Physics Letters B 769 (2017) 213–218

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

Tensor-optimized antisymmetrized molecular dynamics as a successive variational method in nuclear many-body system

Takayuki Myo [a,b,*], Hiroshi Toki [b], Kiyomi Ikeda [c], Hisashi Horiuchi [b], Tadahiro Suhara [d]

[a] General Education, Faculty of Engineering, Osaka Institute of Technology, Osaka 535-8585, Japan
[b] Research Center for Nuclear Physics (RCNP), Osaka University, Ibaraki 567-0047, Japan
[c] RIKEN Nishina Center, Wako, Saitama 351-0198, Japan
[d] Matsue College of Technology, Matsue 690-8518, Japan

ARTICLE INFO

Article history:
Received 5 September 2016
Received in revised form 28 November 2016
Accepted 25 March 2017
Available online 30 March 2017
Editor: J.-P. Blaizot

Keywords:
Nucleon–nucleon interaction
Antisymmetrized molecular dynamics
Tensor correlation
Short-range correlation
Successive variational method

ABSTRACT

We study the tensor-optimized antisymmetrized molecular dynamics (TOAMD) as a successive variational method in many-body systems with strong interaction for nuclei. In TOAMD, the correlation functions for the tensor force and the short-range repulsion and their multiples are operated to the AMD state as the variational wave function. The total wave function is expressed as the sum of all the components and the variational space can be increased successively with the multiple correlation functions to achieve convergence. All the necessary matrix elements of many-body operators, consisting of the multiple correlation functions and the Hamiltonian, are expressed analytically using the Gaussian integral formula. In this paper we show the results of TOAMD with up to the double products of the correlation functions for the *s*-shell nuclei, ^{3}H and ^{4}He, using the nucleon–nucleon interaction AV8′. It is found that the energies and Hamiltonian components of two nuclei converge rapidly with respect to the multiple of correlation functions. This result indicates the efficiency of TOAMD for the power series expansion in terms of the tensor and short-range correlation functions.

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 [1,2]. 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 of nucleon motion in nuclei. It is necessary to treat the high-momentum components induced by the tensor force in the nuclear wave function. The tensor force also produces the characteristic D-wave state of a nucleon pair in nuclei, which comes from the strong S-D coupling of the tensor force. This D-wave state is spatially compact as compared with the S-wave state due to the high-momentum component of the tensor correlation [3]. The high-momentum component in nuclei coming from the tensor correlation has been investigated experimentally with the (p,d) reaction [4].

So far, we have described the tensor correlation with high-momentum components on the shell model basis, which we name "tensor-optimized shell model" (TOSM) [5,6]. 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 is essential to achieve convergence of the contributions of tensor force. This property is related to the inclusion of the spatially compact D-wave state with high momentum in the wave function.

The clustering of nucleons is one of the important aspects in the nuclear structure, such as the two-α state in ^{8}Be and the Hoyle state in ^{12}C as the triple-α state [7,8]. Those clustering states can coexist with shell model-like states in a nucleus such as ^{12}C, the ground state of which is considered to be the shell model-like state. Theoretically, it is generally difficult to describe the clustering states in the shell model type approach, while the shell model-like states are fairly described [6,9,10]. It is also known that the α cluster itself contains the large contribution of the tensor force [5,11]. The relation between the NN interaction and the co-

* Corresponding author at: General Education, Faculty of Engineering, Osaka Institute of Technology, Osaka 535-8585, Japan.
E-mail address: takayuki.myo@oit.ac.jp (T. Myo).

http://dx.doi.org/10.1016/j.physletb.2017.03.059

existence of the clustering states and the shell model-like states is unclear.

It is important to understand the nuclear clustering phenomena from the viewpoint of the *NN* interaction and the tensor force. One of the theoretical approaches to describe the nuclear clustering is the antisymmetrized molecular dynamics (AMD) [12,13]. The AMD wave function consists of the Gaussian wave packet for each nucleon, which is suitable to express the formation of cluster with spatial localization of some of nucleons in a nucleus. So far, AMD has shown the successful results in the description of various clustering states in finite nuclei from light mass to medium mass region [8]. However, this model cannot treat the tensor force and/or short-range repulsion, and it is necessary for the AMD analysis to rely on the effective interaction of mild central force and *LS* force without the tensor force.

For the clustering description of nuclei based on the *NN* interaction, the unitary correlation operator method (UCOM) has been developed to treat the short-range and tensor correlations [14,15]. Using the Fermionic molecular dynamics (FMD) with UCOM, they have discussed the clustering phenomena [16]. In UCOM, the unitary-transformed Hamiltonian is truncated up to the two-body operator, while the exact transformation produces many-body operators. This truncation seems reasonable for short-range repulsion because of the short-range character, but tensor force has a long-range character and many-body operators should be important for the tensor correlation to work correctly. The many-body operators are also important for the consistent treatment of the variational principle starting from the *NN* interaction.

In our study of TOSM, only the short-range part of UCOM is adopted to describe the short-range correlation in the shell-model type basis states, while the tensor correlation is explicitly treated using the full 2p2h excitation in the wave function. The method of TOSM+UCOM nicely works to describe the shell model-like states with the correct order of the energy level in the *p*-shell nuclei, while the α clustering states such as those in ^{8}Be and ^{12}C are difficult to describe quantitatively [10,17].

Toward the nuclear clustering description from the *NN* interaction, we have proposed a new variational theory [18]. We employ the antisymmetrized molecular dynamics (AMD) [12,13] as the basis state. We introduce two-kinds of correlation functions of the tensor-operator type for the tensor force and the central-operator type for the short-range repulsion. This physical concept is similar to UCOM [15]. The correlation functions are multiplied to the AMD wave function as the correlated basis states and superposed with the AMD wave function. We name this framework "tensor-optimized antisymmetrized molecular dynamics" (TOAMD) [18]. In TOAMD, the products of the Hamiltonian and correlation functions become the series of the many-body operators, which are exactly treated using the cluster expansion. We take all the necessary many-body operators without any truncation, which enable us to determine the correlation functions variationally. The formulation of TOAMD is common for all nuclei with various mass numbers. The scheme of TOAMD is extendable by taking the series of the multiple product of correlation functions as the power expansion. This is done systematically and successively in TOAMD and necessary formulas are published [18].

In this paper, we take up to the double products of correlation functions of tensor and short-range types, and investigate the convergence of the solutions with respect to the multiples of correlation functions and discuss the role of each term. To demonstrate the new successive variational method, we take the *s*-shell nuclei, ^{3}H and ^{4}He, using the AV8′ *NN* interaction.

2. Tensor-optimized antisymmetrized molecular dynamics (TOAMD)

We explain the basic formulation of TOAMD, while all the details are given in Ref. [18]. We start from the AMD wave function, which is expressed by using the Slater determinant of the Gaussian wave packets of nucleons with mass number A. The AMD wave function $\Phi_{\rm AMD}$ is explicitly given as:

$$\Phi_{\rm AMD} = \frac{1}{\sqrt{A!}} \det\left\{\prod_{i=1}^{A}\phi_i\right\} , \tag{1}$$

$$\phi(\vec{r}) = \left(\frac{2\nu}{\pi}\right)^{3/4} e^{-\nu(\vec{r}-\vec{D})^2}\chi_\sigma\,\chi_\tau . \tag{2}$$

The single-nucleon wave function $\phi(\vec{r})$ consists of a Gaussian wave packet with a range parameter ν and a centroid position $\vec{D}$, the spin part χ_σ and isospin part χ_τ. In this study of *s*-shell nuclei, χ_σ is fixed as up or down component and χ_τ is proton or neutron component. The range ν is common for all nucleons and this condition factorizes the center-of-mass wave function from $\Phi_{\rm AMD}$. The range ν also contributes to the spatial size of $\Phi_{\rm AMD}$.

In TOAMD we include two-kinds of correlations induced by the tensor force and short-range repulsion, which are difficult to treat in the AMD wave function $\Phi_{\rm AMD}$. Following the concept given in Ref. [19,20], we introduce the pair-type correlation functions F_D for tensor force and F_S for short-range repulsion and multiply them to the AMD wave function. This choice of the TOAMD wave function is motivated by the success of TOSM [5,10]. We superpose these components with the original AMD wave function. Here we define the basic TOAMD wave function as:

$$\Phi^{\rm basic}_{\rm TOAMD} = (1+F_D)(1+F_S)\times\Phi_{\rm AMD} , \tag{3}$$

$$F_D = \sum_{t=0}^{1}\sum_{i<j}^{A} f_D^t(r_{ij})\,O_{ij}^t\,r_{ij}^2 S_{12}(\hat{r}_{ij}) , \tag{4}$$

$$F_S = \sum_{t=0}^{1}\sum_{s=0}^{1}\sum_{i<j}^{A} f_S^{t,s}(r_{ij})\,O_{ij}^t\,O_{ij}^s , \tag{5}$$

with relative coordinate $\vec{r}_{ij}=\vec{r}_i-\vec{r}_j$, $O_{ij}^t=(\vec{\tau}_i\cdot\vec{\tau}_j)^t$ and $O_{ij}^s=(\vec{\sigma}_i\cdot\vec{\sigma}_j)^s$. Here t and s represent the isospin and spin channel of a pair, respectively. The correlation functions F_D and F_S affect only the relative motion of nucleon pairs in $\Phi_{\rm AMD}$, and do not excite the center-of-mass motion. The center-of-mass motion is completely removed in TOAMD. The function F_D induces the relative D-wave transition via the tensor operator S_{12}:

$$S_{12}(\hat{r}_{ij}) = 3(\vec{\sigma}_i\cdot\hat{r}_{ij})(\vec{\sigma}_j\cdot\hat{r}_{ij}) - \vec{\sigma}_i\cdot\vec{\sigma}_j . \tag{6}$$

The functions F_D and F_S are scalar operator and do not change the total angular-momentum state of $\Phi_{\rm AMD}$. In general, two functions F_D and F_S are not commutable. Physically, 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. This formulation of TOAMD is independent of the mass number A and commonly used for all nuclei.

We state here the essential difference of TOAMD from the Green's function Monte-Carlo (GFMC) method [1]. In the GFMC method, the standard concept of correlation function is used, where it is expressed by a product:

$$F_S^{\rm GFMC} = \prod_{i<j}^{A}\left(1+\sum_{t=0}^{1}\sum_{s=0}^{1} f_S^{t,s}(r_{ij})\,O_{ij}^t\,O_{ij}^s\right) . \tag{7}$$