The tensor-optimized high-momentum antisymmetrized molecular dynamics with bare interaction and its application in $^4$He nucleus

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We formulate the “tensor-optimized high-momentum antisymmetrized molecular dynamics (TO-HMAMD)” framework for $ab\ initio$ calculations of nuclei by hybridizing the tensor-optimized (TO-) and high-momentum (HM-) AMD approaches. This hybrid approach has advantages in both analytical simplicity and numerical efficiency comparing with other AMD-based methods which treat the bare interaction, especially for heavier nuclear systems. In this work, the s-shell nucleus $^4$He is calculated with TO-HMAMD by including up to double product of nucleon-nucleon ($NN$) correlations, described by using high-momentum pairs and spatial correlation functions of nucleons. The total energy and radius of $^4$He nucleus are well reproduced using the AV8′ interaction. The spin-isospin channel dependence is also discussed for $NN$-correlations, which are found to be mostly contributed in the even-state channels, especially the triplet-even channel. Analyses of the analytical formation and numerical results suggest that TO-HMAMD could be a promising framework for general nuclear systems.
I. INTRODUCTION

The bare nucleon-nucleon (NN) interaction has been determined phenomenologically in high precision by reproducing the NN scattering data [1]. In recent years, it is in active progress to predict the NN interaction from the underlying Quantum Chromodynamics (QCD) [2]. The strong tensor force and short-range repulsion in bare NN interaction have been observed in both phenomenological models and underlying field theory. In nuclei, strong NN-correlations, including tensor and short-range correlations, are induced by tensor force and short-range repulsion, respectively [3]. In ab initio calculations, accurate description of NN correlations are crucial for both exact solution of nuclear wave functions and properties and the examinations of the underlying QCD predictions for nucleon systems. Usually, in ab initio calculations, correlation functions based on the Jastrow type or unitary transformation with exponential form are multiplied to the reference nuclear state [1, 4].

In the present and previous works [5], we propose the “tensor-optimized high-momentum antisymmetrized molecular dynamics” (TO-HMAMD) for ab initio calculations of nuclear system, which is a hybridization of the “tensor-optimized antisymmetrized molecular dynamics” (TOAMD) method [6–10] and the “high-momentum antisymmetrized molecular dynamics” (HMAMD) method [11–13]. These three methods are based on the framework of “antisymmetrized molecular dynamics” (AMD), which has been very successful in microscopic description of light nuclei, especially for the cluster states [14, 15]. In the TOAMD approach, the variational correlation functions in operator forms are explicitly formulated for both central and tensor channels and then their multiple products successively act on the AMD basis state. The TOAMD method is applied in ab initio calculations of s-shell nuclei by using the AV8’ bare interaction, and reproduces well the total energies and radii of 3H and 4He nuclei [7]. In Ref. [10], it is found that using the AV6 interaction, the TOAMD wave function provides better energies for s-shell nuclei comparing with the variational wave functions with the Jastrow type NN-correlations. In the HMAMD approach, the NN correlations are directly described by using the NN-pairs with large momentum in their relative motion [11, 12], which are called ”high-momentum pairs”. With these high-momentum pairs both tensor and short-range correlations can be described. This approach is very similar to the one used in sSMT [16] and AQCM-T [17], in which the tensor correlation is treated. In Ref. [12], energies and radii of the of 4H nucleus are calculated through HMAMD approach using multi high-momentum pairs and the AV4’ interaction having central short-range repulsions. It is found that solutions obtained in TOAMD and HMAMD approaches converge exactly with each other and nicely reproduce the Green’s function Monte Carlo results [12].

From the convergence behavior of the solutions for light nuclei between TOAMD and HMAMD, it is concluded that the correlation function in the TOAMD method and the high-momentum NN pairs in the HMAMD method essentially provide the same description of NN correlation [12]. However, there are differences of both physical concepts and mathematical expressions between these two methods. If these methods are combined, we expect to get a better description of many-body correlations in ab initio studies of nuclei, where many kinds of NN correlations can be included in the wave function. We try to integrate the analytical simplicity of the HMAMD approach and numerical efficiency of the TOAMD approach. Hence, the hybridized nature of TO-HMAMD could be a promising framework for general nuclear system. In our previous work, we have applied the TO-HMAMD method to the ab initio calculation of the simple 3H nucleus, and discussed the accuracy and flexibility of the method. In this work, we perform the detailed comparison between the formulations of TO-HMAMD with HMAMD and TOAMD, and apply the TO-HMAMD method to ab initio calculation of much more complicated nuclei 4He using the AV8’ bare interaction.

This paper is organized as follows. In Sec. [II] we introduce the cluster expansion of the multiple products of the NN-correlations. We also explain the HMAMD and TOAMD methods and then the formulation of the hybridized TO-HMAMD approach. We discuss in detail the advantages of the TO-HMAMD method in comparison with HMAMD and TOAMD. In Sec. [III] we present the numerical results and discussions of the ab initio calculations for 4He nucleus by using the TO-HMAMD method. In Sec. [IV] we discuss the spin-isospin channel dependence of NN-correlations in the wave function of TO-HMAMD. The last Sec. [V] contains the conclusion.

II. FORMULATION

We introduce the framework of TO-HMAMD by explaining first the AMD wave function and next the cluster expansion of the products of NN-correlations, and then formulate successively HMAMD, TOAMD and TO-HMAMD approaches.
A. Antisymmetrized Molecular Dynamics (AMD)

These HMAMD, TOAMD and TO-HMAMD methods are based on the AMD wave function which is defined as Slater determinant of A-nucleons,

$$\{|\Phi_{\text{AMD}}\rangle = \text{det}\{\phi_1(r_1) \cdots \phi_A(r_A)\}\}. \quad (1)$$

Here the single-nucleon states $\phi(r)$ are expressed in Gaussian wave packet form with range parameter $\nu$ and centroid $R$ multiplied by the spin-isospin component $\chi_{\tau,\sigma}$,

$$\phi(r) \propto e^{-\nu(r-R)^2} \chi_{\tau,\sigma}. \quad (2)$$

The Gaussian centroids $R$ are usually determined by the cooling process as discussed in Refs. [14, 15]. For $s$-shell nuclei $^3\text{H}$ and $^4\text{He}$, the centroids are optimized to be $R = 0$ which is obtained in the previous studies of TOAMD [7], and corresponding AMD wave functions are reduced to the $s$-wave states.

B. Description of $NN$ correlations in cluster expansion

In the AMD wave function $\Phi_{\text{AMD}}$, there is no explicit description of $NN$-correlation, and it is energetically unfavorable in nuclei, when there are strong tensor force and short-range repulsion in bare $NN$-interactions. In $ab\ initio$ calculations, the $NN$-correlations are introduced by multiplying the correlation functions to the basis state [10]. In TOAMD, HMAMD and TO-HMAMD methods, we adopt the AMD wave function as the basis state and treat the correlations between nucleons in terms of “cluster expansion”, where many-body wave function of nuclear system can be expanded into power series of $NN$-correlations [10,12]. In Fig. 1, we show the first and second orders of correlation diagrams of $^4\text{He}$ wave functions corresponding to HMAMD, TOAMD and TO-HMAMD methods, respectively. In these diagrams, the $NN$-correlations are denoted by connections of particle lines and presented in different colors according to their mathematical descriptions as introduced in the following paragraphs. The column entitled “[12]” contains the two-body diagrams in which only the nucleons labeled “1” and “2” are correlated. The “[12:23]” denotes the connected three-body diagrams with double product of the $NN$-correlations connecting “[12]” and “[23]”, which belong to the second order in the cluster expansion. The “[12:34]” denotes disconnected four-body diagrams with double product of correlations “[12]” and “[34]”. Some other diagrams, such as the ladder term “[12:12]”, are not included in this figure. The cluster expansion in TOAMD approach is explained in detail in Ref. [9].

To obtain the total wave function of nuclei, the original AMD wave function and the correlated bases described by diagrams in cluster expansion, to the first or second order, are superposed. When only single $NN$-correlation such as “[12]” is included in HMAMD or TOAMD method, we call the corresponding method “single HMAMD” or “single TOAMD”, respectively. When additional second order diagrams with double product of $NN$-correlations are also included, these two methods are named as “double HMAMD” or “double TOAMD”, respectively [9,12]. In the TO-HMAMD method, we include at least first and second order diagrams.

C. High-momentum Antisymmetrized Molecular Dynamics (HMAMD)

In the HMAMD method, the $NN$ correlations are described by introducing high-momentum excitations of nucleon pairs into AMD wave function, utilizing the imaginary parts of the Gaussian centroids [11,12,16,17]. For $s$-shell nuclei, we denote the excited pairs according to their spin-isospin combinations:

$$\begin{align*}
1 : D_{p\uparrow,n\uparrow}, & \quad 2 : D_{p\uparrow,n\downarrow}, & \quad 3 : D_{n\uparrow,n\downarrow}, & \quad 4 : D_{p\uparrow,p\downarrow},
\end{align*} \quad (3)$$

where the subscripts denote two nucleons in each pair with their spins in $z$-direction. The vector symbol $D$ denotes the imaginary shifts of Gaussian centroids for the paired nucleons as

$$\begin{align*}
R_i & \to R_i + iD, \\
R_j & \to R_j - iD,
\end{align*} \quad (4)$$

where subscripts $i$ and $j$ denote each nucleon in the $NN$ pair introduced in Eq. (3). The vector $D$ excites only the relative motion between two nucleons. Both plus and minus signs are included in Eq. (4) to ensure the parity symmetry. The first three cases 1, 2 and 3 in Eq. (3) should be included in the wave function of $^3\text{H}$ nucleus, and the $^4\text{He}$ nucleus requires additional case 4. The symmetric spin-isospin states, such as $D_{p\uparrow,p\uparrow}$, are dropped to ensure the
FIG. 1. Part of the correlation diagrams for the wave functions in HMAMD, TOAMD and TO-HMAMD methods. Vertical lines indicate the particles, numbering from the left side as 1, 2, 3, 4. The red connections entitled “HM” denote NN-correlations described by the high-momentum pairs of nucleons. The blue connections entitled “F” denote NN-correlations described by the TOAMD correlation functions in the central or tensor channels. The green connection entitled “F or HM” stands for either “F” or “HM”. The label with square bracket below each diagram indicates the configuration of particle correlations.

total antisymmetrization for the ground states of s-shell nuclei of which the spatial wave functions are symmetric. This prescription of the correlated pair is extendable to multi-pairs [12].

As discussed in Ref. [12], the imaginary component of the Gaussian centroid Im(\(Z\)) is proportional to the mean value of nucleon momentum as \(\langle k\rangle = 2\nu \cdot \text{Im}(Z)\) in the single-nucleon state described by Eq. (2). The finite \(D\) in Eq. (4) corresponds to a high-momentum excitation of the \(NN\) pairs in Eq. (3), hence they are named as “high-momentum pairs”. In Ref. [11], we examined the physical role of high-momentum pairs in terms of the shell model. It is found that high-momentum pairs provide the equivalent effect of the full amount of the 2p-2h excitations described in tensor-optimized shell model frameworks [18–22]. It is also noted that in Ref. [16], they consider two-deuteron model of \(^4\)He, where one nucleon of each deuteron has a high-momentum component.

In single HMAMD calculations, bases are formulated by introducing a single high-momentum pair in each AMD basis wave function. The imaginary shift in each high-momentum pair is described by Eq. (4) and the vector \(D\) is selected to be in spin parallel \(z\)- and spin perpendicular \(x\)-directions [12]. In double HMAMD calculations, two high-momentum pairs are additionally introduced in each AMD basis wave function, as shown in the connected and disconnected cases in Fig. 1. As an example of two high-momentum pairs for three nucleons, we show the shifted Gaussian centroids for the connected case [10] as

\[
\begin{align*}
R_i &\rightarrow R_i + iD_1 + iD_2, \\
R_j &\rightarrow R_j - iD_1, \\
R_k &\rightarrow R_k - iD_2,
\end{align*}
\]

where \(i, j\) and \(k\) denote three nucleons with two connected high-momentum pairs \(D_1\) and \(D_2\). For the bases with two high-momentum pairs, \(z\) and \(x\)-directions are adopted for the first pair and \(x, y\) and \(z\)-directions are taken for the second pair [12].

For each HMAMD basis, the rotational symmetry is restored by projection of basis \(|\Psi_{\text{HMAMD}}\rangle\) onto eigenstates of
total angular momentum $J$ with the operator $\hat{P}_MK^{JM}$ \cite{29}, as

\[
\begin{align*}
|\Psi_{JM,\text{HMAMD},n}\rangle & = \hat{P}_MK^{JM} |\Psi_{\text{HMAMD},n}\rangle \\
& = \frac{2J+1}{8\pi^2} \int d\Omega D_{MK}^J(\Omega) \hat{R}(\Omega) |\Psi_{\text{HMAMD},n}\rangle,
\end{align*}
\]

where $J$ is the quantum number of total angular momentum, $K$ is the magnetic quantum number in intrinsic state before rotation $\hat{R}(\Omega)$ of Euler angle $\Omega$, and $M$ is the magnetic quantum number after the projection. Subscript $n$ denotes all the parameters in the HMAMD basis including the spin-isospin channels and imaginary shifts $D$ for high-momentum pairs. In numerical calculations, the integration over Euler angles are performed with the Gauss-Legendre quadrature algorithm.

After angular momentum projection, HMAMD bases of different spin-isospin channels and various imaginary shift vector $D$ are superposed with the original AMD basis. It is found that the magnitudes of $|D|$ ranging from 1 fm to 12 fm with interval of 1 fm is sufficient in the superposition to provide the converging energy in single HMAMD calculation \cite{11}. After superposition, $NN$ correlations in nuclei are described precisely, including the tensor correlations \cite{11} and short-range correlations \cite{12}.

One significant advantage of the HMAMD approach is its simplicity in analytical derivations of matrix elements. Due to the fact that all HMAMD bases are merely Slater determinants of shifted Gaussians with complex centroids, all the matrix elements in the HMAMD bases have the same analytical form as those of AMD calculation. Hence, only analytical derivations of AMD matrix elements are necessary. Meanwhile, the formulation of HMAMD bases leads to difficulty in numerical calculation, which is mainly caused by the relative angles between two kinds of vectors for imaginary shifts when two high-momentum pairs are included simultaneously in double HMAMD calculation. For this, six bases corresponding to different combinations of pair directions ($x, z$ for the first pair and $x, y, z$ for the second pair) should be included in model space for each combination of magnitudes $|D_1|$ and $|D_2|$, which significantly enlarges the number of bases.

D. Tensor-optimized Antisymmetrized Molecular Dynamics (TOAMD)

In the TOAMD approach, $NN$ correlation functions are formulated explicitly in operator forms and then multiplied successively to the AMD basis \cite{6}. In the lowest order, the single TOAMD wave function is written as:

\[
(1 + F_D + F_S) \times |\Psi_{\text{AMD}}\rangle,
\]

where the operators $F_D$ and $F_S$ correspond respectively to the tensor and short-range correlations. In practical calculations, they are formulated in the Gaussian expansion form,

\[
\begin{align*}
F_D &= \sum_{m} \sum_{t} C_{D,m}^{t} f_{D,m}^{t}, \\
F_S &= \sum_{m} \sum_{t,s} C_{S,m}^{t,s} f_{S,m}^{t,s},
\end{align*}
\]

where

\[
\begin{align*}
f_{D,m}^{t} &= \sum_{i<j}^{A} \exp(-a_{D,m}^{t} r_{ij}^2) O_{ij}^{t} S_{12}(\hat{r}_{ij}), \\
f_{S,m}^{t,s} &= \sum_{i<j}^{A} \exp(-a_{S,m}^{t,s} r_{ij}^2) O_{ij}^{t} O_{ij}^{s}.
\end{align*}
\]

Here, $s$ and $t$ denote the spin-isospin channels of the two correlated nucleons and $O_{ij}^{t} = (\tau_i \cdot \tau_j)^{t}$, $O_{ij}^{s} = (\sigma_i \cdot \sigma_j)^{s}$. The vector $r_{ij} = r_i - r_j$ is the relative coordinate between correlated two nucleons. Subscript $m$ denotes the different range parameters $a_{D,m}^{t}$ and $a_{S,m}^{t,s}$ in the Gaussian expansion of each channel with the number of $n_G$. The properties of these correlation functions are discussed in Refs. \cite{10} \cite{9}.
In double TOAMD calculations, up to the second order of diagrams are included by using double product of correlation functions $F_S$ and $F_D$, as

$$
(1 + F_D + F_S + F_S F_D + F_D F_S + F_D F_D) \times |\Psi_{AMD}\rangle.
$$

(12)

Parameters in each correlation function $F$ are determined independently and have different coefficients. Comparing with the double HMAMD method, the double TOAMD approach converges faster to the exact solution with the small number of bases. However, this numerical efficiency relies on the enormous efforts on the analytical derivations of matrix elements coming from the double product of $FF$ in Eq. (12). For instance, when calculating the two-body matrix element $\langle \Psi_{AMD} | F^1 F^1 V FF | \Psi_{AMD} \rangle$ for $^4$He, there are 336 diagrams of up to the four-body terms in the cluster expansion of many-body operator $F^1 F^1 V FF$. For each of these diagrams, analytical formulation of matrix element needs to be derived. In addition, it takes efforts for code development.

In Ref. [12], the equivalent results between the correlation functions $F$ and high-momentum pairs are discovered. We compared numerical results from double HMAMD and double TOAMD calculations using AV4′ central interaction with short-range repulsions. In Appendix, we show explicitly the analytical proof for the equivalence between high-momentum pairs and correlation functions $F$ for the central type of $NN$-correlation under some specific conditions.

### E. Tensor-optimized High-momentum Antisymmetrized Molecular Dynamics (TO-HMAMD)

In order to integrate advantages from both HMAMD and TOAMD methods, and balance between the analytical simplicity and numerical efficiency in \textit{ab initio} calculations, we propose the TO-HMAMD method by hybridizing the HMAMD and TOAMD description of $NN$-correlations. The correlation diagrams for the TO-HMAMD approach are shown in the bottom row of Fig. [1]. For the first order of diagrams, such as “[12]”, the $NN$-correlations are described by using either the high-momentum pair with imaginary shift $D$ or the TOAMD correlation function $F_S$ or $F_D$. For the second order diagrams, the $NN$ correlations are described in combination of both high-momentum nucleon pair and the TOAMD correlation function $F$. The TO-HMAMD wave function can be expressed in the following form as

$$
|\Psi_{TO-HMAMD}\rangle = \sum_n C_n (1 + F_{D,n} + F_{S,n}) \times \hat{P}_{MK}^j |\Psi_{HMAMD,n}\rangle,
$$

(13)

where $|\Psi_{HMAMD,n}\rangle$ are HMAMD bases with single high-momentum pair and $F_D$ and $F_S$ are correlation functions in Eq. (5). Subscripts $n$ for $F_D$ and $F_S$ indicate that parameters in $F_{D,n}$ and $F_{S,n}$ are determined independently for each HMAMD basis $|\Psi_{HMAMD,n}\rangle$. Operator $\hat{F}_\mu$ in the second line is selected from the operators $\{1, f^j_{D,m}, f_{S,m}^s\}$ that correspond to three different channels where $f^j_{D,m}$ and $f_{S,m}^s$ are defined in Eqs. (10) and (11). Subscripts $\mu$ denote all the parameters in both $|\Psi_{HMAMD}\rangle$ and $\hat{F}$, including spin-isospin combination and imaginary shift $D$ (including 0) of high-momentum pairs in $|\Psi_{HMAMD,n}\rangle$ and the channel, spin $s$ and isospin $t$ and range parameter $m$ of the operator $\hat{F}_\mu$. $|\Psi_{TO-HMAMD,\mu}\rangle = \hat{F}_\mu |\Psi_{HMAMD,\mu}\rangle$ are defined as TO-HMAMD bases and $\hat{C}_\mu$ are corresponding expansion coefficients. Then the energy and wave function of a nucleus could be obtained by solving the Hill-Wheeler equation, as

$$
\sum_{\mu, \mu'} (H_{\mu\mu'} - EN_{\mu\mu'}) \hat{C}_{\mu'} = 0,
$$

(14)

where $H_{\mu\mu'}$ and $N_{\mu\mu'}$ are the Hamiltonian and norm matrix elements, respectively, as

$$
H_{\mu\mu'} = \langle \Psi_{TO-HMAMD,\mu} | \hat{P}_{MK}^j H | \Psi_{TO-HMAMD,\mu'} \rangle,
$$

(15)

$$
N_{\mu\mu'} = \langle \Psi_{TO-HMAMD,\mu} | \hat{P}_{MK}^j \hat{P}_{MK}^j | \Psi_{TO-HMAMD,\mu'} \rangle.
$$

(16)

Here, $\hat{P}_{MK}^j$ is the angular momentum projection operator. In the above matrix elements, the integrations over Euler angle $\Omega$ in $\hat{P}_{MK}^j$ are performed numerically but the integral kernels such as $\langle \Psi_{TO-HMAMD} | H | \Psi_{TO-HMAMD} \rangle$ are obtained analytically. As discussed in Subsection IIIC, introduction of high-momentum pairs does not require the additional components of the analytical forms of matrix elements. Hence, in analytical derivations of the matrix elements, $\langle \Psi_{TO-HMAMD} | H | \Psi_{TO-HMAMD} \rangle$ is reduced to the matrix element $\langle \Psi_{TOAMD} | H | \Psi_{TOAMD} \rangle$ for single TOAMD.
wave function, which is to be obtained in term of cluster expansion [9]. As an example, in Fig. 2 we show 16 diagrams in cluster expansion associated to two-body operator $V$, in the order of $V$ (a), $F^\dagger V$ (b-d) and $F^\dagger VF$ (e-p) cases. Integral kernels corresponding to each diagram should be derived analytically.

![Diagram](image)

**FIG. 2.** Diagrams of cluster expansions in calculating matrix elements for two-body operator $V$. Diagram (a) is for the operator $V$. Diagrams (b-d) correspond to cluster expansion of operator $F^\dagger V$. Diagrams (e-p) correspond to cluster expansion of operator $F^\dagger VF$. Blue connections indicate the TOAMD correlation functions $F_D$ or $F_S$. Dotted connections indicate the two-body operator $V$. For each diagram, the corresponding integral kernels should be derived analytically.

We get now three methods for the treatment of the correlations among nucleons. In Table I, we compare the analytical and numerical efforts in detail for the new TO-HMAMD method as compared with double HMAMD and double TOAMD approaches. The second row lists the number of diagrams in cluster expansions that need to be derived analytically in the calculation of matrix elements for a two-body operator $V$. In the double HMAMD approach, high-momentum pairs do not change the analytical form of matrix element. Therefore, all the diagrams are reduced to the most simple type as shown in Fig. 2(a), and only one integral kernel for operator $V$ is to be derived analytically. In the double TOAMD method, the number of diagrams is 412, including 16 diagrams shown in Fig. 2, 60 diagrams for $F^\dagger VFF$ and 336 diagrams for $F^\dagger F^\dagger VFF$, as discussed in Ref. [9]. Integral kernel corresponding to each of these diagrams needs to be derived independently. In the new hybridized TO-HMAMD method, the diagrams are reduced to 16 different single TOAMD diagrams as shown in Fig. 2, which significantly simplifies the analytical derivation, comparing with the double TOAMD case. It is therefore clearly shown that in the calculation of two-body operator $V$, TO-HMAMD requires more analytical efforts comparing to double HMAMD, but is still significantly simpler than double TOAMD.

**TABLE I.** Comparison of analytical and numerical settings between double HMAMD, double TOAMD and TO-HMAMD methods in the calculation of $^4$He ($0^+$). In the first row, we compare the number of diagrams in calculating matrix elements for two-body operator $V$. For each diagram, the corresponding integration kernels should be derived analytically. In the second and third rows, we compare the number of bases in the superposition and number of mesh points in numerical integrations for angular momentum projection (AP). Numbers of bases for double HMAMD and double TOAMD are the estimated ones. Definitions of diagrams and bases are explained in the text and Fig. 2.

|                  | Double HMAMD | Double TOAMD | TO-HMAMD |
|------------------|--------------|--------------|----------|
| Diagrams Number  | 1            | 412 [9]      | 16       |
| Bases Number     | 13824        | 1369         | 1813     |
| AP mesh points   | 8000 [12]    | –            | 14       |

Another advantage in the TO-HMAMD approach is that only $z$-direction of imaginary shift $D$ is necessary in the HMAMD part [5]. This is because of the fact that the relative coordinates $r$ between the correlated two nucleons is integrated over the entire space by using the correlation functions of $F_D$ and $F_S$ in Eqs. (8) and (9), which contribute
to the high-momentum excitations for $NN$-pairs in any direction. Hence, all possible relative angles between the two kinds of the correlated $NN$-pairs, described respectively by the high-momentum pairs and $F_{D,S}$, are naturally taken into account. Consequently, the number of bases are significantly smaller in the TO-HMAMD method comparing to the double HMAMD approach, where different orientations of the first and second high-momentum pairs should be taken into account.

In the third row of Table I we compare the number of bases that is required in the numerical calculation among the TO-HMAMD, double HMAMD and double TOAMD methods. The basis number for the double HMAMD calculation is estimated as follows. We set $n_D=12$ with different magnitudes for the imaginary shifts $D$ in two directions $(x$ and $z)$ for both the first and second pairs and select two sets from four kinds of spin-isospin combinations in Eq. (3). Parity doublets for these pairs are also included. The total base number is then estimated to be $(n_D \times 2 \times 2)^2 \times C(4,2)=13824$. For the double TOAMD method, we typically include $n_G=6$ different ranges in Gaussian expansion for each of the 6 channels of correlation function $F$ in Eqs. (3) and (4), and then the total number of bases could be approximated by $(1+6 \times n_G)^2 = 1369$. In TO-HMAMD, we adopt all the 4 possible spin-isospin combinations in Eq. (3) for each high-momentum pair in the HMAMD bases $|\Psi_{\text{HMAMD}}\rangle$ in Eq. (13). Each pair is fixed in $z$ direction with $n_D = 6$ different magnitudes of imaginary shift and their parity doublets are also included. In the correlation functions $F$ in Eq. (13), we include for each of the 6 channels $n_G = 6$ proper ranges for the Gaussian expansion. Hence the total number of TO-HMAMD bases is $(1+4 \times 2 \times n_D) \times (1+6 \times n_G)=1813$. It is observed that the number of bases in TO-HMAMD is similar as in double TOAMD but much smaller than that in double HMAMD method. From this fact, we conclude the numerical efficiency of TO-HMAMD and double TOAMD in describing the exact wave function, as compared to double HMAMD method.

In the application to the $0^+$ ground state of $^4\text{He}$, there is one additional advantage in the TO-HMAMD approach. In this state, the TO-HMAMD wave function has rotational symmetry around $z$-axis and hence the angular momentum projection operator $P_{MK}^J$ in Eq. (13) reduces to

$$P_{00}^0 = \frac{1}{8\pi^2} \int d\beta \sin \beta \hat{R}(\beta),$$

where the rotation over Euler angle $\Omega = \{\alpha, \beta, \gamma\}$ is reduced to single rotation over polar angle $\beta$. This reduces significantly the numerical efforts because integration over angle $\alpha$ and $\gamma$ can be skipped. In TO-HMAMD calculation of $^4\text{He}(0^+)$, we adopt 14 mesh points in the numerical integration over angle $\beta$. This reduction of effort for the angular momentum projection is only valid for the calculation of the $0^+$ states and it is not available for the calculation of $^3\text{H}$ nucleus, ground state of which has spin-parity $1/2^+$. In addition, this reduction relies on the rotational symmetry around $z$-axis, which is broken in the double HMAMD wave function by the high-momentum pairs in $x$-direction. Hence, in this case numerical integration has to be carried out for all of three Euler angles. In the previous double HMAMD calculation, the total number of mesh points for projection is $20 \times 20 \times 20 = 8000$ [12]. In the fourth row of Table I we compare the total number of mesh points for angular momentum projection between double HMAMD and TO-HMAMD calculations, which further illustrates the numerical efficiency in TO-HMAMD approach. In addition, we note that the double TOAMD wave function has intrinsic spin-parity $0^+$ for the ground state of $^4\text{He}$ because of the scalar nature of the correlation functions $F$ in Eqs. (3) and (4). Therefore, angular momentum projection is not necessary for double TOAMD method.

As a balance between the analytical and numerical simplicity, the TO-HMAMD approach can be extended to the $p$-shell nuclei with minimal efforts, which makes it a promising $ab\ initio$ method for general nuclear system.

### III. RESULTS FOR $^4\text{He}$ NUCLEUS

We perform the $ab\ initio$ calculation of $^4\text{He}$ nucleus with the TO-HMAMD method using the AV8' bare interaction. The Gaussian range parameter $\nu$ in Eq. (1) is variationally optimized as $\nu=0.20$ fm$^{-2}$. The corresponding energy curve of $^4\text{He}$ by successively adding high-momentum pairs, and correlation functions $F_D$ and $F_S$ is presented in Fig. 3. It is observed that both addition of high-momentum pairs and correlation functions $F_{S,D}$ significantly improve the total energy of $^4\text{He}$, and the final TO-HMAMD result converges with the double TOAMD calculation.

In Fig. 3 and Table I we show the evolution of Hamiltonian components and radius of $^4\text{He}$ with successive addition of high-momentum pairs and correlation functions. We found that both the central (red curve) and tensor (green curve) terms are improved by the first inclusion of high-momentum pairs, especially for the central term where the improvement is as large as 48.8 MeV. This means that both the tensor and short-range correlations are treated by using high-momentum pairs. It is interesting that the spin-orbit term remains almost 0 MeV for the AMD case, showing that the spin-orbit correlation can only be well described by the second order of correlation diagrams. In the next introduction of tensor correlation function $F_D$, the tensor term is more significantly improved by 42.5 MeV comparing to the central term. In addition, contribution from the spin-orbit term arises with a finite value -3.46 MeV as expected,
FIG. 3. Energy of the $^4$He nucleus calculated with TO-HMAMD using the bare interaction AV8′ by successively adding the high-momentum pairs (+HM), and correlation functions $F_D$ and $F_S$.

because of the coupling between the high-momentum pair and tensor correlation function $F_D$. Addition of the last correlation function $F_S$ contributes to all the Hamiltonian components. For each addition of high-momentum pairs and correlation functions, we observe significant increases of the kinetic energy, which correspond to the high-momentum excitations induced by the short-range repulsion and tensor attraction in the AV8′ bare interaction.

FIG. 4. Hamiltonian components of the $^4$He nucleus calculated with TO-HMAMD using the bare interaction AV8′ by successively adding the high-momentum pairs (+HM), and correlation functions $F_D$ and $F_S$. “K/2” denotes a half of kinetic component. “C”, “T” and “LS” denote central, tensor and spin-orbit components, respectively.

TABLE II. Total energies, Hamiltonian components and root-mean-square radii of $^4$He (0+) calculated with TO-HMAMD using the bare interaction AV8′ by successively adding the high-momentum pairs (+HM), and correlation functions $F_D$ and $F_S$. The units of energies and radii are MeV and fm, respectively.

|        | AMD | +HM | +FD | +FS |
|--------|-----|-----|-----|-----|
| Energy | 48.64 | -0.01 | -20.14 | -24.74 |
| Kinetic | 37.32 | 53.11 | 82.99 | 95.17 |
| Central | 11.31 | -37.50 | -41.61 | -52.33 |
| Tensor  | 0.00  | -15.55 | -58.05 | -63.80 |
| LS      | 0.00  | -0.07  | -3.47  | -3.77  |

|        |        |
|--------|--------|
| Radius | 1.68   |
|        | 1.71   |
|        | 1.58   |
|        | 1.51   |

We compare the TO-HMAMD results of $^4$He nucleus with the double TOAMD and GFMC methods by listing the total energy, Hamiltonian components and the root-mean-square radius obtained from each method in Table III. Nice agreements are found for each component between the TO-HMAMD and other two methods. The TO-HMAMD
method is found to reproduce exactly the same total energy of $^4$He nucleus as the double TOAMD calculation, showing that these two methods describe almost the same wave function. Comparing with the double TOAMD results, the kinetic energy in TO-HMAMD results is slightly smaller. This indicates that the high-momentum components are slightly underestimated in the current calculation. When the TO-HMAMD calculation is performed with larger model space, it is expected that small difference between current result and precise solution can be further reduced.

**TABLE III.** Total energies, Hamiltonian components and root-mean-square radius of $^4$He (0$^+$) calculated with TO-HMAMD using AV8′ potential in comparison with TOAMD and GFMC methods. “$F^2$-TOAMD” denotes double TOAMD method. The units of energies and radii are MeV and fm, respectively.

| Method      | Energy (MeV) | Kinetic (MeV) | Central (MeV) | Tensor (MeV) | LS (MeV) | Radius (fm) |
|-------------|--------------|---------------|---------------|--------------|----------|-------------|
| TO-HMAMD    | -24.74       | 95.17         | -52.33        | -63.80       | -3.77    | 1.51        |
| $F^2$-TOAMD | -24.74       | 97.06         | -53.12        | -64.84       | -3.83    | 1.50        |
| GFMC        | -25.93       | 102.3         | -55.05        | -68.05       | -4.75    | 1.49        |

**IV. SPIN-ISOSPIN CHANNEL DEPENDENCE OF THE $NN$-CORRELATION**

We further discuss the spin-isospin channel dependence of $NN$-correlations in both descriptions using high-momentum pairs or correlation functions $F$. In Fig. 5, we show the spin-isospin channel dependence for the $NN$-correlations described by the correlation function $F$ in single TOAMD and TO-HMAMD calculation of $^4$He. In this figure, we project the correlation functions $F_S$ and $F_D$ in Eqs. (8) and (9) into spin-isospin eigenstates of correlated two nucleons, and add these correlation functions successively in the order of triplet-even (TE), singlet-even (SE), triplet-odd (TO) and singlet-odd (SO) channels. As shown by the red curve in Fig. 5, which corresponds to the single TOAMD calculation, the even channels contribute to the entire energy improvements from the AMD basis, while the odd channels have exactly no effect. This originates from the total even parity of the s-wave AMD basis state of $^4$He, and single correlation function $F$ should be in even channel to preserve the parity of the AMD basis state. In the case of TO-HMAMD calculation (green curve), we observe similar dominance of the even channels. However, in this case, contributions from the odd channels are very small but finite, because of the coupling terms between odd TOAMD correlation functions and odd channels of high-momentum pairs. Furthermore, the triplet-even channel contributes to about 95% of the total energy improvement, which agrees with the prediction from the one-pion-exchange process. In Fig. 6, we show similar channel dependence of the correlation functions $F$ in $^3$H nucleus where total energy is obtained as -7.64 MeV with AV8′ interaction.

The $NN$-correlation is also described by the high-momentum pairs of nucleons in TO-HMAMD calculation. In Fig. 7, we show the energy contribution from each successive addition of various spin-isospin combinations for the
high-momentum pairs in Eq. (3). It is found that in both single HMAMD and TO-HMAMD calculations, the \((p \uparrow, n \uparrow)\) high-momentum pairs contribute to most of the energy improvements comparing with the original AMD or single TOAMD basis. On the other hand, \((n \uparrow, n \downarrow)\) and \((p \uparrow, p \downarrow)\) pairs have smaller contribution to the total energy, especially in the TO-HMAMD calculations. Considering that the \((p \uparrow, n \uparrow)\) pair contains both the triplet-even and triplet-odd channels, while \((n \uparrow, n \downarrow)\) and \((p \uparrow, p \downarrow)\) pairs contain only triplet-odd but no triplet-even channels, we may conclude that the triplet-even channel also dominates the NN-correlations in the description using the high-momentum pairs, as like the previous discussion for correlation functions \(F\). Similar spin-isospin dependence is also shown for the \(^3\text{H}\) nucleus in Fig. 8. We also notice that contributions from the \((n \uparrow, n \downarrow)\) and \((p \uparrow, p \downarrow)\) pairs are finite in Fig. 8 instead of the negligible results reported in Ref. [11]. This is because of the fact that the \((n \uparrow, n \downarrow)\) and \((p \uparrow, p \downarrow)\) pairs improve descriptions of short-range correlation induced by the AV8' interaction in this calculation, while for the calculation in Ref. [11], no short-range repulsion is included in the central interaction.

In future \textit{ab initio} calculations with the TO-HMAMD method, information of the spin-isospin channel dependence can be utilized for more effective description of \(NN\)-correlations in nuclei.

\textbf{V. CONCLUSION}

In conclusion, we propose the variational “TO-HMAMD” framework for \textit{ab initio} calculation of general nuclei by hybridizing the tensor-optimized and high-momentum AMD approaches (TOAMD and HMAMD). The wave function of nuclei is formulated by using the AMD reference state and the additional \(NN\)-correlations expressed in the form of cluster expansion. The correlation diagrams are included up to the second order and described by the product

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure6}
\caption{Energy convergence with respect to the spin-isospin channels of the correlation functions \(F_D\) and \(F_S\) in TO-HMAMD and single TOAMD calculations of \(^3\text{H}\) nucleus.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure7}
\caption{Energy convergence with respect to the spin-isospin combinations of the high-momentum pairs in TO-HMAMD and single HMAMD calculations of \(^4\text{He}\) nucleus.}
\end{figure}
of high-momentum pairs and spatial correlation functions. Comparing with other two AMD based methods (double HMAMD and double TOAMD), it is found that the newly proposed TO-HMAMD approach has an advantage in balancing analytical simplicity and numerical efficiency, which is ideal for the future extensions to $p$-shell nuclei. Through the TO-HMAMD approach, the $^4$He nucleus is calculated using the AV8' bare interaction. It is found that the total energy, Hamiltonian components and root-mean-square radius of $^4$He nucleus are well reproduced comparing to the double TOAMD and GFMC results. We also discuss the spin-isospin channel dependence of $NN$-correlations in TO-HMAMD, and observe dominance of even channels, especially the triplet-even channel, in the description of $NN$ correlations within the ground state of $^4$He. In future studies, application of the TO-HMAMD approach will be extended to $p$-shell and heavier nuclear systems. Because of its flexibility in describing the $NN$-correlations and its advantages in analytical and numerical efficiency, it is expected that the TO-HMAMD can be used as a general $ab$ $initio$ framework for nuclear systems.

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Appendix: Comparison between HMAMD and TOAMD

We compare single HMAMD and single TOAMD wave functions for the central-type correlation. The single HMAMD wave function with imaginary shift $D$ is written as

$$\Psi_{\text{HMAMD}}^{I \pi}(D) = \sum_{i<j}^A C_{ij} P^{J \pi} A \left\{ \phi_i(r_i, iD) \phi_j(r_j, -iD) \cdot \prod_{p \neq i,j}^A \phi_p(r_p) \right\}, \quad (A.1)$$

where $A$ is an antisymmetrizer. $\phi_i$, $\phi_j$ and $\phi_p$ are single-nucleon states, where $\phi_i$ and $\phi_j$ have imaginary shifts $\pm iD$ as shown in Eq. (2) and $\phi_p$ is single-nucleon state expressed by Eq. (1). $P^{J \pi}$ denotes angular momentum and parity projections.

When only central correlation $F_S$ is included, for one Gaussian function term of $F_S$ in Eq. (9) with range parameter $a$, we can express the corresponding single TOAMD wave function as

$$\Psi_{\text{TOAMD}} = F_S \Psi_{\text{AMD}}$$

$$= \sum_{i<j}^A f_{ij} P^{J \pi} A \left\{ \prod_{p=1}^A \phi_p(r_p) \right\}, \quad (A.2)$$

FIG. 8. Energy convergence with respect to the spin-isospin combinations of the high-momentum pairs in TO-HMAMD and single HMAMD calculations of $^3$H nucleus.
where the pair function \( f_{ij} = e^{-a(r_i - r_j)^2} \).

We consider two assumptions in HMAMD below:

1. Superpose all the basis states having high-momentum pairs with an equal weight, namely, \( C_{ij} = 1 \).

2. Integrate over the vector \( D \) corresponding to the momentum, with Gaussian weight with the range \( b \), namely,

\[
\Psi_{\text{HMAMD}}^{J\pi} = \int dD e^{-bD^2} \Psi_{\text{HMAMD}}(D)
\]  

(A.4)

Under these assumptions, we consider the relation between the wave functions of HMAMD and TOAMD. The integrated HMAMD wave function can be expressed as

\[
\Psi_{\text{HMAMD}}^{J\pi} = \int dD e^{-bD^2} e^{2\nu D \cdot (r_i - r_j)} e^{2\nu D^2} \prod_p \phi_p(r_p)
\]  

(A.5)

As \( s \)-wave configuration, we limit the case of \( R = 0 \) for all real components of centroid \( R \) for \( \phi_i, \phi_j \) and \( \phi_p \). Hence from Eq. (2), we have relation

\[
\phi_i(r_i, iD) \phi_j(r_j, -iD) = \phi_i(r_i) \phi_j(r_j) \times e^{2\nu D \cdot (r_i - r_j)} e^{2\nu D^2}
\]  

(A.6)

and substitute into the single HMAMD wave function, as

\[
\Psi_{\text{HMAMD}}^{J\pi} = \sum_{i<j} P^{J\pi} A \left\{ f_{ij} \prod_p \phi_p(r_p) \right\} 
\]  

(A.7)

\[
= \sum_{i<j} P^{J\pi} A \left\{ e^{-a(r_i - r_j)^2} \prod_p \phi_p(r_p) \right\} 
\]  

(A.8)

where \( a' = \frac{a}{2\nu} \). Considering that \( b \) is adjustable parameter, we may choose appropriate \( b \) to obtain \( a' = a \) using pair function \( f_{ij} \), and

\[
\Psi_{\text{HMAMD}}^{J\pi} = \sum_{i<j} P^{J\pi} A \left\{ f_{ij} \prod_p \phi_p(r_p) \right\} 
\]  

(A.9)

\[
= \sum_{i<j} P^{J\pi} \sum_p \epsilon(P) f_{P_1, P_2} \phi_1(r_{P_1}) \phi_2(r_{P_2}) \cdots \phi_A(r_{P_A})
\]  

(A.10)

\[
= P^{J\pi} \sum_p \epsilon(P) \left( \sum_{i<j} f_{P_1, P_2} \right) \phi_1(r_{P_1}) \phi_2(r_{P_2}) \cdots \phi_A(r_{P_A}).
\]  

(A.11)

Here \( \epsilon(P) \) is a sign for the permutation

\[
P : \begin{pmatrix} 1 & 2 & \cdots & A \\ P_1 & P_2 & \cdots & P_A \end{pmatrix}
\]  

(A.12)

From the symmetry of \( f_{ij} \) we have the following relation

\[
\sum_{i<j} f_{P_1, P_2} = \sum_{i<j} f_{ij}.
\]  

(A.13)

Hence, this scalar factor can be factorized from the antisymmetrization and \( J\pi \) projection operator, as

\[
\Psi_{\text{HMAMD}}^{J\pi} = \sum_{i<j} f_{ij} \cdot P^{J\pi} A \left\{ \prod_p \phi_p(r_p) \right\} 
\]  

(A.14)

\[
= F_S \Psi_{\text{AMD}}
\]  

(A.15)

\[
= \Psi_{\text{TOAMD}}.
\]  

(A.16)

With this equation, we have shown the equivalence of the wave functions of single HMAMD and single TOAMD for \( s \)-wave configuration under two conditions.
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