新学術科研費
「素核宇融合による計算基礎科学物理学の進展研究会」
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A New Computational Approach for Radiative Capture Reaction Rate

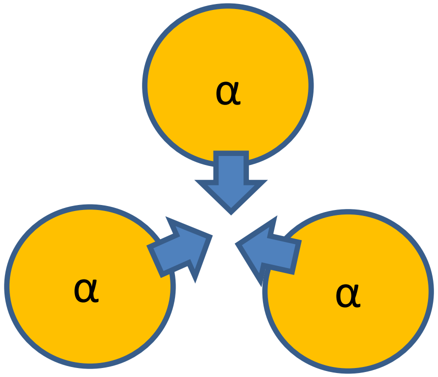
K. Yabana

University of Tsukuba

In collaboration with
Y. Funaki, T. Akahori

I will talk on our work towards…

$$3\alpha \rightarrow {}^{12}\mathrm{C}$$



In astrophysical environment,

- reaction starts in total angular momentum L=0
- proceeds either resonant (Hoyle state) or nonresonant
- emission of E2 gamma-ray to yield bound 2^+ state ^{12}C at 4.44MeV

Computational approach is important

- since experiment is not possible
- but serious calculation was achieved only recently.

Recent 3α -> ^{12}C reaction rate calculation by CDCC method
The first serious 3-body direct capture calculation below barrier energy

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

Kazuyuki OGATA,[1,*)] Masataka KAN[1,**)] and Masayasu KAMIMURA[1,2]

[1] *Department of Physics, Kyushu University, Fukuoka 812-8581, Japan*
[2] *RIKEN Nishina Center, Wako 351-0198, Japan*

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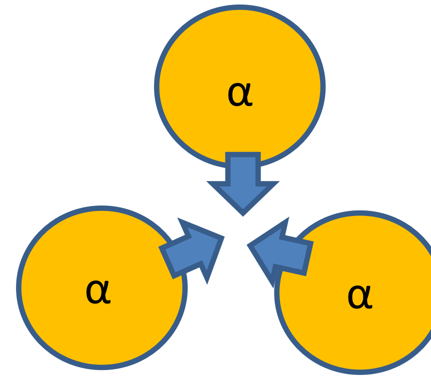
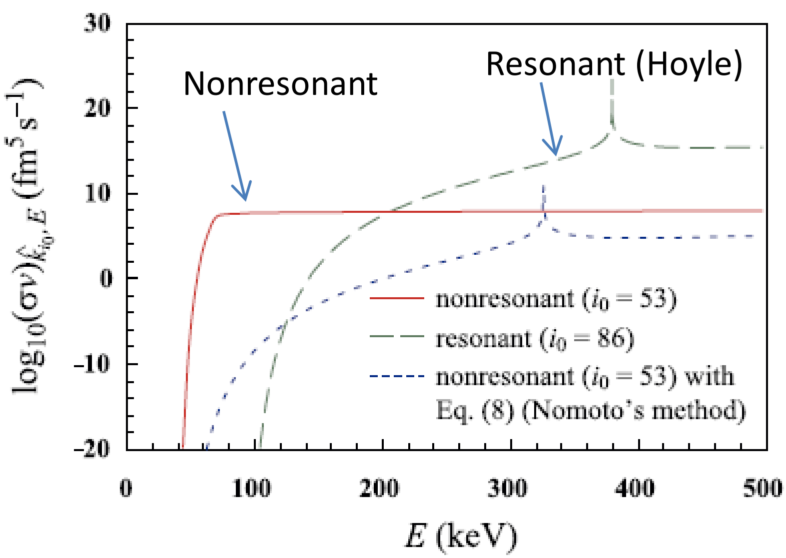
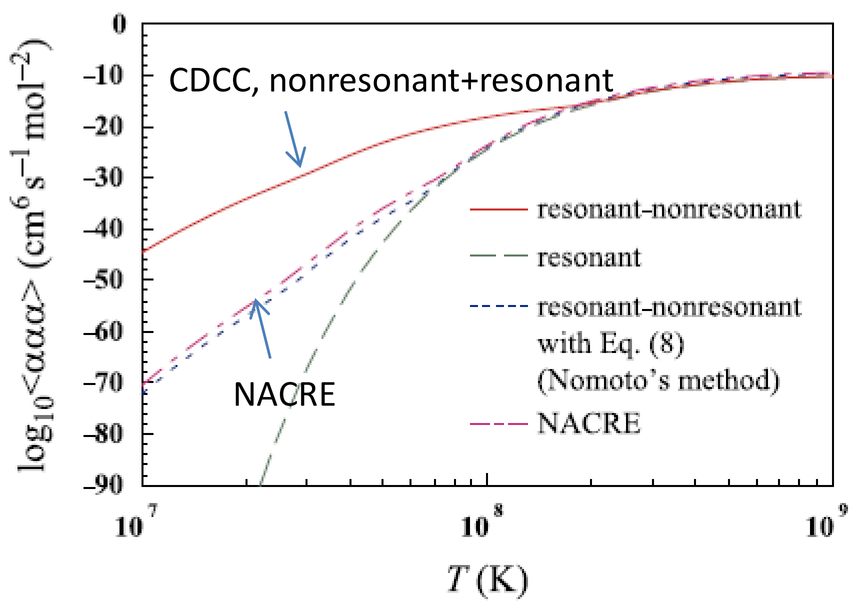


Large direct capture cross section at low energy



Dominant and large contribution of Direct capture process at low temperature, 10^7-10^8K



Need to solve up to R=2500-5000fm, 3-body boundary condition?, Jacobi coord. L=l=0 only.

Large reaction rate below 10^8K by Ogata et.al. has significant astrophysical implications

- Shortening or disappearance of the red giant phase of low mass star.

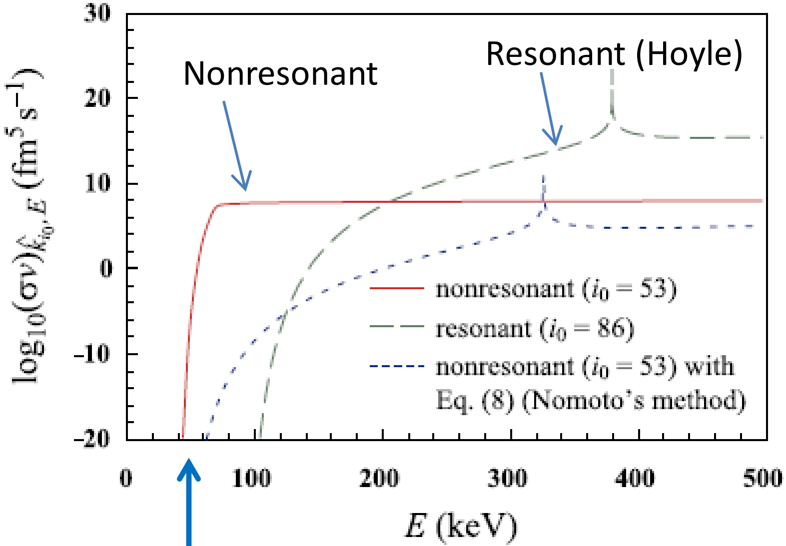
Independent examination of 3α reaction rate is quite important, but…

- Analytic asymptotic form of the wave function for three-charged particles is not known.

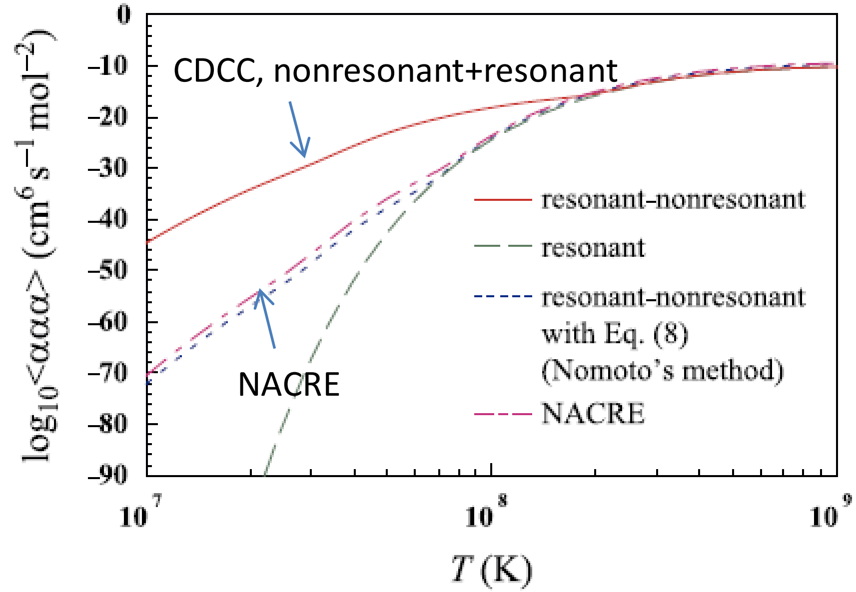
- One must solve three-body tunneling problem in huge space (several thousands fm?).

- ‘Ogata’ and ‘Kamimura’ are well-known experts of 3-body reaction

Large direct capture cross section at low energy

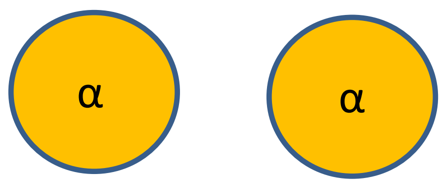


Dominant and large contribution of Direct capture process at low temperature, 10^7-10^8K



Need to solve up to R=2500-5000fm, 3-body boundary condition?, Jacobi coord. L=l=0 only.

50keV



$$\frac{2\cdot 2\cdot e^2}{R} = 50\ \mathrm{keV} \quad \Rightarrow \quad R = 120\ \mathrm{fm}$$

c.f. α-decay 50fm

Our idea to overcome the first difficulty.

- Analytic asymptotic form of the wave function for three-charged particles is not known.

Erase the 3-body scattering state employing spectral representation of the 3-body Hamiltonian,

we then obtain 'imaginary-time Schroedinger equation starting from final (bound) wave function'.

2-body case:

Thermal reaction rate at temperature $\beta = 1/kT$

散乱状態

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

Combining two expressions, we may erase initial scattering states

散乱状態

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

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

$$\boxed{e^{-\beta H} = \sum_n e^{-\beta E_n} \phi_n(\vec{r}) \phi_n^*(\vec{r}\,') + \frac{1}{(2\pi)^3} \int d\vec{k}\ \exp\left(-\beta \frac{\hbar^2 k^2}{2\mu}\right) \phi_{\vec{k}}(\vec{r}) \phi_{\vec{k}}^*(\vec{r}\,')}$$

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

Projector to remove bound states in the intial channel

Imaginary-time method for reaction rate

$$\left\langle v\sigma_{fi}\right\rangle \propto \left\langle \phi_f \left| M_{\lambda\mu} \underbrace{e^{-\beta\hat{H}}\left(\hat{H}-E_f\right)^{2\lambda+1}\hat{P}M_{\lambda\mu}{}^{+}\left|\phi_f\right.}_{\psi\,(\vec{r},\beta)}\right.\right\rangle \qquad \hat{P}=1-\sum_n\left|\phi_n\right\rangle\left\langle\phi_n\right| \qquad M_{\lambda\mu}=\sum_{i\in p} r_i^{\lambda}Y_{\lambda\mu}(\hat{r}_i)$$

Algorithm:

1. Prepare β=0 wave function from 'final' state

$$\psi(\vec{r},\beta=0)=\left(\hat{H}-E_f\right)^{2\lambda+1}\hat{P}M_{\lambda\mu}{}^{+}\phi_f(\vec{r})$$

2. Solve imaginary time equation

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

3. Take overlap with β=0 wave function
   to obtain reaction rate

$$r(\beta)\propto\int d\vec{r}\,\psi^{*}(\vec{r},0)M_{\lambda\mu}\psi(\vec{r},\beta)$$

Taylor expansion method

$$\psi(\vec{r},\beta+\Delta\beta)=\hat{P}e^{-\Delta\beta H}\psi(\vec{r},\beta)$$

$$\approx\hat{P}\sum_k\frac{(-\beta)^k}{k!}H^k\psi(\vec{r},\beta)$$

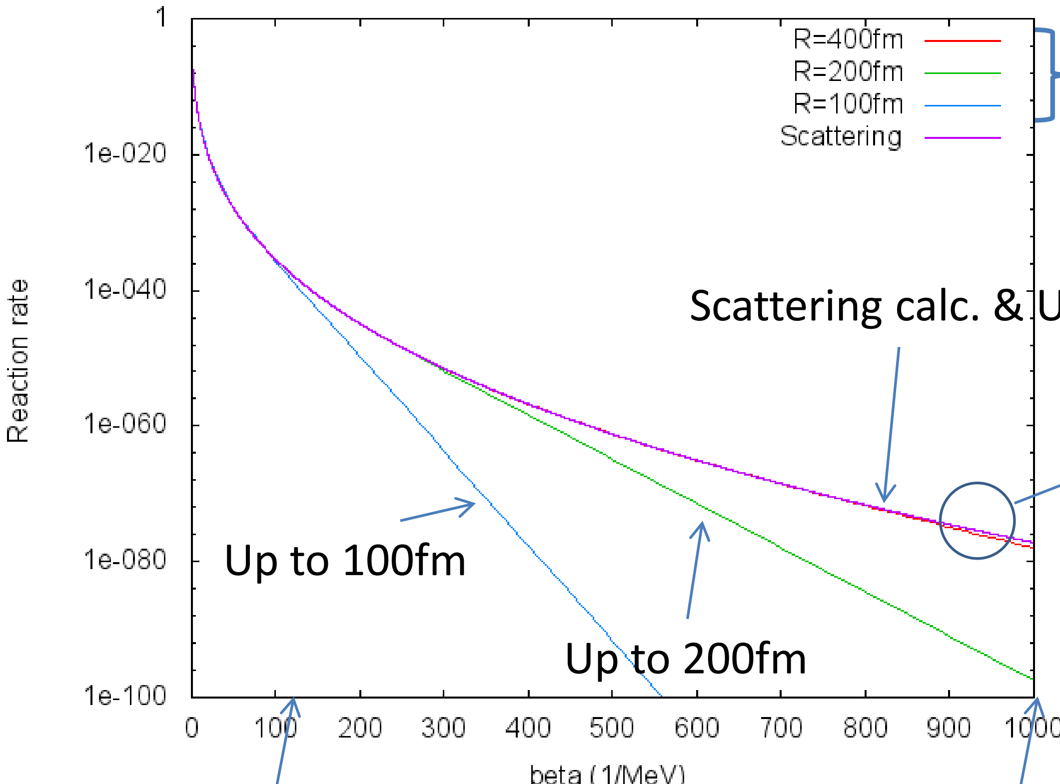
Three-body scattering states are removed.

Next problem, how large space we need to solve the equation, several hundred (thousand?) fm?

Test calculation: $^{16}O(\alpha,\gamma)^{20}Ne$
(2-body reaction, Simple potential model)

$$\psi\left(\vec{r},\beta\right)=\frac{u_l(r)}{r}Y_{lm}(\theta,\phi) \qquad -\frac{\partial}{\partial\beta}u_l(r,\beta)=\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2\mu r^2}+V(r)\right\}u_l(r,\beta)$$

２通りの計算の比較。①散乱問題を解く ②虚時間法



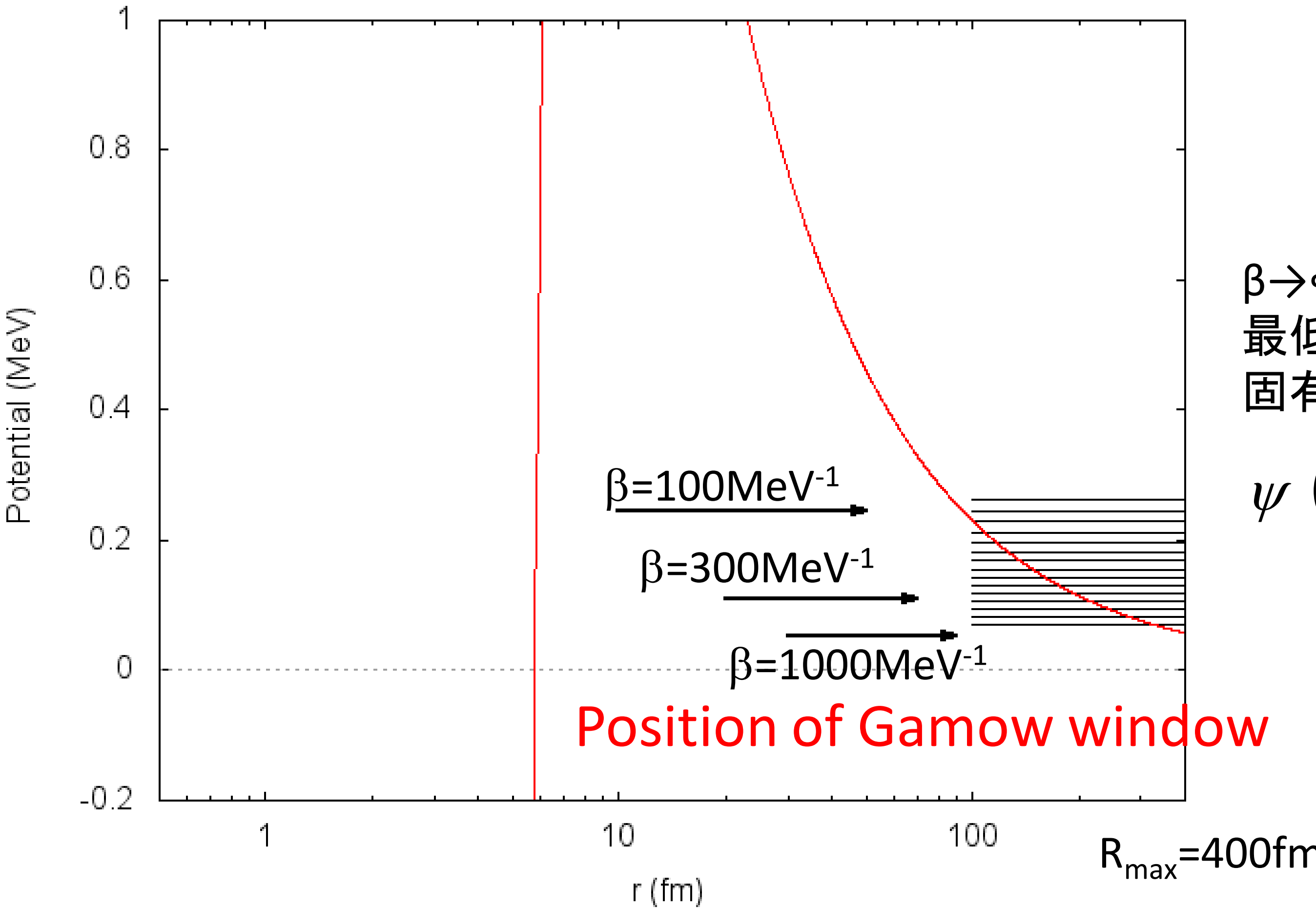
Spatial box size
for imaginary-time calculation

Calculation by ordinary method
and imaginary-time method
coincide each other
If we calculate up to 400fm.

10^8K $\qquad$ 10^7K

For a given temperature β, how far we need to solve the equation?

$$\psi\left(\vec{r},\beta\right)=\frac{u_l(r)}{r}Y_{lm}(\theta,\phi) \qquad -\frac{\partial}{\partial\beta}u_l(r,\beta)=\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+\frac{\hbar^2 l(l+1)}{2\mu r^2}+V(r)\right\}u_l(r,\beta)$$



β→∞では、
最低エネルギーの
固有状態に

$$\psi\left(\vec{r},\beta\right)\rightarrow e^{-\beta E}\varphi_E\left(\vec{r}\right)$$

Imaginary-time evolution of the wave function

- decrease in β-evolution by 10^{80}
- 10^{20} difference in r at T=10^7K

Algorithm:

1. Prepare initial wave function

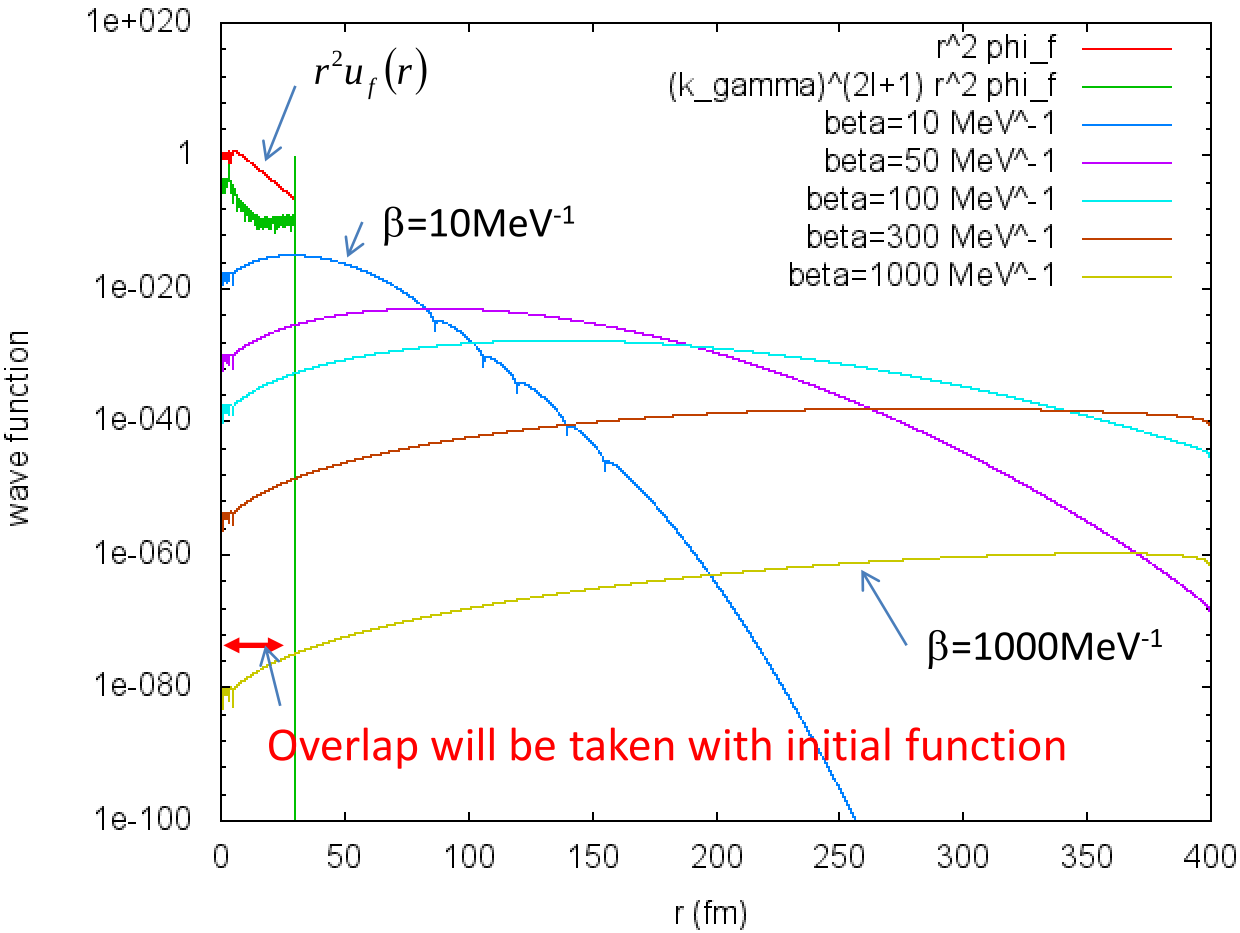
$$\psi(\vec{r},\beta=0)=\left(\frac{\hat{H}+|E_f|}{\hbar c}\right)^{2\lambda+1}\hat{P}M_{\lambda\mu}{}^{+}\phi_f(\vec{r})$$

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

$$r(\beta)\propto\int d\vec{r}\psi^{*}(\vec{r},0)M_{\lambda\mu}\psi(\vec{r},\beta)$$



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Independent examination of 3α reaction rate is quite important, but…

- Analytic asymptotic form of the wave function for three-charged particles is not known. ⇒ Imaginary time method

- One must solve three-body tunneling problem in huge space (several thousands fm?). ⇒ Probably 200-300fm

- 'Ogata' and 'Kamimura' are well-known experts of 3-body reaction

Final problem,
How to calculate 3-body imaginary-time problem?

$$\langle v\sigma_{fi}\rangle \propto \langle \phi_f | M_{\lambda\mu} e^{-\beta\hat{H}} \left(\hat{H} - E_f\right)^{2\lambda+1} \hat{P} M_{\lambda\mu}{}^{+} | \phi_f \rangle \qquad M_{\lambda\mu} = \sum_{i\in p} r_i{}^{\lambda} Y_{\lambda\mu}(\hat{r}_i)$$

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

ϕ_f 3-body wave function for 2^+ 4.44 MeV excited state of ^{12}C confined within 30fm.

$$H = -\frac{1}{2}\left(\Delta_1 + \Delta_2 + \Delta_3\right) + \left(\frac{2}{r_{12}} + \frac{2}{r_{23}} + \frac{2}{r_{31}}\right)$$

3-body Hamiltonian. Probably, nuclear force is not important.

What is the efficient representation for the wave function and algorism to evolve it ?
- decrease in β-evolution by 10^{80}
- 10^{20} difference in coordinate space r

Summary

Triple-alpha reaction rate.
Toward examining Ogata, Kan, Kamimura calculation:
10^{20} increase in reaction rate at low temperature.

- Imaginary-time method: rate calculation without scattering solution
- For 2-body problem, it works.
- large space, 200-400fm
  (Coulomb potential is below the Gamow window)

- How to solve 3-body imaginary-time evolution?