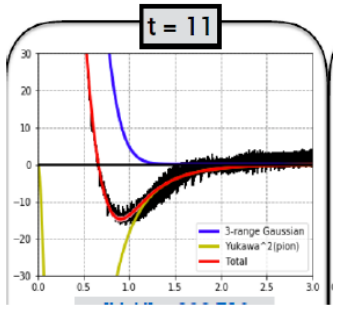
Gaussian Expansion method and future perspective

Emiko Hiyama (Tohoku Univ./RIKEN/Paris-Saclay Univ.)

Computational science is essential to develop many fields of physics.

- elementary particle physics, nuclear physics

  Schroedinger equation, Einstein equation, Lattice QCD
  Many-body quantum physics, Heavy ion collisions, …



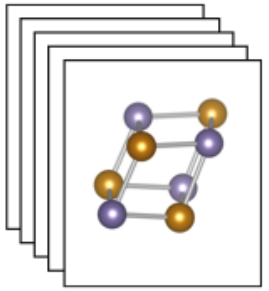
Lattice
QCD simulation

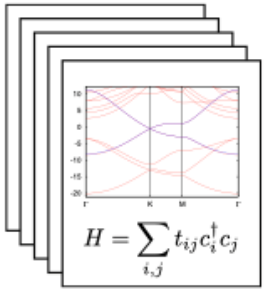
- condensed matter physics, atomic physics

  Electron dynamics, 1st principle calculation, Molecular dynamics,
  Phase transition, Symmetry and topology, …

- materials science, functional materials

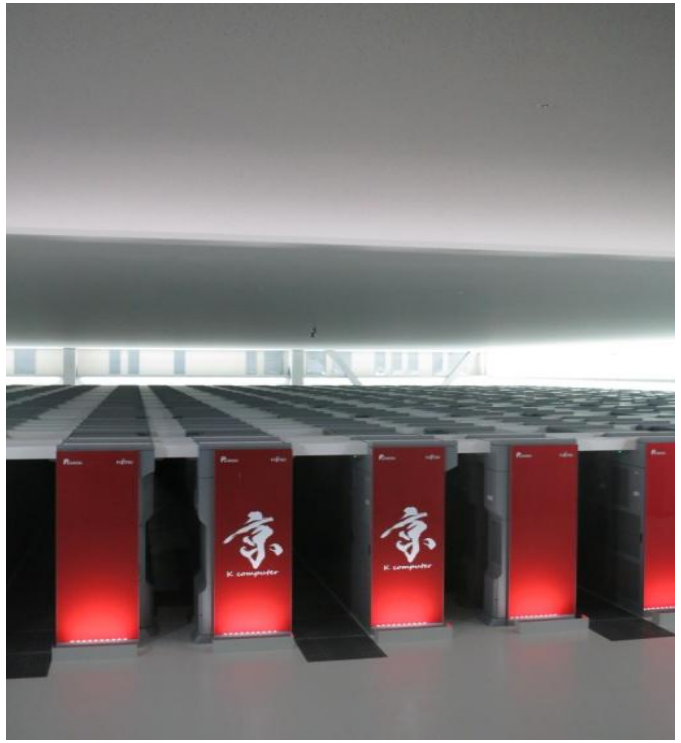
  Many-body quantum physics, Nano-technology,
  Spintronics,





To perform experiment, its cost is expensive. Thus, before the experiment,
a reliable theoretical prediction with high accuracy is very important.

Fast development of Super computer systems in Japan



‘Kei’(2009-2019)

‘Fugaku’(2020-)

Now, AI and quantum computers are getting into the research tools …
=> become important for predicting new phenomena and materials.

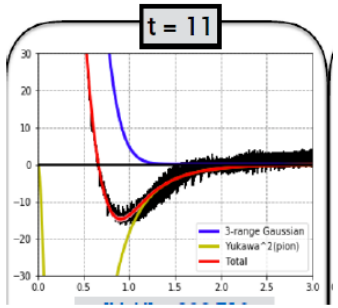
In this way, numerical simulation is getting significant year by year.

Computational science is essential to develop many fields of physics.

My research field

- elementary particle physics, nuclear physics

  Schroedinger equation, Einstein equation, Lattice QCD
  Many-body quantum physics, Heavy ion collisions, …



Lattice QCD simulation

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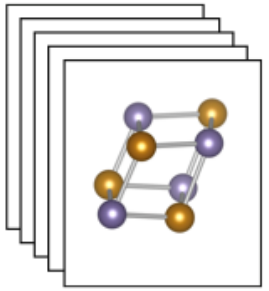
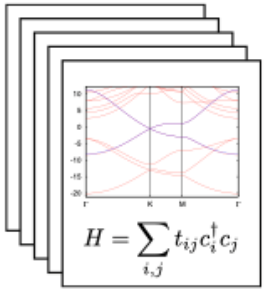
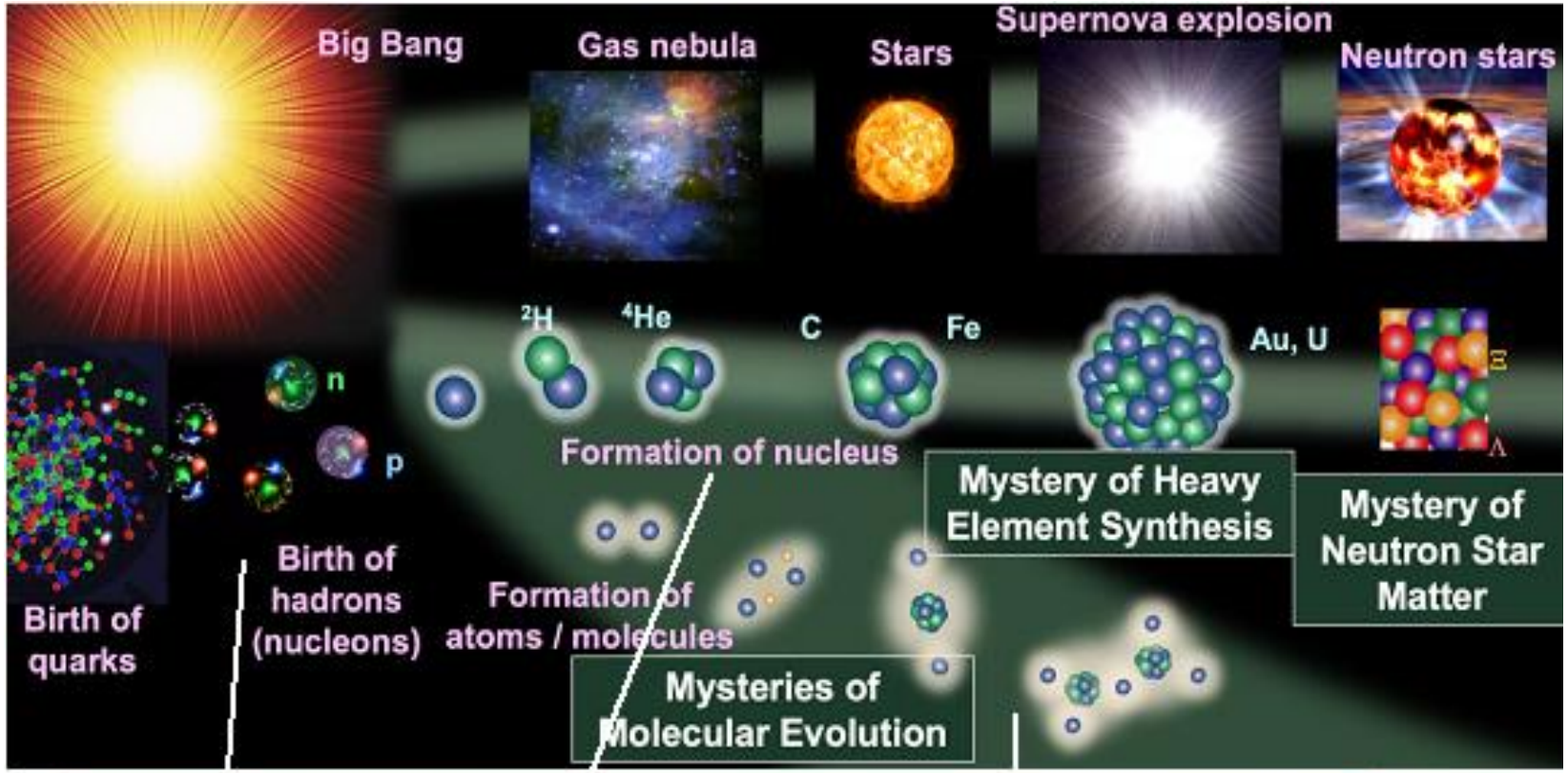
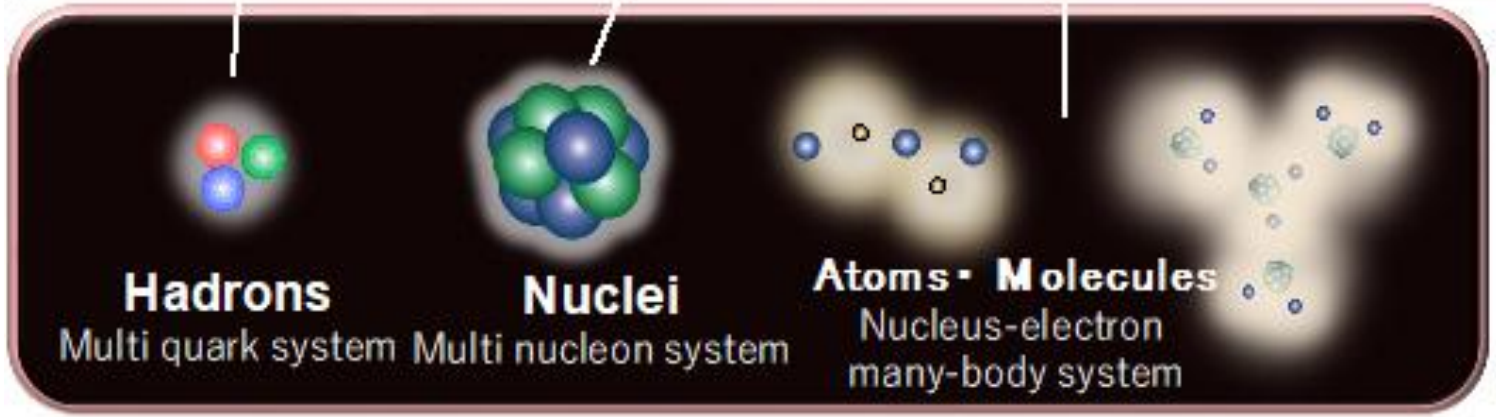




To perform experiment, its cost is expensive. Thus, before the experiment,
a reliable theoretical prediction with high accuracy is very important.

One of the major goal in nuclear physics
: to understand evolution of quantum matter in the universe





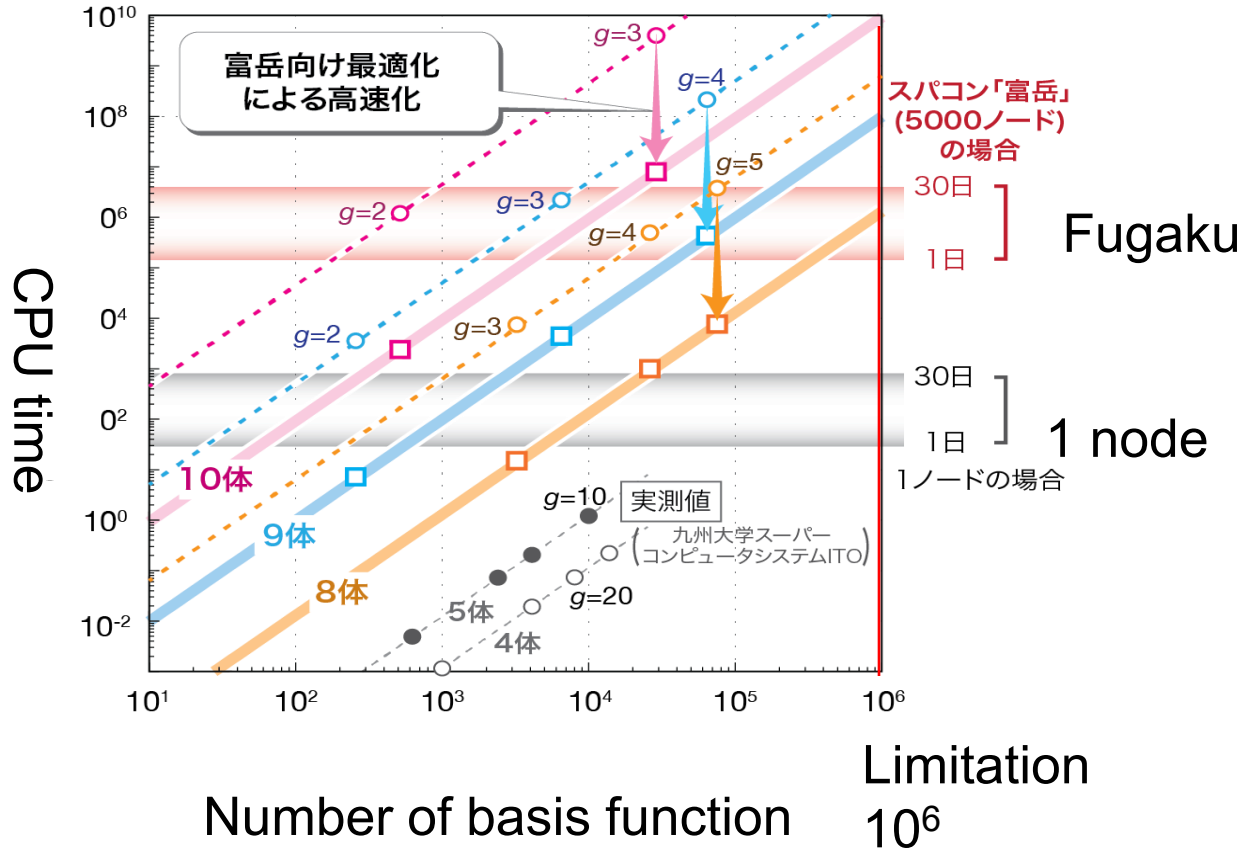
(1) Study of interior of neutron star
(2) Nucleosynthesis

To achieve the goals,
we need to solve many-body Schroediner equation accurately.
Now, in our fields, many people are developing their methods to many-body problem calculation.

One of my research goal:

- To develop my method, Gaussian Expansion Method up to 10-body systems and apply to many research fields.
  - The codes are open for public, so that everyone can use easily for each field.
  - The wavefuctions by GEM should be applied to reaction theory.=>Ogawa san's talk.

Why 10-body system?

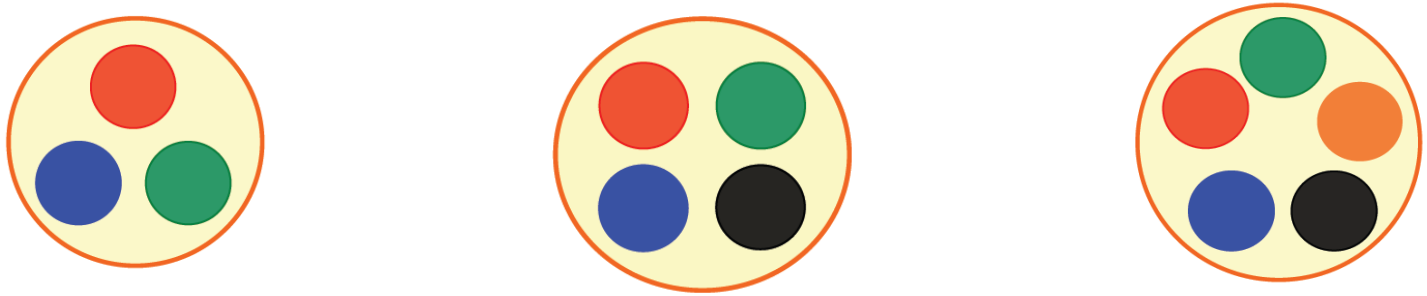


Rather than Memory, limitation of CPU time reaches in the case of 10-body calculation.
Can we calculate more than 10-body problem accurately?
This is our goal.

Introduction

- Gaussian Expansion Method
- Application to 4He atomic system (Up to 5-body)
- future plan
  -What is difficulty? How do we overcome it?

Gaussian Expansion Method



Our few-body caluclation method

Gaussian Expansion Method (GEM) , since 1987

- A variational method using Gaussian basis functions
- Take all the sets of Jacobi coordinates

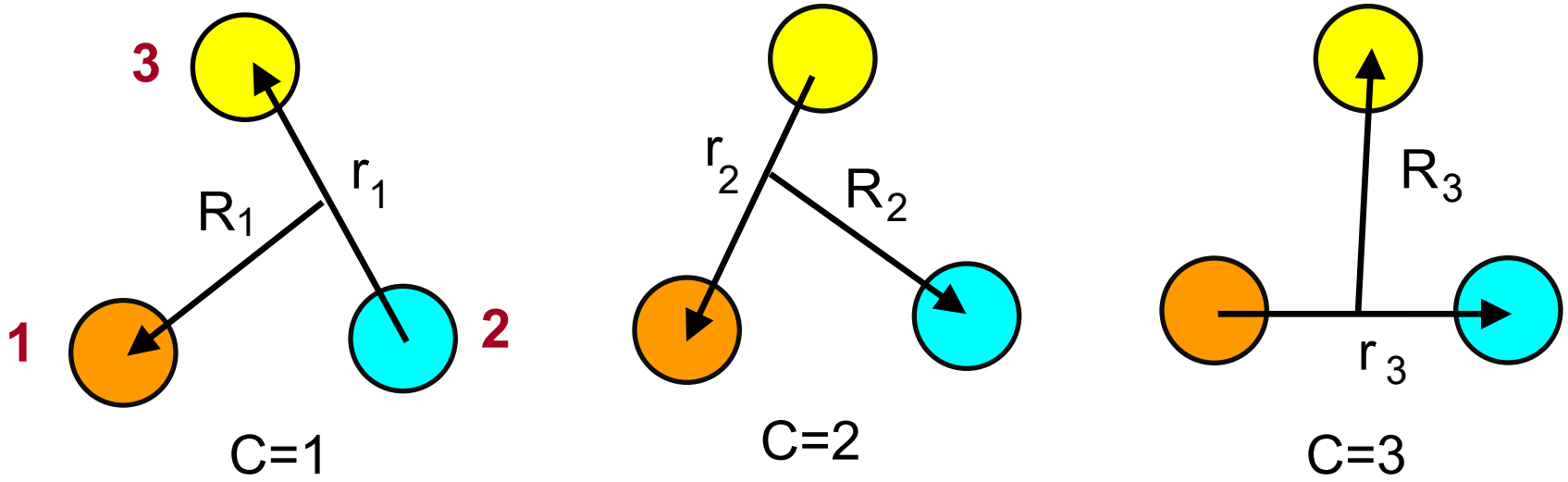
Developed by Kyushu Univ. Group,
Kamimura and his collaborators.

Review article :
E. Hiyama, M. Kamimura and Y. Kino,
Prog. Part. Nucl. Phys. 51 (2003), 223.

High-precision calculations of various 3- and 4-body systems:

Exotic atoms / molecules , Light hypernuclei,
3- and 4-nucleon systems, 3-quark systems,
multi-cluster structure of light nuclei,

I shall explain this method briefly.

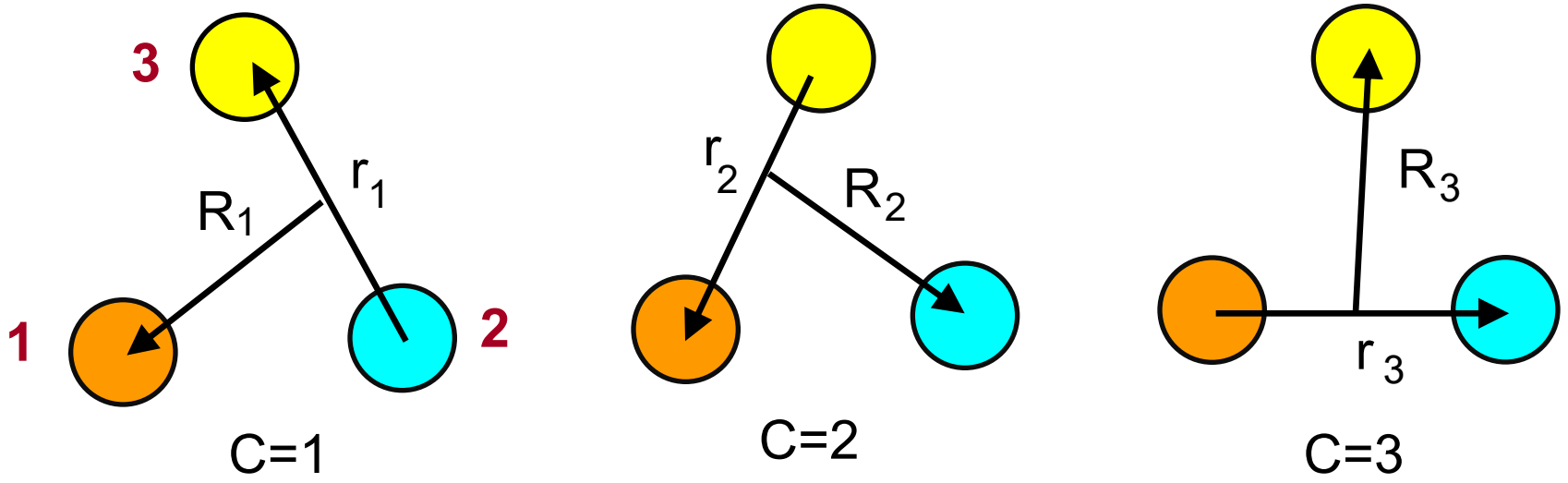


$$(H - E)\Psi_{JM} = 0$$

$$H = T + V_1(r_1) + V_2(r_2) + V_3(r_3)$$

$$T = -\frac{\hbar^2}{2\mu_{r_c}}\nabla^2_{\mathrm{r_c}} - \frac{\hbar^2}{2\mu_{R_c}}\nabla^2_{\mathrm{R_c}} \qquad (c = 1, 2, \text{ or } 3)$$

$$\Psi_{JM} = \Phi^{(1)}_{JM}(\mathrm{r}_1, \mathrm{R}_1) + \Phi^{(2)}_{JM}(\mathrm{r}_2, \mathrm{R}_2) + \Phi^{(3)}_{JM}(\mathrm{r}_3, \mathrm{R}_3)$$



$$\Psi_{JM} = \Phi^{(1)}_{JM}(\mathrm{r}_1, \mathrm{R}_1) + \Phi^{(2)}_{JM}(\mathrm{r}_2, \mathrm{R}_2) + \Phi^{(3)}_{JM}(\mathrm{r}_3, \mathrm{R}_3)$$

Basis functions of each Jacobi coordinate

$$\phi^{(c)}_{nl}(r_c)\, Y_{lm}(\hat{\mathrm{r}}_c), \quad \psi^{(c)}_{NL}(R_c)\, Y_{LM}(\widehat{\mathrm{R}}_c), \quad (c = 1, 2, 3)$$

(θ, ϕ) (Θ, Φ)

$$\Phi^{(c)}_{JM}(\mathrm{r}_c, \mathrm{R}_c) = \sum_{nl,NL} A^{(c)}_{nl,NL}\, \phi^{(c)}_{nl}(r_c)\, \psi^{(c)}_{NL}(R_c) \left[Y_l(\hat{\mathrm{r}}_c) \otimes Y_L(\widehat{\mathrm{R}}_c) \right]_{JM}$$

in the next slide

Determined by diagonalizing H

An important issue of the variational method is how to select a good set of basis functions.

What is good set of basis functions?

Using them,

(1) we can describe well the properties of wave function:

a) short-ranged correlation,
b) long-range tail behaviour,
c) highly oscillatory character

(2) we can easily calculate the matrix elements of Hamiltonian

$$H_{in} = \langle \Phi_i | H | \Phi_n \rangle, \quad N_{in} = \langle \Phi_i | 1 | \Phi_n \rangle$$

For this purpose, we have been using the following basis function:

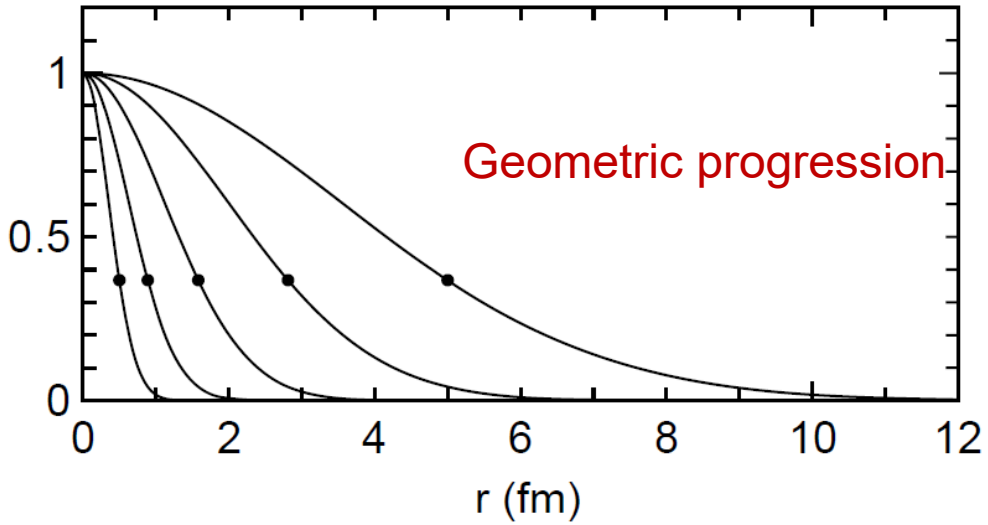
$$\phi_{nlm}(\mathbf{r}) = r^l e^{-\nu_n r^2} Y_{lm}(\hat{\mathrm{r}})$$

$$\nu_n = \frac{1}{r_n^2}$$

$$r_n = r_1 a^{n-1} \qquad (n = 1, \ldots, n_{\max})$$

Geometric progression 等比數列

The Gaussian basis function is suitable not only for the calculation of the matrix elements but also for describing short-range correlations and long-range tail behaviour.



Benchmark-test calculation of the 4-nucleon bound state

Our GEM provides accurate results together with other few-body methods.

Good agreement among 7different methods

In the binding energy, r.m.s. radius and wavefunction density

TABLE I. The expectation values $\langle T \rangle$ and $\langle V \rangle$ of kinetic and potential energies, the binding energies E_b in MeV, and the radius in fm.

Method	$\langle T \rangle$	$\langle V \rangle$	E_b	$\sqrt{\langle r^2 \rangle}$
FY	102.39(5)	−128.33(10)	−25.94(5)	1.485(3)
GEM	102.30	−128.20	−25.90	1.482
SVM	102.35	−128.27	−25.92	1.486
HH	102.44	−128.34	−25.90(1)	1.483
GFMC	102.3(1.0)	−128.25(1.0)	−25.93(2)	1.490(5)
NCSM	103.35	−129.45	−25.80(20)	1.485
EIHH	100.8(9)	−126.7(9)	−25.944(10)	1.486

ours

very different techniques and the complexity of the nuclear force chosen. Except for NCSM and EIHH, the expectation values of T and V also agree within three digits. The NCSM results are, however, still within 1% and EIHH within 1.5% of the others, but note that the EIHH results for T and V are

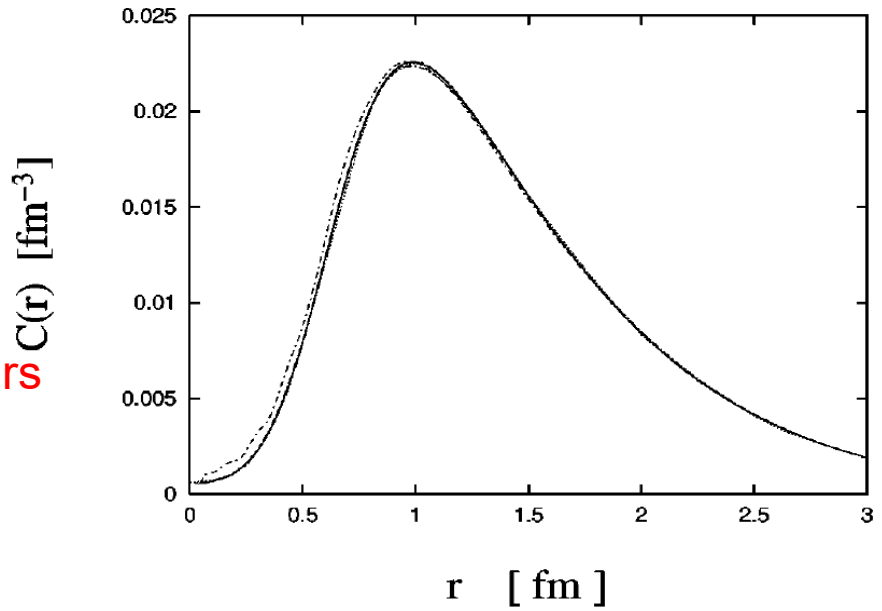


FIG. 1. Correlation functions in the different calculational schemes: EIHH (dashed-dotted curves), FY, CRCGV, SVM, HH, and NCSM (overlapping curves).

・Gaussian Expansion Method

・Application to 4He atomic system (Up to 5-body)

・future plan
-What is difficulty? How do we overcome it?

Why atomic system?

One of my research goal:

- To develop my method, Gaussian Expansion Method up to 10-body systems and apply to many research fields.

・The codes are open for public, so that everyone can use easily for each field.

・The wavefuctions by GEM should be applied to reaction theory.=>Ogawa san's talk.

Why 10-body system?

Application of 10-body problem to atomic, molecular, nuclear and quark systems.

For instance, if I apply the method to nuclear physics, ・・・

$$\Psi_{JM} = (\text{Isospin}) \times (\text{spin}) \times (\text{spatial})$$

For multi-quark systems,

$$\Psi_{JM} = (\text{color}) \times (\text{Isospin}) \times (\text{spin}) \times (\text{spatial})$$

Number of configuration is increasing and it might be difficult to calculate for 10-body systems.

Therefore, I start to make this project for atomic physics.

$$\Psi_{JM} = (\text{Spatial})$$

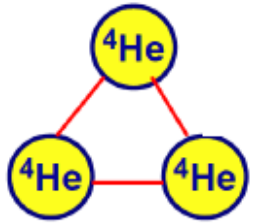
It is NOT interesting to develop the method to 10-body systems only.
We need to explore some new physics.=>4He Bosonic systems

Application to ^{4}He atoms

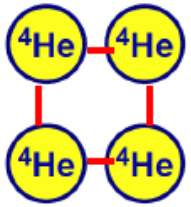
One of the most fundamental theoretical issues from the view point of few-body problems:

to perform accurate calculations of the 3- and 4-body ^{4}He-atom systems using realistic ^{4}He-^{4}He potentials.

This subject has been intensively studied by nuclear physicists, atomic physicists and quantum chemists.

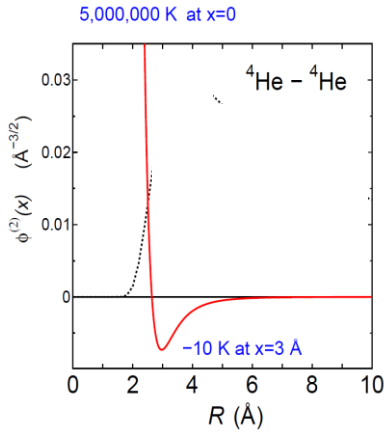


trimer



tetramer

Realistic potential



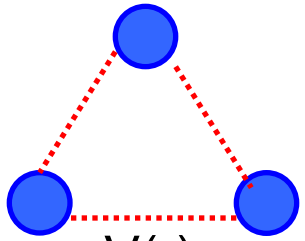
Van del waals potential

In 1970, Efimov predicted the following phenomenon,

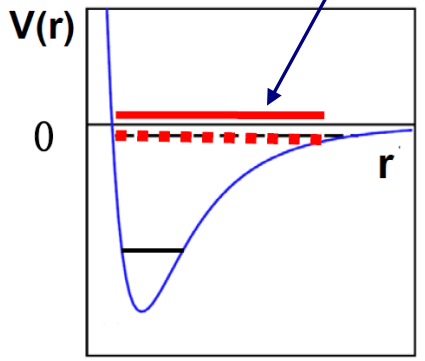
Efimov effect ;

in 3-body systems, if 2-body short-range interactions

support a bound state or resonant state near the threshold,



then,



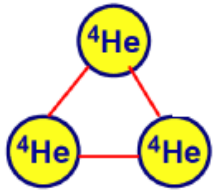
(in other words,
if the s-wave
scattering length
is very large)

1) a large number of 3-body weakly-bound states (Borromean states)
can be formed even when the interaction is too weak to have
a two-body bound state,

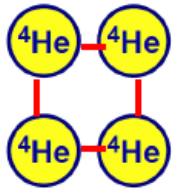
2) all the low-energy properties of 3-body systems
do NOT depend on details of the interactions at short distance:
[this is called "universality"].

4He-atom clusters --- Level structure known before our calculation :

dimer



trimer



tetramer

0.0 mK

4He + 4He

0^+_1

-1.30348 mK

4He + 4He + 4He

dimer + 4He

0^+_2

-2.2706

4He + 4He + 4He + 4He

0.0 mK

Efimov states

0^+_1

-126.40 mK

trimer + 4He

?

There are many 3-body calculations for 4He trimer.

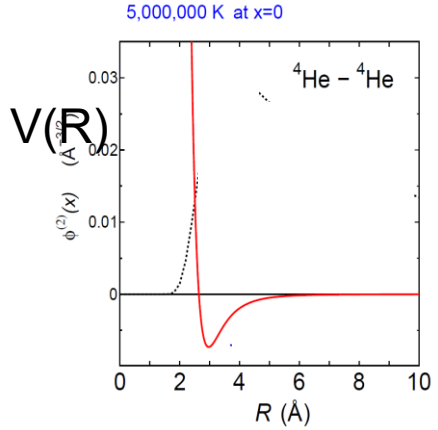
0^+_1

≈ -558 mK

There was no reliable calculation for very weakly bound state near the trimer +4He threshold.

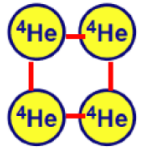
← Numerical difficulty:

The difficulty for the 4-body calculations of the 4He tetramer is



1) the realistic 4He–4He potential has an extremely strong repulsive core.

The core part of the atomic potential is ~1000 times higher than that of the nucleon-nucleon potential.



tetramer

^{4}He + ^{4}He + ^{4}He + ^{4}He

0.0 mK

2) the very weakly-bound excited state should have a very long-range tail, which is also difficult to treat.

trimer + ^{4}He

?

0^+_1 ≈ -558 mK

There are 5 calculations of tetramer using realistic pair potentials (LM2M2, TTY) .

^{4}He tetramer binding energies

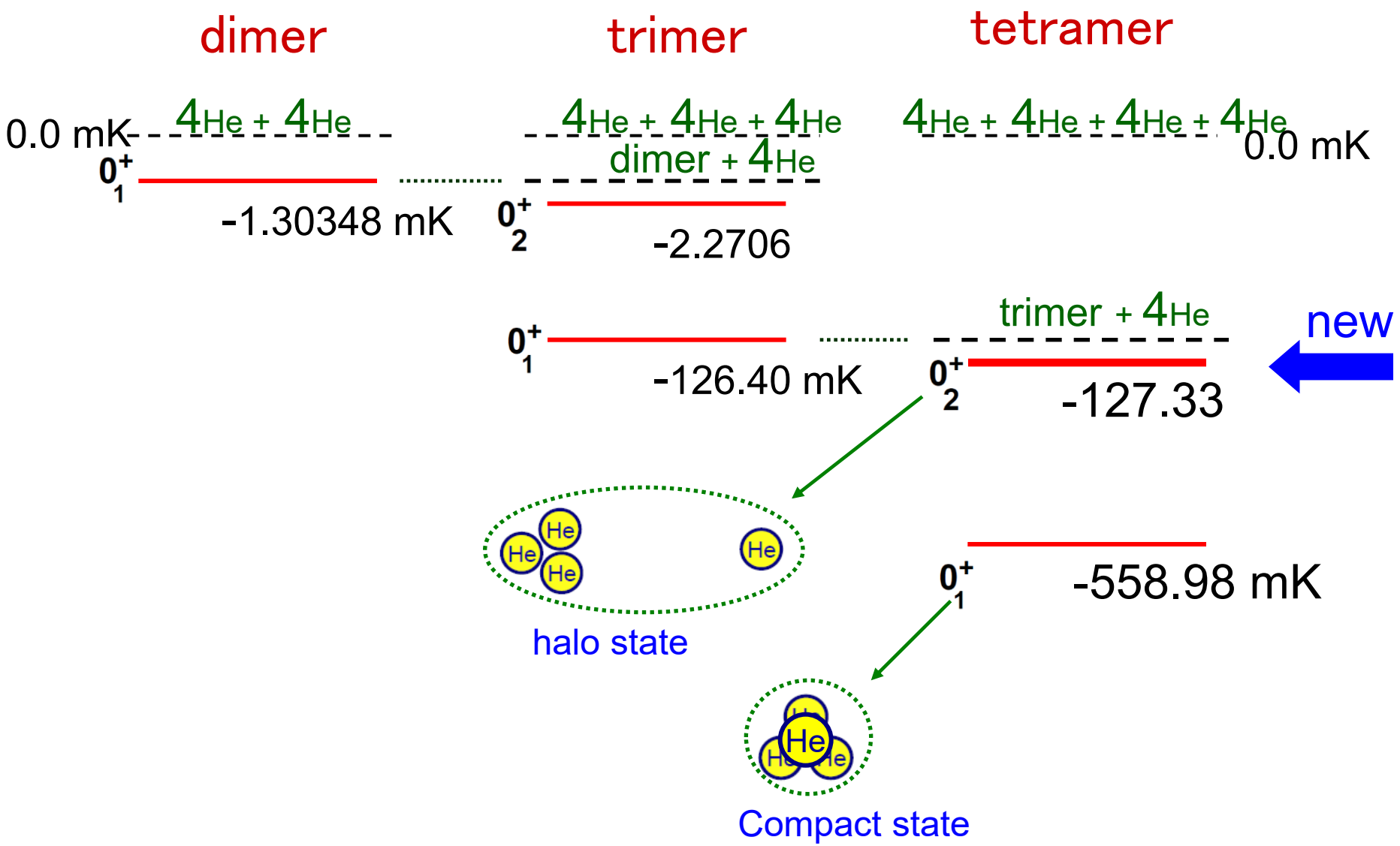
Method	Reference	potential	ground state (mK)	excited state (mK)
Monte Carlo	Lewerenz (1977)	TTY	558	
Monte Carlo	Bressanini *et al.* (2000)	TTY	559.1	
Monte Carlo	Blume and Greene (2000)	LM2M2	557	133
Faddeev	Lazauskas and Carbonell (2006)	LM2M2	557.5	127.5
Correlated potential harmonic expansion	Das *et al.* (2011)	TTY	558	178

cf. Trimer g.s. = 126.40

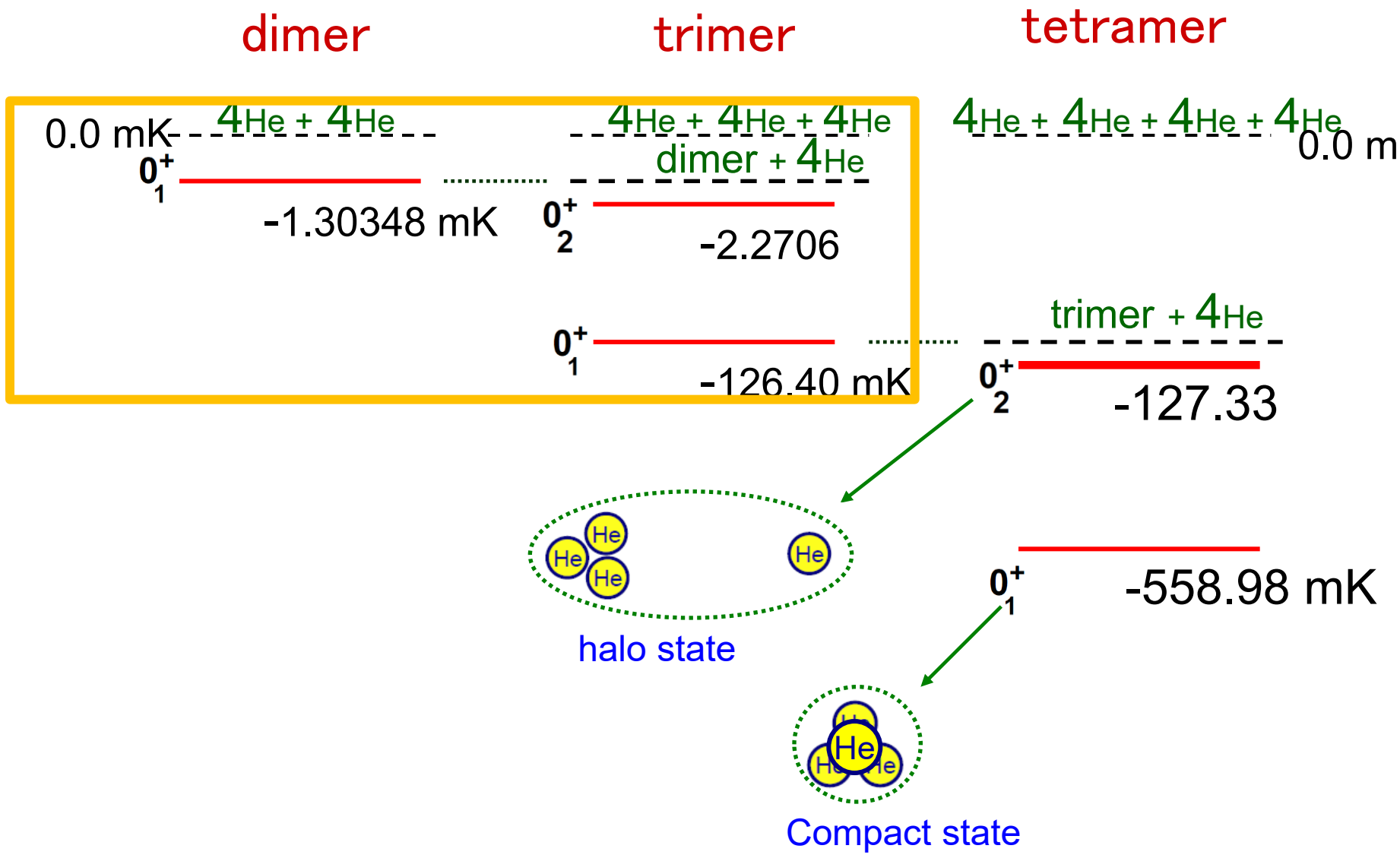
This value was not obtained by bound-state calculation, but was extrapolated from atom-trimer scattering calculation.

So, we intended to confirm this value by our bound-state calculation.

We confirmed this level structure of 4He-atom clusters (2012).

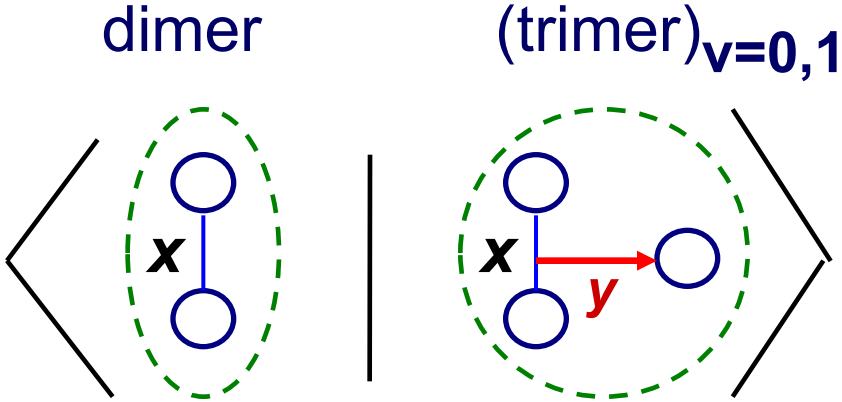


To explore ‘universality’ is one of interesting subject.
especially, we are interested in the first excited states which are nearby threshold.



Overlap function

$$\mathcal{O}_v^{(3)}(\boldsymbol{y}) = \int \phi_{00}^{(2)*}(\mathbf{x}_1)\,\Psi_v^{(3)}\,d\mathbf{x}_1 =$$



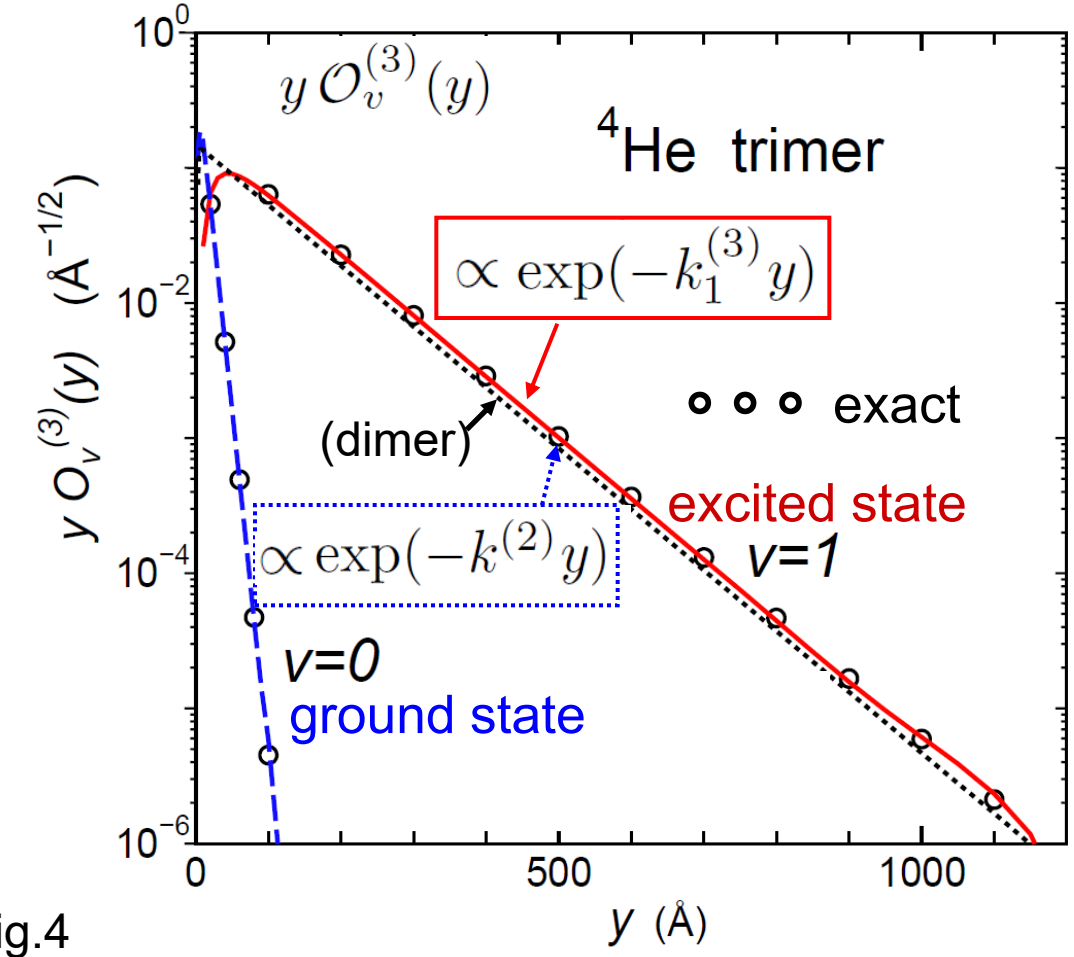


Fig.4

1) Asymptotic behavior of the
trimer excited state
is exactly decaying
up to ~1000 Å.

2) Two lines are parallel.
Decaying constants are
the same to each other.

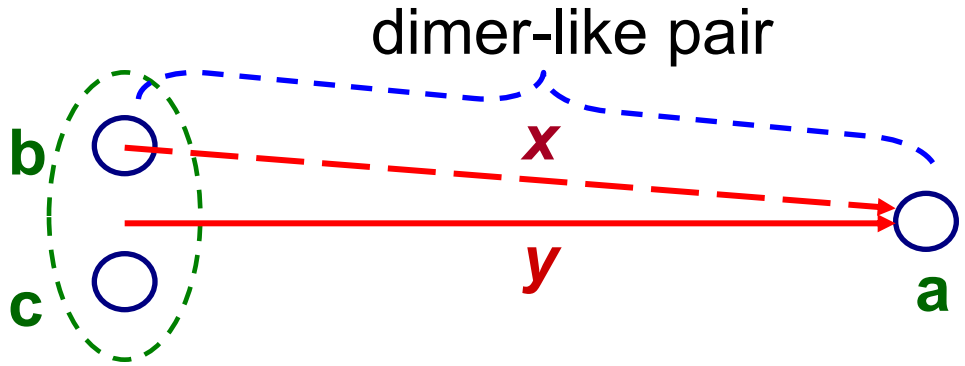
$$k_1^{(3)} = k^{(2)}$$

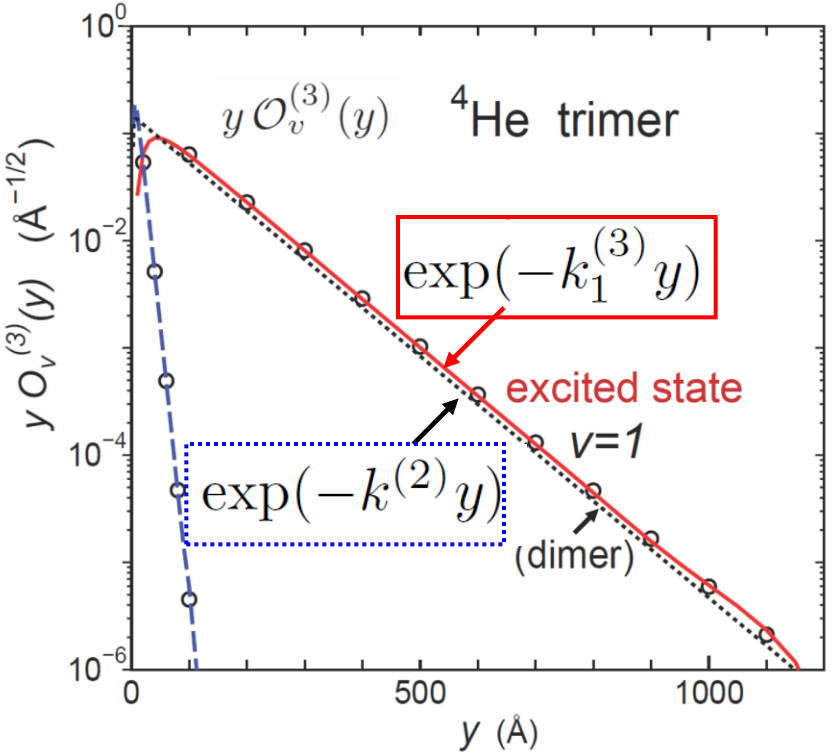
decaying constant

This is unexpected,
but, understandable
from the following model:

Dimer-like pair model

for asymptotic behavior of trimer excired state





1) Particle **a** (located far from loosely-bound **b** and **c**) is not affected by the interaction between **b** and **c**,

2) Therefore, the pair **a**-**b** at a relative distance ***x*** is asymptotically dimer-like.

3) Since $x \approx y$ asymptitically, the amplitude of particle **a** along ***y*** is dimerlike, $k_1^{(3)} = k^{(2)}$

If we accept this model, we can estimate

$\Delta B_1^{(3)} (= B_1^{(3)} - B^{(2)})$ binding energy of trimer excited state measured from dimer.

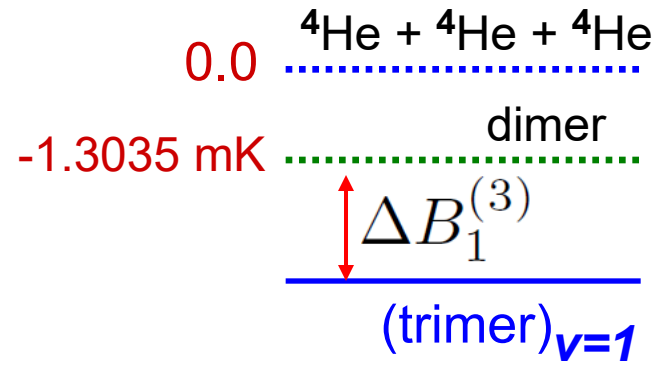
by using $B^{(2)}$ only.

The binding energies are written as

$$B^{(2)} = \frac{\hbar^2}{2\mu_x}(k^{(2)})^2$$

$$\Delta B_1^{(3)} = \frac{\hbar^2}{2\mu_y}(k_1^{(3)})^2$$

where $\mu_x = \frac{1}{2}m$ and $\mu_y = \frac{2}{3}m$,



If we take this relation $k_1^{(3)} = k^{(2)}$, then we have

$$\Delta B_1^{(3)} = \frac{3}{4}B^{(2)} = 0.978\text{mK}$$

$$B_1^{(3)} = 2.281 \text{ mK}.$$

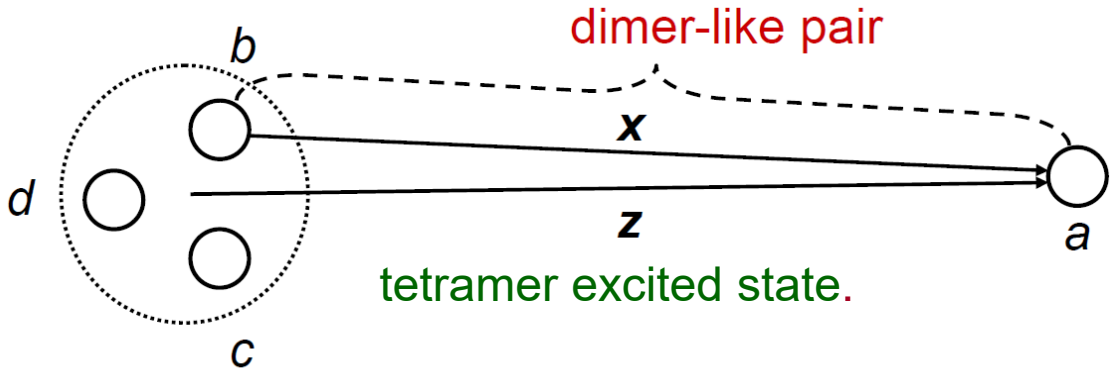
0.967 mK

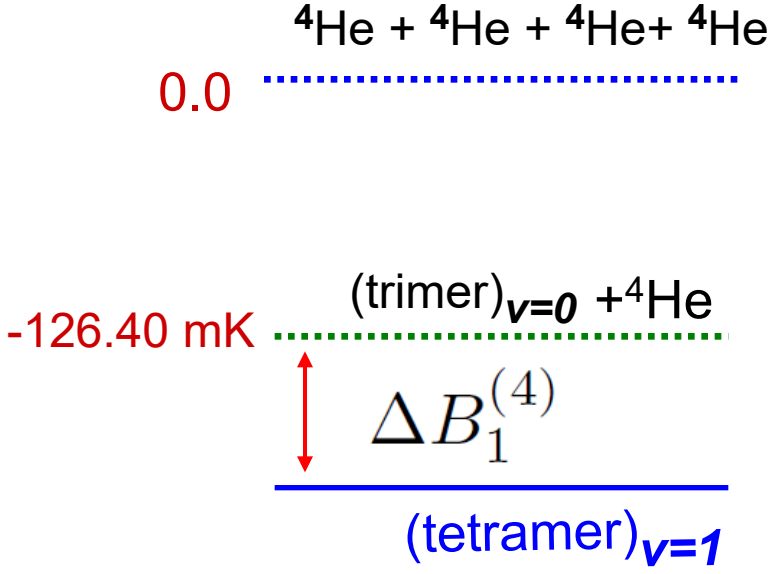
2.2706 mK

Good model !

3-body calculation

Also, if we accept this
dimer-like pair model
for the asymptotic behavior of
the tetramer excited state.





then, we can predict the binding energy

$$\Delta B_1^{(4)} (= B_1^{(4)} - B_0^{(3)})$$

of the tetramer excited state with respect to the
trimer ground state
as follows:

We can predict this binding energy

$$\Delta B_1^{(4)} (= B_1^{(4)} - B_0^{(3)})$$

using the relation

$$B^{(2)} = \frac{\hbar^2}{2\mu_x} (k^{(2)})^2 \qquad \mu_x = \frac{1}{2} m$$

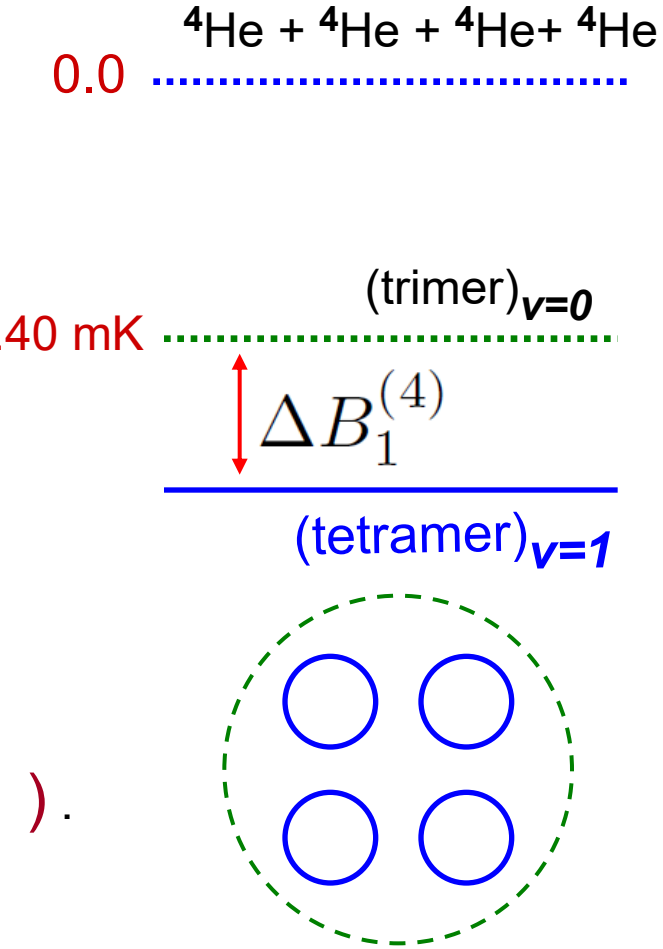
$$\Delta B_1^{(4)} = \frac{\hbar^2}{2\mu_z} (k_1^{(4)})^2 \qquad \mu_z = \frac{3}{4} m$$

and the dimer-like model ($k_1^{(4)} = k^{(2)}$).

We have

$$\Delta B_1^{(4)} = \frac{2}{3} B^{(2)} = 0.87 \text{ mK}$$

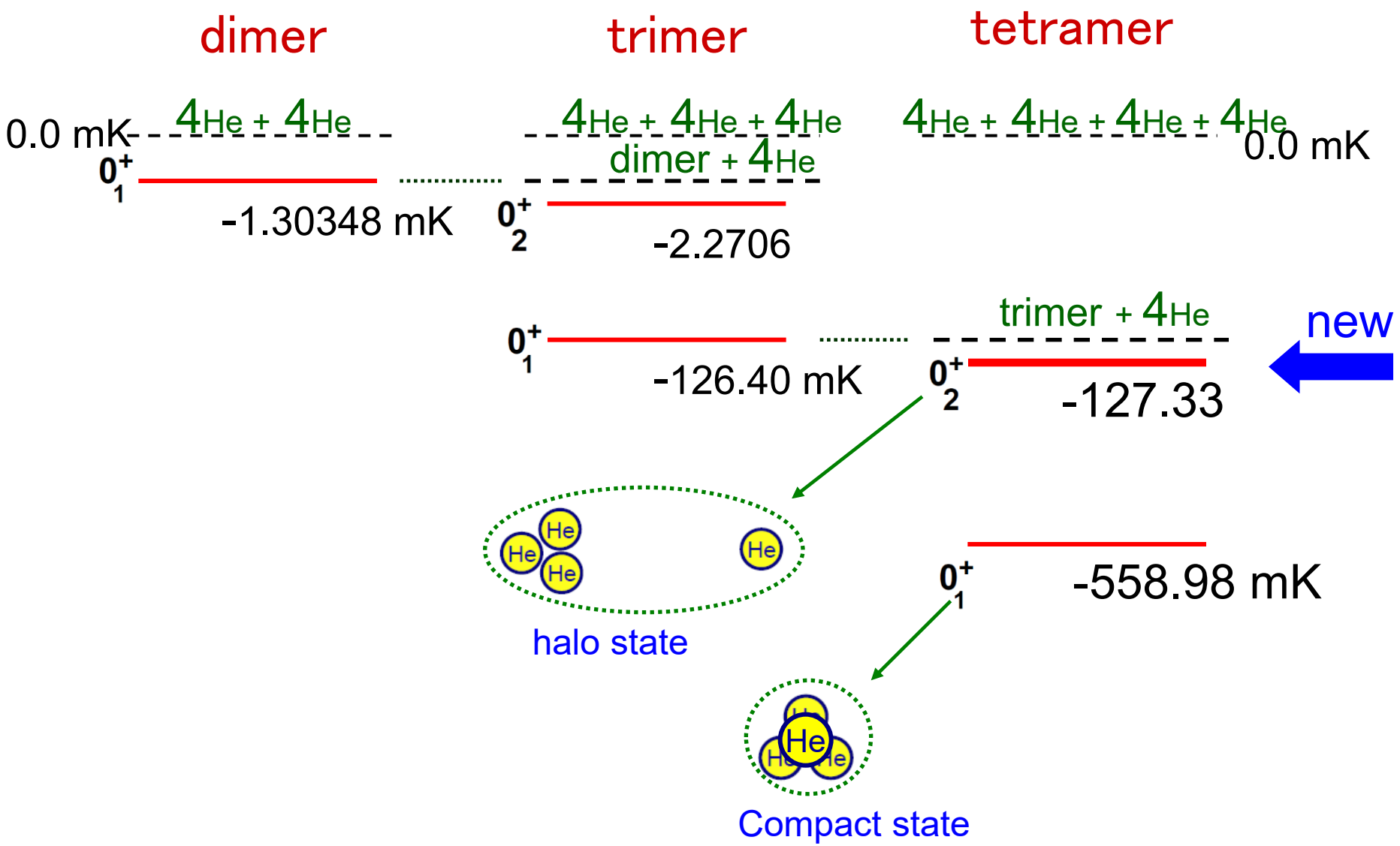
hence $B^{(4)} = 127.27 \text{ mK}$



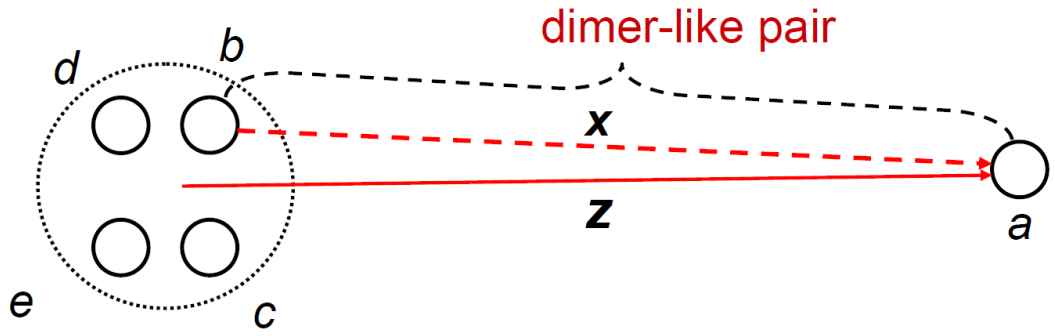
0.93mK
127.33mK

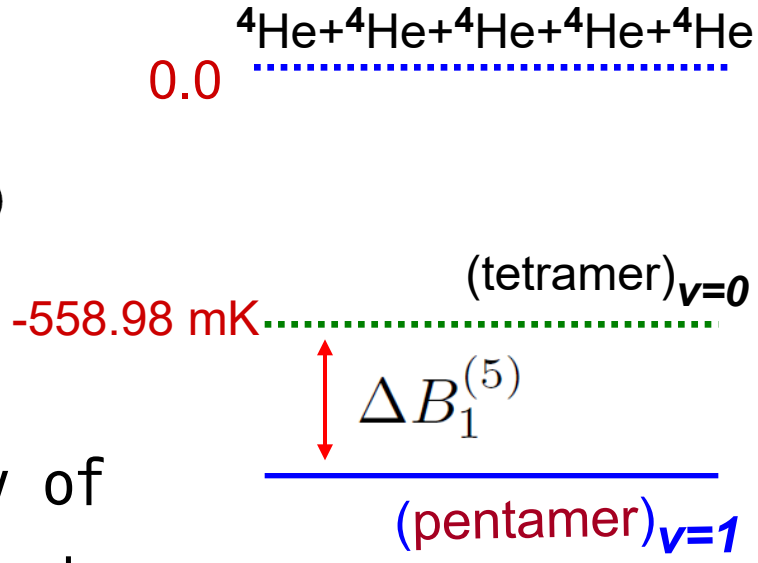
4-body calculation

We confirmed this level structure of 4He-atom clusters (2012).



Pentamer ($^4He_5$) excited bound state





We predict that the binding energy of the pentamer excited state, measured from the tetramer ground state, will be

$$\Delta B_1^{(5)} (= B_1^{(5)} - B_0^{(4)}) = \tfrac{5}{8} B^{(2)} = \boxed{0.81 \text{ mK}}$$

Generally, dimer-like pair model predicts, for *N*-atom system

$$\Delta B_1^{(N)} (= B_1^{(N)} - B_0^{(N-1)}) = \frac{N}{2(N-1)} B^{(2)}$$

$B^{(2)}$ ← dimer

What about calculation of 5-body calculation of 4He done so far?

JOURNAL OF CHEMICAL PHYSICS VOLUME 112, NUMBER 18 8 MAY 2000

Monte Carlo hyperspherical description of helium cluster excited states

D. Blume[a] and Chris H. Greene
Department of Physics and JILA, University of Colorado, Boulder, Colorado 80309-0440

(Received 16 November 1999; accepted 11 February 2000)

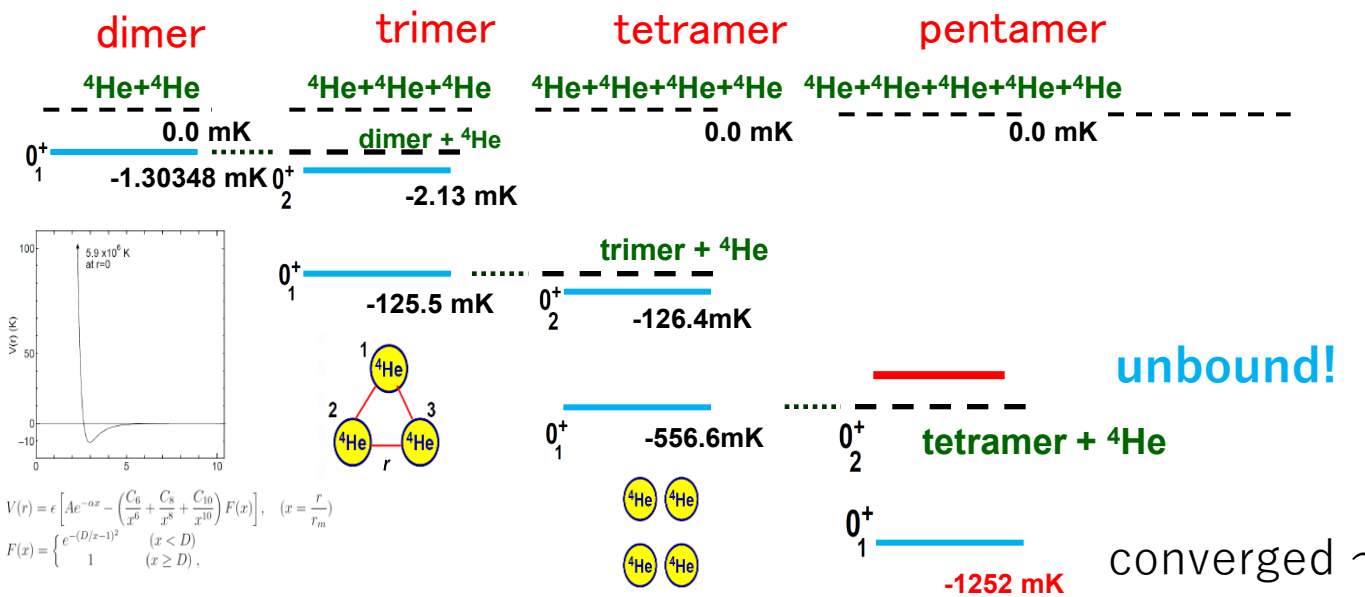
N=3 to 10 (ground states)

Using TTY potentials: diffusion MonteCarlo
For the ground state 1296.3mK
Born Oppenheimer Method for the excited state
656mK

M. Gattobigio, A. Kievsky, PRA90,012502(2014)

One-range Gaussian potential:$V\exp(-r/a)^2$ +3-body repulsive +4-body repulsive force
Potential parameters tuned so as to reproduce dimer energy, trimer and tetramer with LM2M2
Potentials done by me.
They discussed on universalities for the excited states of many-body systems.
They obtained bound excited bound states for 5-,6- 10-body systems.

Spectra of 2- 6-body systems in ^{4}He using 'Fugaku' computer

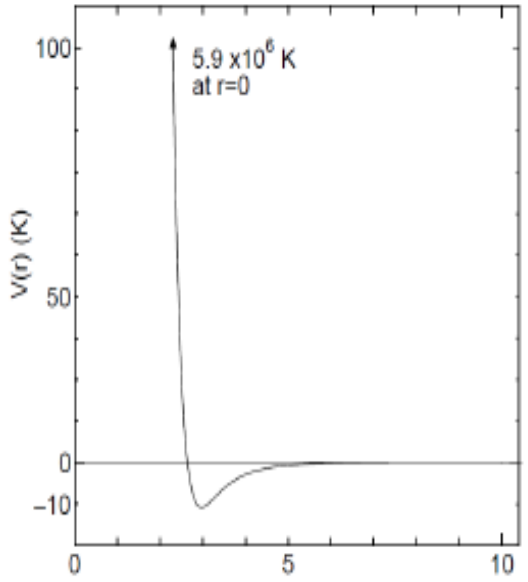


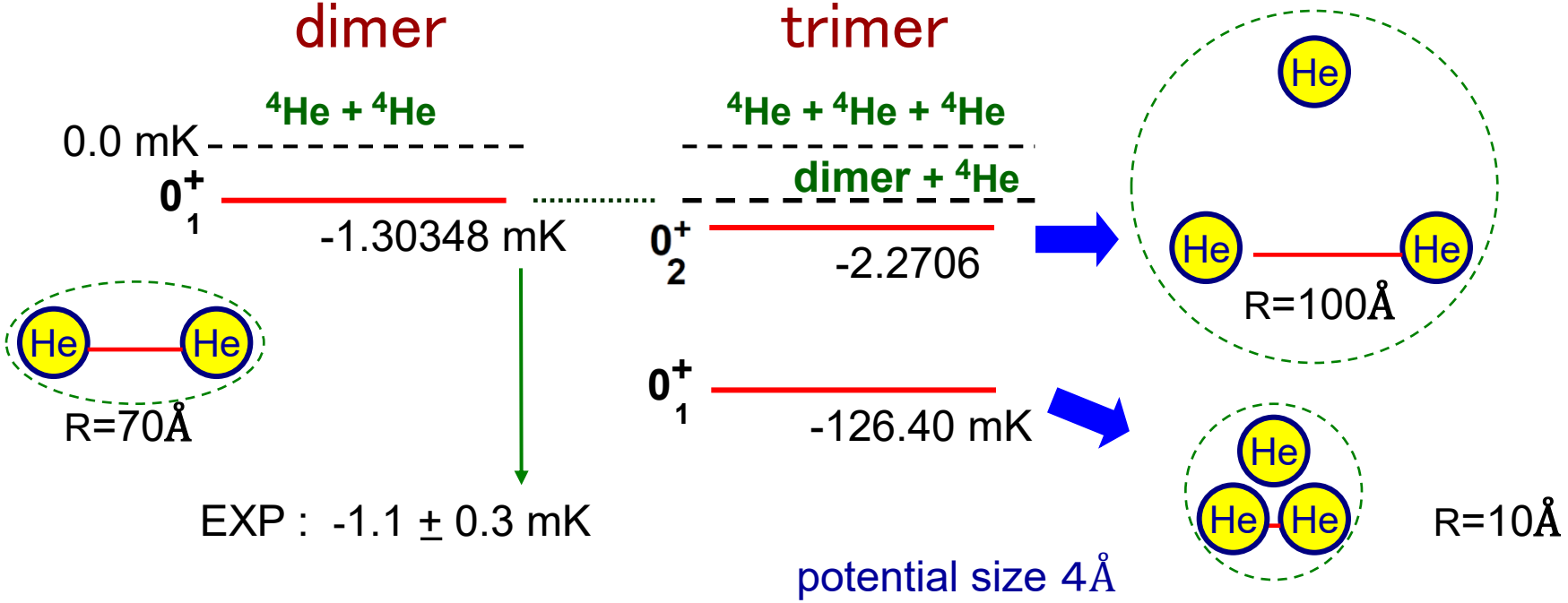
Pentamer ground state
1296mk J. Chem Phys. 112, 8053(2000)
1300mk RA10101501(R)(2020)
1310mk J.ChemPhys.124,084307(2009)

converged ～10mk Riams'cal:1281mK

Why we do not have excited bound state?

Answer : Whether or not to have a bound excited state is strongly dependent on height of repulsive core of 4He-4Hepotential.



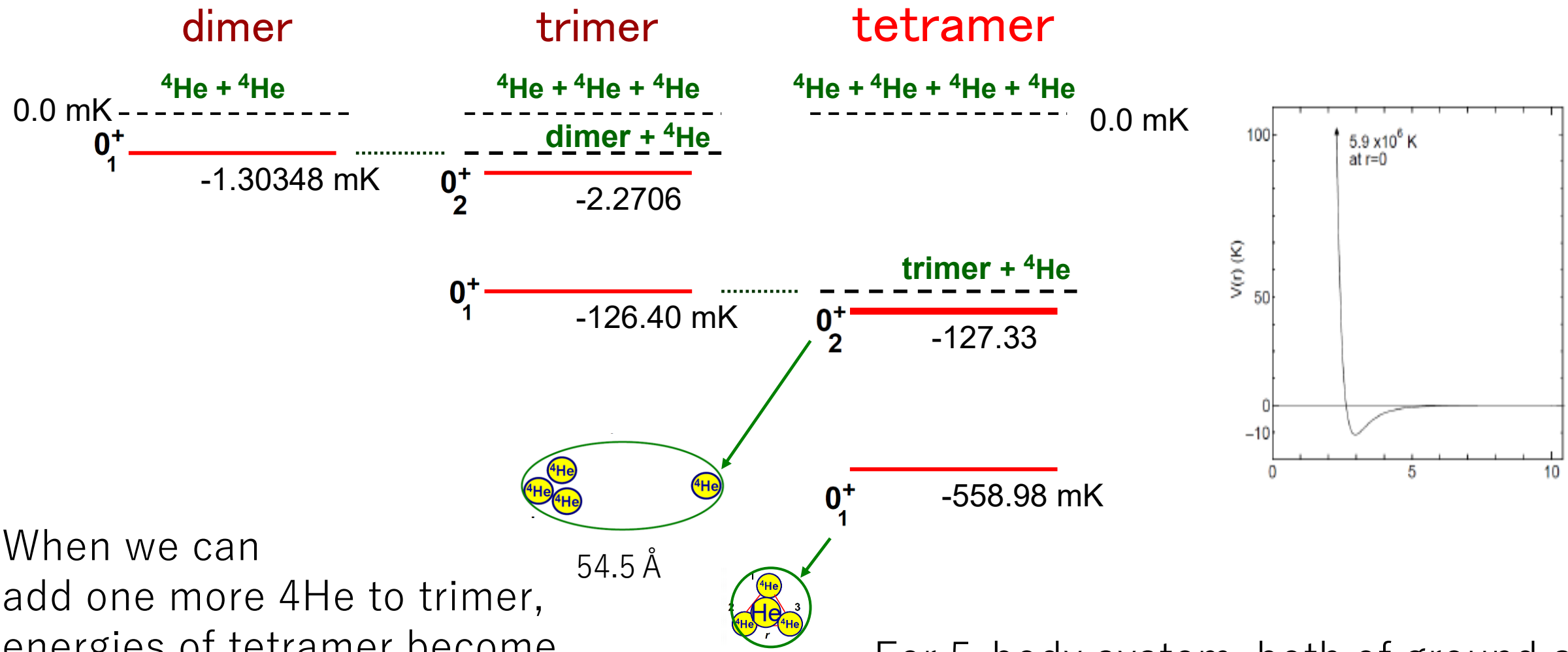


$$V(r) = \epsilon \left[A e^{-\alpha x} - \left(\frac{C_6}{x^6} + \frac{C_8}{x^8} + \frac{C_{10}}{x^{10}} \right) F(x) \right], \quad (x = \frac{r}{r_m})$$

$$F(x) = \begin{cases} e^{-(D/x-1)^2} & (x < D) \\ 1 & (x \geq D) \end{cases},$$

However, the repulsive core affects slightly affect to the ground state of trimer and does not affect to the excited state of . trimer.
Because, distance is still away from repulsive core.

LM2LM2 potential has along range tail.
Due to this tail, there is one weakly bound state.
Once one more 4He is added to dimer, We have 2 bound states:
One is deeply bound state and the other is weakly bound state which Is close to dimer+4He threshold.



When we can
add one more 4He to trimer,
energies of tetramer become
deeper. Especially, ground state
of tetramer is affected much by
repulsive core of 4He-4He potential.

For 5-body system, both of ground and excited states are affected by repulsive core.

To investigate effect of repulsive core of 4He-4He potential,
I use 2-range Gaussian potentials:
V(R) = V1 exp(-(R/s1)^2) - V2 exp(-(R/s2)^2)

	V1(K)	s1	V2	s2
(1)	1000	1.	6.36495	3.66484
(2)	2000.	1.	8.28233d0	3.48813d0
(3)	3000	1.	9.72031	3.38891
(4)	4000	1.	10.9346	3.31922
(5)	5000	1.	12.0180	3.26500
(6)	6000	1.	12.9382	3.22563
(7)	7000	1.	13.8253	3.19000
(8)	8000	1.	14.6652	3.15875
(9)	9000	1.	15.4845	3.12999
(10)	10000	1.	16.2047	3.10750

scattering length and effective range

100.224	Å
7.32587	

(1) V1=1000 K
dimer -1.3mK
trimer -127.52 mK -2.9mK
Tetramer -571.4mK -128.68mK
pentamer -1350.5mK -571.8mK =>0.4mK bound

No change for dimer energies
No change for the excited state of trimer

(2) V1=2000K
dimer -1.29mK
trimer -125.56 mK -2.15mK
tetramer -557.58mK -126.46 mK
Pentamer -1308.20mk -557.73mK => 0.15 mK weakly bound

Small affected for ground state of trimer

(3)V1=3000K
dimer -1.3mK
trimer -124.49mK -2.12mK
Tetramer -550.0mK -125.27 mK
Pentamer -1285.34 mk -550.mK on the threshold

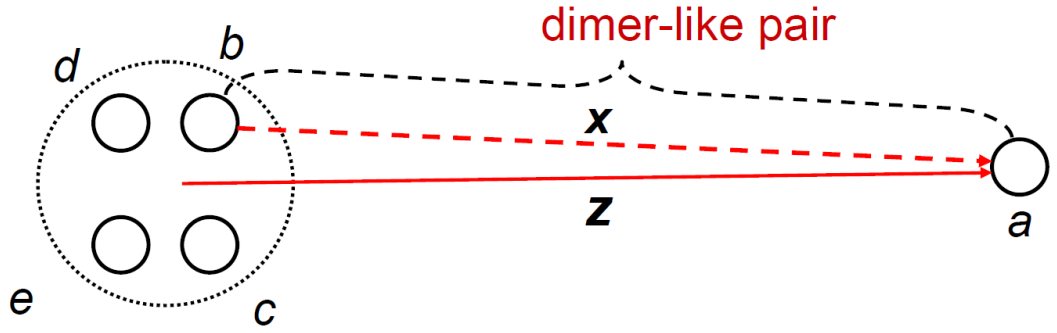
Energies of ground state in tetramer
Are dependent on height of repulsive core.
The similar for the excited states of tetramer.

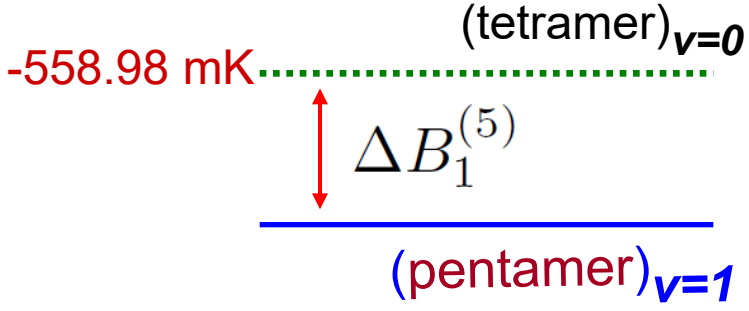
(4) V1=4000K
dimer -1.3mK
trimer -123.80mK -2.12 mK
tetramer -546.13mK -124.51mK
Pentamer -1270mK -544.52mK unbound

We see strong affection of
repulsive core for pentamers.
As increasing height of repulsive core,
the excited energies of Pentamer
go up and finally, we have no bound state.

Pentamer ($^4He_5$) excited bound state

Conclusion:
For beyond 5-body bosonic systems,
It is difficult to keep the below universality
due to high repulsive core of 4He-4He potential.





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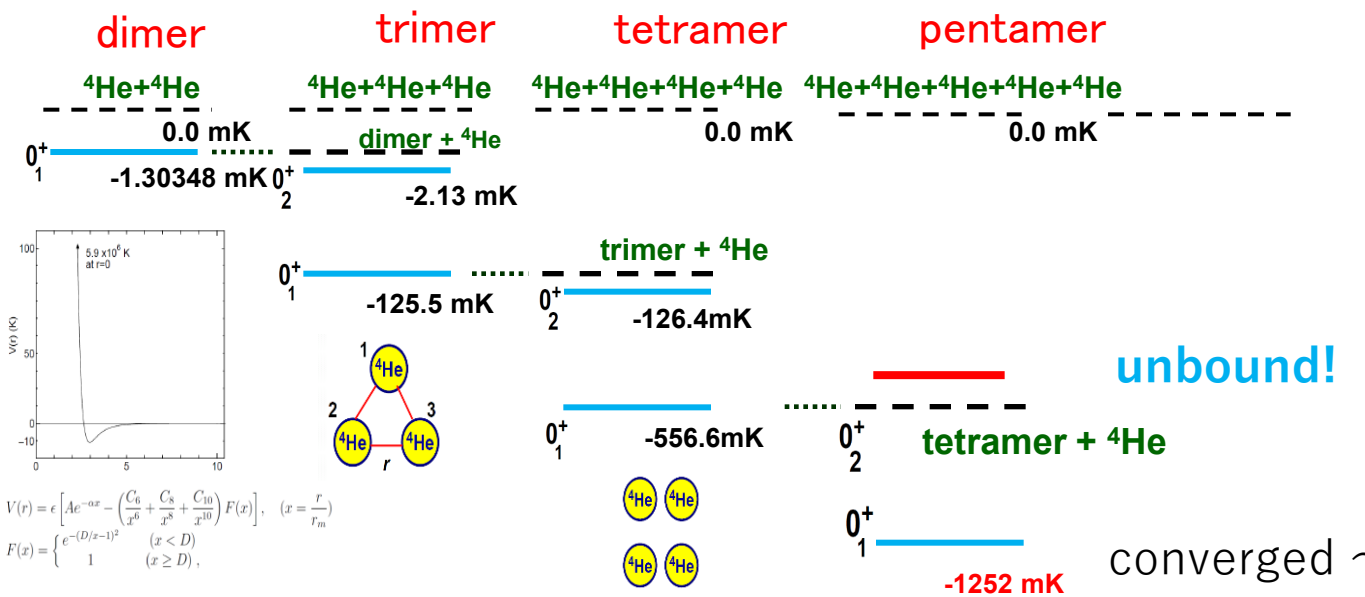

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1310mk J.ChemPhys.124,084307(2009)

Conclusion: for beyond 5-body 4He bosonic system, there is only one bound system and it is important to treat repulsive core of 4He-4He potential. Otherwise, we mislead physics.

Conclusion and perspective

- To develop my method, Gaussian Expansion Method up to
10-body systems and apply to many research fields.
・The codes are open for public, so that everyone can use easily for each field.
Up to 5-body problem (Bosonic system), I and collaborators are trying to open for public.

We could obtain eigen energies accurately. However, how should I check accuracy of wavefunction?

・One of the way is to calculate reaction using the wavefuction by GEM.
How should I calculate? => one of tool is CDCC
=>Ogawa san' talk(Next talk)

Question

・To produce to many-body problem, we need huge memory and CPU time.
How should I reduce them?
SVM, machine learning, GPU?? Anything else?

・To apply our wavefunction to reaction.
What kind of reaction is applicable?
As the first stage, I started to collaborate with Ogawa san using CDCC.
Probably, this discussion would be better after his talk.

Thank you!

Another research: how to obtain information on the interaction

Fundamental equation of quantum three-body problem (Schrodinger equation)

$$\left[a\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+A\left(\frac{\partial^2}{\partial X^2}+\frac{\partial^2}{\partial Y^2}+\frac{\partial^2}{\partial Z^2}\right)\right.$$

$$\left. +V(x,y,z,X,Y,Z)-E\right]\Psi(x,y,z,X,Y,Z)=0$$

In the case that V has a lot of ambiguity

Using the V, we can obtain E and Ψ accurately.

⇕ compare

Experiment: To observe E, Ψ accurately

If $E_{exp} \neq E_{cal}$., we improve the following interactions.