Global Sensitivity Analysis of Bulk Properties of an Atomic Nucleus

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Presenting work from collaboration with

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Sean Miller
Thomas Papenbrock
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Achim Schwenk
Zhonghao Sun
Isak Svensson
Sarah Wesolowski

Progress in Ab Initio Techniques in Nuclear Physics, March 3-6, 2020, TRIUMF

CHALMERS UNIVERSITY OF TECHNOLOGY

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Overview

- Fast and accurate emulation using eigenvector continuation (EC)
- Sub-space projected coupled cluster theory (SP-CC)
- Global sensitivity analysis of the ground-state energy/radius of 16-Oxygen
- Recent developments:SP-CC and excited states, Bayesian parameter estimation, GPUs

Physics questions

- How do properties of atomic nuclei depend on the underlying interaction between protons and neutrons?
- What is the predictive power of ab initio nuclear theory?
- Some interaction models work better than others, but only for selected types of observables and in limited regions of the nuclear chart, e.g. NNLO_{sat}, 1.8/2.0 (EM), $\Delta\text{NNLO}_{\text{go}}$. **Why?**

Summary

The sub-space projected coupled-cluster method enables **emulation of nuclear observables** at different values of the coupling constants in chiral Hamiltonians at unprecedented speed:

- Ground-state energy
- Ground-state radius
- Excited state energies

A global sensitivity analysis indicates that the NNLO description of the radius of 16-O depends sensitively on higher order correlations between the LECs.

Bayesian inference in nuclear physics is rapidly moving forward.

Outlook: sophisticated statistical computation in ab initio nuclear theory!

(Next talk by C. Forssén)

Bayesian inference: from likelihood & prior to posterior.

- Collect N data points that we gather in a data vector **D**
- Propose some model **M** to explain the data, depending on the parameter vector **α**
- Apply Bayes' theorem

Posterior — **Likelihood** — Prior

$$P(\vec{\alpha}|D,M) = \frac{P(D|\vec{\alpha},M)\cdot P(\vec{\alpha}|M)}{P(D|M)}$$

Marginal likelihood

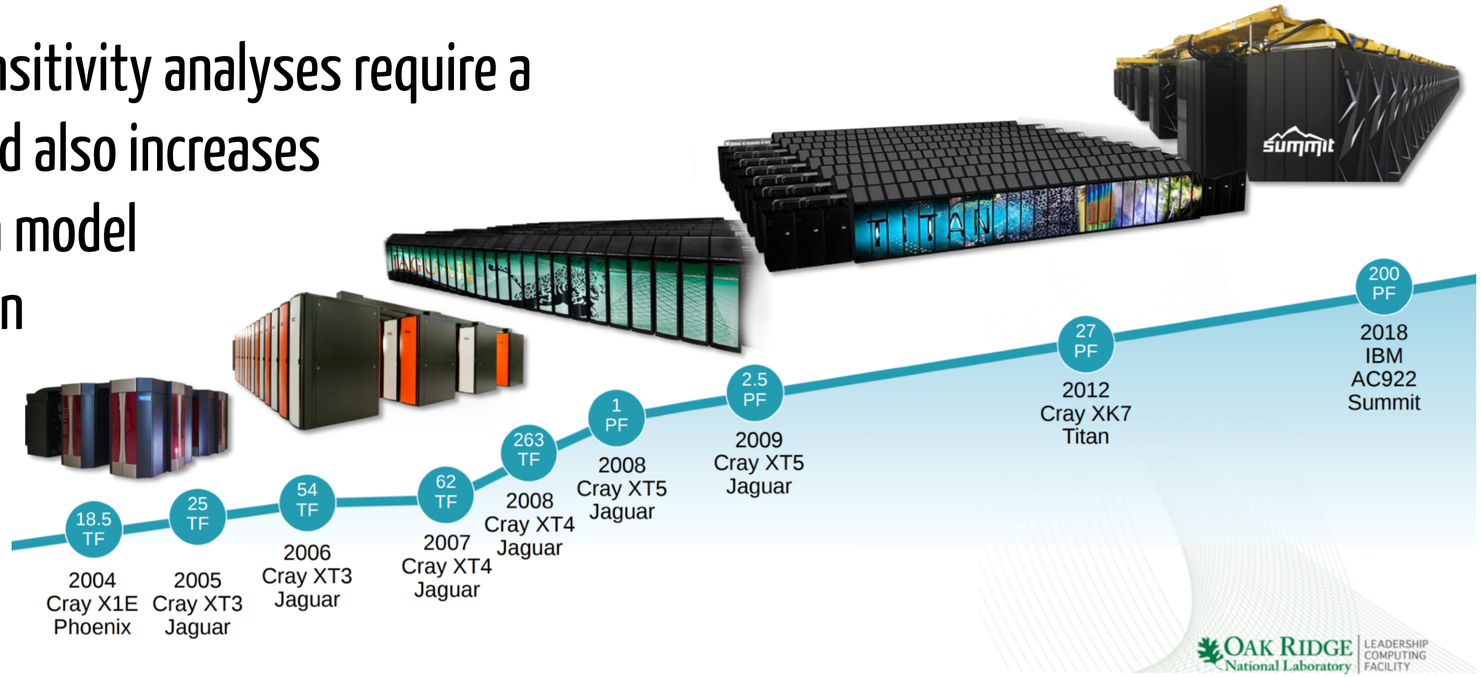
- The **prior** encodes our knowledge about the parameter values before analyzing the data
- The **likelihood** of the data given a set of parameters
- The **marginal likelihood** (or model evidence) provides normalization of the posterior
- The **posterior** is the complete inference and resulting probability density for the parameters **α**

Computing nuclei: the curse of dimensionality

Solving the Schrödinger equation for a large collection of strongly interacting nucleons is an interesting challenge that typically requires substantial high-performance computing resources.

$$\hat{H}|\Psi_i\rangle = E_i|\Psi_i\rangle$$

Rigorous uncertainty quantification and sensitivity analyses require a large number of model samples. The demand also increases exponentially with the number of uncertain model parameters. Clearly, this is not feasible given the computational cost of existing many-body methods.



“Eigenvector Continuation as an Efficient and Accurate Emulator for Uncertainty Quantification”

S. König, et al. arXiv:1909.08446 [nucl-th]

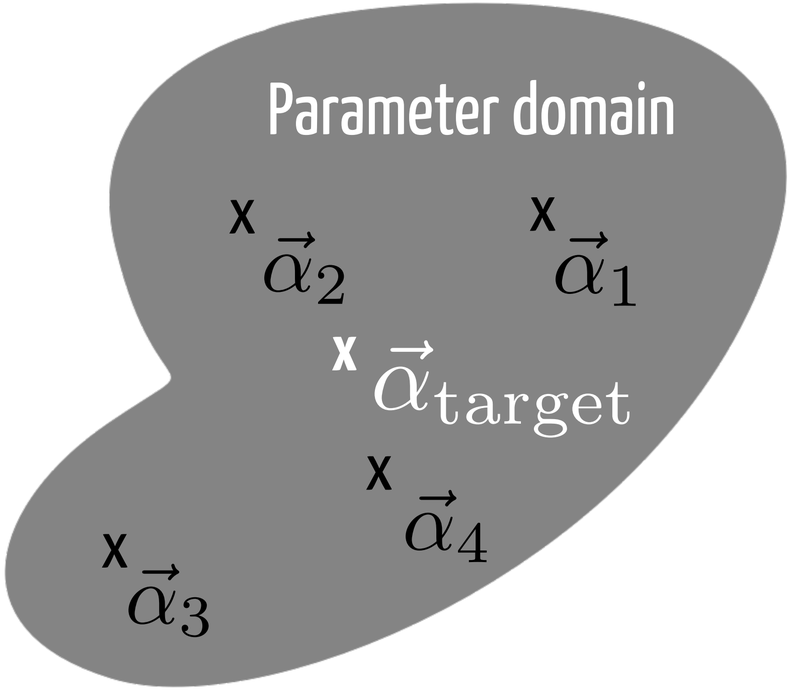
(See S. König talk)

Eigenvector continuation: emulating nuclei

We have a Hamiltonian that depends smoothly on some LECs $\hat{H}(\vec{\alpha})$

For the potential models we can often write the LEC dependence as $\hat{H}(\vec{\alpha}) = \hat{H}_0 + \sum_{i=1}^{N} \alpha_i \hat{H}_i$

We seek the lowest energy and wavefunction in a given symmetry class for some target value $\vec{\alpha}_{\rm target}$



Project each term $\hat{H}_i$ to the eigenvector subspace, represented here by a 4-by-4 matrix, and **quickly** solve for the eigenvalues and eigenvectors at any $\vec{\alpha}_{\rm target}$

Tremendous gain: replaced original large space eigenvalue problem with a generalized eigenvalue problem of considerably smaller dimension.

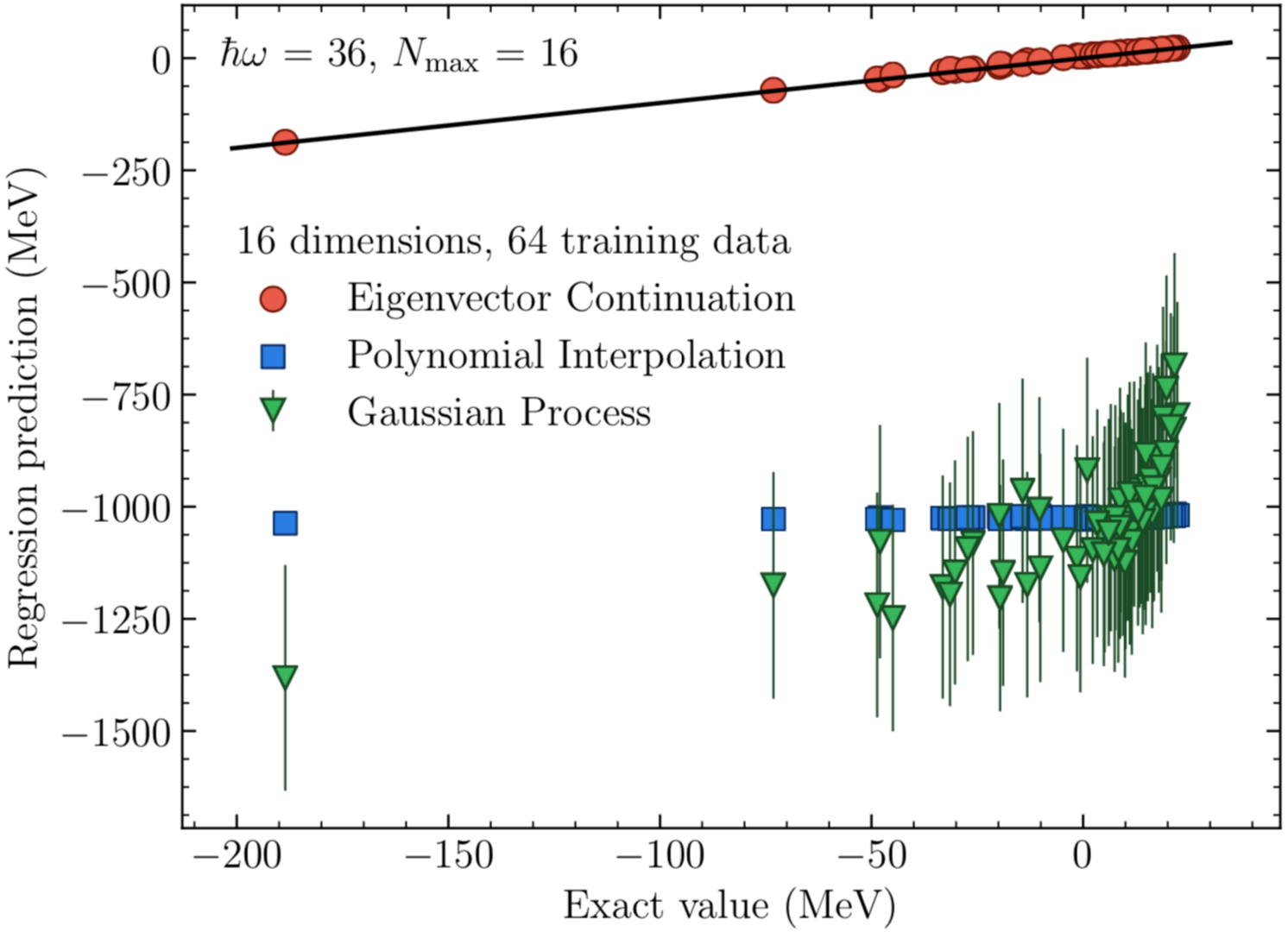
$$\tilde{H}|\tilde{\Psi}(\vec{\alpha}_{\rm target})\rangle = E_{\rm target} N |\tilde{\Psi}(\vec{\alpha}_{\rm target})\rangle$$

D. Frame, et al. Phys. Rev. Lett. 121, 032501 (2018)

S. König, et al. arXiv:1909.08446 [nucl-th]

(See S. König talk)

Eigenvector continuation: example ($N_{parameters}$=16)



^{4}He
NNLO(450)

S. König, et al. arXiv:1909.08446 [nucl-th]

What about heavier systems?

“Global Sensitivity Analysis of Bulk Properties of an Atomic Nucleus”

A. Ekström and G. Hagen Phys. Rev. Lett. **123**, 252501 (2019)

Sub-space projected coupled-cluster theory

The no-core shell-model for nuclei corresponds to fully diagonalizing the nuclear Hamiltonian.
Straightforward, although computationally expensive with increasing mass number.

Coupled-cluster (CC) theory exploits a similarity transformed Hamiltonian $\bar{H}(\vec{\alpha}) = e^{-T(\vec{\alpha})} H(\vec{\alpha}) e^{T(\vec{\alpha})}$

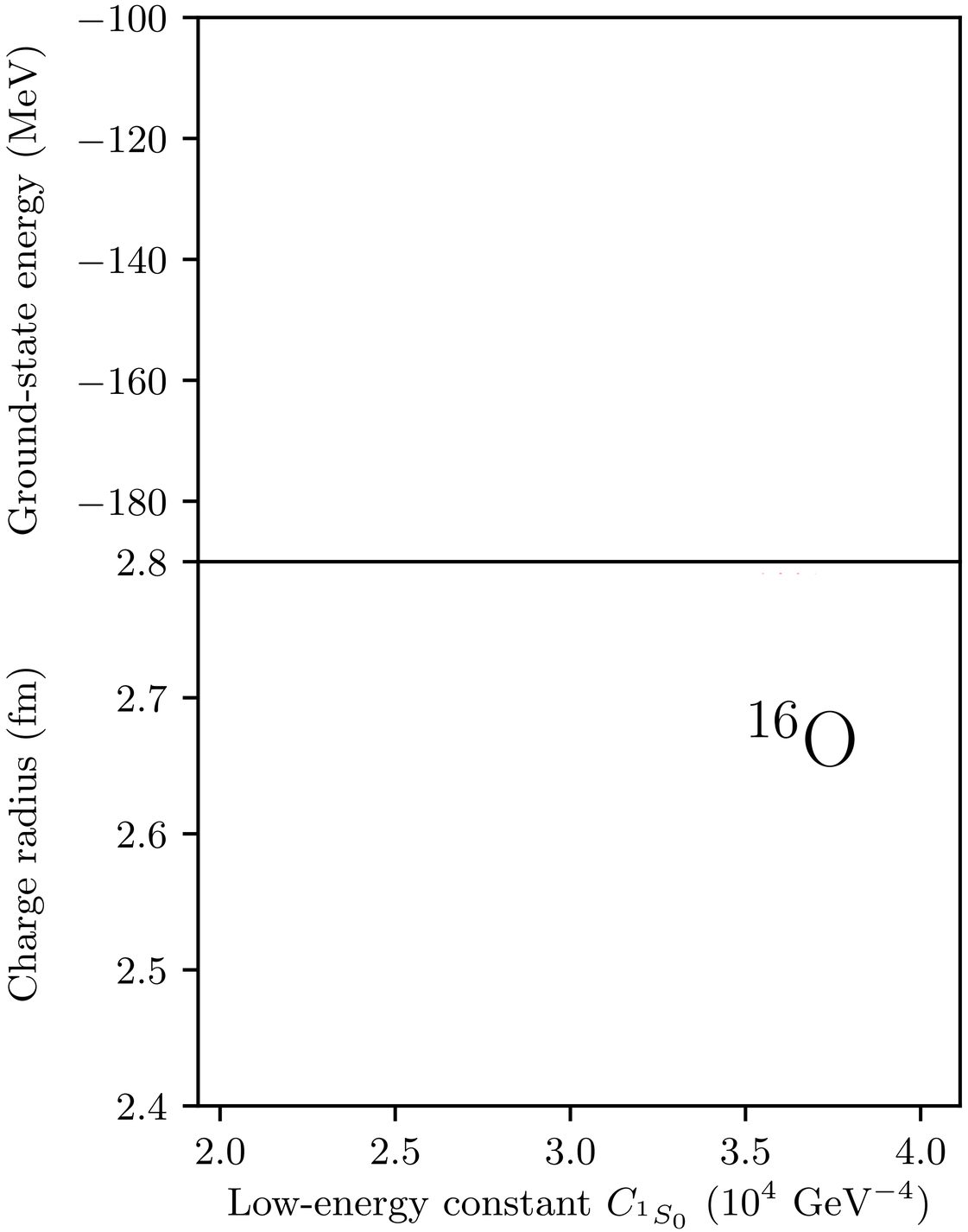
Where in the singles and doubles approximation (CCSD) the cluster operator is $T(\vec{\alpha}) = T_1(\vec{\alpha}) + T_2(\vec{\alpha})$

The sub-space projected coupled-cluster (SP-CC)Hamiltonian, which we end up diagonalizing,
is non-hermitian and given by

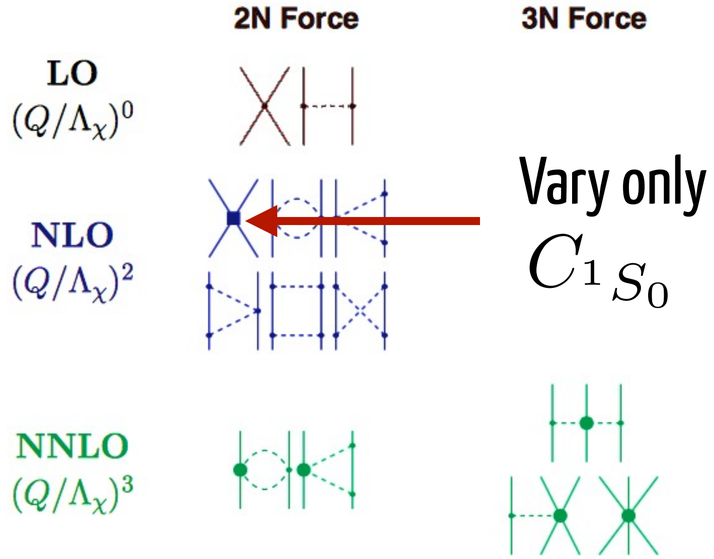
$$\langle \tilde{\Psi}' | H(\vec{\alpha}_{\text{target}}) | \Psi \rangle = \langle \Phi_0 | (1 + \Lambda(\vec{\alpha}')) e^{-T(\vec{\alpha}') + T(\vec{\alpha})} \bar{H}(\vec{\alpha}_{\text{target}}) | \Phi_0 \rangle$$

Large-space CCSD states
at $\vec{\alpha}'$ and $\vec{\alpha}$

A. Ekström and G. Hagen Phys. Rev. Lett. **123**, 252501 (2019)

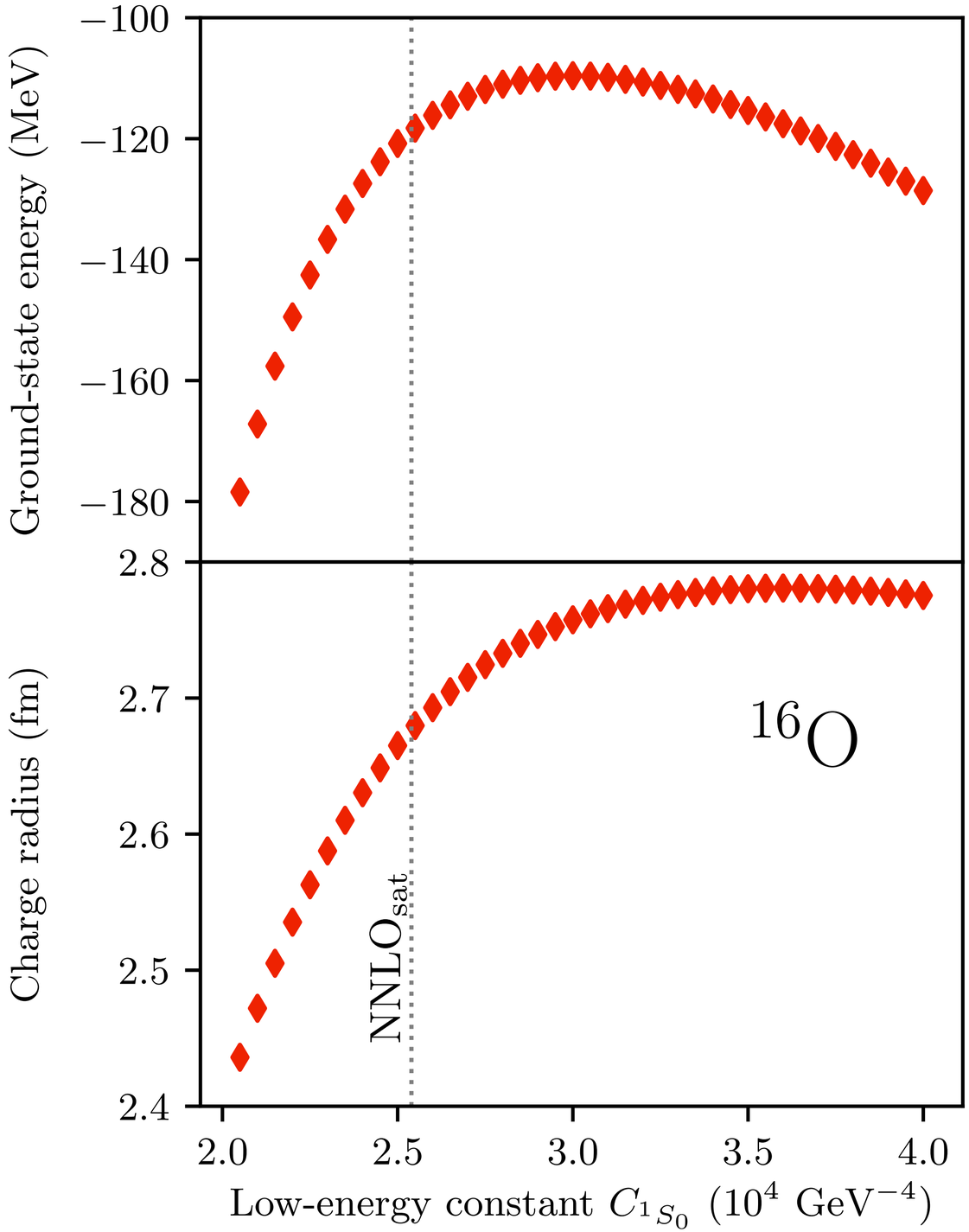


Exact coupled cluster calculations at the singles and doubles level



Vary only C_{1S_0}

A. Ekström and G. Hagen Phys. Rev. Lett. **123**, 252501 (2019)



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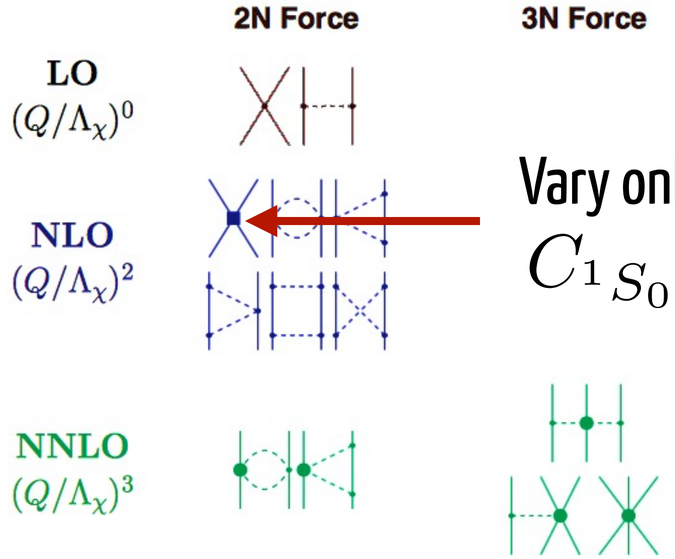

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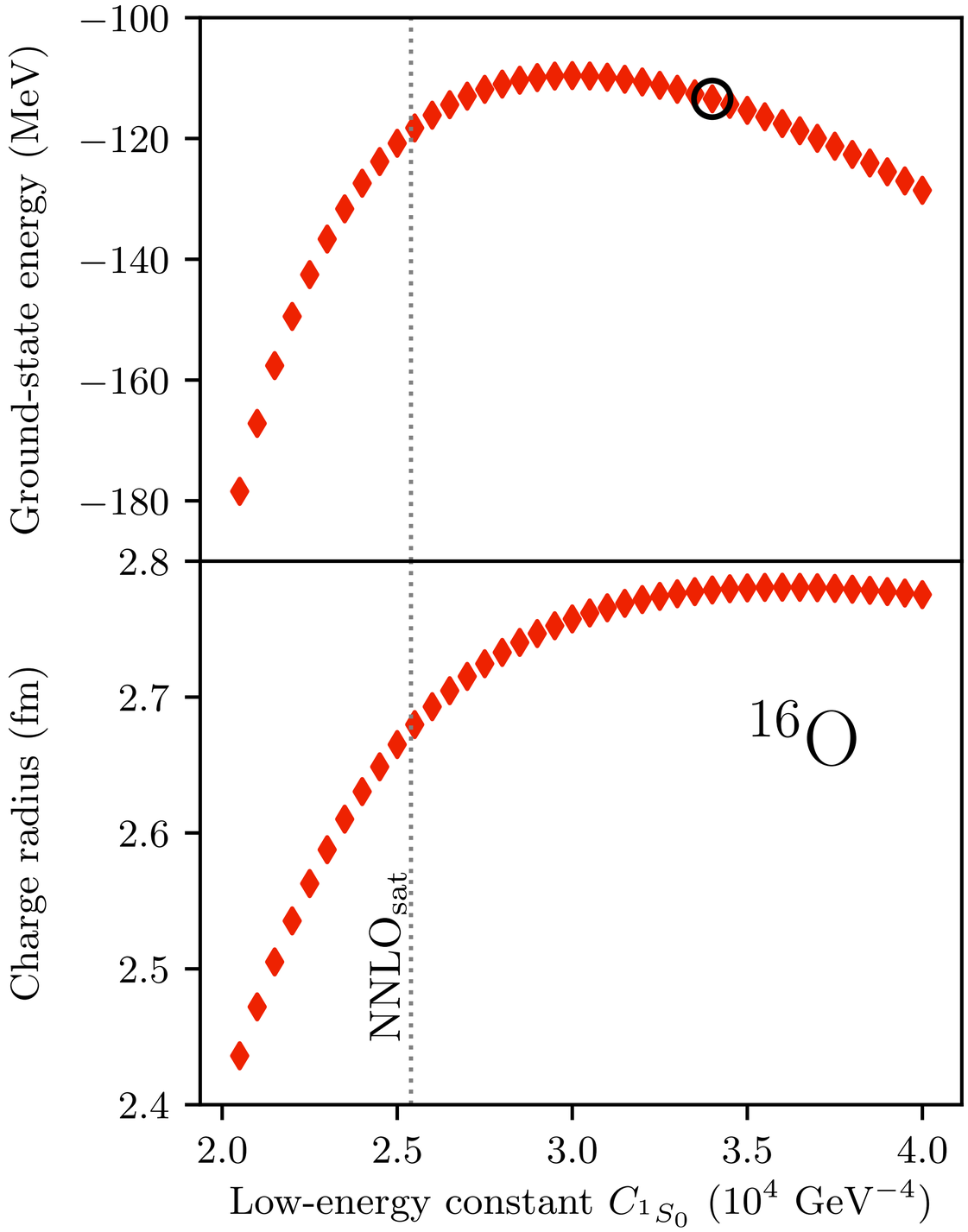

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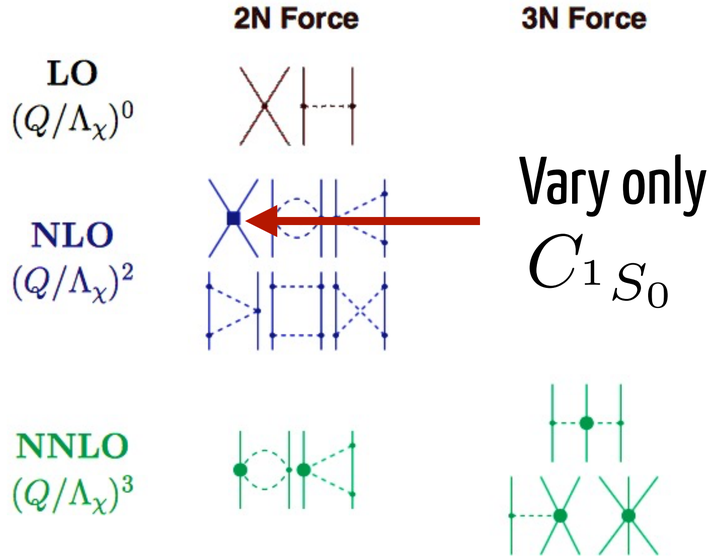

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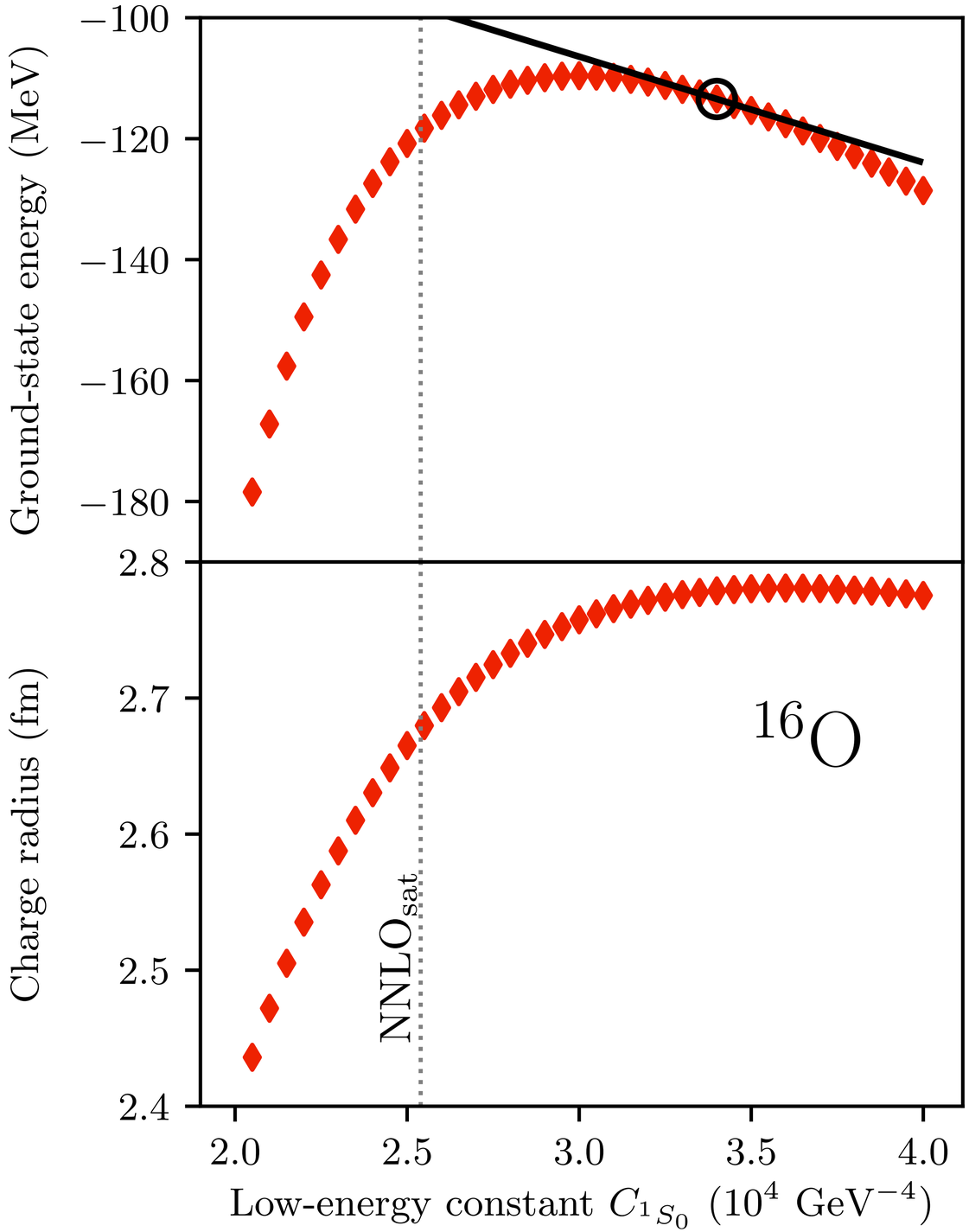

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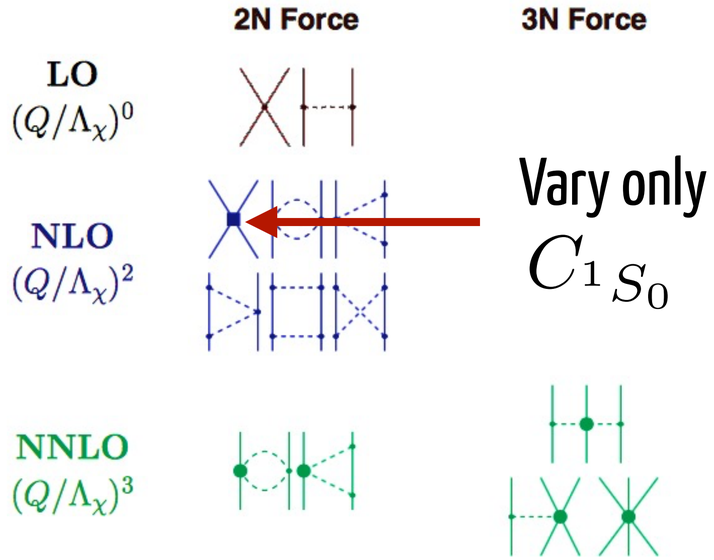

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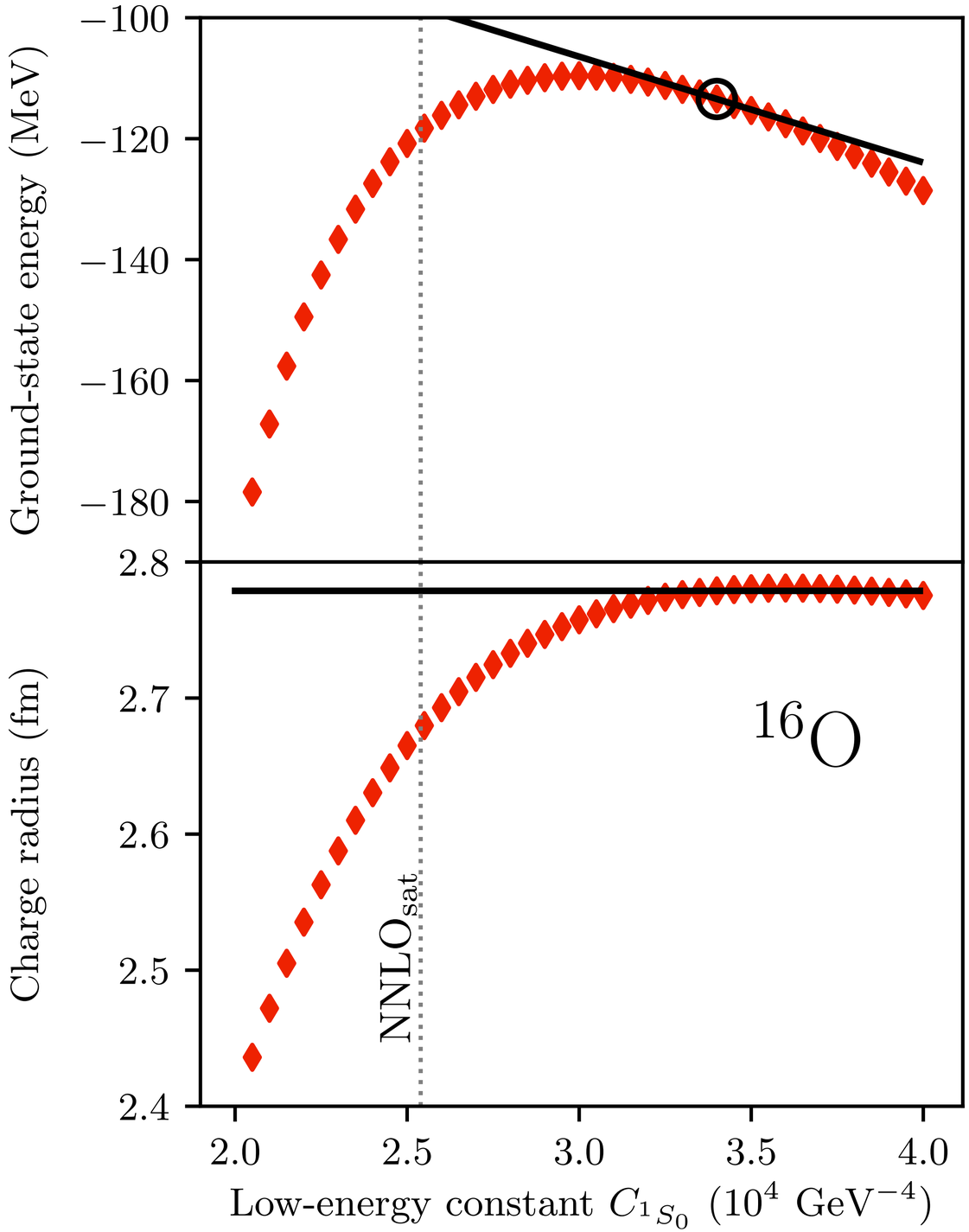

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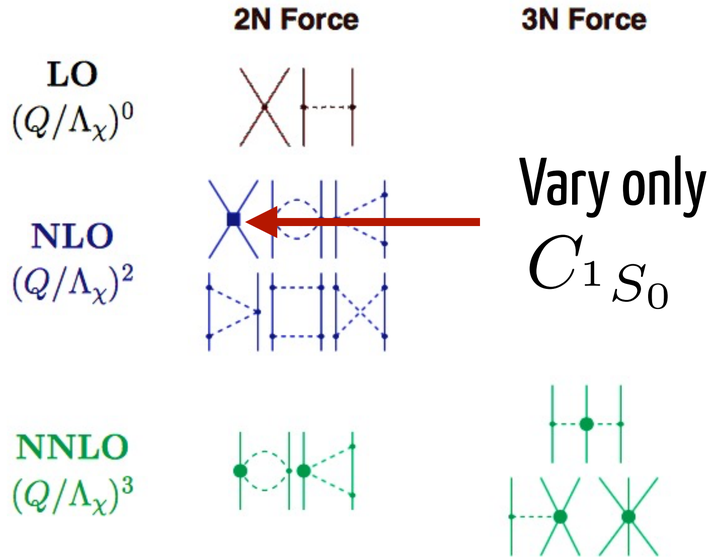

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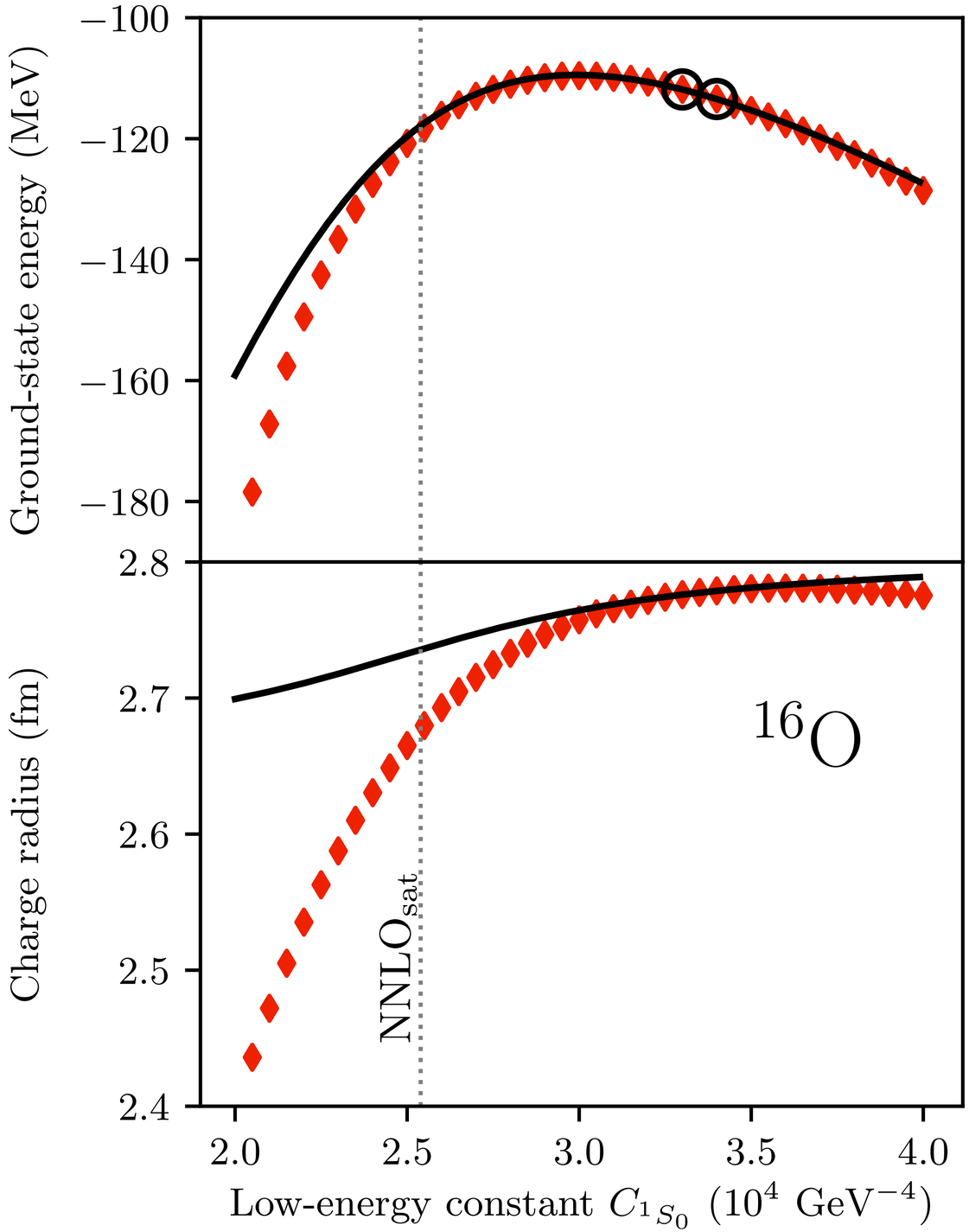

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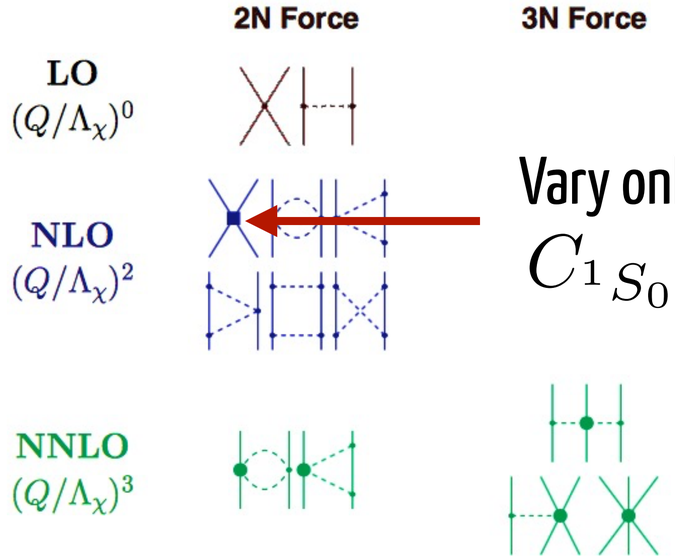

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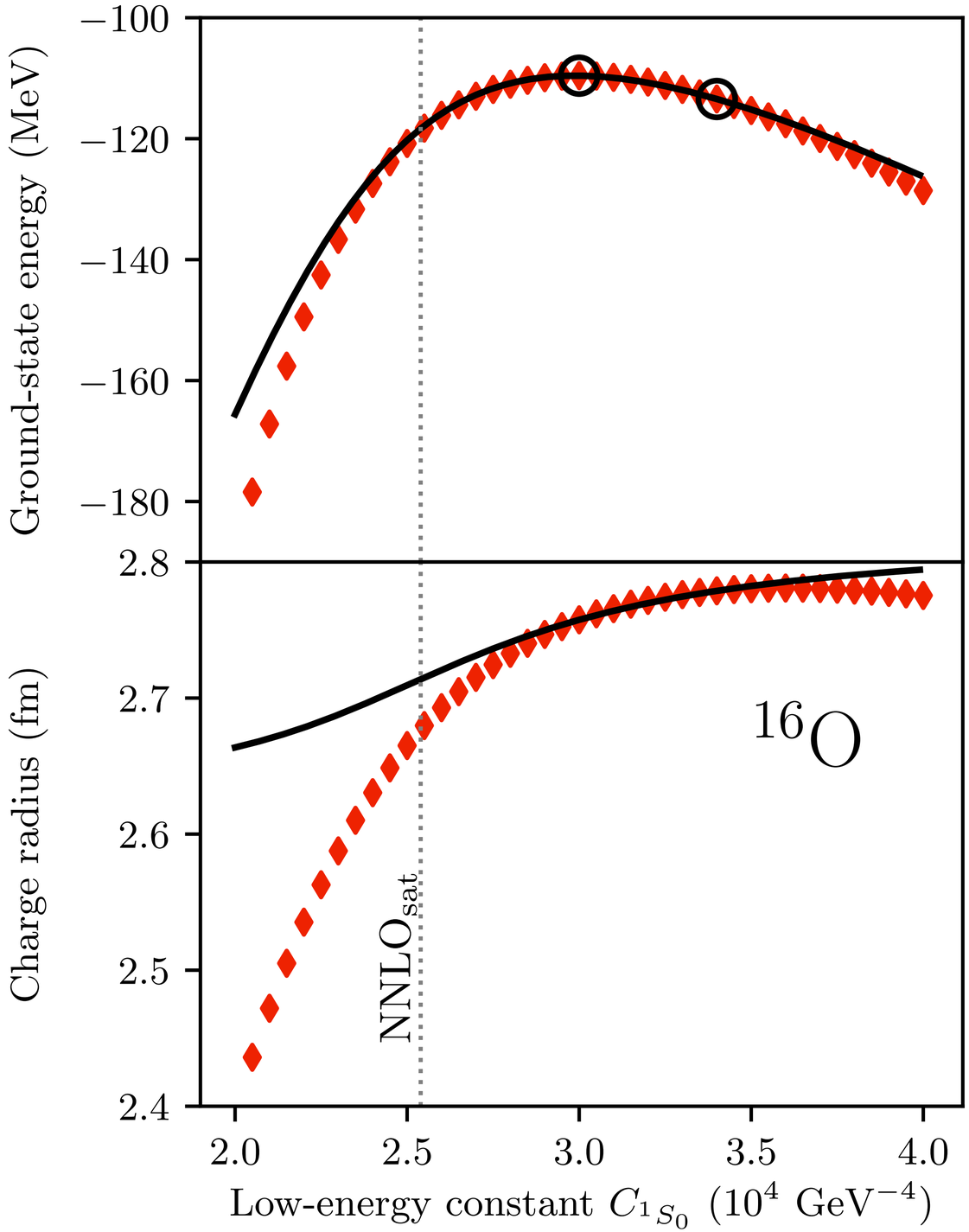

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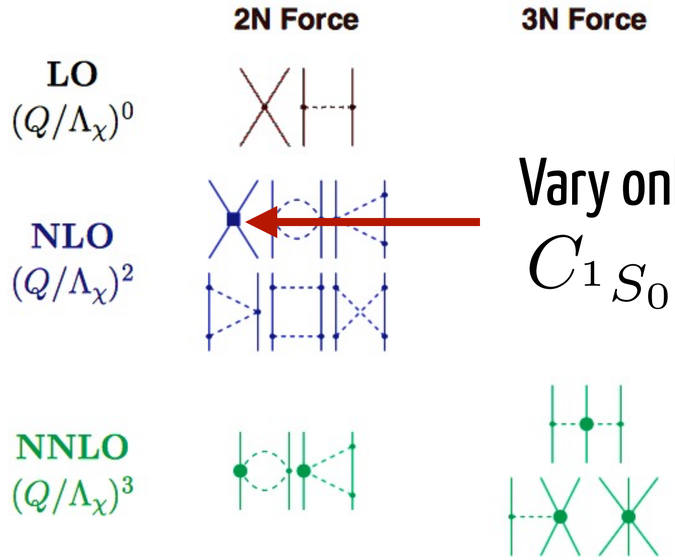

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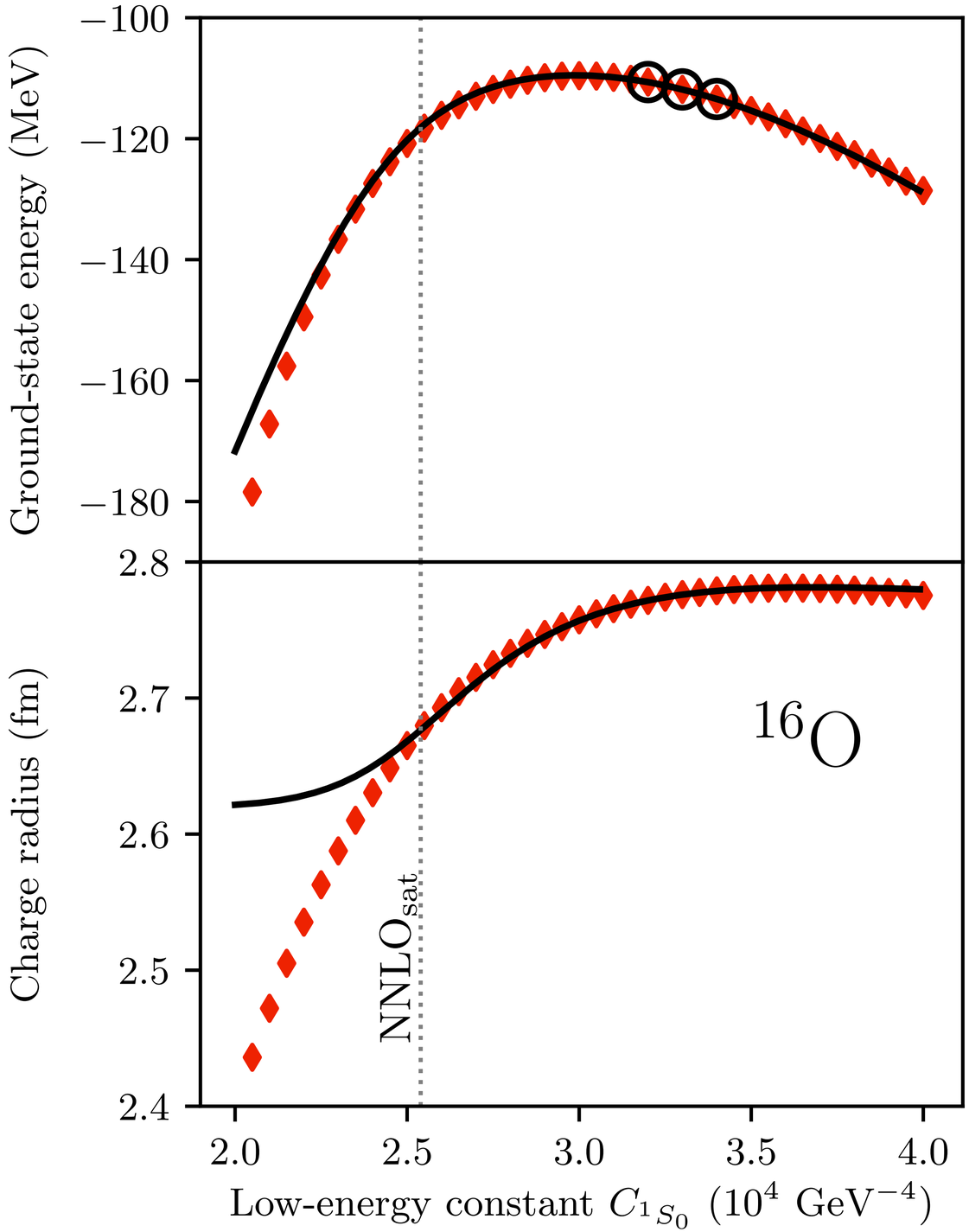

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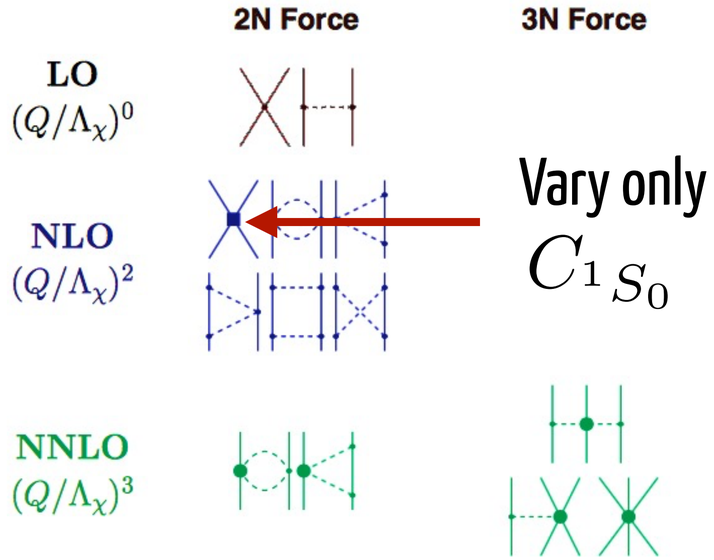

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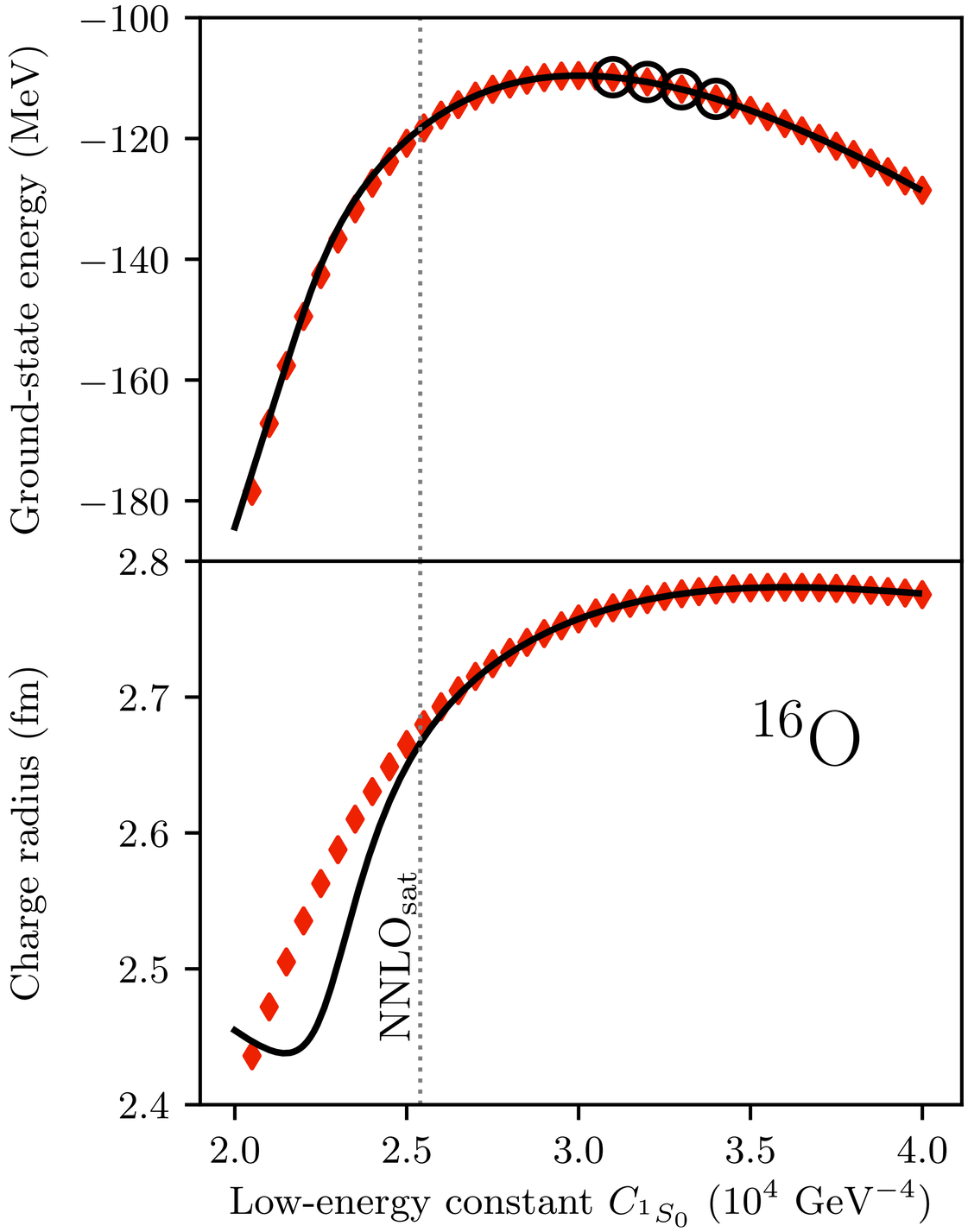

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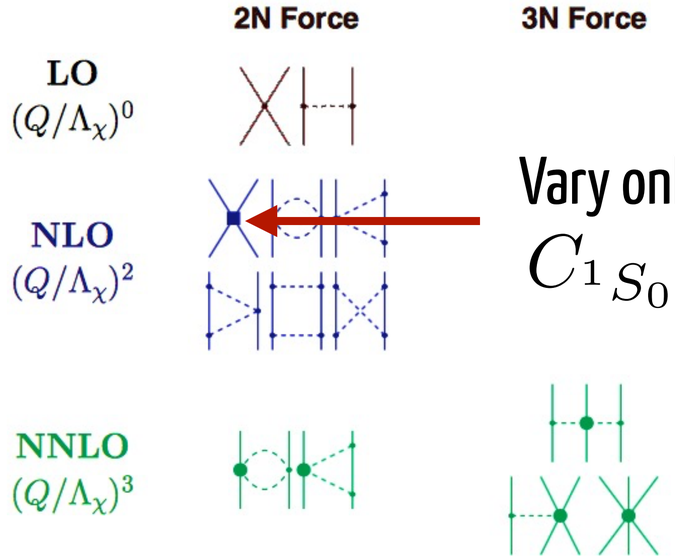

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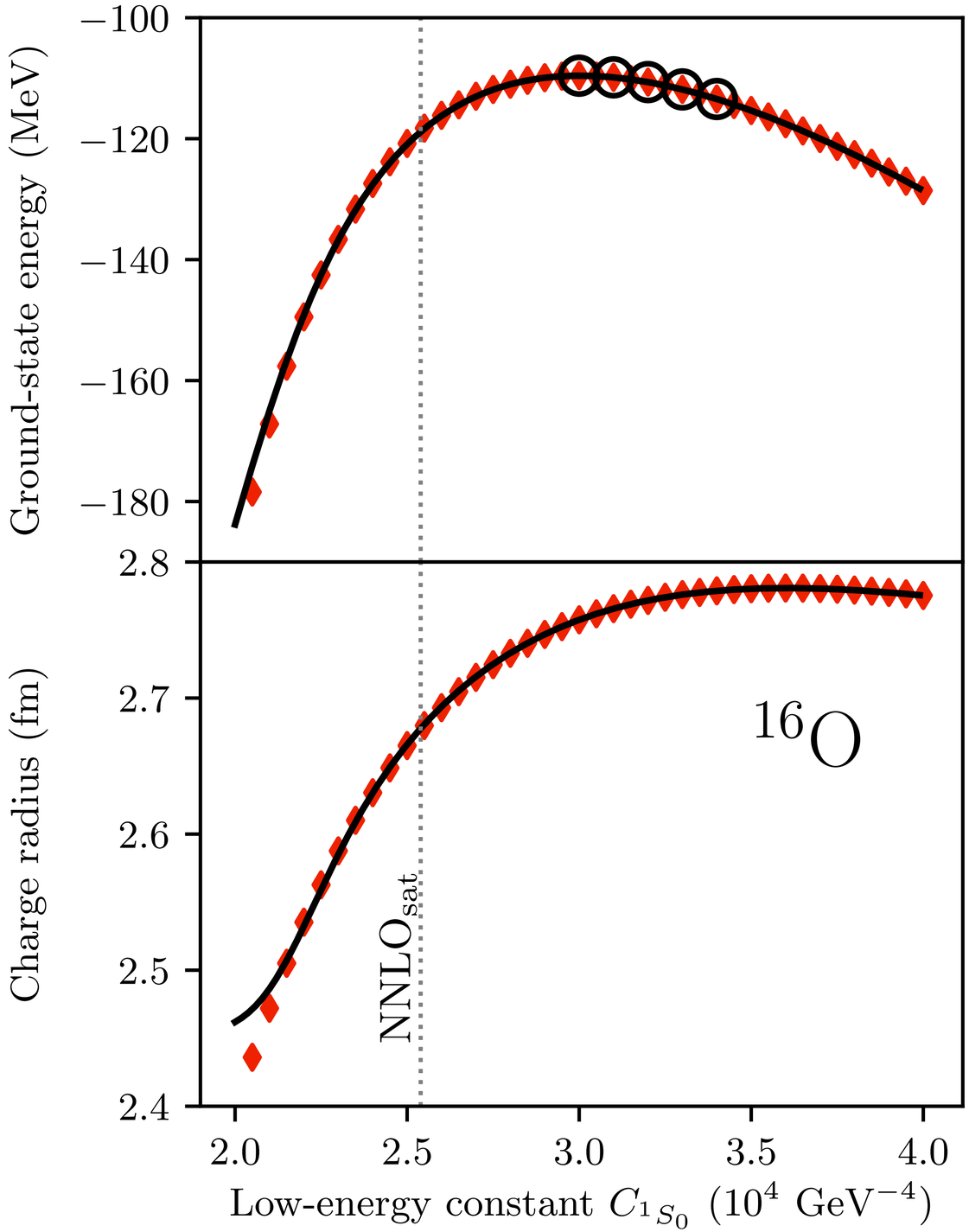

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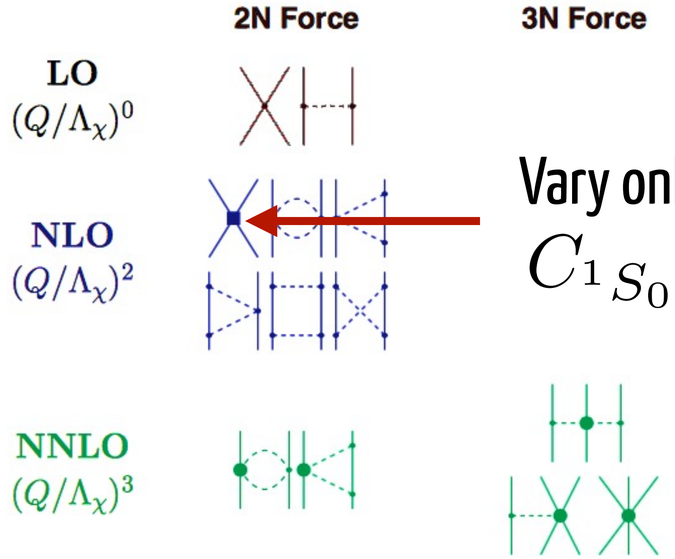

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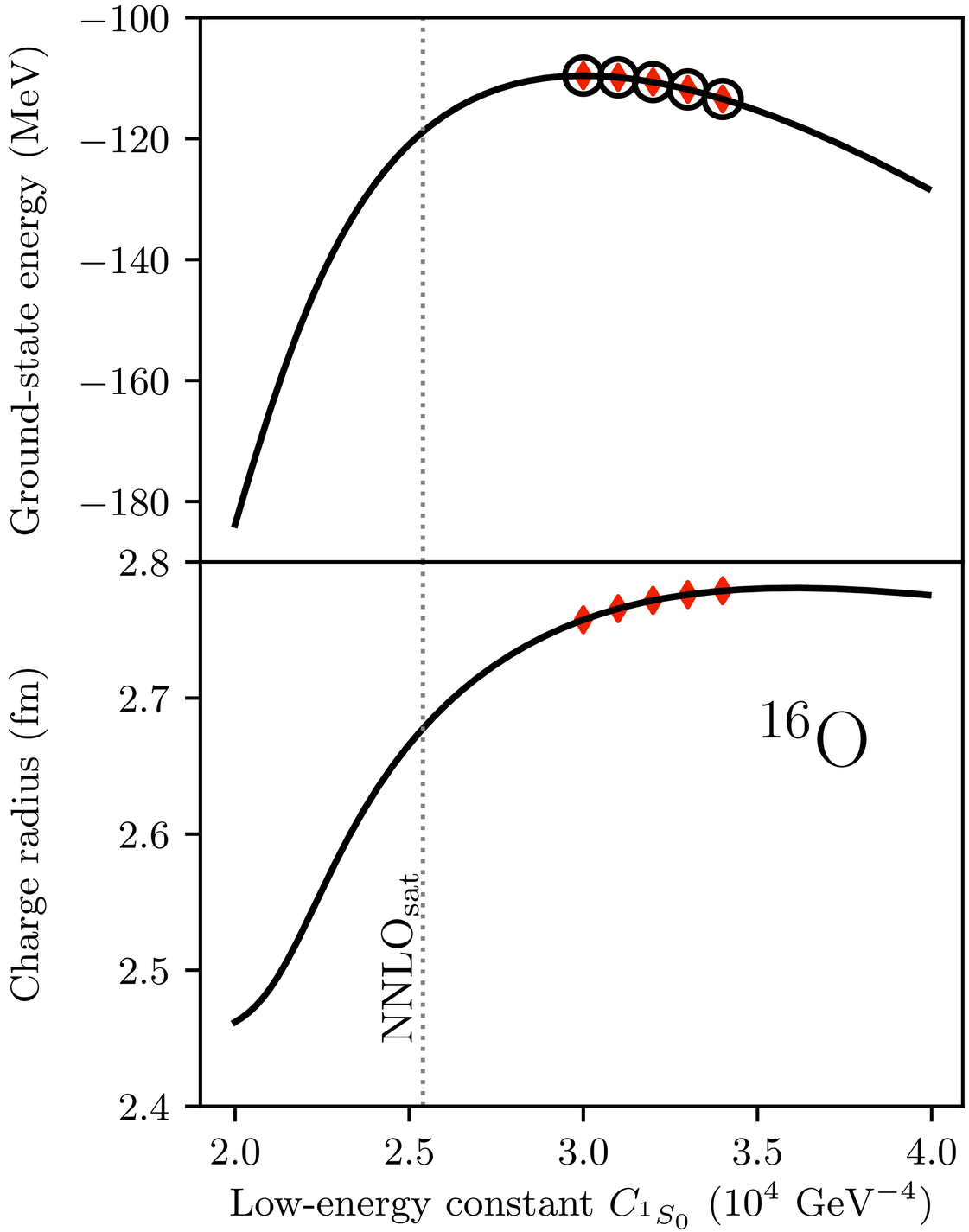

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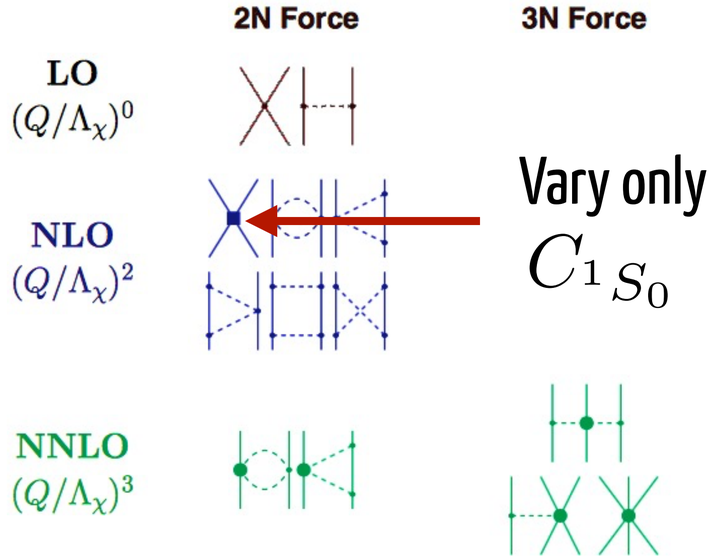

Vary only C_{1S_0}

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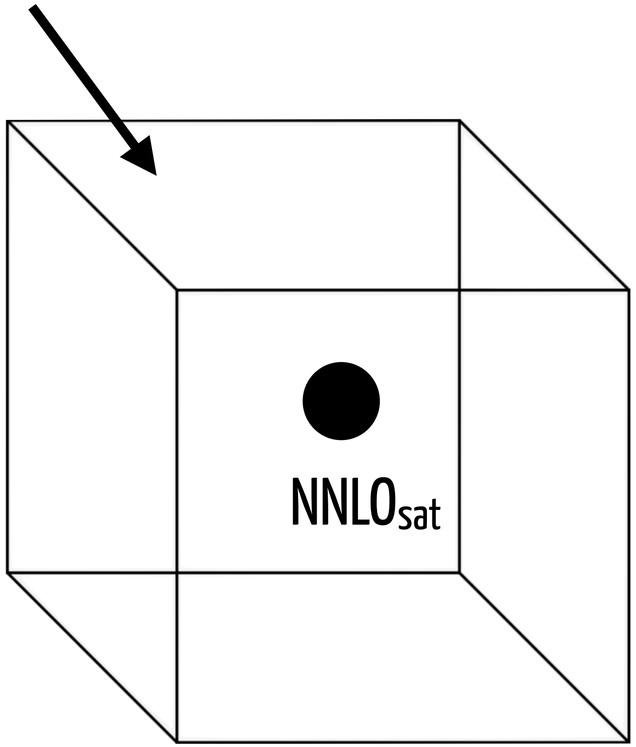
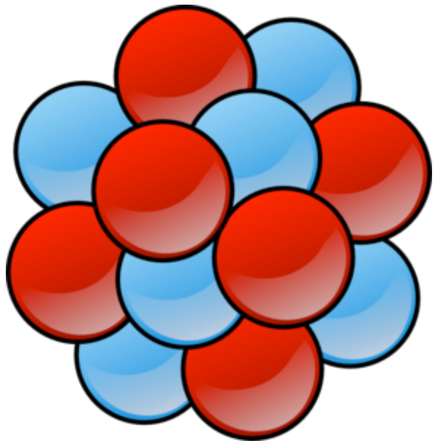
Realistic application: ^{16}O with an NNLO Hamiltonian

Huge α-space



±20% variation in all parameters
with respect to a well-know point



Two sets of exact CCSD calculations to setup
two sub-space projected CCSD Hamiltonians

SPCC(64)
SPCC(128)

Takes a few milliseconds
to diagonalize exactly

Incorporate prior information: $H_{\mathrm{nn}} \approx H_{\mathrm{np}} \approx H_{\mathrm{pp}}$

Coupled-cluster singles and doubles approximation CCSD

N_{max}=10, hw=16 MeV, E_{3max}=14

Harmonic oscillator basis

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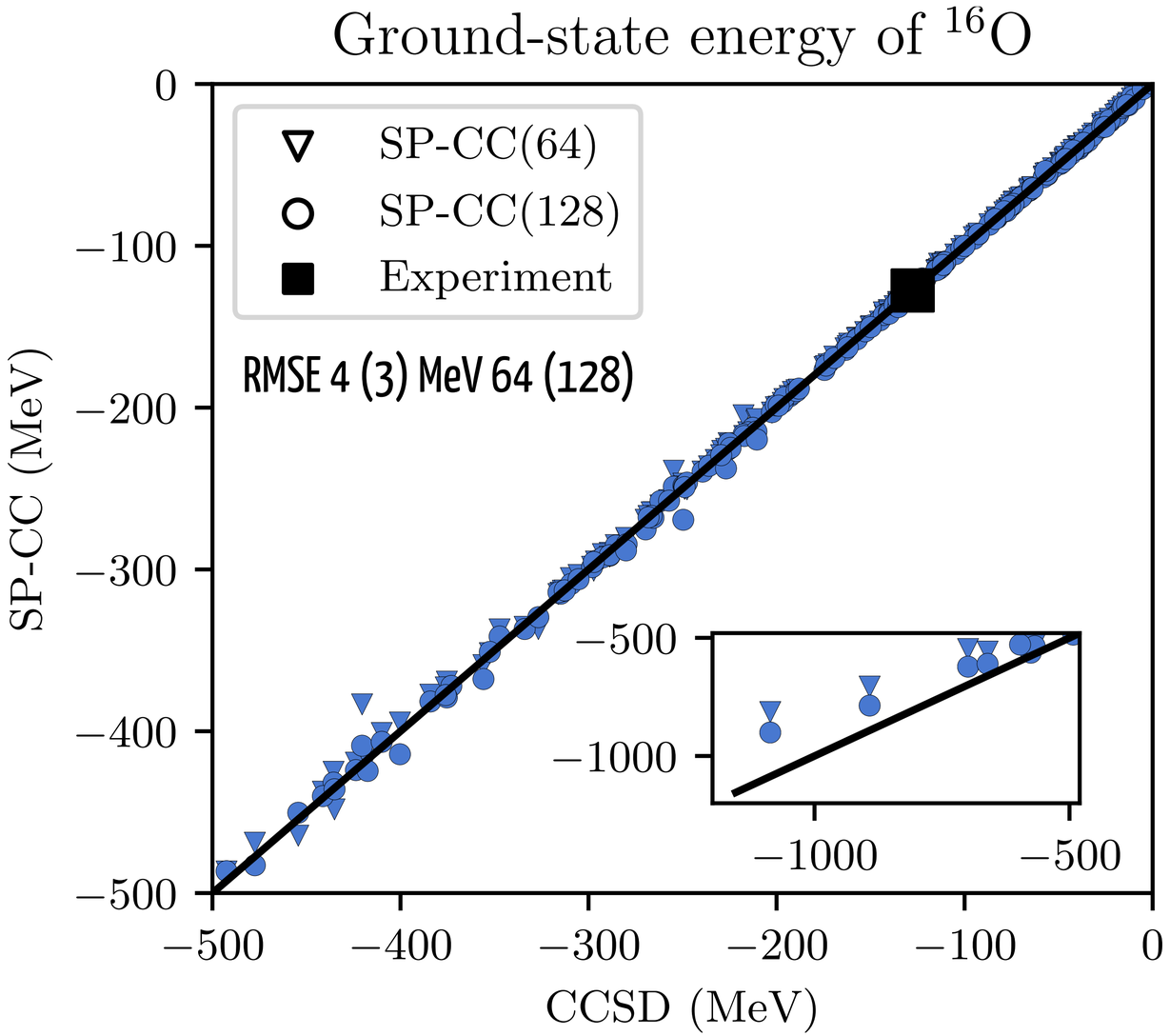
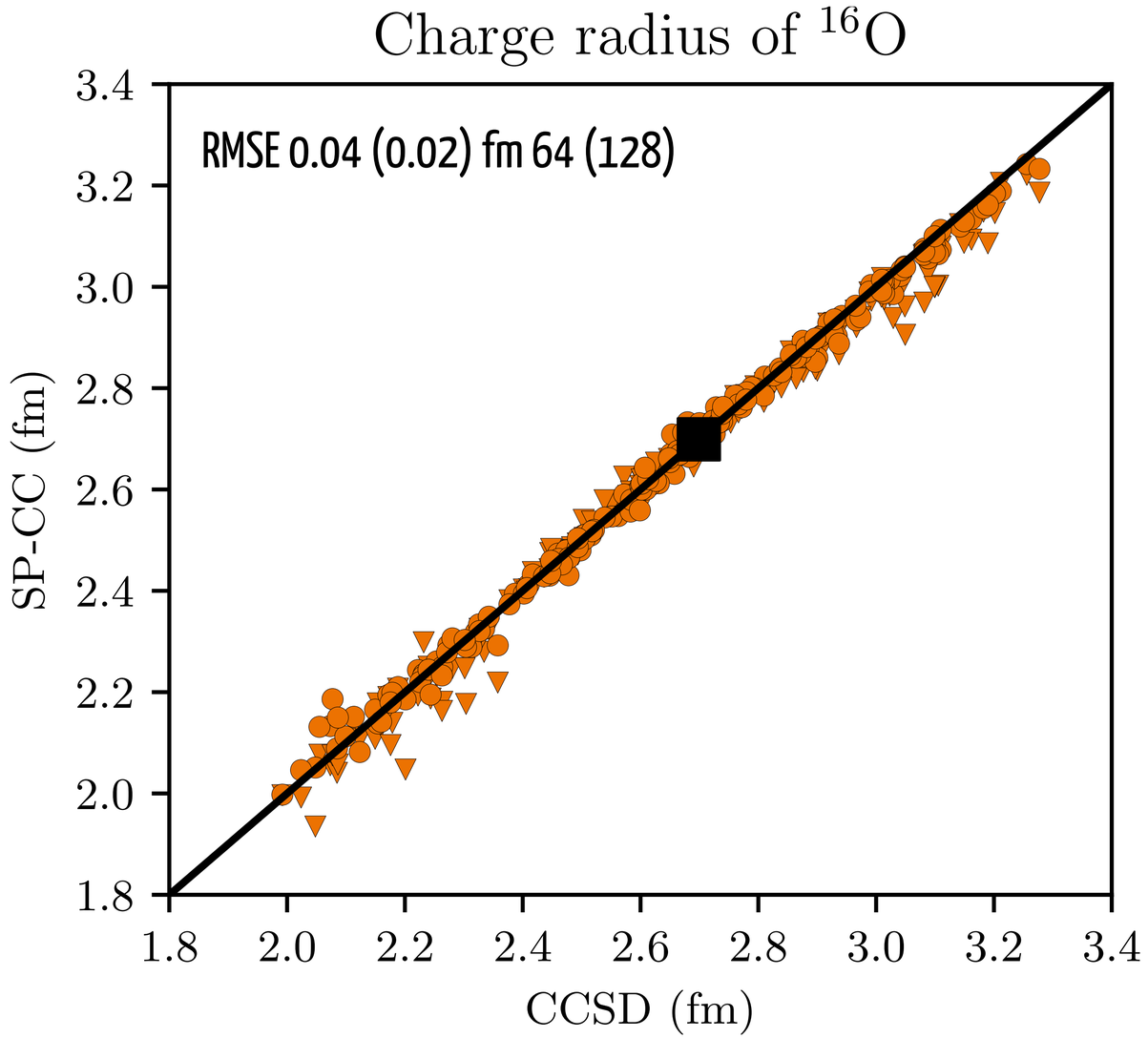
SPCCSD matrices for ^{16}O available

Cross-validation





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Global sensitivity analysis (GSA)

Sensitivity analysis addresses the question ‘How much does each model parameter contribute to the uncertainty in the prediction?’

Uncertainty analysis addresses the question ‘How uncertain is the prediction?’

Variance-based methods for GSA decompose the variance of a certain model output in terms of each input and their combinations.

Global methods deal with the uncertainties of the outputs due to input variations over the whole domain.

A. Saltelli et al. Global sensitivity analysis: the primer, John Wiley & Sons

Sobol sensitivity analysis

Given models for some observable(s)

$$E = f_E(\alpha_1, \alpha_2, \ldots, \alpha_N)$$
$$R = f_R(\alpha_1, \alpha_2, \ldots, \alpha_N)$$

Decompose the total variance:

$$\mathrm{Var}[Y] = \sum_i^N V_i + \sum_{i<j}^N V_{ij} + \ldots$$

Basically requires multiple model evaluations across some pre-determined parameter domain

Compute the variance integrals using MC sampling, which is the computationally expensive part

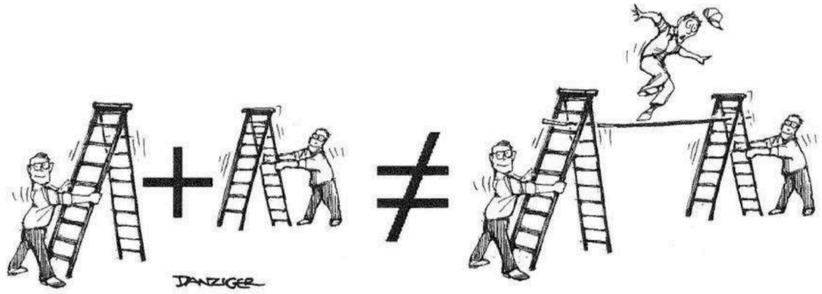
$$V_i = \mathrm{Var}[\mathbb{E}_{\vec{\alpha}\sim\alpha_i}[Y|\alpha_i]]$$
$$V_{ij} = \mathrm{Var}[\mathbb{E}_{\vec{\alpha}\sim(\alpha_i,\alpha_j)}[Y|\alpha_i,\alpha_j]] - V_i - V_j$$

We find it necessary to do ~1 Million computations of ^{16}O to extract statistically significant variances

With SPCCSD(68), 1 hour on my MacBook Pro (2016)

I. M. Sobol Mathematic and Computers in in Simulation **55**, 271 (2001)

Sensitivity indices



$$S_i = \frac{V_i}{\mathrm{Var}[Y]}$$ "Main effect" A number between 0 and 1

$$S_{ij} = \frac{V_{ij}}{\mathrm{Var}[Y]}$$ Second order index Another number between 0 and 1

$$1 = \sum_{i=1}^{N} S_i + \sum_{i<j} S_{ij} + \sum_{i<j<k} S_{ijk} + \dots$$

$$S_{Ti} = S_i + S_{ij} + S_{ijk} + \dots$$ "Total effect"

Easier to compute the sum progressively more difficult to compute

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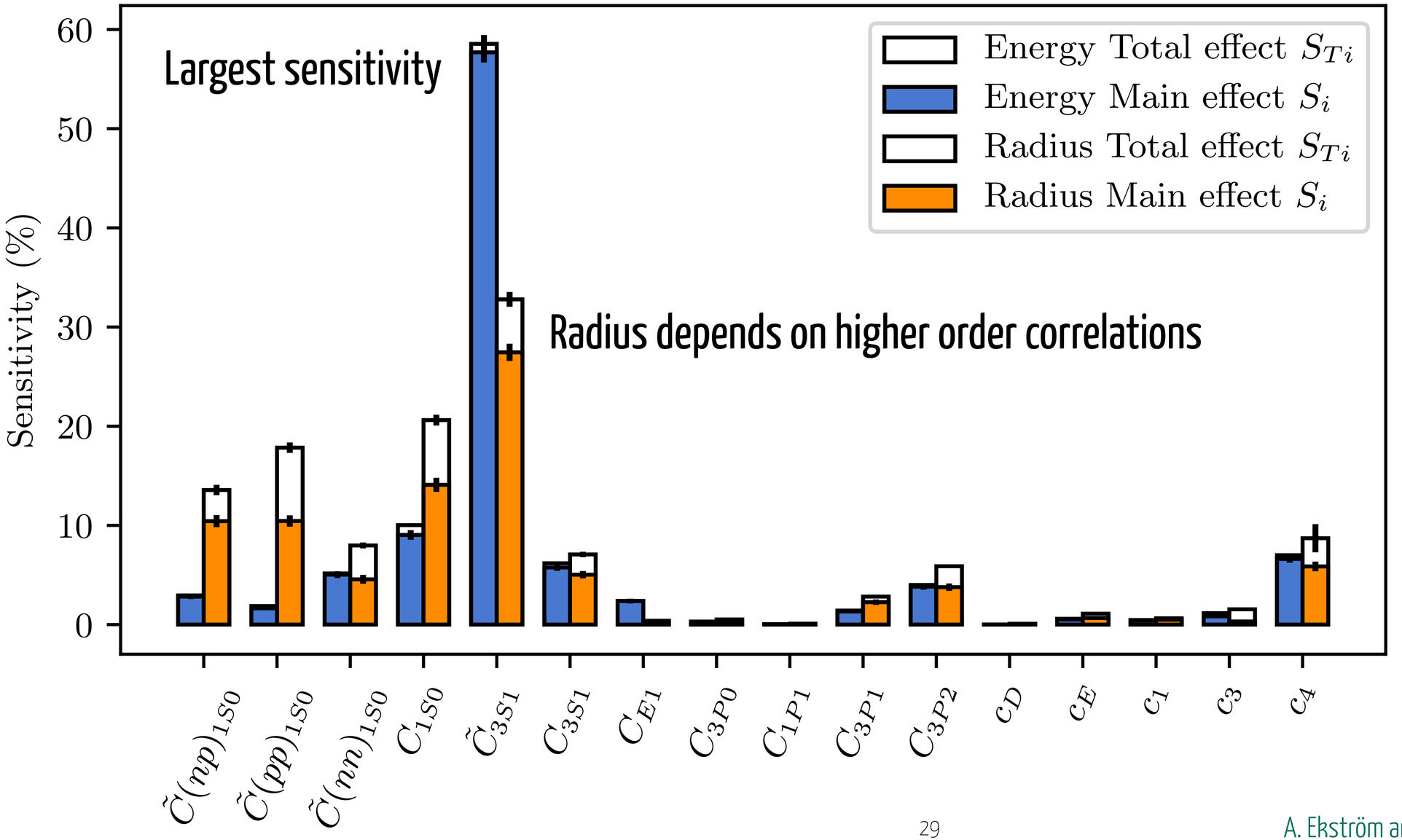
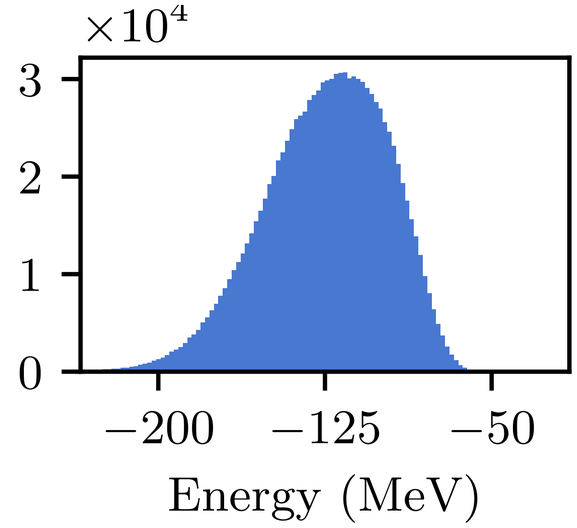
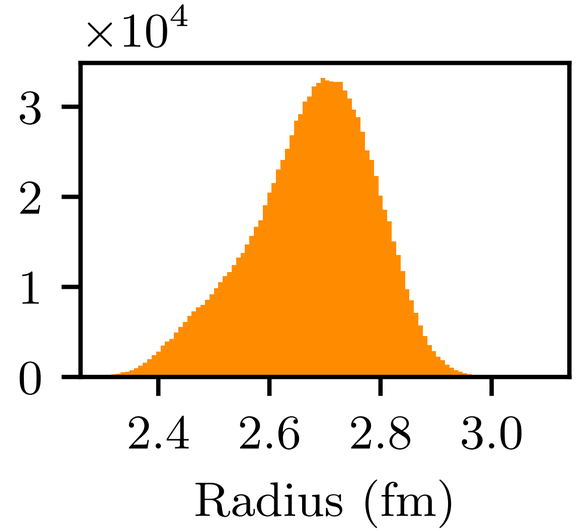
Global sensitivity analysis: results

1 million SPCC computations!







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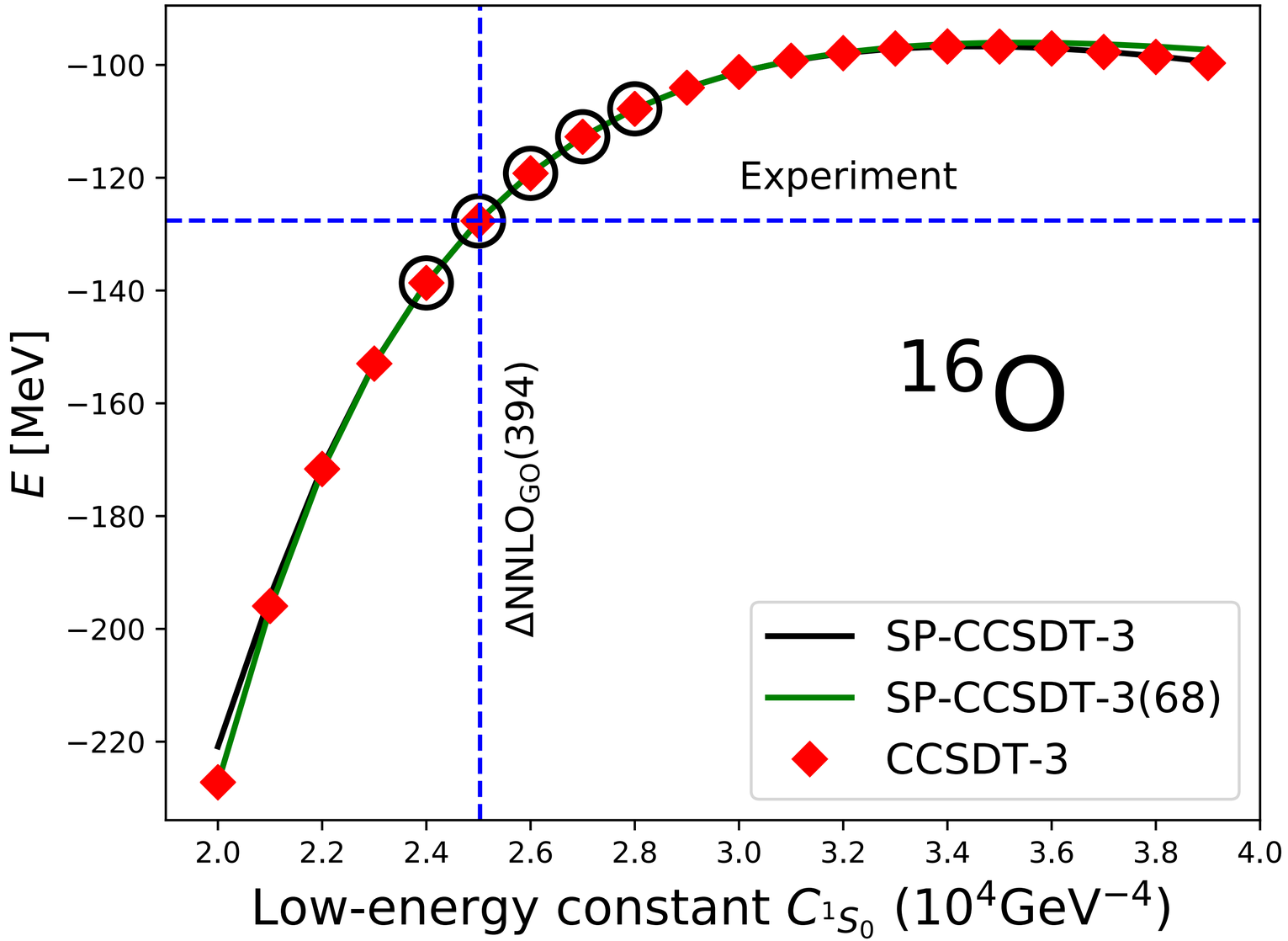
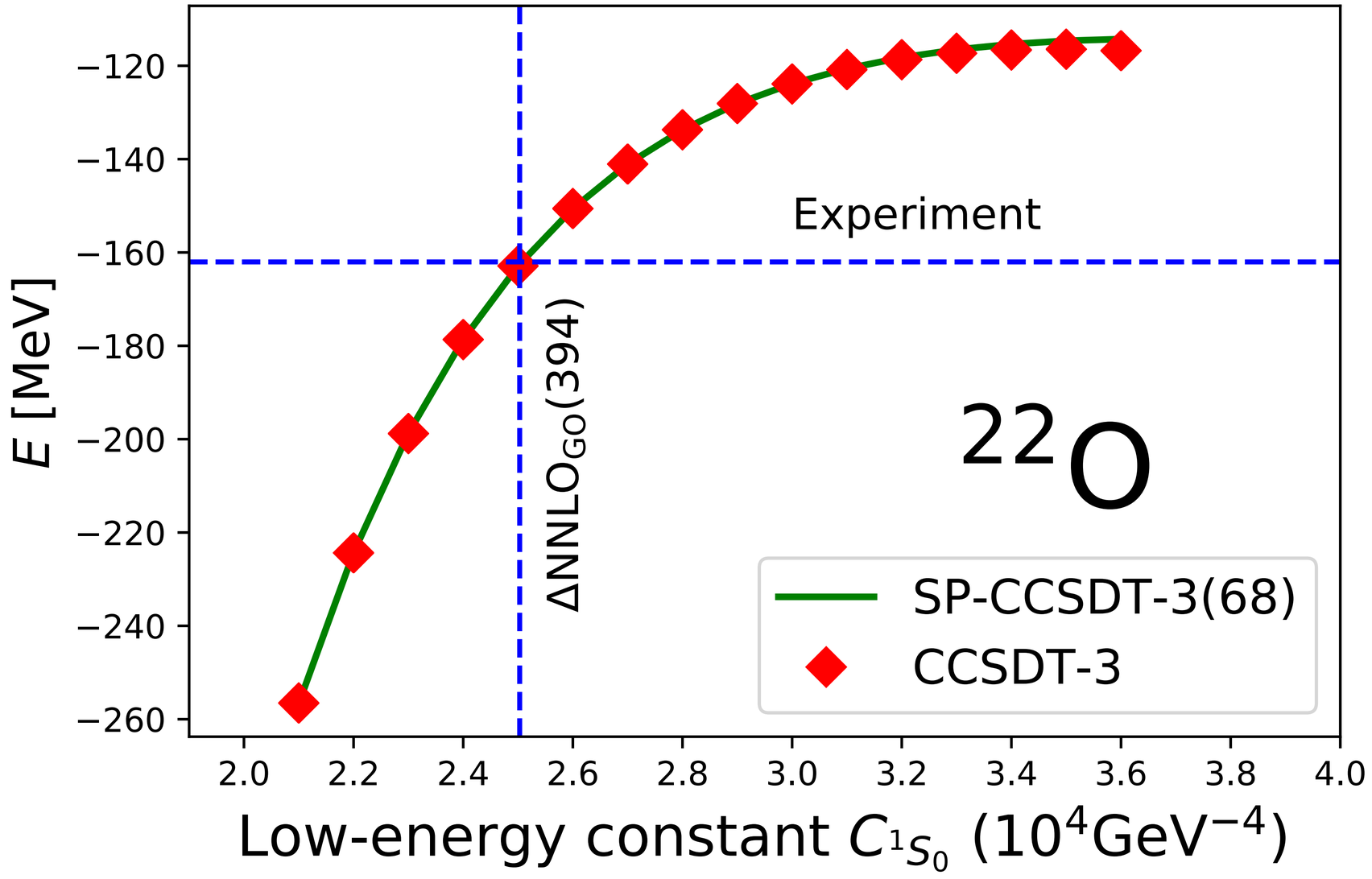
More recent developments

Including Δ-isobars and CC triples: ground states



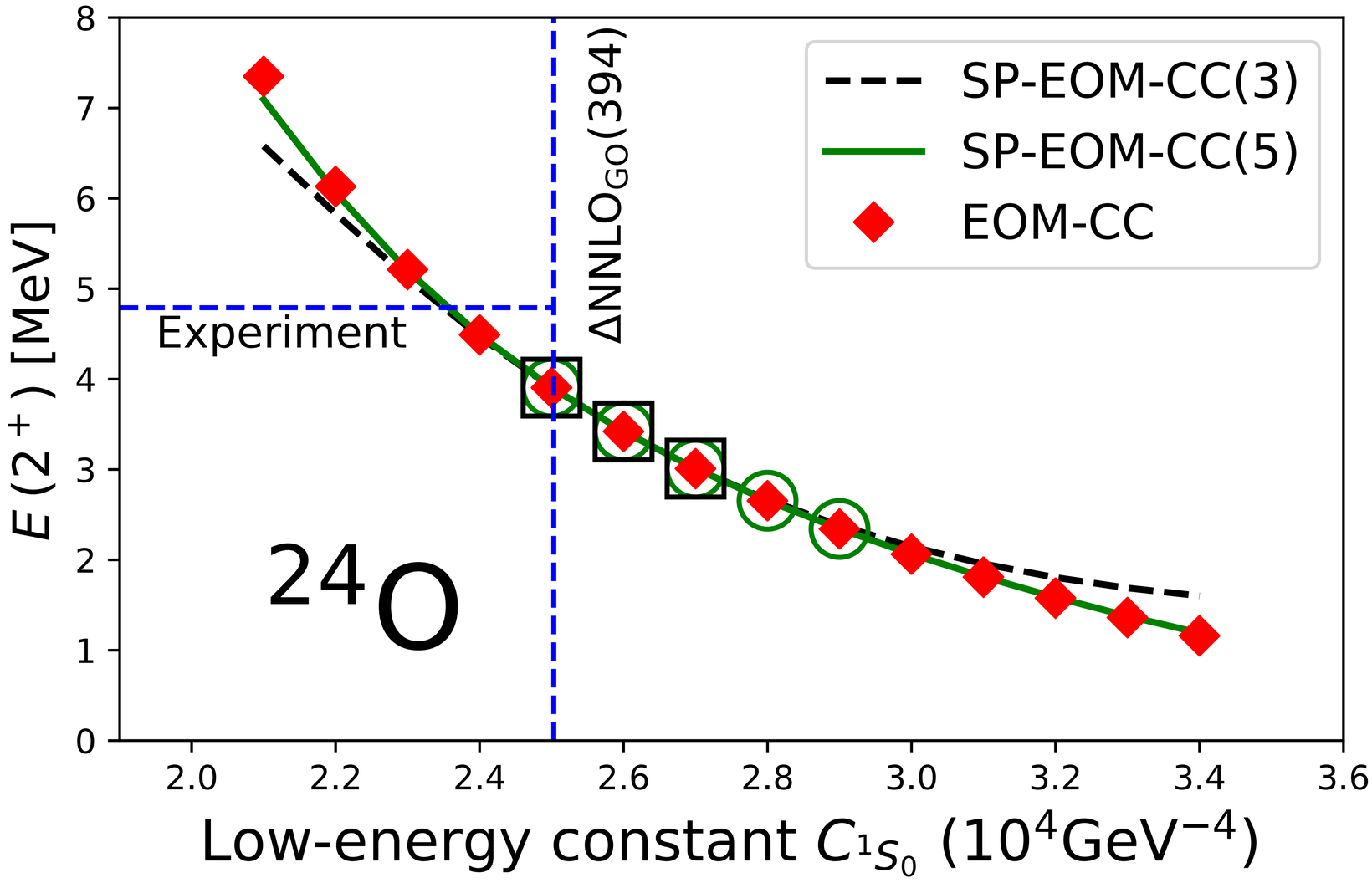
(See C. Forssén talk for details)

Including Δ-isobars and CC triples: ground states



(See C. Forssén talk for details)

Including Δ-isobars and CC triples: excited states

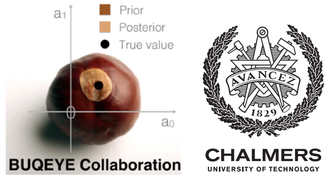


(See C. Forssén talk for details)

N_{max}=6 proof-of-principle calculation

In progress, and preliminary

Bayesian estimation of c_D and c_E



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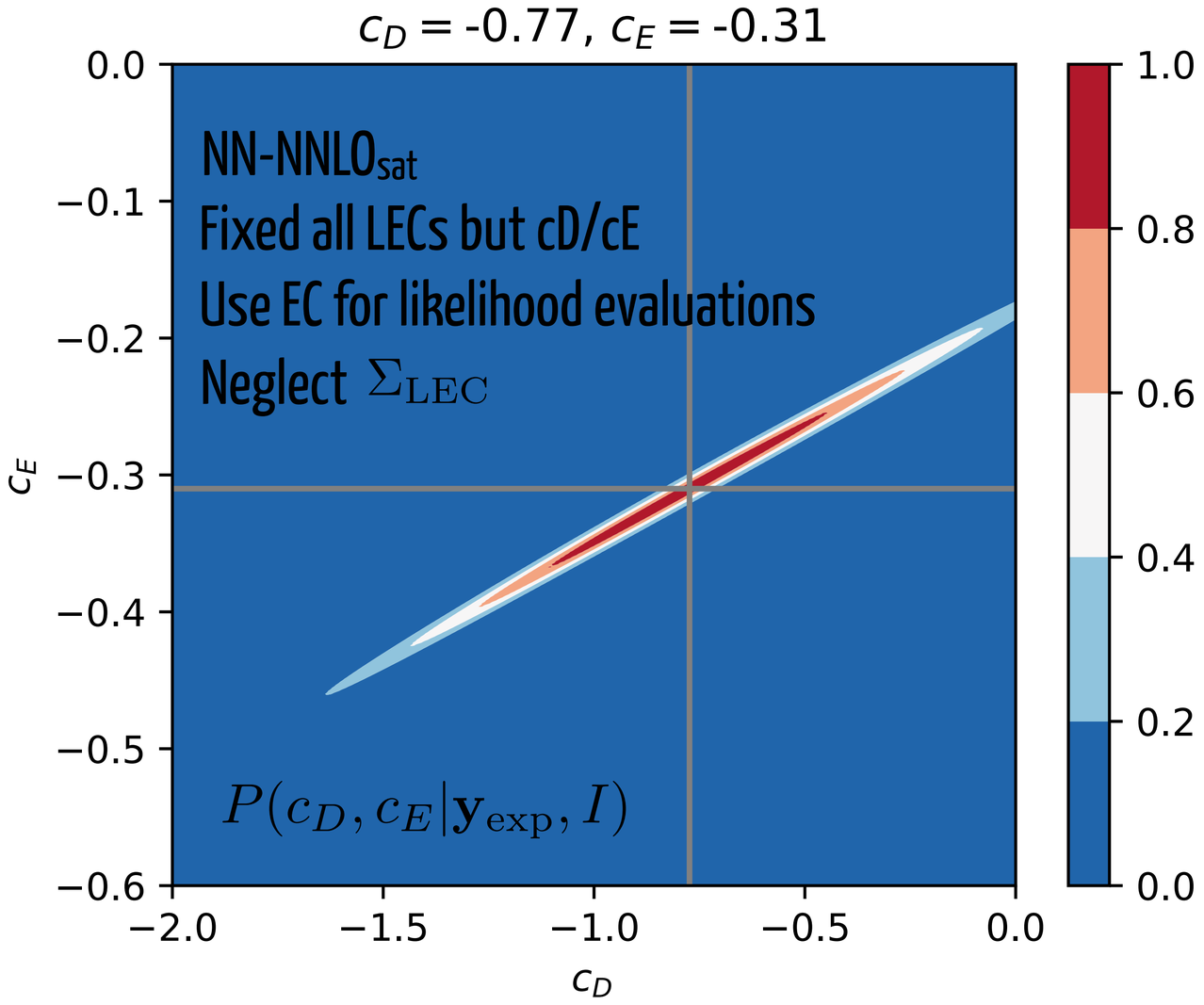
S. Wesolowski, Chalmers, et al.



Data: energy/radius of ^{4}He, energy of ^{3}H

Potential model: NNLO, only vary c_D & c_E (Using EC)

Log-likelihood proportional to:

$$(\mathbf{y}_{\rm exp} - \mathbf{y}_{\rm th})^T (\mathbf{\Sigma}_{\rm exp} + \mathbf{\Sigma}_{\rm th})^{-1} (\mathbf{y}_{\rm exp} - \mathbf{y}_{\rm th})$$

Assume uncorrelated LEC and truncation errors

$$\mathbf{\Sigma}_{\rm th} = \mathbf{\Sigma}_{\rm LEC} + \mathbf{\Sigma}_{\rm truncation}$$

$$(\mathbf{\Sigma}_{\rm th})_{ij} = (\mathbf{\Sigma}_{\rm LECs})_{ij} + \left[\frac{\bar{c}_i^2 (y_{\rm ref})_i^2 Q_i^2}{1 - Q_i^2}\right] \delta_{ij}$$

$$Q = \frac{m_\pi}{\Lambda_b}, \quad \Lambda_b = 600\,\text{MeV}, \quad \bar{c}_i = 1 \text{ for all } i$$

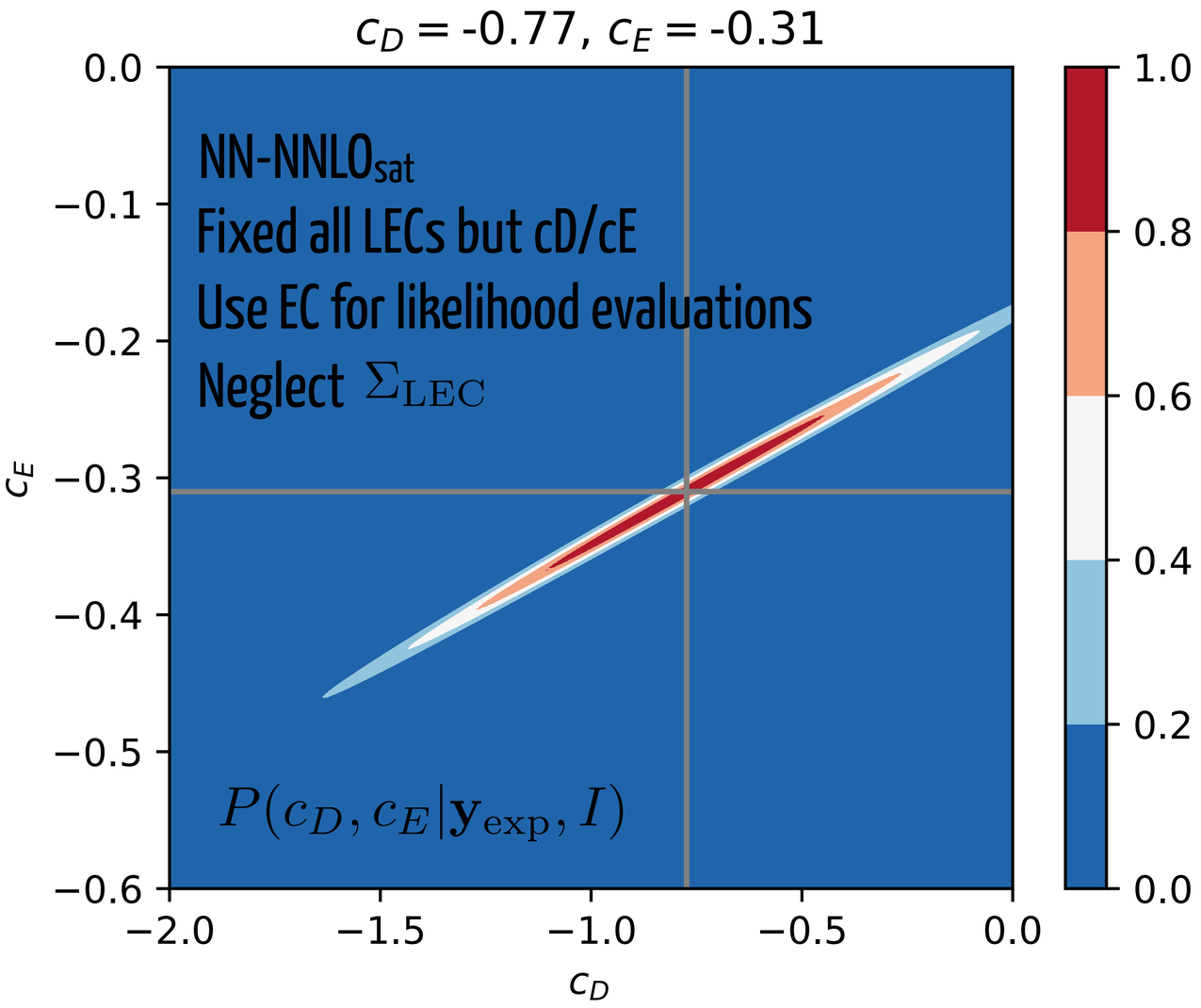
ToDo: add LEC errors

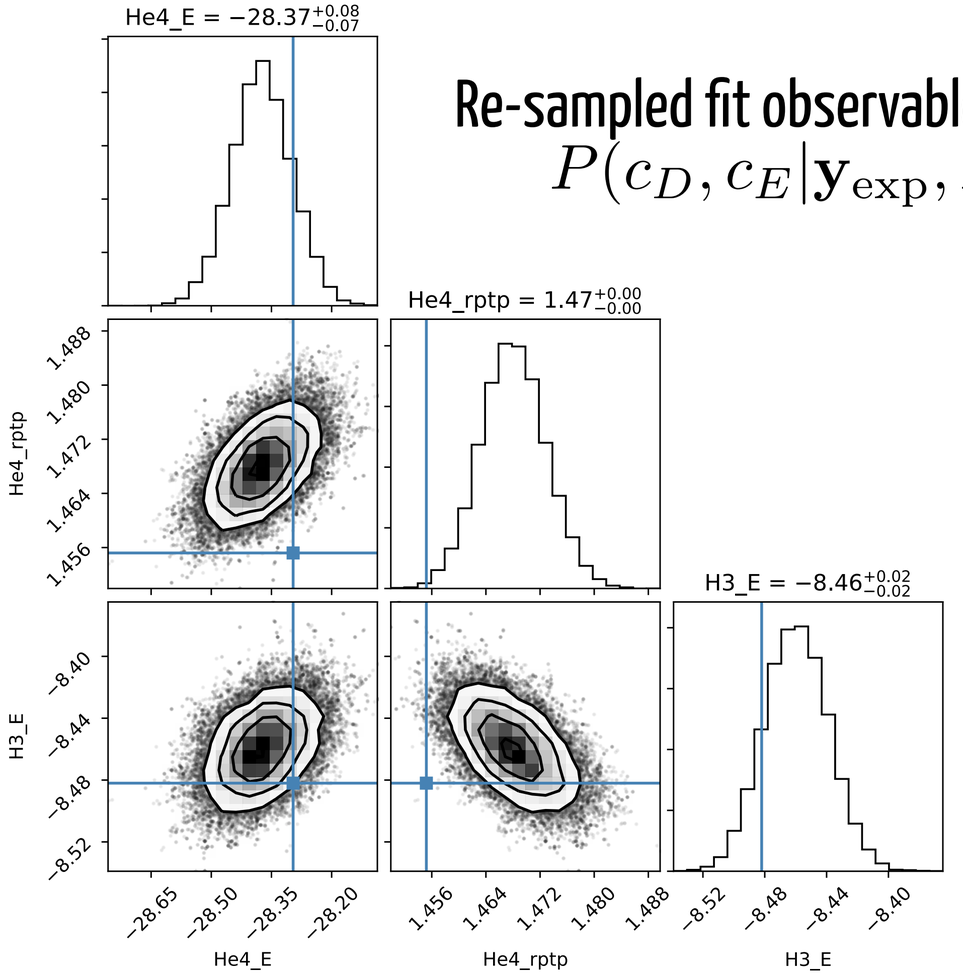
study prior dependencies

S Wesolowski et al., J. Phys. G: Nucl. Part. Phys. 46, 045102 (2019)

In progress, and preliminary

Observable posteriors

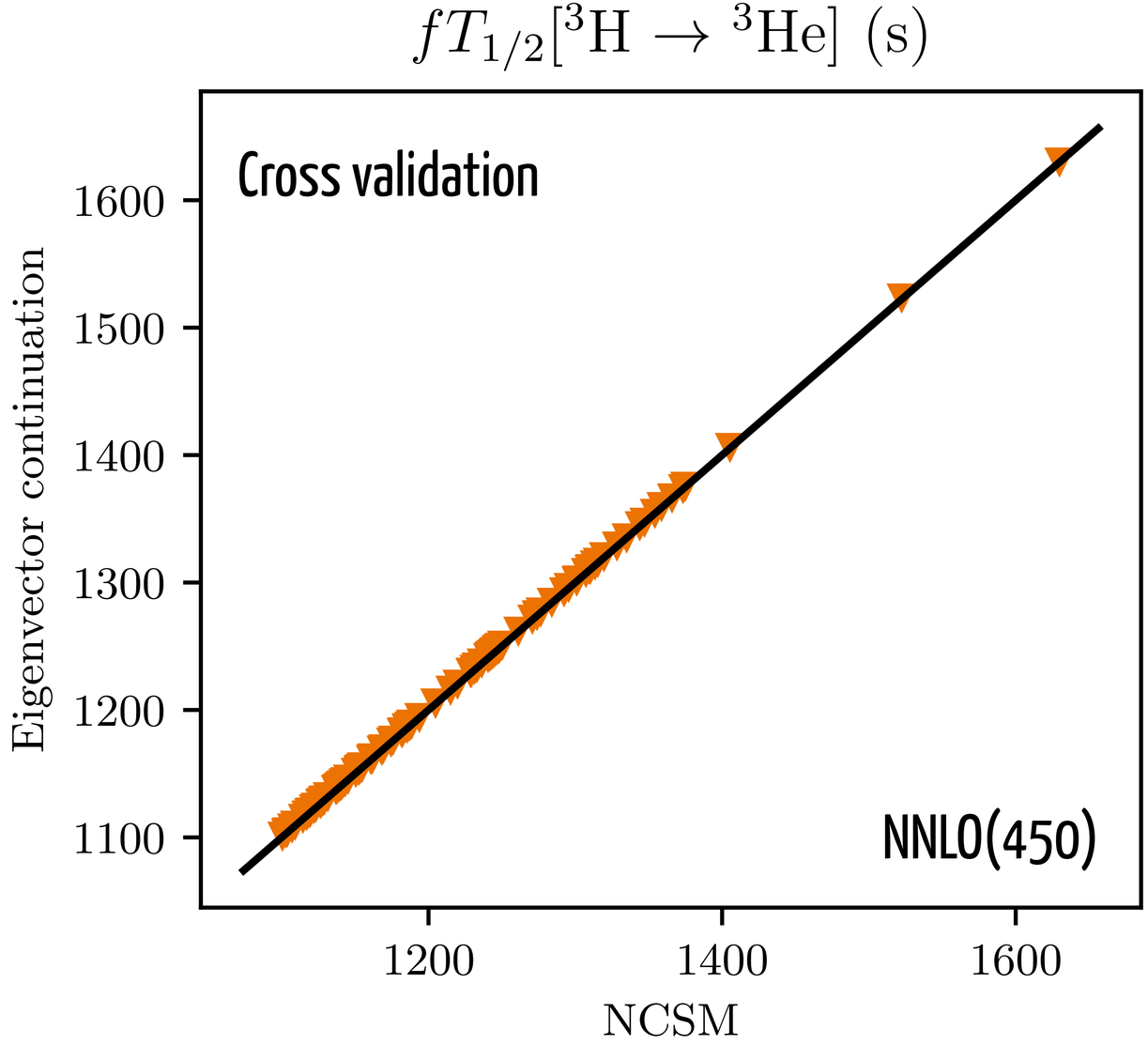




Re-sampled fit observables over
$P(c_D, c_E|\mathbf{y}_{\rm exp}, I)$

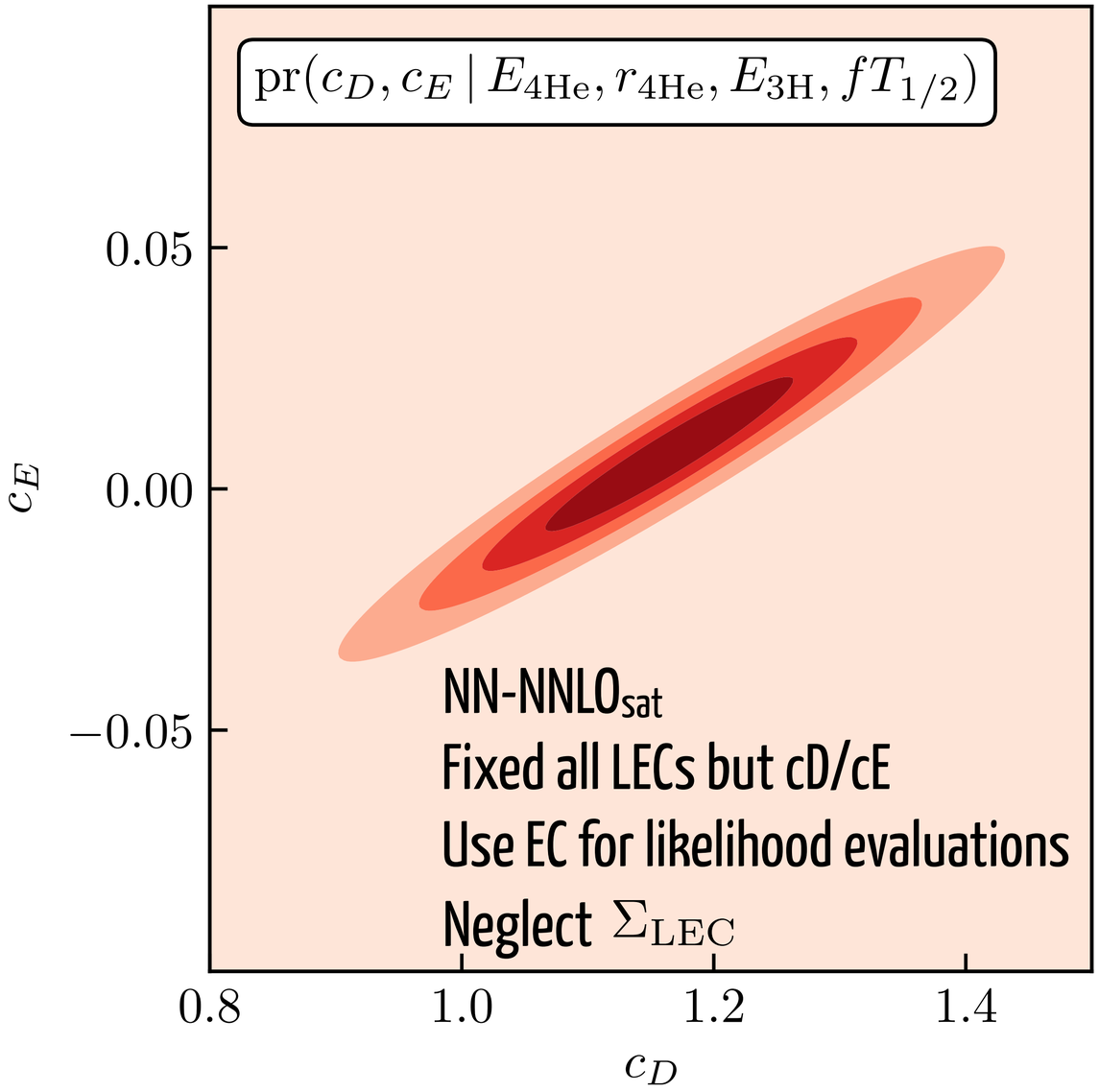
ToDo: predictions with theory errors
bound state momentum scale?

EC emulation of NCSM calculations of triton beta-decay

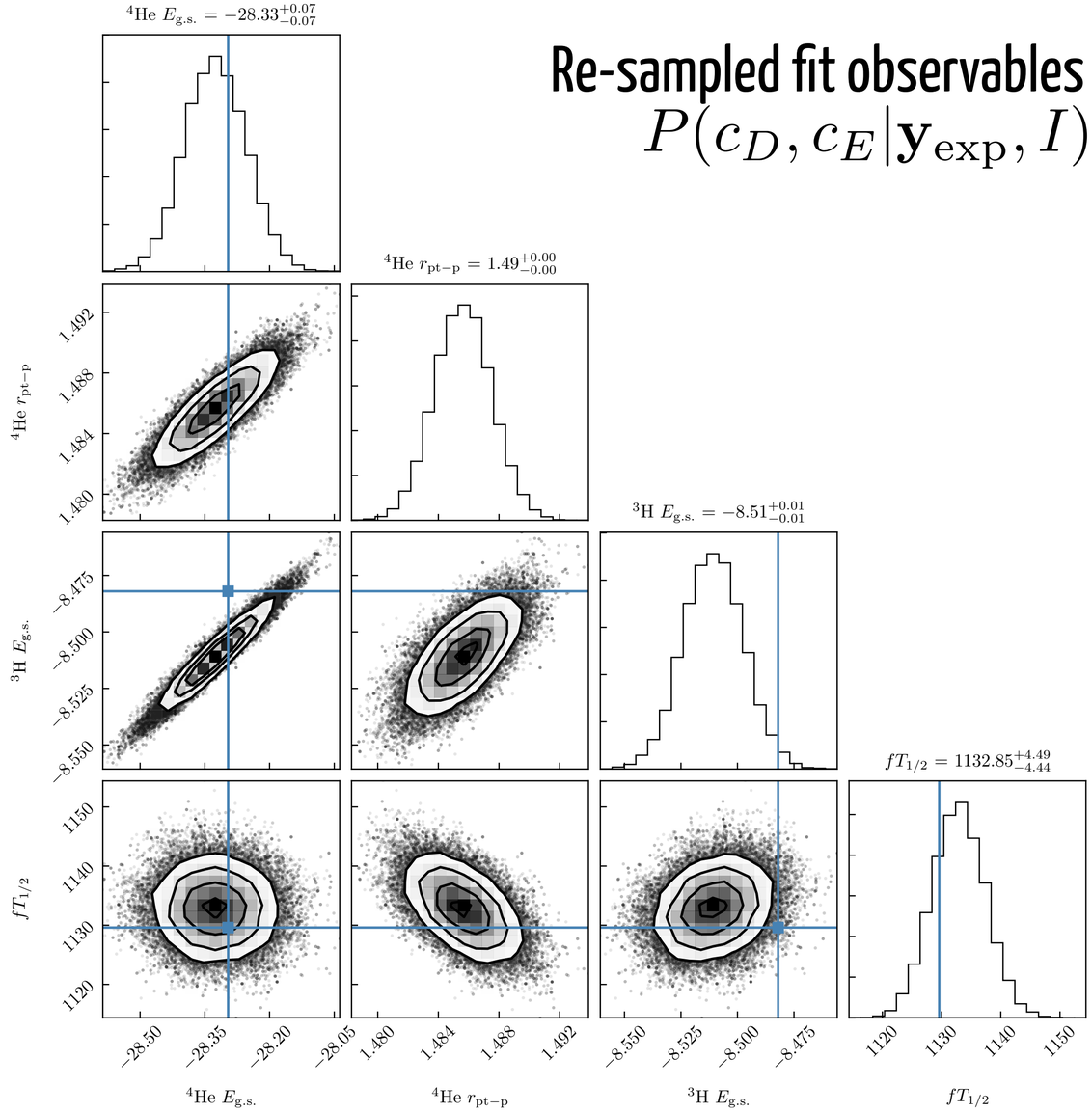


In progress, and preliminary

Including triton beta decay



Re-sampled fit observables over
$P(c_D, c_E | \mathbf{y}_{\mathrm{exp}}, I)$



Bayesian LEC estimation using HMC

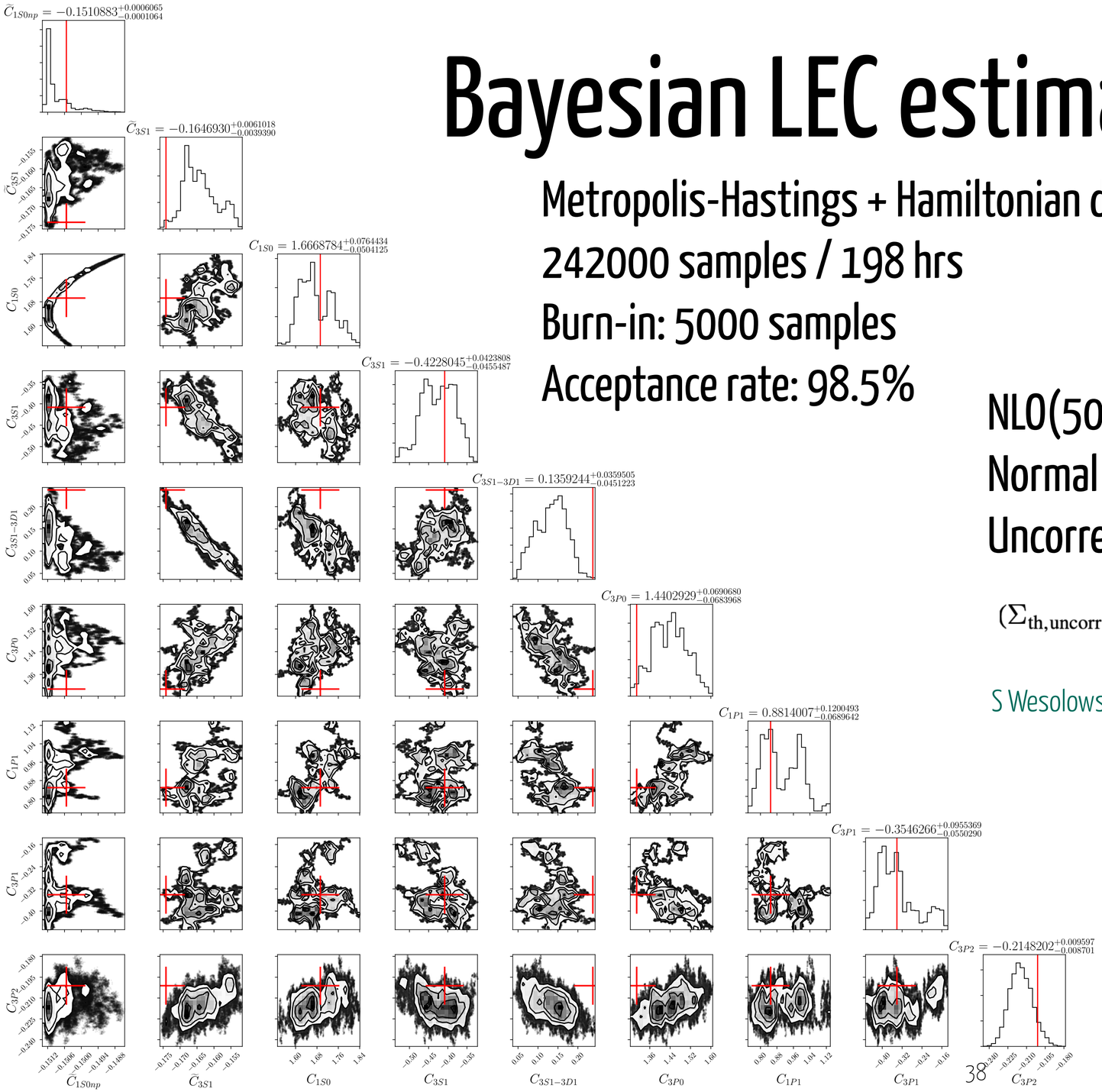
Isak Svensson

Metropolis-Hastings + Hamiltonian dynamics

242000 samples / 198 hrs

Burn-in: 5000 samples

Acceptance rate: 98.5%



NLO(500), select np scattering data with T_{lab}<100 MeV

Normal LEC prior: mean=0,variance=5

Uncorrelated truncation errors $\bar{c} = 1.55$

$$(\Sigma_{\text{th,uncorr.}})_{ij} = (y_{\text{ref}})_i^2\, \bar{c}^2 \sum_{n=k+1}^{k_{\max}} Q_i^{2n}\, \delta_{ij} \underset{k_{\max}\to\infty}{\longrightarrow} \frac{(y_{\text{ref}})_i^2\, \bar{c}^2\, Q_i^{2k+2}}{1 - Q_i^2}\, \delta_{ij}$$

S Wesolowski et al., J. Phys. G: Nucl. Part. Phys. 46, 045102 (2019)

Questions/ToDo:

HMC/MCMC convergence diagnostics

Identifying multiple modes (History Matching?)

Posterior predictive distribution with theory errors

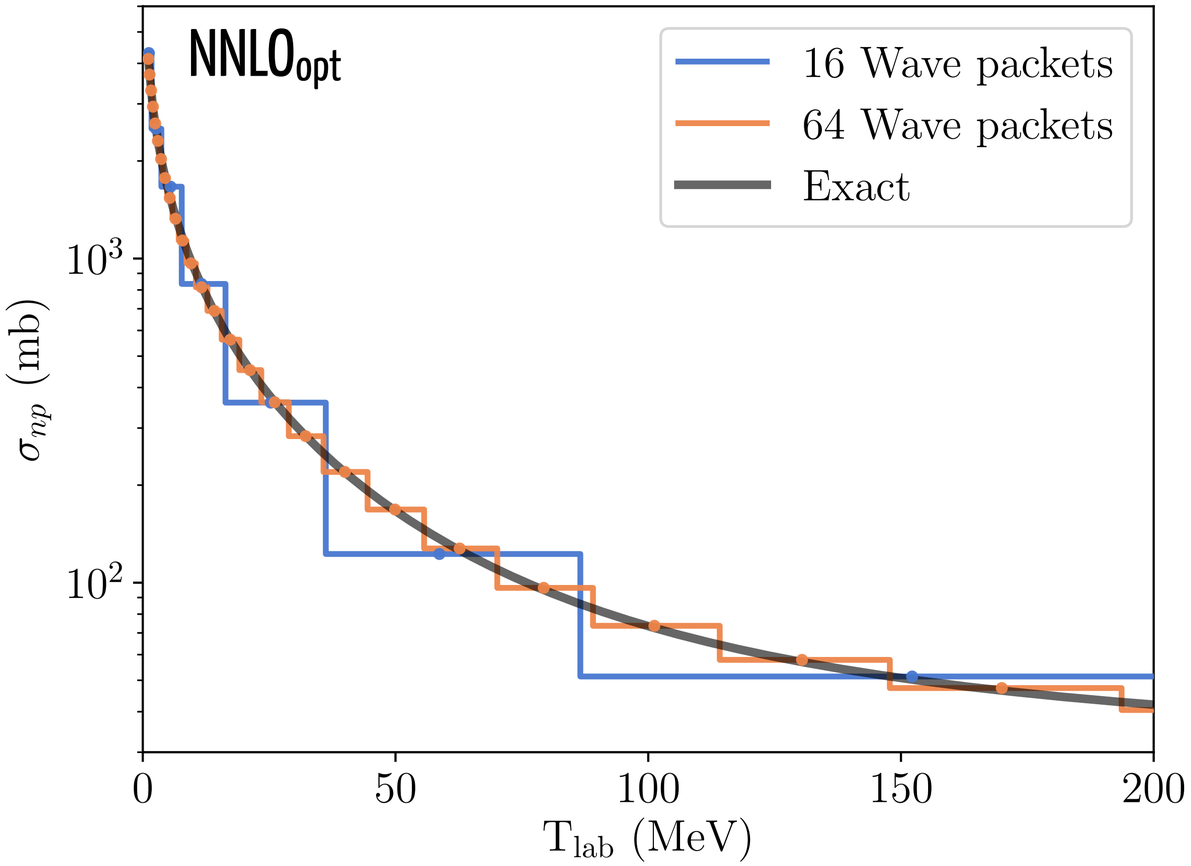
In progress, and preliminary

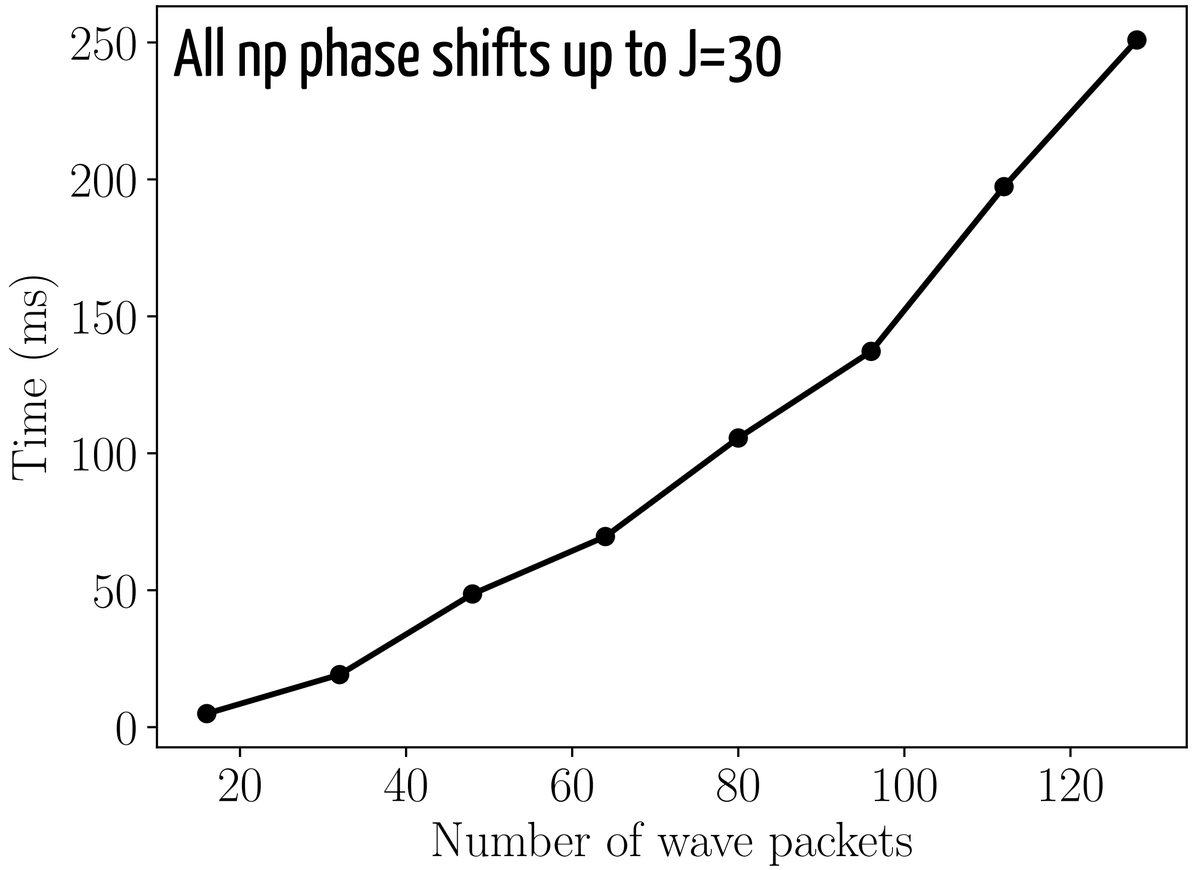
GPU/Wave-packet computation of NN scattering cross sections

Sean Miller

"Computation via an approximate method and batched CUDA calls"

GPU challenge: efficient diagonalization of many small (< '100 x 100') matrices



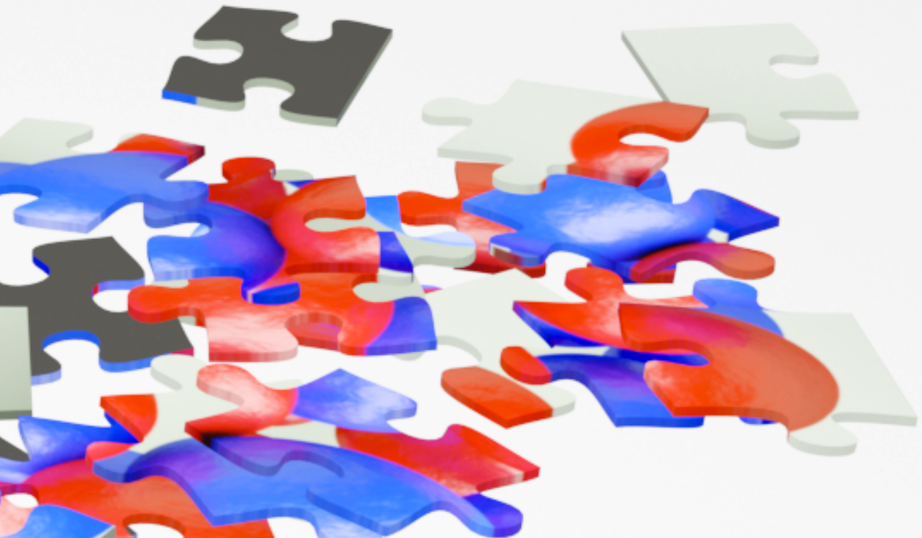


In progress, and preliminary

O. A. Rubtsova et al. Annals of Physics 360, 613–654, (2015)

Looking ahead

The SP-CC method and eigenvector continuation enables sophisticated statistical computation in ab initio nuclear theory. This can help reveal which data would reduce the uncertainty in Hamiltonian models the most and provide key insights for understanding how the properties of atomic nuclei depend on the underlying interaction between protons and neutrons.



Summary

The sub-space projected coupled-cluster method enables **emulation of nuclear observables** at different values of the coupling constants in chiral Hamiltonians at unprecedented speed:

- Ground-state energy
- Ground-state radius
- Excited state energies

A global sensitivity analysis indicates that the NNLO description of the radius of 16-O depends sensitively on higher order correlations between the LECs.

Bayesian inference in nuclear physics is rapidly moving forward.

Outlook: sophisticated statistical computation in ab initio nuclear theory!

Thank You for Your Attention!

(Next talk by C. Forssén)

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