Quantum Three-Body Calculation of the Nonresonant Triple-α Reaction Rate at Low Temperatures

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Triple-α reaction rate is re-evaluated by directly solving the three-body Schrödinger equation. The resonant and nonresonant processes are treated on the same footing using the continuum-discretized coupled-channels method for three-body scattering. An accurate description of the α-α nonresonant states significantly quenches the Coulomb barrier between the first two α-particles and the third α-particle. Consequently, the α-α nonresonant continuum states below the resonance at 92.04 keV, i.e., the ground state of $^8\text{Be}$, give a markedly larger contribution at low temperatures than that reported in previous studies. We show that Nomoto’s method for three-body nonresonant capture processes, which is adopted in the NACRE compilation and many other studies, is a crude approximation of the accurate quantum three-body model calculation. We find an increase in triple-α reaction rate by about 20 orders of magnitude around $10^7$ K compared with the rate of NACRE.

After the Big Bang, all elements surrounding us have been created in the cosmos. Among them, $^{12}\text{C}$ is one of the most important nuclei because it is an essential element of life. In this sense, understanding the origin of $^{12}\text{C}$ would be equivalent to knowing “where we came from”. In view of nuclear physics, the second $0^+$ state of $^{12}\text{C}$ at 7.65 MeV above its ground state was predicted by Hoyle in 1953 to explain the abundance of $^{12}\text{C}$ or the existence of humans; this challenging prediction was soon confirmed experimentally,1) and the newly discovered $0^+_2$ state is called the Hoyle resonance. Since this historic discovery of the Hoyle resonance, the $^{12}\text{C}$ reaction, i.e., the so-called triple-α reaction, has been described as a series of the following two reactions:2)

$$\alpha + \alpha \rightarrow ^8\text{Be}, \quad \alpha + ^8\text{Be} \rightarrow ^{12}\text{C}(2^+_1) + \gamma.$$  

(1)

In the latter, $^{12}\text{C}$ in the $2^+_1$ state is formed by a $\gamma$-decay from the Hoyle resonance, and then decays into the ground state of $^{12}\text{C}$, while emitting $\gamma$ again. This picture of the triple-α reaction, which is realized at temperatures higher than a few $10^8$ K in helium burning stars, successfully describes the present abundance of $^{12}\text{C}$.

At low temperatures, however, the energy of the three-α system cannot reach a resonance energy of 379.5 keV above the three-α threshold. The formation process through nonresonant three-α continuum states, i.e., the nonresonant triple-α process,

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then becomes dominant. The formation rate of $^{12}$C at low temperatures is crucial for studies of helium burning in accreting white dwarfs and neutron stars,\textsuperscript{3,4} and is considered to strongly affect the evolution of primordial stars.\textsuperscript{5} In Ref. 3) Nomoto proposed a method of evaluating the contribution of the nonresonant triple-$\alpha$ process using resonance formulae, with an energy shift for the Hoyle resonance, to describe the two reactions in Eq. (1). This method, which we call Nomoto’s method in this paper, was found to give a significantly larger triple-$\alpha$ reaction rate at low temperatures\textsuperscript{3,6} than that obtained using a naive resonance formula without the energy shift. Nomoto’s method has been a standard method of describing the nonresonant triple-$\alpha$ reaction. Note, however, that Nomoto’s method does not explicitly describe the role of the nonresonant continuum states in the triple-$\alpha$ process.

In the present study, we evaluate nonresonant triple-$\alpha$ reaction rate by directly solving the Schrödinger equation of the three-$\alpha$ system. The three-$\alpha$ scattering wave function is obtained by the continuum-discretized coupled-channels method (CDCC),\textsuperscript{7} which was proposed and developed by the Kyushu group more than 20 years ago, and has been successfully applied to studies of various three-body reaction processes, see, e.g., Refs. 7–9). In CDCC, the resonant and nonresonant states of the $\alpha$-$\alpha$ system, as well as those of the three-$\alpha$ system, are treated on the same footing. This is one of the most important advantages of the present calculation.

As for previous three-body calculations of the triple-$\alpha$ reaction, Kamimura and Fukushima\textsuperscript{10} firstly showed, using the microscopic three-$\alpha$ resonating group method, the importance of the couplings between the $\alpha$-$\alpha$ resonant channel and the $\alpha$-$\alpha$ nonresonant channels for reproducing the properties of the Hoyle resonance and for understanding the processes shown in Eq. (1). This finding was confirmed by Descouvemont and Baye\textsuperscript{11)} using the microscopic three-$\alpha$ generator coordinate method; they derived triple-$\alpha$ reaction rate down to $10^7$ K. In these studies, however, the treatment of the $\alpha$-$\alpha$ nonresonant continuum was very primitive; only a few discretized nonresonant states were included. More importantly, $\alpha$-$\alpha$ nonresonant continuum states below the resonance at 92.04 keV, which play essential roles in the nonresonant triple-$\alpha$ process as shown below, were completely missed. Thus, it is evident that these models cannot accurately describe the nonresonant triple-$\alpha$ process at low temperatures, say, $T \lesssim 10^8$ K.

CDCC is well known as one of the most accurate reaction models for describing three-body reactions. It works even in cases where Coulomb interactions play dominant roles and requires a detailed description of low-energy continuum states. In the present study, we use the three-$\alpha$ scattering wave function obtained by CDCC, and evaluate the triple-$\alpha$ reaction rate at temperatures of $10^7$ K $\leq T \leq 10^9$ K. Emphasis is on the reaction rate at low temperatures for $T \leq 10^8$ K, where the contribution of the nonresonant triple-$\alpha$ process is dominant. We show that Nomoto’s method\textsuperscript{3,6} used in the NACRE compilation\textsuperscript{12)} and many other studies is a crude approximation of the accurate quantum three-body model calculation. At $T = 10^7$ K, typically, our new result is more than 20 orders of magnitude larger than that of NACRE.\textsuperscript{12)}

In the present calculation, we work with the three-$\alpha$ system shown in Fig. 1 based on the Jacobi coordinates ($\mathbf{r}, \mathbf{R}$). The relative energy of $\alpha_1$ and $\alpha_2$ is denoted by $\epsilon_{12}$ and the relative energy between $\alpha_3$ and the center of masses (c.m.) of $\alpha_1$ and
\( \alpha_2 \) is denoted by \( \epsilon_3 \); the total energy \( E \) in the three-\( \alpha \) c.m. frame is \( \epsilon_{12} + \epsilon_3 \). We obtain triple-\( \alpha \) reaction rate by directly solving the three-body Schrödinger equation

\[
[T_R + T_R + v(r) + v(R_1) + v(R_2) - E] \psi(r, R) = 0,
\]

where \( T_R \) and \( T_R \) are the kinetic energy operators associated with \( r \) and \( R \), respectively, and \( v \) is the interaction between two \( \alpha \)-particles consisting of the nuclear and Coulomb parts.

Following the standard continuum-discretization procedure called the \textit{average method}, we first discretize the continuum states of the \( \alpha_1-\alpha_2 \) subsystem into momentum bins. We prepare \( L^2 \)-integrable \( \alpha_1-\alpha_2 \) wave functions \( \hat{u}_i(r) \) \((i = 1-i_{\text{max}})\) by

\[
\hat{u}_i(r) = \frac{\int_{k_i}^{k_{i+1}} f_i(k) u(k, r) dk}{\left[ \int_{k_i}^{k_{i+1}} |f_i(k)|^2 dk \right]^{1/2}},
\]

where \( u(k, r) \) is the \( \alpha_1-\alpha_2 \) scattering wave function with the relative momentum \( k \), and \( f_i(k) \) is a weight function set to be constant and the Breit-Wigner function for nonresonant and resonant bin states, respectively. The normalization of \( u(k, r) \) is defined by \( \int u^*(k', r) u(k, r) dr = \delta(k' - k) \), which makes \( \hat{u}_i(r) \) satisfy \( \int \hat{u}_i^*(r) \hat{u}_j(r) dr = \delta_{ij} \). The average momentum (energy) of the \( i \)th bin state of the \( \alpha_1-\alpha_2 \) system is denoted by \( k_i \) \((\epsilon_{12,i})\). The total wave function of the three-\( \alpha \) system with CDCC is given by

\[
\psi^{0+}_{k_{i_0}, E}(r, R) = \sqrt{\frac{2}{\pi}} \frac{1}{32\pi^2} \frac{\hat{u}_i(r)}{r} \hat{\chi}^{(i_0)}_{i}(R),
\]

where \( \hat{\chi}^{(i_0)}_{i}(R) \) describes the relative motion between \( (\alpha_1-\alpha_2) \) in \( \hat{u}_i \) and \( \alpha_3 \) with the relative momentum \( \hat{K}_i \) that is obtained by the energy conservation of the three-\( \alpha \) system. The index \( i_0 \) represents the incident channel. Note that we consider only s-waves of \( \hat{u}_i \) and \( \hat{\chi}^{(i_0)}_{i}(R) \), since we are interested in reactions at very low energies. Furthermore, we have dropped all phase factors in \( \psi^{0+}_{k_{i_0}, E} \) giving no contribution to the reaction probability shown below. The coupled-channel (CC) equations for \( \hat{\chi}^{(i_0)}_{i}(R) \) \((i = 1-i_{\text{max}})\) are given by

\[
[T_R + V_{ii'}(R) - (E - \epsilon_{12,i})] \hat{\chi}^{(i_0)}_{i}(R) = -\sum_{i' \neq i} V_{ii'}(R) \hat{\chi}^{(i_0)}_{i'}(R),
\]
which are solved under a conventional boundary condition for $\hat{\chi}_{i0}(R)$. The coupling potential $V_{ii'}(R)$ is defined by

$$V_{ii'}(R) = \left\langle \frac{\hat{u}_i(r)}{r} | v(R_1) + v(R_2) | \frac{\hat{u}_{i'}(r)}{r} \right\rangle_r.$$  \hspace{1cm} (5)

The reaction probability $(\sigma v)_{k_{i0},E}$ of the triple-$\alpha$ process due to the electric quadrupole (E2) transition to the $2^+_1$ state is given by

$$(\sigma v)_{k_{i0},E} = \frac{2(2\pi)^7}{75\hbar} \left( \frac{\hbar \omega}{\hbar c} \right)^5 \sum_M \left| \left\langle \Psi^{2+}_M | O^{E2}_M | \Psi^{0+}_{k_{i0},E} \right\rangle \right|^2,$$

where $\Psi^{2+}_M$ is the wave function of the $2^+_1$ state of $^{12}$C with $M$ as the projection of the total spin, $O^{E2}_M$ is the E2 transition operator, and the photon energy $\hbar \omega$ is given by 2.8358 + $E$ MeV. Note that we use the symbol $(\sigma v)$ for the reaction probability following NACRE; \cite{12} it is actually the E2 transition probability divided by the normalization factor $1/(2\pi)^6$ for the three-$\alpha$ scattering wave function in free space. The triple-$\alpha$ reaction rate $\langle \alpha\alpha\alpha \rangle(T)$, as a function of $T$, is obtained by taking the average $(\sigma v)_{k_{i0},E}$ with the Maxwell-Boltzmann distribution for the velocity of each $\alpha$:

$$\langle \alpha\alpha\alpha \rangle(T) = 3N_A^2 \frac{4}{\pi(k_B T)^3} \int \left\{ \sum_{i_{i0}=1}^{i_{\text{max}}} w_{i_{i0}} (\sigma v)_{k_{i0},E} \right\} \exp \left( -\frac{E}{k_B T} \right) dE \hspace{1cm} (6)$$

with

$$w_{i_{i0}} = \frac{2\hat{\epsilon}_{12,i_{i0}}}{k_{i0}} \sqrt{\hat{\epsilon}_{12,i_{i0}}(E - \hat{\epsilon}_{12,i_{i0}})},$$

Fig. 2. $\alpha_1$-$\alpha_2$ momentum bin states included in the present CDCC calculation.
where $k_B$ is Boltzmann’s constant and $N_A$ is Avogadro’s number. Factor 3 in Eq. (6) comes from the fact that the three-$\alpha$ system is symmetric with respect to the exchange of each pair of alpha particles.\[12]

In numerical calculation, we discretize the $k$-continuum of the $\alpha_1$-$\alpha_2$ system from 0.008 fm$^{-1}$ ($\epsilon_{12} = 0.668$ keV) to 0.130 fm$^{-1}$ ($\epsilon_{12} = 176$ keV) with a width of 0.001 fm$^{-1}$, which results in $i_{\text{max}} = 122$. A schematic illustration of the $\alpha_1$-$\alpha_2$ bin states taken in the CDCC calculation is shown in Fig. 2. This discretization is sufficiently precise for the present purpose. The 86th bin corresponds to the $\alpha_1$-$\alpha_2$ resonance. The maximum $r$ is 5,000 fm with an increment $\Delta r$ of 0.1 fm.

As for the nuclear potential between two $\alpha$-particles, we use the following two-range Gaussian form (with depth in MeV):

$$v_{\text{nucl}}(x) = 100.0e^{-(x/1.00)^2} - 30.35e^{-(x/2.13)^2},$$

(7)

where $x$ is the displacement of the two $\alpha$-particles in fm. The first repulsive part simulates the Pauli exclusion principle, i.e., nucleons in an $\alpha$ cannot occupy the nucleon s-orbit in the other. This potential gives $\alpha$-$\alpha$ resonance at 92.0 keV with a width of 4.8 eV, which reproduces well the corresponding experimental values, i.e., 92.04 $\pm$ 0.05 keV and 5.57 $\pm$ 0.25 eV.\[13] It is known\[14] that this type of $\alpha$-$\alpha$ potential with a repulsive core is not suitable for describing the $0^{+}_1$ or $2^{+}_1$ state of $^{12}$C, in which the three $\alpha$-particles are closely bound. However, it can be successfully applied to the $0^{+}_2$ state, in which the three $\alpha$-particles are loosely coupled. Therefore, we consider that the simulation of the Pauli principle by introducing the repulsive part is justified in describing the three-$\alpha$ scattering states. In fact, it is numerically confirmed that even if we put $v_{\text{nucl}}(x) = 0$ in the calculation of $V_{ii'}(R)$ given by Eq. (5), the resulting reaction rate $\langle \alpha \alpha \alpha \rangle(T)$ for $T \leq 10^8$ K changes by only about 2%, at most.

Equation (4) is numerically integrated up to $R_{\text{max}} = 2,500$ fm with $\Delta R = 0.25$ fm, and $\hat{\chi}_i(0)(R) (i = 1-i_{\text{max}})$ are connected to a conventional asymptotic form. The total energy $E$ is varied from 1 to 500 keV with $\Delta E = 1$ keV; around the Hoyle resonance at $E = 379.5$ keV, we put $\Delta E = 0.1$ keV. In the evaluation of the coupling potentials $V_{ii'}(R)$ given by Eq. (5), we reduce $v_{\text{nucl}}$ by 1.5% so that the $(\alpha_1$-$\alpha_2$)-$\alpha_3$ system in the $i = 86$ channel, with $i_0 = 86$, forms a resonance at $\epsilon_3 = 287.5$ keV.

In the calculation of $\Psi_{2+}^{i_0}$, the use of the potential of Eq. (7) is not appropriate, as mentioned above. Instead, we adopt a sophisticated three-$\alpha$ wave function\[15,16] that was obtained on the basis of the orthogonality condition model\[17] for describing the Pauli principle with the three $\alpha$-particles symmetrized. In this semimicroscopic calculation, $\alpha$-$\alpha$ potential was derived by folding an effective nucleon-nucleon force\[18] into $\alpha$-particle density.

We show in Fig. 3 the discretized continuum wave functions $\hat{u}_i(r)$ of the $(\alpha_1$-$\alpha_2$ system (upper panel) and the Coulomb parts of the diagonal coupling potentials $V_{ii}^{\nu}(R)$ (lower panel). We use the logarithmic scale for the horizontal axis in each panel. The solid, dashed, and dotted lines correspond to the $\alpha_1$-$\alpha_2$ continuum states with average energies $\hat{\epsilon}_{12,i}$ of 38.2 keV ($i = 53$), 92.0 keV ($i = 86$), and 152 keV ($i = 113$), respectively. One sees that the resonant wave function has a dominant amplitude in the interaction region ($r \lesssim 10$ fm), while the nonresonant wave functions

\[60x429\]
have appreciable amplitudes only at larger $r$. This clear difference in $\hat{u}_i(r)$ markedly affects $V^C_{ii}(R)$, as shown in the lower panel. One sees that the Coulomb barrier height $V^C_{ii}(R)$ for the $\alpha_1$-$\alpha_2$ nonresonant bins is much lower than that for the resonant bin. Thus, $\alpha_3$ can easily approach the $\alpha_1$-$\alpha_2$ system when $\alpha_1$-$\alpha_2$ is in nonresonant states. This important feature has not been considered in previous studies using Nomoto’s method.

Figure 4 shows the calculated results of $(\sigma v)_{k_{ii0},E}$. To show the difference between the resonant and nonresonant results clearly, no CC effects are included here. The solid (dashed) line corresponds to $i_0 = 53$ (86). One sees that the solid line has a completely different energy dependence from the dashed line. The nonresonant reaction probability $(\sigma v)_{k_{ii0},E}$ is almost constant (on the scale of the vertical axis in Fig. 4) above $E \sim 70$ keV, and dominates the resonant one for $E \lesssim 200$ keV. Note that for $i_0 = 53$, $E = 70$ keV corresponds to $\epsilon_3 = 31.8$ keV, which agrees well with the quenched Coulomb barrier height shown by the solid line in Fig. 3 (lower panel).

If we unphysically disregard the channel dependence of coupling potential $V_{ii'}(R)$ and take only the diagonal components, by using the replacement

$$V_{ii'}(R) \rightarrow V_{86,86}(R)\delta_{ii'},$$

we can simulate the evaluation of $(\sigma v)_{k_{ii0},E}$ by Nomoto’s method; note that the 86th bin corresponds to the $\alpha_1$-$\alpha_2$ resonant state. This replacement of $V_{ii'}(R)$ in Eq. (4) makes the three-$\alpha$ system form a resonance when $\epsilon_3 = 287.5$ keV, independently of $\epsilon_{12}$. In other words, when $\epsilon_{12} = 92.0 - \Delta\epsilon_{12}$ keV, the three-$\alpha$ system has a resonance at $E = 379.5 - \Delta\epsilon_{12}$ keV. $\Delta\epsilon_{12}$ is nothing but the energy shift in Nomoto’s method. The result for $i_0 = 53$ obtained using Eq. (8) is shown by the dotted line in Fig. 4.
Although it has a peak at $E \sim 326$ keV as expected, its energy dependence is similar to that shown by the dashed line, which results in a much smaller value than the true nonresonant capture probability (solid line) at low energies. Thus, Nomoto’s method is shown to be a crude approximation of the accurate three-body model calculation.

We show using the solid line in Fig. 5 our result of the triple-$\alpha$ reaction rate obtained by CDCC. The triple-$\alpha$ reaction rate of the NACRE compilation\(^{12}\) is shown by the dash-dotted line for comparison. A marked increase in reaction rate at low temperatures is found. The dashed line shows our result including only the resonant capture process, i.e., via the $(\alpha_1-\alpha_2)$-$\alpha_3$ resonance state at $E = 379.5$ keV. The difference between the solid and dashed lines clearly shows the dominant contribution of the nonresonant triple-$\alpha$ process for $T < 2 \times 10^8$ K. As mentioned above, we can simulate the NACRE evaluation, which is essentially based on Nomoto’s method, using Eq. (8); the result of this calculation is shown by the dotted line. As expected, the dotted line reproduces the result of NACRE well. Thus, we conclude that the nonresonant capture process has a much larger contribution than that in previous evaluations,\(^{3,6,12,19}\) as a result of the significant reduction in the Coulomb barrier height between $\alpha_3$ and the nonresonant $\alpha_1-\alpha_2$. This barrier reduction cannot be taken into account if one uses Eq. (8), or, equivalently, if one adopts Nomoto’s method, as mentioned above. Also note the importance of the low-energy $\alpha_1-\alpha_2$ continuum states below the resonance at 92.04 keV, which were completely missed in the preceding three-$\alpha$ model studies.\(^{10,11}\) It is found that almost all of these low-energy states have contributions to total reaction rate (solid line) for $T < 4.0 \times 10^7$ K. Because of the lack of these states, the reaction rate given in Ref. 11), e.g., $5.34 \times 10^{-63}$ cm$^6$ s$^{-1}$ mol$^{-2}$ at $10^7$ K, is markedly smaller than the present result at low temperatures.

For a more detailed comparison, we need to perform renormalization for the CDCC result. We introduce an effective charge $\delta e = 0.77e$ to the E2 transition.
Fig. 5. (color online) Triple-\(\alpha\) reaction rate as a function of temperature. The solid line represents the result of CDCC. The dashed line shows the contribution of resonant capture. The result of CDCC simulating Nomoto’s method with Eq. (8) is shown by the dotted line. The dash-dotted line shows the reaction rate of NACRE.\(^{12}\)

operator, so that our B(E2) value, evaluated at \(E = 379.5\) keV with the \(0^+\) wave function normalized to unity, reproduces the experimental value of \(13.4\) \(e^2\) fm\(^4\)\(^{20}\) as in Ref. 11). Then, we renormalize our result (with \(\delta e\)) to the reaction rate of NACRE at \(T = 10^9\) K, where the resonant capture process through the Hoyle resonance is dominant;\(^{12}\) the renormalization factor obtained is 1.54. From this value, one may estimate the uncertainty of the present calculation to be more or less 50%.

In Table I we show the renormalized triple-\(\alpha\) reaction rate obtained by CDCC, together with its ratio to the rate of NACRE, at some typical temperatures. As

<table>
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<th>(T) ((10^7) K)</th>
<th>(\langle \alpha\alpha\alpha \rangle)</th>
<th>ratio</th>
<th>(T) ((10^7) K)</th>
<th>(\langle \alpha\alpha\alpha \rangle)</th>
<th>ratio</th>
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<td>1.52 [-16]</td>
<td>9.5 [+01]</td>
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expected, for $T \geq 2.5 \times 10^8$ K, the ratio is almost unity, which shows that our calculation, with the renormalization at $10^9$ K, reproduces the temperature dependence of the resonant triple-$\alpha$ process through the Hoyle resonance very well. At low temperatures, on the other hand, the ratio exceeds $10^{20}$, which will affect the helium burning in accreting white dwarfs and neutron stars. Furthermore, even at a rather high temperature of $1.5 \times 10^8$ K, we obtain a reaction rate larger than that of NACRE by almost two orders of magnitude. Note that a broad $2^+_2$ resonance state at $E = 1.75$ MeV with an $\alpha$-decay width of 0.56 MeV\(^{11}\) is included in the NACRE evaluation. In fact, it is shown that this $2^+_2$ state has a significant contribution to the triple-$\alpha$ reaction rate for $T \gtrsim 2 \times 10^9$ K.\(^{12}\) At these high temperatures, the nonresonant triple-$\alpha$ process that we focus on in this study is clearly negligible compared with resonant processes via the $0^+_2$, $2^+_2$, and other possible resonance states\(^{5}\) of \(^{12}\)C. Very recently, it has been reported\(^{21}\) that a stellar evolution model computed with our new reaction rate of the triple-$\alpha$ reaction causes inconsistency with the observations of red giant branches. Further investigation on the implication of this will be very interesting and important.

In summary, we have evaluated the triple-$\alpha$ reaction rate by directly solving the three-body Schrödinger equation with CDCC. We treat the resonant and nonresonant processes on the same footing. The $\alpha$-$\alpha$ continuum states below the resonance at 92.04 keV are shown to play essential roles in the nonresonant triple-$\alpha$ process for $T \lesssim 4.0 \times 10^7$ K. The key of the nonresonant capture process is that the Coulomb barrier between the first two $\alpha$-particles and the third $\alpha$ particle is much quenched compared with that in the resonant capture. This property extremely enhances the nonresonant triple-$\alpha$ process at low temperatures, i.e., $T \lesssim 10^8$ K. The ratio of our triple-$\alpha$ reaction rate to that of the NACRE compilation is more than $10^{26}$ at $10^7$ K; it is about 100 at $1.5 \times 10^8$ K. It is found that Nomoto’s method for three-body nonresonant capture processes, which is used in the NACRE compilation and many other studies, is a crude approximation, with Eq. (8), of the accurate quantum three-body model calculation. The newly evaluated triple-$\alpha$ reaction rate will affect many studies of nuclear astrophysics, namely, those of helium burning in accreting white dwarfs and neutron stars in particular. A detailed description of the theoretical framework together with further discussion on the comparison with other existing methods will be presented in a forthcoming paper.

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