Deuteron-Equivalent Phase-Equivalent Transformation and Its Manifestation in Many-Body Systems

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Abstract

We propose a phase-equivalent transformation of NN interaction of a new type, the DET-PET transformation, which does not affect the wave function of the bound system (deuteron). The DET-PET properties and its manifestation in many-body systems are studied. In particular, we investigate the correlation of the ^{3}H and ^{4}He binding energies (Tjon line) in calculations with NN potentials obtained by means of DET-PET from the JISP16 NN interaction.

Keywords: *Phase-equivalent transformation; NN interaction.*

1 Introduction

One of the best *ab initio* approaches in the theory of light atomic nuclei is the No-core Full Configuration (NCFC) approach [1] based on extrapolation of results obtained in the No-core Shell Model (NCSM) calculations [2]. This approach does not imply any model assumption, a nucleon-nucleon interaction is the only input information utilized by NCFC. The NCFC approach was designed for calculations with the J-matrix Inverse Scattering Potentials (JISP) [3–5], the NN interactions obtained in the J-matrix inverse scattering approach, and was carefully tested in calculations with these NN interactions (see, e. g., Ref. [6–9]). Various versions of JISP interactions are related by phase-equivalent transformations (PETs) which do not affect the NN potential on-shell and hence preserve description of scattering phase shifts and deuteron binding energy, however modify the potential off-shell and therefore the description of few-body systems. A remarkable feature of JISP-type potentials is that they are able to reproduce nuclear properties without three-body nuclear forces reducing significantly the computer resources required for calculations. Up to now, nuclear studies were mostly performed [6–9] with the JISP16 interaction version [5, 10]; a more accurate interaction version JISP16$_{2010}$ providing a better description of the binding energies of $A \geq 10$ nuclei, was introduced [11–13].

Recently we proposed a new type of PETs, a deuteron-equivalent transformation (DET-PET) [14], which properties we discuss here. Contrary to conventional PETs resulting in the modification of potential and bound state wave functions [3, 15–17], DET-PET guarantees that the transformed interaction generates not only the same scattering phase shifts but also the same bound state (deuteron) wave function as the initial untransformed interaction. To the best of our knowledge, such PETs have not been ever discussed in literature. Obviously, DET-PET preserves the description of deuteron observables. DET-PET, as well as any other PET, modifies a two-body interaction off-shell, and hence can be used for fitting potentials to many-body systems without violation of high-quality description of two-body data.

After introducing DET-PET, we discuss the DET-PET modification of the JISP16 NN interaction providing an accurate description of light nuclei [1, 2, 6–9]. A DET-PET manifestation in many-body systems is illustrated by the study ^{3}H and ^{4}He binding energies and their correlation (the so-called Tjon line [18]) in particular.

2 Theory

Two types of PETs are known in scattering theory: local PETs [15] that transform a local potential into another local potential and nonlocal PETs [16] which generate nonlocal potential terms. We focus the discussion here on nonlocal PETs.

The Schrödinger equation

$$H\Psi(E,r) = E\Psi(r) \tag{1}$$

describes a relative motion in two-body quantum system. The wave function $\Psi(r)$ can be expanded in infinite series of $\mathcal{L}^2$ functions which are supposed to form a complete orthonormalized basis. We denote these functions by $|a_n\rangle$, their orthonormalization condition is

$$\langle a_i|a_j\rangle = \delta_{ij}, \tag{2}$$

and the wave function expansion is

$$\Psi(E,r) = \sum_{n=0}^{\infty} c_n(E)|a_n\rangle. \tag{3}$$

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

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

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

A phase-equivalent transformation of Hamiltonian H can be defined by means of a unitary transformation,

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

where $[H]$ is the Hamiltonian H matrix in basis $\{|a_n\rangle\}$. The infinite unitary matrix $[U]$ is supposed to be of the form

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

where $[I]$ is an infinite unit matrix and $[U^0]$ is a finite matrix mixing only a few low-lying states in a given basis. The Hamiltonian $\tilde{H}$ is defined through its matrix $[\tilde{H}]$ in the initial basis $\{|a_n\rangle\}$.

Obviously, the Hamiltonians $\tilde{H}$ and H have identical eigenvalue spectra and their eigenfunctions $\tilde{\Psi}(E,r)$ and $\Psi(E,r)$ differ by a linear combination of a finite number of functions $\{|a_n\rangle\}$. Any superposition of a finite number of $\mathcal{L}^2$ functions does not affect asymptotics of scattering wave functions, hence the Hamiltonian $\tilde{H}$ is phase-equivalent to the initial Hamiltonian H.

The unitary operator U^0 can be written as

$$U^0 = \sum_{i,j\leqslant N'} |a_i\rangle \tilde{U}^0_{ij}\langle a_j|. \tag{7}$$

$|a_i\rangle$ in Eq. (7) can be any $\mathcal{L}^2$ function, e. g., any oscillator function φ_l or any linear combination of oscillator functions φ_l. We shall use DET-PETs with the functions $|a_i\rangle$ defined as

$$|a_i\rangle = \sum_{l\leqslant N''} \alpha_i^l \varphi_l, \tag{8}$$

supposing that they fit the orthonormalization condition (2).

The transformation (5) becomes a DET-PET, i. e. it does not affect the deuteron wave function $|d\rangle$, when each of the functions $|a_i\rangle$ in Eq. (7) is orthogonal to $|d\rangle$:

$$\langle a_i|d\rangle = 0. \tag{9}$$

At this stage, we assert that we have obtained our DET-PET defined through the unitary transformation (5) with additional constraints (2), (7)–(9). 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 $\det U^0 = +1$ (we will use the index $^+$ to denote these transformations) or with a rotation by the angle β combined with reflection when $\det U^0 = -1$ (these type of transformations will be denoted by the index $^-$).

We need to specify not only the unitary matrix but also the vectors $|a_1\rangle$ and $|a_2\rangle$ to define completely the simplest DET-PET. We use the deuteron wave function $|d\rangle$ to construct these vectors.

The function $|d\rangle$ can be expanded in infinite series of oscillator functions φ_i,

$$|d\rangle = \sum_{i=0}^{\infty} d_i \varphi_i, \tag{10}$$

where, generally, all the coefficients d_i are non-zero,

$$d_i \neq 0. \tag{11}$$

Since the vectors $|a_1\rangle$ and $|a_2\rangle$ should fit Eq. (9), none of them can be one of the basis functions φ_i due to Eq. (10)-(11). The simplest way to construct the vectors $|a_1\rangle$ and $|a_2\rangle$ is to define each of them as a linear combination of two different oscillator functions φ_1 and φ_2,

$$|a_1\rangle = a_1^n\,\varphi_n + a_1^m\,\varphi_m, \tag{12}$$

$$|a_2\rangle = a_2^k\,\varphi_k + a_2^l\,\varphi_l, \tag{13}$$

The normalization of these vectors requires

$$(a_1^n)^2 + (a_1^m)^2 = 1, \tag{14}$$

$$\left(a_2^k\right)^2 + \left(a_2^l\right)^2 = 1. \tag{15}$$

Using Eqs. (9) and (10), we obtain

$$a_1^n\,d_n + a_1^m\,d_m = 0, \tag{16}$$

$$a_2^k\,d_k + a_2^l\,d_l = 0. \tag{17}$$

The solution of Eqs. (14) and (16) can be written as

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

$$a_1^m = -\frac{d_n}{\sqrt{d_n^2 + d_m^2}}; \tag{18b}$$

the same type solution of Eqs. (15) and (17) for the vector $|a_2\rangle$ is

$$a_2^k = +\frac{d_l}{\sqrt{d_k^2 + d_l^2}}, \tag{19a}$$

$$a_2^l = -\frac{d_k}{\sqrt{d_k^2 + d_l^2}}. \tag{19b}$$

We need to find all coefficients a_1^n, a_1^m, a_2^k, a_2^l fitting the orthogonality condition

$$\langle a_2|a_1\rangle = 0. \tag{20}$$

It means that all indexes k, l, m, n should be different, i. e., vectors $|a_1\rangle$ and $|a_2\rangle$ should be superpositions of different oscillator functions.

To define completely the simplest DET-PET, we need to fix the rotation angle β, the index $^{\pm}$ related to the sign of $\det U^0$, and the set of four oscillator functions used to build the vectors $|a_1\rangle$ and $|a_2\rangle$. To distinguish various DET-PET types we use notations like $0s2s1s2d^{\pm}$. In this example, the vector $|a_1\rangle$ 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 $\det U^0 = \pm 1$ respectively.

3 Results

We study modifications of JISP16 NN interaction induced by DET-PET. Vectors $|a_1\rangle$ and $|a_2\rangle$ [see Eqs. (12), (13)] are constructed as various superpositions of two low-lying oscillator functions $0s$, $1s$, $2s$, $3s$, $0d$ and $1d$. It is interesting to explore DET-PETs acting in the s channel only and compare them with DET-PETs mixing s and d channels in different ways. It is interesting also to investigate the transformations associated with both pure rotation and a rotation-reflection combination in case of each DET-PET type.

Plots of the np scattering wave functions in the sd coupled partial waves at laboratory energy $E_{lab} = 10$ MeV are presented in Figs. 1–3 in the K-matrix formalism. We use here the nomenclature and terminology adopted in Ref. [3]. The DET-PET $0s2s1s3s^{\pm}$ modifies significantly the large s wave component as is seen in Fig. 1. The modification of the small s wave component is much less pronounced. The d wave components, as expected, are nearly unaffected by $0s2s1s3s^{\pm}$. We observe modifications of both waves by DET-PETs $0s1s0d1d^{\pm}$ and $1s0d0s1d^{\pm}$ in Figs. 2 and 3, however, unlike the previous case, they are more pronounced in the small components of the scattering wave function since the DET-PETs mix s and d waves in these cases. We see that DET-PETs are able to generate essential modifications of scattering wave functions.

The NCSM calculations involve two basic parameters: the oscillator spacing $\hbar\Omega$ and model space dimension associated with the maximal excitation quanta N_{max}. It has been proposed [1] to use the $\hbar\Omega$ and N_{max} dependences to improve the results of calculations (the NCFC approach). Based on these dependences, we extrapolate the NCSM results to the infinite basis space limit and estimate the accuracy of the extrapolation. NCFC suggests two extrapolation methods: extrapolation A and extrapolation B [1]. The extrapolations A and B usually provide consistent results. We present here only the extrapolation A results based on the NCSM calculations with model spaces up through $N_{max} = 16$; we checked the consistency of our results with the ones obtained by extrapolation B in a number of cases. The evaluated 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 $N_{\max} = 18$ to obtain the binding energies with uncertainty of about 10 keV.

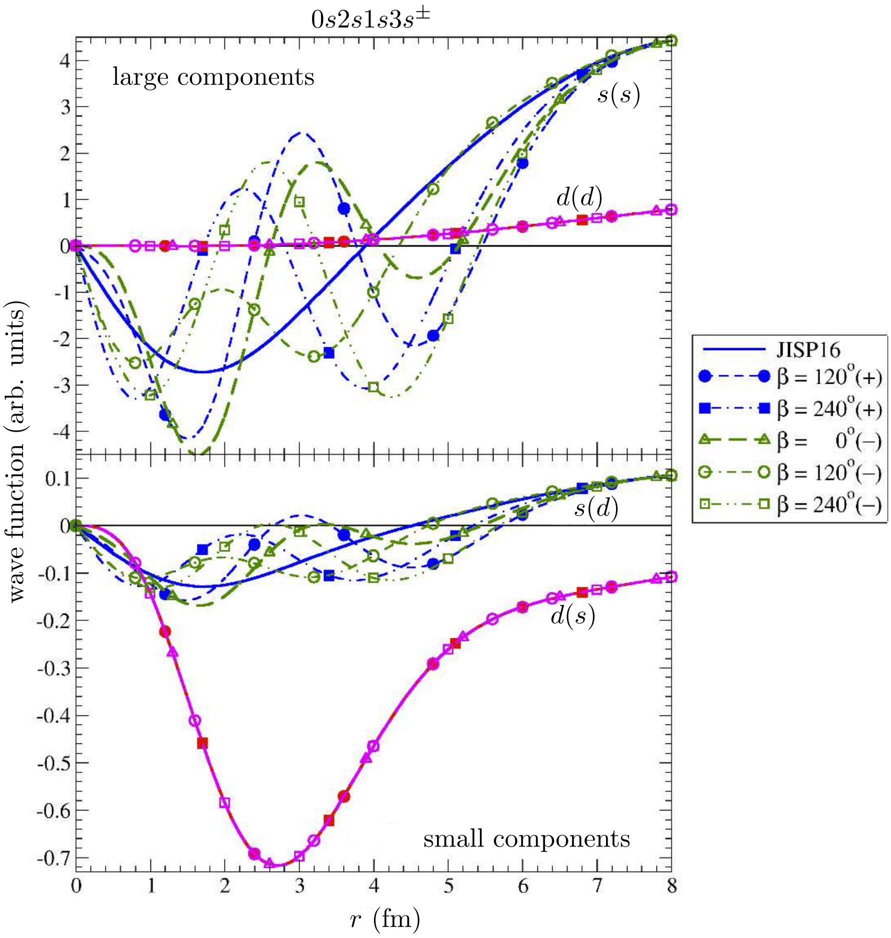

Figure 1: Large and small components of the np scattering wave function at the laboratory energy $E_{\text{lab}} = 10$ MeV in the sd coupled partial wave in the K-matrix formalism (see Ref. [3] for details and nomenclature) generated by JISP16 and NN interactions obtained from JISP16 by means of DET-PET $0s2s1s3s^{\pm}$. The sign of $\det U^0$ is given in the legends in parenthesis after the value of rotation angle β.

The binding energies of ^{3}H and ^{4}He nuclei were calculated with JISP16 NN interaction modified by DET-PETs $0s2s1s3s^{\pm}$, $0s1s0d1d^{\pm}$ and $1s0d0s1d^{\pm}$. The ranges of ^{3}H and ^{4}He binding energy variations for each DET-PET type are shown in Table 1. We see that the ^{4}He binding energy E_α can be varied by DET-PETs on the interval from 21.25 through 30.41 MeV, i. e., DET-PET can change E_α by more than 7 MeV

Table 1: Ranges of ^{3}H and ^{4}He 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	^{3}H	^{4}He
$0s2s1s3s^+$		$0s1s0d1d^+$		$1s0d0s1d^+$	
7.2–8.37	21.25–28.49	7.67–8.41	23.50–28.83	7.98–8.64	25.79–30.36
$0s2s1s3s^-$		$0s1s0d1d^-$		$1s0d0s1d^-$	
7.25–8.35	21.46–28.59	7.68–8.39	23.46–28.91	8.05–8.67	26.18–30.41
JISP16				Experiment	
8.369(1)	28.299(1)			8.482	28.296

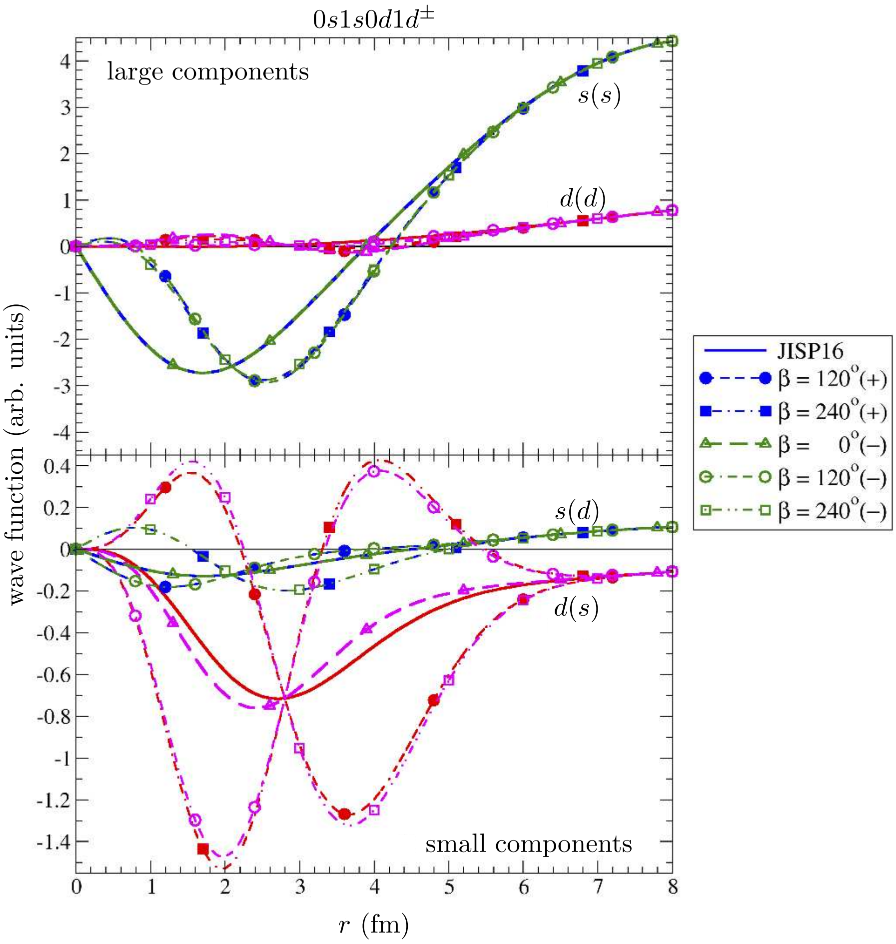

Figure 2: Same as Fig. 1 but for DET-PET $0s1s0d1d^{\pm}$.

from its original value provided by the original JISP16 interaction. In the case of ^{3}H the range of the DET-PET binding energy variation is $7.21 \leq E_t \leq 8.67$, i. e., the ^{3}H binding energy E_t can be shifted by DET-PET by 1 MeV from its original JISP16 value.

The Tjon line [18] is a correlation of the ^{3}H and ^{4}He binding energies which was usually studied using results obtained with various NN interaction models allowing for two-nucleon forces only or various combinations of NN and NNN interactions (see, e. g., Ref. [19]). Here we study the Tjon line using families of NN potentials generated by DET-PET with continuous parameter which generate the same deuteron wave function. Two types of Tjon lines are shown in the each of Figs. 4-6. For each of DET-PETs mixing a particular combination of partial wave components, one of the Tjon line types corresponds to the case of pure rotation while the other corresponds to the rotation-reflection transformation. The symbols at the curves present the results obtained with different values of the angle β in the range from 0° through 360°. We use the step 60° for smooth regions of the curves and 30° in some cases around extremums of the ^{3}H and ^{4}He binding energies which are found usually around 180° and 360°. In addition to our results, we present in the figure also the experimental value and results of Refs. [19, 20, 21], obtained with other potential models which involve either two-nucleon forces only or combinations of two-nucleon and three-nucleon interactions.

We begin the discussion of the Tjon lines from the results obtained with the $1s0d0s1d^{\pm}$. It is seen from the Fig. 4 that our results are concentrated close to the Tjon line connecting the points extracted from other interactions. We recall here

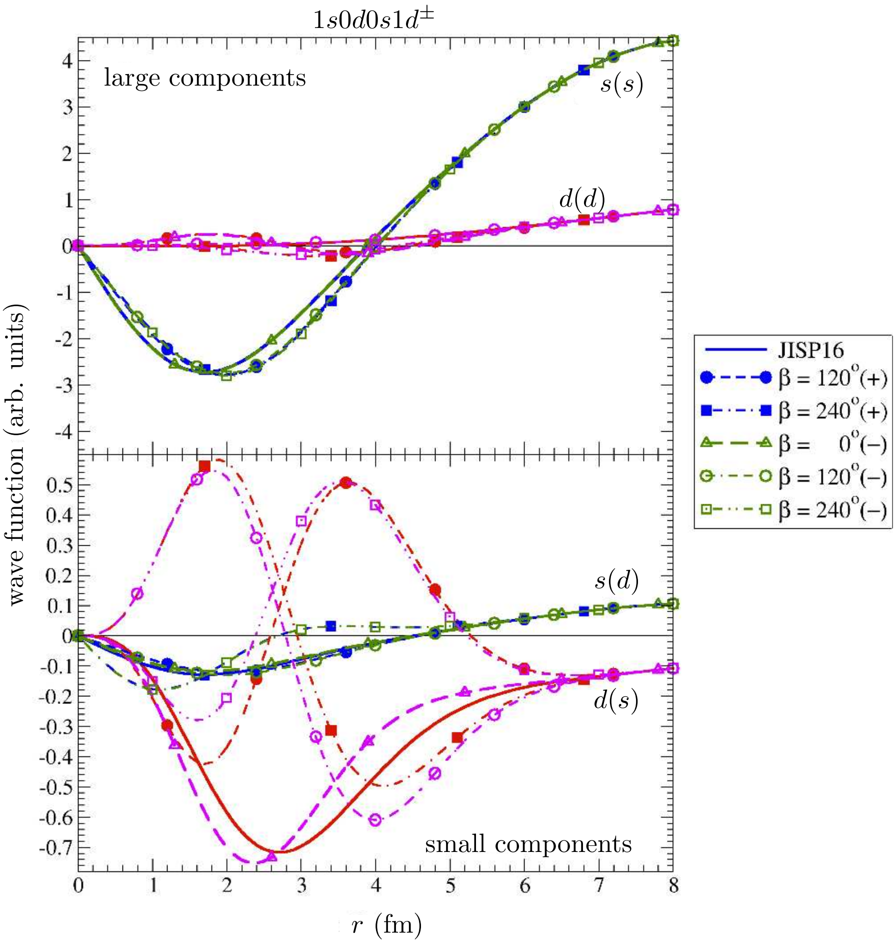

Figure 3: Same as Fig. 1 but for DET-PET $1s0d0s1d^{\pm}$.

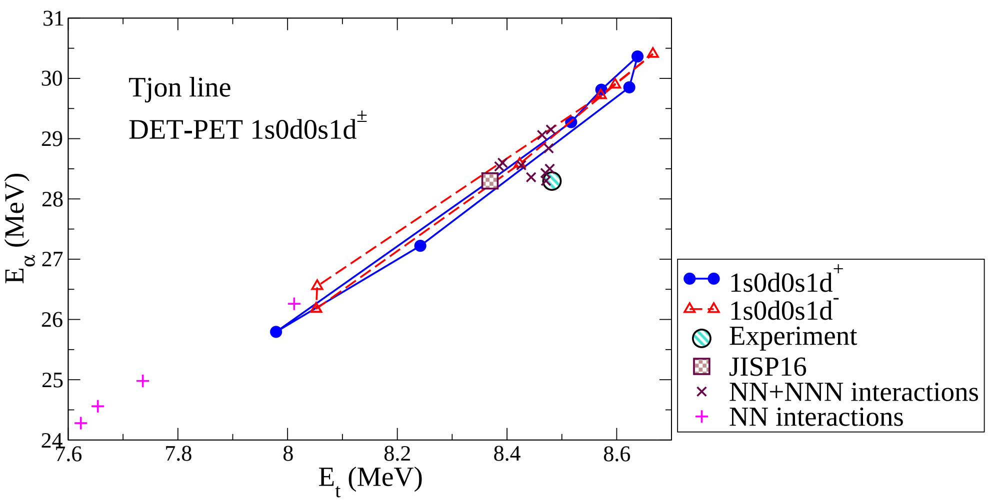

Figure 4: Tjon line obtained with DET-PET $1s0d0s1d^{\pm}$ in comparison with results obtained with various NN and $NN+NNN$ interaction models from Refs. [19, 20, 21].

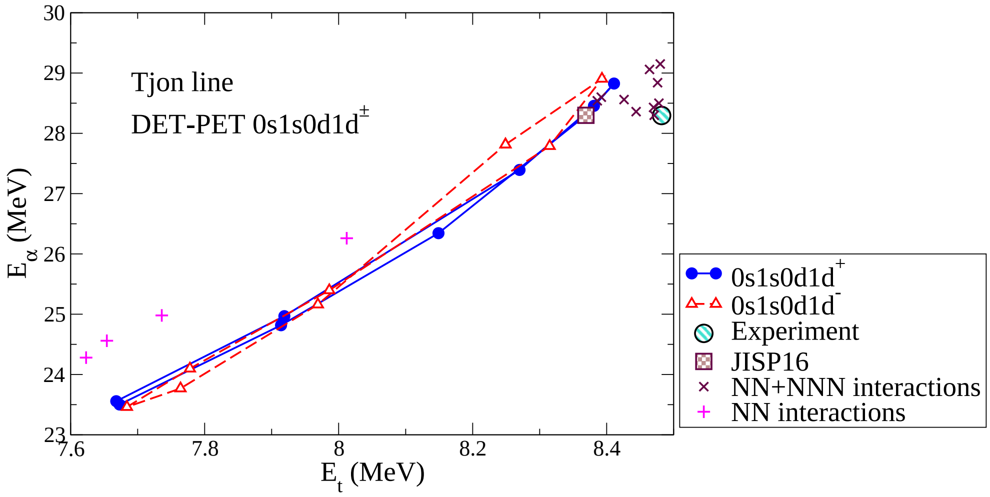

Figure 5: Same as Fig. 4 but for DET-PET $0s1s0d1d^{\pm}$.

that this DET-PET leave the large wave function components nearly unchanged while modifies essentially the small components as is seen from Fig. 3; such transformations correspond to strong modification of the tensor component of NN interaction.

Now we turn the discussion to the DET-PET $0s1s0d1d^{\pm}$. In this case, the DET-PET results in a very different range of binding energies variations (see the Table 1 and Fig. 5). The binding energies in this case are also correlated along a nearly straight line, however this line has a very different slope. As a result, our binding energy correlations around the maximal ^{3}H and ^{4}He binding energies accessible by this DET-PET are consistent with the correlations derived from other interaction models; however our correlations deviate from those obtained with other interactions as the binding energies decrease and the difference between our correlations and derived from other potential models become essential around the minimal binding energies. We have also a strong modification of the tensor component of the NN force in this case as seen in Fig. 2.

Let us discuss now the DET-PET $0s2s1s3s^{\pm}$. It results in the ^{3}H and ^{4}He binding energy correlation shown in Fig. 6. We see that in this case the Tjon lines transform

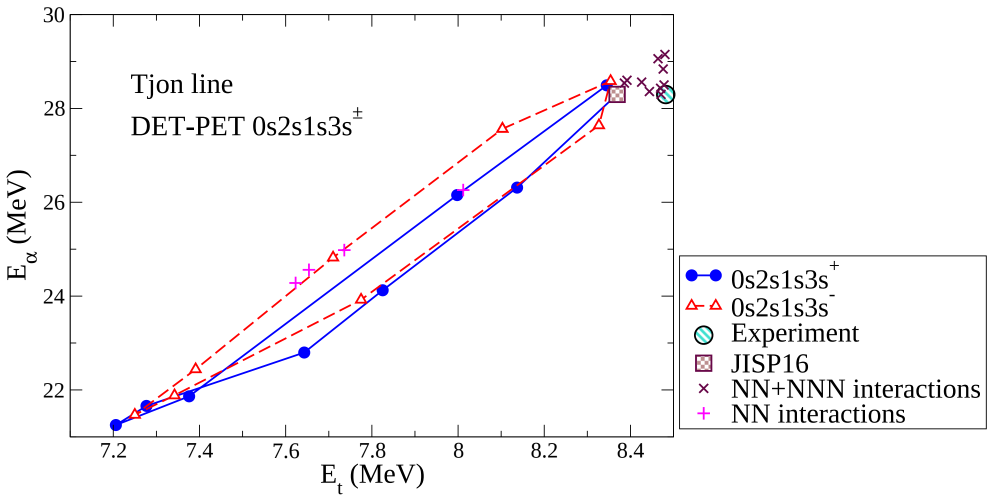

Figure 6: Same as Fig. 4 but for DET-PET $0s2s1s3s^{\pm}$.

into closed-loop curves surrounding large enough areas. In the case of the DET-PET $0s2s1s3s^-$ our Tjon curve surrounds the line derived from other NN interactions. The DET-PET $0s2s1s3s^+$ generates the Tjon curve shifted down from the Tjon line suggested by other interactions. This DET-PET $0s2s1s3s^\pm$ mixes only s-waves and does not affect the tensor component of the NN forces (see Fig. 1.)

4 Conclusions

We have introduced [14] a new type of phase-equivalent transformations, DET-PET, preserving the deuteron wave function and investigated transformations of the JISP16 NN interaction induced by few DET-PET versions mixing oscillator components in various combinations. We demonstrated that DET-PETs are able to modify significantly the np scattering wave functions. We studied DET-PET manifestations in the binding energies of ^{3}H and ^{4}He nuclei and found out that these bindings can be significantly changed by DET-PETs. We investigated also the correlation of these binding energies and found out that DET-PETs with some values of their parameters can significantly modify this correlation; more, in some cases, this correlation is washed out by DET-PET as compared with the conclusions based on the results obtained with other potential models. We speculate that DET-PET can be helpful in the further development of JISP-like NN interactions. It would be interesting to study DET-PET manifestations in binding energies and other observables of heavier nuclei.

Acknowledgements

This work was supported in part by the Ministry of Education and Science of the Russian Federation through the Contract 14.V37.21.1297 and by the Dynasty Foundation and Russian Foundation for Basic Research. This work was also supported in part by the US DOE Grants DESC0008485 (SciDAC-3/NUCLEI) and DE-FG02-87ER40371. AMS is also supported by the American Physical Society through the International Travel Grant Award Program. Calculations were performed on the supercomputers Hopper (NERSC) and Lomonosov (Moscow State University).

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