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# Binding in light nuclei: Statistical NN uncertainties vs Computational accuracy[1]

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**Abstract.** We analyse the impact of the statistical uncertainties of the the nucleon-nucleon interaction, based on the Granada-2013 np-pp database, on the binding energies of the triton and the alpha particle using a bootstrap method, by solving the Faddeev equations for $^3$H and the Yakubovsky equations for $^4$He respectively. We check that in practice about 30 samples prove enough for a reliable error estimate. An extrapolation of the well fulfilled Tjon-line correlation predicts the experimental binding of the alpha particle within uncertainties.

Nuclear structure *ab initio* calculations are notoriously difficult and computationally demanding and have thus so far been limited to light nuclei, although recently, these calculations have been extended to more complex systems [1, 2, 3]. Besides giving important input for applications such as astrophysically relevant nuclear reactions, these calculations are important tests of current nuclear interactions. To this aim, not only the result itself is important but also the uncertainty (see e.g. the special issue [4].) From a theoretical point of view and the inferred predictive power uncertainties can be grouped into three main categories

- The input information: the basic nucleon-nucleon (NN) interaction should describe a relevant piece of the NN scattering data and the simplest two-body bound state: the deuteron. We will call this the statistical uncertainty for reasons to be justified below.
- The solution method: the way the multinucleon problem is solved once the NN interaction is represented. This requires some sufficiently high precision which makes computations costly. We will call these the numerical uncertainty.
- The representation problem: the way the input NN data are represented theoretically. Normally potentials are used, but the form of the potential in the short range region, below $2-3$fm, is generally not universal, and they are often tailored to make the solution of the many body problem as simple as possible. We will call these the systematic uncertainty [2].

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[2] This includes in particular any theoretically based expansion of the interaction rooted or inspired by QCD such as chiral perturbation theory or large $N_c$ expansions were some renormalization scheme dependence is unavoidable.

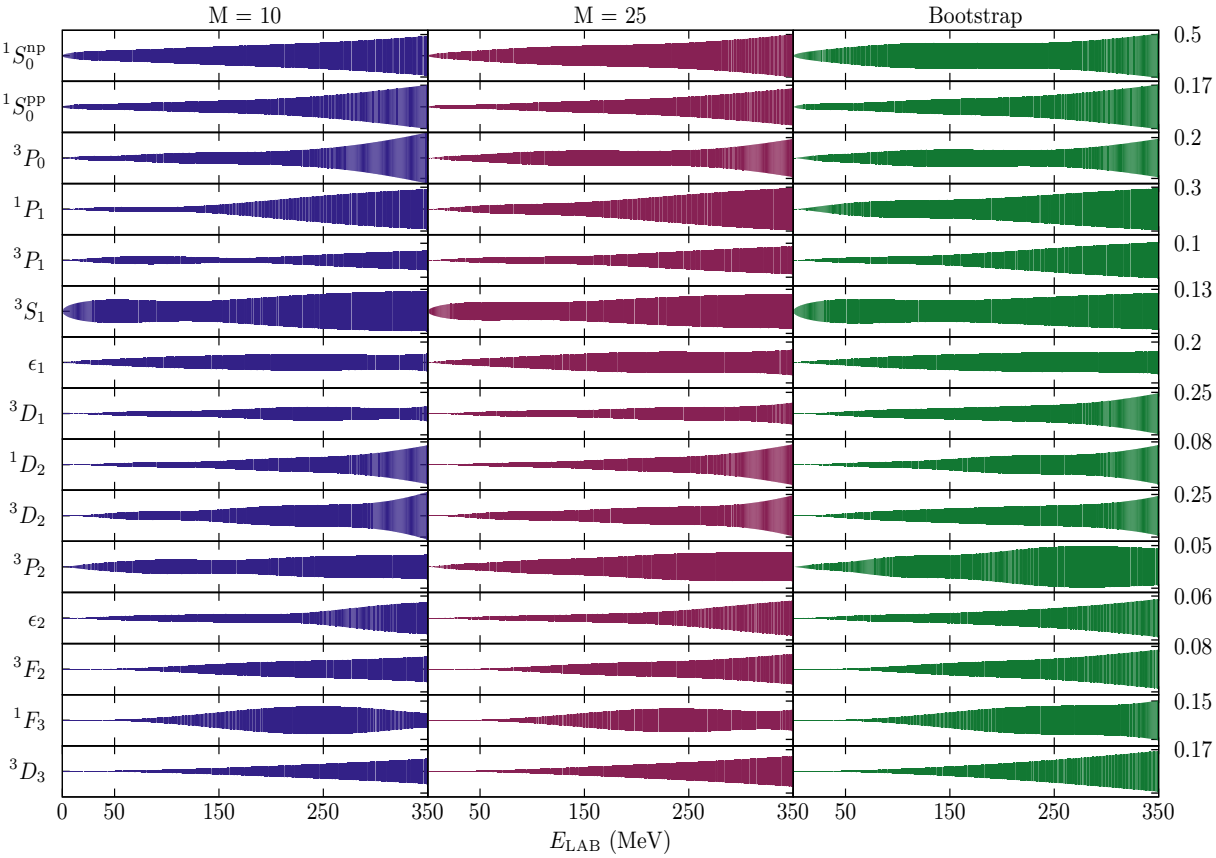


**Figure 1.** (Color online) Phaseshift statistical error bands (in degrees) for the $\delta$-shell potential [5]. The error bands on the first two columns where obtained using a MonteCarlo family of $\delta$-shell potentials where potential parameters are random numbers following the multivariate normal distribution determined by the original fit covariance matrix. The columns use a sample size of $M = 10$ (left column) and $M = 25$ (middle column). The right column is the error bar obtained from the Bootstrap to experimental data presented in [6] with $M = 1000$. All phase shifts are np unless otherwise indicated.

Assuming that these sources of error are independent of each other, we expect the total uncertainty to be given, as usual, by

$$\Delta E^2 = \Delta E^2_{\rm stat} + \Delta E^2_{\rm num} + \Delta E^2_{\rm syst} \tag{1}$$

Clearly, the total error is dominated by the largest one. So, it makes sense either to reduce the largest source of uncertainty or to tune all uncertainties to a similar level. This sets the limit of predictive power in *ab initio* calculations. While numerical accuracy has been a goal in itself in few-body calculations, the *physical* accuracy is given by *all* possibles sources of uncertainties.

In this talk, we discuss the relation between the statistical uncertainties stemming from the finite experimental accuracy of NN scattering data [7, 8, 9, 10] and the currently available numerical accuracy with which the few body problem can be solved. A pioneering work was carried out in [11] where the so-called statistical regularization was used to evaluate the impact of errors on the binding energies of the $A = 3, 4$ systems. The analysis was based on the Paris potential which has $\chi^2$/d.o.f. $\sim 2$.

The recent Granada-2013 $3\sigma$-self consistent database comprises 6713 np and pp scattering data below $E_{\rm LAB} = 350$MeV and has a $\chi^2$/d.o.f $= 1.04$ [12, 5]. The procedure to propagate

uncertainties is based in spirit on the bootstrap analysis proposed in [6] where the 6713 np and pp scattering data are randomized and multiple ($M = 1020$) $\chi^2$-fits yield a multivariate distribution of fitting parameters. This provides a sample enabling a random evaluation of any observable. We monitor the size $M$ of the needed sample by looking for statistical stability of the output. The result for the errors in the corresponding phase shifts is compared in Fig. 1 for different Monte Carlo generated sample sizes following a gaussian multivariate distribution dictated by the parameter's covariance matrix. As we see $M = 25$ already gives a result rather close to the full bootstrap method.

We have built a simple and smooth gaussian potential which can be used in most few- and many-body calculational schemes and which provides an acceptable $\chi^2$/d.o.f. = 1.06 [13], so it can be considered to be statistically equivalent to the original delta-shells potential [8, 5]. As we will put forward here, and in agreement with previous findings using either the hyperspherical harmonics (HSH) method for $A = 3$ [14] and no-core full configuration shell model calculations [15], these estimates already suggests that the numerical accuracy is close to optimal given the statistical uncertainty. We will use here the Faddeev equations for the $A = 3$ case and the Yakubovsky equations for the $A = 4$ situation. As a first step we will consider only NN forces explicitly and leave out 3N and 4N forces for future developments. The multiple evaluations for the triton are shown in Fig. 2. As in [14] we bin the distribution according to the numerical accuracy, $\Delta E_t^{\rm num} \sim 1$keV [3].

In a Monte Carlo approach many variations of the parameters produce irrelevant changes. A principal component analysis looks for eigenvalues and eigenvectors of the computed observable and provides valuable information on the most relevant changes of the input parameters but has seldomly been investigated in nuclear physics (see however Ref. [16] and references therein). In Fig. 3, we show the results of such an analysis applied to the coefficients of the gaussian potential of Ref. [8] implemented in a Monte Carlo fashion. We found that the number of principal components to obtain most of the uncertainty in $E_t$ is around 10. This indicates that regarding $\Delta E_t^{\rm stat}$ a fit to the NN scattering data base could be done with less parameters, if the fit were to be designed in terms of relevant parameters only.

The tiny error band suggests that the discrepancy between our number $E_t^{\rm th} = -7.6669 \pm 0.0124$MeV and the $E_t^{\rm exp} = -8.4820 \pm 0.0001 MeV$ has to be sought in missing three-nucleon forces (3NFs). It is well known that 3NFs give an important contribution to nuclear bindings [17, 18]. This raises the question of how much of this statistical uncertainty will be absorbed into variations in the parameters of the 3NFs. In order to implement some 3N information, we invoke the empirical linear correlation displayed by the Tjon line [17] [4].

In the Monte Carlo method, any choice of parameters $\mathbf{p}$ determines a value of the triton binding energy. Given the variations of the triton binding energy, we expect, when determining the $\alpha$ particle binding energy, a Tjon-like linear correlation of the form $E_\alpha(\mathbf{p}) = aE_t(\mathbf{p}) + b$. The values found are $a = 4.7(1)$ and $b = 11.4$. Thus we expect a Tjon-like correlation would give $\Delta E_\alpha^{\rm stat} = 4.7(1) \times \Delta E_t^{\rm stat} = 50(5)$keV which is mainly determined by the channels involving relative S-waves. In Fig. 4, we show our results for the $^3$H and $^4$He binding energy. The yellow band shows the fit including the uncertainty. The error bars show the numerical uncertainty. Whereas the variation of the binding energies is rather large, the linear correlation indicates that most of this variation will be eventually absorbed into a properly adjusted 3NFs. We take the band width as an indication for the remaining error induced by the uncertainty of NN data. As one can see, the band width and the numerical errors are comparable. Therefore, we deduced

[3] One of the advantages of the present method over the HSH expansion employed in [14] is that the determination of avoided crossings are difficult to identify rigorously; an effect which has to be assisted by visual inspection and, if mistaken, has a repulsive effect. This explains the longer tails of the triton binding energies distributions. We thank Eduardo Garrido for noting this.

[4] See [19, 20] for a Similarity Renormalization Group analysis yielding the simple formula $E_\alpha = 4E_t - 3E_d$.

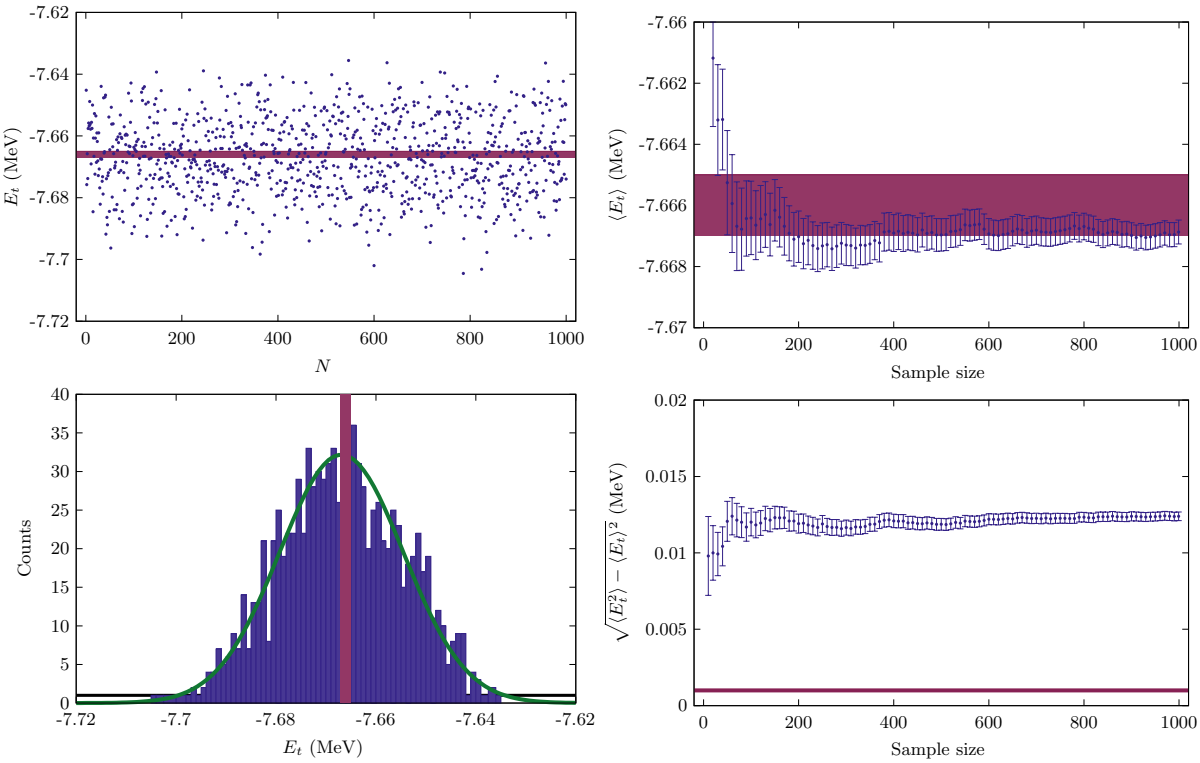


**Figure 2.** (Color online) Distribution (top left) and histogram (bottom left) representing the triton binding energy (in MeV) for a sample of 1000 Monte Carlo generated gaussian potential parameters. Finite sample estimates for the population mean (top right) and population standard deviation (bottom right) of the triton binding energy as a function of the sample size $M$ of the gaussian potential parameters are also shown. In all panels the red band represents the value obtained with the most likely parameters $E_t(\mathbf{p}_0) = 7.666 \pm 0.001$MeV and its width is the numerical error. We take the bin size equal to the numerical precision.

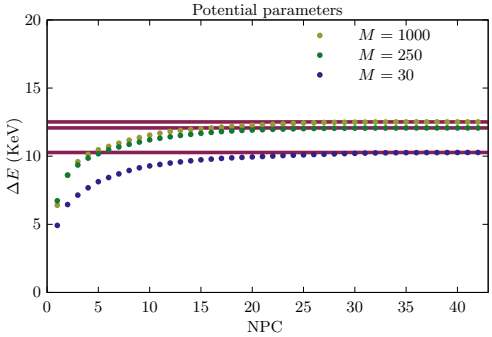


**Figure 3.** (Color online) Number of principal components contributions of gaussian parameters for samples of size $M = 30, 250, 1000$ (from bottom to top) to the triton binding energy uncertainty.

that this uncertainty is comparable to the statistical one. Strong efforts to increase the numerical accuracy are therefore not desired. For this analysis, we used a moderate sample of only M=30, the smallness of which is justified from the analysis of Fig. 2, as far as uncertainty estimates are concerned. In order to have a tighter predicted extrapolated band one would need to reduce the numerical error in $E_\alpha$ in harmony with the Tjon slope $\Delta E_\alpha^{\rm num} \sim 4.7 \Delta E_t^{\rm num} \sim 5$keV. Further details will be presented in a forthcoming publication.

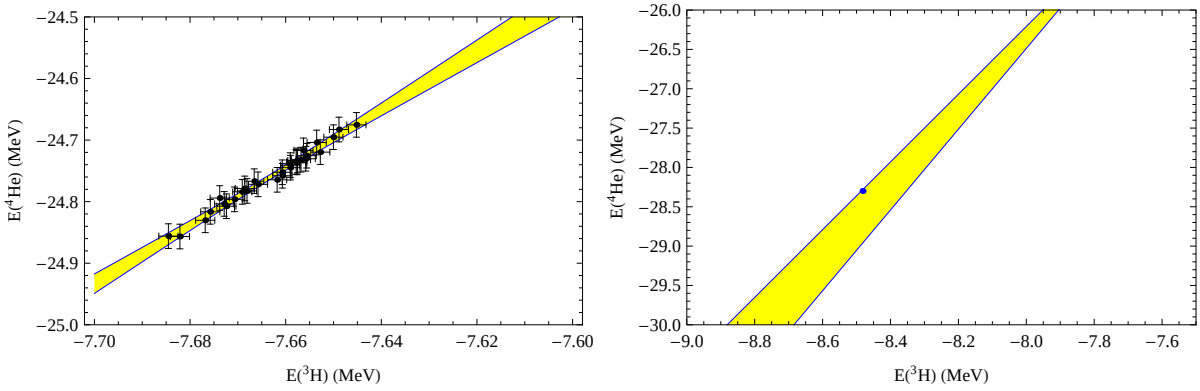


**Figure 4.** (Color online) Tjon type analysis of the $^4$He binding energy vs the $^3$H binding energy. We show the fit to the sample of $N = 30$ Monte Carlo generated binding energies both in a small scale (left panel) and extrapolated in a larger scale (right panel) compared with the experimental point (blue dot). We take $\Delta E_t^{\rm num} = 1\,$keV and $\Delta E_\alpha^{\rm num} = 20\,$keV.

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