Triton binding energy with realistic precision

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We compute the binding energy of triton with realistic statistical errors stemming from NN scattering data uncertainties and the deuteron and obtain $E_t = -7.638(15)$ MeV. Setting the numerical precision as $\Delta E_{\text{num}} \lesssim 1$ keV we obtain the statistical error $\Delta E_{\text{stat}} = 15(1)$ keV which is mainly determined by the channels involving relative S-waves. This figure reflects the uncertainty of the input NN data, more than two orders of magnitude larger than the experimental precision $\Delta E_{\text{exp}} = 0.1$ keV and provides a bottleneck in the realistic precision that can be reached. This suggests an important reduction in the numerical precision and hence in the computational effort.

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One of the main challenging goals in theoretical Nuclear Physics is the ab initio determination of binding energies of atomic nuclei. The accepted protocol consists of undertaking a quantum multinucleon calculation from the knowledge of few-body forces. The simplest case was such a program has been most often investigated is the binding energy of triton, a stable system consisting of two neutrons and a proton with an experimental mass defect given currently by $M_t - 2m_n - m_p = E_t^{\exp} = -B_t^{\exp} = -8.4820(1)$ MeV. Already in the mid 1930’s quantum mechanical theoretical studies of triton binding allowed to establish essential properties of the nuclear force: its finite range as well as the existence of neutron-neutron interactions (see e.g. Refs. [1, 2] for early reviews). The increasing precision in our knowledge of the two body interaction has strongly motivated the developments in solving the computationally expensive 3N problem (see e.g. [3–6]). While this was partly aimed at establishing the need of 3N forces, high numerical precision in conjunction with realistic and precise nucleon-nucleon interactions has become a major issue by itself in few-body computational methods. In Refs. [7–9] benchmarking precisions of $\Delta E_{\text{num}} = 10, 0.1, 0.01$ keV have been achieved within different schemes.

However, nucleon-nucleon potentials determined from data inherit statistical fluctuations that propagate to the triton theoretical energy into a genuine statistical error $\Delta E_{\text{stat}}$. A pioneering and forgotten attempt already looked at the consequences for triton binding based on an analysis of the inverse scattering in the $^1S_0$ channel [10]. In the present paper we quantify for the first time the uncertainty of triton energy $\Delta E_{\text{stat}}$ stemming from a complete statistical analysis of 6713 selected nucleon-nucleon scattering data.

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The main and most reliable source of information for the NN interaction are the deuteron energy and the more than 8000 np and pp scattering data below pion production threshold published during the last 65 years. These will be denoted as $O_i^{\exp} \pm \Delta O_i$, with $i = 1, \ldots, N$ and will be regarded as normally distributed variables. In the classical statistical approaches one proposes a given NN interaction $V_{NN}(\bm{p})$ depending on a set of parameters $\mathbf{p} = (p_1, \ldots, p_P)$ which, by solving the two body Schrödinger equation, generates a set of scattering observables $O_i(\mathbf{p})$ with $i = 1, \ldots, N$. The parameters are determined by a least squares $\chi^2$ fit:

$$\min_{\mathbf{p}} \chi^2(\mathbf{p}) = \min_{\mathbf{p}} \sum_{i=1}^{N} \left( \frac{O_i^{\exp} - O_i(\mathbf{p})}{\Delta O_i^{\exp}} \right)^2 \equiv \chi^2(\mathbf{p}_0).$$

A high quality potential is one verifying $\chi^2/v \sim 1$, with $v = N - P$. Since the Nijmegen group analysis in 1993 [11] a set of high quality potentials have emerged fitting their contemporary databases [12–21]. However, the self-consistency of the $\chi^2$ approach requires the residuals to be normally distributed,

$$R_i = \frac{O_i^{\exp} - O_i(\mathbf{p}_0)}{\Delta O_i^{\exp}} \sim \mathcal{N}(0,1),$$

a condition which, even if elementary, has only recently been addressed [21] and checked in the previous analyses [18–20]. The total number of np and pp data was $N = 6713$. This is almost twice as in the 1993 Nijmegen analysis [11] that lacked a normality test. The normality property of the residuals has been exploited to extract the effective interaction parameters and corresponding counterterms [22] and to replicate via Monte Carlo bootstrap simulation as a means to gather more robust information on the uncertainty characteristics of fitting parameters [23]. We stress that the verification of normality, Eq. (3), is essential for a meaningful propagation of the statistical error, since the uncertainty inherited from the fitted scattering data $\Delta O_i^{\exp}$ corresponds to a genuine statistical fluctuation. This allows to determine the $1\sigma$ error of the...
parameters \( p = p_0 \pm \Delta p^{\text{stat}} \) and hence the error in the potential
\[
V_{NN} = V_{NN}(p_0) \pm \Delta V_{NN}^{\text{stat}}
\]
which generates in turn the error in the NN phase-shifts \( \delta = \delta(p_0) \pm \Delta \delta^{\text{stat}} \) and mixing angles. Once the NN-potential is determined the three body problem can be solved for the triton binding energy,
\[
\left[ \sum_i T_i + \sum_{i<j} V_{NN}(ij) \right] \Psi = E_t \Psi
\]
where
\[
E_t = E_t(p_0) \pm \Delta E_t^{\text{stat}}.
\]

Direct methods to determine \( \Delta p^{\text{stat}} \), \( \Delta V_{NN}^{\text{stat}} \) and \( \Delta E_t^{\text{stat}} \) proceed either by the standard error matrix or Monte Carlo methods (see e.g. \cite{24}). In Ref. \cite{23} we have shown that the latter method is more convenient for large number of fitting parameters (typically \( P = 40 - 60 \)), and consists of generating a sufficiently large sample drawn from a multivariate normal probability distribution
\[
P(p_1, p_2, \ldots, p_P) = \frac{1}{\sqrt{(2\pi)^P \det \mathbf{\Sigma}}} e^{-\frac{1}{2}(p-p_0)^T \mathbf{\Sigma}^{-1}(p-p_0)},
\]
where \( \mathbf{\Sigma}_{ij} = (\partial^2 \chi / \partial p_i \partial p_j)^{-1} \) is the error matrix. We generate \( M \) samples \( p_\alpha \in P \) with \( \alpha = 1, \ldots, M \), and compute \( V_{NN}(p_\alpha) \) from which the corresponding scattering phase shifts \( \delta(p_\alpha) \) and triton binding energies \( E_t(p_\alpha) \) can be determined.

In our calculations we take \( M = 205 \) samples for the smooth potential described in \cite{21} \(( r_c = 3 \text{ fm})\),
\[
V(\vec{r}) = V_{\text{short}}(r_\text{c} - r) + V_{\text{long}}(r) \theta(r-r_\text{c}).
\]
The long-range piece \( V_{\text{long}}(\vec{r}) \) contains a charge-dependent (CD) one pion exchange (OPE) with fixed \( f^2 = 0.075 \) \cite{23} and electromagnetic (EM) corrections which are kept fixed throughout the fitting process. The short-range component is
\[
V_{\text{short}}(\vec{r}) = \sum_{n=1}^{21} \hat{O}_n \sum_{i=1}^{N} V_{i,n} e^{-r^2/(2a_i^2)},
\]
where \( \hat{O}_n \) are the set of operators in the extended AV18 basis \cite{13,26,28}. \( V_{i,n} \) are fitting parameters and \( a_i = a/(i+1) \) with \( a = 2.3035 \pm 0.0133 \text{ fm} \). For this potential \( \chi^2/\nu = 1.06 \) and normality of residuals is verified. The potential uncertainties \( \Delta V_{NN}^{\text{stat}} \) have been depicted in \cite{21}. We have checked that statistical uncertainties in the phases and mixing angles \( \Delta \delta^{\text{stat}} \) determined by the covariance matrix method (which would correspond to the limit \( M \to \infty \)) are fairly well reproduced by our \( M = 205 \) samples when the variance of the population is used as an estimator. Likewise, the uncertainties of the potential Eq. (8) obtained by the multivariate distribution, Eq. (6) are in fair agreement with our original partial wave analysis to the 3\( \pi \) s consistent database in terms of a delta-shell potential with OPE (DS-OPE) \cite{19} and also with the corresponding bootstrap simulation \cite{23}.

The results for \( B_t \) for each one of the \( M = 205 \) Monte Carlo samples of the potential have been obtained by means of the Hyperspherical Adiabatic Expansion Method described in \cite{29}. The angular part of the Faddeev equations is first solved for fixed values of the hyperradius \( \rho \). The corresponding angular eigenfunctions \( \{ \Phi_n(\rho, \Omega) \} \) form a complete set, and it is used as a basis in order to expand the total three-body wave function \( \Psi \) as
\[
\Psi = \frac{1}{p^{\nu/2}} \sum_n f_n(\rho) \Phi_n(\rho, \Omega),
\]
where \( \Omega \) collects the usual five hyperangles, and where the radial wave functions \( f_n(\rho) \) are obtained in a second step by solving a coupled set of differential radial equations where the eigenvalues of the angular part enter as effective potentials (see Ref. \cite{23} for details).

When solving the angular part, the eigenfunctions \( \Phi_n(\rho, \Omega) \) are expanded in terms of the Hyperspherical Harmonics (HH), which contain the dependence on the quantum numbers \( \{ \ell_x, \ell_y, L, s_x, s_y, S \} \) of the different components included in the calculation. Obviously, \( \ell_x \) and \( s_x \) are the relative orbital angular momentum and spin of one of the two-body systems in the triton, \( \ell_y \) is the relative orbital angular momentum between the third particle and the center of mass of the two-body system, and \( s_y \) is the spin of the third particle. The angular momenta \( \ell_x, \ell_y \) couple to \( L \), and \( s_x, s_y \) couple to the total spin \( S \). Finally, \( L \) and \( S \) couple to the total angular momentum \( 1/2 \) of the triton ground state. Together with these quantum numbers the HH depend on the hyperrandom \( K = 2\nu + \ell_x + \ell_y \) \( (\nu = 0, 1, 2, \cdots ) \).

Therefore, the convergence of the three-body wave function \( \Psi \) has to be achieved at three different levels. First, in terms of the adiabatic channels included in the expansion explicitly written in Eq. (9). Second, in terms of the components (with quantum numbers \( \{ \ell_x, \ell_y, L, s_x, s_y, S \} \) included in the expansion of the angular functions \( \{ \Phi_n \} \). And third, in terms of the maximum value of the hyperrandom, \( K_{\text{max}} \), used for each of the components. In the calculations presented here we have included up to 12 adiabatic terms in the expansion in Eq. (9) (typically, four or five terms are enough to get a good convergence for bound states). All the partial waves with \( \ell_x, \ell_y \leq 5 \) have been included (when increasing the number of components to \( \ell_x, \ell_y \leq 8 \) no substantial difference has been observed). Finally, three different sets of \( K_{\text{max}} \)-values have been considered. We shall refer to them as sets (i), (ii), and (iii). In set (i), about 500 HH are used in total, and \( K_{\text{max}} = 50 \) for the most relevant component in the three-body wave function (which corresponds to \( \ell_x = 0 \) and \( s_x = 1 \) between the proton and one of the neutrons, and \( \ell_y = 0 \)). In set (ii) we multiply all the \( K_{\text{max}} \)-values by 2 (which means about 1000 HH in the three-body wave function and \( K_{\text{max}} = 100 \) for the dominating component). Finally, in set (iii) we again multiply all the \( K_{\text{max}} \)-values by 2 (therefore, about 2000 HH in the three-body wave function and \( K_{\text{max}} = 200 \) for the dominating component). An appropriate choice of the \( K_{\text{max}} \)-values is crucial in order to optimize the computing time. An increase of the total number of HH in the calculation by a certain factor implies an increase of the computing time of basically the same factor.
is added depending on the relative orbital angular momenta $(L, l)$ of a NN pair or the third spectator nucleon respectively (denoted as $(l_s, l_s)$ in the HH expansion above). As one can see one needs the $S_s, D_s, D_s$ channels to get a bound triton $E_t = -7.0117$ MeV. Within this reduced Hilbert space we get

$$\Delta B_t^{\text{stat}}(S_s + D_s + D_s) = 20 \text{ keV}$$ (11)

When the $Pp$ channel is added, we obtain $\Delta B_t^{\text{stat}}(S_s + D_s + D_s + Pp) = 19 \text{ keV}$. So, about 75% of the statistical uncertainty comes from the lowest $S_s + D_s + D_s$ channels.

One interesting aspect from the present analysis concerns the statistical correlation analysis of the NN gaussian potential parameters, as this helps to pin down what does fix the current precision. We find that correlations are never larger than 0.4, but since the gaussian potential parameters themselves are strongly correlated there is still the possibility that more global parameters such as volume integrals or low energy scattering parameters would show a clearer pattern.

The precision has been a recurrent topic within the present context, and much of the effort was originally directed with the purpose of establishing the need of 3N-forces within the numerical precision of the calculations. For instance, one needs 34 channels up to angular momentum $J_{\text{pair}} \leq 4$ to obtain $\Delta E_t^{\text{num}} = 10$ keV [7]. Within this numerical precision the triton binding energy obtained by Faddeev calculations has been found to be $8.00, 7.62, 7.63, 7.62, 7.72$ MeV for the CD Bonn [30], Nijm-II, Reid93, Nijm-I and AV18 [31] respectively. The covariant spectator model has produced the closest binding energy $8.57$ MeV to experiment precisely when the NN $\chi^2$ becomes smallest. The spread of values in $B_t$, allowed by the theorem of Glöckle and Polyzou [32], is coming from off-shell ambiguities. The theorem however, does not predict quantitatively the dispersion, which yields $B_t = 7.85(34)$ MeV (exp. $B_t = 8.4820(1)$ MeV). The similarity of the databases but the different potential forms suggests calling this a systematic error, i.e. $\Delta B_t^{\text{sys}} = 340$ keV. In previous estimates a value of $B_t = 7.62(1)$ was obtained using the NijmII, AV18 and Reid93 local potentials fitted to the same database [31].
This was extrapolated to be $B_t = 7.6(1)$ from an inverse scattering analysis of Nijmegen phases up to $T_{LAB} = 300\text{MeV}$ based on a local potential, the error stemming from the high energy extrapolation. We note that these are essentially systematic error estimates.

A high precision calculation with the AV18 potential using the HH expansion method was carried out by the Pisa group leading to the sequence of values $B_t = 7.59267, 7.61227, 7.61786, 7.61809, 7.61812\text{MeV}$ for $N_c = 8, 14, 18, 22, 26$ channels respectively. According to our error estimate of $\Delta B_t = 0.02\text{MeV}$ one could stop already at $N_c = 8$ for a realistic precision. Similar remarks apply to $\Delta P$ where $\Delta P_{num} = 0.1\text{keV}$. Based on general arguments, attempts have also been made to quantify the systematic uncertainties in nuclear bindings stemming from NN scattering yielding $\Delta E_{sys}/A = 100-500\text{keV}$ in rough agreement with the more sophisticated three-body calculations. This suggests to use the present calculation as a benchmark in approximate error estimates sidestepping the full fledged calculation.

From a more general perspective, there is an ongoing effort to quantify the uncertainties in nuclear physics as a means to establish the real predictive power of the theory. While this topic is presently in its infancy, from a theoretical point of view and the inferred predictive power, errors in \textit{ab initio} calculations can be grouped into three main categories: i) the input information (in our case the NN scattering experimental data), ii) the method of solution and its numerical precision and iii) the form (e.g. local or non-local) of the interaction in the unknown region. We have denoted these errors as $\Delta E_{stat}$, $\Delta E_{num}$ and $\Delta E_{syst}$ respectively. Assuming that these sources of error are independent of each other we expect the total theoretical uncertainty to be given by

$$ (\Delta E_{th})^2 = (\Delta E_{stat})^2 + (\Delta E_{num})^2 + (\Delta E_{syst})^2 $$  \hspace{1cm} (12)

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 a realistic limit of predictive power in \textit{ab initio} calculations, which we find to be $\Delta E_{th} \geq 15(1)\text{keV}$. While the use of realistic potentials has been a must in few body calculations, we note that the physical precision of the calculation is finite and will definitely have sizeable consequences in large scale calculations in nuclear physics. Given the large systematic uncertainties, the theoretical calculation of the triton binding energy provides a good example of a precise but inaccurate quantity.

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