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Imaginary-time formalism for triple- α reaction rates

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Using imaginary-time formalism, it is shown that the triple- α reaction rate can be reliably calculated without the need to solve scattering problems involving three charged particles. The calculated reaction rate is found to agree well with the empirical NACRE rate, which is widely adopted in stellar evolution calculations. The reason for this is explained using R -matrix theory. Extremely slow convergence is found to occur when a coupled-channel expansion is introduced, which helps to explain the very different reaction rates obtained using a coupled-channel approach.

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The triple- α reaction is a key process that influences the production of all heavy elements in the universe. Accurate knowledge of the reaction rate is essential for understanding stellar evolution and nucleosynthesis. Since experimental measurements are not feasible for this reaction, theoretical evaluation of the reaction rate is crucially important.

In the triple- α process, the importance of ^{12}C and ^8Be resonances is well recognized [1,2]. At high temperature, the reaction proceeds dominantly through a resonant 0^+ state of ^{12}C at 7.65 MeV, which is known as the Hoyle state. At lower temperatures, processes that do not involve the Hoyle state become important. An empirical reaction rate assuming successive two-body reactions of α - α and α - ^8Be has been derived [3–5] and is adopted in the NACRE compilation [6] as the standard rate to be used in stellar evolution calculations.

However, the validity of the empirical rate formula should be confirmed by calculations based on microscopic quantum theories. Several theoretical attempts to calculate the rate using quantum theory involving three α particles have recently been undertaken. The first was conducted by Ogata and coworkers [7], and employed continuum-discretized coupled-channel (CDCC) theory, which is a well-established theory for direct nuclear reactions [8]. A surprisingly high value for the reaction rate was found at low temperatures, and at $T = 0.01$ GK it was larger than the NACRE value by 26 orders of magnitude [6]. Soon after this report was published, the consequences of the new rate for the present understanding of stellar evolution were investigated [9–11]. It was pointed out that such a high rate would not be compatible with the standard picture of stellar evolution; for example, the red giant phase disappears if the rate is adopted [9,11]. Following the report by Ogata *et al.*, calculations using different quantum three-body approaches have been carried out [12–17]. Unfortunately, there is a large degree of scatter in the reported rates at low temperatures, which vary between the NACRE rate [6] and that determined by the CDCC calculation [7]. In view of the number of successful achievements of nuclear three-body reaction theories, this huge discrepancy among the reported rates is both surprising and puzzling. However, two possible explanations can be put forward. The first is the lack of a rigorous scattering theory for three charged particles. The

second is related to the quantum-tunneling nature of the process: the α particle travels through the Coulomb barrier over a long distance, typically a few hundred femtometers, causing the reaction rate to be extremely small, and to vary by 60 orders of magnitude within the range of astrophysically relevant temperatures.

Recently, we proposed a new theoretical approach for determining the radiative capture reaction rate, which we refer to as imaginary-time formalism [18]. In this formalism, imaginary time is identified with inverse temperature as is often used in quantum many-body theories of nonequilibrium systems. A related approach has been developed for the theory of chemical reaction rates [19]. In this Rapid Communication, we report the application of the imaginary-time formalism to the determination of the triple- α reaction rate. In the past, several theoretical frameworks have been put forward for the triple- α process to overcome difficulties related to the Coulomb three-body scattering problem [12–17]. As will be shown below, the imaginary-time formalism provides a natural and useful framework for the triple- α process, avoiding any scattering problems to be solved.

The following expression describes the triple- α reaction rate [18]:

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

where $\beta = 1/k_B T$ is the inverse temperature, M_α is the mass of an α particle, H is the Hamiltonian for three α particles, Φ_f is the wave function for ^{12}C in the final state after 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 for the final state. $M_{\lambda\mu}$ is the multipole transition operator for γ -ray emission with a multipolarity λ . The reaction of three α particles with total angular momentum $J = 0$ is considered, which leads to the emission of a γ ray with $\lambda = 2$, and the 2^+ state of ^{12}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. It can easily be shown that Eq. (1) exactly coincides with the expression for the triple- α reaction rate, Eqs. (2)–(5) of [20], by inserting a completeness relation for a functional space of three α particles into Eq. (1).

In practice, to evaluate the reaction rate using Eq. (1), it is necessary to calculate $\Psi(\beta) = e^{-\beta H} M_{\lambda\mu}^\dagger \Phi_f$. This is achieved by evolving the wave function along the imaginary-time axis,

$$-\frac{\partial}{\partial\beta}\Psi(\beta) = H\Psi(\beta), \quad (2)$$

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

$$\langle\alpha\alpha\alpha\rangle \propto \sum_{M_f\mu} \left\langle \Psi\left(\frac{\beta}{2}\right) \left| \left(\frac{H - E_f}{\hbar c} \right)^5 \right| \Psi\left(\frac{\beta}{2}\right) \right\rangle. \quad (3)$$

The numerical calculations are carried out using the model space and the three-body Hamiltonian described below. In the calculations, the α particles are treated as point particles. The assumption of dominant $J = 0$ contribution is expected to be valid below $T < 1.0$ GK [20,21]. A Jacobi coordinate system is used, defined by $r = r_1 - r_2$ and $R = (r_1 + r_2)/2 - r_3$, where r_i ($i = 1-3$) are the coordinates of the 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, only the $L = 0$ component is considered, since this is expected to be the most important at low temperature. Ogata *et al.* adopted the same model space for their CDCC calculations [7]. The radial variables R and r are discretized with a grid size $\Delta R = \Delta r = 0.5$ fm, and radial grid points are employed up to the maximum values, R_{\max} and r_{\max} . The differential operators in the Hamiltonian are treated using a nine-point finite difference formula. To solve Eq. (2), the Taylor expansion method is used for short-time evolution with a step size of $\Delta\beta = 0.004$ MeV $^{-1}$.

The Hamiltonian H for the three α particles is constructed as follows. For the potential between two α particles, the Ali-Bodmer potential is used, considering only the $l = 0$ angular momentum channel [22]. The potential parameter is modified slightly so that it accurately reproduces the resonance corresponding to the ground state of ${}^8\text{Be}$ at 92.08 keV. A three-body potential among the three α particles is added, and is given by $V_{3\alpha}(r_1, r_2, r_3) = V_3 e^{-\mu(r_{12}^2 + r_{23}^2 + r_{31}^2)}$ with $\mu = 0.15$ fm $^{-2}$. The value of V_3 is chosen so that the resonance energy of the Hoyle state, the 0_2^+ state of ${}^{12}\text{C}$, is reproduced at 379.8 keV above the three- α threshold. The final wave function Φ_f for ${}^{12}\text{C}$ $J^\pi = 2^+$ at 4.44 MeV is constructed using the orthogonality condition model [23].

In Fig. 1, the calculated triple- α reaction rates for different spatial areas specified by R_{\max} and r_{\max} are compared. The NACRE rate [6] is also shown for comparison. It can be seen that when R_{\max} and r_{\max} are larger than 400 fm, a fully converged reaction rate is obtained in the entire temperature region, and this rate coincides well with the NACRE rate. Calculations within smaller spatial areas yield a rate which is valid only in limited higher-temperature regions.

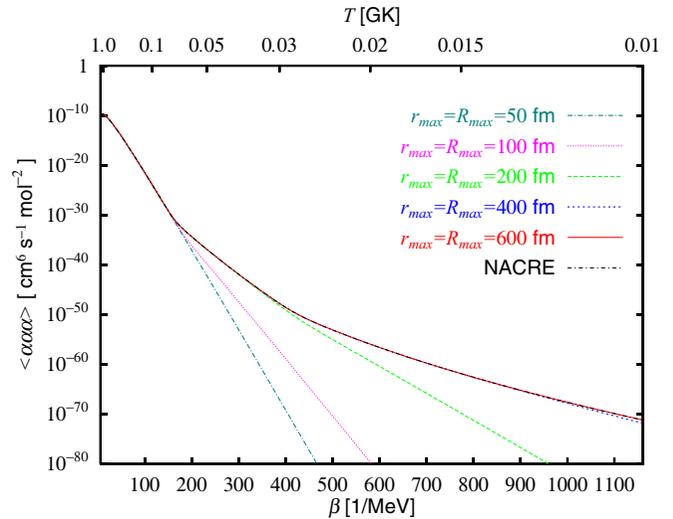


FIG. 1. (Color online) Calculated triple- α reaction rates for different choices of radial cutoff distances, r_{\max} and R_{\max} . The NACRE rate is also shown for comparison.

We also checked the convergence with respect to the truncation of angular momentum L . In Fig. 2 we show the convergence behavior of the reaction rate for the inclusion of the partial waves up to L_{\max} . The convergence is very quick and only the $L = 2$ term makes a sizable contribution. The converged reaction rate increases by at most two orders of magnitude at low temperatures and still is in good coincidence with the NACRE rate. We note that the symmetry property of the wave function due to identical α particles, which is not satisfied in our approach, is recovered by increasing L_{\max} .

In the empirical NACRE formula, there are three temperature regions that are distinguished by different reaction mechanisms [24]: $T > 0.074$ GK dominated by the Hoyle state process, $0.074 > T > 0.028$ GK dominated by the α - ${}^8\text{Be}$

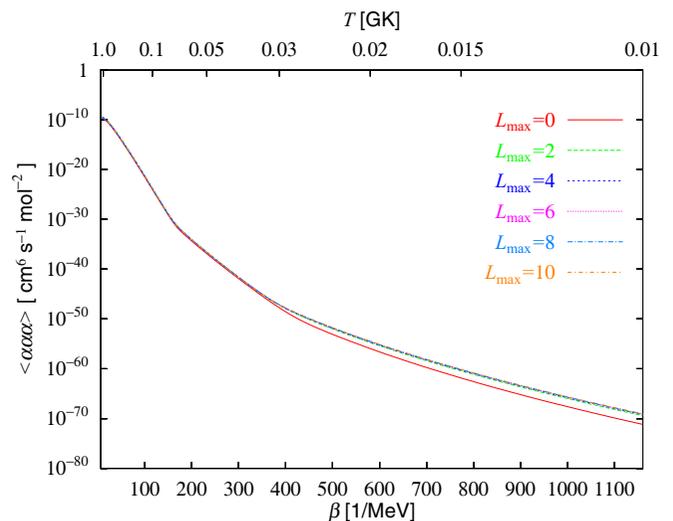


FIG. 2. (Color online) Calculated triple- α reaction rate for different choices of maximal angular momentum of the partial wave, L_{\max} .

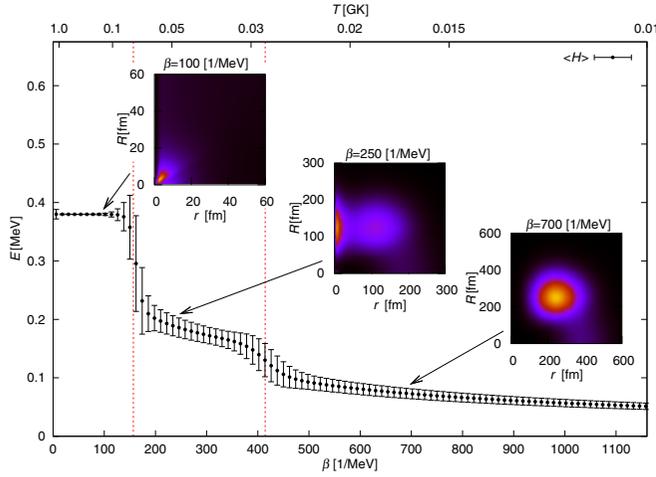


FIG. 3. (Color online) Energy expectation value and variance as function of temperature. The insets show density distributions for three different temperatures.

two-body nonresonant process, and $T < 0.028$ GK dominated by a nonresonant process involving three α particles. A careful look at Fig. 1 reveals that the calculated rate curves show changes in slope at exactly the same temperatures.

To illustrate this more clearly, Fig. 3 shows the energy expectation value and the variance, defined by $\bar{E} = \langle \Psi(\beta/2) | H | \Psi(\beta/2) \rangle / \langle \Psi(\beta/2) | \Psi(\beta/2) \rangle$ and $(\Delta E)^2 = \langle \Psi(\beta/2) | (H - \bar{E})^2 | \Psi(\beta/2) \rangle / \langle \Psi(\beta/2) | \Psi(\beta/2) \rangle$, as a function of the inverse temperature, respectively. The insets show the density distribution, $\rho(R, r, \beta/2) = u_{L=0}(R, r, \beta/2)^2 / R^2 r^2$, for three typical temperatures.

In the high-temperature region $T > 0.074$ GK, the energy expectation value coincides with the resonance energy of the Hoyle state, $\bar{E} = 379.8$ keV, indicating the dominance of the Hoyle state process. In addition, the density $\rho(R, r, \beta/2)$ is localized within a small R and r region, which is consistent with the resonant picture. In the medium-temperature region, $0.074 > T > 0.028$ GK, most of the density is contained within a small r region, $r < 10$ fm, whereas it is extended along the R direction. This indicates that two of the α particles are forming a ${}^8\text{Be}$ resonance, with the third remaining outside. In the lowest temperature region, $T < 0.028$ GK, the density extends in both the R and r directions, indicating the nonresonant character of the reaction.

The agreement between the calculated and NACRE rates, not only in terms of the magnitude, but also with regard to the change in reaction mechanism, indicates that the imaginary-time formalism provides quantum-mechanical support for the conventional description. An analytic investigation based on microscopic three-body theory was next carried out to determine if the empirical formula [3,6] is justified.

In the empirical formula, it is assumed that successive α - α and α - ${}^8\text{Be}$ reactions occur, and the reaction cross sections are described using Breit-Wigner formulas. It will be shown that it is possible to derive a formula quite similar to the empirical one starting from Eq. (1), by assuming that the three-body Hamiltonian is separable, and then approximating it using R -matrix theory [25].

The separability assumption for the three-body Hamiltonian is written as $H = h_{\alpha\alpha}(r) + h_{\alpha\text{Be}}(R)$, where the α - α Hamiltonian, $h_{\alpha\alpha}(r) = T_r + V_{\alpha\alpha}(r)$, has a resonance at $E_r^{\alpha\alpha} = 92.08$ keV. The normalized wave function for the resonance is expressed as $\phi_r^{\alpha\alpha}(r)$. In addition, a simple potential model is assumed for the α - ${}^8\text{Be}$ relative motion, so that $h_{\alpha\text{Be}}(R) = T_R + V_{\alpha\text{Be}}(R)$. The potential $V_{\alpha\text{Be}}(R)$ is chosen so as to give a resonance at $E_r^{\alpha\text{Be}} = 287.7$ keV with the normalized wave function of $\phi_r^{\alpha\text{Be}}(R)$. The Hoyle state is then described by the wave function product, $\phi_r^{\alpha\alpha}(r)\phi_r^{\alpha\text{Be}}(R)$, at the summed resonance energy of $E_r^{\alpha\alpha} + E_r^{\alpha\text{Be}} = 379.8$ keV.

The following approximation is then introduced. The problem of potential scattering in either the α - α or α - ${}^8\text{Be}$ system is considered. The resonance energy is denoted as E_r and its normalized radial wave function as $u_r(r)$. Using R -matrix theory [25], the radial wave function at an energy E around a resonance with an asymptotic form of $u_E(r) \rightarrow (2\mu/\pi\hbar^2k)^{1/2} \sin(kr + \delta)$ can be approximated by

$$u_E(r) = u_r(r) \sqrt{L(E, E_r, \Gamma_r(E))}, \quad (4)$$

where $L(E, E_r, \Gamma_r)$ is a Lorentzian function given by

$$L(E, E_r, \Gamma_r(E)) = \frac{1}{2\pi} \frac{\Gamma_r(E)}{(E - E_r)^2 + \Gamma_r(E)^2/4}. \quad (5)$$

Here the shift of the resonance energy is ignored. The energy-dependent width $\Gamma_r(E)$ is related to the width at the resonance energy Γ_r by $\Gamma_r(E) = \Gamma_r P_l(E)/P_l(E_r)$, where $P_l(E)$ is the penetrability.

Using Eq. (4), any function $f(H)$ of the three-body separable Hamiltonian H can be approximated as

$$f(H) = |\phi_r^{\alpha\alpha}(r)\rangle\langle\phi_r^{\alpha\alpha}(r)| \cdot |\phi_r^{\alpha\text{Be}}(R)\rangle\langle\phi_r^{\alpha\text{Be}}(R)| \cdot \int dE_{\alpha\alpha} \int dE_{\alpha\text{Be}} L(E_{\alpha\alpha}, E_r^{\alpha\alpha}, \Gamma_r^{\alpha\alpha}(E_{\alpha\alpha})) \times L(E_{\alpha\text{Be}}, E_r^{\alpha\text{Be}}, \Gamma_r^{\alpha\text{Be}}(E_{\alpha\text{Be}})) f(E_{\alpha\alpha} + E_{\alpha\text{Be}}), \quad (6)$$

where $\Gamma_r^{\alpha\alpha}$ and $\Gamma_r^{\alpha\text{Be}}$ are the α -decay widths of the α - α and α - ${}^8\text{Be}$ resonances, respectively. Substituting this into Eq. (1) gives

$$\langle\alpha\alpha\alpha\rangle = 6 \times 3^{3/2} \left(\frac{2\pi\beta\hbar^2}{M_\alpha} \right)^3 \times \int dE_{\alpha\alpha} \int dE_{\alpha\text{Be}} L(E_{\alpha\alpha}, E_r^{\alpha\alpha}, \Gamma_r^{\alpha\alpha}(E_{\alpha\alpha})) \times L(E_{\alpha\text{Be}}, E_r^{\alpha\text{Be}}, \Gamma_r^{\alpha\text{Be}}(E_{\alpha\text{Be}})) e^{-\beta E_{\alpha\alpha} - \beta E_{\alpha\text{Be}}} \times \Gamma_\gamma({}^{12}\text{C}; 0_2^+) \left(\frac{E_{\alpha\alpha} + E_{\alpha\text{Be}} - E({}^{12}\text{C}; 2^+)}{E_r({}^{12}\text{C}; 0_2^+) - E({}^{12}\text{C}; 2^+)} \right)^5, \quad (7)$$

where $\Gamma_\gamma({}^{12}\text{C}; 0_2^+)$ is the radiative decay width of the Hoyle state and $E({}^{12}\text{C}; 2^+)$ is the excitation energy of the first 2^+ state of ${}^{12}\text{C}$. The rate expression given in Eq. (7) is almost equivalent to the empirical NACRE formula [6]. Thus, a formula quite close to the NACRE formula could be successfully derived, starting with a microscopic three-body Hamiltonian.

However, a question still remains regarding the validity of assuming that the three-body Hamiltonian is in fact separable. To resolve this, a numerical investigation was carried out to

determine how much this assumption changes the calculated reaction rate. It was found that using the separable Hamiltonian when solving Eq. (2) changed the reaction rate by only a factor of 2 or less. This indicates that if the Hamiltonian is constructed such that the ^8Be ground state and ^{12}C Hoyle state resonances are reasonably described, the separability approximation does not seriously affect the reaction rate.

The largest numerical difference between Eq. (7) and the NACRE expression is associated with the width $\Gamma_r^{\alpha\text{Be}}$. In the derivation used in the present paper, this quantity represents the decay width of the α - ^8Be resonance, while in the NACRE derivation it is the particle decay width of the Hoyle state, which may include both α - α and α - ^8Be decay.

Although the above results indicate that the NACRE rate is supported by our quantum three-body calculations, we should be aware that different theoretical approaches have yielded widely different reaction rates at low temperatures as mentioned before. For example, Refs. [14,16] employing the elaborated R -matrix theory with screening in the hyperspherical harmonic basis reported a substantial enhancement of the reaction rate at low temperature. On the other hand, Ref. [15] employing the Faddeev theory reported no enhancement at low temperature, giving results quite close to the NACRE rate. In those works, the symmetry property of the wave function due to identical α particles is correctly treated, while in the present work it is approximate. The origin of the large discrepancy between Refs. [14,16] and Ref. [15] is still unknown and needs further investigation.

The CDCC calculation of Ref. [7] reported a reaction rate which differs by 26 orders of magnitude at low temperature from the NACRE rate and our calculation. Since it employed almost the same model space as that with $L_{\text{max}} = 0$ in the present paper, it is possible to make a straightforward comparison by carrying out the imaginary-time evolution of Eq. (2) in terms of the coupled-channel scheme. We next show that the discrepancy between Ref. [7] and ours comes from a slow convergence of the coupled-channel expansion.

In the coupled-channel approach, the eigenvalue problem for α - α relative motion described by the Hamiltonian $h_{\alpha\alpha}(r)$ is first solved. Discretizing the radial variable r in 0.5-fm steps up to 600 fm gives 1200 grid points for this coordinate. Diagonalizing the radial Hamiltonian then gives 1200 eigenfunctions, $w_n(r)$ ($n = 1$ –1200). Eigenstates associated with 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 the 14th eigenstate. In the coupled-channel approach, the wave function is expanded in the form $u(R, r, \beta) = \sum_n v_n(R, \beta) w_n(r)$ and the imaginary-time evolution of $v_n(R, \beta)$ is calculated in the form of a matrix differential equation. It was first numerically confirmed that, employing all 1200 eigenstates in the expansion, the calculated rate exactly matches the result shown in Fig. 1, as is expected. However, if the number of basis functions in the expansion is truncated, the results depend on the degree of truncation. The dependence of the convergence behavior on the number of basis functions is shown in Fig. 4. In each coupled-channel calculation, the strength of the three-body potential among the three α particles is adjusted so that the Hoyle state always appears at 379.8 keV.

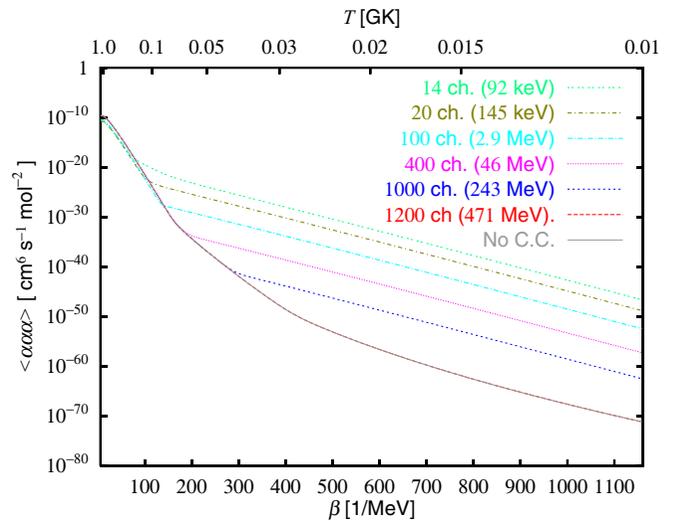


FIG. 4. (Color online) Calculated triple- α reaction rate using coupled-channel expansion for different numbers of channels, n_{max} . The energy eigenvalue of the α - α system corresponding to the n_{max} channel is indicated in the parentheses.

Employing states below the ^8Be ground state ($n_{\text{max}} = 14$), the reaction rate is much higher than that given by the fully converged calculation, and the difference is 24 orders of magnitude at $T = 0.01$ GK. This can be easily understood because low-energy eigenstates of $h_{\alpha\alpha}(r)$ are characterized by a large separation between two α particles outside the Coulomb barrier. The Coulomb barrier for the third α particle is then very small in these channels, yielding a high reaction rate. This artificial enhancement of the calculated reaction rate for a small channel number is reduced by off-diagonal coupling terms as the number of channels increases. However, as seen in Fig. 4, convergence is extremely slow. We note that, in [7], the channels are truncated at very low excitation energy, 176 keV. It is considered that this indicates a difficulty in numerically expressing exponentially small functions in the tunneling process using the basis expansion method.

In summary, imaginary-time formalism was applied to determine the triple- α reaction rate. Since the formalism does not require solving any scattering problems, it is quite suitable for the triple- α process. Indeed, a converged reaction rate was obtained without any numerical problems. The calculated rate agreed well with the conventional NACRE rate, not only in terms of the magnitude, but also in terms of the critical temperature where the dominant reaction mechanism changes. No enhancement of the rate was found at low temperature. The reason for the good agreement was analytically clarified using R -matrix theory. It was found that extremely slow convergence occurs if a coupled-channel expansion of the wave function is used, which helps to explain the very different reaction rates obtained with a coupled-channel approach. However, since there still remain discrepancies among different theoretical approaches, further investigations along the lines of the present paper employing a more realistic Hamiltonian will be required.

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