Deuteron-equivalent and phase-equivalent interactions within light nuclei

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Background: Phase-equivalent transformations (PETs) are well known in quantum scattering and inversescattering theory. PETs do not affect scattering phase shifts and bound-state energies of a two-body system but are conventionally supposed to modify two-body bound-state observables such as the rms radius and electromagnetic moments.

Purpose: In order to preserve all bound-state observables, we propose a new particular case of PETs, a deuteronequivalent transformation (DET-PET), which leaves unchanged not only scattering phase shifts and bound-state (deuteron) binding energy but also the bound-state wave function.

Methods: The construction of DET-PET is discussed; equations defining the simplest DET-PETs are derived. We apply these simplest DET-PETs to the JISP16 NN interaction and use the transformed NN interactions in calculations of ³H and ⁴He binding energies in the no-core full configuration (NCFC) approach based on extrapolations of the no-core shell model (NCSM) basis space results to the infinite basis space.

Results: We demonstrate the DET-PET modification of the np scattering wave functions and study the DET-PET manifestation in the binding energies of ³H and ⁴He nuclei and their correlation (Tjon line).

Conclusions: It is shown that some DET-PETs generate modifications of the central component while the others modify the tensor component of the NN interaction. DET-PETs are able to modify significantly the np scattering wave functions and hence the off-shell properties of the NN interaction. DET-PETs give rise to significant changes in the binding energies of ³H (in the range of approximately 1.5 MeV) and ⁴He (in the range of more than 9 MeV) and are able to modify the correlation patterns of binding energies of these nuclei.

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I. INTRODUCTION

Phase-equivalent transformations (PETs) of two-body interactions are well known in quantum-scattering theory [1]. PETs play an important role in the inverse-scattering theory giving rise to ambiguities in the derived potentials. Currently, there is intensive research on supersymmetric transformations (see reviews [2,3]) which are a particular case of PETs [4] associated with removing or adding bound states to the system.

More traditional PETs which do not change the onshell properties of the two-body interaction, i.e., two-body scattering phase shifts and the energies of the two-body discrete spectrum states, but modify the interaction off-shell, were used to study manifestations of off-shell properties of two-nucleon interactions in many-nucleon systems. For example, a correlation between the nuclear matter binding energy and its equilibrium density (the so-called Coester line) was studied with phase-equivalent NN interactions in Ref. [5]. PETs were used to modify the nucleon-cluster interaction in order to obtain a correct description of the nuclear binding energies in cluster model studies of Refs. [6,7]. Various versions of the realistic JISP NN interaction (JISP6 [8] and JISP16 [9,10]) were obtained by means of PETs applied to the initial ISTP NN interaction [11] obtained in the *J*-matrix inverse scattering approach with the aim of improving the description of binding energies of many-nucleon systems. The interaction JISP16 [9,10] provides an accurate description of light nuclei [9,12–21] and was used to predict the binding energy and spectrum of the exotic ¹⁴F nucleus [22] which were confirmed later in the first experimental observation of this isotope [23].

We propose here a new type of PET, a deuteron-equivalent transformation (DET-PET). Contrary to conventional PETs resulting in the modification of bound-state and scattering wave functions [1,4,5,11], DET-PET guarantees that the transformed interaction generates not only the same scattering phase shifts and two-body binding energy (or, more generally, bound state energies) but also the same bound state (deuteron) wave function as the initial untransformed interaction. The same method easily generalizes to preserve a set of bound-state wave functions. DET-PET has the advantage of preserving the deuteron ground-state observables. On the other hand, DET-PET, as well as any PET, modifies a two-body interaction off-shell, and hence manifests itself in many-body systems.

One may naturally inquire whether PETs lead to a better understanding of the appropriate off-shell behavior for the NNinteraction. We note that what is appropriate depends on the adopted theoretical framework for the NN interaction. Since the interaction is not an observable, all approaches (meson exchange, EFT, lattice gauge, inverse scattering, etc.) build in-model assumptions (e.g., form factors, regulators, cutoffs, etc.). Given those model assumptions, there are additional unexplored off-shell freedoms and we will show below how to explore those freedoms with constraints tied to NN boundstate observables.

After introducing the formulas defining DET-PET, we apply DET-PET to the JISP16 NN interaction and illustrate various versions of DET-PET by respective modifications of scattering wave functions at a few values of the DET-PET continuous parameter. A DET-PET manifestation in many-body systems is illustrated by the study of binding energies of ³H and ⁴He binding energies and their correlation (the so-called Tjon line [24]).

It is known [25] that when any PET, DET-PET in particular, is applied to NN interaction, the binding energy of a threebody (or heavier) system can be restored by additional threenucleon NNN (or higher-order) interaction(s). Our initial ³H applications reveal the residual role of the NNN interaction for the ground state energy and how that role changes with the DET-PET selected. Similarly, our initial ⁴He applications reveal the residual roles for the combined NNN and NNNNinteractions on the ground state energy. Given the numerical challenges of treating NNN, NNNN, etc., interactions in many-body applications, it is natural to try to minimize their effects. In this context, DET-PETs are a potentially useful tool in future searches for an NN interaction consistent with many-body data.

II. DET-PET TRANSFORMATION

Two types of PETs are known in scattering theory: local PETs [1] that transform a local potential into another local potential and nonlocal PETs [5] which generate nonlocal potential terms. The local PETs always result in some modification of bound-state wave functions [1,4]. Therefore we focus the discussion here on nonlocal PETs.

The Schrödinger equation

describes a relative motion in two-body quantum system. The state $|\Psi_E\rangle$ can be expanded in infinite series of \mathscr{L}^2 states $|a_n\rangle$,

$$|\Psi_E\rangle = \sum_{n=0}^{\infty} c_n(E) |a_n\rangle.$$
⁽²⁾

The states $|a_n\rangle$ are supposed to form a complete orthonormalized basis,

$$\langle a_i | a_j \rangle = \delta_{ij}. \tag{3}$$

Using expansion (2) we obtain an infinite set of algebraic equations defining the expansion coefficients $c_n(E)$,

$$\sum_{n'=0}^{\infty} (H_{nn'} - \delta_{nn'} E) c_{n'}(E) = 0, \qquad (4)$$

where $H_{nn'} = \langle a_n | H | a_{n'} \rangle$ are the Hamiltonian matrix elements.

A Hamiltonian \tilde{H} phase-equivalent to H can be defined through its matrix $[\tilde{H}]$ in the basis $\{|a_n\rangle\}$. This matrix $[\tilde{H}]$ can be obtained from [H], the matrix of the Hamiltonian H in the basis $\{|a_n\rangle\}$, by means of a unitary transformation,

$$[\tilde{H}] = [U][H][U^{\dagger}]. \tag{5}$$

The infinite unitary matrix [U] is supposed to be of the form

$$[U] = [U^0] \oplus [I] = \begin{bmatrix} [U^0] & 0\\ 0 & [I] \end{bmatrix},$$
 (6)

where [I] is an infinite unit matrix and $[U^0]$, a nontrivial submatrix of [U], is a finite matrix mixing only a few selected basis functions. It is clear that Hamiltonians H and \tilde{H} have identical eigenvalue spectra. Their eigenstates $|\tilde{\Psi}_E\rangle$ and $|\Psi_E\rangle$, differ by a linear combination of a finite number of \mathscr{L}^2 basis states. Any superposition of a finite number of \mathscr{L}^2 functions must decrease at large distances. Therefore at positive energy E associated with scattering, the oscillating asymptotics of wave functions $\langle \vec{r} | \tilde{\Psi}_E \rangle$ and $\langle \vec{r} | \Psi_E \rangle$ at large distances are the same. In other words, the scattering phase shifts defined through asymptotic behavior of functions $\langle \vec{r} | \tilde{\Psi}_E \rangle$ and $\langle \vec{r} | \Psi_E \rangle$ are also the same, i.e., the Hamiltonians H and \tilde{H} are phase-equivalent.

The unitary operator U^0 can be written as

$$U^{0} = \sum_{i,j \leq N} |a_{i}\rangle U^{0}_{ij} \langle a_{j}|.$$
⁽⁷⁾

The transformation (5)–(7) leaves the bound state $|d\rangle$ unchanged, i.e., becomes a DET-PET, when each of the \mathcal{L}^2 vectors $|a_i\rangle$ entering the nontrivial submatrix $[U^0]$ of the infinite unitary matrix [U] through Eq. (7), is orthogonal to $|d\rangle$,

$$\langle a_i | d \rangle = 0, \quad i \leqslant N. \tag{8}$$

At this stage, we assert that we have obtained our DET-PET defined through the unitary transformation (5)–(7) with vectors $|a_i\rangle$ fitting the conditions (3) and (8). In order to obtain a non-local interaction \tilde{V} deuteron-equivalent and phase-equivalent to the initial interaction V, we add to V the two-body relative kinetic energy operator T to obtain the Hamiltonian H,

$$H = T + V, \tag{9}$$

calculate its matrix [*H*] in the basis $\{|a_n\rangle\}$, obtain the matrix $[\tilde{H}]$ by means of DET-PET unitary transformation, and obtain the matrix

$$[\tilde{V}] = [\tilde{H}] - [T].$$
(10)

Here [T] is the infinite kinetic energy matrix in the basis $\{|a_n\rangle\}$. The interaction \tilde{V} is defined through its matrix $[\tilde{V}]$ in the basis $\{|a_n\rangle\}$.

The simplest DET-PET is obtained with arbitrary unitary matrix $[U^0]$ of the rank 2. In this case, $[U^0]$ is associated either with a rotation by the angle β when det $U^0 = +1$ or with a rotation by the angle β combined with reflection when det $U^0 = -1$. We also need to define the \mathcal{L}^2 vectors $|a_1\rangle$ and $|a_2\rangle$ in Eq. (7).

We define here the vectors $|a_1\rangle$ and $|a_2\rangle$ as linear combinations of oscillator states $|\varphi_i\rangle$,

$$|a_i\rangle = \sum_{i' \leqslant N'} \alpha_i^{i'} |\varphi_{i'}\rangle, \qquad (11)$$

which fit the orthonormality condition (3). We expand the deuteron eigenstate $|d\rangle$ in an infinite series of oscillator states,

$$|d\rangle = \sum_{i=0}^{\infty} d_i |\varphi_i\rangle, \qquad (12)$$

where, generally, all the coefficients d_i are nonzero,

$$d_i \neq 0. \tag{13}$$

Since the vectors $|a_1\rangle$ and $|a_2\rangle$ should fit Eq. (8), the expansion (11) of each of them involves at least two different basis states $|\varphi_i\rangle$ due to Eqs. (12) and (13). In this simplest case we have

$$|a_1\rangle = a_1^n |\varphi_n\rangle + a_1^m |\varphi_m\rangle, \qquad (14a)$$

$$|a_2\rangle = a_2^k |\varphi_k\rangle + a_2^l |\varphi_l\rangle. \tag{14b}$$

The normalization of these vectors requires

$$(a_1^n)^2 + (a_1^m)^2 = 1,$$
 (15a)

$$(a_2^k)^2 + (a_2^l)^2 = 1,$$
 (15b)

while the orthogonality of the vectors $|a_1\rangle$ and $|a_2\rangle$,

$$\langle a_2 | a_1 \rangle = 0, \tag{16}$$

is guaranteed when these vectors are constructed from different basis states, i.e., all the basis states $|\varphi_n\rangle$, $|\varphi_m\rangle$, $|\varphi_k\rangle$, $|\varphi_l\rangle$ entering Eqs. (14) are different. Using expansions (11) and (12) we obtain

$$a_1^n d_n + a_1^m d_m = 0, (17a)$$

$$a_2^k d_k + a_2^l d_l = 0. (17b)$$

The solutions of Eqs. (15), (17) are

$$a_1^n = \frac{d_m}{\sqrt{d_n^2 + d_m^2}},$$
 (18a)

$$a_1^m = -\frac{d_n}{\sqrt{d_n^2 + d_m^2}},$$
 (18b)

$$a_2^k = \frac{d_l}{\sqrt{d_k^2 + d_l^2}},$$
 (18c)

$$a_2^l = -\frac{d_k}{\sqrt{d_k^2 + d_l^2}}.$$
 (18d)

To define completely the simplest DET-PET discussed above we need to fix the rotation angle β , the sign of det U^0 and the set of four oscillator states used to build the states $|a_1\rangle$ and $|a_2\rangle$. To distinguish various DET-PET types we use notations like $0s2s1s2d^{\pm}$. In this example, the state $|a_1\rangle$ is a linear combination of the oscillator states 0s and 2s, the vector $|a_2\rangle$ is a linear combination of the oscillator states 1s and 2d, and the index \pm corresponds to the sign of det $U^0 = \pm 1$.

III. DET-PET PROPERTIES AND MANIFESTATION IN FEW-NUCLEON SYSTEMS

In this section, we study modifications of the JISP16 NN interaction [9] induced by various DET-PETs. The modifications of a nonlocal interaction can be illustrated by modifications of its wave functions. The deuteron wave function is unaffected by DET-PET. Therefore we present below the DET-PET induced transformation of the JISP16 np scattering wave function in the *sd* coupled partial wave.

It is interesting to explore a DET-PET which acts only in a single channel, say, in the *s* channel, and compare it with DET-PETs mixing components of the *s* and *d* channels in different ways. Therefore vectors $|a_1\rangle$ and $|a_2\rangle$ [see Eqs. (14)] were constructed as various superpositions of two low-lying oscillator states of the *np* relative motion 0*s*, 1*s*, 2*s*, 3*s*, 0*d*, and 1*d* with $\hbar\Omega = 40$ MeV. For each type of the DET-PET we investigate the transformations associated with both pure rotation and a rotation-reflection combination.

Plots of the JISP16 np scattering wave functions in the sd coupled partial wave at laboratory energy $E_{lab} = 10$ MeV and plots for their $0s2s1s3s^{\pm}$, $0s1s0d1d^{\pm}$, and $1s0d0s1d^{\pm}$ DET-PET partners are given in Figs. 1, 2, and 3, respectively. We use the *K*-matrix formalism (see Ref. [11] for details and nomenclature adopted here). The advantage of the *K*-matrix formalism is that the radial wave functions in the scattering domain defined according to their standing wave asymptotics are real contrary to the more conventional *S*-matrix formalism with complex radial wave functions which are asymptotically a superposition of ingoing and outgoing spherical waves.

The DET-PET $0s2s1s3s^{\pm}$ mixes various *s* wave components of the wave function that is equivalent to modification of the central part of the JISP16 interaction in the *s* wave. This results in significant changes of the large *s* wave component as is seen in Fig. 1. The modification of the small *s* wave component is less pronounced. The *d* wave components, as expected, are nearly unaffected by $0s2s1s3s^{\pm}$.

The DET-PET $0s1s0d1d^{\pm}$ explicitly mixes *s* and *d* waves; the DET-PET $1s0d0s1d^{\pm}$ also mixes *s* and *d* waves but in a different manner. This corresponds to an essential modification of the tensor component of the JISP16 *NN* interaction. As a result, we observe an essential modification of small scattering wave function components which are generated by the tensor *NN* interaction as is seen in Figs. 2 and 3.



FIG. 1. (Color online) Large (a) and small (b) components of the *np* scattering wave function at the laboratory energy $E_{lab} = 10$ MeV in the *sd* coupled partial wave in the *K*-matrix formalism (see Ref. [11] for details and nomenclature) generated by JISP16 and *NN* interactions obtained from JISP16 by means of DET-PET $0s2s1s3s^{\pm}$. The sign of det U^0 is given in the legends in parenthesis after the value of rotation angle β .

Modifications of the large wave function components are much less pronounced.

We see that DET-PET generates essential modifications of scattering wave functions without any change of scattering phase shifts and scattering observables (cross sections, polarization observables, etc.). It is worth noting here that the deuteron wave function and deuteron observables (rms radius, quadrupole moment, etc.) are unaffected by DET-PET due to the nature of this transformation. The alteration of scattering wave functions is an indicator for the variation of the off-shell properties of the interaction arising from DET-PET. The modification of the the NN interaction off-shell should manifest itself in properties of many-nucleon systems. Therefore, we investigate the DET-PET-induced changes of the ³H and ⁴He binding energies.

We calculate ³H and ⁴He in the *ab initio* no-core full configuration (NCFC) [17] approach. Within the NCFC approach, we start with the no-core shell model [26,27]

calculations using the code MFDn [28-31] with a few values of the oscillator frequency $\hbar\Omega$ and in a few basis spaces characterized by the maximum oscillator quanta N_{max} allowed in the many-body basis above the minimal configuration. Next, we extrapolate the sequence of finite basis space results to the infinite basis space limit. This makes it possible to obtain basis space independent results for binding energies and to evaluate their numerical uncertainties. NCFC suggests two extrapolation methods: a global extrapolation based on the calculations in four successive basis spaces and five $\hbar\Omega$ values in a 10 MeV interval (extrapolation A), and extrapolation B based on the calculations at various fixed $\hbar\Omega$ values in three successive basis spaces and defining the most reliable $\hbar\Omega$ value for the extrapolation. We present here only the extrapolation A results based on the NCSM calculations with basis spaces up through $N_{\text{max}} = 16$. The extrapolations A and B usually provide consistent results [17], and we checked this consistency for our results in a number of cases. The evaluated



FIG. 2. (Color online) Same as Fig. 1 but for DET-PET $0s1s0d1d^{\pm}$.



FIG. 3. (Color online) Same as Fig. 1 but for DET-PET $1s0d0s1d^{\pm}$.

uncertainties of results for binding energies presented here are less then 10 keV in most cases; in a few cases, we performed the NCSM calculations up to $N_{\text{max}} = 18$ to obtain the binding energies with uncertainty of about 10 keV.

The binding energies of ³H nucleus E_t and of ⁴He nucleus E_{α} were calculated with JISP16 interaction modified by DET-PETs $0s2s1s3s^{\pm}$, $0s1s0d1d^{\pm}$, and $1s0d0s1d^{\pm}$ varying angle β from 0° through 360° in steps of 60°. We observe variations of E_t and E_{α} due to DET-PETs. In some cases, when the ³H and ⁴He binding energies were close to their maximal or minimal values for a given DET-PET type, we decreased the step of β to investigate the behavior of E_t and E_{α} around their extremal values in more detail.

The ranges of ³H and ⁴He binding energy variations for each DET-PET type are shown in Table I. We see that DET-PETs can cause essential modification of both ³H and ⁴He binding energies. For example, in the case of the ⁴He nucleus, E_{α} can be varied by DET-PETs on the interval from 21.25 through 30.41 MeV, i.e., the DET-PET *NN* interaction can change E_{α} by more than 7 MeV from its original value provided by the original JISP16 interaction. In the case of ³H, the range of the DET-PET binding energy variation is $7.21 \le E_t \le 8.67$ MeV, i.e., the binding energy can be shifted by more than 1 MeV from its original JISP16 value.

We study also a correlation of the ³H and ⁴He binding energies, the so-called Tjon line [24]. The Tjon line is usually

studied using results obtained with different *NN* interactions and different combinations of *NN* and *NNN* interactions (see, e.g., Ref. [32]). We note here also an investigation of Jurgenson *et al.* [33] where the ³H and ⁴He binding energy correlation was studied with *NN* interactions SRG evolved to various values of momentum parameter λ . An interesting observation mentioned by various authors (see, e.g., Refs. [24,32]) is that these results obtained with different interaction models form nearly a straight line on the plot E_{α} vs E_t . Here we study the E_t-E_{α} correlation using families of *NN* potentials generated by various DET-PET types from the JISP16 interaction, i.e., all *NN* interactions provide not only algebraically identical *NN* phase shifts but also identical deuteron wave functions that should give rise to specific *np* correlations in three- and four-nucleon systems.

We begin the discussion of the Tjon lines from the results obtained with the $1s0d0s1d^{\pm}$ DET-PET presented in Fig. 4 where we show also the results from Refs. [32,34,35] obtained with various modern *NN* and *NN* + *NNN* interaction models. It is seen that the DET-PET E_t-E_{α} correlation generally follows the trend suggested by other interactions: our results are concentrated close to the Tjon line connecting the points extracted from Refs. [32,34,35] and extend it to larger ³H and ⁴He bindings. We recall here that the $1s0d0s1d^{\pm}$ DET-PET is associated with modification of the tensor component of *NN* interaction.

TABLE I. Ranges of ³H and ⁴He binding energy variations (in MeV) caused by various types of DET-PET in comparison with the binding energies obtained with JISP16 and their experimental values.

³ H	⁴ He	³ H	⁴ He
	$0s2s1s3s^+$	0s2s1s3s	_
7.21-8.37	21.25-28.49	7.25-8.35	21.46-28.59
	$0s1s0d1d^+$	0s1s0d1d	_
7.67-8.41	23.50-28.83	7.68-8.39	23.46-28.91
	$1s0d0s1d^{+}$	1s0d0s1d	_
7.98-8.64	25.79-30.36	8.05-8.67	26.18-30.41
	JISP16	Experiment	nt
8.369(1)	28.299(1)	8.482	28.296



FIG. 4. (Color online) Tjon line obtained with DET-PET $1s0d0s1d^{\pm}$ in comparison with results obtained with various NN and NN + NNN interaction models from Refs. [32,34,35].

Another DET-PET modifying the tensor component of the JISP16 NN interaction, is the DET-PET $0s_1s_0d_1d^{\pm}$. This DET-PET results in a very different range of E_t and E_{α} variations (see Table I). The DET-PET ³H and ⁴He binding energies are also correlated along a nearly straight line (see Fig. 5). However this line has a slope very different from the slope of the Tjon line obtained with other interaction models. Around the maximal ³H and ⁴He binding energies accessible by this DET-PET, it suggests correlations consistent with those derived using modern NN + NNN interaction models. However, for smaller binding energies, this DET-PET suggests much less bound ⁴He at the same ³H bindings as provided by modern purely two-nucleon interactions.

The DET-PET $0s2s1s3s^{\pm}$ modifies the central *s*-wave component of the *NN* interaction. It results in the ³H and ⁴He binding energy correlation shown in Fig. 6. We see that in this case the results do not concentrate as tightly around some straight line. That is, they are more spread out on



FIG. 5. (Color online) Same as Fig. 4 but for DET-PET $0s1s0d1d^{\pm}$.



FIG. 6. (Color online) Same as Fig. 4 but for DET-PET $0s2s1s3s^{\pm}$.

the $E_t - E_\alpha$ plane. The DET-PET Tjon lines transform into closed-loop curves surrounding elongated areas. In the case of the DET-PET $0s2s1s3s^-$, the Tjon curve surrounds many points obtained with various *NN* interactions. The DET-PET $0s2s1s3s^+$ generates the Tjon curve shifted down from the Tjon line suggested by other interactions. Both $0s2s1s3s^+$ and $0s2s1s3s^-$ DET-PETs essentially extend the range of the ³H and ⁴He binding energy variations to smaller bindings.

IV. CONCLUSIONS

We have introduced a new type of phase-equivalent transformations, DET-PET, preserving the deuteron wave function. The suggested theory of DET-PET can be easily reformulated to preserve scattering wave functions at a given energy instead of the bound state wave function. We investigated transformations of the JISP16 NN interaction induced by DET-PETs mixing oscillator components in various combinations. One of these DET-PETs generates modifications of the central component of the NN interaction, the others modify the tensor NNinteraction component. We demonstrated that DET-PETs are able to modify significantly the np scattering wave functions and hence the off-shell properties of the NN interaction while the on-shell interaction properties are preserved.

DET-PETs impact the binding energies of many-nucleon systems. We found that the ³H and ⁴He binding energies can be significantly changed by DET-PETs. The investigated DET-PETs modifying tensor NN interaction, correlate the ³H and ⁴He bindings along some lines that may differ in slope from the Tjon line obtained with modern NN and NNN interactions. The DET-PET $0s2s1s3s^{\pm}$ modifying the central *s* wave NN interaction, weakens the E_t-E_{α} correlation spreading the results on the E_t-E_{α} plane.

It would be interesting to study DET-PET manifestations in binding energies and other observables of heavier nuclei. We speculate that DET-PET can be helpful in the further development of JISP-like NN interactions.

DET-PETs can be also used to design an interesting approach to effective interactions. In particular, DET-PETs can be applied to a modern *NN* realistic interaction to reduce

their high momentum components (and hence to improve the convergence of *ab initio* calculations). At the same time, we are preserving the deuteron wave function and *NN* correlations in other partial waves at some energy by using the extension of DET-PET to preserve the scattering wave function. Such an effective interaction can be very interesting for many-body nuclear applications.

It is also possible to extend the DET-PET concept to NNN interactions. The corresponding set of transformations would then involve changing the interior part of the NNN wave function in such a manner as to preserve the NNN ground state wave function and to preserve the asymptotic NNN

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wave function. This could provide a useful tool to explore the off-shell freedoms available in *NNN* interactions without requiring repeated fits to the *NNN* bound state properties.

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