Low-Temperature Triple-Alpha Rate in a Full Three-Body Nuclear Model

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A new three-body method is used to compute the rate of the triple-alpha capture reaction, which is the primary source of ¹²C in stars. In this Letter, we combine the Faddeev hyperspherical harmonics and the *R*-matrix method to obtain a full solution to the three-body $\alpha + \alpha + \alpha$ continuum. Particular attention is paid to the long-range effects caused by the pairwise Coulomb interactions. The new rate agrees with the Nuclear Astrophysics Compilation of Reaction rates for temperatures greater than 0.07 GK, but a large enhancement at lower temperature is found ($\approx 10^{12}$ at 0.02 GK). Our results are compared to previous calculations where additional approximations were made. We show that the new rate does not significantly change the evolution of stars around one solar mass. In particular, such stars still undergo a red-giant phase consistent with observations, and no significant differences are found in the final white dwarfs.

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The triple-alpha reaction is key to the production of elements with mass $A \ge 12$. It plays a key role in many astrophysical processes, from stellar evolution to explosive scenarios. Since the early days when Fred Hoyle postulated that there should be a 0^+ resonance close to the 3α threshold to justify the observed abundances of 12 C in stars [1], a state experimentally confirmed by Dunbar et al. [2], the accepted mechanism for the triplealpha capture has been sequential: $\alpha + \alpha \rightarrow {}^{8}\text{Be}(0^{+}_{1})$ followed by ${}^{8}Be(0^{+}_{1}) + \alpha \rightarrow {}^{12}C(0^{+}_{2})$. However, if the energy of the alpha particles in the stellar environment is insufficient to populate the narrow resonances, a direct threebody capture becomes the favored path. The most recent compilation of charge-particle induced thermonuclear rates (Nuclear Astrophysics Compilation of Reaction rates) [3] extrapolates the sequential model to low energy, an approach that should be questioned [4,5]. Recent theoretical works [4,5] predict enhancements in the triple-alpha rate by 7 to 20 orders of magnitude when compared to NACRE, for temperatures around 0.02 GK. Because the triple-alpha rate, even at these low temperatures, can have dramatic and widespread effects in astrophysics, it is critical to resolve the large discrepancies found between Refs. [3–5]. This is the aim of the present Letter.

The Hoyle resonance dominates the triple-alpha rate at $T \sim 0.1$ GK, while other resonances play a role at $T \sim 1$ GK, relevant in explosive environments. At these high temperatures, a ${}^{12}C(0_3^+)$ state around 3 MeV above the 3α threshold [6] contributes significantly to the rate, but the main path for the capture is through a high-lying ${}^{12}C(2_2^+)$ resonance, which decays directly to the ground state of ${}^{12}C$ [7]. Uncertainties in the properties of this 2_2^+ state have been recently addressed [8]. It is important to note that this 2^+ resonance has little influence at very low temperatures. Even if the triple-alpha resonant rate remains more uncertain than desired [9], it is far better understood than the nonresonant counterpart.

At temperatures below $T \approx 0.07$ GK, the 3 α -particles, having no access to intermediate resonances, fuse directly. The description of this process requires a good solution to the three-body scattering equation including Coulomb effects. A recent work by the Kyushu group [4] makes use of the continuum discretized coupled channel (CDCC) method [10], which expands the full three-body wave function in terms of the continuum states in the two-body subsystem (in this case ⁸Be). In this method, resonant and nonresonant processes are treated on the same footing. The CDCC method has been widely used in nuclear reactions, but the application to the triple-alpha capture is particularly challenging because the charged particle reaction occurs at large distances and is dominated by the Coulomb interactions. The CDCC results [4], when compared to NACRE, show a 20 orders of magnitude increase in the reaction rate at T = 0.02 GK. Soon after these results became available, numerous astrophysical studies were performed to understand the implications of such a dramatic change. Stellar evolution calculations [11,12] demonstrate that the CDCC rate suppresses He flashes in the asymptotic giant branch and can result in the disappearance of the red giant phase in low- and intermediate-mass stars. Studies of He ignition in accreting white dwarfs [13] and neutron stars [14,15] show that the CDCC rate is barely consistent with observations of type Ia supernovae and type I x-ray bursts, respectively.

The CDCC calculations in Ref. [4] represent the first attempt to take into account nonresonant contributions to the triple-alpha cross section at very low relative energies, where it is expected to dominate. The main drawback of the CDCC method is that, in general, the truncated CDCC wave function does not have the correct asymptotic form for the scattering of three charged particles [16]. It is known that the asymptotic form is naturally expressed in terms of hyperspherical coordinates [16]. Recent attempts to solve the $\alpha + \alpha + \alpha$ problem by the Madrid-Aarhus collaboration [17,18] employ the hyperspherical adiabatic expansion method. Limitations in the numerical techniques did not allow for determining the rate below $T \approx 0.1$ GK. In this Letter, we discuss another method based on the hyperspherical coordinates that does provide improved accuracy and enables us to reach temperatures down to 0.01 GK.

An alternative and rather schematic approach was recently proposed [5]. Inspired by the low-energy extrapolation of the sequential process implemented in NACRE, Ref. [5] proposed an extrapolation of the three-body Breit-Wigner form for the contribution to the three-body capture that does not go through the ⁸Be resonance. This method is referred to as BW(3B) here. Results for the triple-alpha reaction rate in Ref. [5] show a modification of the temperature dependence of the rate at low temperatures amounting to a 7 orders of magnitude increase of the triple-alpha rate at 0.02 GK when compared to NACRE.

The studies in Refs. [4,5,18] approach the triple-alpha reaction as a three-body problem. Presently, a fully microscopic approach to the nonresonant triple-alpha capture is not feasible. In this Letter, we also follow the three-body approach, and expect the microscopic corrections to this approach to be small compared to the three-body effects discussed in Refs. [4,5].

The reaction rate R_{abc} for $a + b + c \rightarrow D + \gamma$ at a given energy *E* can be related to the cross section for photo-dissociation σ_{γ} through

$$R_{abc}(E) = p! N_A^2 G_{abc,D} \frac{\hbar^3}{c^2} \frac{8\pi}{(\mu_{ab}\mu_{ab,c})^{3/2}} \frac{E_{\gamma}^2}{E^2} \sigma_{\gamma}(E_{\gamma}) \quad (1)$$

with E_{γ} the photon energy, *E* the three-body energy, μ_{ab} and $\mu_{ab,c}$ the reduced masses of the a + b and (ab) + csystems, respectively, *p* the number of identical particles, N_A Avogadro's number, and $G_{abc,D}$ a statistical factor depending on the spins of the nuclei *a*, *b*, *c*, and *D* [5]. The energies are related by $E_{\gamma} = E + |E_D|$, where E_D is the energy of the bound final state of *D* relative to the 3α threshold. The relevant astrophysical quantity is the energy averaged reaction rate $\langle R_{abc} \rangle(T)$ obtained by integrating $R_{abc}(E)$ over the Maxwell-Boltzmann distribution.

At low energies, the photo-dissociation process is usually dominated by a single transition of multipolarity λ , so

$$\sigma_{\gamma} = \frac{(2\pi)^3(\lambda+1)}{\lambda[(2\lambda+1)!!]^2} \left(\frac{E_{\gamma}}{\hbar c}\right)^{2\lambda-1} \frac{dB(E\lambda)}{dE}$$
(2)

depending on the corresponding electromagnetic transition strength $dB(E\lambda)/dE$. For the triple-alpha reaction at low energies, the reaction proceeds through a quadrupole transition from the 0⁺ continuum to the 2⁺₁ bound state in ¹²C.

In order to calculate the transition strength dB(E2)/dEat low relative energies, we need to solve the bound threebody problem to obtain the 2_1^+ state and the full scattering three-body problem for the 0^+ triple-alpha continuum. To solve the three-body Faddeev equation, we use the hyperspherical harmonic (HH) method [19]. Hyperspherical coordinates (hyper-radius $\rho = \sqrt{x_i^2 + y_i^2}$ and hyperangle $\theta_i = \tan \frac{x_i}{y_i}$) are introduced as functions of the scaled Jacobi coordinates x_i , y_i , with i = 1, 2, 3 [19]. The HH method expands the three-body wave function as sums of products of hyper-radial functions $\chi_{\gamma}(\rho)$ and angular functions $\Omega_{\gamma}(\theta, \hat{\vec{x}}, \hat{\vec{y}})$, where $\gamma = \{i, K_i, l_{x_i}, l_{y_i}\}$. This expansion introduces a new quantum number, the hypermomentum K_i , and sufficiently many K_i values need to be used to obtain convergence. The orbital angular momenta l_{x_i} , l_{y_i} refer to the Jacobi coordinates x_i , y_i . Introducing the HH expansion in the Faddeev equations gives the set of coupled channel equations in the hyper-radius coordinate:

$$\left(\frac{\hbar^2}{2m} \left[\frac{d^2}{d\rho^2} - \frac{\Delta_i(\Delta_i + 1)}{\rho^2}\right] + E\right) \chi_{\gamma}(\rho) = \sum_{\gamma'} V_{\gamma\gamma'}(\rho) \chi_{\gamma'}(\rho),$$
(3)

where $\Delta_i = K_i + 3/2$ and *m* is a scaling mass. The coupling potentials are defined as the sum of three pairwise interactions $V_{jk}(\rho, \theta)$ plus a three-body force $V_{3b}(\rho)$, integrated over all variables but ρ :

$$V_{\gamma\gamma'}(\rho) = \langle \Omega_{\gamma}(\theta, \hat{\vec{x}}, \hat{\vec{y}}) | \sum_{k>j=1}^{3} V_{jk} + V_{3b} | \Omega_{\gamma'}(\theta, \hat{\vec{x}}, \hat{\vec{y}}) \rangle.$$
(4)

We take the same interactions for the three-body Hamiltonian as in Ref. [17]. After minor adjustments, this reproduces the ⁸Be ground state, and the ¹²C 2_1^+ bound state and 0_2^+ Hoyle resonance. We explicitly take into account the symmetrization of the system, thereby reducing the set of coupled equations.

The solution for the 2^+_1 bound state is obtained by solving Eq. (3) for negative energy E. The numerical method is implemented in the code FACE[20], which is specifically designed for three-body bound states. The 0^+ continuum states are found by using the *R*-matrix method in the HH basis (HHR), originally developed in the context of core + n + n scattering [21], a problem with different symmetries and no Coulomb interactions. The HHR method generates an orthonormal basis set to solve Eq. (3) in a box with hyper-radius ρ_m by fixing the logarithmic derivative there. We expand χ_{γ} in terms of the HHR basis. Due to the long-range Coulomb forces, numerical solutions are needed out to the very large distances $(\rho \gg 100 \text{ fm})$, where it becomes safe to ignore off-diagonal couplings, and matching to known Coulomb functions can be performed [16]. Extending the orthonormal basis to the required large ρ would be impractical, so we use an

R-matrix propagation technique [22] out to an asymptotic $\rho_a \gg \rho_m$. We divide the interval from ρ_m to ρ_a into sectors labeled *p*, the sizes of which are sufficiently small so that the interactions within can be taken as constant. The propagating functions G^p are then given in terms of complex exponentials [22], and used to propagate from sector p - 1 to the next:

$$-R^{p}_{\gamma\gamma'} = G^{p}_{\gamma\gamma'}(\rho^{p}_{R}, \rho^{p}_{R}) + \sum_{\alpha,\beta} G^{p}_{\gamma,\alpha}(\rho^{p}_{R}, \rho^{p}_{L})$$
$$\times [R^{p-1} - G^{p}(\rho^{p}_{L}, \rho^{p}_{L})]^{-1}_{\alpha,\beta} G^{p}_{\beta,\gamma'}(\rho^{p}_{L}, \rho^{p}_{R}).$$
(5)

This gives the *R*-matrix on the right side of the boundary R^p from R^{p-1} on the left. The coordinate subscripts ρ_R , ρ_L imply the evaluations on the right and the left sides of the boundary, respectively. While without Coulomb this propagation method was numerically stable, including Coulomb interaction introduced numerical instabilities in the threebody scattering wave function in the turning-point region. To overcome these instabilities, we introduced screening in the off-diagonal potentials Eq. (4) using a Woods-Saxon multiplying factor $(1 + \exp[(\rho - \rho_{\text{screen}})/a_{\text{screen}}])^{-1}$. Our calculations use a sufficiently large screening radius such that dB(E2)/dE for E = 0.05 - 0.5 MeV becomes independent of ρ_{screen} and a_{screen} .

Convergence of dB(E2)/dE was checked for all the relevant parameters. At relative energies $\approx 0.1 \text{ MeV}$, dB(E2)/dE picks up contributions from the wave functions at hyper-radii $\rho = 5 - 30$ fm. However, in order to get a reliable three-body scattering wave function, matching to the asymptotic form needs to be performed at $\rho \gg \rho_{\text{screen}}$. The results here presented include up to K = 26 in the HH expansion, 50 poles in the *R*-matrix expansion, an R-matrix box size of 50 fm, and R-matrix propagation out to 3000 fm. In addition, we use $\rho_{\text{screen}} =$ 800 fm and $a_{\text{screen}} = 10$ fm to screen the off-diagonal couplings. The only limiting factor for full convergence is the truncation in K_{max} . We carefully studied the exponential behavior of dB(E2)/dE as a function of K_{max} for the relative energy range E = 0.01 - 0.15 MeV (the relevant region for rates below 0.07 GK). We conclude that our results with $K_{\text{max}} = 26$ differ from those obtained from the extrapolation of $K_{\text{max}} \rightarrow \infty$ by a factor of at most 2. Our energy-averaged rates are plotted in Fig. 1 as a function of temperature (solid line). The factor of 2 error on the rate at low energy cannot be seen, given the scales in Fig. 1.

Our method to determine the three-body scattering state can be checked for the pure Coulomb case. In that case, no resonances are present in either the two-body or three-body systems, and the capture is necessarily direct. For the pure Coulomb case, the propagation technique is stable, and we were able to unambiguously determine that no error is introduced by screening the off-diagonal couplings. In addition, there is an analytic solution of Eq. (3) for the pure diagonal Coulomb couplings, which we use to test our implementation. The rate for diagonal Coulomb differs



FIG. 1 (color online). Different evaluations of the triple-alpha reaction rate: comparing the hyperspherical harmonic *R*-matrix method (solid) with NACRE (dotted), CDCC (dashed), and the three-body Breit Wigner (dot-dashed) methods.

from the full rate by 10 orders of magnitude, thus demonstrating the importance of including the Coulomb effects correctly. The off-diagonal Coulomb couplings are important, but their major contribution to the rates in the range T = 0.01-1.00 GK occurs for $\rho < 100$ fm.

In Fig. 1, we compare our results (solid) with those obtained previously. The rate obtained from the full solution of the HHR equations agree with NACRE (dotted line) above 0.07 GK. Although there is a slight reduction of the rate below 0.07 GK, we find a pronounced increase of the rate for T < 0.06 GK, accompanied by a very different temperature dependence. In some ways, the results obtained by assuming a rate extrapolated with a three-body Breit-Wigner form BW(3B) (dot-dashed line) [5] are qualitatively similar, but the BW(3B) treatment enhances the rate to a smaller degree. Although we do find a strong enhancement at low energy, it is not as strong as that seen in the CDCC result of Ref. [4] (long-dashed line). While the deviation of the CDCC results from NACRE is seen all the way up to 0.11 GK, the HHR result agrees with NACRE for T > 0.07 GK. This aspect turns out to be crucial in the repercussions for astrophysics.

The kink observed (Fig. 1) in the full rate around $T \approx 0.06$ GK is a signature of two processes with different temperature dependence. Above $T \approx 0.06$ GK the process through the Holye state dominates, while below there is mostly nonsequential (direct) capture. The calculations in Ref. [5] exhibit this same feature. Temperature dependence is best illustrated by evaluating $d \ln \langle R_{\alpha\alpha\alpha} \rangle / d \ln T$, as shown in Table I. For T < 0.06 GK the HHR rate has a much weaker temperature dependence than the NACRE rate, as is evident in Fig. 1. For T > 0.06 GK, the HHR rate follows that of NACRE, and their temperature sensitivities are basically equal (Table I).

We have tested the sensitivity of the rate to the nuclear interaction and the three-body force by using the same Hamiltonian as Ref. [4] to calculate the 0^+ continuum.

IADLE I.	Temperature sensitivity of unpre-arpita rate	
T (GK)		$d\ln\langle R_{\alpha\alpha\alpha}\rangle/d\ln T$
	HHR	NACRE
0.01	34.1	56.5
0.02	23.3	45.5
0.04	18.5	47.7
0.08	51.7	48.3
0.16	24.4	24.4

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The introduction of a three-body interaction was necessary to reproduce the relevant Hoyle state. This modified Hamiltonian increases the rates at T = 0.02 GK by 4 orders of magnitude, compared to those obtained with the Ali-Bodmer interaction [23]. However, while the Ali-Bodmer interaction used in Ref. [17] and also here reproduces the α - α phase shifts, that of Ref. [4] does not.

Next, we study the effect of the strong enhancement of the triple-alpha rate at low temperatures on stellar evolution. We use the MESA (Modules for Experiments in Stellar Astrophysics, version 3635) code library [24], but replace the NACRE rate by the HHR rate for T < 0.1 GK. We explore the evolution of progenitors with mass M = $0.8M_{\odot}$, $1.0M_{\odot}$, and $1.25M_{\odot}$, all with a standard solar composition, using the setups described in Sec. 7.1 of Ref. [24]. In general, He burning occurs in low-mass stars only for T > 0.07 GK, and therefore the changes to the stars are minimal. Figure 2 illustrates the post main sequence evolutionary track in the luminosity-effective temperature plane for a star of mass $1M_{\odot}$. Tracks for the standard NACRE rate (dashed line) and the HHR rate (solid line) are shown. Both stars go through a red-giant phase until He ignites in the semidegenerate core, unlike the case calculated with the CDCC rate, for which the redgiant phase vanishes [11]. Only after cessation of core He burning and the onset of H and He thermal shell flashes do small differences appear (shown in Fig. 2): the enhanced HHR rate at T < 0.06 GK tends to produce a slightly larger convective zone during helium shell flashes. Both rates lead to final white dwarfs with identical masses and carbon-oxygen ratios. The evolutionary tracks for a $1.25M_{\odot}$ star behave similarly to the $1M_{\odot}$ case, while the tracks for the $0.8M_{\odot}$ star are identical for both the NACRE and HHR rates. Further astrophysical studies to understand the implications of the new rate in explosive scenarios will be carried out in the near future.

In summary, we have developed a framework combining the hyperspherical method, the *R*-matrix expansion, and the *R*-matrix propagation and screening technique (named here HHR) to calculate the triple-alpha reaction rate at low temperatures, T < 0.1 GK. Our results show a strong enhancement of the rate below 0.06 GK, while reproducing the NACRE rate at higher temperatures. A longer publication with a detailed account of the method and further analysis of the reaction dynamics is under way.



FIG. 2 (color online). Evolutionary track (luminosity vs. surface effective temperature) of a one solar—mass star with solar composition, for the HHR rate (*solid line*) and the NACRE rate (*dashed line*). The evolution is identical for both from when H fuses to He in the core ("main sequence") through the formation of a degenerate He core ("giant branch") and the ignition of He in the core ("core He flash"). Small differences are seen when thermally unstable H and He burning occurs in a shell about a degenerate C/O core ("thermal pulses"), but there is no difference in the final white dwarf's mass or composition.

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