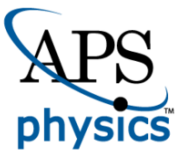

Global Sensitivity Analysis of Bulk Properties of an Atomic Nucleus

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Phys. Rev. Lett. **123**, 252501 — Published 20 December 2019

DOI: 10.1103/PhysRevLett.123.252501

Global sensitivity analysis of bulk properties of an atomic nucleus

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(Dated: November 12, 2019)

We perform a global sensitivity analysis of the binding energy and the charge radius of the nucleus ^{16}O to identify the most influential low-energy constants in the next-to-next-to-leading order chiral Hamiltonian with two- and three-nucleon forces. For this purpose we develop a subspace-projected coupled-cluster method using eigenvector continuation [Frame D. *et al.*, Phys. Rev. Lett. 121, 032501 (2018)]. With this method we compute the binding energy and charge radius of ^{16}O at more than one million different values of the 16 low-energy constants in one hour on a standard laptop. For relatively small subspace projections, the root-mean-square error is about 1% compared to full space coupled-cluster results. We find that 58(1)% of the variance in the energy can be apportioned to a single contact-term in the $^3S_1$-wave, whereas the radius depends sensitively on several low-energy constants and their higher-order correlations. The results identify the most important parameters for describing nuclear saturation, and help prioritize efforts for uncertainty reduction of theoretical predictions. The achieved acceleration opens up for an array of computational statistics analyses of the underlying description of the strong nuclear interaction in nuclei across the Segré chart.

Introduction.- How do properties of atomic nuclei depend on the underlying interaction between protons and neutrons? Recent *ab initio* computations of nuclei [1–16] have revealed that observables such as binding energies, radii, spectra, and decay probabilities are very sensitive to the values of the low-energy constants (LECs) in chiral Hamiltonian models with two- and three-nucleon forces [17–19]. Certain interaction models work better than others, but only for selected types of observables and in limited regions of the Segré chart. It is not clear why. The NNLO$_{\rm sat}$ interaction [20] reproduces experimental binding energies and charge radii for nuclei up to mass $A \sim 50$ [4, 5, 9, 16], while the 1.8/2.0 (EM) interaction [21, 22] reproduces binding energies and low-lying energy spectra up to mass $A \sim 100$ [4, 7, 8, 10, 12, 15] while radii are underestimated.

To improve theoretical predictions requires rigorous uncertainty quantification and sensitivity analyses that are grounded in the description of the underlying nuclear Hamiltonian. Unfortunately, the number of model samples required for statistical computing increases exponentially with the number of uncertain LECs. A global sensitivity analysis of the ground-state energy and charge radius ^{16}O, based on a realistic next-to-next-to-leading order (NNLO) chiral Hamiltonian with 16 LECs, requires more than one million model evaluations. Similar numbers can be expected for Markov Chain Monte Carlo sampling of Bayesian marginalization end evidence integrals [23–25]. Clearly, this is not feasible given the computational cost of existing state-of-the-art *ab initio* many-body methods applied to medium-mass and heavy nuclei.

In this Letter we solve this problem by utilizing eigenvector continuation [26] to develop a subspace-projected coupled-cluster (SP-CC) method as a fast and accurate approximation to the corresponding full-space coupled-cluster (CC) method [27–33]. The SP-CC method generalizes the eigenvector-continuation formalism in Ref. [34] to non-Hermitian problems and enables accelerated computation of nuclear observables across the Segré chart for any target value $\vec{\alpha}_\odot$ of the LECs in the underlying Hamiltonian. See Fig. 1 for a demonstration of the SP-CC method applied to ^{16}O and the variation of a single LEC (details are given below). We will use SP-CC to analyze the description of the ^{16}O ground-state energy and charge radius across a large domain of relevant LECs. This way we can for the first time clearly identify the LECs that have the biggest impact on binding energy and radius predictions, which in turn impacts saturation properties of nuclear matter [8, 35, 36].

Method.– Following Ref. [34] we start by representing the chiral Hamiltonian at NNLO $H(\vec{\alpha})$ as a linear combination with respect to all the LECs $\vec{\alpha}$; i.e. $H(\vec{\alpha}) = \sum_{i=0}^{N_{\rm LECs}=16} \alpha_i h_i$, with the zeroth term given by $h_0 = t_{\rm kin} + V_0$ and $\alpha_0 = 1$. Here $t_{\rm kin}$ is the intrinsic kinetic energy and V_0 denotes a constant potential contribution that does not depend on any of the considered LECs; for example the one-pion exchange interaction, the leading two-pion exchange, and terms proportional to pion

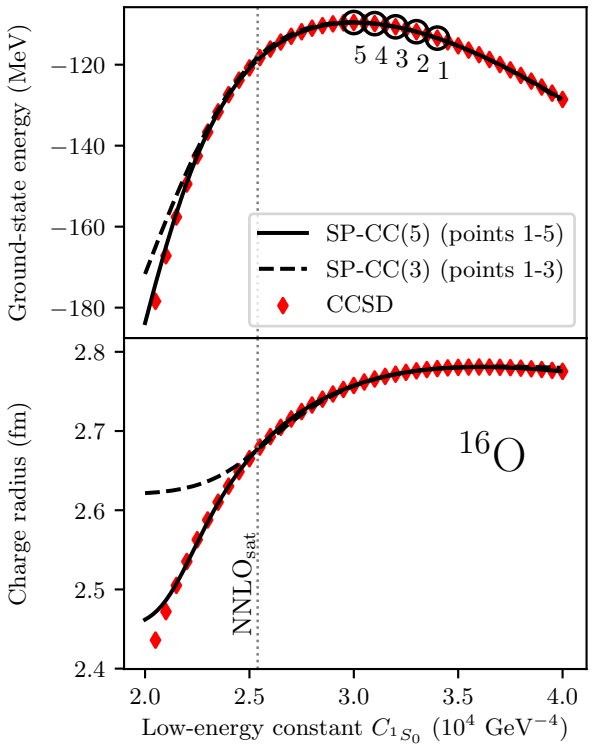

FIG. 1. (Color Online) SP-CC results for ^{16}O, using three or five subspace vectors, for different values of the low-energy constant (LEC) $C_{^1S_0}$. The red diamonds indicate exact CC calculations at the singles and doubles level (CCSD). The NNLO$_{\rm sat}$ point is indicated with a dashed vertical line.

and nucleon masses. The analytical form of the NNLO Hamiltonian is identical to the one of NNLO$_{\rm sat}$ [20], including the regularization scheme, which means that for a particular value $\vec{\alpha} = \vec{\alpha}_\star$ the Hamiltonian $H(\vec{\alpha}_\star)$ will reproduce the binding energy and radius predictions of NNLO$_{\rm sat}$. The SP-CC Hamiltonian for a target value $\vec{\alpha} = \vec{\alpha}_\circledcirc$ is constructed by projecting $H(\vec{\alpha}_\circledcirc)$ onto the subspace spanned by CC wavefunctions obtained at $N_{\rm sub}$ different values for $\vec{\alpha}$. SP-CC is a controlled approximation to the full-space CC method, and allows for rapid and accurate solutions to the many-nucleon problem necessary for statistical computing. In this Letter we use the CC method in the singles- and doubles approximation (CCSD).

The workhorse of the CC method is the similarity transformed Hamiltonian $\overline{H}(\vec{\alpha}) = e^{-T(\vec{\alpha})}H(\vec{\alpha})e^{T(\vec{\alpha})}$, where in the CCSD approximation the cluster operator is truncated at one-particle-one-hole and two-particle-two-hole excitations, i. e. $T(\vec{\alpha}) = T_1(\vec{\alpha}) + T_2(\vec{\alpha})$. For clarity, we have indicated the implicit dependence on $\vec{\alpha}$. The CCSD similarity transformation is non-unitary and renders $\overline{H}(\vec{\alpha})$ non-Hermitian, and we thus introduce $N_{\rm sub}$ bi-orthogonal left and right CC ground-states,

$$\langle\tilde{\Psi}| = \langle\Phi_0|(1+\Lambda(\vec{\alpha}))e^{-T(\vec{\alpha})}, \;\; |\Psi\rangle = e^{T(\vec{\alpha})}|\Phi_0\rangle. \qquad (1)$$

Here $\Lambda(\vec{\alpha}) = \Lambda_1(\vec{\alpha}) + \Lambda_2(\vec{\alpha})$ is a linear expansion in one-particle-one-hole and two-particle-two-hole de-excitation operators, and we have bi-orthonormality according to $\langle\tilde{\Psi}|\Psi\rangle = 1$. For notational simplicity we will from here on omit the explicit $\vec{\alpha}$ dependence in the (de)-excitation operators and set $T(\vec{\alpha}) = T$ and $\Lambda(\vec{\alpha}) = \Lambda$, respectively. The reference state $|\Phi_0\rangle$ is built from harmonic oscillator single-particle states, and we solve the CCSD equations in a model-space comprising 11 major oscillator shells with a frequency $\hbar\Omega = 16$ MeV. The matrix-elements of the three-nucleon interaction that enters the Hamiltonian are truncated by the energy cut $E_{3\rm max} \leq 14$. The CCSD result for ^{16}O with NNLO$_{\rm sat}$ in this model-space is -118.76 MeV, which is within 1 MeV of the converged CCSD value using a Hartree-Fock basis.

Using the $N_{\rm sub}$ different CCSD ground-state vectors in Eq. (1), the matrix elements of the target Hamiltonian in the subspace and the corresponding norm matrix are given by,

$$\begin{aligned}\langle\tilde{\Psi}'|H(\vec{\alpha}_\circledcirc)|\Psi\rangle &= \langle\Phi_0|(1+\Lambda')e^{-T'}H(\vec{\alpha}_\circledcirc)e^{T}|\Phi_0\rangle \\ &= \langle\Phi_0|(1+\Lambda')e^{X}\overline{H}(\vec{\alpha}_\circledcirc)|\Phi_0\rangle, \qquad (2)\\ \langle\tilde{\Psi}'|\Psi\rangle &= \langle\Phi_0|(1+\Lambda')e^{X}|\Phi_0\rangle, \qquad (3)\end{aligned}$$

respectively. Here we also introduced $e^X = e^{-T'+T}$, and $\overline{H}(\vec{\alpha}_\circledcirc)$ is the similarity transformed target Hamiltonian. The left ground-state $\langle\tilde{\Psi}'| = \langle\Phi_0|(1+\Lambda')e^{-T'}$ is obtained from $H(\vec{\alpha}')$, and the right ground-state $e^T|\Phi_0\rangle$ is obtained from $H(\vec{\alpha})$, respectively. We can now solve the generalized non-Hermitian $N_{\rm sub} \times N_{\rm sub}$ eigenvalue problem for the SP-CC target Hamiltonian to obtain the ground-state energy and wavefunction in the subspace. With the SP-CC wavefunction we can also calculate the expectation value of any subspace-projected operator with matrix elements $\langle\tilde{\Psi}'|O|\Psi\rangle$. Equations (2) and (3) can be evaluated using Wick's theorem and closed form algebraic expressions are given in the Supplementary Material. Note that in general the reference states for the $N_{\rm sub}$ different subspace CC wavefunctions in Eq. (1) are non-orthogonal. This is a non-trivial case and would require the generalized Wick's theorem [37, 38] in order to evaluate the matrix elements of the SP-CC Hamiltonian and the norm matrix.

Results.– The SP-CC predictions for the energy and charge radius in ^{16}O as a function of the LEC $C_{^1S_0}$ in the Hamiltonian are shown in Fig 1. Using $N_{\rm sub} = 5$ exact CCSD ground-state vectors, from a small region of $C_{^1S_0}$ values, points 1-5 in Fig. 1, the SP-CC method extrapolates to the exact CCSD results across a large $C_{^1S_0}$ range. With $N_{\rm sub} = 3$ CCSD vectors, points 1-3 in Fig. 1, the radius extrapolation deteriorates far away from the exact solutions, while the energy predictions remain more accurate.

We now move to the challenging case where all 16 LECs at NNLO can vary. In the following we analyze two SP-CC Hamiltonians based on $N_{\rm sub} = 64$ and $N_{\rm sub} = 128$

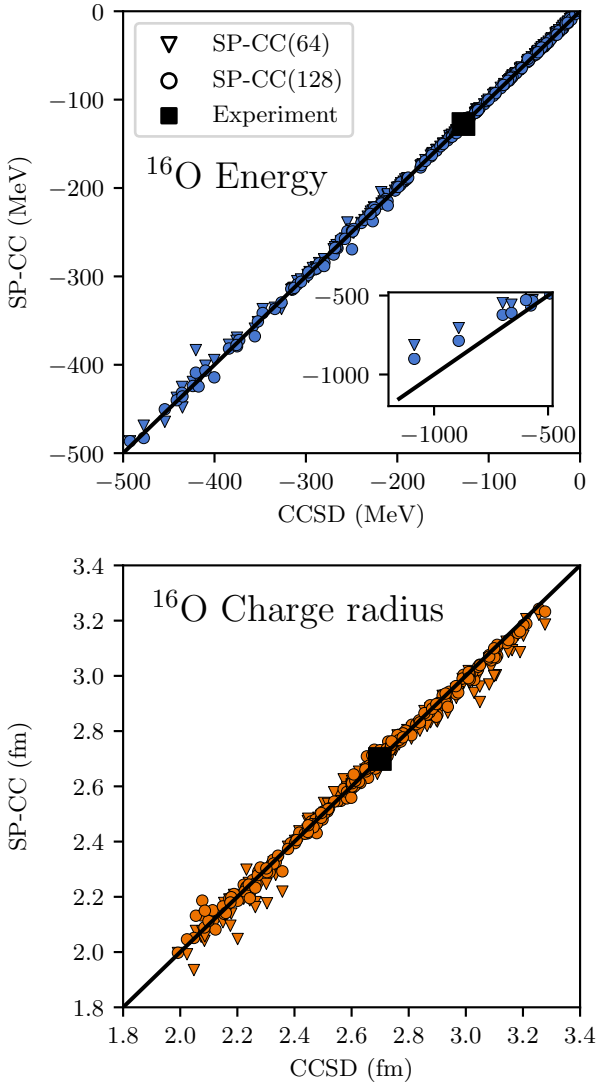

FIG. 2. (Color Online) Cross-validation of SP-CC(64) and SP-CC(128) for the ground-state energy (top) and charge radius (bottom) using 200 exact CCSD calculations. The inset shows energy predictions below -500 MeV. Only radii for negative-energy states shallower than -500 MeV are included.

CCSD ground-state vectors, referred to as SP-CC(64) and SP-CC(128), respectively. The ground-state vectors are obtained at $N_{\rm sub}$ points in a domain of LEC values that surrounds the nominal LEC values of NNLO$_{\rm sat}$ within $\pm 20\%$ relative variation. This domain spans a rather large interval of ground-state energies and charge radii in ^{16}O. The three-nucleon contact-LEC $c_E \approx 0.0395$ in NNLO$_{\rm sat}$ is small compared to the values of the remaining 15 LECs, we therefore scaled c_E with a factor of 20. In accordance with observation, we also constrained the leading-order isospin-breaking $^1S_0$ LECs ($\tilde{C}$) to exhibit small isospin-breaking. We draw $N_{\rm sub}$ values for $\vec{\alpha}$ using a space-filling latin hypercube design and solve for the exact CCSD wavefunction at each point. We have verified that the SP-CC(64) and SP-CC(128) Hamiltonians reproduce the energies and radii of the exact CCSD calculations for all $N_{\rm sub}$ choices of $\vec{\alpha}$.

Figure 2 shows the cross-validation with respect to an additional set of 200 randomly drawn exact CCSD calculations in the same 20% domain. From the cross-validation we extract a root mean-squared error (RMSE) of SP-CC(64): 4 MeV and 0.04 fm for the ground-state energy and charge radius, respectively. With SP-CC(128) the RMSE values are 3 MeV and 0.02 fm. Using more subspace vectors gives better predictions. The present results are within the expected accuracy of CCSD. The non-hermiticity of the CCSD equations yields SP-CC Hamiltonians that do not obey a variational bound with respect to the exact CCSD calculations. From Fig. 2 we see that this is a minute effect.

We use SP-CC(64) and global sensitivity analysis (GSA) to analyze how the *ab initio* predictions for the energy and charge radius in ^{16}O explicitly depend on the LECs in the NNLO nuclear interaction. GSA is a very powerful, although computationally demanding, method for learning how much each unknown model parameter contributes to the uncertainty in a model prediction [39]. As opposed to an uncertainty analysis, which addresses the question of how uncertain the prediction itself is. With SP-CC we can carry out the large amount of model evaluations that is required to extract statistically significant GSA results. In the following, we treat the ground-state energy or radius of ^{16}O as an output $Y = f(\vec{\alpha})$ of a model f, given here by the SP-CC(64) Hamiltonian and its eigendecomposition. In the GSA we decompose the total variance Var$[Y]$ as

$$\mathrm{Var}[Y] = \sum_{i=1}^{N_{\rm LECs}} V_i + \sum_{i<j}^{N_{\rm LECs}} V_{ij} + \ldots, \tag{4}$$

where the partial variances are given by

$$\begin{aligned} V_i &= \mathrm{Var}[E_{\vec{\alpha}\sim(\alpha_i)}[Y|\alpha_i]] \\ V_{ij} &= \mathrm{Var}[E_{\vec{\alpha}\sim(\alpha_i,\alpha_j)}[Y|\alpha_i,\alpha_j]] - V_i - V_j \end{aligned} \tag{5}$$

and $\mathrm{Var}[E_{\vec{\alpha}\sim(\alpha_i)}[Y|\alpha_i]]$ denotes the variance of the conditional expectation of Y, and $\vec{\alpha} \sim (\alpha_i)$ denotes the set of all LECs excluding α_i, and correspondingly for the second-order term. The variance integrals are evaluated using quasi Monte Carlo (MC) sampling and we extract a 95% confidence interval of the final result via bootstrap with 100 re-samples [40]. The first- and second-order sensitivity indices are defined as

$$S_i = \frac{V_i}{\mathrm{Var}[Y]}, \; S_{ij} = \frac{V_{ij}}{\mathrm{Var}[Y]}. \tag{6}$$

The first-order sensitivity, S_i, is often referred to as the main effect. It apportions the total variance in the model output to an individual model parameter α_i. The higher-order indices, e.g. S_{ij}, apportion the variance in the model output to the combination of parameters α_i

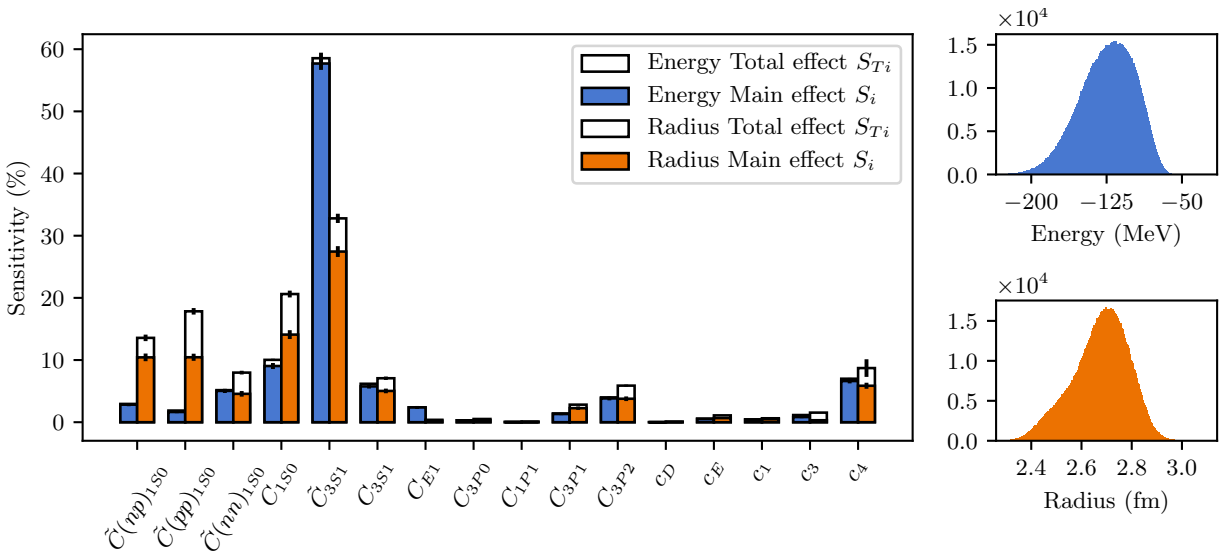

FIG. 3. (Color Online) (Left panel) Main and total effects (in %) for the ground-state energy (left bar) and charge radius (right bar) in ^{16}O, grouped per LEC. The main and total effects were computed from $(16+1)\cdot 2^{16} = 1,114,112$ quasi MC evaluations of the SP-CC(64) Hamiltonian. The vertical lines on each bar indicate bootstrapped 95% confidence intervals. A larger sensitivity value implies that the corresponding LEC is more critical for explaining the variance in the model output. (Right panels) Histograms of the ground-state energy (top) and charge radius (bottom) from which total variances are decomposed.

and α_j. The number of higher-order indices grow exponentially with the number of parameters in the model. Fortunately, it is possible to compute the sum of all sensitivity indices for each α_i, i.e. $S_{Ti} = S_i + S_{ij} + S_{ijk} + \ldots$. This is referred to as the total effect, and it quantifies the total sensitivity of Var$[Y]$ to parameter α_i including all of its higher-order parameter combinations [41]. We always have that $S_{Ti} \geq S_i$, and equality for purely additive models. In this analysis, we do not calibrate the model to reproduce data. We study the behavior and response of the model itself, and assume all LECs to be independent of each other and uniformly distributed. In future studies one could draw LECs from a Bayesian posterior distribution.

Figure 3 shows the results from the GSA of the ^{16}O energy and radius using an SP-CC(64) chiral NNLO Hamiltonian. To limit the model response of the energy and radius to a physically reasonable interval we only sample a LEC domain corresponding to 10% variation around the NNLO$_{\text{sat}}$ values. The LEC c_E is still scaled with a factor of 20. The MC sample size required for carrying out a reliable GSA depends on: i) the complexity of the model, and ii) the number of parameters in the model. We have to use $(16+1)\cdot 2^{16} = 1,114,112$ quasi MC samples to extract statistically significant main and total effects of the energy and radius for all LECs. With SP-CC(64) this took about 1 hour on a standard laptop, while an equivalent set of exact CCSD computations would require 20 years. We find that 58(1)% of the variance in the energy can be attributed to the leading order LEC $\tilde{C}_{^3S_1}$ and all main and total effects are nearly identical, which signals that the energy is nearly additive in all LECs. We would like to point out that $\tilde{C}_{^3S_1}$ is directly proportional to the deuteron binding energy. However, to calibrate realistic nuclear interactions requires additional data, partly from heavier-mass nuclei, see e.g [20]. For the radius, the main effects are distributed across several LECs and they differ from the total effects. Indeed, second-order correlations between the LECs are responsible for almost 14% of the variance in the radius. This result also reflects the challenge, and importance, of optimizing chiral NNLO Hamiltonians to reproduce radii of medium-mass atomic nuclei and consequently saturation properties of nuclear matter. Our analysis also reveals that the energy and radius of ^{16}O are not sensitive to the short-ranged parts of the three-nucleon interaction in this domain. Of the long-ranged πN LECs, $c_{1,3,4}$, only c_4 exhibits a non-negligible main-effect for the energy and radius. This LEC contributes to the tensor force in the nucleon-nucleon interaction. As expected, only $P-$wave LECs with large spin-weights contribute to the ^{16}O wavefunction. There also seems to be a larger sensitivity of the radius to the isospin- breaking terms in the interaction. Constraining the πN LECs to within the limits of the recent Roy-Steiner analysis [42] does not alter the sensitivity pattern or our conclusions. The GSA results guide future uncertainty reduction efforts for specific observables by identifying non-influential LECs, which is also useful for e.g. calibration. The SP-CC method will significantly leverage statistical computation for analyzing correlations between different observables in different nuclei across the Segré chart.

Summary and outlook.– We have developed the SP-CC method for evaluating nuclear observables at different values of the LECs in chiral Hamiltonians at unprecedented speed. With a modest number of subspace vectors, $N_{\rm sub} = 64$, we reached 1% accuracy relative to exact CCSD solutions in ^{16}O. CC can generate subspace vectors also for heavier nuclei, and according to the theoretical underpinnings of eigenvector vector continuation, smooth changes of the wavefunction should mostly live in a low-dimensional manifold. Therefore, we expect the SP-CC method to scale well with larger A. From a GSA we conclude that the variance of the ground-state energy in ^{16}O is additive in all LECs of the NNLO chiral Hamiltonian, and that the charge radius depends sensitively on the combination of several LECs. The SP-CC method enables sophisticated statistical computation [43–46] in *ab initio* nuclear theory to reveal which new data would best reduce the uncertainty in Hamiltonian models and for understanding how properties of atomic nuclei depend on the underlying interaction between protons and neutrons. The stability of ^{16}O with respect to breakup into ^{4}He clusters is a relevant example [35, 47–49]. The SP-CC method also enables straightforward computation of derivatives with respect to the LECs using e.g. algorithmic differentiation. SP-CC Hamiltonians occupy very little disk space, and can easily be shared within the nuclear community.

We thank Michael Grosskopf, Sebastian König, Dean Lee, Titus Morris, and Thomas Papenbrock for fruitful discussions. G. H. acknowledges the hospitality of Chalmers University of Technology where most of this work was carried out. This work was supported by the European Research Council (ERC) under the European Unions Horizon 2020 research and innovation programme (Grant agreement No. 758027), the Office of Nuclear Physics, U.S. Department of Energy, under grants desc0018223 (NUCLEI SciDAC-4 collaboration) and by the Field Work Proposal ERKBP72 at Oak Ridge National Laboratory (ORNL). Computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This research used resources of the Oak Ridge Leadership Computing Facility located at ORNL, which is supported by the Office of Science of the Department of Energy under Contract No. DE-AC05-00OR22725.

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