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Short-Range and Tensor Correlations in Light Nuclei Studied with Antisymmetrized Molecular Dynamics

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We developed a new variational framework of "tensor–optimized antisymmetrized molecular dynamics" (TOAMD) for finite nuclei. In TOAMD, we multiply the correlation functions of the short-range repulsion and tensor force to the AMD basis state in the power series expansion. Each correlation function in every term is independently treated in the energy minimization. The total energy and the Hamiltonian components in TOAMD nicely reproduce the results in the few-body calculations for *s*-shell nuclei. The total energies in TOAMD are also shown to be lower than the values of the variational Monte Carlo using the Jastrow's product-type correlation functions. This indicates that the power series expansion using the independent correlation functions in TOAMD describes the nuclei better than the Jastrow approach.

KEYWORDS: nuclear force, short-range correlation, tensor correlation, antisymmetrized molecular dynamics

1. Introduction

Nucleon-nucleon (*NN*) interaction has a strong short-range repulsion and a strong tensor force [1]. Recently, we have developed a new variational approach to treat the characteristics of *NN* interaction in nuclei [2–10]. We use the antisymmetrized molecular dynamics (AMD) for nuclear wave function and adopt two kinds of two-body correlation functions with the central- and tensor-operator types. These correlation functions are multiplied to the AMD wave function in the power series form, in which the power of the multiple products of the correlation functions can be increased successively. We call this method "tensor–optimized antisymmetrized molecular dynamics" (TOAMD).

We show the results of TOAMD for *s*-shell nuclei using the *NN* interaction within the double products of the correlation functions. It is shown that TOAMD nicely reproduces the results of few-body calculations. The TOAMD wave function has a power series form of the correlation functions, where each correlation function is independently optimized in the energy minimization. This property is different from the variational method using the Jastrow ansatz, where the common correlation function is multiplied for every pair in nuclei. We discuss the merit of the independent correlation functions in TOAMD in comparison with the Jastrow method.

2. Tensor–optimized antisymmetrized molecular dynamics (TOAMD)

We explain TOAMD [2, 6]. The basis wave function of AMD, $\Phi_{\rm AMD}$, is given as a Slater determinant of the Gaussian wave packets for A-nucleon system:

$$\Phi_{\rm AMD} = \frac{1}{\sqrt{A!}}\det\left\{\prod_{i=1}^{A}\phi_i\right\}, \qquad \phi(\boldsymbol{r}) = \left(\frac{2\nu}{\pi}\right)^{3/4} e^{-\nu(\boldsymbol{r}-\boldsymbol{D})^2}\chi_\sigma\chi_\tau. \tag{1}$$

The nucleon wave function $\phi(\boldsymbol{r})$ is a Gaussian having a range parameter ν, centroid $\boldsymbol{D}$. The spin part χ_σ is the up or down component, and the isospin part χ_τ is a proton or a neutron.

We adopt two kinds of two-body correlation functions; F_S for short-range repulsion and F_D for tensor force with D-wave transition. The form of each correlation function is given as

$$F_S = \sum_{t=0}^{1}\sum_{s=0}^{1}\sum_{i<j}^{A} f_S^{t,s}(r_{ij})\,(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)^t\,(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)^s, \quad F_D = \sum_{t=0}^{1}\sum_{i<j}^{A} f_D^t(r_{ij})\,r_{ij}^2\,S_{12}(\hat{\boldsymbol{r}}_{ij})\,(\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j)^t, \tag{2}$$

with a relative coordinate $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$ and the tensor operator $S_{12}(\hat{\boldsymbol{r}})$. The spin-isospin dependence is described with s and t for two nucleons. The pair functions $f_S^{t,s}(r)$ and $f_D^t(r)$ are determined variationally and can excite two nucleons to the high-momentum state. These correlation functions are multiplied to the AMD wave function $\Phi_{\rm AMD}$. We take the power series expansion using F_S and F_D and currently consider up to the double products of the correlation functions in TOAMD as

$$\Phi_{\rm TOAMD} = (1 + F_S + F_D + F_SF_S + F_SF_D + F_DF_S + F_DF_D)\times\Phi_{\rm AMD}\,. \tag{3}$$

In Eq. (3), there are five kinds of F_S and F_D, which are independently determined in the total-energy minimization, where we briefly express the common symbols F_S and F_D.

The total energy E in TOAMD is calculated based on the AMD wave function as

$$E = \frac{\langle\Phi_{\rm TOAMD}|H|\Phi_{\rm TOAMD}\rangle}{\langle\Phi_{\rm TOAMD}|\Phi_{\rm TOAMD}\rangle} = \frac{\langle\Phi_{\rm AMD}|\tilde{H}|\Phi_{\rm AMD}\rangle}{\langle\Phi_{\rm AMD}|\tilde{N}|\Phi_{\rm AMD}\rangle}\,. \tag{4}$$

The operators $\tilde{H}$ and $\tilde{N}$ in the last equation indicate the correlated Hamiltonian and norm, respectively. The correlated operators include the products of the correlation functions such as $F^\dagger HF$, where F represents F_S and F_D. These operators are classified into many-body operators using the cluster expansion [2, 6], and we treat all of them in TOAMD from the variational viewpoint. The forms of the pair functions $f_S^{t,s}(r)$ and $f_D^t(r)$ in Eq. (2) are expanded with the Gaussian functions as

$$f_S^{t,s}(r) = \sum_{n=1}^{N_G} C_n^{t,s} e^{-a_n^{t,s}r^2}, \qquad f_D^t(r) = \sum_{n=1}^{N_G} C_n^t e^{-a_n^t r^2}. \tag{5}$$

The Gaussian number N_G is taken to be seven after confirming the energy convergence. We determine the values of $a_n^{t,s}$ and a_n^t in a wide range to cover the radial correlation [6]. The expansion coefficients $C_n^{t,s}$ and C_n^t are obtained in the diagonalization of the Hamiltonian matrix.

3. Results

We use the AV8′ bare NN potential [1, 11] and discuss the results of s-shell nuclei in TOAMD. In the AMD part, the range parameters ν are optimized as 0.095 fm^{-2} for ^{3}H and 0.22 fm^{-2} for ^{4}He. We obtain $\boldsymbol{D}_i = \boldsymbol{0}$ variationally as an s-wave state in two nuclei [3, 6].

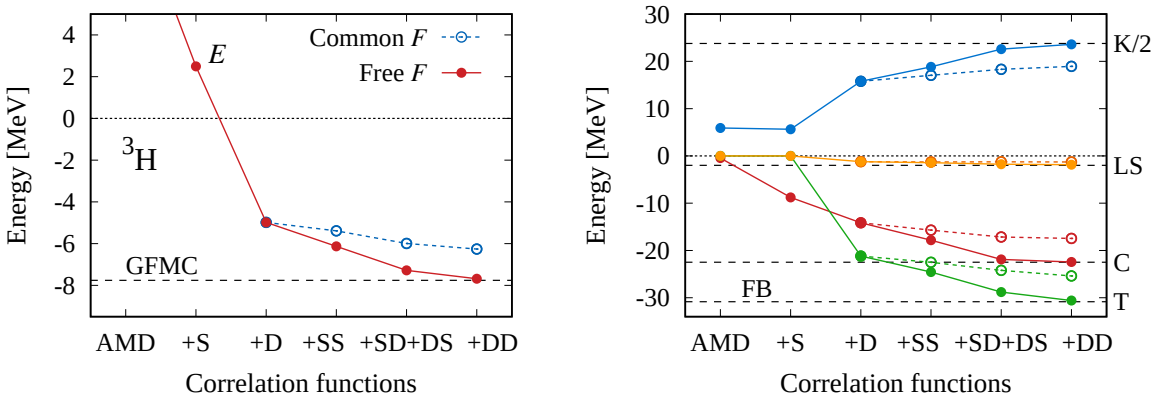

Fig. 1. Left: Convergence of total energy E of ^{3}H with the AV8′ potential in TOAMD by adding terms successively. Right: Hamiltonian components of ^{3}H. A half-value is shown for the kinetic energy using the symbol of K/2. The other symbols C, T, and LS indicate the central, tensor, and LS forces, respectively. In two figures, solid (open) circles show the results with the fully-optimized (common) correlation functions. Horizontal dashed lines are the results of other methods.

In Table I, we list the results of TOAMD by successively adding the correlation functions. We use the simple labels S for F_S and D for F_D. The symbol +S indicates the result with the wave function of $(1 + F_S) \times \Phi_{\rm AMD}$. The symbol +DD is the full calculation of TOAMD with the wave function in Eq. (3). It is found that the energies of ^{3}H and ^{4}He are converged to the values of Green's function Monte Carlo (GFMC) [1]. This behavior is clearly confirmed in Figs. 1 and 2. The matter radius in TOAMD is 1.75 fm for ^{3}H and 1.50 fm for ^{4}He.

In Fig. 1, we show the total energy and the Hamiltonian components of ^{3}H using the solid circles. We obtain a good agreement between TOAMD and other methods for the individual components [1, 12]. We discuss the contributions of the kinetic energy, central, tensor, and LS forces. The contributions from the tensor and LS forces appear after the addition of the tensor correlation F_D as "+D" giving the D-state component in nuclei. Kinetic energy largely increases with the tensor correlation owing to the high-momentum component of the D-state. It is confirmed that a nice convergence of each Hamiltonian component to the values of few-body (FB) calculations [12].

We discuss ^{4}He in Fig. 2. The solid circles indicate the total energy and Hamiltonian components in TOAMD and the behavior is similar to that of ^{3}H. The total energy and each Hamiltonian component show good convergence with successive addition of the correlation terms.

In TOAMD, we can optimize the correlation functions F_S and F_D independently in each term of Eq. (3). This is different from the Jastrow method, in which the correlation function with a common form is multiplied for all pairs in nuclei. It is meaningful to investigate the effect of the independent correlation functions in TOAMD. For this aim, we perform the calculations of TOAMD in the following condition: First, we calculate the nuclei in the wave function of $(1 + F_S + F_D) \times \Phi_{\rm AMD}$ and determine F_S and F_D. Second, keeping F_S and F_D, we calculate the nuclei again with all correlation terms in Eq. (3), where the weights of each correlation term are parameters. In Figs. 1 and 2, the

Table I. Energies of ^{3}H ($\frac{1}{2}^+$) and ^{4}He (0^+) using the AV8′ NN potential by adding each term of TOAMD successively. The units are in MeV.

	AMD	+S	+D	+SS	+SD+DS	+DD	GFMC [1]
^{3}H	11.37	2.58	−4.98	−6.12	−7.27	−7.68	−7.76
^{4}He	56.42	7.90	−14.74	−18.13	−22.44	−24.74	−25.93

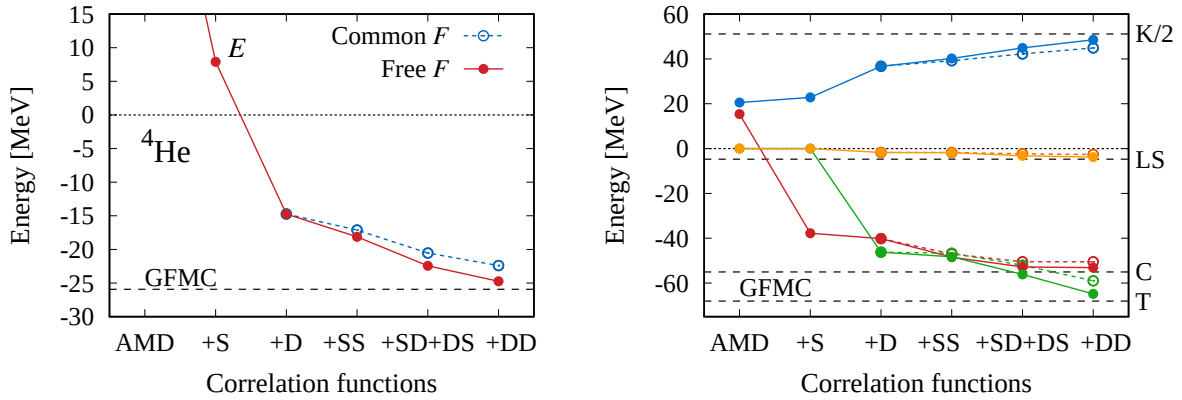

Fig. 2. Results of ^{4}He with the AV8′ potential. Notations are the same as used in Fig. 1.

open circles indicate the results with the above constrained calculations for ^{3}He and ^{4}He, which is named "Common F". We can confirm the energy difference from the original calculation as "Free F". In this condition, the total energies of ^{3}H and ^{4}He are obtained as −6.26 MeV and −22.40 MeV, respectively, which leads to the energy losses from the full calculations of 1.44 MeV for ^{3}H and 2.34 MeV for ^{4}He. These energy differences show the importance of the independent determination of the correlation functions in TOAMD, contributing to the good energy convergence. In Figs. 1 and 2, the Hamiltonian components of "Common F" show smaller values in magnitude than the values of the full calculations.

We compare the results of TOAMD with those of the variational Monte Carlo (VMC) calculation based on the Jastrow approach [13]. We use the AV6 bare NN potential consisting of the central and tensor forces for ^{3}H and ^{4}He. The range parameters ν of $\Phi_{\rm AMD}$ are optimized as 0.11 fm^{-2} for ^{3}H and 0.22 fm^{-2} for ^{4}He, respectively in TOAMD. In Table II, we show the energies and radii for two nuclei in TOAMD in comparison with other methods including VMC. It is found that the energies of ^{3}H and ^{4}He in TOAMD are nicely converged to the values of few-body calculations. It is noted that the energies in TOAMD are lower than those in VMC. This indicates that variational accuracy of TOAMD is better than the VMC case.

We further provide the results of TOAMD with the AV6 potential using the common correlation functions for two nuclei in a similar manner to the "Common F" condition for AV8′. This condition gives the total energy of ^{3}H with −6.04 MeV, close to the VMC value of−6.33 MeV. For ^{4}He, the calculation gives the total energy of −22.29 MeV, which is also close to the VMC value of −22.75 MeV. From the results, it is confirmed that description of the NN correlations in TOAMD is better than VMC based on the Jastrow concept. In TOAMD, the correlation functions in the power series expansion are favored to be different from each other. In Table II, we also see the energy difference between the TOAMD and few-body results. In order to reduce this difference, we can extend TOAMD

Table II. Energies of ^{3}H ($\frac{1}{2}^+$) and ^{4}He (0^+) with the AV6 potential in comparison with other methods. The units of energy and radius are MeV and fm, respectively.

		VMC [13]	GFMC [13]	Few-body [14]	TOAMD [5]
^{3}H	Energy	−6.33(5)	−7.22(12)	−7.15	−7.10
	Radius	1.95(3)	1.75(10)	1.76	1.76
^{4}He	Energy	−22.75(10)	−24.79(20)	−25.40	−24.31
	Radius	1.50(1)	1.50(4)	1.49	1.50

to include the triple products of the correlation functions such as $F_D F_S F_S$ as the next order.

4. Summary

We investigated the s-shell nuclei with a new variational framework of "tensor-optimized antisymmetrized molecular dynamics" (TOAMD) [2–10]. We introduce two kinds of correlation functions for the short-range and tensor correlations to treat the nucleon-nucleon interaction. In TOAMD, the total wave function is expanded in the power series form of the correlation functions, and each correlation function in each power term is optimized independently. This is a different property from the Jastrow concept, in which the correlation functions have a common form.

We showed the results of s-shell nuclei with the AV8′ two-body bare potential in TOAMD with up to the double products of the correlation functions. The total energies and Hamiltonian components of the s-shell nuclei in TOAMD reproduce the results of the few-body calculations. The present results indicate the reliability of TOAMD and the validity of two kinds of correlation functions to treat the bare nuclear forces. We further discussed the effect of the independent optimization of the correlation functions in TOAMD. This treatment provides the better energy than the calculations using common correlation function for all orders. This result indicates that the variational accuracy of TOAMD is beyond the variational Monte Carlo using the common correlation functions.

As an extension of TOAMD, we can superpose the basis states of AMD having various Gaussian centroids [7–10]. Based on the success of TOAMD for the s-shell nuclei, we will investigate the p-shell nuclei from nuclear force.

Acknowledgments

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