Three-body calculation of triple-alpha reaction at low energies

Souichi Ishikawa

Science Research Center, Hosei University, 2-17-1 Fujimi, Chiyoda, Tokyo 102-8160, Japan E-mail: ishikawa@hosei.ac.jp

Abstract. The reaction rate of the triple-alpha (3α) process at low temperatures, where resonant reaction is not dominant, is calculated through the inverse process, the photodisintegration of a ¹²C nucleus. For this, Schrödinger equations in a three-alpha $(3-\alpha)$ model of ¹²C are directly solved by a Faddeev method, which has been successfully applied to three-nucleon problem so far. The nuclear Hamiltonian consists of an α - α potential, which reproduces the ⁸Be resonance state, together with three-body potentials to reproduce ¹²C properties. Our results of the 3α reaction rate are about 10³ times larger at low temperature $(T = 10^7 \text{ K})$ than a standard rate from the Nuclear Astrophysics Compilation of Reaction Rates (NACRE), which means our results are remarkably smaller than recent results of quantummechanical three-body calculations by Ogata *et al.*

1. Introduction

The 3α reaction, ${}^{4}\text{He} + {}^{4}\text{He} + {}^{4}\text{He} (\alpha + \alpha + \alpha) \rightarrow {}^{12}\text{C} + \gamma$, is known to play a significant role in the stellar evolution scenarios. At temperatures higher than 10^{8} K, the reaction is considered to be dominated by so called resonant process [1, 2], which is consisting of two sequential steps:

Here, ⁸Be is the resonant state of α - α system with the energy of $E_r[^8\text{Be}(0^+)] = 91.89 \text{ keV}$ ($\Gamma = 6.8 \pm 1.7 \text{ eV}$) [3], and $^{12}\text{C}(0_2^+)$ is the second 0⁺ resonant state of the carbon nucleus, which is known as Hoyle state, with the energy of $E_r[^{12}\text{C}(0_2^+)] = 379.4 \text{ keV}$ ($\Gamma = 8.3 \pm 1.0 \text{ eV}$) above the 3- α threshold [4].

Since it is impossible to directly perform the 3α reaction in a laboratory, theories of nuclear reactions are expected to provide a crucial information of its reaction rate, which is used as astrophysical inputs. At high temperatures as $T > 10^8$ K, where the resonant process is expected to be dominant, theoretical evaluations of the 3α reaction rate are performed with resonance formulae for the reactions of Eq. (1). On the other hand, at low temperatures as $T \sim 10^7$ K, where the 3α reaction might be important in phenomena of accreting white dwarfs and neutron stars, α particles do not have enough energies to produce the ⁸Be resonant state, and thus the reaction proceeds through "non-resonant process". Nomoto *et al.* [5] evaluated non-resonant 3α reaction rates by extending the resonance formulae to low energy wings of the resonances. Standard reaction rates by the NACRE compilation [6] followed the idea of Nomoto *et al.* with a minor modification.

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On the other hand, theoretical treatments of quantum mechanical three-body reactions have been well developed in a sense that precise numerical calculations are possible by numbers of different methods. Recently, Ogata *et al.* [7] calculated the 3α reaction rate by solving a threebody Schrödinger equation with the method of continuum-discretized coupled-channel (CDCC). Their results (hereafter referred to as the OKK rate) at low temperature are quite different from those given by Refs. [5, 6]: about 10^{26} (10^6) times larger at $T = 10^7$ K (10^8 K) compared to the NACRE rate (see figure 3 below). In this paper, we calculate the 3α reaction rate by solving the three-body Schrödinger equations by a different method from the CDCC, which is based on the Faddeev method [8] improved in the treatment of the Coulomb three-body problem and having been successfully applied to the study three-nucleon scattering systems [9].

In the following, after describing a formalism to calculate the 3α reaction rate shortly in Sec. 2, I will introduce interaction models among the α particles, and show some numerical results in Sec. 3. A summary is given in Sec. 4.

2. Formalism

In the present work, we calculate the inverse reaction of the 3α reaction, namely the E2photodisintegration of the first excited state of ${}^{12}C$, ${}^{12}C(2_1^+)$:

$$^{12}\mathrm{C}(2^+_1) + \gamma \to \alpha + \alpha + \alpha, \tag{2}$$

in which the total angular momentum of the final 3- α state is 0. Using the disintegration cross section $\sigma_{\gamma}(E_{\gamma})$, the 3 α reaction rate $\langle \alpha \alpha \alpha \rangle$ is calculated (See Ref. [10], *e.g.*) by

$$N_{\rm A}^2 \langle \alpha \alpha \alpha \rangle = N_{\rm A}^2 (3)^{3/2} 240 \pi \left(\frac{\hbar}{m_\alpha c}\right)^3 \frac{c}{(k_{\rm B}T)^3} e^{-\frac{E_{\rm C}}{k_{\rm B}T}} \int_{|E_{\rm C}|}^{\infty} E_{\gamma}^2 \sigma_{\gamma}(E_{\gamma}) e^{-\frac{E_{\gamma}}{k_{\rm B}T}} dE_{\gamma},\tag{3}$$

where $N_{\rm A}$ is the Avogadro constant, $k_{\rm B}$ is the Boltzmann constant, m_{α} is the mass of the α particle, E_{γ} is the energy of photon, and $E_{\rm C}$ is the (negative) energy of the ¹²C(2⁺₁) state, which is related with the energy of the final 3- α state E as

$$E = E_{\gamma} + E_{\rm C}.\tag{4}$$

We consider the ¹²C nucleus as a system of three α particles, 1, 2, and 3. Hereafter, we will use indexes (i, j, k) to denote (1,2,3) or its cyclic permutations and an index *i* to indicate the particle *i* or particles *j* and *k*.

The disintegration reaction is calculated by defining a wave function [11]

$$|\Psi\rangle = \frac{1}{E + i\epsilon - H_{3\alpha}} H_{\gamma} |\Psi_{\rm C}\rangle,\tag{5}$$

where $H_{3\alpha}$ is a Hamiltonian of the 3- α system, H_{γ} is the (E2) electromagnetic transition operator, and $\Psi_{\rm C}$ is a wave function of the initial ${}^{12}{\rm C}(2^+_1)$ state.

Since there is no incoming wave in this process, the asymptotic form of the wave function Ψ is given as a purely outgoing wave of the three particles with a breakup amplitude $f^{(B)}$:

$$\Psi(\boldsymbol{x}, \boldsymbol{y}) \to \frac{e^{iK_0R}}{R^{5/2}} f^{(\mathrm{B})}(\Theta, \hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}), \tag{6}$$

where we use a set of Jacobi coordinates $\{x, y\}$ defined as

$$x = r_1 - r_2, \qquad y = r_3 - \frac{1}{2} (r_1 + r_2)$$
 (7)

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with r_i being the position vector of the particle i, and define a hyper radius R and a hyper angle Θ as

$$R = \sqrt{x^2 + \frac{4}{3}y^2},$$
(8)

$$x = R\cos\Theta, \quad y = \sqrt{\frac{3}{4}}R\sin\Theta.$$
 (9)

The variable K_0 is given by

$$K_0 = \sqrt{\frac{m_\alpha}{\hbar^2}E}.$$
(10)

The photodisintegration cross section is given by the breakup amplitude as

$$\sigma_{\gamma}(E_{\gamma}) = \left(\frac{3}{4}\right)^{3/2} \frac{2\hbar K_0}{m_{\alpha}c} \int d\Theta d\hat{\boldsymbol{x}} d\hat{\boldsymbol{y}} \cos^2 \Theta \sin^2 \Theta |f^{(\mathrm{B})}(\Theta, \hat{\boldsymbol{x}}, \hat{\boldsymbol{y}})|^2.$$
(11)

Next, we apply the three-body Faddeev method to Eq. (5) [11]. In the following, we will consider only two-body potential for simplicity, and write the Hamiltonian as

$$H_{3\alpha} = H_0 + \sum_{i=1}^{3} V_i, \tag{12}$$

where H_0 is the internal kinetic energy operator of the three-body system, and V_i is a two-body potential (2BP) between particles j and k.

The wave function Ψ is decomposed into three components:

$$\Psi = \Phi^{(1)} + \Phi^{(2)} + \Phi^{(3)},\tag{13}$$

and these (Faddeev) components satisfy the following Faddeev-type equations:

$$\Phi^{(i)} = G_i(E)H_{\gamma,i}\Psi_{\rm C} + G_i(E)V_i\left(\Phi^{(j)} + \Phi^{(k)}\right) \qquad (i = 1, 2, 3).$$
(14)

Here, we defined a channel Green's function $G_i(E)$ as

$$G_i(E) = \frac{1}{E + i\epsilon - H_0 - V_i},\tag{15}$$

and decomposed the electromagnetic operator as

$$H_{\gamma} = H_{\gamma,1} + H_{\gamma,2} + H_{\gamma,3}.$$
 (16)

Due to a severe singularity in the integral kernel caused by the long-range property of the Coulomb interactions, we solve a modified version of Eq. (14) as described in Ref. [9]. Some technical remarks in solving the Faddeev equations for three-body breakup reactions accommodating three-body potentials are given in Refs. [9, 12].

3. Models and calculations

3.1. Interactions

An interaction potential for the α - α system is taken from Ref. [13]:

$$V(x) = \left(125\hat{P}_{2\alpha,L=0} + 20\hat{P}_{2\alpha,L=2}\right)e^{-(x/1.53)^2} - 30.18e^{-(x/2.85)^2} + \frac{4e^2}{x^2},\tag{17}$$



Figure 1. Calculated α - α scattering phase shifts for L = 0 and L = 2 partial waves with the potential Eq. (17). Experimental data are taken from Ref. [14].

where $\hat{P}_{2\alpha,L}$ is a projection operator on the *L* angular momentum state. This potential is a shallow one that does not contain forbidden states, and produces a L = 0 resonance (⁸Be) at 0.093 MeV with the width of 8 eV. Figure 1 shows the scattering phase shifts for the L = 0 and L = 2 partial waves using this potential.

In order to reproduce some 3- α observables, such as binding energies and resonance energies, we introduce a three-body potential (3BP), which depends on the total angular momentum of the 3- α system, which takes a form given in Ref. [13]:

$$V_{3\alpha} = \sum_{J=0,2} \hat{P}_{3\alpha,J} W_3^{(J)} \exp\left(-\frac{A_{\alpha}R^2}{2b_3^2}\right),\tag{18}$$

where $\hat{P}_{3\alpha,J}$ is a projection operator on the 3- α state with the total angular momentum J, $A_{\alpha} = m_{\alpha}/m_N = 3.97$ and $b_3 = 3.9$ fm, and the strength parameters $W_3^{(J)}$ will be determined in the following.

3.2. Three-body calculations

For the initial state of the E2-photodisintegration, the ${}^{12}C(2_1^+)$ state, we calculate a 3- α bound state by taking into account α - α states of the angular momentum up to 2 with the 2BP, Eq. (17) and the 3BP, Eq. (18). The strength parameter of the 3BP is determined to be $W_3^{(2)} = -56$ MeV, which gives the binding energy of ${}^{12}C(2_1^+)$ state as -2.763 MeV in comparison with the empirical value of -2.8357 MeV [4].

For calculations of $3 - \alpha$ continuum states with zero angular momentum, we take into account the 2BP of L = 0. It turns out that calculated photodisintegration cross sections reveal a sharp peak corresponding to the Hoyle state, and the energy of the peak position strongly depend on the choice of the 3BP strength parameter. Calculated cross sections for $W_3^{(0)} = -169.0$ MeV, -169.5 MeV, and -170.0 MeV, which produce the $3 - \alpha$ resonance energy close to the experimental value, are shown in figure 2. Obtained values of the $3 - \alpha$ resonance energy and the width of the resonance peak as well as the E2 strength function $B(E2; 0_2^+ \rightarrow 2_1^+)$ are shown in table 1. Although the calculations do not reproduce the B(E2) value, we do not introduce an effective charge in the present work.

Calculated 3α reaction rates are shown in figure 3 as a function of the temperature $T_7 = T/(10^7 \text{K})$ together with the NACRE rate and the OKK rate for a comparison. In figure 4, ratios of our calculations to the NACRE rate are shown.

Apparently our results are not consistent with the OKK rate at low temperatures. Compared to the NACRE rate, our results are about 10^3 times larger at $T_7 = 1$ almost independently on the choice of the 3BP strength parameter. At higher temperatures, the results with different



Figure 2. Photodisintegration cross section for the process, Eq. (2), as a function of the photon energy. The solid (black), dashed (red), and dotted (green) lines denote calculations with $W_3^{(0)} = -169.0$ MeV, $W_3^{(0)} = -169.5$ MeV, and $W_3^{(0)} = -170.0$ MeV, respectively.

Table 1. Resonance parameters of the Hoyle state and the E2 strength function B(E2) for the transition from the Hoyle state to ${}^{12}C(2_1^+)$ state for the calculations with $W_3^{(0)} = -169.0$ MeV, -169.5 MeV, and -170.0 MeV. Experimental values are taken from Ref. [4].

$W_3^{(0)}$ (MeV)	$E_r \; ({\rm MeV})$	Γ (eV)	$B(E2; 0_2^+ \to 2_1^+) \ (e^2 \text{fm}^4)$
-169.0	0.396	19.2	9.9
-169.5	0.380	10.2	9.8
-170.0	0.364	5.0	9.9
Exp.	0.3794	$8.3 {\pm} 1.0$	13.3 ± 1.8



Figure 3. 3α reaction rate as a function of the temperature $T_7 = T/(10^7 \text{K})$. The solid (black), dashed (red), and dotted (green) lines denote calculations with $W_3^{(0)} = -169.0$ MeV, $W_3^{(0)} = -169.5$ MeV, and $W_3^{(0)} =$ -170.0 MeV, respectively. The dasheddotted (blue) line denotes the NACRE rate [6]. The dashed-dotted-dotted (purple) line denotes the OKK rate [7].

3BP strength parameters tend to approach to the NACRE rate. The results with $W_3^{(0)} = -169.5$ MeV, which almost reproduces the 3- α resonance energy, are about 30% smaller than the NACRE rate for $T_7 > 10$. This reduction rate almost agrees with that of the E2 strength as compared to the experimental value as demonstrated in table 1, which means that our calculation renormalized by an effective charge to reproduce the E2 strength may reproduce the NACRE rate well at higher temperatures.

The underestimation of the NACRE rate compared to ours at low temperatures is qualitatively consistent with an argument of Ogata *et al.* that it is because of a proper magnification of the Coulomb barrier between an α - α pair and the spectator α particle by the use of resonant α - α wave functions instead of the non-resonant ones. However, the size of its effect in our rates is extremely smaller than that of the OKK rate.



Figure 4. Ratio of the 3α reaction rate to the NACRE rate. The solid (black), dashed (red), and dotted (green) lines denote calculations with $W_3^{(0)} = -169.0$ MeV, $W_3^{(0)} = -169.5$ MeV, and $W_3^{(0)} = -170.0$ MeV, respectively.

4. Summary

In this paper, calculations of the 3α reaction as a quantum mechanical three-body problem are performed. For this, a wave function corresponding to the inverse process, Eq. (2), is defined and solved by applying the Faddeev three-body theory with accommodating long-range Coulomb force effect, which has been successfully applied for three-nucleon systems.

Our results of the 3α reaction rate are consistent with the NACRE rate at higher temperatures of $T_7 > 10$, where the resonant process may be dominant, and are about 10^3 times larger at low temperature of $T_7 = 1$. This means that the ratio of the OKK rate to the present result still exceeds 10^{20} at $T_7 = 1$.

Although the three-body Hamiltonian used in the CDCC calculations and that in the present calculation are not exactly the same, they are essentially the same kind in a sense that potential parameters are determined so as to reproduce the resonance and binding energies of the 2- α and the 3- α systems. Thus the difference might be ascribed to the methods to solve the three-body problem, which should be clarified. Also, it would be interesting to extend the calculations for the use of various α - α and 3- α interaction models including a microscopic cluster model and for higher energies.

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