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Imaginary time formalism of triple-alpha reaction

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Contents

What is the "imaginary time" ?

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

$$\beta = \frac{1}{k_B T}$$

Imaginary time = 1 / Temperature

In nuclear physics, we often use the "imaginary time method"
to calculate ground states of nuclei.

- Mean field calculations
- Ab-initio calculations

$$\lim_{\beta\to\infty} e^{-\beta H}\Psi = \Phi_0$$

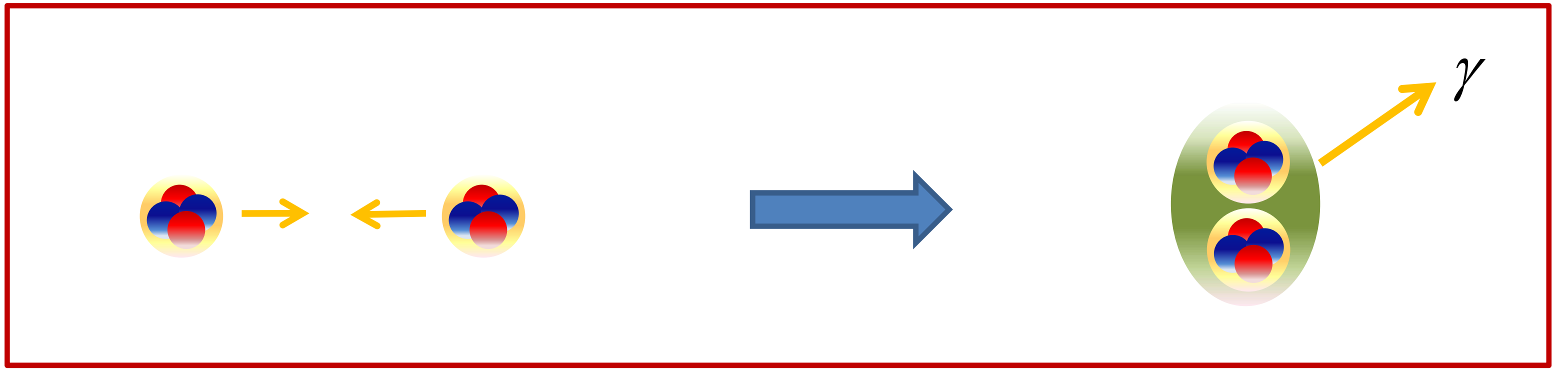
In quantum many-body theory at finite temperature,
Imaginary-time formalism is very popular

We use the "imaginary-time method" for radiative capture reaction rate.

K. Yabana, Y. Funaki, Phys. Rev. C85, 055803 (2012)

Evaluation of radiative capture reaction rate

Ordinary procedure



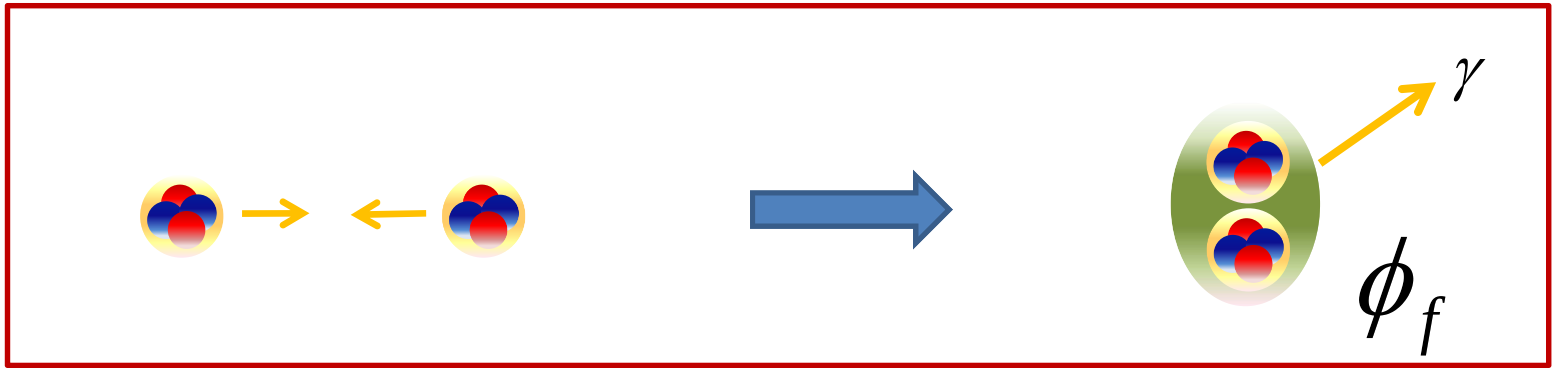
1. Measure/Calculate cross section as a function of energy

$$\sigma_{fi}(E)$$

2. Average with Boltzmann distribution, $\beta = 1/k_B T$

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

Imaginary time method for radiative capture reaction rate



Imaginary time algorithm

1. $\psi(\beta=0)=M_{\lambda\mu}{}^{+}\phi_f \qquad M_{\lambda\mu}=\sum_{i\in p} r_i^{\lambda} Y_{\lambda\mu}(\hat{r}_i)$

2. $\psi(\beta)=e^{-\beta H}\psi(\beta=0) \quad \Rightarrow \quad -\frac{\partial}{\partial\beta}\psi(\beta)=H\psi(\beta)$

   wave function at temperature $\beta=1/k_B T$

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

K. Yabana, Y. Funaki, Phys. Rev. C85, 055803 (2012)

We can skip solving scattering problems.

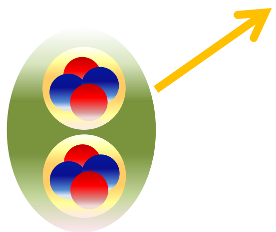
Derive the imaginary time formula.
(3 slides)

Imaginary time method (1/3): Ordinary procedure

Radiative capture process of two nuclei

Initial scattering state $\phi_{\vec{k}}(\vec{r})$

Final bound state $\phi_f(\vec{r})$



photon (λμ)

Cross section

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

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

λ photon multipolarity

Bound state

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

Scattering state

$$\phi_{\vec{k}}(\vec{r}) \to e^{i\vec{k}\vec{r}} + f(\hat{r}) \frac{e^{ikr}}{r}$$

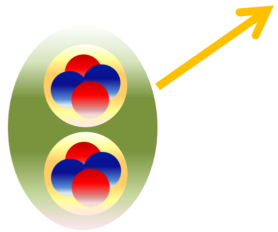
Reaction rate at $\beta = 1/k_B T$

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

Imaginary time method (2/3): Eliminate scattering state

Initial scattering state $\phi_{\vec{k}}(\vec{r})$

Final bound state $\phi_f(\vec{r})$



photon (λμ)

Eliminate scattering wave function

$$\langle v\sigma \rangle \propto \int d\vec{k} e^{-\beta E_k} \left(E_k - E_f\right)^{2\lambda+1} \langle \phi_f | M_{\lambda\mu} | \phi_{\vec{k}} \rangle \langle \phi_{\vec{k}} | M_{\lambda\mu}{}^{+} | \phi_f \rangle$$

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

bound wave function after photo-emission

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

Projector to remove bound states.

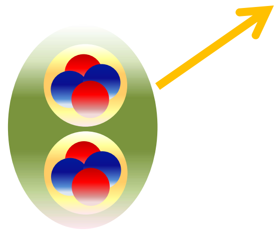
We use spectral representation of the Hamiltonian

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

Imaginary time method (3/3): Imaginary time algorithm

Initial scattering state $\phi_{\vec{k}}(\vec{r})$

Final bound state $\phi_f(\vec{r})$



photon (λμ)

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

Imaginary time algorithm

1. $\psi(\vec{r},\beta=0) = PM_{\lambda\mu}{}^{+}\phi_f(\vec{r})$ Initial wave function = final bound state x multipole operator

2. $\psi(\vec{r},\beta) = e^{-\beta H}\psi(\vec{r},0) \quad \Rightarrow \quad -\dfrac{\partial}{\partial\beta}\psi(\vec{r},\beta) = H\psi(\vec{r},\beta)$

   Imaginary time evolution → wave function at $\beta = 1/k_B T$

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

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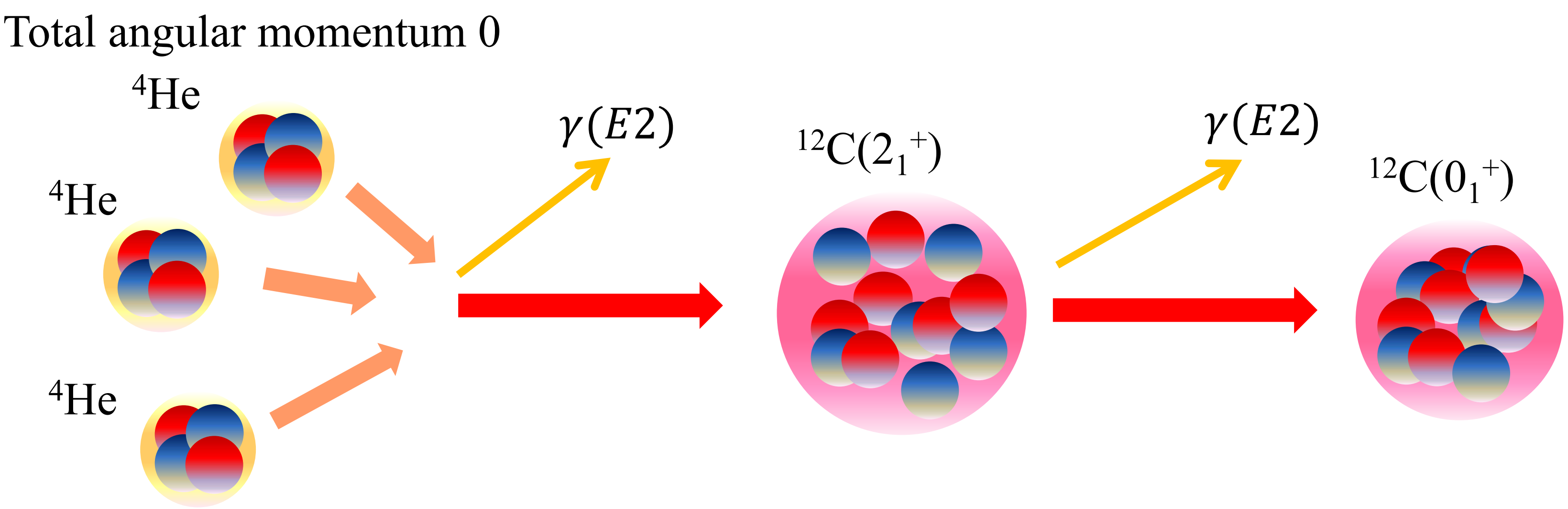
3. “Imaginary time formalism” applied to “triple-alpha reaction rate”

Triple-alpha reaction



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 αα 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.

Nomoto 1985、NACRE 1999:

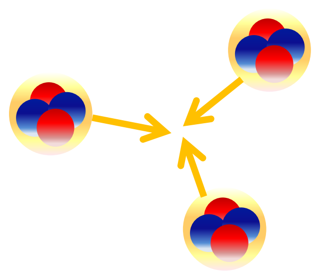
Sequential 2-body process assuming secular equilibrium

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

Three reaction mechanisms discussed in empirical theory

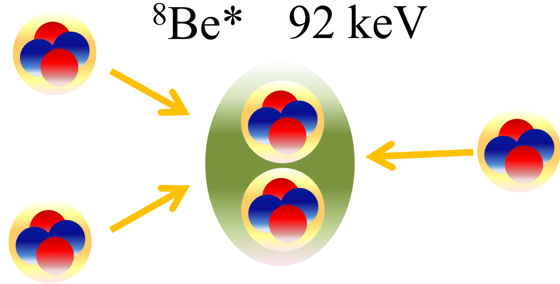
Low Temperature ⟷ High Temperature

Direct 3-alpha collision



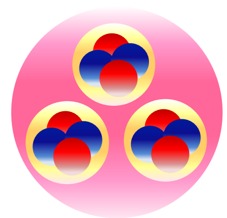
Binary collision
(^{8}Be resonance)

^{8}Be* 92 keV



By way of Holy state
(^{12}C resonance)

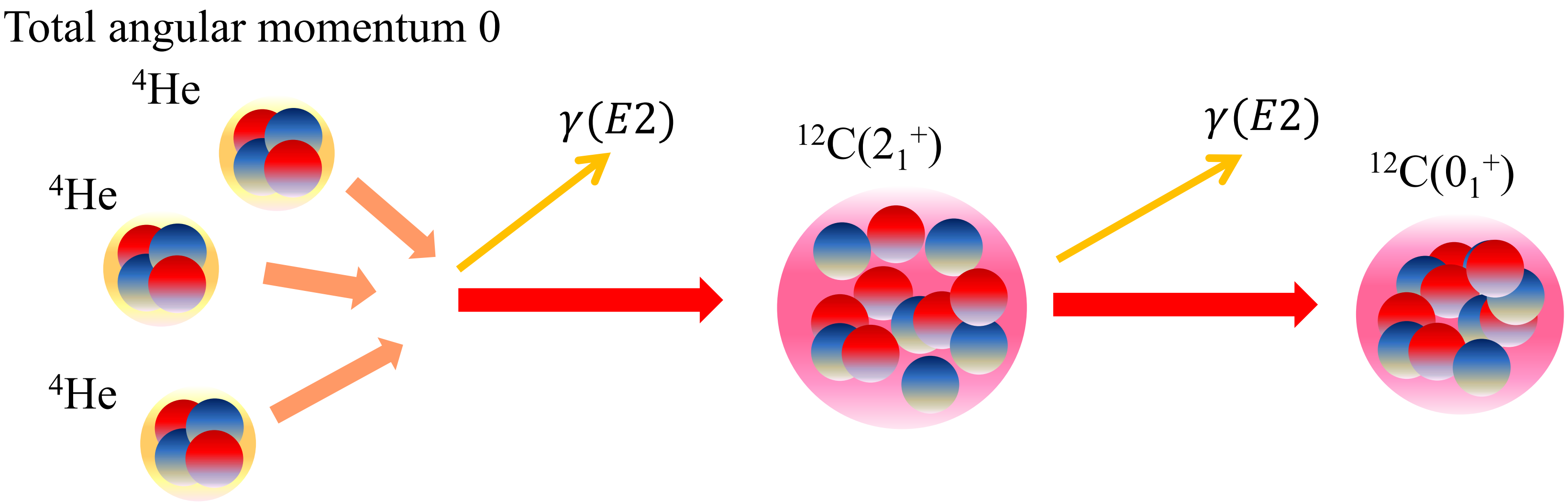
^{12}C*(0_2^+) 379 keV



$T = 2.8 \times 10^7$K

$T = 7.4 \times 10^7$K

Triple-alpha reaction



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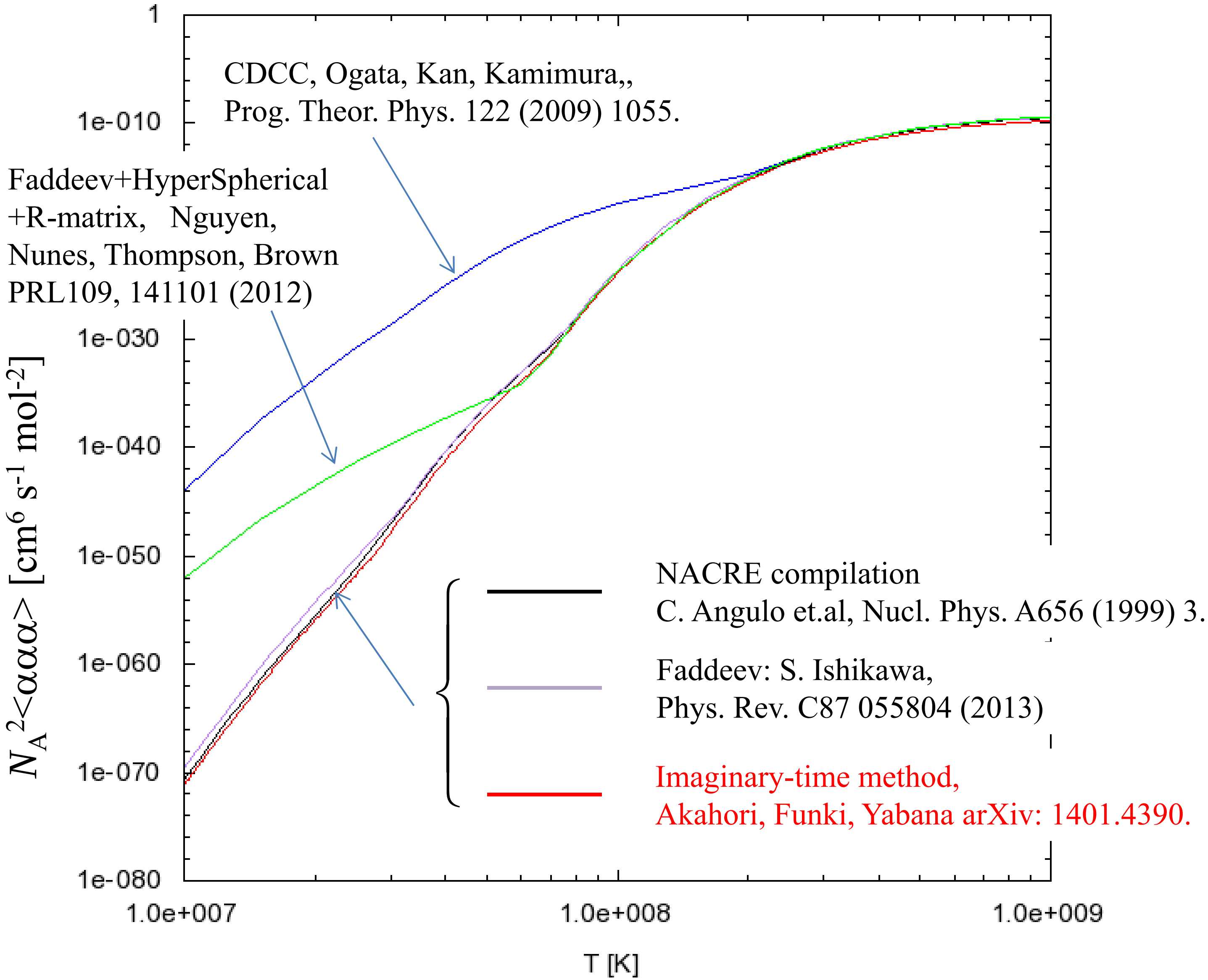
Triple-alpha reaction rate: theoretical controversy

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



Difficulties and theoretical challenges of triple-alpha process

- Experimental measurements are very difficult.

- Scatting problem 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.

Imaginary time method will be suitable
since it does not require any scattering solutions.

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Triple-alpha reaction rate by the imaginary-time theory

T. Akahori, Y. Funaki, K. Yabana, arXiv: 1401.4390

Prepare by OCM
(Orthogonality Condition Model)

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

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

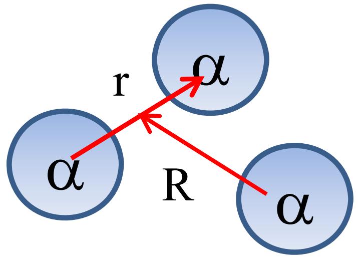
Hamiltonian of 3 alpha particles

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

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

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

Coordinates

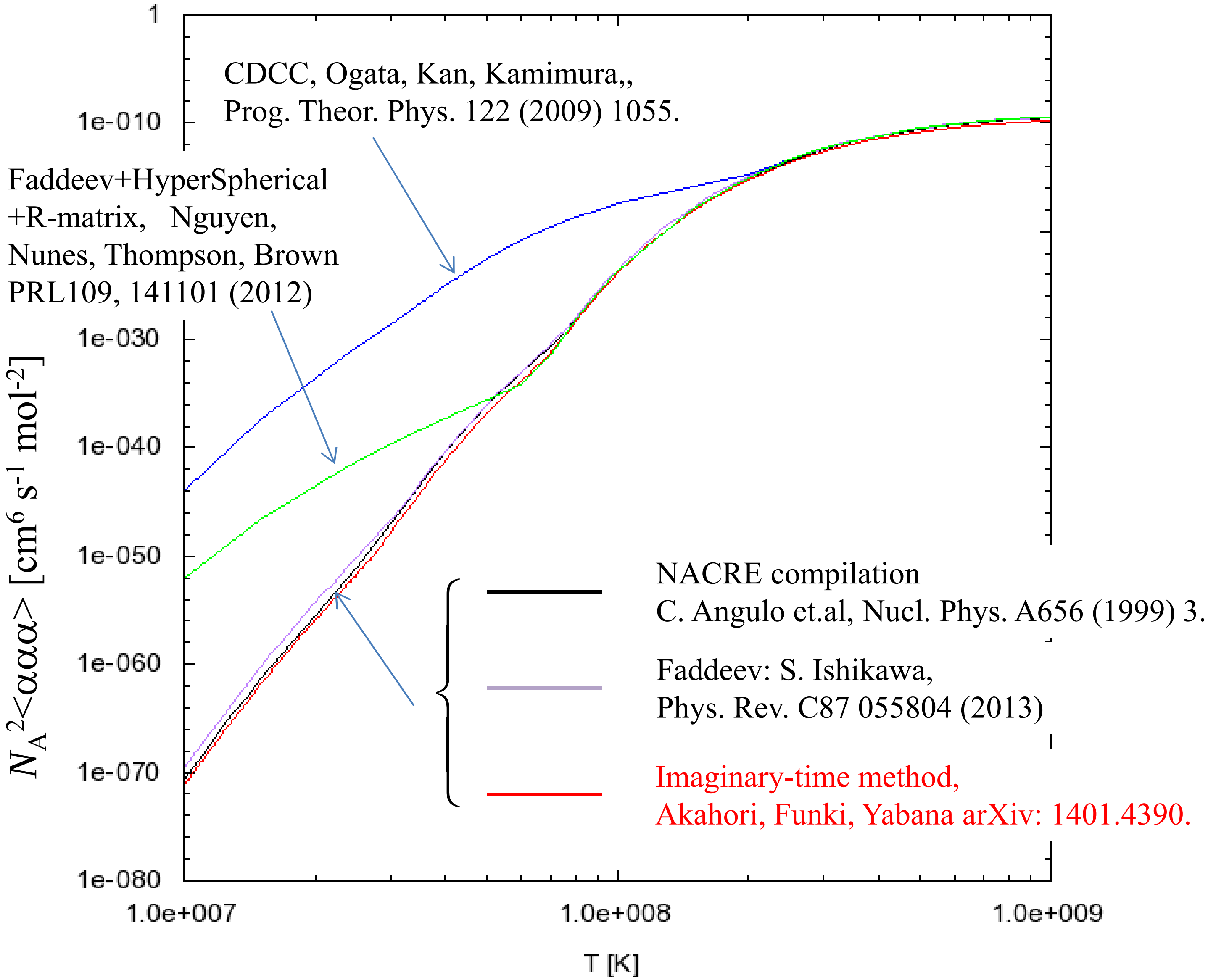


$$\psi(\vec{r},\vec{R},\beta)=\frac{u_{l=L=0}(r,R,\beta)}{rR}\left[Y_{l=0}(\hat{r})Y_{L=0}(\hat{R})\right]_{J=0}$$

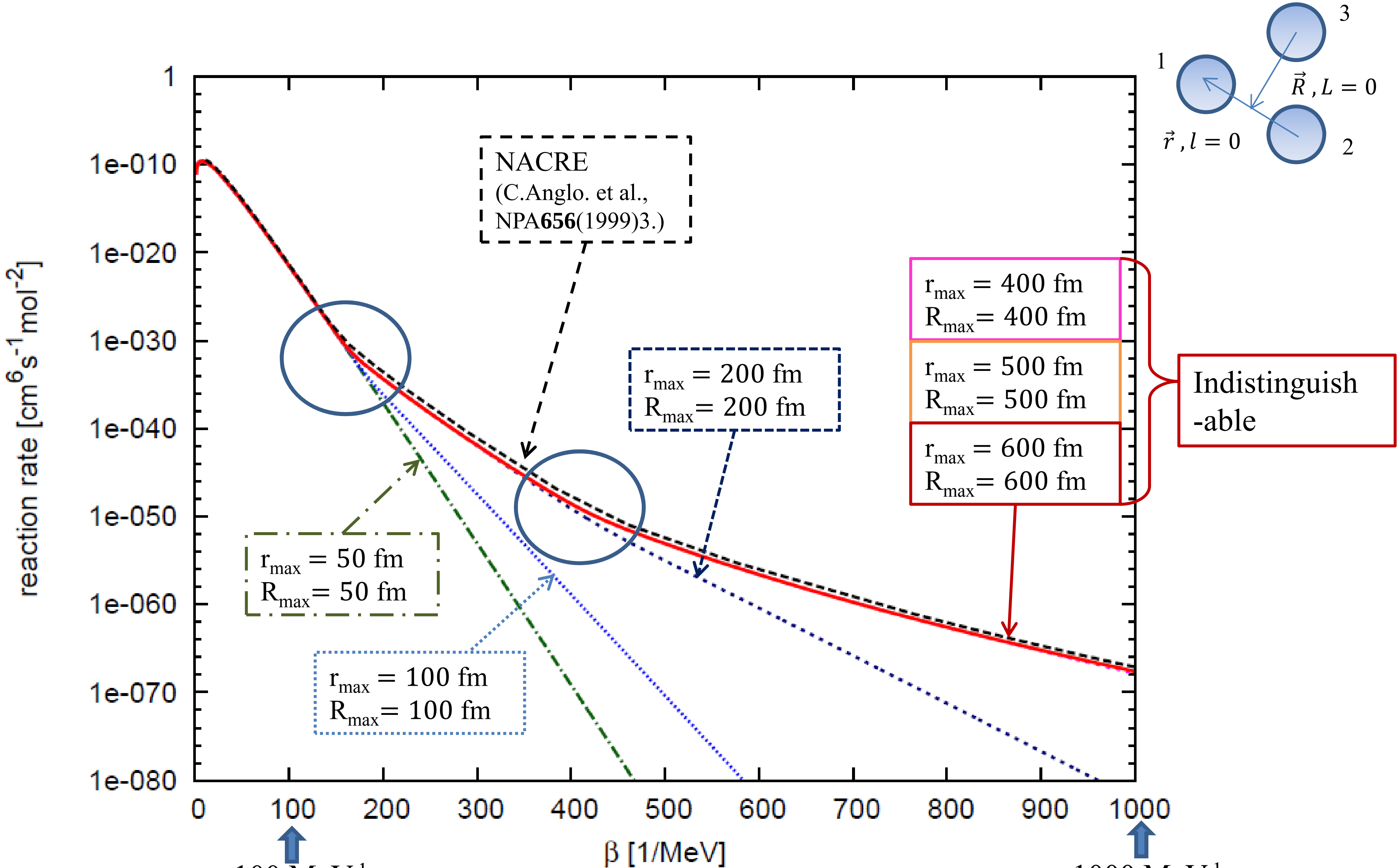
Jacobi coordinate, $l=L=0$ only
Uniform grid for R and r, $\Delta R=\Delta r=0.5$fm

Triple-alpha reaction rate: theoretical controversy

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



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



100 MeV^{-1}
= 1.15 x 10^8 K

$=1/k_B T$

1000 MeV^{-1}
= 1.15x 10^7 K

Nomoto 1985、NACRE 1999 :
Sequential 2-body process assuming secular equilibrium

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

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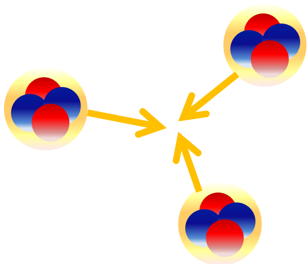
Low Temperature ⟷ High Temperature

Direct 3-alpha collision



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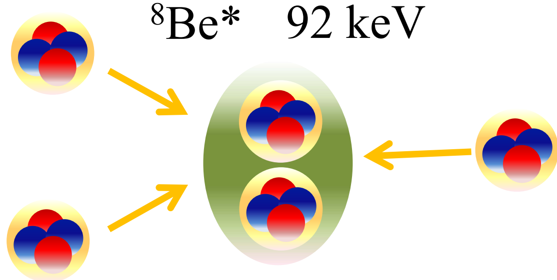

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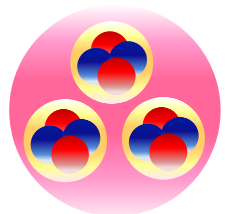

$T = 2.8 \times 10^7$K

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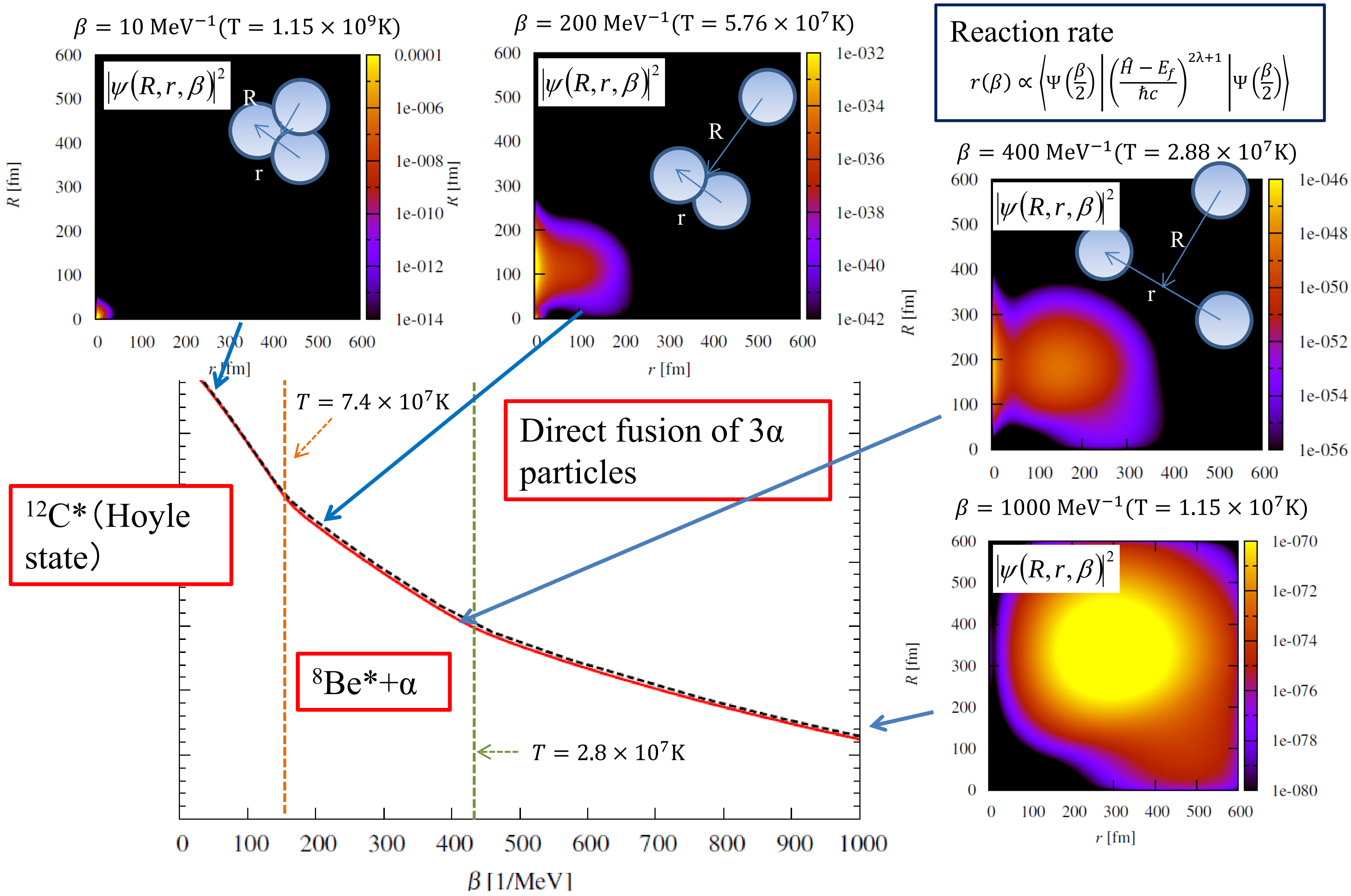
Imaginary time evolution of wave function $\psi(R,r,\beta)$



Gamow peak energy from imaginary time evolution

Reaction rate

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

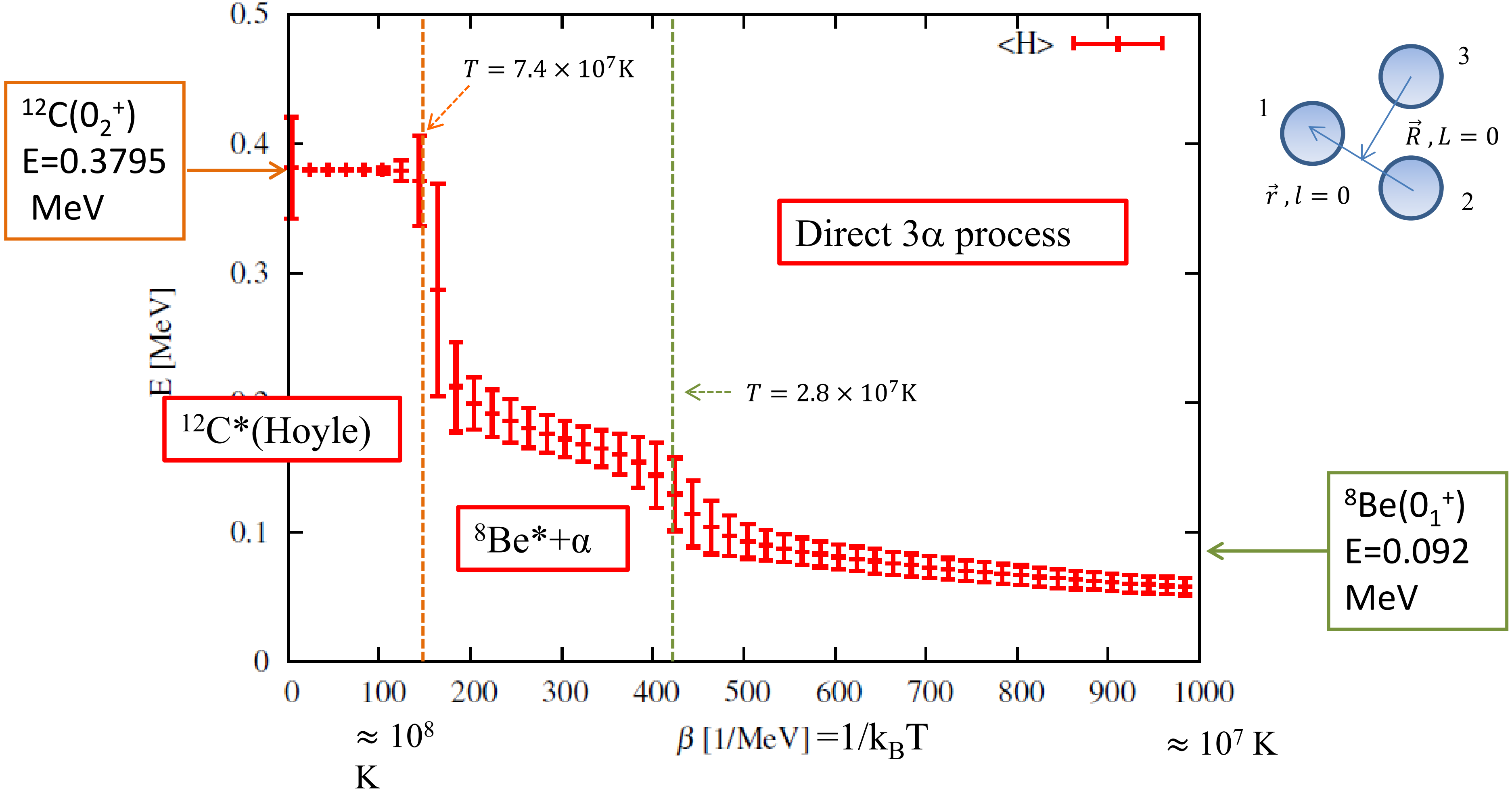
$$\equiv \langle \Psi(\beta/2) | \psi(\beta/2) \rangle$$

Average and variance of energy

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

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

$$\Delta H \equiv \sqrt{\langle H^2 \rangle - \langle H \rangle^2}$$



Though our imaginary time forumula is very different from NACRE, calculated rate is quite close to each other.

Nomoto 1985、NACRE 1999:
Sequential 2-body process assuming secular equilibrium

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

Imaginary time theory

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

We can derive a formula quite close to NACRE making some assumptions.

To derive NACRE-like formula,
we need to assume "separable assumption

1. Three-body Hamiltonian is separable, into α-α and α-^{8}Be parts

$$H = H_{\alpha\alpha} + H_{\alpha\mathrm{Be}}$$

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

$$\Phi_H \simeq \phi_r^{\alpha\alpha}(\vec{r})\phi_r^{\alpha\mathrm{Be}}(\vec{R})$$

Combining R-matrix theory, we may obtain

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

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

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

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

This almost coincides with NACRE formula

Summary

We have developed a new theoretical formalism for radiative capture reaction rate "imaginary time method"

- We evolve wave function, starting with bound wave function after fusion
- It does not require any scattering solution to calculate reaction rate

We have applied the imaginary-time method 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.

Since imaginary time method is used in various nuclear structure calculations, the imaginary time method may be useful to extend them for reaction rate calculations.

Derive "Breit-Wigner formula" for the triple-alpha reaction

Two basic assumptions

1. Three-body Hamiltonian is separable, into α-α and α-^{8}Be parts

$$H = -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial R^2} - \frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + V(r,R) \approx -\frac{\hbar^2}{2M}\frac{\partial^2}{\partial R^2} - \frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2} + V_R(R) + V_r(r)$$

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

$$\Phi_H \simeq \phi_r^{\alpha\alpha}(\vec{r})\phi_r^{\alpha\mathrm{Be}}(\vec{R})$$

Then the spectrum representation of the Hamiltonian is given by、

$$f(\hat{H}) \to |\phi_H\rangle\langle\phi_H| \int dE_{\alpha\alpha} \frac{1}{2\pi} \frac{\Gamma_r({}^8\mathrm{Be}; E_{\alpha\alpha})}{\left(E_r({}^8\mathrm{Be}) + \Delta_r(E_{\alpha\alpha}) - E_{\alpha\alpha}\right)^2 + \Gamma_r(E_{\alpha\alpha})/4}$$
$$\times \int dE_{\alpha^8\mathrm{Be}} \frac{1}{2\pi} \frac{\Gamma_r({}^{12}\mathrm{C}; E_{\alpha^8\mathrm{Be}})}{\left(E_r({}^{12}\mathrm{C}) + \Delta_r(E_{\alpha^8\mathrm{Be}}) - E_{\alpha^8\mathrm{Be}}\right)^2 + \Gamma_r(E_{\alpha^8\mathrm{Be}})/4}$$
$$\times f(E_{\alpha\alpha} + E_{\alpha^8\mathrm{Be}})$$

We put it into the imaginary-time expression of the reaction rate

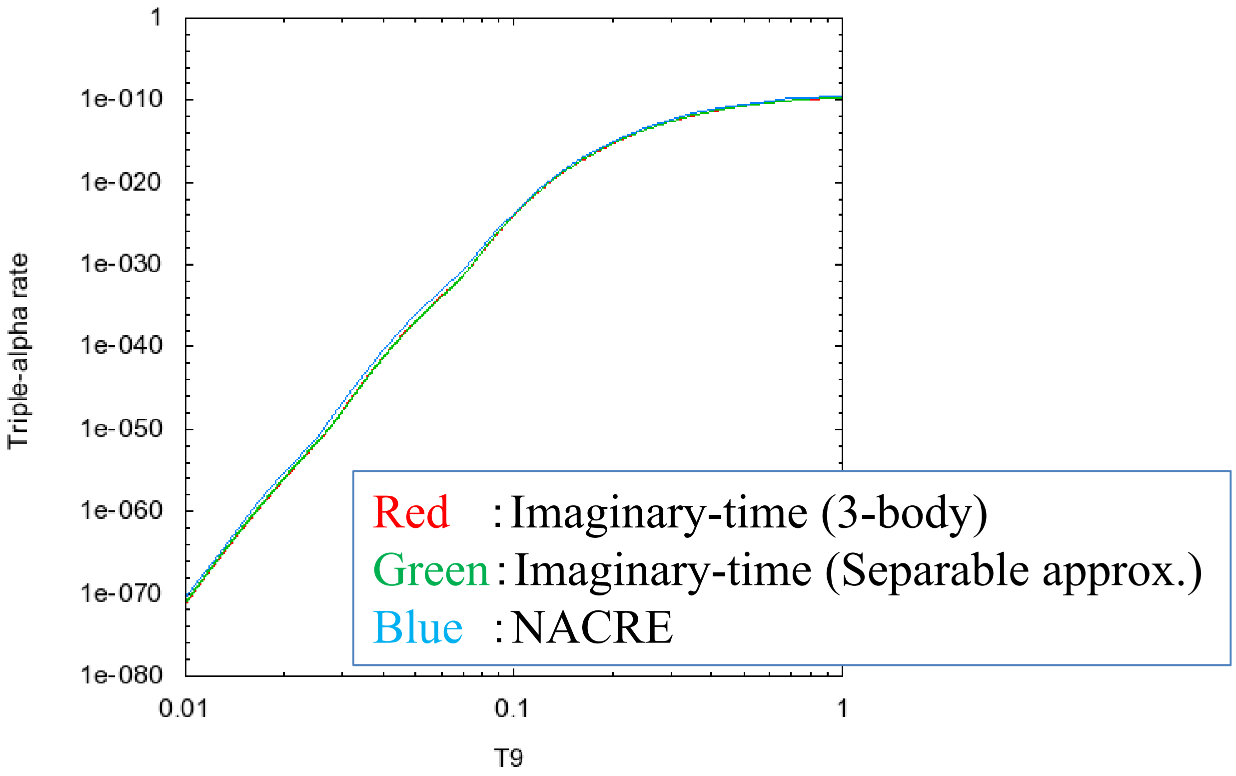
$$\langle \alpha\alpha\alpha \rangle \propto \left\langle \phi_f \middle| M_{\lambda\mu} e^{-\beta\hat{H}} \left(\frac{\hat{H} + |E_f|}{\hbar c} \right)^{2\lambda+1} \hat{P} M_{\lambda\mu}^{+} \middle| \phi_f \right\rangle$$

How good is the separable assumption

$$H(R,r) \overset{?}{\approx} H_{\alpha^8\mathrm{Be}}(R) + H_{\alpha\alpha}(r)$$

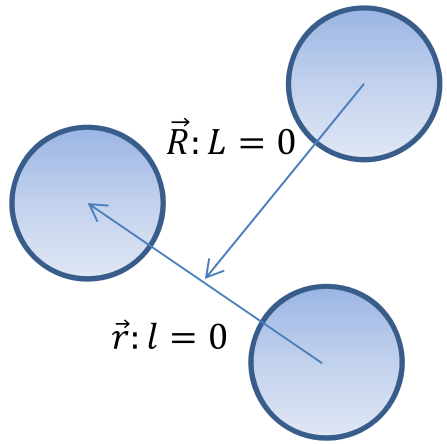
3-body Hamiltonian — Separable approx.

We calculate the triple-alpha reaction rate using separable Hamiltonian.
The separable Hamiltonian is so constructed that resonances of ^{8}Be and ^{12}C(0_2^+) are reproduced



In the imaginary time theory,
we solved radial Schrodinger equation of two variables *R* and *r*.

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



We make a coupled-channels approximation in the imaginary time theory to know the origin of the difference.

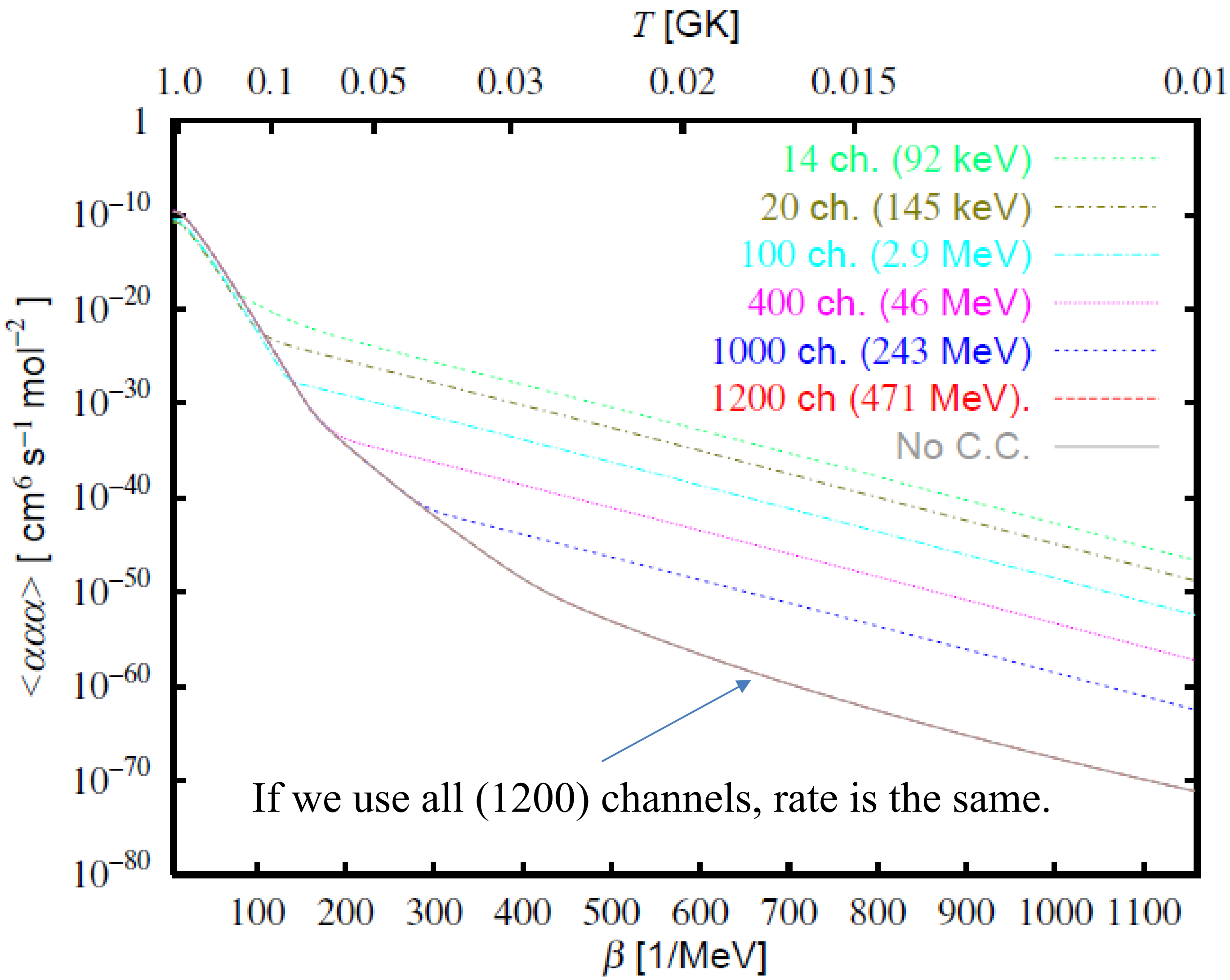
In the coupled-channel approximation,
We solve the αα problem first, and then use the solution as base.

$$\left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}+v_{\alpha\alpha}(r)\right]w_n(r)=\varepsilon_n w_n(r)$$

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

Up to $r_{\max}$=600fm with Δr=0.5fm, we have 1200 eigenfunctions (channels).

Convergence with respect to channels is very slow.



Warn slow convergence of coupled channels approach for tunneling problem.