Imaginary-time theory for triple-alpha thermonuclear reaction rate

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Dominant ¹²C synthesis process depends on temperature





Calculated rates deviates among theories at low temperature 10²⁶ order of magnitude difference at 10⁷ K



Calculation of triple-alpha reaction rate at low temperature Difficulties and theoretical challenges

- Treatment of scatting of three charged particles, (we do not know "Coulomb wave function" for 3-charged particles).
- We need to treat tunneling phenomena of three charged particles. The reaction rate changes 10^{60} in magnitude between $10^7 - 10^9$ K.

Our Attempt: develop a new theory Imaginary-time theory for radiative capture reaction rate

Imaginary-time theory for triple-alpha reaction rate

- 1. Imaginary-time theory for 2-body radiative capture reaction rate K. Yabana and Y. Funaki, Phys. Rev. C85, 055803 (2012).
- 2. Apply the imaginary-time theory for triple-alpha reaction rate Reaction rate, reaction mechanisms
- 3. Why different theories result in different results? Slow convergence in coupled-channels approach
- 4. Derive NACRE formula from the imaginary-time theory R-matrix theory + separable approximation

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What is the imaginary-time theory?

Standard procedure for capture rate

Step 1. Calculate reaction cross section $\sigma(E)$

Step 2. Average over Boltzmann distribution $\langle v\sigma \rangle$

Our new (numerical) method

K.Yabana and Y.Funaki. PRC85,055803(2012)

Identify inverse temperature as imaginary-time as in quantum theory of nonequilibrium systems

$$\beta = \frac{1}{kT}$$

Averaging over Boltzmann distribution

= Evolution of wave function along the imaginary time axis, starting with wave function after capture reaction

(Skip step 1, calculation of $\sigma(E)$)

We can obtain reaction rate without solving any scattering problems



Imaginary-time method (1/3): Ordinary procedure



Reaction rate at temperature $\beta = 1/k_B T$

$$r(\beta) = \langle v\sigma \rangle = \frac{\sum_{i} e^{-\beta E_{i}} v\sigma_{fi}}{\sum_{i} e^{-\beta E_{i}}} = \left(\frac{\beta \hbar^{2}}{2\pi\mu}\right)^{\frac{3}{2}} \int d\vec{k} e^{-\beta \frac{\hbar^{2} k^{2}}{2\mu}} \left(\frac{\hbar k}{\mu}\right) \sigma_{fi}$$

Imaginary-time method (2/3): Eliminate scattering states

Closure relation

 $1 = \sum_{n} \left| \phi_{n} \right\rangle \left\langle \phi_{n} \right| + \int d\vec{k} \left| \phi_{\vec{k}} \right\rangle \left\langle \phi_{\vec{k}} \right|$

Spectral representation of the Hamiltonian

$$f(\hat{H}) = \sum_{n} f(E_{n}) |\phi_{n}\rangle \langle \phi_{n}| + \int d\vec{k} f\left(\frac{\hbar^{2}k^{2}}{2\mu}\right) |\phi_{\vec{k}}\rangle \langle \phi_{\vec{k}}|$$



Projector to remove bound states.

Imaginary-time method (3/3): Computational procedure



- No need to solve scattering problem.
 (No boundary condition required)
- Solving in finite space amounts to bound state approximation.

K.Yabana and Y.Funaki. PRC85,055803(2012)

Test the method in a 2-body problem: Direct capture process of ${}^{16}O(\alpha,\gamma){}^{20}Ne$

$$\sigma_{fi} = \frac{8\pi}{k^2} \frac{1}{\hbar v} \frac{(\lambda+1)(2\lambda+1)}{\lambda((2\lambda+1)!!)^2} \left(\frac{E_i - E_f}{\hbar c}\right)^{2\lambda+1} e^2 \left\{ Z_1 \left(\frac{A_2}{A}\right)^{\lambda} + Z_2 \left(-\frac{A_1}{A}\right)^{\lambda} \right\}^2 \\ \times \sum_{l_i} (2l_i + 1) \left(C_{l_i 0 \lambda 0}^{l_f 0}\right)^2 \left| \int_0^\infty dr u_{n_f l_f}(r) r^{\lambda} u_{k l_i}(r) \right|^2$$

Dominant contribution from l=0(scattering) to l=2(bound)

 $\left\langle u_{n_f l_f=2} \left| r^2 \right| u_{k,l_i=0} \right\rangle$





Astrophysical S-factor for ${}^{16}O(\alpha,\gamma)^{20}Ne$

$$\sigma = \frac{S(E)}{E} e^{-2\pi\eta} \qquad \eta = \frac{Z_1 Z_2 e^2}{\hbar v}$$



Maxwellian-averaged reaction rate



Imaginary-time evolution of the radial wave function -1



R_{max}=400 fm

Imaginary-time algorithm:

- 1. Prepare initial wave function $\psi(\vec{r}, \beta = 0) = \left(\frac{\hat{H} + |E_f|}{\hbar c}\right)^{2\lambda + 1} \hat{P}M_{\lambda\mu}^{+} \phi_f(\vec{r})$
- 2. Solve imaginary time equation $-\frac{\partial}{\partial\beta}\psi(\vec{r},\beta) = H\psi(\vec{r},\beta)$
- 3. Take overlap to obtain reaction rate $r(\beta) \propto \int d\vec{r} \phi_f^*(\vec{r}) M_{\lambda\mu} \psi(\vec{r},\beta)$

Imaginary-time evolution of the radial wave function -2



Imaginary-time algorithm: 1. Prepare initial wave function $\psi(\vec{r}, \beta = 0) = \left(\frac{\hat{H} + |E_f|}{\hbar c}\right)^{2\lambda + 1} \hat{P}M_{\lambda\mu}^{+} \phi_f(\vec{r})$ 2. Solve imaginary time equation $-\frac{\partial}{\partial \beta} \psi(\vec{r}, \beta) = H\psi(\vec{r}, \beta)$ 3. Take overlap to obtain reaction rate $r(\beta) \propto \int d\vec{r} \phi_f^{*}(\vec{r}) M_{\lambda\mu} \psi(\vec{r}, \beta)$

Ordinary calculation vs Imaginary-time calcualtion



Imaginary-time method gives the same reaction rate as that by ordinary method, if calculation is achieved in sufficiently large space.





Maximum radius should be larger than exit (entrance) point in the Coulomb barrier.

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Choice of the Hamiltonian

 α - α potential to reproduce ⁸Be resonance (ground state) energy and width $E_R = 92 \text{ keV} (=\text{Exp}), \Gamma = 5.9 \text{ eV} (\text{Exp 5.6 eV})$

$$V_{\alpha\alpha} = 500.0e^{-(0.7r)^2} - 130.0e^{-(0.475r)^2} + \text{Coulomb}$$

We add "three-body force" among alpha particles to reproduce 0_2^+ (Hoyle state) resonance energy $E_{0+}=379.5$ keV

 $V_{\alpha\alpha\alpha} = -924.43e^{-0.15(r_{12}^2 + r_{23}^2 + r_{31}^2)}$

Final wave function (2⁺ state of ¹²C) Adopted from phenomenological 3-alpha cluster model (Orthogonality Condition Model = OCM)



Coordinate system and model space

The same as those adopted in CDCC calculation K. Ogata et.al, Prog. Theor. Phys. 122, 1055 (2009).

Jacobi coordinate



Taking L = l = 0 angular momentum channel in the imaginary-time evolution.

$$\psi(\vec{r},\vec{R},\beta) = \frac{u_{l=L=0}(r,R,\beta)}{rR} \left[Y_{l=0}(\hat{r}) Y_{L=0}(\hat{R}) \right]_{J=0} = \frac{1}{4\pi} \frac{u(r,R,\beta)}{rR}$$

$$2^{+} \text{OCM wave function}$$

$$r(\beta) \propto \left\langle \Phi_{f} \right| M_{\lambda\mu} \left[e^{-\beta \hat{H}} \left(\frac{\hat{H} - E_{f}}{\hbar c} \right)^{2\lambda + 1} \right] \hat{P} M_{\lambda\mu}^{+} \left| \Phi_{f} \right\rangle \equiv \left\langle \Phi_{f} \right| M_{\lambda\mu} \left| \Psi(\beta) \right\rangle$$

Numerical detail to treat the radial imaginary-time equation

$$-\frac{\partial}{\partial\beta}u_{L=l=0}(R,r,\beta) = \hat{H}_{L=l=0}(R,r)u_{L=l=0}(R,r,\beta)$$
$$\hat{H}_{L=l=0} = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial R^2} - \frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + V(r,R)$$

We simply discretize both radial coordinates with grid spacing $\Delta R = \Delta r = 0.5$ fm up to a certain spatial region, R_{max} and r_{max} .

Differentiation with respect to R and r are treated by high-order finite-difference formula.

Convergence with respect to spatial size (R_{max} and r_{max})



Changes of dominant reaction mechanisms in empirical theory



 $T = 7.4 \times 10^7 \mathrm{K}$

 $T = 2.8 \times 10^7 \mathrm{K}$



Our imaginary-time result shows changes of reaction mechanisms at exactly the same temperatures as those of empirical theory





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We use almost the same Hamiltonian, coordinate system, and the truncation of the partial wave as those adopted by K. Ogata et.al, Prog. Theor. Phys. 122 (2009) 1055. However, the obtained rate is more than 10²⁰ times different at low temperature.

We solve the imaginary-time evolution equation in the finite difference approximation, while in the CDCC method, basis function expansion is introduced.

To clarify the origin of the difference, we solve the imaginary-time equation employing *the coupled-channels method (basis function expansion)*.

Radial Schroedinger equation in imaginary-time

$$-\frac{\partial}{\partial\beta}u(r,R,\beta) = \left[-\frac{\hbar^2}{2M}\frac{\partial^2}{\partial R^2} - \frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + V(r,R)\right]u(r,R,\beta)$$

Up to now, we solved it as a differential equation.

Instead, we solve the equation using basis function expansion. We first solve $\alpha - \alpha$ 2-body problem.

$$\begin{bmatrix} -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + v_{\alpha\alpha}(r) \end{bmatrix} w_n(r) = \varepsilon_n w_n(r)$$
$$\int_0^{r_{\text{max}}} dr w_m(r) w_n(r) = \delta_{mn}$$

We then expand 3-body wave function with the basis

$$u(r, R, \beta) = \sum_{n} \chi_{n}(R, \beta) w_{n}(r)$$
$$-\frac{\partial}{\partial \beta} \chi_{n}(R, \beta) = \left[-\frac{\hbar^{2}}{2M} \frac{\partial^{2}}{\partial R^{2}} + \varepsilon_{n} \right] \chi_{n}(R, \beta) + \sum_{n'} V_{nn'}(R) \chi_{n'}(R, \beta)$$

If we use a complete set $\{w_n(r)\}$, then the coupled-channel calculation gives completely the same result as that we shows previously. However, if we make a truncation, the result may be different.

 $\vec{R}: L = 0$ $\vec{r}: l = 0$

Coupled Channel Calculation [dr = 0.5 fm, Nr = 1200, $r_{max} = 600$ fm]

 2α Energy

- N_{max} =1 (single channel): overestimate by 10¹⁵
- N_{max} =400 (E_{\alpha\alpha}=45.4 MeV): still overestimate by 10¹²
- N_{max} =1200 (all channels) coincides with result without channel expansion.

Very slow convergence with respect to increase of channel number.



Why the single channel calculation so much overestimates the reaction rate?

$$\begin{bmatrix} -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + v_{\alpha\alpha}(r) \end{bmatrix} w_n(r) = \varepsilon_n w_n(r)$$
$$\int_0^{r_{\text{max}}} dr w_m(r) w_n(r) = \delta_{mn}$$



Most wave functions localize outside the Coulomb barrier.

Very small barrier for n=n'=1 channel.

Coulomb barrier for "Channel-1"



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Very small barrier for n=n'=1 channel.



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Though empirical and imaginary-time theories look very different, calculated rate is almost the same.

Nomoto 1985, NACRE 1999:
Sequential 2-body process

$$\langle \alpha \alpha \alpha \rangle = 3 \int_{0}^{\infty} \frac{\hbar}{\Gamma_{\alpha}(\text{Be}, E_{\alpha \alpha})} \frac{d\langle \alpha \alpha \rangle (E_{\alpha \alpha})}{dE_{\alpha \alpha}} \langle \alpha \text{Be}(E_{\alpha \alpha}) \rangle dE_{\alpha \alpha}$$
Imaginary-time theory

$$\langle \alpha \alpha \alpha \rangle \propto \langle \phi_{f} \left| M_{\lambda \mu} e^{-\beta \hat{H}} \left(\frac{\hat{H} + \left| E_{f} \right|}{\hbar c} \right)^{2\lambda + 1} \hat{P} M_{\lambda \mu}^{-+} \right| \phi_{f} \rangle$$



We next examine the relation analytically using R-matrix theory.

Derivation of "Breit-Wigner formula" from imaginary-time theory

We start with the imaginary-time formula for reaction rate

$$r(\beta) = \left(\frac{2\pi\hbar^{2}\beta}{\mu}\right)^{2} \frac{8\pi}{\hbar\lambda((2\lambda+1)!!)^{2}} \sum_{m_{f}\mu} \left\langle \phi_{l_{f}m_{f}} \left| M_{\lambda\mu} e^{-\beta H} \left(\frac{H-E_{f}}{\hbar c}\right)^{2\lambda+1} P M_{\lambda\mu}^{+} \right| \phi_{l_{f}m_{f}} \right\rangle$$

Spectral representation of the Hamiltonian

$$f(\hat{H}) = \sum_{nlm} f(E_n) |\phi_{nlm}\rangle \langle \phi_{nlm} | + \sum_{lm} \int_0^\infty dE f(E) |\phi_{Elm}\rangle \langle \phi_{Elm} | \qquad u_{El}(r) \to \left(\frac{2\mu}{\pi\hbar^2 k}\right)^{\frac{1}{2}} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right)$$

Continuum wave function around resonance energy (R-matrix theory)

$$u_{El}(r) = u_r(r) \left(\frac{1}{2\pi} \frac{\Gamma_r(E)}{(E_r + \Delta_r(E) - E)^2 + \Gamma_r(E)/4} \right)^{\frac{1}{2}} \qquad \Delta_r(E) = -\gamma_r^2 S_l(E) \quad \Gamma_r(E) = 2\gamma_r^2 P_l(E)$$

Approximate spectrum representation of the Hamiltonian effective around resonance

$$f(\hat{H}) \rightarrow \sum_{m} |\phi_{rlm}\rangle \langle \phi_{rlm}| \int dE \frac{1}{2\pi} \frac{\Gamma_r(E)}{(E_r + \Delta_r(E) - E)^2 + \Gamma_r(E)/4} f(E)$$

Putting this relation to the rate expression in the imaginary-time theory, we main obtain the "Breit-Wigner formula" for the reaction rate.

Derive the empirical formula in the imaginary-time theory

Two basic assumptions for microscopic 3-body Hamiltonian 1. The Hamiltonian is separable, into α - α and α -⁸Be parts

$$H = h_{\alpha\alpha} + h_{\alpha^8 B a}$$

2. Hoyle state is described by a product of α - α and α -⁸Be resonant wave functions.

 $\Phi_{H} \approx \phi_{\alpha\alpha}^{res.}(\vec{r}) \phi_{\alpha Be}^{res.}(\vec{R})$

Approximate spectral representation of H using R-matrix theory

$$\begin{split} f(\hat{H}) \to |\phi_{H}\rangle \langle \phi_{H}| \int dE_{\alpha\alpha} \frac{1}{2\pi} \frac{\Gamma_{r}({}^{8}\text{Be}; E_{\alpha\alpha})}{(E_{r}({}^{8}\text{Be}) + \Delta_{r}(E_{\alpha\alpha}) - E_{\alpha\alpha})^{2} + \Gamma_{r}(E_{\alpha\alpha})/4} \\ \times \int dE_{\alpha^{8}\text{Be}} \frac{1}{2\pi} \frac{\Gamma_{r}({}^{12}\text{C}; E_{\alpha^{8}\text{Be}})}{(E_{r}({}^{12}\text{C}) + \Delta_{r}(E_{\alpha^{8}\text{Be}}) - E_{\alpha^{8}\text{Be}})^{2} + \Gamma_{r}(E_{\alpha^{8}\text{Be}})/4} \\ \times f(E_{\alpha\alpha} + E_{\alpha^{8}\text{Be}}) \end{split}$$

Put it in the rate expression of the imaginary-time theory

$$\langle \alpha \alpha \alpha \rangle \propto \langle \phi_f \left| M_{\lambda \mu} e^{-\beta \hat{H}} \left(\frac{\hat{H} - E_f}{\hbar c} \right)^{2\lambda + 1} \hat{P} M_{\lambda \mu}^{+} \right| \phi_f \rangle$$

Triple-alpha reaction rate derived from imaginary-time theory

$$\langle \alpha \alpha \alpha \rangle = 6 \cdot 3^{\frac{3}{2}} \left(\frac{2\pi\hbar^2}{M_{\alpha}kT} \right)^3$$

$$\times \int dE_{\alpha\alpha} \frac{1}{2\pi} \frac{\Gamma_{\alpha} \left({}^8\text{Be}; E_{\alpha\alpha} \right)}{\left(E_r \left({}^8\text{Be}\right) - E_{\alpha\alpha} \right)^2 + \Gamma_{\alpha} \left(E_{\alpha\alpha} \right)/4} \qquad \text{We ignore energy}$$

$$\times \int dE_{\alpha^8\text{Be}} \frac{1}{2\pi} \frac{\Gamma_{\alpha} \left({}^{12}\text{C}; E_{\alpha^8\text{Be}} \right)}{\left(E_r \left({}^{12}\text{C} \right) - E_{\alpha^8\text{Be}} \right)^2 + \Gamma_{\alpha} \left(E_{\alpha^8\text{Be}} \right)/4} \qquad \text{We ignore energy}$$

$$\times \exp\left[-\frac{E_{\alpha\alpha} + E_{\alpha^8\text{Be}}}{kT}\right] \cdot \Gamma_{\gamma} \left({}^{12}\text{C} \left(\frac{E_{\alpha\alpha} + E_{\alpha^8\text{Be}} - E \left({}^{12}\text{C}; 2^+ \right)}{E \left({}^{12}\text{C}; 2^+ \right)} \right)^{2\lambda + 1}$$

This expression mostly coincides with that of NACRE

$$\langle \alpha \alpha \alpha \rangle = 3 \int_0^\infty \frac{\hbar}{\Gamma_\alpha (\text{Be}, E_{\alpha \alpha})} \frac{d \langle \alpha \alpha \rangle (E_{\alpha \alpha})}{dE_{\alpha \alpha}} \langle \alpha \text{Be}(E_{\alpha \alpha}) \rangle dE_{\alpha \alpha}$$

There are a few minor differences.

$$\frac{\Gamma_{\alpha}\left({}^{12}\text{C}; E_{\alpha^{8}\text{Be}}\right)}{\left(E_{r}\left({}^{12}\text{C}\right) - E_{\alpha^{8}\text{Be}}\right)^{2} + \Gamma_{\alpha}\left(E_{\alpha^{8}\text{Be}}\right)/4} \implies \frac{\Gamma_{\alpha}\left({}^{12}\text{C}; E_{\alpha^{8}\text{Be}}\right)}{\left(E_{r}\left({}^{12}\text{C}\right) + E_{r}\left({}^{8}\text{Be}\right) - E_{\alpha^{8}\text{Be}} - E_{\alpha\alpha}\right)^{2} + \Gamma_{\alpha}\left(E_{\alpha^{8}\text{Be}}\right)/4}$$

Imaginary-time theory NACRE

Summary

We have developed the imaginary-time theory for the radiative capture reaction rate.

- It does not require any scattering solution to calculate reaction rate

We have applied the imaginary-time theory to the triple-alpha reaction rate.

- We can calculate a convergent reaction rate.
- The calculated reaction rate accurately coincides with that of NACRE
- Changes of reaction mechanisms occur at exactly the same temperature of
- those of NACRE.
- We clarified that the truncation in the coupled-channel method gives larger reaction rate at low temperature.
- Using R-matrix theory and assuming separable approximation, we may derive an analytical "Breit-Wigner formula" in the imagianry-time theory, which almost coincide with the formula of NACRE

Future task:

- Contributions of high partial wave components
- Calculation imposing exact symmetry of 3-alpha particles.