Clustering aspects in $N = Z$ nucleus $^{24}$Mg studied by antisymmetrized molecular dynamics

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Abstract. Cluster structure of highly excited states of $^{24}$Mg has been investigated by the antisymmetrized molecular dynamics. Imposing the constraints on the expectation values of harmonic oscillator quanta, $\alpha + ^{20}Ne$, $^{12}C + ^{12}C$ and 6$\alpha$ cluster wave functions were generated without any a priori assumption. The isoscalar monopole excitation function is also calculated and reasonably agrees with the observation. It is found that $\alpha + ^{20}Ne$, $^{12}C + ^{12}C$ and 6$\alpha$ clusters appear as the prominent peaks in the strength function.

1. Introduction
The recent development of nuclear structure models has enabled the description of a rich variety of nuclear structure changes and dynamics. Especially, the study of the $N = Z$ sd-shell nuclei such as $^{24}$Mg, $^{24}$Si and $^{32}$S is of particular interest and importance because many exotic clusters will appear as the highly excited states and they will coexist with and couple to the low-lying collective states.

Among the sd-shell nuclei, $^{24}$Mg is the nucleus that has been most intensively studied in detail. The triaxial deformed low-lying collective states have been discussed for a long time [1, 2], and in the highly excited region, many cluster states are expected to exist. According to the Ikeda’s diagram [3], a couple of threshold energies that decompose the system into clusters such as $^{12}C + ^{12}C$, $\alpha + ^{20}Ne$ and 2$\alpha + ^{16}O$ are located at approximately 10 to 20 MeV in excitation energy. Cluster model studies [4, 5, 6, 7] have been devoted to reveal them, but to date, little is known and their existence has not been established well, except for the well-known $^{12}C + ^{12}C$ molecular resonances [8, 9, 10]. It is also noted that very recently Girod and Schuck [11] have pointed out the possible existence of 6$\alpha$ cluster state around 30 MeV based on the Hartree-Fock-Bogoliubov (HFB) calculation.

Thus, the excited states of $^{24}$Mg must contain rich dynamics of nuclear many-body system, triaxial deformed collective states and many clusters. Furthermore, recent new experimental information obtained by the inelastic $\alpha$ scattering sheds new light on the highly excited states of $^{24}$Mg. It is reported that several excited states exist around 10 to 20 MeV, and because their isoscalar (IS) monopole transition strengths are fairly large [12], they may be associated with the cluster states similar to the cases of $^{11}$B [13, 14], $^{12}C$ and $^{16}O$ [15, 16].

Our aim in this theoretical study is to show the existence of many clusters in $^{24}$Mg and to investigate the relationship between those cluster states and the observed large IS monopole strengths. For this purpose, we employ the theoretical framework of antisymmetrized molecular dynamics (AMD) [17, 18], because it is capable of describing the various structures in the
wide energy region without any a priori assumption. We show that AMD is quite successful in explaining the observed IS monopole strengths including the giant resonance and predicts the existence of the $^{12}\text{C}+^{12}\text{C}$, $\alpha+^{20}\text{Ne}$ and $6\alpha$ cluster states with large IS monopole transition strengths.

2. Theoretical Framework

2.1. Constrained energy minimization

We start from the microscopic Hamiltonian with the Gogny D1S effective interaction \cite{19} and use the parity-projected wave function as the variational wave function,

$$
\hat{H} = \sum_i A_i \hat{t}_i - \frac{1}{2} \sum_{ij} \hat{v}_{NN}(ij) + \frac{1}{2} \sum_{ij} \hat{v}_{C}(ij),
$$

(1)

$$
\Phi^\pi = \frac{1 + \pi \hat{P}_x}{2} \Phi_{\text{int}}, \quad \Phi_{\text{int}} = A\{\varphi_1, \varphi_2, \ldots, \varphi_A\},
$$

(2)

$$
\varphi_i = \exp \left\{- \sum_{\sigma=x,y,z} \nu_{\sigma} \left( r_{\sigma} - \frac{Z_{\sigma}}{\sqrt{\nu_{\sigma}}} \right)^2 \right\} (a_i \chi_\uparrow + b_i \chi_\downarrow) \otimes (\text{proton or neutron}),
$$

(3)

where the single particle wave packet $\varphi_i$ describing the motion of each nucleon is represented by the deformed Gaussian \cite{20}, and the parameters $Z_i$, $a_i$, $b_i$ and $\nu_{\sigma}$ are determined by the energy minimization with constraints. To deal with the low-lying quadrupole collectivity and highly excited cluster states simultaneously, we introduce two different constraints. The first is imposed on the nuclear matter quadrupole deformation parameters $\beta$ and $\gamma$ \cite{21, 22} to describe the low-lying collectivity, and we denote the wave functions obtained with it as $\Phi_{\beta,\gamma}$. As the second constraint, the method used in Refs. \cite{23, 24} is extended, and we put the constraint on the following values,

$$
\Delta N = N_x + N_y + N_z - N_0, \quad \lambda = N_z - N_y, \quad \mu = N_y - N_x, \quad (N_z \geq N_y \geq N_x),
$$

(4)

where $N_x, N_y, N_z$ represent the expectation values of the harmonic oscillator quanta in $x, y, z$ directions and $N_0$ is the lowest Pauli-allowed value equal to 28 in the case of $^{24}\text{Mg}$. We denote thus-obtained wave functions as $\Phi_N$. As we see in the next section, $N$-basis successfully describes various cluster states as well as the single-particle excited states.

2.2. Generator coordinate method and isoscalar monopole strength

We further introduce the basis wave functions defined as,

$$
\Phi_{r,x} = (1 - e^{-\mu\hat{O}})\Phi_{\beta,\gamma} \simeq \mu\hat{O}\Phi_{\beta,\gamma}, \quad \hat{O} = \sum_{i=1}^{A} r_i^2,
$$

(5)

where $\mu$ is arbitrary small number and $\hat{O}$ is the IS monopole transition operator. By definition, the wave functions $\Phi_{r,x}$ describe $1p1h$ ($2h\omega$) configuration built on $\Phi_{\beta,\gamma}$ by the IS monopole transition operator. Then, the wave functions generated by energy minimizations and by Eq. (5) are projected to the eigenstate of the angular momentum and superposed to perform the generator coordinate method (GCM),

$$
\Psi_{M\alpha}^{J\pi} = \frac{2J + 1}{8\pi^2} \sum_{K_i} g_{K_i}^{J\pi} \int d\Omega D_{MK}^{J\pi}(\Omega) \hat{R}(\Omega)\Phi^\pi_i.
$$

(6)

Solving the Hill-Wheeler equation, we obtain the eigenenergies $E_{\alpha}^{J\pi}$ and wave functions $g_{K_i}^{J\pi}$ for the ground and excited states of $^{24}\text{Mg}$. 


Using the wave function of the ground and excited $0^+$ states, we calculate the IS monopole transition strength $S(E)$, its sums $m_n$, and reduced transition probability $B(IS0)$,

$$S(E) = |\langle \Psi_n^0(E')|\hat{O}|\Psi_n^0(E)\rangle|^2 E\delta(E' - E), \quad B(IS0; 0^+_n) = |\langle \Psi_n^0|\hat{O}|\Psi_n^0\rangle|^2,$$

$$m_n = \int_0^\infty dE' E'^n |\langle \Psi_n^0(E')|\hat{O}|\Psi_n^0\rangle|^2 \delta(E' - E).$$

We smear the strength function $S(E)$ by Lorentzian of 100 keV width for the sake of the presentation.

3. Results

3.1. Wave functions obtained by energy minimization

Figure 1 shows the density distributions of the various intrinsic wave functions obtained by the energy minimizations. The panels (a) and (b) show typical example of the wave functions $\Phi_{\beta\gamma}$, and they are the dominant components of the ground and the $0^+_2$ states, respectively. Both of them are largely deformed with triaxility showing the importance of the quadrupole collectivity in the low-lying states. Indeed, the GCM calculation with only the basis wave functions $\Phi_{\beta\gamma}$ reasonably explains the low-lying spectrum of $^{24}$Mg as shown in Fig. 2. The ground band, the $\gamma$ and $\beta$ bands built on the $2^+_2$ and $0^+_2$ states are nicely reproduced including their intra- and inter-band $B(E2)$ strengths. It is also noted that there is no cluster state in $\Phi_{\beta\gamma}$ as stated in Ref. [22]. Therefore, by a quick glance of this result, it looks as if there was no room for the clustering in this nucleus.

The use of the constraint on $\Delta N, \lambda$ and $\mu$ reveals the other facet of $^{24}$Mg. It generates various cluster states shown in Fig. 1 (c)-(h) as well as the single-particle excited states that are not on the energy surface of $\Phi_{\beta\gamma}$. It is found that by increasing the value of $\Delta N$, various cluster states start to emerge and their configurations such as inter-cluster distance and orientation of clusters vary depending on the values of $\Delta N, \lambda$ and $\mu$. By applying the constraint of $\Delta N = 2 (2h\omega$ excitation), the $^{12}$C+$^{12}$C cluster states start to appear and they grow by increasing $\Delta N$. 

\[\text{Figure 1. The density distributions of the intrinsic wave functions in the } z = 0 \text{ plane. (a) and (b) show the example of } \Phi_{\beta\gamma} \text{ and (c)-(h) show those of } \Phi_N. \text{ Crosses in the figure show the centroid of the Gaussian wave packet describing nucleons.}\]
Figure 2. The calculated and observed excitation spectra of $^{24}$Mg. The GCM calculation employs only $\Phi_{3\gamma}$ as basis wave functions. Arrows in the figure show the intra and inter-band $E2$ transition strengths.

Figure. 1 (c)-(e) are examples of the $^{12}$C+$^{12}$C cluster states having the excitation energies around 15 MeV obtained by $\Delta N = 6$ and 8. It is noted that the inter-cluster distances and orientations of $^{12}$C clusters are different in Fig.1 (c)-(e) depending on the applied values of $\Delta N$, $\lambda$ and $\mu$.

The $^{20}$Ne+\alpha cluster states also start to appear with $\Delta N = 2$, whose excitation energies are typically around 10 MeV. Similar to the case of the $^{12}$C+$^{12}$C cluster states, the distance and orientation of the clusters depend on the applied constraint as shown in Fig. 1 (f) and (g). It is also noted that the $^{20}$Ne cluster is strongly distorted as confirmed from the density distributions. This may owe to the fact that the $^{20}$Ne cluster itself has the $\alpha+^{16}$O cluster structure. Therefore, for example, the wave function shown in Fig. 1 (g) can be alternatively understood as 2$\alpha+^{16}$O cluster structure. Indeed, if we increase the value of $\Delta N$, the wave function (g) continuously evolves into the pronounced 2$\alpha+^{16}$O cluster structure.

A very exotic and interesting cluster structure composed of six $\alpha$ particles emerges with $\Delta N \geq 8$ as shown in Fig. 1 (h). Five $\alpha$ clusters consist a pentagon and the last $\alpha$ cluster locates on top of it. The six alpha cluster state of $^{24}$Mg is also reported by Girod and Schuck based on the HFB calculation with the constraint on the matter radius [11]. However, those 6$\alpha$ states have different properties. While they reported a hexahedral configuration with larger radius and excitation energy, the present result has a pentagon configuration with smaller radius and excitation energy. The difference may originates in the difference of the applied constraint, and we expect that the hexahedral configuration will be also obtained in our calculation, if we increase the value of $\Delta N$ further.

Thus, without any a priori assumption on nuclear structure, AMD shows the existence of various clusters and demonstrates the evolution of the clustering as function of the excitation energy. It must be emphasised that we just imposed the constraint on the oscillator quanta, nevertheless various cluster structure including very exotic 6$\alpha$ state are obtained. This is an eloquent proof of the fact that the clustering is an important degree-of-freedom of nuclear excitation together with the collective and single-particle excitations.
3.2. Cluster correlations in the low-lying states and duality character of the ground state

We performed the GCM calculation superposing the basis wave functions with and without cluster structure, and calculated the excitation spectrum up to $E_x \sim 40$ MeV. Here, we focus on the properties of the ground and $0^+_2$ states to see how the cluster correlation persists in and affects the low-lying states. Table 1 summarizes the properties of the ground and $0^+_2$ states calculated by using (a) $\Phi_{\beta_2}$, (b) $\Phi_{\beta_2} + \Phi_{r_2}$, and (c) $\Phi_{\beta_2} + \Phi_{r_2} + \Phi_N$ basis functions. As already mentioned, the excitation spectrum is reasonably described by $\Phi_{\beta_2}$ alone indicating the importance of the quadrupole collectivity in the low-lying states. Indeed, the addition of $\Phi_{r_2}$ as basis function rarely changes the properties of the ground and $0^+_2$ states. However, it is found that the low-lying states gain non-negligible additional binding energies by the addition of $\Phi_N$. The ground and $0^+_2$ states gain 0.9 and 1.8 MeV, respectively, that shows the cluster correlations in these states. In particular, the $0^+_2$ state has a large contribution from the $\alpha + ^{20}$Ne cluster shown in Fig. 1 (g) and gains large correlation energy. As a result, the excitation energy of the $0^+_2$ state that is overestimated by $\Phi_{\beta_2}$ is improved by the addition of $\Phi_N$. Therefore, we see that the cluster correlation persists and has non-negligible contribution to the binding energy, even though the quadrupole collectivity dominates these states.

The other point that must be mentioned here is the duality character of the ground state that is known from the early days of the cluster studies [25]. Namely, the shell model (mean-field) wave function with SU(3) symmetry can be rewritten in the form of the cluster model wave function [26], which implies that the degree-of-freedom of cluster excitation is embedded in the ground state. Indeed, it is recently found that the IS monopole transition activates the degree-of-freedom of cluster excitation [15] giving rise to the large IS monopole transition probabilities between the ground and cluster states in many light-mass nuclei [13, 14, 16]. In the present study, it is also found that the ground state has duality character of mean-field and clusters, even though the deviation from SU(3) symmetry is large due to the strong spin-orbit splitting. The ground state has 66 % and 52 % of overlaps with $^{12}$C+$^{12}$C and $^{20}$Ne+$\alpha$ cluster wave functions shown in Fig. 1. This finding suggests a possibility to explore the cluster states by using IS monopole transition as a probe.

Table 1. The energies ($B.E.$), excitation energies ($E_x$) in MeV, root mean square radius $r_{rms}$ (fm) and IS monopole transition probabilities $B(IS0)$ (fm$^4$) calculated by using different basis sets.

| $0^+_1$ | $0^+_2$ | $0^+_2$ |
|---------|---------|---------|
| $\Phi_{\beta_2}$ | $\Phi_{\beta_2}$ | $\Phi_{\beta_2} + \Phi_{r_2}$ | $\Phi_{\beta_2} + \Phi_{r_2} + \Phi_N$ |
| -198.2 | 3.06 | -198.1 | 10.1 | 3.08 | 140 |
| -198.3 | 3.06 | -188.1 | 10.2 | 3.11 | 153 |
| -199.2 | 3.06 | -189.9 | 9.30 | 3.11 | 122 |
| exp. | exp. | -192.9 | 6.43 | - | 180 |

3.3. Isoscalar monopole strength and clusters

Here we demonstrate that the cluster states including $6\alpha$ states can be experimentally explored by using IS monopole excitations. Figure 3 shows the strength functions of the IS monopole mode calculated by using (a) $\Phi_{\beta_2}$ only, (b) $\Phi_{\beta_2} + \Phi_{r_2}$ (c) $\Phi_{\beta_2} + \Phi_{r_2} + \Phi_N$. We first verify the energy weighted sum rule (EWSR) and the position of the giant monopole resonance (GMR) in our results. As clearly seen in Fig. 3 (a), the strength function calculated by only $\Phi_{\beta_2}$ is too weak and exhaust only 35% of the EWSR (Table 2). The addition of $\Phi_{r_2}$ which describes $1p1h$ states built on $\Phi_{\beta_2}$ greatly increases the strengths in the region of $E_x > 20$ that corresponds to the ISGMR. However, it does not largely change the strengths below $E_x < 15$ MeV, and the calculated centroid energy of ISGMR overestimates the observed value. By including cluster
Figure 3. The IS monopole strength functions calculated with (a) $\Phi_{\beta\gamma}$ (b) $\Phi_{\beta\gamma}+\Phi_{r^2}$ (c) $\Phi_{\beta\gamma}+\Phi_{r^2}+\Phi_N$ basis sets. The vertical dashed lines indicate threshold energies of the cluster decays.

Table 2. Calculated and observed energy weighted sum $m_1$ in fraction of EWSR and centroid energy of ISGMR evaluated by $m_1/m_0$ and $\sqrt{m_3/m_1}$ in MeV. (a)-(c) shows the present results obtained by using $\Phi_{\beta\gamma}$, $\Phi_{r^2}$ and $\Phi_N$. Numbers in parenthesis are the energy weighted sum $m_1$ with all of obtained states, while other numbers are calculated by excluding the $0^+_2$ state. These values are compared with the experimental data [29] and the results by the quasi particle random phase approximation [27].

| Basis            | $m_1$   | $m_1/m_0$ | $\sqrt{m_3/m_1}$ |
|------------------|---------|-----------|-------------------|
| (a) $\Phi_{\beta\gamma}$ | 26 (35) | 20.29     | 24.24             |
| (b) $\Phi_{\beta\gamma}+\Phi_{r^2}$ | 101 (116) | 25.61     | 29.26             |
| (c) $\Phi_{\beta\gamma}+\Phi_{r^2}+\Phi_N$ | 90 (103) | 22.24     | 25.18             |
| Exp.             | 82 ± 9  | 21.9$^{+0.3}_{-0.2}$ | 24.7$^{+0.5}_{-0.3}$ |
| Peru et al.      | 94      | 20.57     |                   |

states described by $\Phi_N$, the centroid energy of ISGMR and EWSR are reasonably reproduced simultaneously. Thus, AMD successfully describes IS monopole strength function in a wide energy region. It is also noted that quasi particle random phase approximation (QRPA) calculation [27] also reports very similar results except for the low-energy region of $E_x < 18$ MeV.

As clearly seen in Fig. 3, the addition of $\Phi_N$ changes the structure of strength function below $E_x < 18$ MeV. In particular, it generates prominent peaks at 13.7 and 15.3 MeV which are missing in Fig. 3 (a)(b) and QRPA result [27]. The states at $E = 13.7$ MeV is dominated by the $^{20}\text{Ne}+\alpha$ cluster state shown in Fig. 1 (f) and its $B(IS0)$ is 1.1 W.u. exhausting 2% of EWSR. The $^{12}\text{C}+^{12}\text{C}$ cluster state appears as the peak at 15.3 MeV that is just above the the $^{12}\text{C}+^{12}\text{C}$ threshold. Its $B(IS0)$ is 2.8 W.u. and exhaust 5% of EWSR which is as large as that of the $0^+_2$ state. Very interesting and important point is that these peaks are missing in QRPA calculation [27], but look existing in the observed data [28, 29]. Therefore, it is very tempting to conclude that the $\alpha+^{20}\text{Ne} and ^{12}\text{C}+^{12}\text{C}$ cluster states were successfully populated by the experiment, although further experimental data is needed to confirm it. Finally, we discuss $6\alpha$ cluster state with pentagon shape. By the coupling with other cluster and $1p1h$ states, it is fragmented into two states at 22.4 and 25 MeV that are unfortunately embedded in the broad distribution of ISGMR. However, they are still visible in Fig. 3 (c) and should be experimentally accessible, because they will selectively decay by $\alpha$ particle emission not by neutron emission. Thus, $^{24}\text{Mg}$ has a rich variety of cluster states in the energy range of 10–30 MeV, and many of them should
be detectable by their enhanced IS monopole transition strengths.

4. Summary
We have investigated cluster structure of highly excited states of $^{24}$Mg on the basis of the antisymmetrized molecular dynamics. By imposing the constraints on the expectation values of harmonic oscillator quanta, $\alpha + ^{20}$Ne, $^{12}$C$^{+}$ $^{12}$C and 6$\alpha$ cluster structures were generated without any a priori assumption. We also studied the IS monopole transition strength. By including the cluster states as the basis function, the calculated strength function reasonably agrees with the observation. It is found that $\alpha + ^{20}$Ne, $^{12}$C$^{+}$ $^{12}$C and 6$\alpha$ cluster structures appear as the prominent peaks in the energy range of 10$\sim$30 MeV.

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References
[1] Girod M and Grammaticos B 1983 Phys. Rev. C 27 2317
[2] Bender M and Heenen P H 2008 Phys. Rev. C 78 024309
[3] Ikeda K, Tagikawa N and Horiuchi H 1968 Prog. Theor. Phys. Suppl. Extra Number 464
[4] Matsuse T, Kondô Y and Abe Y 1978 Prog. Theor. Phys. 59 1009
[5] Katô K and Bando H 1979 Prog. Theor. Phys. 62 644
[6] Baye D and Descouvemont P 1984 Nucl. Phys. A 419 397
[7] Descouvemont P and Baye D 1987 Nucl. Phys. A 475 219
[8] Almqvist E, Bromely D A and Kuehner J A 1960 Phys. Rev. Lett. 4 515
[9] Cosman E R et al. 1975 Phys. Rev. Lett. 35 265
[10] Erb K A et al. 1976 Phys. Rev. Lett. 37 670
[11] Girod M and Schuck P 2013 Phys. Rev. Lett. 111 132503
[12] Kawabata T et al. 2012 Prog. Theor. Phys. Suppl. 196 198
[13] Kanada-En’yo Y 2007 Phys. Rev. C 75 024302
[14] Kawabata T et al. 2007 Phys. Lett. B 646 6
[15] Yamada T et al. 2008 Prog. Theor. Phys. 120 1139
[16] Yamada T et al. 2012 Phys. Rev. C 85 034315
[17] Kanada-En’yo Y, Kimura M and Horiuchi H 2003 C. R. Physique 4, 497
[18] Kanada-En’yo Y, Kimura M and Uno A 2012 PTEP 2012 01A202
[19] Berger J F, Girod M and Gogny D 1991 Comput. Phys. Comm. 63 365
[20] Kimura M 2004 Phys. Rev. C 69 044319
[21] Suhara T and Kanada-En’yo Y 2010 Phys. Rev. C 82 044301
[22] Kimura M, Yoshida R and Isaka M 2012 Prog. Theor. Phys. 127 287
[23] Kanada-En’yo Y and Kimura M 2005 Phys. Rev. C 72 064322
[24] Kimura M 2007 Phys. Rev. C 75 034312
[25] Wildermuth K and Kanellopoulos Th 1958 Nucl. Phys. 7 150
[26] Bayman B F and Bohr A 1958/59 Nucl. Phys. 9 596
[27] Peru S and Goutte H 2008 Phys. Rev. C 77 044313
[28] Youngblood D H, Lui Y -W and Clark H L 1999 Phys. Rev. C 60 014304
[29] Youngblood D H, Lui Y -W., Chen X F and Clark H L 2009 Phys. Rev. C 80 064318