Three-nucleon bound states using realistic potential models

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The bound states of ^{3}H and ^{3}He have been calculated by using the Argonne v_{18} plus the Urbana IX three-nucleon potential. The isospin $T=3/2$ state have been included in the calculations as well as the n-p mass difference. The ^{3}H-^{3}He mass difference has been evaluated through the charge-dependent terms explicitly included in the two-body potential. The calculations have been performed using two different methods: the solution of the Faddeev equations in momentum space and the expansion on the correlated hyperspherical harmonic basis. The results are in agreement within 0.1% and can be used as benchmark tests. Results for the charge-dependent–Bonn interaction in conjunction with the Tucson-Melbourne three-nucleon force are also presented. It is shown that the ^{3}H and ^{3}He binding energy difference can be predicted model independently.

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In the past years, great efforts have been made to improve the description of the nucleon-nucleon (NN) interaction. A new generation of potentials including explicitly charge independence breaking terms appeared. These interactions describe the NN scattering data below $T_{lab}=300$ MeV with a nearly perfect $\chi^2/\text{datum}\approx 1$. The charge-dependent–Bonn (CD-Bonn) [1] and Argonne v_{18} (AV18) [2] interactions also allow for charge symmetry breaking (CSB) by providing a neutron-neutron (nn) force, which has been adjusted to the experimental nn scattering length, whereas the Nijmegen interactions [3] are fitted only to proton-proton and proton-neutron data. Recently, the CD-Bonn potential has been updated to CD-Bonn 2000 [4]. In this paper, we only present results for the AV18 and CD-Bonn 2000 interactions. Both are quite different from each other in their functional form, but their description of the NN data is almost equally accurate. Therefore, a comparison of the results will give insights into the model dependence or independence of our understanding of the three-nucleon ($3N$) bound states ^{3}He and ^{3}H.

Following for example the notation of Ref. [2], all these NN potentials can be put in the general form

$$v(NN)=v^{EM}(NN)+v^{\pi}(NN)+v^{R}(NN). \tag{1}$$

The short range part $v^R(NN)$ of all of these interactions includes a certain number of parameters (around 40), which are determined by a fitting procedure to the NN scattering data and the deuteron binding energy (BE), whereas the long range part is represented by the one-pion-exchange potential $v^{\pi}(NN)$ and an electromagnetic (EM) part $v^{EM}(NN)$.

For AV18, $v^{EM}(pp)$ consists of the one- and two-photon Coulomb terms plus the Darwin-Foldy term, vacuum polarization, and magnetic moment interactions. The $v^{EM}(np)$ interaction includes a Coulomb term due to the neutron charge distribution in addition to the magnetic moment interaction. Finally, $v^{EM}(nn)$ is given by the magnetic moment interaction only. All these terms take into account the finite size of the nucleon charge distributions. AV18 additionally includes an energy dependence of the EM coupling constant [5]. In few-body calculations, this energy dependence is often replaced by the orbit-orbit interaction in the pp system $v_{oo}=-(\mathbf{p}_1\cdot\mathbf{p}_2)/M^2\ V(\text{static Coulomb})$, the only term of the one-photon exchange force, which is missing in the definition of AV18. In fact, it would have been quite natural to include the orbit-orbit force in the first place as part of the one-photon exchange in the definition of AV18 and not the peculiar energy dependent choice. Here we will also disregard this energy dependence and give a perturbative estimate of the contribution of v_{oo}. The $v^{EM}(NN)$ for CD-Bonn is much simpler: $v^{EM}(pp)$ is given by the Coulomb force of point protons, whereas $v^{EM}(np)=v^{EM}(nn)=0$. Also the strong part of that force is quite different. It is basically a one-boson-exchange model.

As it is well known, when these interactions are used to describe the $3N$ bound state, an underbinding from about 0.5 MeV to 0.9 MeV depending on the model is obtained (see, for example, Refs. [6,7]). The local potentials lead to less binding than the nonlocal ones, a characteristic related to the bigger D-state probability predicted for the deuteron. Hence, it seems to be not possible to describe the $A>2$ systems without the inclusion of three-nucleon interaction (TNI) terms in the nuclear Hamiltonian. Several TNI models have been studied in the literature mostly based on the exchange of two pions with an intermediate Δ excitation (for a recent review, see Ref. [8]). These interactions include a certain number of parameters not completely determined by theory, therefore some of them can be used to reproduce, for example, the triton BE.

In the following, we show BE results for ^{3}H and ^{3}He. They have been calculated many times before for various NN forces by different calculational schemes (see, for instance, Refs. [8,9]). In Ref. [9], the BE difference $D=B(^3\text{H})-B(^3\text{He})$ has been evaluated perturbatively based on variational Monte Carlo wave functions. A more formal analysis of the contributions to D as a test of the CSB terms in the interaction was performed a decade ago [10,11] before the construction of a new series of interactions, which in-

TABLE I. ^{3}H binding energy B, mean value of the kinetic energy T, S'-, P-, and D-state probabilities, and the probability of the $T=3/2$ state. The Pisa results are displayed in the first four rows. The last four rows show the Bochum results, in this case the modulus of the Faddeev eigenvalue E is also given. For $T=1/2$, differences between B and E arises from a truncation in the representation of the t matrix. All energies are given in MeV. The probabilities are given in percent.

Hamiltonian	$\|E\|$	B	T	$P_{S'}$	P_P	P_D	$P_{T=3/2}$
AV18 ($T=1/2$)		7.618	46.714	1.295	0.066	8.510	
AV18 ($T=1/2,3/2$)		7.624	46.727	1.293	0.066	8.510	0.0025
AV18+UIX($T=1/2$)		8.474	51.262	1.055	0.135	9.301	
AV18+UIX($T=1/2,3/2$)		8.479	51.275	1.054	0.135	9.301	0.0025
AV18 ($T=1/2$)	7.622	7.616	46.73	1.290	0.066	8.510	
AV18 ($T=1/2,3/2$)	7.621	7.621	46.73	1.291	0.066	8.510	0.0025
AV18+UIX($T=1/2$)	8.477	8.470	51.28	1.051	0.135	9.302	
AV18+UIX($T=1/2,3/2$)	8.476	8.476	51.28	1.052	0.135	9.302	0.0025

clude the CSB terms in the fit to the *NN* data for the first time. See also the much earlier investigation in Ref. [12] based on the Reid *NN* potential. Therefore, a reanalysis is in order and might remove uncertainties due to an inaccurate description of the *NN* data. The recent analysis [9] was based only on the AV18+Urbana-IX (UIX) interaction and could not give insight into possible model dependences.

Here we perform a detailed calculation of the $A=3$ system including total isospin states $T=1/2$ and 3/2 and comparing the results of two different interaction models. In addition, particular attention will be given to the BE difference D as a test of the CSB terms present in the interaction. The experimental value of this quantity is 764 keV, from which only 85% correspond to the standard Coulomb potential [10,11,13]. The remaining 15% should come from other CSB terms.

There are further reasons for revisiting the $3N$ bound state problem. The technical challenge to achieve very accurate bound state properties, when *NN* and $3N$ forces are used together, is still high and we would like to present benchmarks based on two quite different calculational schemes, Faddeev equations in momentum space and an hyperspherical expansion method in configuration space. Both methods treat the full Hamiltonian nonperturbatively in all its details. The benchmark calculation is also highly needed because many computational methods, treating nuclear problems for much more complex nuclei, rely on approximate Hamiltonians and calculate the difference of the full Hamiltonian and the approximation as a perturbation. The quality of this approximation has to be checked by comparison to an exactly known result. This paper will provide this result for the $3N$ system.

As mentioned before, an important further reason is the comparison of the two quite different nuclear force models, which is of great interest to provide a hint on possible model dependences or independences of subtle nuclear $A=3$ mass properties like the quantity D.

Since the Coulomb energy scales with the BE of ^{3}H [13], we need $3N$ Hamiltonians, which predict this observable accurately. This can be achieved with properly adjusted TNI's. Then the calculation of D requires reliable solutions of the $3N$ Schrödinger equation including these TNI's. The Bochum group solves the Faddeev equation in momentum space [6,7], whereas the Pisa group uses a decomposition of the wave function in pair-correlated hyperspherical basis functions [14,15]. Both methods were used to find BE's to an accuracy of 2 keV, which means an accuracy better than 0.1%. Such a level of accuracy is nowadays routinely achieved for the $3N$ system by several methods using only *NN* interactions (sometimes simplified versions) [16–19]. Here we show that the same level of accuracy is obtained when TNI terms are taken into account.

We start by considering ^{3}H. The calculations have been done for three identical fermions using the isospin formalism. We used an averaged nucleon mass M with the value $\hbar^2/M=41.471$ MeV fm^2 (the contribution of the n-p mass

TABLE II. Same as in Table I for ^{3}He.

Hamiltonian	$\|E\|$	B	T	$P_{S'}$	P_P	P_D	$P_{T=3/2}$
AV18 ($T=1/2$)		6.917	45.669	1.531	0.064	8.468	
AV18 ($T=1/2,3/2$)		6.925	45.685	1.530	0.065	8.467	0.0080
AV18+UIX($T=1/2$)		7.742	50.194	1.242	0.131	9.249	
AV18+UIX($T=1/2,3/2$)		7.750	50.211	1.242	0.132	9.248	0.0075
AV18 ($T=1/2$)	6.936	6.915	45.70	1.515	0.065	8.465	
AV18 ($T=1/2,3/2$)	6.923	6.923	45.68	1.524	0.065	8.466	0.0081
AV18+UIX($T=1/2$)	7.759	7.738	50.23	1.229	0.132	9.248	
AV18+UIX($T=1/2,3/2$)	7.746	7.746	50.21	1.235	0.132	9.248	0.0075

TABLE III. Contribution of the proton and neutron mass difference to the ^{3}H and ^{3}He BE. The Pisa results are displayed in the first two rows. The last two rows show the Bochum results.

Hamiltonian	^{3}H	^{3}He
AV18	6 keV	−6 keV
AV18+*U*IX	7 keV	−7 keV
AV18	6 keV	−6 keV
AV18+*U*IX	7 keV	−7 keV

difference will be given separately). The AV18 and AV18 $+U$IX have been used to calculate the binding energy B, the mean value of the kinetic energy T, as well as the S', P-, and D-state probabilities. The results are given in Table I corresponding to two different calculations: (i) for total isospin limited to $T=1/2$ and (ii) including also $T=3/2$. The occupation probability $P_{T=3/2}$ of this state is given in the last column of Table I. The first four rows of the table show the Pisa group results, whereas the last four show the Bochum group results. In the latter case, the BE $|E|$ is determined from the eigenvalue spectrum of the Faddeev equations. Additionally, we present the absolute value of the expectation value of the Hamiltonian B. In Table II, the same set of results are given for ^{3}He. For the $T=3/2$ calculations, we find good agreement for the BE results and the wave function properties for both nuclei. The BE's are in agreement within 4 keV or 0.1%. The deviations for the wave function properties, especially for $P_{S'}$, are slightly bigger, but remain below 0.4%. This is below our numerical error bounds and confirms the reliability of both methods, even in presence of a TNI. The tables also reveal a small, but appreciable, contribution of the $T=3/2$ state to the BE. Its inclusion produces 5–6 keV (8 keV) more binding in ^{3}H (^{3}He). It should be noted that the $T=1/2$ results depend on the numerical method. The truncation of the Hilbert space to $T=1/2$ leads to average pp (nn) and np matrix elements in the isospin $t=1$ NN channels. This averaging is performed for the potential matrix elements in case of the Pisa calculations, but for the t matrix in case of the Bochum scheme. This explains the visible deviation of $|E|$ and B for $T=1/2$ Faddeev calculations because B is based on matrix elements of the potential, whereas $|E|$ is based on the t matrix. The small, but visible differences show that benchmarks to this accuracy require the comparison of fully charge-dependent calculations.

The contribution of the n-p mass difference is visible, but sufficiently small to be treated perturbatively. Therefore, we show only perturbative estimates in Table III. The positive sign in the tritium case indicates a slightly more bound system, conversely the ^{3}He results slightly less bound. Again we find an encouraging agreement between the Pisa and Bochum results.

The numbers given up to now do not yet include the contribution of the orbit-orbit interaction. This contribution will be given below. Taking into account the contribution of the n-p mass difference and averaging the Pisa and Bochum results, the final values of the BE's for the AV18+UIX are $B(^3\mathrm{H})=8.485(3)$ MeV and $B(^3\mathrm{He})=7.741(3)$ MeV. This is to be compared with the experimental values: $B_{exp}(^3\mathrm{H})=8.482$ MeV and $B_{exp}(^3\mathrm{He})=7.718$ MeV. Therefore, the AV18+UIX potential overbinds the tritium only by 3 keV, whereas the ^{3}He is overbound by 23 keV. This can be better analyzed looking at the predicted BE difference $D=744$ keV, which is 20 keV smaller than the experimental value.

TABLE IV. Contributions of the various terms of the interaction to the ^{3}H-^{3}He mass difference D. The AV18+UIX potential has been used.

Interaction term	D (keV)
Nuclear CSB	65
Point Coulomb	677
Full Coulomb	648
Magnetic moment	17
Orbit-orbit force	7
n-p mass difference	14
Total (theory)	751
Experiment	764

Since this paper also serves as a benchmark, we would like to point to the small difference of our BE to the result 8.46(1) of a recent GFMC study [20].

The contributions to D of different parts of the interaction have been studied calculating the ^{3}H and ^{3}He BE's omitting these parts and comparing to the full calculations. Note that this is not perturbative. The results for the AV18+UIX potential including isospin states $T=1/2$ and 3/2 states based on hyperspherical calculations are collected in Table IV. We distinguish (i) the nuclear CSB terms, (ii) the point Coulomb interaction, (iii) the complete pp and np Coulomb interaction, which includes the finite size charge distributions, the one- and two-photon terms, and the Darwin-Foldy and vacuum polarization interactions, (iv) the magnetic moment interaction, and (v) the n-p mass difference. Here, we also include the orbit-orbit interaction, which leads to an even improved description of D.

Due to the rather high statistical errors of GFMC calculations, a perturbative estimate of D is more accurate in this scheme. This compares well with our results if the GFMC propagation is done for the ^{3}He nucleus to calculate the expectation value. In this way, GFMC obtains for the Coulomb force expectation value 648 keV [21]. The expectation value for the mass difference depends slightly on the used propagator: using the propagator for ^{3}H results in an expectation value of 762 keV, whereas for ^{3}He, the GFMC result is 753 keV [21,20]. The latter one is in excellent agreement with our result.

From inspection of Table IV, it can be noted that the magnetic moment terms and the difference of full Coulomb and point Coulomb visibly contributes to D and cannot be neglected. This raises the interesting question, whether CD-Bonn 2000, coming without an elaborate EM force, can also describe D.

To this aim, we performed $3N$ BE calculations in the Faddeev scheme using the CD-Bonn 2000 interaction. The

TABLE V. $3N$ BE's $|E|$ for CD-Bonn 2000 with and without TM-TNI compared to the experimental values. Results are shown for ^{3}H, ^{3}He, and their BE difference D. Additionally, we show the kinetic energies T. All results are given in MeV

	^{3}H		^{3}He		
	$\|E\|$	T	$\|E\|$	T	D
CD-Bonn 2000	8.005	37.64	7.274	36.81	0.731
CD-Bonn 2000+TM	8.482	39.39	7.732	38.54	0.750
Expt.	8.482		7.718		0.764

results are given in Table V. Again, the NN interaction underbinds the $3N$ nuclei. Therefore, we augmented the Hamiltonian by the Tucson-Melbourne (TM) TNI [22–24]. The strength of the original model has been adjusted to reproduce the experimental ^{3}H BE as described in Ref. [7]. It results the πNN cutoff value $\Lambda = 4.795\ m_\pi$. Again ^{3}He is overbound. The mass difference D of 750 keV is slightly improved as compared to our result for AV18 and UIX.

In Ref. [25], it has been observed that D is only sensitive to CSB in the S wave. Unfortunately, nn scattering is only poorly known experimentally. There is only one datum for the scattering length, which is still controversial [26–33]. AV18 is adjusted to $a_{nn} = -18.82$ fm, whereas for CD-Bonn 2000 a_{nn} results in -18.97 fm. Its charge dependence is based on theoretical predictions of the full Bonn model [4]. To pin down the origin of the difference of the predictions of both models, we modified the $^1S_0$ nn interaction of CD-Bonn 2000 by a factor λ and calculated the resulting nn scattering length a_{nn}, the ^{3}H BE, and D. We found a strong linear correlation of a_{nn} and D shown in Table VI and Fig. 1. Moreover, the prediction of AV18+UIX perfectly fits into the results obtained from CD-Bonn 2000 and TM (see the dashed-dotted marks in the figure). This shows that the dependence of D on the interaction can be traced back to different predictions for the nn scattering length. The very different treatment of EM interactions and the differences of the CSB in higher partial waves do not appreciably affect D. Please note that the orbit-orbit term is not included here. It is now interesting to shift the straight line in Fig. 1 by the 7 keV upwards coming from the orbit-orbit term and to read off from the experimental value of D the corresponding a_{nn} result. This would be about -19.15 fm. We refrain, however, from proposing this a_{nn} value because the deviation of the NN+TNI force predictions of D to the experimental value might be caused, as stated before, by CSB TNI terms not considered in the present description or by other relativistic effects than those included in the EM interaction. A recent investigation, for instance, using boosted NN forces (see Ref. [34], and references quoted therein) showed that those specific relativistic effects reduce the BE by 300–400 keV. Additional effects might change that result. Therefore, it is premature to read off from Fig. 1 the value of a_{nn}, but the scaling behavior will very likely survive an improved dynamical input. However, we would like to note that the $a_{nn} \approx -16.3$ fm found in Refs. [31,32] would worsen our description of the $3N$ BE difference significantly.

TABLE VI. Strength factor λ for the $^1S_0$ nn force, resulting ^{3}H BE $|E|$ in MeV, the BE difference of ^{3}He and ^{3}H D in keV, and nn scattering length a_{nn} in femtometer. The calculations are based on the CD-Bonn 2000 potential modified by the strength factor in the $^1S_0$ partial wave and the TM-TNI.

λ	$\|E\|$	D	a_{nn}
0.9990	8.474	742	−18.75
0.9995	8.478	746	−18.86
1.0000	8.482	750	−18.97
1.0005	8.486	754	−19.08
1.0010	8.491	759	−19.19
1.0020	8.499	767	−19.42

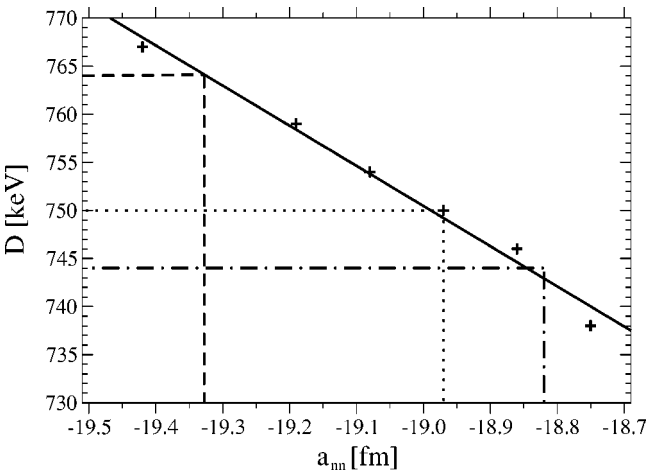

FIG. 1. Difference of the ^{3}He and ^{3}H BE's D dependent on the nn scattering lengths a_{nn}. The crosses are based on the calculations shown in Table VI and the solid line is a linear fit to the crosses. The dashed, the dotted, and the dashed dotted lines mark pairs of D and a_{nn}, which belong to the experimental D (a_{nn} is an estimation based on the linear fit in this case), the predictions of CD-Bonn 2000 and AV18, respectively.

In summary, we have calculated the ^{3}H and ^{3}He BE's based on modern NN interaction models including TNI terms of different types and using two different numerical methods. Our results showed the stability and reliability of both schemes. We use only NN forces, the BE's are too small, calling for TNI terms. These led by construction to the experimental ^{3}H BE. We found that the BE difference of ^{3}H and ^{3}He is predicted nearly model independently. We could trace back the remaining model sensitivity to the differences in the predictions for the nn scattering length. However, uncertainties arising from CSB TNI terms and relativity do not allow us to extract the scattering length from the ^{3}H and ^{3}He BE difference. The model dependence arising from the different forms of the used interactions is extremely small.

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