Quantum few-body calculation method and its application to neutron-rich nuclei

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Section 1

Introduction

One of my research purpose is to develop My method for three-body-5body problem

We call 3-5 problem as ‘few-body problem’.

What is ‘few-body problem’?

I shall explain this word in the terms of ‘Human science’.

Section 2

Individual and Group

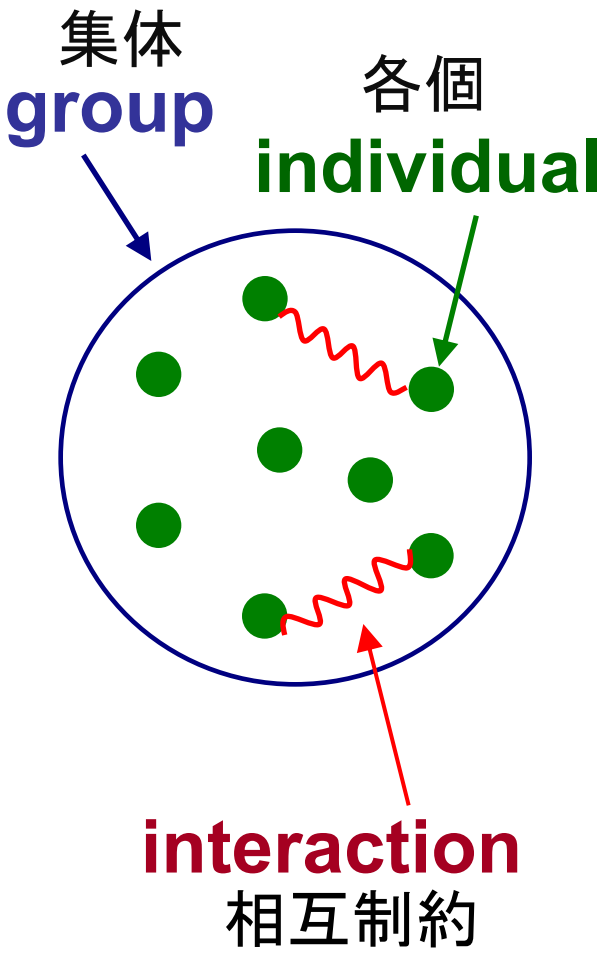
in the microscopic world

Physics: **Few-Body Problems in Physics**

(many-body)

||

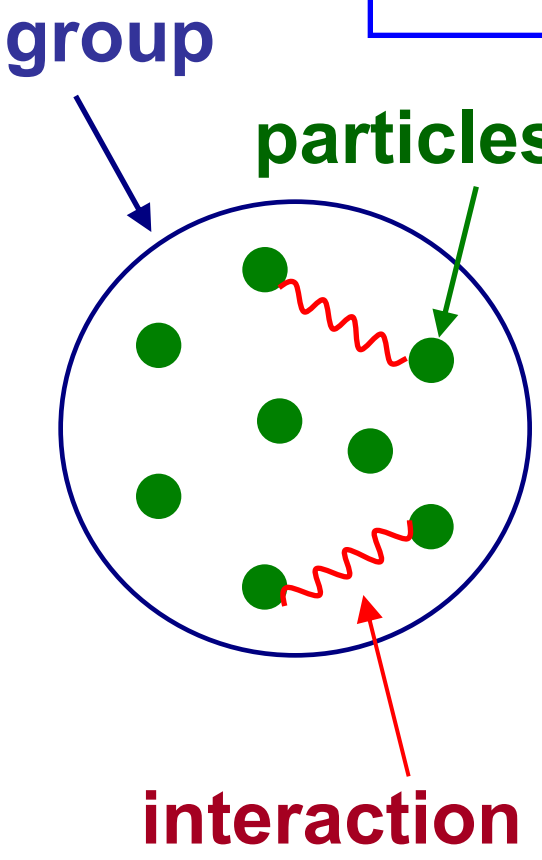
Social Science: **Individual and Group Behavior** based on the interaction between individuals



A typical problem :
the group may act collectively to achieve a goal that differs from what individuals would act alone.

In physics, this problem is called …

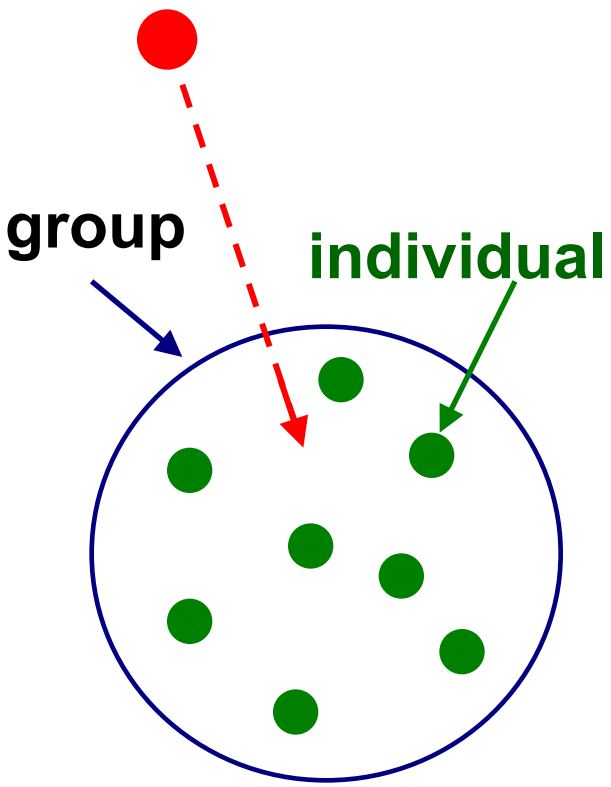
Few-Body (Many-Body) Problems:
to disscuss about the group behavior
starting from the interaction
between constituent particles.



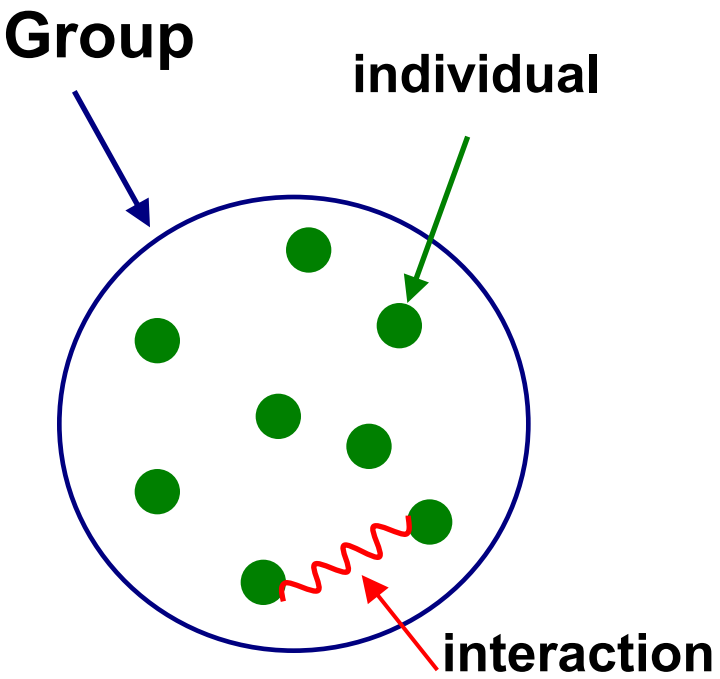
To study such problems,
we need any good research methods
to clarify the dynamics of
individual and group behavior.

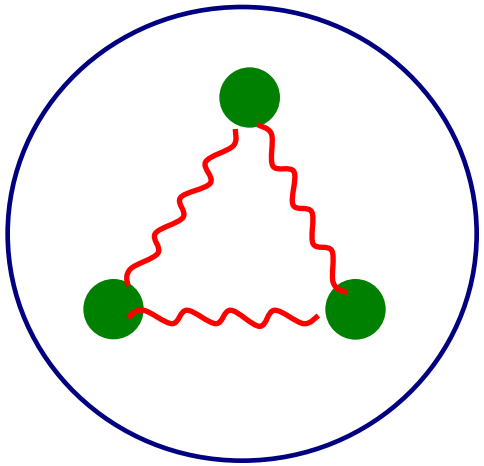
My research goal is
1) to establish such a method
2) to apply it to various kinds of interesting, important problems.

侵入者
strange intruder



One of my research subjects:
To study how the group responds, as a whole, against a strange intruder coming into the community.





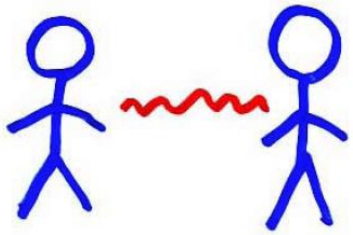
3-body model

The simplest is
‘3-body problem’.

But, it seems difficult to solve
this problem.

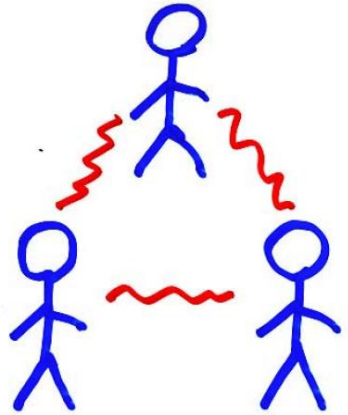
Next, let’s consider
why ‘3-body problem’ is difficult.

2-body problem



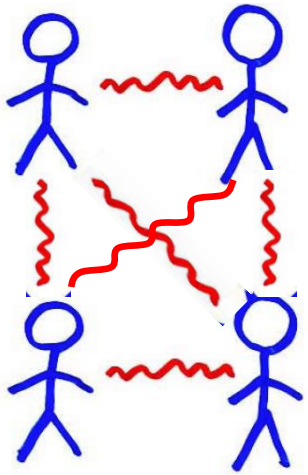
Some Issues are easily solved.

3-body problem



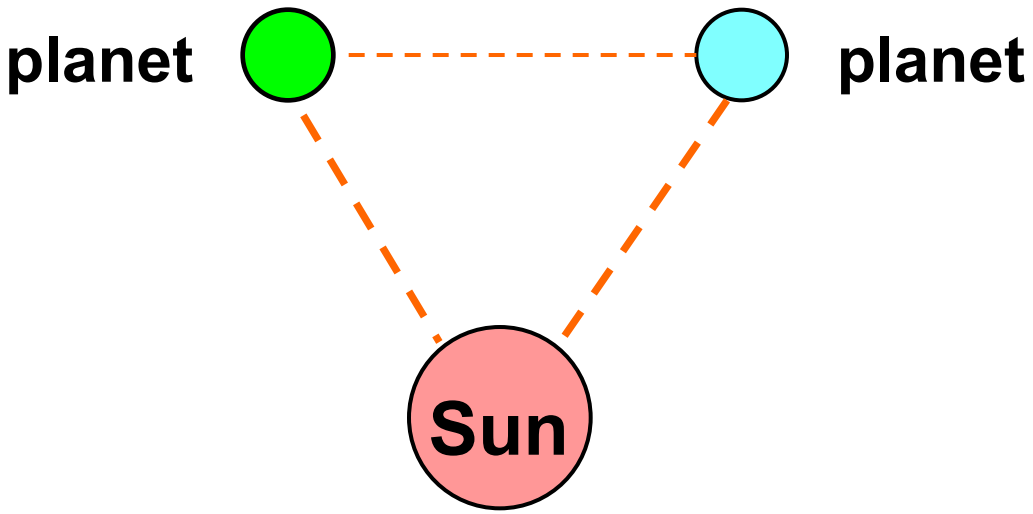
Become complicated due to the presence of the 3-rd person

4-body problem



Much more complicated !

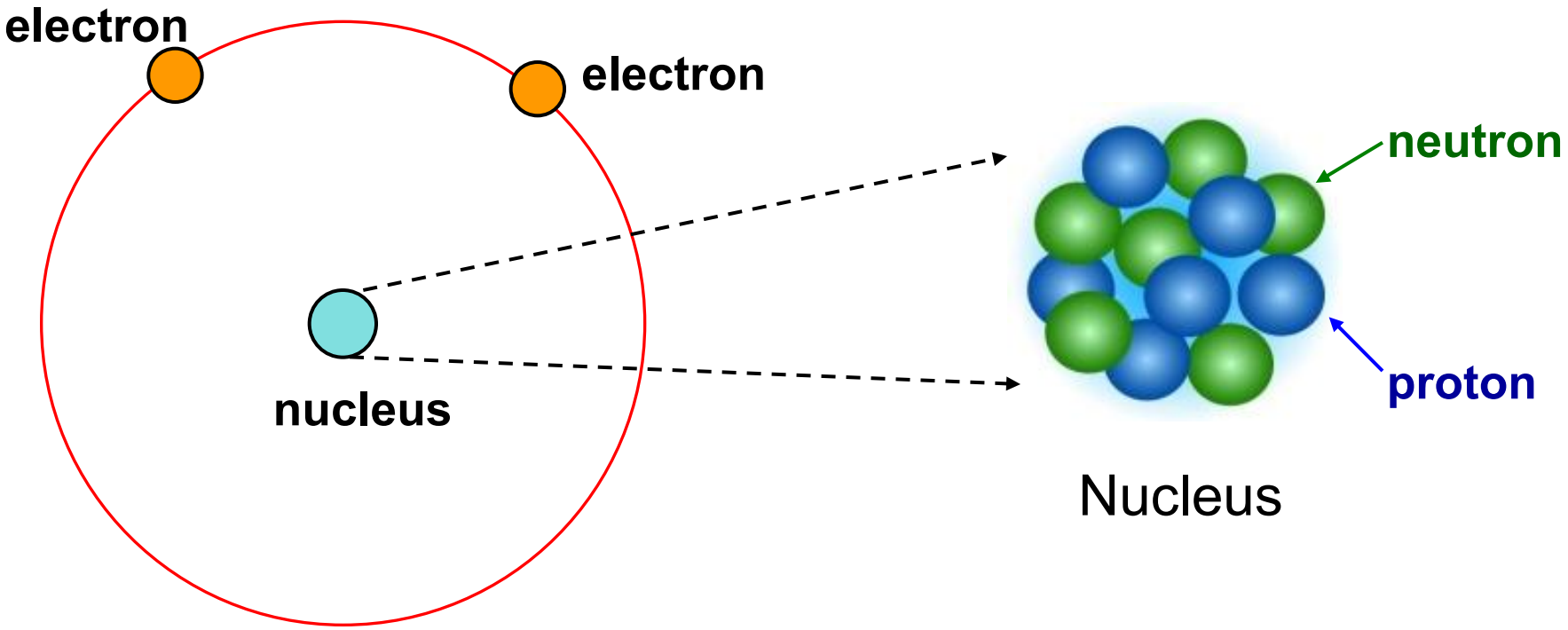
3-body problem in macroscopic (astro-)physics :



You might know, it is difficult to solve accurately the 3-body Newton equation that has chaotic solutions sometime.

How about is the microscopic 3-body problems such as in atomic and nuclear physics ?

A 3-body problem in atomic physics

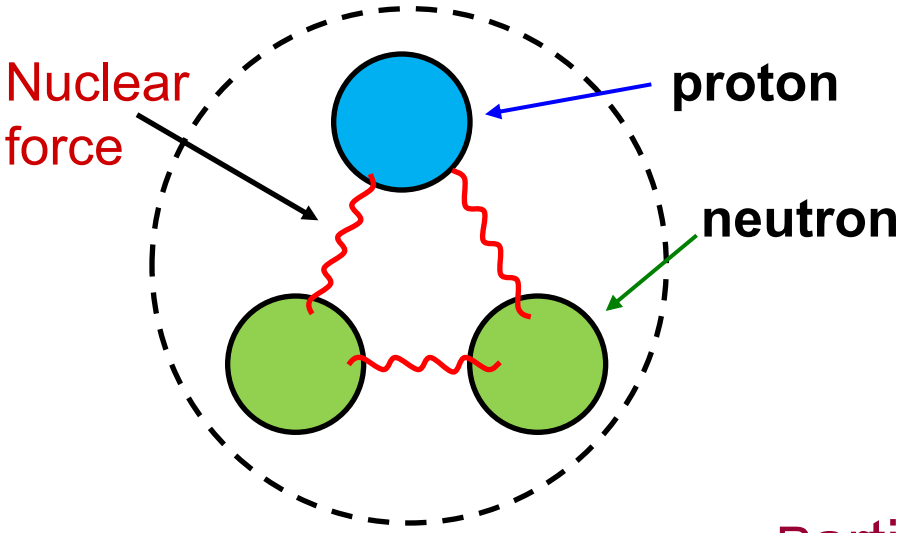


Atom = **Nucleus + Electrons**

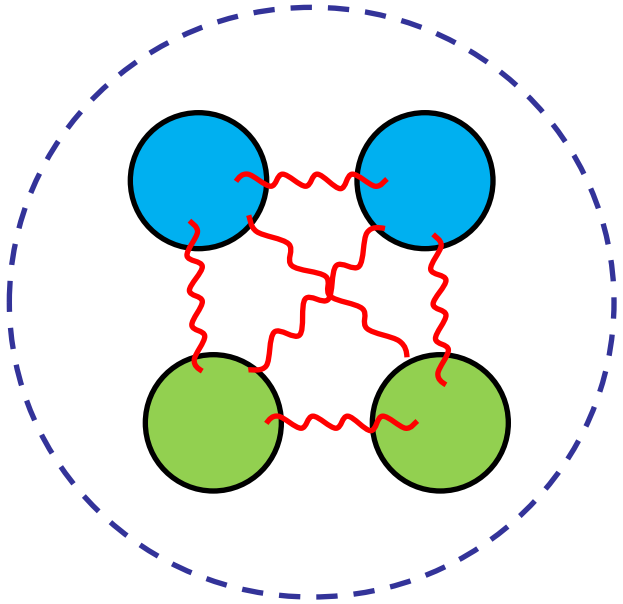
A typical 3-body problem in nuclei

A typical 4-body problem in nuclei

Triton Nucleus



Helium-4 Nucleus



Particles are moving fast.

It is difficult to solve nuclear 3- and 4-body problems accurately.

Question: Why is it difficult to solve ‘many-body problem’ accurately?

Many important problems in physics can be attributed to solving accurately Schrödinger equation

$$(\mathbf{H} - \mathbf{E})\Psi = 0$$

for 3- and 4-body systems.

By solving the equation,

i) we can predict various observable before measurement, and

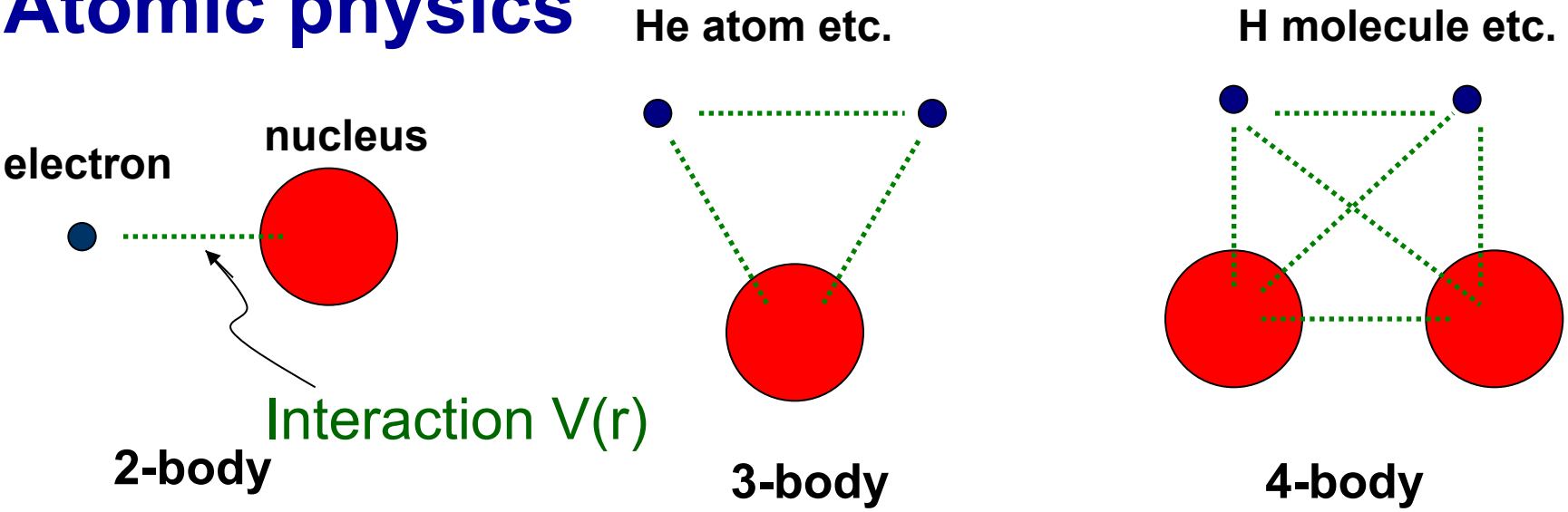
ii) we can obtain new understandings by comparing the observed data and our theoretical prediction.

For this purpose, it is necessary

i) to develop the method to calculate 3- and 4-body problems precisely, and

ii) to apply to various fields such as nuclear physics as well as atomic physics.

Atomic physics



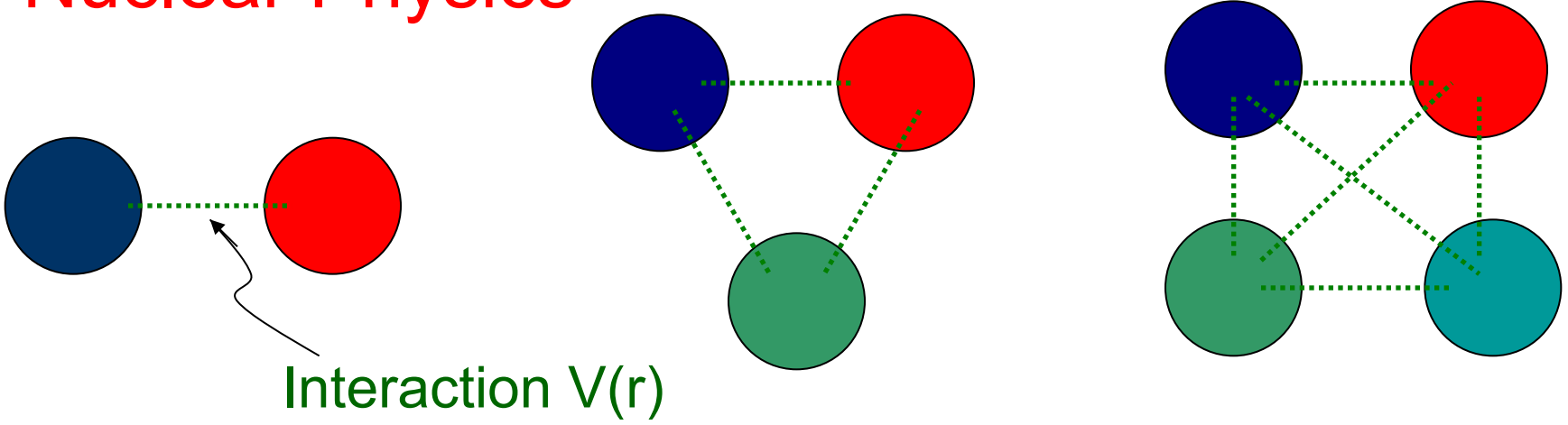
In atomic physics,
constituent particles are electrons and nuclei.

$m_{electron} << m_{nucleus}$

Coulomb interaction is weak, therefore,

for example, using adiabatic approximation,
we can perform 3- and 4-body calculations more easily
than those in the case of nuclear physics.

Nuclear Physics



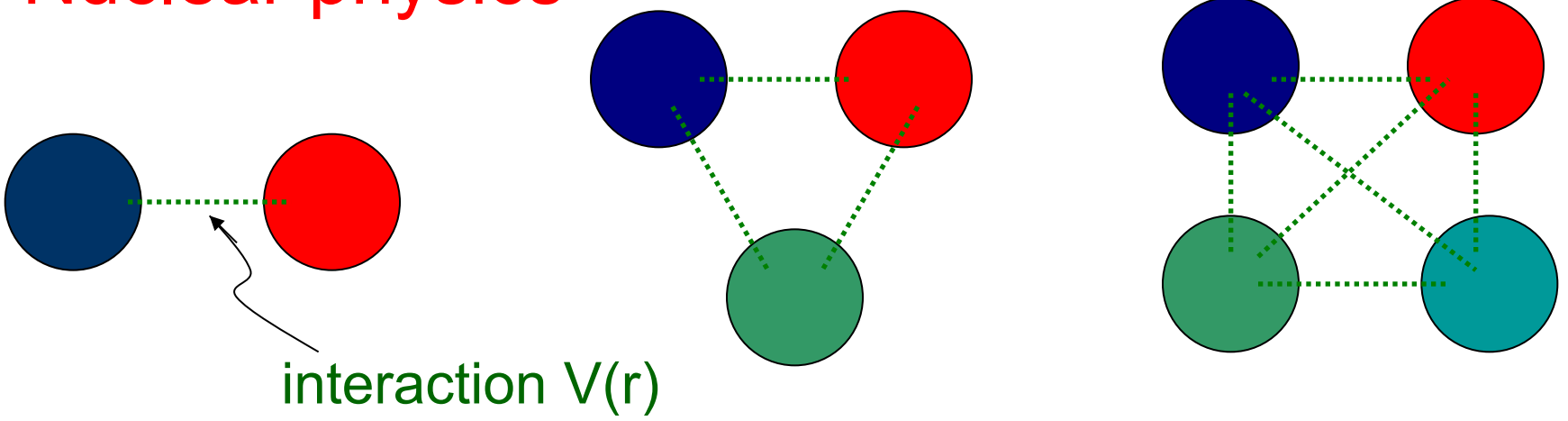
Two-body **Three-body** **Four-body**

However, in nuclear physics, since interaction between nucleon and nucleon is strong, we have no approximation method to solve three- and four-body problems accurately.

Then,

We should develop the method for solving various few-body problem accurately.

Nuclear physics



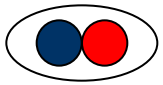
2-body **3-body** **4-body**

In the 2-body problem, since how to calculate 2-body Schrödinger equation is written in the textbook of quantum mechanics, everybody can calculate the 2-body problem exactly.

i) However, it is usually difficult to calculate 3-body and 4–body problem since the interaction is strong.

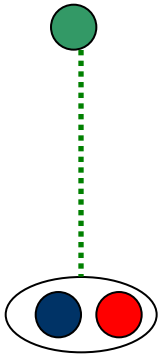
ii) In 3-body system, there are many rearrangement channels.

Simple in two-body system



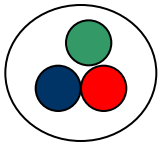
Strongly coupling

Loosely coupling

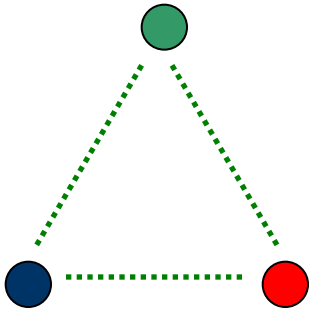


If one more particle is added to….

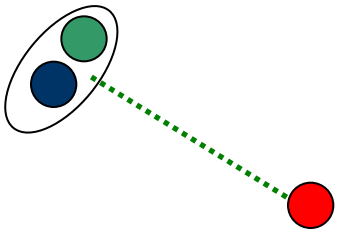
3-body problem : commplicated!

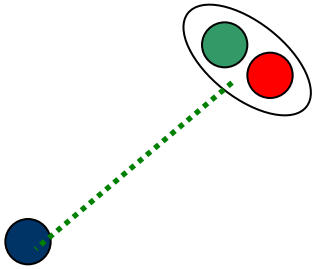


Strongly coupling



Loosely coupling



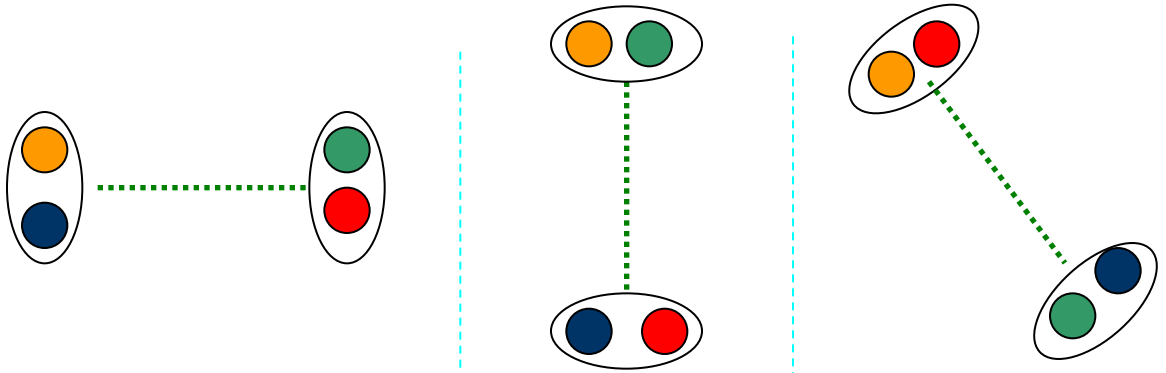


(2+1) coupling

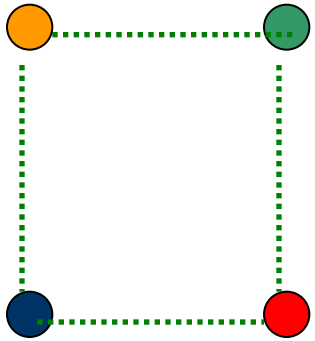
Three-types

4-body problem is more complicate.

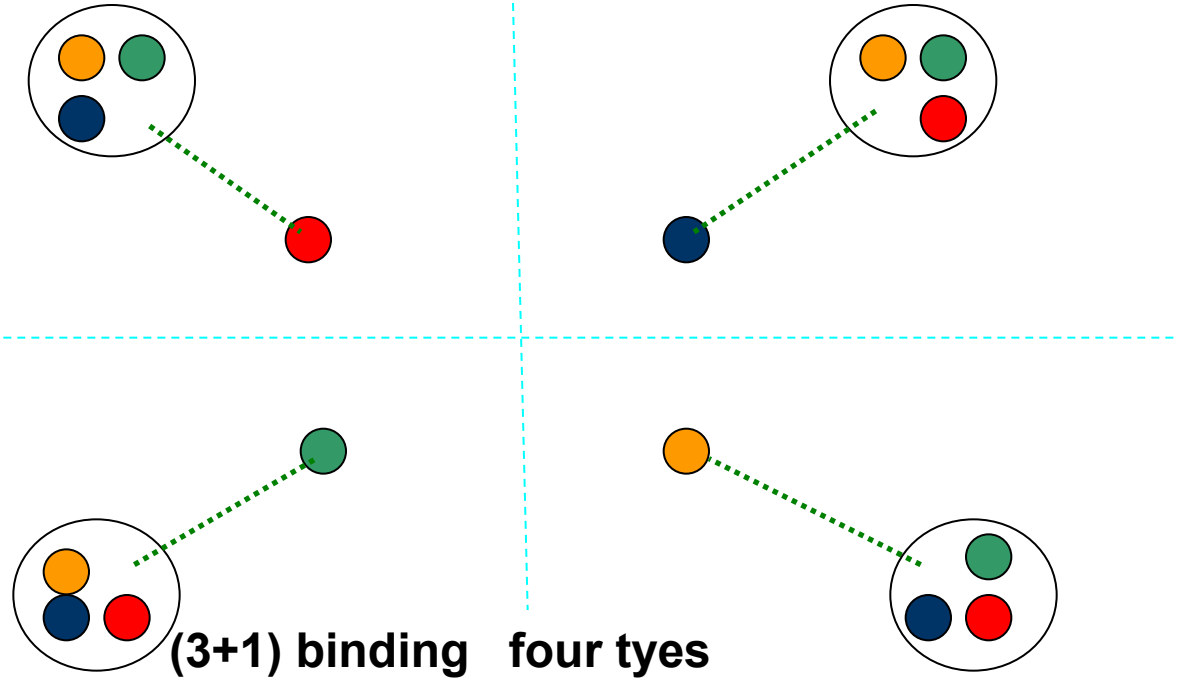
(2+2)binding three types



Strongly binding



Loosely binding



(3+1) binding four tyes

We should take account of these rearrangement and solve accurately.

Few-body research group to solve four-body problem

7 methods in the world!

- Gaussian Expansion method: RIKEN & Tohoku.(Japan)
- SVM Osaka metropolitan Univ.(Japan)
- Fadeev Yakbovsky Ruhr Univ. (Germany)
- Hypersherical method Pisa Univ. (Italy)
- No core shell model
- Green Function monte Carlo (U.S.A.)
- EHH

5-Body problem

Only 5 or 6 methods

- RIKEN & Tohoku Univ.(Japan)
- Osaka metropolitan Univ.(Japan):SVM
- TRIUMF &Livermore (U.S.A.):No core shell model
- Argonne National Laboratory &Los Alamos (U.S.A.) GFMC
- Faddeev calculation

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

In order to solve the **Schrödinger equation, we use Rayleigh-Ritz variational method (変分法)and we obtain eigen value E and eigen function Ψ.**

$$(\mathbf{H} - \mathbf{E})\,\Psi = 0$$

Here, we expand the total wavefunction in terms of a set of L^2-integrable basis function $\{\Phi_n : n=1,\ldots,N)\}$

$$\Psi = \sum_{n=1}^{N} C_n \Phi_n$$

The Rayleigh-Ritz variational principle leads to a generalized matrix eigenvalue problem.

$$\left\langle \Phi_i \middle| H - E \middle| \sum_{n=1}^{N} C_n \Phi_n \right\rangle = 0\,, \qquad (i = 1, \ldots, N)$$

$$\Psi$$

Where the energy and overlap matrix elements are given by

$$H_{in} = \langle \Phi_i | H | \Phi_n \rangle$$

$$N_{in} = \langle \Phi_i | 1 | \Phi_n \rangle$$

Next, by solving eigenstate problem, we get eigenenergy E and unknown coefficients C_n .

$$\left(\left(H_{in} \right) - E \left(N_{in} \right) \right) \left(\mathbf{c_n} \right) = 0$$

Variational method（変分法） for Schroedinger Eq.

$$(H - E)\,\Psi = 0 \qquad \langle\, \Psi \mid \Psi \,\rangle = 1$$

We check the energy of a trial function Ψ

Suppose that we have a ortho-normal complete set $\{\phi_n\}$

$$H\phi_n = E_n\phi_n \quad (n = 0, 1, 2, ..., N) \qquad E_0 \le E_1 \le E_2 \le, ..., \le E_N$$

$$\langle\, \phi_n \mid \phi_{n'} \,\rangle = \delta_{n\,n'} \qquad \sum_{n=1}^{N} \mid \phi_n \,\rangle\langle\, \phi_n \mid = 1 \qquad \langle\, \phi_n \mid H \mid \phi_{n'} \,\rangle = E_n\delta_{n\,n'}$$

Expectation value of H

$$\langle\, \Psi \mid H \mid \Psi \,\rangle = \sum_{n\,n'} \langle\, \Psi \mid \phi_n \,\rangle\langle\, \phi_n \mid H \mid \phi_{n'} \,\rangle\langle\, \phi_{n'} \mid \Psi \,\rangle$$

$$= \sum_n E_n \langle\, \Psi \mid \phi_n \,\rangle\langle\, \phi_n \mid \Psi \,\rangle \geqq \sum_n E_0 \langle\, \Psi \mid \phi_n \,\rangle\langle\, \phi_n \mid \Psi \,\rangle = E_0 \langle\, \Psi \mid \Psi \,\rangle = E_0$$

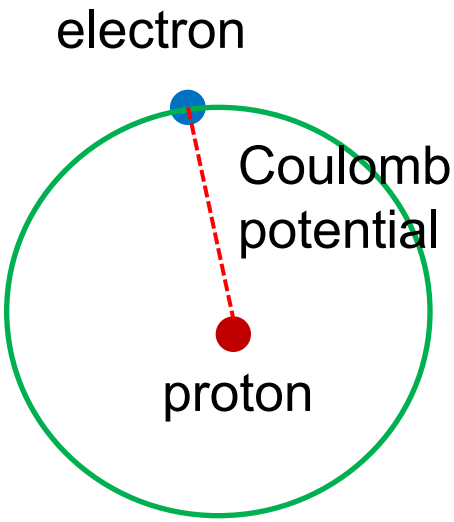
$$\langle\, \Psi \mid H \mid \Psi \,\rangle \geqq E_0$$

How to find accurate Ψ ? This can be $=$, when $\Psi = \phi_0$.

Example of the simple variational method

Calculation of the ground-state energy of Hydrogen atom

$$\left[-\frac{\hbar^2}{2m_e}\nabla^2 - \frac{e^2}{r} - E \right] \psi_{lm}(\mathbf{r})$$



Atomic unit

$$\left[-\frac{1}{2}\nabla^2 - \frac{1}{r} - E \right] \psi_{lm}(\mathbf{r})$$

H

Trial function

1) Gaussian function exp(-ar^2)

2) Exponential function exp(-ar)

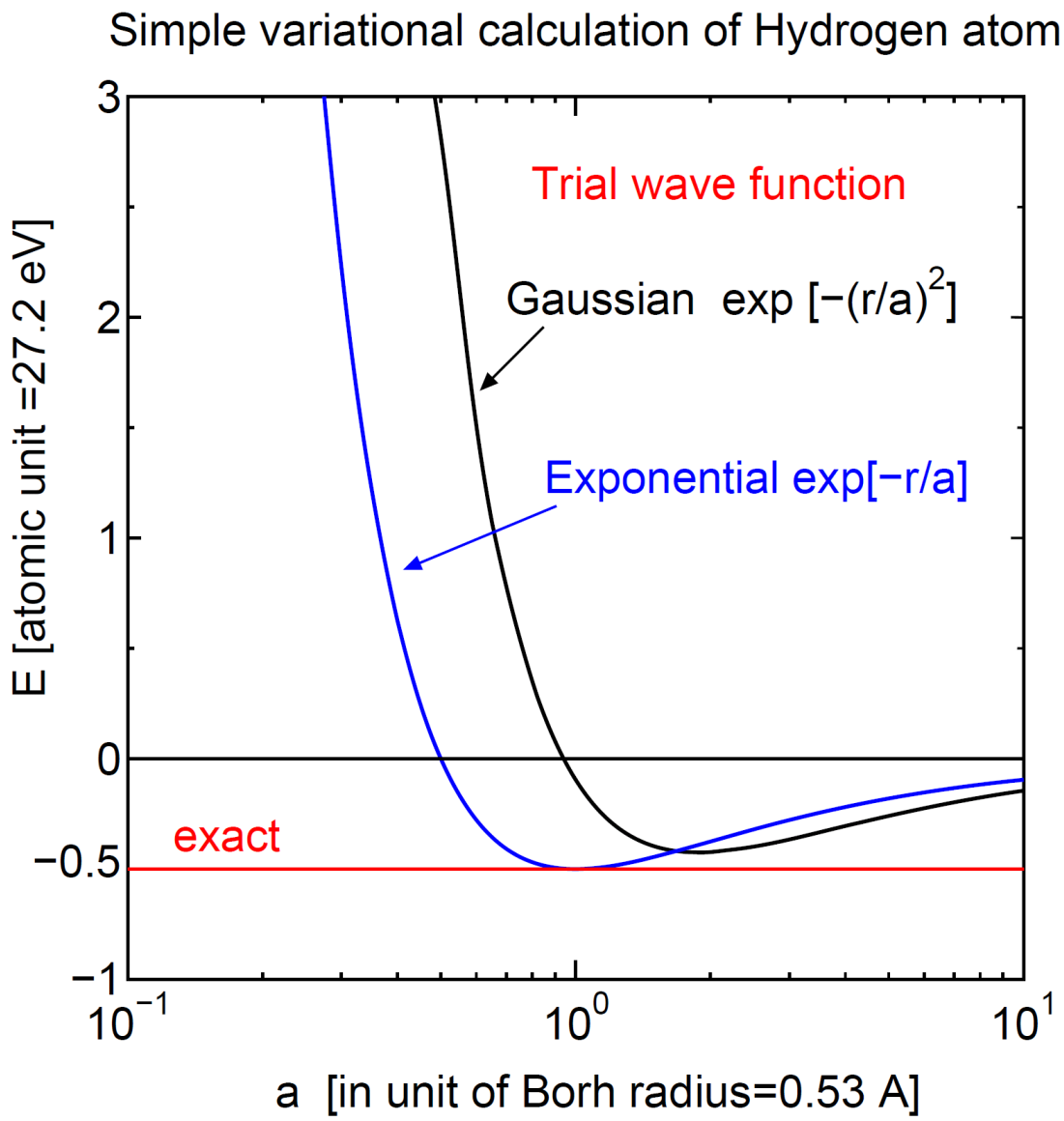
Atomic unit

Distance in unit of Bohr radius

$$a_0 = \frac{\hbar^2}{m_e e^2} = 0.5291 \text{ Å}$$

Energy in atomic unit

$$E_0 = \frac{m_e e^4}{\hbar^2} = 27.3 \text{ eV}$$

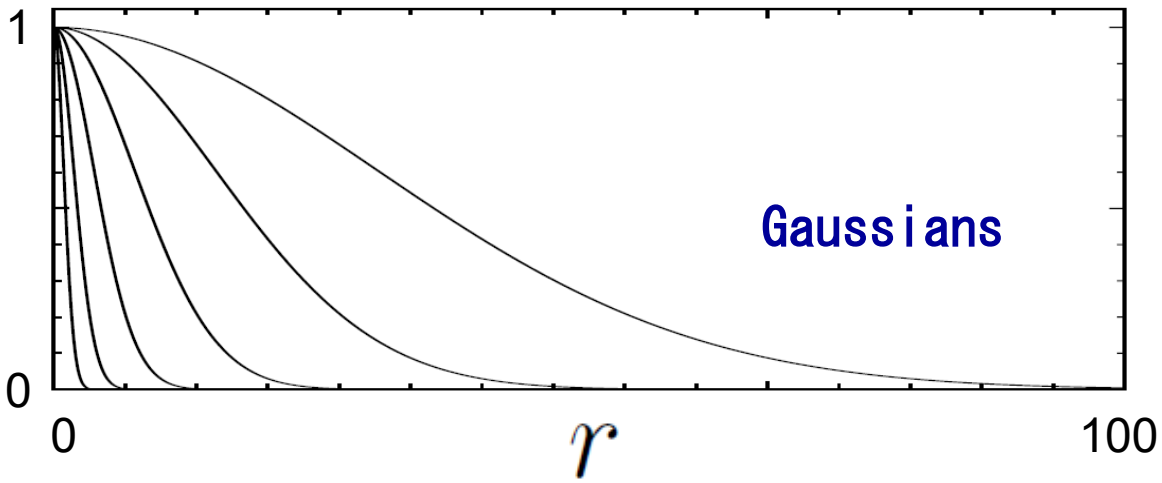

Simple variational calculation of Hydrogen atom
Trial wave function
Gaussian exp [−(r/a)^2]
Exponential exp[−r/a]
exact
E [atomic unit =27.2 eV]
a [in unit of Borh radius=0.53 A]
3
2
1
0
−0.5
−1
10^−1
10^0
10^1

Section 3

jewel
寶石

Gaussian Expansion Method (GEM)

for Few-Body Systems



Rayleigh-Ritz variational method

can be accurate for the ground state and some excited states

$$(\mathbf{H} - \mathbf{E})\,\Psi = 0$$

Here, we expand the total wavefunction in terms of a set of L^2-integrable non-orthogonal basis function $\{\Phi_n: n=1,\ldots,N)\}$

$$\Psi = \sum_{n=1}^{N} C_n \Phi_n$$

More general than orthogonal basis

The Rayleigh-Ritz variational principle leads to a generalized matrix eigenvalue problem.

$$\langle \Phi_i | \mathbf{H} - \mathbf{E} | \sum_{n=1}^{N} C_n \Phi_n \rangle = 0\,, \qquad (i = 1, \ldots, N)$$

$$\Psi$$

Where the energy and overlap matrix elements are given by

$H_{in} = \langle \Phi_i | H | \Phi_n \rangle$ (i, n =1,…,N)

$N_{in} = \langle \Phi_i | 1 | \Phi_n \rangle$ --- non-orthogonal basis

Next, we get eigenenergy E and coefficients C_n
by solving generalized matrix eigenvalue problem,

$$(H - E)\Psi = 0 \qquad \Psi = \sum_{n=1}^{N} C_n \Phi_n$$

$$\left((H_{in}) - E (N_{in}) \right) \left(C_n \right) = 0$$

solution $\Psi = \Psi_0, \Psi_1, \Psi_2, \ldots, \Psi_N$

$E = E_0, \; E_1, \; E_2, \; \ldots, E_N$

$$\Psi = \sum_{n=1}^{N} C_n \Phi_n$$

$$\Phi_n = \phi_{nl}^{G}(r) Y_{lm}(\hat{\mathbf{r}})$$

θ,φ

$$\phi_{nl}^{G}(r) = N_{nl}\, r^l\, e^{-\nu_n r^2},$$

$$N_{nl} = \left(\frac{2^{l+2}(2\nu_n)^{l+\frac{3}{2}}}{\sqrt{\pi}\,(2l+1)!!} \right)^{\frac{1}{2}} \qquad (n = 1 - n_{\max}),$$

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

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

Let's calculate Hydrogen atomic system. Code name is bound-coul.f

Test in hydrogen atom

$$[\, -\frac{\hbar^2}{2m_{\rm e}}\nabla^2 - \frac{e^2}{r} - E\,]\,\psi_{lm}(\mathbf{r})$$

E in atomic unit of $\boldsymbol{m_{\rm e}e^2/\hbar^2 = 27.21}$ eV

R in atomic unit $\hbar^2/(m_{\rm e}e^2) = 0.5291\text{Å}$ (Bohr radius)

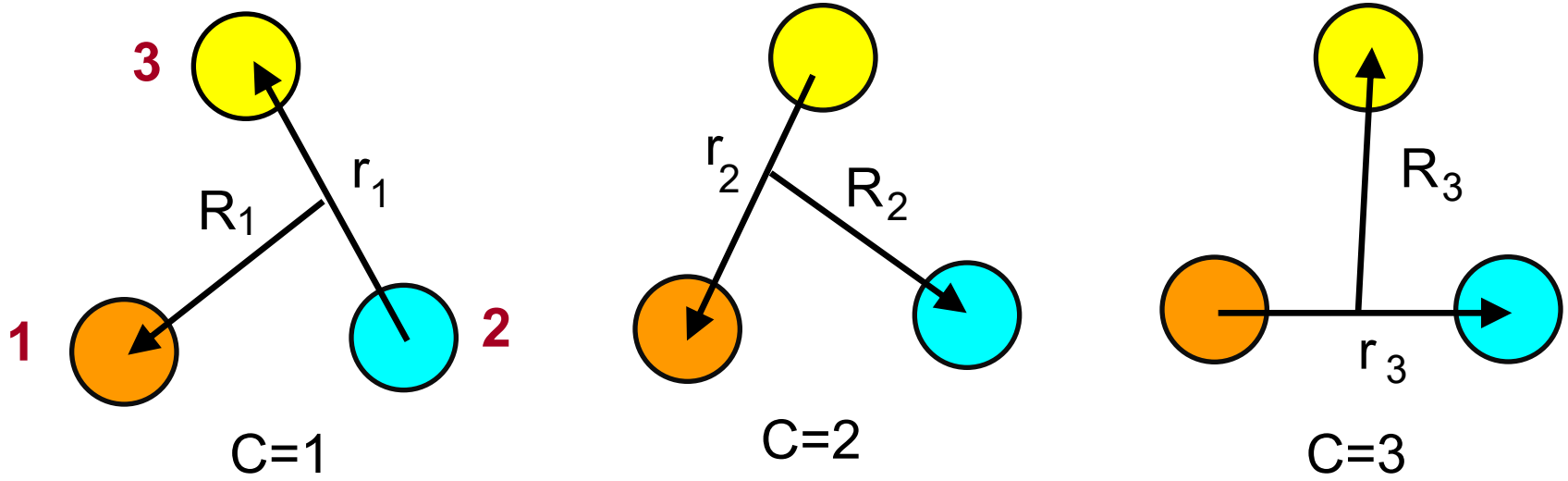
$$[\, -\frac{1}{2}\nabla^2 - \frac{1}{r} - E\,]\,\psi_{lm}(\mathbf{r})$$

$n_{\rm max} = 20,$

$r_1 = 0.1$ a.u.,

$r_{n_{\rm max}} = 80$ a.u.

k	$E^{(k)}$ (GEM)	$E^{(k)}$ (Exact)
1	−0.499982	−0.500000
2	−0.124998	−0.125000
3	−0.055555	−0.055556
4	−0.031249	−0.031250
5	−0.019998	−0.020000
6	−0.013883	−0.013889
7	−0.010203	−0.010204



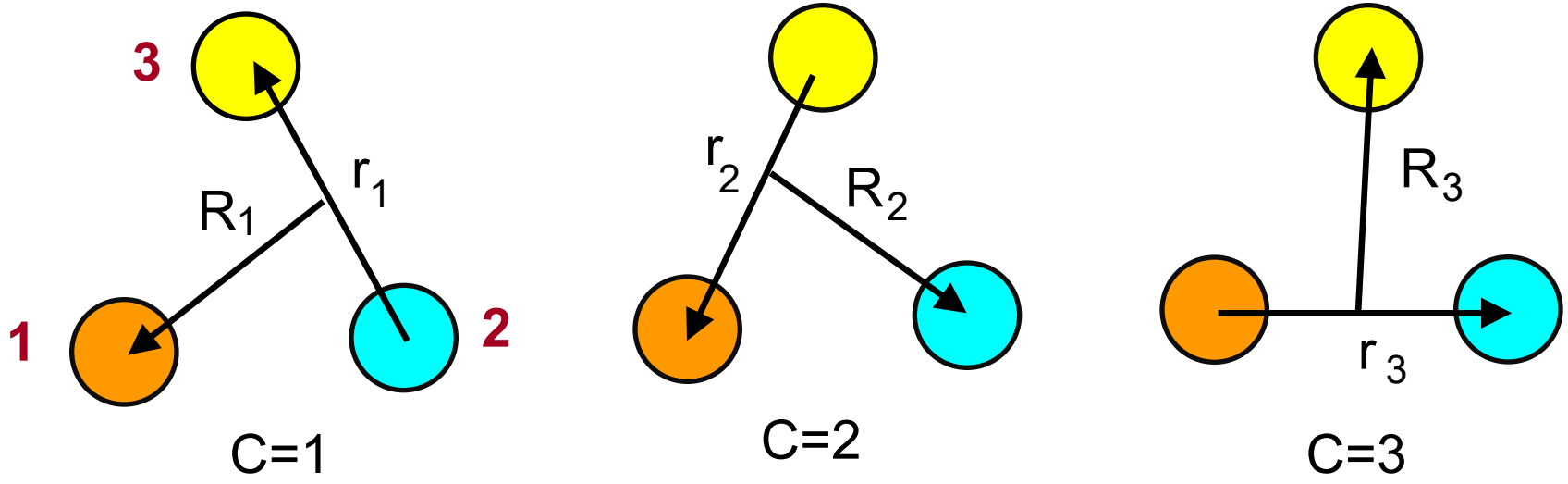
$$(H - E)\Psi_{JM} = 0$$

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

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

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

Why we take 3-channels?



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

Basis functions of each Jacobi coordinate

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

$Y_{lm}(\hat{\mathrm{r}}_c)$: (θ, ϕ) — $Y_{LM}(\hat{\mathrm{R}}_c)$: (Θ, Φ)

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

in the next slide

Determined by diagonalizing H

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

$$\left[Y_l(\hat{\mathrm{r}}) \otimes Y_L(\hat{\mathrm{R}}) \right]_{JM} = \sum_{m,K} (lmLK|JM)\, Y_{lm}(\hat{\mathrm{r}})\, Y_{LK}(\hat{\mathrm{R}})$$

(θ, ϕ)

Clebsh-Gordon coefficient in order to couple two angular momenta l and L to J.

Spherical harmonics

$$Y_{lm}(\theta, \phi) = \sum_{j=0}^{[\frac{l-m}{2}]} A_{lmj}\ \cos^{l-m-2j}\theta\ \sin^{m+2j}\theta\, e^{im\phi}$$

$$A_{lmj} = \left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right]^{\frac{1}{2}} \frac{(l+m)!}{2^m} \frac{(-)^j}{4^j\, j!(m+j)!(l-m-2j)!}$$

Complicated !

$$Y_{21}(\theta, \phi)\ \propto \cos\theta \sin\theta\, e^{i\phi}$$

Section 3

Gaussian basis functions

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

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

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

Using this three-body basis function, we calculate the matrix element of Hamiltonian.

Channel a　　Channel b

$$\langle\, \phi^{(a)}_{nl}(r_a)\, \psi^{(a)}_{NL}(R_a)\, [\, Y_\ell(\hat{\mathbf{r}}_a) \otimes Y_L(\widehat{\mathbf{R}}_a)\,]_{JM} \,|\, H \,|\, \phi^{(b)}_{nl}(r_b)\, \psi^{(b)}_{NL}(R_b)\, [\, Y_\ell(\hat{\mathbf{r}}_b) \otimes Y_L(\widehat{\mathbf{R}}_b)\,]_{JM} \rangle$$

The key point of solving 3-body problem:

To propose basis functions to calculate the matrix elements easily between basis functions of different channels

The suited basis function is

Gaussian basis function proposed by Kyushu Univ. Group

(afterwards, we shall propose more improved 'infinitesimally Gaussian Lobe basis functions').

For this purpose, we use the following basis function:

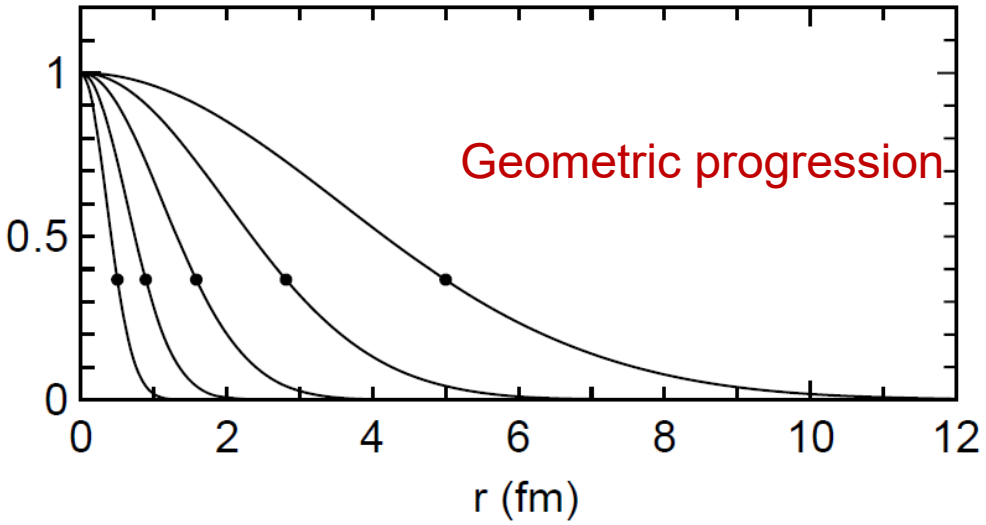
$$\phi_{nlm}(\mathbf{r}) = r^l e^{-\nu_n r^2} Y_{lm}(\hat{\mathrm{r}})$$

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

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

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.



Gaussian basis function proposed by Kyushu Univ. Group

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

$$\downarrow$$

$$(\theta, \phi)$$

If the interaction between constituent particles is central force, we can calculate the 3-body matrix element easily (but not easy for beginners).

The method has been applied to nuclear physics successfully.

However, it is very difficult to apply to

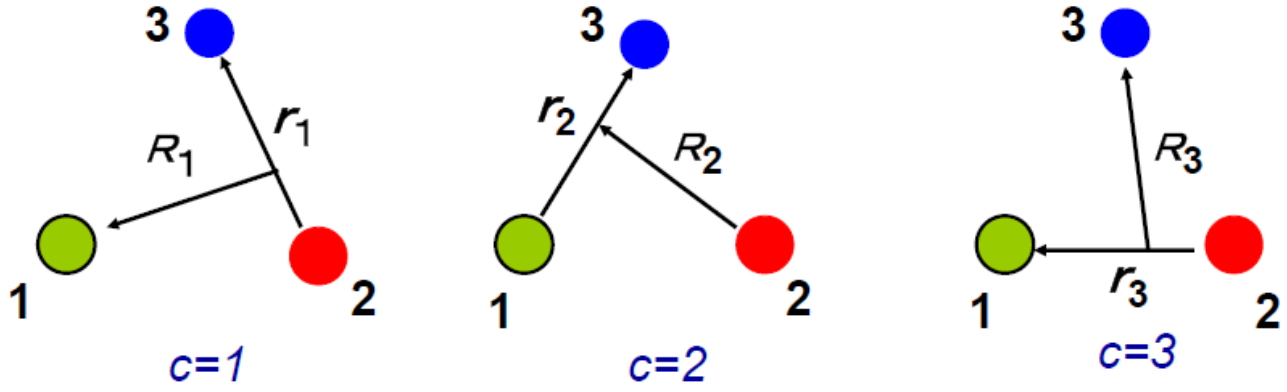
i) 3-body problem with complicated interaction such as spin-orbit forces and tensor forces.

ii) 4-body problems.

Why difficult?

I shall explain why.

In the morning on 30 July



General case of 3-body matrix calculation

c=1 c=3 c=2

$$\langle \Phi^{(1)}_{JM}(\vec{r}_1, \vec{R}_1) \mid V_0 e^{-\nu r_3^2} \mid \Phi^{(2)}_{JM}(\vec{r}_2, \vec{R}_2) \rangle_{\boldsymbol{r}_3, \boldsymbol{R}_3}$$

$$\Phi^{(1)}_{JM}(\vec{r}_1, \vec{R}_1) = r_1^l e^{-\nu r_1^2} R_1^L e^{-\lambda R_1^2} [Y_l(\hat{\mathbf{r}_1}) \otimes Y_L(\hat{\mathbf{R}_1})]$$

$$\Phi^{(2)}_{JM}(\vec{r}_2, \vec{R}_2) = r_2^l e^{-\nu r_2^2} R_2^L e^{-\lambda R_2^2} [Y_l(\hat{\mathbf{r}_2}) \otimes Y_L(\hat{\mathbf{R}_2})]$$

座標変換

c=1 to c=3

$$\mathbf{r}_1 = \alpha_{13}\mathbf{r}_3 + \beta_{13}\mathbf{R}_3$$

$$\mathbf{R}_1 = \gamma_{13}\mathbf{r}_3 + \delta_{13}\mathbf{R}_3$$

c=2 to c=3

$$\mathbf{r}_2 = \alpha_{23}\mathbf{r}_3 + \beta_{23}\mathbf{R}_3$$

$$\mathbf{R}_2 = \gamma_{23}\mathbf{r}_3 + \delta_{23}\mathbf{R}_3$$

座標変換　　c=1 to c=3

$$\mathbf{r}_1 = \alpha_{13}\mathbf{r}_3 + \beta_{13}\mathbf{R}_3 \qquad \mathbf{R}_1 = \gamma_{13}\mathbf{r}_3 + \delta_{13}\mathbf{R}_3$$

$$Y_{lm}(\theta,\phi) = \sum_{j=0}^{[\frac{l-m}{2}]} A_{lmj}\,\cos^{l-m-2j}\theta\,\sin^{m+2j}\theta\,e^{im\phi}$$

Complicated transformation of $Y_{lm}(\theta,\phi)$

Y- 2個

$$r_1^l Y_{lm}(\widehat{\boldsymbol{r}_1}) = \sum_{\lambda=0}^{l} \left[\frac{4\pi(2l+1)!}{(2\lambda+1)!(2\lambda-2l+1)!}\right]^{\frac{1}{2}} (\alpha_{13}r_{13})^{\lambda}(\beta_{13}R_3)^{l-\lambda}[Y_{\lambda}(\widehat{\mathbf{r}_3}) \otimes Y_{l-\lambda}(\widehat{\mathbf{R}_3})]_{lm}$$

Similarly for $Y_{lm}(\widehat{\mathbf{r}_2})$, $Y_{LM}(\widehat{\mathbf{R}_1})$, $Y_{LM}(\widehat{\mathbf{R}_2})$ → Y- 6個

Radial part:　c=1 to c=3

$$e^{-\nu r_1^2} = e^{-ar_3^2 - bR_3^2 + 2c\mathbf{r}_3\cdot\mathbf{R}_3}$$

Y- 2個

$$= e^{-ar_3^2-bR_3^2} \sum_{\lambda} 4\pi I_{\lambda}(cr_3R_3)\left[Y_l(\widehat{\mathbf{r}_3}) \otimes Y_l(\widehat{\mathbf{R}_3})\right]$$

Modified Bessel function

Total number of Y-functions =10　**Y- 共計10個**

In 3-body problems, we meet these angle-intergrations including at least **10** shperical harmonics,

$$\int\int d\theta\, d\phi\, Y_{\ell_1 m_1}(\theta,\phi) Y_{\ell_2 m_2}(\theta,\phi) Y_{\ell_3 m_3}(\theta,\phi) Y_{\ell_4 m_4}(\theta,\phi) Y_{\ell_5 m_5}(\theta,\phi)$$
$$\times \int\int d\Theta\, d\Phi\, Y_{L_1 M_1}(\Theta,\Phi) Y_{L_2 M_2}(\Theta,\Phi) Y_{L_3 M_3}(\Theta,\Phi) Y_{L_4 M_4}(\Theta,\Phi) Y_{L_5 M_5}(\Theta,\Phi)$$

24 shperical harmonics in 4-body problems

$$\int\int d\theta\, d\phi\, Y_{\ell_1 m_1}(\theta,\phi) Y_{\ell_2 m_2}(\theta,\phi) Y_{\ell_3 m_3}(\theta,\phi) Y_{\ell_4 m_4}(\theta,\phi) Y_{\ell_5 m_5}(\theta,\phi) \times Y_{\ell_6 m_6}(\theta,\phi) Y_{\ell_7 m_7}(\theta,\phi) Y_{\ell_8 m_9}(\theta,\phi)$$
$$\times \int\int d\Theta\, d\Phi\, Y_{L_1 M_1}(\Theta,\Phi) Y_{L_2 M_2}(\Theta,\Phi) Y_{L_3 M_3}(\Theta,\Phi) Y_{L_4 M_4}(\Theta,\Phi) Y_{L_5 M_5}(\Theta,\Phi) \times Y_{L_6 M_6}(\Theta,\Phi) Y_{L_7 M_7}(\Theta,\Phi) Y_{L_8 M_8}(\Theta,\Phi)$$
$$\times \int\int d\theta'\, d\phi'\, Y_{\ell'_1 m'_1}(\theta',\phi') Y_{\ell'_2 m'_2}(\theta',\phi') Y_{\ell'_3 m'_3}(\theta',\phi') Y_{\ell'_4 m'_4}(\theta',\phi') Y_{\ell'_5 m'_5}(\theta',\phi') \times Y_{\ell'_6 m'_6}(\theta',\phi') Y_{\ell'_7 m'_7}(\theta',\phi') Y_{\ell'_8 m'_9}(\theta',\phi')$$

This calculation is very difficult, especially for beginners such as master-course students. The result is

The 3-body interaction matrix element : Gaussian potential $e^{-\mu r_3^2}$

$$\langle \Phi^{(1)}_{JM}(\boldsymbol{r}_1,\boldsymbol{R}_1)| \; e^{-\mu r_3^2} \; | \Phi^{(2)}_{JM}(\boldsymbol{r}_2,\boldsymbol{R}_2)\rangle$$

$$= \langle r_1^{l} R_1^{L} e^{-\nu r^2} e^{-\lambda R^2} [Y_l(\hat{r}_1) \times Y_L(\hat{R}_1)]_{JM} | \; e^{-\mu r_3^2} \; |$$
$$\times r_2^{l} R_2^{L} e^{-\nu r^2} e^{-\lambda R^2} [Y_l(\hat{r}_2) \times Y_L(\hat{R}_2)]_{JM} \rangle$$

$$= \sum\sum\sum\sum \gamma^{\lambda} \delta^{l-\lambda} \gamma'^{\Lambda} \delta^{L'-\lambda}$$

$$\times \sqrt{(2l-1)!(2L'-1)!/(2\lambda!)(2(l'-\lambda)!)(2\Lambda)!(2(L'-\Lambda)!(2l+1)!(2J+1)!}$$

$$\times \begin{Bmatrix} \Lambda & l'-\lambda & l' \\ \Lambda & L'-\Lambda & L' \\ l & K & J \end{Bmatrix} (-)^{l+l+J} (\lambda\Lambda 00|l0)\,(l'-\lambda\; L'-\lambda|K0)$$

9j symbol

Clebsch-Gorgon coefficent

Racah coeffiient

$$\times \sum W(llKL;jJ)\,(KL00|j0)\,(ll00|j0)(2m+2j+1)!!/2^{m+j+n+4}\, m!(\xi-\xi^2/\eta)^{j+n+j/2}$$

$$\times \sum (2p+2j+2n+1)!!/(2P+2j+1)!! \begin{bmatrix} m \\ p \end{bmatrix} (\xi^2/(\zeta\eta-\xi^2))^p$$

Summerizing, **3-body matrix elements**

$$\langle \phi_{nl}^{(a)}(r_a)\,\psi_{NL}^{(a)}(R_a)\,[\,Y_\ell(\hat{\mathbf{r}}_a)\otimes Y_L(\widehat{\mathbf{R}}_a)\,]_{JM}\,|\,H\,|\,\phi_{nl}^{(b)}(r_b)\,\psi_{NL}^{(b)}(R_b)\,[\,Y_\ell(\hat{\mathbf{r}}_b)\otimes Y_L(\widehat{\mathbf{R}}_b)\,]_{JM}\rangle$$

It is laborious to integrate over the angular coordinate of spherical harmonics $Y_{lm}(\theta,\phi)$

a) In the case of calculating the matrix element of central force, we have 10 spherical harmonics'.
This is hard for beginner.

b) In the case of complicated interaction such as spin-orbit force and tensor force, we have more than 10 spherical harmonics'. This is hard even for experts.

c) In the case of four-body problem, we have 24 spherical harmonics at least. This is hard even for experts.

Difficult points using $r^{\ell} e^{-\nu_n r^2} Y_{\ell m}(\hat{\mathbf{r}})$

a) 3-body problem using complicated interactions

b) 4-body problem

It is difficult even for expert to apply the method to a) and b) cases.

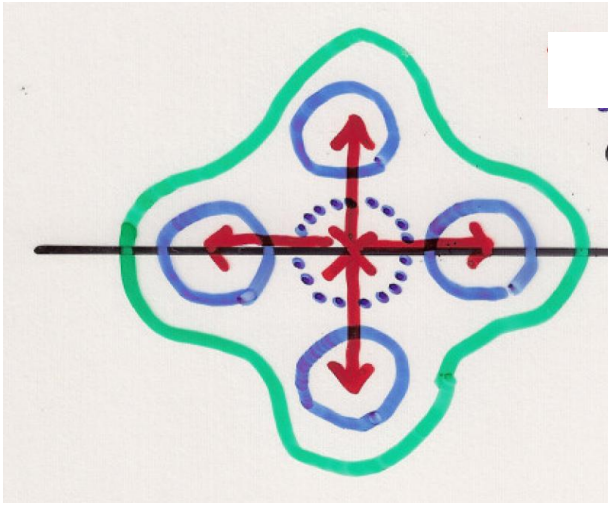
We should overcome this difficulty and make the method to be applicable for beginners such as master course students.

I proposed (1994):
Infinitesimally shifted Gaussian Lobe basis function

Section 3.1

無限小　位移

Infinitesimally Shifted Gaussian Lobe basis function



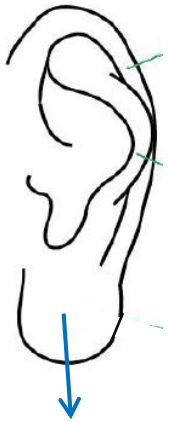
無限小 位移
Infinitesimally shifted Gaussian Lobe basis function

What is Lobe ?

Lobe = something
roundly sticking out

圓的突出部

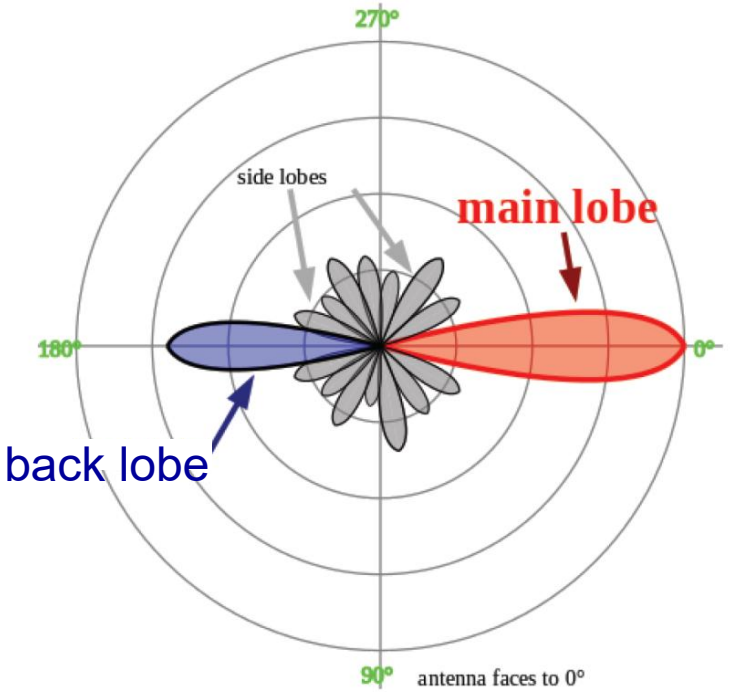
Ear 耳



Ear-Lobe

耳垂

來自天線的電波輻射的圖形

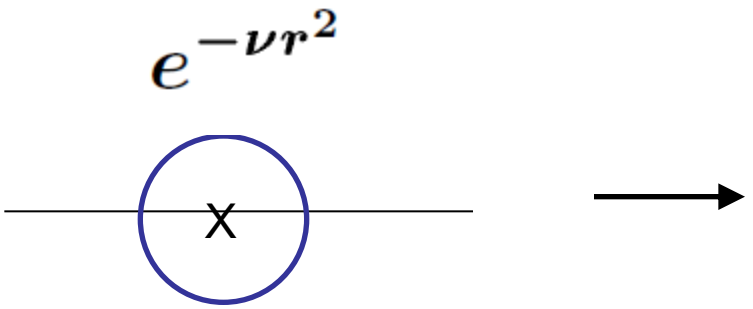


Radiation pattern of antennas shows a pattern of *Lobes* at various angles.

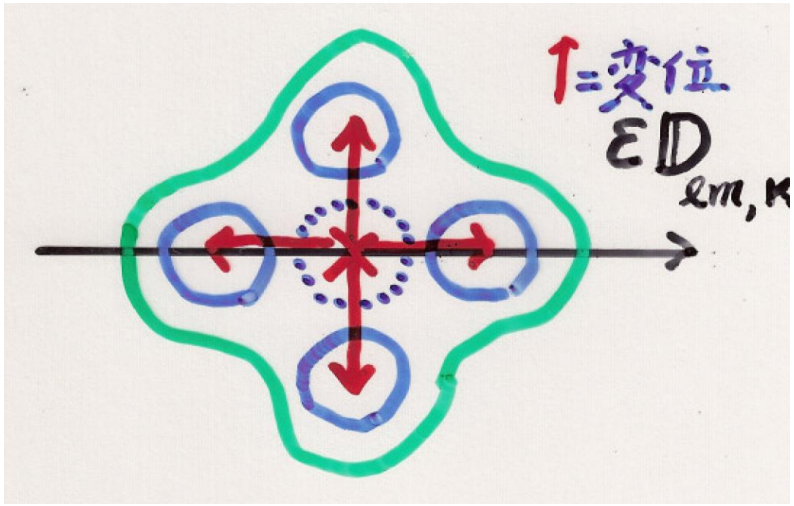
Infinitesimally Shifted Gaussian Lobe (ISGL) basis Function

$$r^l e^{-\nu r^2} Y_{\ell m}(\theta,\phi) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^l} \sum_{k=1}^{k_{\max}} C_{lm,k}\, e^{-\nu(\boldsymbol{r} - \varepsilon \boldsymbol{D}_{lm,k})^2}$$

位移



A Gaussian function around the origin



Describe angular dependence by sum of **shifted** Gaussian functions (without spherical harmonics)

The simplest example

↓

Shifted parameter *C*, ***D*** can be easily determined.

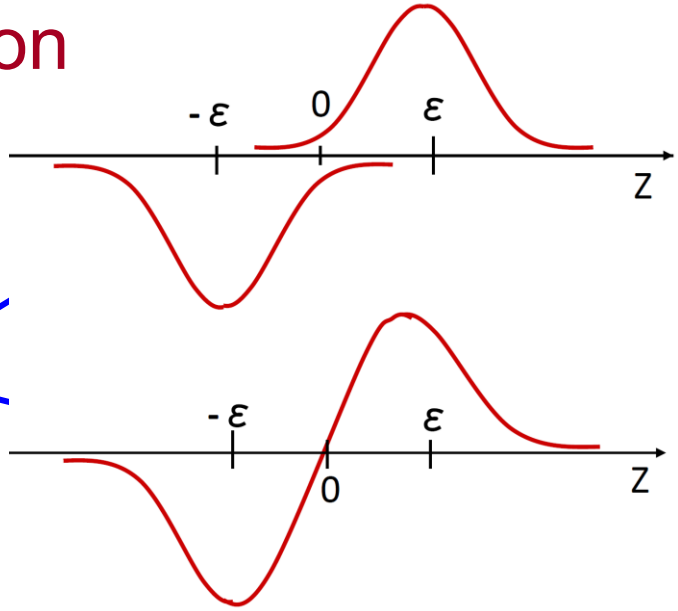
Construction of the ISGL function

Simple example: l=1,m=0

roughly

$$e^{-\nu r^2}\, r\, Y_{10}(\hat{\mathbf{r}}) \quad \propto \quad z e^{-\nu z^2}$$

$$e^{-\nu(z-\varepsilon)^2} - e^{-\nu(z+\varepsilon)^2}$$



In detail

$$\frac{1}{\varepsilon}\left[e^{-\nu(z-\varepsilon)^2} - e^{-\nu(z+\varepsilon)^2}\right] = \frac{1}{\varepsilon} e^{-\nu(z^2+\varepsilon^2)}\left[e^{2\nu\varepsilon z} - e^{-2\nu\varepsilon z}\right]$$

Taylor expansion

$$= \frac{1}{\epsilon} e^{-\nu(z^2+\epsilon^2)}\left[1 + (2\epsilon\nu z) + \frac{(2\epsilon\nu z)^2}{2!} + \frac{(2\epsilon\nu z)^3}{3!} + \cdot\cdot\right]$$

$$- \frac{1}{\epsilon} e^{-\nu(z^2+\epsilon^2)}\left[1 - (2\epsilon\nu z) + \frac{(2\epsilon\nu z)^2}{2!} - \frac{(2\epsilon\nu z)^3}{3!} + \cdot\cdot\right]$$

$$= \frac{1}{\varepsilon} e^{-\nu(z^2+\varepsilon^2)}\left[4\varepsilon\nu z + \frac{2}{3}(2\varepsilon\nu z)^3 + \cdot\cdot\cdot\cdot\cdot\right] \overset{\varepsilon\to 0}{\longrightarrow} 4\nu\, z\, e^{-\nu z^2}$$

Mixture of L=3

$$r\, e^{-\nu r^2}\, Y_{10}(\hat{\mathbf{r}}) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \sum_{k=1}^{2} C_{10,k}\, e^{-\nu(\mathbf{r} - \varepsilon\, \mathbf{D}_{10,k})^2}$$

$$C_{10,k} = \frac{(-1)^{k-1}}{8\nu}\sqrt{\frac{3}{\pi}} \qquad \mathbf{D}_{10,k} = (-1)^{k-1}\mathbf{e_z} \qquad (k=1,2)$$

Unit vector for Z-axis

$$r^l e^{-\nu r^2} Y_{\ell m}(\theta,\phi) = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^l} \sum_{k=1}^{k_{\max}} C_{lm,k}\, e^{-\nu(\boldsymbol{r} - \varepsilon \boldsymbol{D}_{lm,k})^2}$$

For any angular momentum (l, m),

using the mathematical formura

$$r^l\, Y_{\ell m}(\theta,\phi) = \sum_{j=0}^{[\frac{l-m}{2}]} A_{lm,j}\, z^{l-m-2j}\, (x+iy)^{m+j}\, (x-iy)^j$$

simple factor

we can easily derive

the shift parameters $C_{lm,k}$ and $\mathrm{D}_{lm,k}$

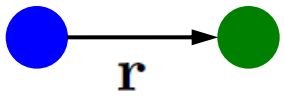
Details is written in

E. Hiyama *et al*. Prog. Part. Nucl. Phys. **51** (2003) 223.

Calculation of 2-body norm matrix element

It is too simple but very instructive.

2体問題



Normal Lobe

$$\Phi_{lm}(\nu,\mathbf{r}) = r^l e^{-\nu r^2} Y_{lm}(\hat{\mathbf{r}}) = \lim_{\varepsilon\to 0} \Phi_{lm}(\varepsilon,\nu,\mathbf{r})$$

$$\Phi_{lm}(\varepsilon,\nu,\mathbf{r}) = \frac{1}{\varepsilon^l}\sum_{k=1}^{k_{\max}} C_{lm,k}\, e^{-\nu(\mathbf{r}-\varepsilon\mathbf{D}_{lm,k})^2}$$

Norm matrix element

$$\langle \Phi_{lm}(\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\nu',\mathbf{r})\rangle = \lim_{\varepsilon,\varepsilon'\to 0} \langle \Phi_{lm}(\varepsilon,\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\varepsilon',\nu',\mathbf{r})\rangle$$

(straightforward integaration)

$$= A \lim_{\varepsilon,\varepsilon'\to 0} \frac{1}{(\varepsilon\varepsilon')^l} \sum_k \sum_{k'} C^*_{lm,k} C_{lm,k'}\, e^{-\alpha\,\varepsilon\varepsilon'(\mathbf{D}^*_{lm,k}\cdot\mathbf{D}_{lm,k'})}$$

$$A = \left(\frac{\pi}{\nu+\nu'}\right)^{3/2} \qquad \alpha = \frac{2\nu\nu'}{\nu+\nu'}$$

=1
(for $\nu = \nu'$)

$$\langle \Phi_{lm}(\nu, \mathbf{r})| \quad 1 \quad |\Phi_{lm}(\nu', \mathbf{r})\rangle = \lim_{\varepsilon,\varepsilon' \to 0} \langle \Phi_{lm}(\varepsilon, \nu, \mathbf{r})| \quad 1 \quad |\Phi_{lm}(\varepsilon', \nu', \mathbf{r})\rangle$$

$$= A \lim_{\varepsilon,\varepsilon' \to 0} \frac{1}{(\varepsilon\varepsilon')^l} \sum_k \sum_{k'} C^*_{lm,k} C_{lm,k'} \; e^{-\alpha\, \varepsilon\, \varepsilon'} \, (\mathbf{D}^*_{lm,k} \cdot \mathbf{D}_{lm,k'})$$

$=1$

(for $\nu = \nu'$)

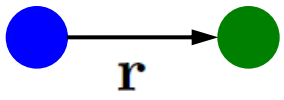
Finite value of ε,ε'->mixture of angular momenta
Small value of ε,ε'-> round-off error

What is round-off error?

Calculation of 2-body norm matrix element

It is too simple but very instructive.

2体問題



Normal Lobe

$$\Phi_{lm}(\nu,\mathbf{r}) = r^l e^{-\nu r^2} Y_{lm}(\hat{\mathbf{r}}) = \lim_{\varepsilon\to 0} \Phi_{lm}(\varepsilon,\nu,\mathbf{r})$$

$$\Phi_{lm}(\varepsilon,\nu,\mathbf{r}) = \frac{1}{\varepsilon^l}\sum_{k=1}^{k_{\max}} C_{lm,k}\, e^{-\nu(\mathbf{r}-\varepsilon\mathbf{D}_{lm,k})^2}$$

Norm matrix element

$$\langle \Phi_{lm}(\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\nu',\mathbf{r})\rangle = \lim_{\varepsilon,\varepsilon'\to 0} \langle \Phi_{lm}(\varepsilon,\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\varepsilon',\nu',\mathbf{r})\rangle$$

(straightforward integaration)

$$= A \lim_{\varepsilon,\varepsilon'\to 0} \frac{1}{(\varepsilon\varepsilon')^l} \sum_k \sum_{k'} C^*_{lm,k} C_{lm,k'}\, e^{-\alpha\,\varepsilon\varepsilon'(\mathbf{D}^*_{lm,k}\cdot\mathbf{D}_{lm,k'})}$$

$$A = \left(\frac{\pi}{\nu+\nu'}\right)^{3/2} \qquad \alpha = \frac{2\nu\nu'}{\nu+\nu'}$$

=1
(for $\nu = \nu'$)

$$\langle \Phi_{lm}(\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\nu',\mathbf{r})\rangle = \lim_{\varepsilon,\varepsilon'\to 0} \langle \Phi_{lm}(\varepsilon,\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\varepsilon',\nu',\mathbf{r})\rangle$$

$$= A \lim_{\varepsilon,\varepsilon'\to 0} \frac{1}{(\varepsilon\varepsilon')^l} \sum_k \sum_{k'} C^*_{lm,k} C_{lm,k'} \; e^{-\alpha\,\varepsilon\,\varepsilon'} \, (\mathbf{D}^*_{lm,k} \cdot \mathbf{D}_{lm,k'})$$

$=1$ (for $\nu = \nu'$)

We calculate $e^{-\alpha\varepsilon\varepsilon'}$ in Fortran code as DEXP(-αεε').

a) This generates serious mixture of $Y_{lm}(\hat{\mathbf{r}})$ with higher ℓ for a finite value of ε

To avoid the mixture of $Y_{lm}(\hat{\mathbf{r}})$

For example, we take =0.00001. The matrix element =1.00022333.

Then, ε =0.000000001. But, the matrix element =1.223333333! Why?

This phenomena is round-off error.

けた落ち

In calculation by computers, usually numbers are given in **15** significant figures (digits) .

有効数字

no problem

15

1.000000000000123
+) 1.000000000000121

2.000000000000244

有効数字=15

however

15

1.000000000000123
-) 1.000000000000121

0.000000000000002

$= 2 \times 10^{-14}$

Only one **significant** figure !

有効数字=1

Be careful when subtracting nearly the same numbers.

So far, I though that this new basis function was my original idea.
However, I found that text the similar basis function was introduced in quantum chemistry textbook.
According to the textbook,
It mentioned that when ε have some value, we have mixture of higher angular momentum. When ε=>0,
We have serious round-off error.

Then, due to this difficulty,

the old Gaussian Lobe method (1960's) was NOT

used in actual calculations and was

soon forgotten (only used as exercise for student) .

I was so shocked to read the textbook. And I lost the motivation to do research for one week.

But, some 30 years after, this difficulty was solved by Hiyama [3,6,7] by introducing the ISGL basis functions with properly taking $\lim_{\varepsilon \to 0}$ **after** performing the analytical integration of the matrix elements.

Hiyama's new method (at the time of MC student, 1994)

Infinitesimally Shifted Gaussian Lobe (ISGL) basis Function

$$\Phi_{lm}(\varepsilon,\nu,\mathbf{r}) = \frac{1}{\varepsilon^{\,l}} \sum_{k=1}^{k_{\max}} C_{lm,k}\; e^{-\nu(\mathbf{r}-\varepsilon\mathbf{D}_{lm,k})^2}$$

Norm matrix element

$$\langle\, \Phi_{lm}(\nu,\mathbf{r})|\quad 1\quad |\Phi_{lm}(\nu',\mathbf{r})\rangle = \lim_{\varepsilon,\varepsilon'\to 0} \langle\, \Phi_{lm}(\varepsilon,\nu,\mathbf{r})|\quad 1\quad |\Phi_{lm}(\varepsilon',\nu',\mathbf{r})\,\rangle$$

$$= A \lim_{\varepsilon,\varepsilon'\to 0} \frac{1}{(\varepsilon\varepsilon')^l} \sum_k \sum_{k'} C^*_{lm,k} C_{lm,k'}\; e^{-\alpha\,\varepsilon\,\varepsilon'\,(\mathbf{D}^*_{lm,k}\cdot\mathbf{D}_{lm,k'})}$$

$= 1$
(for $\nu = \nu'$)

Dangerous if we use FUNCTION EXP (….)

$e^{\varepsilon\varepsilon' x}$

Taylor expansion with very small ε and ε'

$$e^{\varepsilon\varepsilon' x} = 1 + (\varepsilon\varepsilon' x) + \frac{1}{2!}(\varepsilon\varepsilon' x)^2 + \cdots\cdots\cdots$$

If we take the full terms, it causes serius round-off error as is expected. But,

$$\frac{1}{(\varepsilon\varepsilon')^l}\sum_k\sum_{k'} C^*_{lm,k}C_{lm,k}\ e^{\varepsilon\varepsilon' x}$$

$$e^{\varepsilon\varepsilon' x} = \cancel{1} + \cancel{(\varepsilon\varepsilon' x)} + \frac{1}{2!}(\varepsilon\varepsilon' x)^2 + \cdots\cdots\cdots$$

But, I tried to omit the first term, namely "1" (I took $l = 2$).
I thought the term is the bad origin in the round-off error.
My superviser said -- "It is very stupid because, in the Talor expansion, the first term is the most important and the higher-order terms are less important".
I answered --"We shall never know the result, unless we try"

The result became slightly better, but not good.

Then, I omitted the second term too.
Surprisingly, we obtained the exact result, namlely Norm =1.0

What happened ???

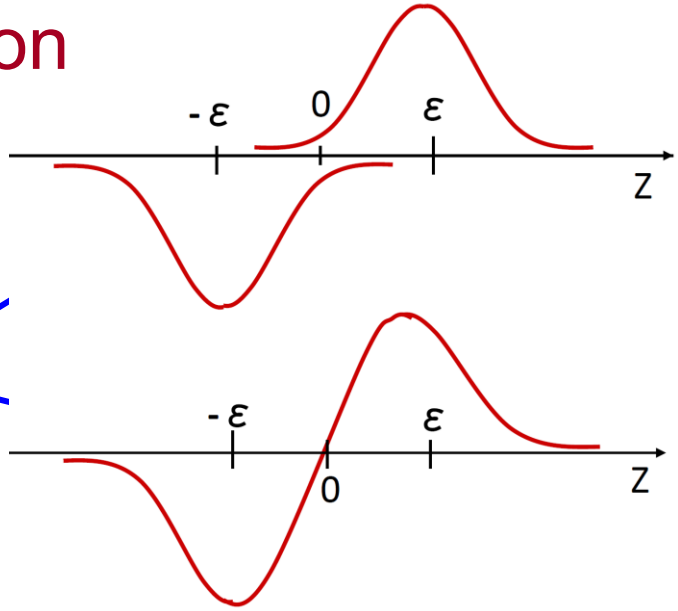
Construction of the ISGL function

Simple example: l=1,m=0

roughly

$$e^{-\nu r^2}\, r\, Y_{10}(\hat{\mathbf{r}}) \quad \propto \quad z e^{-\nu z^2}$$

$$e^{-\nu(z-\varepsilon)^2} - e^{-\nu(z+\varepsilon)^2}$$



In detail

$$\frac{1}{\varepsilon}\left[e^{-\nu(z-\varepsilon)^2} - e^{-\nu(z+\varepsilon)^2}\right] = \frac{1}{\varepsilon} e^{-\nu(z^2+\varepsilon^2)}\left[e^{2\nu\varepsilon z} - e^{-2\nu\varepsilon z}\right]$$

Taylor expansion

$$= \frac{1}{\epsilon} e^{-\nu(z^2+\epsilon^2)}\left[1 + (2\epsilon\nu z) + \frac{(2\epsilon\nu z)^2}{2!} + \frac{(2\epsilon\nu z)^3}{3!} + \cdot\cdot\right]$$

$$- \frac{1}{\epsilon} e^{-\nu(z^2+\epsilon^2)}\left[1 - (2\epsilon\nu z) + \frac{(2\epsilon\nu z)^2}{2!} - \frac{(2\epsilon\nu z)^3}{3!} + \cdot\cdot\right]$$

First power of ε

$$= \frac{1}{\varepsilon} e^{-\nu(z^2+\varepsilon^2)}\left[4\varepsilon\nu z + \frac{2}{3}(2\varepsilon\nu z)^3 + \cdot\cdot\cdot\cdot\right] \overset{\varepsilon\to 0}{\longrightarrow} 4\nu\, z\, e^{-\nu z^2}$$

Mixture of L=3

$$e^{\varepsilon\varepsilon' x} = 1 + (\varepsilon\varepsilon' x) + \frac{1}{2!}(\varepsilon\varepsilon' x)^2 + \cdots\cdots\cdots \qquad 2$$

Second power is remained.

$$\frac{1}{(\varepsilon\varepsilon')^l} \sum_k \sum_{k'} C^*_{lm,k} C_{lm,k'} \, e^{-\alpha\,\varepsilon\,\varepsilon'\,(\mathbf{D}^*_{lm,k}\cdot\mathbf{D}_{lm,k'})}$$

Taylor expansion

$$\sum_{j=l}^{\infty} \sum_{k=1}^{k_{\max}} \sum_{k'=1}^{k_{\max}} C_{lm,k}\, C_{lm,k'} \frac{1}{j!} \left(\nu_n \varepsilon\varepsilon'\, \mathrm{D}^*_{lm,k} \cdot \mathrm{D}_{lm,k'}\right)^j .$$

$$= 0 \quad (j < l)$$

The shift parameters were so constructed at the beginning.

The terms with $j > l$ can be neglected for small ε

It is sufficient to pickup the terms with $j = l$

Thus, my method solved the Gauss-Lobe's difficulty (since 1960's in quantum chemistry):

1) higher-angular-momentum mixing
2) severe round-off error.

The method using ISGL function is applicable for especially nuclear physics with high accuracy.

The merit of this method:

(1) To calculate the few-body matrix elements very easily.

(2) To calculate the energy of few-body bound state very accurately.

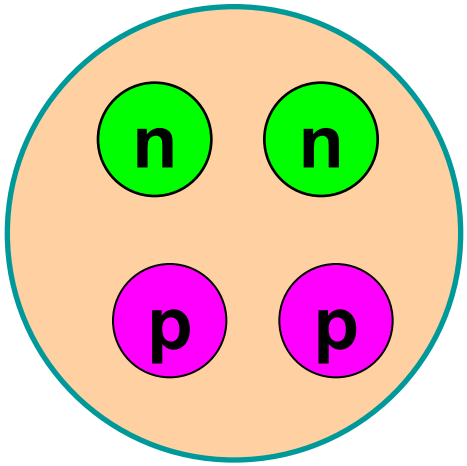
(3) To calculate the wave function very precisely both in the short-range region and long-range region.

Section 4

A successful example:

Benchmark-test calculation to solve

the 4-nucleon bound state



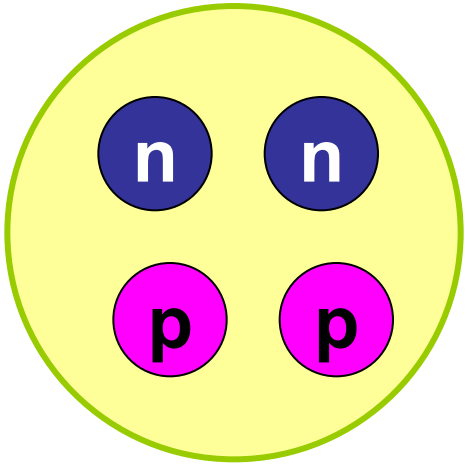
PRC **64**, 044001(2001)

Benchmark-test calculation to solve the 4-nucleon bound state

7 different groups (18 co-authors)

1. Faddeev-Yakubovski (Kamada et al.)
2. Gaussian Expansion Method (Hiyama and Kamimura)
3. Stochastic varitional (Varga et al.)
4. Hyperspherical variational (Viviani et al.)
5. Green Function Variational Monte Carlo (Carlson at al.)
6. Non-Core shell model (Navratil et al.)
7. Effective Interaction Hypershperical HarmonicsEIHH (Barnea et al.)

^{4}He

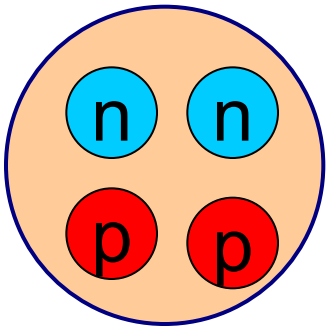


4-nucleon bound state
NN: AV8’

Benchmark-test calculation of the 4-nucleon bound state

Within the 7 groups

1）subject: Let's solve the 4-body problem and obtain the binding energy and wavefunction of ^{4}He by using their own calculation methods.



^{4}He

2）We all should send our results to Prof. Gloeckle at Ruhr Univ. until 1st February, 2001 by e-mail. Therefore, we all know ONLY our own result and do not know other groups' results (a blind-calculation test)

3）As soon as Prof. Gloeckle got all results, he wrote the paper and submitted it to Physical Review C (PRC). We all knew each other's results after this paper was submitted to PRC (What a terrible test !).

This competition is very severe and stressful !

Happiest	All of our results are in good agreement with each other.
Happier	All of our results are different from each other. We do not know which one is correct.
Happy	Divided into 2 groups. We do not know which group give the correct result.
unhappy	The groups except me give the correct result. My result only is wrong!

Benchmark-test 4-body calculation : Phys. Rev. C64 (2001), 044001

Benchmark test calculation of a four-nucleon bound state

by 7 groups

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M. Kamimura
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③ K. Varga
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Y. Suzuki
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⑥ Steven C. Pieper and R. B. Wiringa
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W. Leidemann and G. Orlandini
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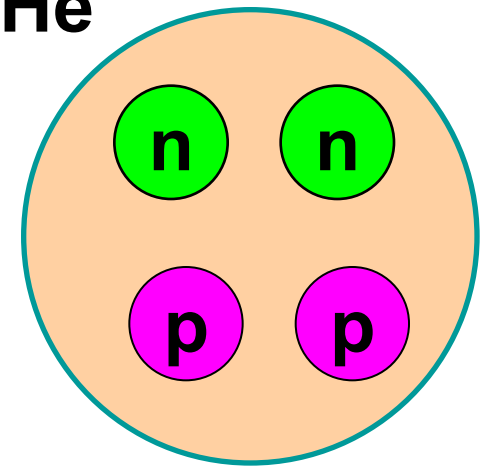
^{4}He



4 nucleon bound state

Realistic NN force: AV8'

Benchmark-test calculation of the 4-nucleon bound state

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

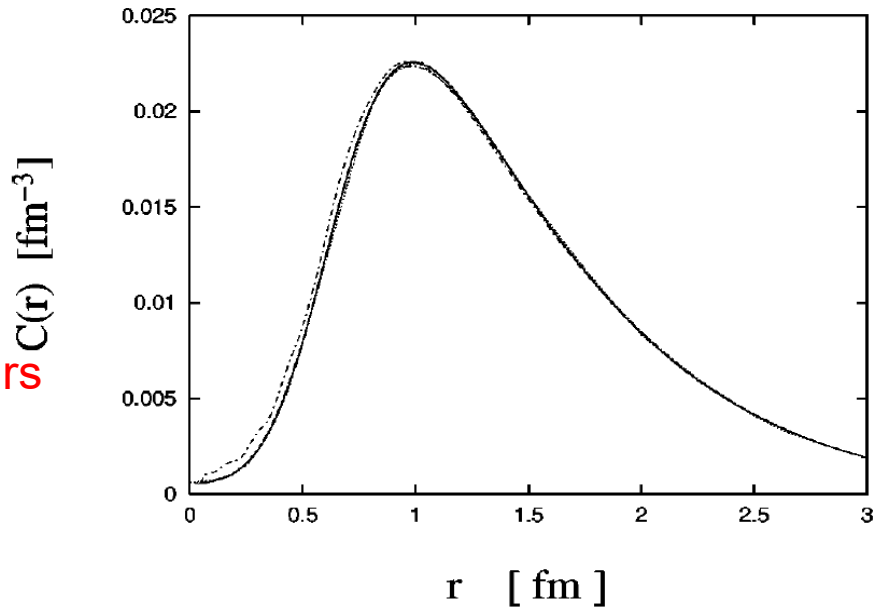


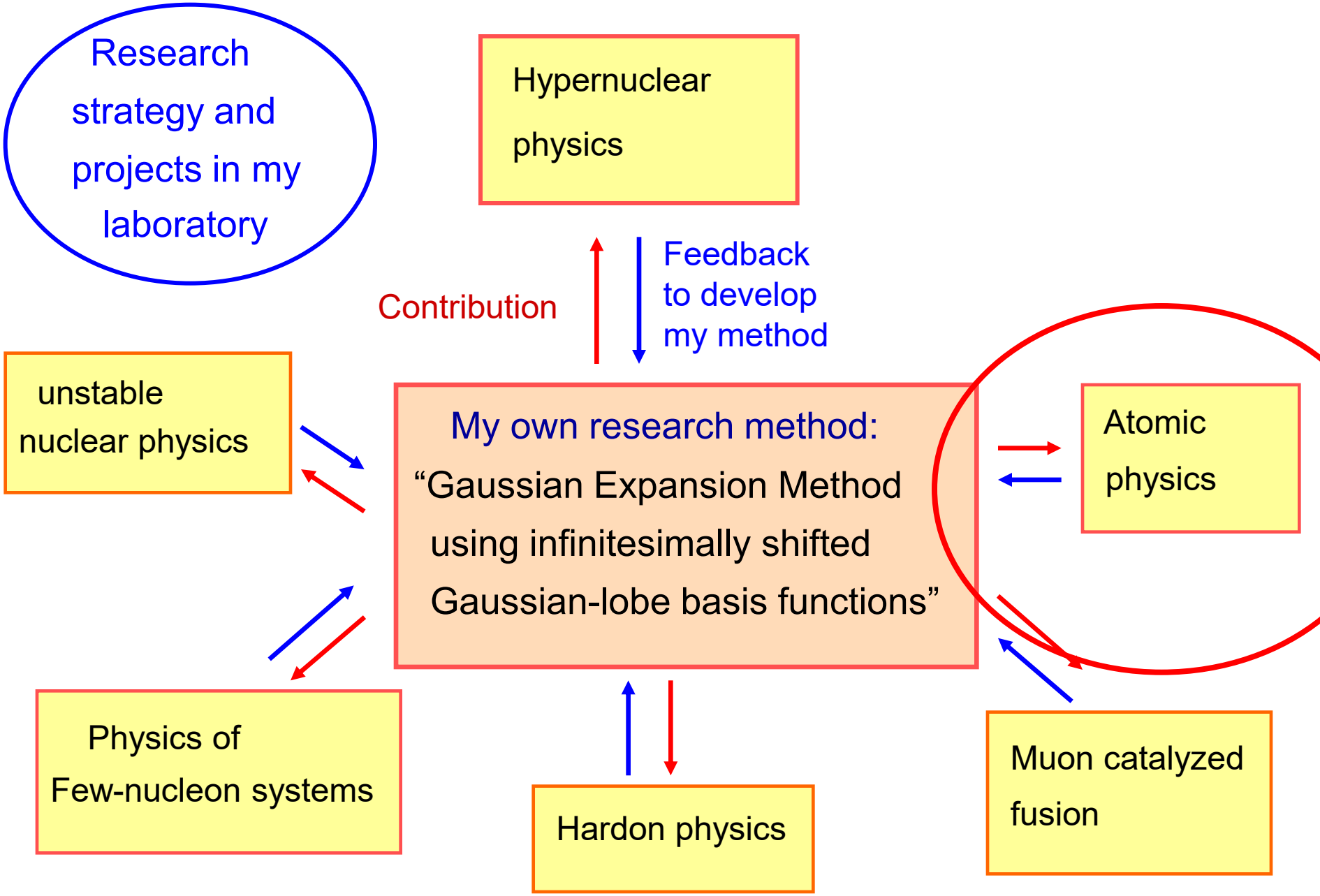
FIG. 1. Correlation functions in the different calculational schemes: EIHH (dashed-dotted curves), FY, CRCGV, SVM, HH, and NCSM (overlapping curves).

Congratulations!! I was very happy

Here, let me emphasize that

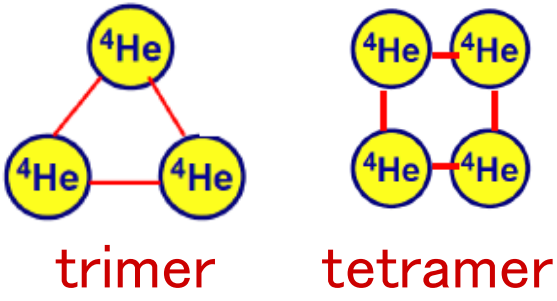
1) All the calculation methods from the 7 groups
   are all accurate and reliable.

2) The community of Few-Body Problems in Physics
   works so severely by checking
   their research results with each other.


Research strategy and projects in my laboratory
Hypernuclear physics
Contribution
Feedback to develop my method
unstable nuclear physics
My own research method:
"Gaussian Expansion Method using infinitesimally shifted Gaussian-lobe basis functions"
Atomic physics
Physics of Few-nucleon systems
Hardon physics
Muon catalyzed fusion

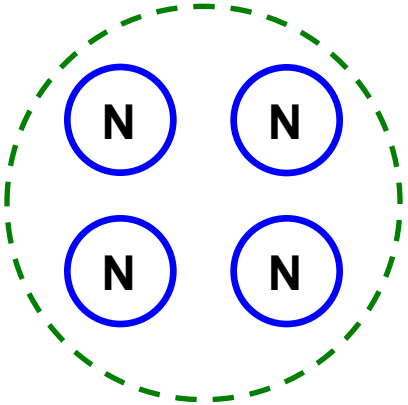
Section 5

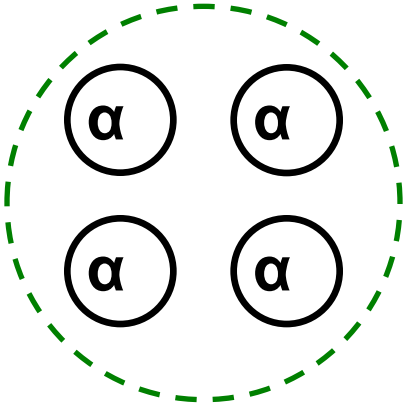
4He atomic three- and four-body systems



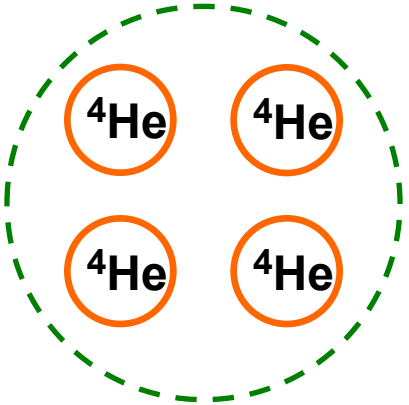
Nucleus

α= ^{4}He nucleus





Atom



^{4}He nucleus
(4 - Nucleon)

^{16}O nucleus
(4-**α**)

^{4}He - atom tetramer

Structure of nuclei

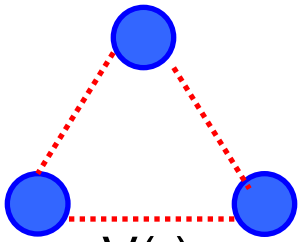
Structure of this system from view point of 'Efimov Physics'

In 1970, Efimov predicted the following phenomenon,

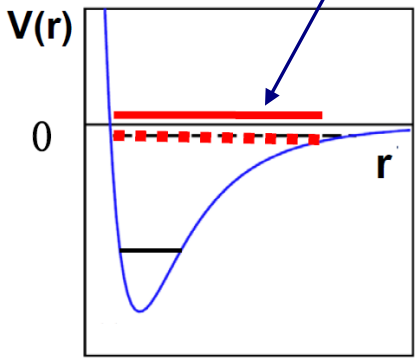
Efimov effect ;

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"].

Efimov effects in 4He atoms

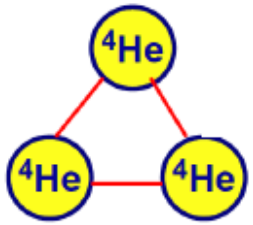
One of the most fundamental theoretical issues

from the view point of few-body problems:

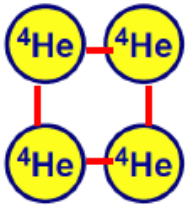
to perform accurate calculations of the

3- and 4-body 4He-atom systems

using realistic 4He-4He potentials.



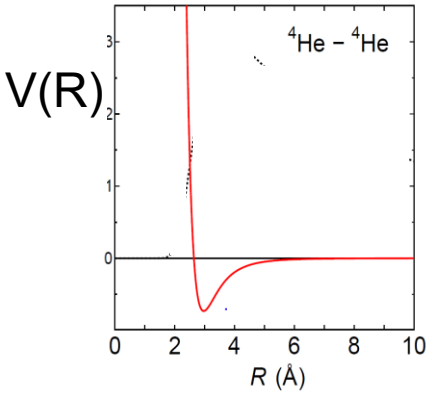
trimer



tetramer

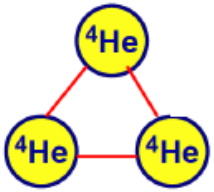
This subject has been intensively studied by nuclear physicists, atomic physicists and quantum chemists.

Realistic potential

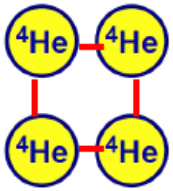


^{4}He-atom clusters --- Level structure known before our calculation :

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 — ?

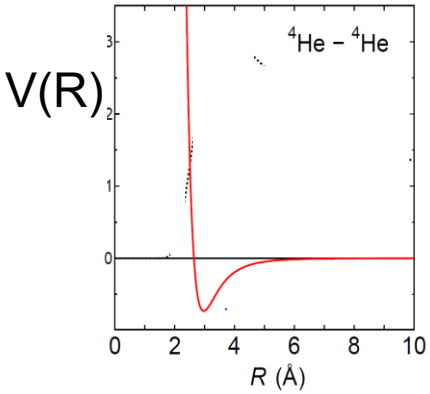
There are many 3-body calculations for 4He trimer.

0^+_1 ≈ -558 mK

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

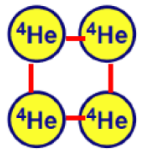
← Numerical difficulty:

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

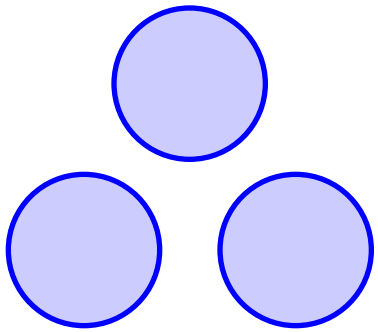
Method	Reference	potential	ground state (mK)	excited state (mK)
Monte Carlo	Lewerenz (1977)	TTY	558	
Monte Carlo	Bressanini *et al.* (2000)	TTY	559.1	
Monte Carlo	Blume and Greene (2000)	LM2M2	557	133
Faddeev	Lazauskas and Carbonell (2006)	LM2M2	557.5	127.5
Correlated potential harmonic expansion	Das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

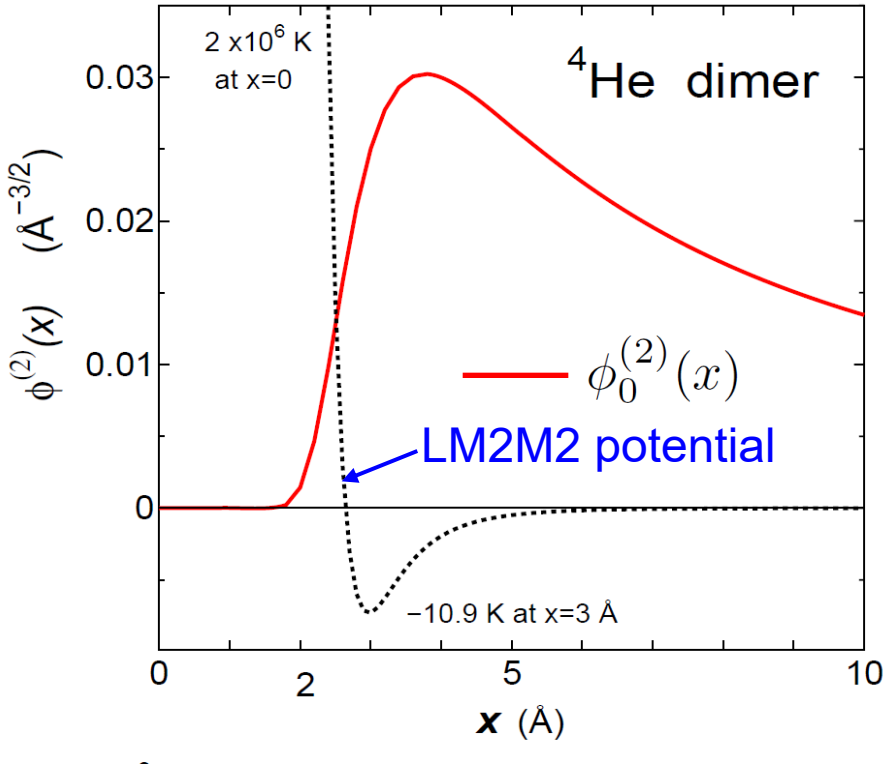
So, we intended to confirm this value by our bound-state calculation.

^{4}He Trimer and tetramer systems using LM2M2 potential



^{4}He Dimer

$$B^{(2)} = 1.30348 \text{ mK and } \sqrt{\langle x^2 \rangle} = 70.93 \text{ Å},$$
the same as those obtained in literature.



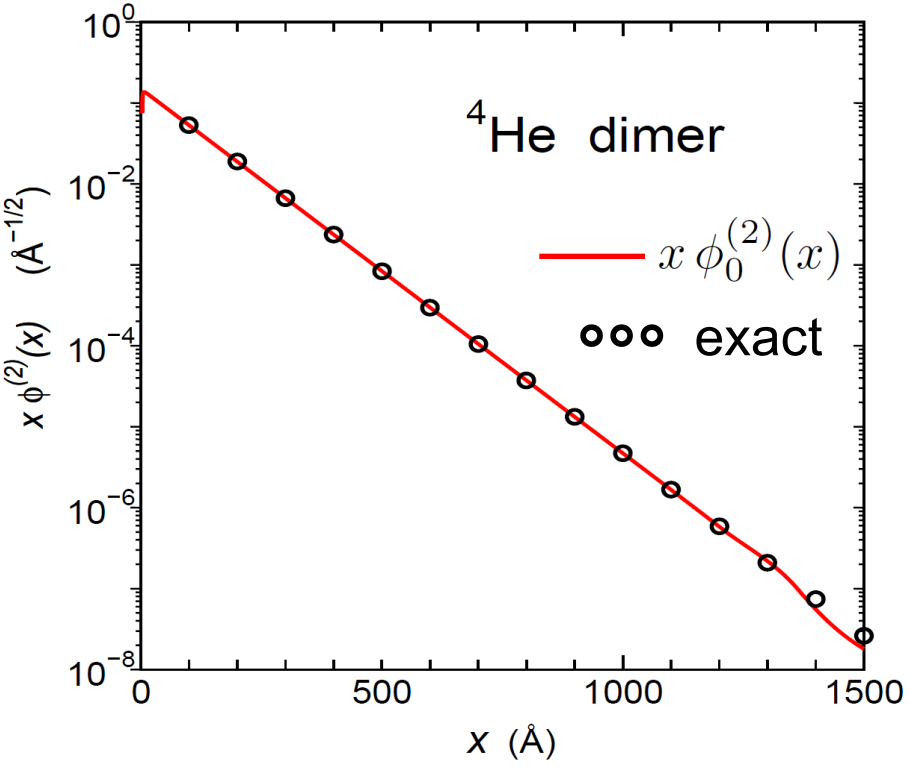
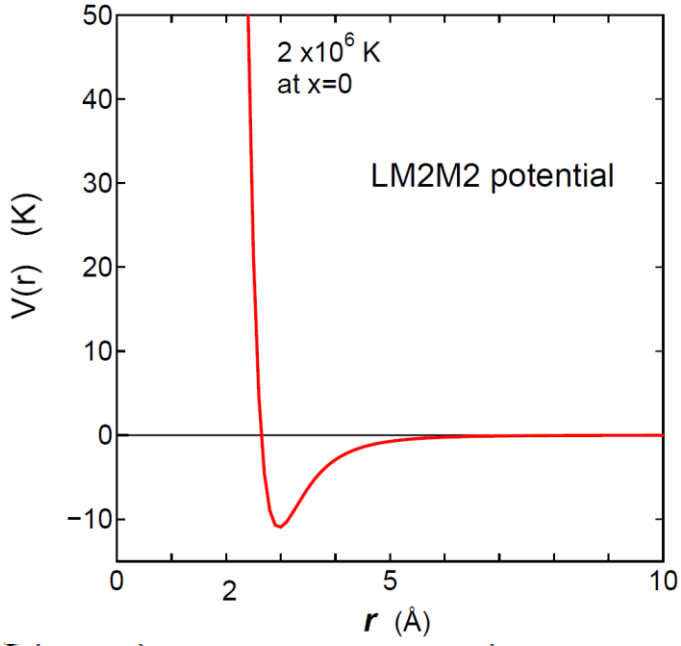


Fig.2

Gaussian expansion method for

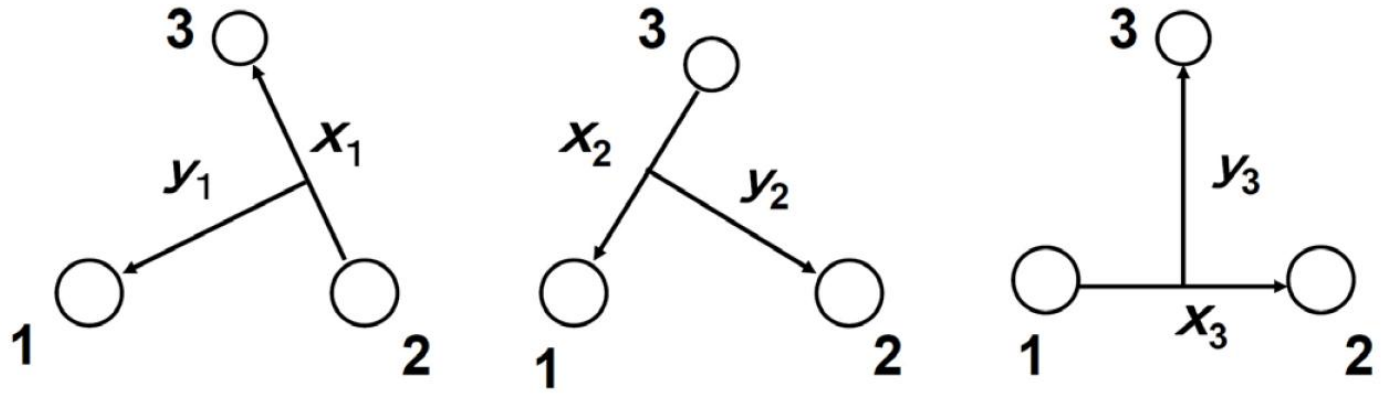
1) three identical spinless particles
2) very weakly bound states,
3) using realistic potential (LM2M2)



$$(H - E)\Psi^{(3)} = 0.$$

$$H = -\frac{\hbar^2}{2\mu_x}\nabla_x^2 - \frac{\hbar^2}{2\mu_y}\nabla_y^2 + \sum_{1=i<j}^{3} V(r_{ij}), \qquad)$$

We take all the three sets of Jacobi coordinates:



Trimer ground state

(LM2M2 potential)

Present result excellently agree with literature.

trimer	ground state			
	present	Ref.[7]	Ref.[8]	Ref.[9]
binding energy $B_0^{(3)}$ (mK)	126.40	126.39	126.4	126.40
$\langle T \rangle$ (mK)	1660.4	1658	1660	
$\langle V \rangle$ (mK)	−1786.8	−1785	−1787	
$\sqrt{\langle r_{ij}^2 \rangle}$ (Å)	10.96	10.95	10.96	
$\langle r_{ij} \rangle$ (Å)	9.616	9.612	9.636	
$\langle r_{ij}^{-1} \rangle$ (Å^{-1})	0.134	0.135		
$\langle r_{ij}^{-2} \rangle$ (Å^{-2})	0.0228	0.0230		
$\sqrt{\langle r_{iG}^2 \rangle}$ (Å)	6.326		6.49	6.32

[7] R. Lazauskas and J. Carbonell, Phys. Rev. A **73** (2006) 062717.

[8] P. Barletta and A. Kievsky, Phys. Rev. A **64** (2001) 042514.

[9] V.A. Roudnev, S.L. Yakovlev and S.A. Sofianos, Few-Body Syst. **37** (2005) 179.

Trimer **excited** state

(LM2M2 potential)

Present result excellently agree with literature.

trimer	excited state			
	present	Ref.[7]	Ref.[8]	Ref.[9]
binding energy $B_1^{(3)}$ (mK)	2.2706	2.268	2.265	2.2707
$\langle T \rangle$ (mK)	122.15	122.1	121.9	
$\langle V \rangle$ (mK)	−124.42	−124.5	−124.2	
$\sqrt{\langle r_{ij}^2 \rangle}$ (Å)	104.5	104.3		
$\langle r_{ij} \rangle$ (Å)	84.51	83.53	83.08	
$\langle r_{ij}^{-1} \rangle$ (Å^{-1})	0.0265	0.0267		
$\langle r_{ij}^{-2} \rangle$ (Å^{-2})	0.00216	0.00218		
$\sqrt{\langle r_{iG}^2 \rangle}$ (Å)	60.33			59.3

[7] R. Lazauskas and J. Carbonell, Phys. Rev. A **73** (2006) 062717.

[8] P. Barletta and A. Kievsky, Phys. Rev. A **64** (2001) 042514.

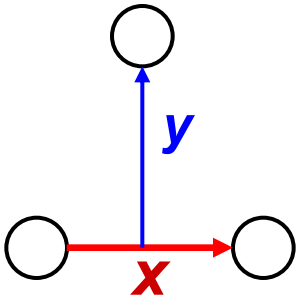
[9] V.A. Roudnev, S.L. Yakovlev and S.A. Sofianos, Few-Body Syst. **37** (2005) 179.

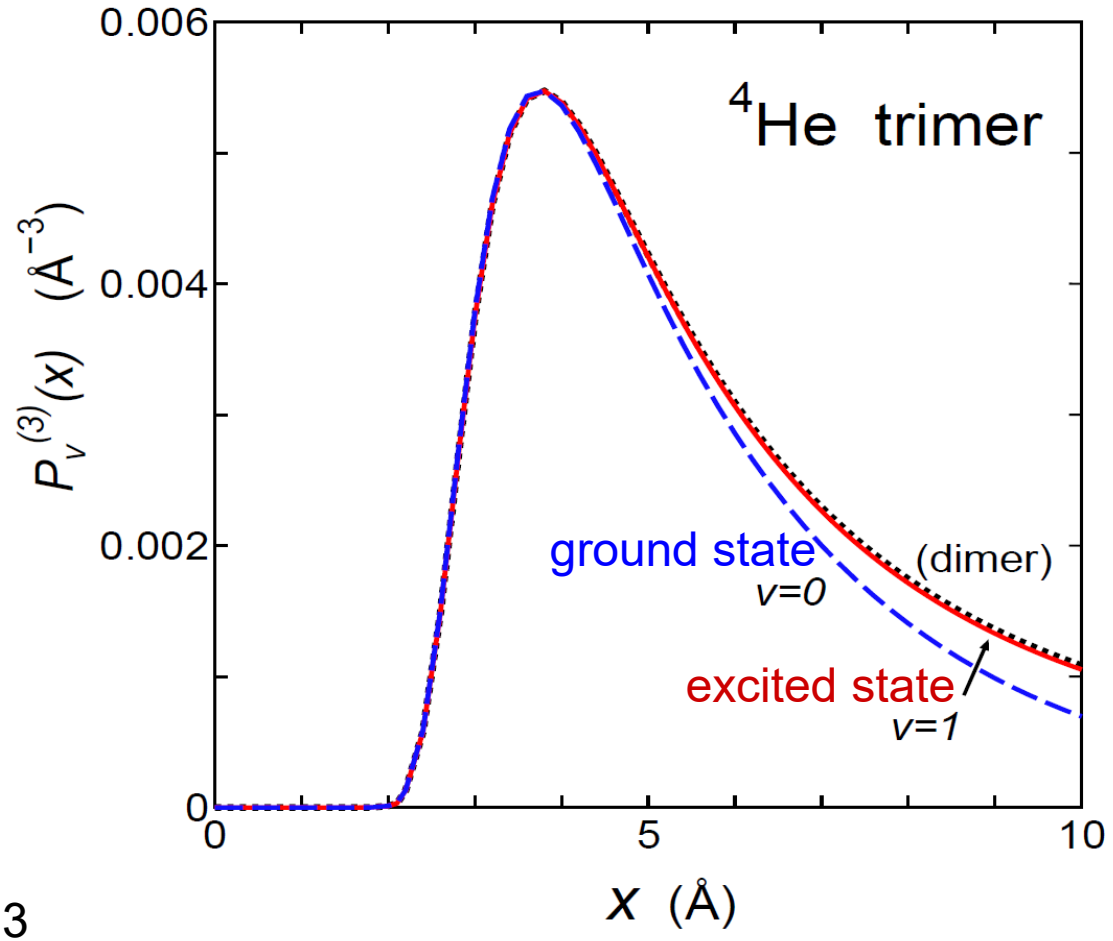
Strong short-range correlation

Pair correlation (distribution) function

$$P_v^{(3)}(\boldsymbol{x}) = \int |\Psi_v^{(3)}|^2 \mathrm{d}\mathbf{y}$$

probability of finding two particles at $\boldsymbol{x}$.





Already multiplied by

——— x 14.5

····· x 6.0

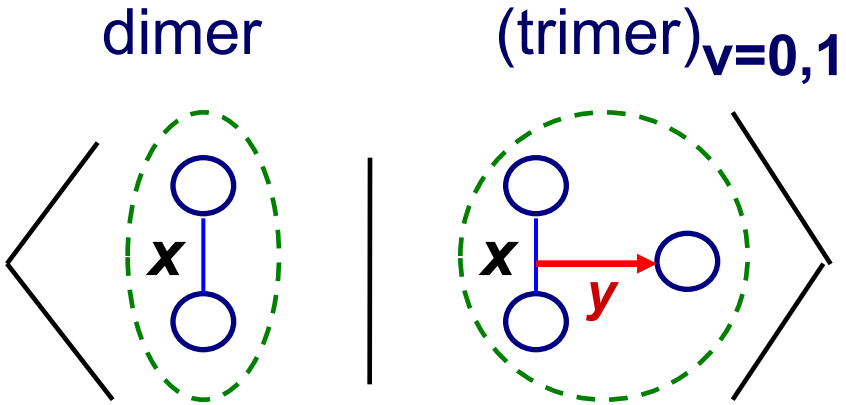
to be normalized at the peak

Precisely the same shape of the short-range correlations (x<4 A) appear in all the states.

Fig.3

Overlap function

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



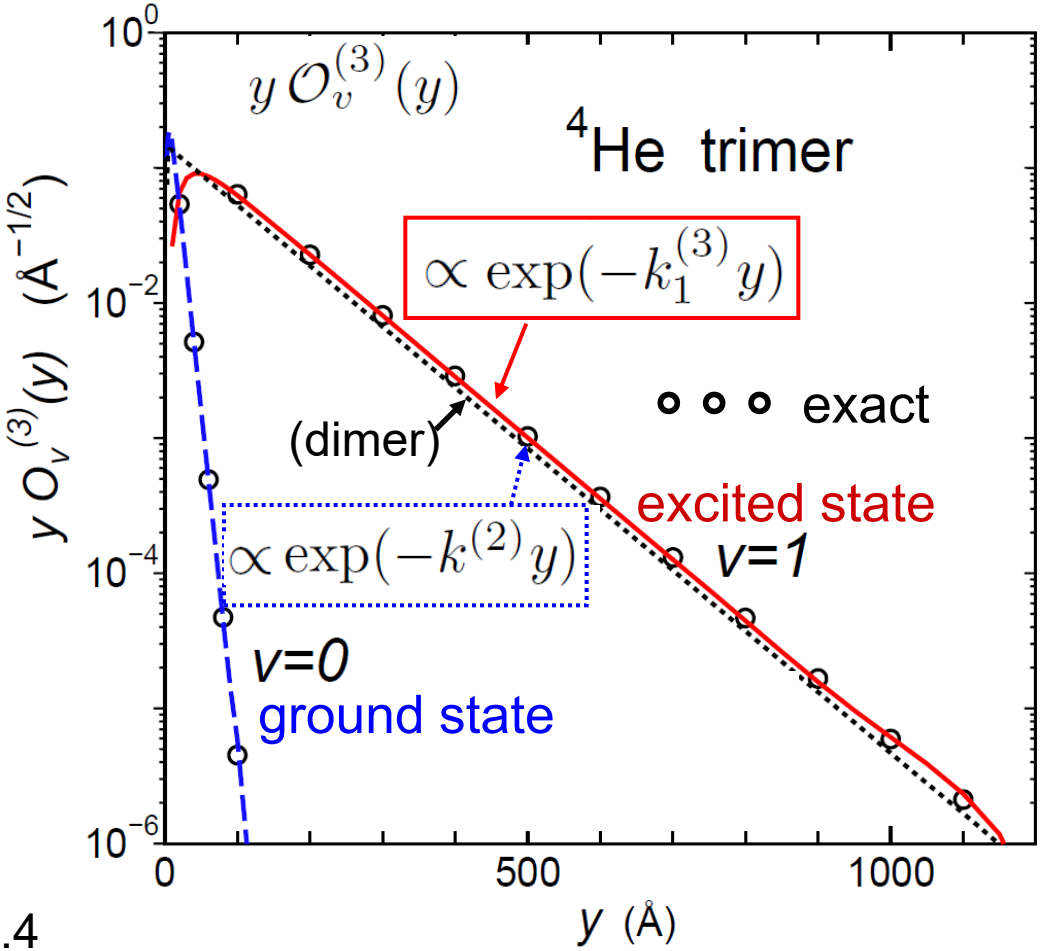


Fig.4

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.

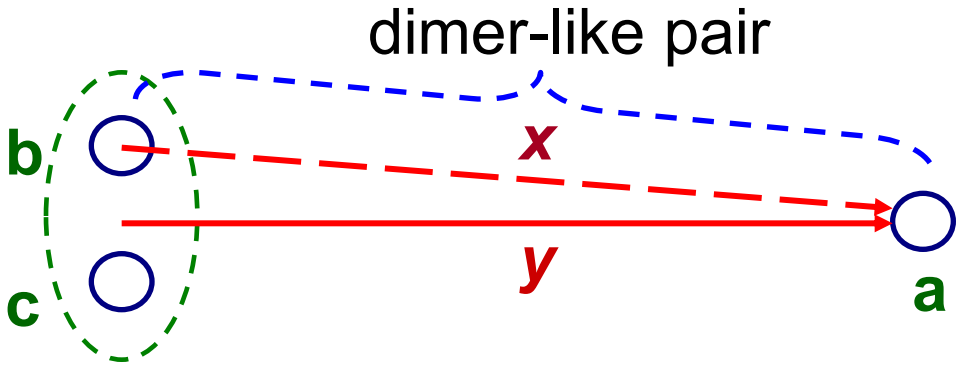
$$k_1^{(3)} = k^{(2)}$$

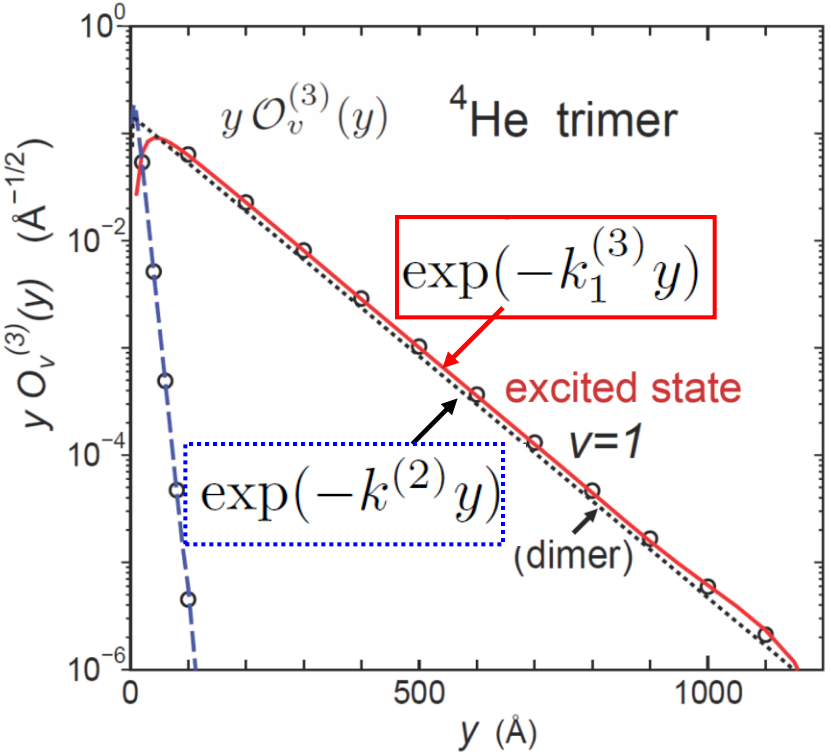
decaying constant

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.

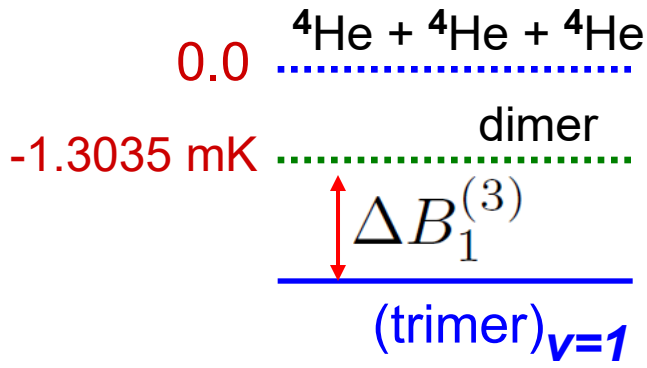
by using $B^{(2)}$ only.

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

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

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

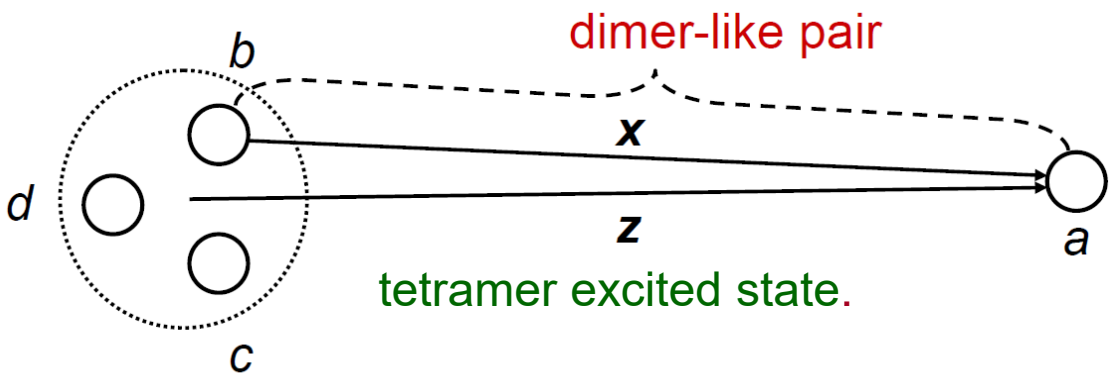
0.967 mK

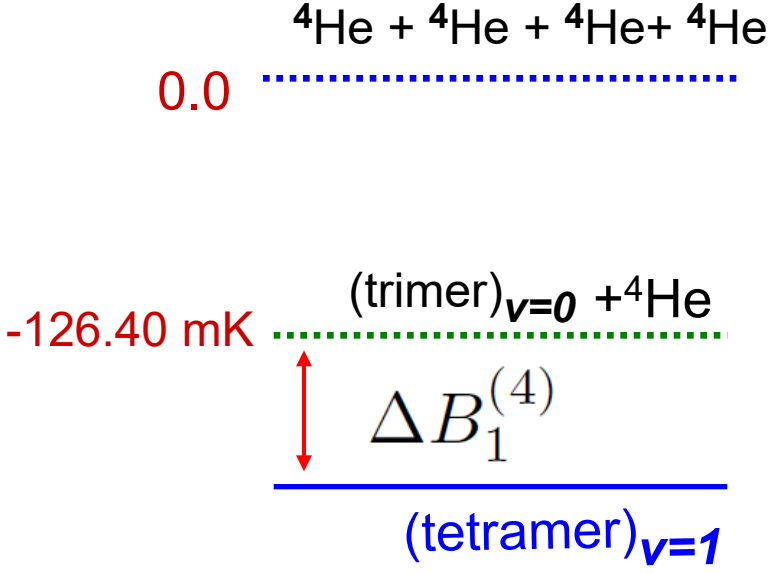
2.2706 mK

3-body calculation

Good model !

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





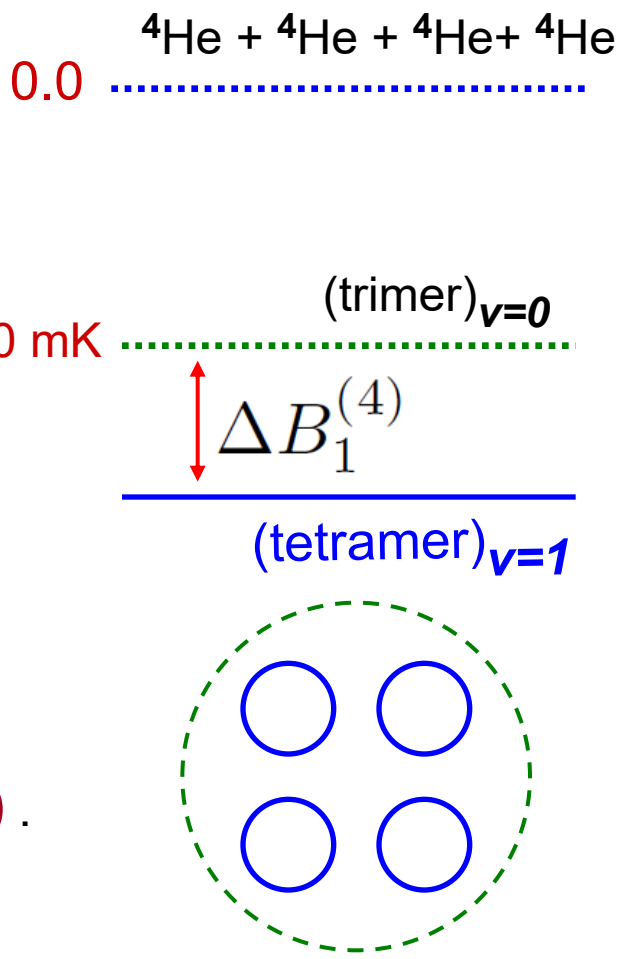
then, we can predict the binding energy

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

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

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

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

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

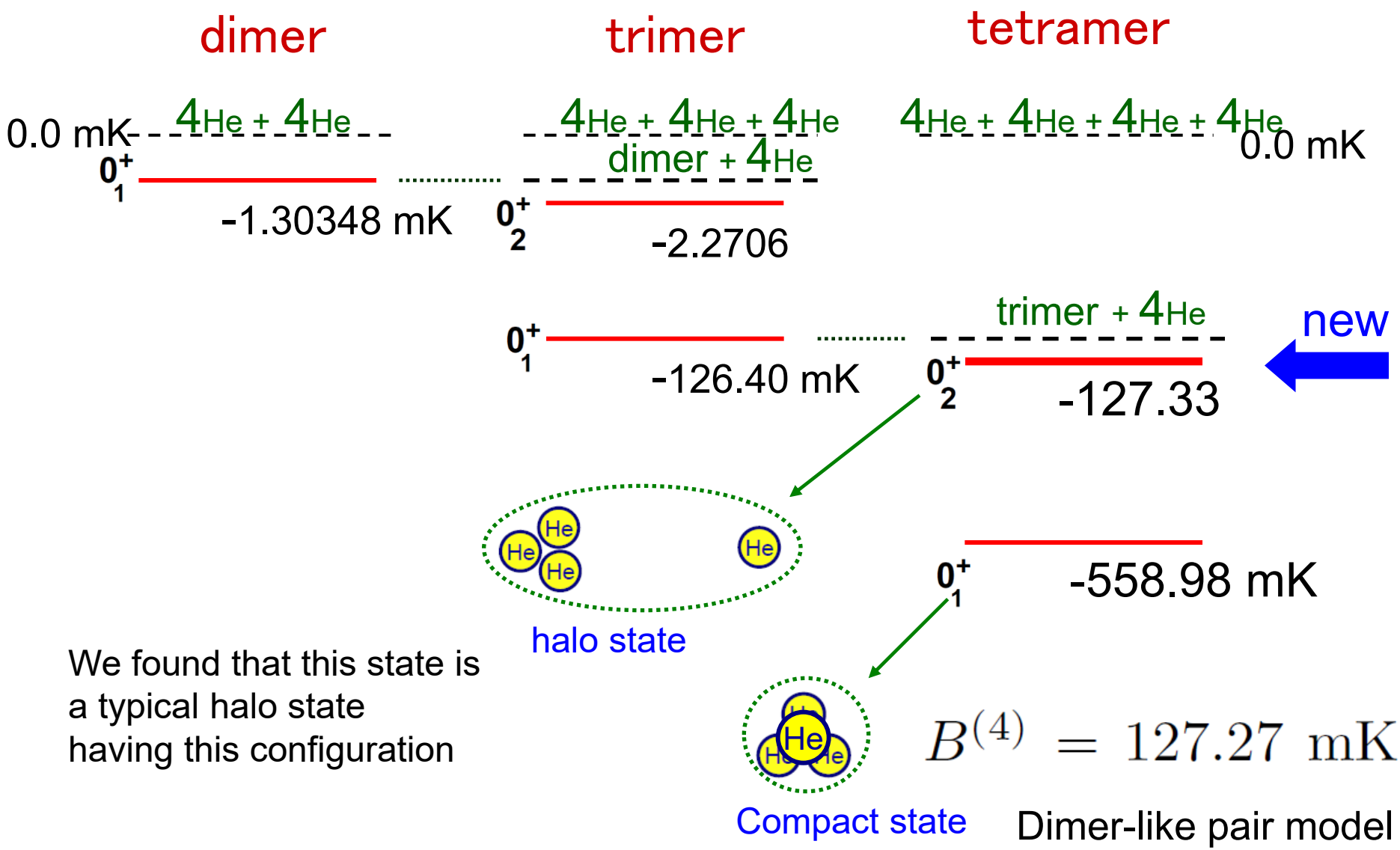
We have

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

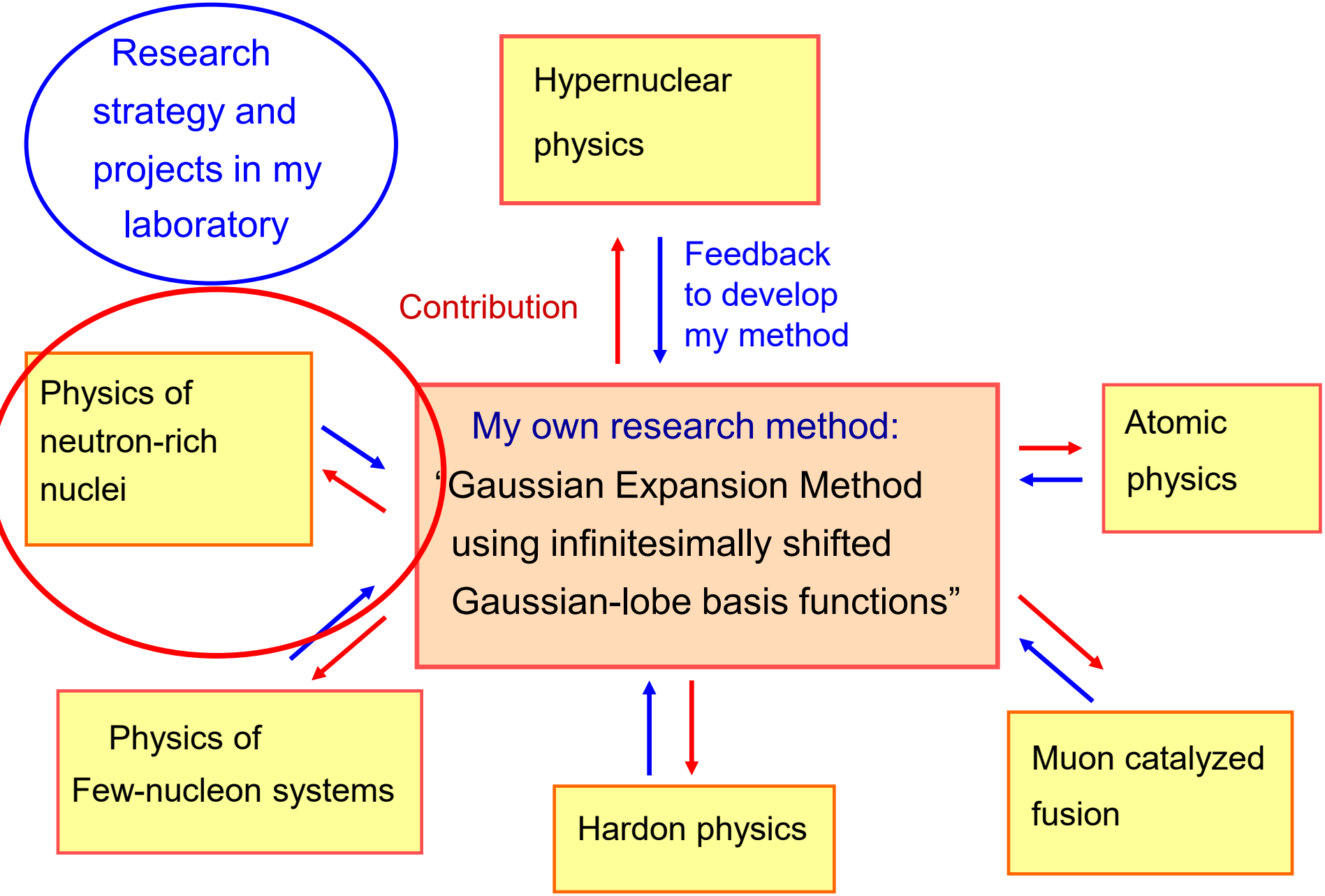
hence $B^{(4)} = 127.27$ mK

We shall check this by the four-body calculation.

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



We found that this state is
a typical halo state
having this configuration



Morning on 22 May

4n system and ^{7}H

Thank you!

Application to ^{4}He atoms

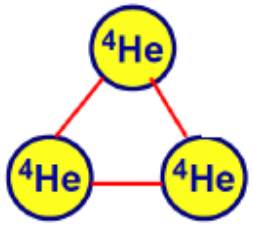
One of the most fundamental theoretical issues

from the view point of few-body problems:

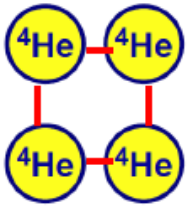
to perform accurate calculations of the

3- and 4-body ^{4}He-atom systems

using realistic ^{4}He-^{4}He potentials.



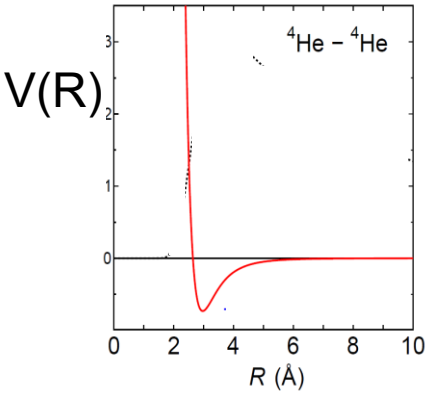
trimer



tetramer

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

Realistic potential

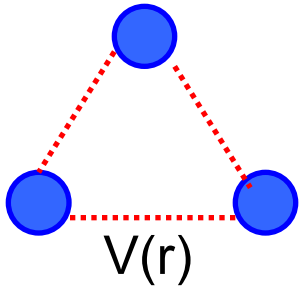


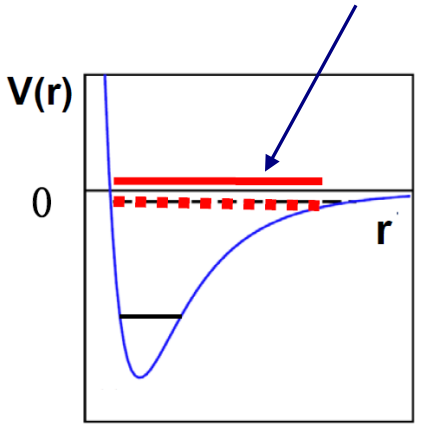
In 1970, Efimov predicted the following phenomenon,

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)

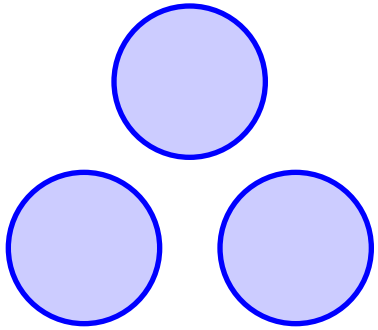
1) a large number of 3-body weakly-bound states (Borromean states) can be formed even when the interaction is too weak to have a two-body bound state,

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"]. As an example, I study 4He systems.

^{4}He Trimer

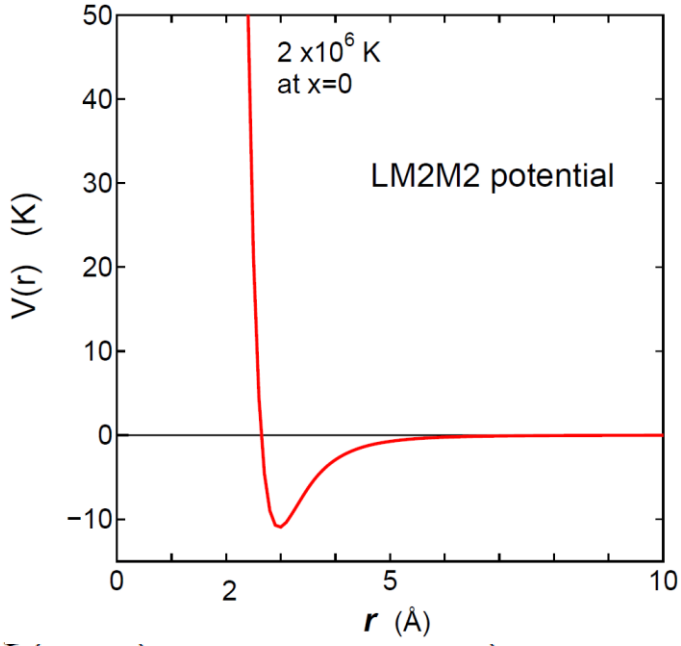
ground and excited states

using LM2M2 potential



Gaussian expansion method for

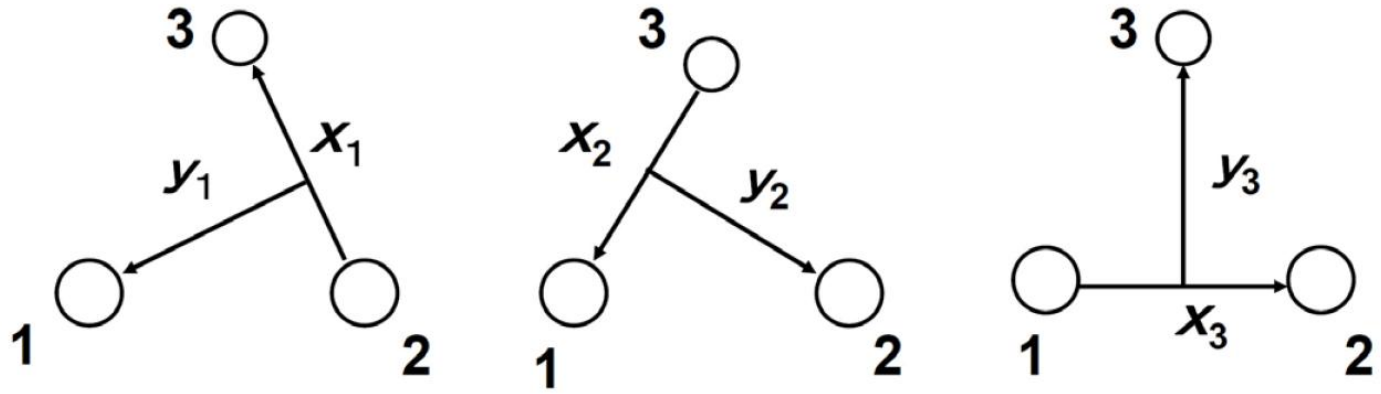
1) three identical spinless particles
2) very weakly bound states,
3) using realistic potential (LM2M2)



$$(H - E)\Psi^{(3)} = 0.$$

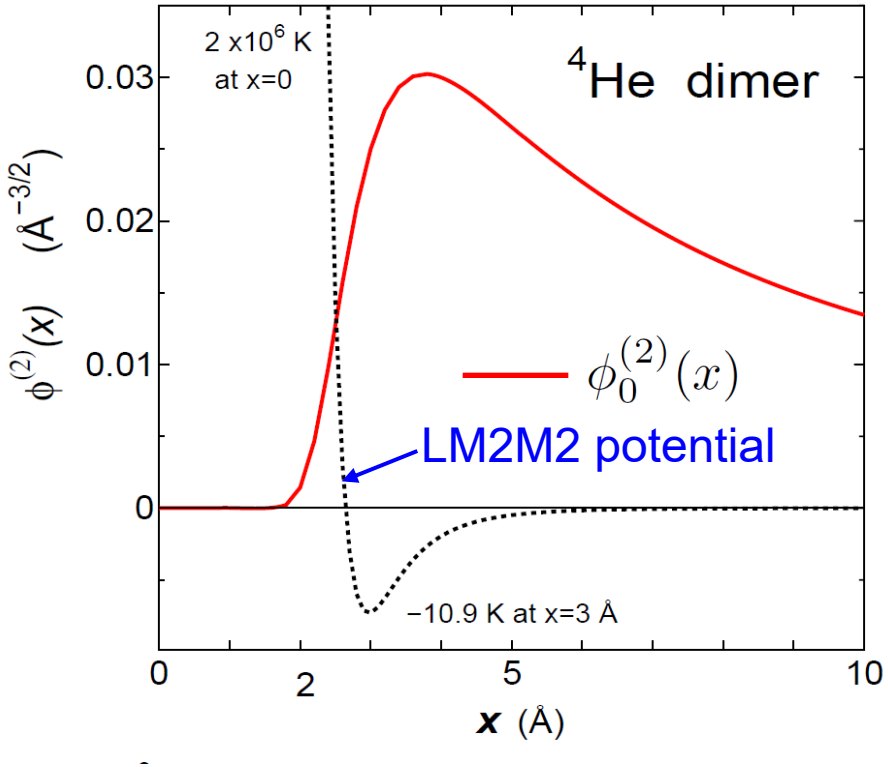
$$H = -\frac{\hbar^2}{2\mu_x}\nabla_x^2 - \frac{\hbar^2}{2\mu_y}\nabla_y^2 + \sum_{1=i<j}^{3} V(r_{ij}), \qquad)$$

We take all the three sets of Jacobi coordinates:



^{4}He Dimer

$$B^{(2)} = 1.30348 \text{ mK and } \sqrt{\langle x^2 \rangle} = 70.93 \text{ Å},$$
the same as those obtained in literature.



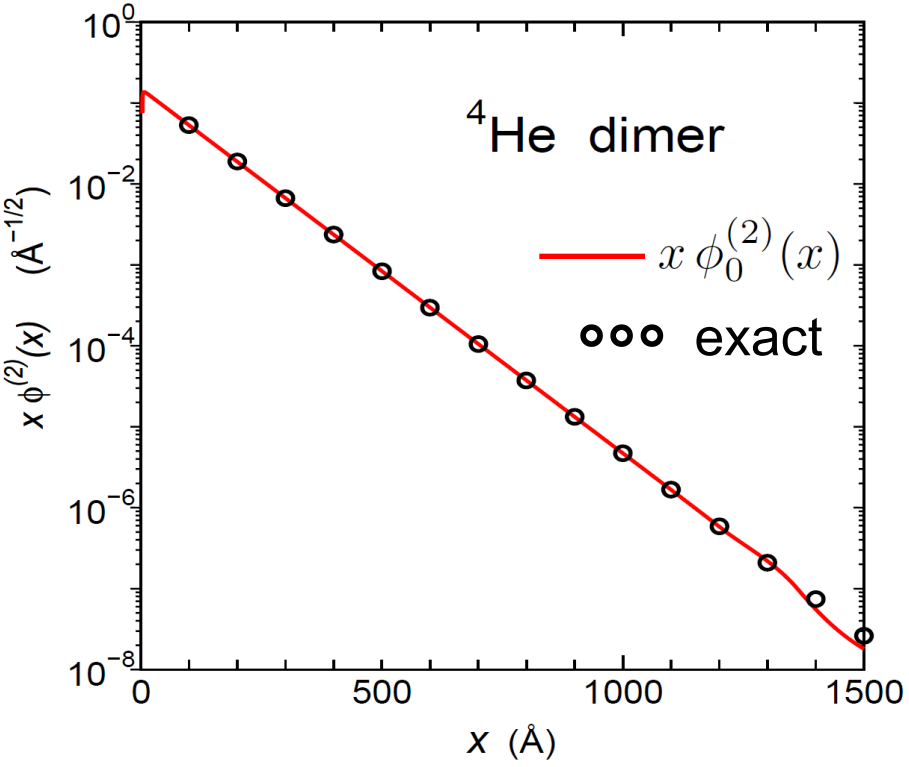


Fig.2

Trimer ground state

(LM2M2 potential)

Present result excellently agree with literature.

trimer	ground state			
	present	Ref.[7]	Ref.[8]	Ref.[9]
binding energy $B_0^{(3)}$ (mK)	126.40	126.39	126.4	126.40
$\langle T \rangle$ (mK)	1660.4	1658	1660	
$\langle V \rangle$ (mK)	−1786.8	−1785	−1787	
$\sqrt{\langle r_{ij}^2 \rangle}$ (Å)	10.96	10.95	10.96	
$\langle r_{ij} \rangle$ (Å)	9.616	9.612	9.636	
$\langle r_{ij}^{-1} \rangle$ (Å^{-1})	0.134	0.135		
$\langle r_{ij}^{-2} \rangle$ (Å^{-2})	0.0228	0.0230		
$\sqrt{\langle r_{iG}^2 \rangle}$ (Å)	6.326		6.49	6.32

[7] R. Lazauskas and J. Carbonell, Phys. Rev. A **73** (2006) 062717.

[8] P. Barletta and A. Kievsky, Phys. Rev. A **64** (2001) 042514.

[9] V.A. Roudnev, S.L. Yakovlev and S.A. Sofianos, Few-Body Syst. **37** (2005) 179.

Trimer **excited** state

(LM2M2 potential)

Present result excellently agree with literature.

trimer	excited state			
	present	Ref.[7]	Ref.[8]	Ref.[9]
binding energy $B_1^{(3)}$ (mK)	2.2706	2.268	2.265	2.2707
$\langle T \rangle$ (mK)	122.15	122.1	121.9	
$\langle V \rangle$ (mK)	−124.42	−124.5	−124.2	
$\sqrt{\langle r_{ij}^2 \rangle}$ (Å)	104.5	104.3		
$\langle r_{ij} \rangle$ (Å)	84.51	83.53	83.08	
$\langle r_{ij}^{-1} \rangle$ (Å^{-1})	0.0265	0.0267		
$\langle r_{ij}^{-2} \rangle$ (Å^{-2})	0.00216	0.00218		
$\sqrt{\langle r_{iG}^2 \rangle}$ (Å)	60.33			59.3

[7] R. Lazauskas and J. Carbonell, Phys. Rev. A **73** (2006) 062717.

[8] P. Barletta and A. Kievsky, Phys. Rev. A **64** (2001) 042514.

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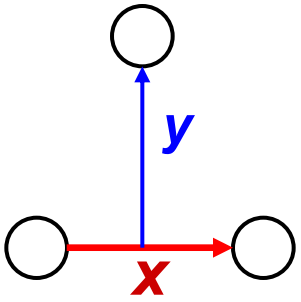
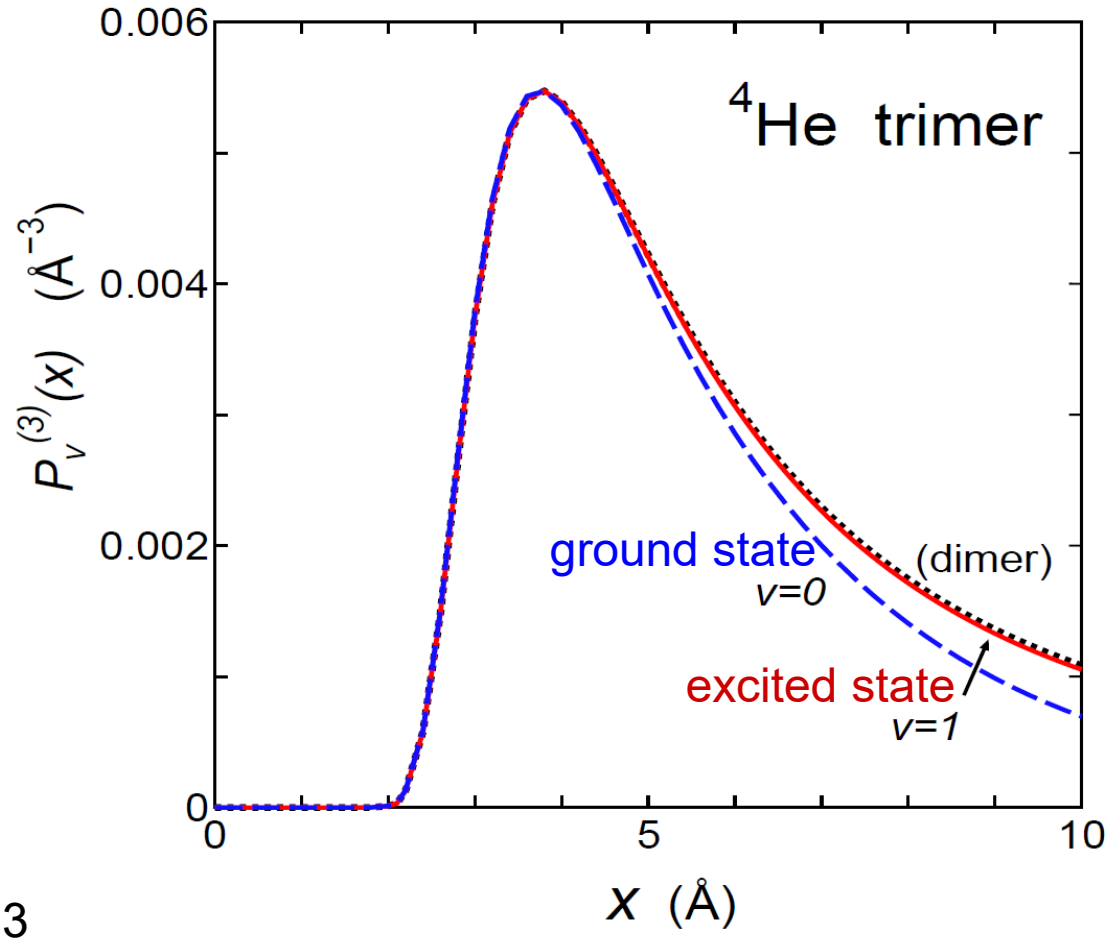
Strong short-range correlation

Pair correlation (distribution) function

$$P_v^{(3)}(\boldsymbol{x}) = \int |\Psi_v^{(3)}|^2 \mathrm{d}\mathbf{y}$$

probability of finding two particles at $\boldsymbol{x}$.





Already multiplied by

——— x 14.5

····· x 6.0

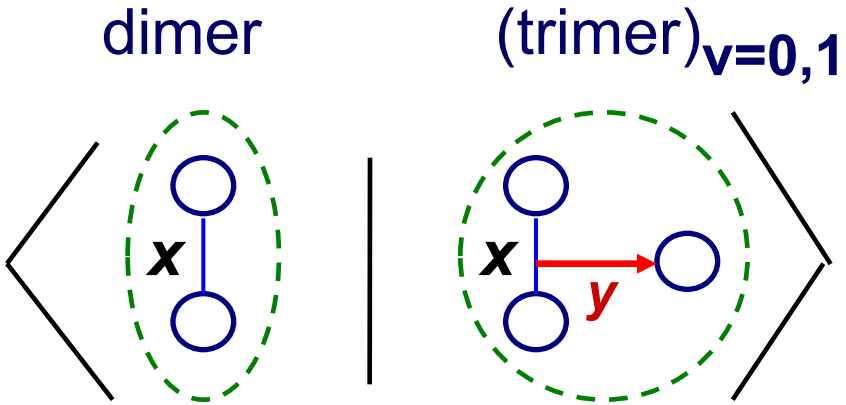
to be normalized at the peak

Precisely the same shape of the short-range correlations (x<4 A) appear in all the states.

Fig.3

Overlap function

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



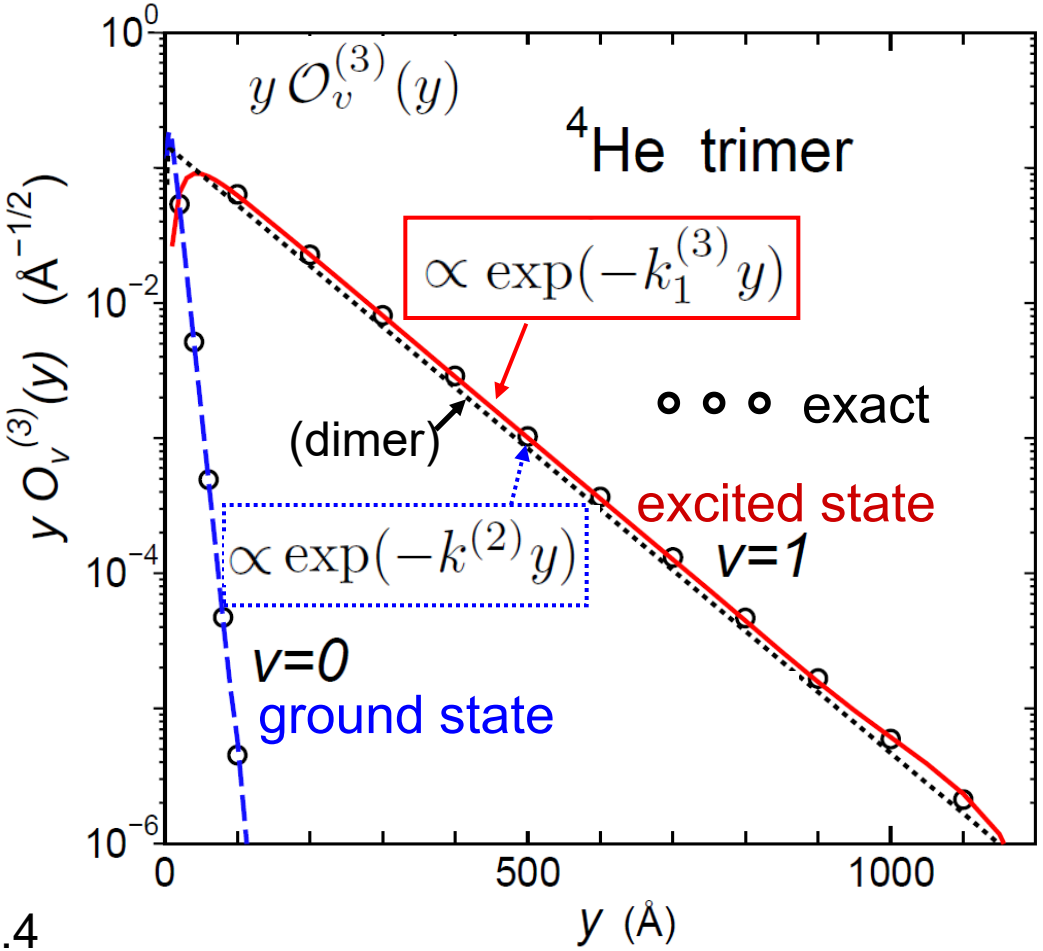


Fig.4

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

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

Dimer-like pair model

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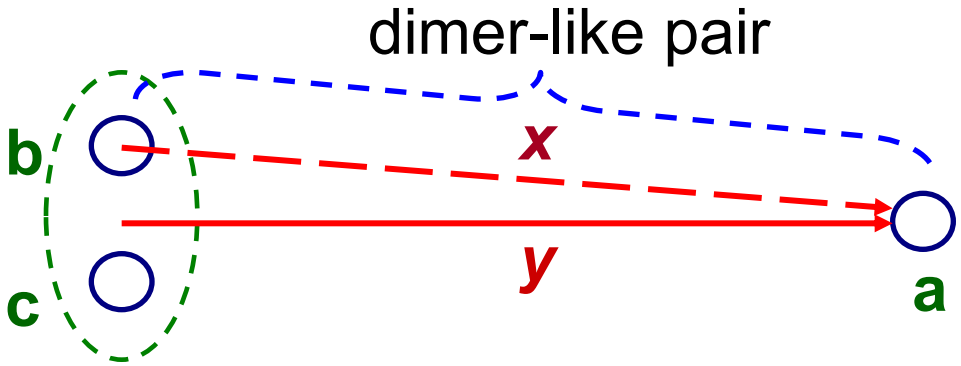

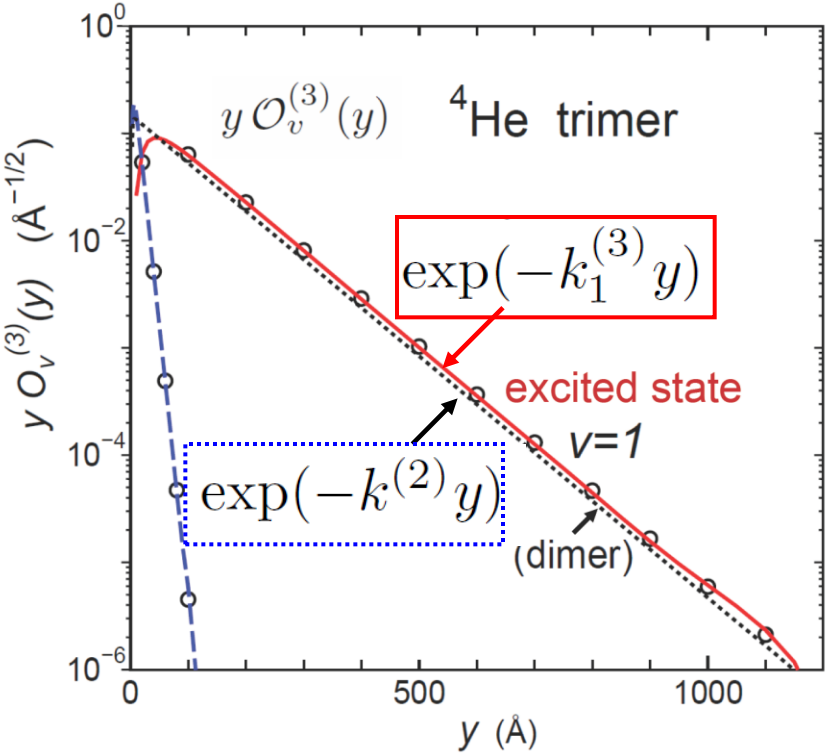

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binding energy of trimer excited state measured from dimer.

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

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

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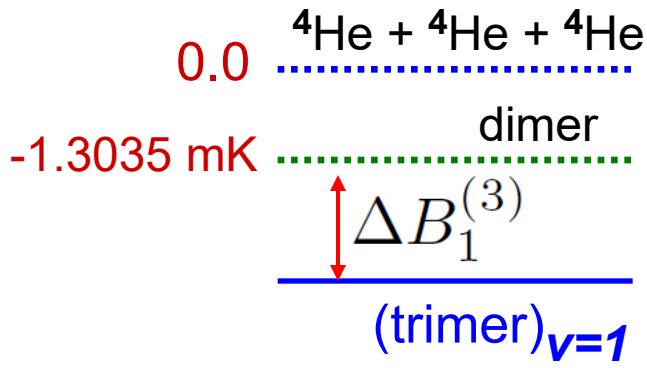

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0.967 mK

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3-body calculation

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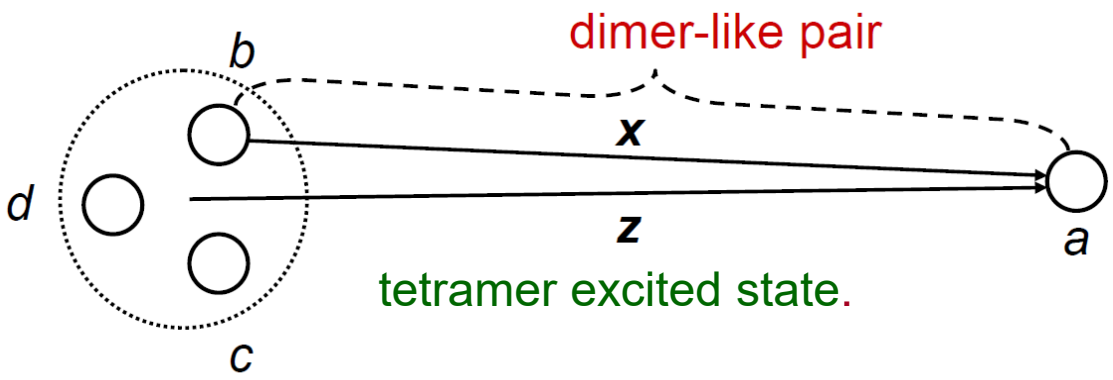

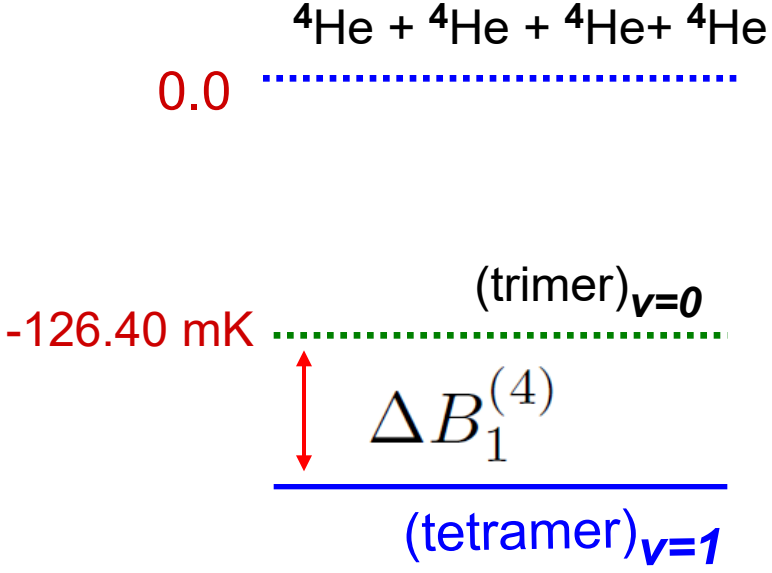

then, we can predict the binding energy

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

of the tetramer excited state with respect to the
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We can predict this binding energy

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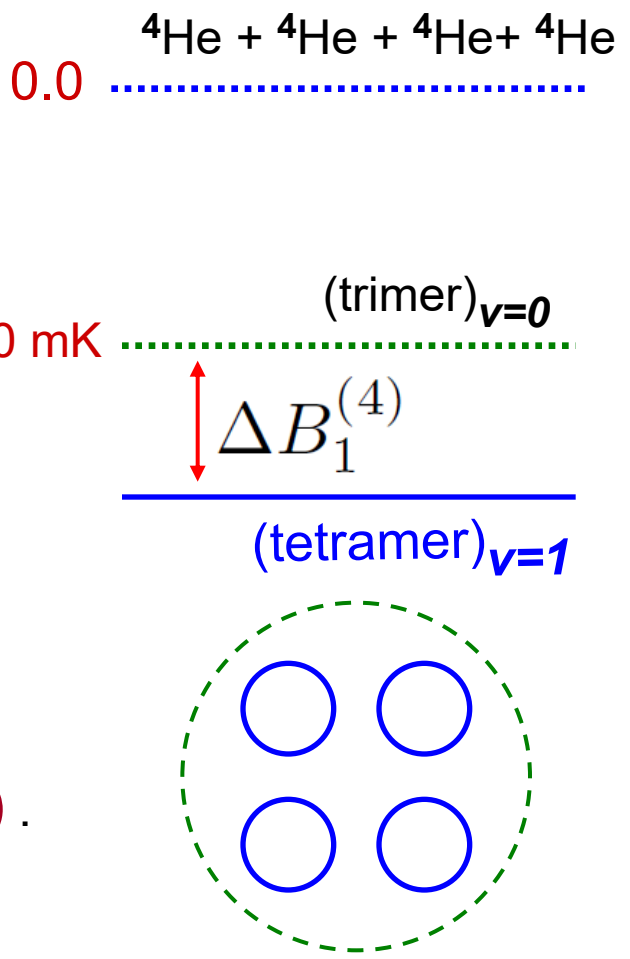

using the relation

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

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

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

We have

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

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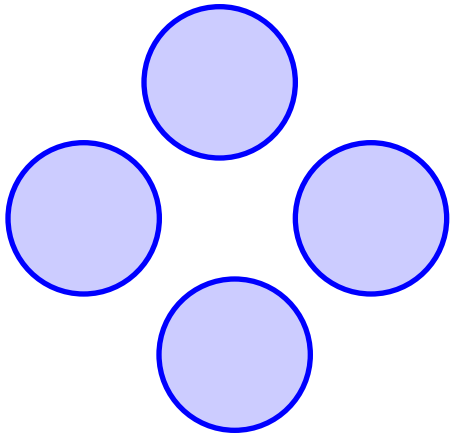
We shall check this by the four-body calculation.

^{4}He Tetramer

ground and excited states

using LM2M2 potential



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

^{4}He tetramer binding energies			ground state	excited state
Method	Reference	potential	(mK)	(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

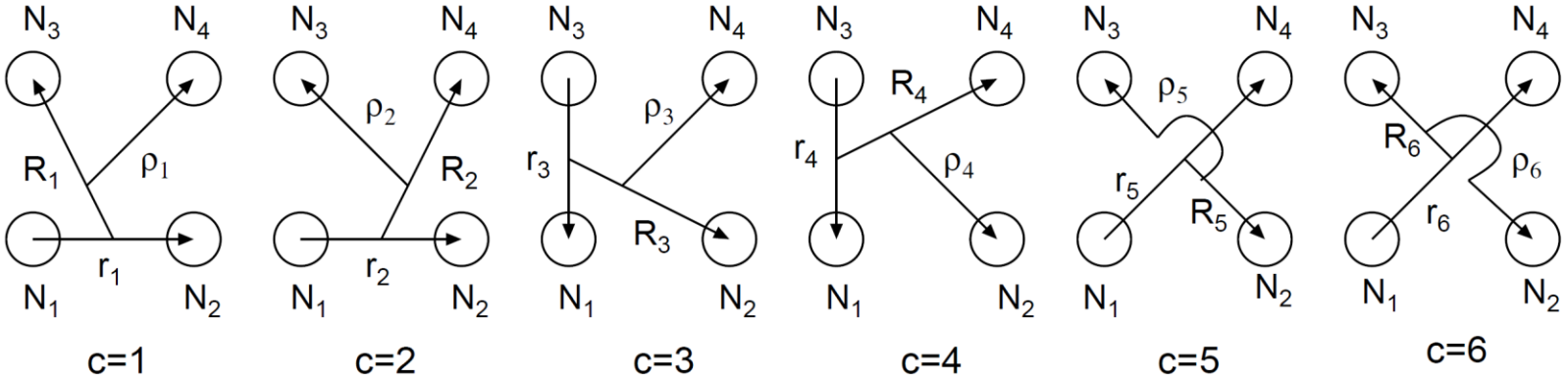
cf. Trimer g.s. = 126.40

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

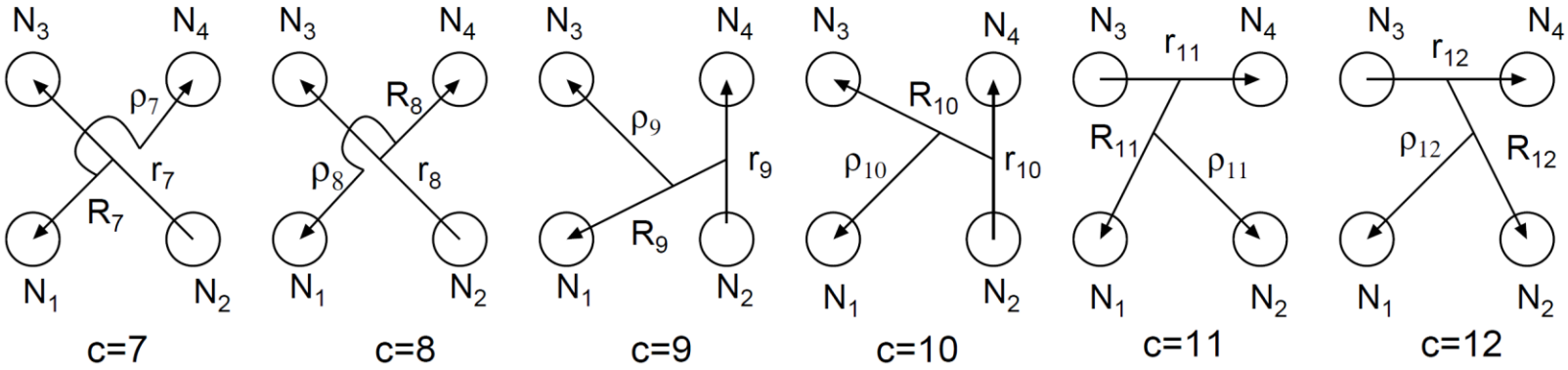
So, we intended to confirm this value by our bound-state calculation.

Full 18 sets of Jacobi coordinates for 4-body systems

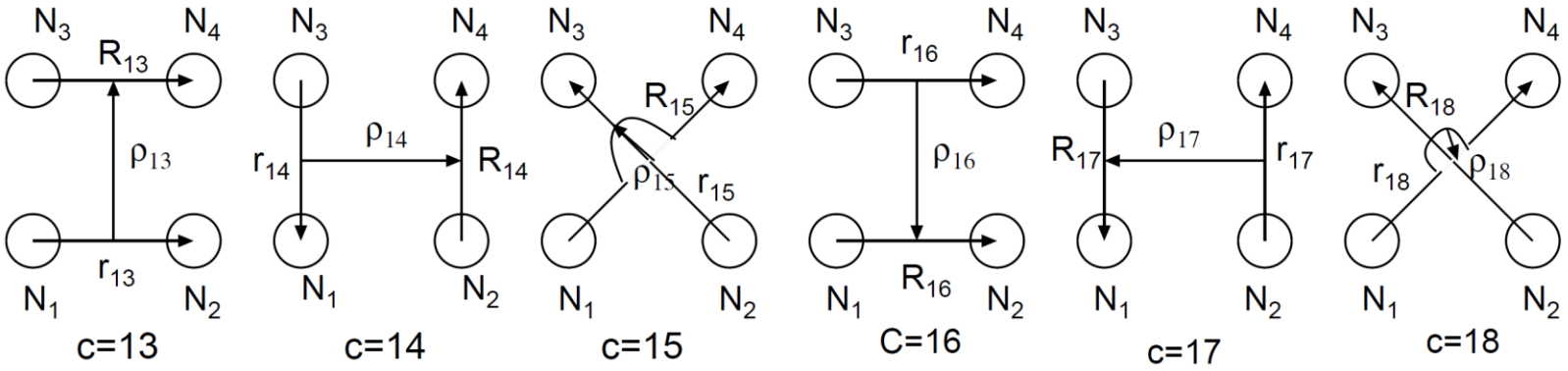
K-type



K-type



H-type



Tetramer : Convergence of the binding energy with respect to maximum ang.-momentum (l_{max})

tetramer	present				Faddeev [7]
	$B_0^{(4)}$ (mK)		$B_1^{(4)}$ (mK)		$B_0^{(4)}$ (mK)
l_{max}	K+H	(K)	K+H	(K)	
	ground		excited		ground
0	500.71	(185.96)	–	(–)	348.8
2	558.29	(508.62)	127.24	(–)	505.9
4	558.98	(532.56)	127.33	(–)	548.6
6					556.0
8					557.7

Only 0.93 mK (=127.33 - 126.40) below the trimer ground state

In our calculation, l_max =4 is sufficient with totally 29000 symmetric 4-body basis functions.

[7] R. Lazauskas and J. Carbonell, Phys. Rev. A **73** (2006) 062717.

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

Method	Reference	potential	^{4}He tetramer binding energies 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 ←	Das *et al.* (2011)	TTY	558	178
.....				
GEM	Present (2011)	LM2M2	558.98	127.33

We confirmed that there is a very shallow excited bound state of ^{4}He tetramer.

(a) Tetramer --- binding energies and mean values

tetramer	ground state		excited state	
	present	Faddeev [7]	present	Faddeev [7]
$B^{(4)}$ (mK)	558.98	557.7	127.33	127.5*)
$\langle T \rangle$ (mK)	4282.2	4107	1639.2	
$\langle V \rangle$ (mK)	−4841.2	−4665	−1766.5	
$\sqrt{\langle r_{ij}^2 \rangle}$ (Å)	8.43	8.40	54.5	34.4*)
$\langle r_{ij} \rangle$ (Å)	7.70		35.8	
$\langle r_{ij}^{-1} \rangle$ (Å^{-1})	0.155		0.0792	
$\langle r_{ij}^{-2} \rangle$ (Å^{-2})	0.0285		0.0117	
$\sqrt{\langle r_{iG}^2 \rangle}$ (Å)	5.16		33.3	

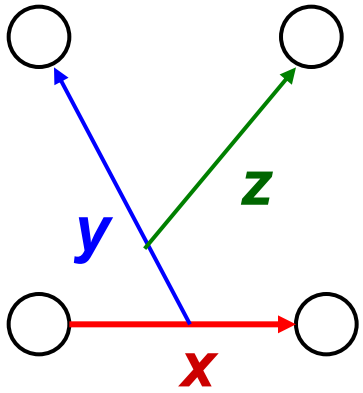
*) As for the excited state, Faddeev bound-state calculation was not performed, but these results were extrapolated from the low-enegy scattering calculation.

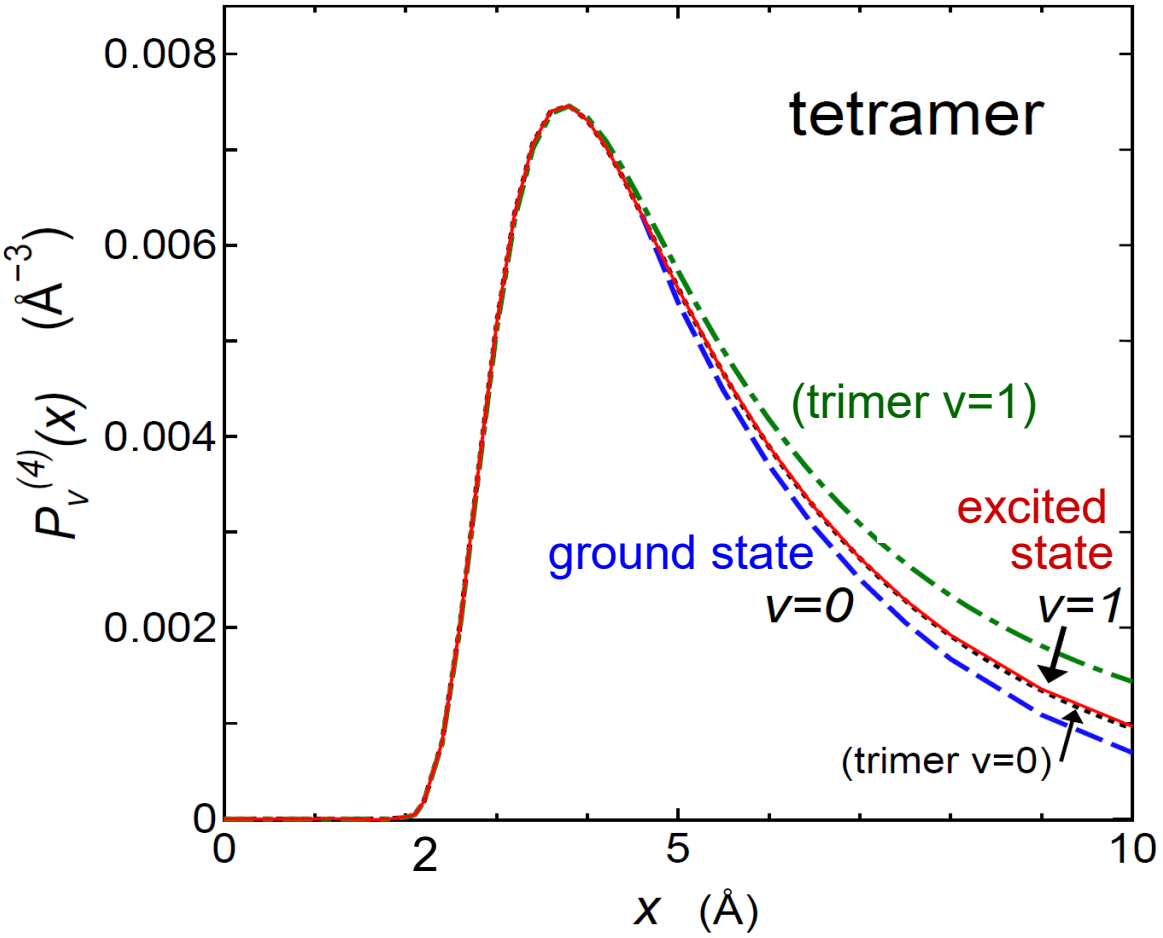
[7] R. Lazauskas and J. Carbonell, Phys. Rev. A **73** (2006)

Strong short-range correlation

Pair correlation function along ***x*** :

$$P_v^{(4)}(\boldsymbol{x}) = \int |\Psi_v^{(4)}|^2 \mathrm{d}\mathbf{y}\mathrm{d}\mathbf{z} \quad (v=0,1)$$





Already multiplied by

x 2.76

x 1.36

x 19.8

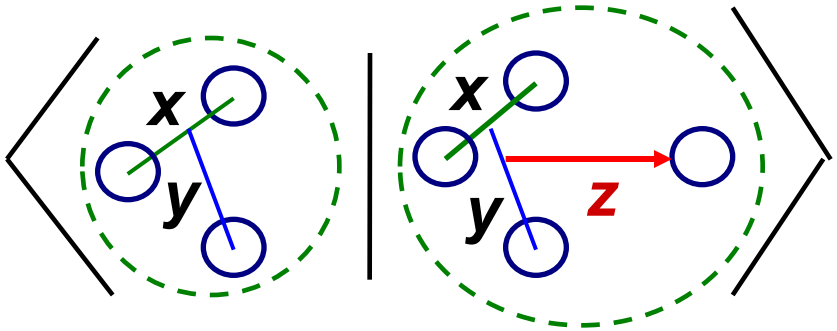
to be normalized at the peak.

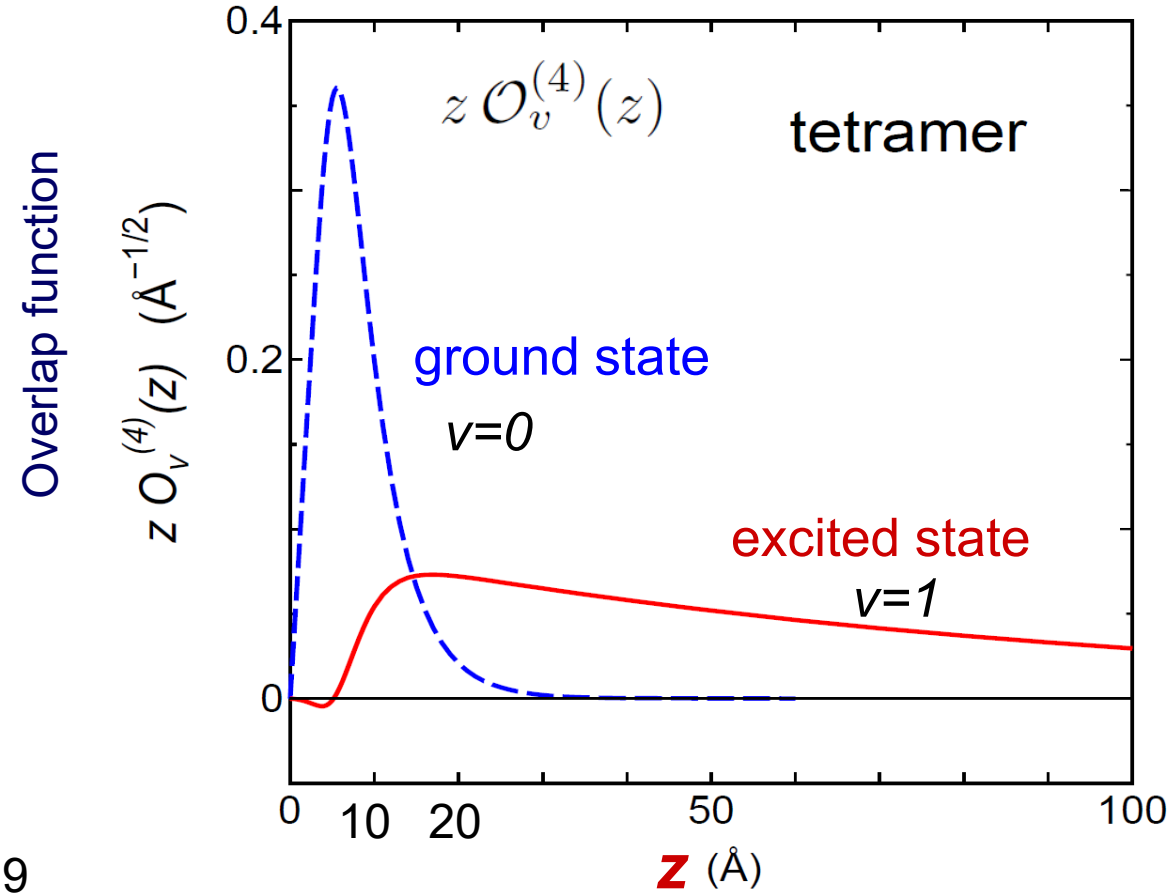
Precisely the same shape of the short-range correlations (x< 4 A) appear in all the states.

Overlap function

$$\mathcal{O}_v^{(4)}(z) = \int \Psi_0^{(3)*}\,\Psi_v^{(4)}\,\mathrm{d}x\,\mathrm{d}y =$$

$(\text{trimer})_{v=0}$ $(\text{tetramer})_{v=0,1}$





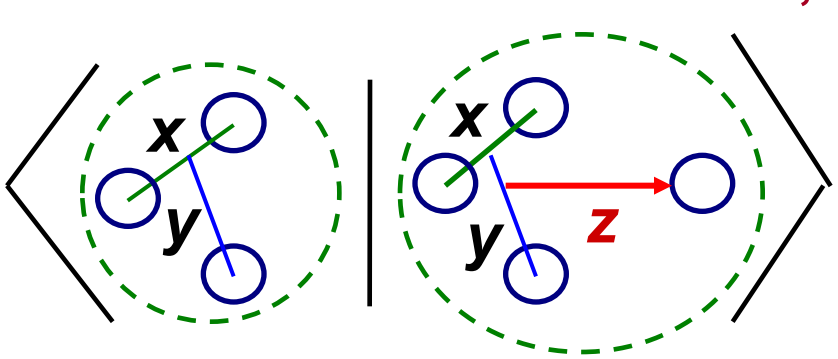
The excited state is much more dilute state than the ground state.

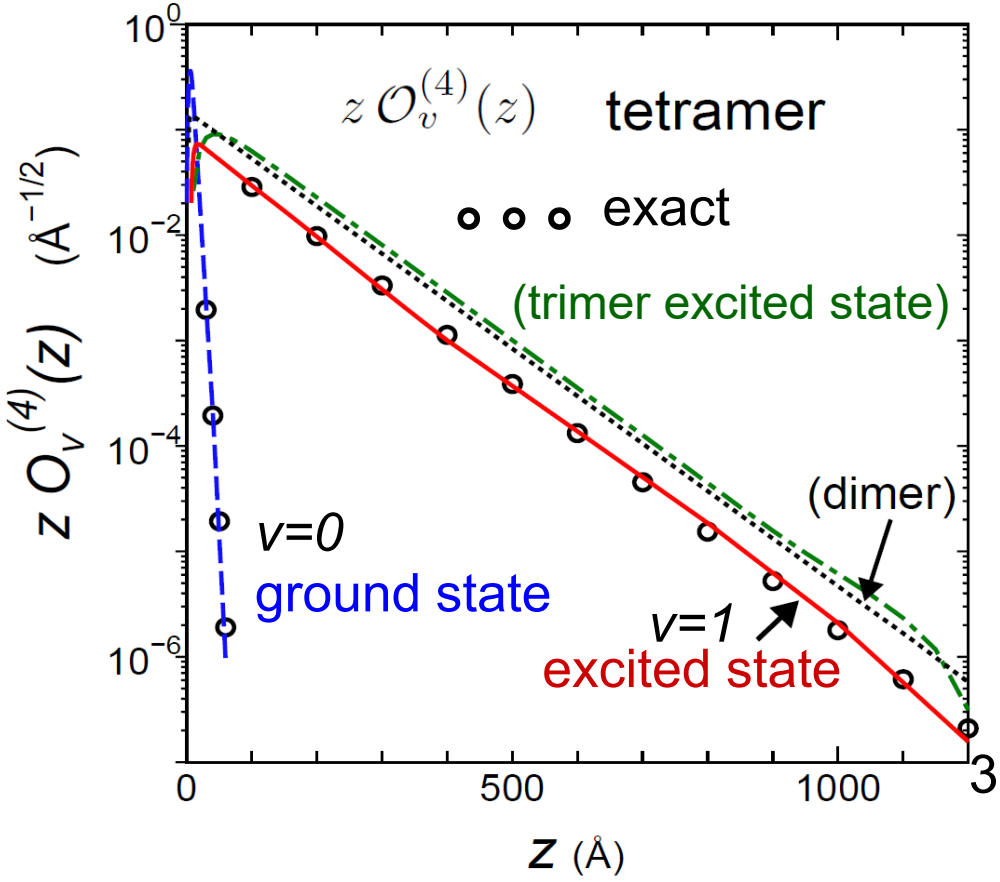
Fig.9

Overlap function

asymptotic region

$$\mathcal{O}_v^{(4)}(z) = \int \Psi_0^{(3)*}\, \Psi_v^{(4)}\, \mathrm{dx\, dy} =$$





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

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

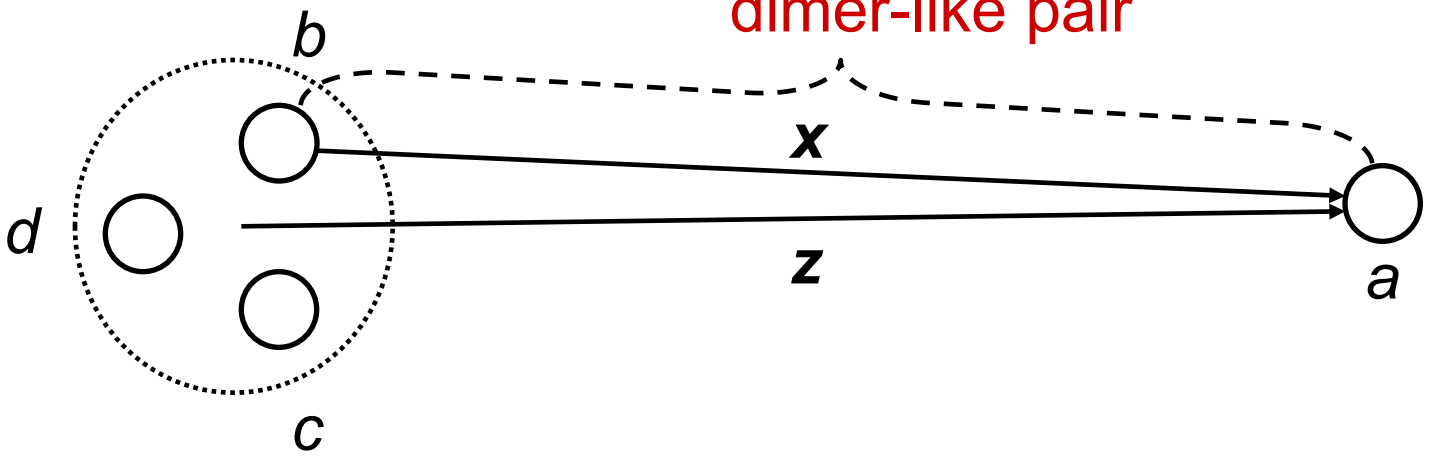
$$k_1^{(4)} = k_1^{(3)} = k^{(2)}$$

3) Dimer-like pair model in asymptotic region works well.

Fig.10

Dimer-like pair model in the asymptotic region

tetramer excited state



As I mentioned before, the dimer-like pair model predicts

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

$$B_1^{(4)} = 127.27\ \mathrm{mK}$$

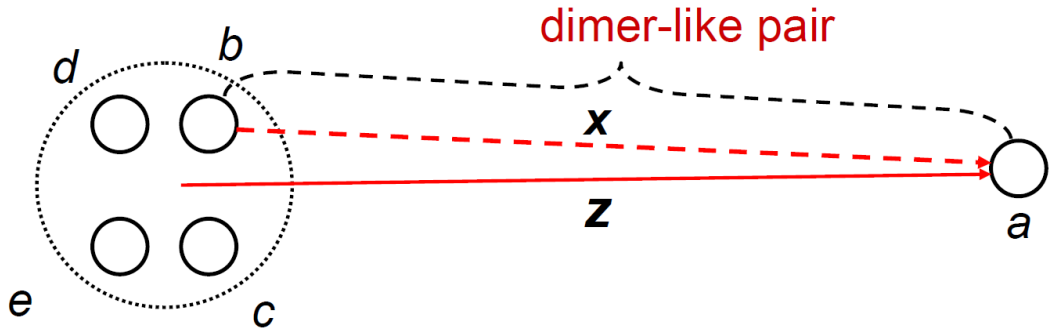
Our 4-body calculation

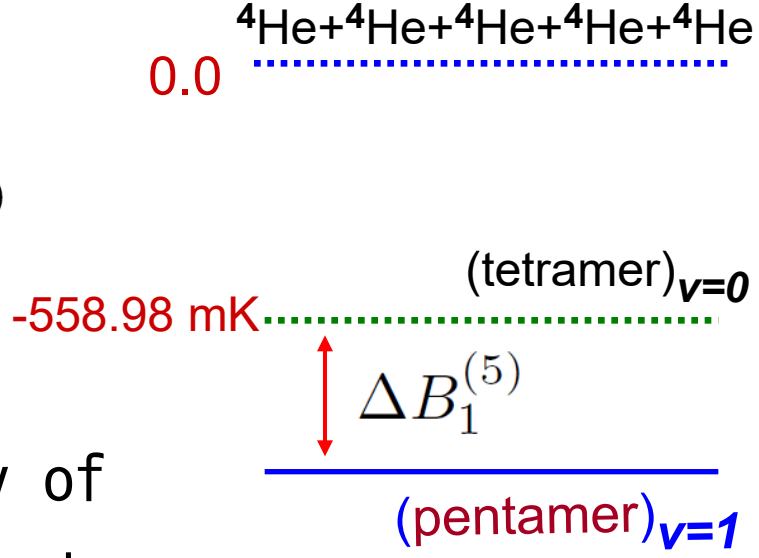
$0.93\ \mathrm{mK}$

$127.33\ \mathrm{mK}$

Very good!

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

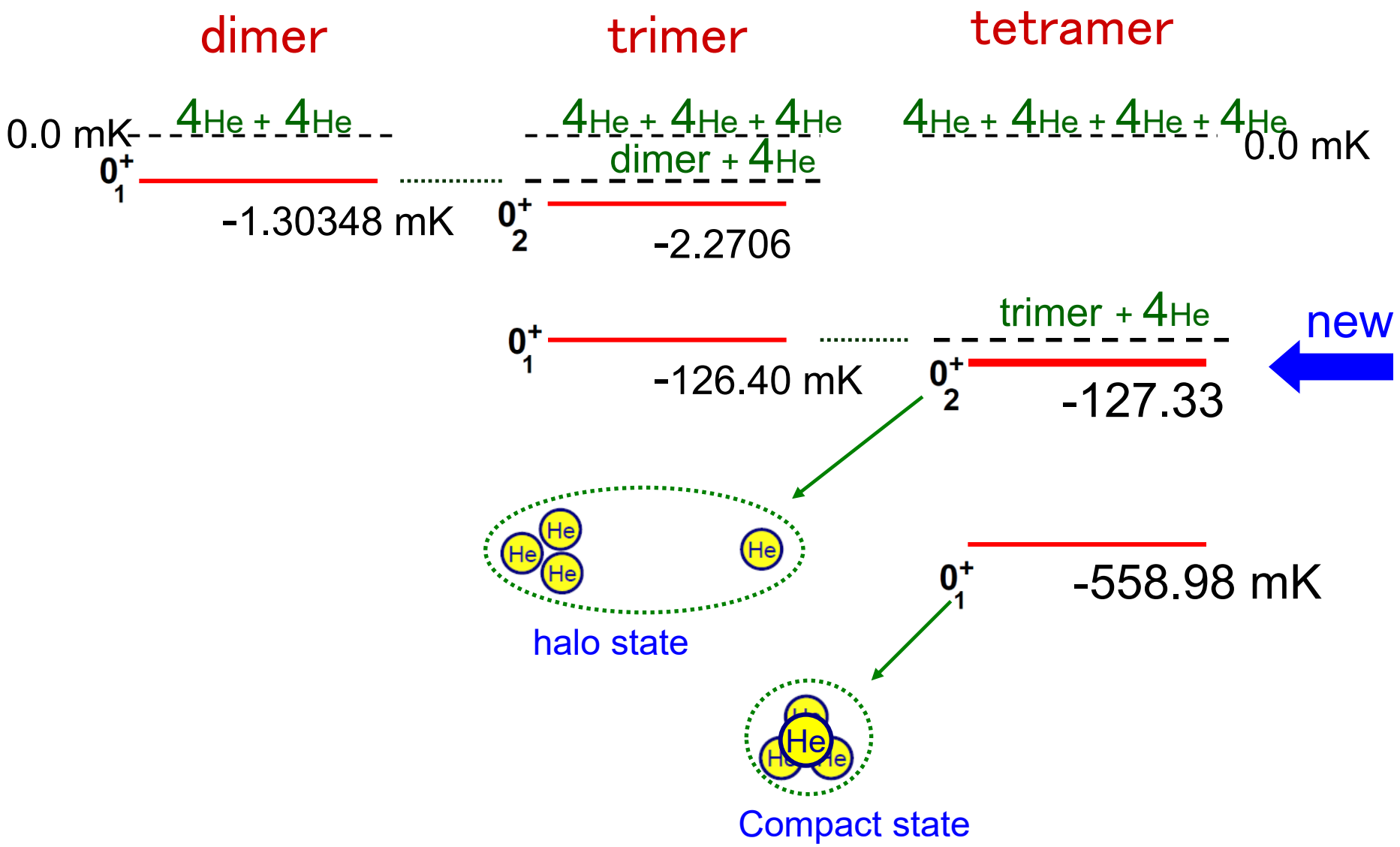
$$\Delta B_1^{(5)} (= B_1^{(5)} - B_0^{(4)}) = \frac{5}{8} B^{(2)} = \boxed{0.81 \text{ mK}}$$

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

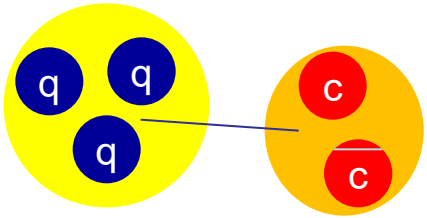
$$\Delta B_1^{(N)} (= B_1^{(N)} - B_0^{(N-1)}) = \frac{N}{2(N-1)} B^{(2)}$$

$B^{(2)}$ ← dimer

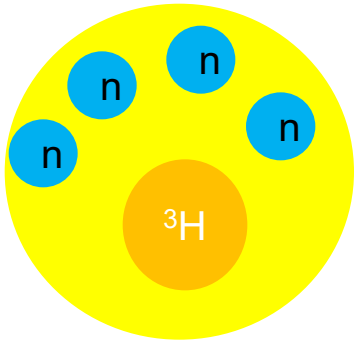
We confirmed this level structure of 4He-atom clusters (2012).



Our method is applicable to 5-body systems with bound and resonant states.



Resonance for penta quark system



We have obtained energy and decay width.

Resonant state of super-Heavy hydrogen nucleus

Next step is beyond 6-body problem calculation.

To go beyond 6-body problem,

Critical points:

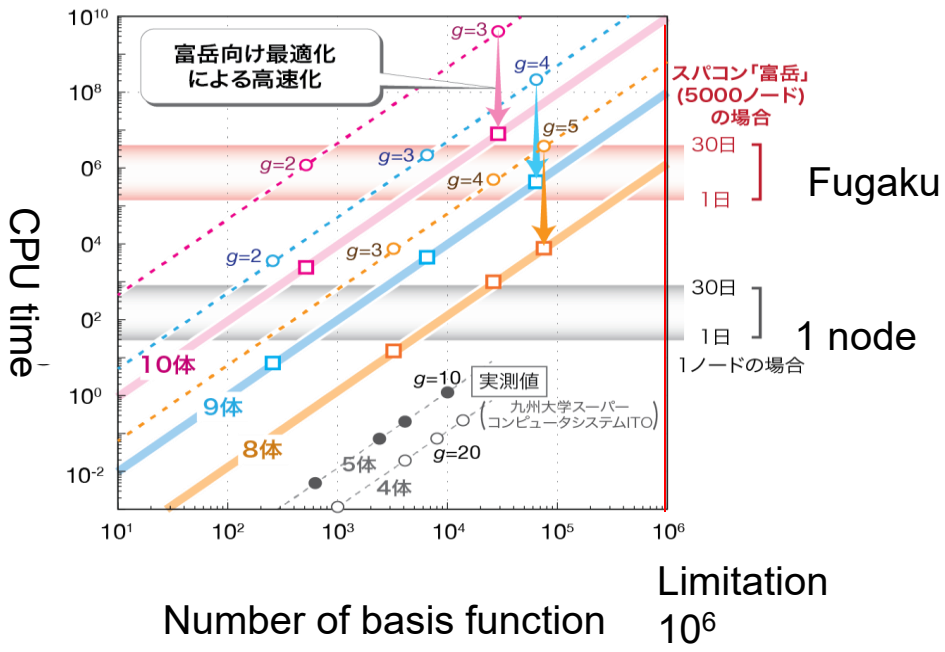
Many CPU time

Huge memory

$$\left(\left(H_{in} \right) - E \left(N_{in} \right) \right) \left(\mathbf{c_n} \right) = 0$$

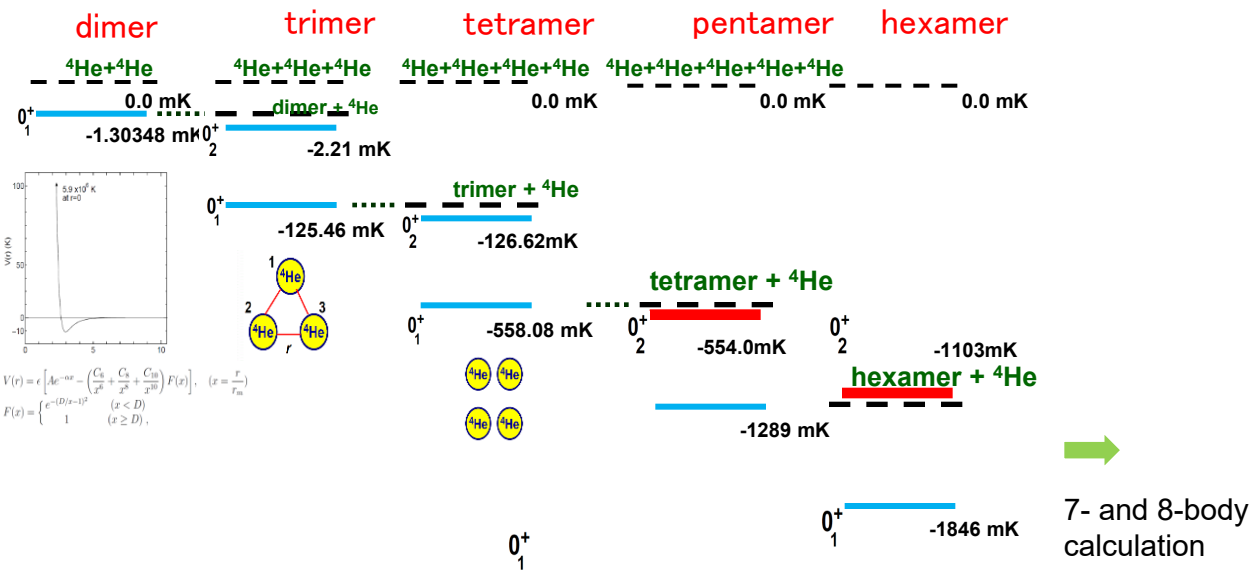
$$\begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & & \neq 0 & \end{pmatrix}$$

There are many non-zero matrix element.
Increasing number of particles, we need many basis functions.
Thus, we need huge computation time to calculate
matrix elements.
In addition, to diagolanize Hamiltonian, we need huge Memory.



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.

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



Fugaku computer

Future perspective in my research

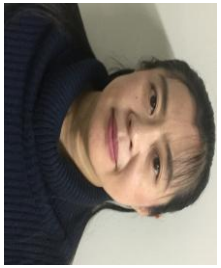
Grant-in-Aid for Transformative Research Areas (2025 April to 2030 march, 5 years)

Quantum Matter Science in the Universe Opened Up by Precise Numerical Calculations

about 8.0×10^6 USDs for 5 years

1USD=150JPY

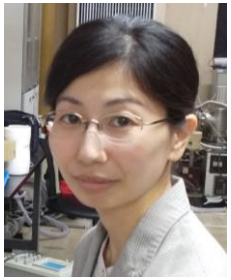
A01 : E. Hiyama
(Tohoku Univ./RIKEN



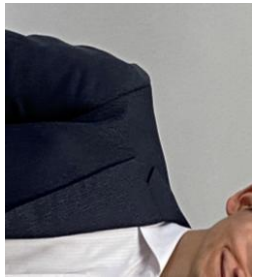
A02 : K. Yoshida
(Osaka Univ.)

A03 : I. Kanamori
(RIKEN)

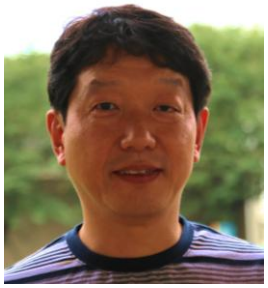
B01 : K. Iwakuni
(Electro-Comm. Univ.)



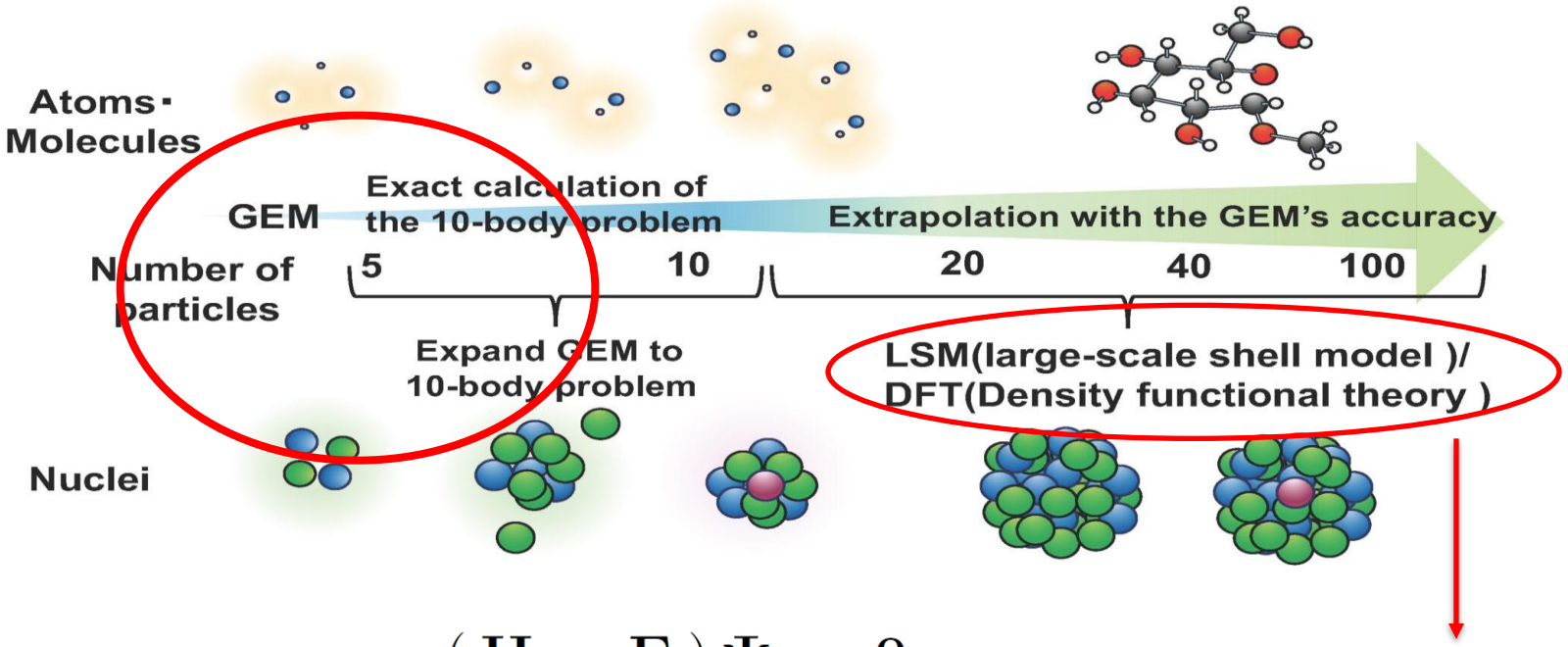
B02 : K. Miwa
(Tohoku Univ.)



B03 : S. Nishimura
(RIKEN)



B04 : S. Kawasaki
(KEK)



$$(\mathrm{H} - \mathrm{E})\,\Psi = 0$$

Fugaku supercomputer　D-wave quantum computer

DFT is also applicable
for material science etc.

統一プラットフォームを活用した宇宙の量子物質の研究

有限量子多体系計算
統一プラットフォーム

A01 GEM
A01 LSM
A02 DFT
A03 計算科学

B01

精度保証

プロトン化分子(H_3^+, H_5^+)の
精密スペクトルの決定

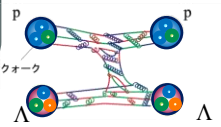
H_3^+

星間分子の研究
(陽子の量子効果の解明)

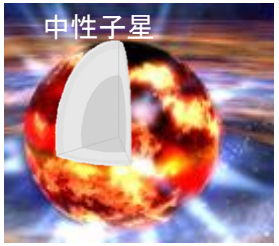
B02

インプット

重粒子間相互作用の決定
(精密散乱実験)



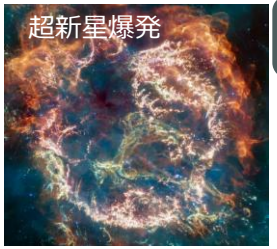
中性子星内部の研究
(高密度物質の構造の解明)



精度保証

B03

重い原子核の質量の決定



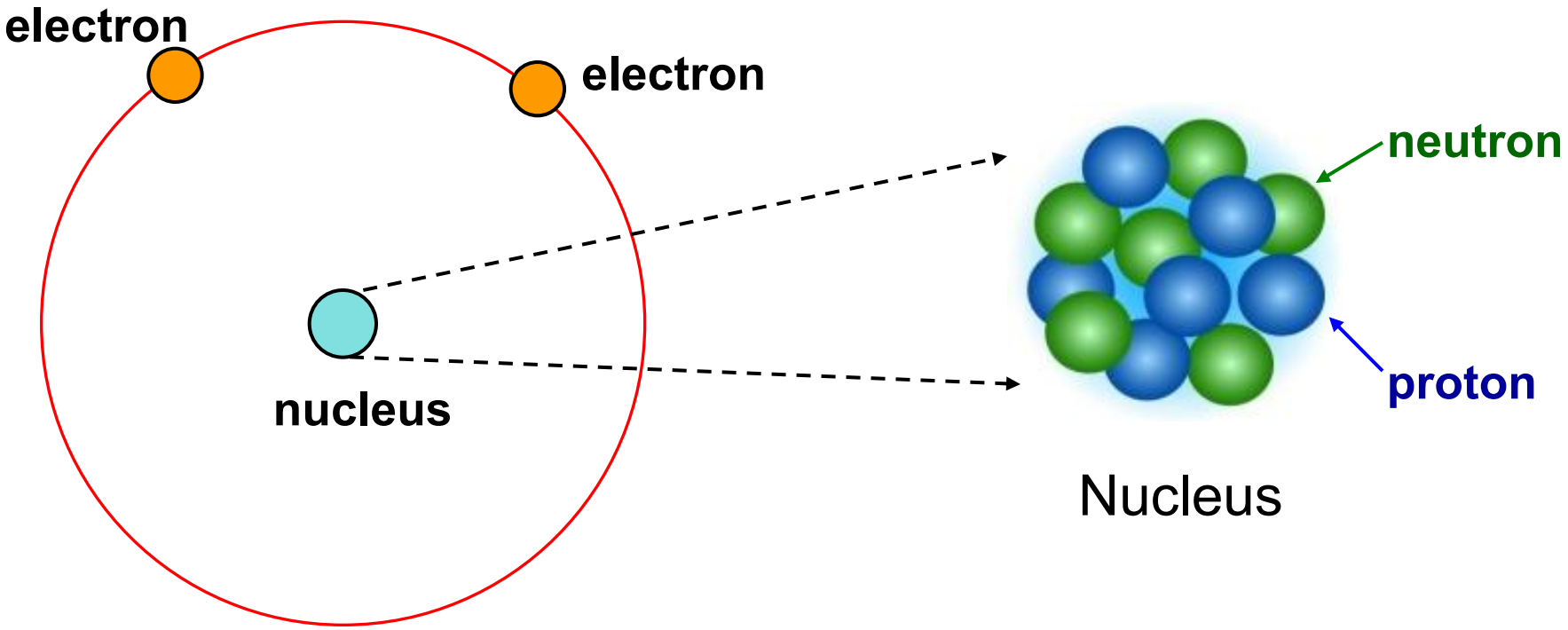
元素合成過程の解明

B04

産学連携(小型中性子源)

Challenge to beyond 5-body problem

A 3-body problem in atomic physics



Atom = **Nucleus + Electrons**

表 1.1 強い相互作用によって崩壊しない安定な素粒子

レプトン（軽粒子）B（バリオン数）$= 0$

粒子	記号	質量 (MeV/c^2)	寿命（秒）	スピン	L_e	L_μ	L_τ
電子	e^-	0.511	安定	1/2	+1	0	0
ミュオン	μ^-	106	2.2×10^{-6}	1/2	0	+1	0
タウ	τ^-	1784	3.4×10^{-23}	1/2	0	0	+1
電子ニュートリノ	ν_e	0	安定	1/2	+1	0	0
ミュオンニュートリノ	ν_μ	0	安定	1/2	0	+1	0
タウニュートリノ	ν_τ	0	安定	1/2	0	0	+1

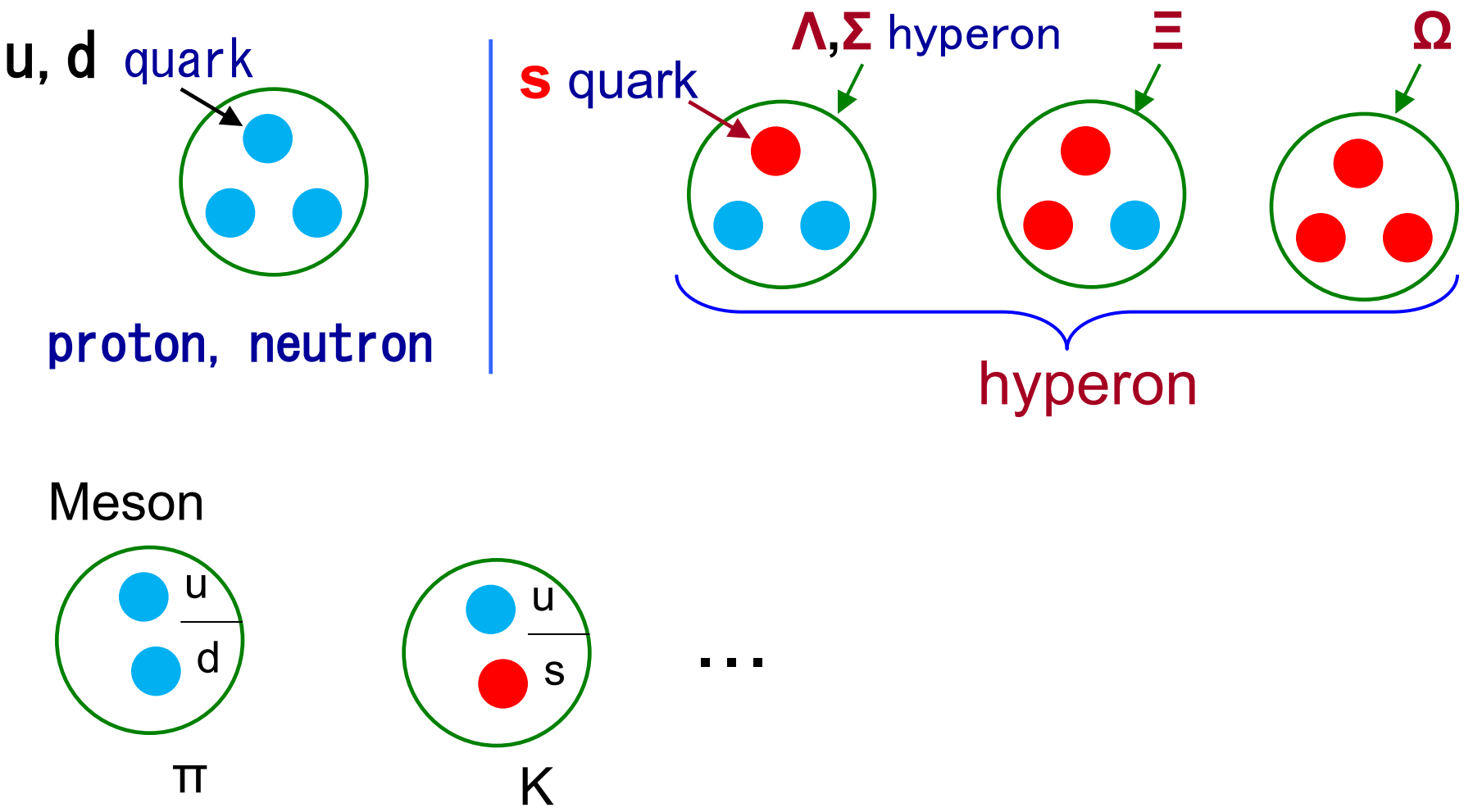
メソン（中間子）$B = L_e = L_\mu = L_\tau = 0$

粒子	記号	質量 (MeV/c^2)	寿命（秒）	スピン	S	Y	I	I_3
π 中間子	π^+	140	2.6×10^{-8}	0	0	0	1	+1
	π^0	135	8.7×10^{-17}					0
	π^-	140	2.6×10^{-8}					−1
K 中間子	K^+	494	1.2×10^{-8}	0	+1	+1	1/2	+1/2
	K^0	498	9×10^{-11}, 5×10^{-8}					−1/2
η 中間子	η^0	549	6×10^{-19}	0	0	0	0	0

バリオン（重粒子）$B = +1$, $L_e = L_\mu = L_\tau = 0$

粒子	記号	質量 (MeV/c^2)	寿命（秒）	スピン	S	Y	I	I_3
陽子	p	938.3	安定	1/2	0	+1	1/2	+1/2
中性子	n	939.6	889					−1/2
ラムダ	Λ^0	1116	2.6×10^{-10}	1/2	−1	0	0	0
シグマ	Σ^+	1189	8.0×10^{-11}	1/2	−1	0	1	+1
	Σ^0	1193	6×10^{-20}					0
	Σ^-	1197	1.5×10^{-10}					−1
グザイ	Ξ^0	1315	2.9×10^{-10}	1/2	−2	−1	1/2	+1/2
	Ξ^-	1321	1.6×10^{-10}					−1/2
オメガ	Ω^-	1672	8.2×10^{-11}	3/2	−3	−2	0	0

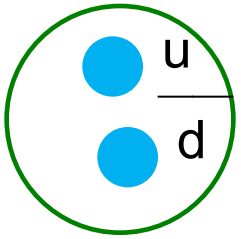
In 1950's, we observed many baryons and mesons.



Quarks are currently elementary particles.
To describe these baryons and mesons, theoretically, they
Use Lattice QCD which is abinitio calculation.

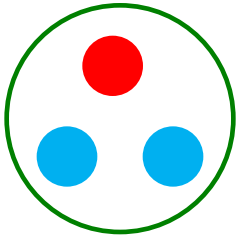
Some use quark model for these baryons and mesons. Namely,

Meson



π

It is considered that meson is composed of two quarks.



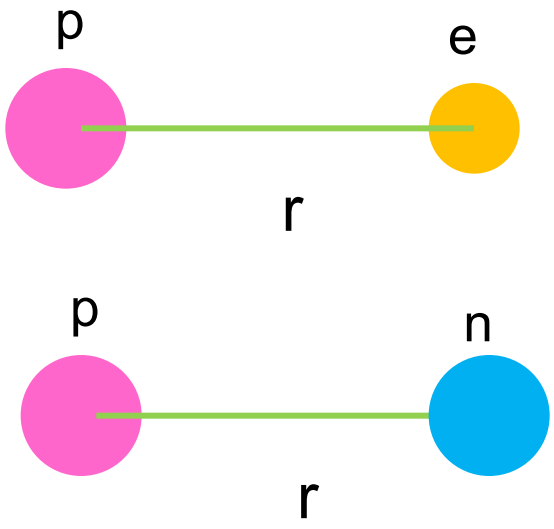
Λ

It is considered that baryon is composed of three quarks.

How do we calculate two and three quarks systems?
Let's solve these systems.

First, let's consider wavefunction of meson and baryon systems.

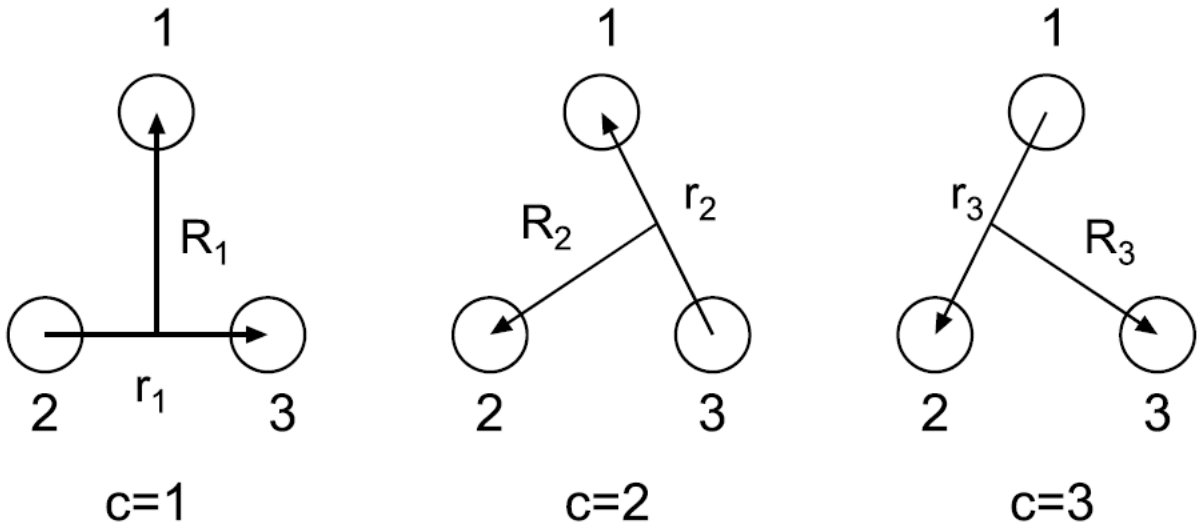
Cf. Hydrogen: wavefunction: spatial part only



Deuteron: wavefunction: isospinxspinxspatial

Meson:wavefunction:
colorxisospinxspinxspatial

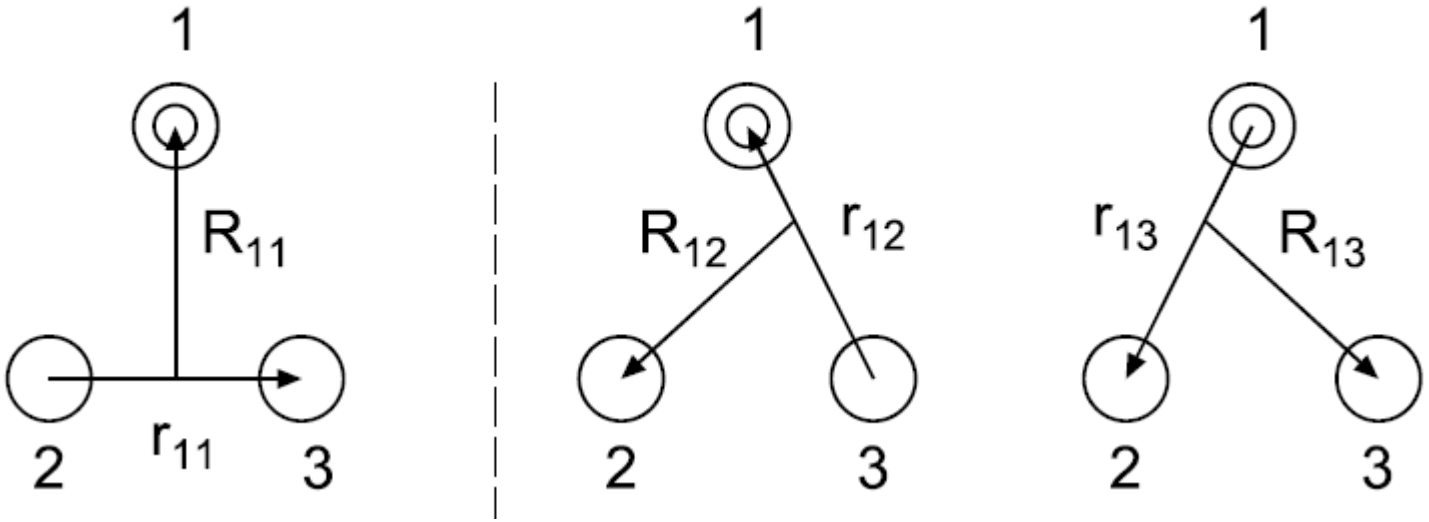
Let's go to three-body problem.



$$\Phi^{(c=k)}_{JMTT_z,\xi} = \left[\left[[\chi_{\frac{1}{2}}(i)\ \chi_{\frac{1}{2}}(j)]_s \chi_{\frac{1}{2}}(k) \right]_S \left[\phi_{nl}(\boldsymbol{r}_k)\ \psi_{NL}(\boldsymbol{R}_k) \right]_I \right]_{JM}$$
$$\times \left[[\eta_\tau(i)\ \eta_\tau(j)]_t \eta_\tau(k) \right]_{TT_Z}, \qquad \xi \equiv \{s, S, n, l, N, L, I, t\}$$

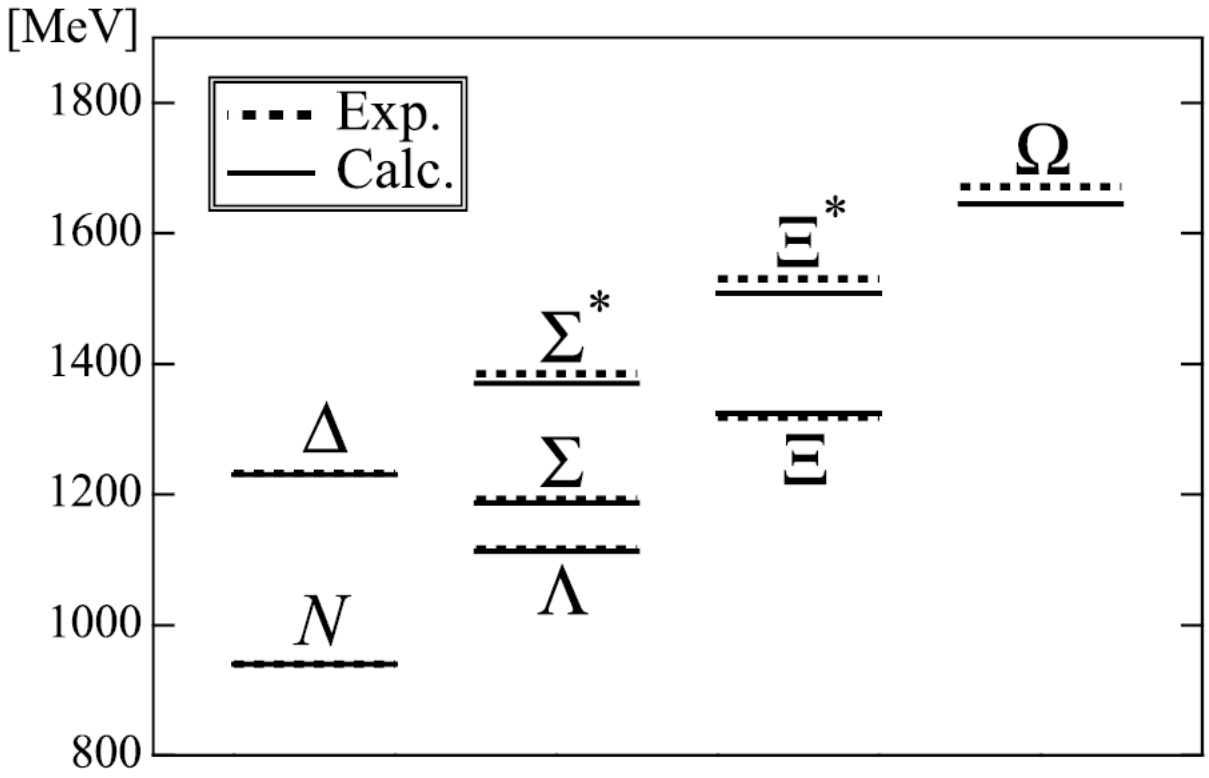
$$\Phi_{JMTT_z,\,\xi} = \Phi(\text{color singlet}) \sum_{c=1}^{3} \Phi^{(c)}_{JMTT_z,\,\xi} \,.$$

We just consider this part only.



$$\Phi^{(\gamma,\,c)}_{JMTT_z,\,\xi} = \left[\left[\left[\chi_{\frac{1}{2}}(\alpha)\chi_{\frac{1}{2}}(\beta) \right]_s \chi_{\frac{1}{2}}(\gamma) \right]_S \left[\phi_{nl}(\boldsymbol{r}_{\gamma c})\psi_{NL}(\boldsymbol{R}_{\gamma c}) \right]_I \right]_{JM}$$

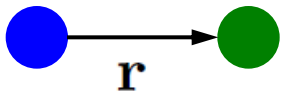
$$\times \left[[\eta_\tau(\alpha)\eta_\tau(\beta)]_t \eta_{\tau_\gamma}(\gamma) \right]_{TT_z}, \qquad \xi \equiv \{s, S, n, l, N, L, I, t\},$$


[MeV]
1800
1600
1400
1200
1000
800
Exp.
Calc.
Δ
N
Σ*
Σ
Λ
Ξ*
Ξ
Ω

Calculation of 2-body norm matrix element

It is too simple but very instructive.

2体問題



Normal Lobe

$$\Phi_{lm}(\nu,\mathbf{r}) = r^l e^{-\nu r^2} Y_{lm}(\hat{\mathbf{r}}) = \lim_{\varepsilon\to 0} \Phi_{lm}(\varepsilon,\nu,\mathbf{r})$$

$$\Phi_{lm}(\varepsilon,\nu,\mathbf{r}) = \frac{1}{\varepsilon^l}\sum_{k=1}^{k_{\max}} C_{lm,k}\, e^{-\nu(\mathbf{r}-\varepsilon\mathbf{D}_{lm,k})^2}$$

Norm matrix element

$$\langle \Phi_{lm}(\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\nu',\mathbf{r})\rangle = \lim_{\varepsilon,\varepsilon'\to 0} \langle \Phi_{lm}(\varepsilon,\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\varepsilon',\nu',\mathbf{r})\rangle$$

(straightforward integaration)

$$= A \lim_{\varepsilon,\varepsilon'\to 0} \frac{1}{(\varepsilon\varepsilon')^l} \sum_k \sum_{k'} C^*_{lm,k} C_{lm,k'}\, e^{-\alpha\,\varepsilon\varepsilon'(\mathbf{D}^*_{lm,k}\cdot\mathbf{D}_{lm,k'})}$$

$$A = \left(\frac{\pi}{\nu+\nu'}\right)^{3/2} \qquad \alpha = \frac{2\nu\nu'}{\nu+\nu'}$$

=1
(for $\nu = \nu'$)

$$\langle \Phi_{lm}(\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\nu',\mathbf{r})\rangle = \lim_{\varepsilon,\varepsilon'\to 0} \langle \Phi_{lm}(\varepsilon,\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\varepsilon',\nu',\mathbf{r})\rangle$$

$$= A \lim_{\varepsilon,\varepsilon'\to 0} \frac{1}{(\varepsilon\varepsilon')^l} \sum_k \sum_{k'} C^*_{lm,k} C_{lm,k'} \; e^{-\alpha\,\varepsilon\,\varepsilon'} \, (\mathbf{D}^*_{lm,k} \cdot \mathbf{D}_{lm,k'})$$

=1

(for $\nu = \nu'$)

Finite value of ε,ε'->mixture of angular momenta

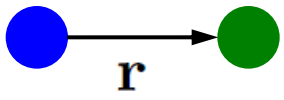
Small value of ε,ε'-> round-off error(けた落ち)

What is round-off error?

Calculation of 2-body norm matrix element

It is too simple but very instructive.

2体問題



Normal Lobe

$$\Phi_{lm}(\nu,\mathbf{r}) = r^l e^{-\nu r^2} Y_{lm}(\hat{\mathbf{r}}) = \lim_{\varepsilon\to 0} \Phi_{lm}(\varepsilon,\nu,\mathbf{r})$$

$$\Phi_{lm}(\varepsilon,\nu,\mathbf{r}) = \frac{1}{\varepsilon^l}\sum_{k=1}^{k_{\max}} C_{lm,k}\, e^{-\nu(\mathbf{r}-\varepsilon\mathbf{D}_{lm,k})^2}$$

Norm matrix element

$$\langle \Phi_{lm}(\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\nu',\mathbf{r})\rangle = \lim_{\varepsilon,\varepsilon'\to 0} \langle \Phi_{lm}(\varepsilon,\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\varepsilon',\nu',\mathbf{r})\rangle$$

(straightforward integaration)

$$= A \lim_{\varepsilon,\varepsilon'\to 0} \frac{1}{(\varepsilon\varepsilon')^l} \sum_k \sum_{k'} C^*_{lm,k} C_{lm,k'}\, e^{-\alpha\,\varepsilon\varepsilon'(\mathbf{D}^*_{lm,k}\cdot\mathbf{D}_{lm,k'})}$$

$$A = \left(\frac{\pi}{\nu+\nu'}\right)^{3/2} \qquad \alpha = \frac{2\nu\nu'}{\nu+\nu'}$$

=1
(for $\nu = \nu'$)

$$\langle \Phi_{lm}(\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\nu',\mathbf{r})\rangle = \lim_{\varepsilon,\varepsilon'\to 0} \langle \Phi_{lm}(\varepsilon,\nu,\mathbf{r})| \quad 1 \quad |\Phi_{lm}(\varepsilon',\nu',\mathbf{r})\rangle$$

$$= A \lim_{\varepsilon,\varepsilon'\to 0} \frac{1}{(\varepsilon\varepsilon')^l} \sum_k \sum_{k'} C^*_{lm,k} C_{lm,k'} \; e^{-\alpha\,\varepsilon\,\varepsilon'} \, (\mathbf{D}^*_{lm,k} \cdot \mathbf{D}_{lm,k'})$$

$=1$ (for $\nu = \nu'$)

We calculate $e^{-\alpha\varepsilon\varepsilon'}$ in Fortran code as DEXP(-αεε').

a) This generates serious mixture of $Y_{lm}(\hat{\mathbf{r}})$ with higher ℓ for a finite value of ε

To avoid the mixture of $Y_{lm}(\hat{\mathbf{r}})$

For example, we take =0.00001. The matrix element =1.00022333.

Then, ε =0.000000001. But, the matrix element =1.223333333! Why?

This phenomena is round-off error.

けた落ち

In calculation by computers, usually numbers are given in **15** significant figures (digits) .

有効数字

no problem

15

1.000000000000123
+) 1.000000000000121

2.000000000000244

有効数字=15

however

15

1.000000000000123
-) 1.000000000000121

0.000000000000002

$= 2 \times 10^{-14}$

Only one **significant** figure !

有効数字=1

Be careful when subtracting nearly the same numbers.

So far, I though that this new basis function was my original idea.
However, I found that text the similar basis function was introduced in quantum chemistry textbook.
According to the textbook,
It mentioned that when ε have some value, we have mixture of higher angular momentum. When ε=>0,
We have serious round-off error.

Then, due to this difficulty,

the old Gaussian Lobe method (1960's) was NOT

used in actual calculations and was

soon forgotten (only used as exercise for student) .

I was so shocked to read the textbook. And I lost the motivation to do research for one week.

But, some 30 years after, this difficulty was solved by Hiyama [3,6,7] by introducing the ISGL basis functions with properly taking $\lim_{\varepsilon \to 0}$ **after** performing the analytical integration of the matrix elements.

Hiyama's new method (at the time of MC student, 1994)

Infinitesimally Shifted Gaussian Lobe (ISGL) basis Function

$$\Phi_{lm}(\varepsilon,\nu,\mathbf{r}) = \frac{1}{\varepsilon^{\,l}} \sum_{k=1}^{k_{\max}} C_{lm,k}\; e^{-\nu(\mathbf{r}-\varepsilon\mathbf{D}_{lm,k})^2}$$

Norm matrix element

$$\langle\, \Phi_{lm}(\nu,\mathbf{r})|\quad 1\quad |\Phi_{lm}(\nu',\mathbf{r})\rangle = \lim_{\varepsilon,\varepsilon'\to 0} \langle\, \Phi_{lm}(\varepsilon,\nu,\mathbf{r})|\quad 1\quad |\Phi_{lm}(\varepsilon',\nu',\mathbf{r})\,\rangle$$

$$= A \lim_{\varepsilon,\varepsilon'\to 0} \frac{1}{(\varepsilon\varepsilon')^l} \sum_k \sum_{k'} C^*_{lm,k} C_{lm,k'}\; e^{-\alpha\,\varepsilon\,\varepsilon'\,(\mathbf{D}^*_{lm,k}\cdot\mathbf{D}_{lm,k'})}$$

$= 1$
(for $\nu = \nu'$)

Dangerous if we use FUNCTION EXP (….)

$e^{\varepsilon\varepsilon' x}$

Taylor expansion with very small ε and ε'

$$e^{\varepsilon\varepsilon' x} = 1 + (\varepsilon\varepsilon' x) + \frac{1}{2!}(\varepsilon\varepsilon' x)^2 + \cdots\cdots\cdots$$

If we take the full terms, it causes serius round-off error as is expected. But,

$$\frac{1}{(\varepsilon\varepsilon')^l}\sum_k\sum_{k'} C^*_{lm,k}C_{lm,k}\ e^{\varepsilon\varepsilon' x}$$

$$e^{\varepsilon\varepsilon' x} = \cancel{1} + \cancel{(\varepsilon\varepsilon' x)} + \frac{1}{2!}(\varepsilon\varepsilon' x)^2 + \cdots\cdots\cdots$$

But, I tried to omit the first term, namely "1" (I took $l = 2$).
I thought the term is the bad origin in the round-off error.
My superviser said -- "It is very stupid because, in the Talor expansion, the first term is the most important and the higher-order terms are less important".
I answered --"We shall never know the result, unless we try"

The result became slightly better, but not good.

Then, I omitted the second term too.
Surprisingly, we obtained the exact result, namlely Norm =1.0

What happened ???

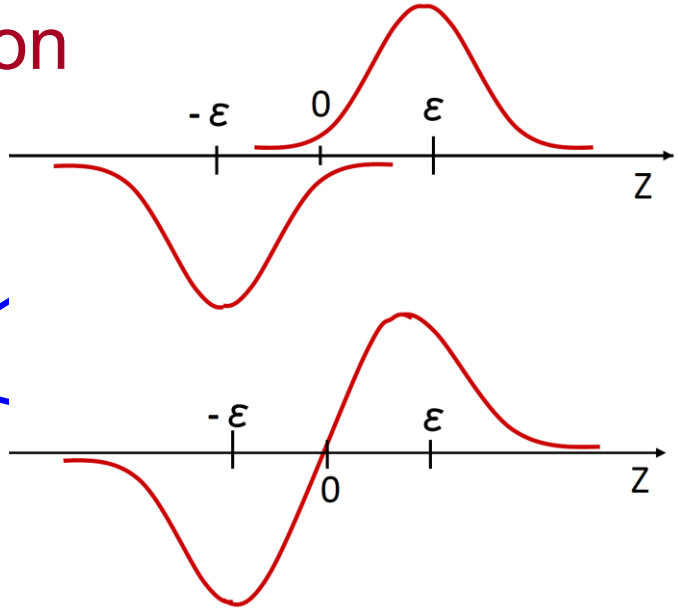
Construction of the ISGL function

Simple example: l=1,m=0

roughly

$$e^{-\nu r^2}\, r\, Y_{10}(\hat{\mathbf{r}}) \quad \propto \quad z e^{-\nu z^2}$$

$$e^{-\nu(z-\varepsilon)^2} - e^{-\nu(z+\varepsilon)^2}$$



In detail

$$\frac{1}{\varepsilon}\left[e^{-\nu(z-\varepsilon)^2} - e^{-\nu(z+\varepsilon)^2}\right] = \frac{1}{\varepsilon} e^{-\nu(z^2+\varepsilon^2)}\left[e^{2\nu\varepsilon z} - e^{-2\nu\varepsilon z}\right]$$

Taylor expansion

$$= \frac{1}{\epsilon} e^{-\nu(z^2+\epsilon^2)}\left[1 + (2\epsilon\nu z) + \frac{(2\epsilon\nu z)^2}{2!} + \frac{(2\epsilon\nu z)^3}{3!} + \cdot\cdot\right]$$

$$- \frac{1}{\epsilon} e^{-\nu(z^2+\epsilon^2)}\left[1 - (2\epsilon\nu z) + \frac{(2\epsilon\nu z)^2}{2!} - \frac{(2\epsilon\nu z)^3}{3!} + \cdot\cdot\right]$$

First power of ε

$$= \frac{1}{\varepsilon} e^{-\nu(z^2+\varepsilon^2)}\left[4\varepsilon\nu z + \frac{2}{3}(2\varepsilon\nu z)^3 + \cdot\cdot\cdot\cdot\right] \overset{\varepsilon\to 0}{\longrightarrow} 4\nu\, z\, e^{-\nu z^2}$$

Mixture of L=3

$$e^{\varepsilon\varepsilon' x} = 1 + (\varepsilon\varepsilon' x) + \frac{1}{2!}(\varepsilon\varepsilon' x)^2 + \cdots\cdots\cdots \qquad 2$$

Second power is remained.

$$\frac{1}{(\varepsilon\varepsilon')^l} \sum_k \sum_{k'} C^*_{lm,k} C_{lm,k'} \, e^{-\alpha\,\varepsilon\,\varepsilon'\,(\mathbf{D}^*_{lm,k}\cdot\mathbf{D}_{lm,k'})}$$

Taylor expansion

$$\sum_{j=l}^{\infty} \sum_{k=1}^{k_{\max}} \sum_{k'=1}^{k_{\max}} C_{lm,k}\, C_{lm,k'} \frac{1}{j!} \left(\nu_n \varepsilon\varepsilon'\, \mathrm{D}^*_{lm,k} \cdot \mathrm{D}_{lm,k'}\right)^j .$$

$$= 0 \quad (j < l)$$

The shift parameters were so constructed at the beginning.

The terms with $j > l$ can be neglected for small ε

It is sufficient to pickup the terms with $j = l$

Thus, my method solved the Gauss-Lobe's difficulty (since 1960's in quantum chemistry):

1) higher-angular-momentum mixing
2) severe round-off error.

Benchmark-test calculation of the 4-nucleon bound state

This benchmark test was so stressful!

Because, if I give a different result from other groups,

then, general readers in the world will consider that

my calculational method is not reliable.

If so, I must decide to quit my research.

And I would really regret to join this bench-mark test.

But, my superviser, Prof. M. Kamimura
who is co-author, said to me,

“You do not need to quit your research!

You should continue surviving in this research field.

Because you are young.

Instead, I will quit my research, since I shall soon retire from Kyushu Univ. within 2 years.

This would give much less damage to us.”

I said, “NO! Great professor, please do not say so!
I will quit my research.”

Professor said, “I will quit my research”