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Cluster Structure of Light Nuclei Superposing Multiple Slater Determinants

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Two topics related to ^{12}C nucleus

1. Structure of ^{12}C nuclei in excited states

   --- Cluster Structure of Light Nuclei Superposing Multiple Slater Determinants ---

   We develop a new computational approach for structure of light nuclei.

   We apply the method to ^{12}C

   Y. Fukuoka, S. Shinohara, Y. Funaki, T. Nakatsukasa, K. Yabana, Phys. Rev. C88, 014321(2013)

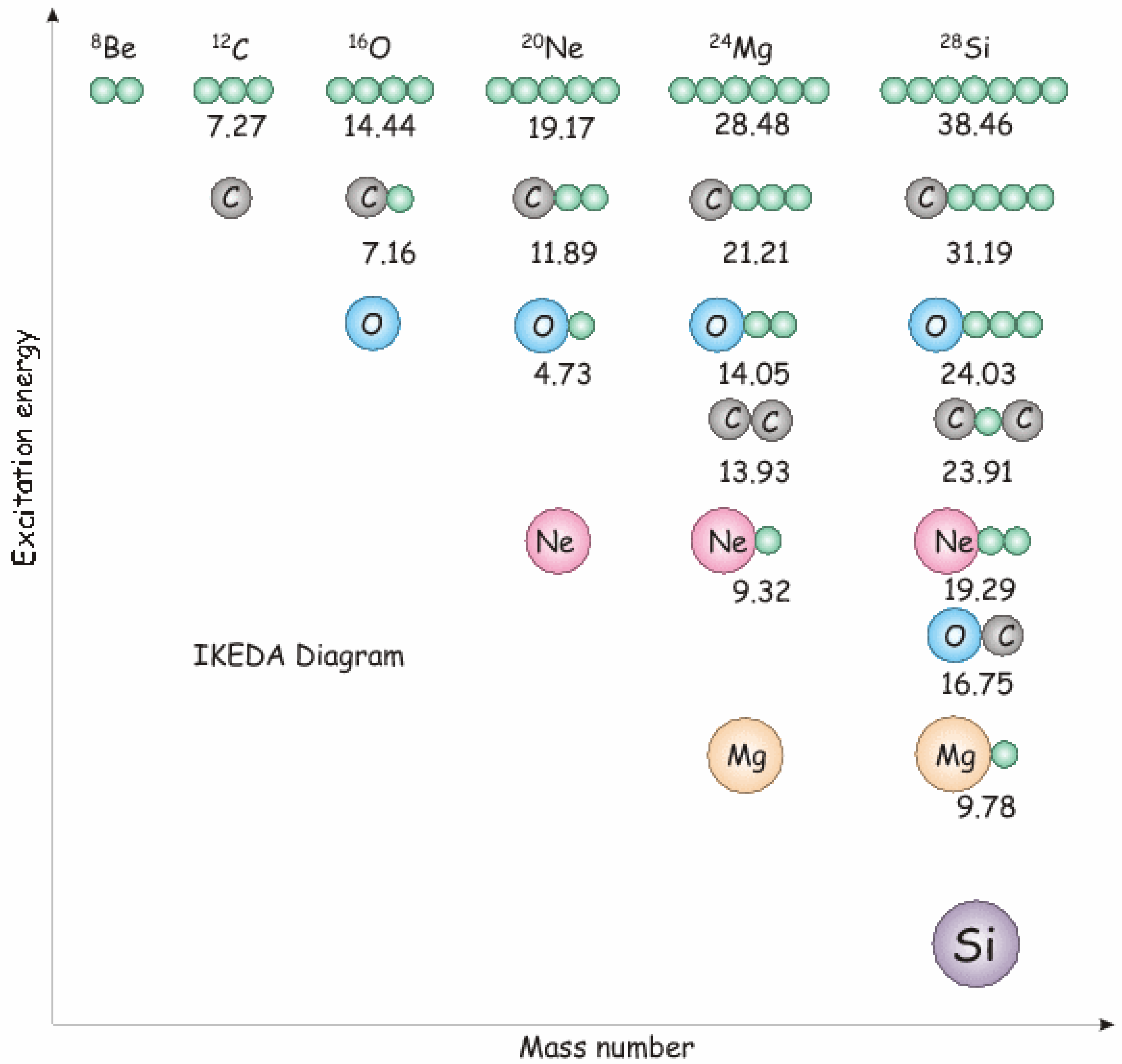
2. Reaction to produce ^{12}C nuclei

   --- Triple-alpha reaction rate in astrophysical environment ---

   Reaction rate calculation of three charged particles without solving scattering problems.

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

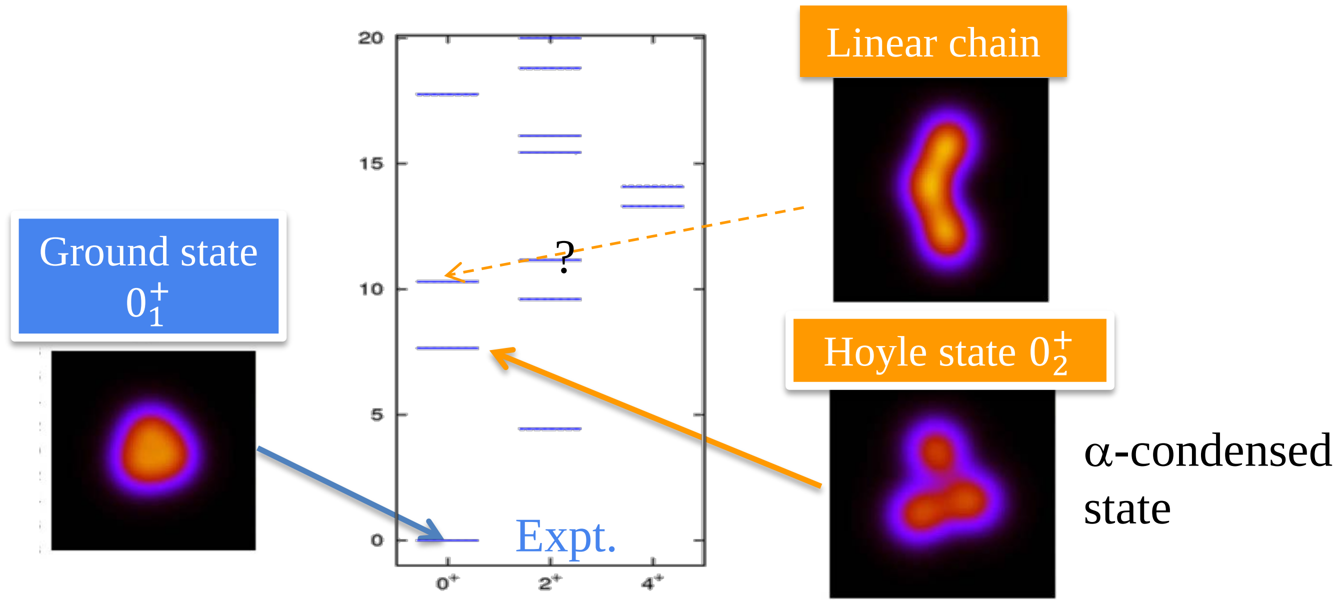
In light nuclei, various cluster structures are known to appear.



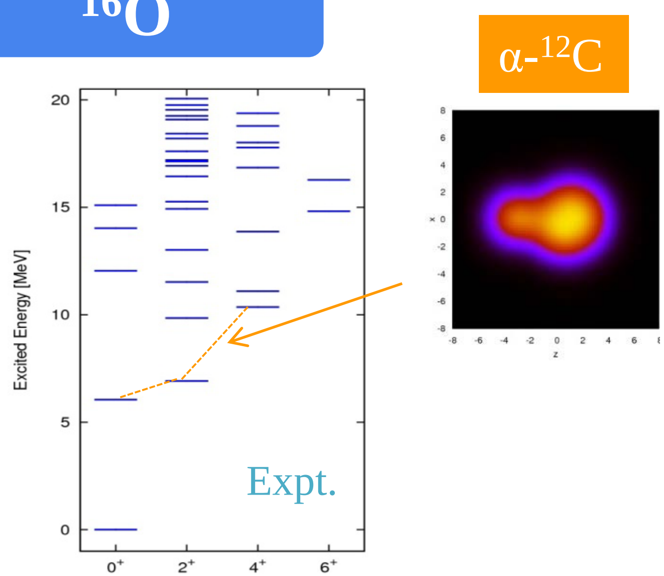
Ikeda diagram, 1968

Typical examples of cluster structures

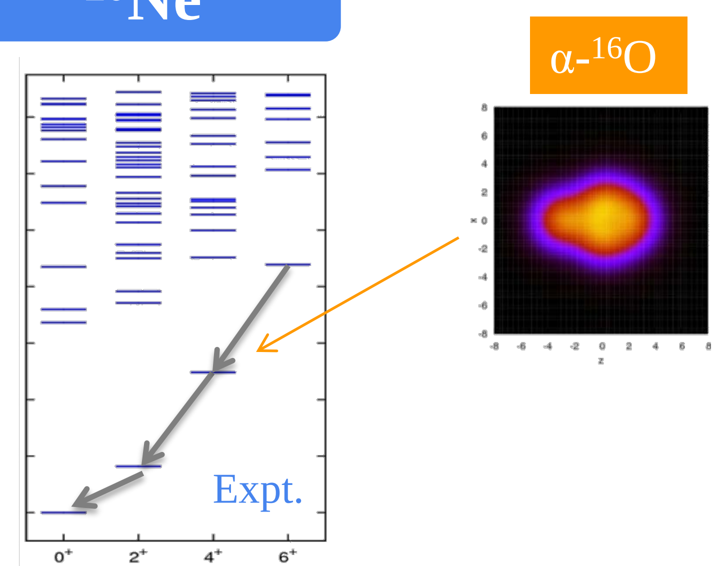
^{12}C



^{16}O



^{20}Ne



Descriptions of clustering states require large model space

- Spatially extended, large deformation
  $\Rightarrow$ We will use 3D grid representation

- Correlated wave function
  $\Rightarrow$ We superpose a number of Slater determinants which show different correlation structures

Starting with empirical (Skyrme or Gogny) interactions,
we attempt to calculate energy spectra and other physical quantities convergent with respect to configurations.

Formalism

0. Set up effective Hamiltonian

1. Prepare Slater determinants

2. Parity and angular mom. projections

3. Diagonalize Hamiltonian

We use Skyrme or Gogny interactions

$$\hat{V}_{Skyrme}(\vec{r}_1, \vec{r}_2) = t_0 \left(1 + x_0 P_\sigma\right) \delta\left(\vec{r}_1 - \vec{r}_2\right) + \frac{1}{6} t_3 \rho^\alpha \left(1 + x_3 \hat{P}_\sigma\right) \delta\left(\vec{r}_1 - \vec{r}_2\right)$$

$$+ \frac{1}{2} t_1 \left(1 + x_1 \hat{P}_\sigma\right) \left(\vec{k}^2 - \vec{k}^2\right) \delta\left(\vec{r}_1 - \vec{r}_2\right) + t_2 \left(1 + x_2 \hat{P}_\sigma\right) \overleftarrow{k} \cdot \delta\left(\vec{r}_1 - \vec{r}_2\right) \overrightarrow{k}$$

$$+ iW_0 \left(\vec{\sigma}_1 + \vec{\sigma}_2\right) \cdot \overleftarrow{k} \times \delta\left(\vec{r}_1 - \vec{r}_2\right) \overrightarrow{k},$$

$$\overrightarrow{k} = \frac{\overrightarrow{\nabla}_1 - \overrightarrow{\nabla}_2}{2i}, \quad \overleftarrow{k} = -\frac{\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2}{2i}$$

Formalism

0. Set up effective Hamiltonian

1. Prepare Slater determinants

2. Parity and angular mom. projections

3. Diagonalize Hamiltonian

Imaginary-time method

$\left\{\psi_i^{(0)}\right\}$ Set up initial orbitals

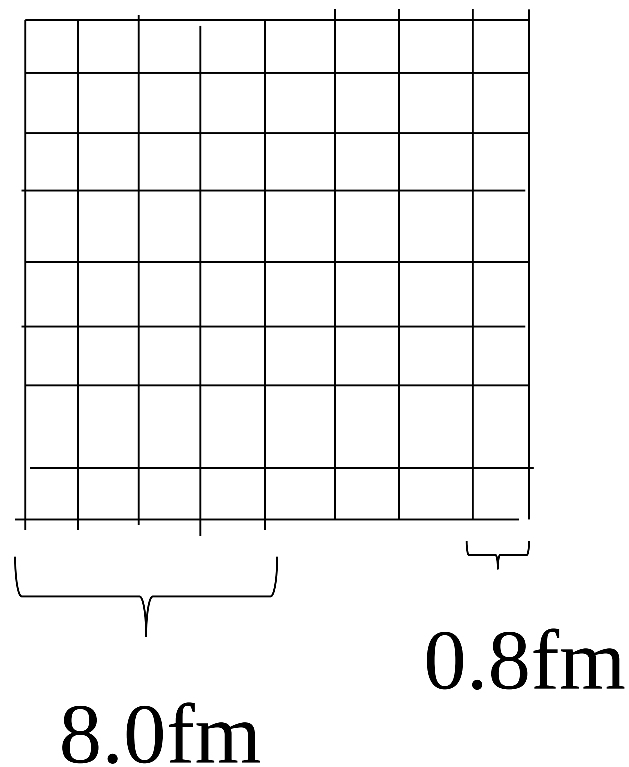
$\rho^{(n)} = \sum_i \left|\phi_i\right|^2$ Update density

Imaginary-time evolution

$$\tilde{\psi}_i^{(n+1)} = \psi_i^{(n)} - \Delta T \cdot h\left[\rho^{(n)}\right]\psi_i^{(n)} \quad (n = 0,1,2,\cdots)$$

$\tilde{\psi}_i^{(n+1)}$ Orthonormalization

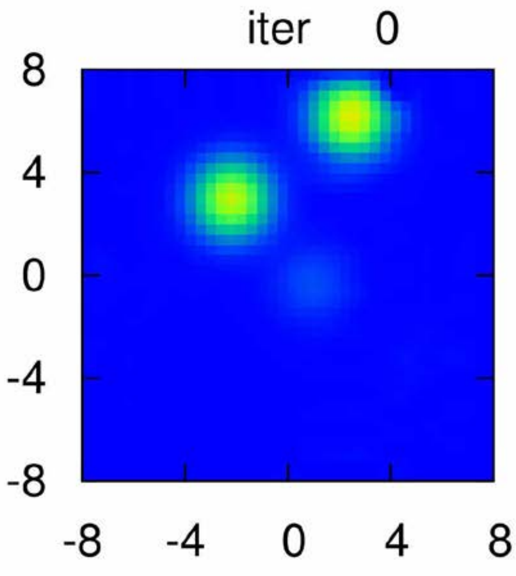
Real-space grid representation

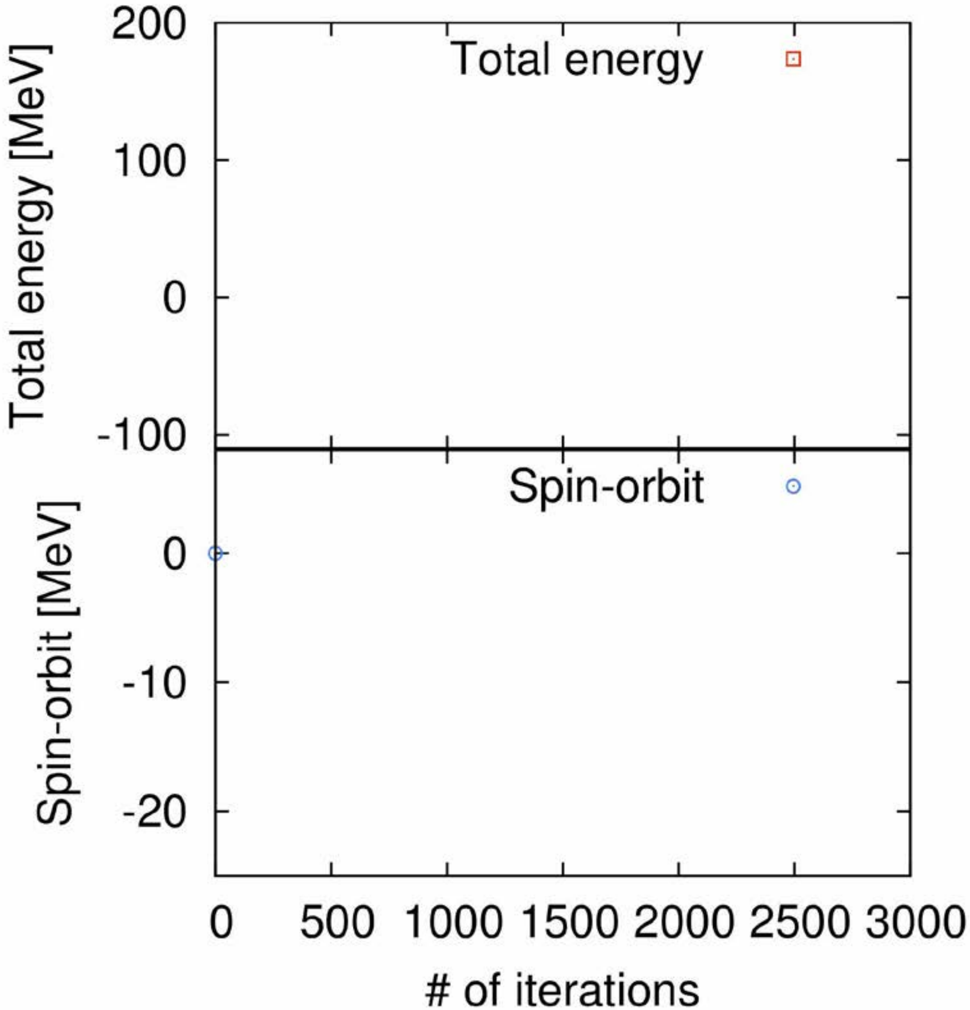


Cluster correlation seen in the density functional calculation (imaginary-time evolution)

- Prepare initial orbitals (Randomly distributed Gaussian functions)
- Imaginary-time iteration to obtain self-consistent solution
  (A steepest descent solver for the Kohn-Sham problem)

^{12}C

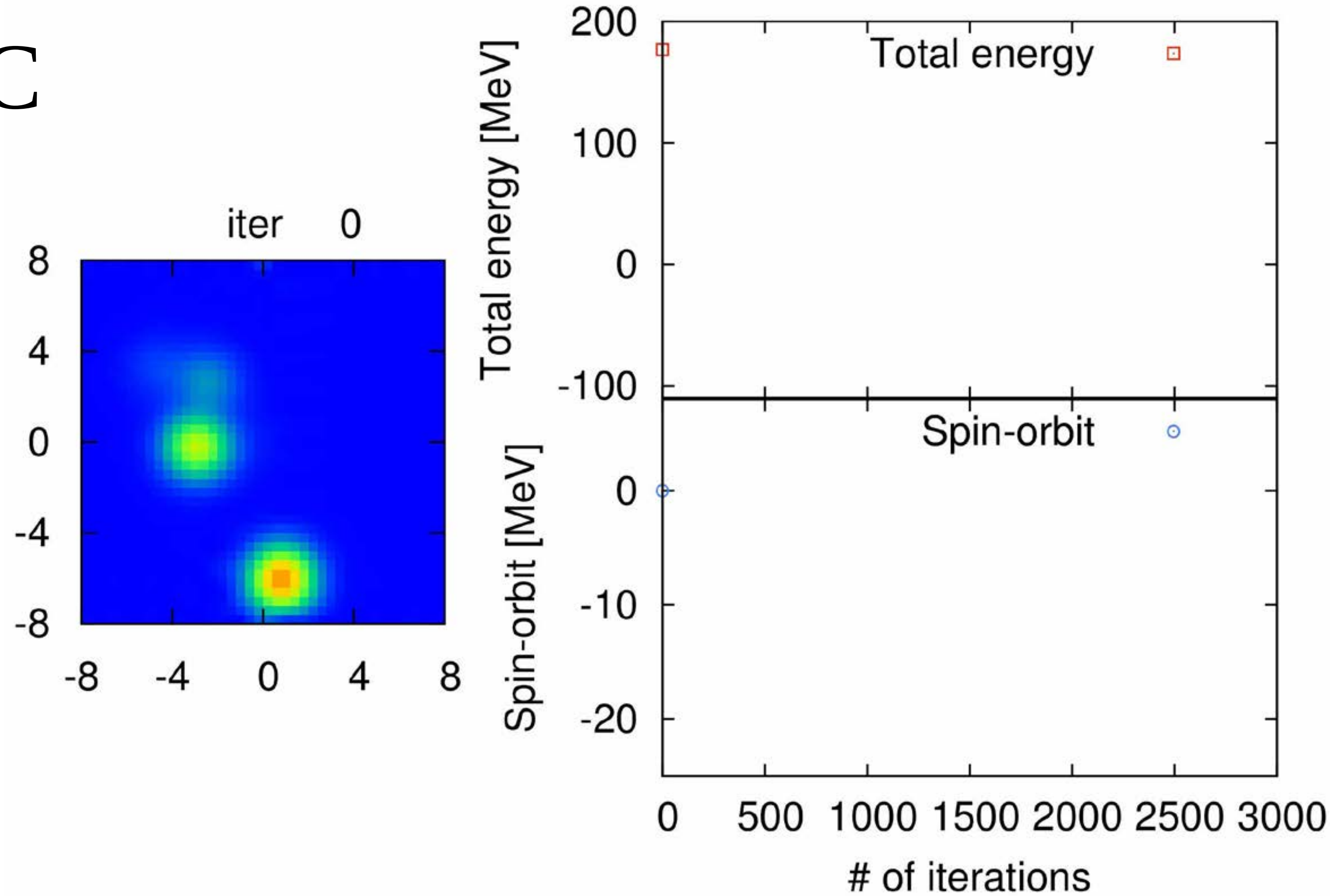




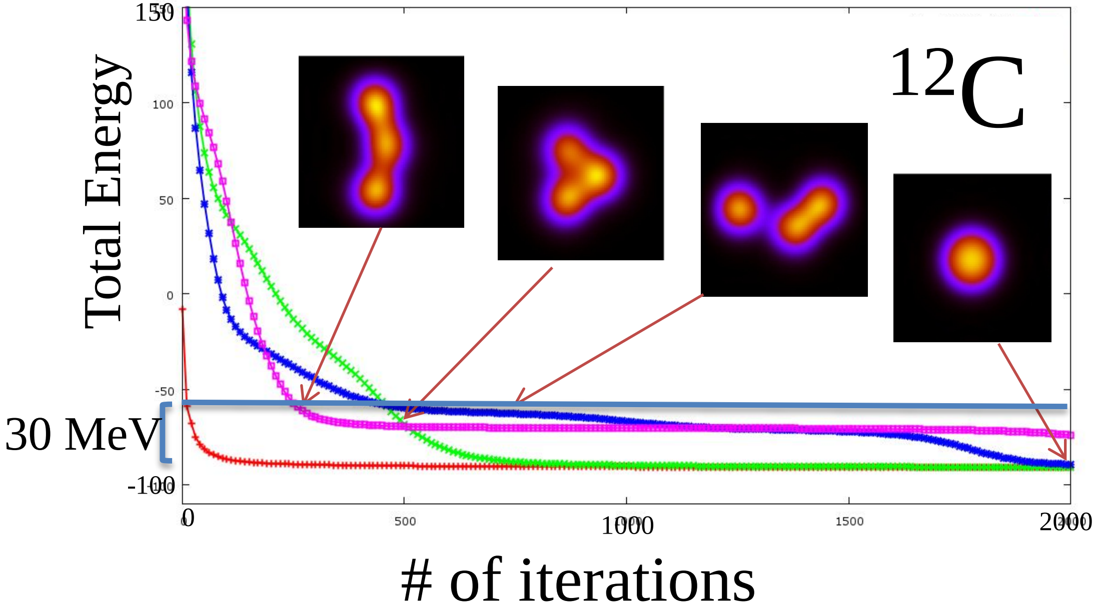
Cluster correlation seen in the imaginary-time evolution (2)

- Prepare initial orbitals (Randomly distributed Gaussian functions)
- Imaginary-time iteration to obtain self-consistent solution
  (A steepest descent solver for the DFT Kohn-Sham problem)

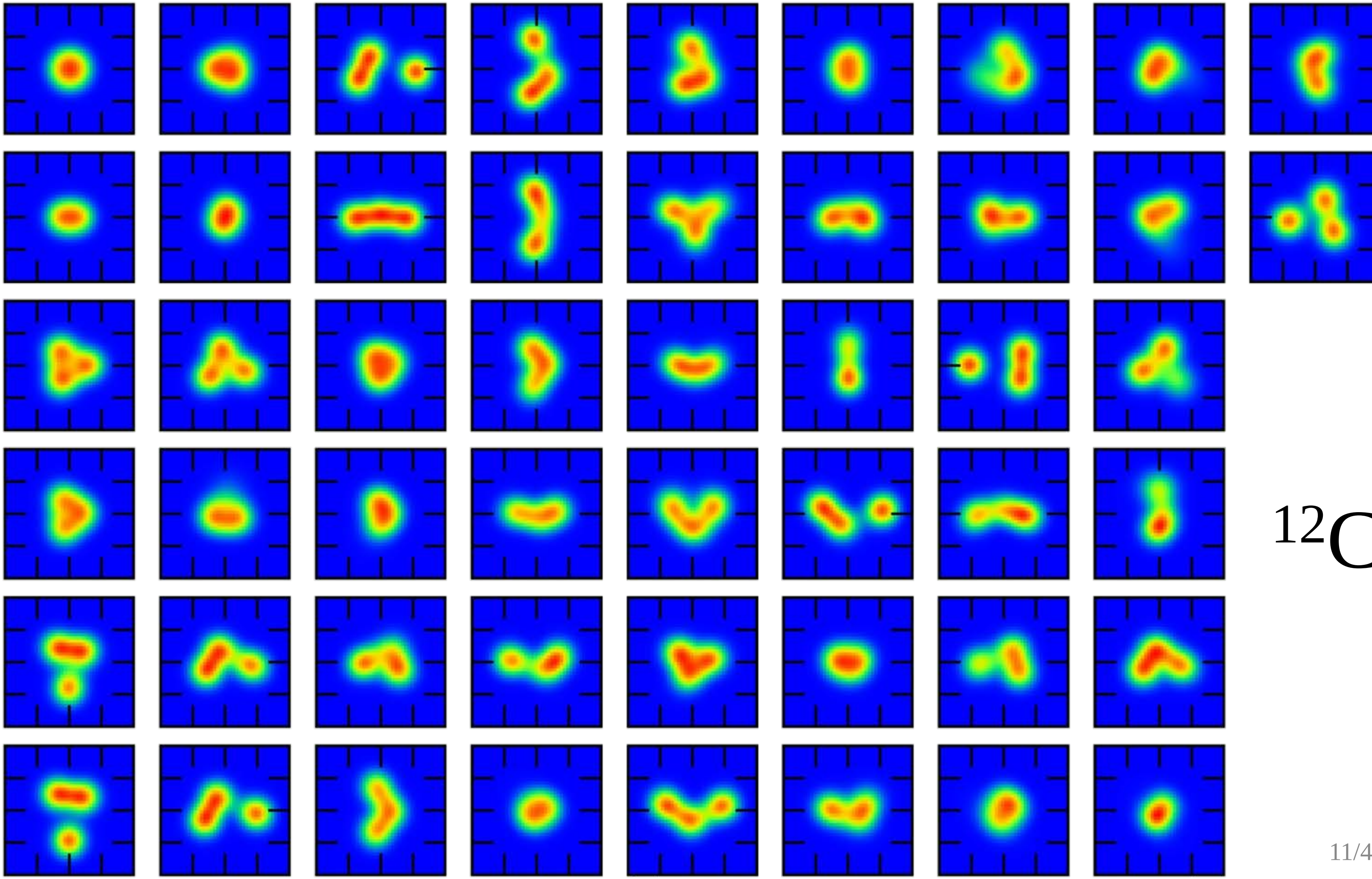
^{12}C



- Repeat imaginary-time calculations from different initial configuration.
- Select and store Slater determinants which show different correlation structures.



Selected Slater determinants for ^{12}C (50 Slater dets will be used)



^{12}C

Formalism

0. Set up effective Hamiltonian

1. Prepare Slater determinants

2. Parity and angular mom. projections

3. Diagonalize Hamiltonian

$$\hat{\mathrm{P}}^{J}_{MK}\hat{\mathrm{P}}^{\pm}\left|\Phi_n\right\rangle$$

3D Angular momentum projection

$$\hat{\mathrm{P}}^{J}_{MK} = \frac{2J+1}{8\pi^2}\int \mathrm{d}\Omega \mathrm{D}^{\mathrm{J}*}_{\mathrm{MK}}\hat{\mathrm{R}}(\Omega)$$

$$(\hat{\mathrm{R}} = e^{-i\alpha\hat{J}_z}e^{-i\beta\hat{J}_y}e^{-i\gamma\hat{J}_z})$$

Parity projection

$$\hat{\mathrm{P}}^{\pm} = \frac{1}{2}(1+\hat{\mathrm{P}}_r)$$

Formalism

0. Set up effective Hamiltonian

1. Prepare Slater determinants

2. Parity and angular mom. projections

3. Diagonalize Hamiltonian

diagonalize the Hamiltonian in the projected space
(Configuration mixing calculation)

$$\left\{h^{(\pm)}_{iK,jK'} - E^{J(\pm)} n^{(\pm)}_{iK,jK'}\right\} g_{jK'} = 0$$

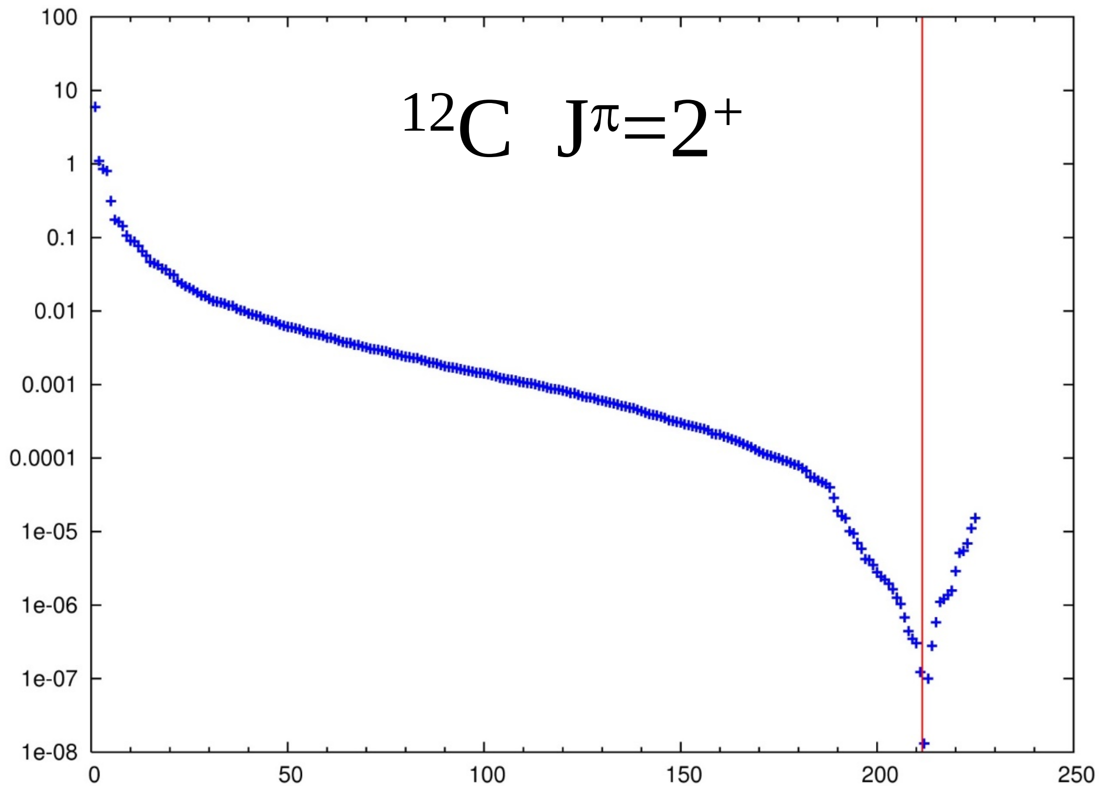
$$\begin{cases} h_{iK,jK'} \equiv \langle \Psi_i | \hat{H}\, \hat{P}^J_{KK'} \hat{P}^{(\pm)} | \Psi_j \rangle \\ n_{iK,jK'} \equiv \langle \Psi_i |\, \hat{P}^J_{KK'} \hat{P}^{(\pm)} | \Psi_j \rangle \end{cases}$$

Difficulty in superposing non-orthogonal Slater determinants

Many configurations are characterized by small (even negative) norm eigenvalues.
We discard these configurations.

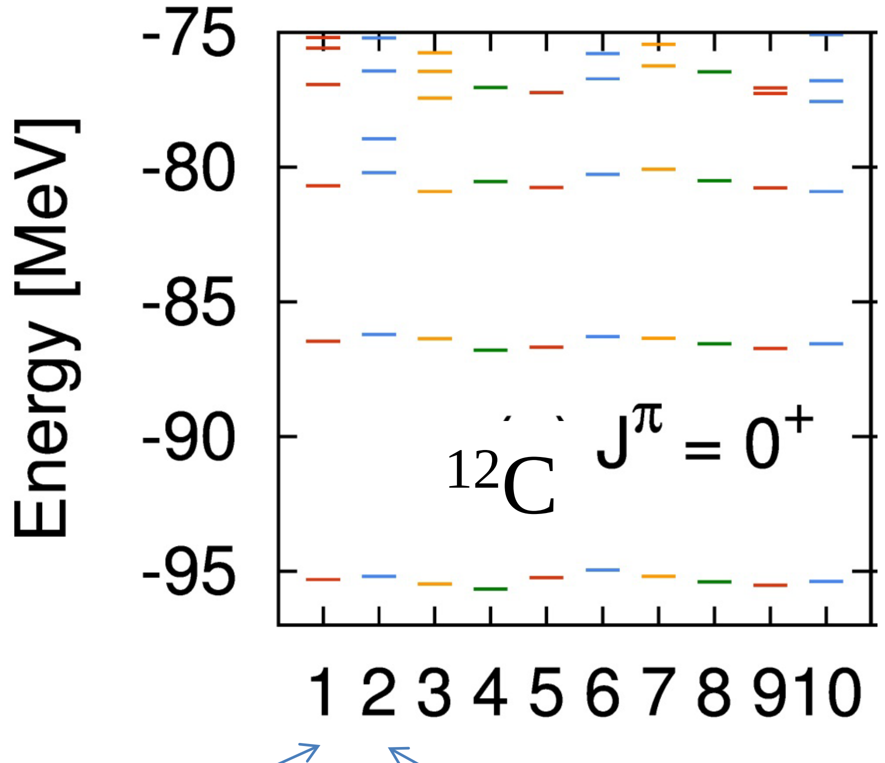
Eigenvalues of $n_{iK,jK'} \equiv \langle \Psi_i | \hat{P}^J_{KK'} \hat{P}^{(\pm)} | \Psi_j \rangle$ (J=2, ij=1-45)

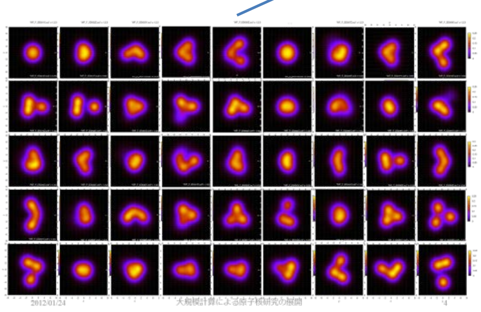
Absolute values of eigenvalues of norm matrix



Basis index

We compare calculations of different sets of Slater determinants to examine reliablility of the calculations.





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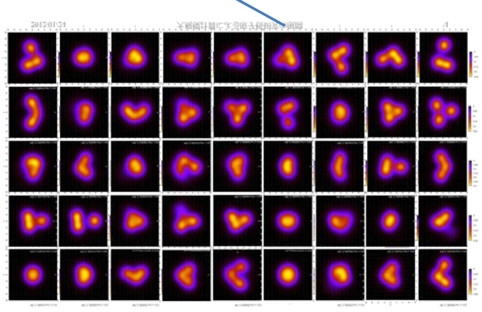


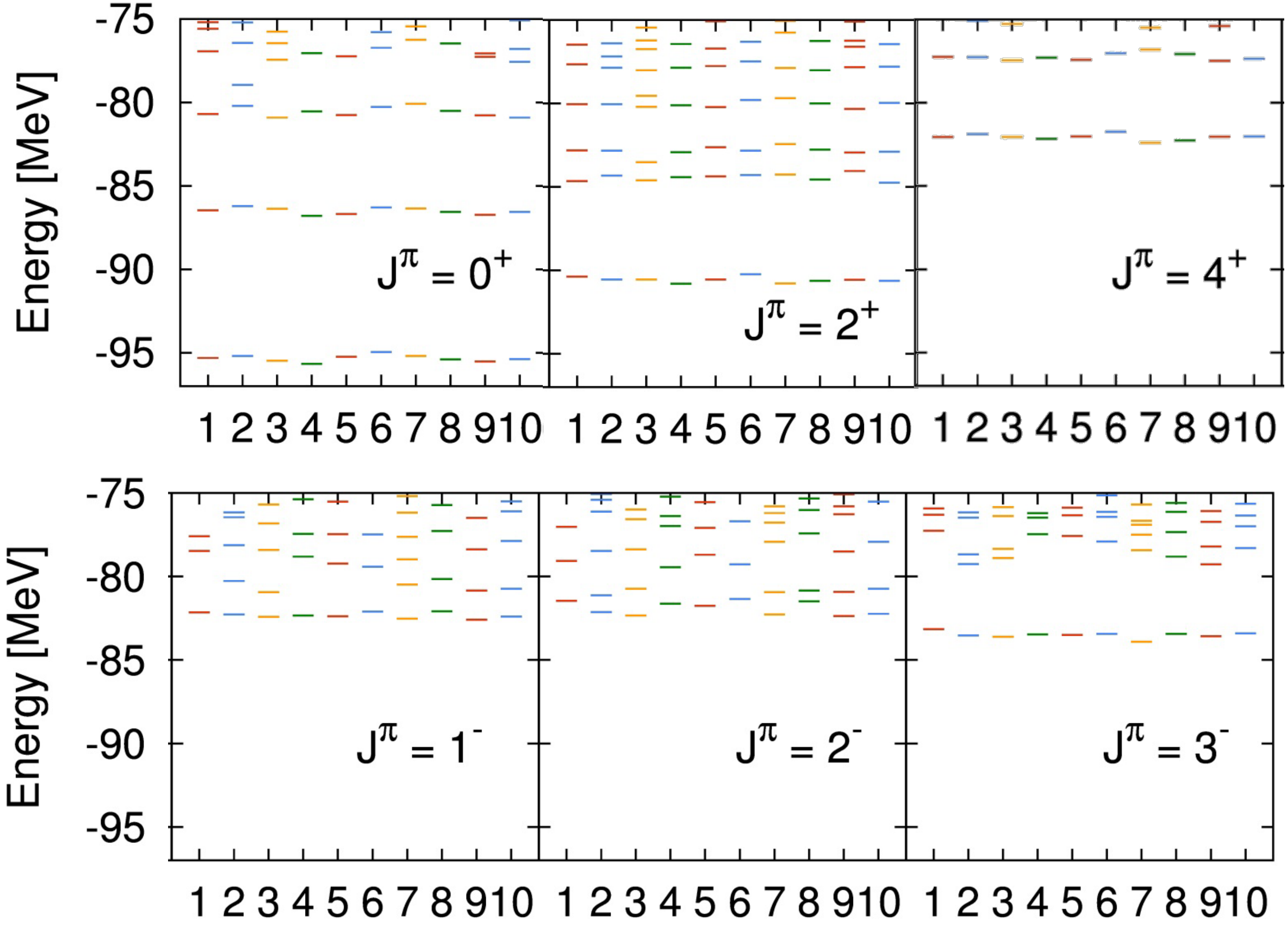
, …….(10 sets)

Comparison among 10 sets of Slater determinants.

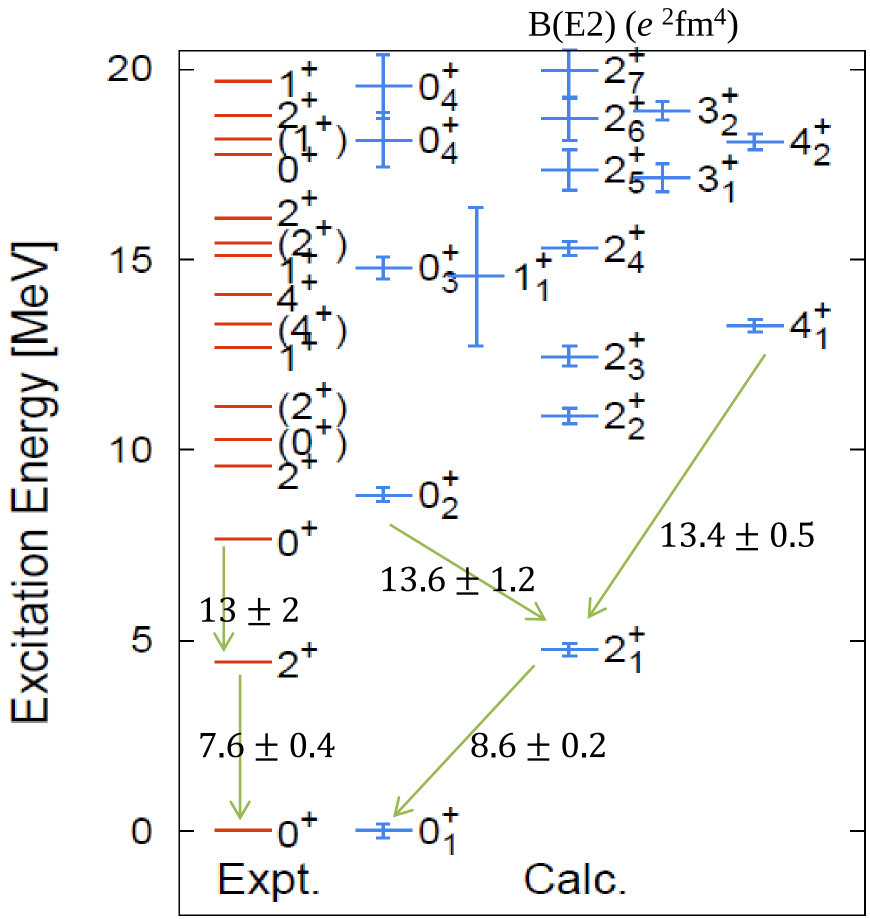
A few low-lying excitations for each parity and angular momentum are reliably obtained.

^{12}C

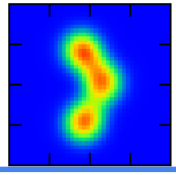
SLy4
50SDs



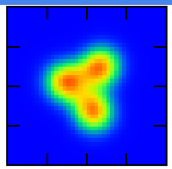
^{12}C Positive Parity



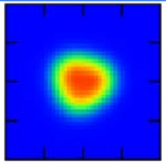
linear chain (0_3^+)



Hoyle state (0_2^+)



Ground state (0_1^+)

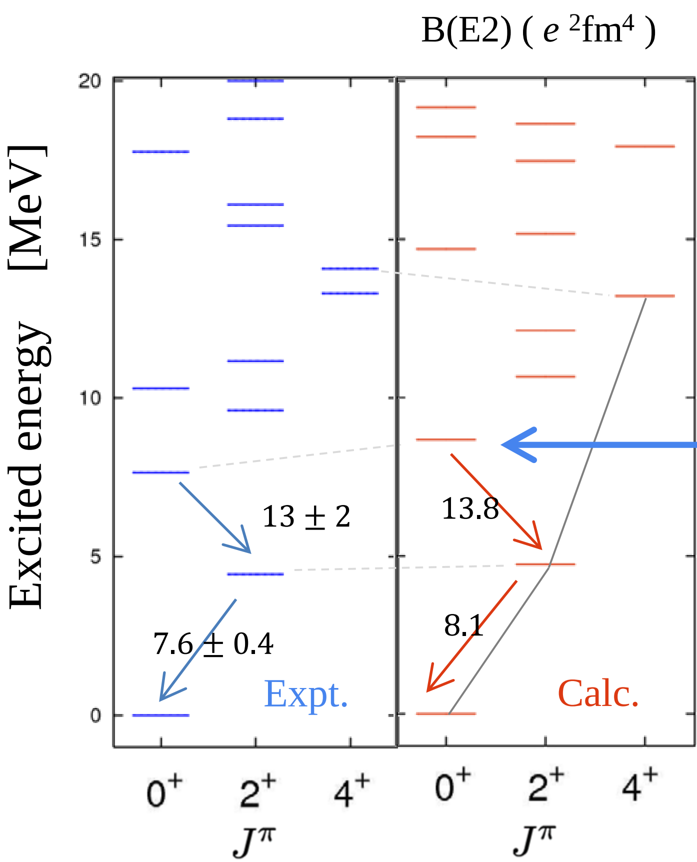


- SLy4 Skyrme interaction
- Total energy

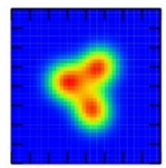
  Calc. : -95.3 MeV
  Expt. : -92.1 MeV

  cf. HF : -90.6 MeV

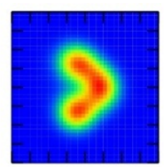
^{12}C Positive Parity



Hoyle state (0_2^+)



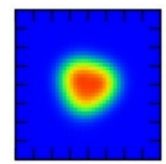
1. 46.3%



2. 44.7%
3. 41.2%
4. 39.4%
5. 38.9%

⋮

Ground state (0_1^+)



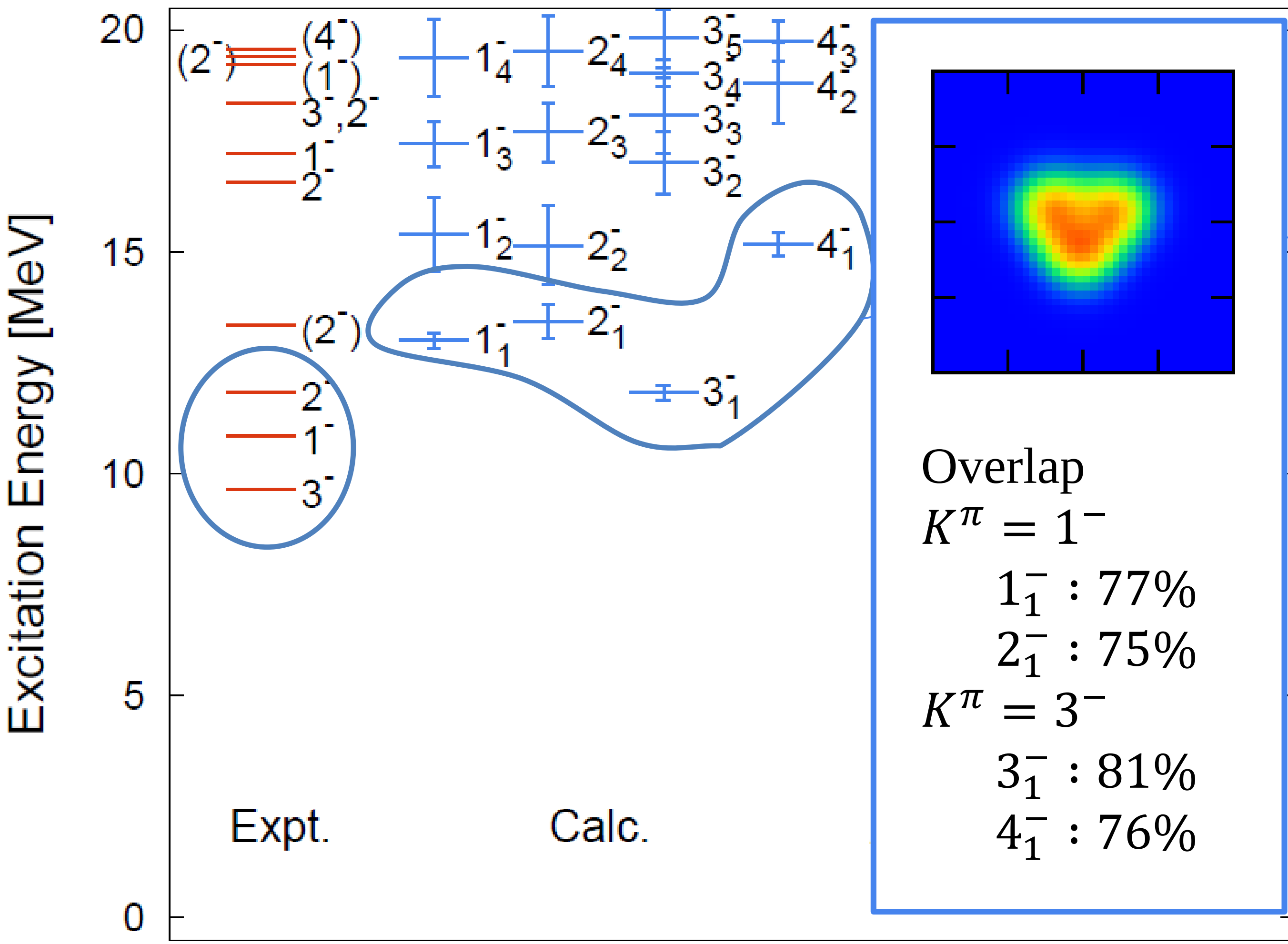
1. 90.4%
2. 87.4%
3. 84.8%
4. 84.8%
5. 81.7%

⋮

Definition of overlaps

$$\left|\frac{\langle \Psi_n^{J\pi}|\hat{P}^J_{MK}\hat{P}^\pi|\Phi_i\rangle}{\sqrt{\langle \Phi_i|\hat{P}^J_{MK}\hat{P}^\pi|\Phi_i\rangle}}\right|^2$$

^{12}C Negative Parity



Overlap
$K^{\pi} = 1^{-}$
1^{-}_{1} : 77%
2^{-}_{1} : 75%
$K^{\pi} = 3^{-}$
3^{-}_{1} : 81%
4^{-}_{1} : 76%

^{12}C

Summary of part 1

--- Cluster Structure of Light Nuclei Superposing Multiple Slater Determinants ---

Starting with empirical (mean-field) Hamiltonian, we attempted to calculate ground and excited states convergent with respect to configurations superposing a number of Slater determinants with different correlations.

Imaginary-time method is used to produce Slater determinants.
Parity and 3D angular momentum projections, then configuration mixing.

For ^{12}C, ground state, Hoyle (0_2^+) state, linear-chain state (0_3^+) are reasonably reproduced.

Two topics related to ^{12}C nucleus

1. Structure of ^{12}C nuclei in excited states

   --- Cluster Structure of Light Nuclei Superposing Multiple Slater Determinants ---

   A new computational approach for structure of light nuclei, applying to ^{12}C

   Y. Fukuoka, S. Shinohara, Y. Funaki, T. Nakatsukasa, K. Yabana, Phys. Rev. C88, 014321(2013)

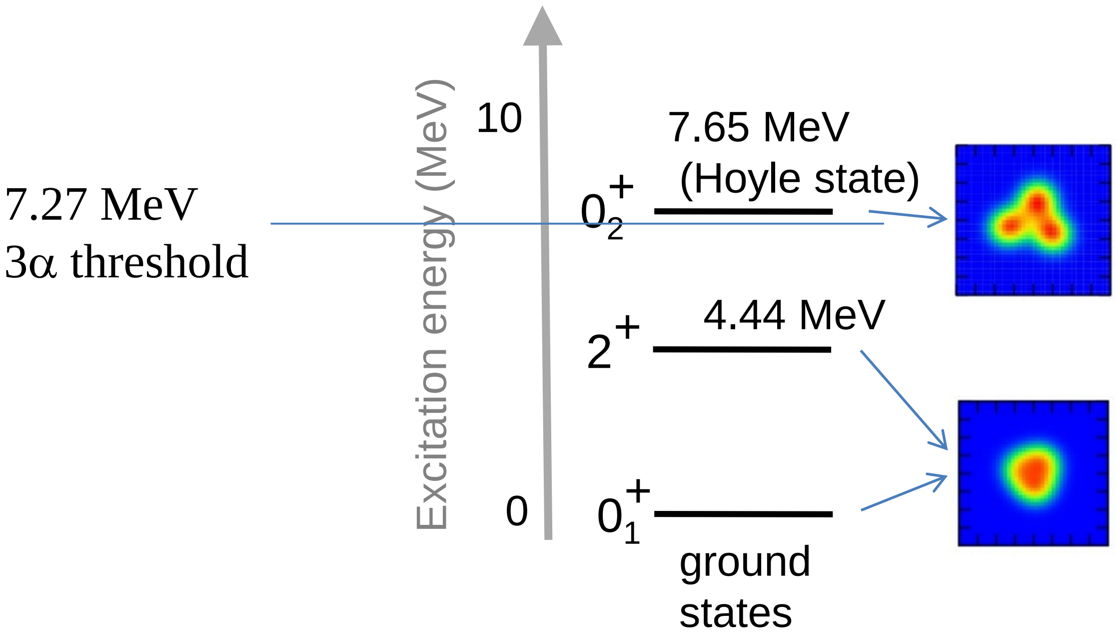
2. Reaction to produce ^{12}C nuclei

   --- Triple-alpha reaction rate in astrophysical environment ---

   Reaction rate calculation of three charged particles without solving scattering problems.

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

Excited states of ^{12}C relevant to astrophysical synthesis by triple-alpha reaction

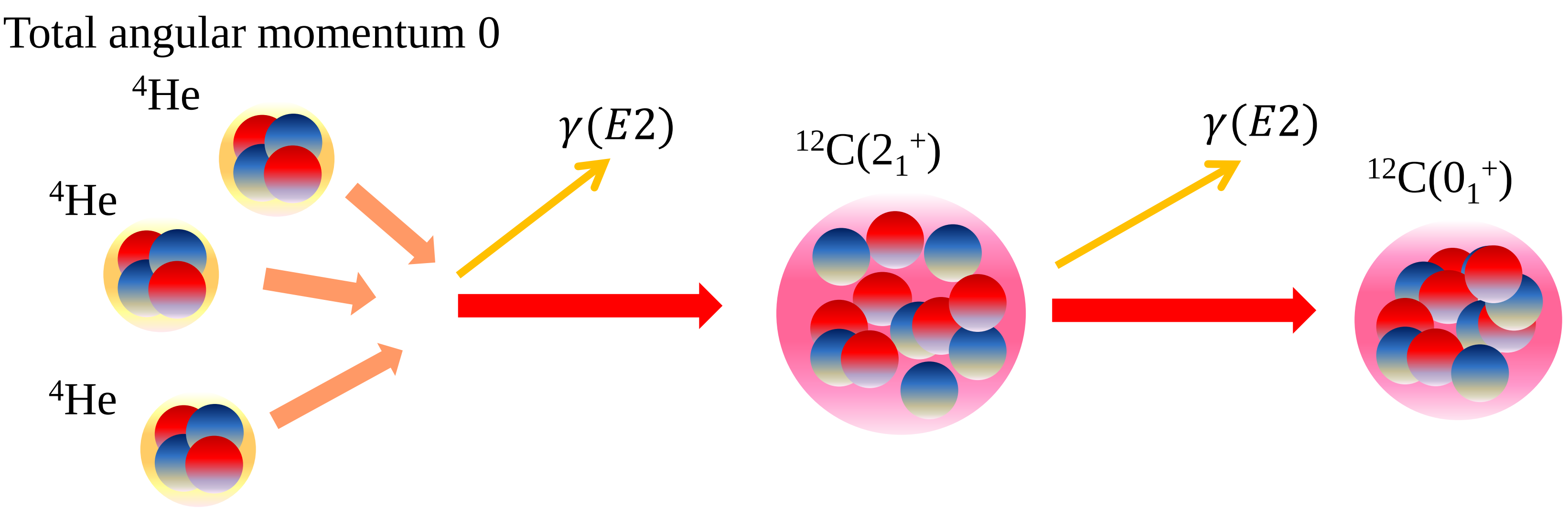


Hoyle state: 0_2^+ (7.65 MeV)

- predicted by F. Hoyle (1952), to explain ^{12}C stellar-synthesis and later confirmed its existence experimentally.

- Interpreted as 3-apha Bose condensed state
  Tohsaki, Horiuchi, Schuck, Roepke, PRL87, 192501 (2002).
  Funaki, Tohsaki, Horiuchi, Schuck, Roepke, PRC67, 051306 (2003).

Triple-alpha process



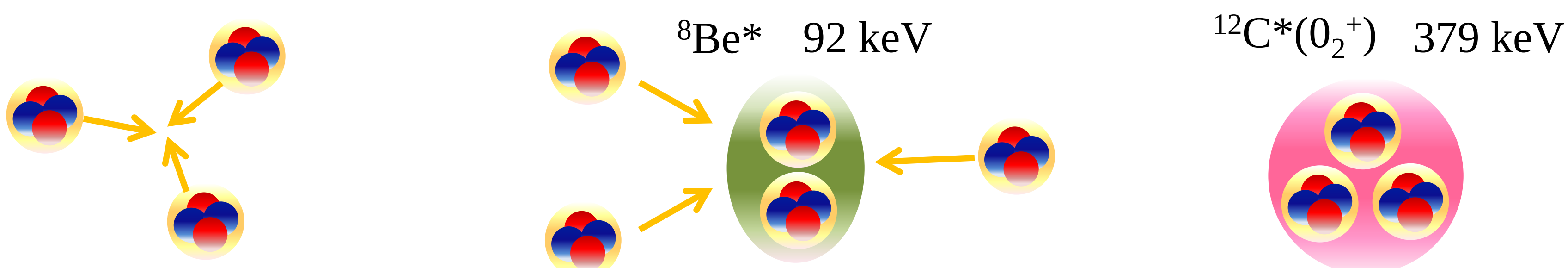
Low Temperature

Direct 3-alpha collision

Binary collision
(^8Be resonance)

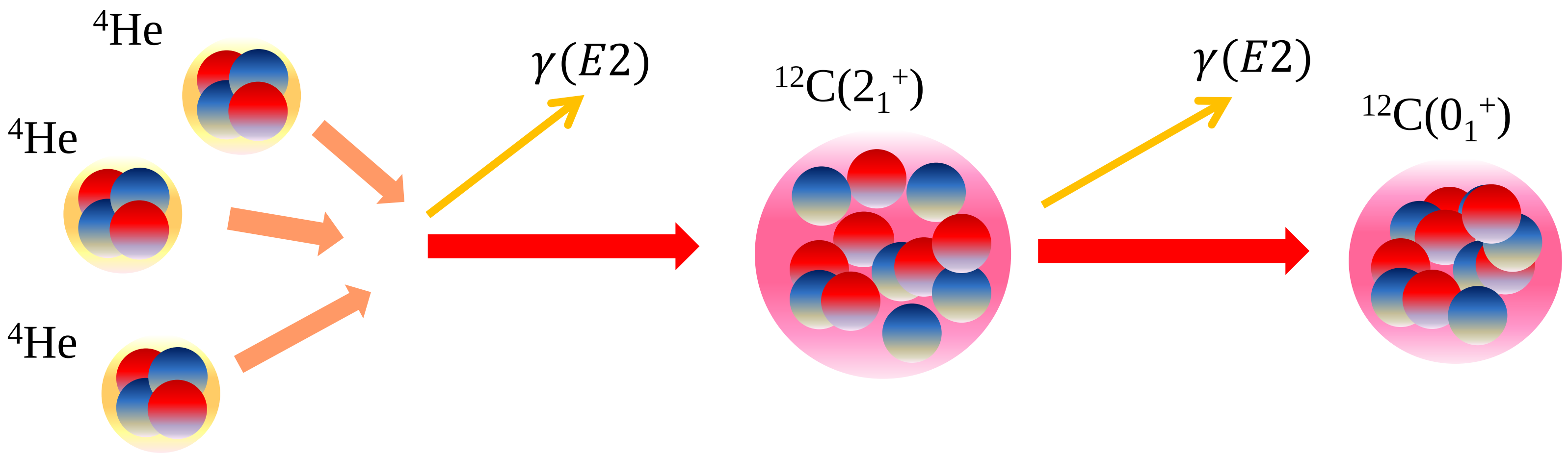
High Temperature

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



History of theoretical investigation

Total angular momentum 0



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

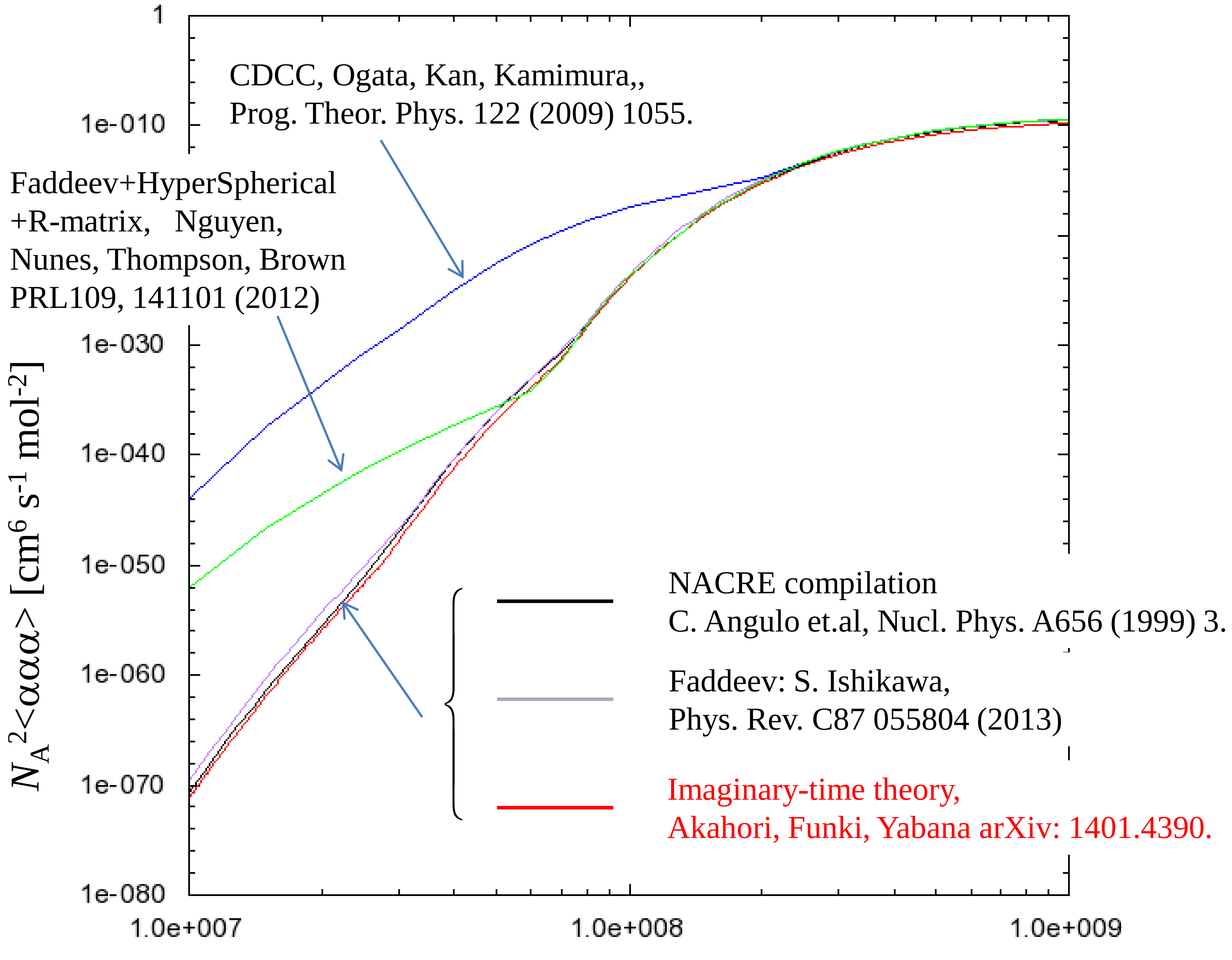
1985 K. Nomoto proposed an empirical formula applicable at low temperature, assuming sequential αα and α^{8}Be reactions. (adopted in NACRE)

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

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

Calculated rates deviates among theories at low temperature

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



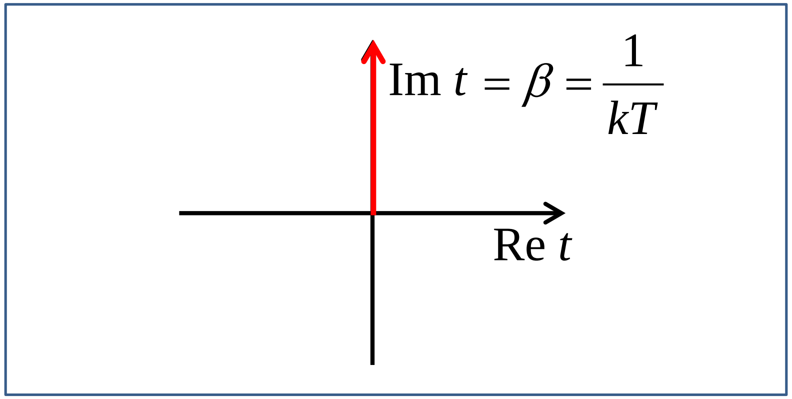
Difficulties and theoretical challenges of triple-alpha process

- Experimental measurements are very difficult.
- Difficulty of treating 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

What is the "imaginary time" ?



Popular method in thermal quantum many-body theory
(Matsubara Green's function, Kadanoff-Baym theory)

Difference from ordinary calculation

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)

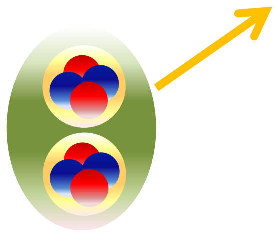
We directly calculate reaction rate, $<v\sigma>$, without solving any scattering problem.

Imaginary time 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

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

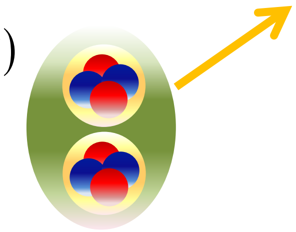
Reaction rate at $\beta = 1/k_B T$

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

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.

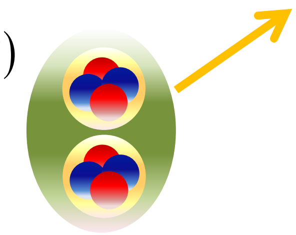
We use spectral representation of the Hamiltonian

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

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

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

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

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

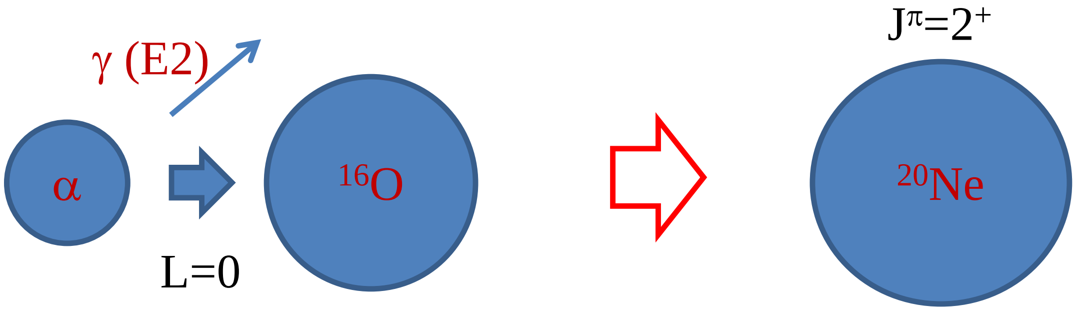
We never need any solution of scattering problem (Coulomb wave function).

Test calculation (2-body problem)
Direct capture process of $^{16}O(\alpha,\gamma)^{20}Ne$

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

Assume a potential model for ^{16}O and α

Dominant contribution from L=0(scattering state) to L=2(bound state)

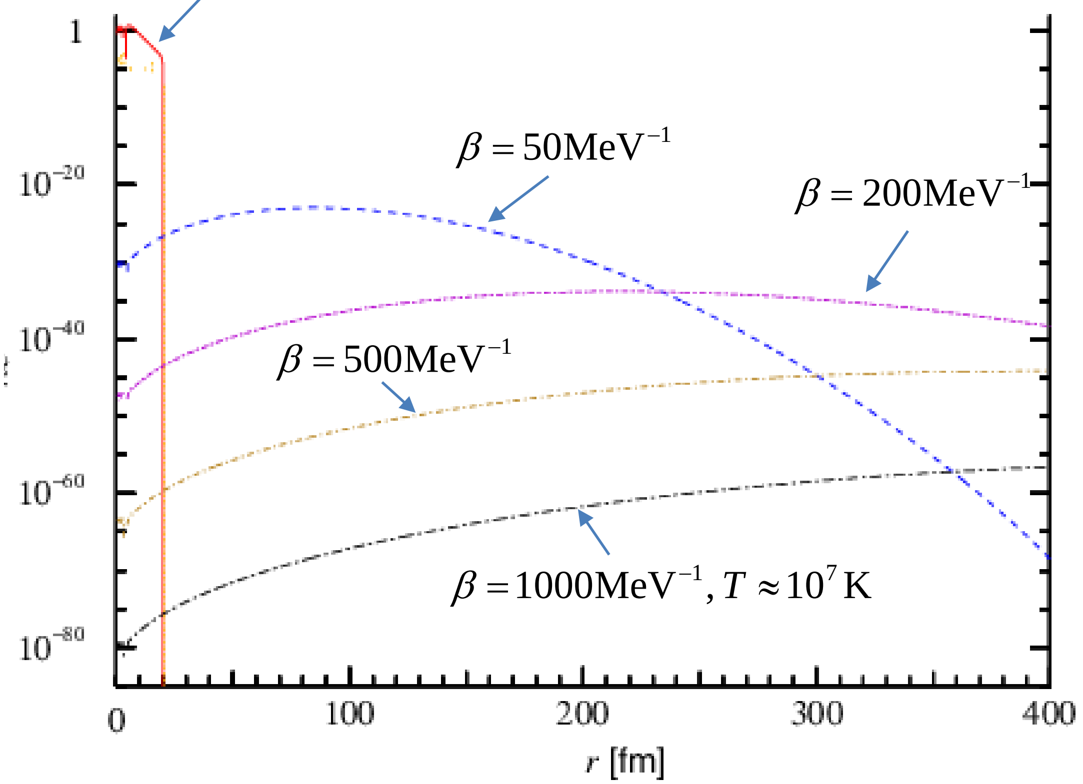


Imaginary-time theory: We calculate "wave function at temperature T"

$$\psi(\vec{r},\beta) = \frac{u_l(r,\beta)}{r} Y_{lm}(\hat{r}) \qquad -\frac{\partial}{\partial\beta} u_l(r,\beta) = H u_l(r,\beta)$$

Initial wave function = final bound state of ^{20}Ne 2^+

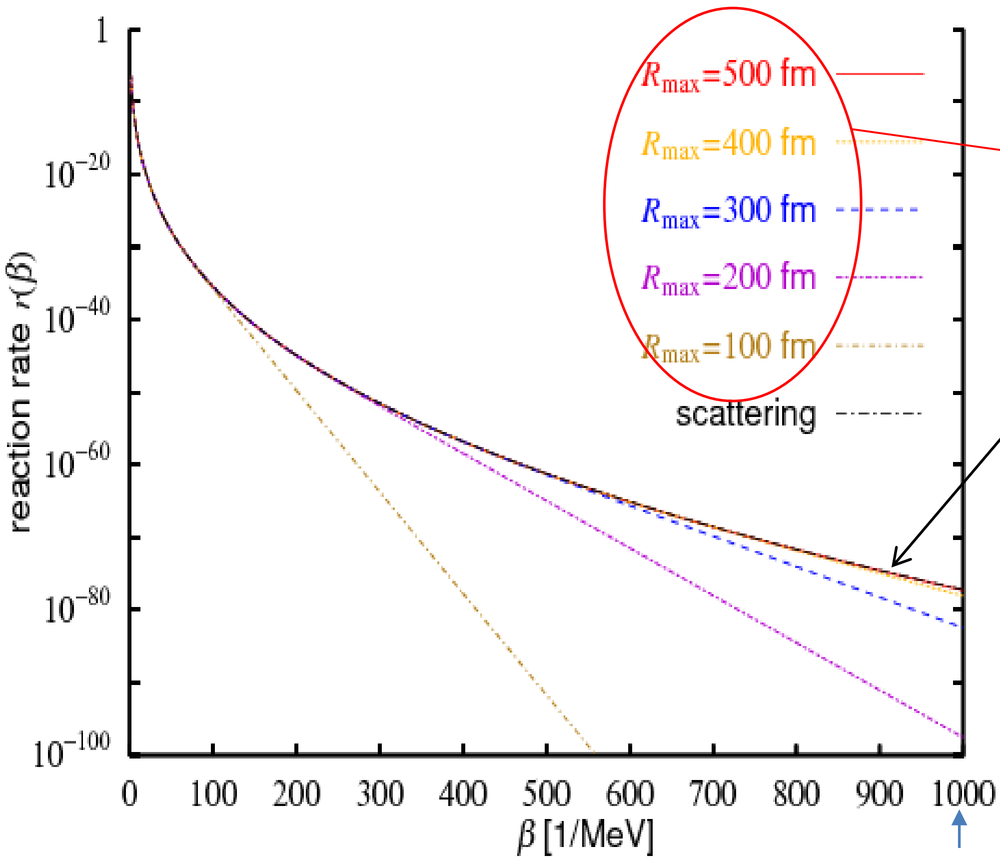
$\beta = 0$, multiplied by E2 operator.



Imaginary time calculation of reaction rate

Test example: α-^{16}O, L=0

$$\langle v\sigma \rangle \propto \left\langle u_l\left(\frac{\beta}{2}\right) \middle| \left(H - E_{2^+}\right)^5 \middle| u_l\left(\frac{\beta}{2}\right) \right\rangle$$



$T \approx 10^7$ K

Spatial size in solving the imaginary-time evolution

Ordinary method, first calculate σ(E) and then take thermal average
= Imaginary-time method (R_{max}>400fm)

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

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

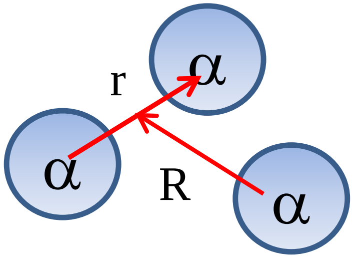
Hamiltonian of 3 alpha particles

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

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

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

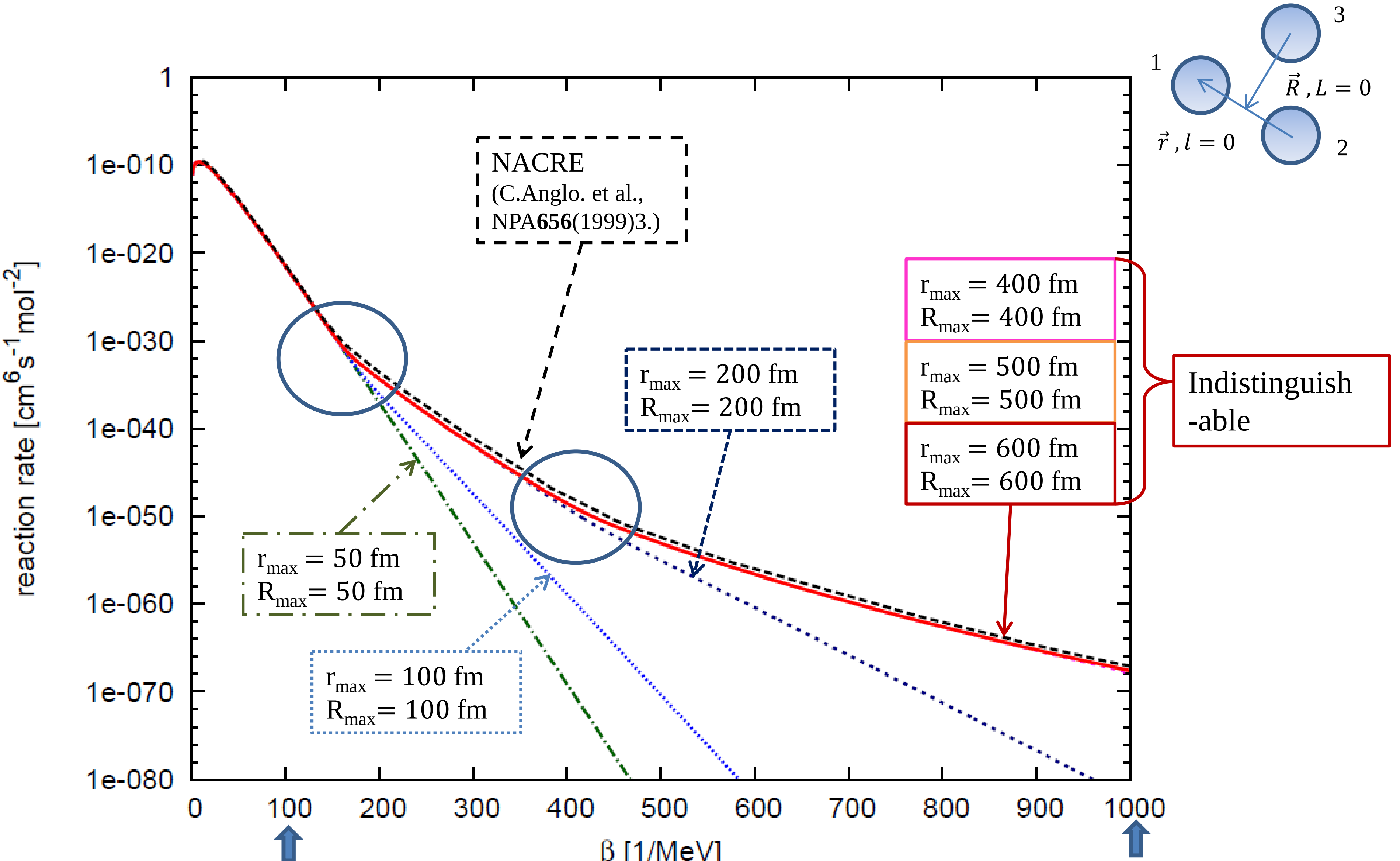
Coordinates



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

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

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



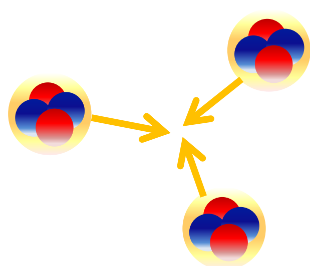
100 MeV^{-1}
= 1.15 x 10^8 K

$=1/k_BT$

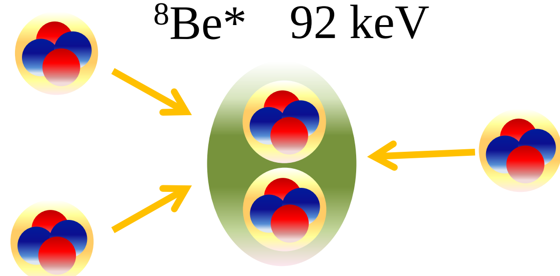
1000 MeV^{-1}
= 1.15x 10^7 K

Changes of dominant reaction mechanisms discussed in empirical theory

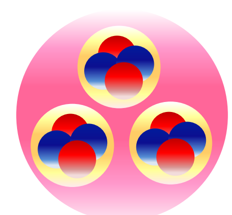
Low Temperature	⟷	High Temperature
Direct 3-alpha collision	Binary collision (^{8}Be resonance)	By way of Holy state (^{12}C resonance)



^{8}Be* 92 keV



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

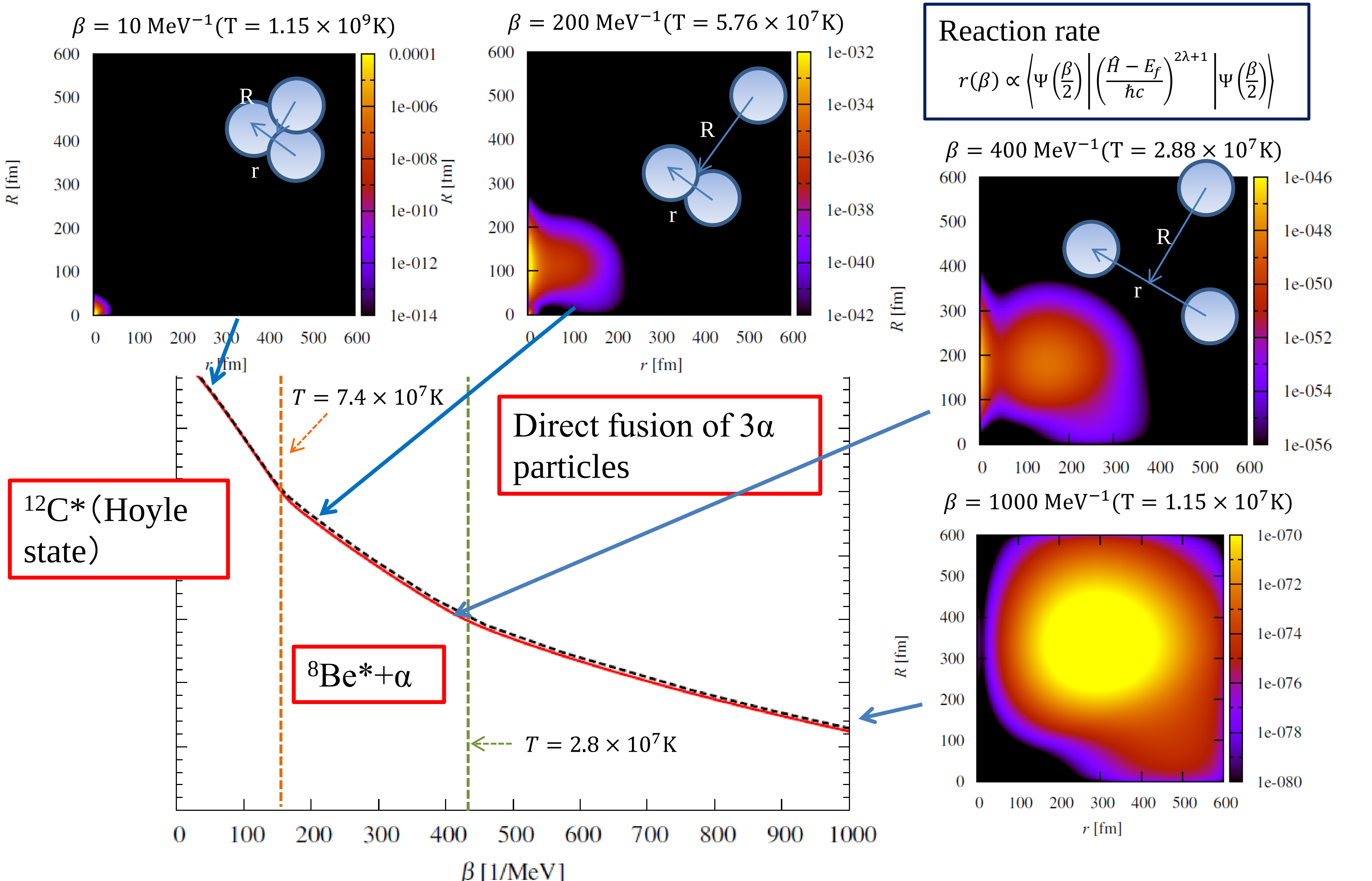


$T = 7.4 \times 10^{7}$K $\quad$ $T = 2.8 \times 10^{7}$K

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

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

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



Gamow peak energy from imaginary time evolution

Reaction rate

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

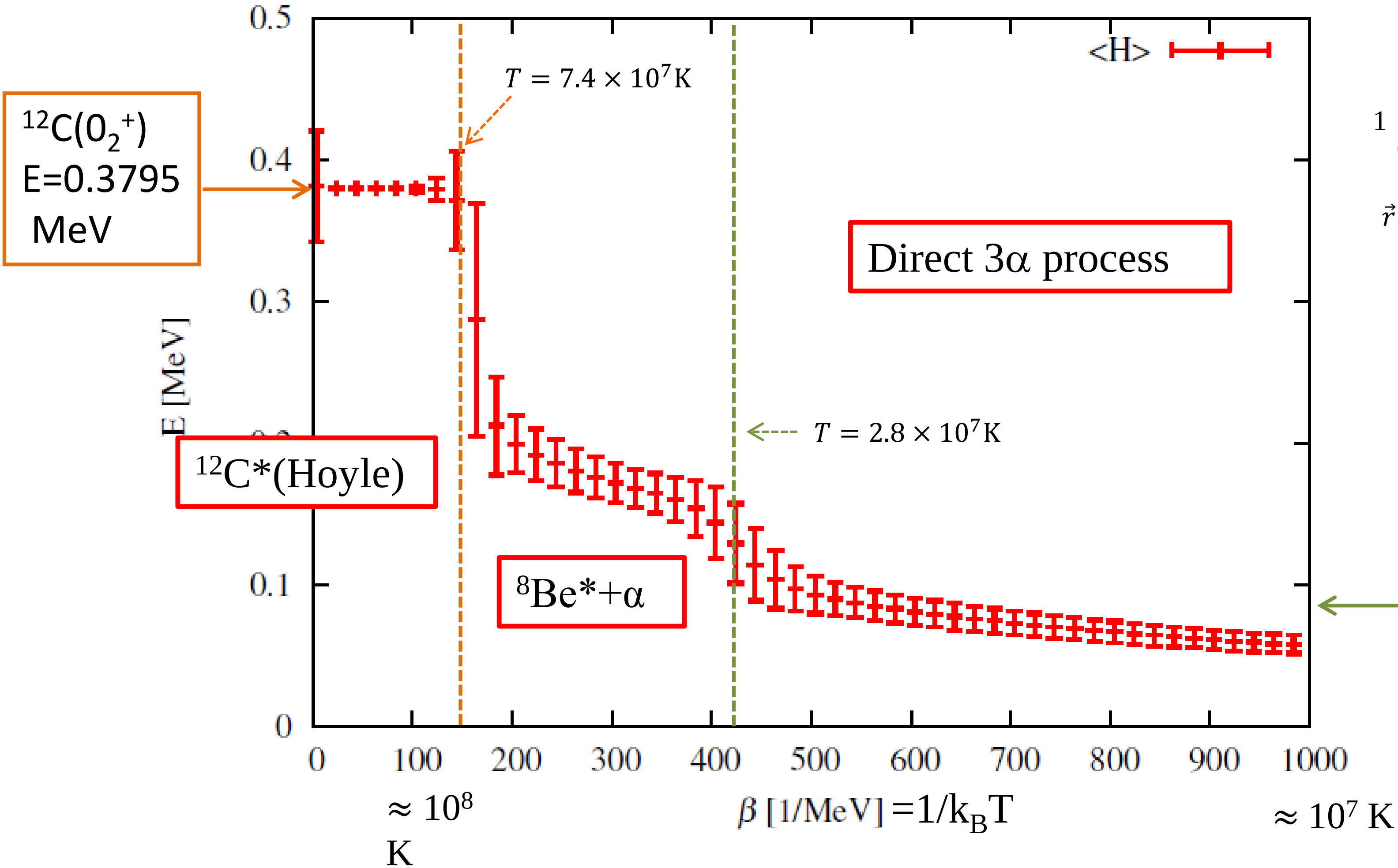
$$\equiv \langle \Psi(\beta/2) | \psi(\beta/2) \rangle$$

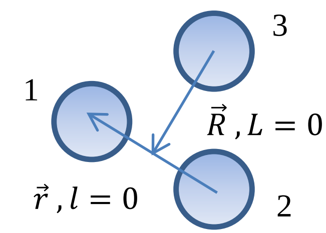
Average and variance of energy

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

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

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





Summary of part 2

--- Triple-alpha reaction rate in astrophysical environment ---

We propose a new theory – imaginary-time theory - for radiative capture process.

We may calculate reaction the triple-alpha rate without solving any scattering problems of three charged particles.

Since the imaginary-time evolution of many-body wave function is the basic ingredient, we hope the method wil be useful for ab-initio type calculations.