Error estimates on Nuclear Binding Energies from Nucleon-Nucleon uncertainties

R. Navarro Pérez, J.E. Amaro and E. Ruiz Arriola
Departamento de Física Atómica, Molecular y Nuclear and Instituto Carlos I de Física Teórica y Computacional
Universidad de Granada, E-18071 Granada, Spain.

(Dated: March 1, 2012)

Despite great theoretical efforts the NN interaction can only be determined with a finite precision, implying an error upper bound for nuclear masses. We analyze for the first time the problem of estimating the systematic errors related to the form of the potential and their impact on nuclear binding. To this end we exploit the concept of coarse grained interactions to typical nuclear wavelengths. Our estimate gives an error $\Delta B/A \sim 0.1 \ldots 0.4$ MeV for the binding energy per particle and paves the way for ab initio calculations tailored to such a precision.

PACS numbers: 13.75.Cs,21.10.Dr,06.20.Dk
Keywords: NN interaction, Nuclear Binding, Error analysis

Since the early days of Nuclear Physics the NN interaction has played a major role in the description of the properties of finite nuclei. While abundant sets of np and pp data have been collected along the years and accurate theoretical analyses have been carried out since the mid-nineties [1–5], the impact of the NN uncertainties in the Nucleon Many Body Problem remains an open challenge. This is of utmost importance as it determines a priori a lower bound on the inaccuracy of first principles calculations [6] and might help to advantageously optimize the computational cost. While Nuclear binding energies are experimentally known to high accuracy $\Delta B = 0.01 \ldots 10$ KeV, liquid-drop model inspired mass fit formulae yield a lower theoretical accuracy $\Delta B = 0.6$ MeV (see e.g. Refs. [7, 8] and references therein). In the present work we face the problem squarely from the NN side by deducing and propagating two-body systematic errors to provide a first theoretical a priori estimate of binding energy uncertainties.

Error analysis of NN phase-shifts for several partial waves became first possible when the Nijmegen group [1] carried out a Partial Wave Analysis (PWA) fitting about 4000 experimental np and pp data (after rejecting further 1000 of 36 mutually inconsistent data) with $\chi^2/\text{dof} \sim 1$. The fit fixed the form of the potential to be an energy dependent square well located at a distance of 1.4 fm, a One-Pion-Exchange (OPE) and Charge-Dependent (CD) contribution starting at 1.4 fm and a One-Boson-Exchange (OBE) piece operating below 2 – 2.5 fm. Unfortunately, the required energy dependence becomes messy for Nuclear Structure calculations. At present there are a variety of NN (energy independent) potentials fitting a large body of scattering data with $\chi^2/\text{dof} \sim 1$ [1–5], but surprisingly error estimates on potential parameters are not given. Whereas all these modern potentials share the verifiable and local OPE and CD tail and include electromagnetic effects, the unknown short range components of these potentials display a variety of forms and shapes, local potentials [2], or nonlocal ones implementing angular momentum dependence [3], energy dependence [1] or linear momentum dependence [2, 4, 5]. While in principle $p-, L-, E-$ non-localities are on-shell equivalent (see e.g. Ref. [9] for a proof in a $1/M_N$ expansion) they reflect truly different physical effects and generally one should consider them as independent quantities; any specific choice is biased and hence becomes a source of systematic errors.

We distinguish as usual in error analyses two sources of uncertainties: statistical errors stemming from the data uncertainties for a fixed form of the potential, and systematic errors arising from the different most-likely forms of the potentials. Clearly, the total uncertainty corresponds to adding both in quadrature. In what follows it is advantageous to take the viewpoint of considering any of the different potentials as an independent but possibly biased way to measure the scattering amplitudes and/or phase-shifts. Because the biases introduced in all single potential are independent on each other, a randomization of systematic errors makes sense. Thus, the overall spread between the various phenomenological models with $\chi^2/\text{dof} \sim 1$ provides the scale of the uncertainty.

In Fig. 1 we show the absolute (mean-square) errors for np partial wave phase shifts due to the different potentials fitting scattering data with $\chi^2/\text{dof} \sim 1$ [1–5] as a function of the LAB energy. As one naturally expects the uncertainties grow with energy and decrease with the relative angular momentum which semiclassically corresponds to probing an impact parameter $b \sim (L+1/2)/p$, with $p = \sqrt{M_N E_{\text{LAB}}}/2$ the CM momentum, making peripheral waves to be mostly determined from OPE. These analyses stop at the pion production threshold so that one probes distances till $b_{\text{min}} \sim 1/\Lambda = 0.5$ fm with $\Lambda = \sqrt{m_\pi M_N}$. Generally, the PWA statistical errors [1] turn out to be smaller than the systematic bands displayed in Fig. 1. This counter-intuitive result relies not only on the specific forms of potentials which treat the mid- and short-range behaviour of the interaction differently but also on the fact that the fits are mainly done to scattering amplitudes rather than to the phase-shifts themselves. Our purpose is to quantify the impact of uncertainties in Fig. 1 on Nuclear Binding energies.

The most direct way of analyzing binding energy uncertainties from randomized systematic errors would be to undertake large scale ab initio calculations using the different forms of the set of $N$ two-body potentials, say $V_1^{(i)}$ with $i = 1, \ldots, N$, yielding $B^{(i)}(A)$ whence a mean $\bar{B}(A)$ and a standard deviation $\Delta B(A)$ can be constructed. For instance, the
triton binding energy obtained by Faddeev calculations is 8.00, 7.62, 7.63, 7.62, 7.72 MeV for the CD Bonn [10], Nijm- II, Reid93, Nijm-I and AV18 [11] respectively. More recently, the covariant spectator model has produced the closest binding energy 8.50 MeV to experiment precisely when the NN $\chi^2$/dof is smallest. This yields in all $B_3 = 7.85(34)$MeV (exp. $B_3 = 8.4820(1)$MeV) i.e. $AB_3/3 = 0.11$MeV. Of course, in doing so even for the triton or the $\alpha$-particle there is typically a flagrant need for three-body interactions which account for the missing 1MeV and 4MeV to the binding energy respectively. On the other hand, the definition of the three- and higher-body interaction depends on the two body potential, so any uncertainty in the two-body interaction will carry over to the three-body interaction. Thus, even if we fix it say in the $A = 3$ system, there will always be a residual uncertainty in the $A + 1 = 4$ calculation. Thus, estimating the two-body uncertainty provides a lower bound on the total uncertainty if the correlations between the two- and three-body forces are ignored. The argument generalizes trivially to any $A$–body interactions and $A + 1$–nuclei.

Unfortunately, the procedure outlined above of using different potentials stops beyond the $A = 4$ nucleus, due to computational and theoretical difficulties related to the form of the potential. From an ab initio viewpoint, only Monte Carlo calculations may go up to $A = 10$ when potentials are fixed to be $r$–dependent with a nonlocality in terms of the relative angular momentum operator [12, 13]. For that good reason the Argonne potential saga has been constructed sticking to this representation and culminating in the AV18 potential [3], an updated version of AV14 containing charge-independence-breaking (CIB) terms and a complete electromagnetic interaction and fitted directly to 4301 pp and np data from the 1993 Nijmegen partial-wave analysis [1] with the requested $\chi^2$/dof $\sim 1$. The AV18 and AV18+UIX have become standard Hamiltonians for ab initio calculations of light nuclei [6] and dense matter [14]. Note that even if statistical errors on potential parameters would have been estimated in Ref. [3], the question on the systematic errors remains. We motivate below an approximate method to address these issues.

One of the outstanding features of the AV18-potential is the presence of the short distance core in the central part, $V_C(r)$, for distances below $a_{core} = 0.5$fm, which demands sizeable and fine-tuned short distance correlations [6]. However, for a closed-shell nucleus one has schematically

$$\langle V_2 \rangle_A = \frac{A(A-1)}{2} \int d^3 r P_2(r) V_C(r),$$

where $P_2(r)$ is the probability of finding two particles at a distance $r$ that turns out to be fairly independent of the particle number. In particular, for $r \lesssim a_{core}$ one has $V_C(r) \gg B/A$ and one is left with a two-body problem with $A = 2$ spectators; in the classically forbidden region an exponential suppression, $P_2(r) \sim \exp(-2\int_r^{a_{core}} dr/\sqrt{2\mu V_C(r)})$ is expected semi-classically. Thus the contribution from the core is small, precisely in the region where the NN force is not well determined from the PWA probing $r \geq b_{min}$. For our error estimate we propose to side-step this core complication by introducing a coarse grained potential where the cancellation of the product $P_2(r) V_C(r)$ comes from a vanishing potential below $a_{core}$.

The previous argument was suggested long ago by Afnan and Tang [13] who realized that for $A = 3, 4$ systems the relevant NN-scattering energies do not probe the core explicitly. Soft core potentials, fitted to NN low partial waves up to $E_{LAB} = 100$MeV, provided reasonable binding energies. Furthermore the hard core can be made into a soft core by introducing (linear-momentum) nonlocalities in terms of the kinetic energy operator by a unitary phase-preserving transformation [16]. Actually, this is the physics behind the so-called $V_{lowk}$ potentials based in the definition of an effective truncated Hilbert space below a given cut-off $\Lambda \sim \sqrt{M_N m_\pi}$ [17, 18]. Recently, we have shown how a similar idea can be implemented in coordinate space using a coarse grained potential [19, 20], i.e. an average potential over a given wavelength resolution $\Delta r \sim b_{min}$; that means specifying the potential information in a finite number of points. The form of the potential is not important but calculations become
simple by taking delta-shells in the region below 3fm. For the partial wave $2s_{1/2}$, the potential reads

$$V_{1s}(r) = \frac{1}{2\mu} \sum_{n=1}^{N} (\lambda_n)^2 \delta(r - r_n), \quad r \leq r_c,$$

with $\mu$ the reduced pn-mass and $r_c = 3$fm. In practice $N \leq 5$ for any given partial wave. For $r > 3$fm we use the customary CD OPE-electromagnetic interactions. The main novelty is a determination of the, so far, missing errors in the potential parameters (in this case $(\lambda_n)^2$) from the uncertainties depicted in Fig. 1 and corresponding to all $\chi^2/\nu$ close to 1 fits [1–5]. For instance, we found [2] by using the $^3S_1$, $^3D_1$ and $E_1$ uncertainties of Fig. 1 that for the deuteron $\Delta B_{1H}/2 = 0.105$MeV compared to the experimental $\Delta B_{1H}/2 = 0.050$MeV.

In our previous calculation [19], we showed how our approach is competitive not only as a way of determining the phase shifts but also with more sophisticated approaches to Nuclear Structure [16]. This was checked with oscillator wave functions in the case of $^4$He, $^{16}$O and $^{80}$Ca which reproduces experiment at the $20 - 30$%-level provided the phase-shifts are fitted to about 100MeV [19]. This is a tolerable accuracy as we just intend to make a first estimate on the systematic uncertainties and then compute the change in the binding energy from the simple formulas,

$$\Delta B_{1H} = \langle \Delta V \rangle_{1H} = 3\langle 1s | \frac{1}{2} (\Delta V_{1s} + \Delta V_{3s}) | 1s \rangle,$$

$$\Delta B_{4He} = \langle \Delta V \rangle_{4He} = 6\langle 1s | \frac{1}{2} (\Delta V_{1s} + \Delta V_{3s}) | 1s \rangle,$$

where $|1s\rangle$ is the Harmonic oscillator relative wave function with the corresponding $b-$ oscillator parameter reproducing the physical charge radius. The numbers in front are Talmi-Moshinsky coefficients and correspond in this particular case to the number of pairs interacting through a relative s-wave. Errors are computed by adding individual contributions $(\Delta \lambda_n)^2$ from Eq. (2) in quadrature. By propagating the PWA errors in Eq. (3) we find $\Delta B_{1H}/4 = 0.07 - 0.085$MeV depending on the fitting cut-off LAB energy, 100-350 MeV respectively, in good agreement with the Faddeev estimates given above. For the $\alpha$-particle Eq. (4) yields $\Delta B_{4He}/4 = 0.10 - 0.13$MeV. Along the lines of Ref. [19] we also find $\Delta B_{16O}/16 = 0.26$MeV and $\Delta B_{80Ca}/40 = 0.32$MeV.

A simple estimate on the impact of errors due to the two body interaction uncertainty can be done using Skyrme effective interactions (for a review see [2])

$$\frac{\Delta B}{A} = \frac{3}{8A} \Delta t_0 \int d^3x \rho(x)^2,$$

where we get $t_0 = (\pi/\mu) \sum_n r_n^2 (\lambda_1^2 + \lambda_3^2)$. Using the two-body interaction of Eq. (2) and propagating errors we get $t_0 = 0.92(1)$GeV/fm$^3$. As a check on the size of $t_0$ we note that from a fit to the equation of state used by the Trento group [23] at low densities we obtain a value $t_0 \sim -0.9(1)$GeV/fm$^3$, whereas a coarse graining of NN interactions in CM momentum space down to $A \sim 0.3$GeV gives a compatible value, $t_0 \sim -4\pi^2/(MN\Lambda)$ [24]. For nuclear matter at saturation, $\rho_0 = 0.17$fm$^{-3}$, our $\Delta t_0 = 10$MeV/fm$^3$ implies

$$\frac{\Delta B}{A} = \frac{3}{8} \Delta \rho_0 = 0.63\text{MeV}.$$

We may implement finite size effects by using a Fermi-type shape for the matter density $\rho(r) = C/(1 + e^{(r-R)/a})$ with $R = r_0 A^{1/3}$ and $r_0 = 1.1$fm and $a = 0.7$fm and normalized to the total number of particles $A = \int d^3x \rho(x)$ we get

$$\Delta B_{1H}/A = 0.1 - 0.4\text{MeV},$$

which depends on the value of $A$ for $4 \leq A \leq 208$.

One may reasonably doubt that the core effects and the corresponding short distance correlations can be reliably monitored by a simple shell model calculation as given by Eq. (3) and Eq. (4) for $^3$H and $^4$He respectively. We show now that for the purpose of error estimate this is however not so. In order to check this we take advantage of a recent analysis using the AV18-potential [21] where the dependence of nuclear binding on the potential parameters is analyzed in much detail for mass numbers $A = 2, \ldots, 8$. Relative 1% variations of two-body potential parameters are considered yielding changes in binding energies in the range of $0.1 - 20$MeV for $^4$He. This

\[\text{FIG. 2. AV18 phase shifts in the } ^1S_0 \text{ (upper panel) and } ^3S_1 \text{ (lower panel) partial waves as a function of the CM momentum when the parameters are varied as specified in Ref. [21]. We also depict the band corresponding to the spread of values obtained with 7 high quality potentials [1–5] containing One-Pion-Exchange (OPE) and Charge Dependence (CD) tail and fit scattering data with } \chi^2/\nu \sim 1.}\]
is a much larger range than our estimated errors. We note here that the largest sensitivity is on the short range potential, whereas the pion mass variation in the OPE piece yields a tiny effect. We may test our strategy by proceeding as follows. For any variation of the $\text{AV18}$-potential parameters there is a corresponding change in the phase shifts. In Fig. 2 we show as an illustration the changes in the most important $1_S0$ and $3_S1$ waves due to several changes in parameters as explained in Ref. [23]. As we see these changes are indeed larger than the systematic errors depicted in Fig. 1 that is enough for our error analysis. In other words, our coarse grained potential, Eq. (2), as to reproduce such a change and then use Eqs. (3,4). We show our results in table I depending on the fitted maximal $E_{\text{LAB}}$. The disagreement of our results with those of AV18 in the case of changing the pion mass in the OPE potential is not very important since the net result is rather small anyhow and the pion mass is well known. We note, however, a larger sensitivity of the $\text{AV18}$ potential with respect to the short distance variations which is the relevant aspect for our error analysis. In other words, our coarse grained calculation reproduces $ab\text{ initio}$ $\Delta B$’s at the 20% accuracy.

We summarize our points. Nuclear Binding energies are a crucial test for the Nuclear Many Body Problem. While first principles calculations are hampered by computational difficulties, we note that nuclear force uncertainties may have a useful impact on these calculations. The present theoretical estimates are in the range $\Delta B/A \sim 0.1 - 0.4\text{MeV}$ exceeding two or three orders of magnitude the available precision of $ab\text{ initio}$ Monte Carlo calculations achieved up to date for $A \leq 10$. The prospective of increasing the particle number keeping the computational cost provides strong reasons to go beyond NN uncertainties as done here and to consider also errors in 3N and 4N forces. Finally, one should keep in mind that agreement between theory and experiment could also be declared even when the theory is less precise than the experiment, as it so frequently happens in Nuclear Physics, provided of course both error bands overlapp.

This work is supported by Spanish DGI (grant FIS2011-24149) and Junta de Andalucía (grant FQM225). R.N.P. is supported by a Mexican CONACyT grant.

![Table I. Changes of ground state energies of lightest nuclei $^A$2,3,4 in MeV for the coarse-grained potentials with oscillator shell model when $^1S_0$ and $^3S_1$ phase shifts are fitted up to LAB energies $E_{\text{LAB}} = 100\text{MeV}$ and $E_{\text{LAB}} = 350\text{MeV}$ used in this work compared to the $ab\text{ initio}$ Monte Carlo calculations [23] (labeled as AV18 here and using their notation). The changes correspond to the variation of the total energy when the mass parameter is either increased or decreased by 1%. For instance the label $m_0$ corresponds to $B(1.0 m_N) - B(0.99 m_N)$.](image)

| Parameter | $\epsilon_Y$ | $\epsilon_Y$ (AV18) | $^2H$ | $^2H$ (AV18) | $^3H$ (100) | $^3H$ (350) | $^3H$ (AV18) | $^4He$ (100) | $^4He$ (350) | $^4He$ (AV18) |
|-----------|--------------|---------------------|-----|--------------|-------------|-------------|-------------|--------------|-------------|--------------|
| $m_N$     | -0.0445      | -0.0444             | -0.3997 | -0.3960 | -1.0030 | -1.1606 | -0.9797 | -1.6820 | -1.9973 | -2.1945 |
| $m_N + \delta_N$ | -0.1602 | -0.1612 | -0.7986 | -0.7928 | -2.7817 | -3.8063 | -2.6560 | -5.2395 | -7.2887 | -6.5230 |
| $\delta_\Delta$ | 0.1350 | 0.1359 | 0.4641 | 0.4609 | 2.0690 | 3.0778 | 1.9504 | 4.1380 | 6.1555 | 5.0380 |
| $m_\sigma$ (OPE) | -0.0051 | -0.0051 | 0.0289 | 0.0623 | 0.0140 | -0.1676 | 0.0730 | 0.0280 | -0.1461 | 0.1045 |
| $m_\sigma$ (+TPE-s) | 0.0706 | 0.0705 | 0.2665 | 0.2981 | 1.1205 | 1.1770 | 1.1055 | 2.2409 | 2.3540 | 2.8105 |
| $m_\sigma$ (+TPE-L) | – | – | 0.2683 | 0.2999 | 1.1229 | 1.1812 | 1.1025 | 2.2459 | 2.3623 | 2.7830 |
| $m_\nu$ | -0.4757 | -0.5079 | -1.8692 | -1.8571 | -7.9517 | -10.3458 | -7.6743 | -15.9034 | -20.6916 | -19.9870 |

References:

[1] V. Stoks, R. Kompl, M. Rentmeester, and J. de Swart, Phys.Rev. C48, 792 (1993).
[2] V. Stoks, R. Klomp, C. Terheggen, and J. de Swart, Phys.Rev. C49, 2950 (1994).
[3] R. B. Wiringa, V. Stoks, and R. Schiavilla, Phys.Rev. C51, 38 (1995).
[4] R. Machleidt, Phys.Rev. C63, 024001 (2001).
[5] F. Gross and A. Stadler, Phys. Rev. C78, 014005 (2008).
[6] S. C. Pieper and R. B. Wiringa, Ann. Rev. Nucl. Part. Sci. 51, 53 (2001).
[7] J. Toivanen, J. Dobaczewski, M. Kortelainen, and K. Mizuyama, Phys.Rev. C78, 034306 (2008).
[8] J. Dudek, B. Szpak, M.-G. Porquet, and B. Fornal, Journal of Physics: Conference Series 267, 012062 (2011).
[9] A. Amghar and B. Desplanques, Nucl.Phys. A585, 657 (1995).
[10] R. Machleidt, F. Sammarruca, and Y. Song, Phys. Rev. C53, 1483 (1996).
[11] J. L. Friar, G. L. Payne, V. G. J. Stoks, and J. J. de Swart (1993), Phys.Lett. B 311, 4 (1993).
[12] I. Lagaris and V. Pandharipande, Nucl.Phys. A359, 331 (1981).
[13] R. B. Wiringa, R. Smith, and T. Ainsworth, Phys.Rev. C29, 1207 (1984).
[14] A. Akmal and V. Pandharipande, Phys.Rev. C56, 2261 (1997).
[15] I. Afnan and Y. Tang, Phys.Rev. C75, 1337 (1968).
[16] T. Neff and H. Feldmeier, Nucl.Phys. A713, 311 (2003).
[17] S. Bogner, T. Kuo, and A. Schwenk, Phys.Rep. 386, 1 (2003).
[18] S. Bogner, R. Furnstahl, and A. Schwenk, Prog.Part.Nucl.Phys. 65, 94 (2010).
[19] R. Navarro Perez, J. Amaro, and E. Ruiz Arriola (2011), arXiv:1111.4328 [nucl-th].
[20] R. Navarro Perez, J. Amaro, and E. Ruiz Arriola (2012), arXiv:1202.2689 [nucl-th].
[21] V. Flambaum and R. B. Wiringa, Phys.Rev. C76, 054002 (2007).
[22] M. Bender, P.-H. Heenen, and P.-G. Reinhard, Rev.Mod.Phys. 75, 121 (2003).
[23] S. Gandolfi, A. Illarionov, S. Fantoni, J. Miller, F. Pederiva, et al., Mon.Not.Roy.Astron.Soc. 404, L35 (2010).
[24] E. Ruiz Arriola (2010), arXiv:1009.4161 [nucl-th].