Cluster Structure of Light Nuclei Superposing Multiple Slater Determinants

K. Yabana[a,b], Y. Fukuoka[b], Y. Funaki[c] and T. Nakatsukasa[a,b,c]

[a] *Center for Computational Sciences, University of Tsukuba, Tsukuba 305-8577, Japan*
[b] *Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba 305-8571, Japan*
[c] *RIKEN Nishina Center, Wako, 351-0198, Japan*

Abstract

We develop a computational approach superposing a number of Slater determinants to describe cluster-like as well as shell-model-like structures of light nuclei simultaneously. The Slater determinants are prepared using imaginary-time method starting with stochastically prepared initial configurations. A microscopic many-body Hamiltonian of Skyrme interaction is then diagonalized in the space spanned by Slater determinants with parity and angular momentum projections. The method is applied to ^{12}C. It is shown that low-lying excited states of both cluster-like and shell-model-like states are reasonably described.

Keywords: *Cluster structure; Skyrme interaction; multiple Slater determinants*

1 Introduction

It has been well-known that various cluster structures appear in excited states of light nuclei [1]. Although shell-model approaches have been successful for low-lying excited states in a wide mass region, it is difficult to describe cluster states since they require a number of many-particle and many-hole configurations across the major shell.

To describe both cluster-like and shell-model-like states simultaneously, we have been developing a new configuration mixing approach [2, 3]. In this approach, we start with a many-body Hamiltonian with an empirical nucleon-nucleon interaction. We attempt to calculate low-lying excited states as well as the ground state which are converged with respect to configurations included in the calculation. To prepare configurations which are sufficient to describe cluster-like states, we employ the imaginary-time method which is usually employed to obtain self-consistent solutions in the mean-field calculations. During the iterations before reaching the self-consistent solution, there often appear various cluster-like configurations in the imaginary-time calculations. We make use of this fact and employ them as basis functions.

In the following, we describe the outline of the method. Then we show an application to the ^{12}C nucleus [2].

2 Formalism

2.1 Preparation of Slater determinants

As a first step of our calculation, we prepare a set of Slater determinants, typically 50, which will be used for the configuration mixing calculation at the next step. The set of Slater determinants is constructed by the following procedure [2, 3].

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http://www.ntse-2014.khb.ru/Proc/Yabana.pdf.

As the Slater determinant which is labeled as no. 1, we choose the self-consistent solution from the mean field calculation. We obtain it as a final convergent solution in the imaginary-time method. Other Slater determinants are obtained in the following recursive procedure. Assuming that we have already N Slater determinants, the next $(N+1)$-th Slater determinant is obtained as follows. We prepare a Slater determinant in which each single-particle orbital is a Gaussian wave packet whose position is determined by random numbers. We then apply the imaginary-time method with the Slater determinant composed of Gaussian wave packets as the initial one. During the iteration before reaching the self-consistent solution, we examine whether the Slater determinant includes a new configuration which will be useful for configuration mixing calculations. In practice, if the expectation value of the Hamiltonian with respect to the Slater determinant is sufficiently close to the energy of the ground state (less than 30 MeV excitation), we calculate the overlap between the present Slater determinant and all Slater determinants which are already selected. If the maximum absolute value of the overlaps is sufficiently small, we adopt it as the $(N+1)$-th Slater determinant. During one imaginary-time iteration, a few Slater determinants are selected in this procedure. As the number of selected Slater determinants increases, it becomes more and more difficult to find a new one which satisfies the overlap criteria.

We note that cluster structures arise often during the imaginary-time iterations. Figure 1 shows energy expectation values obtained during imaginary-time iterations starting from different initial Slater determinants. Calculations are performed for the ^{12}C nucleus. At the initial stage of iterations, the energy expectation values decrease rapidly. In some cases, it is seen that the energy expectation values stay almost unchanged for a long period of iterations. In these flat regions, we find appearances of cluster structures. These configurations are not stable, however. Eventually the Slater determinants converge to the self-consistent ground state solution.

We show in Fig. 2 density distributions of several Slater determinants describing the ^{12}C nucleus obtained by the above procedure. In all calculations presented in this paper, we employ Skyrme SLy4 interaction. In the case of the 1st Slater determinant which is the self-consistent solution, a spherical shape is seen. A triangular shape is seen in the 3rd one and a linear-chain like structure is seen in the 14th one. In this way, various structures including both cluster-like and shell-model-like configurations may be efficiently obtained in this procedure.

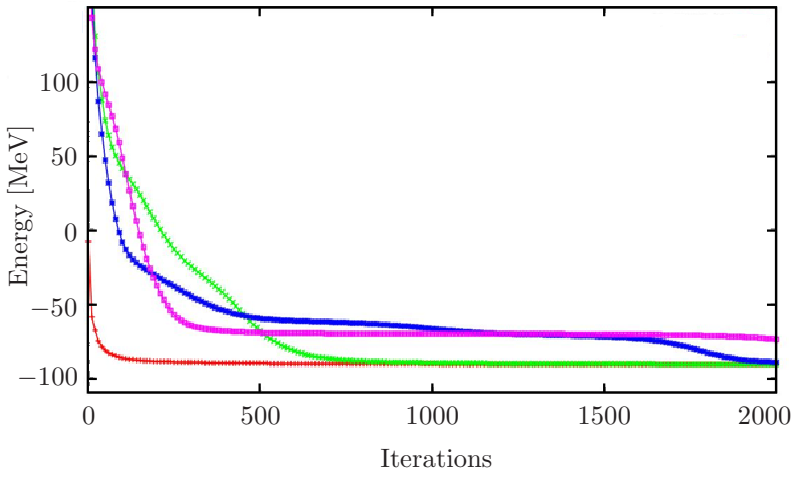

Figure 1: Energy expectation values of the Hamiltonian for ^{12}C nucleus during imaginary-time iterations are shown. Different curves show energy expectation values obtained starting from different initial configurations.

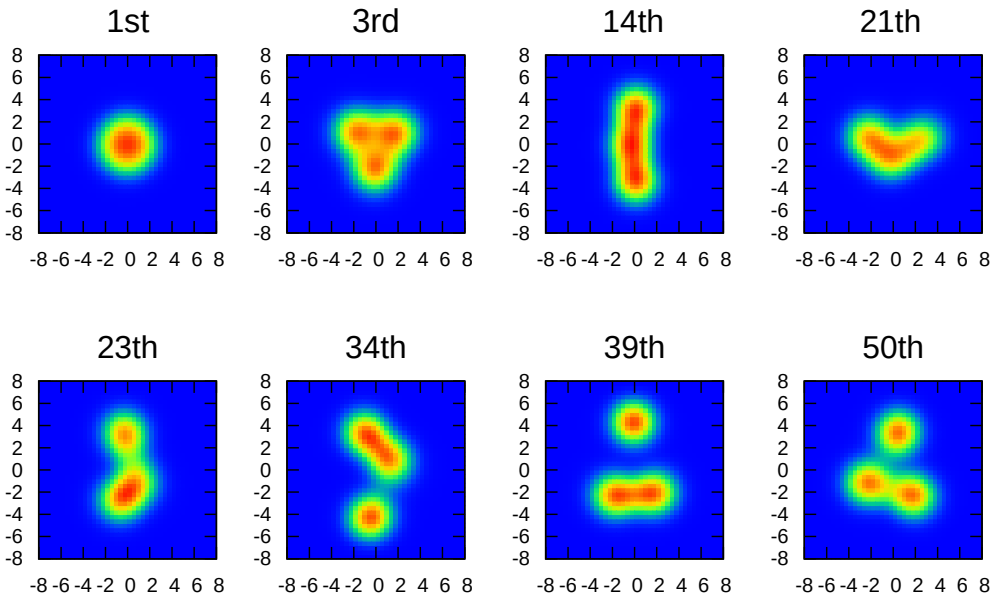

Figure 2: Density distribution in the ^{12}C nucleus corresponding to selected Slater determinants obtained in the imaginary-time calculations. The distance from the center of the nucleus is given in fm. Taken from Ref. [2].

2.2 Projection and configuration mixing calculations

We make a configuration mixing calculation in the space spanned by a set of Slater determinants. Since the microscopic Hamiltonian is invariant under parity and rotational operations, we carry out the projections with respect to the parity and angular momentum before the configuration mixing calculation.

In carrying out the configuration mixing calculations, it is essential to employ configurations which are linearly independent. As mentioned above, we only select those Slater determinants which have small overlaps with each other. However, after the projections, it usually happens that there appears a number of configurations which are not sufficiently independent.

The linear independence of the configurations may be examined using eigenvalues of the norm matrix. The norm matrix elements after parity and angular momentum projections are defined as

$$n^{J\pi}_{iK,jK'} \equiv \int d\Omega\, D^{J*}_{KK'}(\Omega) \langle \Phi_i | e^{-i\alpha \hat{J}_x} \hat{P}^\pi e^{-i\beta \hat{J}_y} e^{-i\gamma \hat{J}_x} | \Phi_j \rangle, \tag{1}$$

where J is the total angular momentum, π is the parity, i and j distinguish Slater determinants, K and K' are angular momentum components along the body-fixed z-axis, $\Omega = (\alpha\beta\gamma)$ is the set of Euler angles, $D^J_{KK'}(\Omega)$ is the Winger's D function.

In Fig. 3, we show the eigenvalues of the norm matrix for ^{12}C, $J^\pi = 2^+$. For 45 Slater determinants, there are 225 states in total. As seen from the figure, only a few eigenvalues have magnitude of order unity. Most of the eigenvalues are small and some of them are even negative (the eigenvalues starting from the number 212). From the definition, the eigenvalues of norm matrix are positive definite. The negative eigenvalues appear due to numerical errors. We need to remove the configurations associated with small and negative eigenvalues for stability of the configuration mixing calculations. In Refs. [2, 3], we describe in detail how we remove the configurations which cause small and even negative eigenvalues.

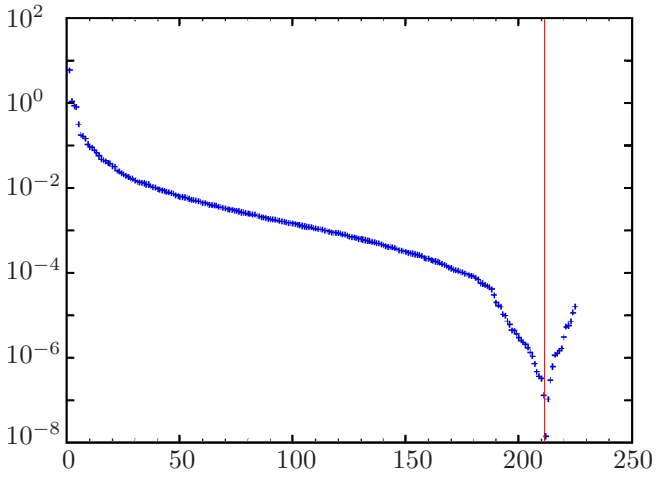

Figure 3: Absolute values of eigenvalues of the norm matrix for ^{12}C nucleus after parity and angular momentum projection.

3 Results for ^{12}C

^{12}C is a nucleus receiving substantial interests in different aspects. It is a key nucleus in nucleosynthesis producing heavy elements. The triple-alpha reaction is a key process to produce ^{12}C in which the 0_2^+ state, the so-called Hoyle state, plays a decisive role. Recently, we have reported a microscopic calculation of the triple-alpha reaction rates [4]. Regarding the structure of the 0_2^+ state, it has been recognized that this state can be understood as a Bose-condensed state composed of three alpha particles [5].

The structure of the ^{12}C nucleus has been extensively investigated within microscopic and semi-microscopic cluster models [1, 6–8]. In Figs. 4 and 5, we show our results for energy spectra of positive and negative parities, respectively.

In the figures, we show our results (Present), in comparison with measured spectra

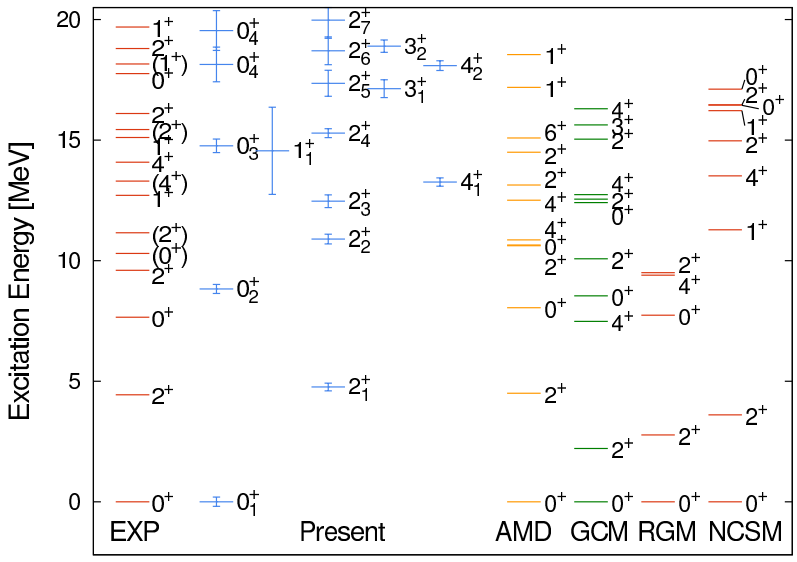

Figure 4: Excitation energies of positive parity levels of ^{12}C nucleus. The energies are obtained by averaging over ten sets of configurations. Taken from Ref. [2].

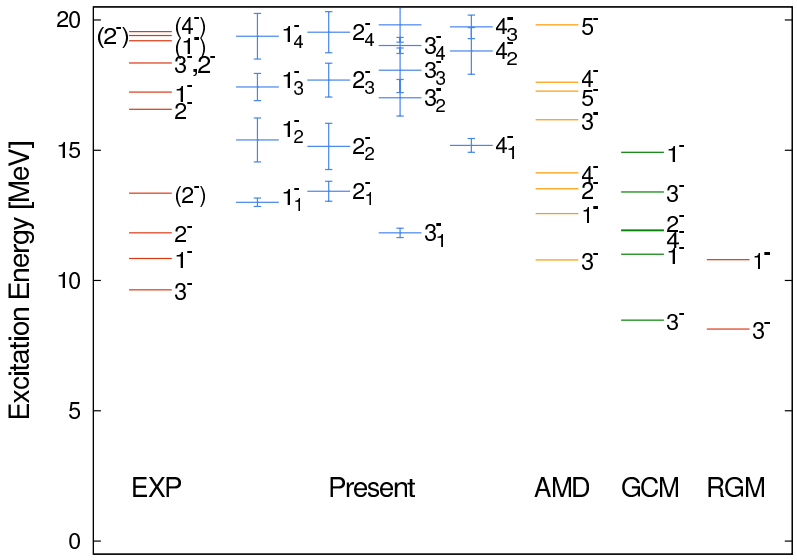

Figure 5: Excitation energies of negative parity levels of ^{12}C nucleus. Taken from Ref. [2].

(Exp) and other theoretical methods including antisymmetrized molecular dynamics method (AMD) [8], generator coordinate method (GCM) [6], resonating group method (RGM) [7], and ab-initio no-core shell model (NCSM) [9]. In the spectrum of our calculation, error bars are attached to the energy. The error bars indicate uncertainly in our calculated spectrum [2]. We carry out 10 different calculations employing different sets of Slater determinants. As mentioned in the section describing the formalism, we prepare 50 Slater determinants in which stochastically prepared initial Slater determinants of Gaussian wave packets are used. By changing the random numbers to generate the initial Slater determinants, we may obtain different sets of Slater determinants. A small error bar indicates that the deviation of energy eigenvalues among 10 different sets is small and that the results are reliable.

As seen from the figure, we may obtain a few low-lying states reliably for each parity and angular momentum. For example, for 0^+ states, three states, the 0^+_1 ground state, the 0^+_2 state which corresponds to the Hoyle state, and the 0^+_3 state are calculated with small uncertainties. The calculated energy levels with small error bars reproduce reasonably the measured spectra. They also coincide well with the results of the AMD calculation. It has been known that the no-core shell model calculations fail to describe the Hoyle state and higher 0^+ states. The GCM and RGM calculations underestimate the energies of 2^+_1 and 4^+_1 states, primarily due to insufficient treatments of spin-orbit interactions.

Regarding the negative parity levels, the lowest energy 3^-, 1^- and 2^- states are reasonably described, although the excitation energies are slightly too high as compared with measurements.

4 Conclusion

We developed a new method to calculate ground and low-lying excited states starting from a microscopic Hamiltonian with empirical two-body interactions. Applying the method to the ^{12}C nucleus, we demonstrate that it is possible to obtain low-lying spectra which are converged with respect to configurations. Both cluster-like and shell-model-like states are described simultaneously. There are two possible directions to extend the present approach. One is to apply the present approach to a wide mass

region and to neutron/proton-rich unstable nuclei, which are now under progress. The other is to employ a Hamiltonian with realistic nucleon-nucleon interactions.

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