Tensor correlations in light nuclei with tensor-optimized antisymmetrized molecular dynamics

T Myo\textsuperscript{1,2}, H Toki\textsuperscript{2}, K Ikeda\textsuperscript{3}, H Horiuchi\textsuperscript{2} and T Suhara\textsuperscript{4}

\textsuperscript{1} General Education, Faculty of Engineering, Osaka Institute of Technology, Osaka, Osaka 535-8585, Japan
\textsuperscript{2} Research Center for Nuclear Physics (RCNP), Osaka University, Ibaraki, Osaka 567-0047, Japan
\textsuperscript{3} RIKEN Nishina Center, Wako, Saitama 351-0198, Japan
\textsuperscript{4} Matsue College of Technology, Matsue 690-8518, Japan

E-mail: myo@ge.oit.ac.jp takayuki.myo@oit.ac.jp

Abstract. We investigate the light nuclei using the nucleon-nucleon interaction. We describe the tensor and short-range correlations with the new variational theory named “tensor-optimized antisymmetrized molecular dynamics” (TOAMD). In TOAMD, the correlation functions for the tensor force $F_D$ and the short-range repulsion $F_S$ and their multiples are multiplied to the AMD wave function and the total wave function is expressed as the sum of all the components. We take all the necessary matrix elements of many-body operators coming from the products of the multiple correlation functions and the Hamiltonian. We use the interaction AV8' and discuss the effect of tensor and short-range correlations in the $s$-shell nuclei, $^3$H and $^4$He.

1. Introduction

One of the central issues in nuclear physics is to understand the nuclear structure from the nucleon-nucleon ($NN$) interaction. The $NN$ interaction has a strong tensor force at long and intermediate distances and a strong repulsion at short distance [1]. It is important to investigate the nuclear structure considering the above characteristics of the $NN$ interaction. The origin of the tensor force is the one-pion exchange interaction, which brings the high momentum components in nuclei. It is necessary to treat the high-momentum components induced by the tensor force in the nuclear wave function. So far, we have included the high-momentum components in nuclei based on the shell model type approach, which we name ”tensor-optimized shell model” (TOSM) [2, 3]. In TOSM, we fully optimize the two-particle two-hole (2p2h) states in the wave function. There is no truncation for the particle states in TOSM. In particular, the spatial shrinkage of the particle states with high momentum is essential to achieve convergence of the contributions of tensor force.

The clustering of nucleons is one of the important aspects in the nuclear structure, such as the two-\(\alpha\) state in $^8$Be and the Hoyle state in $^{12}$C with the triple-\(\alpha\) state. It is difficult to describe the clustering states in the shell model type approach, while the shell model-like states are fairly described in TOSM [3, 4]. Furthermore, the relation between the $NN$ interaction and the clustering mechanism is unclear, although it is known that the $\alpha$ cluster itself contains the
large contribution of the tensor force \cite{2, 5}. It is important to understand the nuclear clustering phenomena from the viewpoint of the $NN$ interaction and the tensor force.

In this report, we propose the new theory to investigate the nuclear clustering using the $NN$ interaction. We employ the antisymmetrized molecular dynamics (AMD) \cite{6} as the basis states. We introduce two-kinds of the correlation functions of the tensor-operator type for the tensor force and the scalar-operator type for the short-range repulsion. These correlation functions are multiplied to the AMD basis states. We name this framework “tensor-optimized antisymmetrized molecular dynamics” (TOAMD) \cite{7}. We show how the TOAMD describes the light nuclei with the $NN$ interaction.

2. Tensor Optimized Antisymmetrized Molecular Dynamics (TOAMD)

We use the $NN$ interaction, AV8' in this study \cite{1}. We explain the basic formulation of TOAMD while the detailed part is given in Ref. \cite{7}. We employ the AMD wave function expressed by the Gaussian wave packets of nucleons, which nicely describes the nuclear clustering \cite{6}. We multiply the pair-type correlation functions $F_D$ for tensor force and $F_S$ for short-range repulsion to the AMD wave function, respectively, and superpose them with the AMD wave function $\Phi_{AMD}$. In TOAMD, we can systematically increase the order of the correlation functions by using the products of the correlation functions such as the $F_S F_D$ term. The TOAMD wave function with mass number $A$ is explicitly given as

$$\Phi_{TOAMD} = (1 + F_S + F_D + F_S F_S + F_S F_D + F_D F_S + F_D F_D) \times \Phi_{AMD}, \quad (1)$$

$$\Phi_{AMD} = A \left\{ \prod_{i=1}^{A} \phi_i \right\}, \quad \phi(\vec{r}) = \left( \frac{2\nu}{\pi} \right)^{3/4} e^{-\nu (\vec{r} - \vec{D})^2} \chi_{\sigma \tau}, \quad (2)$$

$$F_D = \sum_{t=0}^{1} \sum_{i<j} A f_D^{t}(r_{ij}) O_{ij}^t r_{ij}^2 S_{12}(\vec{r}_{ij}) , \quad F_S = \sum_{t=0}^{1} \sum_{i<j} \sum_{s=0}^{A} f_S^{t,s}(r_{ij}) O_{ij}^t O_{ij}^s , \quad (3)$$

with $O_{ij}^t = (\vec{r}_i \cdot \vec{r}_j)^t$ and $O_{ij}^s = (\vec{\rho}_i \cdot \vec{\rho}_j)^s$. The single nucleon wave function $\phi(\vec{r})$ in $\Phi_{AMD}$ has a Gaussian function with a range parameter $\nu$ and a centroid position $\vec{D}$ and the spin-isospin part $\chi_{\sigma \tau}$. The function $F_D$ induces the relative $D$-wave transition via $S_{12}$. The functions $F_D$ and $F_S$ can excite two nucleons in the AMD state to the high-momentum region corresponding to the 2p2h excitation in the shell model. In Eq. (1) we write terms up to two correlation functions, with which we can show numerical results step by step by adding each term successively. At the same time, we are able to add more correlation terms if necessary.

The energy in TOAMD is given as

$$E_{TOAMD} = \frac{\langle \Phi_{TOAMD} | \hat{H} | \Phi_{TOAMD} \rangle}{\langle \Phi_{TOAMD} | \Phi_{TOAMD} \rangle} = \frac{\langle \Phi_{AMD} | \hat{H} | \Phi_{AMD} \rangle}{\langle \Phi_{AMD} | \Phi_{AMD} \rangle} . \quad (4)$$

The correlated Hamiltonian $\hat{H}$ and norm $\hat{N}$ include the products of correlation functions, such as $F_D^{t} \hat{H} F_D$ and $F_S^{t} \hat{V} F_D$, and become the series of many-body operators. In the case of the two-body interaction $\hat{V}$, $F_D^{t} \hat{V} F_D$ is expanded from two-body to six-body operators with various combinations of particle coordinates. We classify many-body operators according to the cluster expansion method. We take the matrix elements of all the resulting many-body operators with the AMD wave function.

The radial forms of $F_D$ and $F_S$ are optimized to minimize the energy $E_{TOAMD}$ under the variational principle. We use the Gaussian expansion method to express the relative motion of the pair functions $f_D^{t}(r)$ and $f_S^{t,s}(r)$ in Eq. (3) for spin-isospin channels, given as

$$f_D^{t}(r) = \sum_{n=1}^{N} C_n^{t} \exp(-a_n^{t} r^2), \quad f_S^{t,s}(r) = \sum_{n=1}^{N} C_n^{t,s} \exp(-a_n^{t,s} r^2). \quad (5)$$
Here, $a_{n}^{t}$, $a_{n}^{t,s}$, $C_{n}^{t}$ and $C_{n}^{t,s}$ are variational parameters. The Gaussian basis number $N$ is taken as seven at most until the solutions are converged. For the ranges $a_{n}^{t}$, $a_{n}^{t,s}$, we search for the optimized values to gain the total energy. The coefficients $C_{n}^{t}$ and $C_{n}^{t,s}$ are linear parameters in the wave function and determined by diagonalization of the Hamiltonian matrix elements. The positions of the Gaussian wave packets, $\mathbf{D}_{i}$ ($i = 1, \ldots, A$) are determined variationally. In the calculation of the matrix elements of many-body operators, we adopt the Fourier transformation of the Gaussian forms of the correlation function and the $NN$ interaction \cite{7}, which decomposes the many-body operators expressed in terms of the relative coordinates into the separable form in the single particle coordinates.

3. Results of TOAMD

3.1. Single correlation function

We discuss first the TOAMD results for $^3$H and $^4$He with the single correlation function in Eq. (1), namely, $\Phi_{\text{TOAMD}} = (1 + F_{S} + F_{D})\Phi_{\text{AMD}}$. In the variation of the AMD wave function, the range $\nu$ in Eq. (2) is determined to minimize the energy of each nuclei. The nucleon positions $\mathbf{D}$ in Eq. (2) become zero for these nuclei and the $s$-wave configurations are favored in the AMD part. The correlation functions $F_{D}$ and $F_{S}$ are optimized for each nuclei. The energies are $-5.05$ MeV for $^3$H and $-15.37$ MeV for $^4$He, which are underbound in comparison with the Green’s function Monte Carlo (GFMC) results; $-7.76$ MeV for $^3$H and $-25.93$ MeV for $^4$He. We overcome this problem next with the double correlation functions in TOAMD. It is interesting to note that these nuclei are not bound for the case where only the short range correlation $F_{S}$ is included, namely, $\Phi_{\text{TOAMD}} = (1 + F_{S})\Phi_{\text{AMD}}$.

In the calculation, the many-body operators up to four-body terms are considered in the correlated Hamiltonian $\hat{H}$. Up to the two-body terms of $\hat{H}$, we cannot obtain the energy minimum and the variational principle is not satisfied. This indicates the inevitable role of the many-body operators in the correlated Hamiltonian. This is related to the spatial ranges of the correlation functions of $F_{D}$ and $F_{S}$, which are extended and increase the contributions of the three- and four-body terms in the correlated Hamiltonian.

3.2. Double correlation function

We include the double correlation functions given in Eq. (1). In Fig. 1, we show the energy of $^3$H successively by adding various double correlation functions one by one, where $\nu = 0.10$ fm$^{-2}$ variationally. For example, “1+D+S” indicates the calculation within the single correlation...
functions and “+SS” indicates the energy by adding $F_S F_S$ component. The components of $F_S F_D$ and $F_D F_S$ are found to give almost identical effect on the energy, and we add two components simultaneously as “+SD+DS”. It is found that the final energy up to $F_D F_D$ (+DD) almost reproduces the GFMC results within 80 keV difference. It is also confirmed that the contributions of the kinetic energy, central and tensor forces are reproduced as shown in Fig. 2. From these results, we can learn the accuracy and power of TOAMD and the efficiency of correlation functions $F_D$ and $F_S$ to treat the $N N$ interaction.

For $^4$He, we show preliminary results in Fig. 3 with the increase of Gaussian basis number $N$ in Eq. (5) from $N = 1$ to $N = 4$ for the case of $\nu = 0.18$ fm$^{-2}$. The convergence of the energy for $N$ is confirmed at each level of the correlation functions. At $N = 4$ with full components up to $F_D F_D$, the energy is obtained as $-24.32$ MeV in TOAMD. In order to reach the exact energy, we can increase the order of correlation functions such as the triple component $F_S F_D F_D$. This extension of more correlation functions can be handled systematically in TOAMD.

4. Summary

We propose the new variational theory of “tensor optimized antisymmetrized molecular dynamics” (TOAMD) to describe the nuclear structure with the $N N$ interaction. In TOAMD, the tensor- and central-type correlation functions are multiplied to the AMD wave function. The necessary many-body operators in the correlated Hamiltonian and norm are treated without any truncation. The TOAMD results reproduce the $^3$H energy using double correlation functions and provide a good binding energy for $^4$He. Based on the success for the $s$-shell nuclei, we shall apply TOAMD to the $p$-shell nuclei with three-body interaction.

Acknowledgments

This work was supported by JSPS Grant: JP15K05091, JP15K17663, JP16K05351.

References
[1] Pieper S C and Wiringa R B 2001 Annu. Rev. Nucl. Part. Sci 51 53
[2] Myo T, Toki H and Ikeda K 2009 Prog. Theor. Phys. 121 511
[3] Myo T, Umeya A, Toki H and Ikeda K 2011 Phys. Rev. C 84 034315
[4] Myo T, Umeya A, Hori K, Toki H and Ikeda K 2014 Prog. Theor. Exp. Phys. 2014 033D01
[5] Kamada H et al. 2001 Phys. Rev. C 64 044001
[6] Kanada-En’yo Y and Horiuchi H 2001 Prog. Theor. Phys. Suppl. 142 205
[7] Myo T, Toki H, Ikeda K, Horiuchi H and Suhara T 2015 Prog. Theor. Exp. Phys. 2015 073D02