α-cluster structure of ^{12}C and ^{16}O in the covariant density functional theory with a shell-model-like approach*

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Abstract: The α-cluster structures for ^{12}C and ^{16}O are investigated in the framework of the covariant density functional theory, where the pairing correlation is treated with a particle number conserving shell-model-like approach. The ground states of ^{12}C and ^{16}O have been calculated and the density distributions demonstrate an equilateral triangle 3α clustering for ^{12}C and a regular tetrahedron 4α clustering for ^{16}O. The existence of linear $n\alpha$ chain structure of both ^{12}C and ^{16}O is revealed at high quadrupole deformation.

Key words: pairing correlation, α-cluster, covariant density functional theory, shell-model-like approach

PACS: 24.10.Jv, 21.10.Gv, 21.60.Jz **DOI:** 10.1088/1674-1137/36/9/004

1 Introduction

Clustering is a universal phenomenon in the nuclear, atomic, molecular, and cosmic worlds [1]. In both stable and unstable nuclei, clustering is one of the essential features and comprises one of the central subjects. It is known that the clustering structures appear in the light nuclei with $N = Z$ or in their neighborhoods [2–6].

When describing the α-cluster structure in nuclei, the antisymmetrized molecular dynamics (AMD) [6] and Fermionic molecular dynamics (FMD) [7] are two of the successful frameworks. Moreover, the covariant density functional theory (CDFT) is also applied to investigate the α-cluster structure [8, 9] and ring nuclei [10] due to its successful description of lots of nuclear phenomena [11, 12]. Most recently, the theoretical framework of CDFT and its applications for nuclear ground states and excited states, as well as a couple of topics in interdisciplinary fields are reviewed in Ref. [13]. There exist a number of attractive features in the CDFT, especially in its practical applications in the self-consistent relativistic mean-field (RMF) framework. It naturally gives the spin-orbit potential and the relativistic effects are responsible for the pseudospin symmetry [14–16] in the nuclear single-particle spectra. Moreover, it is of particular importance that the CDFT includes nuclear magnetism [17], i.e., a consistent description of currents and time-odd fields, which plays an important role in the nuclear rotations [18–21].

In the RMF model, the Bardeen-Cooper-Schrieffer (BCS) approximation and Bogoliubov transformation have become standard literature to treat pairing correlation in both stable and exotic nuclei [12, 22]. As the approximation product of the quasiparticle wave functions in quasiparticle formalism breaks the gauge symmetries connected with the particle number, a particle number conserving (PNC) method has been proposed [23] and successfully employed to investigate the rotational bands [24–26]. This combination of particle number conserving shell-model-like approach with RMF (RMF+SLAP) has been introduced in Ref. [8]. The RMF+SLAP avoids the difficulties encountered in BCS approximation and Bogoliubov transformation and takes into

Received 28 March 2012

* Supported by Major State Basic Research Development (973) Program (2007CB815000), NSFC (11175002, 11105005) and Research Fund for the Doctoral Program of Higher Education (20110001110087)

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account the Pauli blocking effects strictly by diagonalizing the pairing Hamiltonian directly in a reasonable configuration space. In such a way, both the ground state and the low-lying spectra can be obtained.

In the previous work, the RMF+SLAP model was successfully applied in describing the ground states of Sn [27] and C [28] isotopes. Other applications including the description of the excited states can also be found in Ref. [8]. In particular, the clustering phenomenon in ^{8}Be has also been studied in the framework of RMF+SLAP [29]. As an extension of the previous work, we study the α-cluster structures of ^{12}C and ^{16}O in this work. In Section 2, the theoretical framework for the RMF+SLAP is briefly outlined. The numerical details, results, and discussion of ^{12}C and ^{16}O are presented in Sec. 3. Finally, a brief summary is given in Sec. 4.

2 Theoretical framework

The theoretical framework of RMF is explained in Refs. [11, 12] in detail. In Ref. [23], the particle number conserving method is introduced following the idea of the shell model. The formulation of the combination of the RMF model and the shell-model-like approach can be found in Ref. [8]. In the following, we briefly present the framework of the RMF+SLAP model.

The starting point of the RMF theory is an effective Lagrangian density where nucleons are described as Dirac spinors which interact via the exchange of several mesons (the isoscalar scalar σ, the isoscalar vector ω, and isovector vector ρ) and the photon [11, 12]. The detailed formulation of this Lagrangian density can be found in Refs. [11, 12].

The classical variation principle leads to the Dirac equation

$$\{\mathrm{i}\boldsymbol{\alpha}\cdot\nabla+V(\boldsymbol{r})+\beta[M+S(\boldsymbol{r})]\}\psi_i=\epsilon_i\psi_i, \tag{1}$$

for the nucleons and the Klein-Gordon equations

$$\begin{cases}[-\Delta+m_\sigma^2]\,\sigma(\boldsymbol{r})=-g_\sigma\rho_{\mathrm{s}}(\boldsymbol{r})-g_2\sigma^2(\boldsymbol{r})-g_3\sigma^3(\boldsymbol{r}),\\ [-\Delta+m_\omega^2]\,\omega^\mu(\boldsymbol{r})=g_\omega j^\mu(\boldsymbol{r})-g_4(\omega^\nu\omega_\nu)\omega^\mu(\boldsymbol{r}),\\ \left[-\Delta+m_\rho^2\right]\rho^\mu(\boldsymbol{r})=g_\rho j^\mu(\boldsymbol{r}),\\ [-\Delta A^\mu(\boldsymbol{r})]=ej_p^\mu(\boldsymbol{r}),\end{cases} \tag{2}$$

for the mesons. Here the potentials $V(\boldsymbol{r})$ and $S(\boldsymbol{r})$ are connected in a self-consistent way to the various meson fields $\sigma(\boldsymbol{r})$, $\omega(\boldsymbol{r})$, and $\rho(\boldsymbol{r})$ which can be obtained from Klein-Gordon equations with the source terms $\rho_s(\boldsymbol{r})$, $j^\mu(\boldsymbol{r})$, $j^\mu(\boldsymbol{r})$, and $j_p^\mu(\boldsymbol{r})$, for details see Refs. [11, 12]. Following the definition of the Dirac spinors in Ref. [8], the densities can be represented as

$$\rho_{s,v}=2\sum_{i>0}n_i\left[(|f_i^+|^2+|f_i^-|^2)\mp(|g_i^+|^2+|g_i^-|^2)\right], \tag{3}$$

where f_i and g_i represent respectively the large and small components of the Dirac state i, and the corresponding occupation probability is denoted by n_i.

Based on the single-particle levels and wave functions obtained from the RMF theory, SLAP is adopted to treat the pairing correlations. The Hamiltonian reads

$$H=\sum_\nu\varepsilon_\nu a_\nu^\dagger a_\nu-G\sum_{\mu,\nu>0}^{\mu\neq\nu}a_\mu^\dagger a_{\bar\mu}^\dagger a_{\bar\nu}a_\nu, \tag{4}$$

with ε_ν the single-particle energy obtained from the RMF and G the constant average pairing strength.

As in Ref. [8], the multi-particle-configurations (MPC) are constructed as a basis to diagonalize the Hamiltonian in Eq. (4). In realistic calculation, the MPC space has to be truncated and a cutoff energy E_{c} is introduced. Only the configurations with energies $E_i-E_0\leqslant E_{\mathrm{c}}$ are chosen to diagonalize the Hamiltonian H in Eq. (4), where E_i and E_0 are the energies of the ith configuration and the lowest configuration, respectively. According to the obtained wave functions, one can readily have occupation probability of the ith level (see Eq. (15) in Ref. [8]). The SLAP is thus connected to the RMF theory by substituting the obtained occupation probability into Eq. (3) to calculate the various densities.

3 Results and discussion

In the present work, the RMF+SLAP calculations for ^{12}C and ^{16}O are performed with the effective interaction PK1 [30]. The Dirac equation Eq. (1) and the Klein-Gordon equations (2) are solved by expansion in the harmonic oscillator basis with 14 oscillator shells for both the fermion fields and the boson fields. The oscillator frequency of the harmonic oscillator basis is fixed as $\hbar\omega_0=41\ A^{-1/3}$ MeV. The cutoff energy E_{c} of the MPC space is fixed to $E_{\mathrm{c}}=50$ MeV. The pairing strength $G_\tau=0.4$ MeV ($\tau=\mathrm{p,n}$) is adopted according to the experimental odd-even mass difference.

We chose the deformation of harmonic oscillator basis β_0 as -0.3 and 0 to obtain the lowest energy for the ground states of ^{12}C and ^{16}O, respectively. Fig. 1 shows the density distributions of the ground states for ^{12}C (upper panels) and ^{16}O (lower panels) calculated by RMF+SLAP with pairing strength $G=0$ MeV (left panels) and $G=0.4$ MeV (right panels).

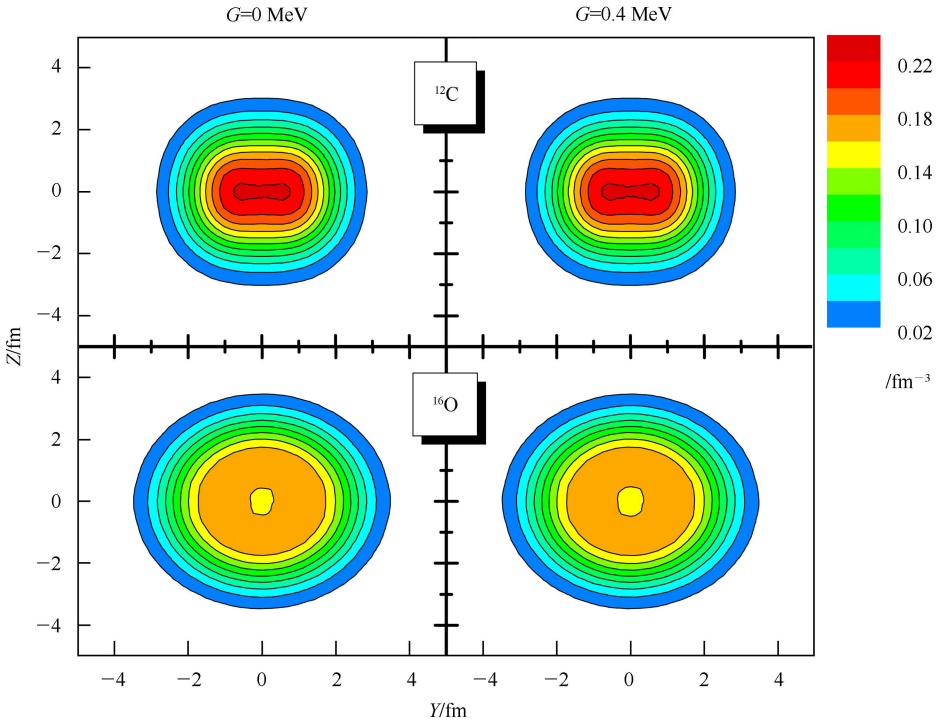

Fig. 1. (color online) The density distributions for the ground states of ^{12}C (upper panels) and ^{16}O (lower panels) calculated by RMF+SLAP with PK1 at $G=0$ MeV (left panels) and $G=0.4$ MeV (right panels).

For the ground state of ^{12}C, although energy increases by 0.176 MeV when pairing correlation is considered, its density distribution is barely changed. One could see that the ground state of ^{12}C undergoes an oblate shape with $\beta=-0.32$. Similar to the results obtained in Ref. [9], this is associated with the 3α cluster of an equilateral triangle structure. One should note here that although the density distributions of ^{12}C show a smooth variation from the center to the periphery in the Y-Z plane, the cluster's structure would be distinctly seen in the plane perpendicular to the symmetry axis Z.

For the ground state of ^{16}O, pairing correlation is negligible since it is a doubly magic nucleus and, as expected, it undergoes a spherical shape. Furthermore the density distribution, as shown in the lower panels of Fig. 1, depicts a circular around the center and a hollowness at the center picture. This is also consistent with the results obtained in Ref. [9], which means that in a three-dimensional space, the 4α particles in ^{16}O form a regular tetrahedron.

In order to obtain the excited state of ^{12}C, the deformation of the harmonic oscillator basis β_0 is chosen as 2.3. Thus, a self-consistent solution (an excited state) is evaluated, whose energy is larger than the ground state energy by $\sim$17 MeV. In Fig. 2, the corresponding density distributions for this excited state are shown. It should be noted that the inclusion of the pairing correlations leads to a decrease of $\sim$0.25 MeV for the excitation energy, whereas the density distribution is not sensitive to the pairing correlations. It is found that the excited state always has a large quadrupole deformation with $\beta=2.4$ no matter whether the pairing strength is 0.4 MeV or zero. Moreover, the 3α chain structure is clearly illustrated in the present calculations. Such structure can also be well reproduced by many other calculations (e.g., Ref. [3]), although it is still questionable with which state the 3α chain might be connected [4].

To obtain the excited state of ^{16}O, the deformation of the harmonic oscillator basis β_0 is chosen as 2.6. The obtained self-consistent solution corresponds to an excited state with the excitation energy $\sim$ 37 MeV. In Fig. 3, the corresponding density distributions for this excited state are shown. Similar to the case of ^{12}C, the inclusion of the pairing correlations leads to a decrease of the excitation energy by $\sim$ 0.55 MeV, whereas the density distribution is not sensitive to the pairing correlations. The excited state always has a large quadrupole deformation with $\beta=3.6$ no matter whether the pairing strength is 0.4 MeV or zero. Moreover, our calculations clearly depict a linear 4α chain structure of ^{16}O at such a high deformation. Such structure has also been discussed in Ref. [31], where its existence of a region of angular momentum is also provided.

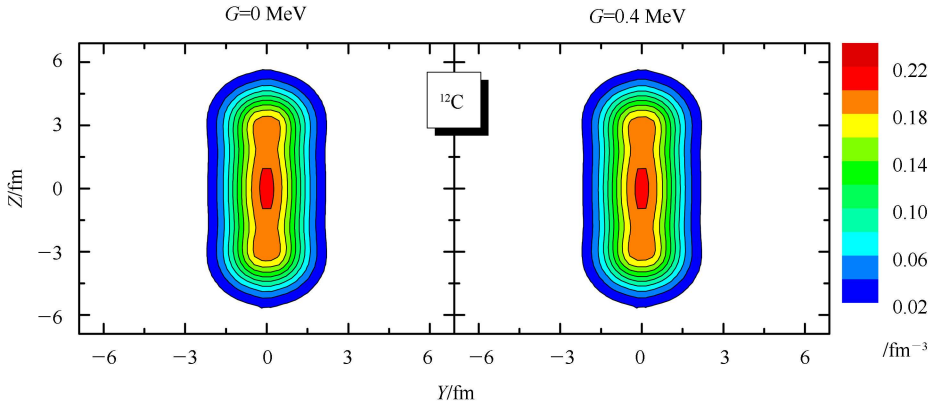

Fig. 2. (color online) The density distributions calculated by RMF+SLAP with PK1 for the excited state of ^{12}C with (right panel) and without (left panel) pairing.

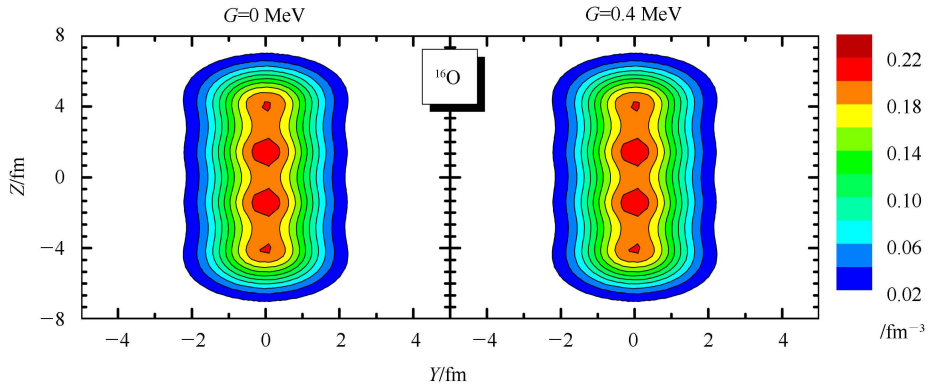

Fig. 3. (color online) The same as Fig. 2 but for ^{16}O.

As an extension of our investigation, it is interesting to explore the border nuclei where the linear nα chain structure could exist. By adding another α particle into ^{16}O, i.e., ^{20}Ne, the linear 5α chain configuration has not been found in the present RMF+SLAP framework so far.

4 Summary

In summary, the α-cluster structures for ^{12}C and ^{16}O are investigated in the framework of covariant density functional theory, where the pairing correlation is treated with a particle number conserving shell-model-like approach. The ground states of ^{12}C and ^{16}O have been calculated and the density distributions demonstrate an equilateral triangle 3α clustering for ^{12}C and a regular tetrahedron 4α clustering for ^{16}O. The RMF+SLAP calculations present the existence of linear nα chain structure of both ^{12}C and ^{16}O at high quadrupole deformation. It should be mentioned that investigations of such α-cluster structures based on different functionals, e.g., point-coupling functionals [32], are also encouraged.

The authors are indebted to Professor MENG Jie for his valuable suggestions and critical review.

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