Phase-equivalent transformations of realistic NN interaction

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Abstract

Muti-channel local and non-local phase equivalent transformations continuous with the identity, are developed and applied to realistic Nijmegen II NN interactions. The effect of the transformations on deuteron observables is discussed. We also study the effect of the transformations on the ^{3}H and ^{4}He binding energies using, as an example, a semi-realistic Malfliet-Tjon NN interaction.Varying the transformation parameters improves the simultaneous description of trinucleon and four-nucleon systems.

1 Introduction

The most popular models of NN interaction are meson exchange potentials like Bonn [1], Paris [2], Argonne [3], Nijmegen [4], etc., conventionally referred to as "realistic NN potentials". Modern versions of realistic potentials and the Moscow NN potential [5] based on quark phenomenology, are carefully fitted to the existing experimental data on deuteron and NN scattering up to energies of $\sim$500 MeV or higher. Unfortunately, none of the known NN interactions provides a satisfactory description of the trinucleon and other light nuclei. To overcome this deficiency, several avenues would appear open. One may introduce (A) phenomenological three-body forces [6], or (B), excitations of the nucleons, or (C), phenomenological off-shell variations of the NN interaction. Indeed there is overlap and possible competition among these choices. Picklesimer *et al.* [7] have shown that the triton binding energy contribution from three-nucleon interactions originating in Δ excitations is canceled by dispersive effects in the two-body channel.

In this paper we examine option (C). We propose searching for new realistic NN potentials that will provide proper triton binding and also improve the description of light nuclei. For this purpose, we generate parameter-dependent families of NN potentials phase-equivalent to realistic NN interactions. In other words, the generated parameter-dependent potentials are equivalent on-shell to the known high-quality realistic NN potentials but have different off-shell properties. All of the potentials give off-shell variations that are continuous with the identity. Our general aim is to fit the potential parameter(s) to the properties of lightest nuclei.

Phase-equivalent potentials can be generated by means of local transformations well-known from inverse scattering theory [8]. However, these local transformations are designed for single-channel problems and cannot be used in the case of a realistic NN interaction with tensor forces. We generalize this transformation to the multi-channel case. Our generalization is based on ideas exploited in Ref. [9] where a multi-channel supersymmetry transformation was suggested. This supersymmetry transformation appears to be a particular case of our local transformation for a special choice of the transformation parameters. We use the multi-channel version of the local phase-equivalent transformation to obtain some examples of local potentials that are equivalent on-shell to the realistic Nijmegen II NN force.

In addition to phase-equivalent families of local potentials, we propose a generalization of the non-local phase-equivalent transformation suggested independently in Refs. [10] and [11] to the multi-channel case, and use it to generate parameter-dependent families of non-local phase-equivalent interactions. We find the non-local potentials to be more flexible and provide better prospects for the simultaneous description of several light nuclei.

To check the possibility of the simultaneous fitting of NN scattering data and deuteron, ^{3}H and ^{4}He binding energies, we performed microscopic ^{3}H and ^{4}He calculations in the framework of the no-core shell model [12, 13] with various phase-equivalent potential families. The families of potentials are generated by applying both local and non-local transformations to a semi-realistic Malfliet-Tjon IV NN interaction [14].

2 Multi-channel phase-equivalent transformations

2.1 Local transformation

Let us consider a multi-channel Schrödinger equation,

$$\sum_j \left(H_{ij} - E\delta_{ij}\right) \varphi_j(E,r) = 0, \tag{1}$$

where indexes i and j label the channels, and E is the energy. The Hamiltonian is

$$H_{ij} = \frac{\hbar^2}{2m}\left[-\frac{d^2}{dr^2} + \frac{l_i(l_i+1)}{r^2}\right]\delta_{ij} + V_{ij}(r), \tag{2}$$

where m is the reduced mass and l_i is the angular momentum in the channel i. We take the potential $V_{ij}(r)$ to be Hermitian and at large distances to approach a diagonal constant matrix,

$$V_{ij}(r) \underset{r\to\infty}{\longrightarrow} \epsilon_i\delta_{ij}, \tag{3}$$

where ϵ_i is a threshold energy in the channel i. We also assume that there is at least one bound state at energy E_0 with normalized wave function, $\varphi_j(E_0,r)$,

$$\sum_i \int\limits_0^\infty \varphi_i{}^*(E_0,s)\,\varphi_i(E_0,s)\,ds = 1. \tag{4}$$

We define the transformed potential

$$\tilde{V}_{ij}(r) = V_{ij}(r) + v_{ij}(r), \tag{5}$$

where

$$v_{ij}(r) = -2C\,\frac{\hbar^2}{2m}\,\frac{d}{dr}\left(\frac{\varphi_i(E_0,r)\varphi_j{}^*(E_0,r)}{1+C\,\sum_k\int_a^r |\varphi_k(E_0,s)|^2\,ds}\right), \tag{6}$$

with the real parameters C and a to be determined.

The new Hamiltonian $\tilde{H}_{ij}$ contains the transformed potential $\tilde{V}_{ij}(r)$ instead of $V_{ij}(r)$. It can be shown that the new wave function

$$\tilde{\varphi}_i(E,r) = \varphi_i(E,r) - C\varphi_i(E_0,r)\frac{\sum_k\int_a^r \varphi_k{}^*(E_0,s)\varphi_k(E,s)\,ds.}{1+C\,\sum_k\int_a^r |\varphi_k(E_0,s)|^2\,ds}, \tag{7}$$

satisfies the homogeneous Schrödinger equation,

$$\sum_j \left(\tilde{H}_{ij} - E\delta_{ij}\right)\tilde{\varphi}_j(E,r) = 0, \tag{8}$$

if $a = 0$ or $a = \infty$ (in the case of arbitrary a, the function (7) satisfies an *inhomogeneous* multi-channel Schrödinger equation).

The case $a = 0$ is a generalization of the single-channel phase-equivalent transformation of Ref. [8] to the multi-channel case. It is clear from Eq. (7) that the new and old wave functions are phase-equivalent. Since the new wave function should be continuous for all r, the parameter C is restricted to values greater than -1. The normalized transformed bound state wave function can be easily obtained with the help of Eq. (7):

$$\sqrt{1+C}\,\tilde{\varphi}_i(E_0,r) = \frac{\sqrt{1+C}\,\varphi_i(E_0,r)}{1+C\,\sum_j\int_0^r |\varphi_j(E_0,s)|^2\,ds}, \tag{9}$$

where the factor $\sqrt{1+C}$ is necessary for the normalization of the new wave function.

The case $a = \infty$ is identical to the case $a = 0$ with redefinition of the parameter $C \to C/(1-C)$. The normalized bound state wave function for the case $a = \infty$ is

$$\sqrt{1-C}\;\tilde{\varphi}_i(E_0,r) = \frac{\sqrt{1-C}\;\varphi_i(E_0,r)}{1-C+C\;\sum_j \int_0^r |\varphi_j(E_0,s)|^2\,ds}. \tag{10}$$

The particular choice of parameters $C = 1$ and $a = \infty$ corresponds to the supersymmetry transformation proposed in Ref. [9]. Indeed, the denominator in Eq. (10) is seen to be zero at the point $r = 0$. Hence the bound state wave function $\tilde{\varphi}_i(E_0,r)$ does not match the boundary condition at the origin. Note also that in Eq. (10) the normalization factor $\sqrt{1-C} \to 0$ as $C \to 1$. As a result, the phase-equivalent transformation removes the bound state at $E = E_0$. At the same time, for all energies $E \neq E_0$ the zero in the denominator in Eq. (7) at $r = 0$ is canceled by the zero in the numerator and the wave function matches the boundary condition at the origin. So, in this case, the transformation removes the bound state at $E = E_0$ and only this bound state. Since the transformation leaves the S-matrix unchanged, it is a supersymmetry transformation.

If the initial Hamiltonian H_{ij} does not have a bound state at the energy $E = E_0 < 0$, one can make use of the function $\varphi_i(E_0,r)$ that satisfies Eq.(8) and is regular at infinity but irregular at the origin. Equations (5)–(7) with $a = \infty$ and the function $\varphi_i(E_0,r)$ irregular at the origin, define (i) a phase-equivalent transformation that can be applied to a system that does not support a bound state if $L \equiv \max\{l_i\} < 2$ and (ii) an inverse supersymmetry transformation (i. e. the transformation that adds a bound state at the energy $E = E_0$ and does not affect the S-matrix and the energies of bound states at energies $E \neq E_0$) if $L \geq 2$. Therefore, one can construct phase-equivalent single- or multi-channel potentials even in a system without a bound state. If $l_i \leq 1$ for all the channel angular momenta , one can directly apply the transformation with the function $\varphi_i(E_0,r)$ irregular at the origin. If at least one of the channel angular momenta $l_i \geq 2$, one can produce a bound state by means of the inverse supersymmetry, use this bound state for constructing a family of phase-equivalent potentials, and then remove the bound state by the supersymmetry transformation at the last stage.

2.2 Non-local transformation

In order to construct the non-local transformation, we introduce a complete basis of L^2 functions $\{\phi^i_n(r)\}$, $n = 0, 1, 2, \ldots$, in the space of channels labelled by the index i. For the wave function $\varphi(E,r)$ we use the expansion

$$\varphi(E,r) = \sum_i \sum_{n_i=0}^{\infty} a^i_{n_i}(E)\;\phi^i_{n_i}(r)\,. \tag{11}$$

Solutions of the Schrödinger equation can be found by diagonalization of the infinite Hamiltonian matrix $[H]$ with matrix elements $\langle \phi^{i'}_{n'}|H|\phi^i_n\rangle$.

We define the non-local phase-equivalent transformation through a unitary transformation U with matrix $[U]$ which is a direct sum of a finite $N \times N$ matrix $[U_0]$ and an infinite unit matrix $[I]$,

$$[U] = \left(\begin{array}{c|c} [U_0] & 0 \\ \hline 0 & [I] \end{array}\right). \tag{12}$$

We apply this unitary transformation to the Hamiltonian H and define the transformed Hamiltonian $\widetilde{H}$ through its (infinite) matrix $[\widetilde{H}]$ with matrix elements $\langle \phi^{i'}_{n'}|\widetilde{H}|\phi^i_n\rangle$ that can be found from

$$[\widetilde{H}] = [U]\,[H]\,[U^+]\,. \tag{13}$$

Note, that we define the Hamiltonian $\widetilde{H}$ through its matrix $\langle \phi^{i'}_{n'}|\widetilde{H}|\phi^i_n\rangle$ *on the original basis* $\{\phi^i_n(r)\}$ and *not on the basis* $\{\widetilde{\phi^i_n}(r)\}$ obtained by applying the unitary transformation U to the basis $\{\phi^i_n(r)\}$. Thus, the Hamiltonians H and $\widetilde{H}$ are not identical. Since the matrix of H on the basis $\{\widetilde{\phi^i_n}(r)\}$ is identical to the matrix of $\widetilde{H}$ on the basis $\{\phi^i_n(r)\}$ the eigenvalue spectra of H and $\widetilde{H}$ are the same. Due to the special form of the unitary matrix $[U]$ given in (12), only the first N terms in the expansion (11) of the function $\varphi(E,r)$ differ from the first N terms in the corresponding expansion of the transformed function $\widetilde{\varphi}(E,r)$. In other words, the functions $\varphi(E,r)$ and $\widetilde{\varphi}(E,r)$ differ only by a superposition of a finite number of L^2 terms:

$$\widetilde{\varphi}(E,r) = \varphi(E,r) \ + \ \Delta\varphi(E,r) \ , \tag{14}$$

where

$$\Delta\varphi(E,r) = \sum_i \sum_{n_i} \Delta a^i_{n_i}(E)\phi^i_{n_i}(r) \ . \tag{15}$$

As $\Delta\varphi(E,r)$ is an L^2 function, it does not contribute to the asymptotics of $\widetilde{\varphi}(E,r)$ at any energy $E > 0$. Hence the Hamiltonians $\widetilde{H}$ and H are phase-equivalent.

The non-local potentials $\widetilde{V}$, phase-equivalent to the initial potential V, can be expressed as

$$\widetilde{V} = V + \Delta V, \tag{16}$$

where

$$\Delta V = U\,H\,U^{+} - H. \tag{17}$$

The simplest unitary transformation of the type (12) is a rotation-like transformation $U(\theta)$ with diagonal matrix elements $\left\langle \phi^{i_1}_{n_1} \,|\, U(\theta) \,|\, \phi^{i_1}_{n_1} \right\rangle = \left\langle \phi^{i_2}_{n_2} \,|\, U(\theta) \,|\, \phi^{i_2}_{n_2} \right\rangle = \cos\theta$ while all the rest of the diagonal matrix elements $\left\langle \phi^{i}_{n} \,|\, U(\theta) \,|\, \phi^{i}_{n} \right\rangle = 1$, and the only non-zero off-diagonal matrix elements are $\left\langle \phi^{i_1}_{n_1} \,|U(\theta)|\, \phi^{i_2}_{n_2} \right\rangle = -\left\langle \phi^{i_2}_{n_2} \,|\, U(\theta) \,|\, \phi^{i_1}_{n_1} \right\rangle = \sin\theta$. The "angle" θ is the only continuous parameter of the transformation. Other important parameters are channel indexes i_1 and i_2 and the additional labels n_1 and n_2 of the basis functions $\{\phi^i_n(r)\}$ that are mixed by the transformation. Generally speaking, parameters of the basis $\{\phi^i_n(r)\}$ can be also treated as transformation parameters. More complicated non-local transformations with two or more continuous parameters may be obtained, for example, by taking the product of two or more transformations of the type $U(\theta)$.

3 Numerical results and discussion

First we discuss the effect of the local and non-local transformations on the deuteron wave functions. We construct the families of local and non-local potentials phase-equivalent to the realistic non-relativistic NN potential Nijmegen-II [4].

The Nijmegen -II deuteron wave function with total angular momentum $J = 1$, total spin $S = 1$, is represented by its s ($L = 0$) and d ($L = 2$) components shown in Fig. 1 by solid curves. Other curves

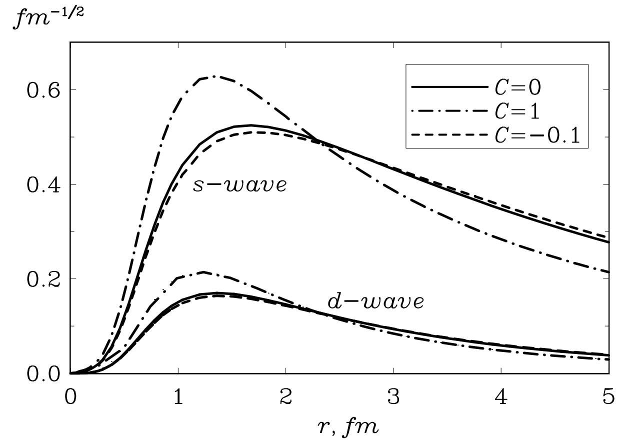

Figure 1: Radial s and d-wave functions of the deuteron for Nijmegen-II (solid curves) and deuteron wave functions arising from local phase-equivalent transformations.

illustrate the effect of the local phase-equivalent transformation with $a = 0$ and a few values of the parameter C. Note that while arbitrarily small changes in the wave functions are feasible, we illustrate large, even unphysical changes here. It is seen from Fig. 1 that the deuteron wave function shifts closer to

Table 1: The variation of the deuteron r.m.s. radius and the contribution of the d component to the deuteron wave function with variation of the parameters of the local and non-local phase-equivalent transformations.

The local transformation			The non-local transformation		
C	*r.m.s.* radius, fm	d state probability, %	θ	*r.m.s.* radius, fm	d state probability, %
-0.8	3.118973	2.896223	-120	1.9415	8.2577
-0.4	2.296052	4.675416	-60	1.9663	21.5352
0.0	1.966778	5.635342	0	1.9669	5.6515
0.4	1.769827	6.280881	60	1.9639	8.2577
0.8	1.633186	6.758014	120	1.9568	21.5352
1.0	1.578558	6.954836	180	1.9350	5.6515

the origin for positive values of C. As a result, the deuteron r.m.s. radius becomes smaller (see Table 1). For $C < 0$ the deuteron r.m.s. radius increases.

As is seen from Eq. (9), both the s and d components of the deuteron wave function are multiplied by the same factor $\sqrt{(1+C)}\left(1 + C\ \sum_j \int_0^r |\varphi_j(E_0,s)|^2\,ds\right)^{-1}$. Nevertheless the relative weight of the components $\varphi_i(E_0,r)$ is changed by the transformation (see Table 1).

The local phase-equivalent transformation guarantees that the deuteron binding energy remains unchanged for any value of the parameter C. However the specific transformations illustrated spoil other observables, for example, the deuteron r.m.s.radius. Hence an appropriate NN potential can be obtained only if the transformation applied to the coupled s and d partial waves has small values of C so that the modifications of the observables are also small and within experimental errors. There are no such restrictions on the parameter C in the case of other coupled and uncoupled partial waves where the NN system does not have a bound state.

The effect of the non-local phase-equivalent transformation $U(\theta)$ (see Section 2.2) is illustrated by Fig. 2. We define this transformation on the basis of oscillator functions $\{\phi_n^i(r)\}$ with the oscillator parameter $\hbar\omega = 300$ MeV. The transformation mixes the lowest oscillator components of triplet s and d coupled partial waves. Because of the large value of $\hbar\omega$, the short distance part of the full wave function is primarily affected.

It is seen from Fig. 2 that the deuteron wave function may be drastically modified by the non-local phase-equivalent transformation. For example, in some cases s or d component (or both) attains a node at short distances. At first glance this may seem surprising since realistic local potentials provide nodeless deuteron wave functions. However, the nonlocality we introduce via the transformation allows the physical possibility of ground state wave functions with nodes[15]. As another example, we remind

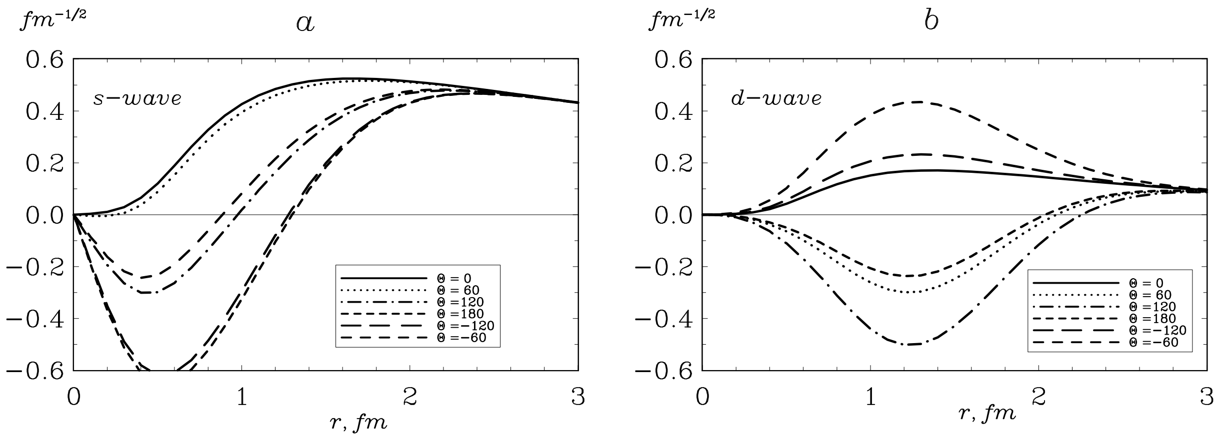

Figure 2: The effect of the non-local phase-equivalent transformation on the deuteron wave function.

the reader of the Moscow potential, a deep attractive potential supporting a low-lying forbidden state, which gives a node to the deuteron wave function at a short distance.

The θ-dependencies of the deuteron r.m.s. radius and of the d state probability for the non-local transformation, are given in the Table 1. It is seen that the variation of the r.m.s. radius is small even for large values of the transformation parameter θ. The variation of the d state probability is very large, however. Note that if the transformation is defined in such a way that it involves only the s wave or only the d wave component of the wave function, it does not affect the d state probability at all. Hence it is possible to have non-local transformations which produce very large short range modifications of the wave function but result in only small modifications of the deuteron observables. A more thorough investigation of these observables (quadrupole moment, form factors, etc.) are motivated by our present work since we argue that such transformations appear to offer good prospects of finding realistic NN interactions consistent with the light nuclei data.

Now we discuss the effect of the local and non-local transformations on the properties of three and four nucleon systems. We use a semi-realistic Malfliet-Tjon IV (MT) NN interaction [14] and neglect the Coulomb interaction. The MT potential is purely central and is known to overbind ^{3}H and ^{4}He. The ^{3}H and ^{4}He ground state energies obtained in no-core shell model calculations with the oscillator parameter $\hbar\omega = 44$ MeV are presented in Fig. 3 and Fig. 4. The calculations were performed in a complete $N\hbar\omega$ model space with the total number of oscillator quanta $N = 10$. To illustrate the convergence of the calculations with no-core model space size, we also present the results obtained with $N = 12$ in the case of ^{3}H and $N = 8$ in the case of ^{4}He. For the case of the local transformation, only the np interaction was modified. The interaction in the nn and pp subsystems does not have a bound state and so was left unchanged. In the case of the non-local transformation, the same transformation $U(\theta)$ mixing the two lowest s wave oscillator components, was applied to np, pp and nn interactions.

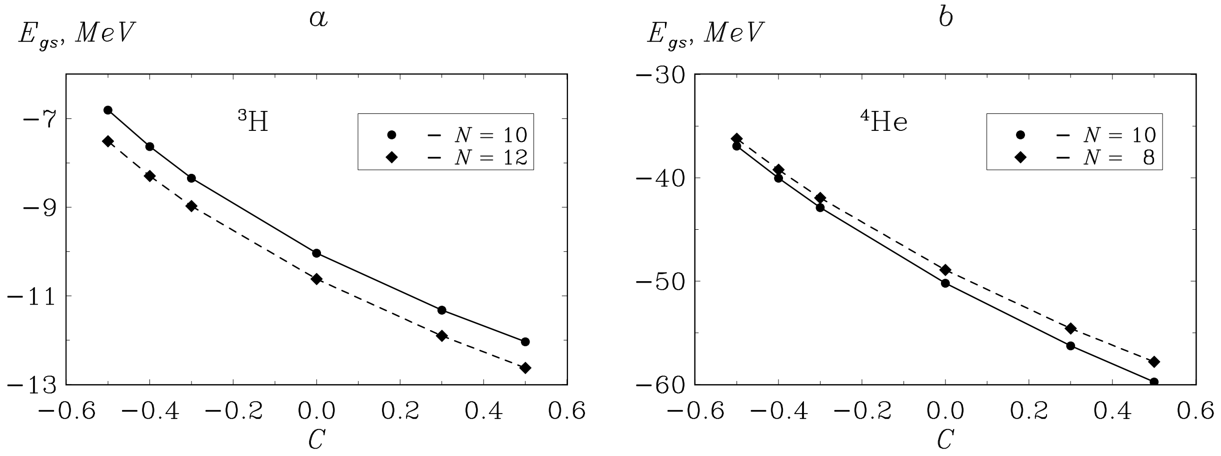

Figure 3: The C-dependences of the ^{3}H (a) and ^{4}He (b) ground state energies in the case of the local phase-equivalent transformation of the MT NN potential.

It is seen that even small modifications of the NN interaction result in significant changes of the binding energies of light nuclei. For example, the local transformation with $C = -0.3$ results in the 1.7 MeV decrease of the ^{3}H binding energy and in the 7.4 MeV decrease of the ^{4}He binding energy. The effect of the non-local transformation is even more impressive: the transformation with $\theta = 0.05$, which is expected to produce small variations of the deuteron observables, causes a decrease in the ^{3}H binding of 1.8 MeV and a decrease in the ^{4}He binding of 10.5 MeV.

These results are very encouraging since the modifications of the binding energies are much more than the discrepancies between the experimental values and the theoretical results obtained with realistic potentials. It thus seems promising that, by means of the phase-equivalent transformations of realistic NN interactions, we will be able to find an interaction accurately describing NN scattering and the properties of the deuteron and ^{3}H simultaneously. It is also encouraging that when the phase-equivalent transformations improve the description of the ^{3}H binding, the description of the ^{4}He binding is also

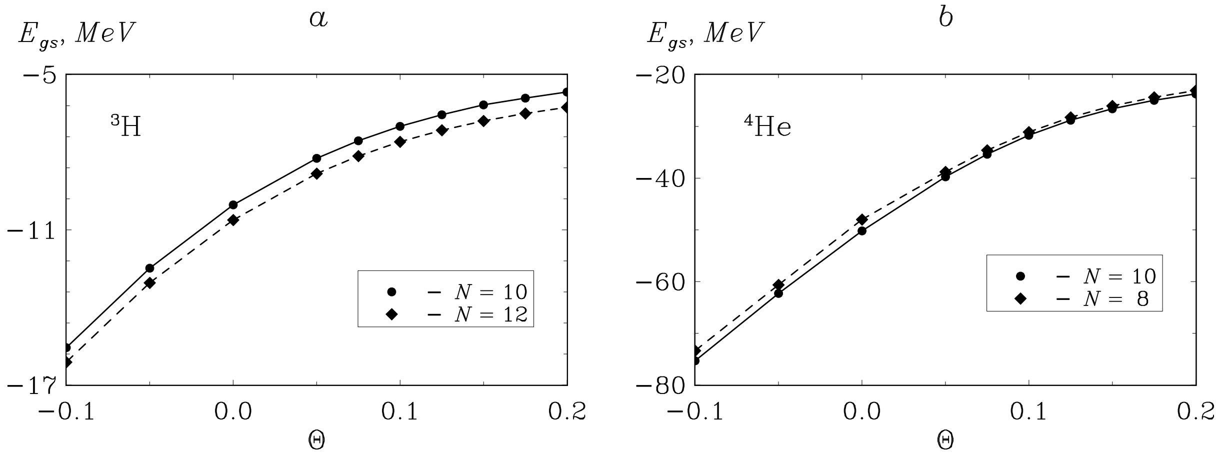

Figure 4: The θ-dependences of the ^{3}H (a) and ^{4}He (b) ground state energies in the case of the non-local phase-equivalent transformation of the MT NN potential.

improved. Because of this, we expect to find an interaction that will improve the theoretical description of light nuclei. The non-local transformation appears to be more promising for this endeavor.

This work was supported in part by Competitive Center on Fundamental Science at St. Petersburg State University, by the State Program "Russian Universities" and by the US Department of Energy, Grant No. DE-FG02-87ER40371. One of the authors (A.M.S.) is thankful for the support by the International Institute of Theoretical and Applied Physics of his stay in Iowa State University and for the hospitality of his colleagues from Iowa where a part of this work was done.

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