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Statistical error propagation in *ab initio* no-core full configuration calculations of light nuclei

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We propagate the statistical uncertainty of experimental NN scattering data into the binding energy of ^{3}H and ^{4}He. We also study the sensitivity of the magnetic moment and proton radius of the ^{3}H to changes in the NN interaction. The calculations are made with the no-core full configuration method in a sufficiently large harmonic oscillator basis. For those light nuclei we obtain $\Delta E^{\rm stat}(^3{\rm H}) = 0.015$ MeV and $\Delta E^{\rm stat}(^4{\rm He}) = 0.055$ MeV.

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I. INTRODUCTION

The quantification of uncertainties in nuclear physics has gained a significant interest in recent years [1–4]. In fact, a special issue of the Journal of Physics G was dedicated entirely to this particular topic [5]. Of course, the concentrated attention is fully justified and the importance of providing theoretical estimates with error bars cannot be overemphasized for several reasons. First, it provides guidance on the relation between the input and the output along with the quantification of the agreement/disagreement between theory and experiment. Second, it sets the standards for the predictive power of the theory. Finally, it helps to determine a balanced experimental program by providing feedback from theory on what data are significant for determining critical aspects of the theory.

The very idea of predictive power is unavoidably related to specifying the links between the input and the output of the calculation. In this paper we are concerned with the impact of the uncertainties of Nucleon-Nucleon (NN) interactions on the structure of the lightest nuclei with $A = 2, 3, 4$. The implementation of such a program requires a scrupulous determination of errors in NN potentials, for which the main source of information has traditionally been the abundant scattering experiments carried up to about the pion production threshold over the last 70 years. In the case of NN scattering, measurements are performed by counting events, giving a Poisson's distribution to the measured observables. However, if the number of events is large enough a standard normal distribution can be safely assumed and experimental error bars can be given as a symmetric 1σ confidence interval. Phenomenological NN potentials assume a specific form for the interaction and adjust a number of parameters to describe a collection of experimental scattering data. The parameter fitting is usually done via a least squares procedure. Since each experimental datum is provided with an error bar, the parameter space contains a confidence region, rather than a single point, where the description of data is considered correct. This region constitutes the *statistical* uncertainty for a particular NN interaction. Different forms are assumed for the phenomenological NN potentials describing correctly the same NN scattering database. These differences are a source of *systematic* uncertainty. A clear sign of this systematic uncertainty is the incompatible predictions in scattering observables for kinematic regions that have not yet been measured [6]. Another clear sign of this systematic uncertainty is the different binding energies and other observables predicted for light nuclei. These differences in properties of finite nuclei are attributable to many-body forces which, in principle, are different for each NN interaction.

We address the specific situation where an NN interaction alone is adopted as an input to make predictions on various observables of light and heavy nuclei. In most cases the NN interaction is taken as exact and only numerical or implementation errors are considered when providing such calculations with an uncertainty. However, both statistical and systematic errors are inherent to phenomenological interactions and should be taken into account when quantifying the total uncertainty of a nuclear structure calculation. For light nuclei the no-core full configuration (NCFC) method [7] provides an *ab initio* approach for extrapolating to an infinite basis expansion of the nuclear wavefunction from a small set of finite basis expansions with increasing size. The purpose of this work is to use the NCFC approach to generate a realistic estimate of the statistical uncertainty stemming from the experimental NN scattering data, leaving the more complex propagation of systematic uncertainties for a future endeavor.

The paper is organized as follows: section II describes the major characteristics of the sum of Gaussians potential which is the phenomenological NN interaction used in these calculations. The theoretical framework to propagate the statistical uncertainties is explained in section III. The NCFC method

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and the corresponding extrapolation uncertainty are shown in section IV. Deuteron properties are calculated in section V in order to test the convergence of the No-Core Shell Model (NCSM) [8] with the sum of Gaussians potential. Section VI shows the NCFC calculations of ^{3}H and ^{4}He binding energy with extrapolation and statistical uncertainties. Finally, our conclusions are summarized in section VII.

II. DESCRIPTION OF THE NN POTENTIAL

The NN interaction used for these nuclear structure calculations is written as the sum of Gaussians potential and was introduced in [9]. This phenomenological interaction has been fitted to the self-consistent Granada database with a total of 2995 neutron-proton and 3717 proton-proton experimental scattering data [10]. The residuals of the potential (see section III) have been shown to follow the standard normal distribution. This allows one to confidently propagate the experimental uncertainty according to this distribution.

The potential has a clear boundary at $r_c = 3.0$ fm separating the short and long range part of the NN interaction by means of

$$V(r) = V_{\text{short}}(r)\theta(r_c - r) + V_{\text{long}}(r)\theta(r - r_c). \tag{1}$$

This differentiates between the purely phenomenological short range part and the field theoretical long range tail which ensures the proper analytic behavior of the scattering amplitude. The short range part consists of a sum of Gaussian functions centered around the origin in an operator basis

$$V_{\text{short}}(r) = \sum_{n=1}^{21} \hat{O}_n \left[\sum_{i=1}^{4} V_{i,n} e^{-\frac{1}{2}\left(\frac{r(1+i)}{a}\right)^2} \right]. \tag{2}$$

The operators $\hat{O}_n$ correspond the AV18 basis plus three additional operators introduced in Appendix A of [10], the strength coefficients $V_{i,n}$ and width parameter a are fitted to describe the self consistent data base of [10]. The values of the fitted parameters can be found in Table VI of [9]. The long range part includes the well known charge dependent one-pion exchange (OPE) potential plus electromagnetic interactions

$$V_{\text{long}}(r) = V_{\text{OPE}}(r) + V_{\text{EM}}(r). \tag{3}$$

We refer to the full interaction in Eq(1) as the Gauss-OPE potential.

III. PROPAGATION OF STATISTICAL UNCERTAINTIES

A chi square minimization scheme corresponds to the trial assumption that the fitted data are independent and normally distributed. When the fitting model is flexible enough to accurately describe the data, this assumption becomes equivalent to the assumption that the discrepancies between theory and experiment follow the standard normal distribution i.e.

$$R_i = \frac{O_i^{\text{exp}} - O_i^{\text{theor}}}{\Delta O_i^{\text{exp}}} \sim N(0,1), \tag{4}$$

where R_i are known as residuals. If the resulting residuals of a fit do not follow the standard normal distribution the trial assumption is invalid and any subsequent error propagation based on normality is at the very least questionable, if not wrong. For the case of the sum of Gaussians potential the normality of residuals has been stringently tested and confirmed [9]. The fitting procedure used to adjust the potential parameters allows one to estimate the corresponding covariance matrix $\mathscr{C}$, which propagates the experimental error bars of the fitted data to the parameters and assumes a multivariate normal distribution for them. The covariance matrix is defined as the inverse of the Hessian matrix H

$$(\mathscr{C}^{-1})_{ij} \equiv H_{ij} = \frac{\partial \chi^2}{\partial p_i \partial p_j}, \tag{5}$$

where $\chi^2 = \sum_i R_i^2$ and $\mathbf{p}$ is the vector containing the fitting parameters. To propagate the statistical uncertainties from the interaction into nuclear structure calculations one could, in principle, directly use the covariance matrix with

$$(\Delta F)^2 = \sum_{ij} \frac{\partial F}{\partial p_i} \frac{\partial F}{\partial p_j} \mathscr{C}_{ij}, \tag{6}$$

where F is any quantity calculated as a function of the potential parameters. However, the level of complexity in most of the nuclear structure numerical methods makes the calculation of the derivatives in Eq. (6) computationally costly; a simple finite differences method at fourth order would require one to make four evaluations of F to calculate the derivative with respect to each parameter. Since the sum of Gaussians potential has 44 independent fitting parameters [1], a total of 176 evaluations would be necessary to propagate the statistical uncertainty to a single quantity. While one could alternatively proceed to differentiate the NN interaction analytically, term by term, and evaluate the single terms separately, we will proceed differently here.

Monte-Carlo techniques provide an efficient approach to study the sensitivity of elaborate nuclear structure calculations to variations on the input interaction. To generate a Monte-Carlo family of potential parameters one simply has to draw random numbers following a multivariate normal distribution according to the covariance matrix $\mathscr{C}$

$$P(p_1, p_2, \ldots, p_P) = \frac{1}{\sqrt{(2\pi)^P \det \mathscr{C}}} e^{-\frac{1}{2}(\mathbf{p}-\mathbf{p}_0)^T \mathscr{C} (\mathbf{p}-\mathbf{p}_0)}, \tag{7}$$

where $\mathbf{p}_0$ has the central values of the fitted parameters. This sampling can be easily done by taking advantage of the Cholesky decomposition $\mathscr{C} = \mathscr{L}\mathscr{L}^T$ and using independent standard normal variates $\mathbf{z} = (z_1, z_2, \ldots, z_p)$ with

$$\mathbf{p} = \mathbf{p}_0 + \mathscr{L} \cdot \mathbf{z}. \tag{8}$$

[1] Although Eq.(2) indicates a total of $21 \times 4 + 1 = 85$ fitting parameters, some of them correspond to linear combinations of others while some others are fixed to zero.

With M different samples of $\mathbf{p}$ one can directly make M evaluations of F and see the resulting spread and distribution. This technique has been recently employed in [11] to estimate the statistical uncertainty of the Triton ground state energy. That particular study was done with $M = 205$, however a much smaller sample of $M = 30$ already gives a fairly similar estimate. A direct bootstrapping of the experimental data has also been used to propagate statistical uncertainties stemming from NN scattering data [12]. The use of a reduced sample has also been checked using larger populations both for triton and the alpha particle using the Faddeev-Yakubovsky equations [13].

IV. NO-CORE FULL CONFIGURATION METHOD

The No-Core Full Configuration (NCFC) method, as an *ab initio* approach, solves the many body Schrödinger equation

$$H\,\Psi_i(\vec{r}_1,\ldots,\vec{r}_A) \;=\; E_i\,\Psi_i(\vec{r}_1,\ldots,\vec{r}_A) \tag{9}$$

by expanding the corresponding wavefunction of Z protons and N neutrons in a $A = Z+N$-body basis of Slater determinants Φ_k of single-particle wave functions $\phi_{nljm}(\vec{r})$

$$\Psi(\vec{r}_1,\ldots,\vec{r}_A) = \sum c_k \Phi_k(\vec{r}_1,\ldots,\vec{r}_A)\,, \tag{10}$$

with

$$\Phi_k(\vec{r}_1,\ldots,\vec{r}_A) = \mathscr{A}\left[\phi_{n_1 l_1 j_1 m_1}(\vec{r}_1)\,\phi_{n_2 l_2 j_2 m_2}(\vec{r}_2)\ldots\phi_{n_A l_A j_A m_A}(\vec{r}_A)\right]$$

and $\mathscr{A}$ the antisymmetrization operation. Even though it is customary to use the harmonic-oscillator (HO) basis for the single-particle wavefunctions, the method can be extended to more general single-particle bases [14]. The single-particle wavefunction labels indicate the quantum numbers: n and l are the radial and orbital HO quantum numbers (with $N_i = 2n_i + l_i$ the number of HO quanta), j is the total spin and m is its projection along the z-axis. Once the basis expansion of the many-body wavefunction has been made Eq. (9) becomes a linear algebra eigenvalue problem with sparse matrices. The many-body Hamiltonian H in Eq. (9) can be expressed in terms of the relative kinetic energy plus 2-body, 3-body, and, in general, up to A-body interaction terms

$$H \;=\; T_{\rm rel} + V_{\rm Coulomb} + V_{\rm NN} + V_{\rm NNN} + \cdots \tag{11}$$

In this work we restrict ourselves to a 2-body (NN) interaction, leaving the inclusion of appropriate 3 and more body forces to future investigations.

Of course the numerical solution of the eigenvalue problem in Eq. (9) requires the truncation of the infinite-dimensional basis expansion. Because of this truncation, the solution gives a strict upper bound for the lowest state with a given spin and parity. The NCFC method establishes the convergence pattern as a functions of the HO energy along with increasing basis space dimension and extrapolates to a complete infinite basis. This requires the solution of eigenvalue problems of considerably large matrices with dimensions well over a billion. Therefore the algorithms used to construct and operate with these matrices are required to make an efficient use of the available computational resources [15–17]

We use the $N_{\rm max}$ truncation, which restricts the total number of HO quanta of the many-body basis: the basis is limited to many-body states with $\sum_A N_i \le N_0 + N_{\rm max}$, where N_i is the number of quanta of each single-particle state; N_0 is the minimal number of quanta for that nucleus; and $N_{\rm max}$ is the truncation parameter. For HO single-particle states, this truncation leads to an exact factorization of the center-of-mass wave function and the relative wave function [8, 14, 18, 19]

A. Extrapolation Method and Extrapolation Uncertainty Quantification

We use the empirical extrapolation introduced in [20] and expanded in [7, 21] for the ground state energy at a fixed value of the oscillator constant $\hbar\Omega$

$$E_{\rm gs}(N_{\rm max}) = a\exp(-cN_{\rm max}) + E_\infty. \tag{12}$$

This type of extrapolation requires one to solve Eq.(9) multiple times to calculate $E_{\rm gs}$ with at least three different values of the cut-off parameter $N_{\rm max}$ in order to fit the a, c and E_∞ parameters. An estimate of the solution of Eq.(9) with a infinitely large basis is given by E_∞.

Given the variational nature of this approach an extrapolation can be improved, by either fitting the parameters in Eq.(12) to a larger number of points or by fitting to ground state energies with larger basis size. With this in mind the extrapolation uncertainty is quantified by direct comparison with extrapolations based on lower $N_{\rm max}$ results. In [7, 21] an extrapolation is made by taking sets of three $E(N_{\rm max})$ values, say $N_{\rm max} = 10,\ 12,\ 14$ while the extrapolation uncertainty is estimated by taking the difference with the extrapolation using $N_{\rm max} = 8,\ 10,\ 12$. For this work we perform all extrapolations by starting with $N_{\rm max} = 8$ and include consecutive even values up to a certain number of points N_p. The extrapolation uncertainty is estimated by comparing with an extrapolation using one point less. For example, an extrapolation with $N_p = 4$ uses $N_{\rm max} = 8,\ 10,\ 12,\ 14$ and the corresponding uncertainty is the difference with the extrapolation using the three points $N_{\rm max} = 8, 10, 12$. These extrapolations with a larger number of points can reduce the extrapolation uncertainty up to two orders of magnitude while keeping the statistical uncertainty within the same order. Also, this approach is self-consistent in the sense that the extrapolation uncertainty decreases as the number of points increases and for a given number of points the extrapolation is within the uncertainty of smaller extrapolations. Although additional methods are available for extrapolating to the ground state energy with an infinite basis from calculations using truncated HO bases [22, 23], the method described here allows us to compare the size of the extrapolation error with the statistical uncertainty.

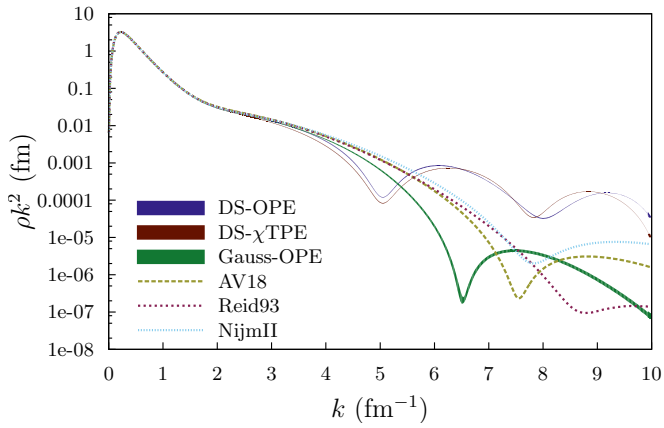

FIG. 1: (Color online) Deuteron momentum distribution for different local potentials. DS-OPE (blue band), DS-χTPE (red band), Gauss-OPE (green band), AV18 (yellow dashed line), Reid93 (red short-dashed line) and NijmII (light blue dotted line).

V. DEUTERON AND CONVERGENCE RATE

In order to get an initial insight into the convergence of NCSM calculations using the Gauss-OPE potential we calculated first the Deuteron momentum distribution using different phenomenological potentials. In particular, we use ArgonneV18 [24], Reid93 [25], NijmII [25], and the delta shell potentials DS-OPE [10, 26] and DS-χTPE [27], in addition to the Gauss-OPE potential [9]. For the DS-OPE, DS-χTPE and Gauss-OPE potentials, we included the results from the Monte-Carlo sampling described in the previous sections to form bands of results. The momentum distributions can be seen in Fig. 1. It is remarkable that the delta-shell potentials contain the largest high-momentum component despite having no repulsive hard core. This is probably due to the discontinuities in which the potential goes from zero to infinity. In fact, these large momentum distributions become manifest when performing NCSM calculations with these two interactions as the convergence rate is significantly slower. Out of the remaining interactions, the Gauss-OPE and Reid93 potentials give the smallest high momentum contribution indicating that they are considerably softer than the other potentials considered. We also note in passing the clearly incompatible high momentum distributions even within the 1σ statistical uncertainty shown as a band for the DS-OPE, DS-χTPE and Gauss-OPE. These incompatibilities are indeed expected and are a signal of the present systematic uncertainties which still need to be quantified.

In order to directly test the convergence of NCSM calculations using the Gauss-OPE potential, we calculated the binding energy and root mean square radius of the Deuteron using different values of the oscillator parameter $\hbar\Omega$ and different basis truncation $N_{\max}$ and compare with the same calculations using the Reid93 potential. The results are shown in Figure 2. As can be seen Gauss-OPE has a faster convergence rate which can be traced to its significantly softer core. All of this is in agreement with our previous Weinberg eigenvalue analyses of these and other local interactions [4].

VI. NCFC CALCULATIONS OF ^{3}H AND ^{4}HE

Once Gauss-OPE has been shown to have an advantageous convergence rate for *ab initio* NCSM calculations of light nuclei we use it to propagate the statistical uncertainty stemming from experimental NN scattering data into the calculation of the binding energy of ^{3}H and ^{4}He. As a first step we looked for the variational minimum of the ground state energy of ^{3}H and ^{4}He as a function of the oscillator parameter $\hbar\Omega$ with the sufficiently large basis size $N_{\max} = 20$ and the central values of the Gauss-OPE potential parameters. The minima were found at $\hbar\Omega = 60$MeV for ^{3}H and $\hbar\Omega = 65$MeV for ^{4}He. Having found the variational minimum, the Monte-Carlo method described in section III was used to generate a family of 33 interactions following the multivariate Gauss distribution of the potential parameters befitting the covariance matrix. With each set of parameters the ground state binding energy of ^{3}H was calculated using different many-body basis space cutoffs $N_{\max} = 8, 10, 12, 14, 16, 18, 20$ with the value of $\hbar\Omega$ fixed at the variational minimum mentioned above. These evaluations allowed us to perform, for sets of $N_{\max}$ values with three to seven entries, 33 extrapolations following Eq.(12) to estimate the corresponding statistical uncertainty. Table I shows the resulting extrapolations for ^{3}H and ^{4}He with different number $N_{\max}$ entries; a clear convergence pattern can be seen as larger basis spaces are included in the extrapolation for the complete space estimate and the corresponding uncertainties. Other observables can be extracted from the resulting many-body wavefunction of the truncated oscillator basis expansion. In particular, we investigated the magnetic moment μ and proton radius r_p of ^{3}H and their sensitivity to the Monte-Carlo sampling of the interaction parameters distribution. For these quantities we find $\mu = 2.610(1)\ \mu_N$ $r_p = 1.4668(8)$fm.

The extrapolations using the seven available $E(N_{\max})$ values and those corresponding to the last row of Table I are shown in Figure 3 as blue lines. As can be seen from the finite basis calculations and the corresponding extrapolations the statistical uncertainty decreases as the cutoff parameter $N_{\max}$ is increased.

We now call attention to the inserts in Figure 3 where we display, on a greatly expanded scale, the extrapolated ground state energies for each of the 33 Monte-Carlo samples. The visual impression is that these results are distributed in a manner that may be consistent with a Gaussian distribution though we do not carry out a detailed study of these limited distributions. These results have some additional impact on the numerical method itself. While in the case of the triton the dominating uncertainty for $N_p = 7$, using calculations up to $N_{\max} = 20$, is the statistical one, in the alpha particle case the situation is just the opposite, indicating that higher $N_{\max}$ values should probably be pursued to confirm the statistical uncertainty. Of course, in both situations there is a mismatch with the experimental binding energies, for which the traditional explanation rests on the inclusion of three- and four-body forces.

In addition, we have restricted the analysis to the statistical

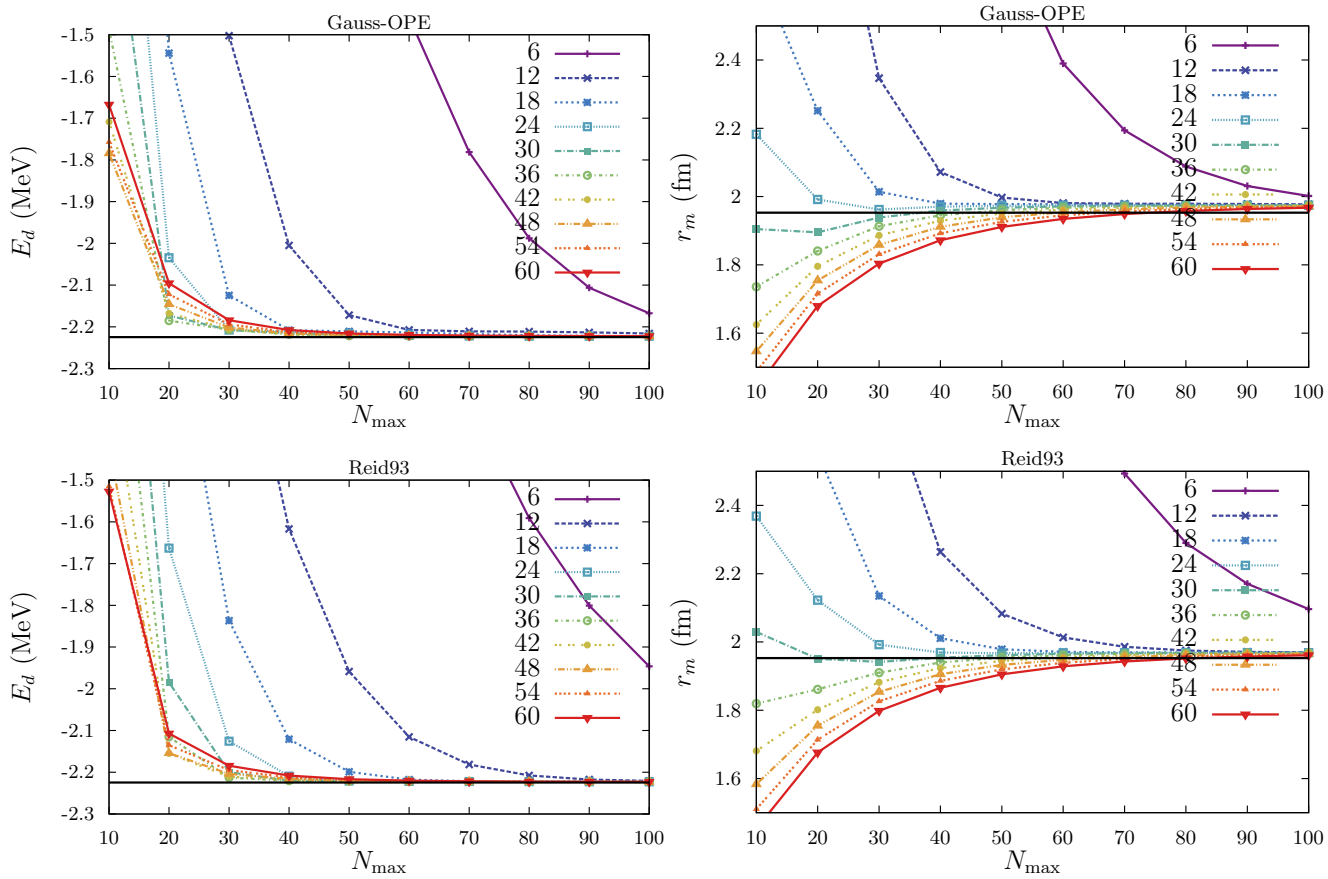

FIG. 2: (Color online) NCSM calculations of the Deuteron binding energy (left panels) and root mean square radius (right panels) as a function of the basis truncation parameter $N_{\max}$ with different values of the harmonic oscillator parameter $\hbar\Omega$ for the Gauss-OPE (top panels) and Reid93 (bottom panels) potentials. The Gauss-OPE potential shows a faster convergence rate in both quantities as evident from the smaller spread with respect to $\hbar\Omega$ at fixed $N_{\max}$.

TABLE I: ^{3}H and ^{4}He ground state energy NCFC extrapolation for the Gauss-OPE potential using different number of $E(N_{\max})$ points N_p according to Eq.(12). All extrapolations start with $N_{\max} = 8$ and include consecutive even values up to the corresponding number of points N_p. E_∞ is the mean of the 33 Monte-Carlo calculations with that number of points, the extrapolation uncertainty $\Delta E_\infty^{\rm ext}$ is the difference between the extrapolation with N_p points listed and the extrapolation with a single point less. The statistical uncertainty $\Delta E_\infty^{\rm stat}$ is given by the standard deviation of the Monte-Carlo extrapolations with the indicated number of entries N_p. For comparison we show experimental values in the last line [28]. Energies are in units of MeV

	^{3}H			^{4}He		
N_p	E_∞	$\Delta E_\infty^{\rm ext}$	$\Delta E_\infty^{\rm stat}$	E_∞	$\Delta E_\infty^{\rm ext}$	$\Delta E_\infty^{\rm stat}$
3	-8.289	–	0.061	-29.224	–	0.226
4	-7.408	0.881	0.020	-25.980	3.244	0.085
5	-7.486	0.078	0.019	-25.417	0.563	0.066
6	-7.421	0.065	0.016	-25.102	0.315	0.058
7	-7.424	0.003	0.015	-24.934	0.168	0.055
$E^{\rm Exp}$	-8.482			-28.296		

uncertainties of the NN interaction stemming directly from the scattering data. In a previous work [29] the role played by the potential representation has been analyzed and it has been found that there are statistically equivalent interactions which, however, produce larger systematic uncertainties by about an order of magnitude in scattering observables. Thus, we expect that when this additional systematic uncertainty is included in the analysis the current numerical uncertainty for $N_p = 7$ will actually be small by comparison.

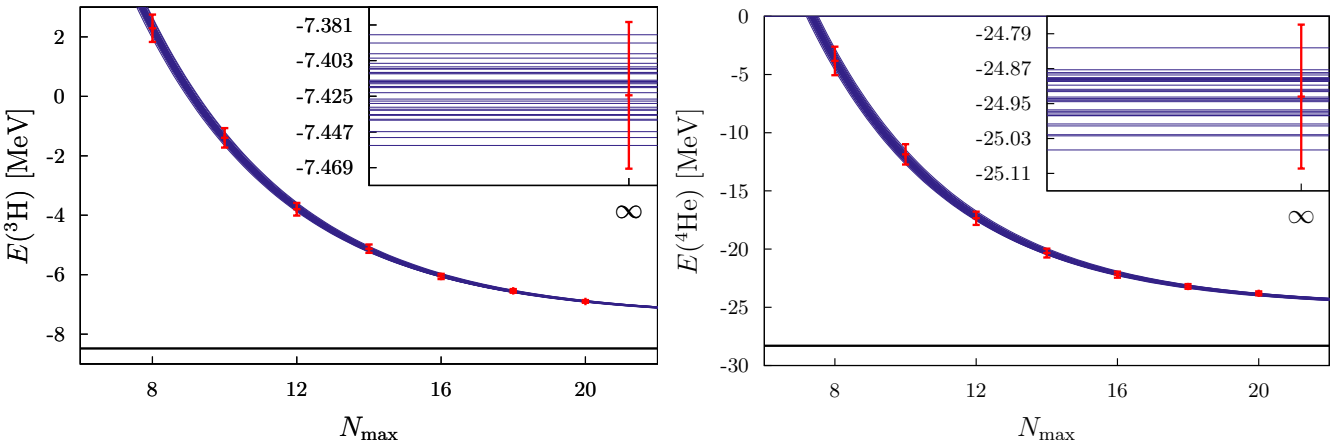

FIG. 3: (Color online) NCSM ground state energy as a function of $N_{\max}$ for ^{3}H at $\hbar\Omega = 60$ MeV (left panel) and ^{4}He at $\hbar\Omega = 65$ MeV (right panel) with the Gauss-OPE potential. The red error bars indicate the mean and 3σ confidence interval of the 33 calculations with different potential parameters (see main text). The blue solid curves give the corresponding 33 extrapolations fitting the a, c and E_∞ of Eq.12 to the calculated values of $E(N_{\max} = 8, 10, \ldots, 20)$. The panels at the top right corners show the extrapolated value at $N_{\max} \to \infty$ from each fit with an error bar indicating the corresponding mean and 3σ confidence interval. The solid black indicates the experimental value.

VII. CONCLUSIONS

We performed NCFC calculations of ^{3}H and ^{4}He combined with Monte-Carlo techniques to extract realistic estimates of the statistical uncertainty originating from uncertainties in experimental NN scattering data. The calculations used the Gauss-OPE potential which showed an appropriate convergence rate for calculations in light nuclei given its soft core nature. The converged result from extrapolation in ^{3}H is in agreement with the previous findings in [11]. In all cases the uncertainty of the NCFC extrapolation was assessed by comparing with extrapolations based on a reduced number of entries for determining the fit function. For the case of ^{3}H it was possible to obtain a result where the extrapolation uncertainty is smaller than the statistical uncertainty. However, this was not possible for the ^{4}He case. Nonetheless one should keep in mind that the *systematic* uncertainty, according to preliminary studies [29], is expected to be an order of magnitude larger than the statistical uncertainty. Therefore, it may not be profitable to reduce the extrapolation uncertainty by performing calculations with an even larger basis size.

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