原子核少数系計算

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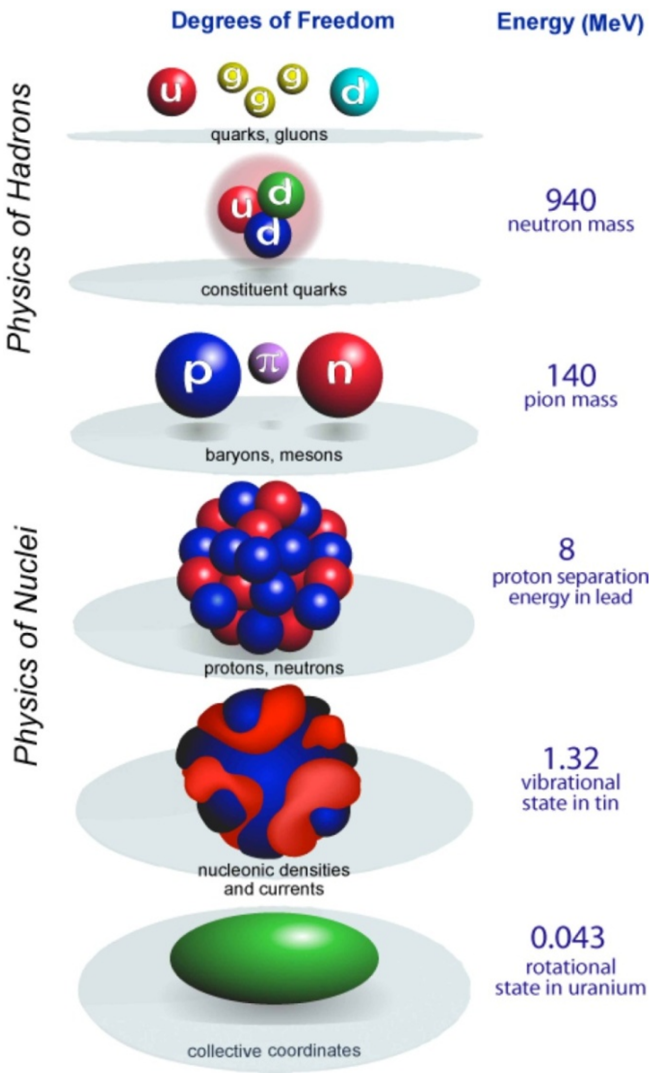
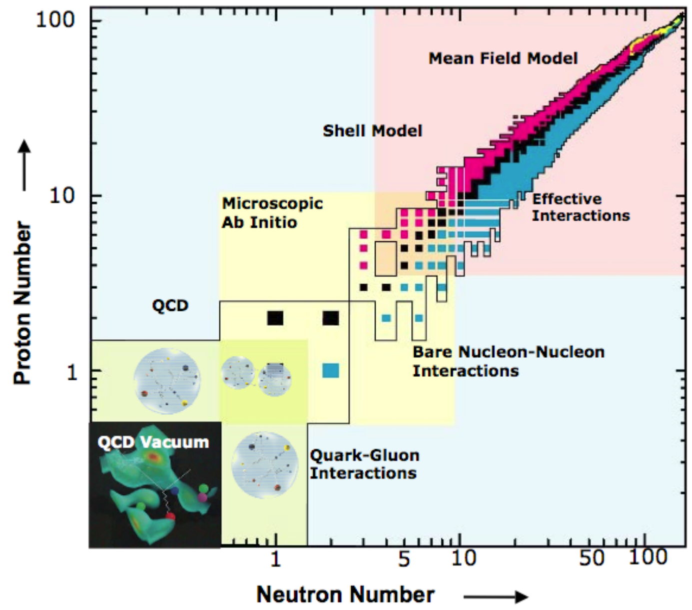
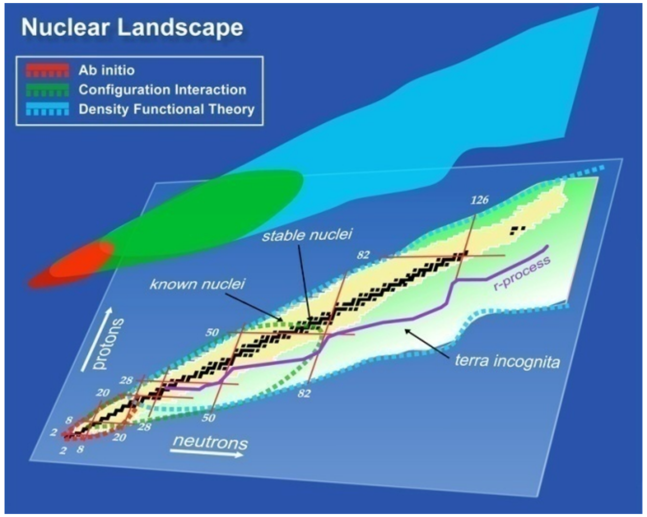
Bridging the nuclear physics scales



QCD

Nuclear
Structure

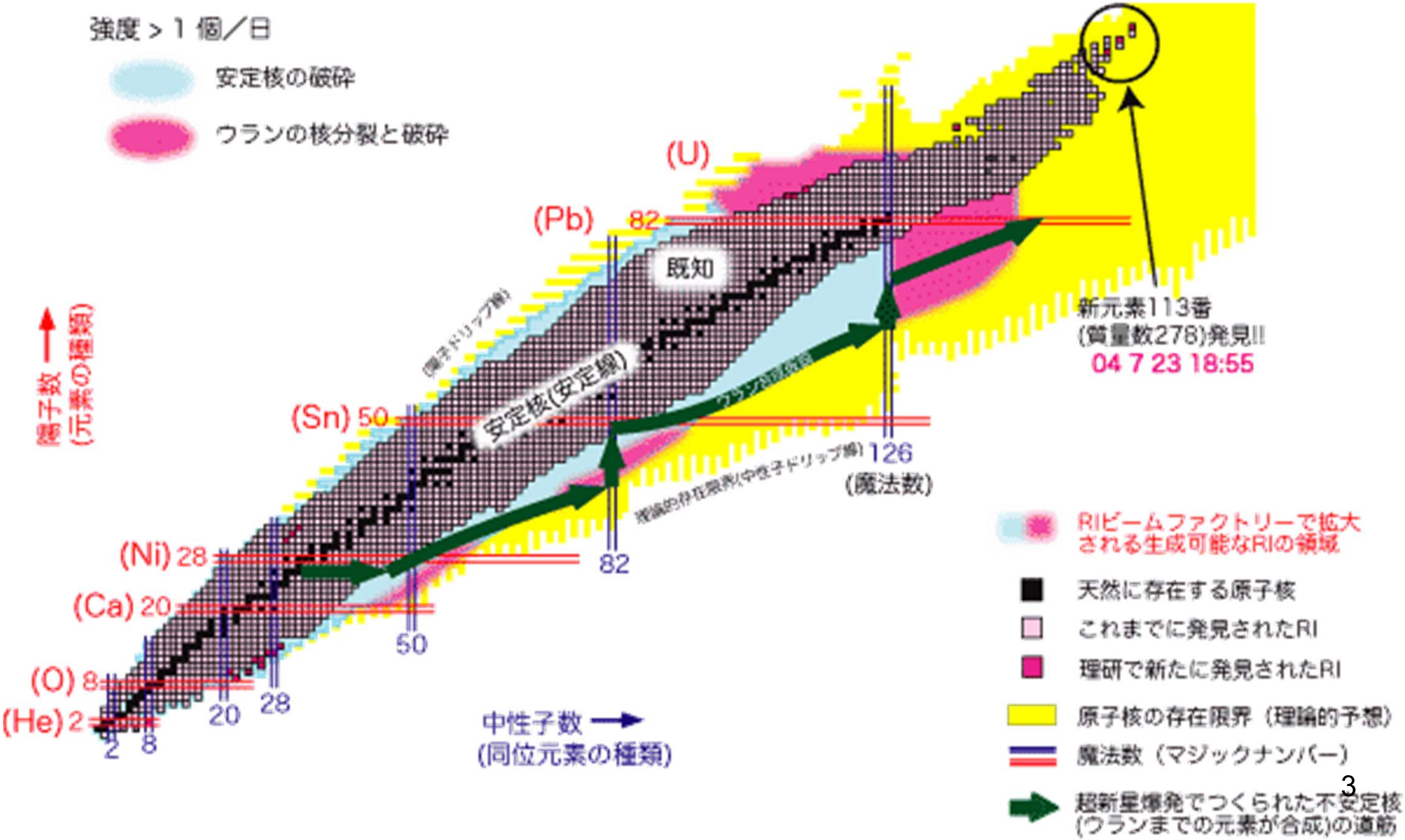




Applications in astrophysics,
defense, energy, and medicine

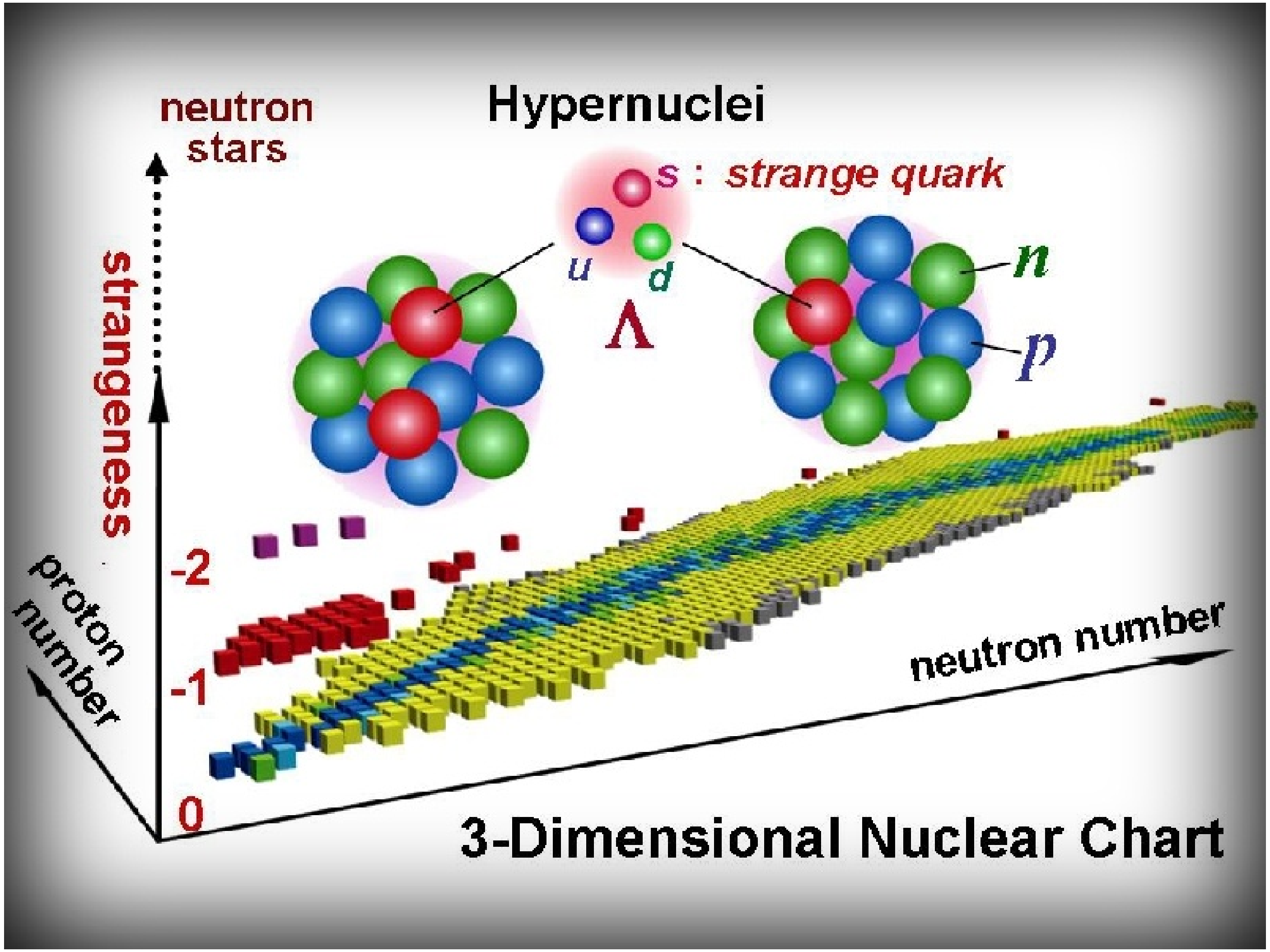
Adapted from D. Dean, JUSTIPEN Meeting, 2009 http://www.rarf.riken.go.jp/pub/newcontents/contents/sisetu/RIBF.html

Table of Nuclides (Nuclear Chart)



http://www.sci.tohoku.ac.jp/mediaoffce_s/_src/sc911/3Dchart.jpg

3D Nuclear Chart



有効相互作用と模型計算

現実的核力（裸の2核子間の相互作用）

$$H = \sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\nabla_i^2\right) + \sum_{i<j}^{A} V(i,j)$$

$$H\Psi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_A) = E\Psi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_A)$$

$$H^{eff} = Pe^{-S}He^{S}P$$

$$PH^{eff}Q = 0$$

$$P + Q = 1, PQ = 0$$

P :全ヒルベルト空間の部分空間（模型空間）への射影演算子

e^S :ユニタリ変換

有効核力

$$H^{eff} = \sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\nabla_i^2\right) + \sum_{i<j}^{A} V^{eff}(i,j)$$

$$H\Phi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_A) = E\Phi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_A)$$

V^{eff} :多くの場合現象論的に決定

Φ :模型波動関数

現実的核力を直接用いた(から出発した直接的)多核子系計算

Ab-initio計算と呼ばれる。

Non-core (MC) shell model

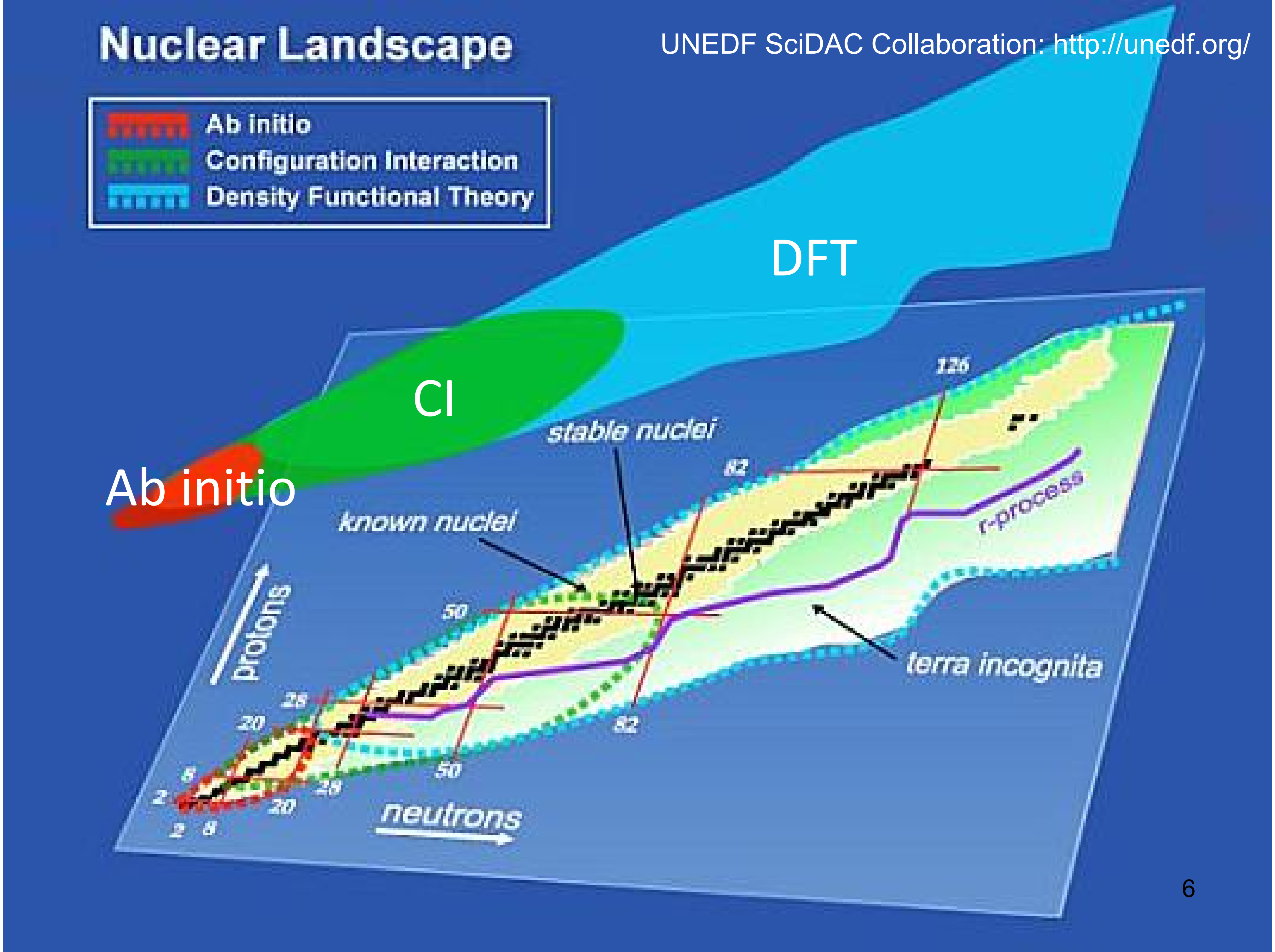
GFMC

SRG

Lattice EFT

…

大規模計算の主戦場


Nuclear Landscape
UNEDF SciDAC Collaboration: http://unedf.org/
Ab initio
Configuration Interaction
Density Functional Theory
DFT
CI
Ab initio
stable nuclei
known nuclei
terra incognita
r-process
protons
neutrons
126
82
50
28
20
8
2
82
50
28
20
8
2

原子核構造模型

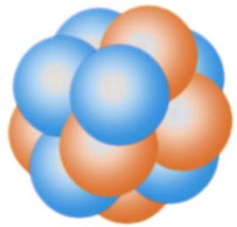
- 液滴模型
- 複合核模型
- 殻模型
- 集団運動模型
- クラスター模型

…

密度の飽和性:

原子核半径: R=1.12 $A^{1/3}$ fm

液滴模型



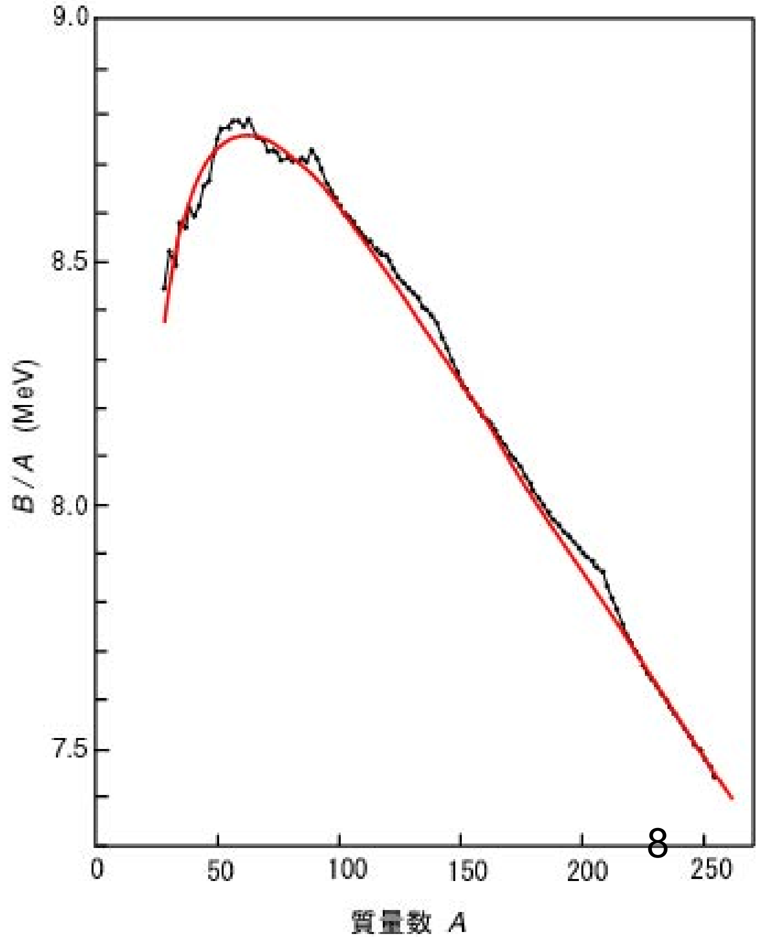
エネルギーの飽和性:

Bethe-Weizaecker mass formula

$$B(Z,N) = C_V A - C_S A^{2/3} - C_C Z^2 A^{-1/3} - C_{sym}\frac{(N-Z)^2}{A} + \delta(A)$$

- Volume: C_V = 15.6 MeV
- Surface: C_S = 17.2 MeV
- Coulomb: C_C = 0.70 MeV
- Asymmetry: C_{sym} = 23.3 MeV
- Pairing: δ(A)

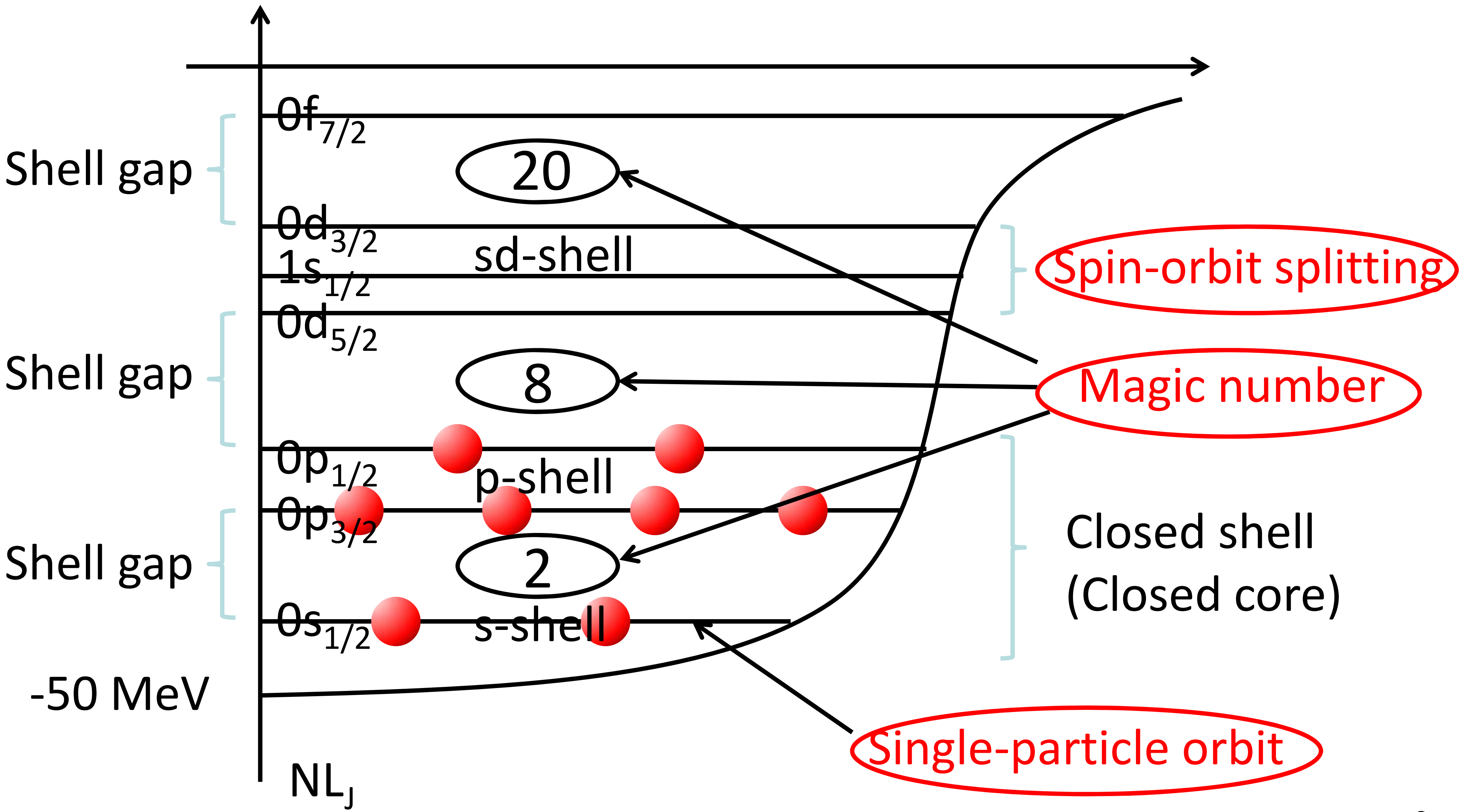
$$\delta(A) = \begin{cases} \frac{12}{\sqrt{A}}\,\mathrm{MeV}, & (Z = \text{偶数}, N = \text{偶数}), \\ 0, & (A = Z + N = \text{奇数}), \\ -\frac{12}{\sqrt{A}}\,\mathrm{MeV}, & (Z = \text{奇数}, N = \text{奇数}) \end{cases}$$



殻模型

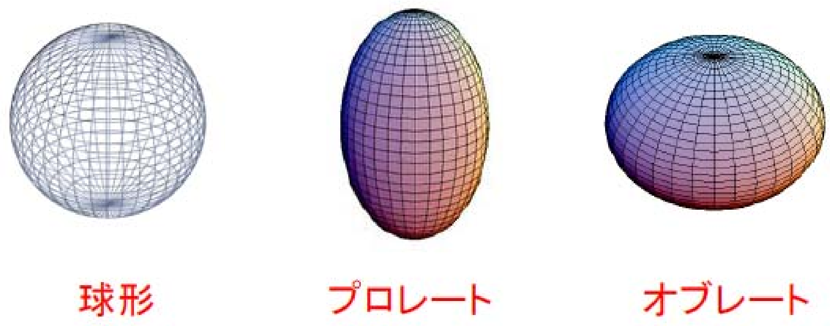
Schematic picture of the single-particle potential

調和振動子的中心力＋スピン・軌道力

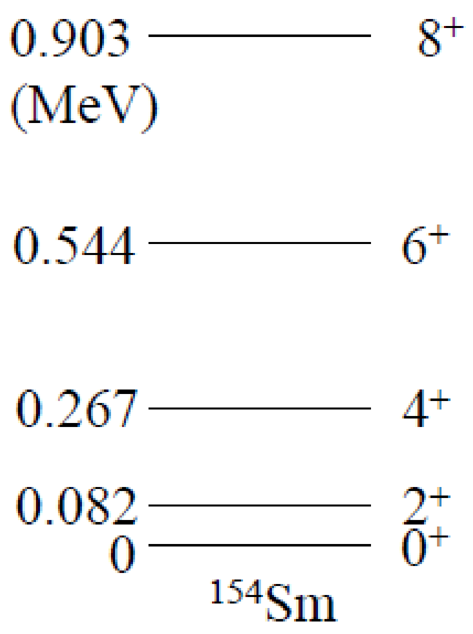


集団運動模型

原子核全体の変形、回転、振動現象を記述する模型



^{154}Sm の励起スペクトル



$$E_I \sim \frac{I(I+1)\hbar^2}{2\mathcal{J}}$$

微視的には平均場模型(Hartree Fock)＋乱雑位相近似
(Random Phase Approximation)

＋ferimi面近傍の2核子対相関(pairing) ``BCS状態''

→ 核子の自由度から出発して理解する

剛体の回転エネルギー(古典力学)

$$E = \frac{1}{2}\mathcal{J}\omega^2 = \frac{I^2}{2\mathcal{J}}$$

$$(I = \mathcal{J}\omega,\ \omega = \dot{\theta})$$

原子核構造模型

- 液滴模型
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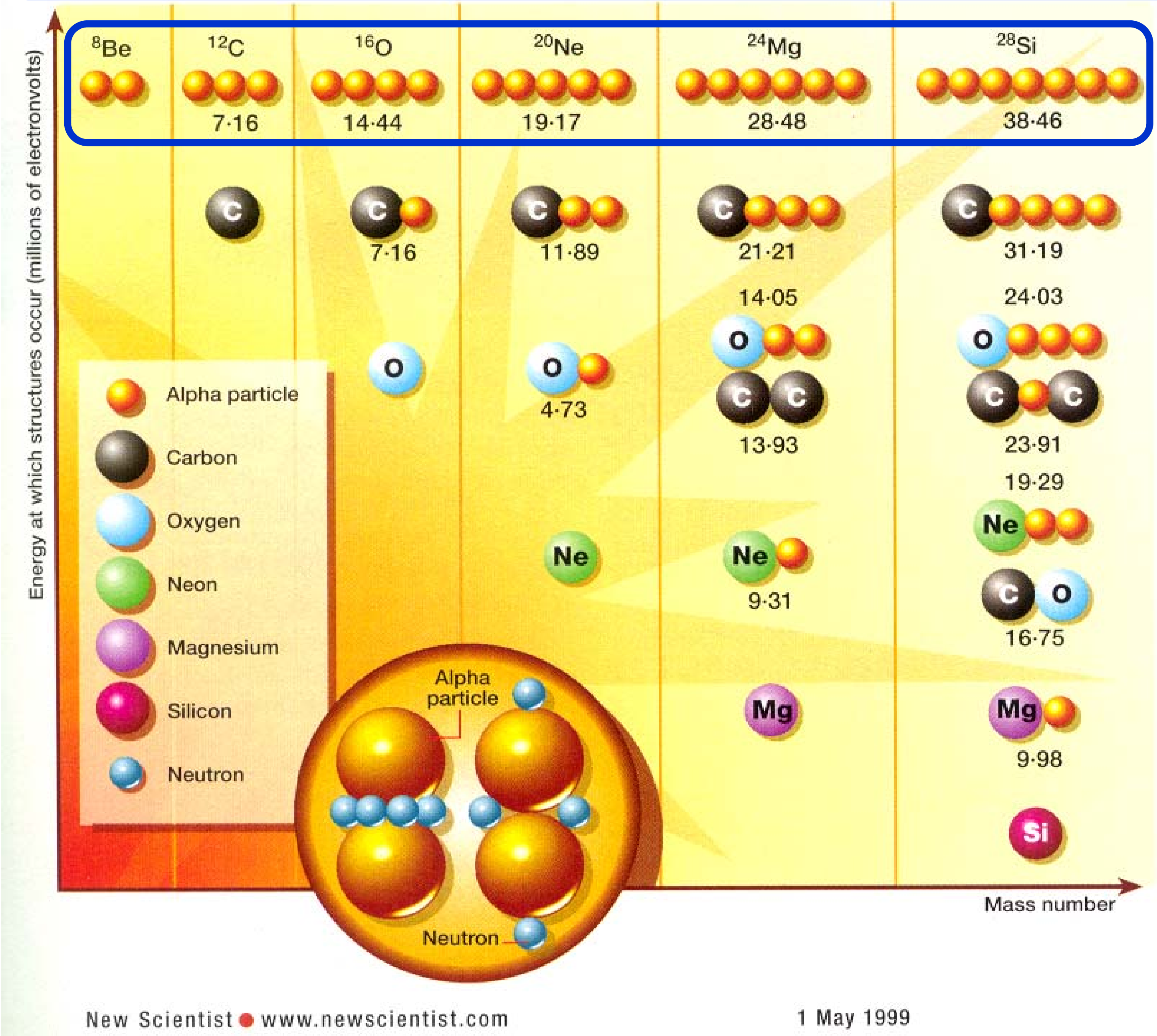
- 集団運動模型
- クラスター模型

…

原子核に現れるクラスター構造 (Ikeda Diagram)



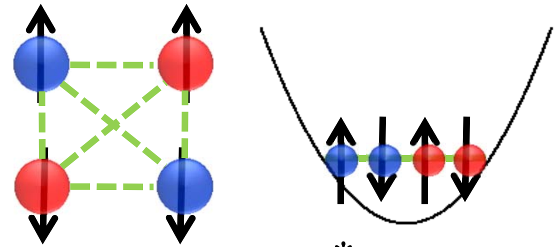
← **Limit of structural change from shell to clusters**

Classified according to the Threshold Rule.

K. Ikeda et al., PTP suppl. Extra num., 464 (1968).

The most tightly bound light cluster

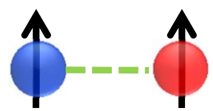
α particle (quartet)



$E/A \sim 7$ MeV $E^* \sim 20$ MeV

stiff

The most elemental subunit in nuclear cluster structures.

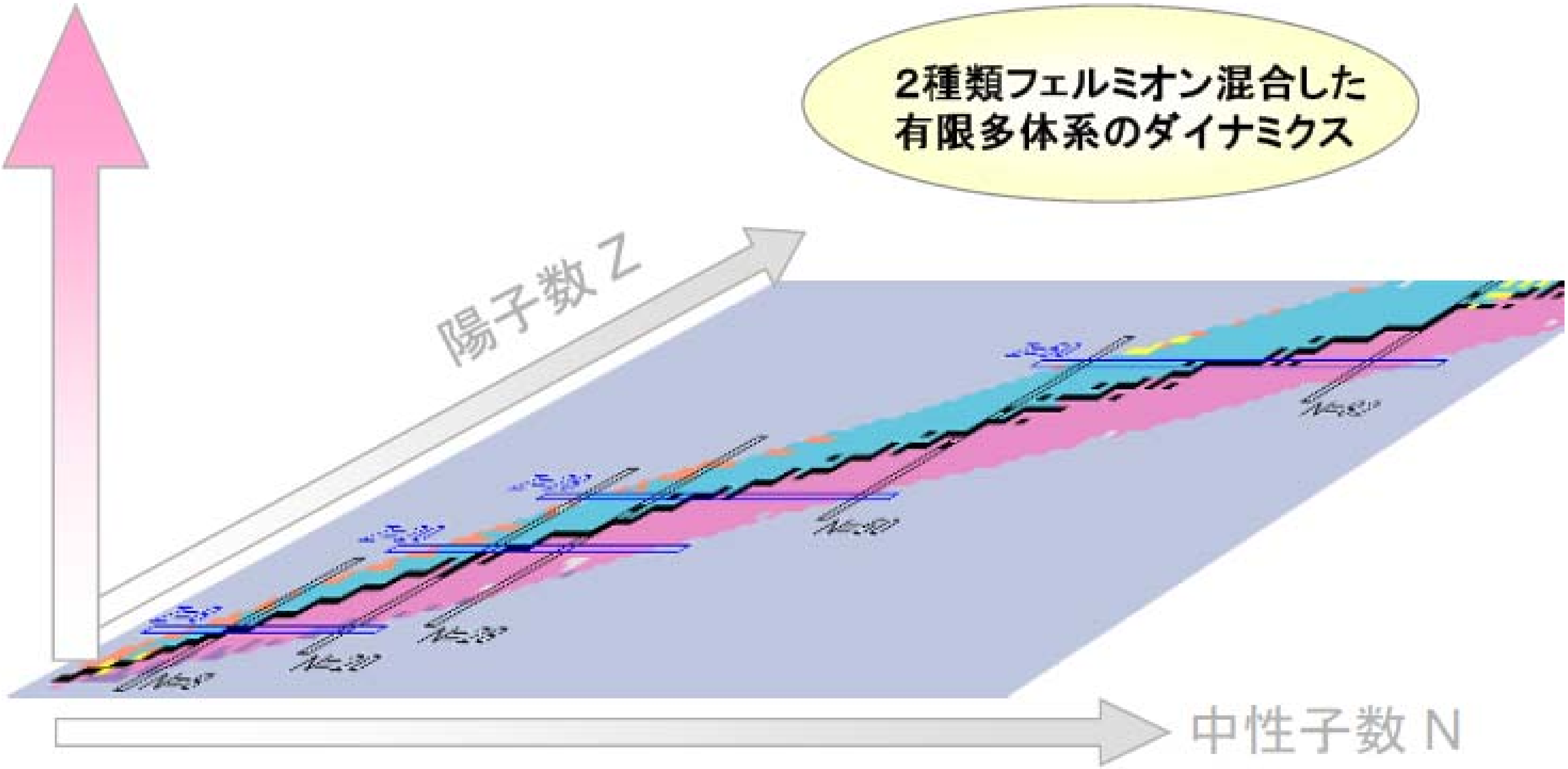


$E/A \sim 1$ MeV

拡がる原子核の世界

3つの軸:
- ・アイソスピンの非対称性
- ・励起エネルギー

2種類フェルミオン混合した有限多体系のダイナミクス



Variational Monte Carlo (ab-initio calculation)　R.B.Wringa et al., (2006)

現実的核力からクラスター構造の存在が示された。

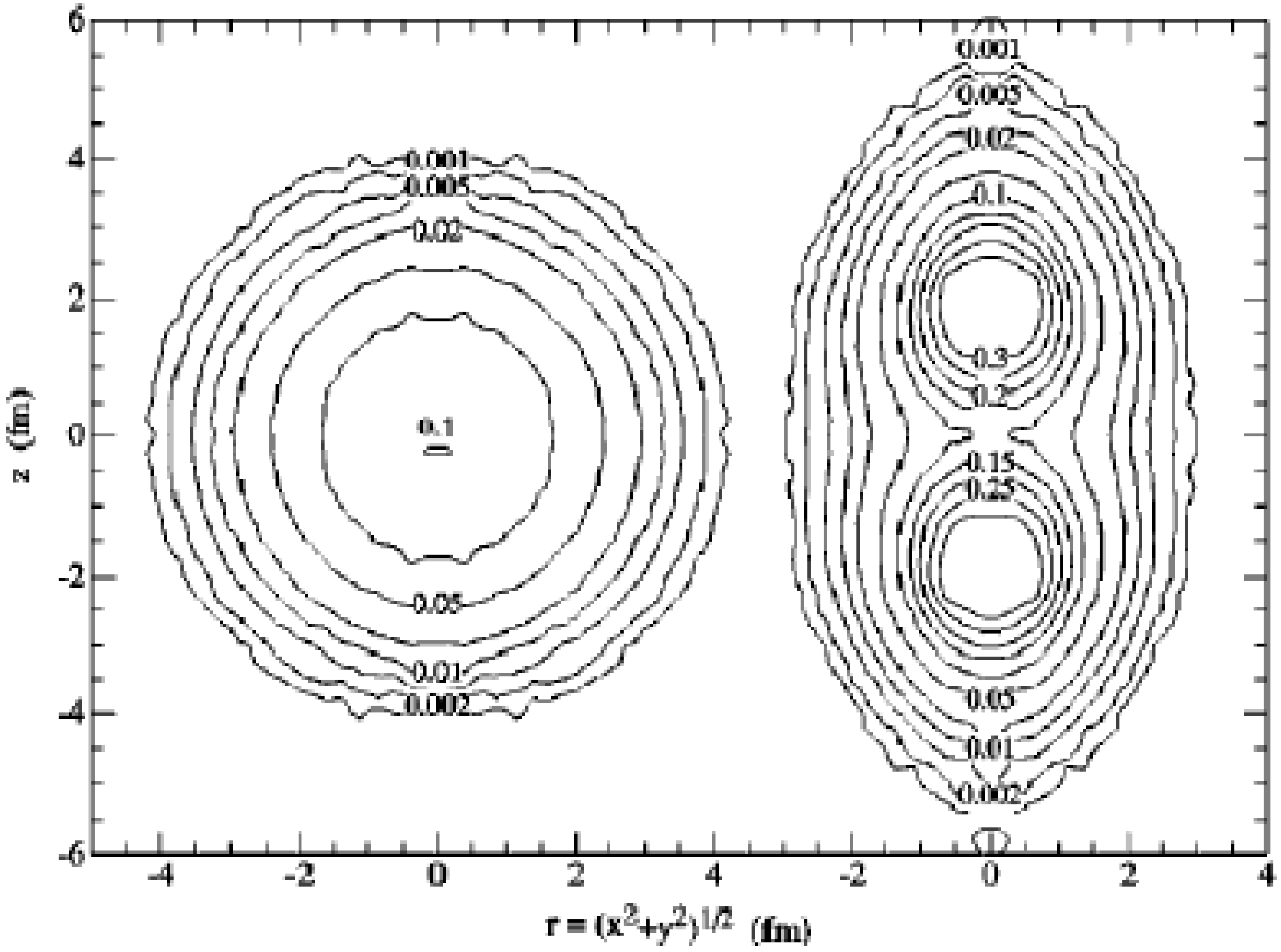


FIG. 15. Contours of constant density, plotted in cylindrical coordinates, for $^8Be(0^+)$. The left side is in the "laboratory" frame while the right side is in the intrinsic frame.

微視的(半微視的)クラスター模型

Brink 模型波動関数(Brink, Bloch, Margenau)

RGM (Resonating Group Method) (Wheeler 1937)

GCM (Generator Coordinate Method) (Griffin, Hill, Wheeler 1957)

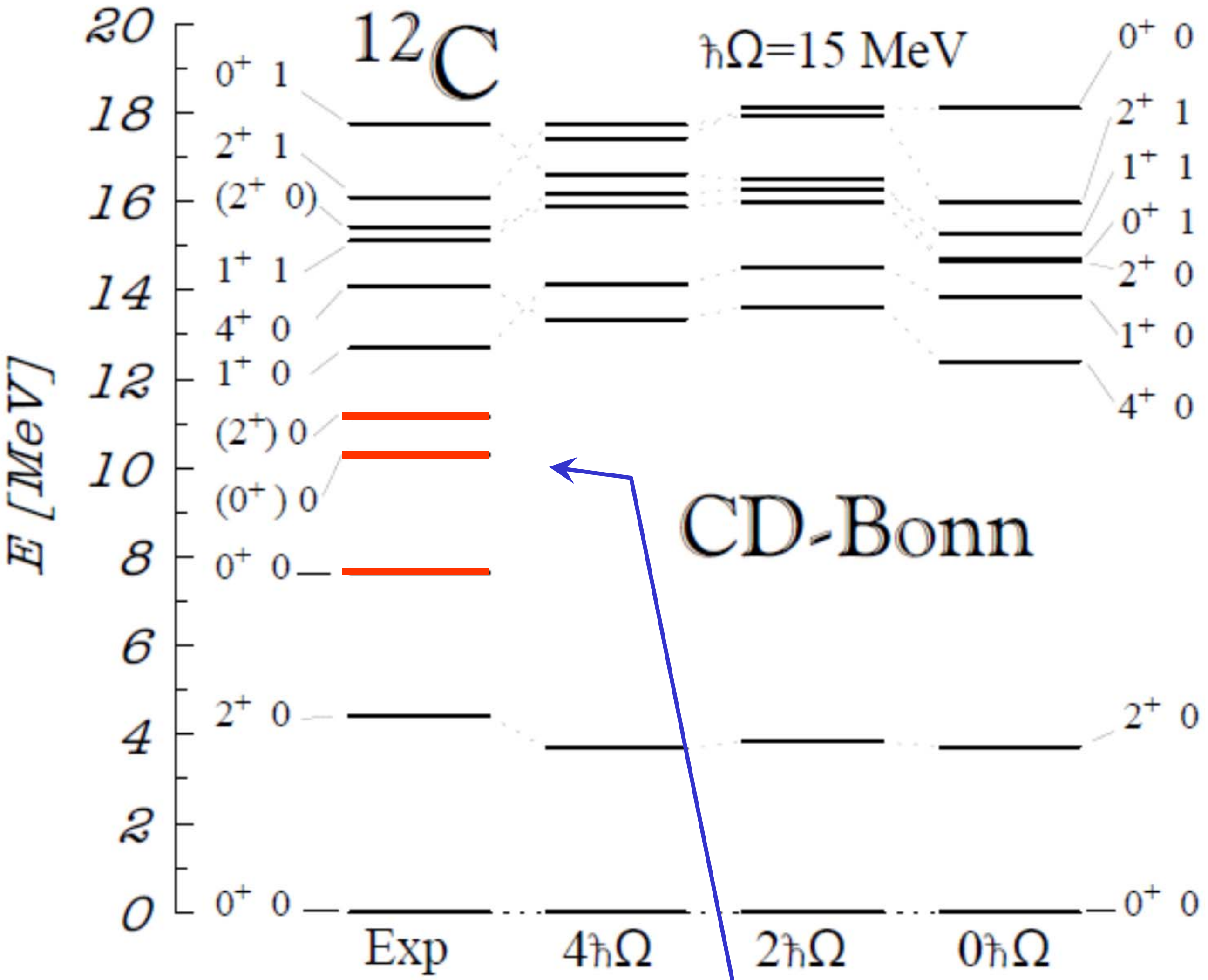
OCM (Orthogonality Condition Model) (Saito 1968)

THSR (alpha condensate model)
(Tohsaki, Horiuchi, Schuck, Roepke 2001)

クラスターを仮定しない微視的模型
AMD(Antisymmetrized Molecular Dynamics)
FMD(Fermionic Molecular Dynamics)
Brink波動関数の核子クラスター版

Typical mysterious 0^+ states in nuclear structure problem

P. Navratil et al., PRL 84, 5728 (2001).



0_2^+ , 2_2^+ , 0_3^+ states : missing

0_2^+ state (Hoyle state):
この状態を再現することが現在のab-initio計算の一つの大きな目標になっている。

Non-core shell model 計算では記述が難しい励起状態

SRG+NCSM

R. Roth, et al., Phys. Rev. Lett. 107, 072501 (2011)

Excitation spectra of carbon-12

First six excited states of positive parity for fixed alpha = 0.08 fm^4

Induced 3N terms
-> over-all compression of the spectrum

Initial (genuine) 3N terms
-> different behavior among the different states

2^+ & 4^+ states: improved
1^+ & 0^+_2 (Hoyle) states: not well described

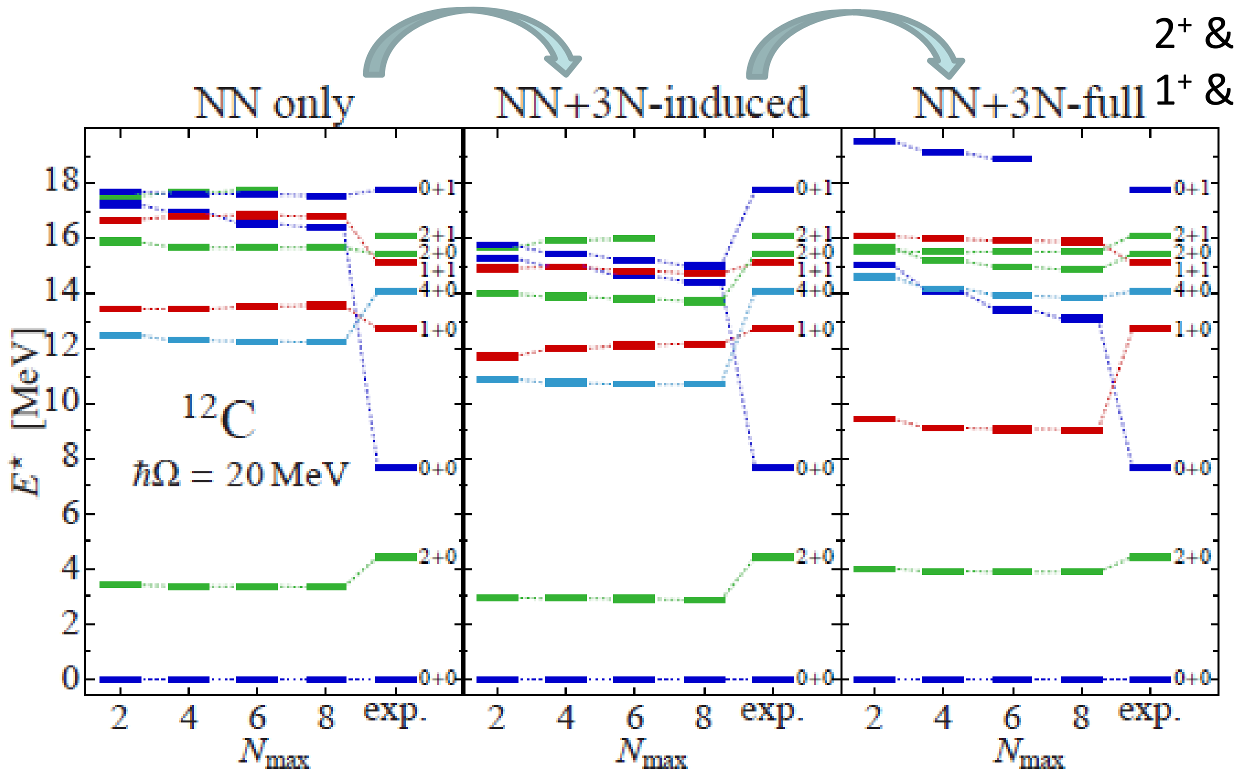


FIG. 4: (color online) Excitation spectrum for the lowest positive-parity states (labelled $J\pi T$) in ^{12}C for the NN-only, the NN+3N-induced, and the NN+3N-full Hamiltonian with $\alpha = 0.08$ fm^4.

Excited states: alpha dependence is much weaker than that in ground states (not shown in Fig.4, though)
~ a few 100 keV for $E^*(0^+_2)$ w/ NN+3N-full -> negligible induced 4N contrib.

模型によって明らかにされた現在のHoyle 状態の理解

α凝縮状態

n α condensate w.f. (THSR模型波動関数)

$$\langle \boldsymbol{r}_1, \cdots, \boldsymbol{r}_{4n} | \Phi_{n\alpha} \rangle = \mathcal{A}\left\{ \Phi(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \boldsymbol{r}_4)\Phi(\boldsymbol{r}_5, \boldsymbol{r}_6, \boldsymbol{r}_7, \boldsymbol{r}_8) \cdots \Phi(\boldsymbol{r}_{4n-3}, \boldsymbol{r}_{4n-2}, \boldsymbol{r}_{4n-1}, \boldsymbol{r}_{4n}) \right\}$$

Variational ansatz (two parameters *B* and *b*)

(THSR ansatz) A. Tohsaki, H. Horiuchi, P. Schuck and G. Röpke et al., PRL **87**, 192501 (2001).

$$\Phi(\boldsymbol{r}_{4i-3}, \cdots, \boldsymbol{r}_{4i}) = e^{-\frac{2}{B^2}(\boldsymbol{X}_i - \boldsymbol{X}_G)^2} \phi_\alpha(\boldsymbol{r}_{4i-3}, \cdots, \boldsymbol{r}_{4i})$$

$$\phi_\alpha \propto e^{-\frac{1}{8b^2}\sum_{k<l}(\boldsymbol{r}_k - \boldsymbol{r}_l)^2}$$

c.o.m. of *i*-th α particle

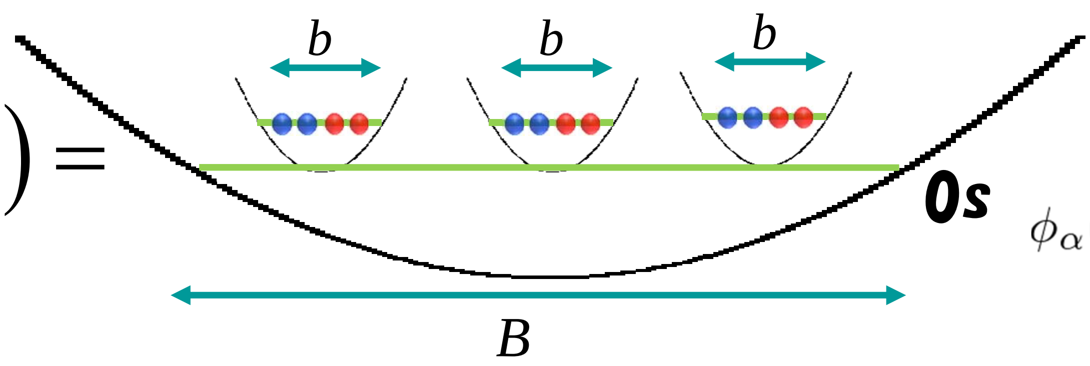
$$\boldsymbol{X}_i = \frac{\boldsymbol{r}_{4i-3} + \cdots + \boldsymbol{r}_{4i}}{4}$$

Total c.o.m.

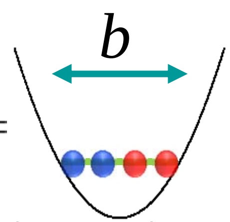
$$\boldsymbol{X}_G = \frac{\boldsymbol{r}_1 + \cdots + \boldsymbol{r}_{4n}}{4n}$$

n=3 case

$$\Phi_{3\alpha}^{THSR}(B, b) =$$



$$\phi_\alpha(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_4) \doteq$$



$(0s)^4$ configuration

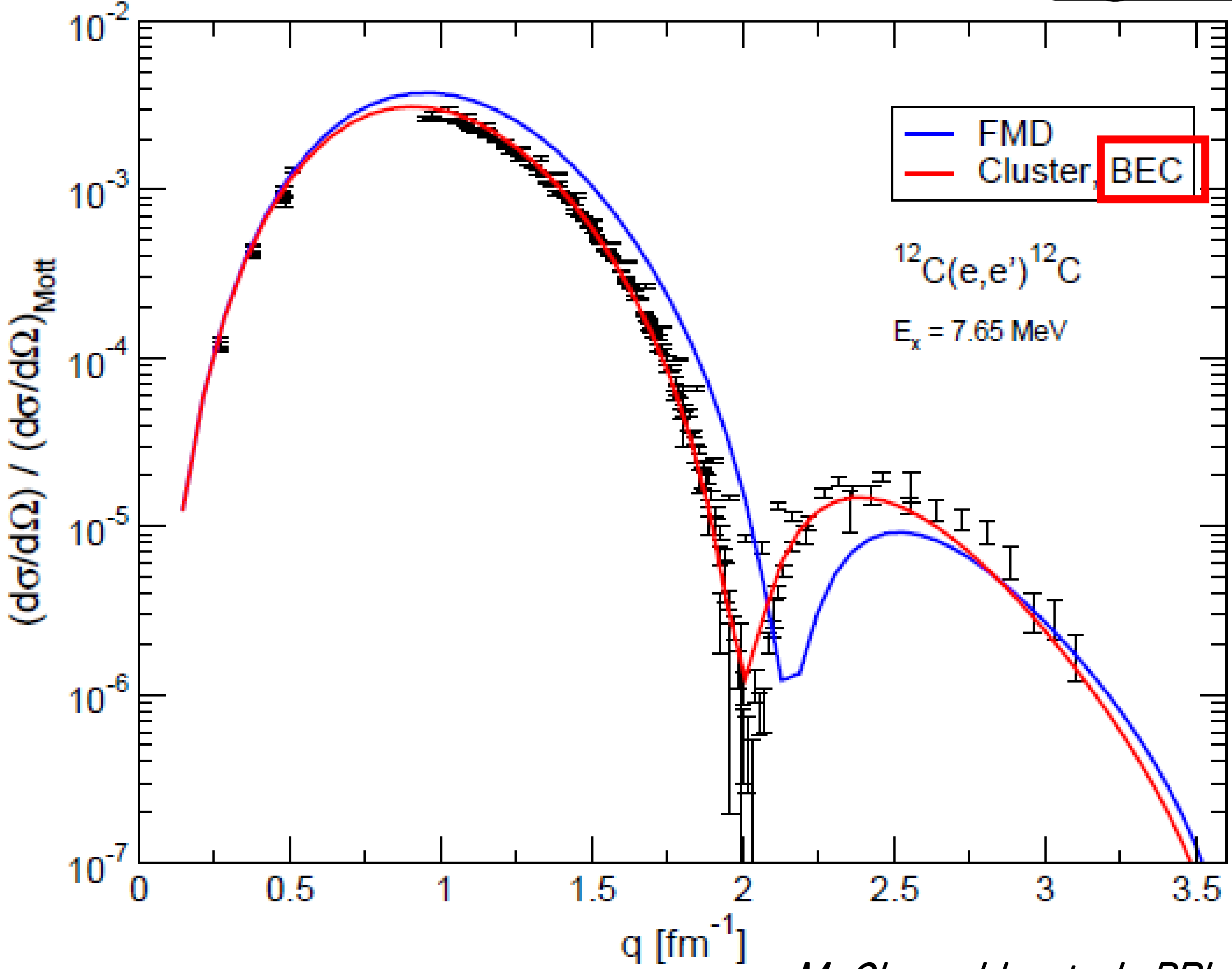
Two limits

***B* =*b*: Slater determinant**

***B* >>*b*: Gas of independent α-particles**

Electron Scattering Data ($0_1^+ \rightarrow 0_2^+$)

Ⓒ T. Neff

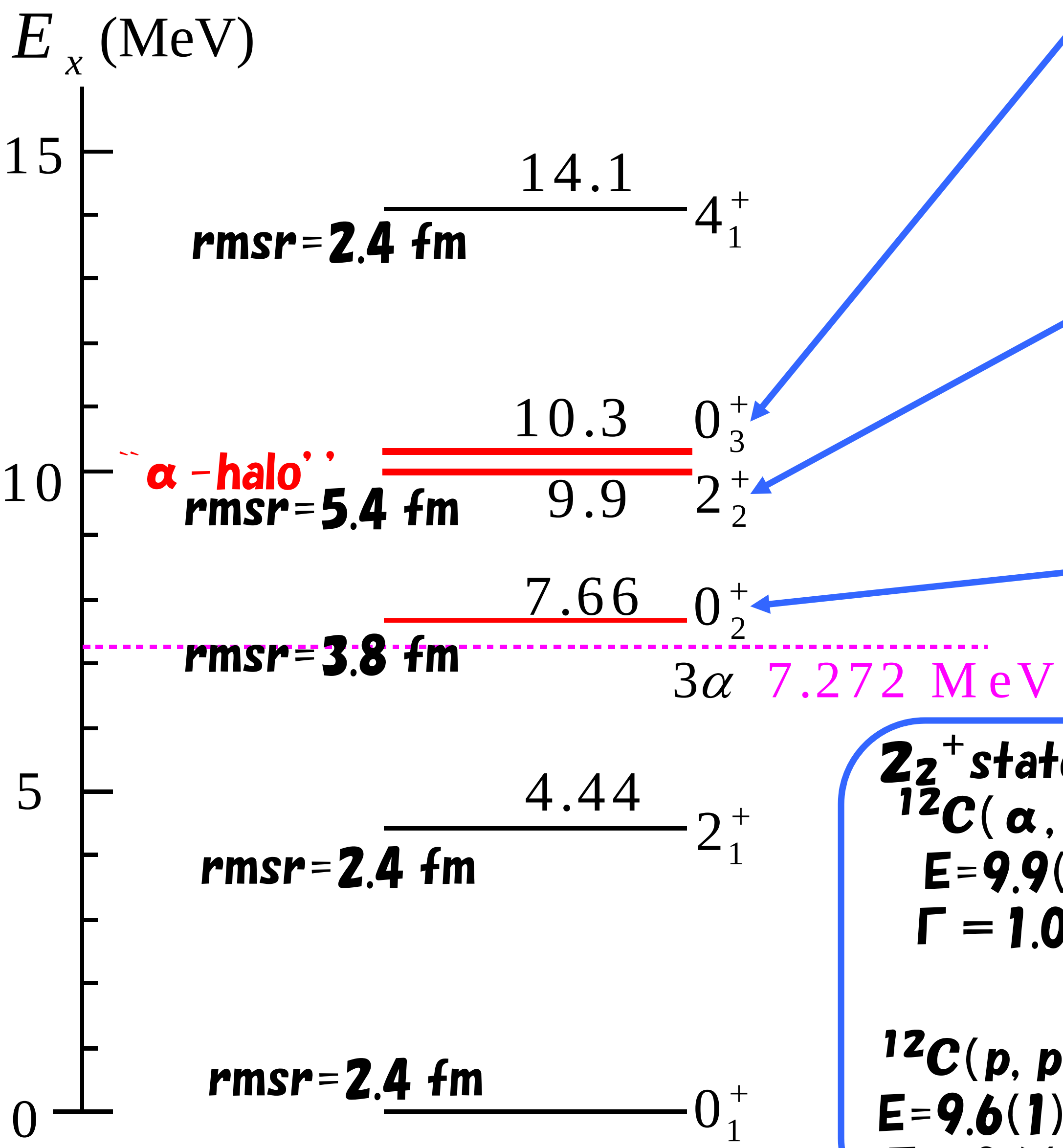


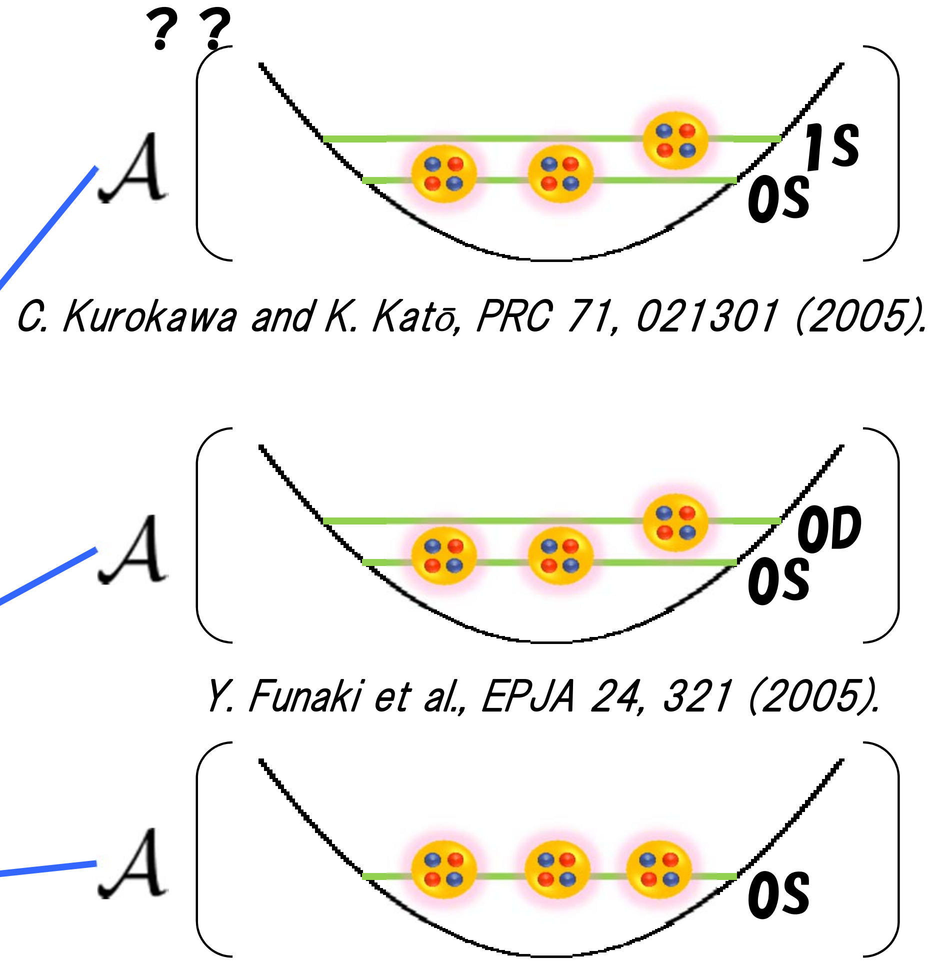
M. Chernykh. et al., PRL 98, 032501 (2007)
also see M. Chernykh et al., arXiv:1004.3877

Very nice reproduction by THSR w.f. (BEC)

``BEC'' from Y.F.et al., EPJA 28, 259(2006)

Observed levels of ^{12}C





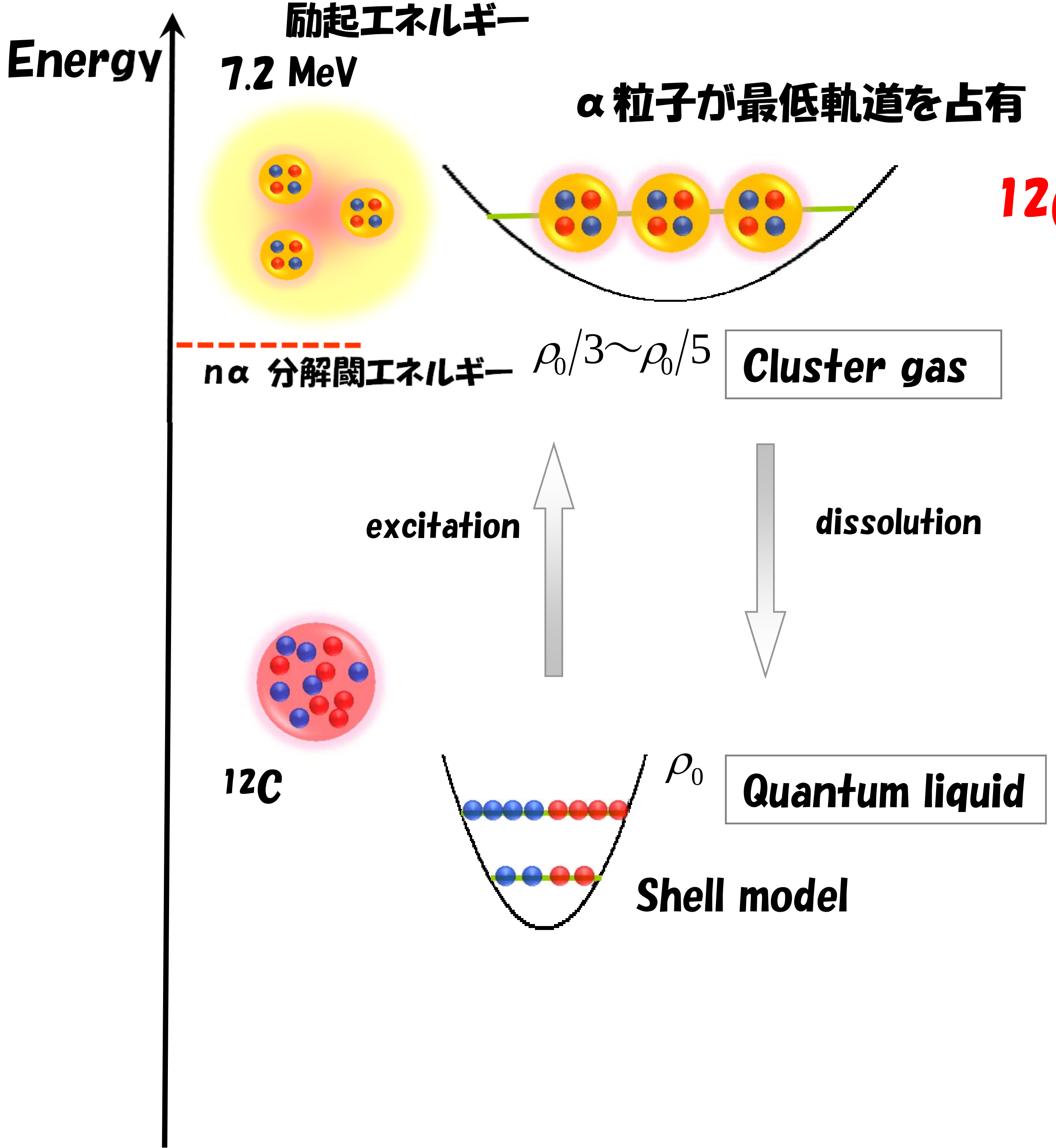
Alpha cond.model
E_{cal}=9.38 MeV
Γ_{cal}=0.64 MeV

2_2^+ state:

$^{12}C(\alpha, \alpha')$
E=9.9(3) MeV
Γ = 1.0(3) MeV
M. Itoh et al., NPA 738, 268 (2004).

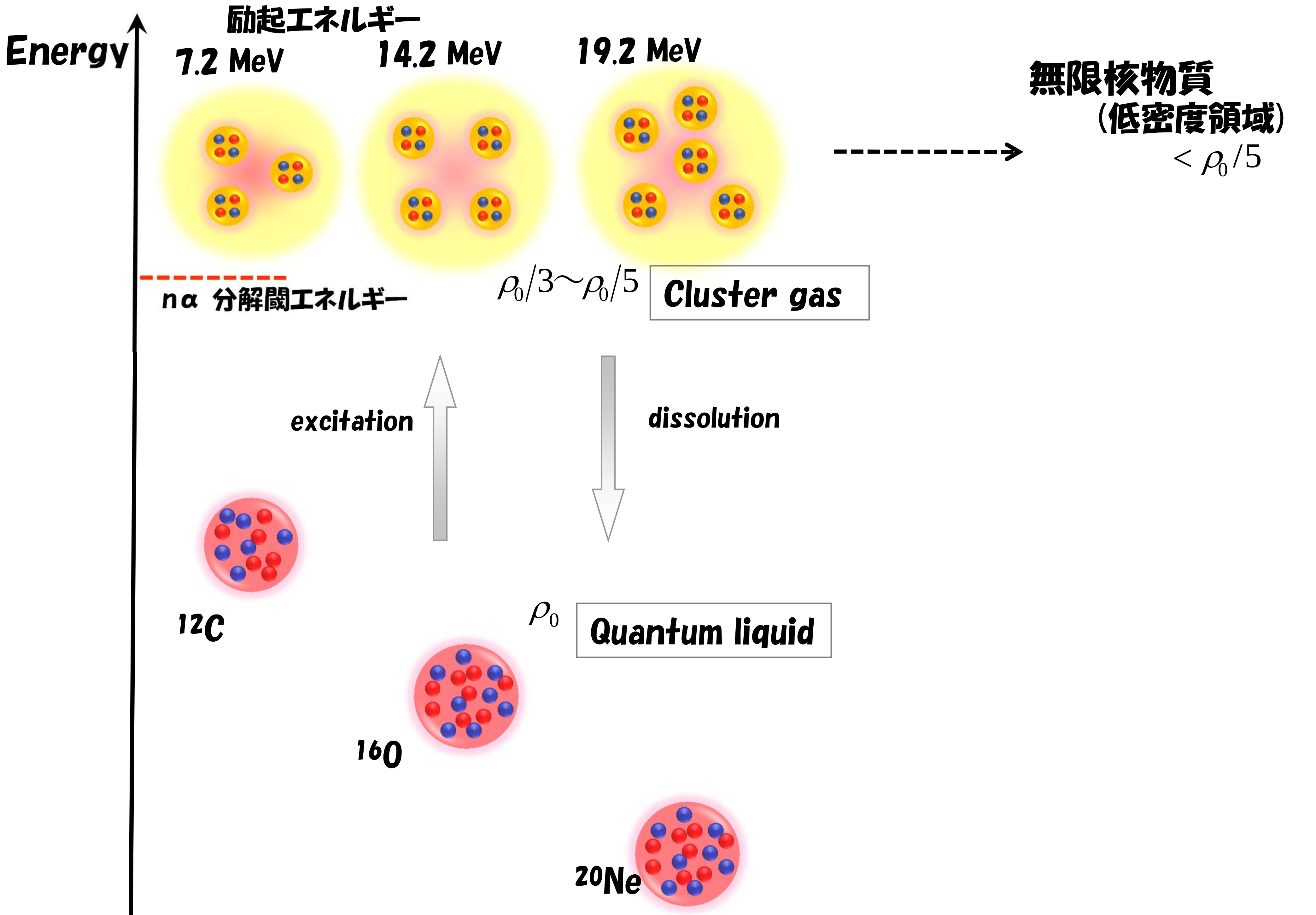
$^{12}C(p, p')$
E=9.6(1) MeV
Γ =0.6(1) MeV *M. Freer et al., PRC80, 041303(R) (2009).*

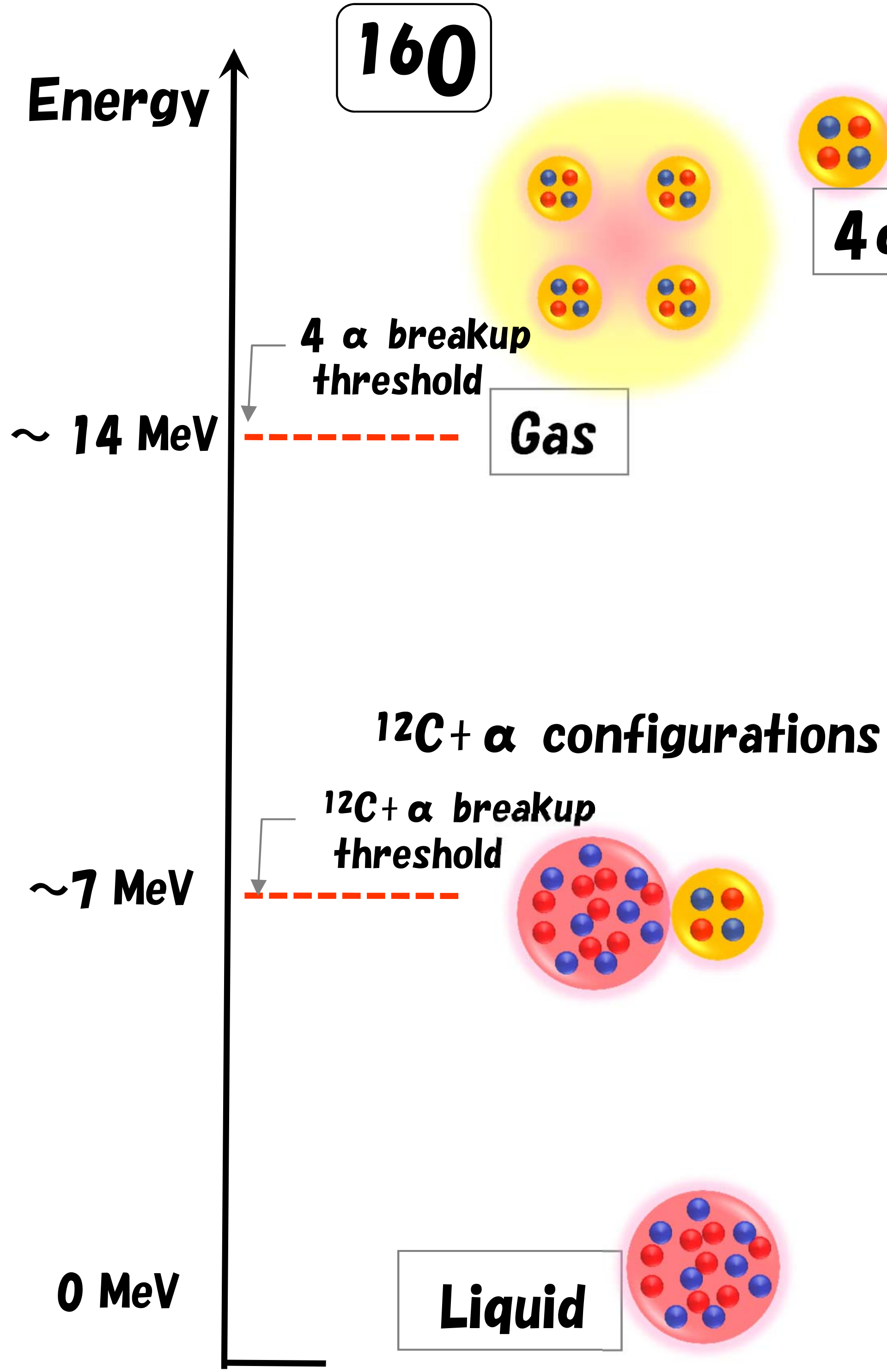
``α condensate'' in finite nuclei



^{12}Cでは十分確立した。

``gas phase'' in finite nuclei





4αクラスター状態を記述するための模型

×平均場模型

平均場とは異質の構造

× ^{12}C+αクラスター模型

○ 4αクラスター模型

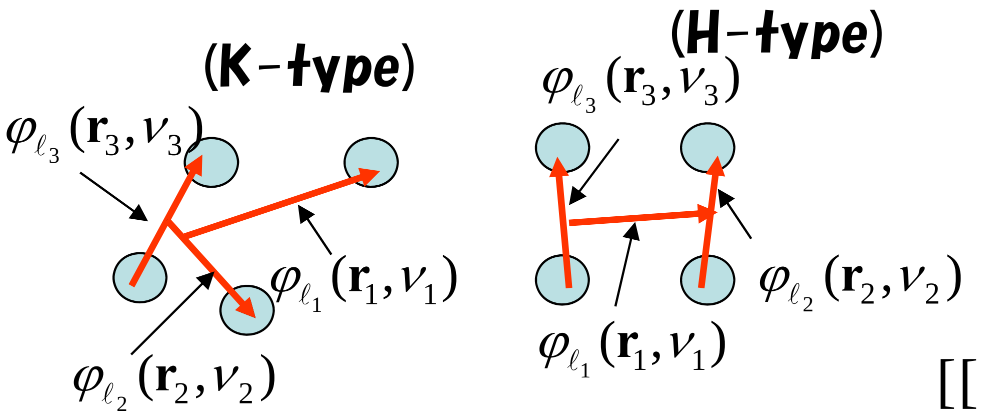
下にある状態(基底状態、^{12}C+α)を正しく記述した上で議論することが決定的に重要

(＜16MeV)αクラスター状態はp-h状態とのカップリングは小さい

^{8}Be+^{8}Be, ^{12}C*+αに崩壊する状態が最近の実験で見えている。

4α直交条件模型(OCM)

模型空間



α間相対運動はガウス関数基底で展開

$$\varphi_{\ell m}(\mathbf{r},\nu)=N_\ell(\nu)r^\ell\exp\left(-\nu r^2\right)Y_{\ell m}(\mathbf{r})$$

$\nu=0.5\sim7.5$ まで8点程度 $\to 8^3=512$

$[[l_3,l_2]_{l_{32}},l_1]_J \;: l=0,1,2,3,4 \to$ 70 channels

計35000次元程度

直線鎖状態や$J^\pi\neq0^+$状態に対しては
高い相対角運動量(l=3,4)が必要

高い相対角運動量を含めた行列要素計算が大変！

$(l_3,l_2,l_1)=(0,0,0),\ (2,2,2),\ (2,2,4)(2,3,3),\ (2,4,4)$

計算コスト　1 ： ～500 ： ～5,000 ： ～100,000

cf) 4核子系やハイパー核4体計算では
低い相対角運動量(l≦2)でOK
(テンソル力: 2核子間相対D波)

2α間相対S波、D波、G波のphase shift を再現するポテンシャル使用

前記の模型空間でHamiltonianを対角化（実対称一般化固有値問題）

$$H = T + \sum_{i<j}\left[V_{2\alpha}(r_{ij}) + V_{2\alpha}^{Coul}(r_{ij})\right] + V_{3\alpha} + V_{4\alpha} + V_{Pauli}$$

射影演算子部分の計算コストがメイン(8割以上)となる

パウリ演算子(パウリ禁止状態除去)

$$V_{Pauli} = \lim_{\lambda\to\infty} \lambda \sum_{2n+\ell<4} \sum_{ij} \left|u_{n\ell}(r_{ij})\right\rangle\left\langle u_{n\ell}(r_{ij})\right|$$

密度演算子

$$\rho(r, r') = \sum_i \left|\delta(r_i - r')\right\rangle\left\langle\delta(r_i - r)\right|$$

ガウス基底が一つ増えたことに相当し、5体系の計算コストがかかる

相対角運動量の高い射影演算子部分の行列要素計算を含んだ4体系計算(4αOCM)

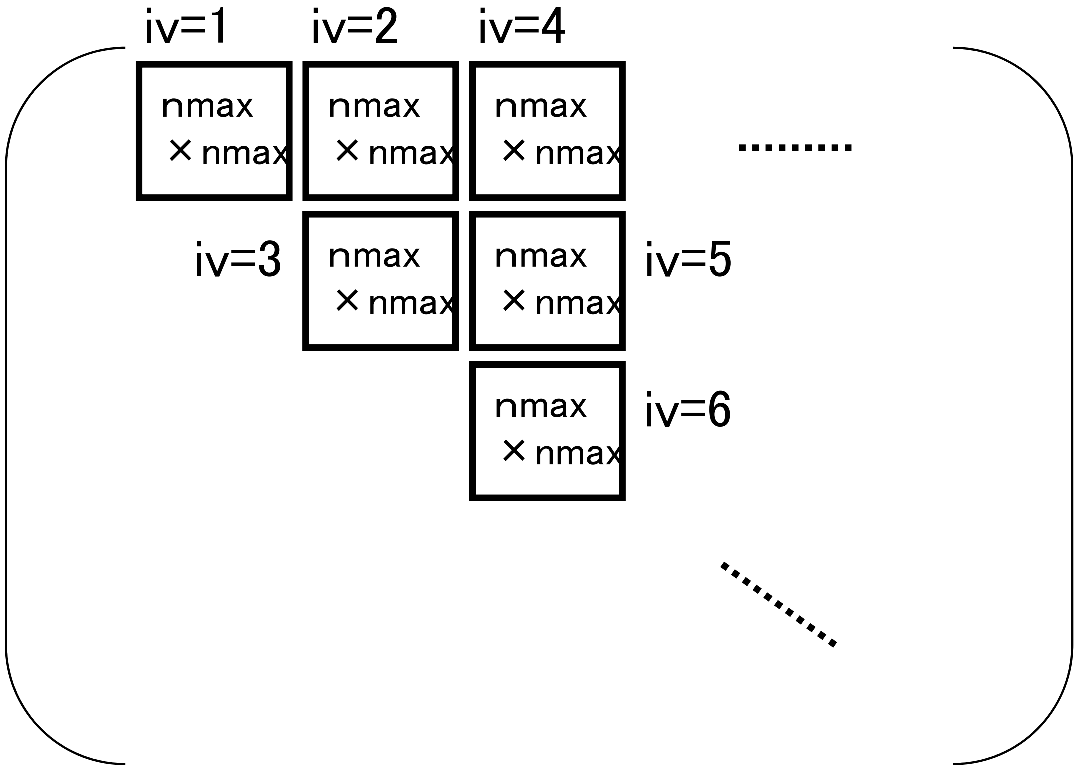
行列要素計算ソースコード

```
call mpi_init(ierr)
call mpi_comm_size(…)
call mpi_comm_rank(…)

 do iv=ista,iend
   do icb=1,nmax
   do ica=1,nmax
             :
     zz(ica,icb,iv)=…
   end do
   end do
 end do

call mpi_gatherv(zz, …)
call mpi_finalize(ierr)
```

iv: ガウス基底展開部分
ica,icb : 角運動量チャンネル部分

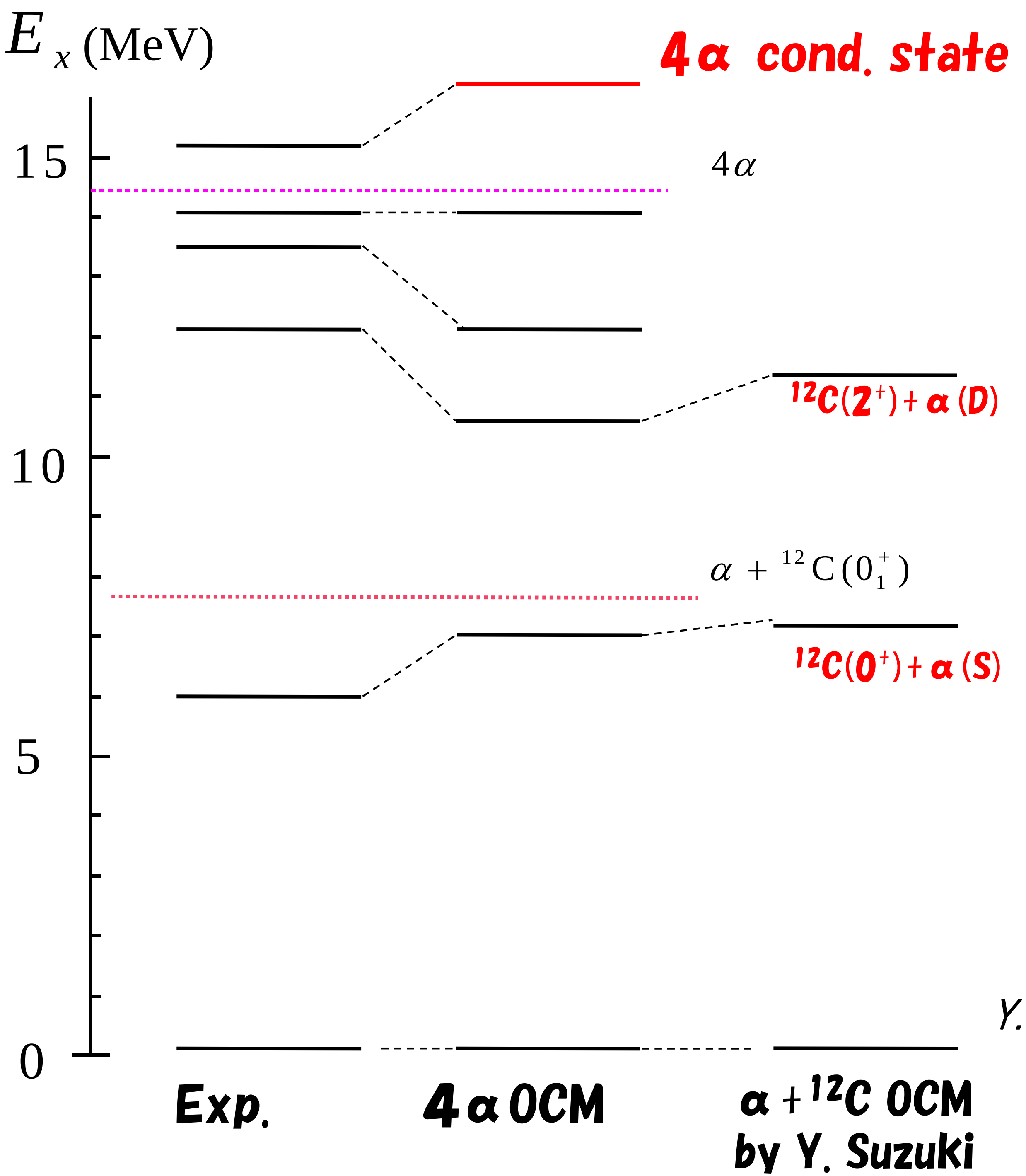


Dim=2560 Calculation time (s)

# of core	1	2	4	8	12
Matrix element	14389	7363	3741	1891	1338

Xeon X5670 (2.93 GHz, 2*6 core)

0^+ spectra, rms radii, monopole matrix elements



0_4^+ state: T. Wakasa, Y. F. et al., PLB 653, 173 (2007).

Y. F. et al., PRL 101, 081502 (2008).

0^+ spectra, rms radii, monopole matrix elements

Large monopole matrix element can be the evidence of cluster states.

T. Yamada, Y. F. et al., PTP120, 1139 (2008).

		Experimental data				4α OCM		
	E_x [MeV]	R [fm]	M(E0) [fm^2]	Γ [MeV]		R [fm]	M(E0) [fm^2]	Γ [MeV]
0^+_1	0.00	2.71				2.7		
0^+_2	6.05		3.55			3.0	3.9	
0^+_3	12.1		4.03			3.1	2.4	
0^+_4	13.6		no data	0.6		4.0	2.4	0.60
0^+_5	14.0		3.3	0.185		3.1	2.6	0.20
0^+_6	15.1		no data	0.166		5.6	1.0	0.14

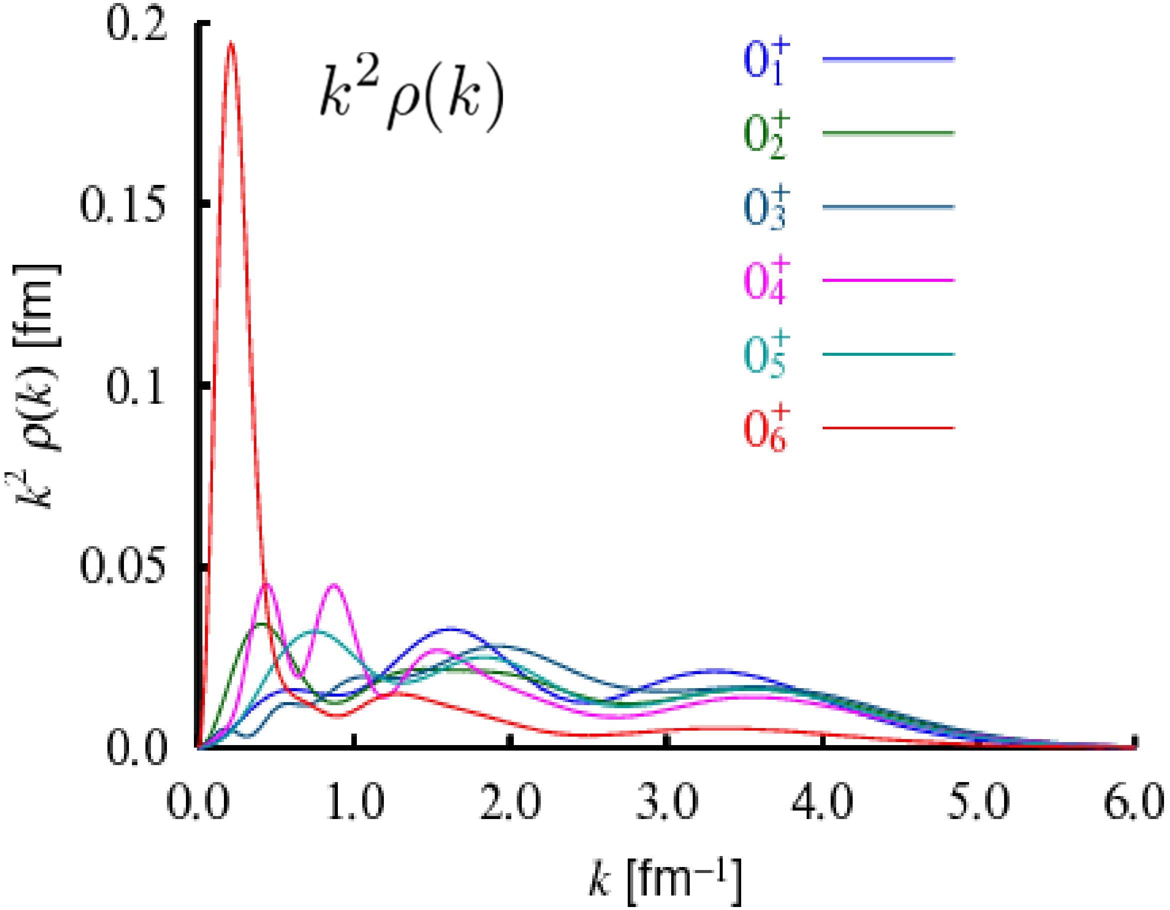
over 15% of total EWSR

20% of total EWSR

Momentum distributions of the α particles

$$\rho(k) = \int d\boldsymbol{r}d\boldsymbol{r}' \frac{e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}}{(2\pi)^{3/2}}\rho(\boldsymbol{r},\boldsymbol{r}')\frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}'}}{(2\pi)^{3/2}}$$

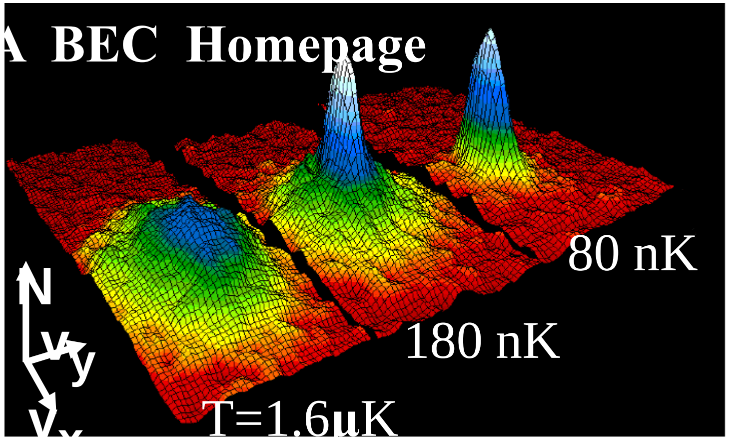
$$\rho(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{4}\sum_{i=1}^{4}\langle\Psi_{\mathrm{OCM}}(0_k^+)|\delta(\boldsymbol{r}_i - \boldsymbol{X}_G - \boldsymbol{r}')\rangle\langle\delta(\boldsymbol{r}_i - \boldsymbol{X}_G - \boldsymbol{r})|\Psi_{\mathrm{OCM}}(0_k^+)\rangle$$



$\boldsymbol{r}_i$: coordinate of the i-th α particle

$\boldsymbol{X}_G$: coordinate of total center-of-mass

BEC in the atomic world



0_6^+: delta-function-like peak at zero momentum

4α condensate state character.

de Broglie w.l. $\lambda = \frac{2\pi}{\sqrt{\langle k^2 \rangle}} \geq 20$ fm

Scalability
(対称密行列)対角化：ScaLapack使用

QRPAコードによる対角化計算

Dim=31965

Calculation time (s)

# of core	256	512	1024
matrix element.	3367	1710	918
diagonalization	610	328	308

Dim=70051

$(70051/31965)^2=4.8$ 918*4.8=4409

$(70051/31965)^3=10.5$ 308*10.5=3242

# of core	1024
matrix element	4061
diagonalization	2597

Dim=104302

$(104302/70051)^2=2.2$

$(104302/70051)^3=3.3$

4061*2.2=9003

2597*3.3=8572

# of core	1024	2048
matrix element.	8788	4336
diagonalization	-	6029

Limit: 21600s

``久保野''図

Cluster Nucleosynthesis(CN) diagram

S. Kubono, PTP96, 275(1996)

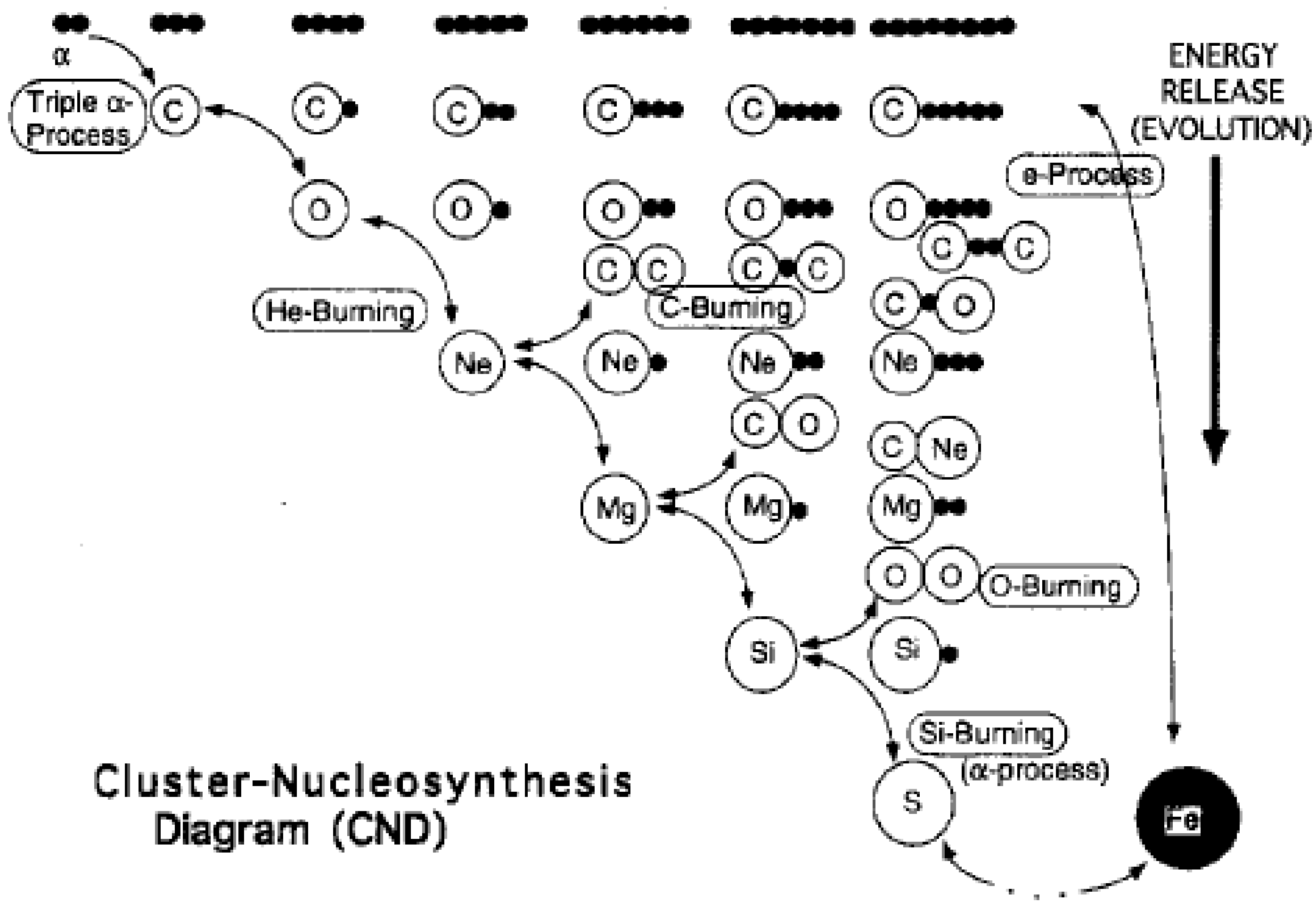
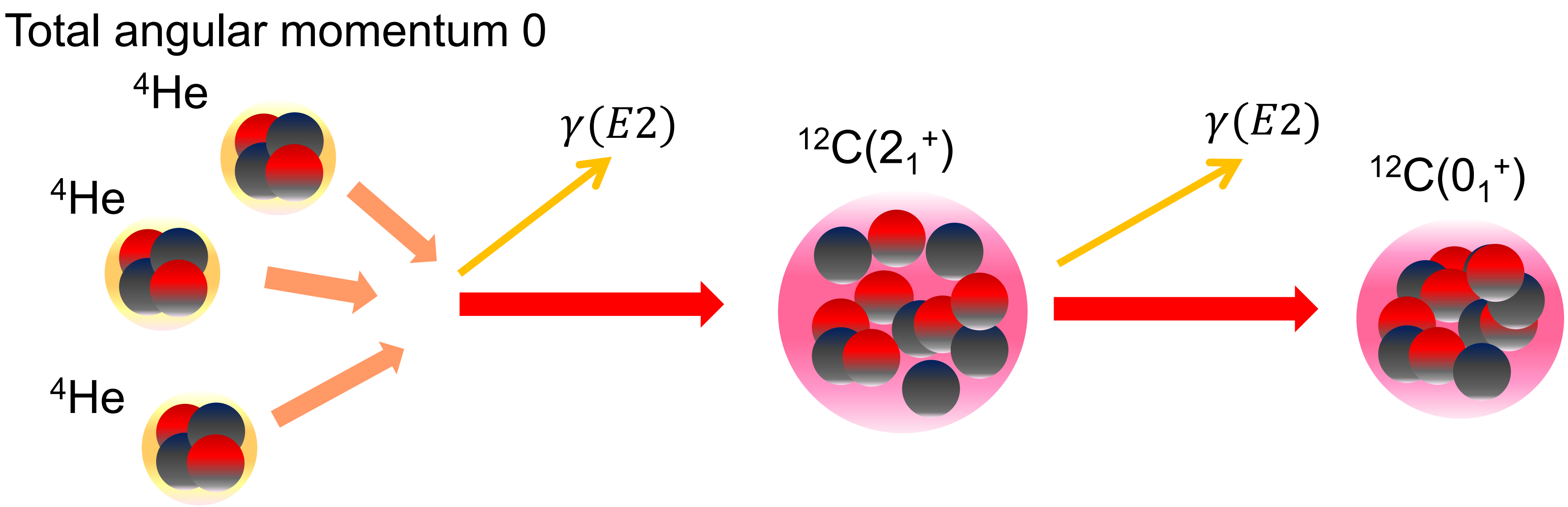


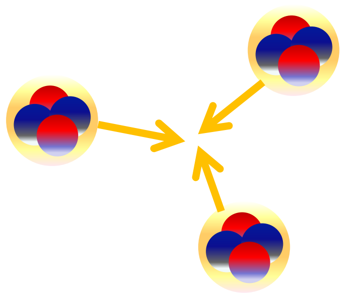
Fig. 8. The Cluster Nucleosynthesis(CN) diagram.[70] Nucleosynthesis to heavy elements flows in the direction from top-left to bottom-right to Fe, releasing the energy to the stellar system.

Dominant ^{12}C synthesis process depends on temperature



Low Temperature

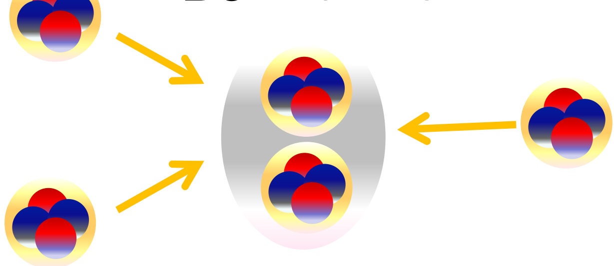
Direct 3-alpha collision



High Temperature

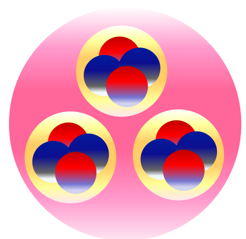
Binary collision
(^8Be resonance)

$^8Be^*$ 92 keV



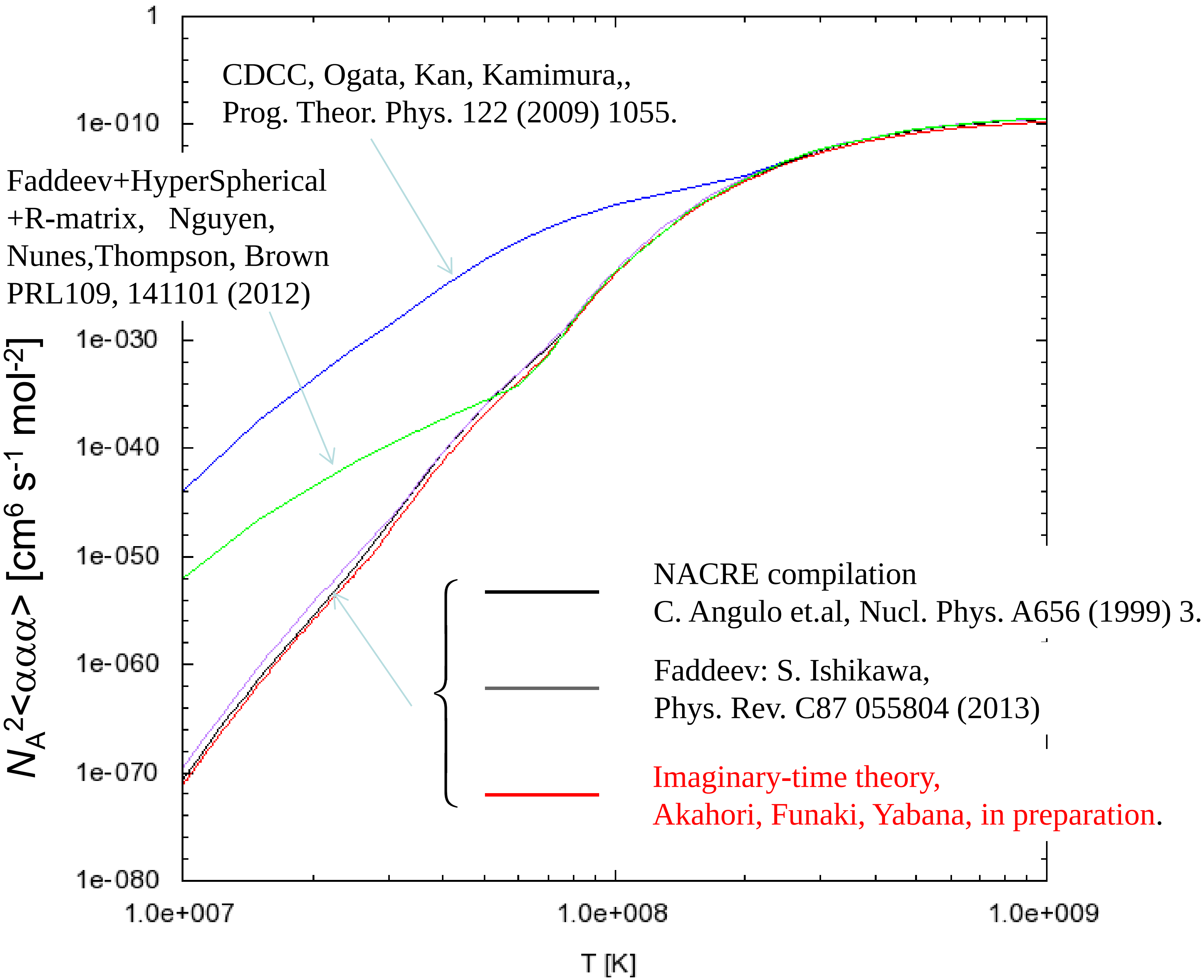
By way of Holy state
(^{12}C resonance)

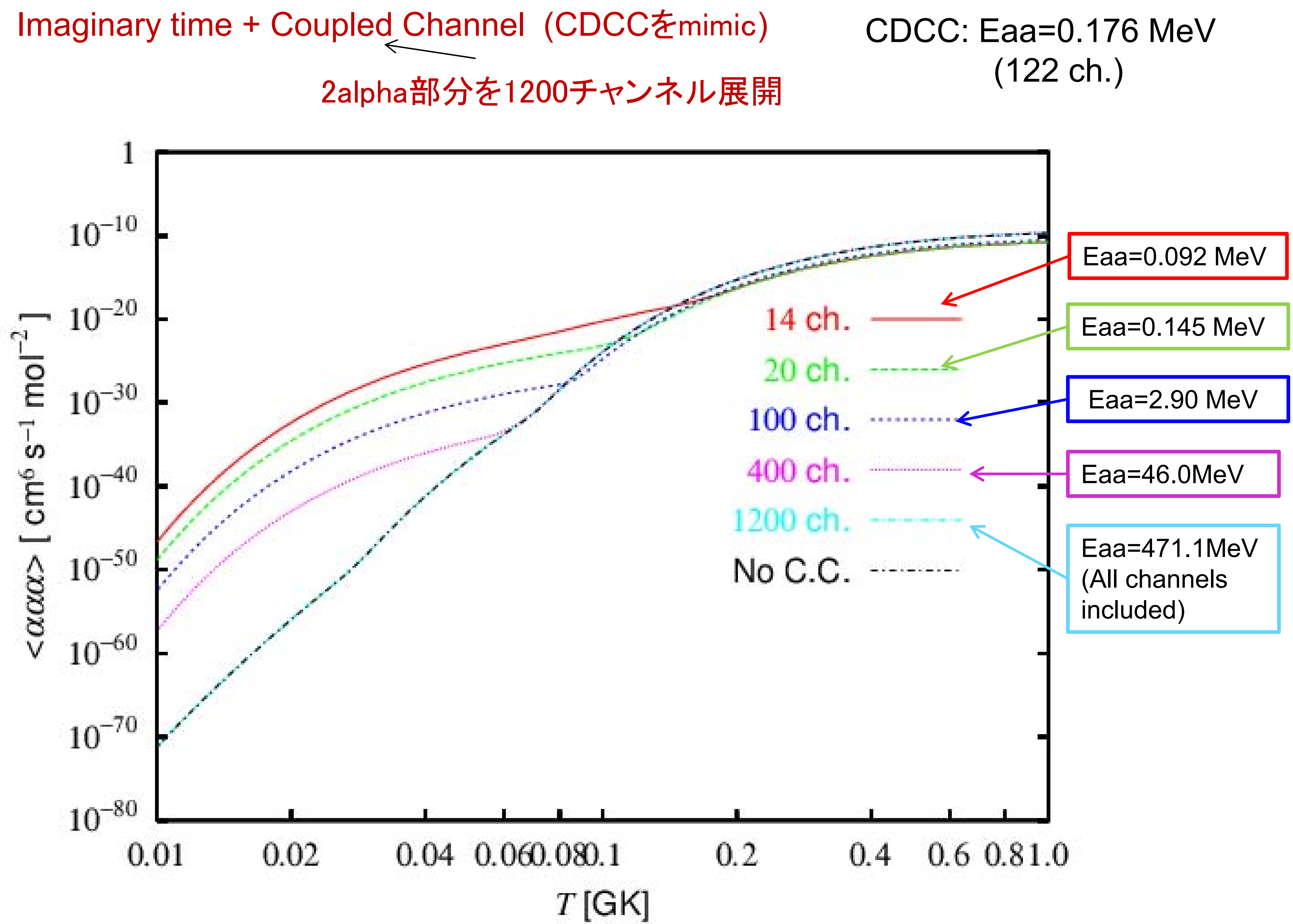
$^{12}C^*(0_2^+)$ 379 keV



Calculated rates deviates among theories at low temperature

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




Imaginary time + Coupled Channel （CDCCをmimic）
2alpha部分を1200チャンネル展開
CDCC: Eaa=0.176 MeV
(122 ch.)
<αααα> [cm^6 s^-1 mol^-2]
1
10^-10
10^-20
10^-30
10^-40
10^-50
10^-60
10^-70
10^-80
0.01
0.02
0.04
0.06
0.08
0.1
0.2
0.4
0.6
0.8
1.0
T [GK]
14 ch.
20 ch.
100 ch.
400 ch.
1200 ch.
No C.C.
Eaa=0.092 MeV
Eaa=0.145 MeV
Eaa=2.90 MeV
Eaa=46.0MeV
Eaa=471.1MeV
(All channels
included)