Imaginary-time theory for triple-alpha reaction rate

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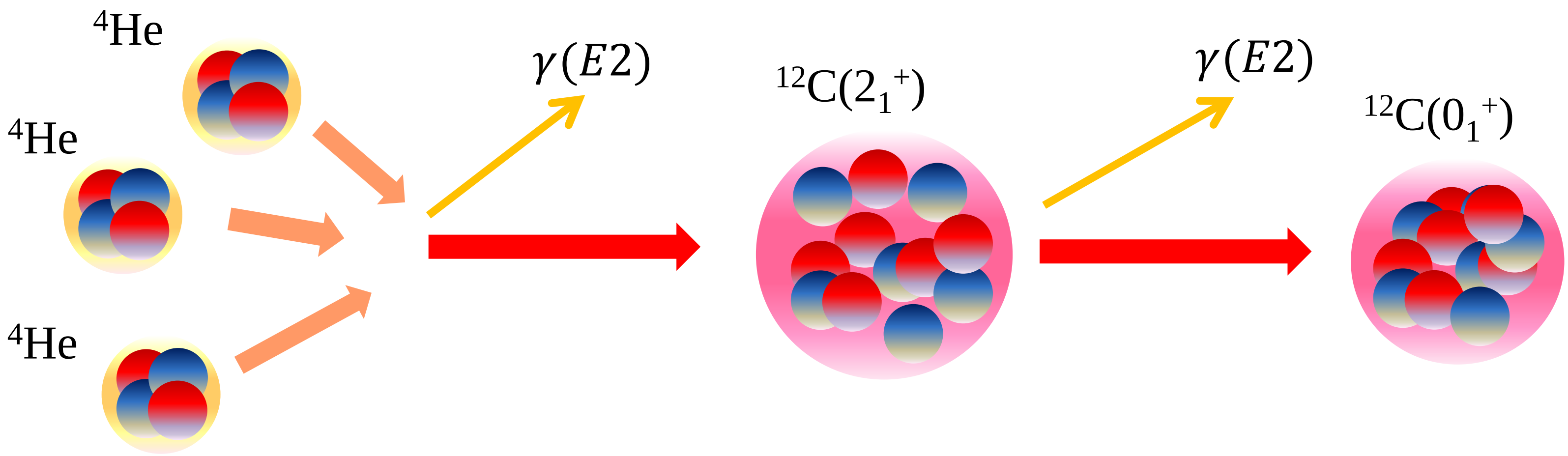
K. Yabana, Y. Funaki, Phys. Rev. C85, 055803 (2012)
"Imaginary-time method for the radiative capture reaction rate"

T. Akahori, Y. Funaki, K. Yabana, Phys. Rev. Lett. (to be accepted)
"Imaginary-time theory for triple-alpha reaction rate"

Triple-alpha process

Total angular momentum 0



1953 F. Hoyle predicted resonance state in ^{12}C and later confirmed experimentally.

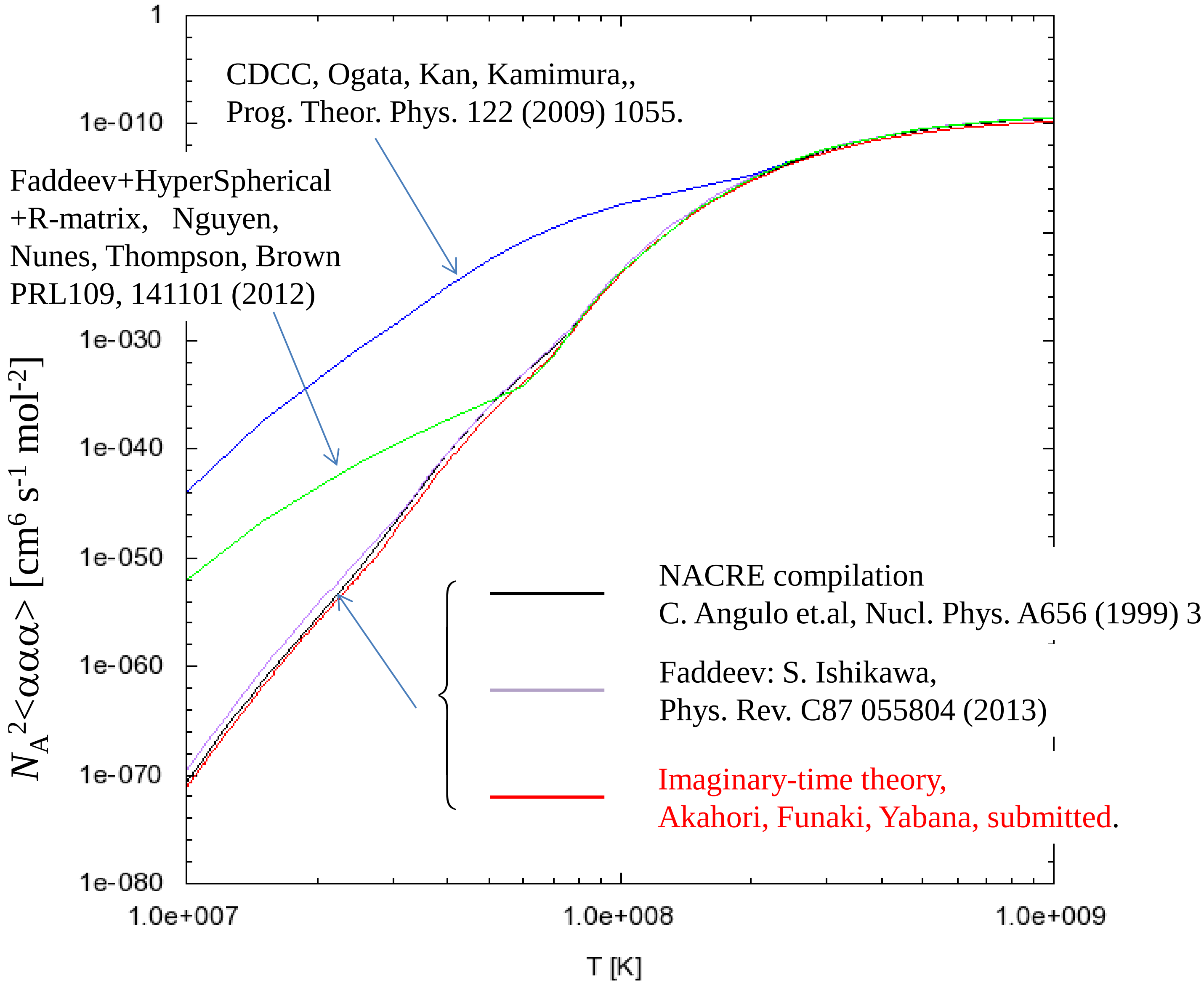
1985 K. Nomoto proposed an empirical formula applicable at low temperature, assuming sequential $\alpha\alpha$ and α^{8}Be reactions. (adopted in NACRE)

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

2009- Serious quantum-mechanical calculations of triple-alpha reaction rate started. At present, controversial among theories.

Calculated rates deviates among theories at low temperature

10^{26} order of magnitude difference at 10^7 K



Difficulties and theoretical challenges of triple-alpha reaction

- Experimental measurement is very difficult.

- Lack of exact theory for scatting of three charged particles,
  (we do not know "Coulomb wave function" for 3-charged particles).

- The reaction rate changes 10^{60} in magnitude between 10^7 – 10^9 K due to quantum tunneling nature of the process..

Develop a new theory: Imaginary-time theory

Contents

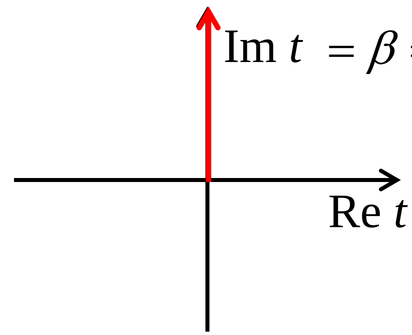
1. Formalism
2. Numerical results
3. Derive empirical formula from the imaginary-time theory
4. Difficulties of coupled-channels approach

What is the “imaginary-time” ?

Identifying inverse temperature with imaginary-time,

A standard procedure in thermal quantum many-body theory

$$\mathrm{Im}\ t = \beta = \frac{1}{kT}$$



Difference from ordinary approach

Standard procedure

Cross section as a function of energy, $\sigma(E)$.

Thermal average to obtain reaction rate, $<v\sigma>$.

Imaginary-time theory

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

We directly calculate reaction rate, $<v\sigma>$, without solving any scattering problem.

Imaginary-time theory: Derivation

Radiative capture cross section

$$M_{\lambda\mu} = \sum_{i \in p} r_i^{\lambda} Y_{\lambda\mu}(\hat{r}_i)$$

λ photon multipolarity

$$v\sigma_{fi} \propto \left(\frac{E_{\vec{k}} - E_f}{\hbar c} \right)^{2\lambda+1} \left| \int d\vec{r}\, \phi_f^*(\vec{r}) M_{\lambda\mu} \phi_{\vec{k}}(\vec{r}) \right|^2$$

Final: bound state

$$\int d\vec{r} \left| \phi_f(\vec{r}) \right|^2 = 1$$

Initial: scattering state

$$\phi_{\vec{k}}(\vec{r}) \to e^{i\vec{k}\vec{r}} + f(\hat{r}) \frac{e^{ikr}}{r} \qquad \text{(2-body)}$$

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

$$\langle v\sigma \rangle \propto \int d\vec{k}\, e^{-\beta E_k} v\sigma_{fi}$$

$$\langle v\sigma_{fi} \rangle \propto \int d\vec{k}\, e^{-\beta E_{\vec{k}}} \left(\frac{E_{\vec{k}} - E_f}{\hbar c} \right)^{2\lambda+1} \langle \phi_f | M_{\lambda\mu} | \phi_{\vec{k}} \rangle \langle \phi_{\vec{k}} | M_{\lambda\mu}^{+} | \phi_f \rangle$$

Eliminate scattering state using spectral representation

$$f(\hat{H}) = \sum_n f(E_n) |\phi_n\rangle\langle\phi_n| + \int d\vec{k}\, f(E_{\vec{k}}) |\phi_{\vec{k}}\rangle\langle\phi_{\vec{k}}|$$

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

$$\hat{P} = 1 - \sum_n |\phi_n\rangle\langle\phi_n|$$

Final expression does not include any scattering states.

Imaginary-time theory : Calculation in practice

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

Start with 2^+ state of ^{12}C
(wave function after radiative capture)
multiplied with E2 operator

$$\psi(\beta=0) = M_{\lambda=2,\mu}^{+}\phi_f\left({}^{12}\mathrm{C},2^+\right)$$

Evolve along imaginary-time axis

$$-\frac{\partial}{\partial\beta}\psi(\beta) = H\psi(\beta)$$

Reaction rate as expectation value

$$\langle v\sigma\rangle \propto \left\langle \psi\left(\frac{\beta}{2}\right) \middle| \left(\frac{\hat{H}-E_f}{\hbar c}\right)^{2\lambda+1} \middle| \psi\left(\frac{\beta}{2}\right)\right\rangle$$

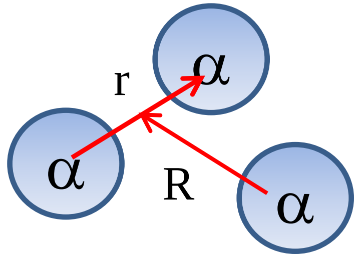
Hamiltonian of 3 alpha particles

$$H = T + V_{12} + V_{23} + V_{31} + V_{123}$$

$V_{\alpha\alpha}$ to reproduce ^{8}Be resonance energy

$V_{\alpha\alpha\alpha}$ to reproduce resonance energy of Hoyle state (0_2^+ of ^{12}C)

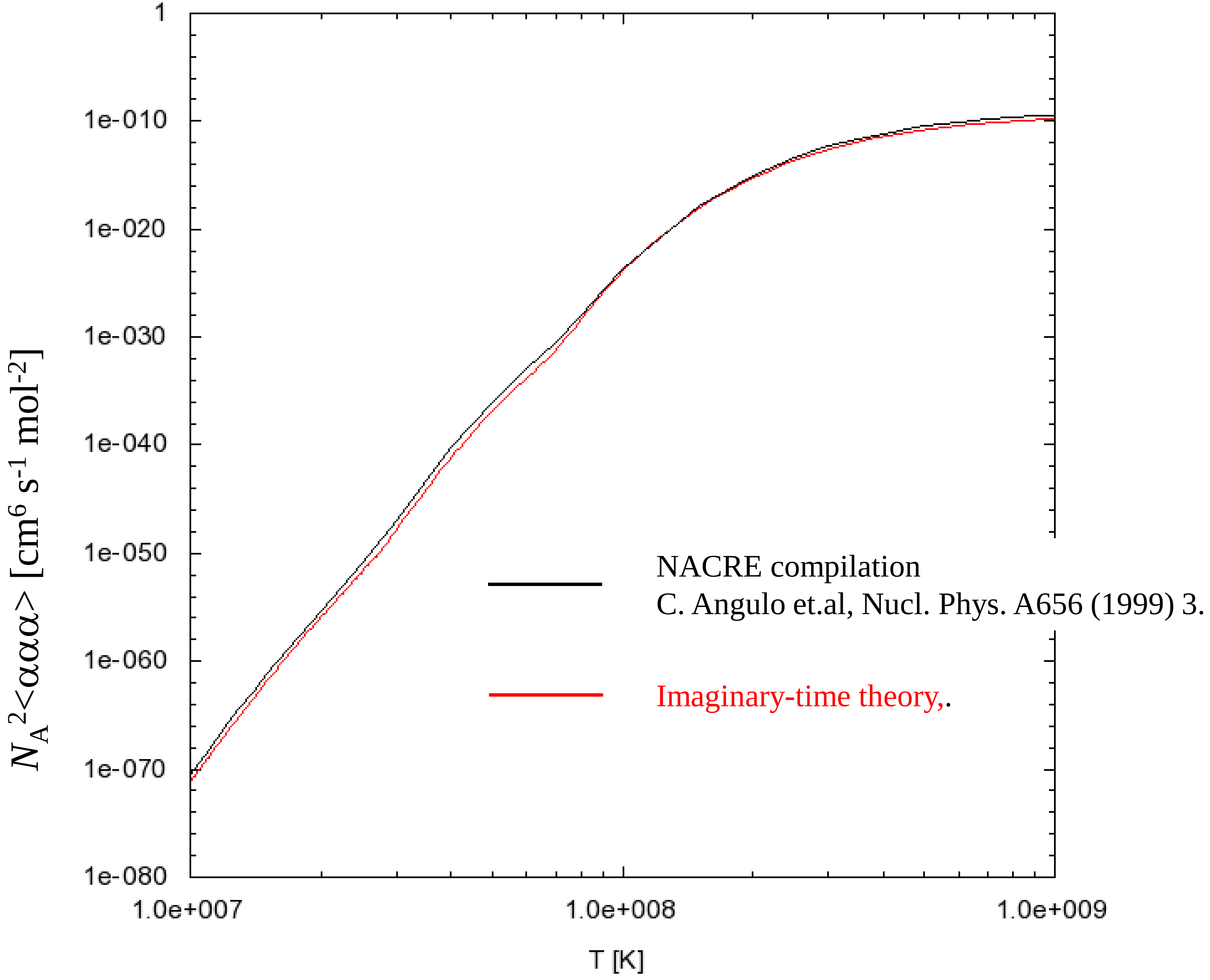
Coordinates



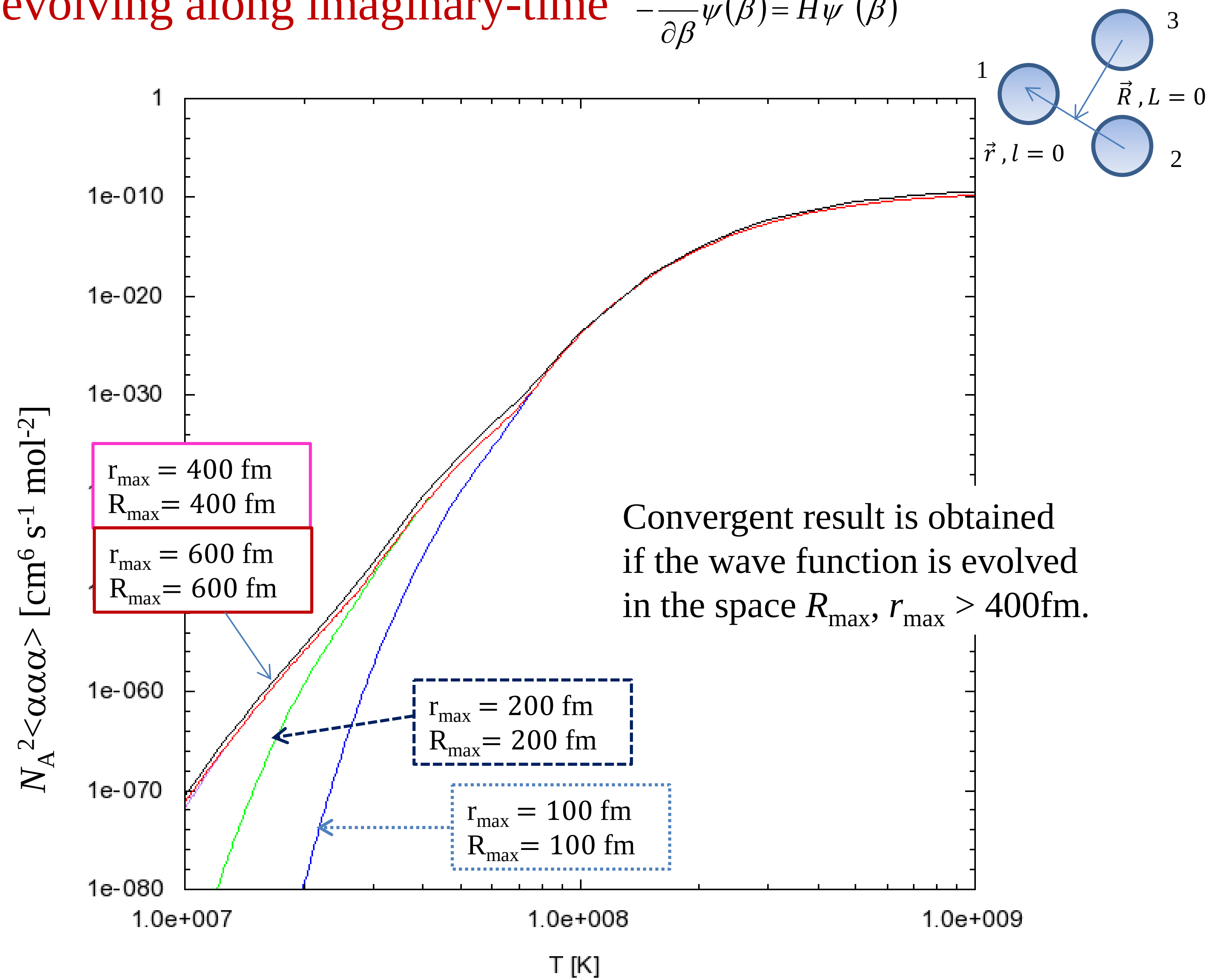
$$\psi(\vec{r},\vec{R},\beta) = \frac{u_{l=L=0}(r,R,\beta)}{rR}\left[Y_{l=0}(\hat{r})Y_{L=0}(\hat{R})\right]_{J=0}$$

Jacobi coordinate, $l=L=0$ only (as in CDCC)
Uniform grid for R and r

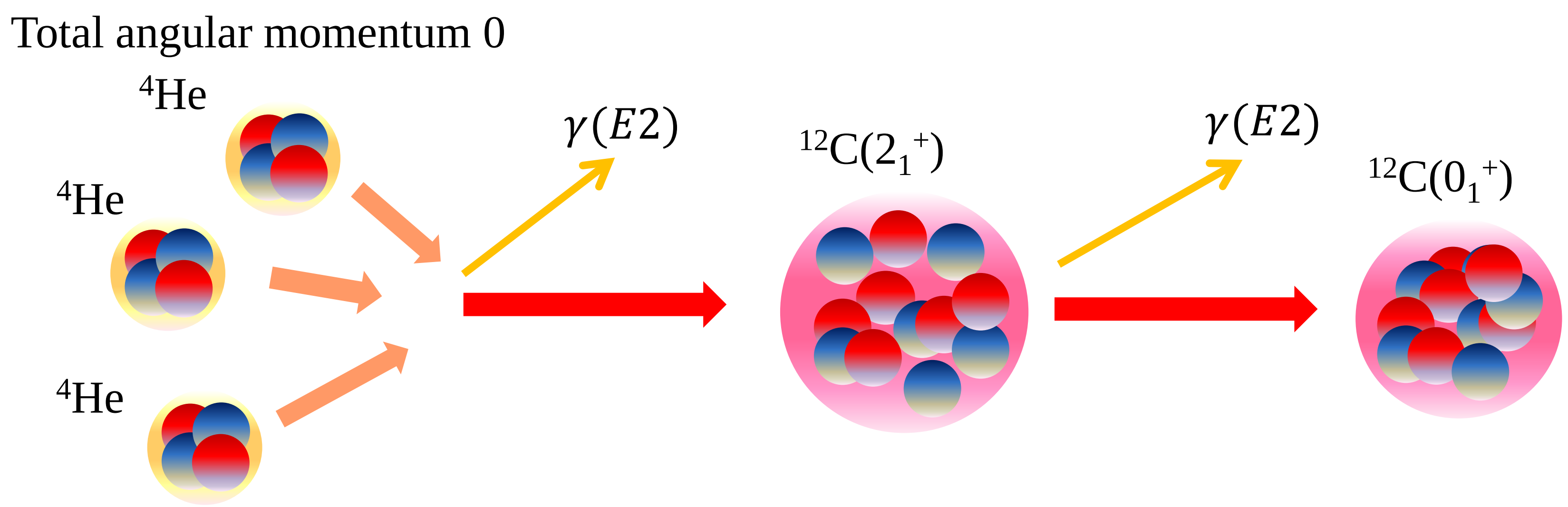
Triple-alpha reaction rate by the imaginary-time theory almost coincides with empirical NACRE rate.

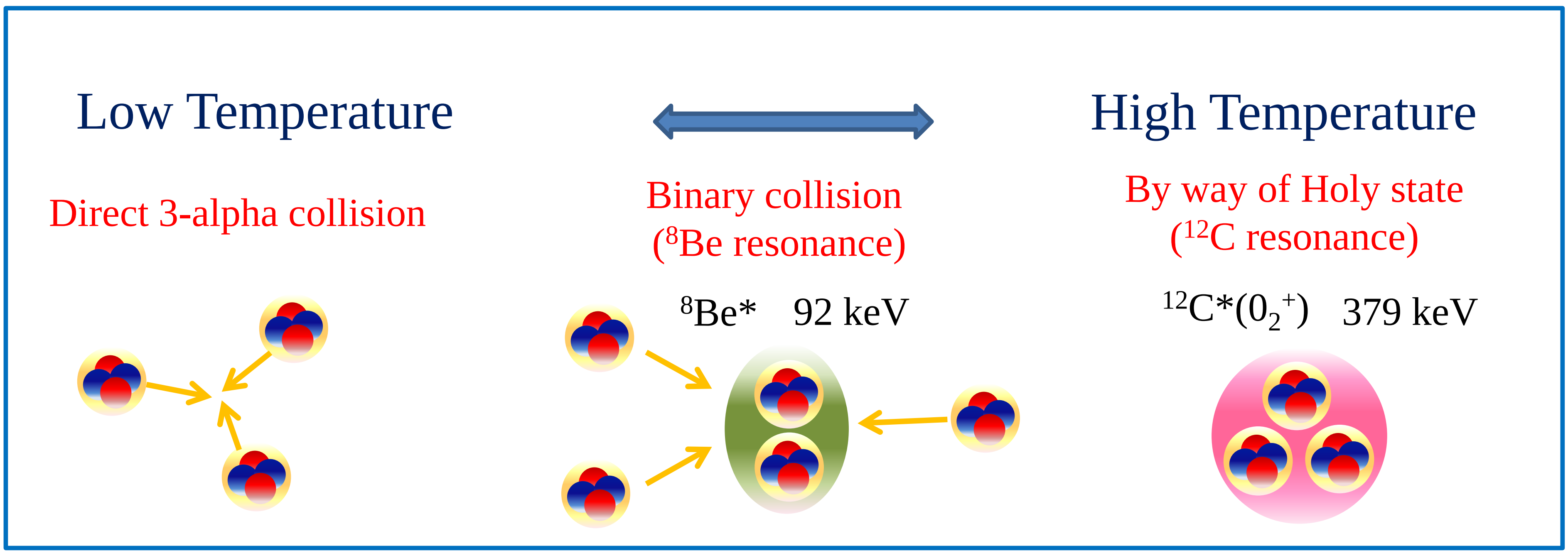


Convergence with respect to spatial size ($R_{\max}$ and $r_{\max}$) in evolving along imaginary-time $-\frac{\partial}{\partial \beta}\psi(\beta) = H\psi(\beta)$



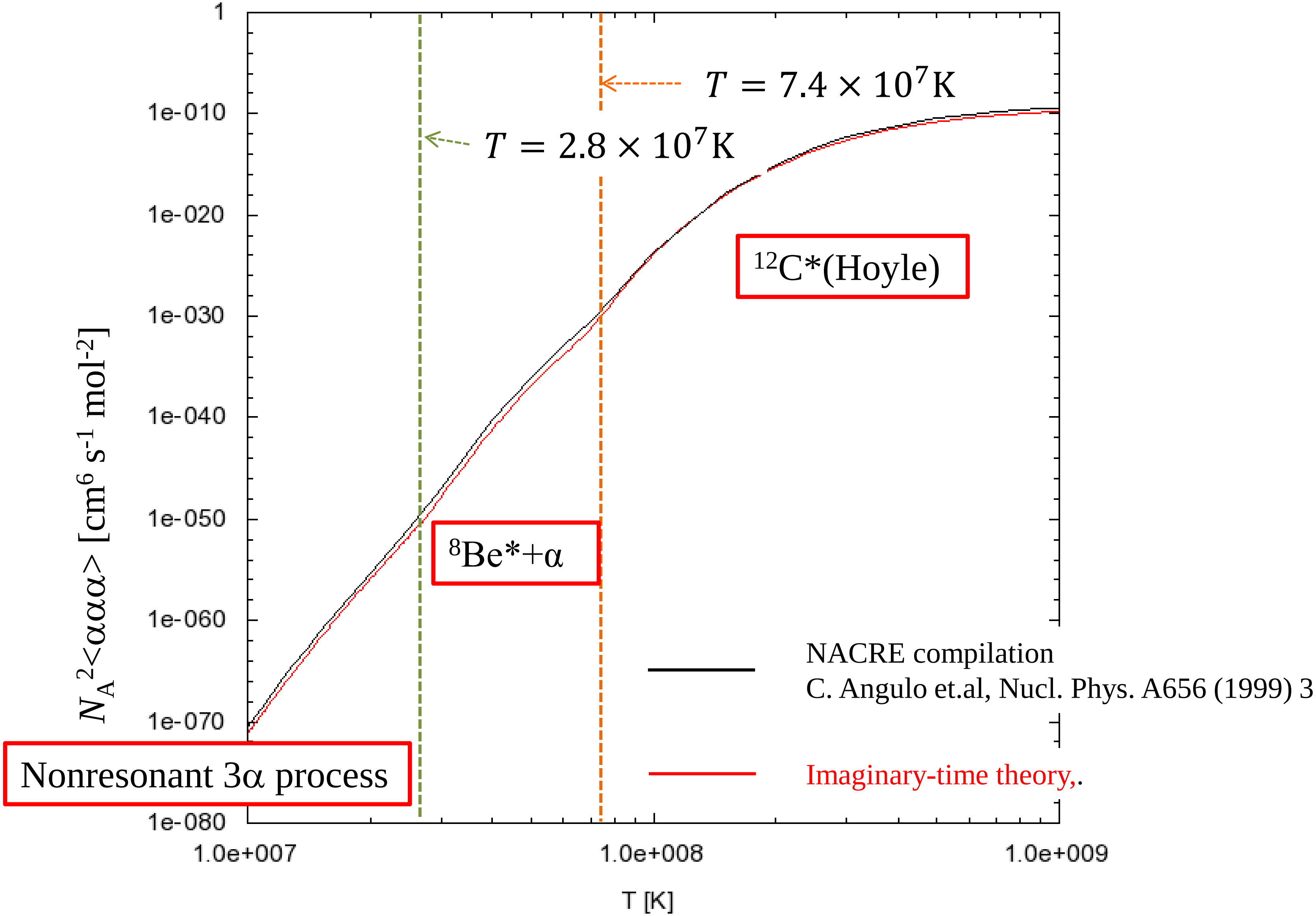
Dominant ^{12}C synthesis process depends on temperature





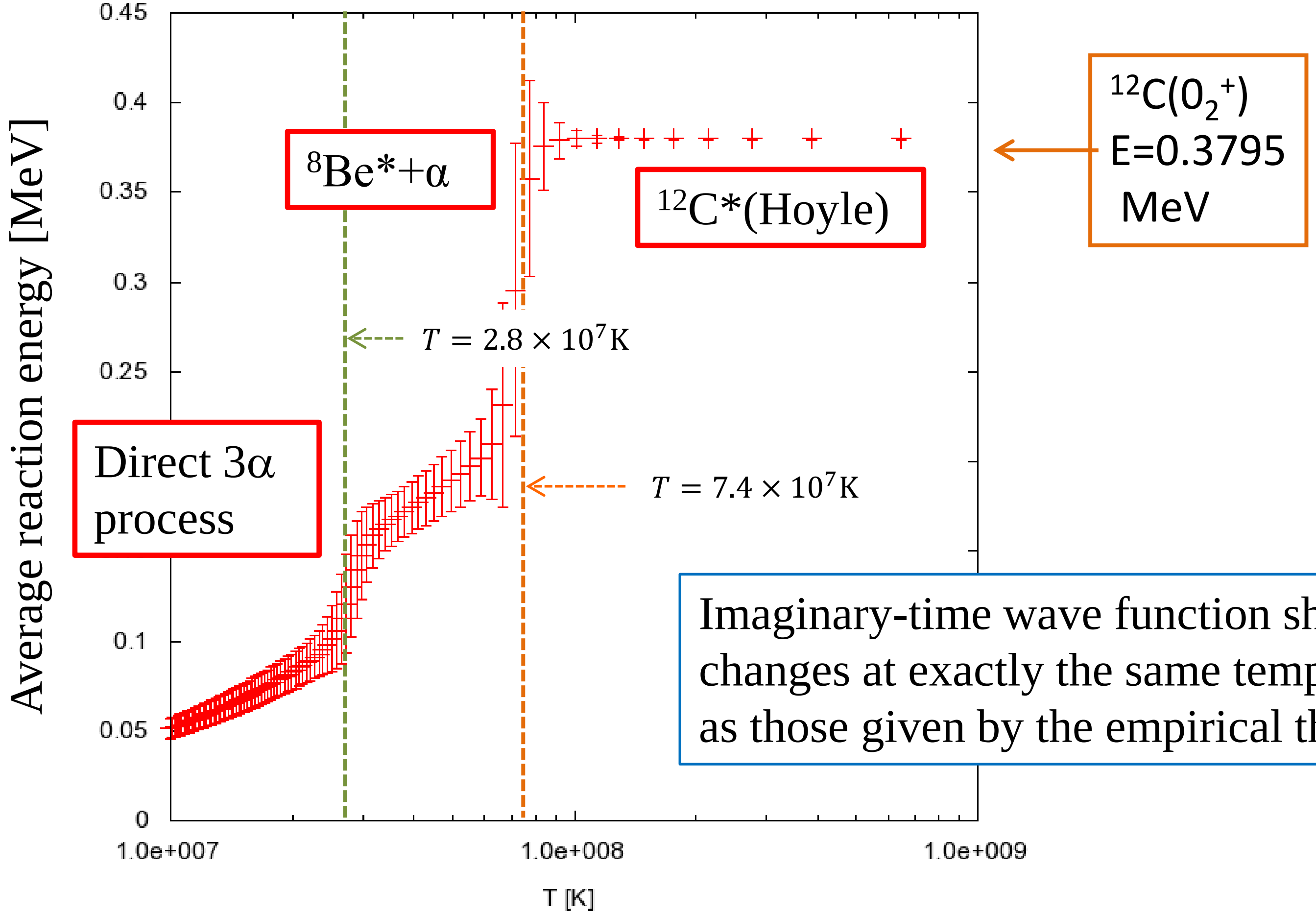
Changes of reaction mechanisms at two temperatures in the empirical theory

K. Nomoto, Astrophys. J. 253, 798 (1982)



Average and variance of reaction energies as a function of temperature

$$\langle H \rangle \equiv \langle \Psi(\beta/2) | \hat{H} | \psi(\beta/2) \rangle$$
$$\langle H^2 \rangle \equiv \langle \Psi(\beta/2) | \hat{H}^2 | \psi(\beta/2) \rangle$$
$$\Delta H \equiv \sqrt{\langle H^2 \rangle - \langle H \rangle^2}$$



Imaginary-time wave function shows changes at exactly the same temperatures as those given by the empirical theory.

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

Nomoto 1985、NACRE 1999：
Sequential 2-body process

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

Imaginary-time theory

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

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

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-^{8}Be parts

$$H = h_{\alpha\alpha} + h_{\alpha^{8}\mathrm{Be}}$$

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

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

Approximate spectral representation of H using R-matrix theory

$$f(\hat{H}) \to |\phi_H\rangle\langle\phi_H| \int dE_{\alpha\alpha} \frac{1}{2\pi} \frac{\Gamma_r({}^{8}\mathrm{Be}; E_{\alpha\alpha})}{\left(E_r({}^{8}\mathrm{Be}) + \Delta_r(E_{\alpha\alpha}) - E_{\alpha\alpha}\right)^2 + \Gamma_r(E_{\alpha\alpha})/4}$$

$$\times \int dE_{\alpha^{8}\mathrm{Be}} \frac{1}{2\pi} \frac{\Gamma_r({}^{12}\mathrm{C}; E_{\alpha^{8}\mathrm{Be}})}{\left(E_r({}^{12}\mathrm{C}) + \Delta_r(E_{\alpha^{8}\mathrm{Be}}) - E_{\alpha^{8}\mathrm{Be}}\right)^2 + \Gamma_r(E_{\alpha^{8}\mathrm{Be}})/4}$$

$$\times f(E_{\alpha\alpha} + E_{\alpha^{8}\mathrm{Be}})$$

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

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

Triple-alpha reaction rate derived from imaginary-time theory

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

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

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

$$\times \exp\left[-\frac{E_{\alpha\alpha} + E_{\alpha^8\mathrm{Be}}}{kT} \right] \cdot \Gamma_\gamma\left({}^{12}\mathrm{C}\right) \left(\frac{E_{\alpha\alpha} + E_{\alpha^8\mathrm{Be}} - E\left({}^{12}\mathrm{C}; 2^+\right)}{E\left({}^{12}\mathrm{C}; 0_2{}^+\right) - E\left({}^{12}\mathrm{C}; 2^+\right)} \right)^{2\lambda+1}$$

We ignore energy shift $\Delta(E)$

This expression mostly coincides with that of NACRE

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

There are a few minor differences.

$$\frac{\Gamma_\alpha\left({}^{12}\mathrm{C}; E_{\alpha^8\mathrm{Be}}\right)}{\left(E_r\left({}^{12}\mathrm{C}\right) - E_{\alpha^8\mathrm{Be}}\right)^2 + \Gamma_\alpha\left(E_{\alpha^8\mathrm{Be}}\right)/4} \Rightarrow \frac{\Gamma_\alpha\left({}^{12}\mathrm{C}; E_{\alpha^8\mathrm{Be}}\right)}{\left(E_r\left({}^{12}\mathrm{C}\right) + E_r\left({}^8\mathrm{Be}\right) - E_{\alpha^8\mathrm{Be}} - E_{\alpha\alpha}\right)^2 + \Gamma_\alpha\left(E_{\alpha^8\mathrm{Be}}\right)/4}$$

Imaginary-time theory

NACRE

(Not symmetric wrt α–α and α-^{8}Be)

Why different theories provide so different reaction rates ?

$$\langle \alpha\alpha\alpha \rangle_{\text{CDCC}} >> \langle \alpha\alpha\alpha \rangle_{\text{Imaginary-Time}} \approx \langle \alpha\alpha\alpha \rangle_{\text{NACRE}}$$

10^{26} order of magnitude difference at 10^7 K

To clarify the origin of theoretical controversy, we use coupled-channel expansion in the imaginary-time formalism

We first solve α–α 2-body eigenvalue problem.

$$h_{\alpha\alpha} w_n(r) = \varepsilon_n w_n(r)$$

$$\int_0^{r_{\max}} dr w_m(r) w_n(r) = \delta_{mn}$$

We then expand 3-body wave function with this basis

$$u(r, R, \beta) = \sum_n \chi_n(R, \beta) w_n(r)$$

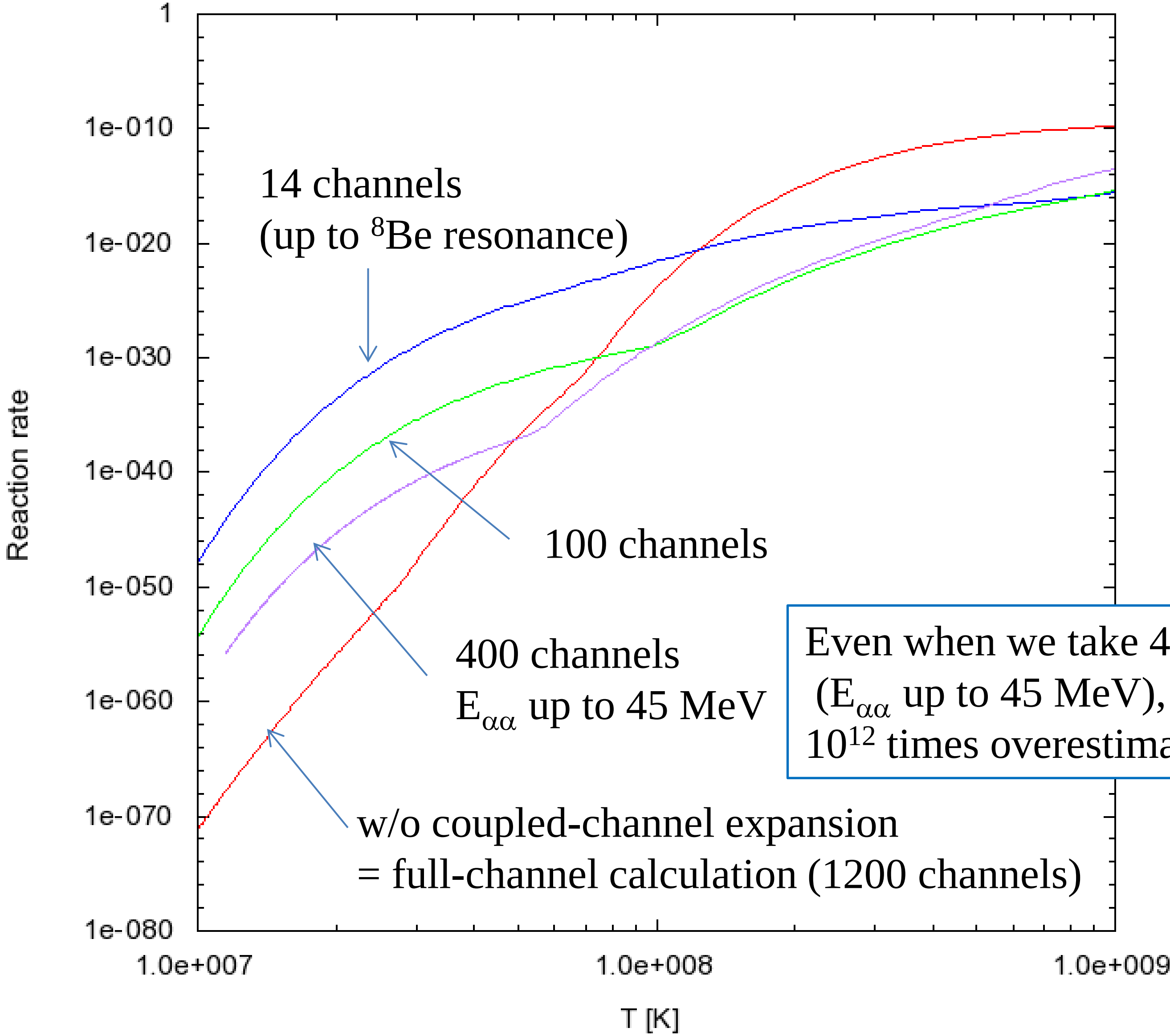
We then solve "coupled-channel imaginary-time equation"

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

Using complete set (all eigenfunction), $\{w_n(r)\}$, results should not change.
However, if we make a truncation, the result may be different.

Convergence of expansion is extremely slow !

Warning the use of coupled-channel method for quantum tunneling



1200 channels
in total

$$h_{\alpha\alpha} w_n(r) = \varepsilon_n w_n(r)$$

$$\int_0^{r_{\max}} dr w_m(r) w_n(r) = \delta_{mn}$$

Even when we take 400 channels ($E_{\alpha\alpha}$ up to 45 MeV), reaction rate is 10^{12} times overestimated.

Conclusion

Imaginary-time theory for radiative capture process

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

Triple-alpha reaction rate using the imaginary-time theory

- We can calculate a convergent reaction rate.
- The calculated reaction rate mostly coincides with that of NACRE
- Changes of reaction mechanisms occur at the same temperature of those of NACRE.

Analytical relation between the imaginary-time theory and the empirical formula

- Using R-matrix theory and assuming separable approximation,
  the imaginary-time theory gives almost the same formula as that of NACRE.

Origin of theoretical controversy

- We find an extremely slow convergence if we make a coupled-channels expansion.