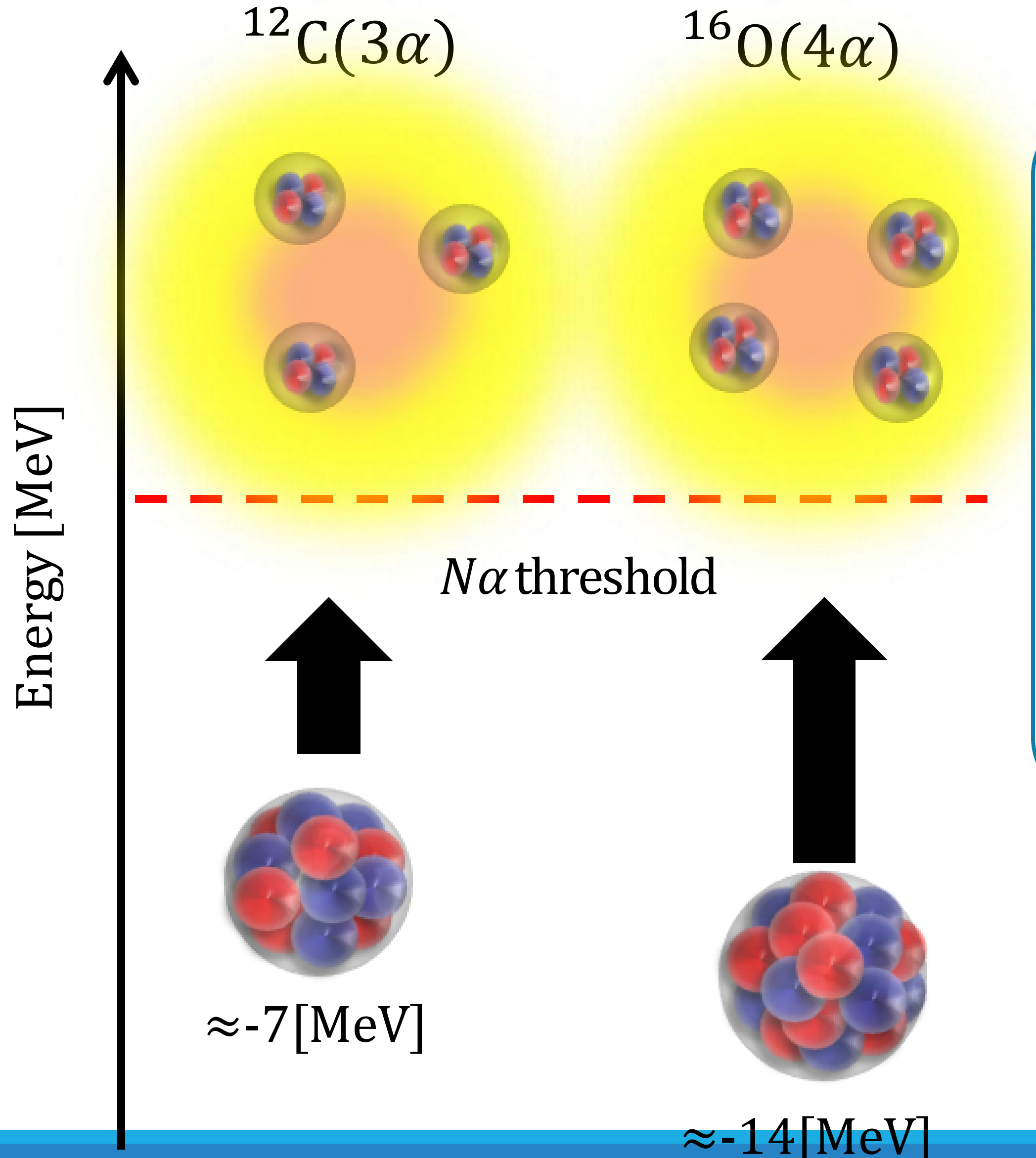
Recent advances and perspectives of cluster physics

M. Kimura (Hokkaido Univ.)

1. A new theoretical approach
   to nuclear structure & reaction problems
2. A new approach to stellar fusion reactions + α
3. Nuclear data evaluation by Machine Learning

Hoyle stateの記述

Introduction Cluster structure and α gas-like states



Recent studies for gas-like stats.

- ^{8}Be(2α), ^{12}C(3α), ^{16}O(4α) are studied in detail

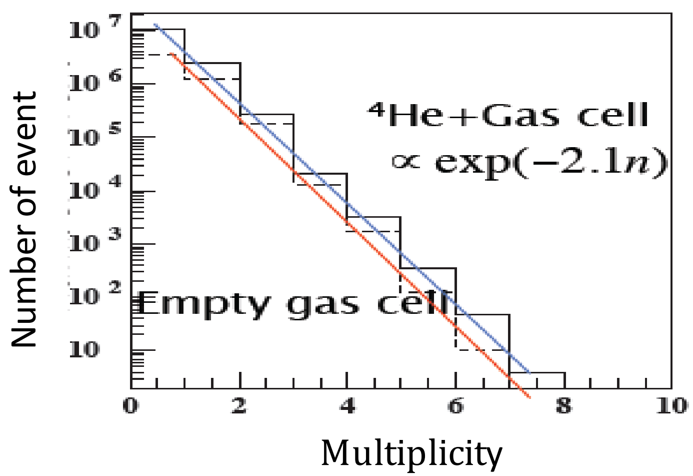
A. Tohsaki et.al PRL, **87**.192501 (2001)
Y. Funaki et.al PRC, **82**.024312 (2010)
Y. Kanada-En'yo PRC, **89**.024304 (2014)

- ^{20}Ne(5α), ^{24}Mg(6α) and heavier systems are also expected to have gas-like state.

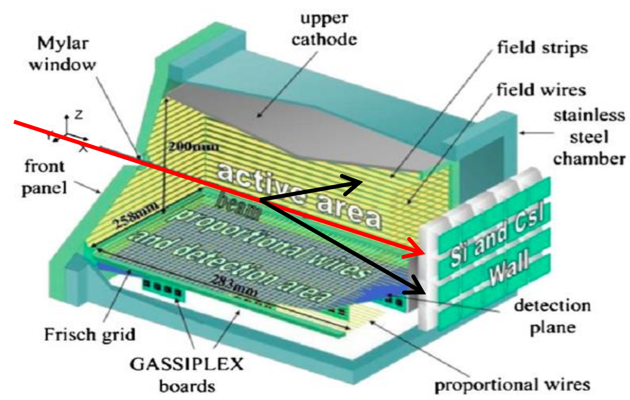
◎ How many α particles can form dilute-gas like state?

Introduction Candidates of 9α and 14α gas-like state

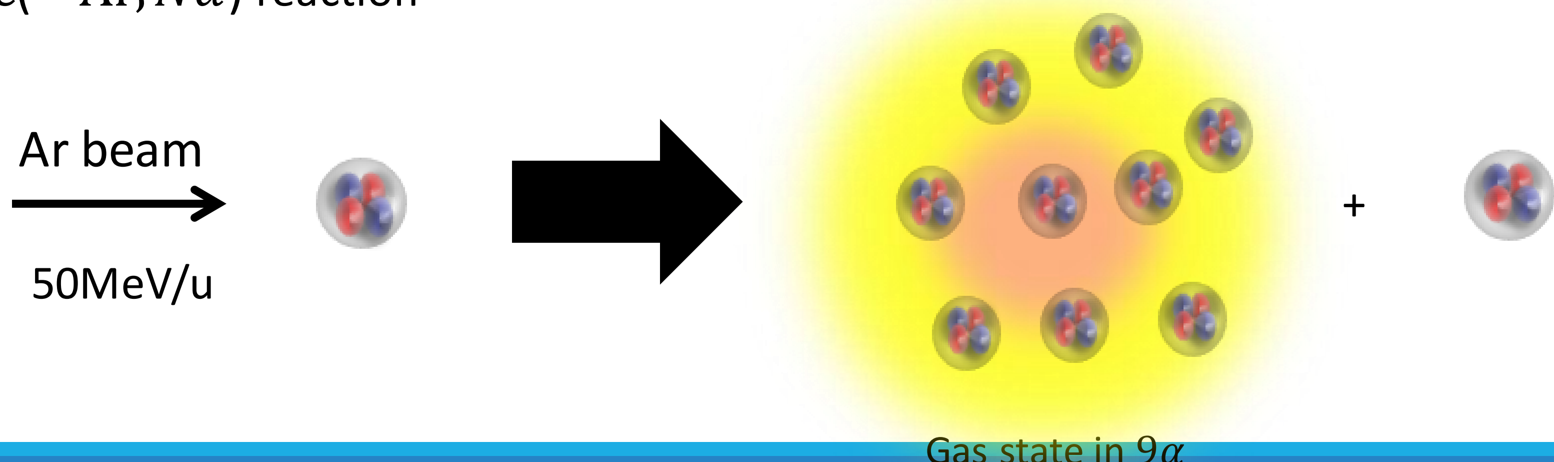
- From $^{4}\mathrm{He}(^{36}\mathrm{Ar}, N\alpha)$ $^{4}\mathrm{He}(^{56}\mathrm{Ni}, N\alpha)$experiment , signature of the 9α and 14α gas-like state.



H.Akimune et.al JPCS **436, 012010** (2013).



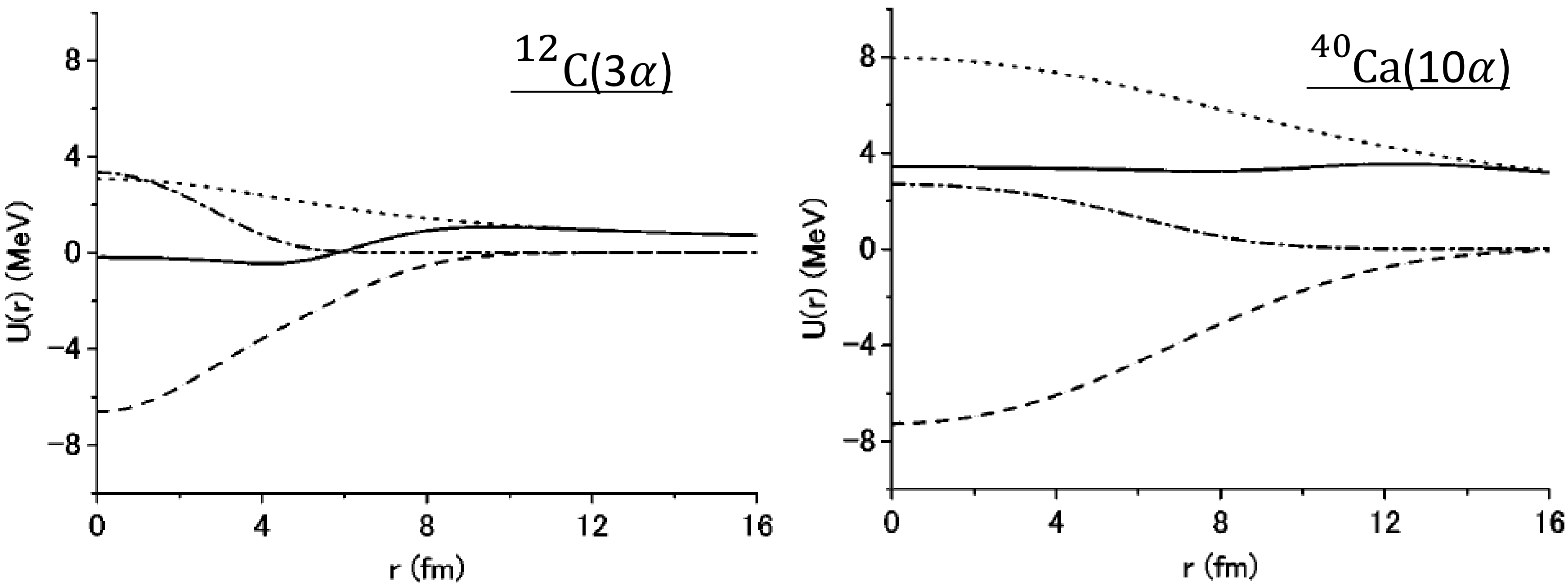
$^{4}\mathrm{He}(^{36}\mathrm{Ar}, N\alpha)$ reaction



Introduction Theoretical study for many α system

T. Yamada and P. Schuck, PRC **69**, 024309 (2004)

◎ Gas-like state possibility exist up to ～10α sysytem .



◎ Boson approximation is applied (Gross-Pitaevskii equation)

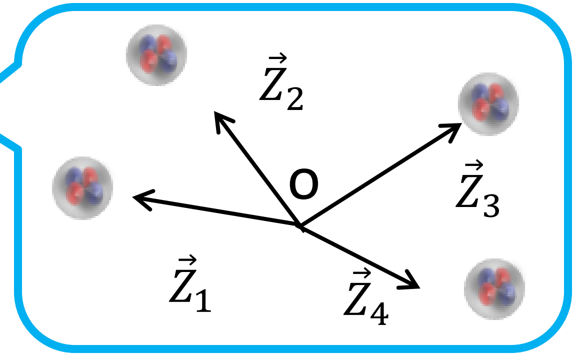
The prediction should be verified by the microscopic cluster model without Boson approximation.

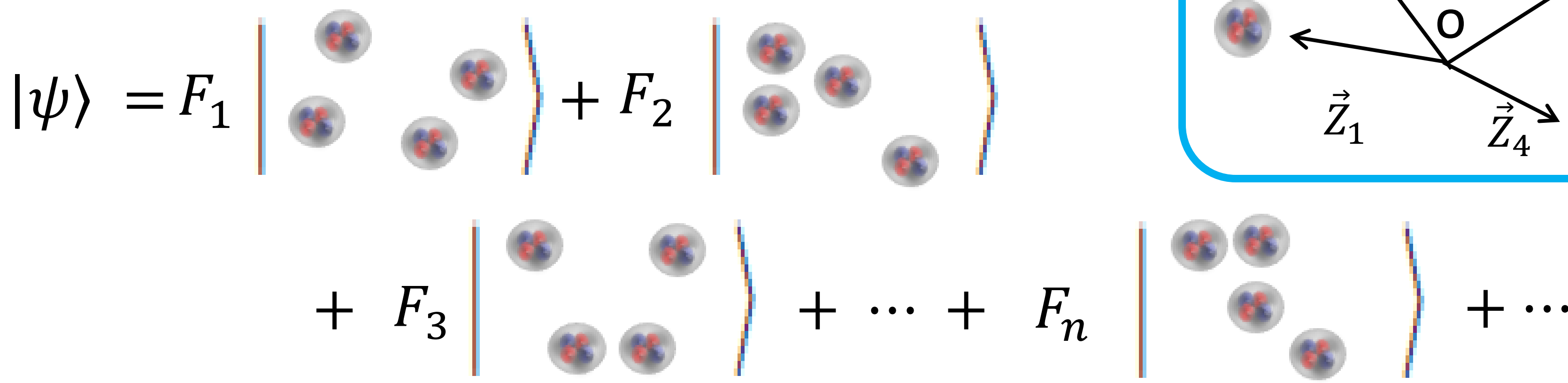
⇒ We need microscopic model that can describe gas-like states of many α particles

Introduction microscopic description of gas-like state

Gas-like state is described by the superposition of "many" Slater determinants

$$\psi(\vec{r}_1,\cdots,\vec{r}_{16}) = \int d\vec{Z}_1\cdots d\vec{Z}_4 F(\vec{Z}_1,\cdots,\vec{Z}_4)\phi(\vec{Z}_1,\cdots,\vec{Z}_4)$$





- Number of Slater determinants becomes huge as the number of α increases

  ⇒ We need effective way to generate basis wave functions.

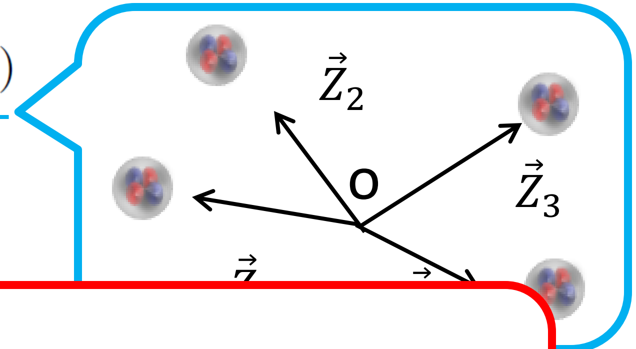
Various methods to genarate $N\alpha$ wave functions

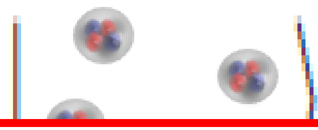
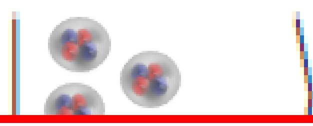
- Random generation — T. Ichikawa et.al PRC, **83**.061301 (2011)
- Imaginary time evolution — Y. Fukuoka et.al PRC, **88**.014321 (2013)
- Real time evolution

Introduction ~~microscopic description of gas-like state~~

Gas-like state is described by the superposition of "many" Slater determinants

$$\psi(\vec{r}_1, \cdots, \vec{r}_{16}) = \int d\vec{Z}_1 \cdots d\vec{Z}_4 F(\vec{Z}_1, \cdots, \vec{Z}_4) \underline{\phi(\vec{Z}_1, \cdots, \vec{Z}_4)}$$



$|\psi\rangle = F_1$  $+ F_2$ 

- In this talk, we introduce a method based on the real time evolution
- The new method is applied to $3\alpha, 4\alpha$ systems

- Number of Slater determinants becomes huge as the number of α increases

  ⇒ We need effective way to generate basis wave functions.

Various methods to genarate $N\alpha$ wave functions

- Random generation — T. Ichikawa et.al PRC, **83**.061301 (2011)
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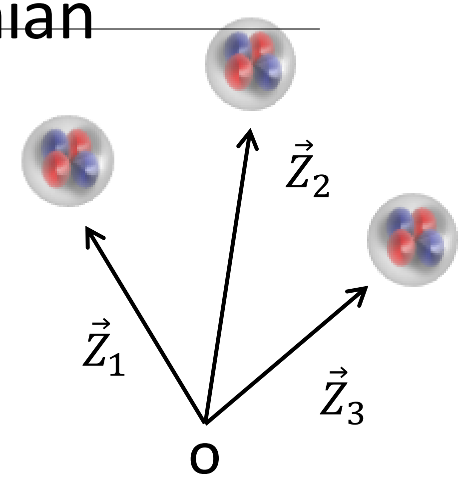
- Real time evolution ⇐ Our method

Framework Wave function and Hamiltonian

Hamiltonian

$$H = \sum_i T_i - t_{c.m} + \sum_{i<j} V_{ij} + \sum_{\text{proton}} V_c$$

Volkov No. 2 Y.Funaki PRC.**92** 021302(2015)



Basis wave function (Brink-wave function)

$$\phi(\vec{Z}_1, \cdots, \vec{Z}_N) = \mathcal{A}\left\{\phi_\alpha(\vec{Z}_1)\phi_\alpha(\vec{Z}_2)\cdots\phi_\alpha(\vec{Z}_N)\right\}$$

$\phi_\alpha(\vec{Z}_i)$; α particle wave function (wave packet) located at $\vec{Z}_i$

Equation of motion for wave packet

$$\delta \frac{\langle \phi \mid i\frac{\partial}{\partial t} - H \mid \phi \rangle}{\langle \phi \mid \phi \rangle} = 0$$

Time dependent variational principle

$$i\hbar \sum_{j,\sigma} C_{i\rho j\sigma} \frac{\partial \vec{Z}_{j\sigma}}{\partial t} = \frac{\partial H}{\partial \vec{Z}^*_{i\rho}}$$

Equation of motion for wave packets

Framework Time evolution of wave packets

$$i\hbar \sum C_{i\rho j\sigma} \frac{\partial \vec{Z}_{j\sigma}}{\partial t} = \frac{\partial H}{\partial \vec{Z}^*}$$

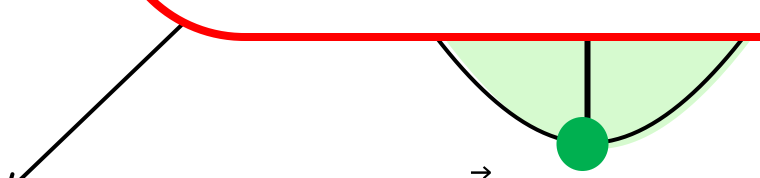
◎Many body wave function represented by wave packet is ⋯

- ○ Ergodic nature. J. Schnack , H. Feldmeier NPA, **601**. (1996)
- ○ Obeying quantum statics. A. Ono , H. Horiuchi PRC.**53**. (1996)

⬇

➢ If the system is evolved long enough, all of important configurations of α particles appear automatically .

⇒ Basis wave functions to describe gas-like state are automatically generated !



Position of center $\vec{Z}$

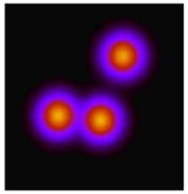
Framework New generator coordinate method

- The time evolution generates all important configurations

Superposition of the wave functions obtained by the time evolution should give a good description for the gas-like state

In other words, we perform GCM calculation using the real time t as the generator coordinate

Step1: Time evolution to generate basis wave function



$$i\hbar \sum_{j,\sigma} C_{i\rho j\sigma} \frac{\partial \vec{Z}_{j\sigma}}{\partial t} = \frac{\partial H}{\partial \vec{Z}^*_{i\rho}}$$

Step2: Superpose basis wave function and solve GCM equation

$$\psi(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_{4N}) = \int_0^\infty dt \underbrace{F^{J\pi}_{MK}(t)}_{\text{Determined by diagonalization of Hamiltonian}} P^{J\pi}_{MK} \phi(\vec{Z}_1(t), \vec{Z}_2(t), \cdots, \vec{Z}_N(t))$$

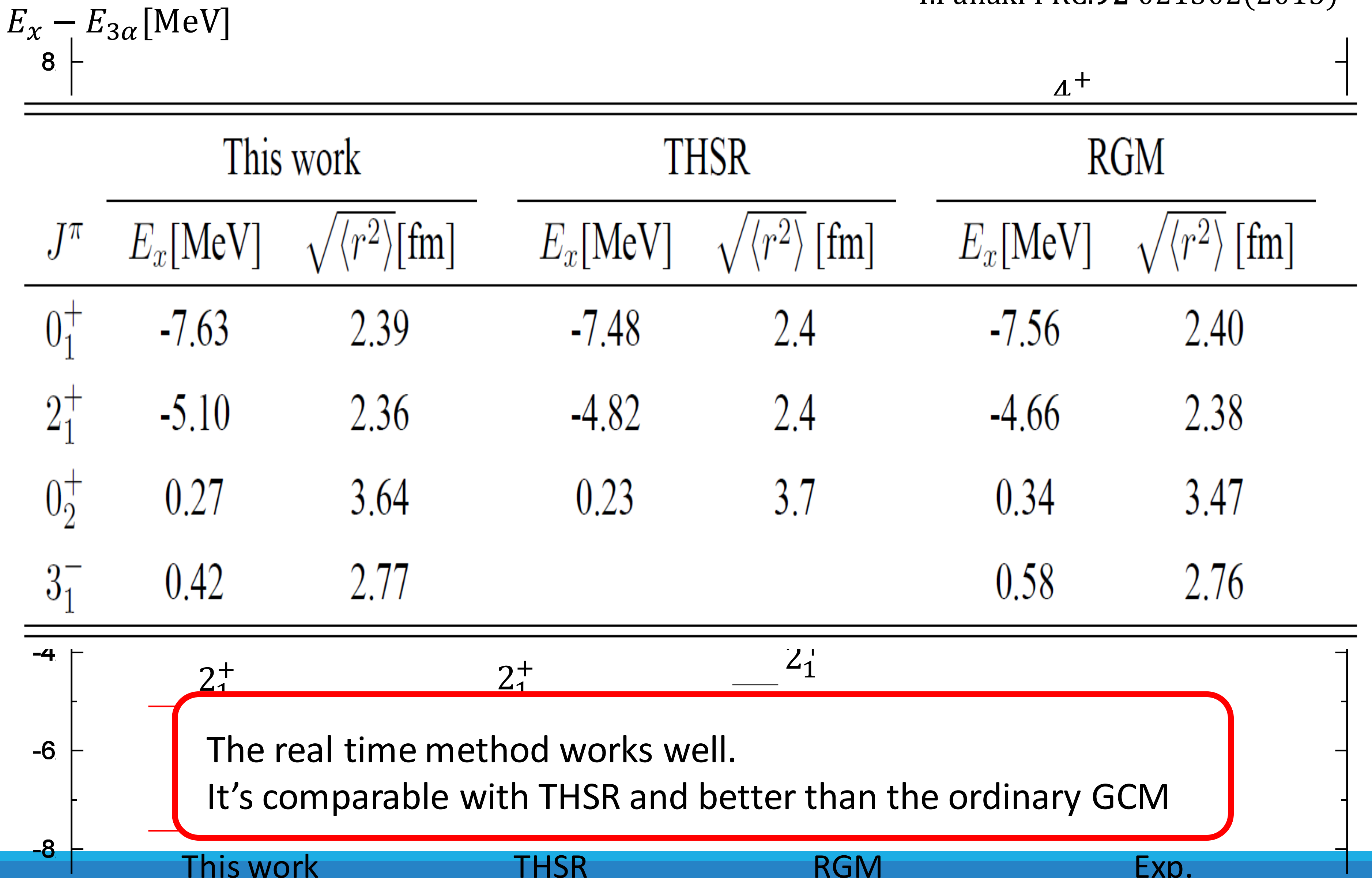
$P^{J\pi}_{MK}$; Projection operator of parity and angler momentum

Results & Discussions for 3α and 4α systems

Result for 3α system (^{12}C)

M.Kamimura NPA.**351**, 456 (1981)
Y.Funaki PRC.**92** 021302(2015)

J^π	This work E_x[MeV]	This work $\sqrt{\langle r^2\rangle}$[fm]	THSR E_x[MeV]	THSR $\sqrt{\langle r^2\rangle}$ [fm]	RGM E_x[MeV]	RGM $\sqrt{\langle r^2\rangle}$ [fm]
0_1^+	-7.63	2.39	-7.48	2.4	-7.56	2.40
2_1^+	-5.10	2.36	-4.82	2.4	-4.66	2.38
0_2^+	0.27	3.64	0.23	3.7	0.34	3.47
3_1^-	0.42	2.77			0.58	2.76



The real time method works well.
It's comparable with THSR and better than the ordinary GCM

Discussion Check of the convergence of calc.

Our method is based on the ergodic nature

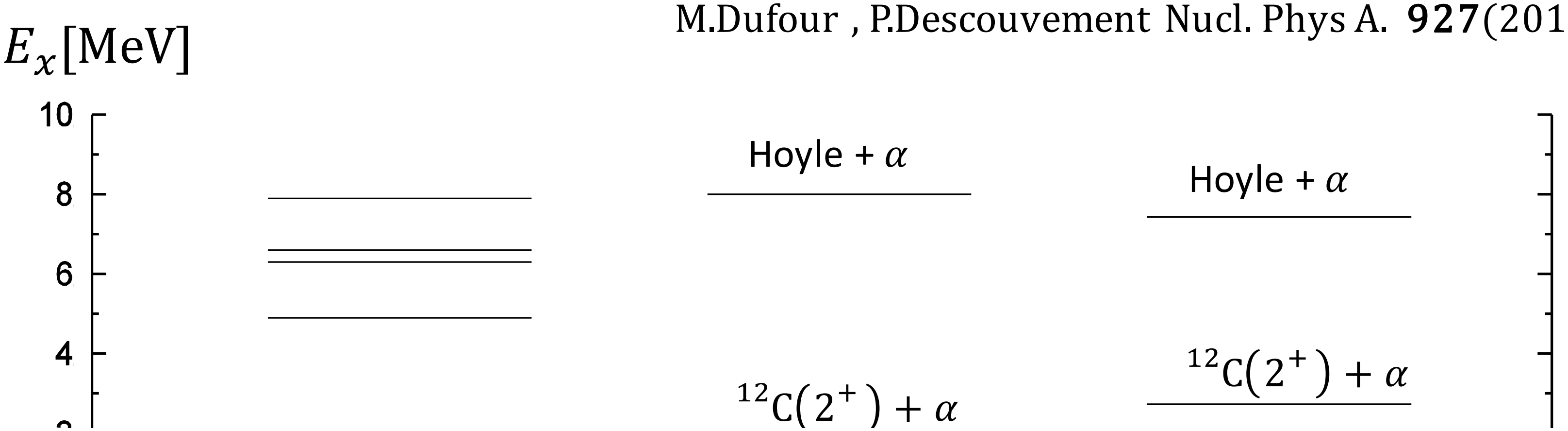
$\Rightarrow$ Following two pointes should be checked

1. When the time evolution is long enough,
   the result should be converged.

2. The result should be independent of
   the initial configuration of α particles at $t = 0$.

Result for 4α system (^{16}O)

M.Dufour , P.Descouvement Nucl. Phys A. **927**(2014). 134-146.



	E_x[MeV]		$\sqrt{\langle r^2 \rangle}$[fm]		$M(E0)$[fm^2]	
J^π	This work	M.Dufour et al	This work	Exp.	This work	Exp.
0_1^+	-17.0	-15.2	2.32	2.71±0.02		
0_2^+	-1.6	-1.1	2.83		5.89	3.55±0.21
0_3^+	2.73	2.1	3.03		3.48	
0_4^+	7.43	8.0	3.40		0.39	

Summary

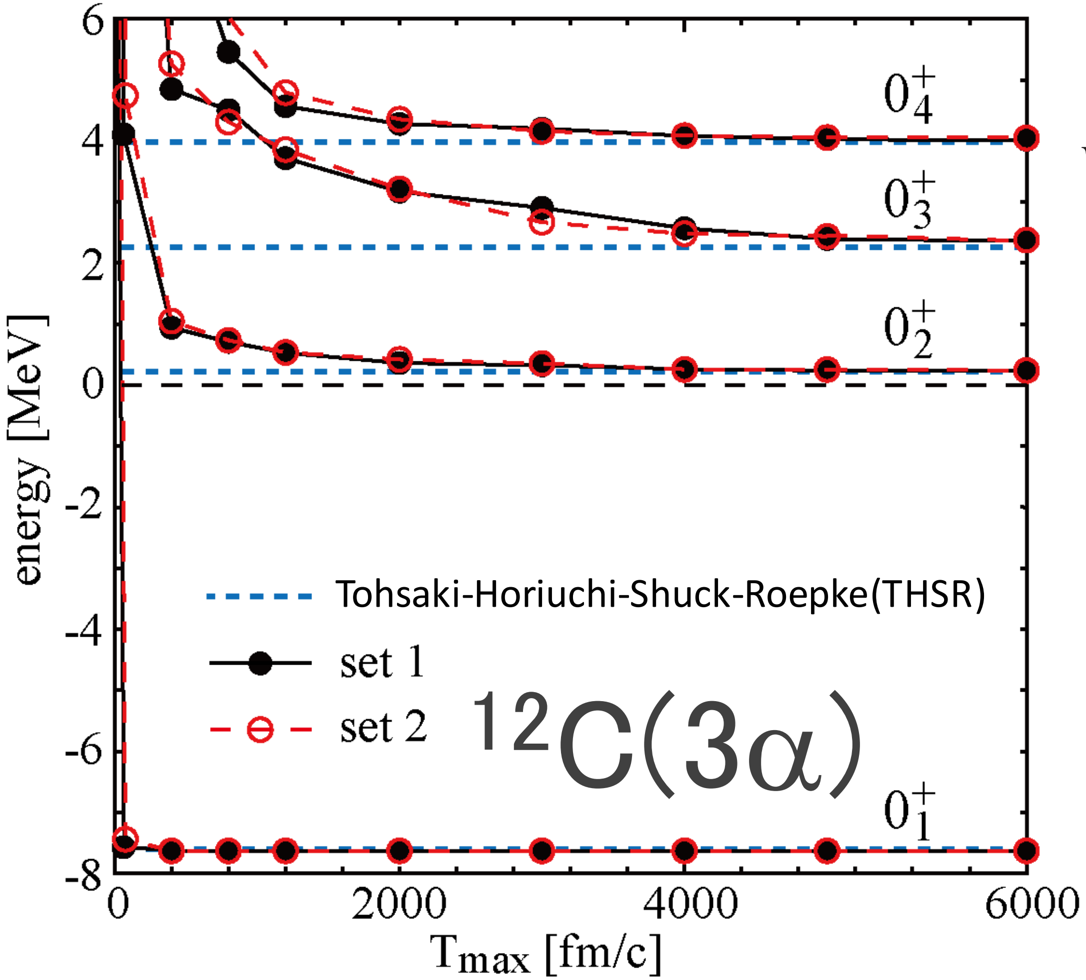
- For $^{8}\mathrm{Be}(2\alpha)$, $^{12}\mathrm{C}(3\alpha)$, $^{16}\mathrm{O}(4\alpha)$, gas state is well known but those of $^{20}\mathrm{Ne}(5\alpha)$, $^{24}\mathrm{Mg}(6\alpha)\cdots$ are not known.
- To solve the difficulty for generating wave function increasing number of α particles, we introduced real time evolution setting time t as a generator coordinate.
- For $^{12}\mathrm{C}(3\alpha)$, $^{16}\mathrm{O}(4\alpha)$ nuclei, this method yielded the results consistent with or better than the previous researches.

Future work

- Separate from continuum state.
- Introduce three-body interaction.

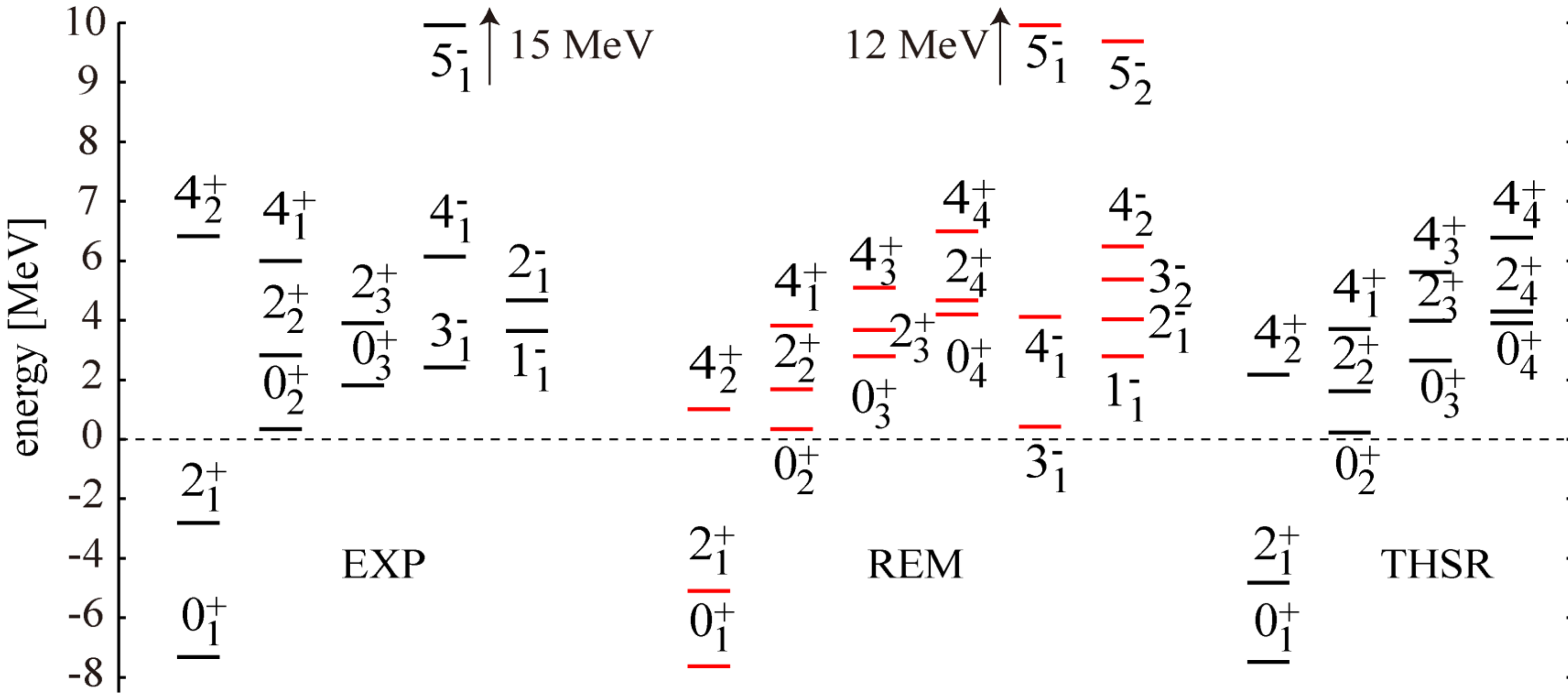
Benchmark calculations for ^{12}C (3α cluster system)

R. Imai, T. Tada and M.K., arXiv:1802.03523



$$\Psi^{J\pi} = \int_0^{T_{max}} dt \;\; f(t)\hat{P}^J_{MK}\Phi(t)$$

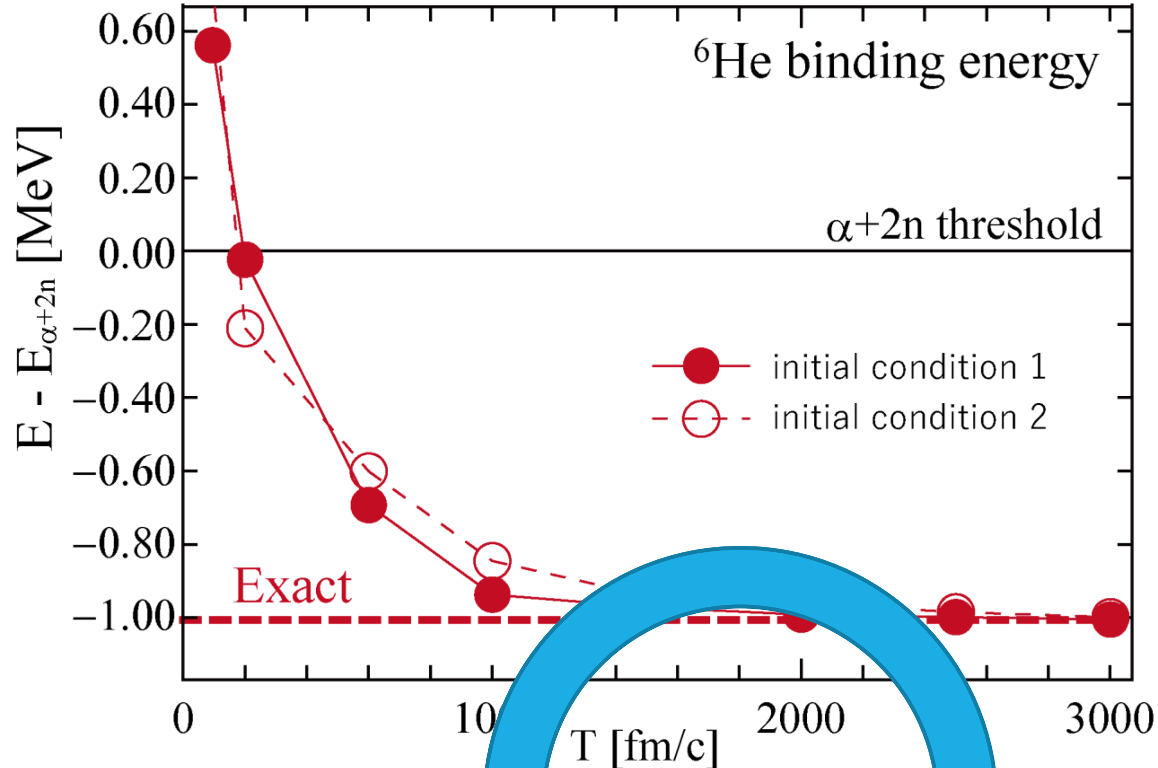
Benchmark calculations for ^{12}C (3α cluster system)



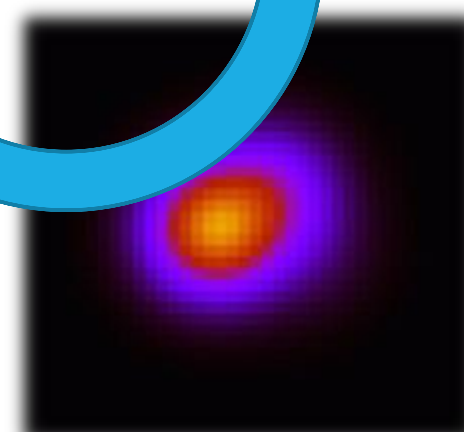
○ All results are consistent with or better than THSR wave function

○ Computational cost is greatly reduced

A new theoretical approach to nuclear structure and reactions



$$i\hbar\frac{d\boldsymbol{Z}_i(t)}{dt} = \sum_j C_{ij}^{-1}\frac{\partial\mathcal{H}}{\partial\boldsymbol{Z}_j^*(t)}$$



Coherent stateの時間発展に関する問題を追加しておく

Motivation

◎ Most of nuclear structure models describes a nuclear state by a superposition of model wave functions

$$\underline{\Psi} = \sum_{n=1}^{N_{max}} c_n \underline{\Phi_n}$$

Nuclear state   Model wave function

Smaller N_{max}	Inaccurate	Accurate	Larger N_{max}
Simple Φ_n	Small CPU cost	Large CPU cost	Accurate Φ_n

Newly developed our method "Real-time evolution method" is a very natural and effective way to choose Φ_n and N_{max}.

It realizes very accurate description of nuclei

Model: Real-Time evolution method

◎ Model wave function (time-dependent wave packets)

○ Slater determinant of nucleon wave packets

$$\Phi(t) = \mathcal{A}\{\,\phi(\boldsymbol{Z}_1(t)), \ldots, \phi(\boldsymbol{Z}_A(t))\,\}$$

$$\phi(\boldsymbol{Z}_i(t)) = \exp\{-\nu(\boldsymbol{r} - \boldsymbol{Z}_i(t))^2\}\,(\alpha_i(t)\,|\uparrow\rangle + \beta_i(t)\,|\downarrow\rangle)$$

○ Dynamical variables of the model (time-dependent parameters)

$\boldsymbol{Z}_i(t)$: Centroids of wave packets (position and momentum)

$\alpha_i(t)$ $\beta_i(t)$: Spin directions

◎ Hamiltonian

$$H = \sum_{i=1}^{A} t(i) - t_{cm} + \sum_{i<j} v(ij)$$

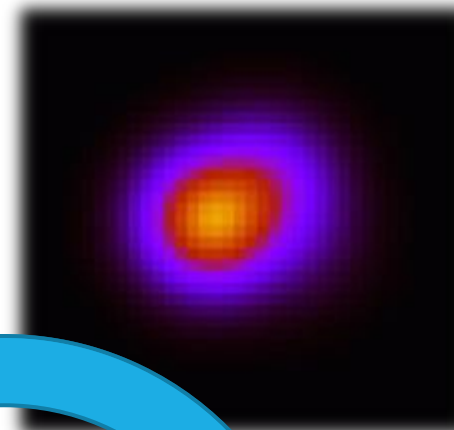
○ Microscopic Hamiltonian with effective/bare NN interactions

Model: Real-Time evolution method

◎ Time-dependent variational principle

$$\delta \int dt \, \frac{\langle \Phi(t) | i\hbar d/dt - H | \Phi(t) \rangle}{\langle \Phi(t) | \Phi(t) \rangle} = 0$$

^{6}He (6 nucleons)

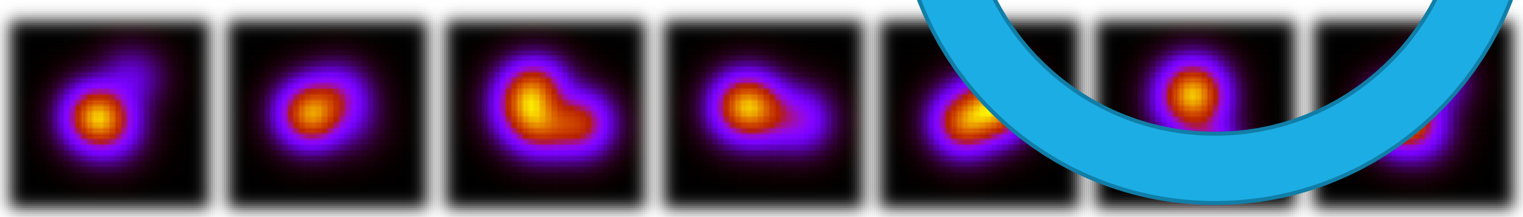


◎ Equation of Motion for nucleon wave packets

$$\Rightarrow \quad i\hbar \frac{d\boldsymbol{Z}_i(t)}{dt} = \sum_j C_{ij}^{-1} \frac{\partial \mathcal{H}}{\partial \boldsymbol{Z}_j^*(t)}$$

$$\mathcal{H} = \frac{\langle \Phi(t) | H | \Phi(t) \rangle}{\langle \Phi(t) | \Phi(t) \rangle}, \quad C_{ij} = \frac{\partial^2}{\partial \boldsymbol{Z}_i^* \partial \boldsymbol{Z}_j} \mathrm{l} \quad \langle \Phi(t) | \Phi(t) \rangle$$

○ By solving EOM, we obtain ensembl f wave functions



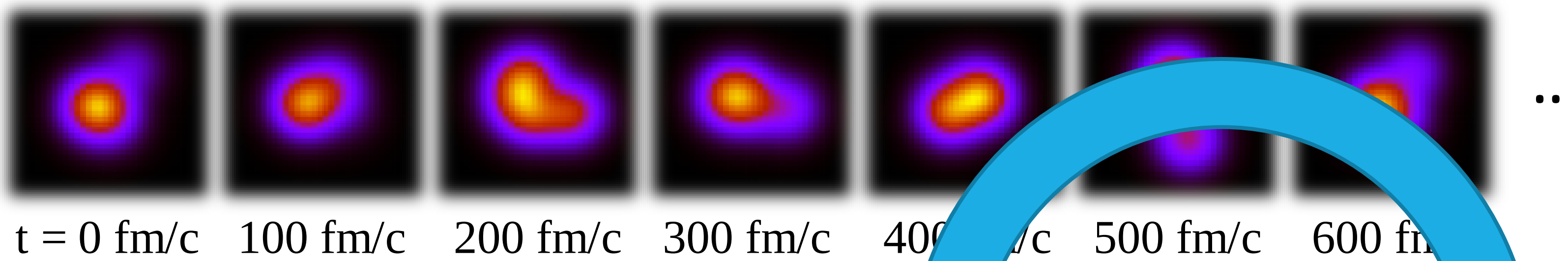
t = 0 fm/c 100 fm/c 200 fm/c 300 fm/c 400 fm/c 500 fm/c 600 fm/c …

Model: Real-Time evolution method

◎ Each wave function is not accurate (Gaussian approx.)

but the ensemble of the wave functions has nice properties

J. Schnack and H. Feldmeier, NPA601, 181 (1996).
A. Ono and H. Horiuchi, PRC53, 845 (1996), PRC53, 2341 (1996).



① The ensemble has ergodicity

All possible quantum states will appea fter long-time prop ation

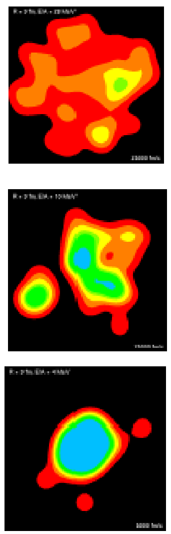
② The ensemble follows *quantum* statisti

Important quantum states appear more frequ

if the excitation energy (temperature) is properly chosen

Model: Real-Time evolution method

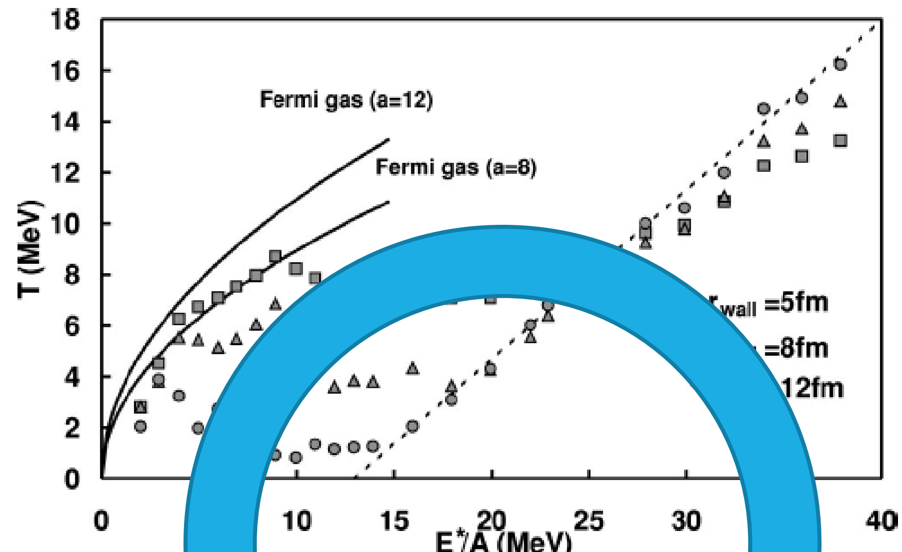
◎ Actually, this ensemble properties (ergodicity & quantum statistcs) have been utilized to discuss Liquid-Gas phase transition of nuclear matter.



$E^* = 28A$ MeV

$E^* = 10A$ MeV

$E^* = 4A$ MeV

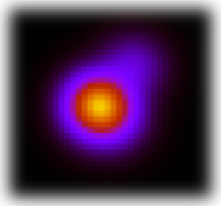
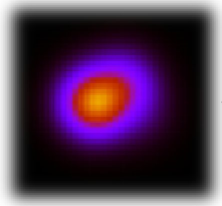
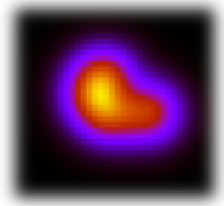
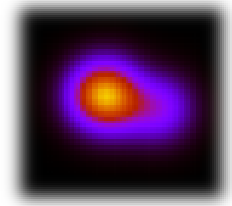


Schnack & Feldmeier PRC59 (1999). Suga and Horiuchi PRC60 (200
Furuta and Ono, PRC79, 014608 (2009).

The ensemble can also be used to desc r structure

Model: Real-Time evolution method

◎ We superpose time dependent wave function and diagonalize the Hamiltonian

$$\Psi^{J\pi} = f_1$$  $$+ f_2$$  $$+ f_3$$  $$+ f_4$$  ...

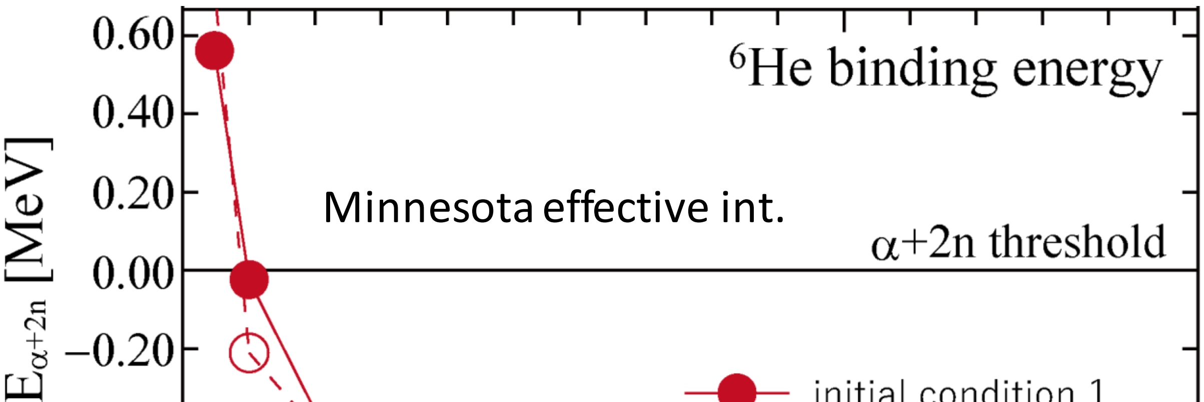
$$= \int_0^{T_{max}} dt \;\; f(t)\hat{P}^J_{MK}\Phi(t)$$

$f_1, f_2, f_3, f_4, \ldots$ are determined by [illegible] diagonalization of Ha[illegible]tonian

○ The result (energy & wave function) [illegible]uld be converge[illegible] after the long-time propagation

○ The result should not depend on the initial co[illegible] at t=0

Benchmark calculations for few-body systems



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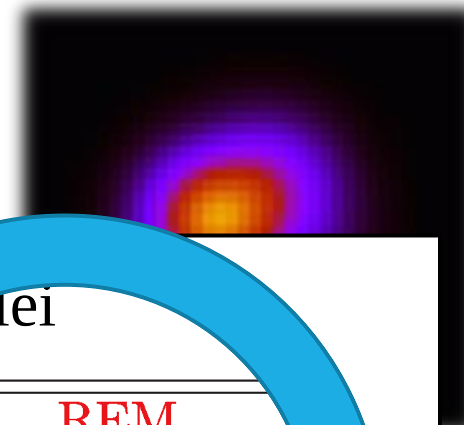


Benchmark: light p-she[illegible]uclei

	GFMC		SV[illegible]		REM	
nuclei	E	$\sqrt{\langle r^2 \rangle}$	E	[illegible]	E	$\sqrt{\langle r^2 \rangle}$
^{3}H	-8.26	1.68	-8.25	[illegible]	-8.25	1.68
^{4}He	-31.3	1.36	-31.4	[illegible]	-31.4	1.39
^{6}He	-66.3	1.50	-66.3	[illegible]	-66.3	1.50
^{7}Li	-	-	-83.4	[illegible]	-83.5	[illegible]

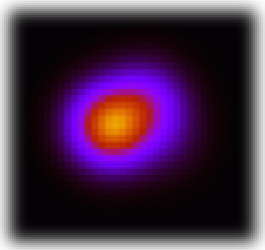
GFMC: Green function Monte Carlo [2] SVM: Stochastic [illegible] method [8]

* An effective potential "Mulfliet-Tjon potential V (MTV)" was used.

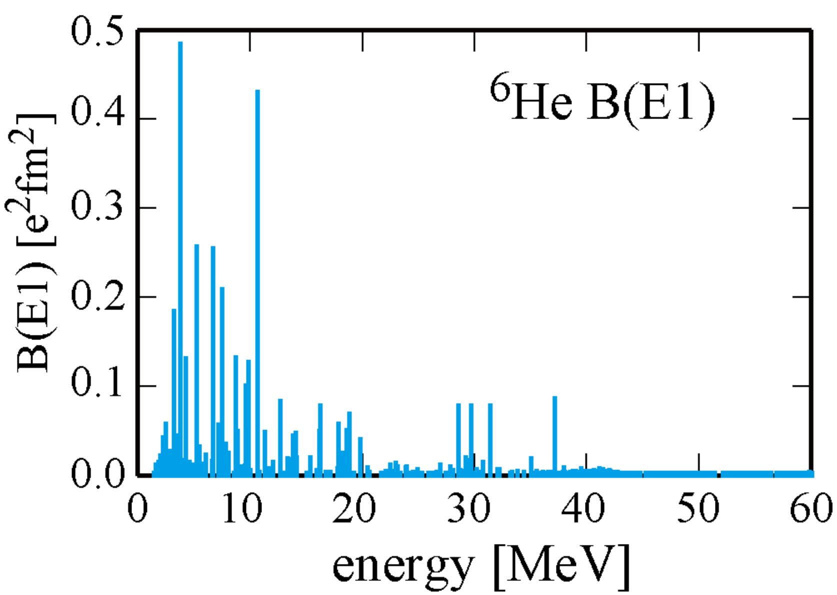
Nuclear response functions

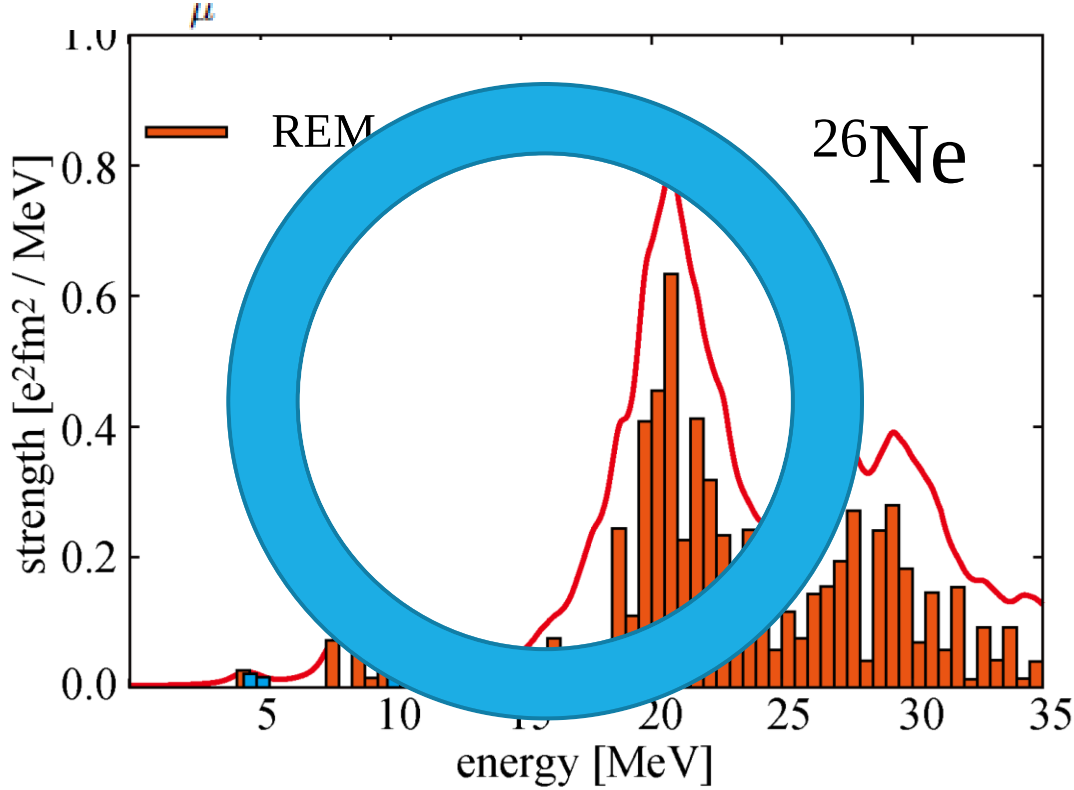
◎ It is also possible to study the nuclear responses

The ensemble of wave function contains
the information of the excited states



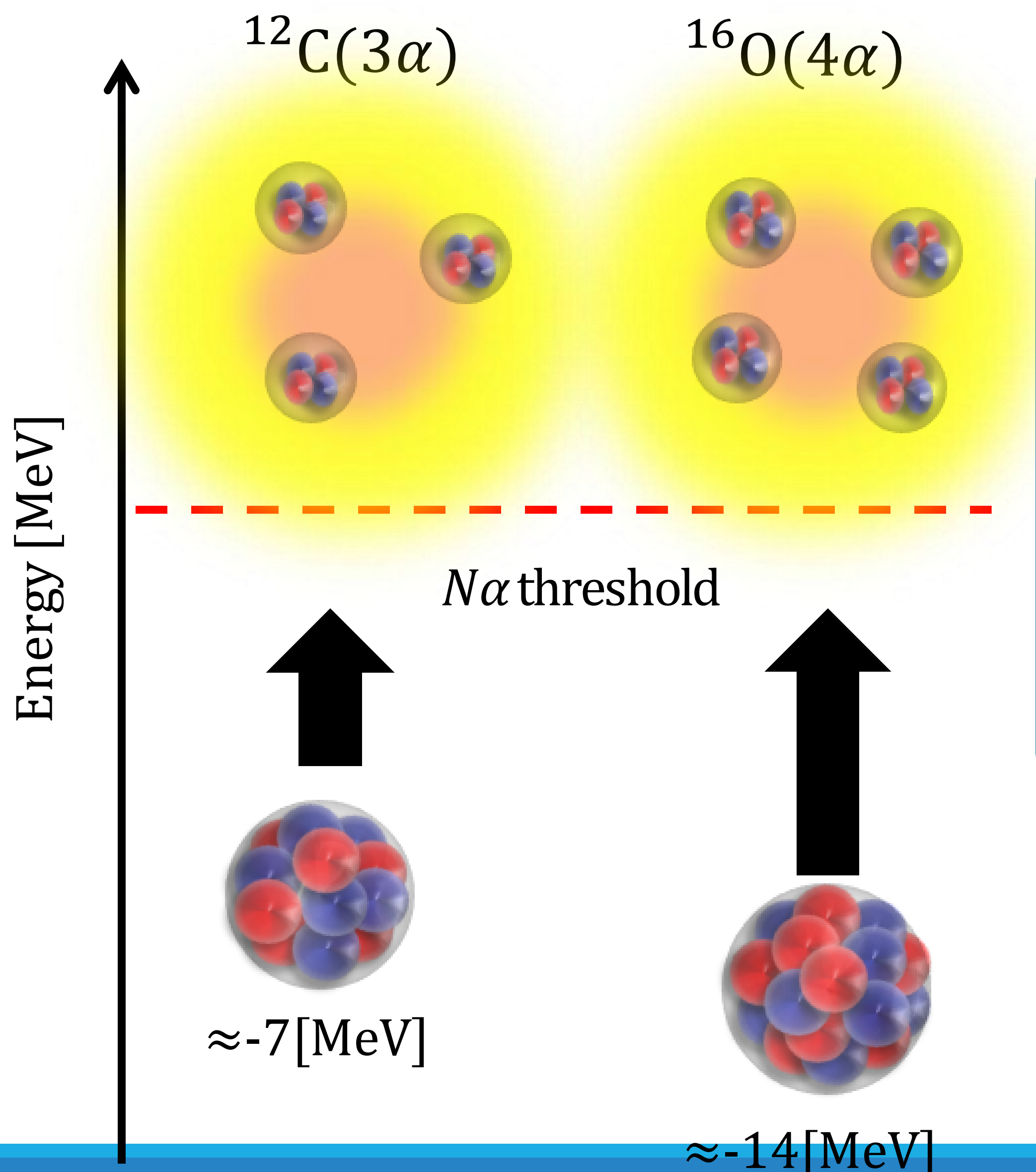
$$B(E1;0_1^+ \to 1_n^-) = \sum_{\mu} |\langle \Psi_n^{1^-\mu} | \mathcal{M}_\mu(E1) | \Psi_1^{0^+0} \rangle|^2$$





Application to the Hoyle state

Introduction Cluster structure and α gas-like states



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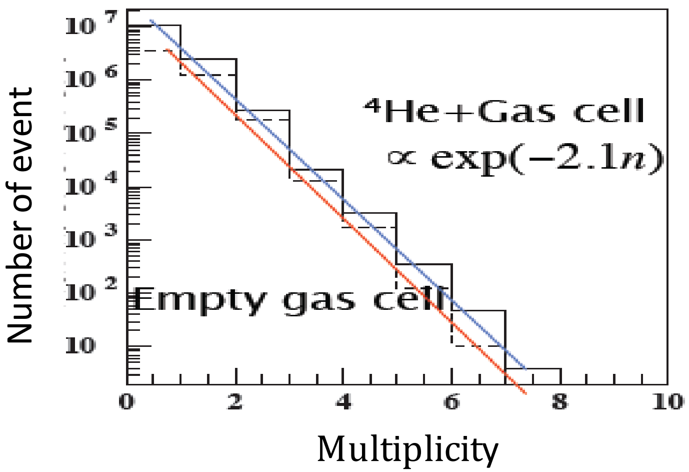
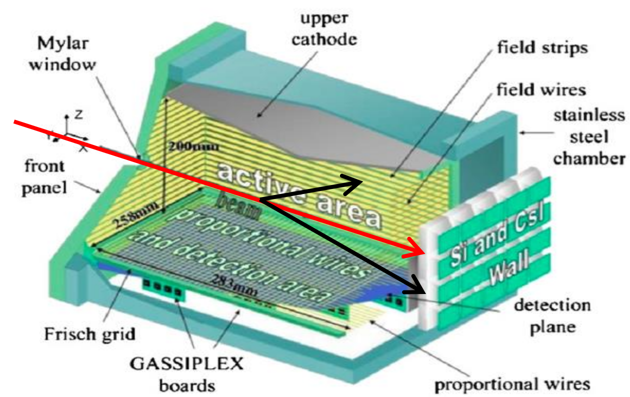
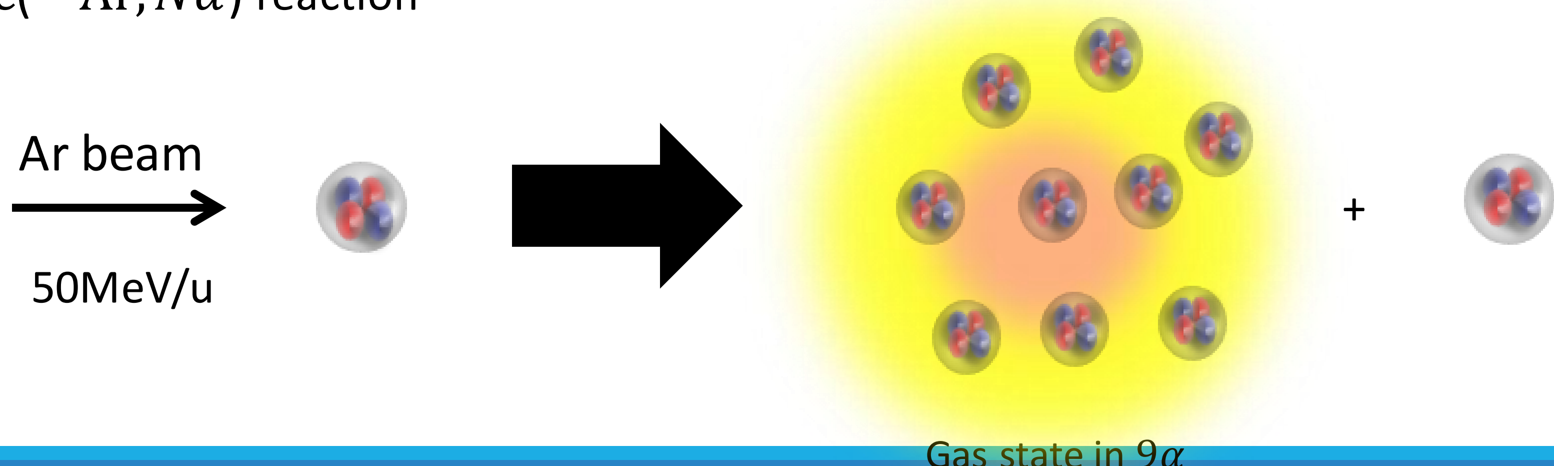
H.Akimune et.al JPCS **436, 012010** (2013).





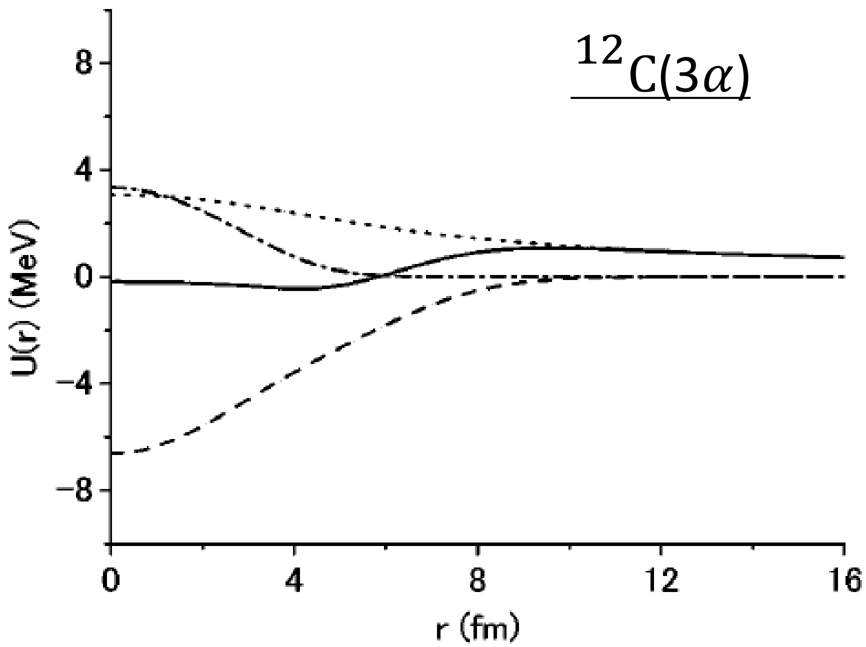
$^{4}\mathrm{He}(^{36}\mathrm{Ar}, N\alpha)$ reaction

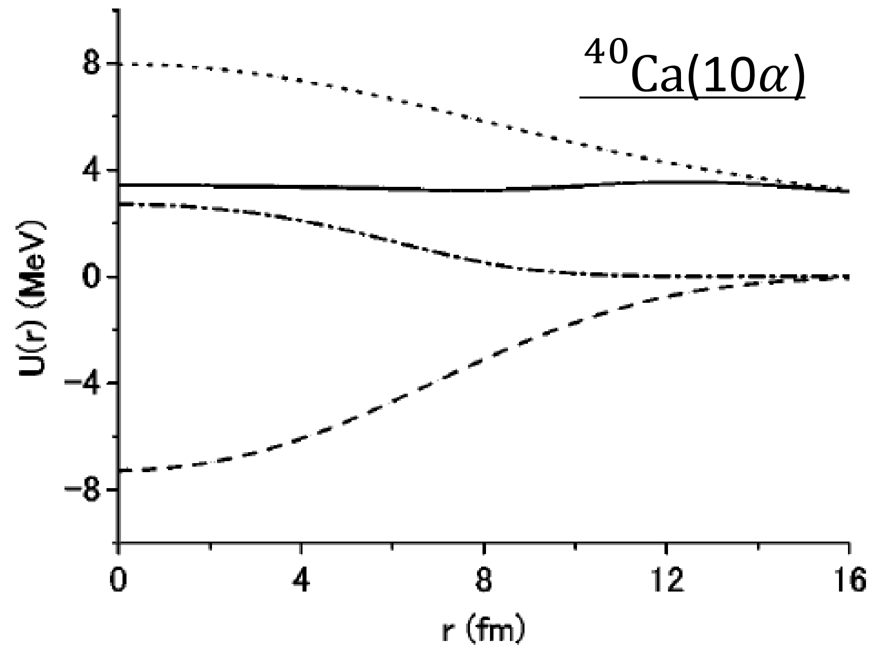


Introduction Theoretical study for many α system

T. Yamada and P. Schuck, PRC **69**, 024309 (2004)

◎ Gas-like state possibility exist up to ～10α sysytem .





◎ Boson approximation is applied (Gross-Pitaevskii equation)

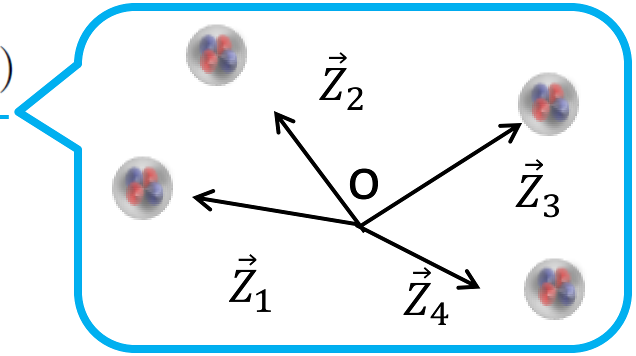
The prediction should be verified by the microscopic cluster model without Boson approximation.

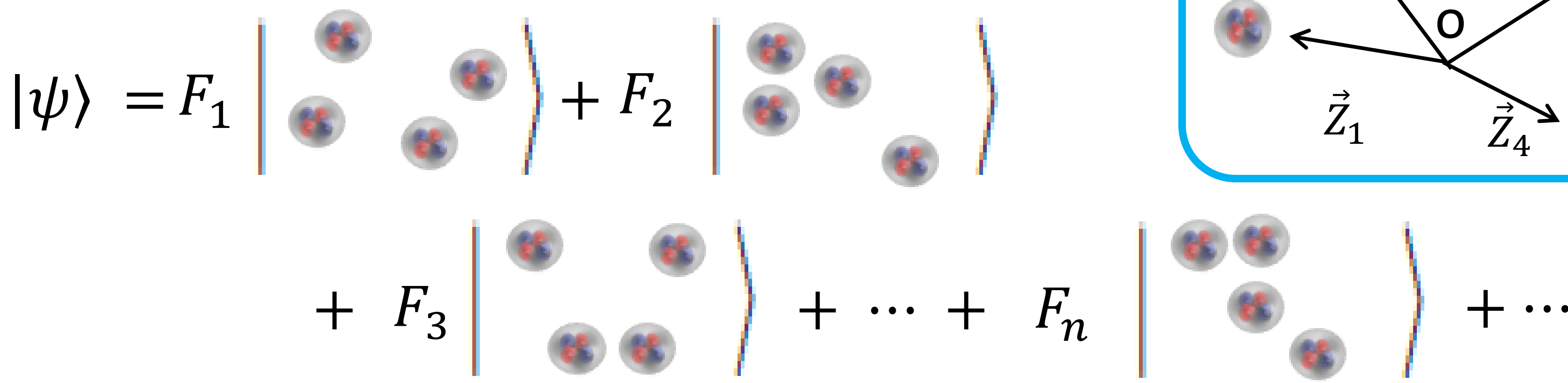
⇒ We need microscopic model that can describe gas-like states of many α particles

Introduction microscopic description of gas-like state

Gas-like state is described by the superposition of “many” Slater determinants

$$\psi(\vec{r}_1,\cdots,\vec{r}_{16}) = \int d\vec{Z}_1\cdots d\vec{Z}_4 F(\vec{Z}_1,\cdots,\vec{Z}_4)\phi(\vec{Z}_1,\cdots,\vec{Z}_4)$$





- Number of Slater determinants becomes huge as the number of α increases

  $\Rightarrow$ We need effective way to generate basis wave functions.

Various methods to genarate $N\alpha$ wave functions

- Random generation — T. Ichikawa et.al PRC, **83**.061301 (2011)
- Imaginary time evolution — Y. Fukuoka et.al PRC, **88**.014321 (2013)
- Real time evolution

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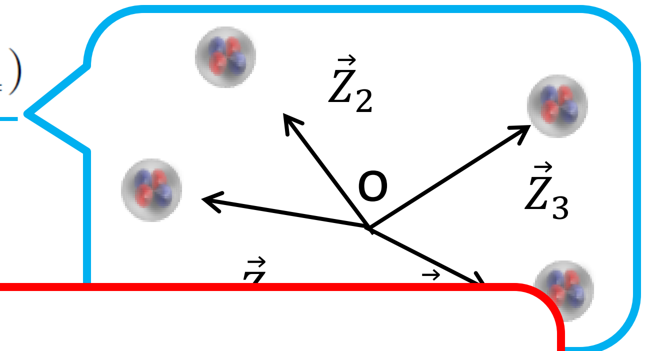

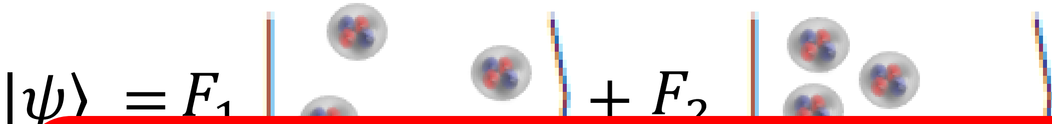

- In this talk, we introduce a method based on the real time evolution
- The new method is applied to 3α, 4α systems

- Number of Slater determinants becomes huge as the number of α increases

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Various methods to genarate $N\alpha$ wave functions

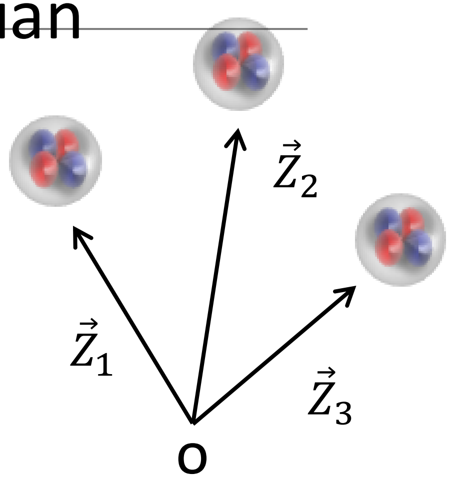
- Random generation — T. Ichikawa et.al PRC, **83**.061301 (2011)
- Imaginary time evolution — Y. Fukuoka et.al PRC, **88**.014321 (2013)
- Real time evolution $\Leftarrow$ Our method

Framework Wave function and Hamiltonian

Hamiltonian

$$H = \sum_i T_i - t_{c.m} + \sum_{i<j} V_{ij} + \sum_{\text{proton}} V_c$$

Volkov No. 2 Y.Funaki PRC.**92** 021302(2015)



Basis wave function (Brink-wave function)

$$\phi(\vec{Z}_1, \cdots, \vec{Z}_N) = \mathcal{A}\left\{\phi_\alpha(\vec{Z}_1)\phi_\alpha(\vec{Z}_2)\cdots\phi_\alpha(\vec{Z}_N)\right\}$$

$\phi_\alpha(\vec{Z}_i)$; α particle wave function (wave packet) located at $\vec{Z}_i$

Equation of motion for wave packet

$$\delta \frac{\langle \phi \mid i\frac{\partial}{\partial t} - H \mid \phi \rangle}{\langle \phi \mid \phi \rangle} = 0 \quad \Rightarrow \quad i\hbar \sum_{j,\sigma} C_{i\rho j\sigma} \frac{\partial \vec{Z}_{j\sigma}}{\partial t} = \frac{\partial H}{\partial \vec{Z}^*_{i\rho}}$$

Time dependent variational principle

Equation of motion for wave packets

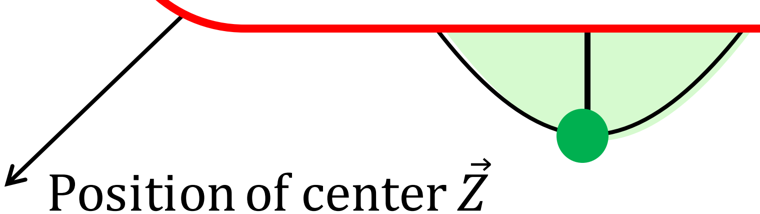
Framework Time evolution of wave packets

$$i\hbar \sum C_{i\rho j\sigma} \frac{\partial \vec{Z}_{j\sigma}}{\partial t} = \frac{\partial H}{\partial \vec{Z}^*}$$

◎Many body wave function represented by wave packet is ⋯

- ○ Ergodic nature. J. Schnack , H. Feldmeier NPA, **601**. (1996)
- ○ Obeying quantum statics. A. Ono , H. Horiuchi PRC.**53**. (1996)

➢ If the system is evolved long enough,
all of important configurations of α particles appear automatically .
⇒ Basis wave functions to describe gas-like state are automatically generated !



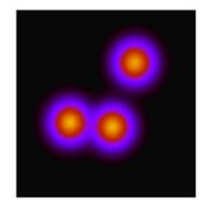
Framework New generator coordinate method

- The time evolution generates all important configurations

Superposition of the wave functions obtained by the time evolution should give a good description for the gas-like state

In other words, we perform GCM calculation using the real time t as the generator coordinate

Step1: Time evolution to generate basis wave function



$$i\hbar\sum_{j,\sigma}C_{i\rho j\sigma}\frac{\partial \vec{Z}_{j\sigma}}{\partial t}=\frac{\partial H}{\partial \vec{Z}^*_{i\rho}}$$

Step2: Superpose basis wave function and solve GCM equation

$$\psi(\vec{r}_1,\vec{r}_2,\cdots,\vec{r}_{4N})=\int_0^\infty dt\,\underbrace{F^{J\pi}_{MK}(t)}_{\text{Determined by diagonalization of Hamiltonian}}P^{J\pi}_{MK}\phi(\vec{Z}_1(t),\vec{Z}_2(t),\cdots,\vec{Z}_N(t))$$

$P^{J\pi}_{MK}$; Projection operator of parity and angler momentum

Results & Discussions for 3α and 4α systems

Result for 3α system (^{12}C)

M.Kamimura NPA.**351**, 456 (1981)
Y.Funaki PRC.**92** 021302(2015)

$E_x - E_{3\alpha}$[MeV]

	This work		THSR		RGM	
J^π	E_x[MeV]	$\sqrt{\langle r^2 \rangle}$[fm]	E_x[MeV]	$\sqrt{\langle r^2 \rangle}$ [fm]	E_x[MeV]	$\sqrt{\langle r^2 \rangle}$ [fm]
0_1^+	-7.63	2.39	-7.48	2.4	-7.56	2.40
2_1^+	-5.10	2.36	-4.82	2.4	-4.66	2.38
0_2^+	0.27	3.64	0.23	3.7	0.34	3.47
3_1^-	0.42	2.77			0.58	2.76

The real time method works well.
It's comparable with THSR and better than the ordinary GCM

This work THSR RGM Exp.

Discussion Check of the convergence of calc.

Our method is based on the ergodic nature

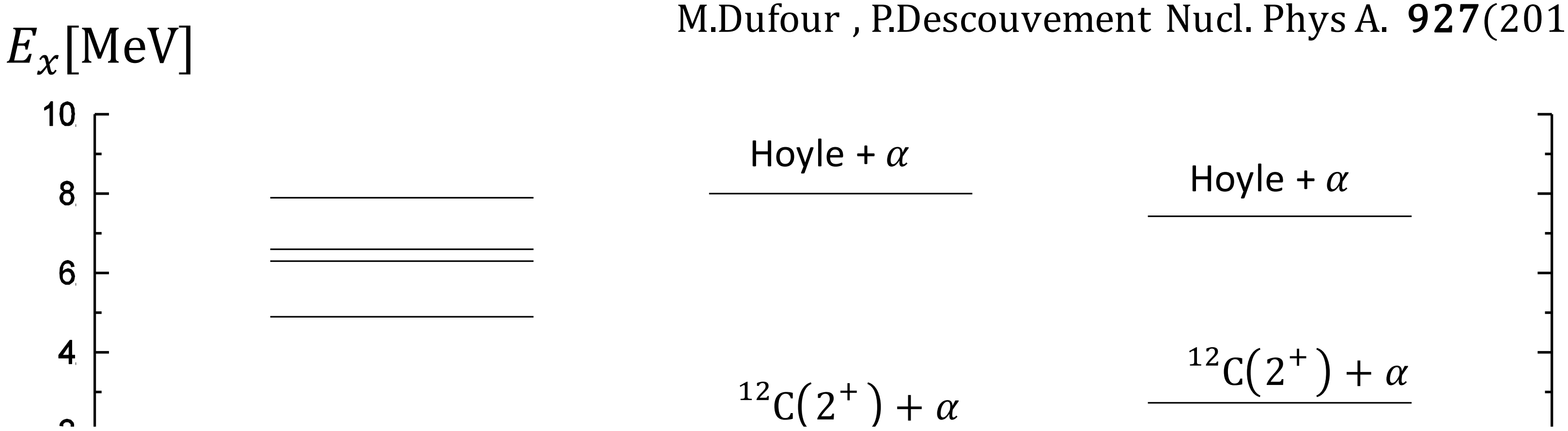
 ⇒ Following two pointes should be checked

1. When the time evolution is long enough,
   the result should be converged.

2. The result should be independent of
   the initial configuration of α particles at $t = 0$.

Result for 4α system (^{16}O)

M.Dufour , P.Descouvement Nucl. Phys A. **927**(2014). 134-146.



	E_x[MeV]		$\sqrt{\langle r^2 \rangle}$[fm]		$M(E0)$[fm^2]	
J^π	This work	M.Dufour et al	This work	Exp.	This work	Exp.
0_1^+	-17.0	-15.2	2.32	2.71±0.02		
0_2^+	-1.6	-1.1	2.83		5.89	3.55±0.21
0_3^+	2.73	2.1	3.03		3.48	
0_4^+	7.43	8.0	3.40		0.39	

Summary

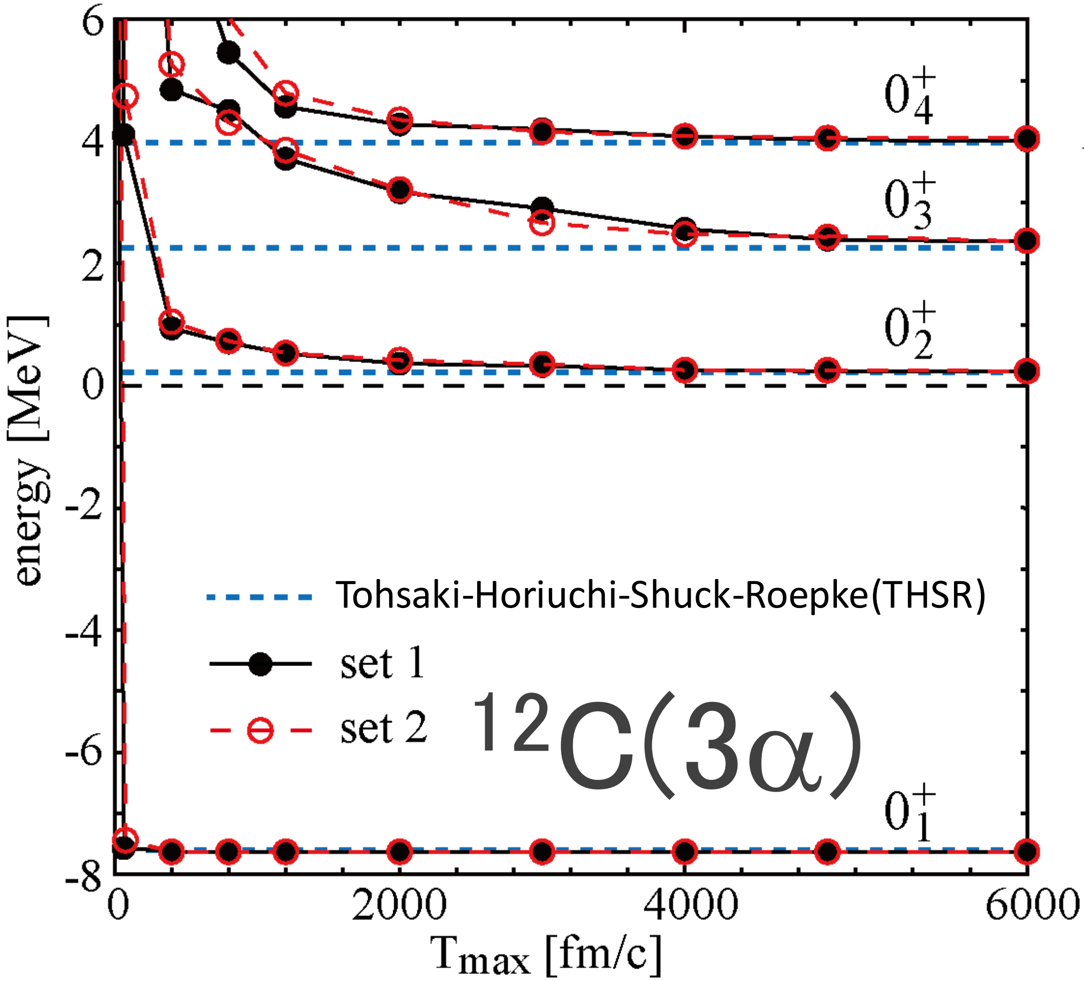
- For $^{8}\mathrm{Be}(2\alpha)$, $^{12}\mathrm{C}(3\alpha)$, $^{16}\mathrm{O}(4\alpha)$, gas state is well known but those of $^{20}\mathrm{Ne}(5\alpha)$, $^{24}\mathrm{Mg}(6\alpha)\cdots$ are not known.
- To solve the difficulty for generating wave function increasing number of α particles, we introduced real time evolution setting time t as a generator coordinate.
- For $^{12}\mathrm{C}(3\alpha)$, $^{16}\mathrm{O}(4\alpha)$ nuclei, this method yielded the results consistent with or better than the previous researches.

Future work

- Separate from continuum state.
- Introduce three-body interaction.

Benchmark calculations for ^{12}C (3α cluster system)

R. Imai, T. Tada and M.K., arXiv:1802.03523



$$\Psi^{J\pi} = \int_0^{T_{max}} dt \;\; f(t)\hat{P}^J_{MK}\Phi(t)$$

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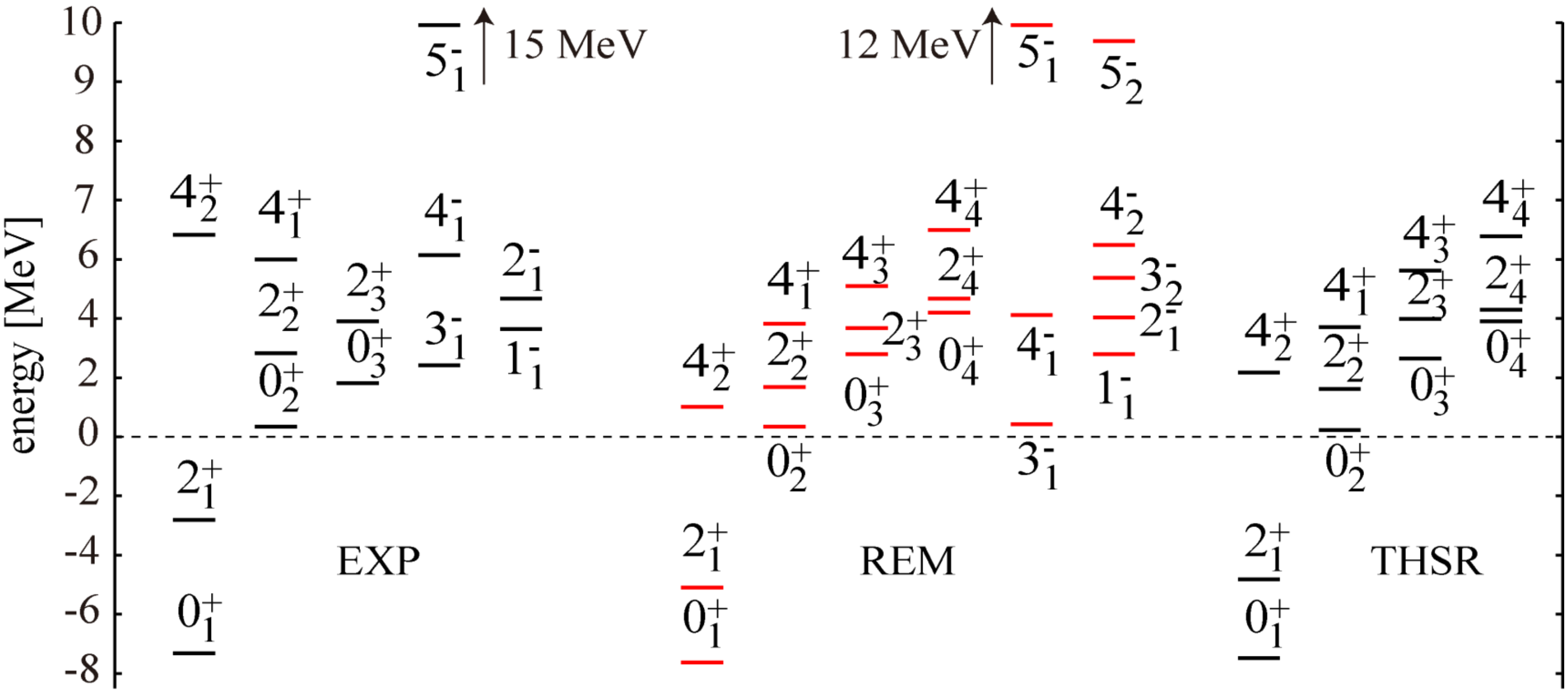

○ All results are consistent with or better than THSR wave function

○ Computational cost is greatly reduced

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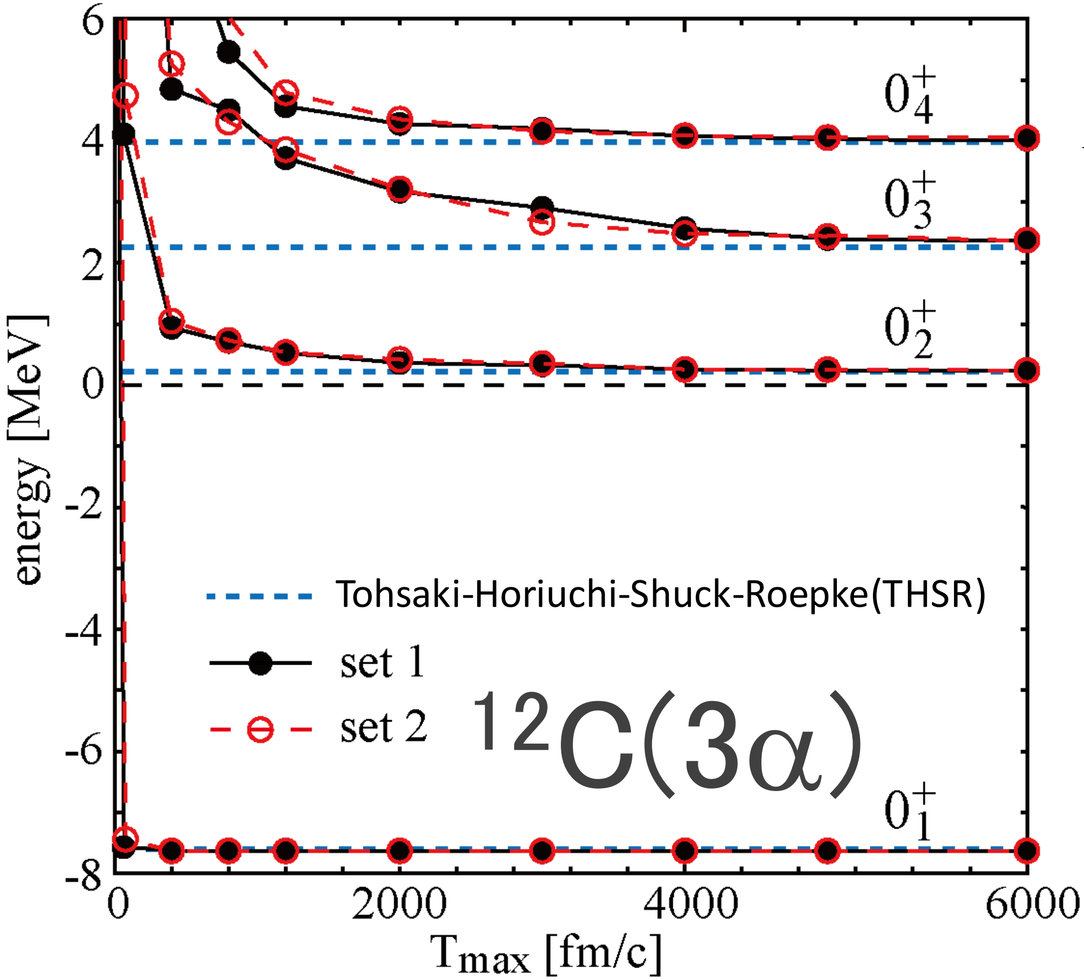

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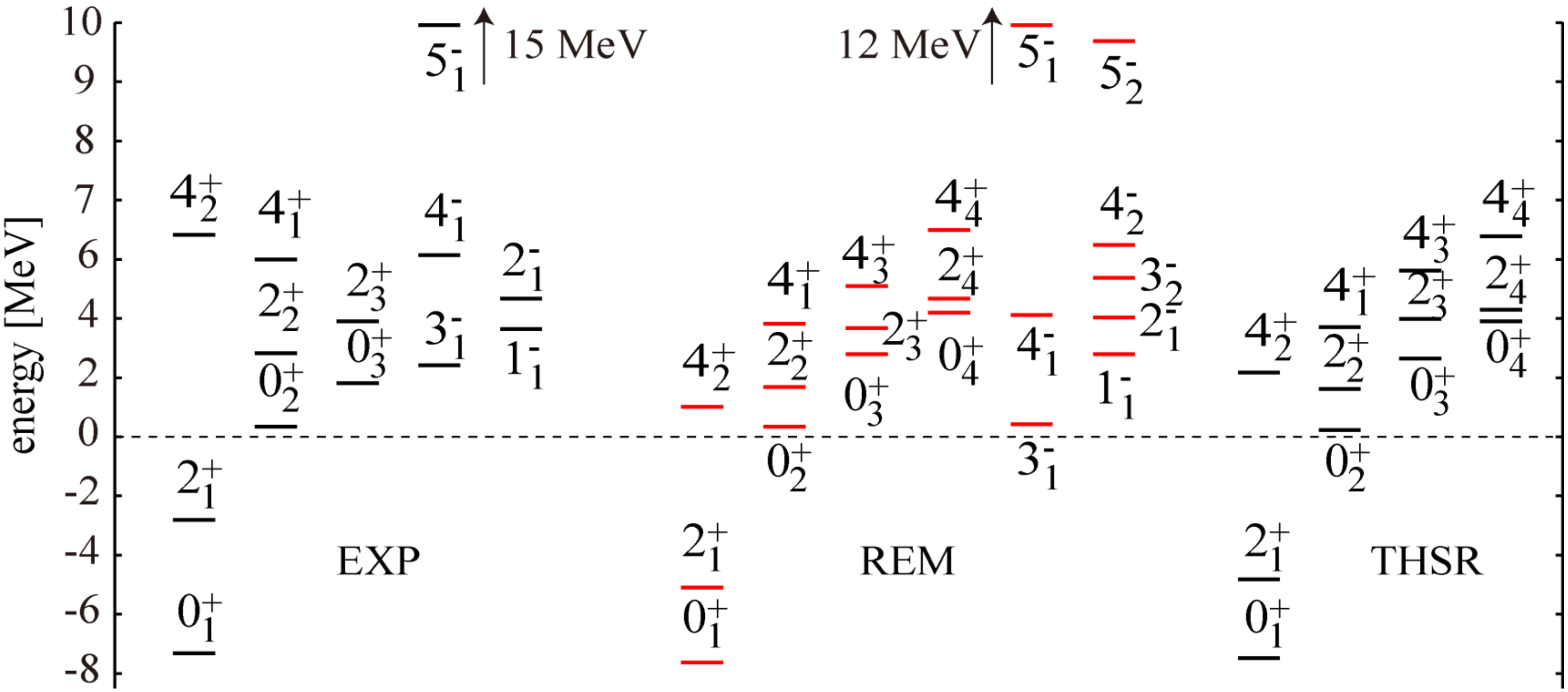

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Collaborators

◎ It is noted that this work was initially motivated by Prof. Yabana

○ Structure and Response of light nuclei
Y. Taniguchi(Kagawa), W. Horiuchi(Hokkaido)

○ Extension to DFT
J. A. Maruhn(Frankfurt)

○ Exotic clusters in neutron-rich nuclei
Zhou Bo (Hokkaido), T. Baba(Kitami), H. Masui(Kitami)

○ Clusters & Astrophysics
K. Ogata(RCNP), Y. Kanada-En'yo(Kyoto), Y. Taniguchi(Kagawa)
Y. Chiba(Osaka-city), K. Yoshida(JAEA)