Feasibility study of a three-nucleon force in the no-core shell model: ^{3}H binding energy

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We investigate the three-nucleon system with a realistic nucleon-nucleon potential and the Tucson-Melbourne (TM) two-pion exchange three-body interaction using a translationally invariant harmonic oscillator basis. In the calculations, the no-core shell-model two-body effective interaction replaces the nucleon-nucleon potential, while the three-nucleon interaction is added without any renormalization. We study the convergence of the approach by changing the basis size. Also the dependence of the binding energies on the TM cutoff parameter Λ is examined. The results show promise for the construction of three-body effective interactions including a three-nucleon interaction, for use in future *ab initio* no-core shell-model nuclear structure calculations for $A>3$ systems.

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I. INTRODUCTION

Recent theoretical and experimental investigations have renewed interest in elucidating the three-body component of the internucleon potential [1–3]. Direct experimental observations of the three-nucleon interaction are lacking (although there are tantalizing hints [4]). It is well known, however, that accurate theoretical calculations of the binding energies of light nuclei with $A\geqslant 3$ yield values that are consistently less than the corresponding experimental values by about 5–10 %, when only two-body potentials are employed [5]. As most modern two-body nucleon-nucleon (*NN*) potentials fit available *NN* scattering data with a satisfactorily high degree of precision, it is reasonable to suspect that we must go beyond two-body interactions if we are to explain this shortfall within the framework of nonrelativistic quantum mechanics. Performing calculations with a three-nucleon interaction (TNI) included in the nuclear Hamiltonian should bring us closer to the ultimate goal of a quantitative *ab initio* theory of nuclear structure.

The purpose of the present investigation is to develop a formalism for calculating the three-body matrix elements of the two-pion-exchange Tucson-Melbourne (TM) three-nucleon interaction in an harmonic-oscillator (HO) basis. This three-nucleon interaction has the operator structure of all local three-nucleon interactions of the two-pion exchange type [6], so our techniques are readily extended to other such three-nucleon interactions currently available. Our aim is to employ eventually this formalism in the determination of the effective three-body interaction that can be utilized in the *ab initio* no-core shell-model (NCSM) calculations for nuclei with $A>3$. Such an approach might yield a method for nuclear structure calculations which utilizes a three-nucleon interaction, and thus, for instance, solves the problem of the aforementioned binding energy deficit observed when effective interactions are derived using only two-body potentials. At the same time, the sensitivity of the nuclear spectra to the different terms of the three-nucleon interaction may provide information on the structure of the three-nucleon interaction itself. A prerequisite for the construction of the three-body effective interaction is the solution of the corresponding three-nucleon system. This is done in the present paper.

Hamiltonians with two- and three-nucleon potentials can be solved very accurately for nuclei with $A\leqslant 4$ by a variety of techniques [7], and the Green's function Monte Carlo (GFMC) method [8] gives very accurate results for energies and other observables of nuclei $A\leqslant 8$ [9]. The latter method has only been applied to local potentials in coordinate space such as the Argonne *NN* potentials and the Urbana and Illinois three-nucleon interactions. It may be limited to such potentials (i.e., those which do not depend on the individual momenta of the interacting nucleons) if the resulting nonlocalities cannot be treated perturbatively. Examples of such nonlocal two-body potentials would be the CD-Bonn potential and, in the three-body case, nonlocal terms from a comprehensive study of the ''Born-term'' parts of the two-pion exchange three-nucleon interaction [10]. The current work is a step toward the development of a promising alternative to the GFMC approach, which may prove to be more versatile (insofar as it could accommodate a variety of two- and three-body potentials), does yield nuclear wave functions in con-

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trast to the GFMC approach, and might also be more easily applicable to heavier nuclei.

To test our formalism we shall apply it to the $A=3$ system, for which calculations with the TM three-nucleon interaction have already been performed using different techniques [5,11–15]. In Sec. II we present our formalism both for the NCSM and for calculating the three-body matrix elements of the TM three-nucleon interaction. The application of our procedure to ^{3}H is given in Sec. III, followed by a discussion and conclusions in Sec. IV.

II. FORMALISM

A. The no-core shell model

In the present study we want to find bound state solutions of the three-nucleon system described by a purely intrinsic Hamiltonian,

$$H_A = T_{\rm rel} + \mathcal{V} = \frac{1}{A}\sum_{i<j}\frac{(\vec{p}_i-\vec{p}_j)^2}{2m} + \sum_{i<j}^{A} V_{NN,ij} + \sum_{i<j<k}^{A} V_{NNN,ijk}, \quad (1)$$

where m is the nucleon mass, $V_{NN,ij}$ is the NN interaction with both strong and electromagnetic components, and $V_{NNN,ijk}$ is the three-nucleon interaction. We work with the HO basis and apply the NCSM approach. First, we modify the Hamiltonian (1) by adding to it the center-of-mass (c.m.) HO Hamiltonian $H_{\rm c.m.}=T_{\rm c.m.}+U_{\rm c.m.}$, where $U_{\rm c.m.}=\frac{1}{2}Am\Omega^2\vec{R}^2$, $\vec{R}=(1/A)\Sigma_{i=1}^{A}\vec{r}_i$. The effect of the HO c.m. Hamiltonian will later be subtracted out in the final many-body calculation so there is no net influence on intrinsic properties of the many-body system. In fact, in the infinite space such a potential has no influence on the intrinsic properties at all. However, this added/subtracted potential facilitates the use of the HO basis for evaluating the effective interactions. The modified Hamiltonian can be cast into the form

$$H_A^\Omega = H_A + H_{\rm c.m.} = \sum_{i=1}^{A} h_i + \sum_{i<j}^{A} V_{ij}^{\Omega,A} + \sum_{i<j<k}^{A} V_{NNN,ijk} = \sum_{i=1}^{A}\left[\frac{\vec{p}_i^{\,2}}{2m}+\frac{1}{2}m\Omega^2\vec{r}_i^{\,2}\right] + \sum_{i<j}^{A}\left[V_{NN,ij}-\frac{m\Omega^2}{2A}(\vec{r}_i-\vec{r}_j)^2\right] + \sum_{i<j<k}^{A} V_{NNN,ijk}. \quad (2)$$

Since we intend to solve the many-body problem in a finite HO basis space, the realistic nuclear interaction in Eq. (2) will yield pathological results unless we use it to derive a model-space dependent effective Hamiltonian. In general, for an A-nucleon system, an A-body effective interaction is needed. Here, we have $A=3$. Therefore, the corresponding effective interaction should be a three-body interaction. However, to construct such an effective interaction is in fact equivalent to solving the full three-body problem, which is our eventual goal. Thus, for the purpose of finding the three-nucleon solutions we resort to a two-body approximation of the effective interaction as was done in majority of the NCSM applications.

The full three-body space is divided into an active (P) model space and an excluded (Q) space, using the projectors P and Q with $P+Q=1$. The model space is spanned by the three-nucleon HO states with the total HO quanta less than or equal to some $N_{\rm max}$. We may ask the question, what is the best two-body effective interaction corresponding to the model space P for the Hamiltonian H_A^Ω (2). In the spirit of the NCSM, we answer that it is such a two-body interaction that will reproduce exactly the two-nucleon eigenstates of the Hamiltonian H_A^Ω, when applied to a two-nucleon system with the sums limited to $A=2$ in Eq. (2), but with A set to three in the HO interaction term. This approach implies that the three-body interaction $V_{NNN,ijk}$ is not used at all when the two-body effective interaction is being derived. It is used, obviously, in the eventual three-body calculation where the two-nucleon interaction is replaced by the two-nucleon effective interaction. A convergence of the three-nucleon eigenstates with respect to the basis-size increase can be achieved in this way, for a tractable size of the model space defined by $N_{\rm max}$, only if the three-nucleon interaction can be considered to be a correction to the dominant two-nucleon interaction. This is indeed the case. We will investigate the convergence issue in Sec. III B.

Details of the process for computing the two-body effective interaction are described fully in, e.g., Ref. [16]; however, for the sake of completeness, the method is briefly revisited here. The two-body effective interaction is derived utilizing the Lee-Suzuki transformation [17–19], which results in a Hermitian effective interaction. Let us write explicitly the two-nucleon Hamiltonian following from Eq. (2) in the two-nucleon relative and c.m. coordinates, e.g.,

$$H_2^\Omega = h_1 + h_2 + V_{12}^{\Omega,A} = H_{02} + H_{2\,\rm c.m.} + V_{12}^{\Omega,A} = \frac{\vec{p}^{\,2}}{2m} + \frac{1}{2}m\Omega^2\vec{r}^{\,2} + H_{2\,\rm c.m.} + V_{NN}(\sqrt{2}\vec{r}) - \frac{m\Omega^2}{A}\vec{r}^{\,2}, \quad (3)$$

where $H_{02}+H_{2\,\rm c.m.}=h_1+h_2$, $\vec{r}=\sqrt{1/2}(\vec{r}_1-\vec{r}_2)$, and $\vec{p}=\sqrt{1/2}(\vec{p}_1-\vec{p}_2)$. The two-nucleon problem is then solved in a relative HO basis space with high precision. The c.m. motion of the two nucleons is not affected by the transformation. Thus, it does not contribute to the effective interaction calculation and cancels out at the end. The A in Eq. (3) is set to 3 in the present application.

The unitary transformation is obtained by choosing an anti-Hermitian two-body operator $S^{(2)}$ determined from the decoupling condition

$$Q_2 e^{-S^{(2)}} H_2^\Omega e^{S^{(2)}} P_2 = 0, \quad (4)$$

and the simultaneous restrictions $P_2 S^{(2)} P_2 = Q_2 S^{(2)} Q_2 = 0$. Note that two-nucleon-state projectors (P_2, Q_2), whose definition follows from the definition of the A-nucleon P and Q projectors, appear in Eq. (4).

The unitary transformation and decoupling condition, introduced by Suzuki and Okamoto and referred to as the unitary-model-operator approach [20], has the solution

$$S^{(2)} = \operatorname{arctanh}(\omega - \omega^\dagger), \tag{5}$$

with ω satisfying $\omega = Q_2 \omega P_2$. Furthermore, we also have

$$Q_2 e^{-\omega} H_2^\Omega e^{\omega} P_2 = 0. \tag{6}$$

With Eq. (5), we obtain for the two-body effective Hamiltonian

$$\overline{H}_{2\text{eff}} = (P_2 + \omega^\dagger \omega)^{-1/2} (P_2 + P_2 \omega^\dagger Q_2) H_2^\Omega (Q_2 \omega P_2 + P_2)(P_2 + \omega^\dagger \omega)^{-1/2}. \tag{7}$$

If the eigensolutions of the Hamiltonian H_2^Ω are given by $H_2^\Omega |k\rangle = E_k |k\rangle$, then the operator ω can be determined as

$$\langle \alpha_Q | \omega | \alpha_P \rangle = \sum_{k \in \mathcal{K}} \langle \alpha_Q | k \rangle \langle \tilde{k} | \alpha_P \rangle, \tag{8}$$

where $|\alpha_P\rangle$ and $|\alpha_Q\rangle$ denote the two-nucleon model- and Q-space basis states, respectively. The tilde in Eq. (8) denotes the inverse of the matrix defined by matrix elements $\langle \alpha_P | k \rangle$, i.e., $\Sigma_{\alpha_P} \langle \tilde{k} | \alpha_P \rangle \langle \alpha_P | k' \rangle = \delta_{k,k'}$ and $\Sigma_k \langle \alpha'_P | \tilde{k} \rangle \times \langle k | \alpha_P \rangle = \delta_{\alpha'_P, \alpha_P}$, for $k, k' \in \mathcal{K}$. Note the sum $\mathcal{K}$ denotes a set of d_P eigenvectors whose properties are exactly reproduced in the model space, with d_P equal to the dimension of the two-nucleon model space.

With the help of the solution for ω (8), we obtain a simple expression for the matrix elements of the Hermitian effective Hamiltonian

$$\langle \alpha_P | \overline{H}_{2\text{eff}} | \alpha'_P \rangle = \sum_{k \in \mathcal{K}} \sum_{\alpha''_P} \sum_{\alpha'''_P} \langle \alpha_P | (P_2 + \omega^\dagger \omega)^{-1/2} | \alpha''_P \rangle \langle \alpha''_P | \tilde{k} \rangle \times E_k \langle \tilde{k} | \alpha'''_P \rangle \langle \alpha'''_P | (P_2 + \omega^\dagger \omega)^{-1/2} | \alpha'_P \rangle. \tag{9}$$

For computation of the matrix elements of $(P_2 + \omega^\dagger \omega)^{-1/2}$, we use the relation

$$\langle \alpha_P | (P_2 + \omega^\dagger \omega) | \alpha''_P \rangle = \sum_{k \in \mathcal{K}} \langle \alpha_P | \tilde{k} \rangle \langle \tilde{k} | \alpha''_P \rangle \quad . \tag{10}$$

Finally, the two-body effective interaction is determined from the two-nucleon effective Hamiltonian, obtained from Eq. (9), as $V_{2\text{eff}} = P_2 (\overline{H}_{2\text{eff}} - h_1 - h_2) P_2$. Apart from being a function of the nucleon number A, $V_{2\text{eff}}$ depends on the HO frequency Ω and on the parameter $N_{\max}$, defining the basis space. It has the important property that $V_{2\text{eff}} \to V_{12}^{\Omega, A}$ for $N_{\max} \to \infty$, following from the fact that $\omega \to 0$ for $P \to 1$.

So, we eventually solve the Schrödinger equation of the three-nucleon system described by the Hamiltonian

$$H^\Omega_{A=3,\text{eff}} = \sum_{i=1}^{3} h_i + \sum_{i<j}^{3} V_{2\text{eff},ij} + \sum_{i<j<k}^{3} V_{NNN,ijk}, \tag{11}$$

by diagonalization using the translationally invariant HO basis. The c.m. dependence is present only in the one-body term of Eq. (11). We remove the c.m. term explicitly from $H^\Omega_{A=3,\text{ eff}}$ by subtracting $H_{\text{c.m.}}$ introduced in Eq. (2). It should be emphasized that the Hamiltonian (11) is applicable only for the $A=3$ system. For $A>3$, the bare three-body interaction must be replaced by a three-body effective interaction, e.g., $(V_{NNN})_{\text{eff},ijk}$ (in fact, the two-body effective interaction will be replaced by a three-body effective interaction as well). This is necessary because of the fact that the convergence with the basis size is rather slow when the bare three-body interaction is used, as will be seen in Sec. III B. Such a three-body effective interaction can be derived in analogy to the derivation of the two-body effective interaction, i.e., using Eq. (9), with the help of three-body solutions obtained using (11). In order to find the three-body solutions by solving the Schrödinger equation with the Hamiltonian (11), we could, in principle, use some perturbative renormalization of $V_{NNN,ijk}$ to speed up the convergence with the basis size. However, this is not really necessary, as we are able to reach sufficiently large basis spaces for the $A=3$ system to achieve a reasonable convergence, as will be shown in Sec. III B.

B. Three-nucleon interactions

The task of extracting a reliable and consistent form for the nuclear three-body interaction has proven to be a difficult one over the years, certainly when compared to the extent to which the precision of empirical two-body potentials has been determined. The wealth of two-nucleon scattering and bound state data starting from the early days of nuclear physics has made it possible to construct empirical *NN* potentials without much constraint from the (approximate) chiral symmetry of the QCD strong interaction. The single exception to this untrammeled empiricism was the long range one-pion exchange potential common to all high-quality potentials; long range due to the tiny pion mass, a direct consequence of the Goldstone-mode realization of chiral symmetry. The three-body force among nucleons, to the contrary, had no such empirical input before the advent of reliable calculations of the $A=3$ bound state and, more recently, of N-d scattering [2] and of heavier nuclei [5,21]. Thus models of the three-nucleon interaction were forced to be more theoretically based than contemporary two-body force models of the same era; indeed the two first papers of which we are aware that discussed the implication of chiral symmetry for

nuclear forces focused first on the three-nucleon force [22] and subsequently on the two-nucleon force [23].

Even with the guidance of chiral symmetry, construction of potentials always involves theoretical choices, since a potential is an unphysical theoretical object, obtained from a subamplitude (an off-mass-shell part of an amplitude) according to a set of prescriptions. Such a subamplitude when iterated (in the Schrödinger equation, for example) produces observables such as on-shell scattering amplitudes or energies. Choices (implicit or explicit) in the definition of a two-body potential that arise naturally in the context of Rayleigh-Schrödinger perturbation theory will also alter the definition of what constitutes a three-body force. None of these definitions is wrong, and consistency considerations relate each one to the others. Expediency and theoretical prejudice are usually our guides in selecting the prescriptions we choose. These general statements were illustrated in a paper by Friar and Coon [24] which clarified the relationship between different two-pion-exchange three-body forces [10,25] obtained from a simple nonlinear chiral Lagrangian. Polyzou and Glöckle [26] have made a similar observation in the context of a Hamiltonian framework; that it is possible to reproduce the binding energy and scattering matrix of a nuclear system from two different Hamiltonians, the two related by a unitary transformation, and consisting of different combinations of two- and three-nucleon interactions. With the advent of an effective field theory of nuclear forces [27], it has become commonplace to think of consistent two- and multibody forces as being ultimately derivable from the low-energy Lagrangian of chiral perturbation theory according to an agreed upon prescription. This prescription may choose to emphasize two-body forces at the expense of three-body forces, a choice of the theorist, but the observables of the theory cannot be changed by his/her choice. Although much progress has been made toward this goal [28], at this moment the *NN* potentials that give the highest precision fit to the nucleon-nucleon data and are used in nuclear structure calculations do not even have a consistent chiral nature with respect to the three-nucleon forces available [10], let alone being derived from the same Lagrangian as the chosen three-body force.

For this study we choose a recent modification (labeled TM′) of the Tucson-Melbourne three-body force, the first of the class of two-pion-exchange three-nucleon forces that incorporate phenomenology from π-N scattering and were constructed in accordance with (approximate) chiral symmetry [29]. This interaction TM′ has been used in several previous studies [5,14,15], thus providing a body of results for comparison with the present method. The two-body interaction that we will apply in this study is the Argonne V18 potential [30]. This potential demonstrates the inconsistency, noted above, between our chosen three-nucleon interaction and the relativistic corrections to the one-pion-exchange potential of our chosen realistic two-nucleon potential. This AV18 potential has no firm value of the arbitrary parameter μ, which can be identified in some other phenomenological *NN* potentials, and has been identified to be -1 (pseudoscalar coupling of the pion to free nucleon spinors) in the TM three-nucleon force [10,31] Nevertheless, the AV18 *NN* potential fits well the two-body data and the TM′ three-body force has the operator structure of the 2π-exchange part of a chiral perturbation theory three-body force. In addition, the latter has strength constants near those expected to arise from a systematic analysis of pion-nucleon scattering [32] and of 2π exchange in *NN* phase shift analyses [33,34]. This combination of two and three-body potentials will suffice for our preliminary studies.

TABLE I. Parameters of the TM′ three-body force for $\Lambda=5.8\mu$. For different values of Λ, the parameter a' varies slightly according to a relation given in Ref. [14].

	$\mu a'$	$\mu^3 b$	$\mu^3 d$	g^2	μ (MeV)
TM′(81)	−0.87	−2.58	−0.753	179.7	139.6
TM′(93)	−0.74	−2.53	−0.72	179.7	138.0
TM′(99)	−1.12	−2.80	−0.72	172.1	138.0

Adapting the original coordinate space derivation [11,12], the TM′ three-nucleon interaction applied in this work has the form

$$W = W_1 + W_2 + W_3, \tag{12}$$

where the W_i each have the same functional form but contain cyclically permuted variables. The analytic form of W_1 is

$$\begin{aligned} W_1 = \left(\frac{g\mu}{8M\pi}\right)^2 \Bigg[& a'(\vec{\tau}_2\cdot\vec{\tau}_3)(\vec{\sigma}_2\cdot\hat{\mathbf{x}}_3)(-\vec{\sigma}_3\cdot\hat{\mathbf{x}}_2)Z_1'(x_3)Z_1'(x_2) + b(\vec{\tau}_2\cdot\vec{\tau}_3)\Bigg((\vec{\sigma}_2\cdot\hat{\mathbf{x}}_3)(-\vec{\sigma}_3\cdot\hat{\mathbf{x}}_2)(-\hat{\mathbf{x}}_3\cdot\hat{\mathbf{x}}_2)\tilde{Z}(x_3)\tilde{Z}(x_2) \\ & + (\vec{\sigma}_2\cdot\hat{\mathbf{x}}_3)(\vec{\sigma}_3\cdot\hat{\mathbf{x}}_3)\tilde{Z}(x_3)\frac{Z_1'(x_2)}{x_2} + (-\vec{\sigma}_2\cdot\hat{\mathbf{x}}_2)(-\vec{\sigma}_3\cdot\hat{\mathbf{x}}_2)\tilde{Z}(x_2)\frac{Z_1'(x_3)}{x_3} + (\vec{\sigma}_2\cdot\vec{\sigma}_3)\frac{Z_1'(x_3)}{x_3}\,\frac{Z_1'(x_2)}{x_2}\Bigg) \\ & + d(\vec{\tau}_3\times\vec{\tau}_2\cdot\vec{\tau}_1)\Bigg((\vec{\sigma}_2\cdot\hat{\mathbf{x}}_3)(-\vec{\sigma}_3\cdot\hat{\mathbf{x}}_2)(-\vec{\sigma}_1\cdot\hat{\mathbf{x}}_3\times\hat{\mathbf{x}}_2)\tilde{Z}(x_3)\tilde{Z}(x_2) + (\vec{\sigma}_2\cdot\hat{\mathbf{x}}_3)(\vec{\sigma}_3\cdot\vec{\sigma}_1\times\hat{\mathbf{x}}_3)\tilde{Z}(x_3)\frac{Z_1'(x_2)}{x_2} \\ & + (-\vec{\sigma}_3\cdot\hat{\mathbf{x}}_2)(-\vec{\sigma}_1\cdot\vec{\sigma}_2\times\hat{\mathbf{x}}_2)\tilde{Z}(x_2)\frac{Z_1'(x_3)}{x_3} + (\vec{\sigma}_1\cdot\vec{\sigma}_2\times\vec{\sigma}_3)\frac{Z_1'(x_3)}{x_3}\,\frac{Z_1'(x_2)}{x_2}\Bigg)\Bigg], \end{aligned} \tag{13}$$

and the correlation functions in this expression are given by

$$Z_1'(r) = -\mu\left(1+\frac{1}{\mu r}\right)\frac{e^{-\mu r}}{\mu r} + \Lambda\left(1+\frac{1}{\Lambda r}\right)\frac{e^{-\Lambda r}}{\mu r} + \frac{(\Lambda^2-\mu^2)}{2\mu}e^{-\Lambda r}$$

$$\tilde{Z}(r) \equiv Z_1''(r) - \frac{Z_1'(r)}{r} = \mu^2\Bigg[\left(1+\frac{3}{\mu r}+\frac{3}{\mu^2 r^2}\right)\frac{e^{-\mu r}}{\mu r} - \frac{\Lambda^2}{\mu^2}\left(1+\frac{3}{\Lambda r}+\frac{3}{\Lambda^2 r^2}\right)\frac{e^{-\Lambda r}}{\mu r}bf - \frac{\Lambda}{2\mu}\left(\frac{\Lambda^2}{\mu^2}-1\right)\left(1+\frac{1}{\Lambda r}\right)e^{-\Lambda r}\Bigg]. \quad (14)$$

Physically W_1 corresponds to a process in which nucleon 1 exchanges pions with each of nucleons 2 and 3. The unit vectors $\hat{\mathbf{x}}_i$ are the unit internucleon coordinates $(\vec{r}_j-\vec{r}_k)/|\vec{r}_j-\vec{r}_k|$, with *i*, *j*, and *k* defined cyclically. $\vec{\sigma}$ and $\vec{\tau}$ represent spin and isospin, respectively, with subscripts denoting the relevant nucleon. Most of the calculations presented in this paper used the constants of Ref. [12]. In that era of the TM force the pion mass was taken to be the charged pion mass and set at 139.6 MeV. The nucleon mass, *M*, is then 6.726μ and g^2 the pion-nucleon coupling constant was taken to be 179.7, a value few percent higher than the $g^2=172.1$ accepted today.

The TM three-nucleon interaction grew out of the observation that the π-*N* scattering amplitude is constrained off-mass-shell by the results of current algebra and the partially-conserved axial current (PCAC) [35]. The combination of off-shell constraints and on-shell values of the invariant amplitudes of pion-nucleon scattering yields a unique input to the TM three-nucleon interaction in the form of the strength constants a', *b*, and *d*. The values of these constants are taken from dispersion relation analyses of pion-nucleon scattering and change as the data base changes [36–38]. These constants roughly correspond to the chiral constants $\{c_i\}$ of the next-to-leading-order chiral Lagrangian of chiral perturbation theory [6], although the TM constants were not derived from a Lagrangian field theory. The specific values we use are given in Table I, where TM′(81) has constants obtained from premeson factory data and TM′(99) is built upon the meson factory data base. (For notation see Ref. [14] and for a PCAC discussion of chiral symmetry and low-energy pion-nucleon scattering consult Ref. [35].) Both a' and *b* contain the pion-nucleon sigma term, a measure of chiral symmetry breaking, whose value is still under discussion after all these years. The constants labeled TM′(81) reflect a sigma term of 69 MeV (i.e., the value of the invariant amplitude at the Cheng-Dashen point) and those of TM′(99) a sigma term of 83 MeV. The latter value is based on a phase shift data base, which may be flawed in the higher partial waves [39]. In any event, we present results with both sets of values, as they are likely to bracket the ''ultimate'' value of the sigma term.

The purely spatial correlation functions in Eqs. (13) and (14), i.e., $Z_1'(r)$ and $Z_1''(r)$, are the first and second derivatives, respectively, of Yukawa functions corresponding to the exchange of a pion between a nucleon pair:

$$Z_1(r) = \frac{4\pi}{\mu}\int \frac{d\vec{q}}{(2\pi)^3}\frac{e^{(i\vec{q}\cdot\vec{r})}F^2(\vec{q}^{\,2})}{(\vec{q}^{\,2}+\mu^2)^1}, \quad (15)$$

modified by a form factor at each πNN vertex,

$$F(\vec{q}^{\,2}) = \frac{\Lambda^2-\mu^2}{\Lambda^2+\vec{q}^{\,2}}, \quad (16)$$

which cuts off the potential at short (pairwise) distances. Because a form factor is not an observable, one is free to change the value of Λ (but not the strength constants which are taken from data) and this is often done. From Eqs. (13)–(16), we see that each term of the potential TM′ of Eq. (13) has the spatial structure of π range in one pair coordinate multiplied by another π range in the other pair coordinate.

The potential TM′ (13) differs from the original TM 2π-exchange three-nucleon potential by the omission of a term in the latter which did not have the spatial structure of π range plus π range but instead that of short range plus π range. If the cutoff factor $\Lambda\to\infty$, this omitted term would have the structure of zero range plus π range familiar from effective field theories. Yet it did not appear in the 2π-exchange three-nucleon force of chiral perturbation theory [6]. This discrepancy was elucidated in Ref. [6] with the aid of a pion field transformation that transmogrifies the form of chiral symmetry chosen for chiral perturbation theory calculations into a form that emulates the current algebra-PCAC constraints adopted by the Tucson-Melbourne group. In that form it became clear that the model ansatz for the off-shell pion-nucleon amplitude of the TM force produced a short range plus π range operator that should have been canceled but was not. Such a cancellation in the current algebra-PCAC technique would require current algebra-PCAC constraints on the subamplitude labeled ''three-nucleon force,'' in addition to the employed constraints on the subamplitude labeled ''off-shell πN amplitude,'' which underlies the TM three-nucleon interaction. This was not understood in the early days, would be technically demanding if not impossible, and seems unnecessary because simply dropping the term makes the modified potential TM′ satisfy all pictures of chiral symmetry. A careful numerical examination [40] showed that the dropping of this spurious term from the TM force has almost no effect on the binding energy of the triton. This is evidently a numerical accident due to the value of its strength parameter and need not be true for all observables. Indeed, the omission of this spurious term does produce a noticeable effect on a polarization observable of elastic proton-deuteron scattering [40].

C. Matrix elements

In order to use the chosen three-nucleon interaction, we must first calculate its matrix elements. We work in the translationally invariant HO basis. We use a standard Jacobi sys-

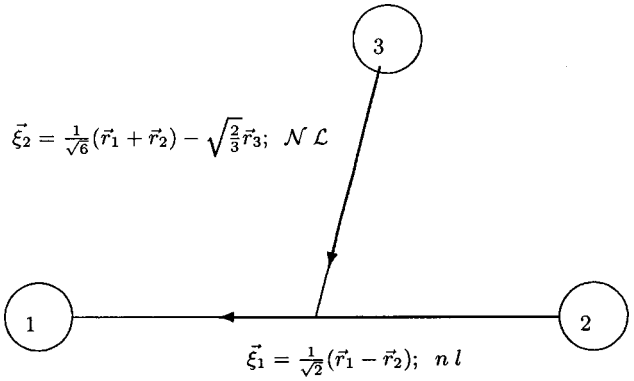

FIG. 1. Coordinate system for the three-body basis set.

tem of coordinates to describe our three-body system. That is, given the three-body system with vector coordinates $\{\vec{r}_1,\vec{r}_2,\vec{r}_3\}$, we define the corresponding Jacobi coordinates,

$$\vec{\xi}_0=\frac{1}{\sqrt{3}}(\vec{r}_1+\vec{r}_2+\vec{r}_3),$$

$$\vec{\xi}_1=\frac{1}{\sqrt{2}}(\vec{r}_1-\vec{r}_2), \tag{17}$$

$$\vec{\xi}_2=\frac{1}{\sqrt{6}}(\vec{r}_1+\vec{r}_2)-\sqrt{\frac{2}{3}}\vec{r}_3.$$

This particular choice of Jacobi coordinates will prove to be useful in the determination of the TM′ three-nucleon interaction matrix elements, as the $\vec{\xi}_1$ coordinate is parallel to the $\hat{\mathbf{x}}_3$ unit vector defined in the interaction in W_1 in Eq. (13). Ignoring the center-of-mass coordinate $\vec{\xi}_0$, we define an HO wave function in each of the remaining two coordinates $\vec{\xi}_1$ and $\vec{\xi}_2$ (as shown in Fig. 1) as the spatial component of the basis functions we employ. With spin and isospin degrees of freedom included, the basis vectors will be designated by their independent quantum numbers $|nl(\vec{\xi}_1)sjt;\mathcal{NL}(\vec{\xi}_2)\frac{1}{2}\mathcal{J}\frac{1}{2};JT\rangle$. Here n,l and $\mathcal{N},\mathcal{L}$ are the HO quantum numbers corresponding to the coordinates $\vec{\xi}_1$ and $\vec{\xi}_2$, respectively. The quantum numbers s,t,j designate the spin, isospin, and total angular momentum for the relative channel of nucleons 1 and 2, while $\mathcal{J}$ is the angular momentum of nucleon 3 relative to the center of mass of nucleons 1 and 2 (see Fig. 1). J,T are the total angular momentum and isospin of the three-body system, respectively. The model space P for our effective interaction calculation shall be the subspace spanned by all those functions with the desired total isospin and total angular momenta, which satisfy $2n+l+2\mathcal{N}+\mathcal{L}\leqslant N_{\max}$. Then $N_{\max}$ defines the size of the model space P—all HO states up to an energy of $N_{\max}\hbar\Omega$ above the ground state are included.

This is not an antisymmetric basis; hence, the first step in our calculation is to antisymmetrize via the calculation of the appropriate coefficients of fractional parentage,

$$|NiJT\rangle=\sum\langle nlsjt;\mathcal{NL}\tfrac{1}{2}\mathcal{J}\tfrac{1}{2}\|NiJT\rangle|nlsjt;\mathcal{NL}\tfrac{1}{2}\mathcal{J}\tfrac{1}{2};JT\rangle, \tag{18}$$

where $N=2n+l+2\mathcal{N}+\mathcal{L}$ and i is an indexing quantum number distinguishing different antisymmetrized states with the same N,J,T. These coefficients are determined by diagonalizing the three-nucleon system antisymmetrizer as described in Refs. [41–43]. In this procedure we are able to eliminate the nonantisymmetrized nonphysical states of the system.

In a next step we recouple the basis from a jj to an LS representation, because in the determination of the TM′ matrix elements we separate spatial and spin components of the three-body potential operator.

Now let us proceed to the determination of the matrix elements of TM′ in the recoupled basis, described above. Of particular note are the spatial components, as these will comprise the bulk of the computational expense. The isospin components of the TM′ three-nucleon interaction are already separated from the remainder of the operator. There are only two cases to be considered, and in the three-body basis being used, the calculation of their matrix-element components is a relatively straightforward exercise in angular momentum recoupling [44],

$$\langle(t\tfrac{1}{2})T|\vec{\tau}_2\cdot\vec{\tau}_3|(t'\tfrac{1}{2})T\rangle = 6\hat{t}\hat{t}'(-1)^{t+t'+T+\frac{1}{2}}\begin{Bmatrix} t & t' & 1\\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix} t & t' & 1\\ \frac{1}{2} & \frac{1}{2} & T\end{Bmatrix} \tag{19}$$

$$\langle(t\tfrac{1}{2})T|\vec{\tau}_3\times\vec{\tau}_2\cdot\vec{\tau}_1|(t'\tfrac{1}{2})T\rangle = 36i\hat{t}\hat{t}'(-1)^{T+t'+\frac{1}{2}}\begin{Bmatrix} t & t' & 1\\ \frac{1}{2} & \frac{1}{2} & T\end{Bmatrix}\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & t'\\ \frac{1}{2} & \frac{1}{2} & t\\ 1 & 1 & 1\end{Bmatrix}. \tag{20}$$

We have followed standard notation in this work, insofar as the ''hat'' notation designates a unit vector when used with the coordinates x_i, but denotes the recoupling factor $\hat{j}=\sqrt{2j+1}$ when applied to the angular momentum quantum numbers of standard recoupling notation.

The spin degrees of freedom cannot be determined quite so easily, because these are, for the most part, coupled to the spatial coordinate unit operators. We perform a recoupling,

$$(\vec{\sigma}_2\cdot\hat{\mathbf{x}}_i)(\vec{\sigma}_3\cdot\hat{\mathbf{x}}_j)=\sum_K(-1)^K(\vec{\sigma}_2\vec{\sigma}_3)^{(K)}\cdot(\hat{\mathbf{x}}_i\hat{\mathbf{x}}_j)^{(K)}, \tag{21}$$

$$(\vec{\sigma}_2\cdot\hat{\mathbf{x}}_3)(\vec{\sigma}_3\cdot\hat{\mathbf{x}}_2)(\hat{\mathbf{x}}_3\cdot\hat{\mathbf{x}}_2)-\sum_{k_1k_2K}(-1)^{k_2}\hat{k}_1\hat{k}_2\begin{Bmatrix}k_1 & k_2 & K\\ 1 & 1 & 1\end{Bmatrix}(\vec{\sigma}_2\vec{\sigma}_3)^{(K)}\cdot[(\hat{\mathbf{x}}_3\hat{\mathbf{x}}_3)^{(k_1)}(\hat{\mathbf{x}}_2\hat{\mathbf{x}}_2)^{(k_2)}]^{(K)}, \tag{22}$$

$$(\vec{\sigma}_2\cdot\hat{\mathbf{x}}_3)(\vec{\sigma}_3\cdot\vec{\sigma}_1\times\hat{\mathbf{x}}_3)=-\sqrt{6}i\sum_{k_1K}(-1)^{K+k_1}\hat{k}_1\begin{Bmatrix}k_1 & K & 1\\ 1 & 1 & 1\end{Bmatrix}[(\vec{\sigma}_1\vec{\sigma}_2)^{(k_1)}\vec{\sigma}_3]^{(K)}\cdot(\hat{\mathbf{x}}_3\hat{\mathbf{x}}_3)^{(K)}, \tag{23}$$

$$(\vec{\sigma}_3\cdot\hat{\mathbf{x}}_2)(\vec{\sigma}_1\cdot\vec{\sigma}_2\times\hat{\mathbf{x}}_2)=-\sqrt{2}i\sum_{K}(-1)^{K}[(\vec{\sigma}_1\vec{\sigma}_2)^{(1)}\vec{\sigma}_3]^{(K)}\cdot(\hat{\mathbf{x}}_2\hat{\mathbf{x}}_2)^{(K)}, \tag{24}$$

$$\begin{aligned}(\vec{\sigma}_2\cdot\hat{\mathbf{x}}_3)(\vec{\sigma}_3\cdot\hat{\mathbf{x}}_2)(\vec{\sigma}_1\cdot\hat{\mathbf{x}}_3\times\hat{\mathbf{x}}_2)=&-\sqrt{6}i\sum_{k_1k_2k_3}(-1)^{k_2+k_3}\hat{k}_1\hat{k}_2\hat{k}_3\begin{Bmatrix}1 & 1 & 1\\ 1 & k_1 & k_2\end{Bmatrix}\begin{Bmatrix}k_2 & k_3 & K\\ 1 & k_1 & 1\end{Bmatrix}\\ &\times[(\vec{\sigma}_1\vec{\sigma}_2)^{(k_1)}\vec{\sigma}_3]^{(K)}\cdot[(\hat{\mathbf{x}}_3\hat{\mathbf{x}}_3)^{(k_2)}(\hat{\mathbf{x}}_2\hat{\mathbf{x}}_2)^{(k_3)}]^{(K)},\end{aligned} \tag{25}$$

leaving the spatial-spin operators in the form $X(\mathbf{x}_2,\mathbf{x}_3)^{(K)}\cdot Y(\vec{\sigma}_1,\vec{\sigma}_2,\vec{\sigma}_3)^{(K)}$. The matrix elements of these separated operators are easily written in terms of the requisite reduced elements,

$$\begin{aligned}&\langle(nl\mathcal{NL})L;(s\tfrac{1}{2})S;J|X(\mathbf{x}_2,\mathbf{x}_3)^{(K)}\cdot Y(\vec{\sigma}_1,\vec{\sigma}_2,\vec{\sigma}_3)^{(K)}|(n'l'\mathcal{N}'\mathcal{L}')L';(s'\tfrac{1}{2})S';J\rangle\\ &\quad=(-1)^{L'+S+J}\begin{Bmatrix}L & S & J\\ S' & L' & K\end{Bmatrix}\langle(nl\mathcal{NL})L\|X(\mathbf{x}_2,\mathbf{x}_3)^{(K)}\|(n'l'\mathcal{N}'\mathcal{L}')L'\rangle\langle(s\tfrac{1}{2})S\|Y(\vec{\sigma}_1,\vec{\sigma}_2,\vec{\sigma}_3)^{(K)}\|(s'\tfrac{1}{2})S'\rangle.\end{aligned} \tag{26}$$

The reduced spin matrix elements are therefore just general cases of the isospin matrix elements noted above in Eqs. (19) and (20),

$$\begin{aligned}&\langle(s\tfrac{1}{2})S\|(\vec{\sigma}_2\vec{\sigma}_3)^{(K)}\|(s'\tfrac{1}{2})S'\rangle\\ &\quad=(-1)^{s}6\hat{s}\hat{s}'\hat{S}\hat{S}'\hat{K}\begin{Bmatrix}s & s' & 1\\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix}s & \frac{1}{2} & S\\ s' & \frac{1}{2} & S'\\ 1 & 1 & K\end{Bmatrix},\end{aligned} \tag{27}$$

$$\begin{aligned}&\langle(s\tfrac{1}{2})S\|[(\vec{\sigma}_1\vec{\sigma}_2)^{(k_1)}\vec{\sigma}_3]^{(K)}\|(s'\tfrac{1}{2})S'\rangle\\ &\quad=6\sqrt{6}\hat{s}\hat{s}'\hat{S}\hat{S}'\hat{k}_1\hat{K}\begin{Bmatrix}\frac{1}{2} & \frac{1}{2} & s\\ \frac{1}{2} & \frac{1}{2} & s'\\ 1 & 1 & k_1\end{Bmatrix}\begin{Bmatrix}s & \frac{1}{2} & S\\ s' & \frac{1}{2} & S'\\ k_1 & 1 & K\end{Bmatrix}.\end{aligned} \tag{28}$$

We are left with the spatial reduced matrix elements of component operators of the form $X(\mathbf{x}_2,\mathbf{x}_3)^{(K)}=[w_3(\mathbf{x}_3)^{(k_1)}w_2(\mathbf{x}_2)^{(k_2)}]^{(K)}$. Here, $w_3(\mathbf{x}_3)$ and $w_2(\mathbf{x}_2)$ represent the decoupled $\hat{\mathbf{x}}_3$ and $\hat{\mathbf{x}}_2$ components determined in Eqs. (21)–(25), along with the corresponding correlation functions for each term, as noted in the expression for W_1; Eq. (13). For example, the first term in W_1 would produce $w_3(\mathbf{x}_3)=\hat{\mathbf{x}}_3^{(1)}Z_1'(x_3)$, from the spherical tensor of order 1 in Eq. (21) and the scalar correlation function $Z_1'(x_3)$ in Eq. (13), and the analogous term $w_2(\mathbf{x}_2)=\hat{\mathbf{x}}_2^{(1)}Z_1'(x_2)$.

The difficulty in the matrix element calculation arises from the $w_2(\mathbf{x}_2)$ piece of this object, as $\mathbf{x}_2$ is not parallel to either of the coordinates $\vec{\xi}_1$, $\vec{\xi}_2$ we have chosen for our HO basis. This problem has been solved by inserting a complete set of states between the w_3 and w_2 operators,

$$\begin{aligned}&\langle(nl\mathcal{NL})L\|[w_3(\mathbf{x}_3)^{(k_1)}w_2(\mathbf{x}_2)^{(k_2)}]^{(K)}\|(n'l'\mathcal{N}'\mathcal{L}')L'\rangle\\ &\quad=\sum_{n''l''\mathcal{N}''\mathcal{L}''L''}(-1)^{L'+K+k_1}\hat{K}\begin{Bmatrix}k_1 & k_2 & K\\ L' & L & L''\end{Bmatrix}\\ &\qquad\times\langle(nl\mathcal{NL})L\|w_3(\mathbf{x}_3)^{(k_1)}\|(n''l''\mathcal{N}''\mathcal{L}'')L''\rangle\\ &\qquad\times\langle(n''l''\mathcal{N}''\mathcal{L}'')L''\|w_2(\mathbf{x}_2)^{(k_2)}\|(n'l'\mathcal{N}'\mathcal{L}')L'\rangle.\end{aligned} \tag{29}$$

Note that the sum over the intermediate HO states in Eq. (29) should be taken to as large a limit as possible (at the least until adequate convergence in the resulting nuclear spectrum is achieved) and not restricted merely to the states permitted in the model space. For a discussion of the summation required to reach this convergence see Sec. III A.

The first spatial matrix element in Eq. (29) is easy, as $w_3(\mathbf{x}_3)$ is diagonal in $|\mathcal{NL}\rangle$, however, the second is not. But we can execute a transformation of the HO basis from one in terms of the $(\vec{\xi}_1,\vec{\xi}_2)$ coordinates (as defined above in Eq. (17)] to $(\vec{\xi}_1',\vec{\xi}_2')$, where these new coordinates are defined by

$$\vec{\xi}_1' = \frac{1}{\sqrt{2}}(\vec{r}_3 - \vec{r}_1),$$

$$\vec{\xi}_2' = \frac{1}{\sqrt{6}}(\vec{r}_3 + \vec{r}_1) - \sqrt{\frac{2}{3}}\,\vec{r}_2. \tag{30}$$

In other words, we have transformed the coordinates to match the second internucleon coordinate of interest. The coordinate transformation is easily determined to be

$$\vec{\xi}_1' = \frac{1}{2}\,\vec{\xi}_1 + \frac{\sqrt{3}}{2}\,\vec{\xi}_2,$$

$$\vec{\xi}_2' = \frac{\sqrt{3}}{2}\vec{\xi}_1 - \frac{1}{2}\,\vec{\xi}_2, \tag{31}$$

and, thus the two HO function basis sets are related by a transformation depending on the Brody-Moshinsky brackets for particles with unequal masses [45]. The ansatz of Ref. [45] defines a parameter d, which is determined from the transformation coefficients: the transformation from coordinates $(\vec{r}_1,\vec{r}_2)$ to $(\vec{r},\vec{R})$ may be written as

$$\vec{r} = \left(\frac{d}{1+d}\right)^{1/2}\vec{r}_1 - (1+d)^{-1/2}\vec{r}_2,$$

$$\vec{R} = (1+d)^{-1/2}\vec{r}_1 + \left(\frac{d}{1+d}\right)^{1/2}\vec{r}_2, \tag{32}$$

which matches Eq. (31) if we set $d=1/3$. Note that a reversal of the ordering of the coordinates in the bracket is required since $\vec{\xi}_1'$ in Eq. (31) corresponds to $\vec{R}$ in Eq. (32), and similarly $\vec{\xi}_2'$ corresponds to $\vec{r}$—thus introducing a phase factor to be included in the final matrix element in Eq. (31). Our reduced spatial matrix element, thus, appears eventually as follows:

$$\begin{aligned}
&\langle (nl\mathcal{N}\mathcal{L})L \| [w_3(\mathbf{x}_3)^{(k_1)} w_2(\mathbf{x}_2)^{(k_2)}]^{(K)} \| (n'l'\mathcal{N}'\mathcal{L}')L' \rangle \\
&= \sum_{n''l''L''n_2l_2\mathcal{N}_2\mathcal{L}_2n_2'l_2'} (-1)^{L+L''+\mathcal{L}'+\mathcal{L}_2+l+l_2'+k_1+k_2+K} \hat{K}\hat{L}\hat{L}'(\hat{L}'')^2 \begin{Bmatrix} k_2 & l_2' & l_2 \\ \mathcal{L}_2 & L'' & L' \end{Bmatrix} \begin{Bmatrix} k_1 & l'' & l \\ \mathcal{L} & L & L'' \end{Bmatrix} \begin{Bmatrix} k_1 & k_2 & K \\ L' & L & L'' \end{Bmatrix} \\
&\times \langle (n_2l_2\mathcal{N}_2\mathcal{L}_2)L'' | (n''l''\mathcal{N}\mathcal{L})L'' \rangle_{d=1/3} \langle (n_2'l_2'\mathcal{N}_2\mathcal{L}_2)L' | (n'l'\mathcal{N}'\mathcal{L}')L' \rangle_{d=1/3} \langle nl \| w_3(\mathbf{x}_3)^{(k_1)} \| n''l'' \rangle \\
&\times \langle n_2l_2 \| w_2(\mathbf{x}_2)^{(k_2)} \| n_2'l_2' \rangle,
\end{aligned} \tag{33}$$

where the subscript 2 denotes the transformed basis in the $\mathbf{x}_2$ coordinate described above.

The remaining one-dimensional integrals can now be easily determined by a standard numerical integration routine (an analytic formulation for these integrals should be possible, but as these take up only a very small part of the actual computation, the benefits of this are negligible). These integrals are noted in the Appendix. Once we calculate these integrals, the determination of each full TM′ matrix element becomes a purely algebraic exercise.

III. RESULTS AND DISCUSSION

To test our formalism we apply it to calculate the ^{3}H binding energy, for which calculations with the TM′ three-nucleon interaction have already been performed using, e.g., the Faddeev technique [5]. We solve the Schrödinger equation with the Hamiltonian (11) by diagonalization using the translationally invariant HO basis applying the approach described in the preceding sections. Our results depend on the HO frequency Ω and on the basis size defined by $N_{\max}$. Concerning the HO frequency Ω, we select it from our ^{3}H calculation with just the two-nucleon interaction. It follows from our previous investigations that $\hbar\Omega = 28$ MeV leads to the fastest convergence when realistic nucleon-nucleon interactions are used [43]. It is important to select the optimal HO frequency Ω in this way, as the nucleon-nucleon interaction is the dominant part of the whole interaction. When we investigate the convergence of the calculation with the three-nucleon interaction on $N_{\max}$ we want to make sure that the two-nucleon part of the interaction is under control. In our present investigation, we use the AV18 *NN* potential [8] together with several versions of the TM′ TNI. The AV18 *NN* potential includes the isospin breaking as well as charge-symmetry breaking terms. In our calculations though, we restrict our basis to $T=\frac{1}{2}$ states. Consequently, we employ the $\frac{1}{3}V_{pn}+\frac{2}{3}V_{nn}$ *NN* potential combination in the $t=1$ two-nucleon channels.

A. Test of convergence for the intermediate sum truncation

As noted above, one limit in the calculations, which must first be established, is that of the intermediate sum in the spatial reduced matrix elements, Eq. (29). These intermediate states should, in theory, be summed over the full infinite dimensional basis space. For practical calculations, however, we must choose a limit to this sum, which hopefully will still be large enough to achieve convergence in the nuclear properties of interest. We choose this limit by defining a parameter $N_{\max}^{\text{int}}$, and allow only those intermediate states whose HO components satisfy $2n''+l''+2\mathcal{N}''+\mathcal{L}'' \leqslant N_{\max}^{\text{int}}$. Then

TABLE II. Energies, in MeV, for the ground and lowest three excited states of ^{3}H from $16\hbar\Omega$-space ($N_{\max}=16$) calculations with the AV18+TM′(81) potential, $\Lambda/\mu=4.756$, using $\hbar\Omega=28$ MeV. Convergence of the results with the $N_{\max}^{\rm int}$ parameter is investigated. For details see text.

E (MeV)	Ground	First	Second	Third
$N_{\max}^{\rm int}=24$	−8.3219	6.2131	12.2709	13.4426
$N_{\max}^{\rm int}=26$	−8.3252	6.2066	12.2598	13.4460
$N_{\max}^{\rm int}=28$	−8.3274	6.2023	12.2516	13.4483
$N_{\max}^{\rm int}=30$	−8.3288	6.2033	12.2553	13.4472
$N_{\max}^{\rm int}=32$	−8.3295	6.2042	12.2565	13.4469
$N_{\max}^{\rm int}=34$	−8.3299	6.2047	12.2553	13.4473
$N_{\max}^{\rm int}=36$	−8.3300	6.2054	12.2549	13.4475
$N_{\max}^{\rm int}=38$	−8.3300	6.2065	12.2551	13.4475

we can study the convergence of nuclear properties as $N_{\max}^{\rm int}$ becomes large and determine an adequate value for this limiting parameter. Table II shows the eigenenergies for the ground and first three excited states of ^{3}H using an intermediate-size $N_{\max}=16$ basis space (which allows us to use large values of $N_{\max}^{\rm int}$) and the AV18+TM′(81) potential for various values of $N_{\max}^{\rm int}$. It should be noted here that these excited states are virtual, unbound eigenstates, useful only as numerical indicators of convergence. We note, though, that the excited states will be required in the determination of an effective three-body interaction for $A>3$. In that case, these states will be bound as the system will be bound in a HO potential obtained by setting $A>3$ in the $V_{ij}^{\Omega,A}$ term of Eq. (2). It is apparent that in the present calculation the excited-state energies are more sensitive to the choice of $N_{\max}^{\rm int}$ than the ground state, and so if a useful spectrum is to be derived, a reasonably large intermediate state expansion will be required. Certainly it appears that convergence has been achieved by the time one reaches $N_{\max}^{\rm int}=36$, as the results change only negligibly between here and using $N_{\max}^{\rm int}=38$. But if one can tolerate a systematic truncation error of less than 4 eV, then using $N_{\max}^{\rm int}=30$ still yields the ground state energy up to about 1 eV, while reproducing the first three excited state energies within this tolerance. A similar series of calculations in other basis spaces shows convergence to this accuracy at $N_{\max}^{\rm int}=N_{\max}+14$. Thus, we will assume that a value for $N_{\max}^{\rm int}$ of $14\hbar\Omega$ above the $N_{\max}$, defining the model space, will provide adequate convergence of this intermediate expansion.

B. Test of convergence for binding energy of ^{3}H

With the HO frequency fixed at $\hbar\Omega=28$ MeV, we performed calculations for ^{3}H both with and without the TNI in the range of basis spaces from $N_{\max}=0$ to $N_{\max}=30$. Figure 2 demonstrates the convergence with the basis size when the Hamiltonian contains the AV18 plus the TM′(81) three-nucleon interaction with the cutoff parameter value of $\Lambda/\mu=4.756$, a value chosen to reproduce closely the experimental ^{3}H and ^{3}He binding energies. Note that the a' parameter is kept fixed here at the value given in Table I (−0.87). Our

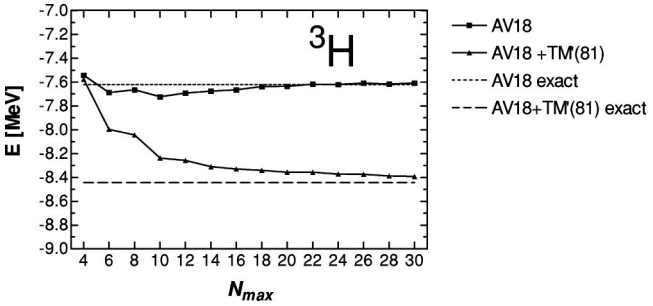

FIG. 2. Convergence of the ^{3}H binding energy with model space size using the AV18 two-body potential both without (squares) and with (triangles) the TM′(81) three-body force ($\hbar\Omega=28$ MeV and $\Lambda/\mu=4.756$). The dotted lines denote the exact binding energies, using the Faddeev method for the AV18 *NN* potential only (−7.623 MeV [5]), and for AV18+TM′(81) (−8.444 MeV [5]).

calculations used these parameters in order to compare with the results of Faddeev calculations by Nogga and co-workers [5], which we take as a benchmark calculation with this Hamiltonian. The binding energies resulting from using only a two-body effective interaction derived from the AV18 *NN* potential, converge very quickly with increasing $N_{\max}$ to the exact AV18-only result (which, as has been noted, underbinds this nucleus by approximately 0.9 MeV). Convergence to the exact Faddeev result of −8.444 MeV [5] when using the combination of the AV18 generated two-body effective interaction and the bare TM′(81) three-nucleon interaction is much slower and indeed has not been quite reached in our calculations. At $N_{\max}=30$, the largest basis size that we were able to reach at present due to technical reasons, we still miss almost 60 keV of the exact result (for a summary of the results see Table III). Obviously, we will improve on this in the future, but even the current result should allow us to construct a reasonably accurate three-body effective interaction usable in calculations for $A>3$ nuclei.

C. Dependence of ^{3}H binding energy on the TM′ cutoff parameter

In this subsection, we investigate the ^{3}H binding energy dependence on the TM′ TNI cutoff parameter Λ for two different versions of the TM′. We note that this type of dependence was investigated in several previous works, e.g., in Refs. [13,14].

In Fig. 3, we present results for the updated Tucson-Melbourne potentials TM′(93) and TM′(99) obtained in one

TABLE III. The ^{3}H ground-state energy, in MeV, obtained in the NCSM and the Faddeev calculations [5] are compared. The cutoff parameter $\Lambda/\mu=4.756$ was used. The NCSM AV18+TM′(81) calculation is not fully converged, see Fig. 2. The result obtained in the largest accessed basis space, $N_{\max}=30$ using the HO frequency $\hbar\Omega=28$ MeV, is presented.

^{3}H $E_{\rm g.s.}$ (MeV)	NCSM	Faddeev [5]	Expt.
AV18	−7.61	−7.623	
AV18+TM′(81)	−8.39	−8.444	−8.482

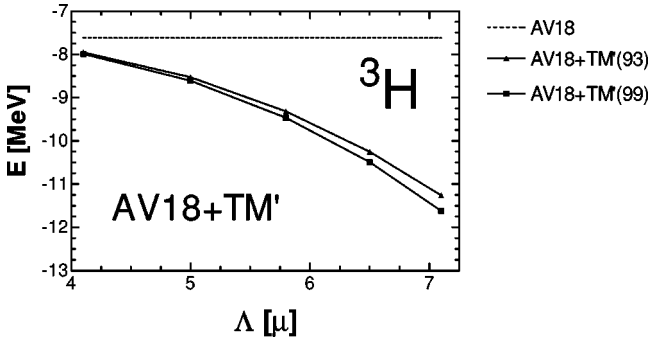

FIG. 3. Dependence of the ^{3}H binding energy, obtained using the AV18 *NN* potential plus the TM′ TNI, on the TM′ cutoff parameter Λ. Results for two different versions of the TM′ TNI are presented. The dotted line shows the result obtained with AV18 *NN* potential only.

of the largest model spaces allowed by our present computing power; $N_{\max}=28$. The HO frequency was again fixed at $\hbar\Omega=28$ MeV. The parameters of the TM′ TNI forces are given in Table I. We note that the a' parameter varies slightly with Λ according to a relation given in Ref. [14]. In general, though, the results are very weakly dependent on the a'. Although convergence has not been quite reached, in particular for larger values of Λ, still these are among the first results with a three-body force which reflect the changing π-N data set. The three-body force TM′(93) uses about the same π-N input parameters (a', b, d) as does TM′(81). The significant difference was the decision to make the range parameters reflect the SU(2) average mass of the pion (138 MeV), rather than the charged pion mass of 139.6 MeV. This minor change reflects the isospin formalism of the potential (13), rather than a charge state formalism. The latest potential incorporates the larger sigma term which may be a result of the π-N data analyses made since the 1980's. One can see from Fig. 3 that the potentials TM′(93) and TM′(99) give about the same binding energy results as a function of Λ/μ. The convergence issue becomes more severe for the larger values of Λ/μ. Our best value for the binding energy of ^{3}H when the TM′(99) is used is only about 0.09 MeV below a benchmark Faddeev calculation for $\Lambda/\mu=5.0$, but the discrepancy rises to about 0.9 MeV for $\Lambda/\mu=7.1$ [46].

IV. CONCLUSIONS

In this work we investigated the three-nucleon system with a realistic nucleon-nucleon potential and the TM′ two-pion-exchange three-body interaction using a translationally invariant harmonic oscillator basis. In the calculations, the no-core shell-model two-body effective interaction replaced the nucleon-nucleon potential, while the three-nucleon interaction was added without any renormalization.

We presented a formalism for calculating the three-body matrix elements of the TM′ interaction in a translationally invariant harmonic oscillator basis. This three-nucleon interaction satisfies all requirements of chiral symmetry including those of the chiral perturbation theory paradigm. It has the operator structure of all local three-nucleon interactions of the 2π-exchange type, so our techniques are readily extended to other such three-nucleon interactions currently available.

We studied the convergence of our approach by changing the basis size. We were able to obtain not yet completely converged three-nucleon solutions that should still be applicable for construction of three-body effective interactions usable for nuclei with $A>3$. In addition, we examined the dependence of the ^{3}H binding energy on the TM′ cutoff parameter Λ.

In summary, we have shown the feasibility of NCSM calculations with free-space three-nucleon interactions. This result, coupled with the work of Navratil and Ormand [47] on effective three-body interactions obtained from free-space *NN* potentials only, clears the way for complete NCSM calculations with full effective three-body interactions in the *p* shell.

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APPENDIX

After applying Eq. (33) to factor the spatial component of the TM′ matrix element, a careful inspection of the interaction (13) reveals that only four cases for each n,l,n'',l'' combination are required:

$$\langle nl\left\|\frac{Z_1'(r)}{r}\right\|n''l''\rangle=\delta_{l,l''}\hat{l}\int_0^\infty R_{nl}(r)\frac{Z_1'(r)}{r}R_{n''l''}(r)r^2dr, \tag{A1}$$

$$\langle nl\|\,\hat{\mathbf{r}}^{(1)}Z_1'(r)\|n''l''\rangle = -\hat{l}\langle l010|l''0\rangle\int_0^\infty R_{nl}(r)Z_1'(r)R_{n''l''}(r)r^2dr, \tag{A2}$$

$$\langle nl\|(\hat{\mathbf{r}}\hat{\mathbf{r}})^{(0)}\tilde{Z}(r)\|n''l''\rangle = -\frac{\hat{l}}{\sqrt{3}}\delta_{l,l''}\int_0^\infty R_{nl}(r)\tilde{Z}(r)R_{n''l''}(r)r^2dr, \tag{A3}$$

$$\langle nl\|(\hat{\mathbf{r}}\hat{\mathbf{r}})^{(2)}\tilde{Z}(r)\|n''l''\rangle = \sqrt{\frac{2}{3}}\hat{l}\langle l020|l''0\rangle\int_0^\infty R_{nl}(r)\tilde{Z}(r)R_{n''l''}(r)r^2dr. \tag{A4}$$

Referring to the example stated in the text between Eqs. (28) and (29), the first term in W_1 yields $w_3(\mathbf{x}_3)=\hat{\mathbf{x}}_3^{(1)}Z_1'(x_3)$ [with a similar expression for $w_2(\mathbf{x}_2)$]. Substituting these into Eq. (33) produces single dimensional integrals of the form (A2) in both coordinates.

[1] H. O. Meyer, Nucl. Phys. News **11**, 15 (2001).
[2] H. Witała, W. Glöckle, J. Golak, A. Nogga, H. Kamada, R. Skibiński and J. Kuroś-Żołnierczuk, Phys. Rev. C **63**, 024007 (2001).
[3] H. Sakai *et al.*, Phys. Rev. Lett. **84**, 5288 (2000); K. Sekiguchi *et al.*, Phys. Rev. C **65**, 034003 (2002); K. Ermisch *et al.*, Phys. Rev. Lett. **86**, 5862 (2001).
[4] H. Witała, W. Glöckle, D. Hüber, J. Golak, and H. Kamada, Phys. Rev. Lett. **81**, 1183 (1998).
[5] A. Nogga, H. Kamada, and W. Glöckle, Phys. Rev. Lett. **85**, 944 (2000); D. Hüber, H. Witała, A. Nogga, W. Glöckle, and H. Kamada, Few-Body Syst. **22**, 107 (1997).
[6] J. L. Friar, D. Hüber, and U. van Kolck, Phys. Rev. C **59**, 53 (1999).
[7] H. Kamada *et al.*, Phys. Rev. C **64**, 044001 (2001).
[8] B. S. Pudliner, V. R. Pandharipande, J. Carlson, Steven C. Pieper, and R. B. Wiringa, Phys. Rev. C **56**, 1720 (1997).
[9] Steven C. Pieper, V. R. Pandharipande, R. B. Wiringa, and J. Carlson, Phys. Rev. C **64**, 014001 (2001).
[10] S. A. Coon and J. L. Friar, Phys. Rev. C **34**, 1060 (1986).
[11] J. Carlson, V. R. Pandharipande, and R. B. Wiringa, Nucl. Phys. **A401**, 59 (1983).
[12] J. L. Friar, B. F. Gibson, G. L. Payne, and S. A. Coon, Few-Body Syst. **5**, 13 (1988).
[13] A. Stadler, J. Adam, Jr., H. Henning, and P. U. Sauer, Phys. Rev. C **51**, 2896 (1995).
[14] S. A. Coon and H. K. Han, Few-Body Syst. **30**, 131 (2001).
[15] V. D. Efros, W. Leidemann, G. Orlandini, and E. L. Tomusiak, Phys. Lett. B **484**, 223 (2000).
[16] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. C **62**, 054311 (2000).
[17] K. Suzuki and S. Y. Lee, Prog. Theor. Phys. **64**, 2091 (1980).
[18] K. Suzuki, Prog. Theor. Phys. **68**, 246 (1982).
[19] K. Suzuki and R. Okamoto, Prog. Theor. Phys. **70**, 439 (1983).
[20] K. Suzuki and R. Okamoto, Prog. Theor. Phys. **92**, 1045 (1994).
[21] R. B. Wiringa, Steven C. Pieper, J. Carlson, and V. R. Pandharipande, Phys. Rev. C **62**, 014001 (2000).
[22] G. E. Brown, A. M. Green, and W. Gerace, Nucl. Phys. **A115**, 435 (1968).
[23] G. E. Brown and J. W. Durso, Phys. Lett. **35B**, 120 (1971).
[24] J. L. Friar and S. A. Coon, Phys. Rev. C **49**, 1272 (1994).
[25] S. Weinberg, Nucl. Phys. **B363**, 3 (1991).
[26] W. N. Polyzou and W. Glöckle, Few-Body Syst. **9**, 97 (1990).
[27] U. van Kolck, Prog. Part. Nucl. Phys. **43**, 337 (1999).
[28] E. Epelbaum, U. G. Meissner, W. Glöckle, C. Elster, H. Kamada, A. Nogga, and H. Witala, Nucl. Phys. **A689**, 111 (2001).
[29] S. A. Coon, M. D. Scadron, P. C. McNamee, B. R. Barrett, D. W. E. Blatt, and B. H. J. McKellar, Nucl. Phys. **A317**, 242 (1979).
[30] R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995).
[31] J. L. Friar, Phys. Rev. C **60**, 034002 (1999).
[32] N. Fettes and U.-G. Meissner, Nucl. Phys. **A693**, 693 (2001).
[33] M. C. M. Rentmeester, R. G. E. Timmermans, J. L. Friar, and J. J. de Swart, Phys. Rev. Lett. **82**, 4992 (1999).
[34] D. R. Entem and R. Machleidt, nucl-th/0202039.
[35] S. A. Coon, Czech. J. Phys. **49**, 1235 (1999).
[36] G. E. Hite, R. J. Jacob, and M. D. Scadron, Phys. Rev. D **14**, 1306 (1976).
[37] G. Höhler, *Pion-Nucleon Scattering*, Landolt-Börnstein, New Series, Group I, Vol. 9, Pt. b2 (Springer-Verlag, Berlin, 1983).
[38] W. B. Kaufmann and G. E. Hite, Phys. Rev. C **60**, 055204 (1999).
[39] J. Stahov, hep-ph/0206041.
[40] H. Kamada, D. Hüber, and A. Nogga, Few-Body Syst. **30**, 121 (2001).
[41] P. Navrátil and B. R. Barrett, Phys. Rev. C **57**, 562 (1998).
[42] P. Navrátil and B. R. Barrett, Phys. Rev. C **59**, 1906 (1999).
[43] P. Navrátil, G. P. Kamuntavičius, and B. R. Barrett, Phys. Rev. C **61**, 044001 (2000).
[44] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, NJ, 1960).
[45] L. Trlifaj, Phys. Rev. C **5**, 1534 (1972).
[46] A. Nogga (private communication).
[47] P. Navrátil and W. E. Ormand, Phys. Rev. Lett. **88**, 152502 (2002).