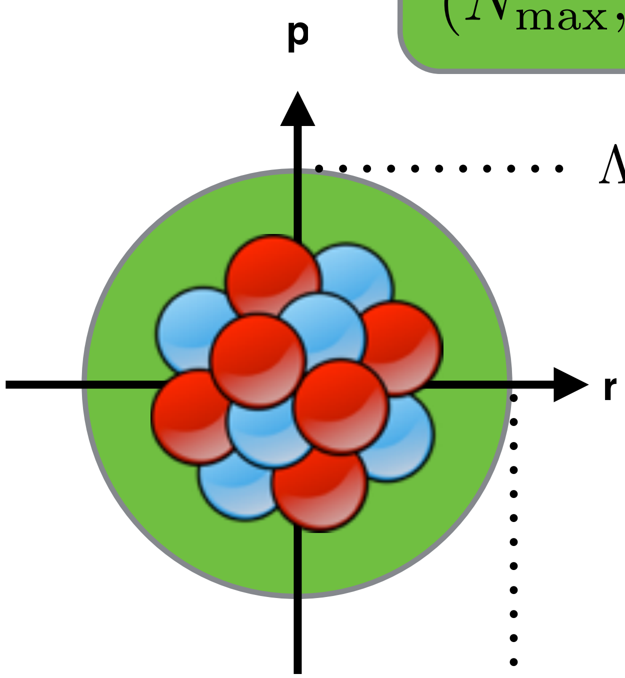
converging heavy nuclei with *ab initio* methods



Nuclei in the Harmonic Oscillator basis

basis parameters

$$(N_{\text{max}}, \omega) \rightarrow (\Lambda_{\text{UV}}, L)$$



$$\Lambda_{UV} \approx \sqrt{2N_{\text{max}}\frac{m\omega}{\hbar}}$$

$$L \approx \sqrt{2N_{\text{max}}\frac{\hbar}{m\omega}}$$

Nucleus needs to fit into the modelspace

$$L > R_{\text{nucleus}}$$

Interaction must be captured

$$\Lambda_{\text{UV}} > \Lambda_{\chi}$$

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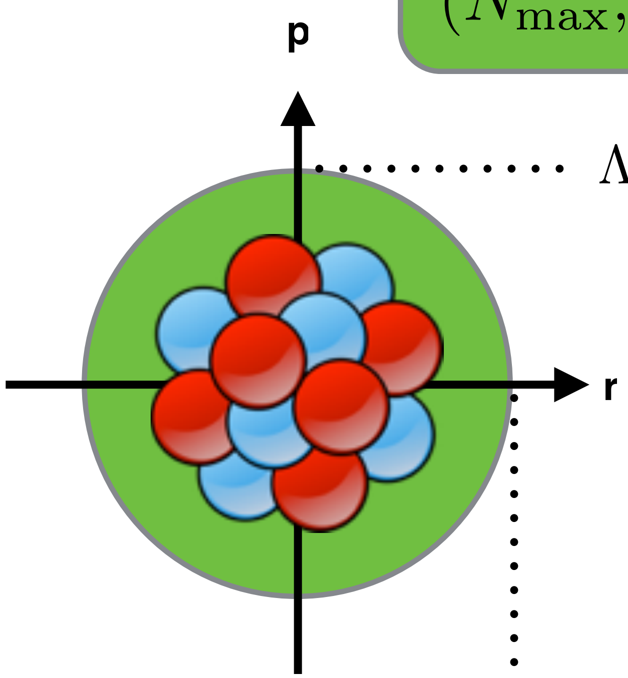

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- *Ab initio* calculations usually carried out at several different oscillator energies hw to gauge the model dependence of the results
- To facilitate calculations in heavy nuclei we propose to ***tailor the EFT interaction to a finite HO basis***

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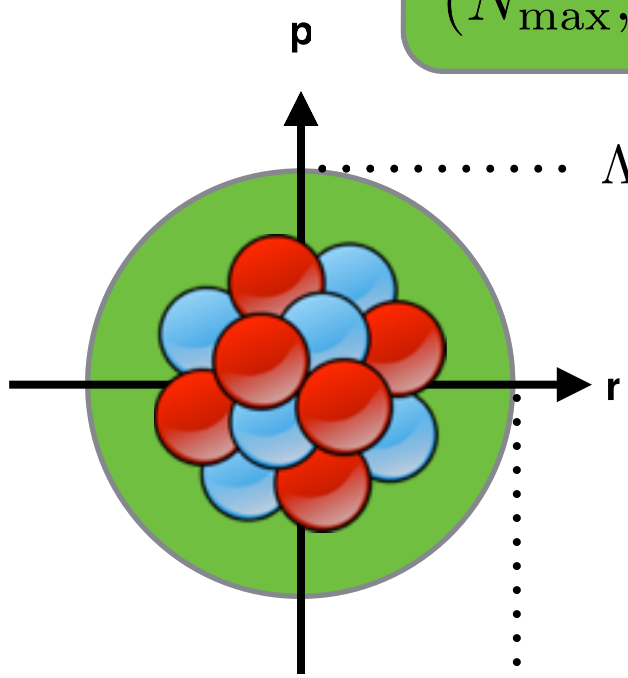

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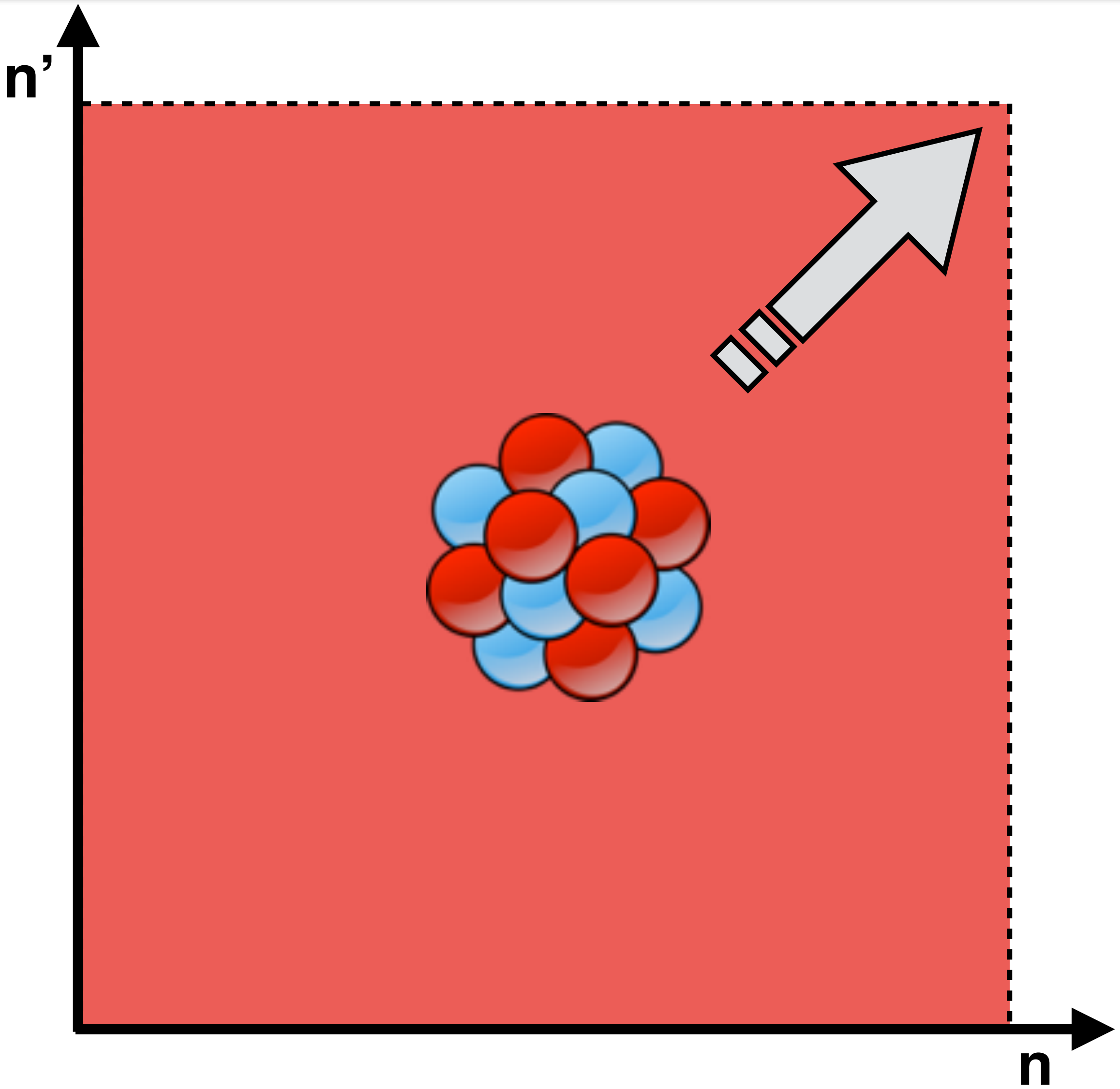
Similar ideas in nuclear physics already exist:

Arizona group developed pionless-EFT in HO basis and studied UV/IR cutoff dependencies. Coupling constants depend on the size of the basis.

Haxton et al. proposed HOBET (HO-based effective theory). “Shell-Model” (Bloch-Horowitz) plus resummed kinetic energy and physics beyond a cutoff absorbed by contact-gradient expansion (like EFT contact potential)

We propose to choose (and fix) an oscillator space and evaluate the *existing* chiral EFT interaction operators in this space. This *projection* requires us to refit the LECs of chiral EFT

EFT interaction in a truncated HO basis



S. Binder, A.Ekstrom, G. Hagen, T Papenbrock, and K .A. Wendt arXiv:1512.03802 [nucl-th]

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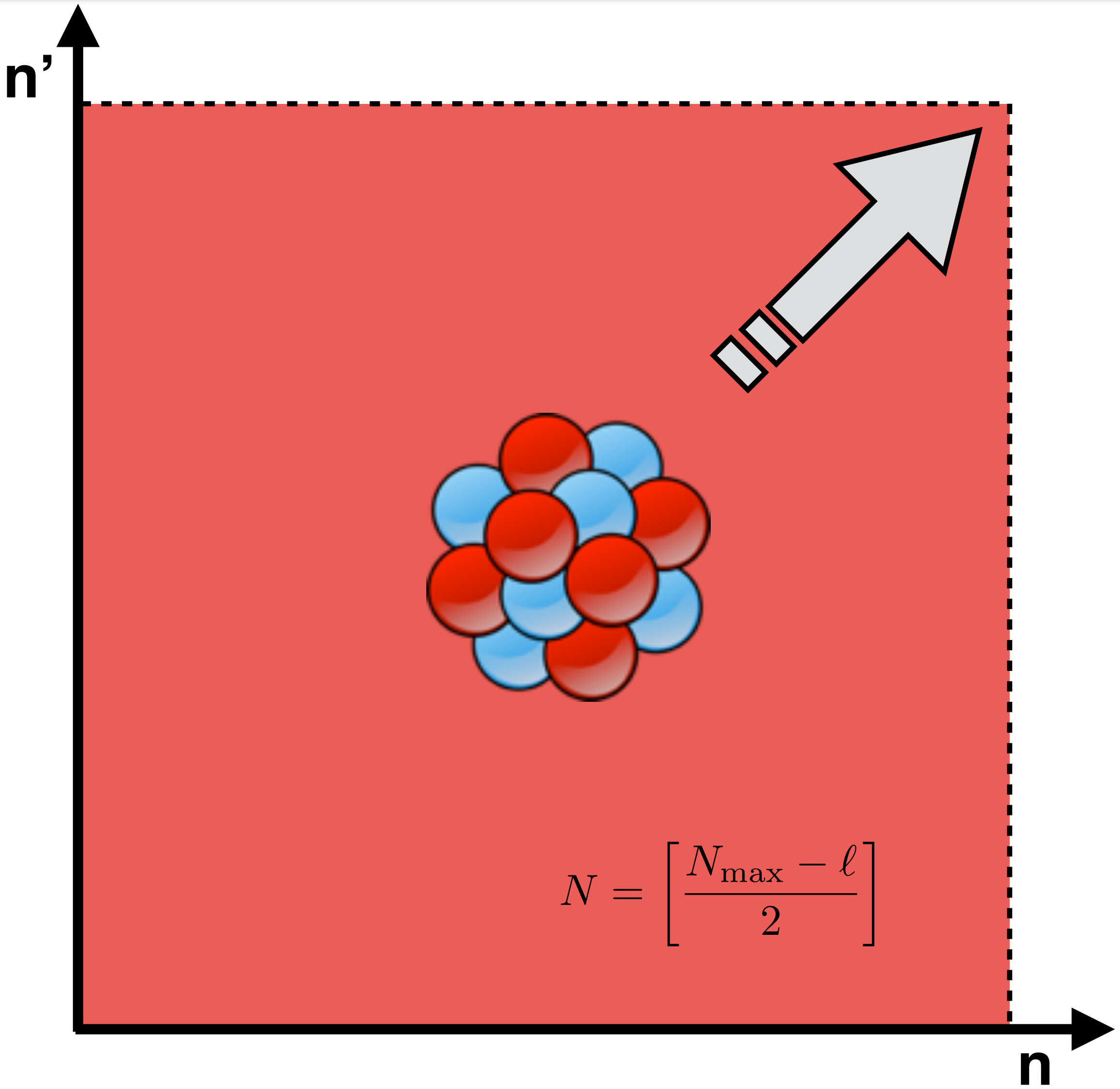

$$N = \left[\frac{N_{\max} - \ell}{2}\right]$$

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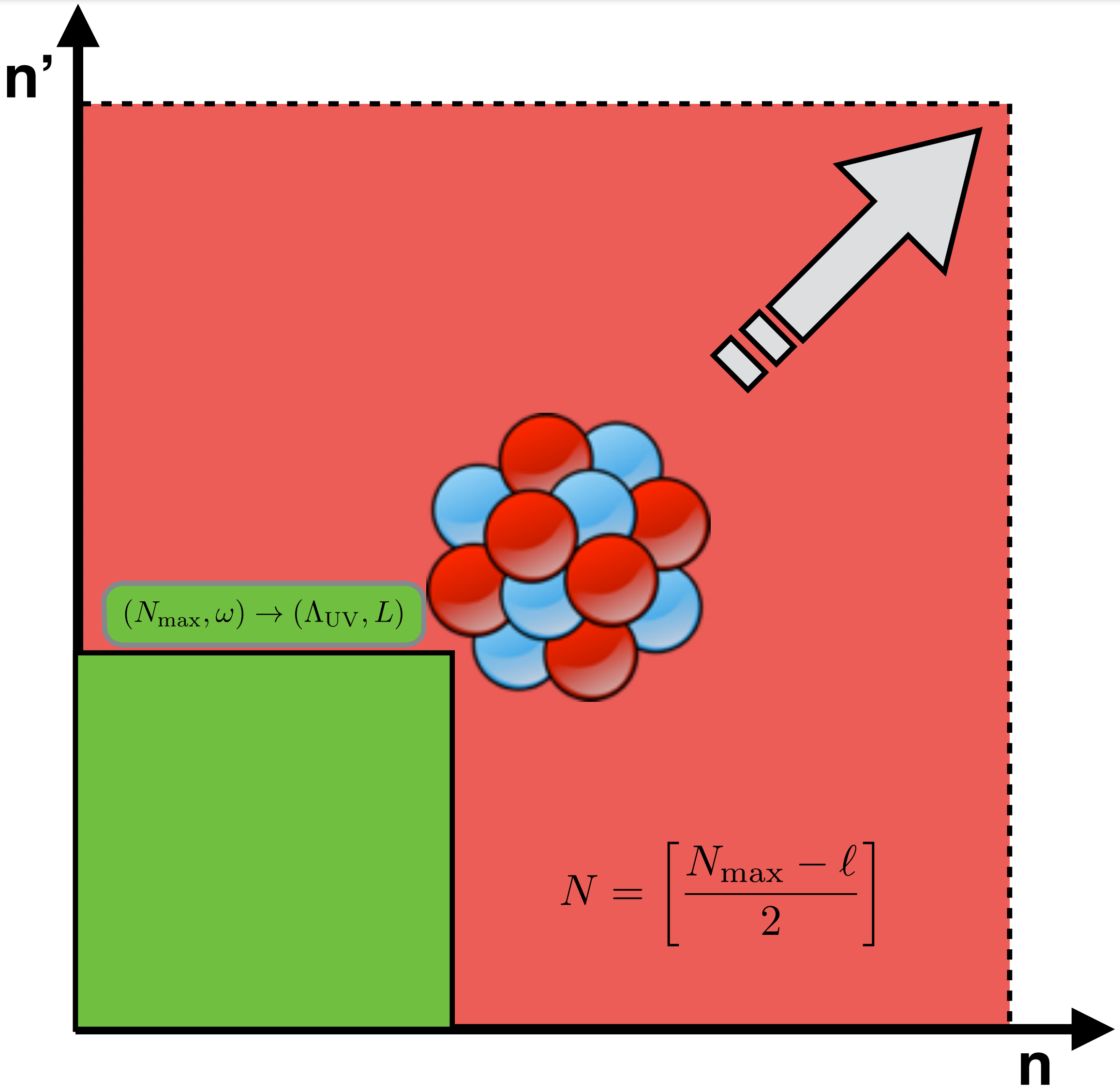

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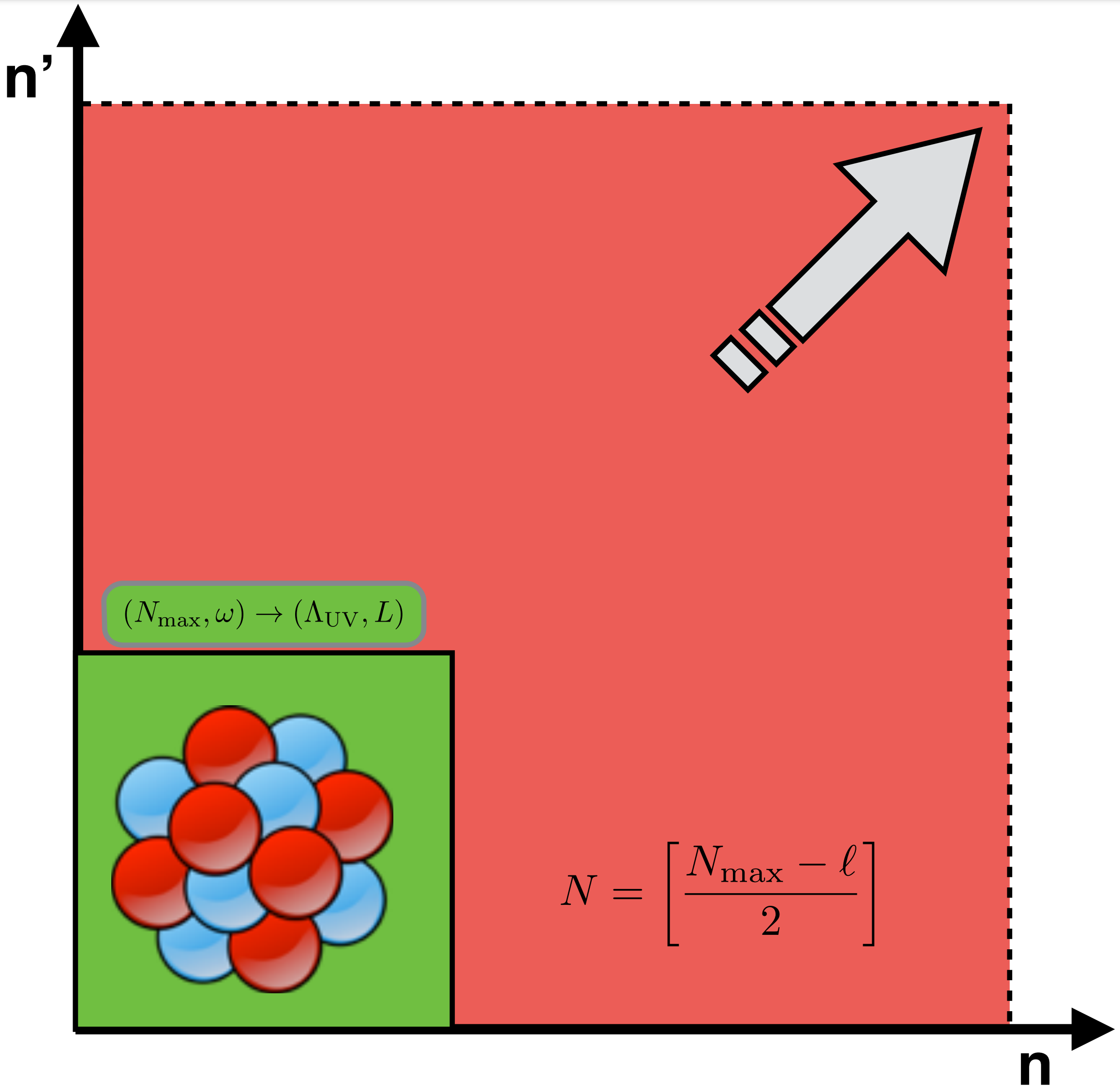

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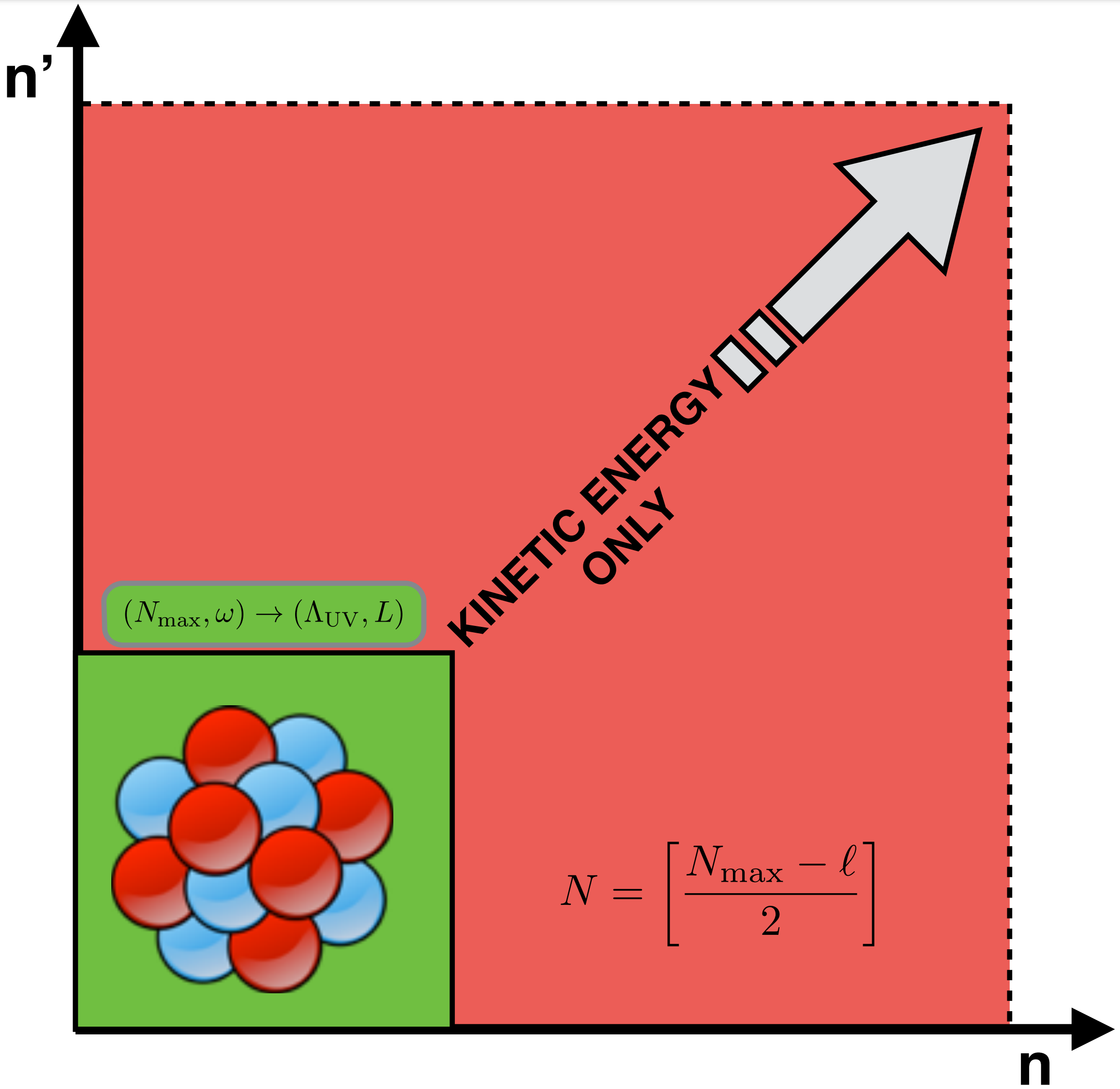

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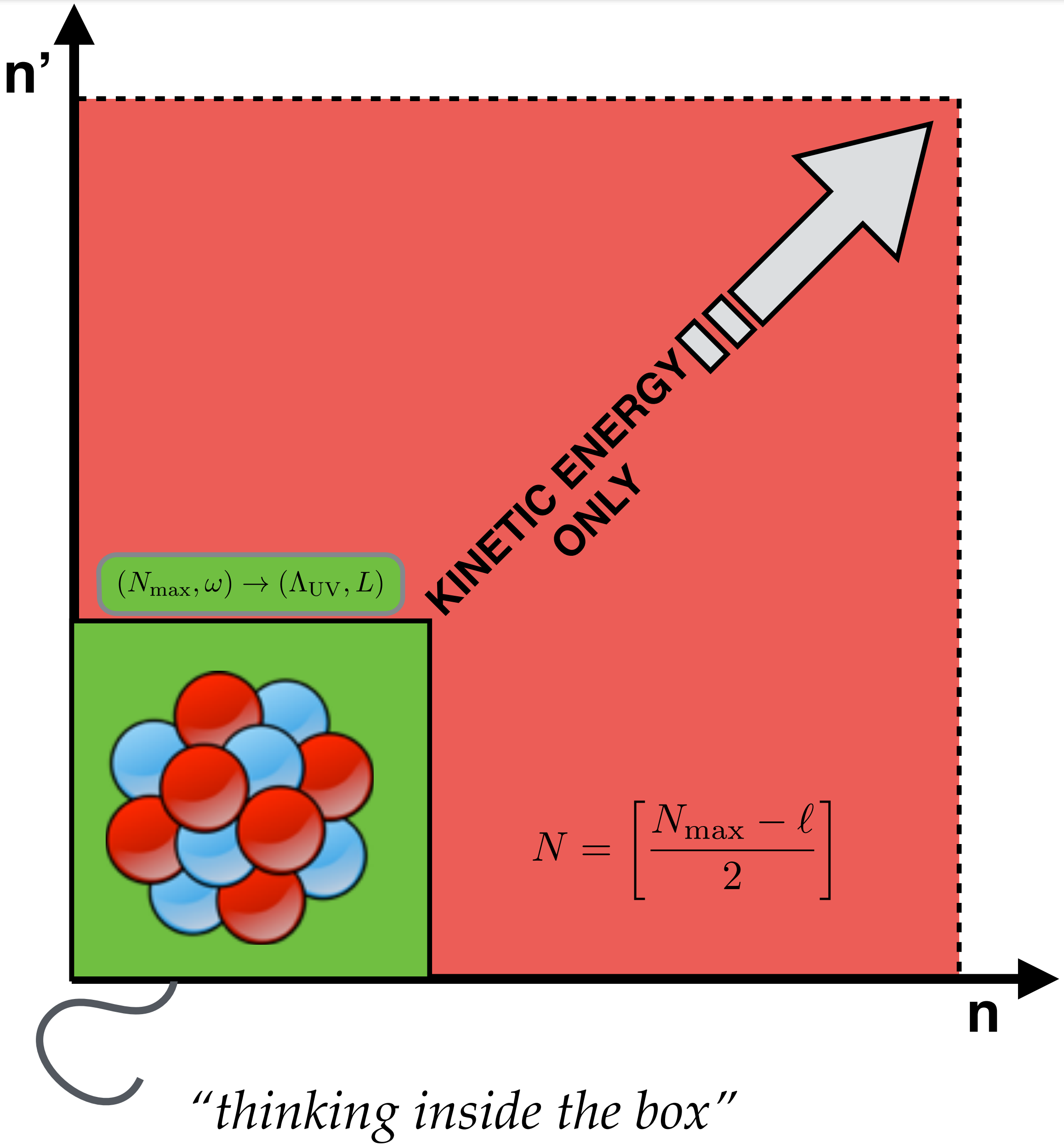
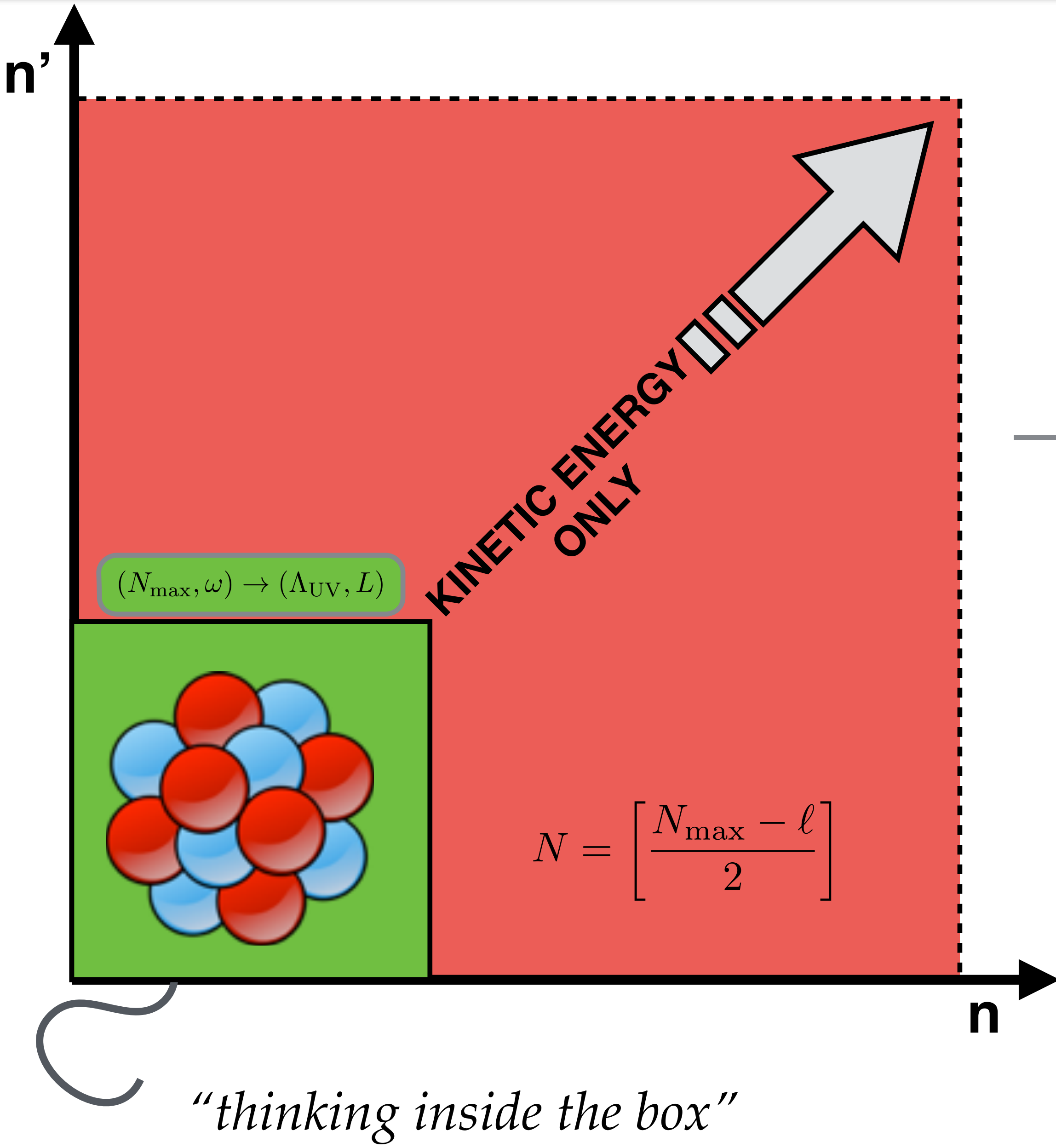


simple picture: choose e.g. $N_{\rm max} = 10, \hbar\omega = 40\,\mathrm{MeV}$

set $\langle n|V|n'\rangle$ to zero outside $N_{\rm max}$

S. Binder, A.Ekstrom, G. Hagen, T Papenbrock, and K .A. Wendt arXiv:1512.03802 [nucl-th]

EFT interaction in a truncated HO basis



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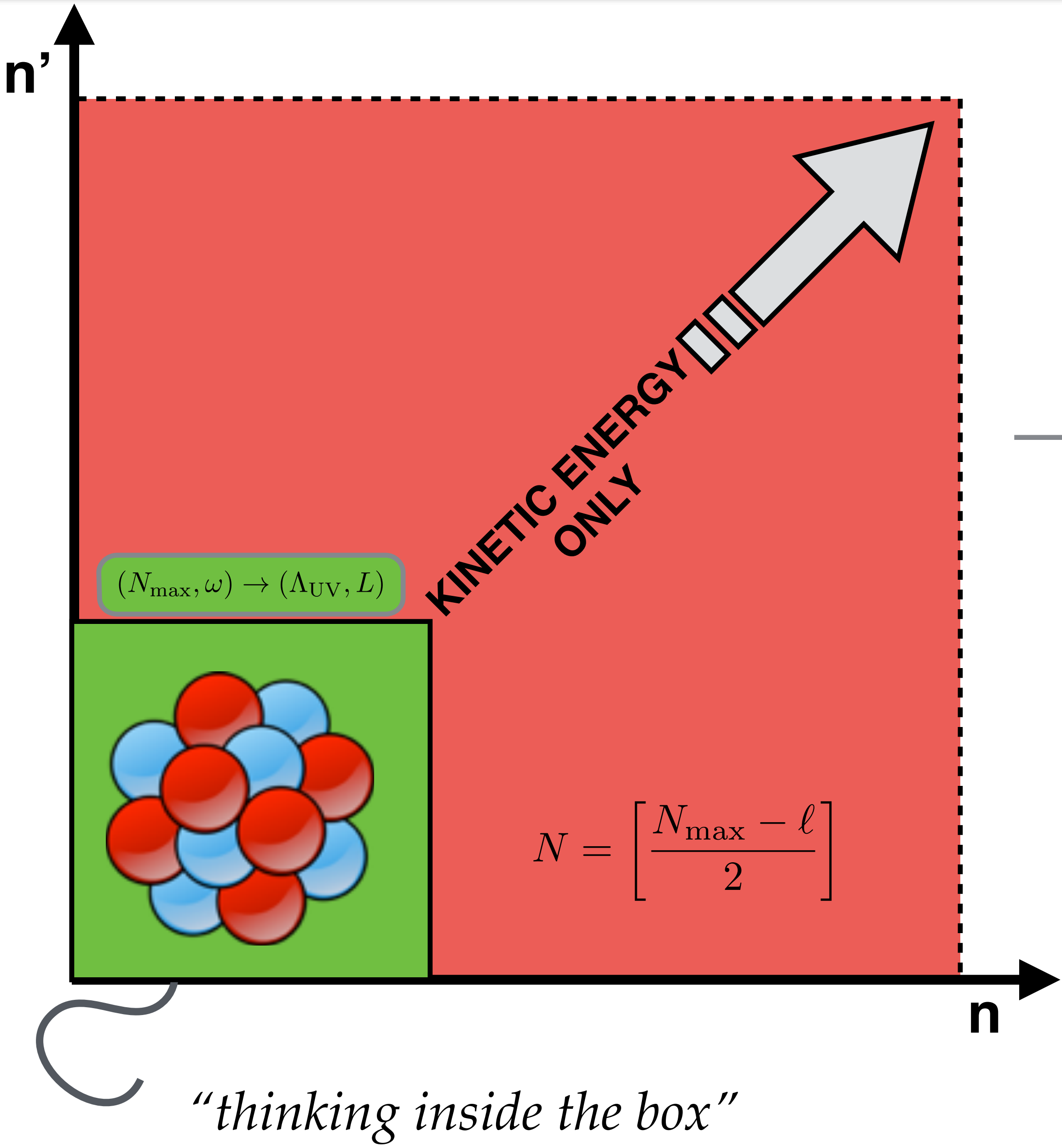

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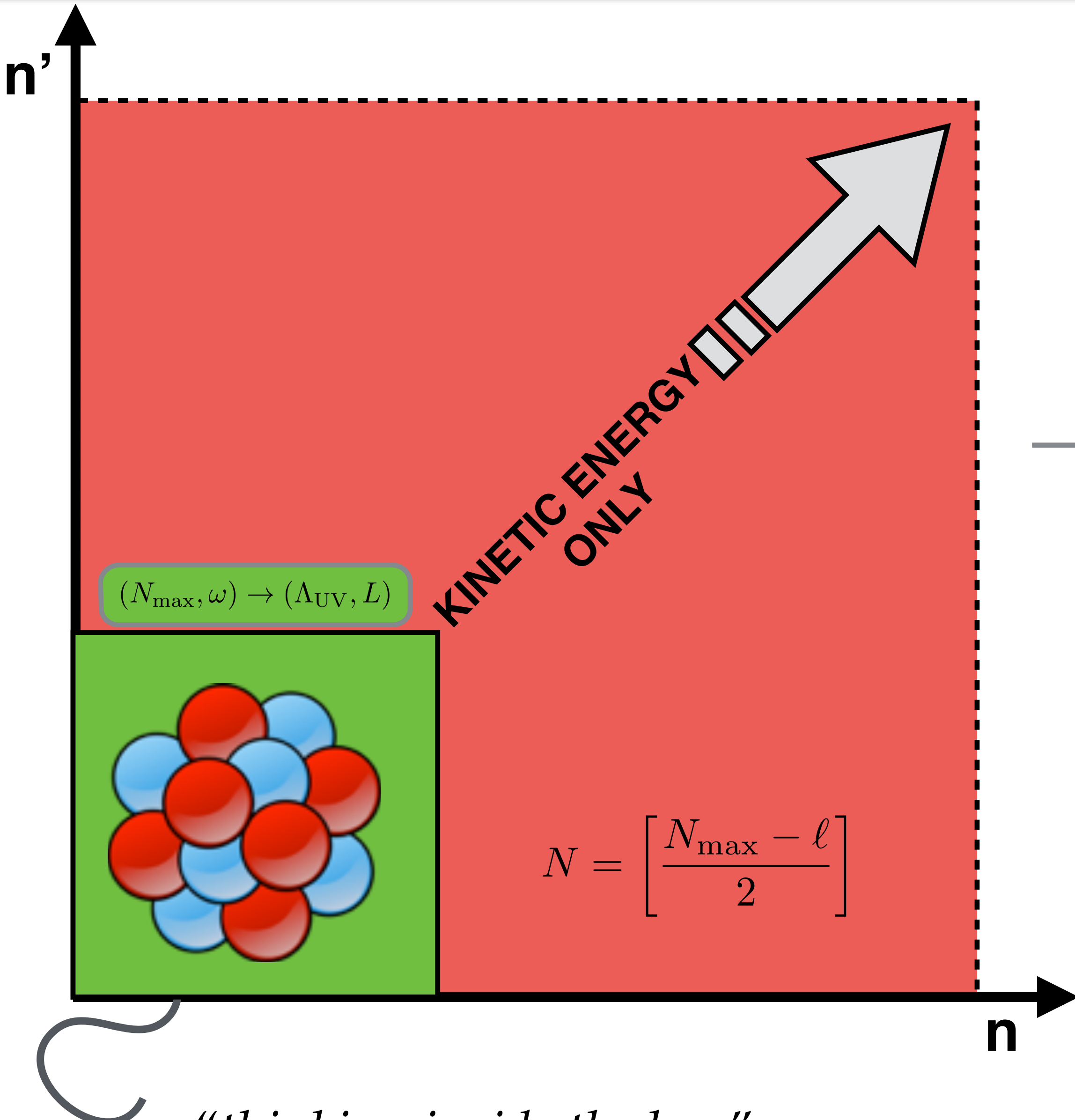

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We start by solving the eigenvalue problem of the squared momentum operator in a finite oscillator space truncated at an energy (N_{max} +3/2)hw. It turns out that momenta $k=k_\mu$ such that $\psi_{N+1}(k)=0$ solve this eigenvalue problem.

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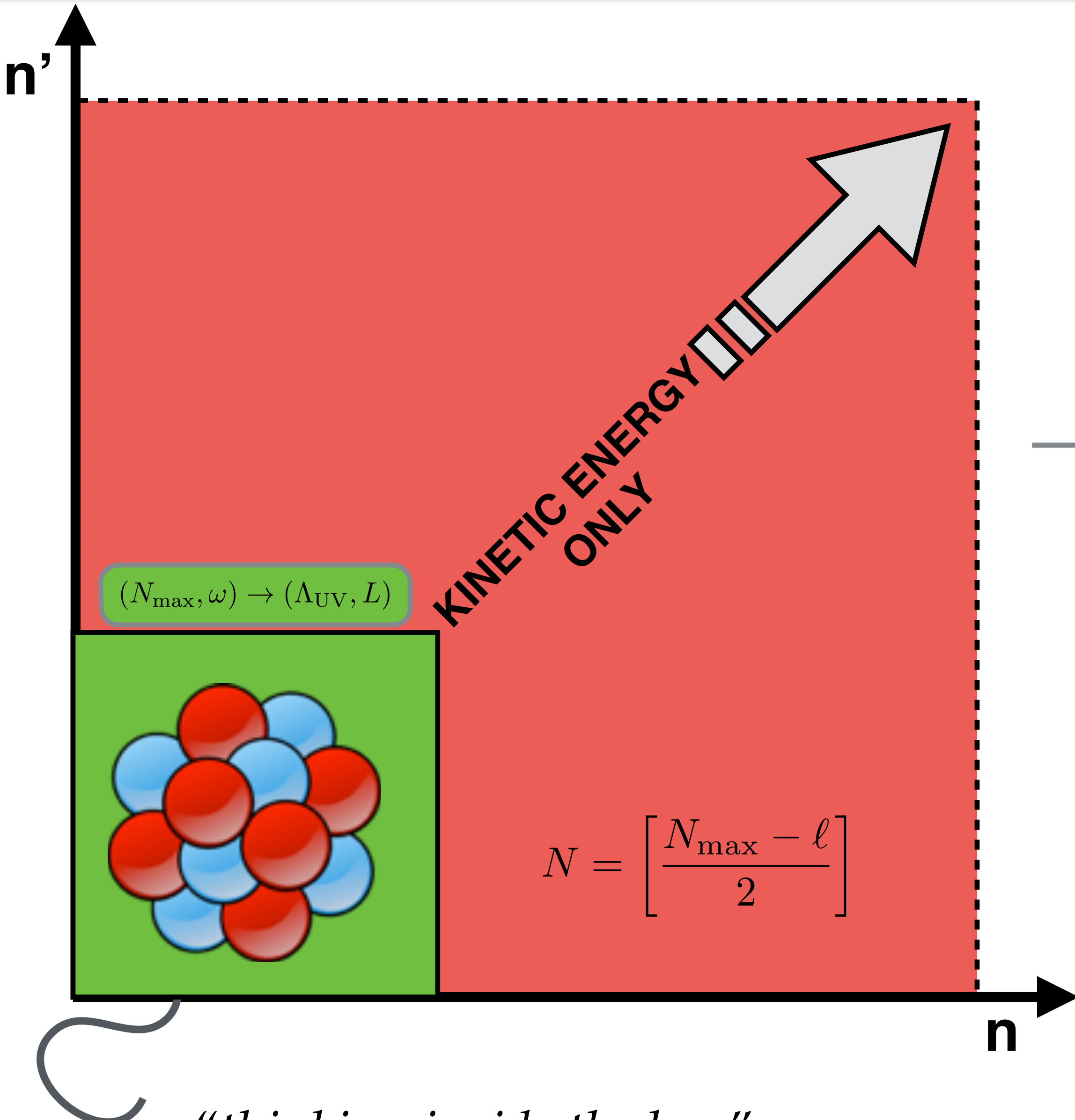

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This has pleasant consequences for most analytical and numerical evaluations!

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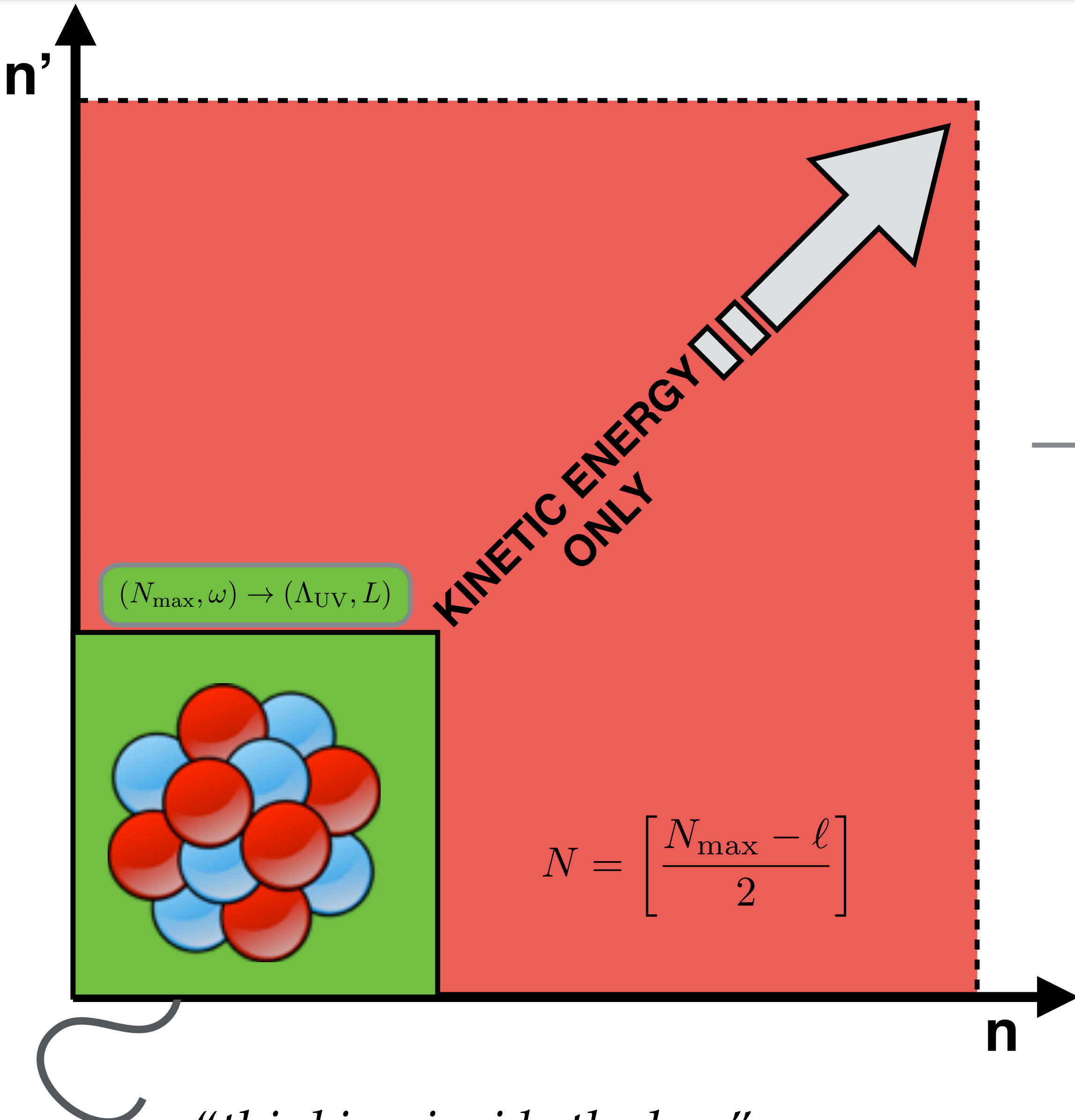

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$$\underbrace{\langle k_{\mu,\ell}, \ell|V|k_{\nu,\ell'}, \ell'\rangle}_{\chi\mathrm{EFT}}$$

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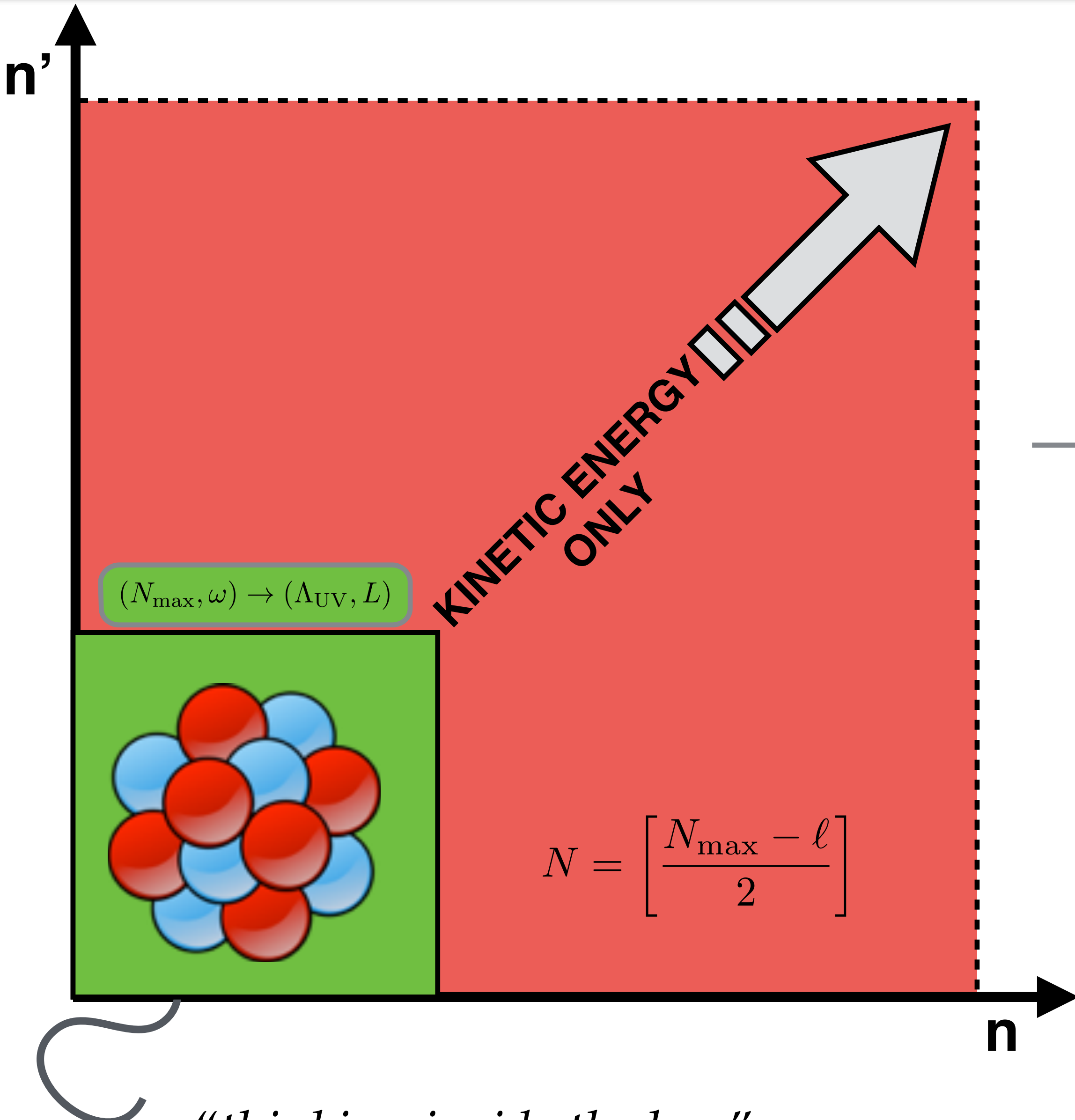

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Idaho-N3LO in the Harmonic Oscillator basis

S. Binder, A.Ekstrom, G. Hagen, T Papenbrock, and K .A. Wendt arXiv:1512.03802 [nucl-th]

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selected proton-neutron phase shifts of Idaho-N3LO(500) projected onto an Nmax=10, hw=40 MeV oscillator space

Λ_{UV} = 700 MeV > Λ_χ = 500 MeV

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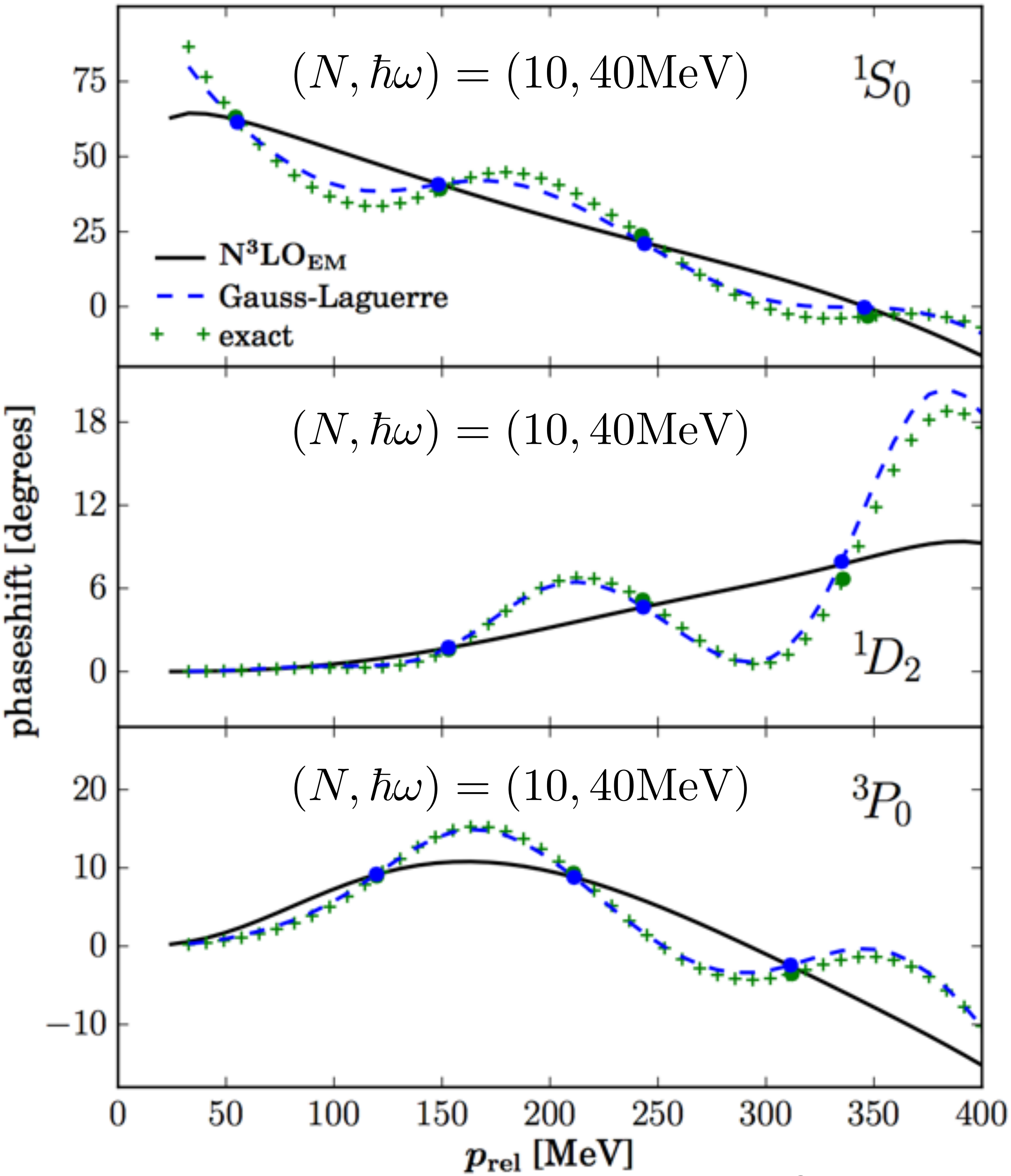

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OBSERVATIONS:

- There are oscillations in the phase shifts
- The period of this oscillation is approximately proportional to the IR cutoff
- Gauss-Laguerre ("HO-EFT") phases exhibits sligthly smaller oscillations than the "exact" phases
- At the energies corresponding to the eigenenergies of the truncated Hamiltonian (solid dots), computed phases are closest to the true N3LO value

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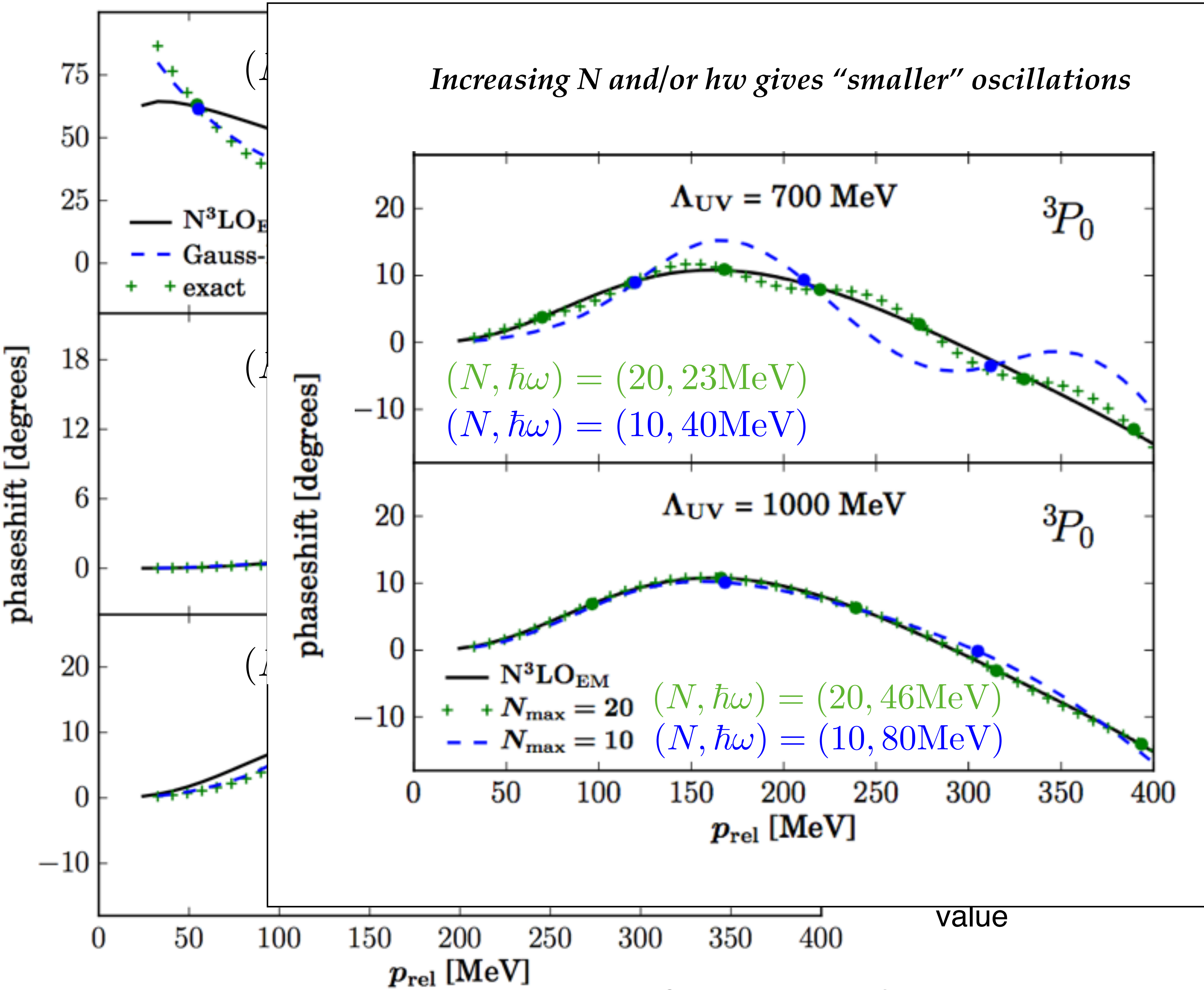

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Refitting the NLO interaction to CD-Bonn phases

**With goal of computing heavy nuclei,
we design a HO-NLO interaction with:**

- small number of oscillator shells Nmax=10
- Lower frequencies, rapid IR convergence
- Lower frequencies, lower UV cutoffs

We choose hw=24 MeV, which gives:
Λ_{UV}=550 MeV, L=9.6 fm.
Considering the tail of the chiral regulator function, we set Λ_χ=450MeV.

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	$N_{\max} = 10$	$N_{\max} = 80$	experiment
E_d [MeV]	−2.227	2.221	−2.225
r_d [fm]	1.984	1.961	1.976
Q_d [fm^2]	0.229	0.259	0.286
P_d	0.026	0.028	
$\tilde{C}^{(np)}_{^1S_0}$	−0.140992	−0.139687	
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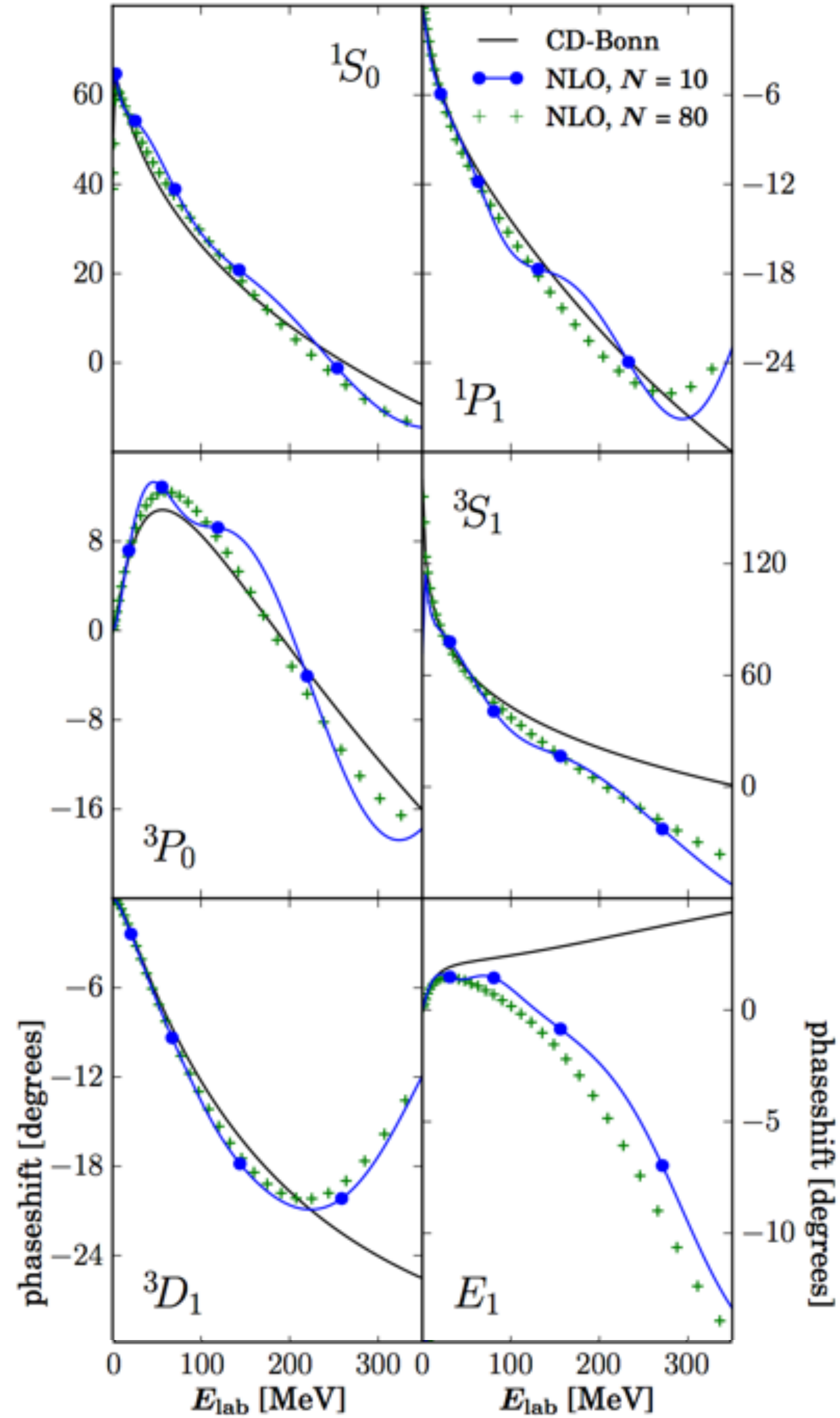

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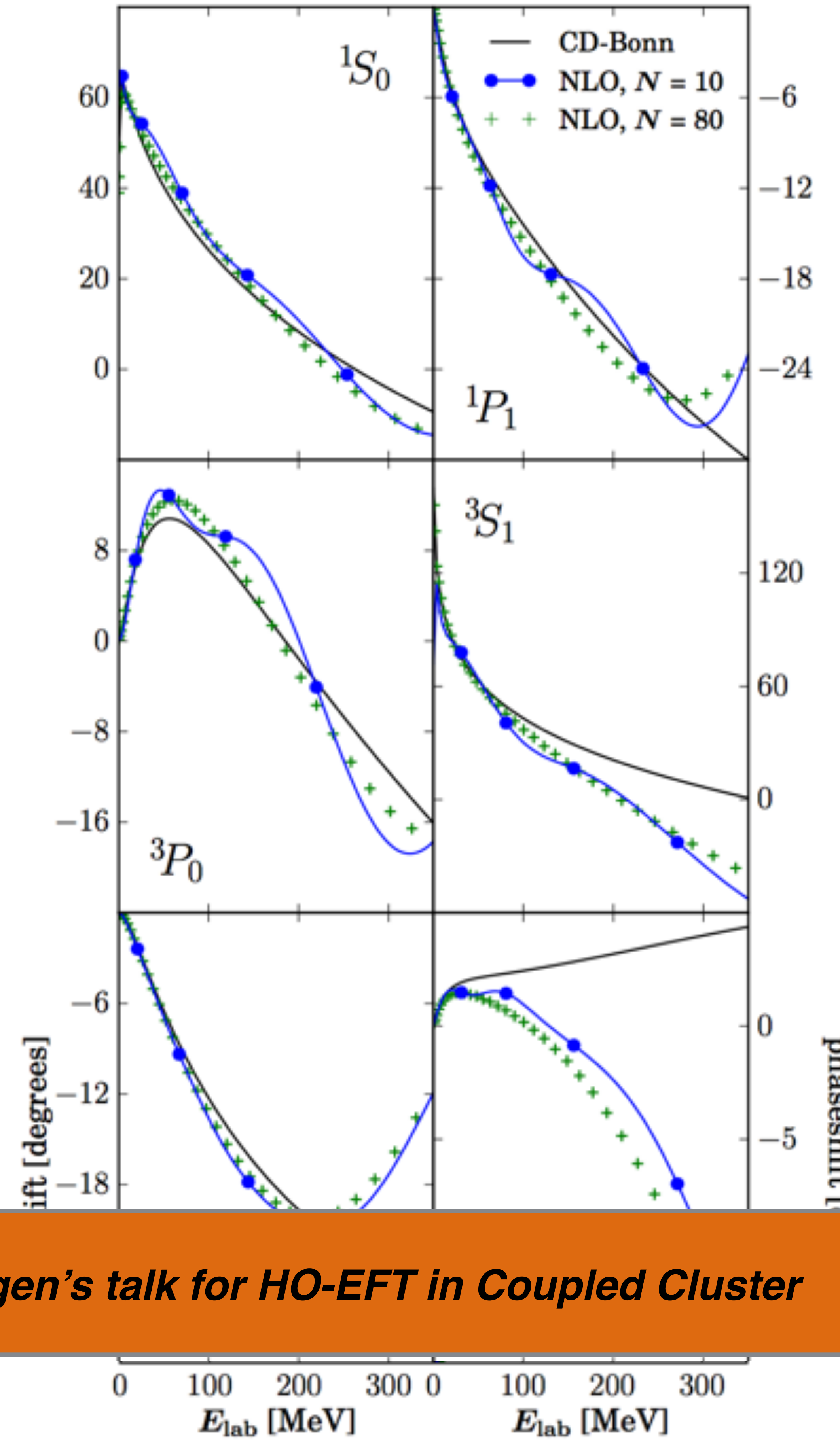

See. G. Hagen's talk for HO-EFT in Coupled Cluster

S. Binder, A.Ekstrom, G. Hagen, T Papenbrock, and K .A. Wendt arXiv:1512.03802 [nucl-th]

Open questions, and next steps

Some open questions that we are currently addressing

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The infrared scale is rather undesirable in a low-energy EFT. Can we get rid of it? It seem like it. At least we can sacrifice the highest momentum point k_N, to better approximate the IR-physics of xEFT.

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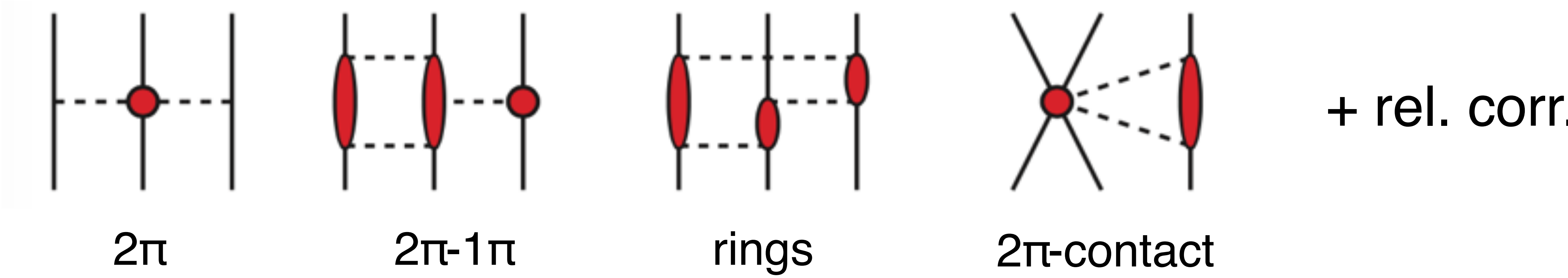
Next step: **HO-NNLO$_{\mathrm{sat}}$**

NNN-N3LO: simple cD/cE scan with Idaho-N3LO



efficient NNN-PWD enabled by K. Hebeler, H. Krebs, et al PRC 91, 044001 (2015)

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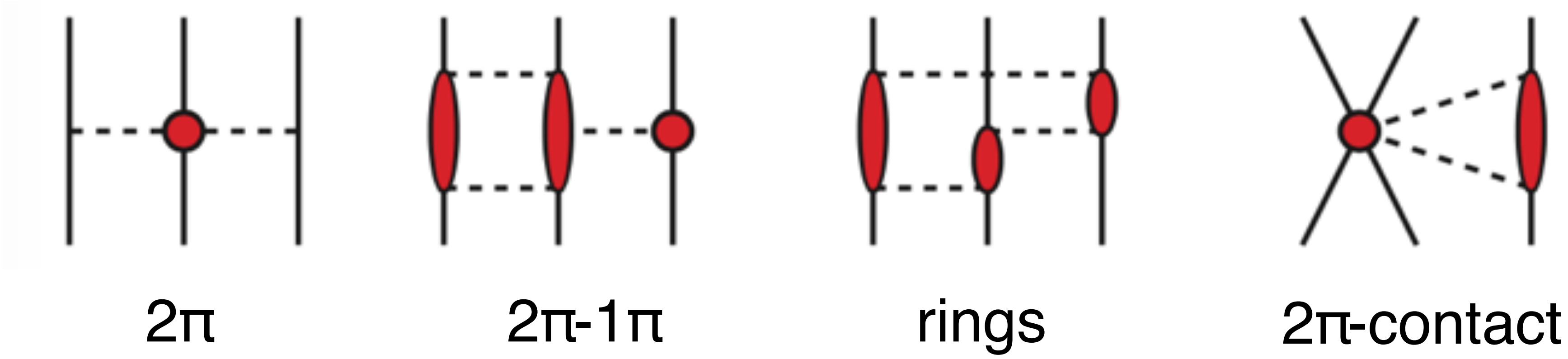

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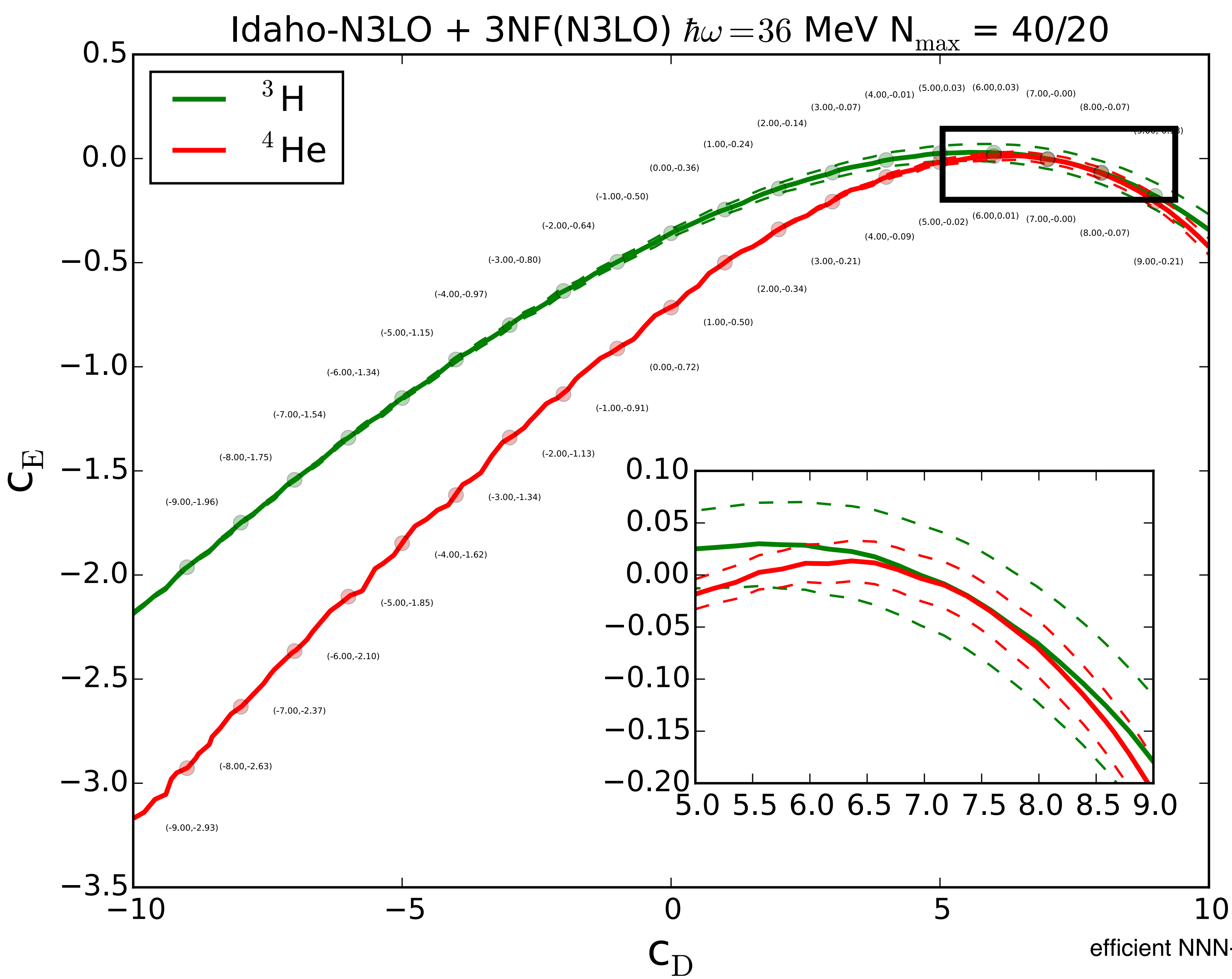

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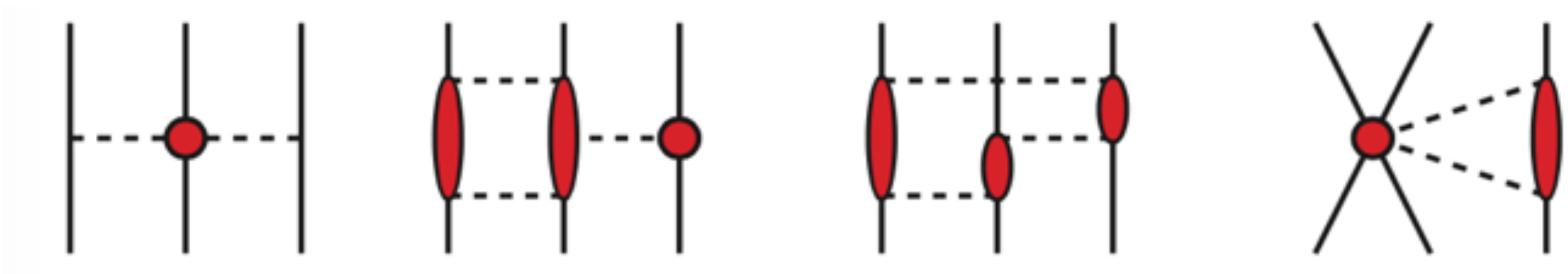
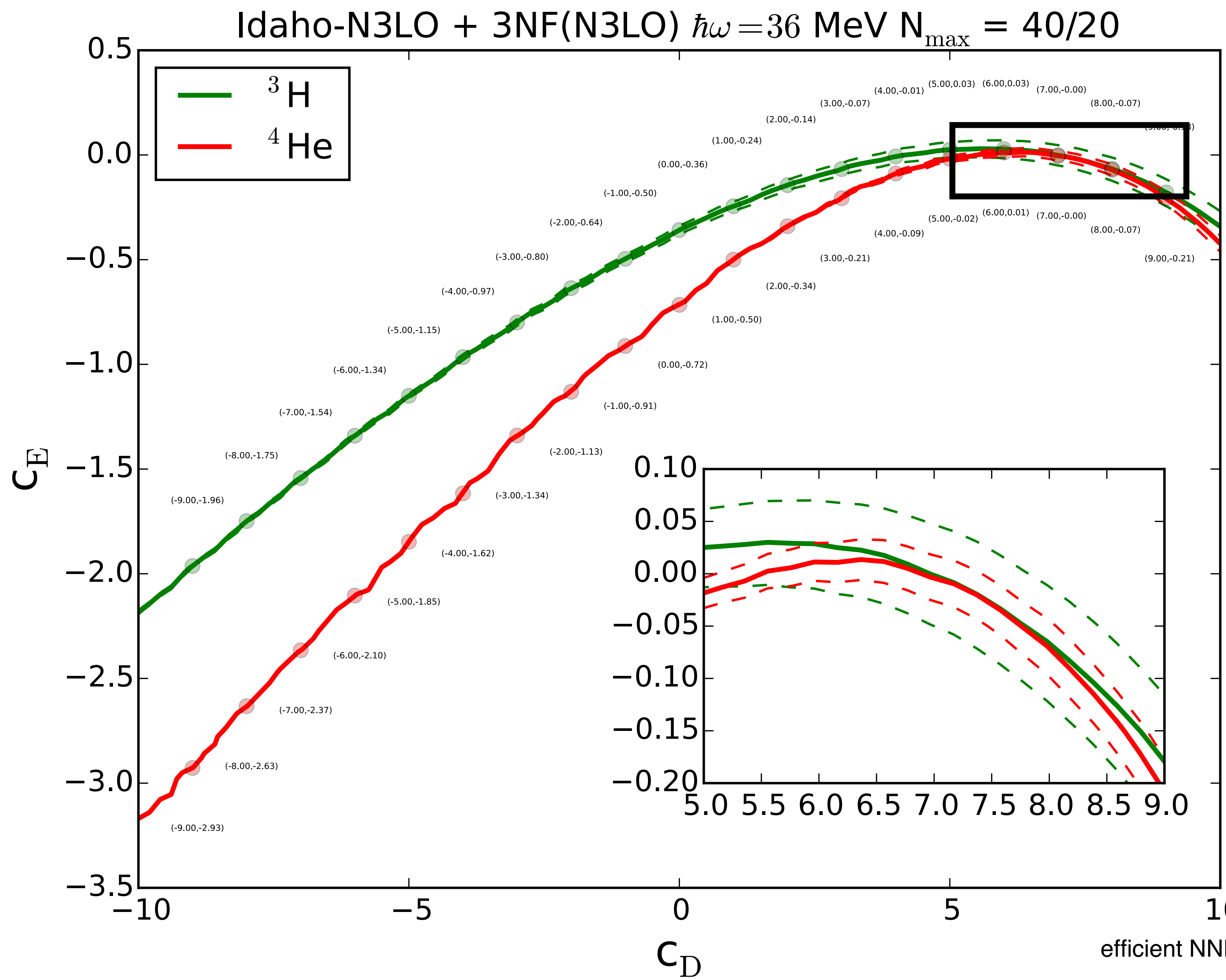


2π　　2π-1π　　rings　　2π-contact

+ rel. corr.



Expectation values (in MeV and fm)

	3H	4He
E_{gs}	**-8.48**	**-28.32**
$r_{pt\text{-}p}$	1.61	1.49
<c1>	-0.14	-0.69
<c3>	-1.29	-6.82
<c4>	0.35	2.16
<cD>	-0.39	-2.16
<cE>	0.02	0.08
<2pi>	-0.40	-2.54
<2pi1pi>	1.22	6.48
<rings>	-0.57	-3.38
<2pi-cont>	0.20	1.25
<rel. corr>	0.24	1.28
N2LO	**-1.45**	**-7.44**
N3LO	**0.68**	**3.09**

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N3LO optimizations are challenging

Work led by B. D. Carlsson (Chalmers)

Initialize by computing phase shifts for 10^5 random contact LEC values for each partial wave and select the ~1000 best values and optimize. This leads to 192 different optima (for cutoff 450 MeV) with respect to phase shifts. (pi-N LECs from sep-optimization)

The A=3 observables weed out several of the S-wave minima, but many P-wave minima remain. Things improve when A=4 is included. But still, several local minima remain.

This is where we stand right now.

Phase shifts from Granada analysis: Navarro Pérez et al PRC 88, 064002 (2013)

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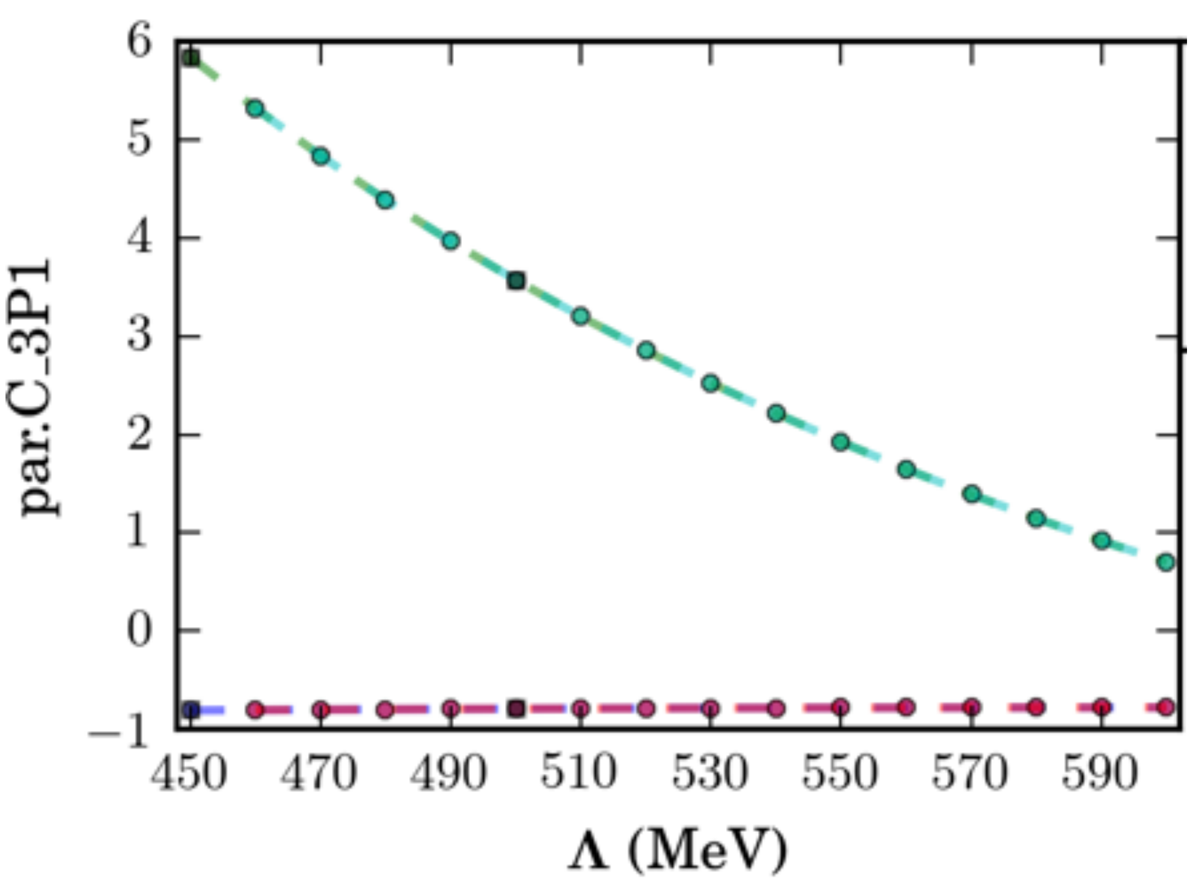

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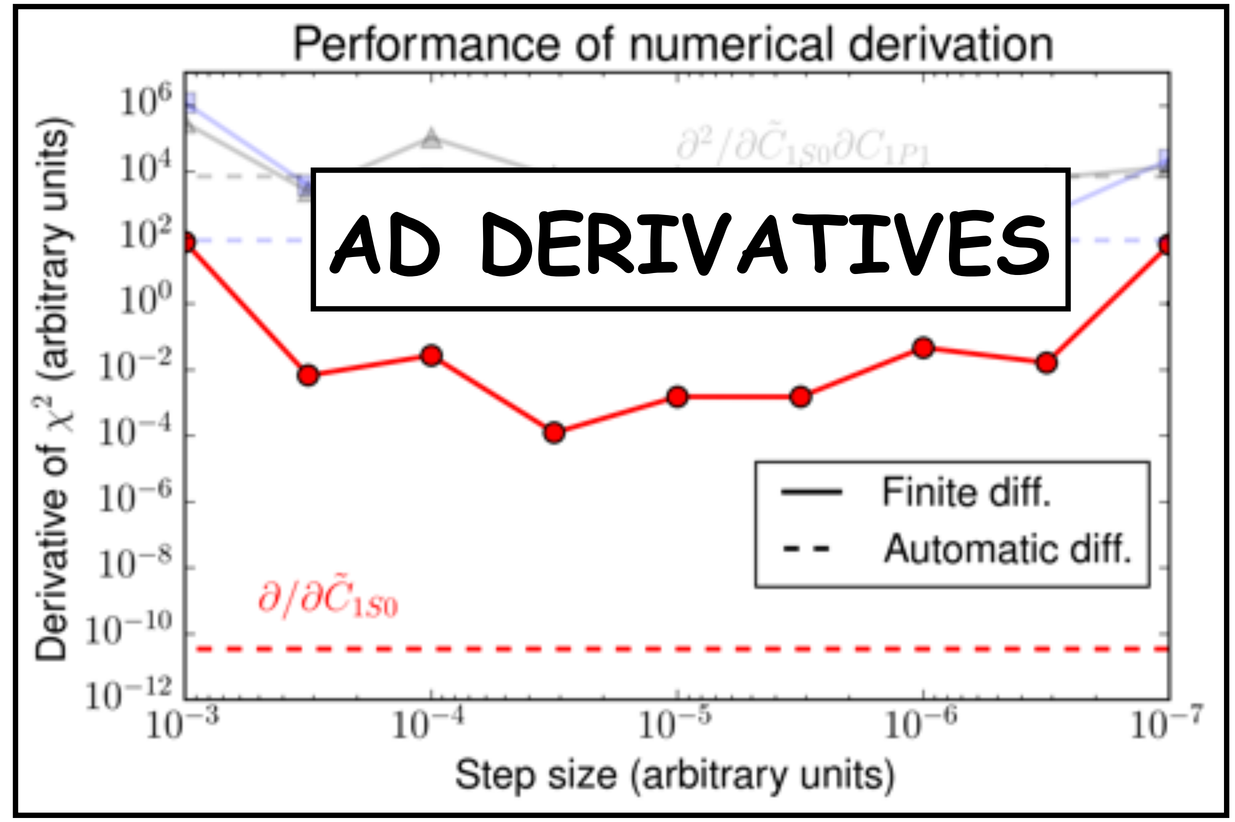

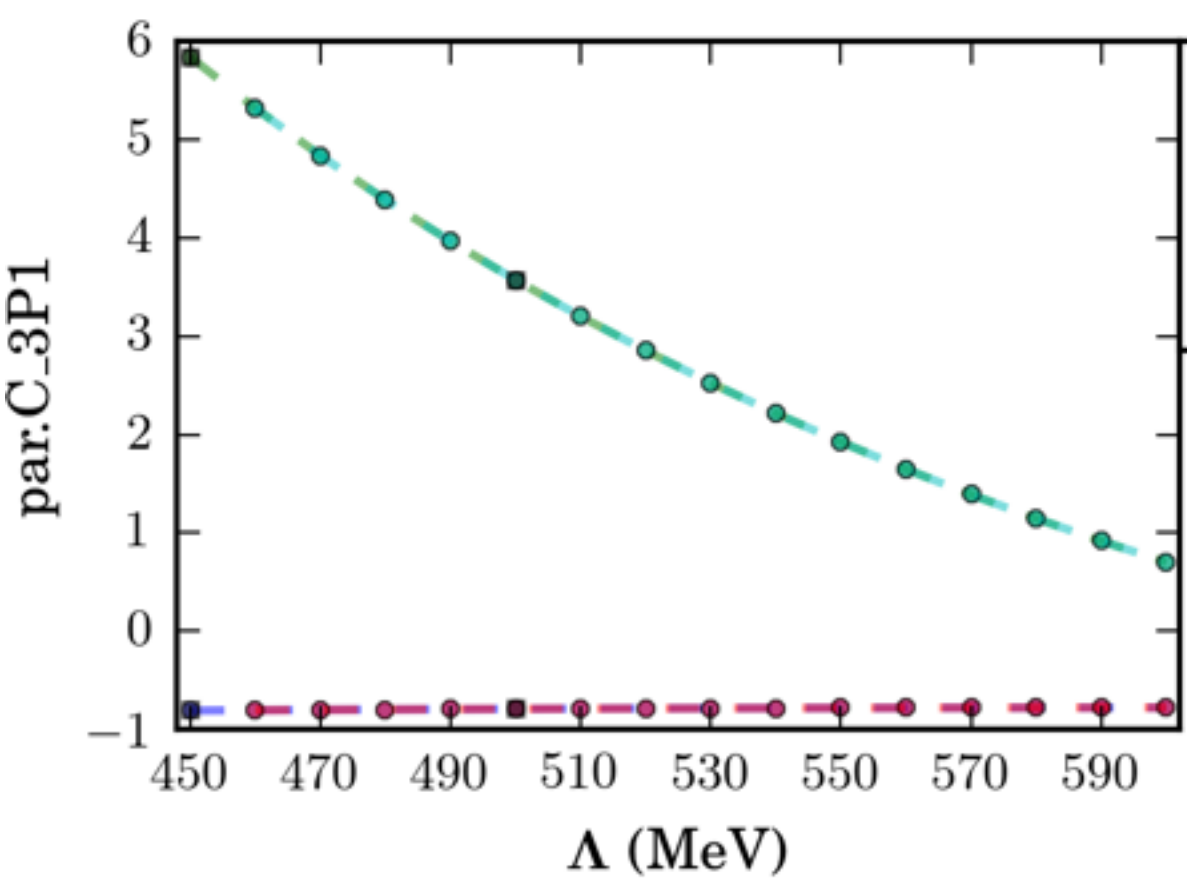

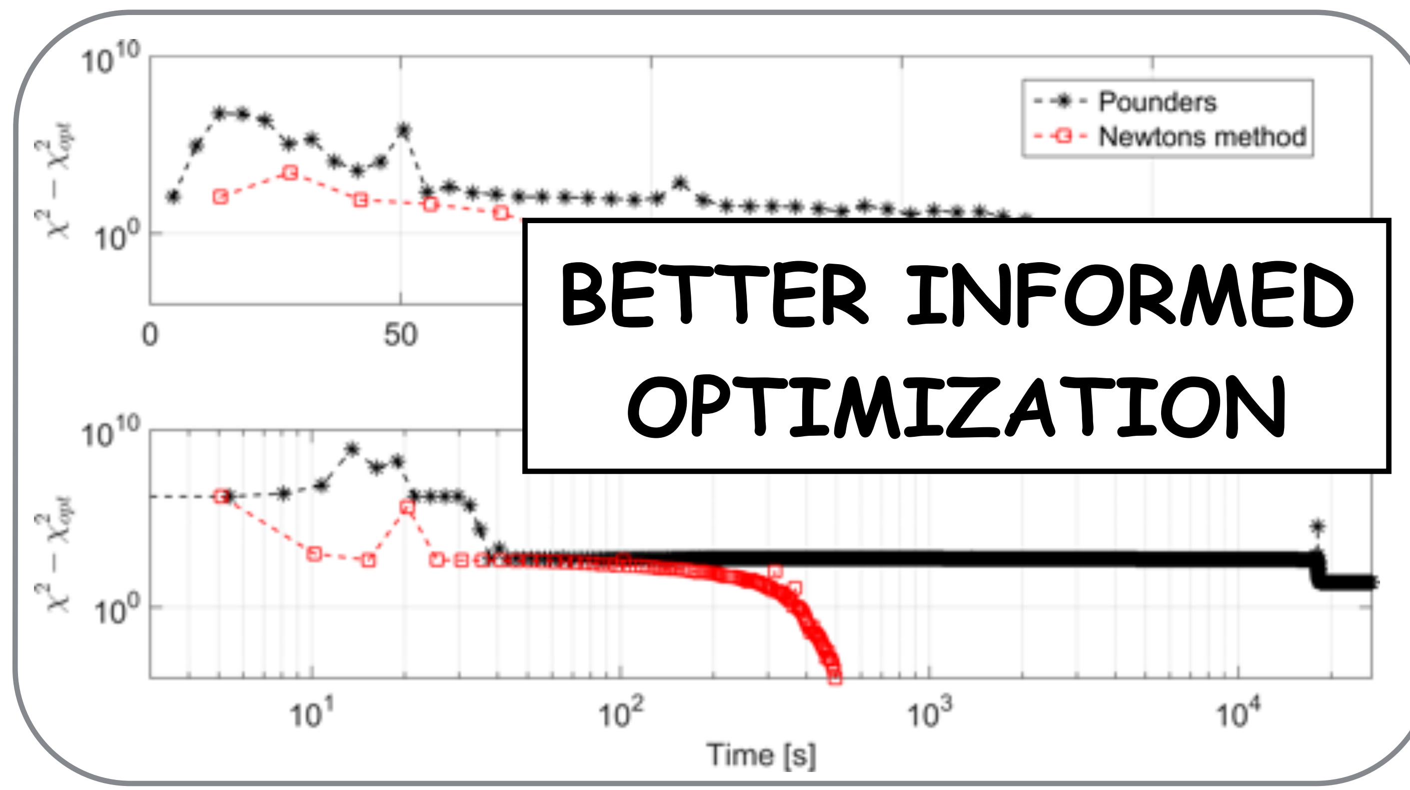

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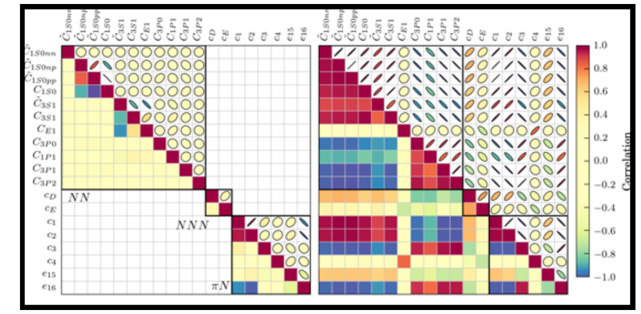
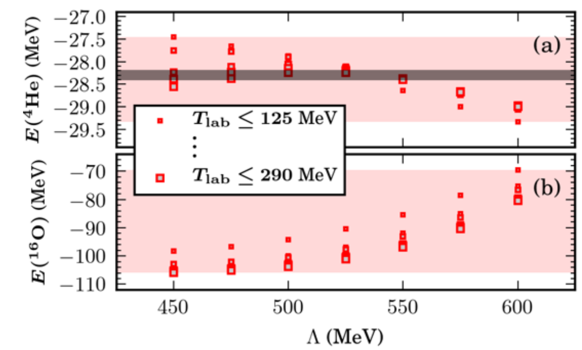
Summary and conclusions

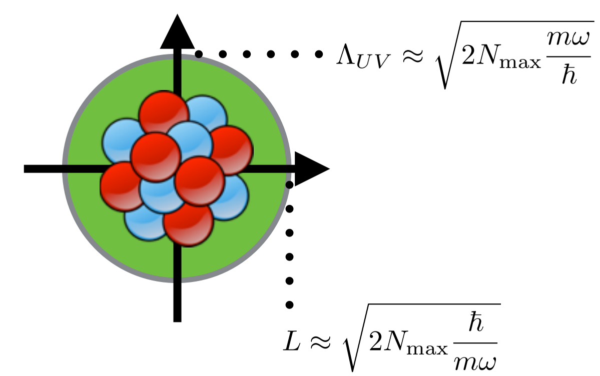
- ***Covariance matrices*** *for optimized LO-NLO-NNLO potentials available for download*



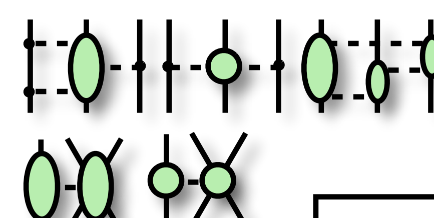
- ***Small variations*** *in the nuclear interaction renders* ***large fluctuations*** *in predictions for heavier nuclei*



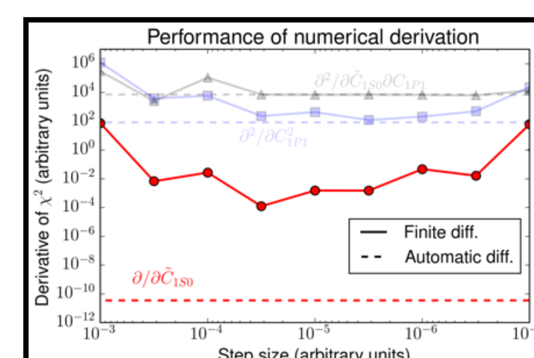
- ***Harmonic Oscillator EFT*** *could be a promising approach for ab initio studies of heavy atomic nuclei*



- ***Non-local 3NF at N3LO*** *is not constrained by A=2,3 data*



- ***N3LO optimizations*** *benefit from gradients*



Thank you for your attention

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