

Cluster states and container picture in light nuclei, and triple-alpha reaction rate

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Abstract. The excited states in ^{12}C are investigated by using an extended version of the so-called Tohsaki-Horiuchi-Schuck-Röpke (THSR) wave function, where both the 3α condensate and $^8\text{Be} + \alpha$ cluster asymptotic configurations are included. We focus on the structures of the “Hoyle band” states, 2_2^+ , and 4_2^+ states, which are recently observed above the Hoyle state, and of the 0_3^+ and 0_4^+ states, which are also quite recently identified in experiment. We show that the Hoyle band is not simply considered to be the $^8\text{Be}(0^+) + \alpha$ rotation as suggested by previous cluster model calculations, nor to be a rotation of a rigid-body triangle-shaped object composed of the 3α particles. We also discuss the rate of the triple-alpha radiative capture reaction, applying the imaginary-time method. Results of the triple-alpha reaction rate are consistent with NACRE rate for both high ($\approx 10^9\text{K}$) and low ($\approx 10^7\text{K}$) temperatures. We show that the rate of the imaginary-time calculation in coupled-channels approach has a large enhancement for low temperatures if we truncate the number of channels.

1. Introduction

The Hoyle state, the second $J^\pi = 0^+$ state at 7.654 MeV in ^{12}C , is a typical example of cluster states. For this state, the aspect of the α condensate, where the 3α clusters occupy an identical S -orbit, has triggered a great interest for recent years, since the so-called Tohsaki-Horiuchi-Schuck-Röpke (THSR) wave function [1], which has the α condensate character, was shown to be equivalent to the Hoyle state wave function obtained by solving the equations of the full 3α resonating group method (RGM) or generator coordinate method (GCM) [2, 3].

The excited states above the Hoyle state have also recently been highlighted by experiments. The 2_2^+ state, which theoretically had been predicted at a few MeV above the Hoyle state as a member of the Hoyle band, was recently confirmed by many experiments [4, 5, 6, 7, 8]. A strong candidate of the member of the Hoyle band with $J^\pi = 4^+$ was also reported by Freer *et al.* [9]. Besides the 2^+ and 4^+ states, quite recently Itoh *et al.* insisted that a broad width 0^+ state at 10.3 MeV should be decomposed into the 0_3^+ and 0_4^+ states [4, 10]. This observation of the two 0^+ states is consistent with theoretical predictions done by using the OCM combined with the CSM [11, 12].

On the other hand, the Hoyle state is known to play a key role in a synthesis of ^{12}C in stellar evolution. At a temperature above 0.1 GK, the Hoyle resonance contributes dominantly [13]. Below 0.1 GK, however, non-resonant contribution is considered to be significant [14, 15, 16]. In a standard compilation NACRE [17], which is used to describe various astronomical phenomena, the non-resonant triple-alpha rate is evaluated by extending the sequential model at high temperatures to low temperatures. Recently, Ogata *et al.* [18] reported that the radiative



capture rate was surprisingly large below 0.1 GK in comparison with NACRE rate ($\approx 10^{26}$ at 0.01 GK) by using the continuum-discretized coupled channels (CDCC) method [19]. We should also mention that some other different techniques are also applied to the calculation of the reaction rate and give large increases of the magnitude at low temperature regions compared to NACRE, for example, $\approx 10^{18}$ in Ref. [21] and $\approx 10^6$ in Ref. [20] at 0.01 GK, whereas the Faddeev calculation gives very similar result to NACRE [22].

The first half of this contribution is devoted to the structure study of the positive parity excited states above the 3α threshold by using an extended version of the THSR wave function [23] so as to include ${}^8\text{Be} + \alpha$ asymptotic configurations with a treatment of resonances. In particular, we focus on the “Hoyle band” (the 0_2^+ , 2_2^+ , and 4_2^+ states, and the 0_3^+ and 0_4^+ states, together with the corresponding experimental data. In the latter half, we discuss the triple-alpha reaction rate by using the imaginary-time method where the radiative capture rate as a function of temperature can be calculated directly by solving an equation that looks like a time-dependent Schrödinger equation along the imaginary-time axis [24, 25].

2. Extended THSR wave function and Hoyle-family states in ${}^{12}\text{C}$

The extended version of the THSR wave function is written as follows:

$$\Phi_{JM}^{\text{THSR}}(\beta_1, \beta_2) = \hat{P}_{MK}^J \mathcal{A} \left[\prod_{i=1}^2 \exp \left\{ -\mu_i \sum_{k=x,y,z} \frac{2(\xi_{ix})^2}{(B_{ik})^2} \right\} \prod_{i=1}^3 \phi(\alpha_i) \right], \quad (1)$$

where $B_{ik}^2 = b^2 + 2\beta_{ik}^2$ with $i = 1, 2$ and $k = x, y, z$. This wave function is characterized by the parameters β_1 and β_2 , which correspond to the sizes of the ${}^8\text{Be}$ core and the remaining α particle c.o.m. motion, respectively. The case of $\beta_1 = \beta_2$ results in the original THSR wave function. Thus this new THSR wave function is a natural extension of the original version, so that taking $|\beta_1| \leq |\beta_2|$ allows for the ${}^8\text{Be} + \alpha$ cluster structure, deviating from the identical 3α -cluster motion for $\beta_1 = \beta_2$. We should note that this THSR wave function includes the ${}^8\text{Be} + \alpha$ asymptotic feature for $|\beta_1| \ll |\beta_2|$, and is also feasible for approaches to resonances like the complex scaling method (CSM) and the analytic continuation of the coupling constant (ACCC) method. In order to obtain the excited states, we solve the Hill-Wheeler equation by this new THSR wave function taking both β_1 and β_2 as the generator coordinates, where axial symmetric deformation is assumed, i.e. $\beta_{i\perp} \equiv \beta_{ix} = \beta_{iy}$. In this calculations we effectively remove spurious continuum components by using a method of the so-called radius constraint method [26, 23]. In Fig. 1(left), the calculated energy spectra are shown. One can see that besides the ground state band, there are many J^π states obtained above the Hoyle state. All these states have large r.m.s. radii (3.7 fm $\sim$ 4.7 fm), and therefore may have gas-like cluster structures. These states seem to appear as the excited states of the Hoyle state that looks like the “ground state” of the gas-like cluster states.

In Fig. 1(right), the $E2$ transition strengths between J and $J \pm 2$ states and monopole transition strengths between $J^\pi = 0^+$ states are also shown with the corresponding arrows. We can see the very strong $E2$ transitions inside the Hoyle band, $B(E2; 4_2^+ \rightarrow 2_2^+) = 591 \text{ e}^2\text{fm}^4$ and $B(E2; 2_2^+ \rightarrow 0_2^+) = 295 \text{ e}^2\text{fm}^4$. The transition between the 2_2^+ and 0_3^+ state is also very large, $B(E2; 2_2^+ \rightarrow 0_3^+) = 104 \text{ e}^2\text{fm}^4$. We should note that the 0_3^+ state is strongly excited from the Hoyle state by monopole transition, whose strength is calculated to be $M(E0; 0_3^+ \rightarrow 0_2^+) = 35 \text{ fm}^2$. In Fig. 1(right), the calculated energy levels are plotted as a function of $J(J+1)$, together with the experimental data. We can say that roughly the 0_2^+ , 2_2^+ , and 4_2^+ states both in theory and experiment follow a $J(J+1)$ trajectory, and therefore, on the one hand, the rotational picture is very good. On the other hand, the $J^\pi = 0^+$ bandhead in experiment seems to be fragmented into the Hoyle state and the 0_3^+ state, and the calculated levels also have similar tendency, where the Hoyle state is located slightly below the $J(J+1)$ line.

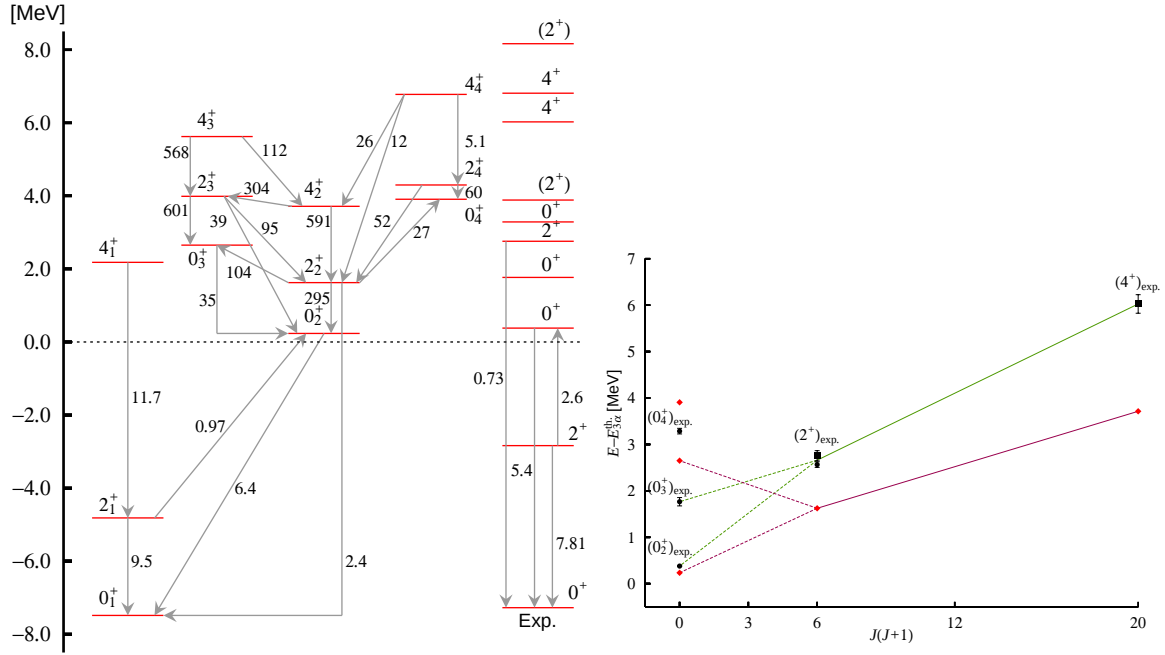


Figure 1. (color online). (Left): Calculated energy levels and electric transition strengths are shown and compared with experiments. (Right): The observed energy levels for the 0_3^+ , 0_4^+ , and 2_2^+ states in Ref. [4], and the 2_2^+ [5] and 4_2^+ [9] states are denoted by black circles and black squares, respectively. The calculated energy levels for the five states are denoted by red diamonds. Figure (right) taken from [23].

Table 1. The S -factors $S_{[I,l]}^2(J^\pi)$ for the five J^π states.

J^π	$S_{[I,l]}^2(J^\pi)$						
	$[I, l]$	$[0, 0]$	$[2, 2]$	$[4, 4]$			
0_2^+		1.85	0.13	0.04			
0_3^+		1.09	0.06	0.03			
0_4^+		0.25	1.47	0.05			
2_2^+	$[I, l]$	$[0, 2]$	$[2, 0]$	$[2, 2]$	$[2, 4]$	$[4, 2]$	$[4, 4]$
		1.24	0.53	0.07	0.03	0.08	0.02
4_2^+	$[I, l]$	$[0, 4]$	$[4, 0]$	$[2, 2]$	$[2, 4]$	$[4, 2]$	$[4, 4]$
		0.88	0.24	0.65	0.06	0.02	0.0

We then discuss the S -factor of the ${}^8\text{Be} + \alpha$ channel, which is defined as $S_{[I,l]}(J) = \int dr (r \mathcal{Y}_{[I,l]J}(r))^2$. Here $\mathcal{Y}_{[I,l]J}(r)$ is the reduced width amplitude (RWA) of the ${}^8\text{Be} + \alpha$ channel. We show in Table 1 the calculated S -factors for these excited states. We can see that except for the 0_4^+ state, all the states have the largest contribution from the $[0, J]_J$ channel. This supports the idea of ${}^8\text{Be} + \alpha$ rotation for the Hoyle band, where the ${}^8\text{Be}$ core is in the 0^+ ground state. On the other hand, the Hoyle state is considered to be the 3α condensate state, where the 3α clusters mutually move in an identical S -wave. Since the ground state of ${}^8\text{Be}$ is composed of weakly interacting 2α clusters coupled loosely in a relative S -wave, it is natural that the Hoyle state, with the α condensate structure, also has a large overlap with the ${}^8\text{Be}(0^+) + \alpha$ structure.

However, the 3α condensate structure in the Hoyle state is not the same as the usual ${}^8\text{Be}(0^+) + \alpha$ rotation, in which the remaining α cluster orbits outside the ${}^8\text{Be}$ core. Namely in the Hoyle state, the remaining α cluster also orbits inside the ${}^8\text{Be}$ core and the independent 3α -cluster motion in an identical $0S$ -orbit is realized. As a result, the Hoyle state gains an extra binding, and hence its energy position is considered to be made lower than the $J(J+1)$ line, as shown in Fig. 1(right). The same effect is also argued in the study of the 4α condensate and ${}^{12}\text{C}(0_2^+) + \alpha$ rotational band [27, 28], where the 4α condensate is mentioned as “complete condensate” and the ${}^{12}\text{C}(0_2^+) + \alpha$ state as “local condensate”. Due to the existence of the “complete condensate”, a higher 0^+ excited state, which has the prominent ${}^8\text{Be}(0^+) + \alpha$ structure, with the remaining α cluster orbiting outside the ${}^8\text{Be}$ core, appears as a higher nodal state, that is the 0_3^+ state, excited by strong monopole transition from the Hoyle state. In Table 1, the 0_4^+ state is shown to have the component of $[2, 2]_0$ channel dominantly. This is consistent with the 0_3^+ state calculated by GCM [2], AMD [29], and FMD [30]. In particular, in AMD and FMD calculations this state is shown to have linear-chain-like intrinsic density. We also mention that the 2_2^+ state also includes non-negligible mixture from the $[2, 0]_2$ channel and 4_2^+ states from the $[2, 2]_4$ channel and smaller amount from the $[4, 0]_4$ channel. These mixtures also deviate the 2_2^+ and 4_2^+ states from a pure ${}^8\text{Be} + \alpha$ rotational structure.

3. Triple-alpha reaction rate

We start with the following expression for the triple-alpha reaction rate [24, 25],

$$N_A^2 \langle \alpha\alpha\alpha \rangle = 6 \cdot 3^{3/2} N_A^2 \left(\frac{2\pi\beta\hbar^2}{M_\alpha} \right)^3 \frac{8\pi(\lambda+1)}{\hbar\lambda((2\lambda+1)!!)^2} \sum_{M_{f\mu}} \langle \Phi_f | M_{\lambda\mu} e^{-\beta H} \left(\frac{H - E_f}{\hbar c} \right)^{2\lambda+1} P M_{\lambda\mu}^\dagger | \Phi_f \rangle, \quad (2)$$

where β is the inverse temperature $\beta = 1/k_B T$, M_α is the mass of the α -particle, H is the Hamiltonian of three α particles, Φ_f is the wave function of ${}^{12}\text{C}$ in the final state after the γ -ray emission, E_f is the energy of the final state measured from the three α threshold, and M_f is the magnetic quantum number of the final state. $M_{\lambda\mu}$ is the multipole transition operator of γ -ray emission with multipolarity λ . We consider reactions of three α -particles in the total angular momentum $J = 0$, emission of $\lambda = 2$ γ -ray, and 2^+ state of ${}^{12}\text{C}$ at 4.44 MeV for the final wave function Φ_f . P is the projection operator which eliminates any bound eigenstates of the three-body Hamiltonian. We may easily show that Eq. (2) exactly coincides with the expression for the triple-alpha reaction rate, Eqs. (2) ~ (5) of [31], if we insert a completeness relation of a functional space of three α -particles in Eq. (2).

To evaluate the rate in practice according to Eq. (2), we need to calculate $\Psi(\beta) = e^{-\beta H} M_{\lambda\mu}^\dagger \Phi_f$. We treat it by evolving the wave function along an imaginary-time axis,

$$-\frac{\partial}{\partial\beta} \Psi(\beta) = H \Psi(\beta), \quad (3)$$

starting with the initial wave function, $\Psi(\beta = 0) = M_{\lambda\mu}^\dagger \Phi_f$. The rate at the temperature specified by β is then evaluated using the wave function at $\beta/2$,

$$\langle \alpha\alpha\alpha \rangle \propto \sum_{M_{f\mu}} \left\langle \Psi \left(\frac{\beta}{2} \right) \left| \left(\frac{H - E_f}{\hbar c} \right)^5 \right| \Psi \left(\frac{\beta}{2} \right) \right\rangle. \quad (4)$$

We have achieved numerical calculations using the model space and the three-body Hamiltonian described below. We treat α -particles as point particles, and consider reactions of three α particles in the space of total angular momentum $J = 0$ as mentioned above,

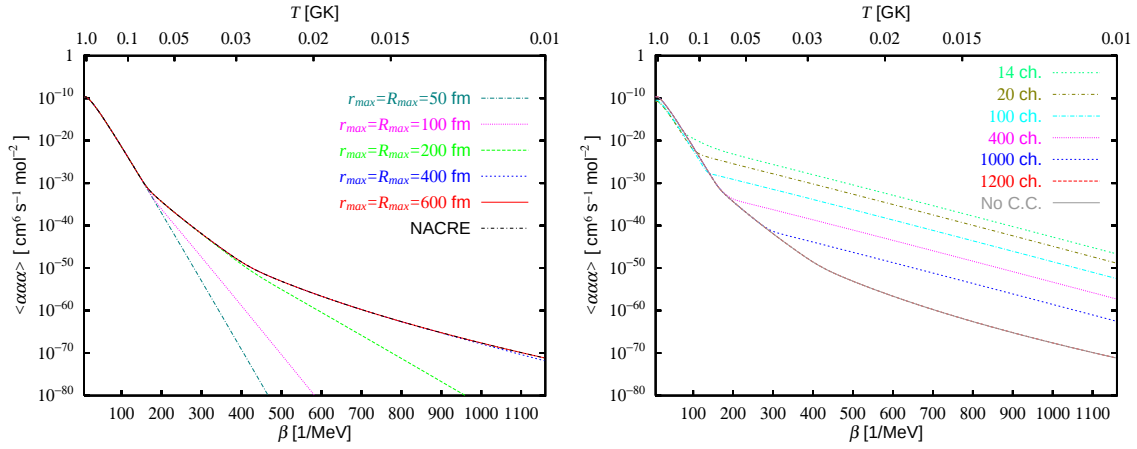


Figure 2. (Color online) (Left): Calculated triple-alpha reaction rates for several choices of radial cutoff distances, $r_{\max}$ and $R_{\max}$, in comparison with the NACRE rate. (Right): Triple-alpha reaction rates employing the coupled-channels expansion. Results of different number of employed channels specified by $n_{\max}$ are compared. Figures taken from Ref. [25].

which should be sufficient below $T < 1.0$ GK [31]. We use a Jacobi coordinate system of two relative coordinates, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2 - \mathbf{r}_3$, with $\mathbf{r}_i$ ($i = 1 - 3$) being coordinates of three α -particles. The three-body wave function is expanded in partial waves, $\Psi(\beta) = \sum_L (u_L(R, r, \beta)/Rr) [Y_L(\hat{R})Y_L(\hat{r})]_{J=0}$. In the present work, we only treat $L = 0$ component which should be the most important at low temperature. We note that the same model space is adopted in the CDCC calculation [18].

The Hamiltonian H of three α -particles is constructed as follows. For the potential between two α -particles, we use the Ali-Bodmer potential of angular momentum $l = 0$ channel. The potential parameter is slightly modified so that it reproduces the resonance corresponding to the ground state of ^8Be at 92.08 keV accurately. We add a three-body potential among three α particles, $V_{3\alpha}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = V_3 e^{-\mu(r_{12}^2 + r_{23}^2 + r_{31}^2)}$ with $\mu = 0.15 \text{ fm}^{-2}$. The value of V_3 is chosen so that the resonance energy of the Hoyle state, 0_2^+ state of ^{12}C , is reproduced at 379.8 keV above the three α threshold. As for the final wave function, Φ_f , of ^{12}C $J^\pi = 2^+$ at 4.44 MeV, we use the one constructed by the orthogonality condition model [32].

In Fig. 2(left), calculated triple-alpha reaction rates adopting different spatial areas specified by $R_{\max}$ and $r_{\max}$ are compared. We also show the NACRE rate [17] for comparison. The figure shows that a convergent reaction rate in the entire temperature region is obtained if we adopt $R_{\max}$ and $r_{\max}$ larger than 400 fm. Calculations in smaller spatial areas provide the rate which is correct in the limited higher temperatures.

We next examine the origin of the discrepancy between the theories: why different theoretical approaches result in so different rates at low temperatures. In particular, the CDCC approach [18] which employs almost the same model space as adopted here, differs by 10^{26} order of magnitude at low temperature from the NACRE rate and ours. To clarify the origin of this discrepancy, we have achieved the imaginary-time evolution of Eq. (3) using the coupled-channels method. In the coupled-channels approach, we first solve the eigenvalue problem of α - α relative motion described by the Hamiltonian $h_{\alpha\alpha}(r)$. Discretizing the radial variable r in 0.5 fm step up to 600 fm, we have 1200 grid points for this coordinate. Diagonalizing the radial Hamiltonian, we obtain 1200 eigenfunctions, $w_n(r)$, ($n = 1 - 1200$). Eigenstates belonging to low eigenvalues are characterized by a large α - α separation outside the Coulomb barrier, except for the resonant state corresponding to the ^8Be ground state which appears as 14th eigenstate. In the coupled-channels

approach, we expand the wave function as $u(R, r, \beta) = \sum_n v_n(R, \beta) w_n(r)$ and calculate the imaginary-time evolution of $v_n(R, \beta)$ in the form of matrix-differential equation. We numerically confirmed that, employing all 1200 eigenstates in the expansion, calculated rate exactly coincides with the result shown in Fig. 2(left), as it should be. However, if we truncate the number of basis in the expansion, results depend on the truncation. Convergence with respect to the number of employed basis functions is shown in Fig. 2(right).

Taking only the lowest state ($n_{\max} = 1$), the reaction rate is much higher than the fully convergent calculation by 10^{16} order of magnitude at $T = 0.01$ GK. This enhancement may be easily understood. In the lowest eigenstate of $h_{\alpha\alpha}(r)$, two α -particles are much apart to each other and stay outside the Coulomb barrier. Then the Coulomb barrier for the third α -particle is very small in this channel, giving large reaction rate. The rate first increases as the number of channels increases. In Fig. 2(right), the rate shows maximum when we include the channel of α - α resonance, the 14th channel, 10^{24} times larger than the convergent value at $T = 0.01$ GK. The artificial enhancement in small-channel calculations should be compensated by off-diagonal coupling terms as we increase the number of channels. However, as is seen from the figure, the convergence is extremely slow. Even with 400 channels, the reaction rate is still 10^{13} times larger than the fully convergent result. We consider it manifests a numerical difficulty of expressing exponentially small function in the tunneling process using the basis expansion method.

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