CNS Summer School 2026 @ CENS, IBS
2026/8/25,26

1. Introduction to nuclear shell-model calculations

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CENTER *for*
NUCLEAR STUDY
THE UNIVERSITY *of* TOKYO

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Outline

August 25 (Tue)

- Lecture I
  Introduction to shell-model calculations

August 26 (Wed)

- Lecture II
  demonstration of the KSHELL code
- Lecture III
  Shell evolution, related topics

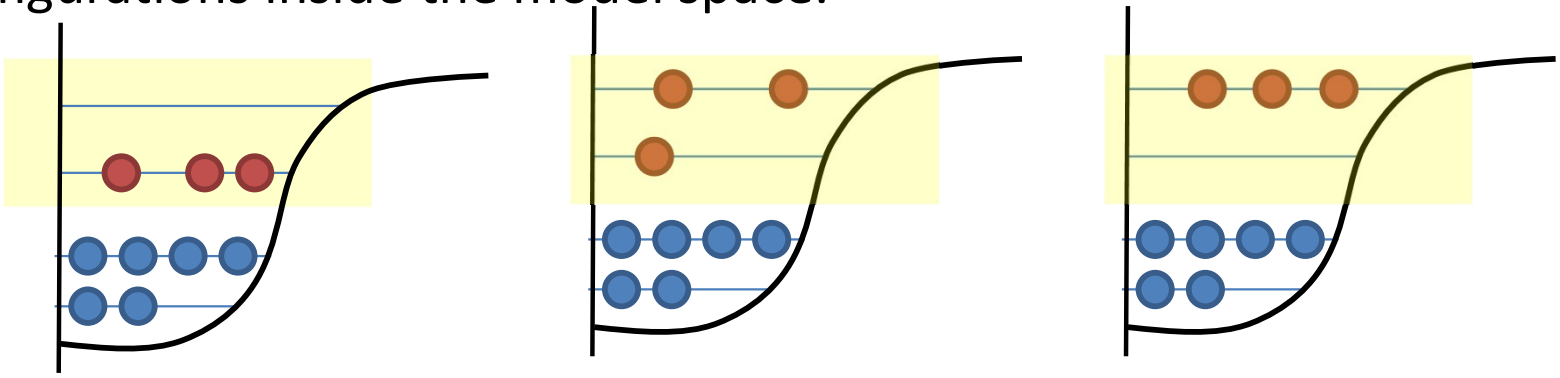
Goal of this lecture :

You can perform shell-model calculations by yourself.

The contents are quite practical.

Large-scale shell model calculation (LSSM)

- Configuration interaction (CI) method
- Assume an inert core and valence space (model space)
- Nuclear wave function is expressed as a linear combination of all configurations inside the model space.



$$|\Psi\rangle = v_1|m_1\rangle + v_2|m_2\rangle + v_3|m_3\rangle + \cdots$$

Solve Schrodinger's equation to obtain the nuclear wave function with configuration mixing

$$H|\Psi\rangle = E|\Psi\rangle \Rightarrow \sum_j \langle m_i|H|m_j\rangle v_j = E v_i$$

Many particle-hole excitations near Fermi surface is fully included.

What it is used for

Spectroscopy

Assigning spins and parities, and interpreting what a measured level actually is.

Shell evolution

Why magic numbers change far from stability — the monopole part of the interaction.

Astrophysics

Electron capture, beta-decay rates and reaction inputs for stellar and explosive burning.

Fundamental symmetries

Nuclear matrix elements for double-beta decay, Schiff moments, and dark-matter searches.

Awkward in nuclear matter, halo structure etc.

Theoretical nuclear chart in 2012

Ab initio:
only from nuclear force

- Green's function Monte Carlo
- no-core shell model calculations
- etc.

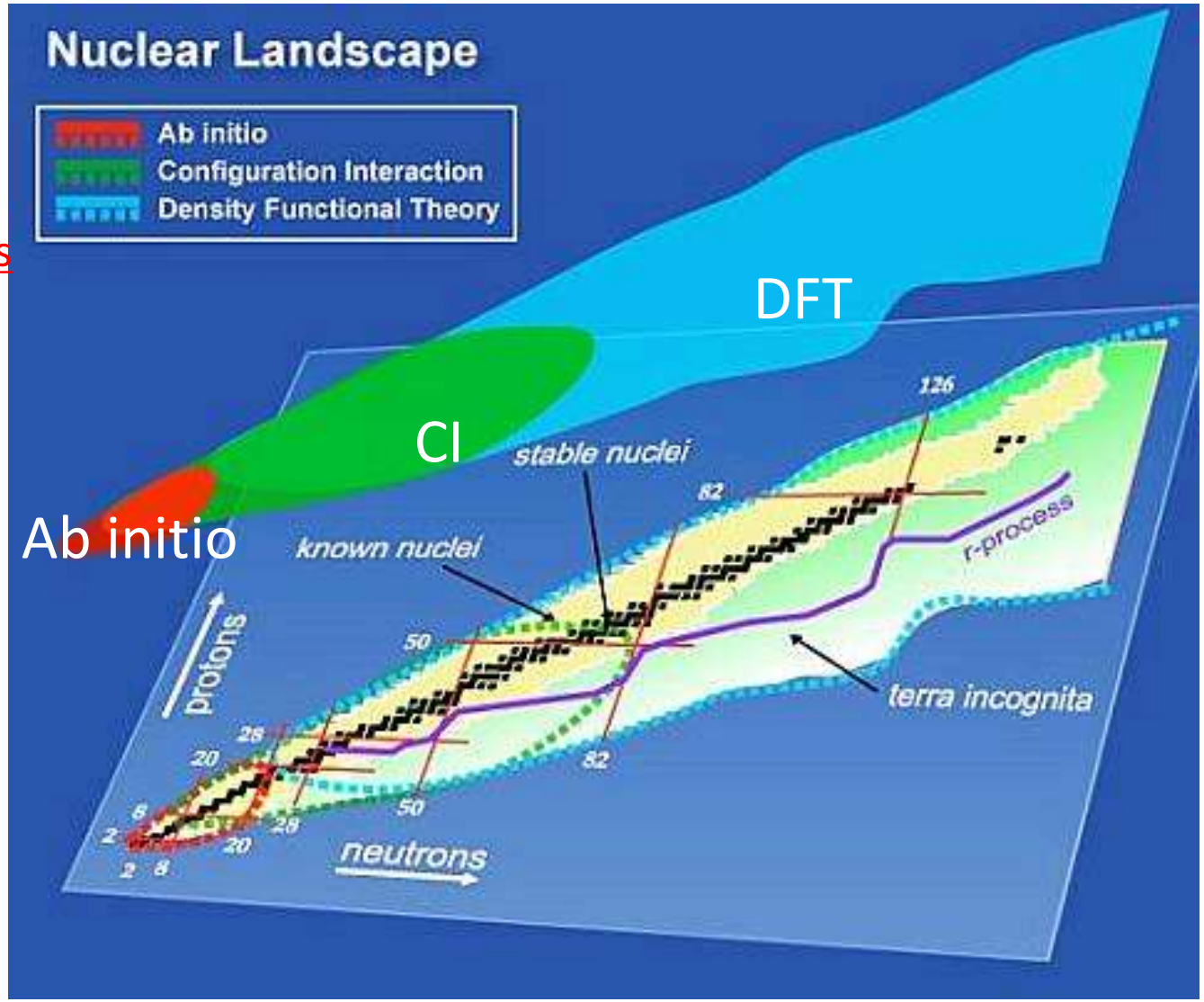
Configuration Interaction:

- Large-scale shell model calc.

with an inert core.
Effective interaction corrected by the medium effect and phenomenology

Density Functional Theory:

- Functional is determined by phenomenology



Modern "ab initio" methods broaden their areas.
Shell-model study is still mainstay especially to understand experimental data.

https://arxiv.org/abs/1205.0227

Shell-model codes

Available on the web

- KSHELL (Tsukuba/Tokyo)
  - *M*-scheme, MPI parallel
- BIGSTICK (SDSU-LLNL)
  - *M*-scheme, MPI parallel, 3-body force for NCSM

Available upon request (?)

- NuShellx@MSU (MSU-Oxford)
  - *J*-scheme, with rich interaction files
- ANTOINE (Strasbourg-Madrid)
  - *M*-scheme

OXBASH, CENS (Oslo), and many others.

Writing a shell-model code is relatively easy, but achieving high performance requires substantial effort.

To do for the lectures tomorrow!

https://sites.google.com/alumni.tsukuba.ac.jp/kshell-nuclear/d

Ref. N. Shimizu *et al.,* Comp. Phys. Comm. 244, 372 (2019)

https://doi.org/10.1016/j.cpc.2019.06.011

"KSHELL" code for nuclear shell-model calculations

Cover page for "KSHELL" code

Download

Links

Download

Nuclear shell-model code "KSHELL"

It is provided as it is and has no warranty.

Any comments, bug reports, suggestions, and collaborations are welcome.

- KSHELL ver.4
- ~~KSHELL ver.3.1~~
- KSHELL ver. 2
- KSHELL ver.1.2g
- 日本語マニュアル(Manual in Japanese) 2022/06/08
- KSHELL Manual in English, 2022/06/08

Download here.

Written by Noritaka Shimizu, Center for Computational Sciences, University of Tsukuba

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NOTE: When any publication is achieved using this software, one of the following papers should be cited

N. Shimizu, T. Mizusaki, T. Utsuno, and Y. Tsunoda, Comp. Phys. Comm. 244, 372 (2019)

https://doi.org/10.1016/j.cpc.2019.06.011

N. Shimizu, "Nuclear shell-model code for massive parallel computation, KSHELL", arXiv:1310.5431 [nucl-th] (2013)

Preparation

https://sites.google.com/alumni.tsukuba.ac.jp/kshell-nuclear/d

Linux:

- Install gfortran, BLAS, LAPACK, and python (or Intel Fortran + MKL)
  (Ubuntu: apt-get install python gfortran liblapack-dev libblas-dev)

- tar xvzf kshell-xxxxxx.tar.gz
  cd kshell-xxxxxx/src
  make
  cd ../test
  ../bin/kshell_ui.py

- MS-Windows : install Ubuntu Linux on Windows (Microsoft Store)

- Mac OS

How to install

tar xvzf kshell-xxxx.tar.gz

cd kshell/src

“modify Makefile to match your system”

make

alias kshell_ui.py=(installed dir)/kshell/bin/kshell_ui.py

That is all, if you are lucky.

Spin-orbit term in mean-field potential

Mayer Jensen introduced

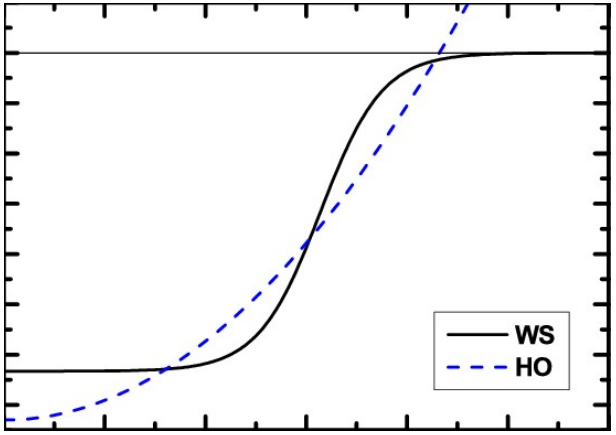
$$[T + U_C(r) + U_{LS}(r)\,\boldsymbol{\ell}\cdot\boldsymbol{s}]\,\phi_i = \varepsilon_i\phi_i$$

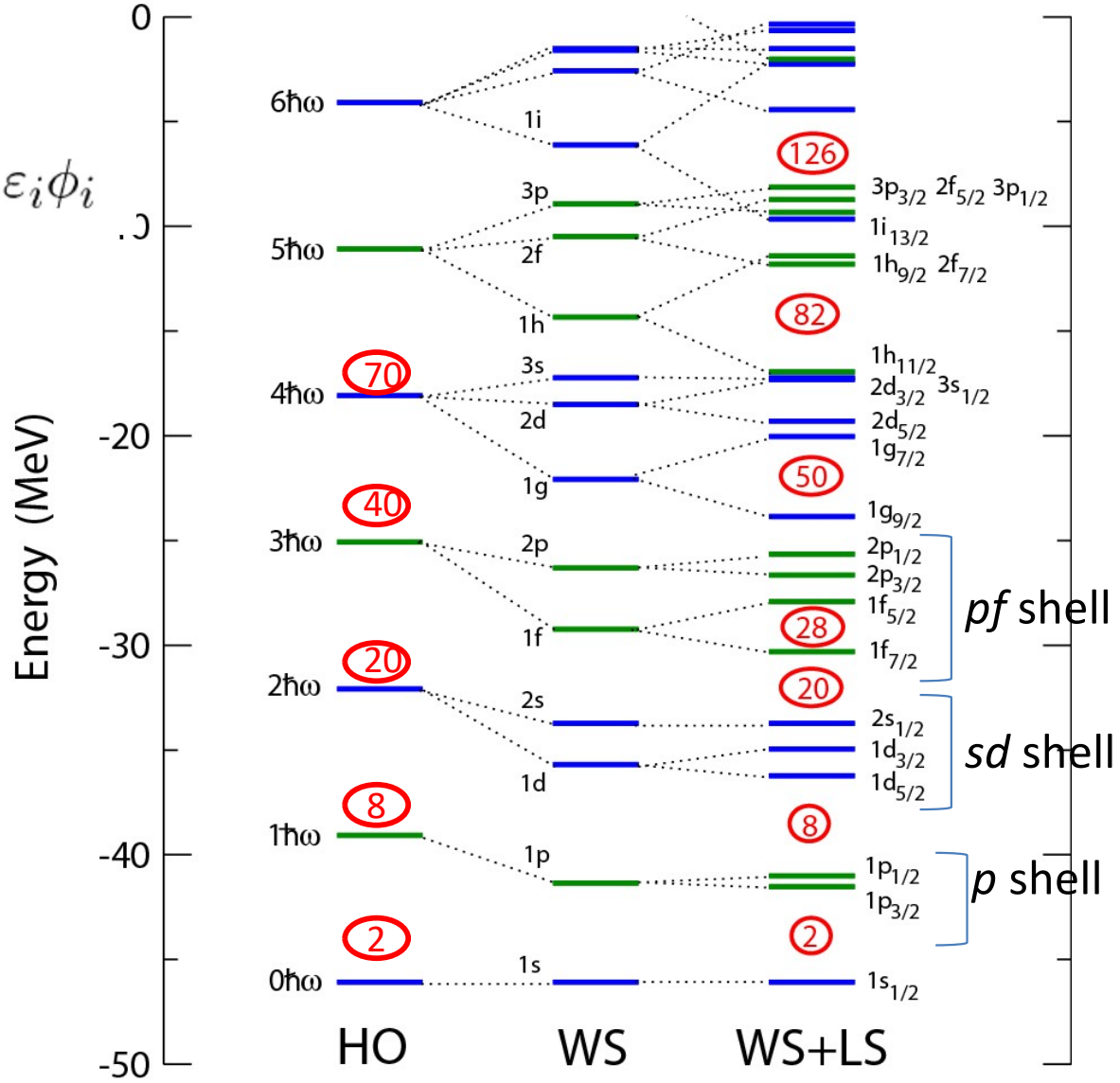
harmonic oscillator (HO)

$$V(r) = -V_0 + \frac{1}{2}M\omega^2 r^2$$

Woods-Saxon potential (WS)

$$V(r) = -\frac{V_0}{1+\exp(\frac{r-R}{a})}$$



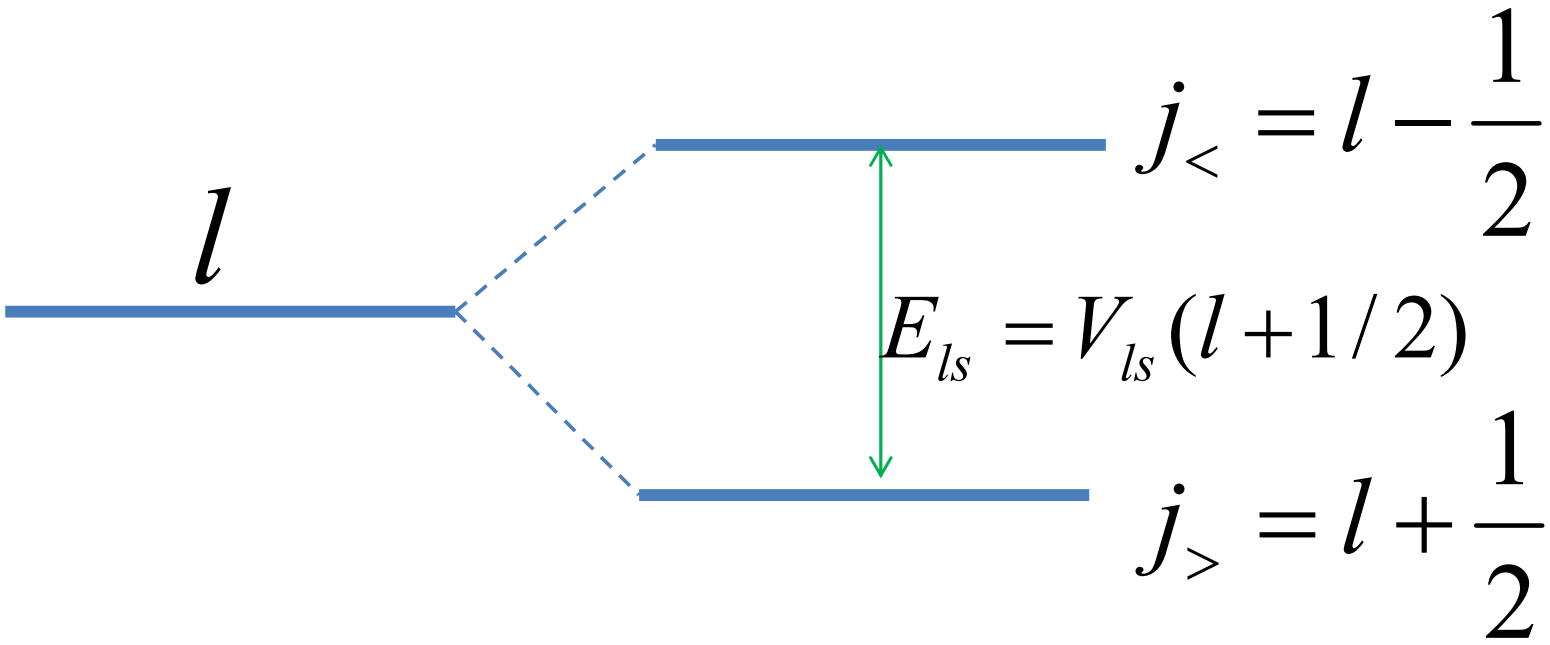


spin-orbit interaction

$$V = -V_{ls}\,\hat{l}\cdot\hat{s}$$

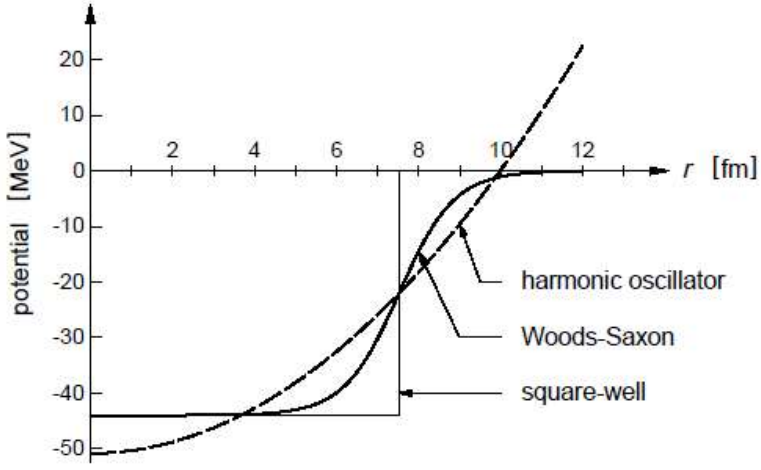
$$\hat{j} = \hat{l} + \hat{s} \qquad s = \frac{1}{2}$$

$$\left\langle j \left| (\hat{l}\cdot\hat{s}) \right| j \right\rangle = \{ j(j+1) - l(l+1) - s(s+1) \} / 2$$



single-particle wave function

- Mean-field potential



- single-particle wave function in 3-dimension harmonic oscillator potential

$$\phi_{n,l,j,m}(r,\theta,\phi) = R_{nl}(r) \sum_{m_l,m_s} \left\langle l, m_l, s, m_s \,\middle|\, j, m \right\rangle Y^l_{m_l}(\theta,\phi)\chi^s_{m_s}$$

$s = 1/2$ $\qquad j = l + s$ $\qquad jj$-coupling scheme

symbol $s, p, d, f, g, h, i, \ldots$

orbital angular momentum $l = 0, 1, 2, 3, 4, 5, 6, \ldots$

$1d_{5/2}$

$n = 1$ (or 0)

$l = 2$

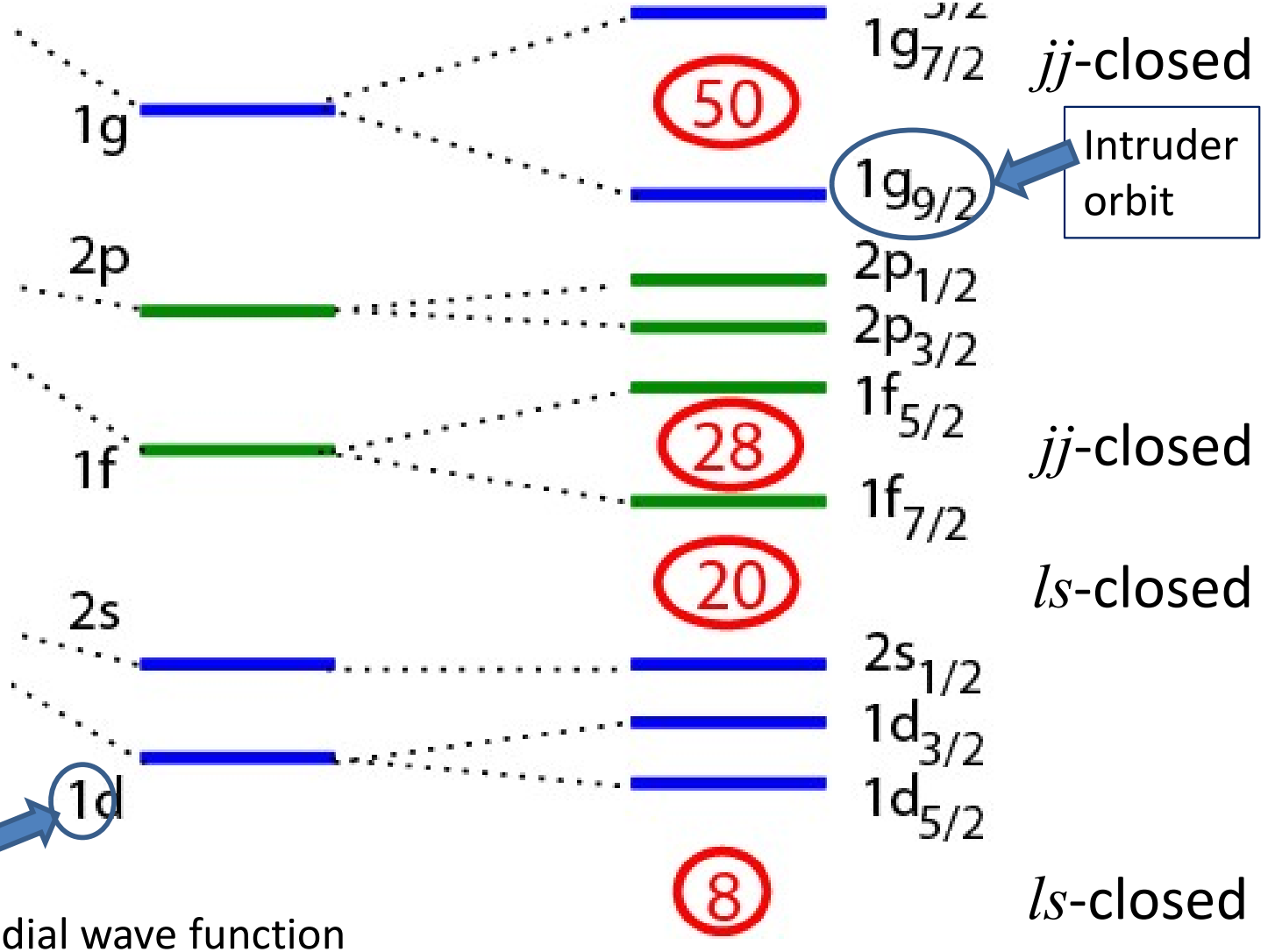
$j = 5/2$

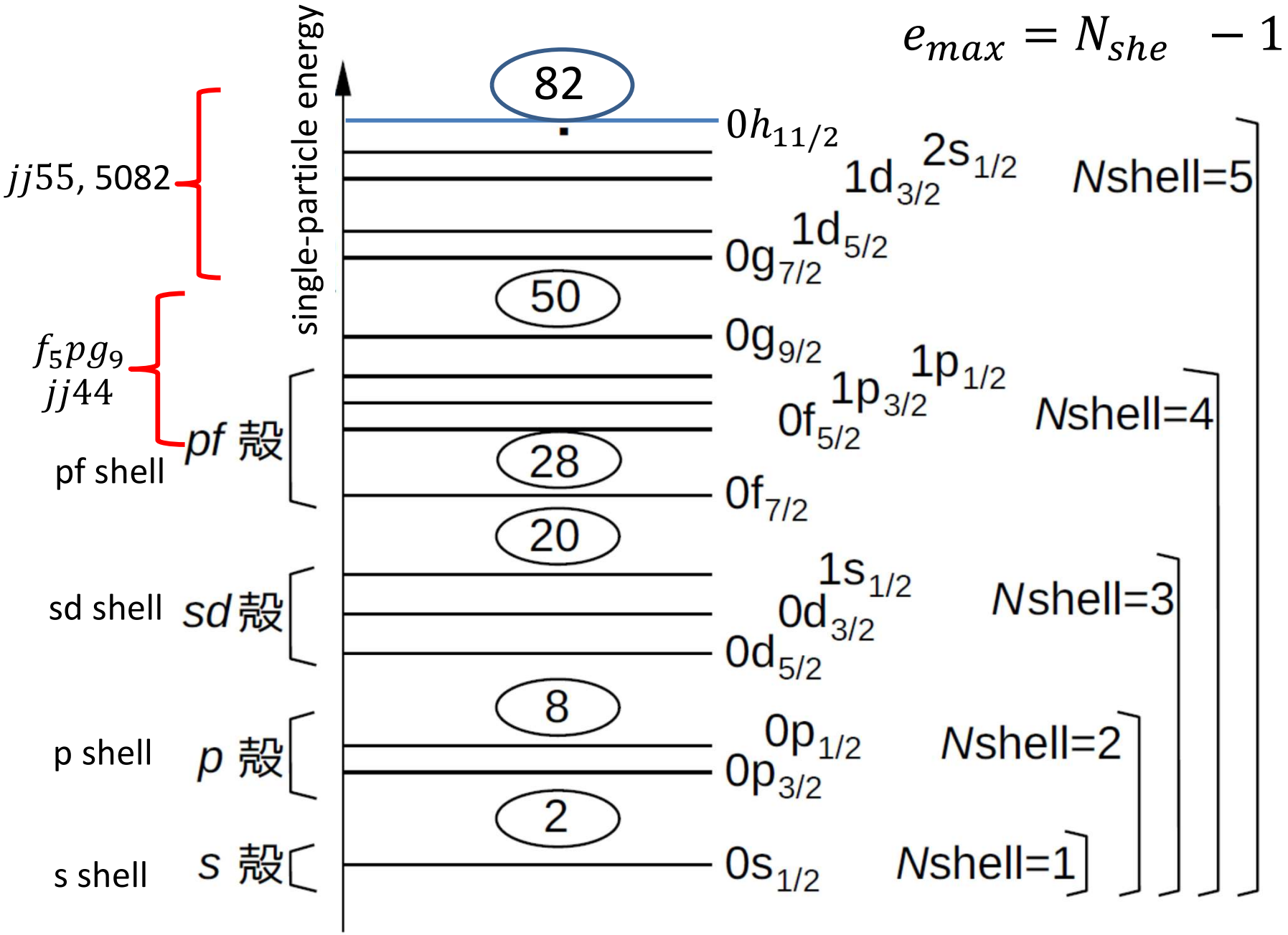
$N = 2n + l$

parity: $\Pi = (-1)^l$

Number of nodes in radial wave function

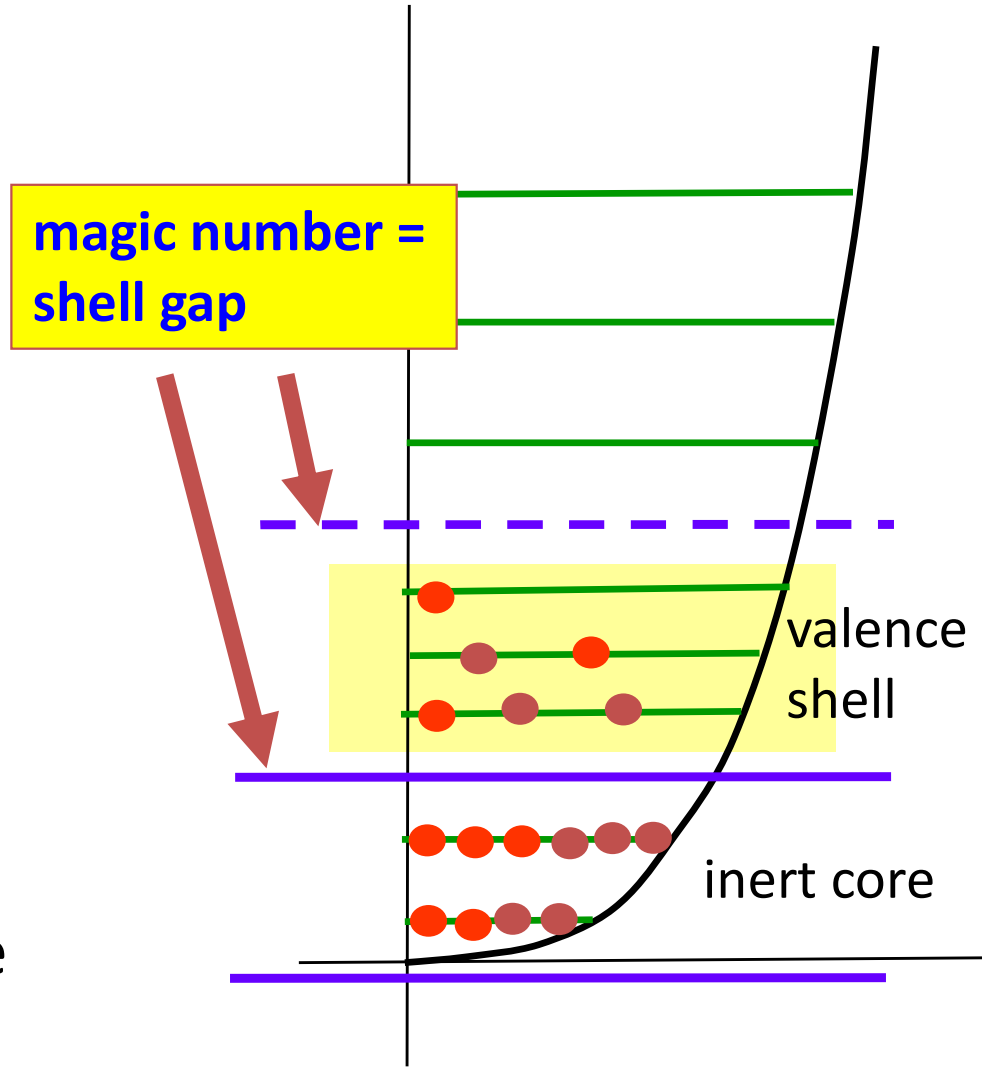
Note : there are two conventions, start from 0 or 1




$e_{max} = N_{she} - 1$
single-particle energy
82
50
28
20
8
2
$0h_{11/2}$
$2s_{1/2}$
$1d_{3/2}$
$1d_{5/2}$
$0g_{7/2}$
$0g_{9/2}$
$1p_{1/2}$
$1p_{3/2}$
$0f_{5/2}$
$0f_{7/2}$
$1s_{1/2}$
$0d_{3/2}$
$0d_{5/2}$
$0p_{1/2}$
$0p_{3/2}$
$0s_{1/2}$
Nshell=5
Nshell=4
Nshell=3
Nshell=2
Nshell=1
$jj55$, 5082
f_5pg_9
$jj44$
pf 殻
pf shell
sd 殻
sd shell
p 殻
p shell
s 殻
s shell

Recipe of LSSM

1. Prepare model space and the interaction file for a given nucleus (*N, Z*).
2. Run a shell-model code to obtain the wave functions, which are eigenstates of the shell-model Hamiltonian.
3. Various observables, such as transition probabilities and moments, are obtained using the wave functions.



Shell model Hamiltonian

Nucleons in a mean potential interacting through residual interactions

- Single particle energy （SPE)
- Two-body matrix element （TBME)

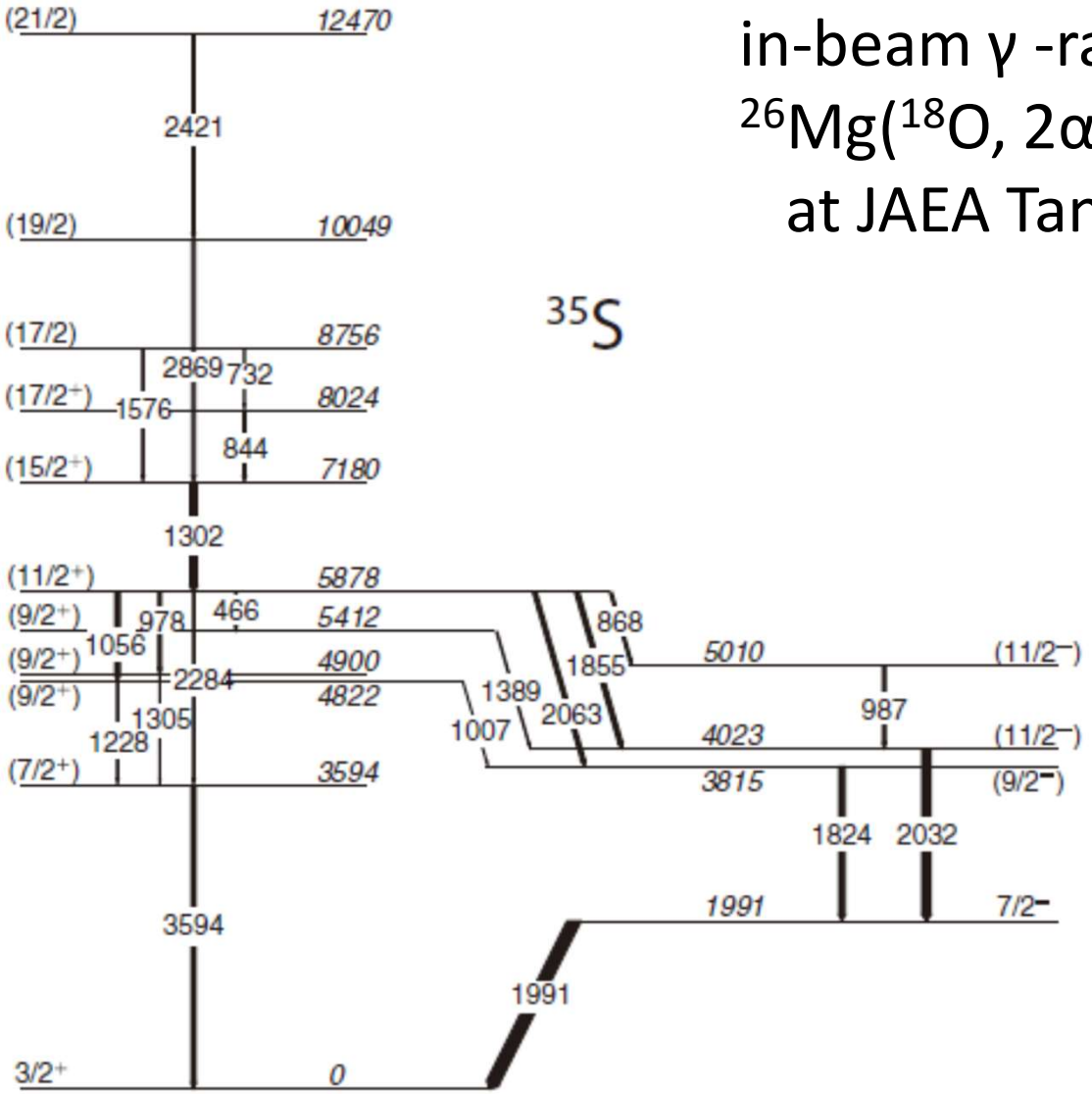
$$H = \sum_a \varepsilon_a n_a + \sum_{a\le b, c\le d, JM} V(abcd;J) A^\dagger_{JM}(a,b) A_{JM}(c,d)$$

$a = (n_a, l_a, j_a, t_{za})$ to specify a single-particle orbit

n_a … number operators of orbit a $\quad n_a = \sum_{m_a} c^\dagger_{a,m_a} c_{a,m_a}$

$$A^\dagger_J(a,b) = \frac{1}{\sqrt{1+\delta_{ab}}}[c^\dagger_a \otimes c^\dagger_b]^{(J)} = \frac{1}{\sqrt{1+\delta_{ab}}} \sum_{m_a,m_b} \langle j_a m_a j_b m_b | JM \rangle c^\dagger_{a,m_a} c^\dagger_{b,m_b}$$

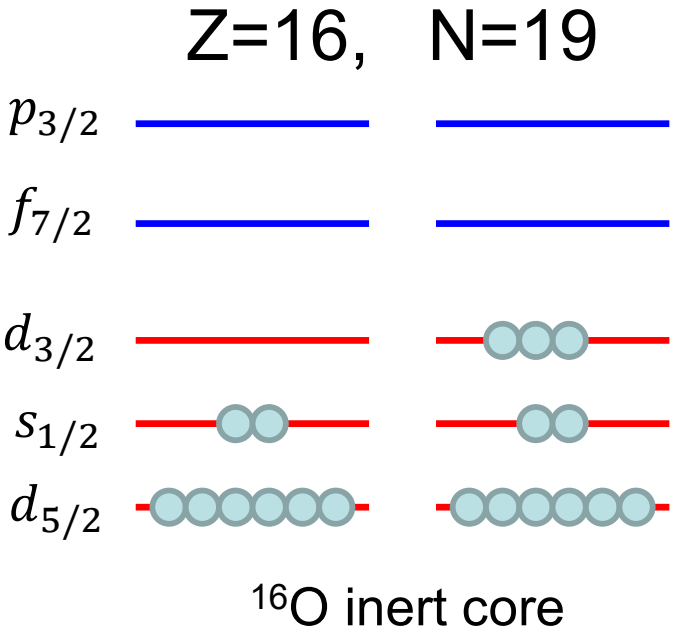
Example of shell-model study: High-spin states in ^{35}S



in-beam γ -ray spectroscopy

^{26}Mg(^{18}O, 2α1n)^{35}S fusion evaporation

at JAEA Tandem, ALTO Tandem



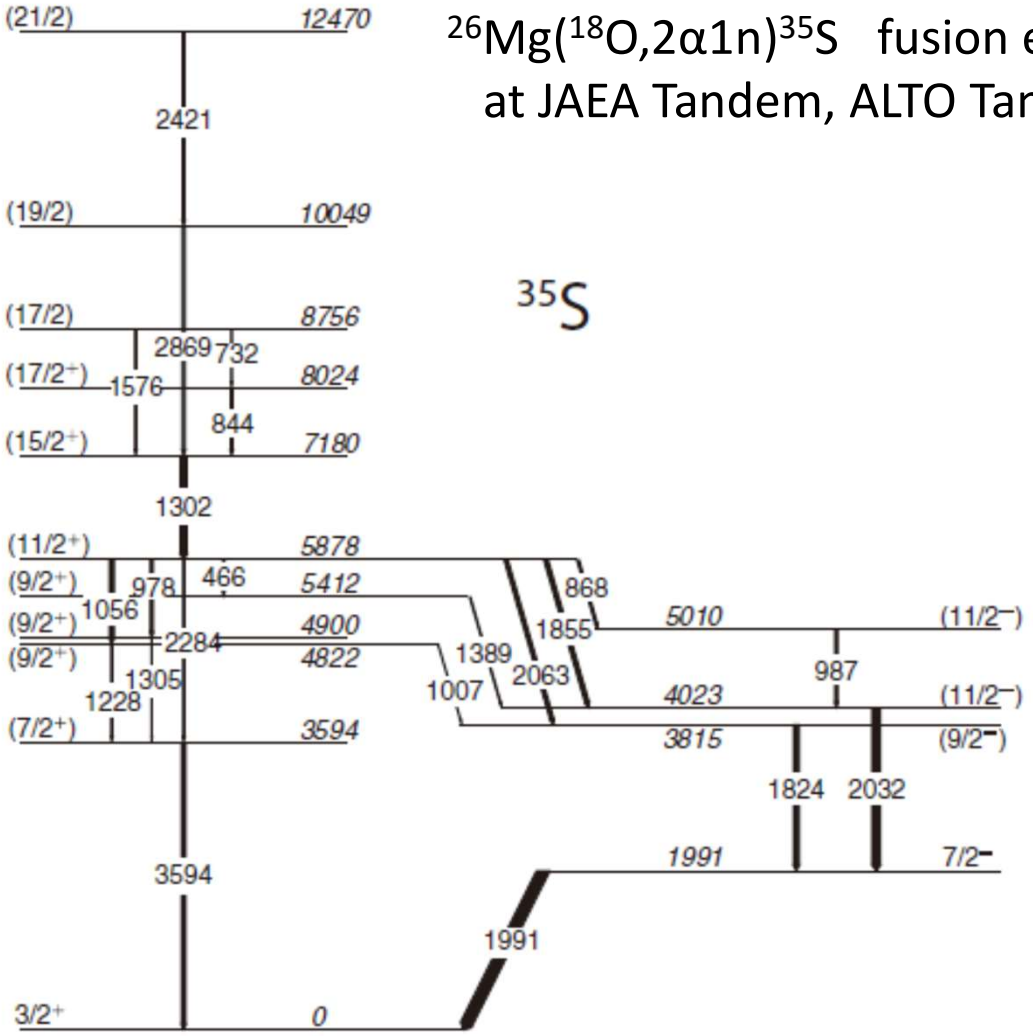
Ref. S. Go, E. Ideguchi, R. Yokoyama *et al.,* Phys. Rev. C 103, 034327 (2021).

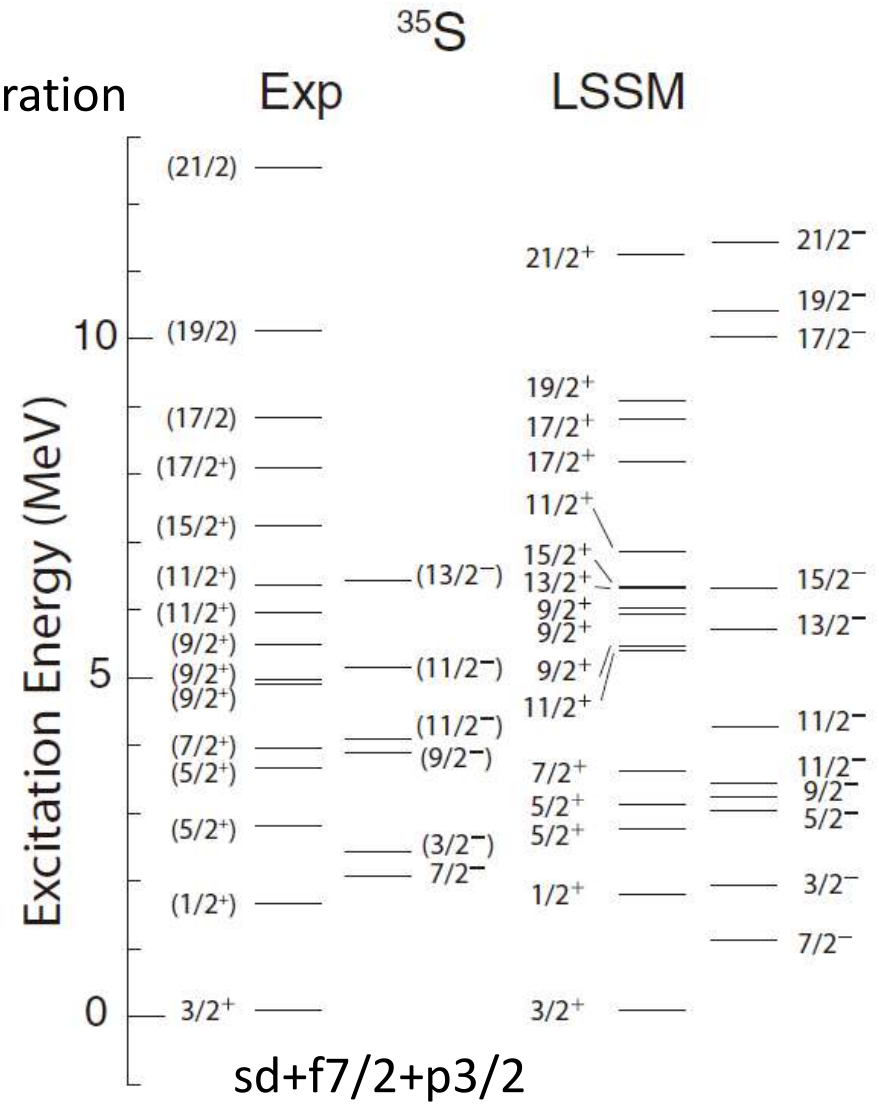
High-spin states in ^{35}S (N,Z)=(19,16)

in-beam γ -ray spectroscopy

^{26}Mg(^{18}O,2α1n)^{35}S fusion evaporation

at JAEA Tandem, ALTO Tandem



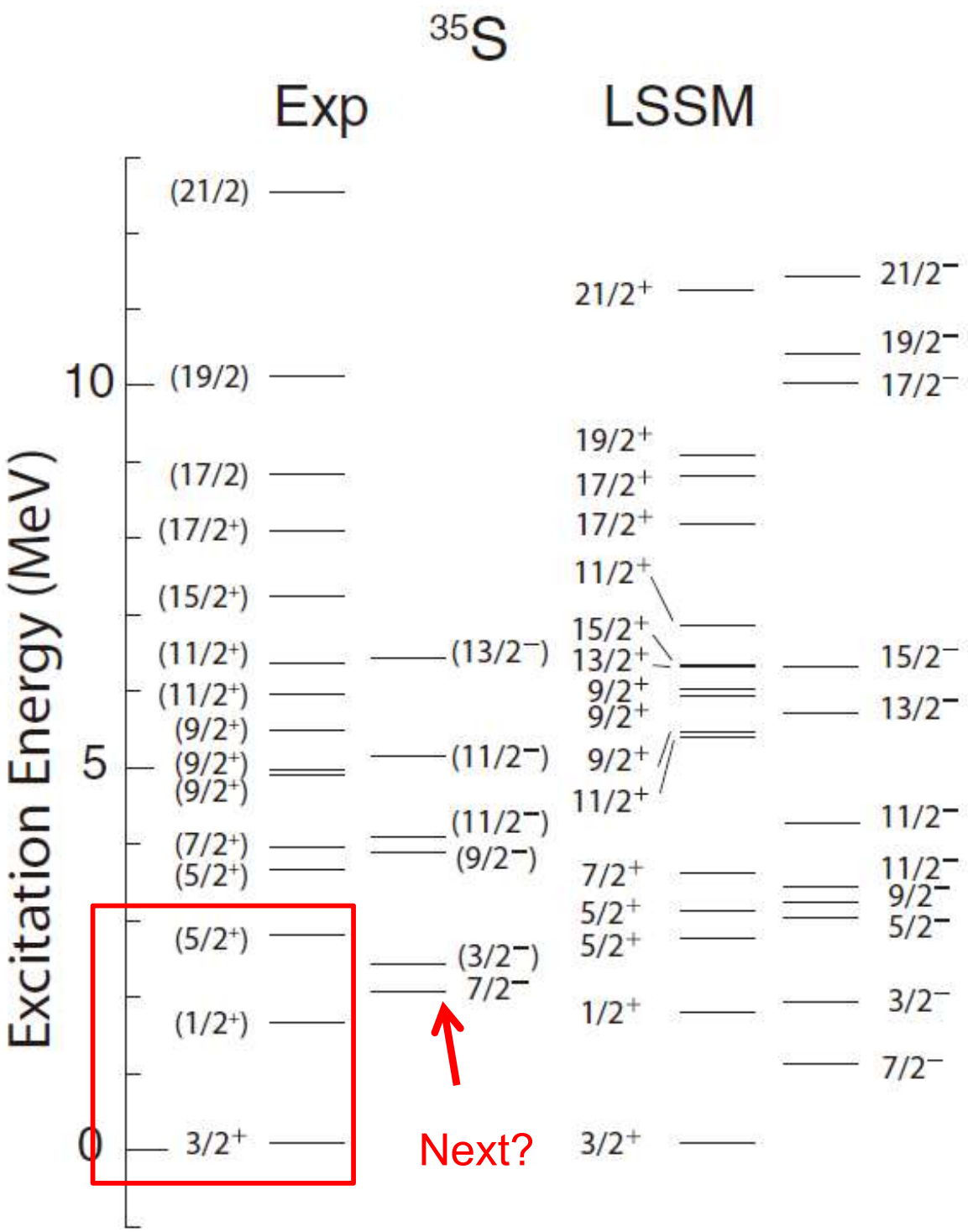


sd+f7/2+p3/2

SDPF-MSD4 interaction

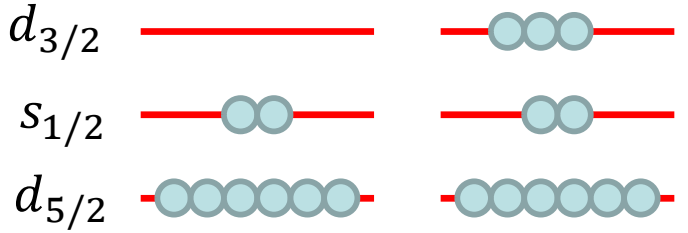
$D_M = 1.02 \times 10^9$

Ref. S. Go, E. Ideguchi, R. Yokoyama *et al.,* Phys. Rev. C 103, 034327 (2021).

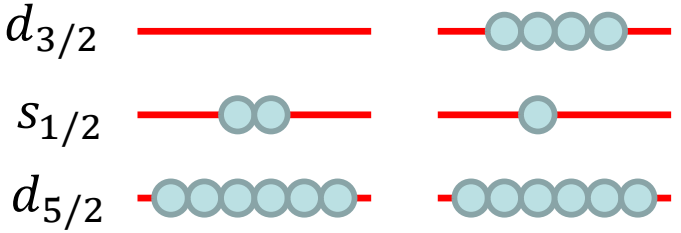


Major configuration

$3/2^+(1)$

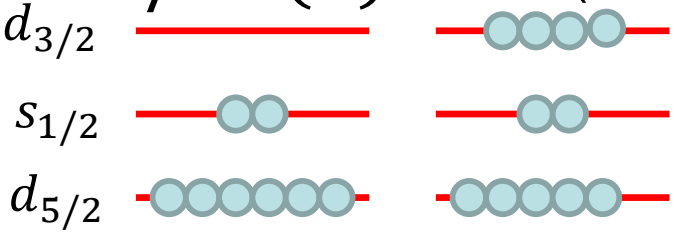


$1/2^+(1)$

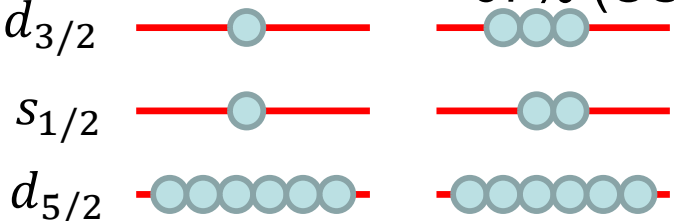


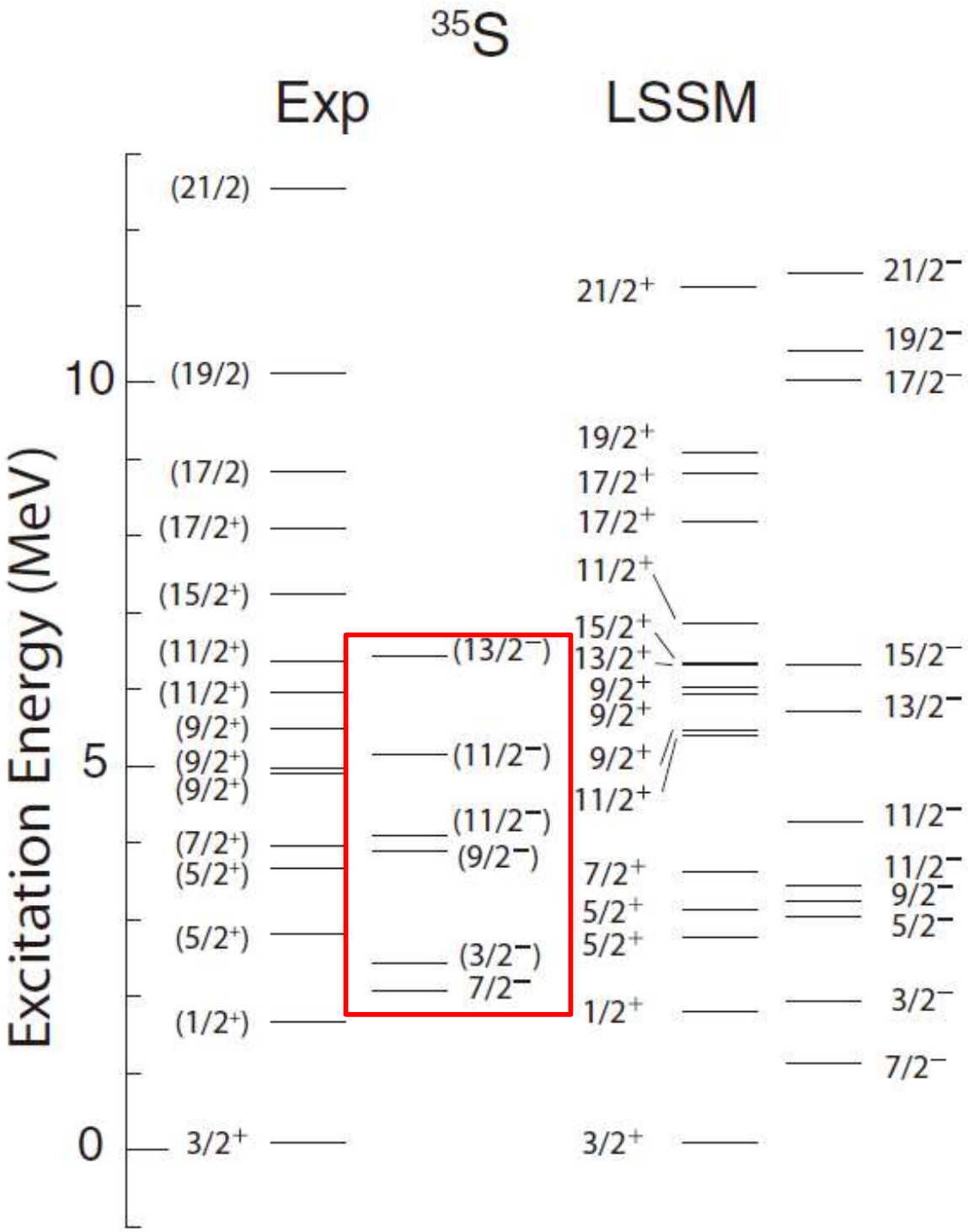
$5/2^+(1)$

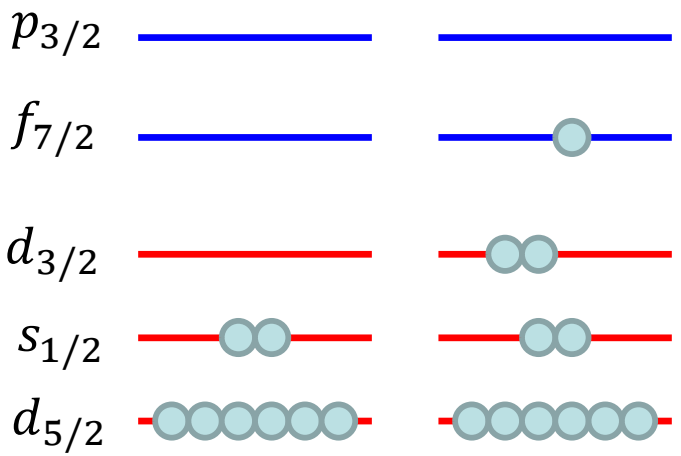
5% (USD)

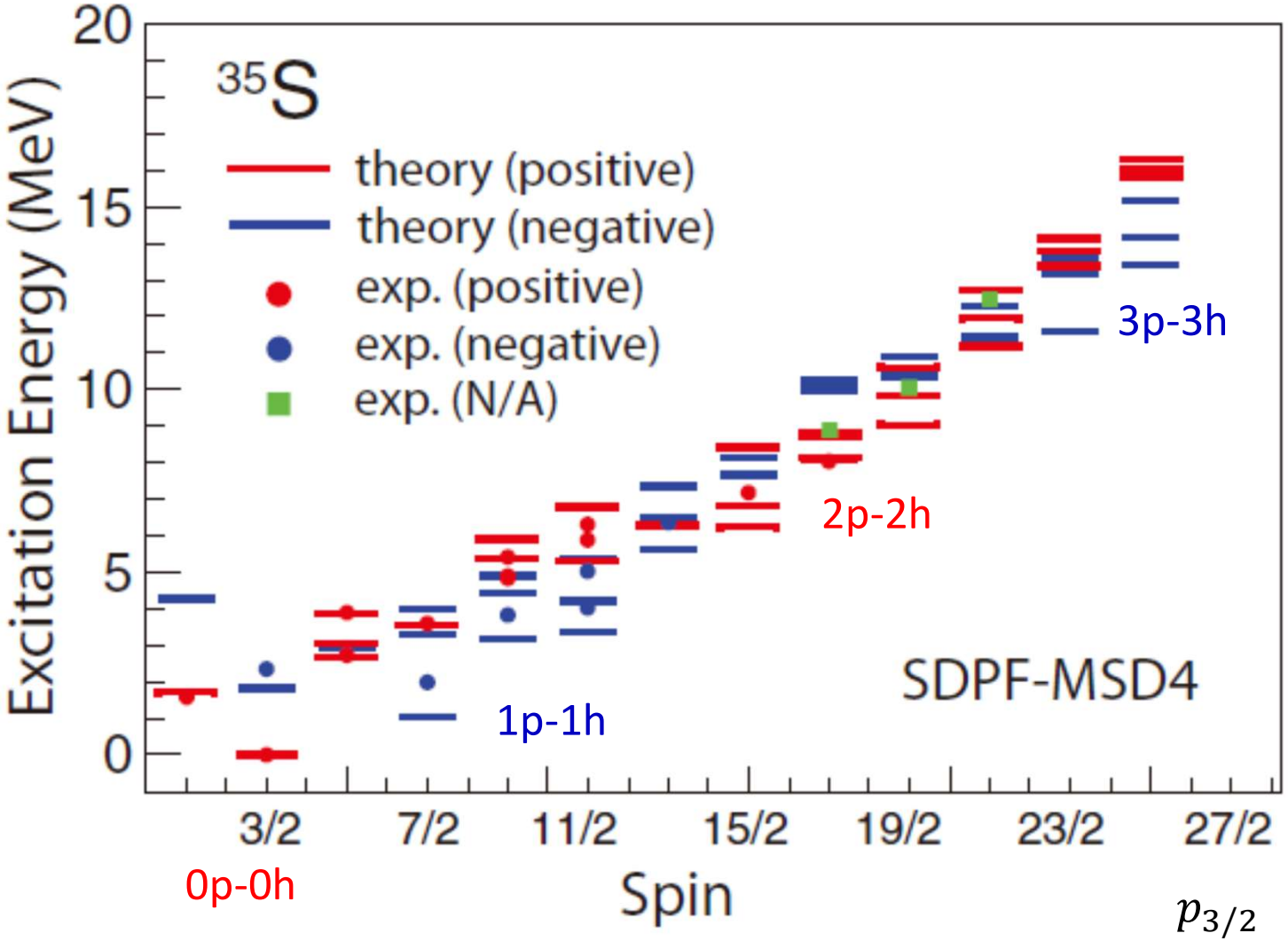


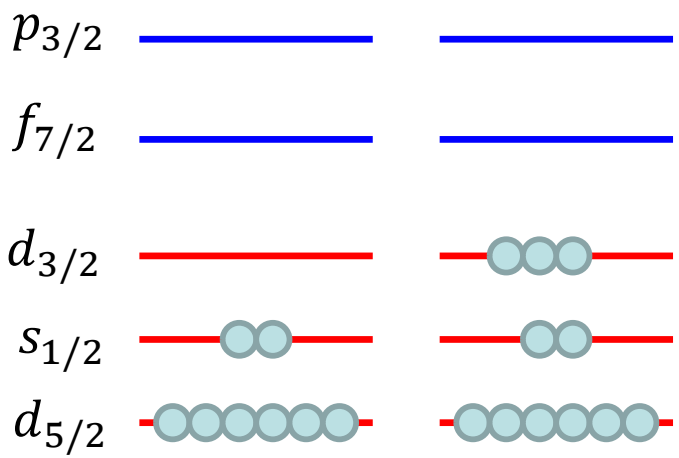
67% (USD)




^{35}S
Exp
LSSM
Excitation Energy (MeV)
10
5
0
(21/2)
(19/2)
(17/2)
(17/2⁺)
(15/2⁺)
(11/2⁺)
(11/2⁺)
(9/2⁺)
(9/2⁺)
(9/2⁺)
(7/2⁺)
(5/2⁺)
(5/2⁺)
(1/2⁺)
3/2⁺
(13/2⁻)
(11/2⁻)
(11/2⁻)
(9/2⁻)
(3/2⁻)
7/2⁻
21/2⁺
19/2⁺
17/2⁺
17/2⁺
11/2⁺
15/2⁺
13/2⁺
9/2⁺
9/2⁺
9/2⁺
11/2⁺
7/2⁺
5/2⁺
5/2⁺
1/2⁺
3/2⁺
21/2⁻
19/2⁻
17/2⁻
15/2⁻
13/2⁻
11/2⁻
11/2⁻
9/2⁻
5/2⁻
3/2⁻
7/2⁻


$p_{3/2}$
$f_{7/2}$
$d_{3/2}$
$s_{1/2}$
$d_{5/2}$

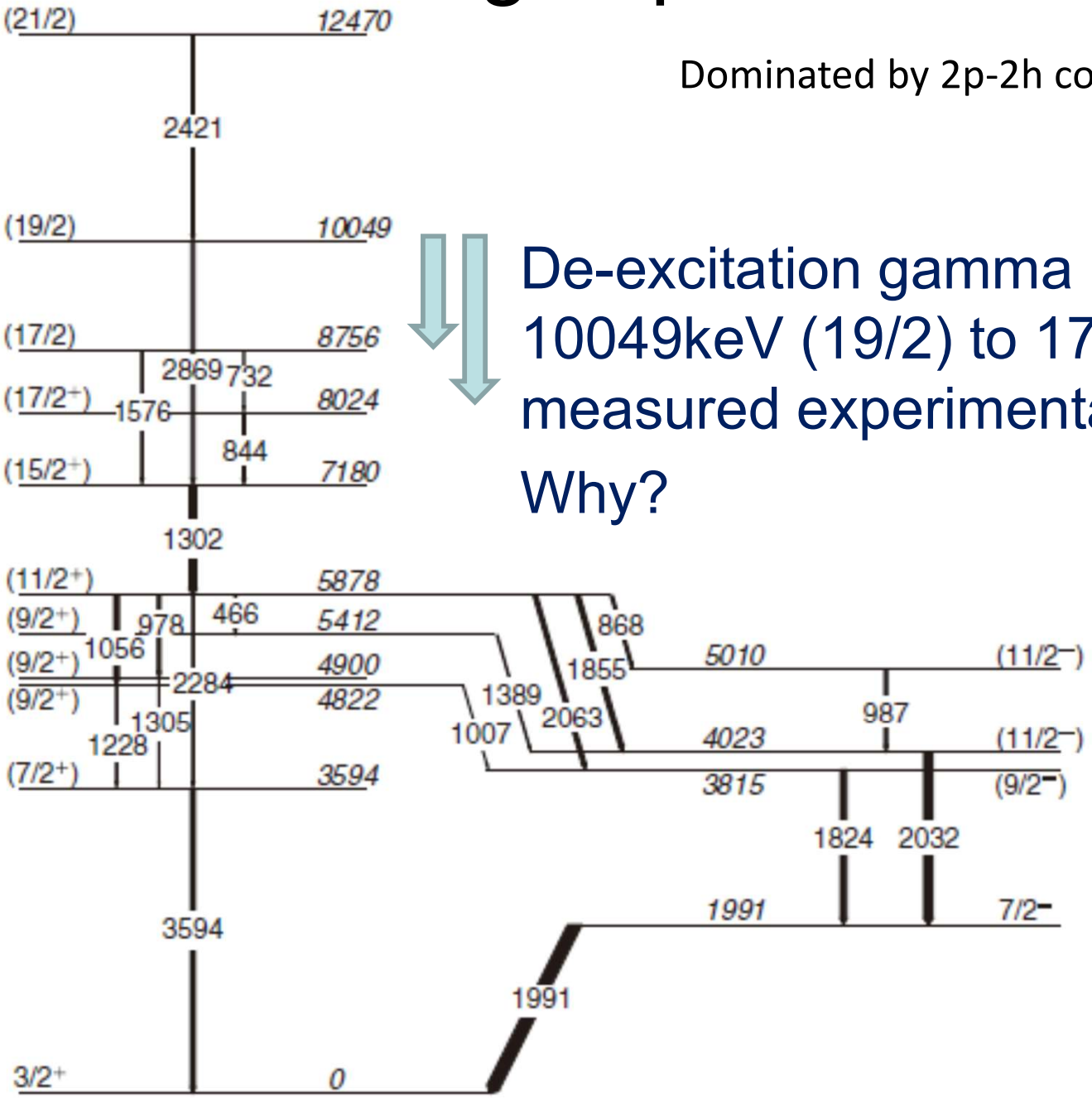




S. Go, E. Ideguchi, R. Yokoyama *et al.*,
Phys. Rev. C 103, 034327 (2021).

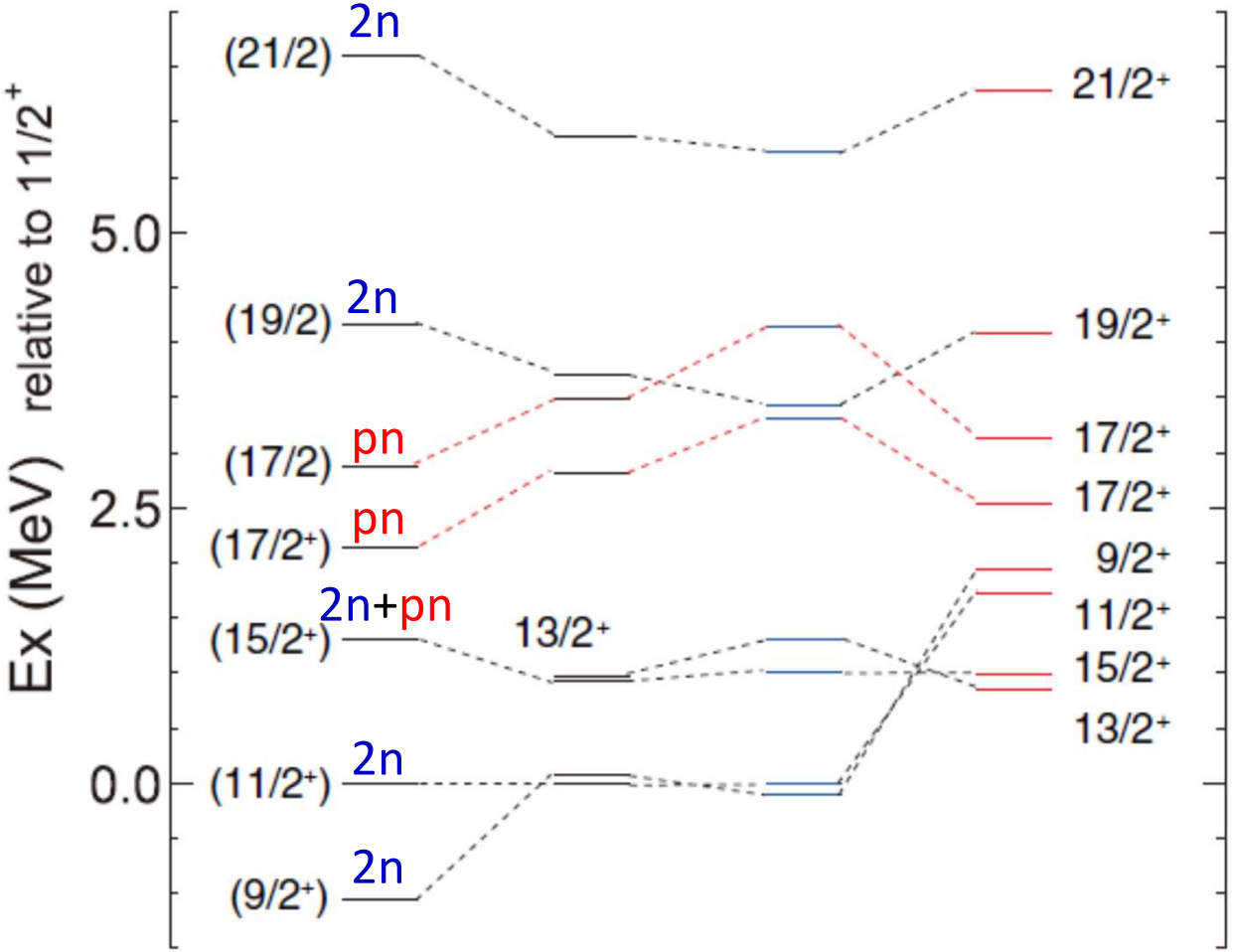
High-spin states of ^{35}S

Dominated by 2p-2h configuration



De-excitation gamma ray from 10049keV (19/2) to 17/2+ was not measured experimentally.

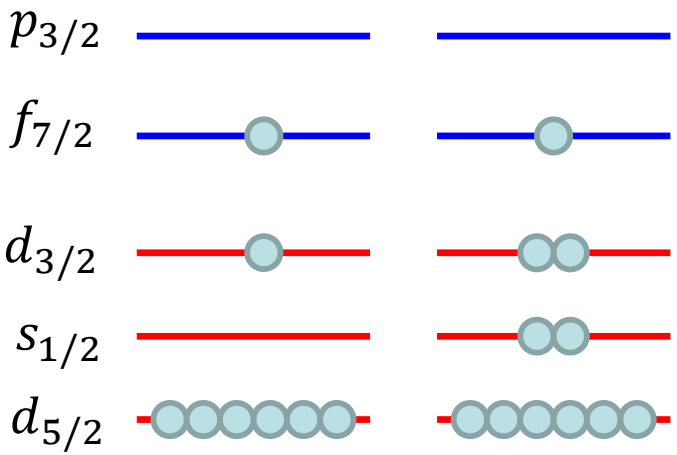
Why?

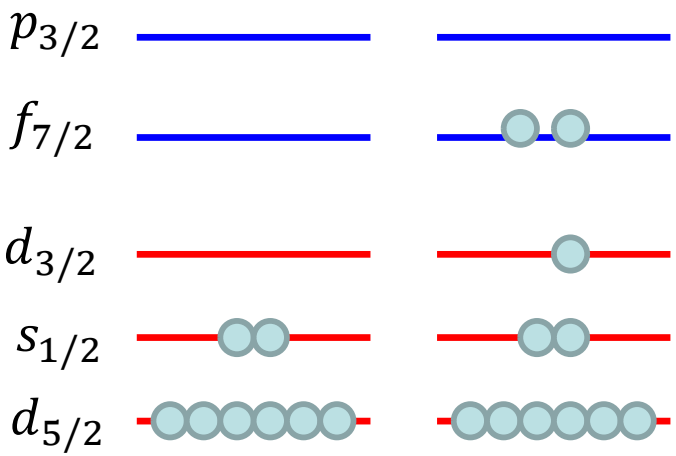


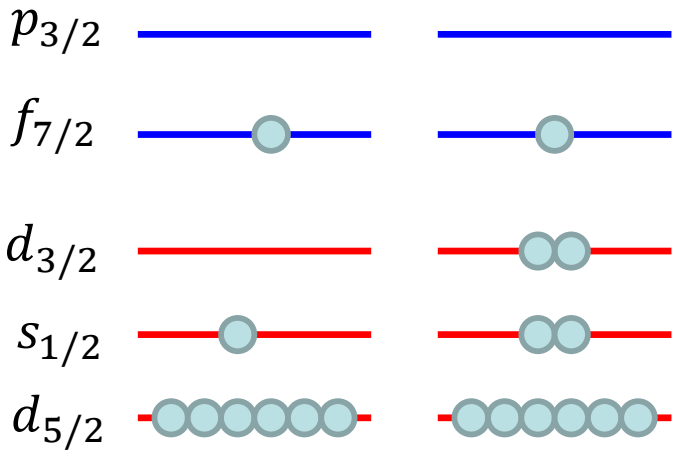
(a) Exp. (b) LSSM (c) 2n (d) pn

"spin-aligned" pn-pair in ^{35}S

$17/2^+ : \left(\pi 0f_{7/2} \times \nu 0f_{7/2}\right)^7 \pi d_{3/2}$



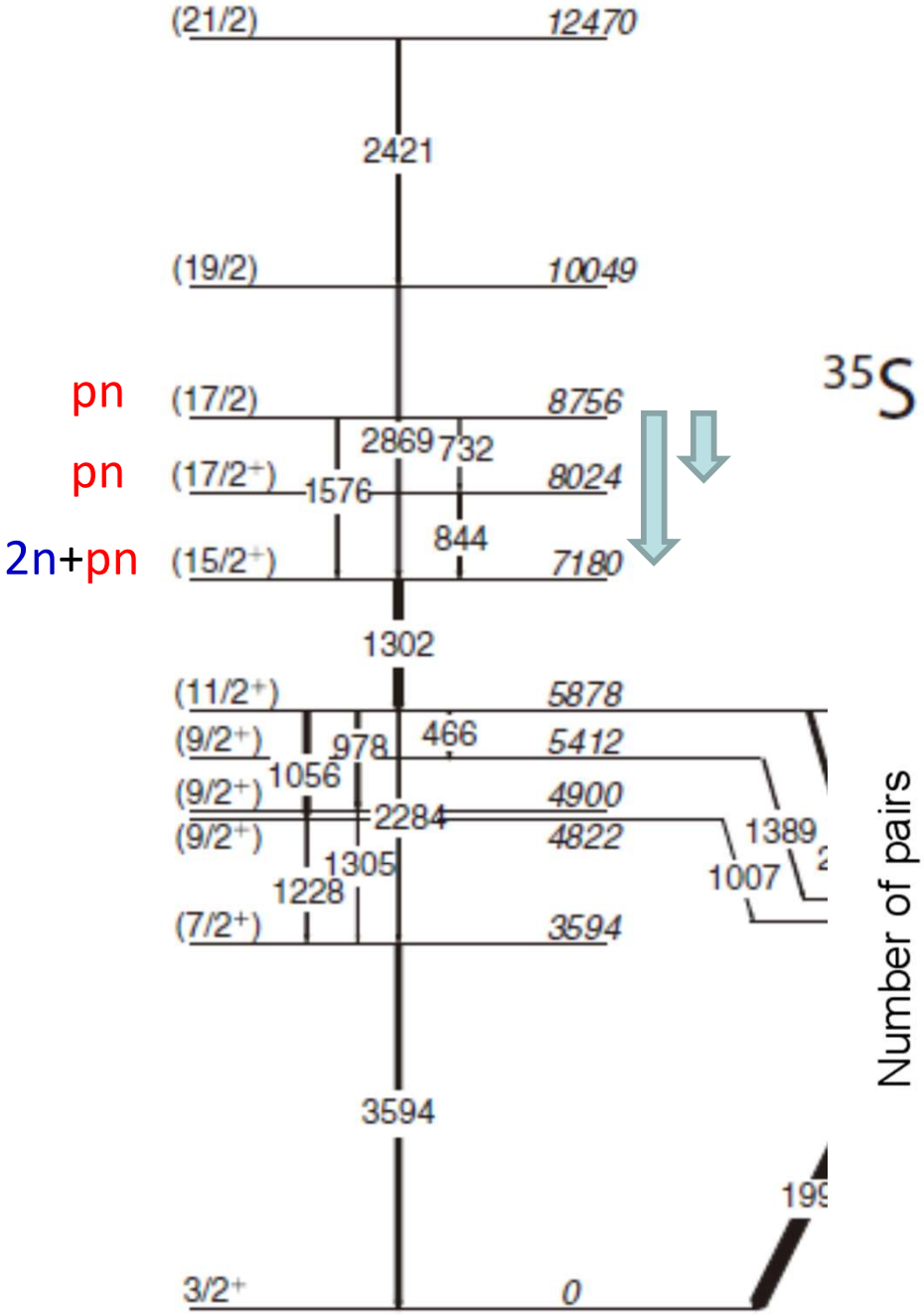




(c) 2n : SM calc. w/ 2n excitation

(d) pn : SM calc. w/ pn excitation

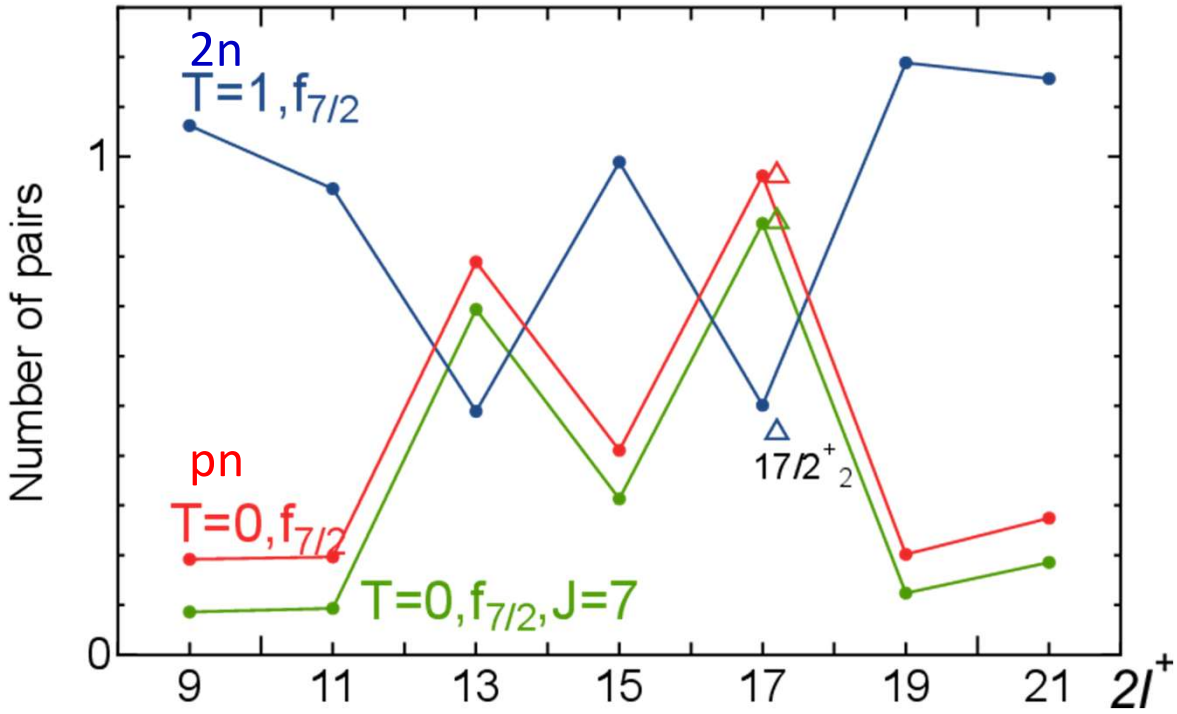
^{35}S branching ratio



^{35}S

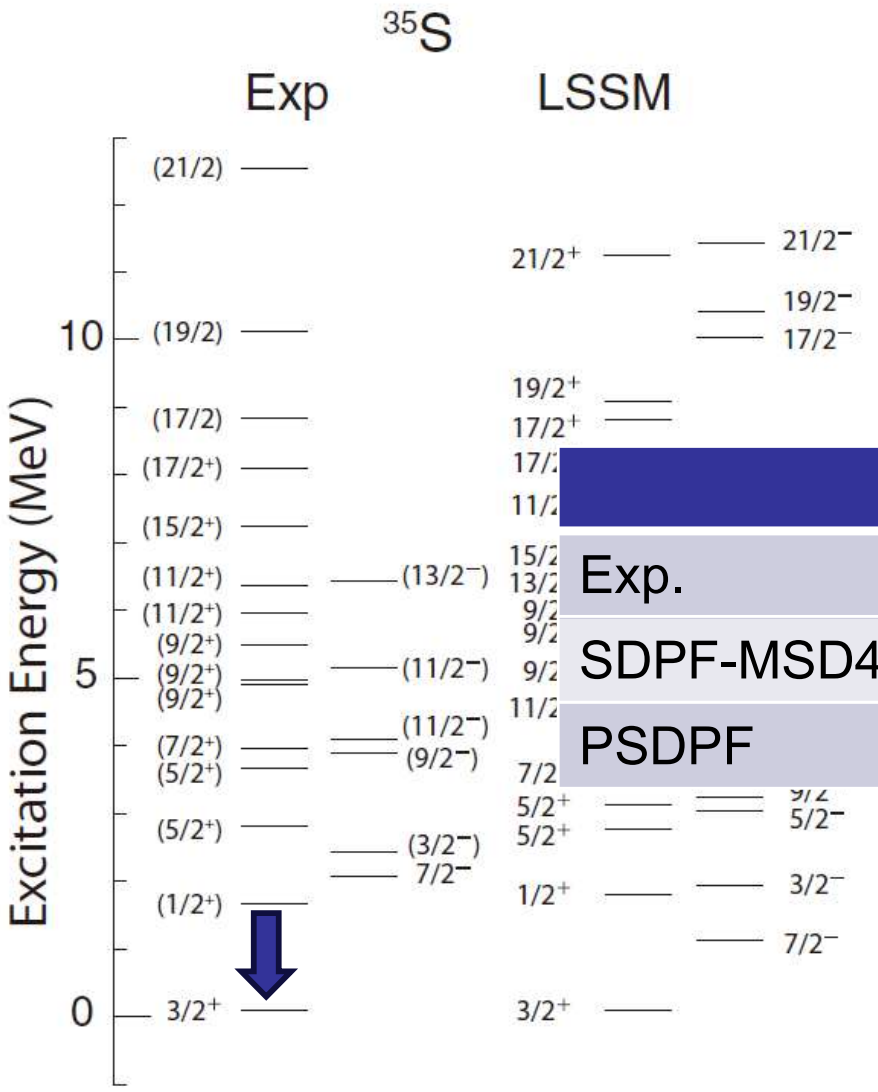
branching ratio (E2 and M1 transitions)

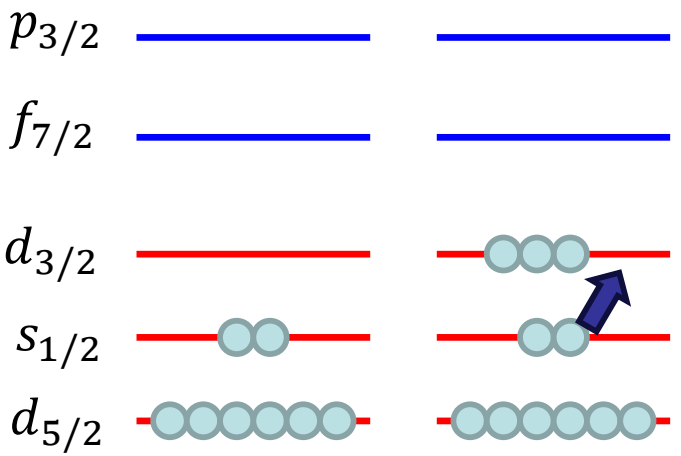
	1576keV	732keV
Exp.	64(18)%	36(15)%
LSSM	59%	41%



L. Grocutt et al., Phys. Rev. C 106, 024314 (2022).

The life time of ½+ (1572keV) was measured: 3.3(5) ps





	B(M1) (μ^2_N)	B(E2) (e^2fm^4)	lifetime
Exp.			3.3(5) ps
SDPF-MSD4	0.003	36.3	1.58 ps
PSDPF	0.0204	35.2	0.55 ps

SDPF-MSD4 : Utsuno (2021)
PSDPF : Boheral (2011)

M1 transition is forbidden
for simple configurations

Configuration mixing

TABLE II. Comparison between experimental and calculated levels for ^{35}S. $n\hbar\omega$ represents n-particle n-hole configurations. The values in the column mean the portion of the wave function for each calculated state. The transition probabilities $B(M1)$ and $B(E2)$ were calculated by the shell-model calculations.

Energy (MeV) Experiment	Theory	J_i^π	J_f^π	$E_\gamma^{\rm exp}$ (keV)	Ratio (%) $0\hbar\omega$	$2\hbar\omega$	$4\hbar\omega$	$B(M1)$ (μ_N^2)	$B(E2)$ (e^2 fm^4)
1.572[a]	1.709	$1/2_1^+$	$3/2_1^+$	1572	57.9	36.9	5.2	0.003	36.3
0.000	0.000	$3/2_1^+$			71.0	26.5	2.4		
2.717[a]	2.672	$5/2_1^+$	$1/2_1^+$	2717	66.0	30.9	3.2		7.7
3.886[a]	3.036	$5/2_2^+$			59.9	35.8	4.3		
3.594	3.538	$7/2_1^+$	$3/2_1^+$	3594	50.8	44.1	5.1		28.8
4.822	5.381	$9/2_1^+$	$7/2_1^+$	1228	0.0	86.2	13.8	0.000	5.4
4.900	5.870	$9/2_2^+$	$7/2_1^+$	1305	0.2	85.2	14.6	0.000	0.6
5.412	5.941	$9/2_3^+$	$5/2_2^+$	1526[a]					11.4
5.878	5.313	$11/2_1^+$	$9/2_1^+$	1056	0.0	86.6	13.4		
					$1\hbar\omega$	$3\hbar\omega$	$5\hbar\omega$		
2.348[a]	1.837	$3/2_1^-$			72.3	25.6	2.1		
	2.946	$5/2_1^-$			69.5	28.1	2.4		
1.911	1.030	$7/2_1^-$			74.6	23.6	1.8		
3.815	3.166	$9/2_1^-$	$7/2_1^-$	1824	78.1	20.5	1.4	0.013	54.7
4.023	3.356	$11/2_1^-$	$7/2_1^-$	2032	74.6	23.7	1.7		60.9
5.010	4.205	$11/2_2^-$	$7/2_1^-$	987	78.4	20.4	1.3		0.3
		$11/2_2^-$	$11/2_1^-$	3019	78.4	20.4	1.3	0.067	31.1
6.352[a]	5.637	$13/2_1^-$	$9/2_1^-$	2536[a]	77.7	21.0	1.4		39.2

Spectroscopic factors of ^{36}S(p,d)^{35}S neutron-removal reaction

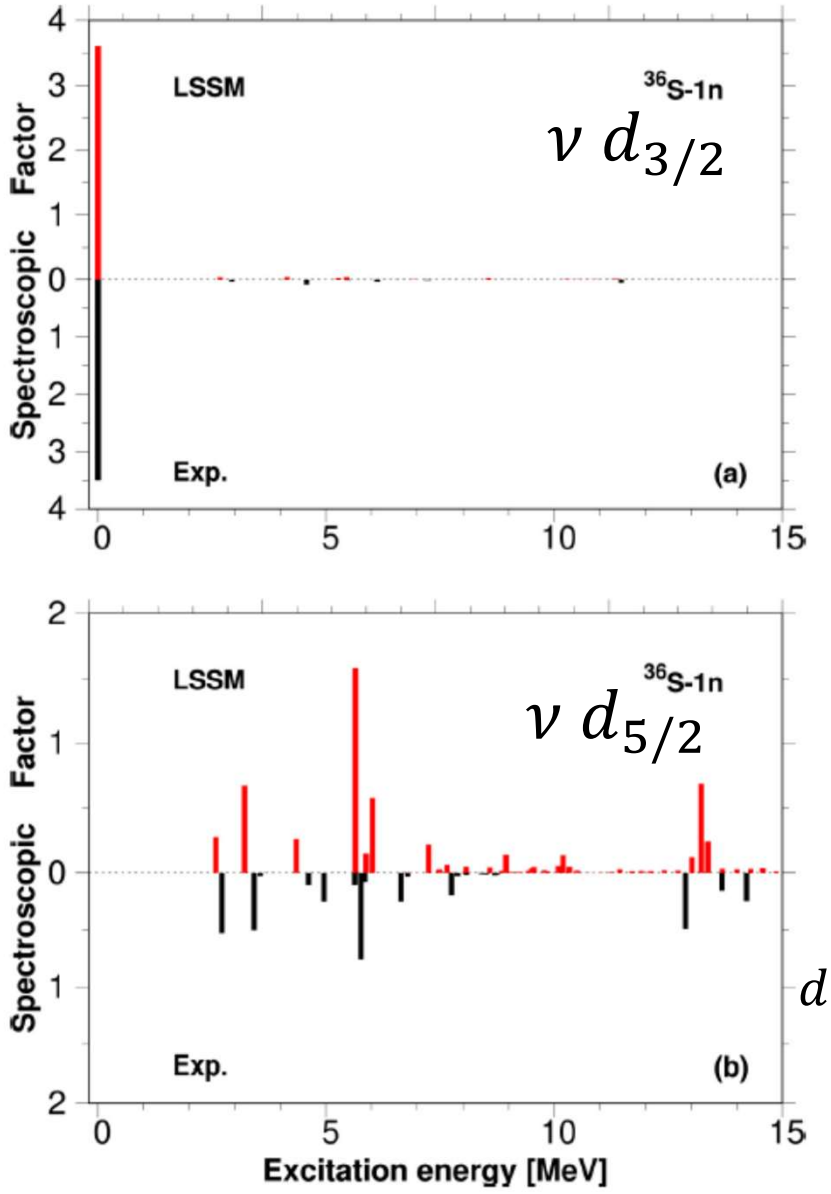
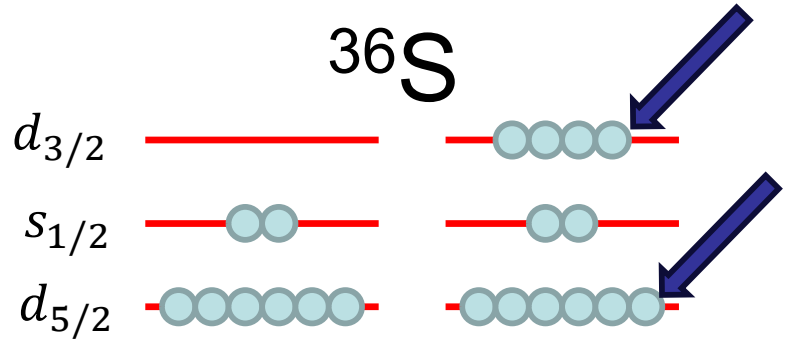


FIG. 8. Comparison of experimental and LSSM $d_{3/2}$ (a) and $d_{5/2}$ (b) spectroscopic factors.

$$A + n \rightleftarrows B$$

$$C^2 S_j = \frac{\left|\langle \Psi_B || a_j^\dagger || \Psi_A \rangle\right|^2}{2J_B + 1}$$

$$= |\langle {}^{36}\mathrm{S}, 0_1^+ | \left| a_j^\dagger \right| | {}^{35}\mathrm{S}, j_i^+ \rangle|^2$$



$d_{5/2}$ hole state is fragmented

$$\Delta_{SO}(1d) = 6.578(44)\mathrm{MeV}$$

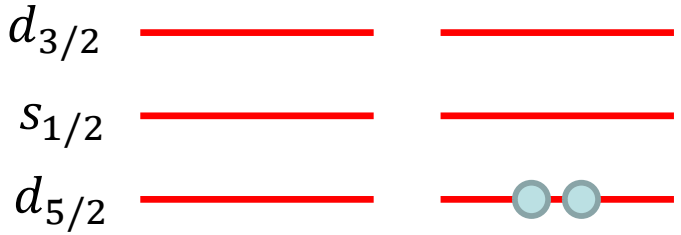
S. Jongile et al., Phys. Rev. C 113, 024323 (2026)

LSSM: SDPF-MIX20 (Nowacki 2026)

Let's us perform a simple example of the shell-model calculations step by step.

^{17}O and ^{18}O, sd shell with ^{16}O inert core

USD interaction (w.snt)



Interaction file in KSHELL (pn formalism)

```
! Wildenthal's USD interaction for sd-shell
! B. A. Brown and B. H. Wildenthal, Annu. Rev. Nucl. Part. Sci. 38, 29 (1988)
! proton-orbit, neutron-orbit, proton core, neutron core
3 3 8 8
! n  l  j  tz
! model space
   3   3     8   8
   1       0   2   3  -1    !  1 = p 0d_3/2
   2       0   2   5  -1    !  2 = p 0d_5/2
   3       1   0   1  -1    !  3 = p 1s_1/2
   4       0   2   3   1    !  4 = n 0d_3/2
   5       0   2   5   1    !  5 = n 0d_5/2
   6       1   0   1   1    !  6 = n 1s_1/2
! one-body interaction
! number of lines, method1
 6   0
   1   1      1.64658
   2   2     -3.94780
   3   3     -3.16354
   4   4      1.64658
   5   5     -3.94780
   6   6     -3.16354
! two-body interaction (TBME)
! # of lines, method2 A mass dependence factor
158    1   18   -0.30000
!   i    j    k    l     J     <i,j| V | k,l>_J
    1    1    1    1     0      -2.18450
    1    1    1    1     2      -0.06650
    1    1    1    2     2       0.61490
    1    1    1    3     2       0.51540
    1    1    2    2     0      -3.18560
    1    1    2    2     2      -1.62210
    1    1    2    3     2      -0.40410
    1    1    3    3     0      -1.08350
    1    2    1    2     1       1.03340
    1    2    1    2     2      -0.32480
    1    2    1    2     3       0.58940
    1    2    1    2     4      -1.44970
...
    5    5    5    5     0      -2.81970
... 158 lines continued
```

USD interaction (w.snt)

$$H = \sum_a \varepsilon_a n_a + \sum_{a \le b, c \le d, JM} V(abcd;J) A^{\dagger}_{JM}(a,b) A_{JM}(c,d)$$

← single-particle space (model space)

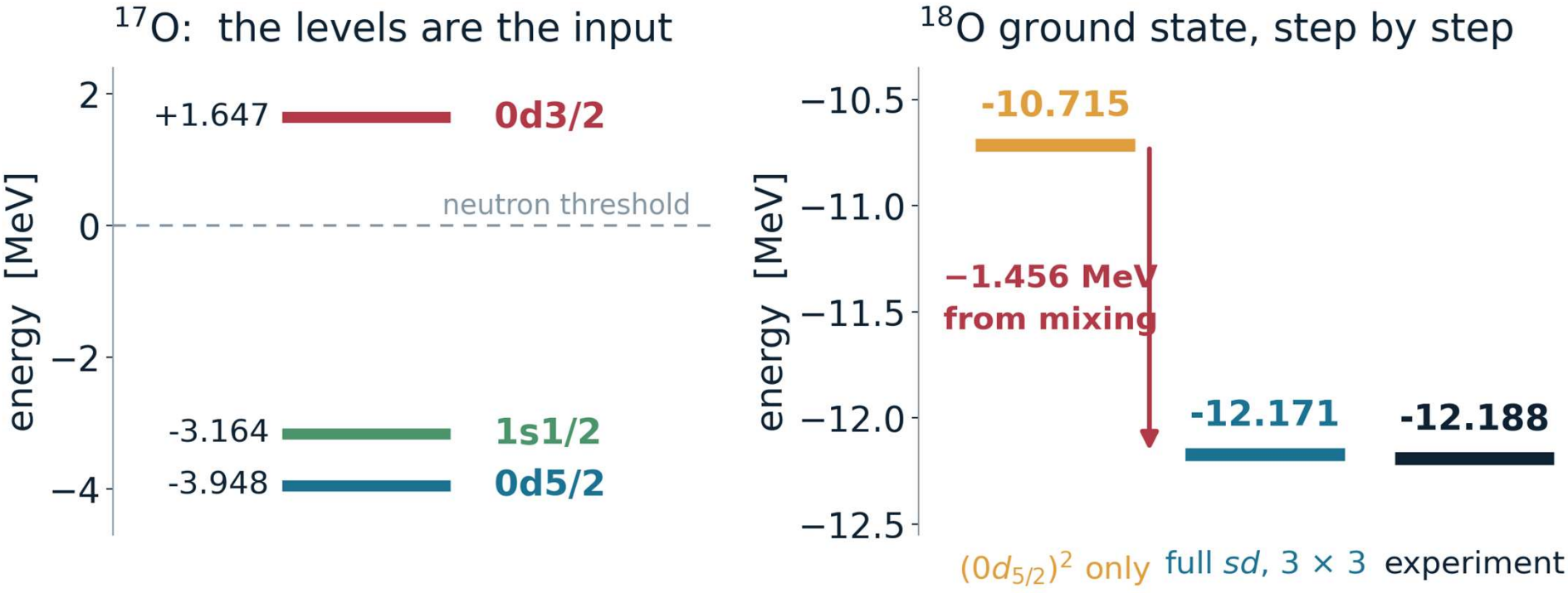
← single-particle energies

$\epsilon_{\nu 0d_{5/2}}$ = -3.94780 MeV

← TBMEs $V(a,b,c,d,J)$

$$\langle \nu 0d_{5/2}, \nu 0d_{5/2} | V | \nu 0d_{5/2}, \nu 0d_{5/2} \rangle_{J=0} = -2.81970 \text{ MeV}$$

^{17}O: the answer is the input



One valence neutron, no two-body term

The three levels are the three single-particle energies, straight from the file.

But they are fitted parameters

Measured S_n is 4.143 MeV, not 3.948 — and the real ^{17}O fragments its d5/2 strength.

^{18}O: two particles, one matrix element

Put both neutrons in 0d5/2 and couple them to J = 0. Then the energy is

$$E = 2\,\varepsilon(0d5/2) + \langle (0d5/2)^2 ; J=0 \mid V \mid (0d5/2)^2 ; J=0 \rangle$$

SPE:

```
5   5     -3.94780
```

TBME :

```
5   5   5   5    0    -2.81970
```

$$\mathbf{E = 2 \times (-3.9478) + (-2.8197) = -10.7153\ MeV}$$

measured S_{2n} = 12.188 MeV

Two lines and no computer — but 1.47 MeV short. Something is missing.

^{18}O: now allow the whole sd shell

Two identical particles coupled to J = 0 must share an orbit — so the basis has exactly three states, and the Hamiltonian matrix is 3 × 3.

	$(0d5/2)^2$	$(1s1/2)^2$	$(0d3/2)^2$
$(0d5/2)^2$	**-10.7153**	-1.3247	-3.1856
$(1s1/2)^2$	-1.3247	**-8.4517**	-1.0835
$(0d3/2)^2$	-3.1856	-1.0835	**+1.1087**

MeV

Look at the corner

The top-left entry is exactly the previous slide's answer.

The simple estimate was this matrix truncated to one row and column.

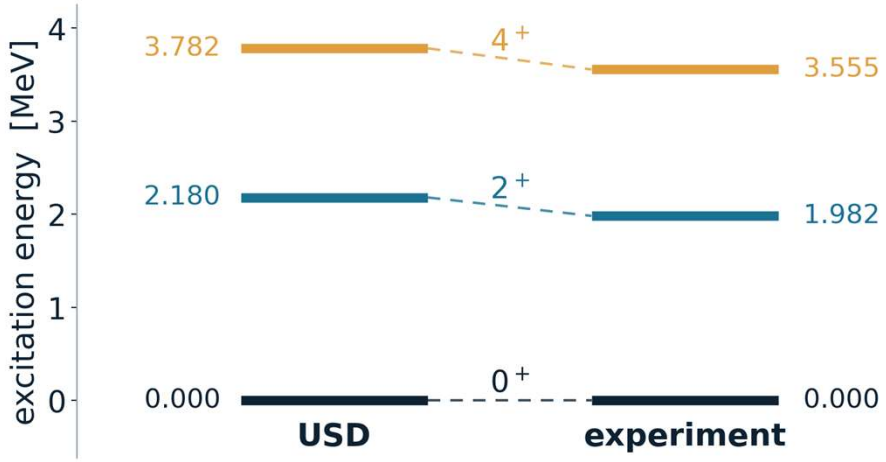
Solve the eigenvalue problem of this 3x3 matrix!

−12.171 MeV
lowest eigenvalue

79.0 %
is $(0d5/2)^2$

−1.456 MeV
gained from mixing

The whole spectrum, from matrices this size



Both excited states come out about 0.2 MeV high. A checkable statement about USD, from matrices you can diagonalise on paper.

J-scheme dimensions

J = 0, 1, 2, 3, 4

D_J = 3, 2, 5, 2, 2

The J = 4 problem is a 2 × 2 you can solve on paper.

The bookkeeping closes

$\Sigma\ (2J+1)\ D_j = 66 = C(12,2)$

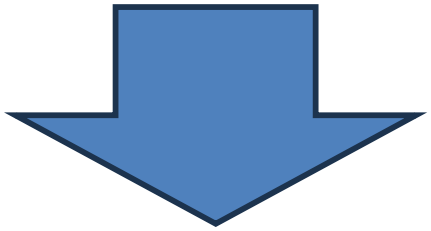
$\Sigma\ D_j = 14$ = the M-scheme dimension at M = 0

More than two valence particles

J-scheme basis state is complicated

c.f.p. (coefficient of fractional parentage)

$$|j^n \alpha J\rangle = \sum_{\alpha_1 J_1} [j^{n-1}(\alpha_1 J_1)_j ; J \; | \} \; j^n \alpha J] \, |j^{n-1}(\alpha_1 J_1)_j ; J\rangle$$



“M-scheme” basis state is easy to be handled,
no recoupling coefficients appear.

M-scheme Slater determinant

- A many-body wave function of *A* particles is expressed as a Slater determinant:

$$\Phi(x_1, x_2, \cdots, x_A) = \frac{1}{\sqrt{A!}} \det \begin{vmatrix} \phi_a(x_1) & \phi_a(x_2) & \cdots & \phi_a(x_A) \\ \phi_b(x_1) & \phi_b(x_2) & \cdots & \phi_b(x_A) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_k(x_1) & \phi_k(x_2) & \cdots & \phi_k(x_A) \end{vmatrix}$$

- A single-particle state is defined as $a = (n_a, l_a, j_a, m_a)$
- In second quantized form, the basis state is expressed as

$$|M_i\rangle = c^\dagger_{a_{i,1}} c^\dagger_{a_{i,2}} \cdots c^\dagger_{a_{i,A}} |-\rangle$$

M-scheme basis state

$$\left|M\right\rangle = c^{\dagger}_{j_1 m_1} c^{\dagger}_{j_2 m_2} \ldots c^{\dagger}_{j_n m_n} \left|-\right\rangle$$

$$M = m_1 + m_2 + \ldots + m_n \qquad \Pi = (-1)^{l_1 + l_2 + \ldots + l_n}$$

- Simple to be treated
- It has good eigenvalues of M angular momentum and parity, but not those of J^2.
- The symmetry of J^2 is automatically restored by diagonalizing the Hamiltonian matrix

J-scheme basis state

- an eigenstate of J^2
- The number of the basis states are reduced by $O\left(10^{-2}\right)$ at most, but the operations are complicated
- $D^{(J)}_{J} = D^{(M)}_{M=J} - D^{(M)}_{M=J+1}$

2. KSHELL code

筑波大学
計算科学研究センター
Center for Computational Sciences

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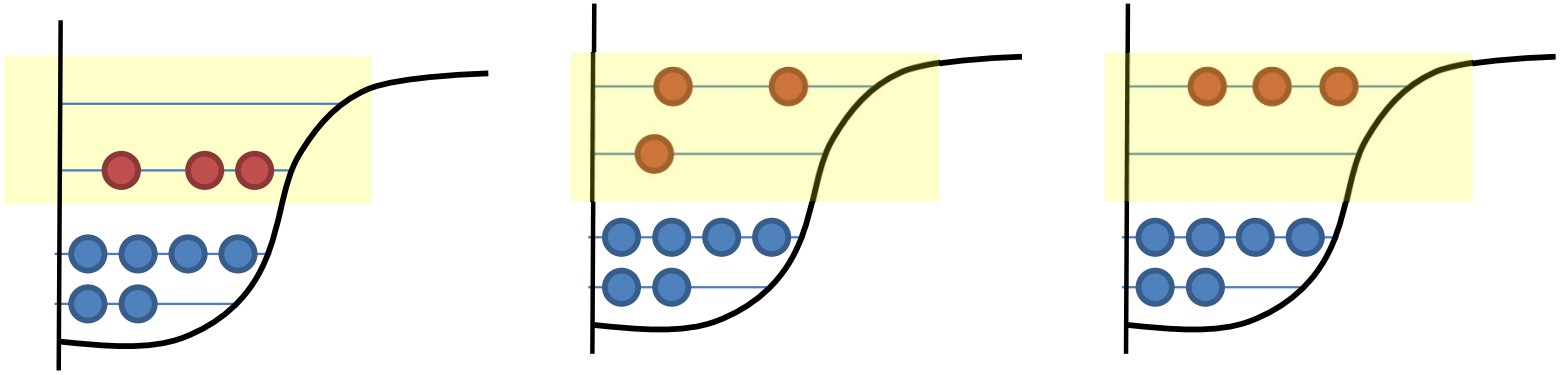
Large-scale shell model calculation (LSSM)

- Consider the inert core and active particles in the valence shells (model space)
- Nuclear wave function is expressed as a linear combination of M-scheme basis states



$$|\Psi\rangle = v_1|m_1\rangle + v_2|m_2\rangle + v_3|m_3\rangle + \cdots$$

$$|\Psi\rangle = \sum_m v_m |m\rangle$$

Schrodinger's equation
... Eigenvalue problem of huge sparse matrix

$$\sum_k \langle m|H|k\rangle v_k = E v_m$$

Solved to obtain low-lying eigenstates

M-scheme basis state on computers

Let us consider ^{42}Ca with ^{40}Ca inert core

2 active neutrons in the $f_{7/2}$ orbit

$$|\phi\rangle = c^{\dagger}_{0f_{7/2},-5/2} c^{\dagger}_{0f_{7/2},-1/2} |-\rangle$$

m = -7/2, -5/2, -3/2 -1/2, 1/2, 3/2, 5/2, 7/2

$8 \times 7 \,/\, 2 = 28$ states

bit representation for a computer

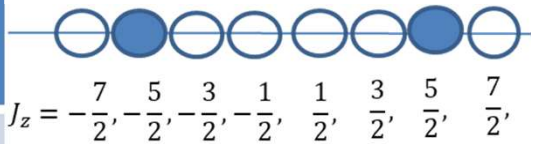
$$|\Psi\rangle = \sum_{i=1}^{28} v_i |M_i\rangle$$

01010000 (bit)

$\Rightarrow$ 10 (decimal)

Configurations of ^{42}Ca, 2 particles in f7/2

	M-scheme dimension	Configurations	*J* components
M=6	1	00000011	J= 6
M=5	1	00000101	J= 6
M=4	2	00001001, 00001010	J= 4,6
M=3	2	00010001, 00001100	J= 4,6
M=2	3	00100001, 00010010, 00010100	J= 2,4,6
M=1	3	01000001, 00100010, 00011000	J= 2,4,6
M=0	4	10000001, 01000010, 00100100, 00011000	J=0,2,4,6
M=-1	3		J= 2,4,6
…	…		…
sum	28		



This space contains all information.

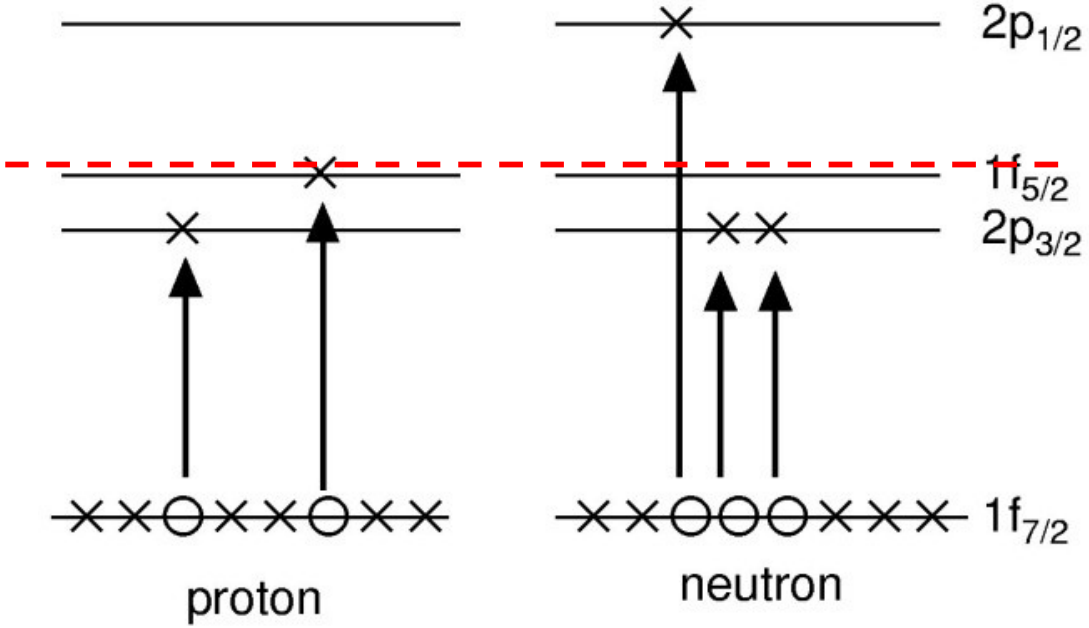
J-scheme dimension

J=0 1
J=2 1
J=4 1
J=6 1

Thanks to $[H, J^2] = 0$, the $M = 0$ subspace is enough to obtain all eigenstate.
In this case, M-scheme dimension is 4.

M-scheme dimension

- ^{56}Ni in pf shell (8 protons 8 neutrons in $1f_{7/2}, 1f_{5/2}, 2p_{3/2}, 2p_{1/2}$)



- How many basis states are required?

$$D = \quad {}_{N_{sps}}C_Z \times_{N_{sps}} C_N$$

For example, ^{56}Ni in pf-shell, ^{40}Ca core

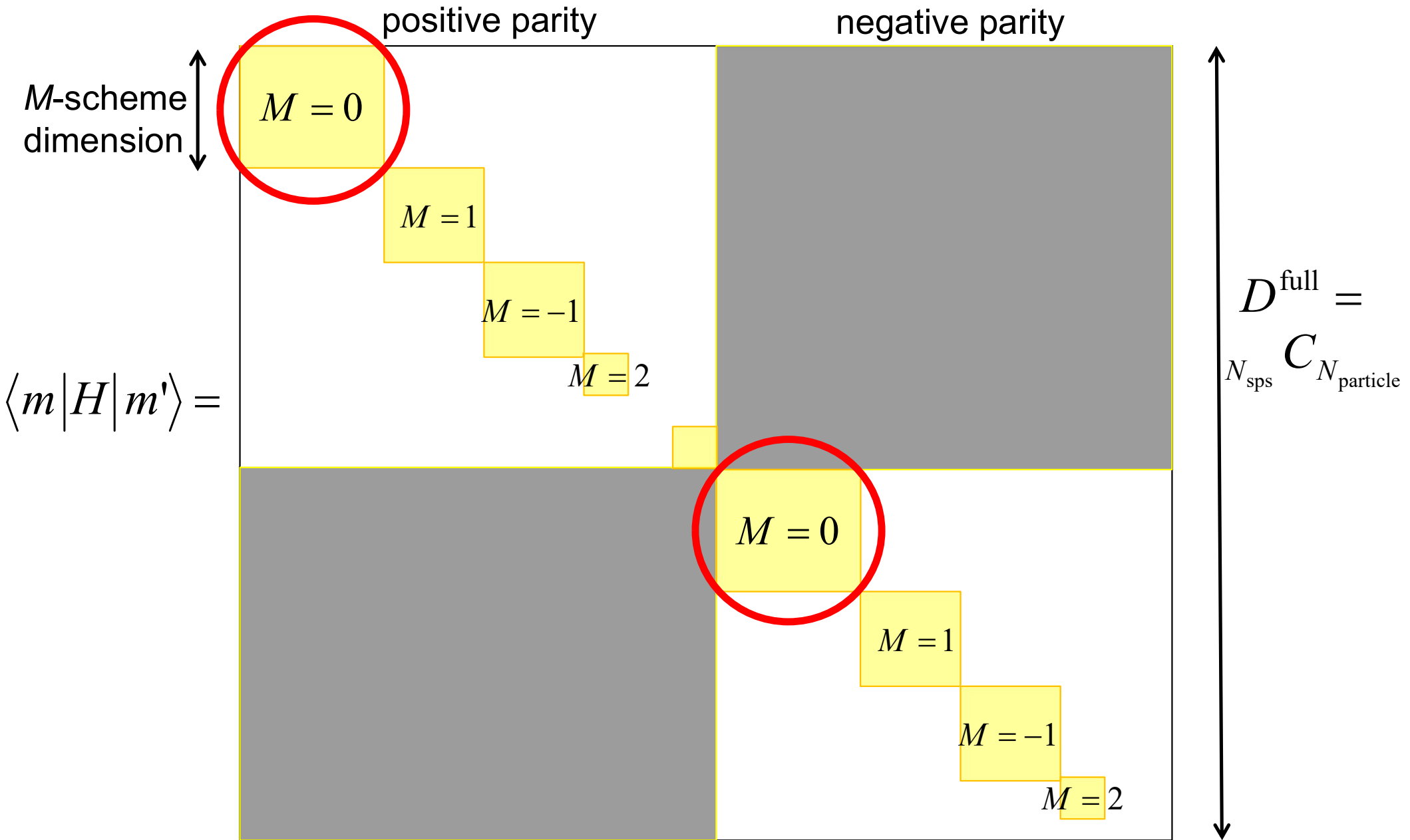
$$D = \quad {}_{20}C_8 \times_{20} C_8 = 1.5 \times 10^{10}$$

In practice, the dimension of M=0 subspace is $D_M = 1.1 \times 10^9$.

M-scheme Hamiltonian matrix element

$i = (n_i, l_i, j_i, m_i)$

$\left| M^{\pi}(i,j,...) \right\rangle = c_i^{\dagger} c_j^{\dagger} ... \left| - \right\rangle$ is an eigenstate of *Jz* (*M*) and parity



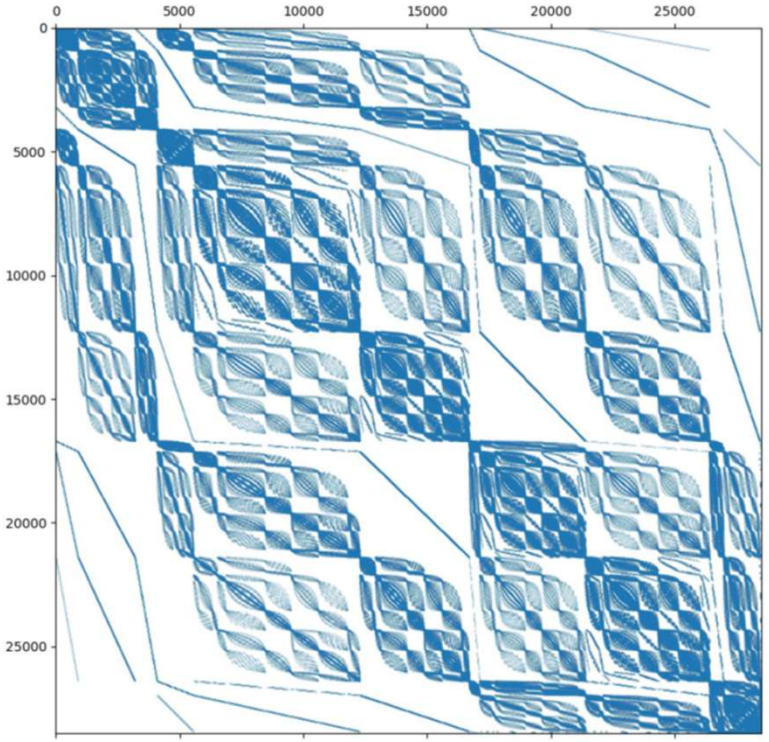
Hamiltonian matrix in the LSSM

⇒ Real symmetric sparse matrix

Nuclide	Space	Basis dim.	Sparsity	Storage (GB)
^{28}Si	sd	9.4×10^4	6×10^{-3}	0.2
^{52}Fe	pf	1.1×10^8	1×10^{-5}	720
^{56}Ni	pf	1.1×10^9	2×10^{-6}	9600

C.W. Johnson *et al.*, CPC 2013

Non-zero matrix elements of
^{24}Mg M=0 space in sd-shell (28,503 dim.)



- Hamiltonian matrix is very sparse because it consists of one- and two-body interactions.
- The Lanczos algorithm is quite efficient to obtain low-lying states.
- In the KSHELL code, the matrix elements of the many-body Hamiltonian is generated on-the-fly every matrix-vector product to suppress the memory usage.

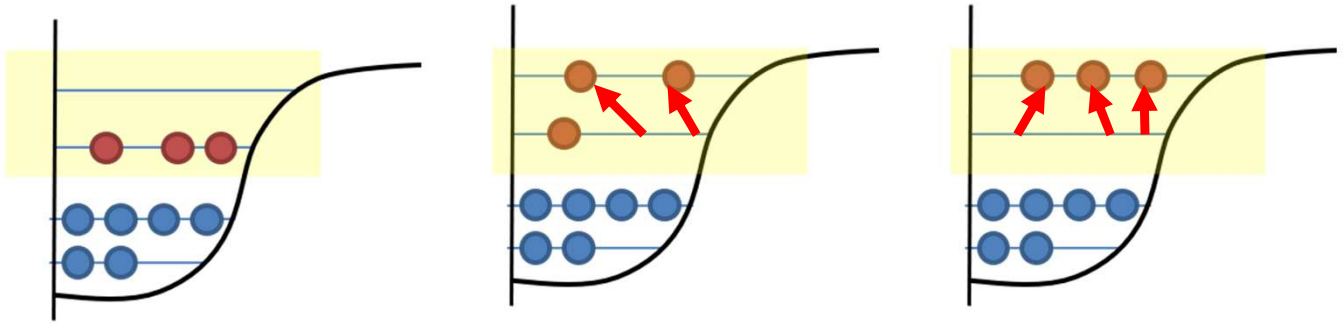
Why is the M-scheme Hamiltonian matrix sparse?

Sparsity of *M*-scheme Hamiltonian matrix

Shell-model Hamiltonian is a two-body interaction

$$H = \sum_a \varepsilon_a a_a^\dagger a_a + \frac{1}{4}\sum_{abcd} V_{abcd} a_a^\dagger a_b^\dagger a_d a_c$$

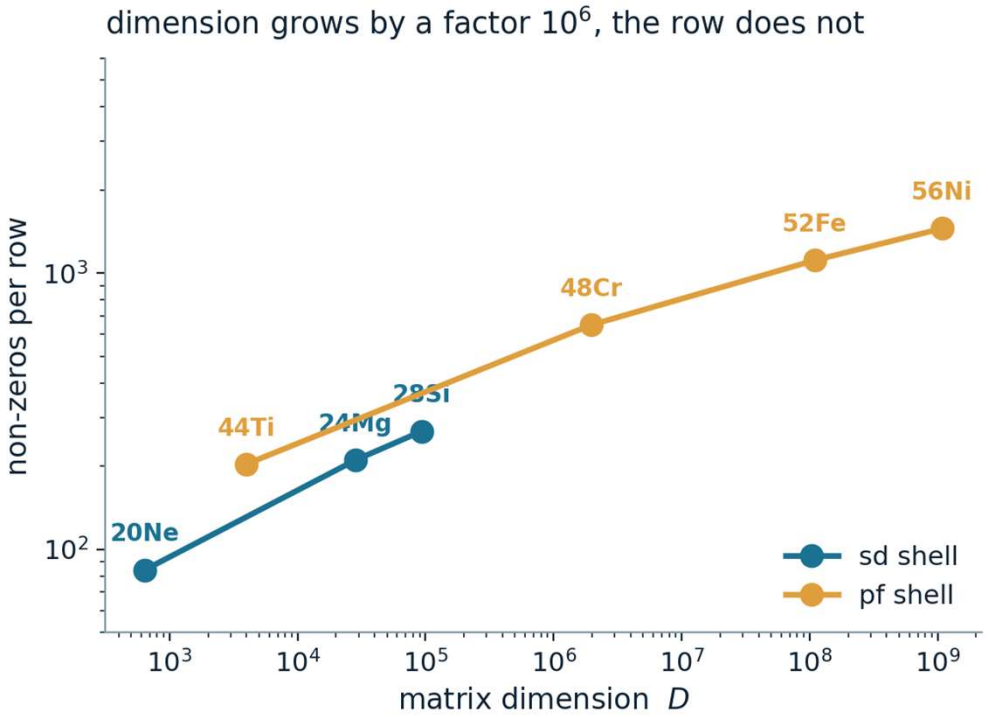
$\langle M|H|M'\rangle \neq 0$ only if $|\mathrm{M}\rangle$ and $|M'\rangle$ differ in at most 2 states

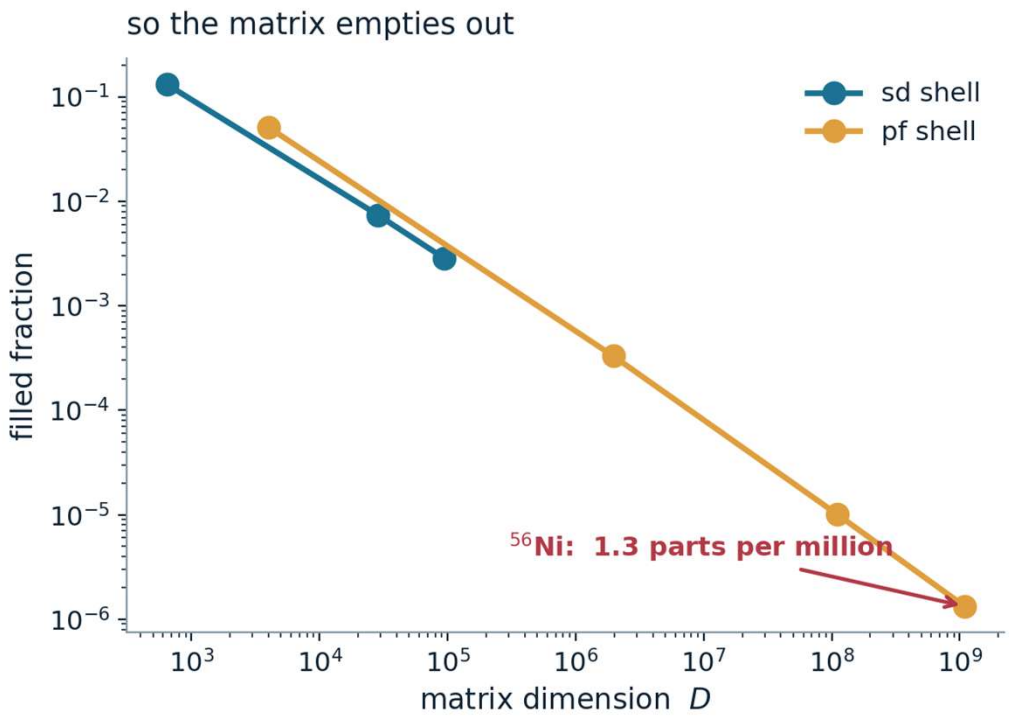


$$|\Psi\rangle = v_1|m_1\rangle + v_2|m_2\rangle + v_3|m_3\rangle + \cdots$$

$\langle m_1|H|m_2\rangle \neq 0,$ but $\langle m_1|H|m_3\rangle = 0$

The row barely grows; the matrix explodes





× 1,700,000
growth in dimension
from ^{20}Ne to ^{56}Ni

× 17
growth in non-zeros
per row over the same range

1.3 ppm
filled fraction
for ^{56}Ni

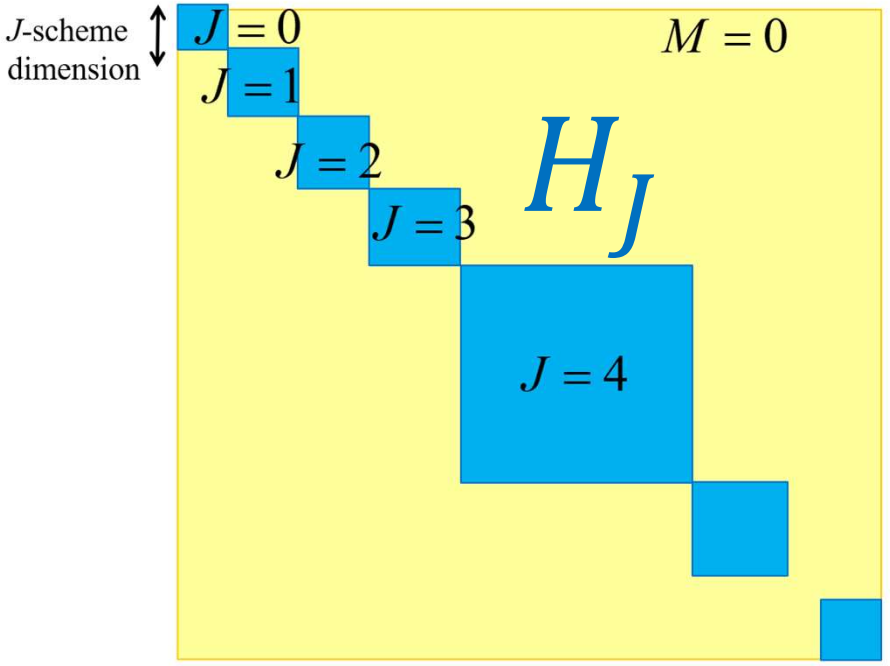
M-scheme vs. *J*-scheme

$$\left|M^{\pi}(i,j,\ldots)\right\rangle = c_i^{\dagger}c_j^{\dagger}\ldots\left|-\right\rangle \quad \text{vs.} \quad \left|J^{\pi},M,\alpha\right\rangle$$

$$U^{\dagger}H_M U = H_J$$

$$D_M^{(M)} = \sum_{J=M}^{J_{max}} D_J^{(J)}$$

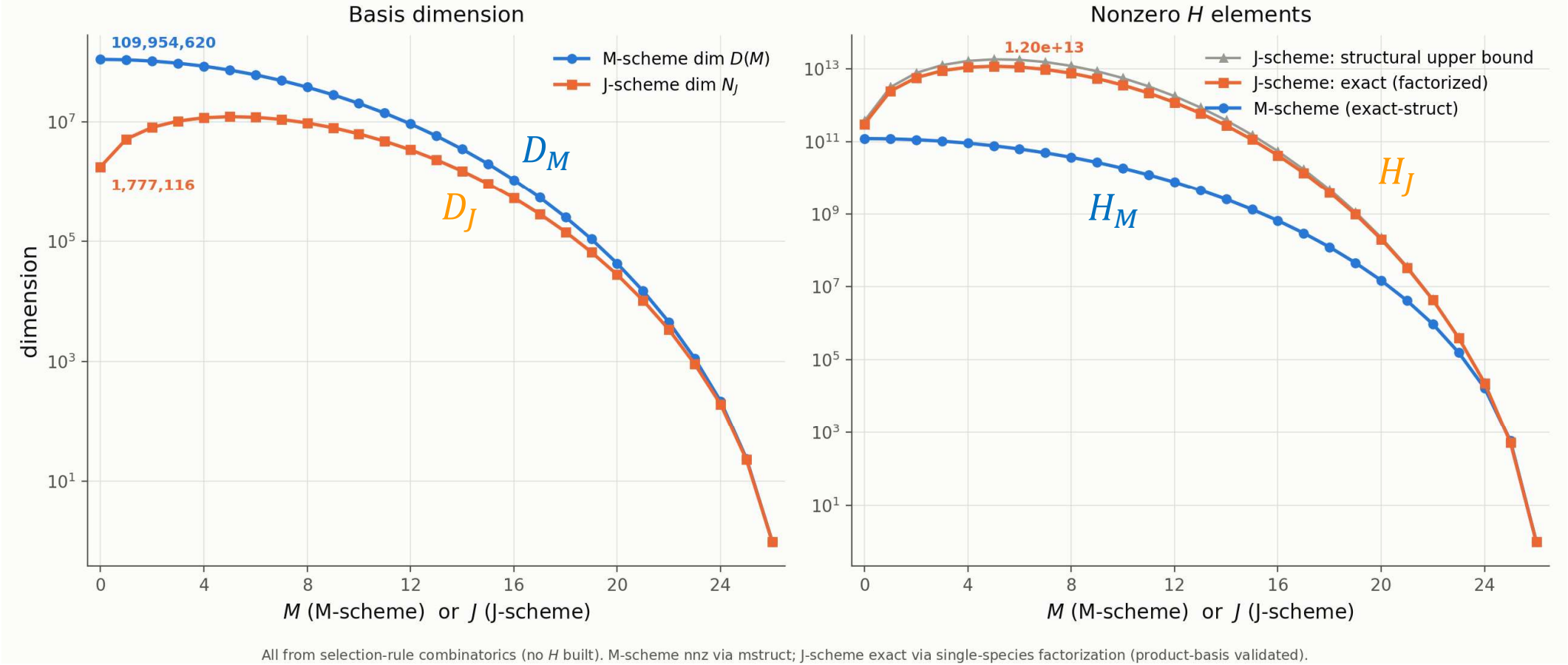
$H_{M=0}$



"Unitary transformation" transforms the M-scheme Hamiltonian to J-scheme Hamltonian.

M-scheme vs. *J*-scheme

^{52}Fe full *pf* shell dimension & nonzero *H*



The *J*-scheme dimension is one order of magnitude smaller than the M-scheme dimension, but the number of nonzero matrix elements is much larger.

Note: Many shell-model codes do not store the Hamiltonian matrix elements explicitly, instead, they factorize it into proton and neutron matrix elements.

Why M and not good J?

What you give up

- States of all J are mixed together.
- The dimension is larger, by roughly 2J+1.
- You must compute $\langle J^2 \rangle$ afterwards to label each state.

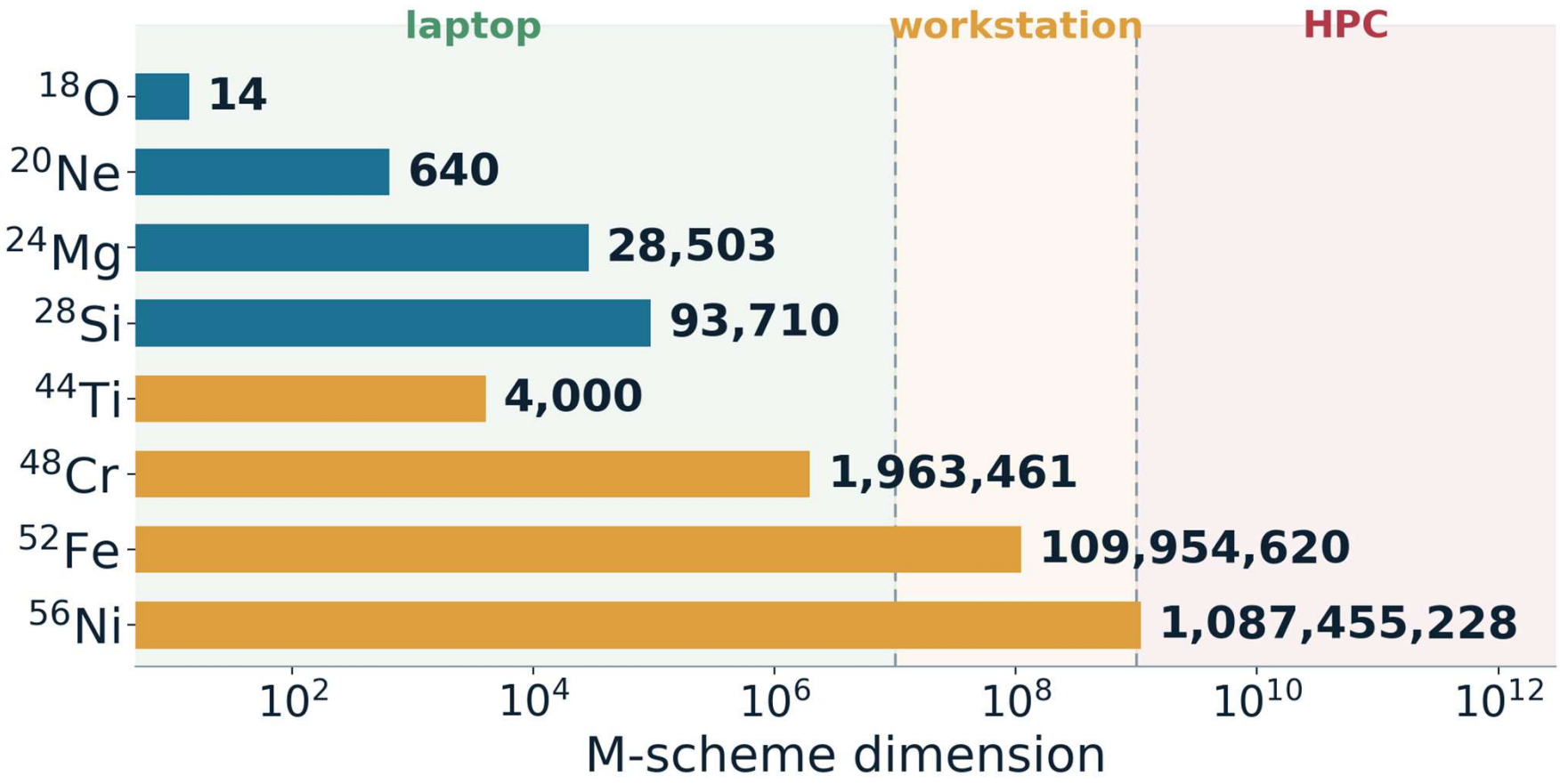
What you gain

- Trivial basis states and trivial matrix elements.
- A far sparser matrix.
- The whole spectrum, all J at once, from one run.

The two schemes are the same physics in different bases. The choice is decided by the third row on the right: what limits a large run is the number of stored non-zeros, not the nominal dimension.

How big does this get?

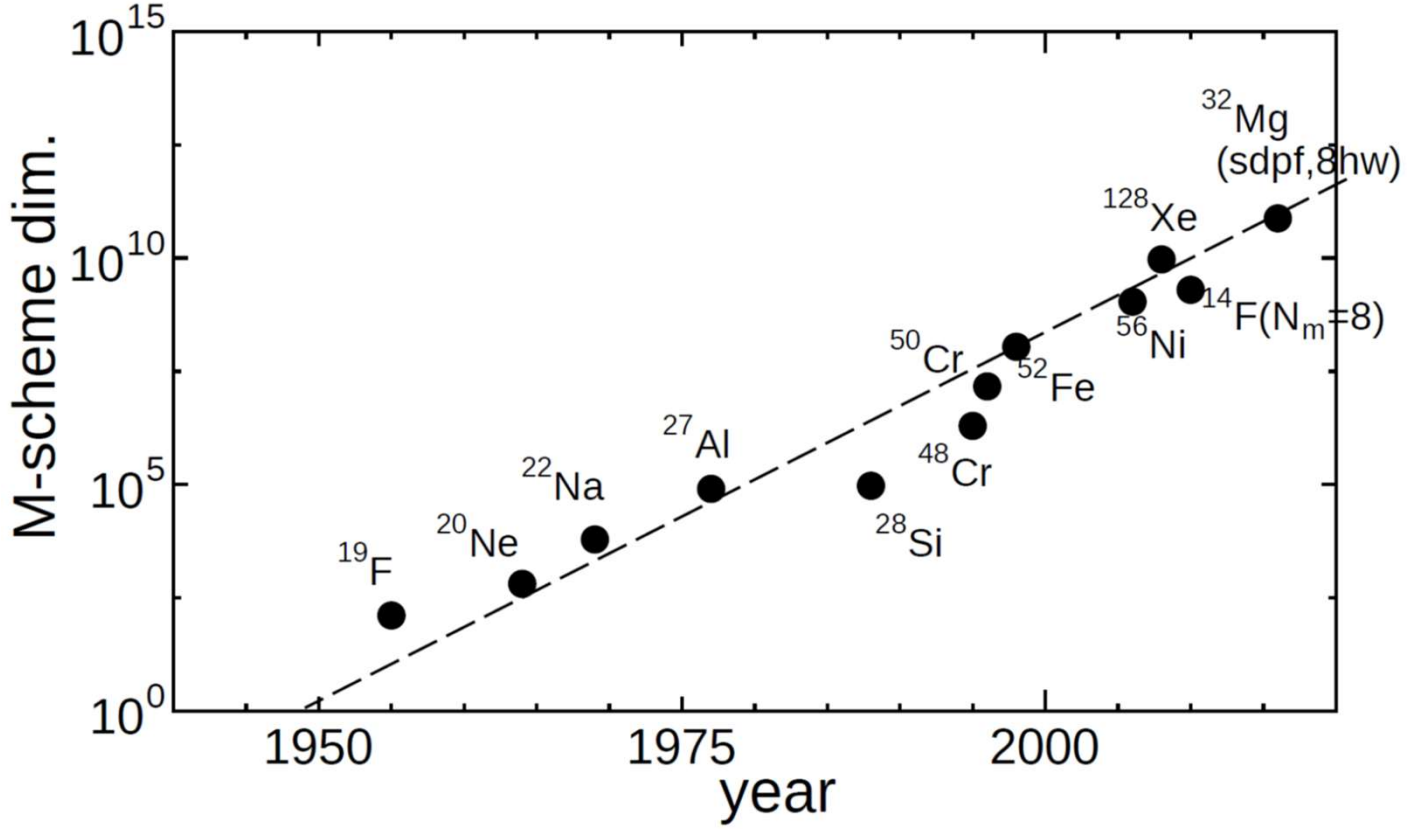
$$D_{M=0} = \sum_{M} D^{\pi}{}_{M} D^{\nu}{}_{-M}$$



sd shell in teal, pf shell in amber; the zones are rough guides

Progress in the large-scale shell-model calculations
M-scheme dimension vs. year

Computation cost is almost proportional to the *M*-scheme dimension

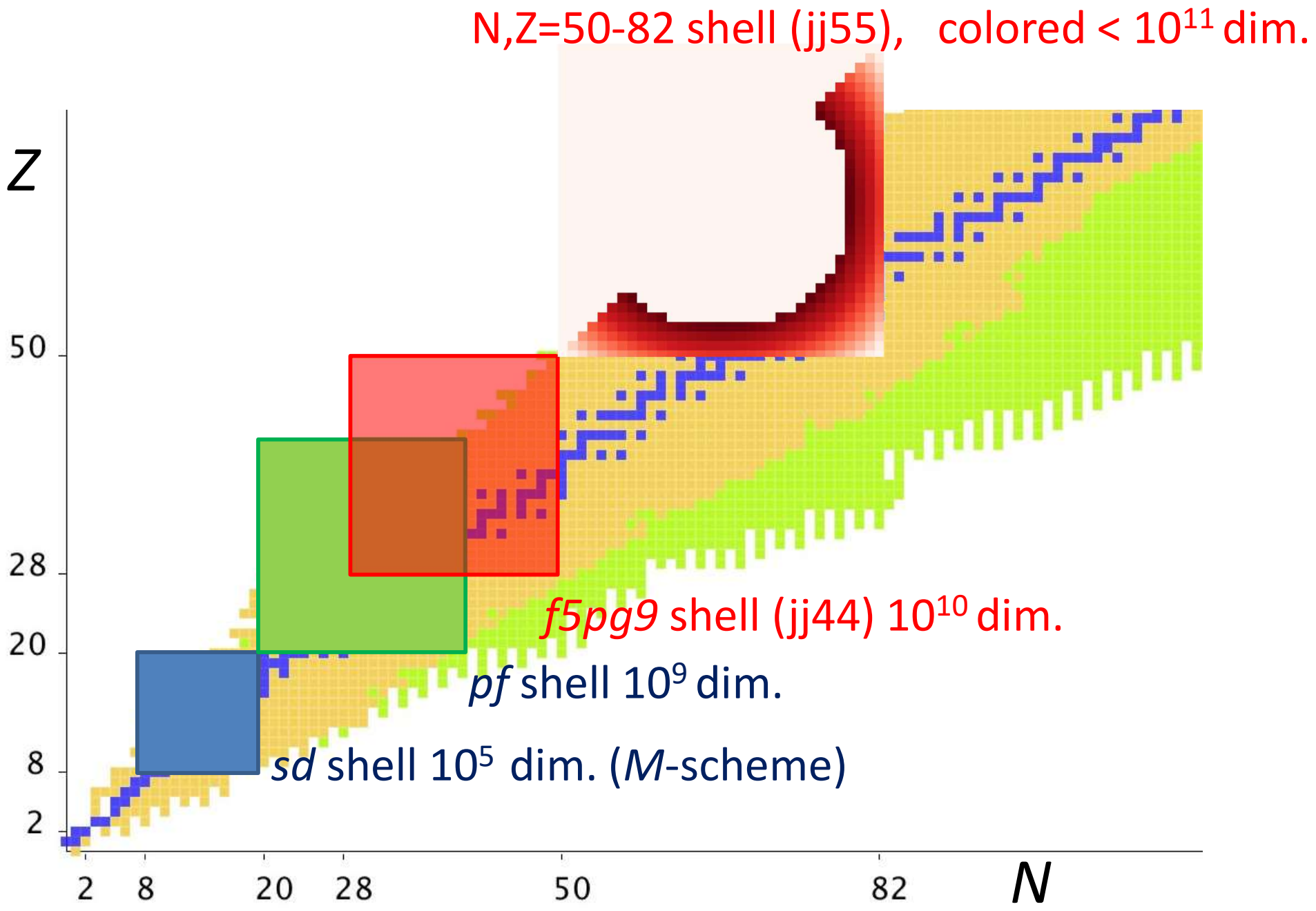


1950 Mayer & Jensen, single-particle SM

Current limit : ~10^{11} M-scheme dim.

⇒ 800 GB / a vector

Applicable region of shell-model calc.



shell-model code “KSHELL”

- *M*-scheme shell-model code

Ref. N. Shimizu, T. Mizusaki, T. Utsuno, and Y. Tsunoda,

Comp. Phys. Comm. 244, 372 (2019)
https://doi.org/10.1016/j.cpc.2019.06.011

- MPI + OpenMP hybrid parallel, also useful for a PC
- Thick-restart block Lanczos method

- Awkward in no-core shell model calc., 3-body force is out of focus

Benchmark

^{46}Ti, pf-shell, KB3 interaction $D_M = 56{,}349$

Elapsed time to obtain 10 lowest *J*=4 states

(J=4, T=4 10 lowest states for OXBASH)

@ Xeon E5-2680v2 2.80GHz, 20 CPU cores

- OXBASH 227.3 sec.
- KSHELL 117.5 sec. 1 thread, block size=1
- KSHELL 8.6 sec. 20 threads, block size=1
- KSHELL 3.5 sec. 20 threads, block size=6

"Thick-restart block Lanczos method"

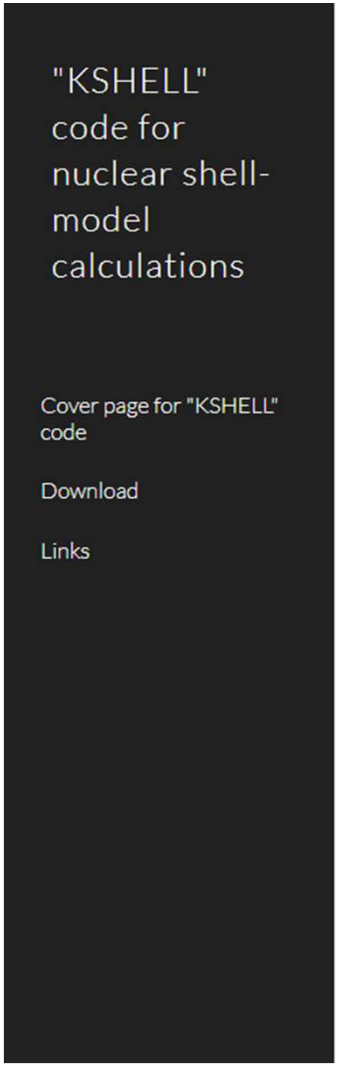
"The computer code OXBASH", BA Brown, A Etchegoyen, WDM Rae, NS Godwin - MSU-NSCL Report, 1988

KSHELL how to

https://sites.google.com/alumni.tsukuba.ac.jp/kshell-nuclear/d

Ref. N. Shimizu *et al.,* Comp. Phys. Comm. 244, 372 (2019)

https://doi.org/10.1016/j.cpc.2019.06.011



Download

Nuclear shell-model code "KSHELL"

It is provided as it is and has no warranty.

Any comments, bug reports, suggestions, and collaborations are welcome.

- KSHELL ver.4
- ~~KSHELL ver.3.1~~
- KSHELL ver. 2
- KSHELL ver.1.2g
- 日本語マニュアル(Manual in Japanese) 2022/06/08
- KSHELL Manual in English, 2022/06/08

Download here.

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Contact: shimizu_at_nucl.ph.tsukuba.ac.jp

NOTE: When any publication is achieved using this software, one of the following papers should be cited

N. Shimizu, T. Mizusaki, T. Utsuno, and Y. Tsunoda, Comp. Phys. Comm. 244, 372 (2019)

https://doi.org/10.1016/j.cpc.2019.06.011

N. Shimizu, "Nuclear shell-model code for massive parallel computation, KSHELL", arXiv:1310.5431 [nucl-th] (2013)

Preparation

https://sites.google.com/alumni.tsukuba.ac.jp/kshell-nuclear/d

Linux:

- Install gfortran, BLAS, LAPACK, and python (or Intel Fortran + MKL)
  (Ubuntu: apt-get install python gfortran liblapack-dev libblas-dev)

- tar xvzf kshell-cpc.tar.gz
  cd kshell-xxxxx/src
  make
  cd ../test
  ../bin/kshell_ui.py

- MS-Windows : install “Windows subsystem for Linux” and gfortran

- Mac OS

How to install

tar xvzf kshell-xxxx.tar.gz

cd kshell/src

“modify Makefile to match your system”

make

alias kshell_ui.py=(installed dir)/kshell-cpc/bin/kshell_ui.py

That is all, if you are lucky.

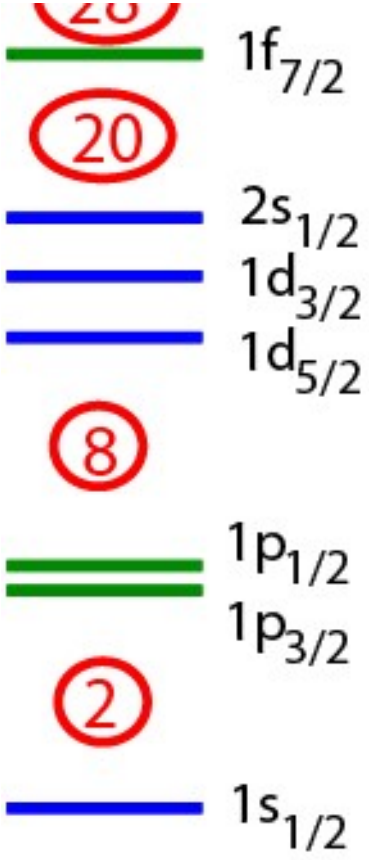
How to run

1. kshell_ui.py

... answer questions to generate a shell script

2. run the generated script

Example: ^{28}Si with USD interaction
6 protons, 6 neutrons with ^{16}O core
model space : sd-shell $(0d_{5/2}, 1s_{1/2}, 0d_{3/2})$
93,710 *M*-scheme dim.



Demonstration

- ^{28}Si in sd-shell

Count shell-model dimensions

- count M-scheme and J-scheme dimensions

kshell/bin/count_dim.exe w.snt Si28_w_p.ptn

```
 Z=  6 N=  6 parity  1


      2*M        M-scheme dim.          J-scheme dim.
dim.    28                    1                     1   1.00x10^ 0  1.00x10^ 0
dim.    26                   18                    17   1.80x10^ 1  1.70x10^ 1
dim.    24                  123                   105   1.23x10^ 2  1.05x10^ 2
dim.    22                  472                   349   4.72x10^ 2  3.49x10^ 2
dim.    20                 1439                   967   1.44x10^ 3  9.67x10^ 2
dim.    18                 3560                  2121   3.56x10^ 3  2.12x10^ 3
dim.    16                 7619                  4059   7.62x10^ 3  4.06x10^ 3
dim.    14                14310                  6691   1.43x10^ 4  6.69x10^ 3
dim.    12                24210                  9900   2.42x10^ 4  9.90x10^ 3
dim.    10                37086                 12876   3.71x10^ 4  1.29x10^ 4
dim.     8                52175                 15089   5.22x10^ 4  1.51x10^ 4
dim.     6                67560                 15385   6.76x10^ 4  1.54x10^ 4
dim.     4                81122                 13562   8.11x10^ 4  1.36x10^ 4
dim.     2                90338                  9216   9.03x10^ 4  9.22x10^ 3
dim.     0                93710                  3372   9.37x10^ 4  3.37x10^ 3

Estimated memory size for single-node mode :         0.002GB
```

N.B. $D_J = D_{M=J} - D_{M=J+1}$

Comput. time is almost proportional to D_M

output : summary_Si28_w.txt

Energy relative to ^{16}O core

Excitation energy

Experiment (Nudat2)

Energy levels

	N	J	prty	N_Jp	T	E(MeV)	Ex(MeV)
0^+_1	1	0	+	1	0	-135.938	0.000
2^+_1	2	2	+	1	0	-133.950	1.987
4^+_1	3	4	+	1	0	-131.279	4.659
0^+_2	4	0	+	2	0	-130.927	5.011
3^+_1	5	3	+	1	0	-129.771	6.167
4^+_2	6	4	+	2	0	-128.901	7.037
0^+_3	7	0	+	3	0	-128.699	7.239
2^+_2	8	2	+	2	0	-128.415	7.522
2^+_3	9	2	+	3	0	-128.032	7.906
1^+_1	10	1	+	1	0	-127.998	7.940

E_{level} (keV)	Jπ
0.0	0+
1779.030 11	2+
4617.86 4	4+
4979.92 8	0+
6276.20 7	3+
6690.74 15	0+
6878.79 8	3-
6887.65 10	4+
7380.59 9	2+
7416.26 9	2+
7799.01 9	3+

B(E2; 2+

B(E2) (> -0.0 W.u.) mass = 28 1 W.u. = 5
e^2

J_i	Ex_i	J_f	Ex_f	dE	B(E	
2+(1)	1.988	0+(1)	0.000	1.987	8	80.1)
4+(1)	4.659	2+(1)	1.988	2.671	11	40.8)
0+(2)	5.011	2+(1)	1.988	3.024	6	2.7)

output : log_Si28_w_m0p.txt

```
 total # of partitions                1679   = 10** 3.23
 total m-scheme dimension            93710   = 10** 4.97
  max. # dim. / a partition                     1156
  max local dim. / proc, average                   93710                    93710

 Memory for one global Lanczos vector:      0.000 GB
 Memory / process is:      0.000 GB x      10 =       0.003 GB
 Total Memory for Lanczos vectors:      0.003 GB
 ...
 ...
 ...
 ------------------------------------------------------------
    1  <H>:  -135.93772  <JJ>:      0.00000  J:  0/2  prty  1
                         <TT>:      0.00000  T:  0/2
  <p Nj>  0.673  4.623  0.704
  <n Nj>  0.673  4.623  0.704
 ------------------------------------------------------------
    2  <H>:  -133.95030  <JJ>:      6.00000  J:  4/2  prty  1
                         <TT>:      0.00000  T:  0/2
  <p Nj>  0.771  4.252  0.977
  <n Nj>  0.771  4.252  0.977
    <Qp>    10.375   <Qn>    10.375   <eQ>     20.751
 ------------------------------------------------------------
 ....
```

Energy

0^+_1

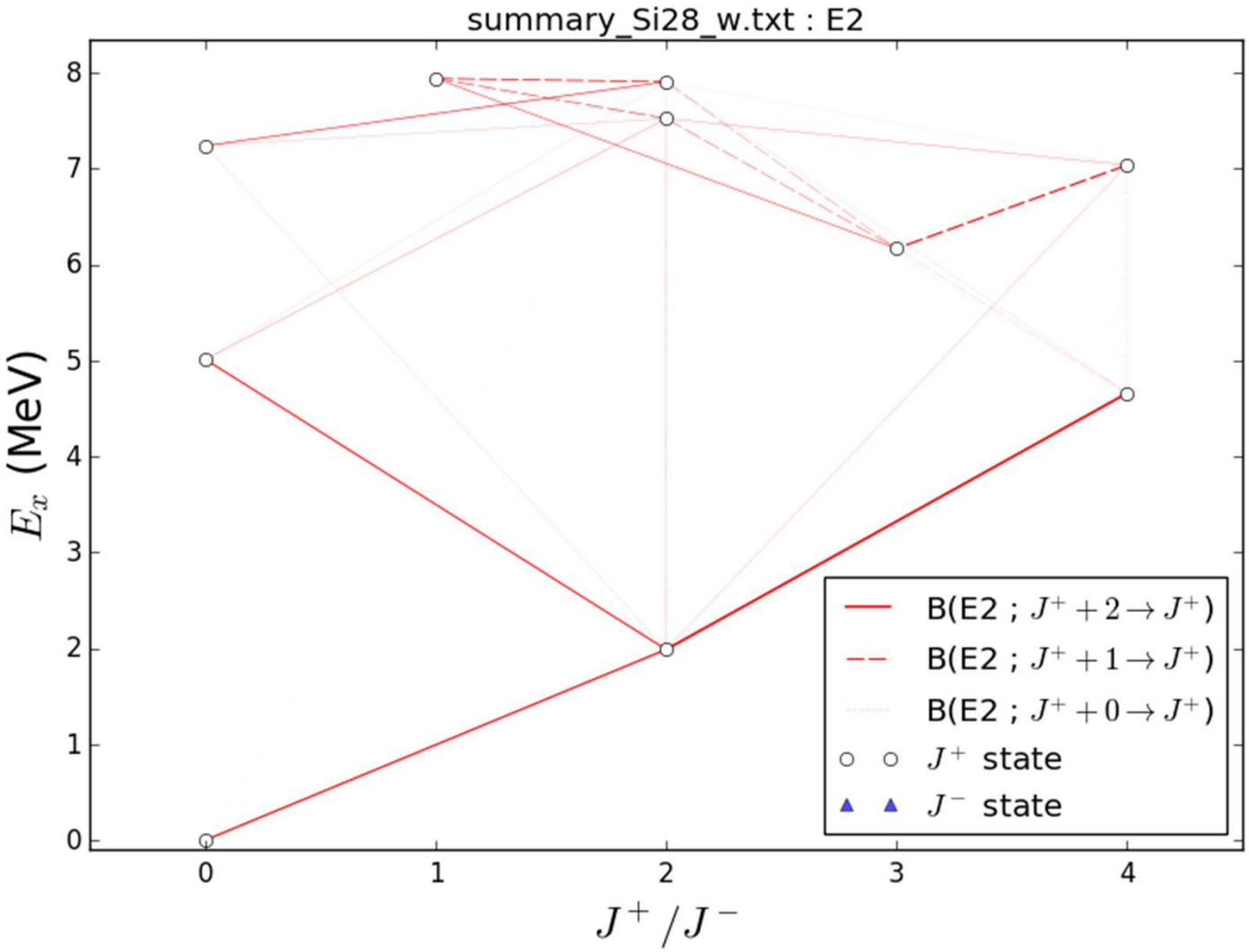
2^+_1

Occupation number of each orbit ($d_{3/2}, d_{5/2}, s_{1/2}$)

Quadrupole moment

E2 map

kshell/bin/map_transit.py summary_Si28_w.txt

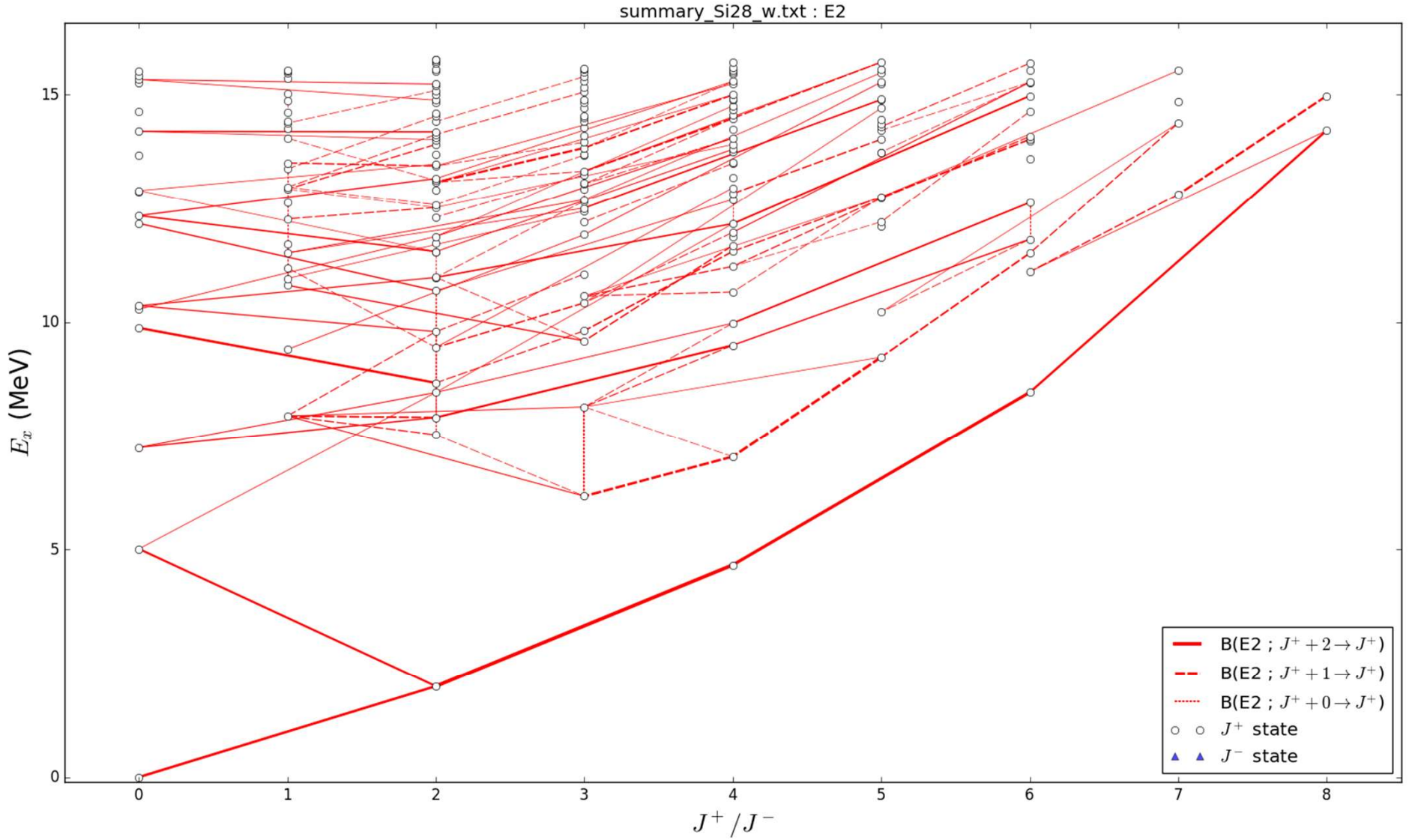


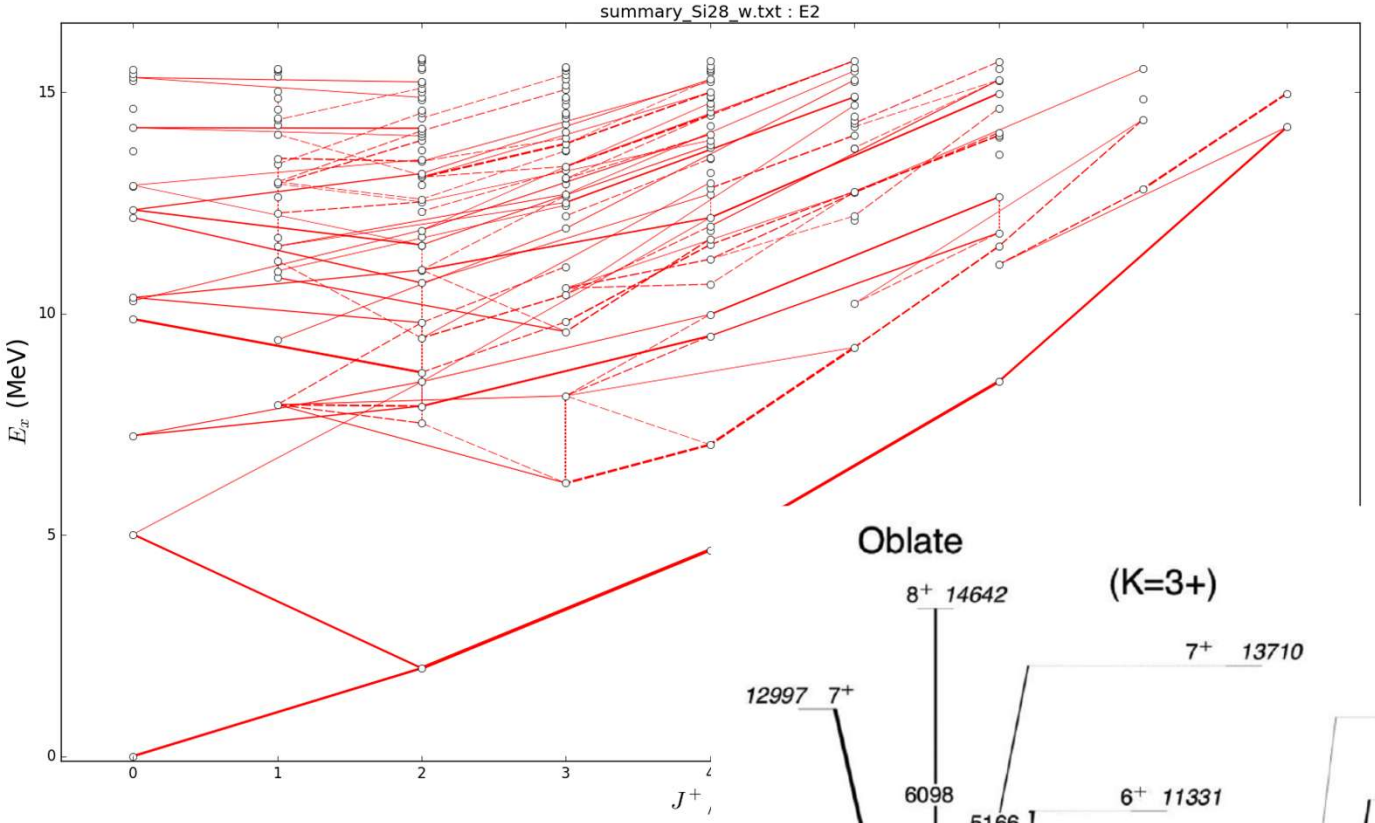
x-axis: J
y-axis : Ex. (MeV)

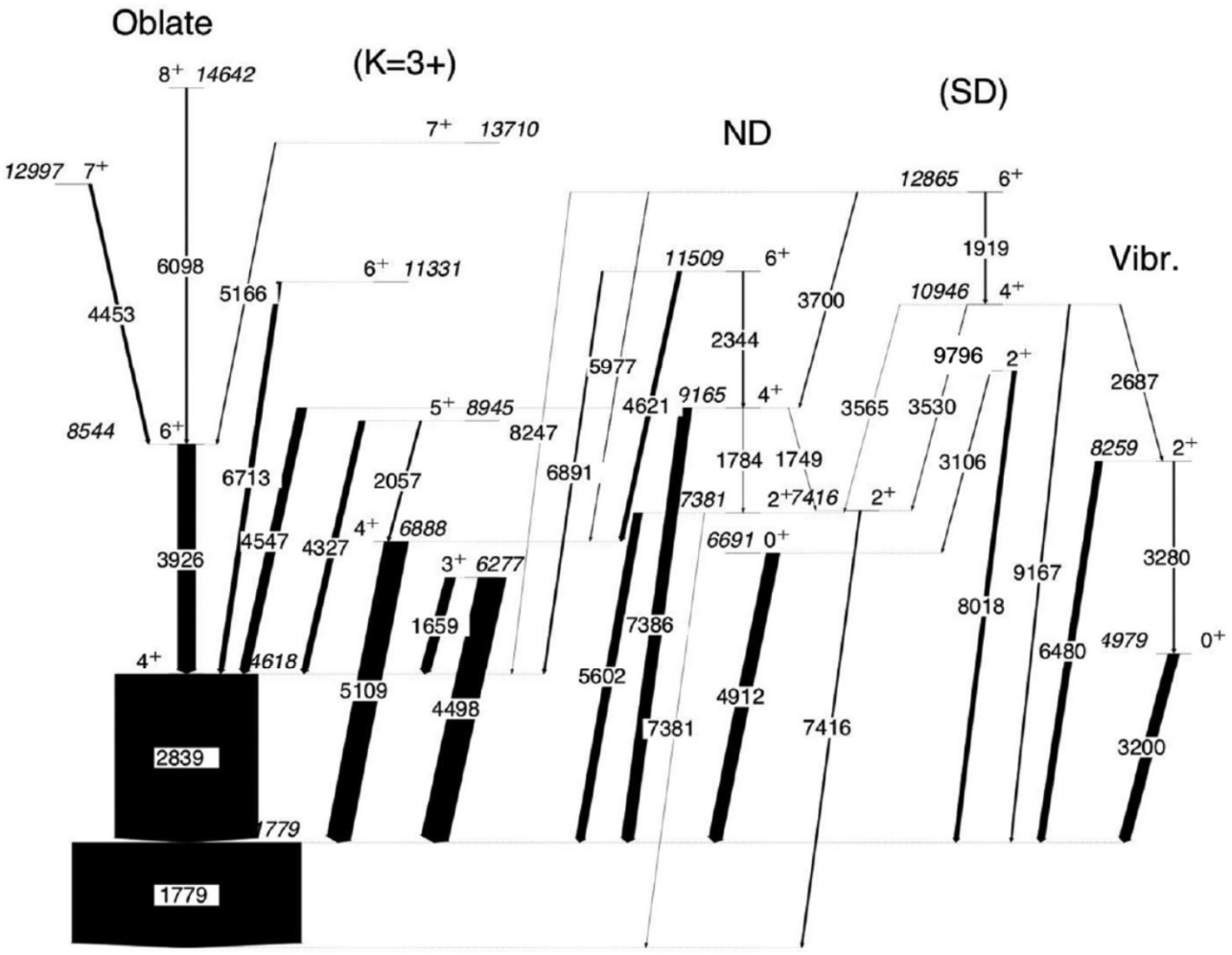
The width of the connected red line is proportional to the B(E2) values.

This figure would help you to find band structures.

E2 map: ^{28}Si, 200 states







D. G. Jenkins et al., Phys. Rev. C 86, 064308 (2012).

interaction and model space

kshell/snt

- w.snt ... Wildenthal's USD interaction (for sd shell)
- gxpf1a.snt ... GXPF1A interaction (for pf shell)
- jun45.snt ... JUN45 interaction (for f5pg9 shell Z,N=28-50)
- sdpf-mu.snt … SDPF-MU interaction (for sdpf shell)
- ysox.snt … YSOX interaction (for p-sd shell)

"snt" file defines model space and its interaction.

You can make your original snt file by yourself.

Some famous interaction files are equipped.

Interaction files in NuShellx@MSU package can be transformed to snt format with "nushell2snt.py"

w.snt (USD interaction)

```
! Wildenthal's USD interaction for sd-shell
! B. A. Brown and B. H. Wildenthal, Annu. Rev. Nucl. Part. Sci. 38, 29 (1988
! proton-orbit, neutron-orbit, proton core, neutron core
3 3 8 8
! n  l j  tz
! model space
    #     n,   l,   2j   2tz
   1       0    2    3   -1     !  1 = p 0d_3/2
   2       0    2    5   -1     !  2 = p 0d_5/2
   3       1    0    1   -1     !  3 = p 1s_1/2
   4       0    2    3    1     !  4 = n 0d_3/2
   5       0    2    5    1     !  5 = n 0d_5/2
   6       1    0    1    1     !  6 = n 1s_1/2
! one-body interaction
! number of lines, method1
 6   0
   1   1       1.64658
   2   2      -3.94780
   3   3      -3.16354
   4   4       1.64658
   5   5      -3.94780
   6   6      -3.16354
```

Model space
(*sd* shell)

Single-particle energy of each orbit
(one-body interaction)

$\mathrm{SPE}(d_{5/2}) = -3.9478$ MeV

w.snt (USD interaction) cont'd

Two-body matrix elements (TBME)

```
! two-body interaction (TBME)
! # of lines, method2 A mass dependence factor
158   1  18  -0.30000
!  i    j    k    l     J     <i,j| V | k,l>_J
   1    1    1    1     0      -2.18450
   1    1    1    1     2      -0.06650
   1    1    1    2     2       0.61490
   1    1    1    3     2       0.51540
   1    1    2    2     0      -3.18560
   1    1    2    2     2      -1.62210
   1    1    2    3     2      -0.40410
   1    1    3    3     0      -1.08350
   1    2    1    2     1       1.03340
   1    2    1    2     2      -0.32480
   1    2    1    2     3       0.58940
   1    2    1    2     4      -1.44970
...
   5    5    5    5     0      -2.81970
... 158 lines continued
```

$\mathrm{SPE}(d_{5/2}) =$ -3.9478 MeV

$$\langle \nu 0d_{5/2}, \nu 0d_{5/2} | V | \nu 0d_{5/2}, \nu 0d_{5/2} \rangle_{J=0}$$
$$= -2.8197 \text{ MeV}$$

Shell-model energy of ^{18}O in d5/2 orbit is

$$-3.9478 * 2 - 2.8197 = -10.715 \text{ MeV}$$

Shell-model energy in full *sd* shell is

$$E = -12.171 \text{ MeV}$$

```
--- input parameter ---
 beta_cm = 0.d0                 # Lawson beta (MeV)
 eff_charge = 1.5, 0.5,         # effective charge
 fn_int = "w.snt"               # snt file
 gl = 1.0, 0.0,                 # g-factor for orbital
 gs = 3.91, -2.678,             # g-factor for spin
 hw_type = 2                    # Harmonic oscillator parameter
 max_lanc_vec = 200             # iteration for Lanczos
 maxiter = 300                  # iteration for TR-Lanczos
 mode_lv_hdd = 1                # Lanczos vector save in HDD or not
 n_restart_vec = 10             # restart vec for TR-Lanczos

modify parameter?
 (e.g.  maxiter = 300 for parameter change
        <CR>          for no more modification ) :
```

n_block = 4 … block size for block Lanczos method for acceleration

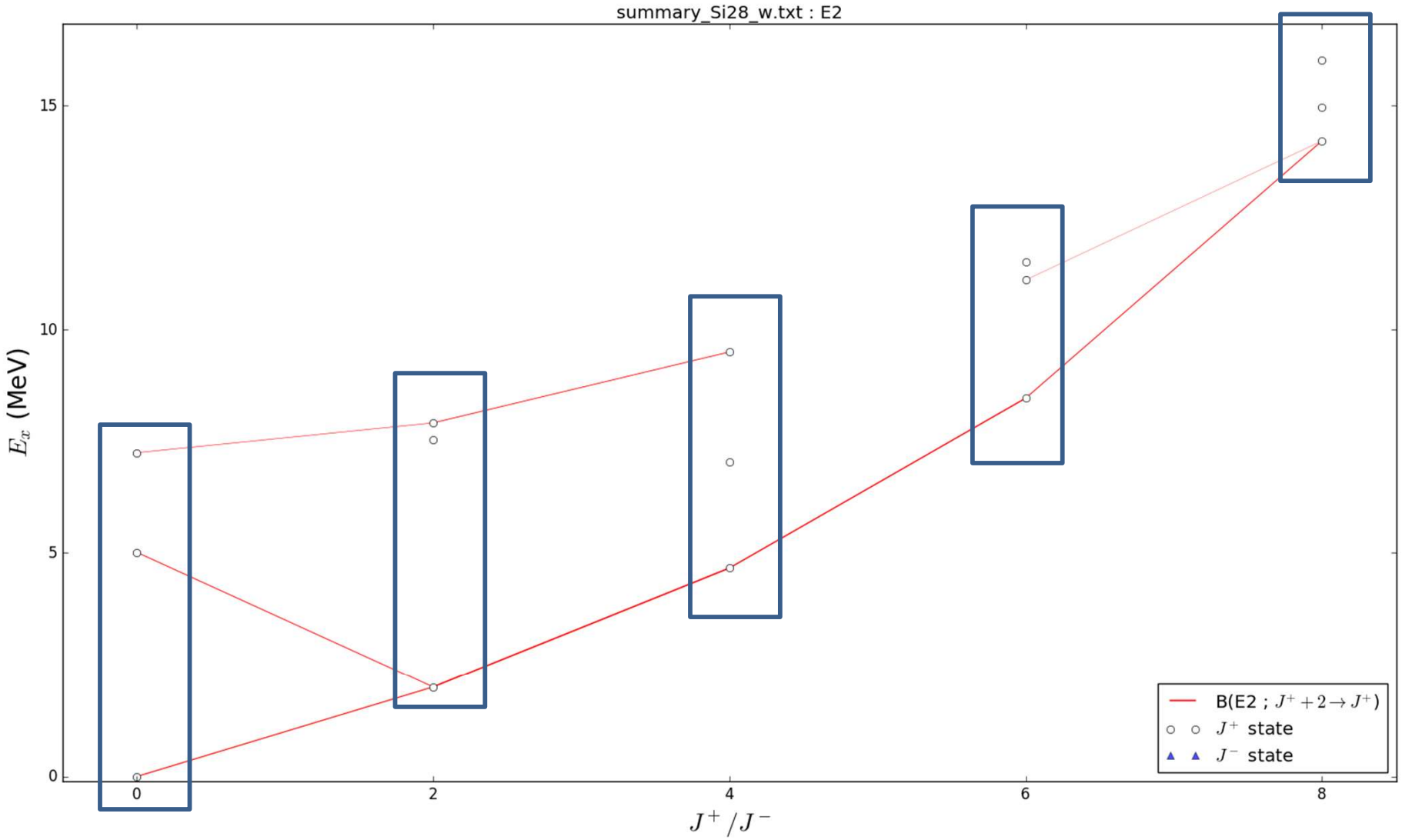
J-projection

- By default, KSHELL diagonalizes the Hamiltonian in $M = 0$ subspace ($M = \frac{1}{2}$ for odd nuclei).
- It can also obtain only specified-*J* states by projecting the Lanczos vectors to good *J* states at every Lanczos iteration nestedly.

```
*************** specify a nuclide ********************


number of valence protons and neutrons
 (ex.  2, 3 <CR> or 9Be <CR>)    <CR> to quit : Si28

number of valence particles  6 6

name for script file (default: Si28_w ):

J, parity, number of lowest states
 (ex. 10           for 10 +parity, 10 -parity states w/o J-proj. (default)
      -5           for lowest five -parity states,
      0+3, 2+1     for lowest three 0+ states and one 2+ states,
      1.5-1, 3.5+3 for lowest one 3/2- states and three 7/2+ states) :
```

0+3, 2+3, 4+3, 6+3, 8+3

E2 map: ^{28}Si, 3 states for each J



KSHELL further

- Input parameters
- Truncation schemes
- Lanczos method for solving the eigenvalue problem.

Input parameters for shell-model calculations

- Model space and Effective interaction
  - look at kshell/snt, or ask shell-model people!
  - Nushellx@MSU contains rich collection of effective interactions (nushell2snt.py)
- effective charges for *Q*-moment, B(E2)
  - $(e_\pi, e_\nu) = (1.5, 0.5)e$ is typical value, caused by the core polarization
- *g*-factor for *M*-moment, B(M1)
  - $g_{l\pi} = 1,\ \mathrm{g}_{l\nu} = 0,\ \mathrm{g}_{s\pi} = 5.586,\ \mathrm{g}_{s\nu} = -3.826$ for free particles
  - spin *g*-factor is typically quenched by 0.7.
- $\hbar\omega$: Energy of the harmonic oscillator quanta
  - $\hbar\omega = 41\mathrm{A}^{-1/3}$ or $\hbar\omega = 45A^{-1/3} - 25A^{-2/3}$ affects E2 and Q-moment, not energies
- Lawson's beta for removing contamination of center-of-mass motion (beyond one-major-shell model space)
  - $\frac{\beta_{CM}\hbar\omega}{A} = 10.$ $\qquad H' = H + \beta_{\mathrm{CM}} H_{\mathrm{CM}}$

Additional notes for KSHELL and LSSM

- TBMEs are often scaled by the mass-dependent factor $\left(\frac{A}{A_c+2}\right)^{-0.3}$ for better agreement with the experimental data.

- Shell-model energy with isospin-symmetric interaction means the relative energy to the core nucleus without Coulomb energy. To estimate it, follow the original paper or estimate with an empirical formula, e.g.,

$$E_C(Z,N) = 0.700\frac{Z(Z-1) - 0.76[Z(Z-1)]^{2/3}}{R_C}\ \text{MeV}$$

$$R_C = e^{1.5/A}A^{1/3}\left(0.946 - 0.573\left(\frac{2T}{A}\right)^2\right)$$

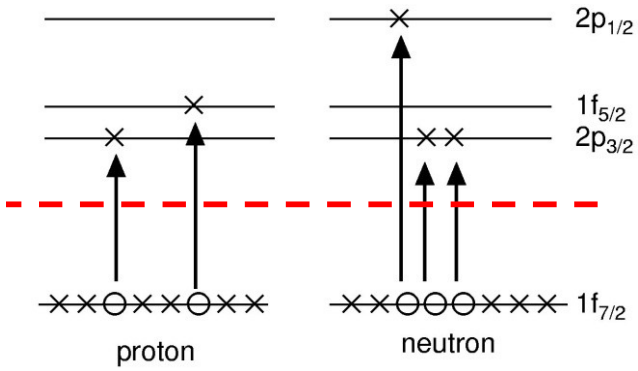
E. Caurier et al., Phys. Rev. C 59, 2033 (1999)

Truncation schemes in KSHELL code

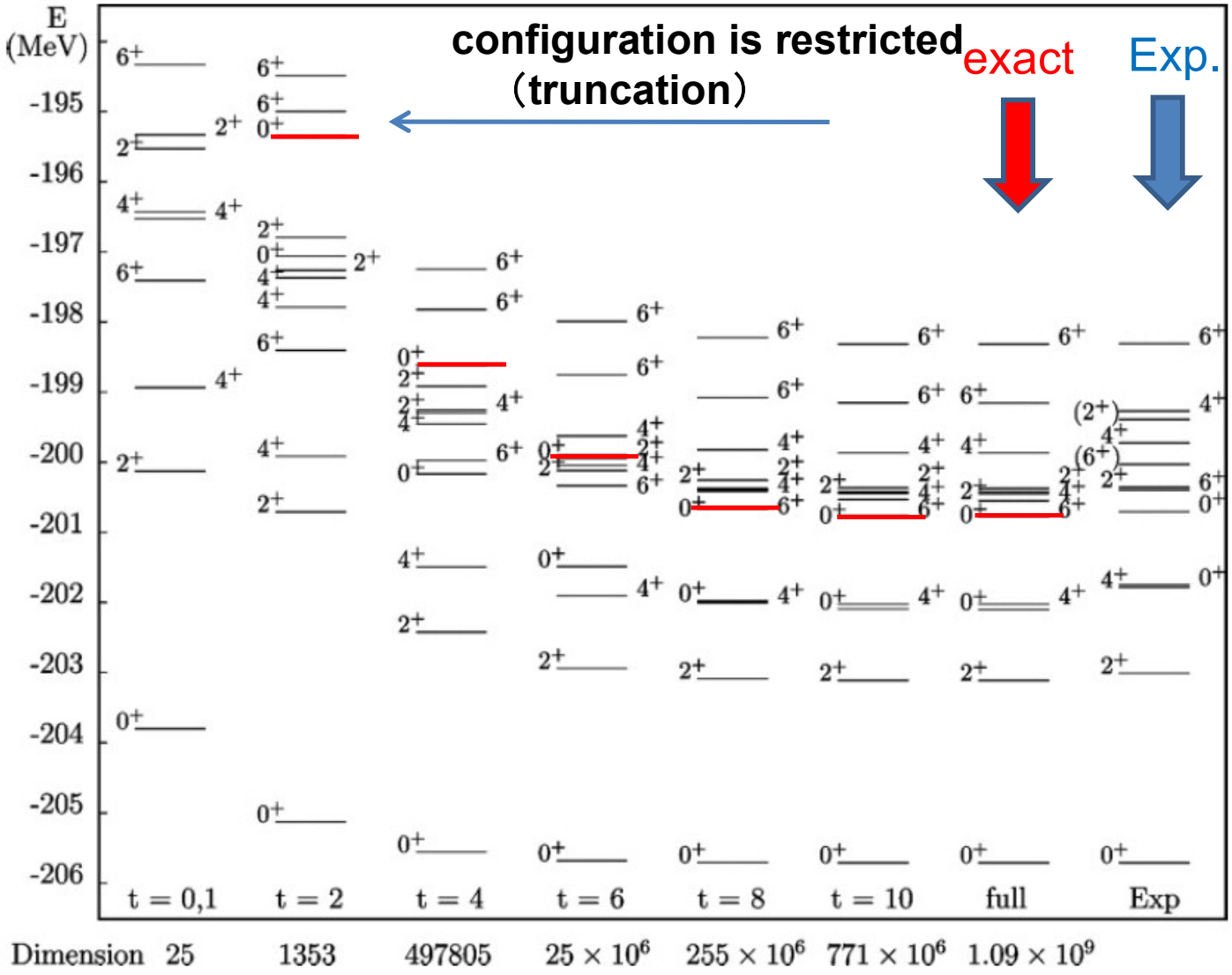
```
truncation scheme ?
      0 : No truncation (default)
      1 : particle-hole truncation for orbit(s)
      2 : hw truncation
      3 : Both (1) and (2)

1
   #     n,   l,   j, tz,     spe
   1     0    3    7  -1    -8.624      p_0f7/2
   2     1    1    3  -1    -5.679      p_1p3/2
   3     0    3    5  -1    -1.383      p_0f5/2
   4     1    1    1  -1    -4.137      p_1p1/2
   5     0    3    7   1    -8.624      n_0f7/2
   6     1    1    3   1    -5.679      n_1p3/2
   7     0    3    5   1    -1.383      n_0f5/2
   8     1    1    1   1    -4.137      n_1p1/2
 specify # of orbit(s) and min., max. occupation numbers for restriction

 # of orbit(s) for restriction?  (<CR> to quit): 2,3,4,6,7,8
 min., max. restricted occupation numbersfor the orbit(s) (or max only) : 0,2

 # of orbit(s) for restriction?  (<CR> to quit):
```

Particle-hole truncation scheme

^{56}Ni ... Z=N=28
doubly closed with
N=Z=28 magic,
truncation of particle-hole excitation is expected to work well

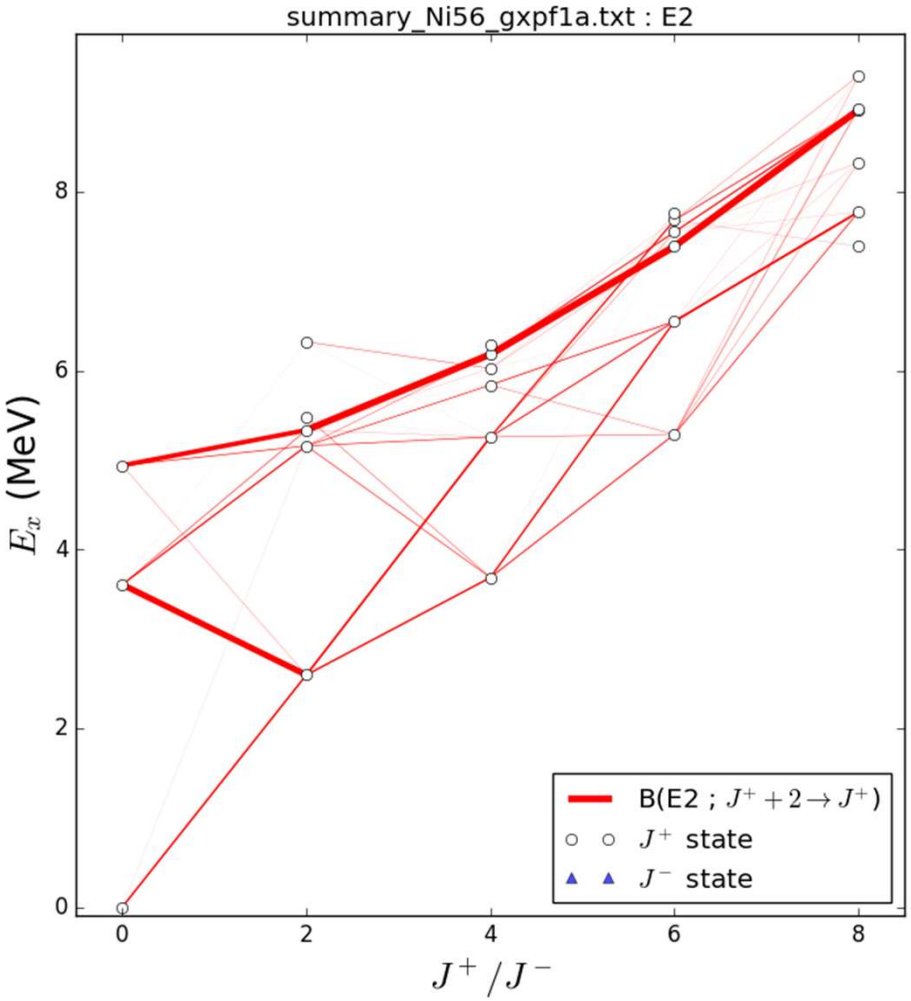


Number of p-h excitations from f7/2 is restricted (*t*)



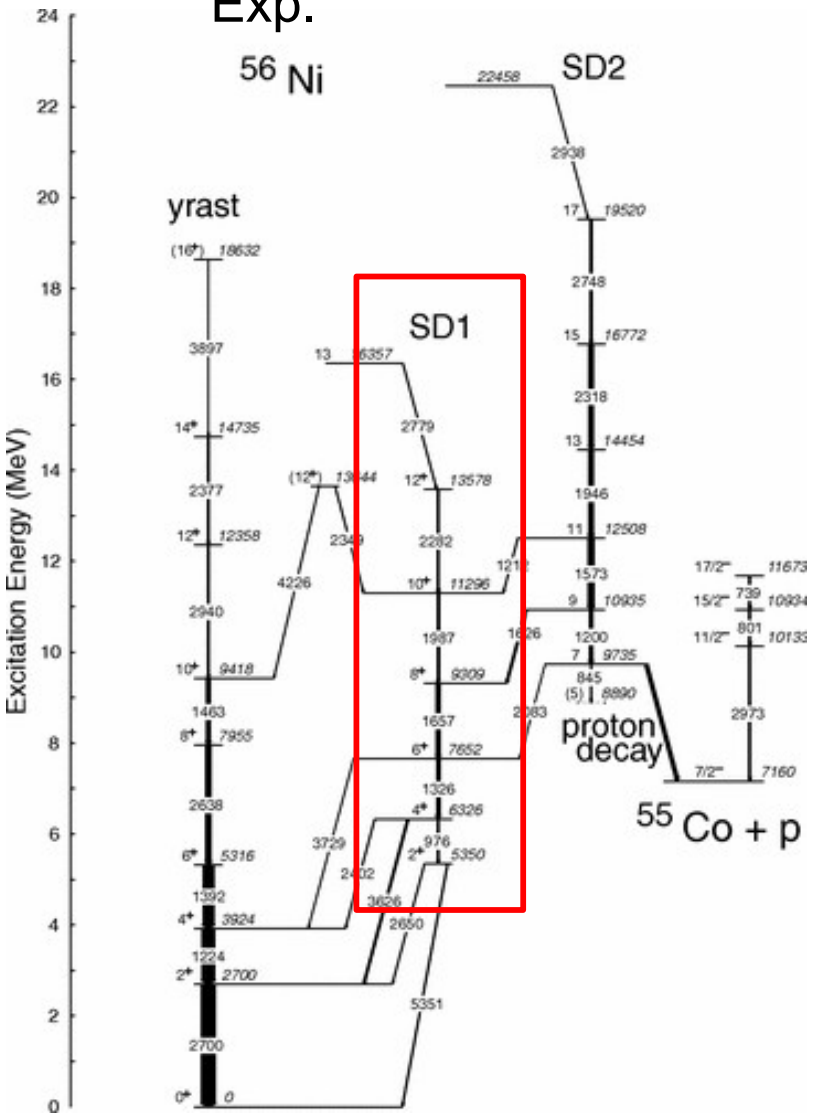
Ref. M. Horoi *et al.*, Phys. Rev. C78, 014318(2008)

Deformed band in ^{56}Ni



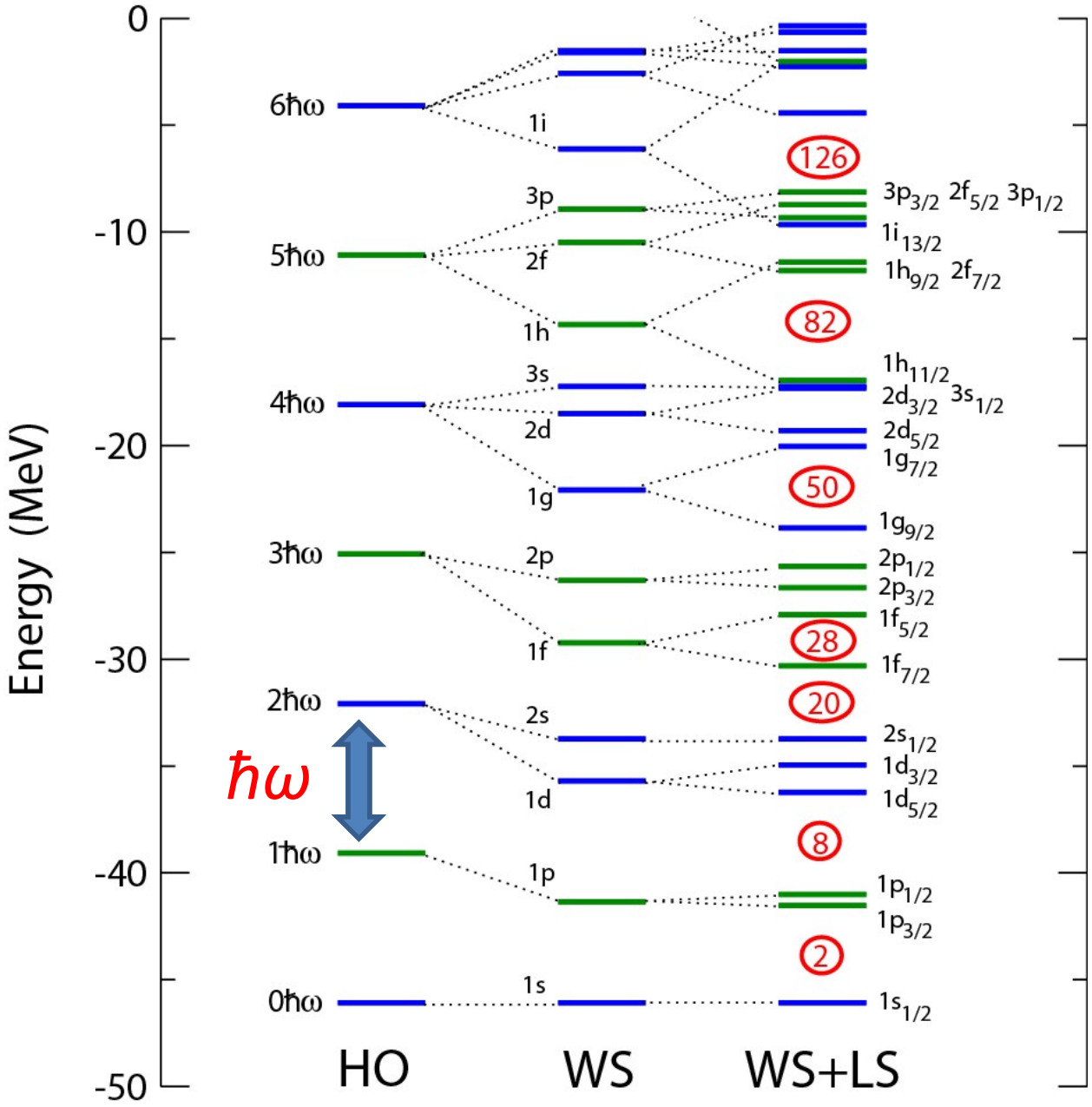
Deformed band by 4-particle 4-hole excitation

Exp.



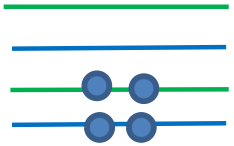
Ref. E. K. Johansson et al., Phys. Rev. C 77 064316 (2008)

Truncation by $N\hbar\omega$ excitation



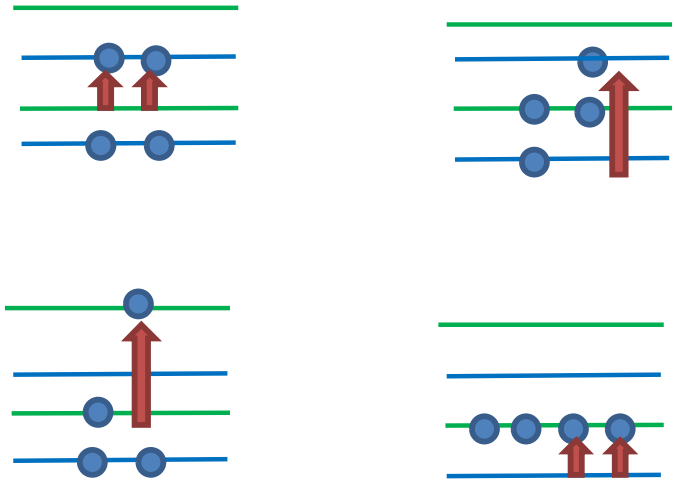
$0\hbar\omega$

no cross shell excitation



$2\hbar\omega$

across 2 shell gaps



$N_{\max}\hbar\omega$ in NCSM

Partition file

- “partition” defines a set of the occupation for each orbit
- foo.ptn file contains a list of the partitions allowed in the model truncation.
- You can make any truncation scheme by preparing the partition file on your own.

```
# partition file of w.snt  Z=8  N=11  parity=+
 8 11 1
# num. of  proton partition, neutron partition
 12 3
# proton partition
     1     0  6  2
     2     1  5  2
     3     1  6  1
     4     2  4  2
     5     2  5  1
     6     2  6  0
     7     3  3  2
     8     3  4  1
     9     3  5  0
    10     4  2  2
    11     4  3  1
    12     4  4  0
# neutron partition
     1     3  6  2
     2     4  5  2
     3     4  6  1
# partition of proton and neutron
36
    1     1
    1     2
    1     3
    2     1
    2     2
```

Lanczos method

- Eigenvalue solver for the lowest eigenvalues of a large real symmetric sparse matrix
- Lanczos method is one of the Krylov-subspace methods

$$\mathcal{K}_{l_m}(H, \boldsymbol{v}_1) = \{\boldsymbol{v}_1, H\boldsymbol{v}_1, H^2\boldsymbol{v}_1, H^3\boldsymbol{v}_1, \cdots, H^{l_m-1}\boldsymbol{v}_1\}$$

- Ritz value ... eigenvalue of the matrix in the Krylov subspace. It is a good approximation to the exact eigenvalue.

Lanczos method : algorithm

- Prepare initial state (e.g. random) u_0
- Iterate

Matrix-vector product, bottle neck!

$$a_k = u_k^T H u_k \qquad b_k = u_k^T H u_{k-1}$$

Gram-Schmidt orthogonalization

$$u'_{k+1} = Hu_k - a_k u_k - b_k u_{k-1}$$

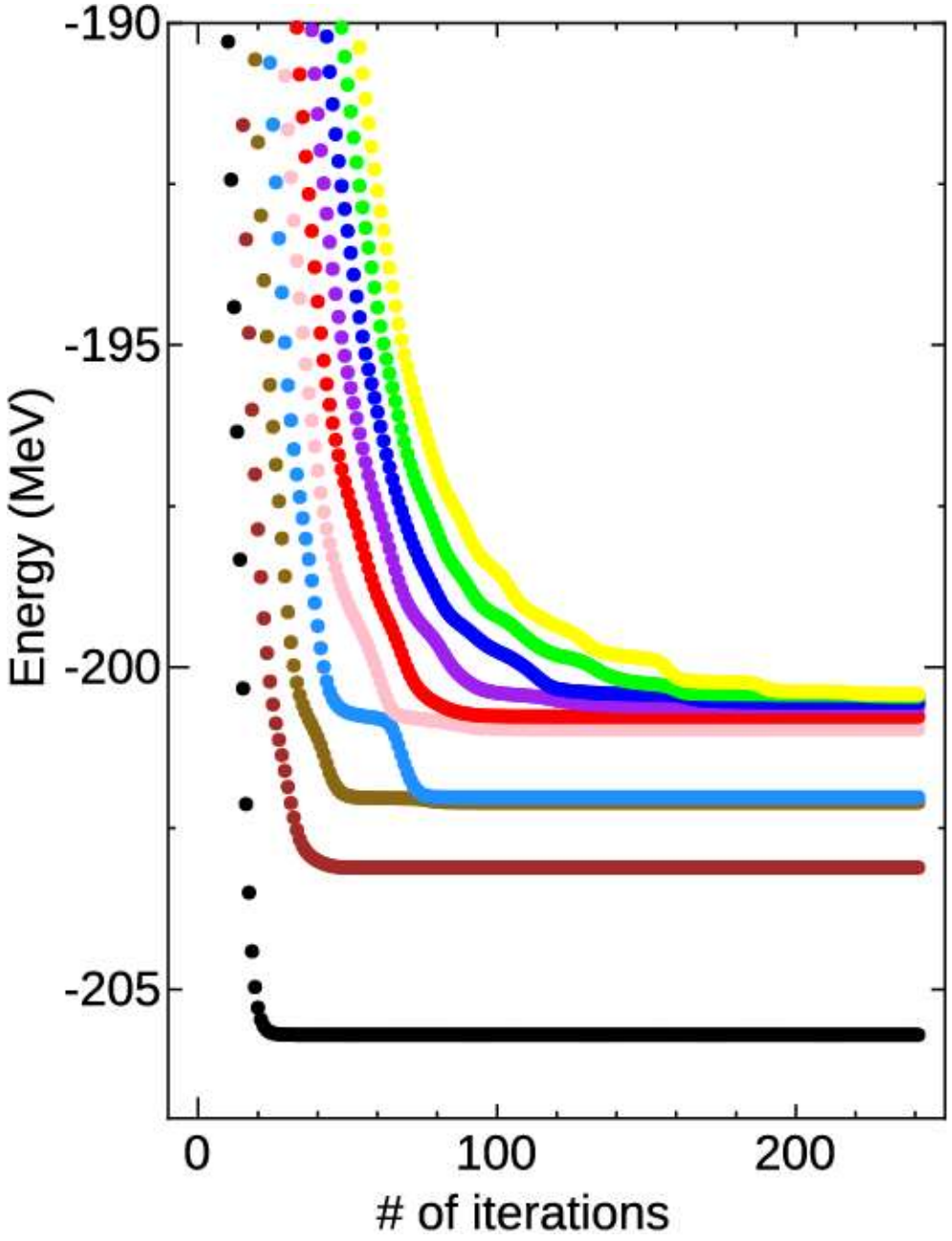
Normalize

$$u_{k+1} = u'_{k+1} / \sqrt{u'^T_{k+1} u_{k+1}}$$

$$T = u_i^T H u_j = \begin{bmatrix} a_0 & b_0 & & & & \\ b_0 & a_1 & b_1 & & & \\ & b_1 & a_2 & b_3 & & \\ & & b_2 & a_3 & b_3 & \\ & & & b_3 & \dots & \dots \\ & & & & \dots & \dots \end{bmatrix}$$

- Solve eigenvalue problem of the tri-diagonal matrix T by bisection method

Convergence of Lanczos method



^{56}Ni shell-model calc.

10^9 M-scheme dimension

241 iterations are required

to obtain 10 lowest eigenvalues

code “KSHELL”
total elapsed time : 35min. 9 sec/iteration
@FX10 supercomputer 240 nodes
(SPARC 64 IXfx, 3840 cores)

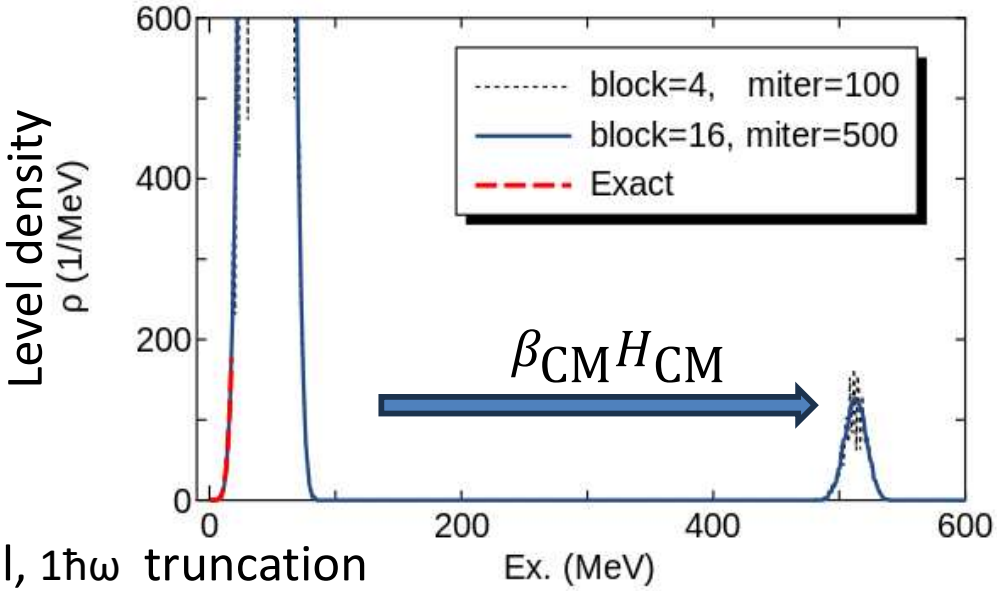
Contamination of center-of-mass motion

- In the model space beyond 0$\hbar\omega$, center-of-mass motion is contaminated.
- Lawson method
  - Lift up spurious center-of-mass excited states by adding CoM Hamiltonian

$$H' = H + \beta_{\mathrm{CM}} H_{\mathrm{CM}}$$

$$H_{\mathrm{CM}} = \frac{\boldsymbol{P}^2}{2AM} + \frac{1}{2} AM\omega^2 \boldsymbol{R}^2 - \frac{3}{2}\hbar\omega$$

$$\frac{\beta_{CM}\hbar\omega}{A} = 10 \text{ MeV}$$

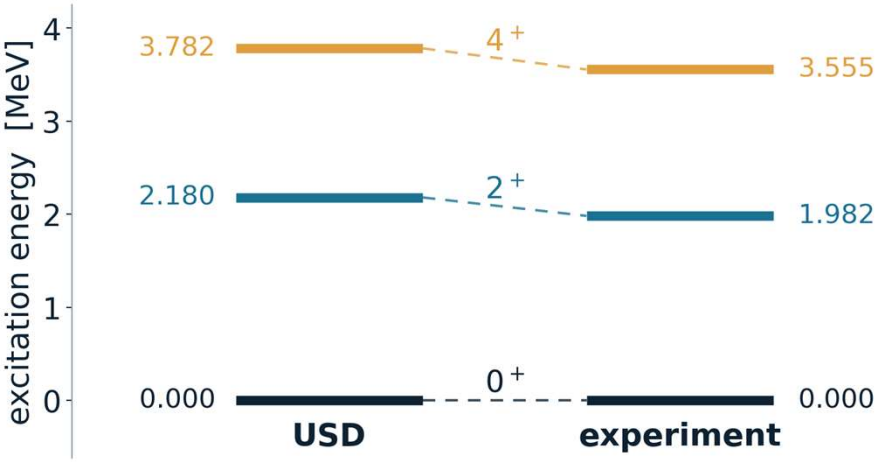


^{48}Ca J=1$^-$, sd-pf-sdg shell, 1ħω truncation

- Center-of-mass motion can be clearly removed in full $N\hbar\omega$ model space
- If not full space, separation is approximately achieved by large β_{CM} ... sometimes problematic

Exercise 1

Compute the 4^+ energy of ^{18}O with USD interaction by hand!



J-scheme dimensions

J = 0, 1, 2, 3, 4

D_J = 3, 2, 5, 2, 2

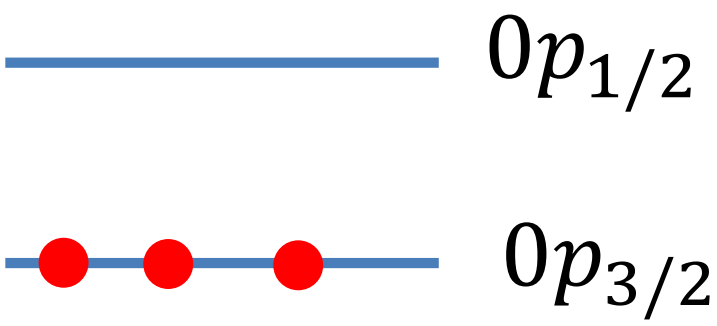
The J = 4 problem is a 2 × 2 you can solve on paper.

Note: 0^+ energy of ^{18}O with USD is -12.171 MeV.

Excitation energy is the difference between 0^+ and 4^+ energies.

Exercise 2

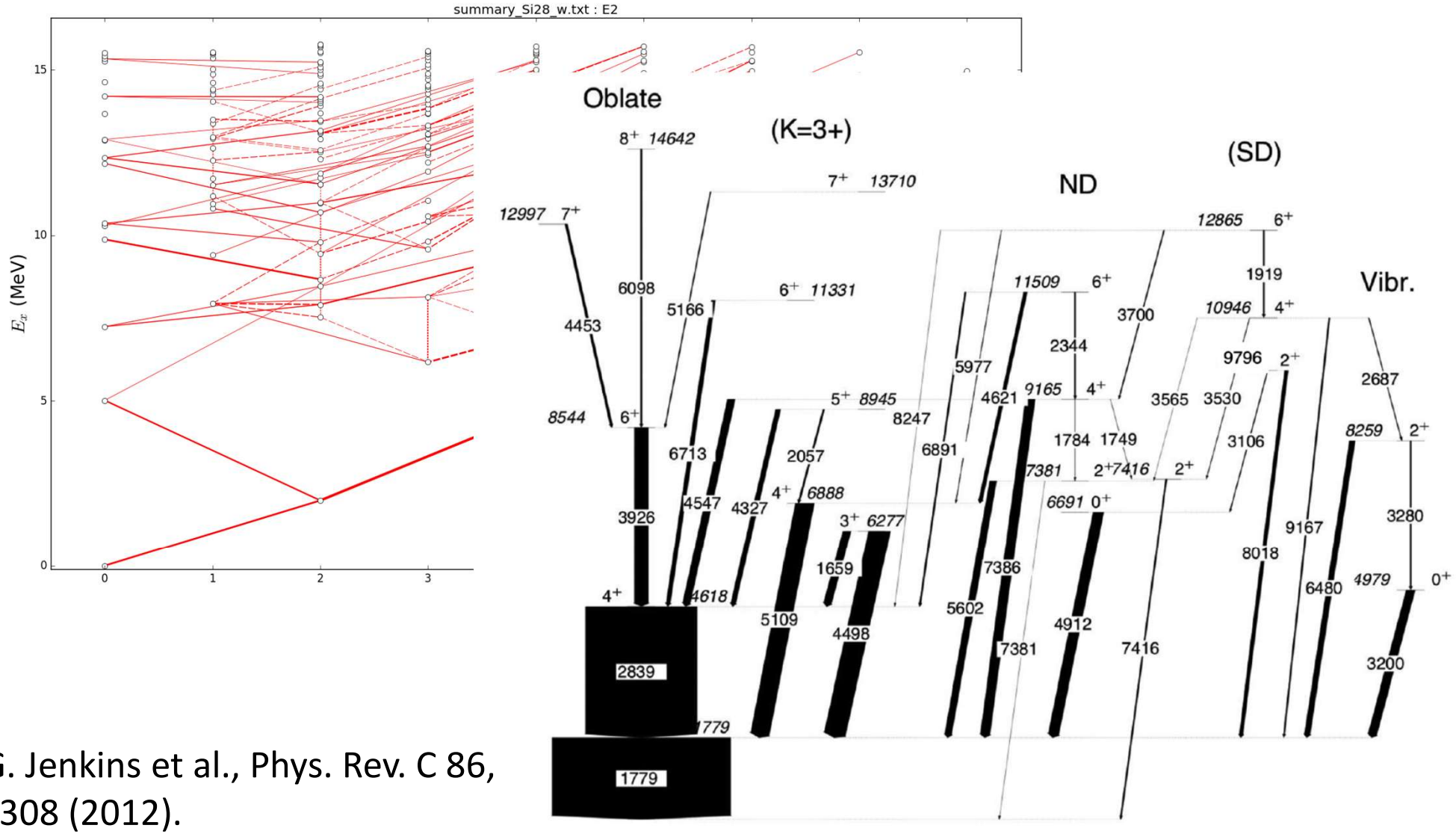
Let us count the M-scheme dimension and J-scheme dimension of ^{7}He with p-shell model space.



And confirm the agreement with the KSHELL output.

Exercise 3

Perform shell-model calculations to obtain 200 levels of ^{28}Si for compassion with the experimental data.
Try “n_block=8, max_lanc_vec=500” for the block Lanczos algorithm.



D. G. Jenkins et al., Phys. Rev. C 86, 064308 (2012).

Exercise 4

Exp. Nudat 2.6
http://www.nndc.bnl.gov/nudat2/

Backbending in ^{48}Cr

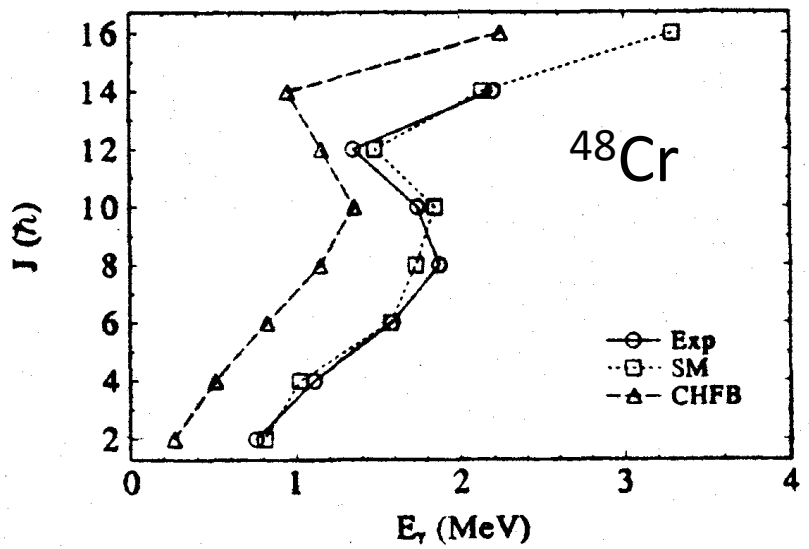
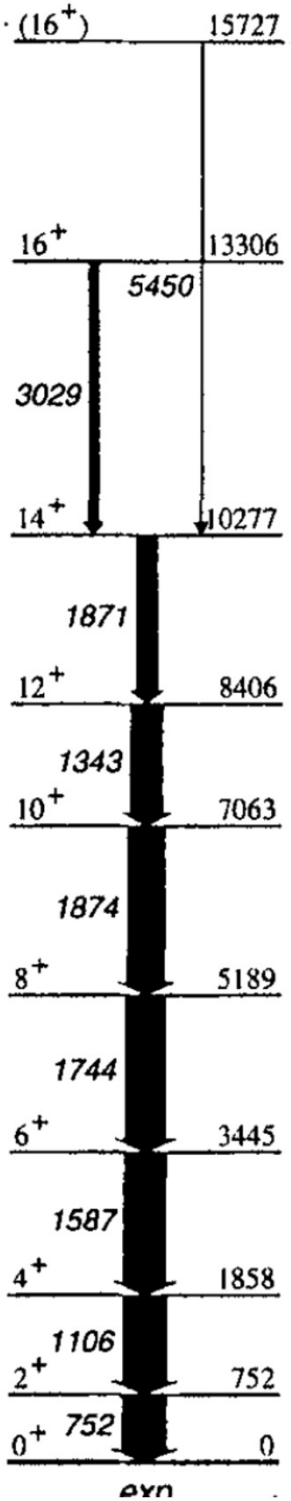


FIG. 1. Yrast energies $E_\gamma = E(J) - E(J-2)$.

E. Caurier et al., PRL75 (1995) 2466



- make backbending plot of ^{48}Cr with GXPF1A
- Try speedup of computation
  - ... J-projection, particle-hole truncation

CNS Summer School 2026 @ CENS, IBS
2026/8/25,26

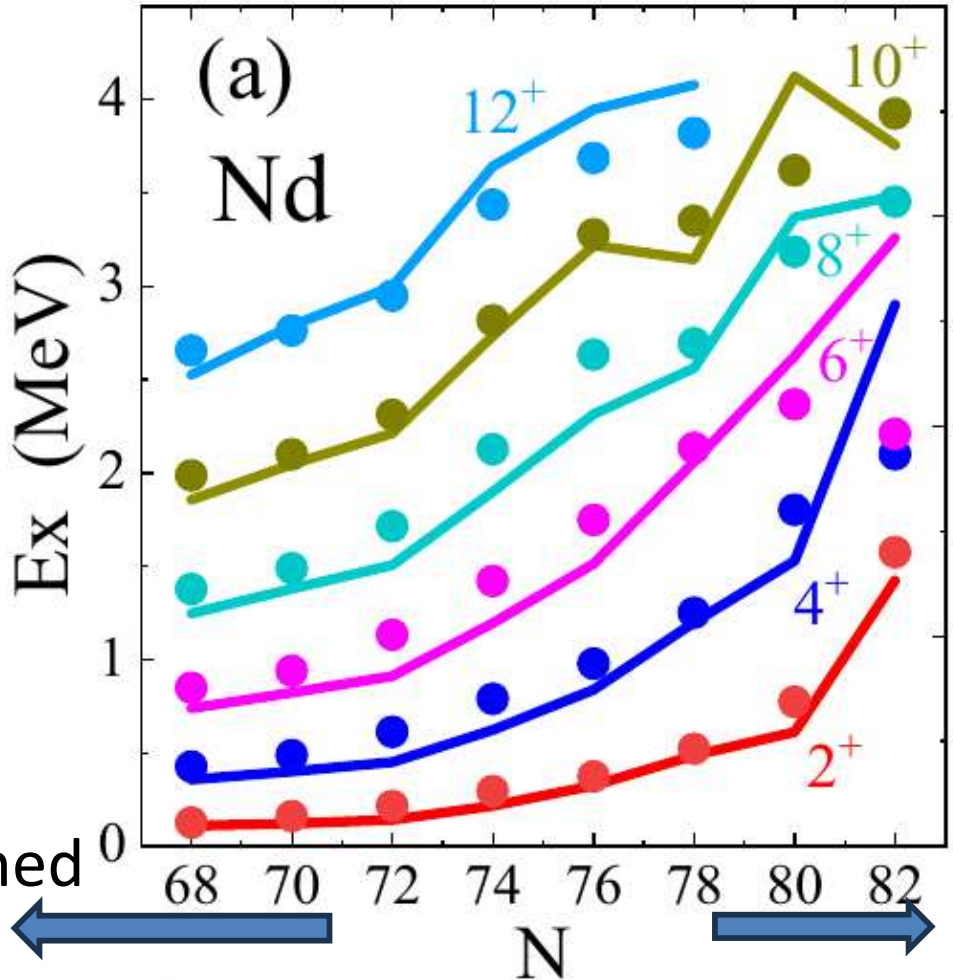
3. Shell-model interaction, monopole interaction and shell evolution

筑波大学
計算科学研究センター
Center for Computational Sciences

Noritaka Shimizu
Center for Computational Sciences, University of Tsukuba

Can ^{130}Nd be computed with the KSHELL code? No, unfortunately

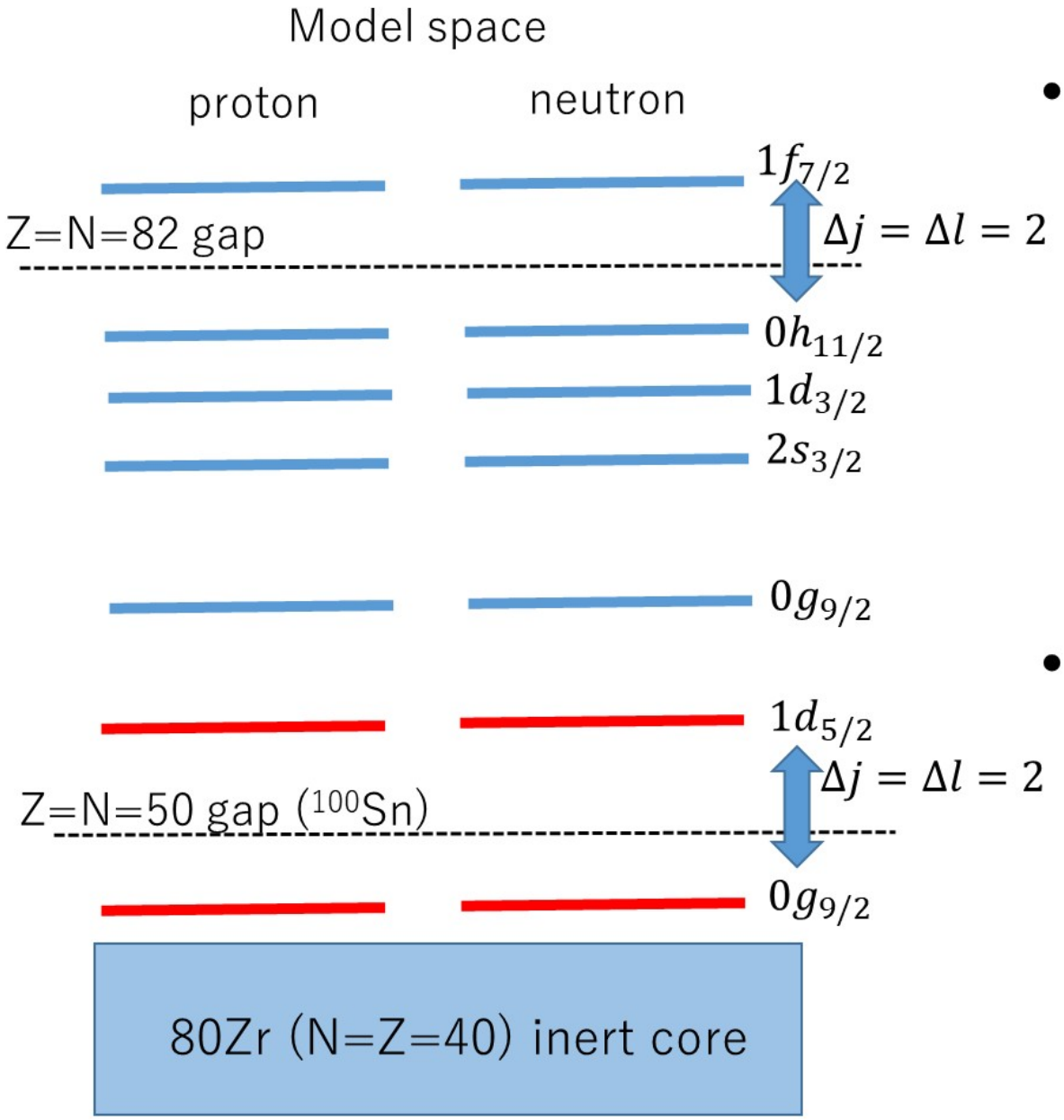
- Large quadrupole deformation in the heavy-mass region
  - The dimension becomes enormous($\gg 10^{11}$) in open-shell nuclei heavier than ^{100}Sn
  - Beyond one major shell is necessary : "Quasi SU(3) coupling" $\Delta l = \Delta j = 2$ pairs
  - Approximation scheme is required, such as PGCM, MCSM, QVSM



deformed

spherical magic

Model space and interaction

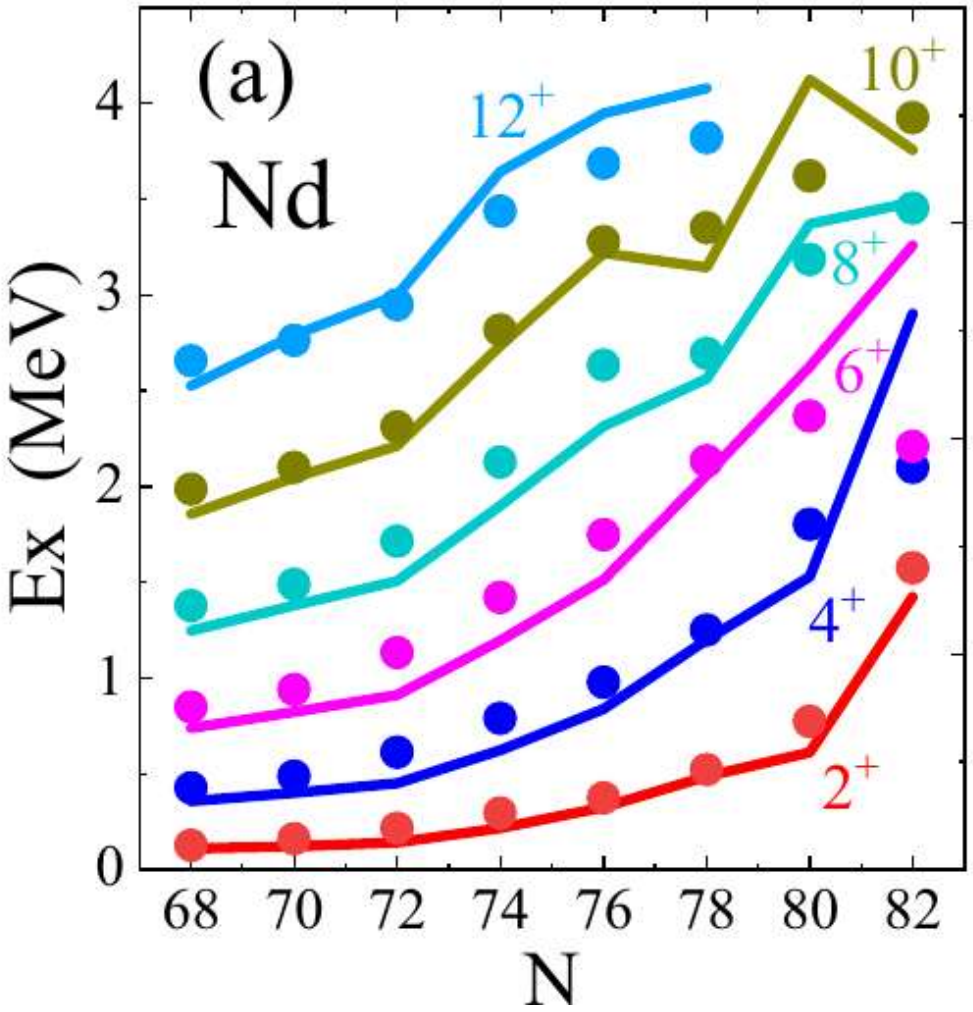


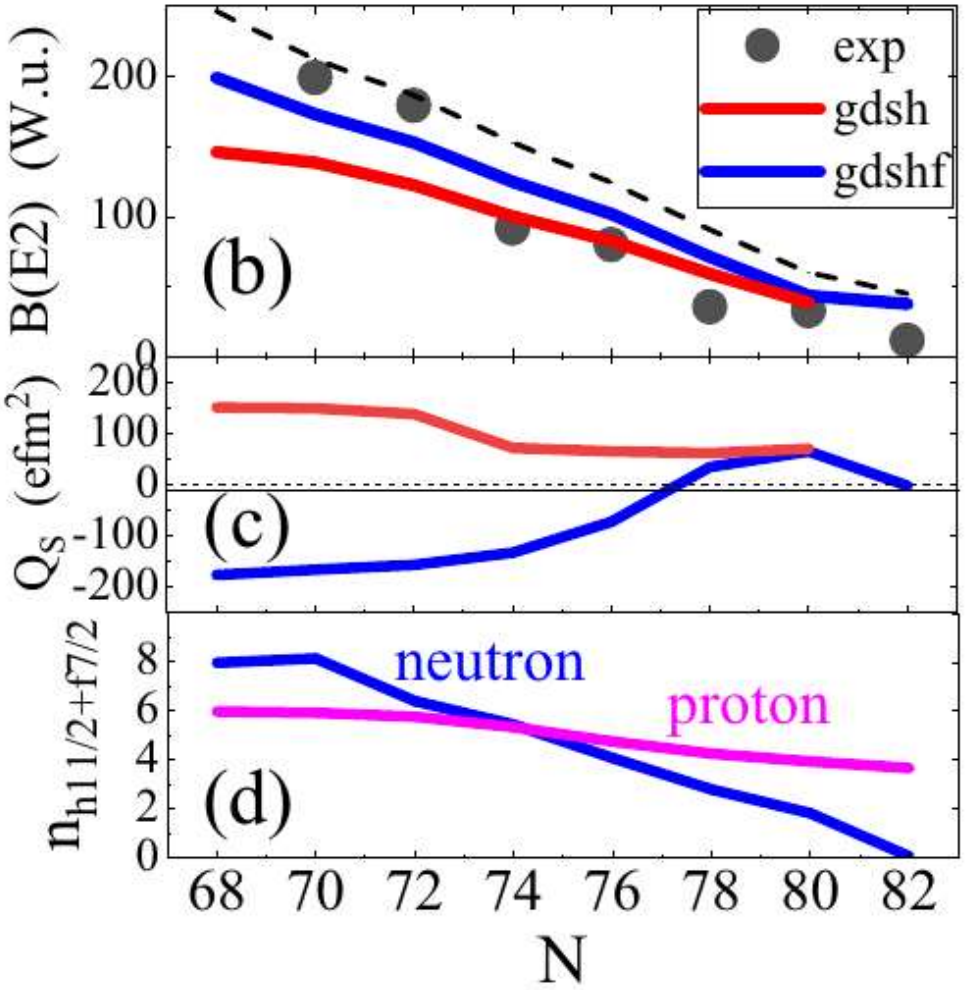
- PMMU interaction is employed (pairing plus multipole Hamiltonian whose monopole part is corrected by V_{MU})

- $0g_{9/2}$ and $1f_{7/2}$ orbits are important for the description of large quadrupole deformation (quasi-SU(3))

A. P. Zuker *et al*., Phys. Rev. C 52, R1741 (1995).

PGCM calc. with PMMU interaction





gdsh : sdg shell + h11/2
gdshf : sdg shell + h11/2 + f7/2

Quasi SU(3) partner orbits are essential for large quadrupole deformation

K. Kaneko, N. Shimizu, T. Mizusaki and Y. Sun, Phys. Rev. C 103 L021301 (2021)

Outline

- History and recipe of constructing shell-model Hamiltonian
- Monopole interaction, ESPE and shell evolution

Realistic shell-model interactions

We have several interactions for each model space

- Model space (sd, pf, sdpf, f5pg9, …)
- Nuclear force (CD-Bonn, AV18, chiral N3LO and its family …)
- Cut-off parameter, Perturbation theory, G-matrix, Vlow-k, SRG, …
- χ^2-fit for the focused area

In the density functional theory, there are many parameter sets of the density functional

- Non-relativistic : UNEDF, SLy4, SkM*, Gogny D1S, …
- Relativistic : PC-PK1, DD-ME2, DD-PC1, NL3, TM1, …

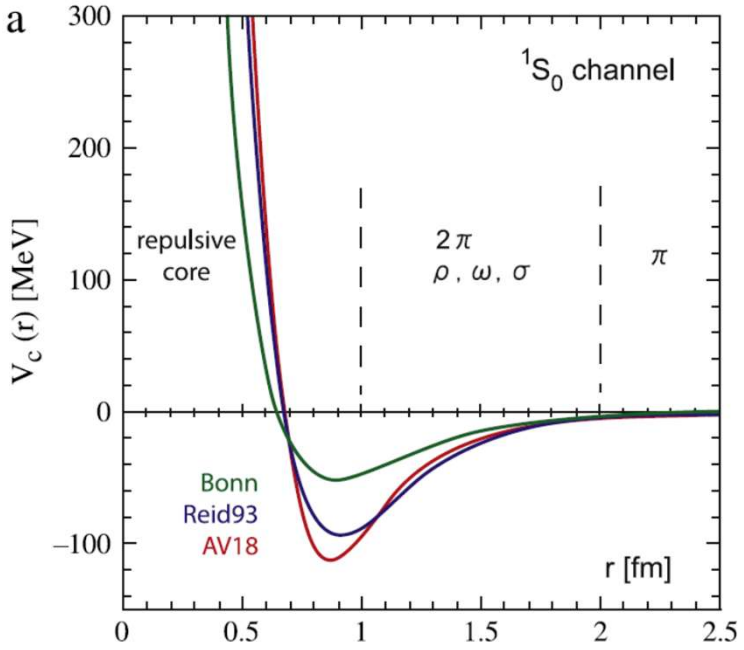
How to construct a realistic shell-model Hamiltonian

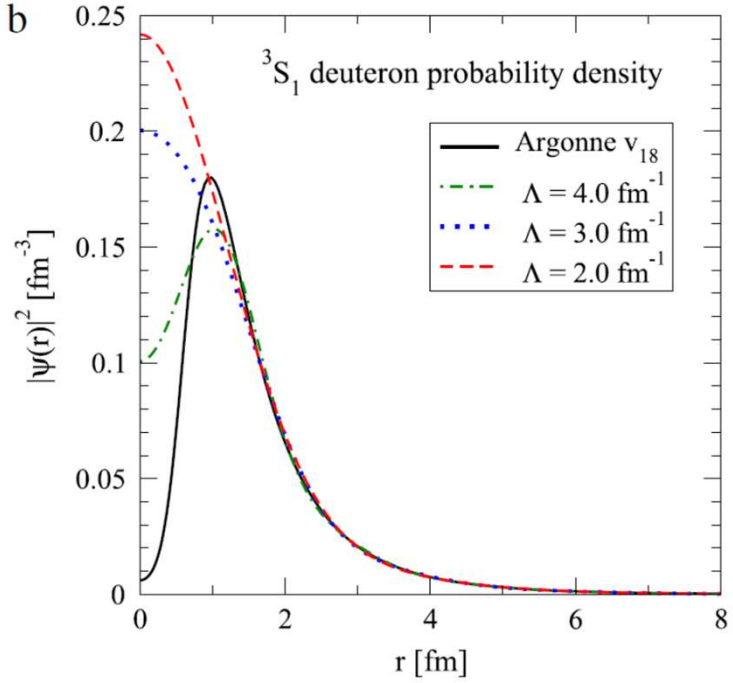
- Some successful interactions (USD, GXPF1A, JUN45, …) are derived by the following procedure.

- SPEs are determined by the experimental levels of the core + 1 nucleus.
  - E.g. ^{41}Ca for SPE of *pf* shell

- TBME is derived by :
  1. Prepare NN interaction (CD-Bonn, chiral N3LO, AV18, …)
  2. Soften short-range replustion (G-matrix, Vlow-k, SRG, …)
  3. Include the effect outside the model by many-body perturbation theory (MBPT)
  4. Phenomenological correction to reproduce the experimental data (χ^2-fit)

Recipe to treat short-range repulsion





Deuteron wave function obtained by V low-k interaction

NN potential

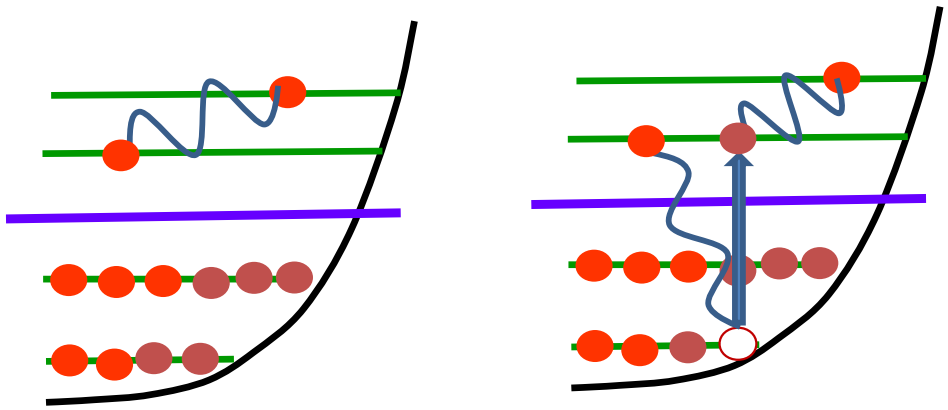
Strong repulsive core causes severe problem in many-body calculations

- G-matrix
- V low-k
- Similarity renormalization group (SRG)
- etc.

S. Bogner, R. J. Furnstahl, and A. Schwenk, Prog. Part. Nucl. Phys. 65, 94 (2010).

Core polarization

- Shell-model Hamiltonian is derived from the NN interaction using the many-body perturbation theory to include the effect outside the model space.
- “Core polarization” plays a crucial role



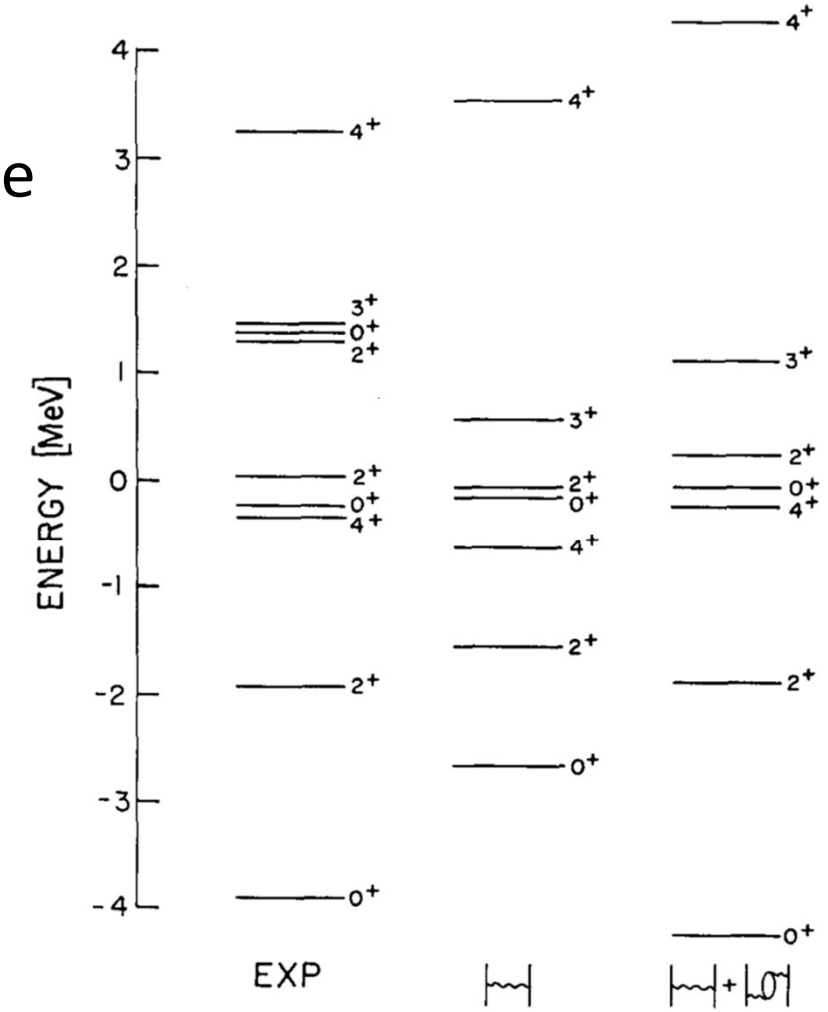
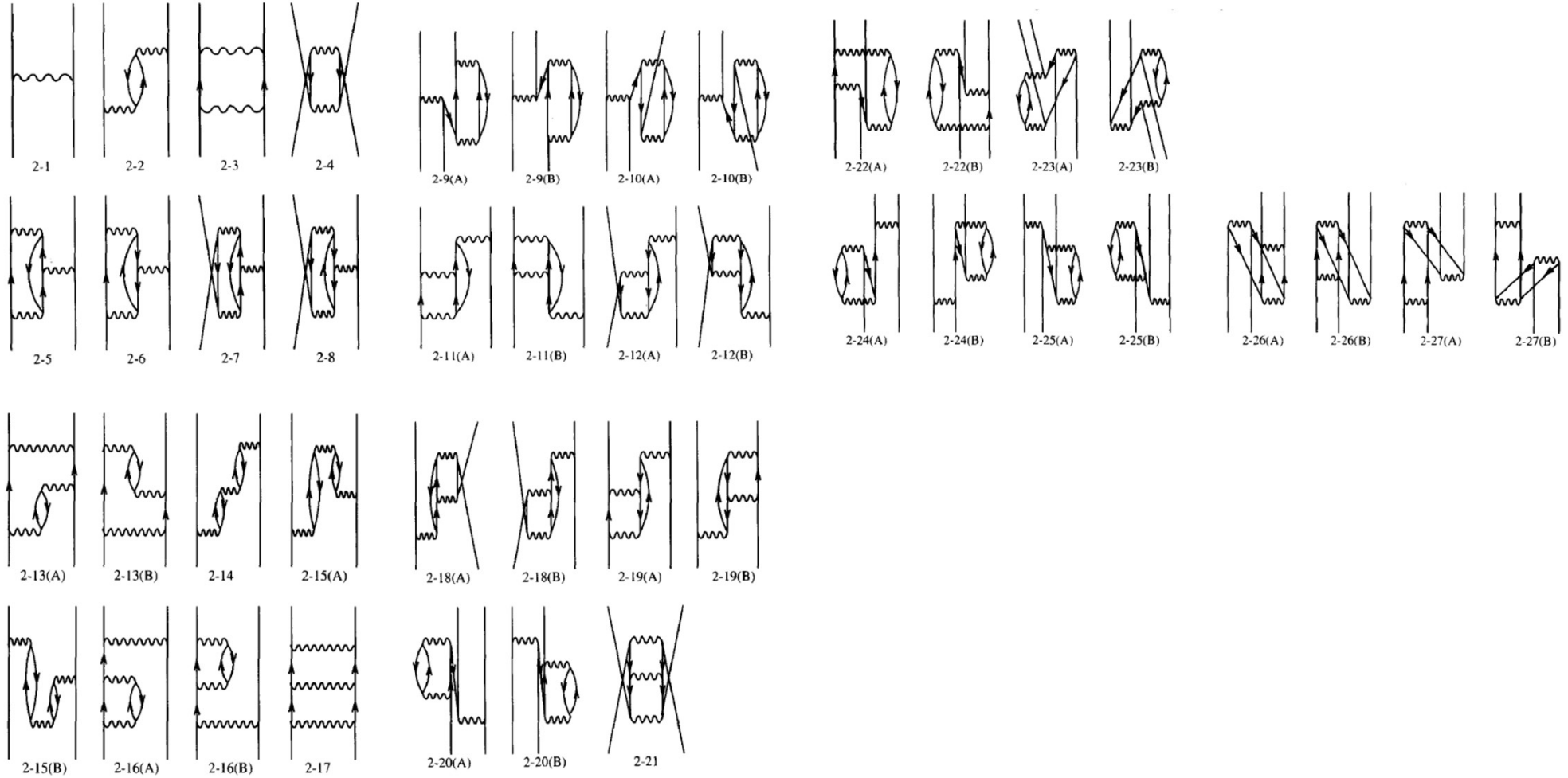


Fig. 13. The spectra of ^{18}O.

T. T. S. Kuo and G. E. Brown, Nucl. Phys. 85, 40 (1966)

Many-body perturbation theory



https://github.com/ManyBodyPhysics/CENS

M.H-Jensen, T.T.S. Kuo, and E Osnes, Phys. Rep. 261, 125 (1995)

- s.p.e .... taken from experiment
- TBME ... chi-square fit for exp. data

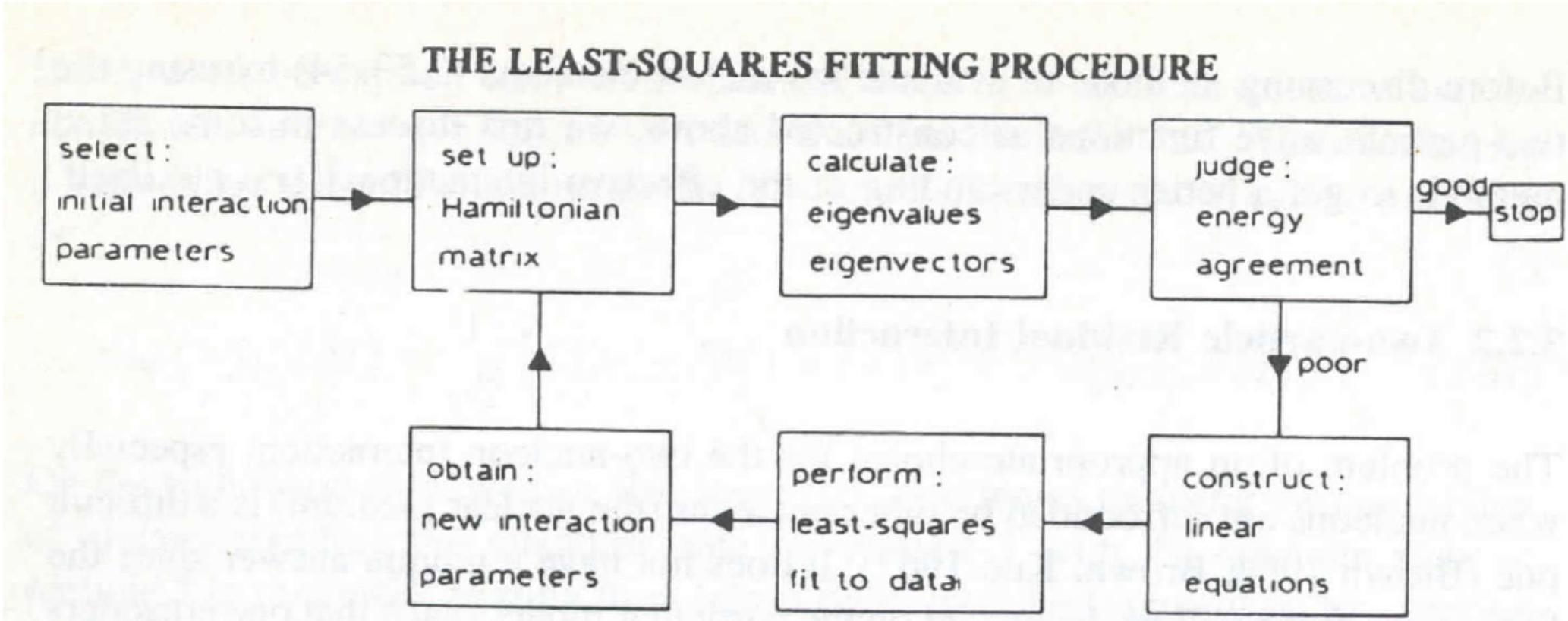


Fig. 3.20. Illustration of the various steps necessary in order to deduce an effective interaction (the two-body matrix elements $\langle j_1 j_2; J|V_{1,2}|j_3 j_4; J\rangle$ and single-particle energies ε_{j_i}) along the method discussed in Sect. 3.2.2a. Thereby a fit to experimental excitation energies and/or electromagnetic properties can be imposed [taken from (Brussaard 1977)]

USD interaction

B. A. Brown and B. H. Wildenthal, Annu. Rev. Nucl. Part. Sci. 38, 29 (1988)

file: w.snt

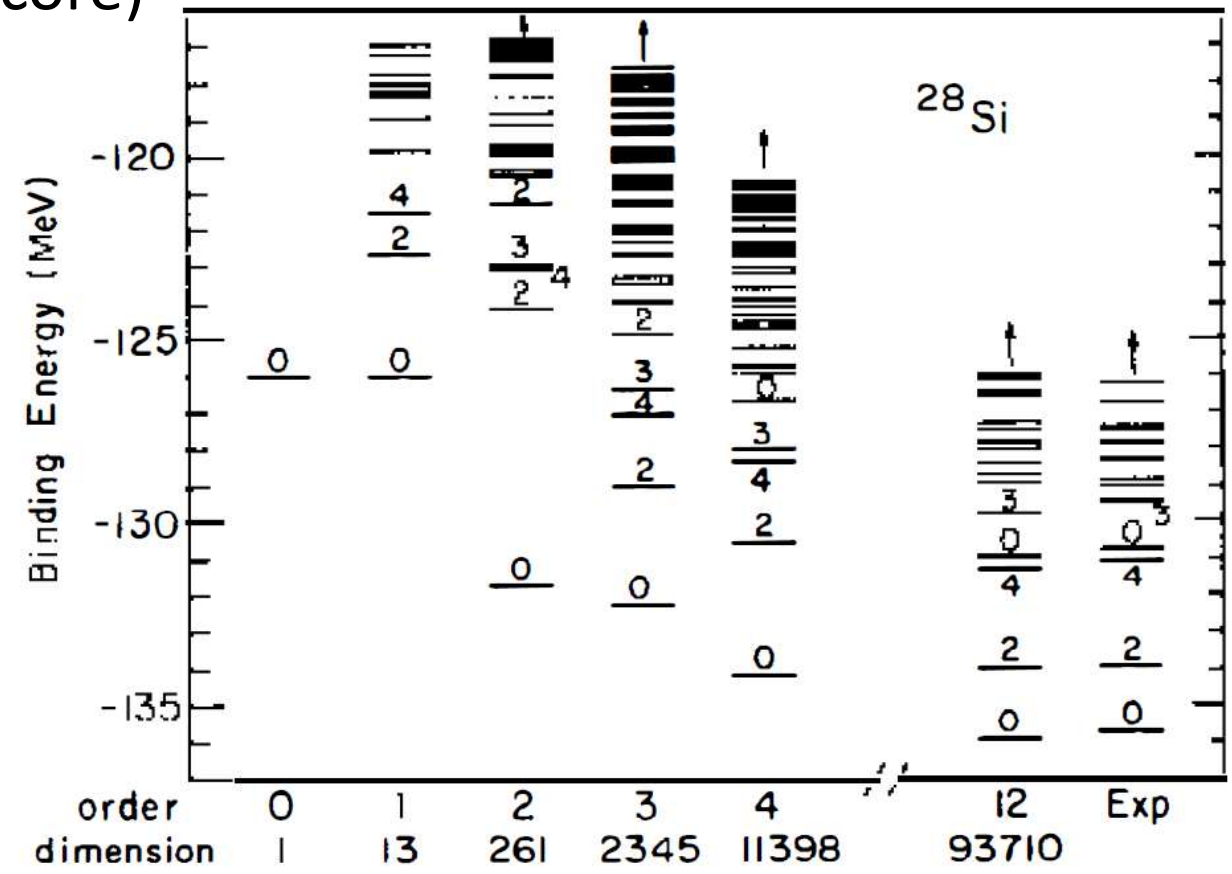
model space : sd-shell

(0d5/2, 0d3/2, 1s1/2, ^{16}O core)

Isospin-symmetric

63 TBME chi-square fitted

phenomenologically



KB3 interaction

A. Abzouzi, E. Caurier, and A. P. Zuker, Phys. Rev. Lett. 66, 1134 (1991)

file: kb3.snt

model space : pf-shell

0f7/2, 0f5/2, 1p3/2, 1p1/2

^{40}Ca core

Isospin-symmetric

Hamada-Johnston pot.

+ core-polarization

+ modification of monopole part

^{52}Fe

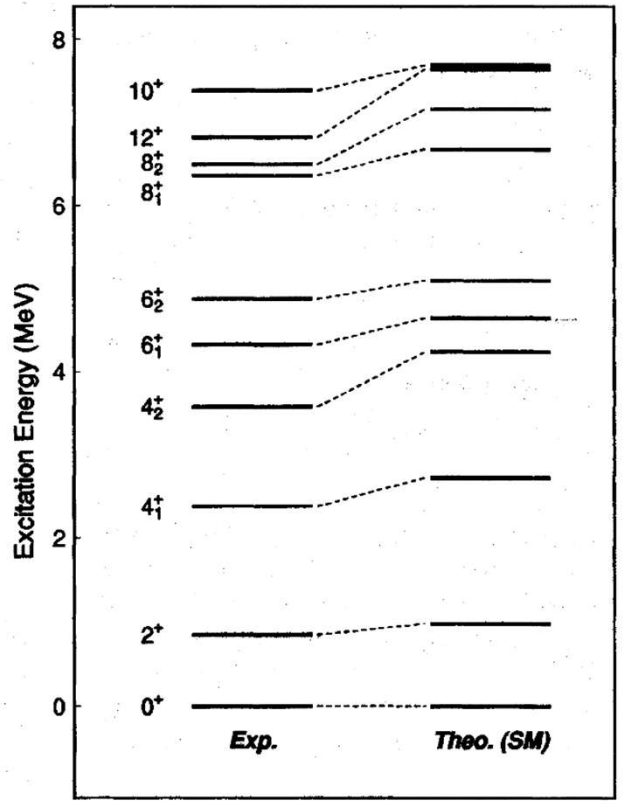


FIG. 5. Comparison between the experimental and the shell model positive parity energy levels in ^{52}Fe. Dashed lines connect the experimental levels with their calculated counterpartners.

C. A. Ur et al., PRC58 (1998) 3163

GXPF1, GXPF1A interaction

M. Honma, et al., Phys. Rev. C 65, 061301(R) (2002)

file: gxpf1.snt, gxpf1a.snt

model space : pf-shell

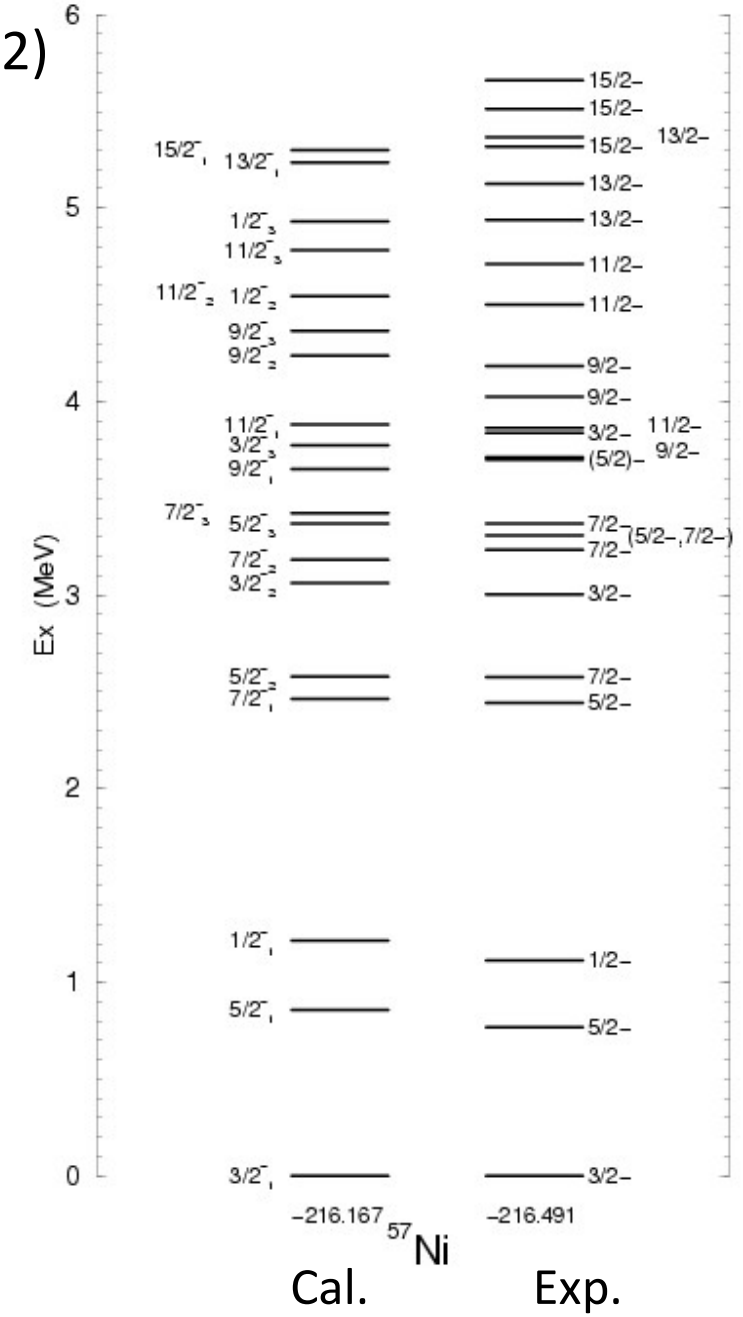
0f7/2, 0f5/2, 1p3/2, 1p1/2

^{40}Ca core

isospin-symmetric

G-matrix + 3rd order Q-box

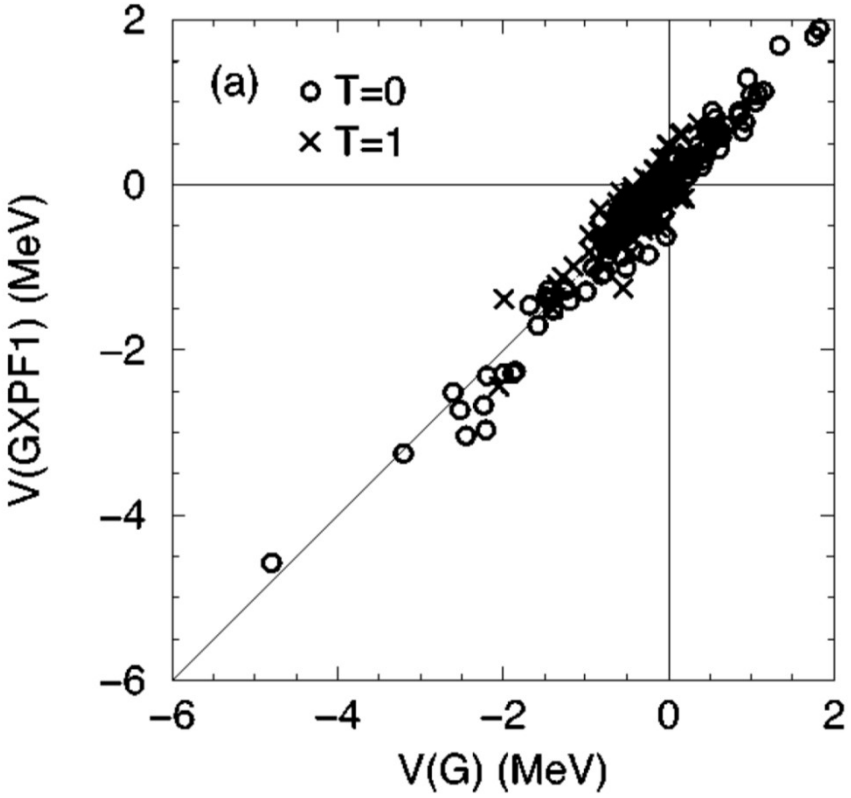
+ chi2 fit for 699 data



Phenomenological correction by χ^2-fit

The GXPF1 interaction

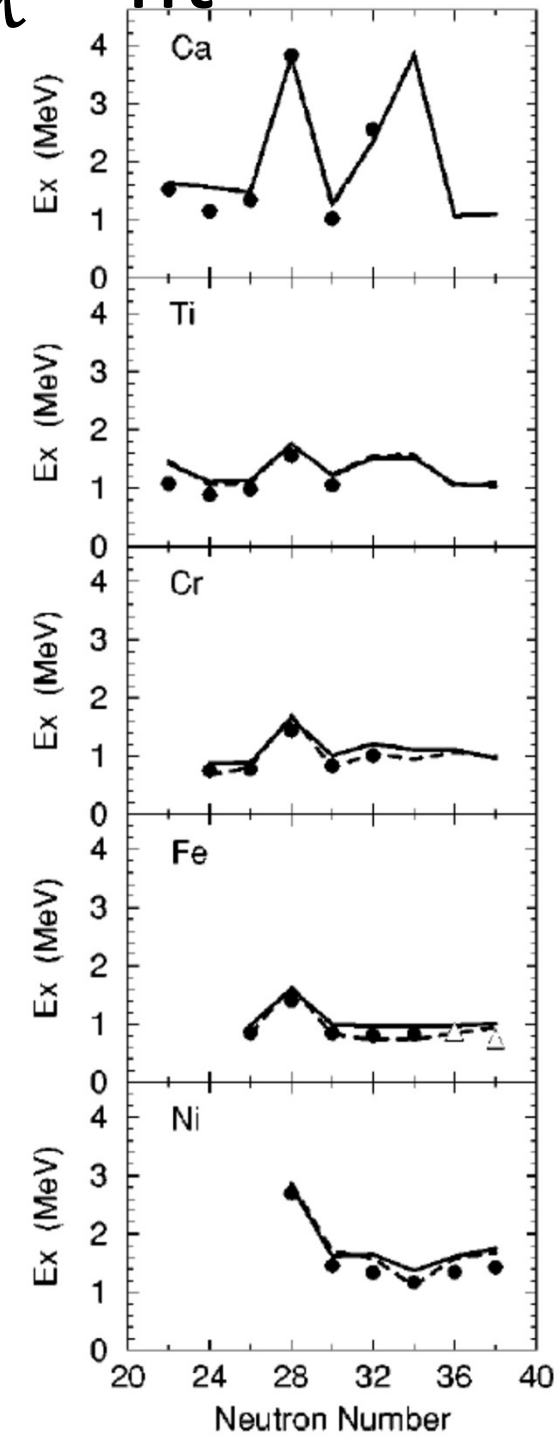
model space : *pf* shell $0f_{7/2},\ 1p_{3/2}, 1p_{1/2},\ 0f_{5/2}$



4 SPEs and 195 TBMEs

699 data of the binding energies and excitation energies are χ^2-fitted by the linear combination method.

~200 keV deviation



Ref. M. Honma, T. Otsuka, B. A. Brown, and T. Mizusaki,

Phys. Rev. C 65, 061301(R) (2002)

What is the microscopic origin of this correction?

JUN45 interaction

M. Honma, et al., Phys. Rev. C 80, 064323 (2009)

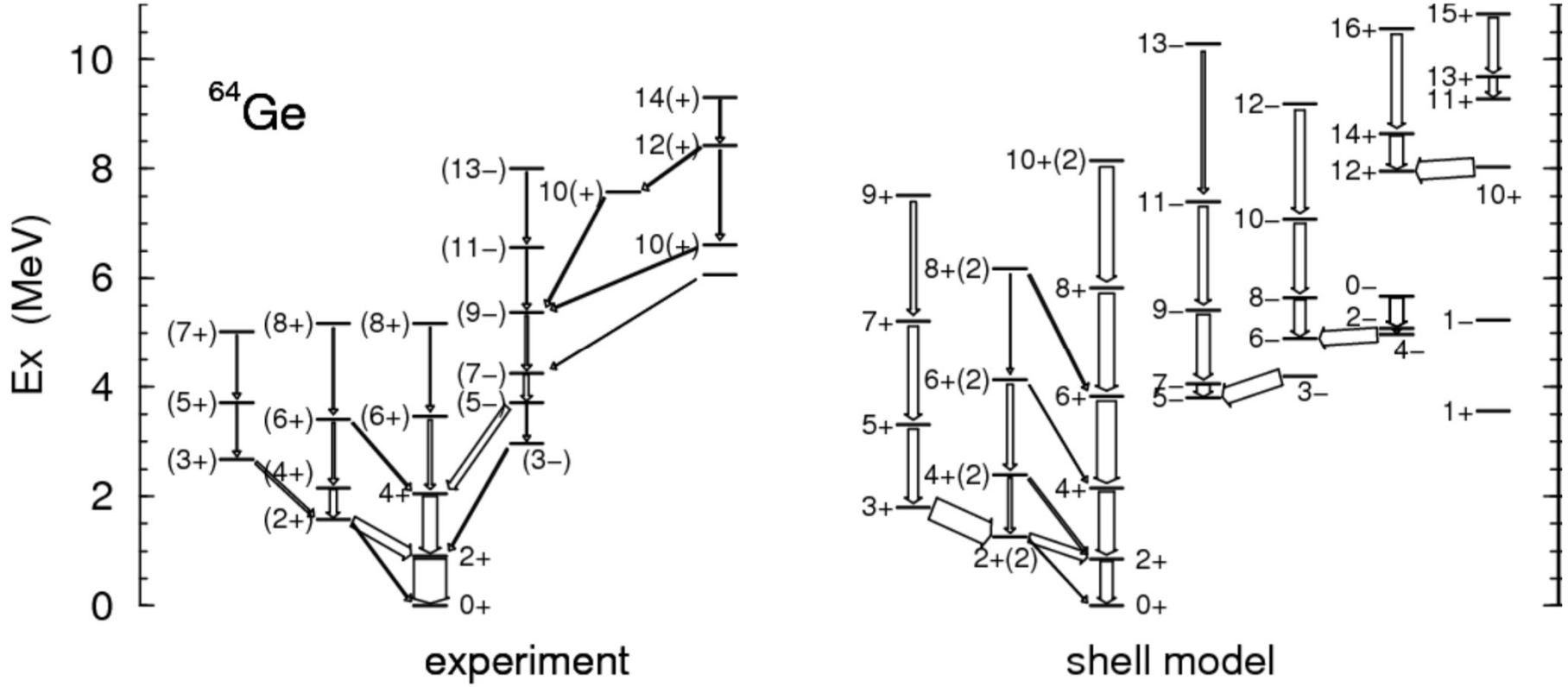
file : jun45.snt

model space : f5pg9-shell (28-50)

0f5/2, 1p3/2, 1p1/2 ^{56}Ni core

isospin-symmetric

G-matrix + 3rd order Q-box + chi2 fit for 400 data



SDPF-M interaction

Y. Utsuno *et al.,* Phys. Rev. C 60, 054315 (1999)

file: sdpf-m.snt

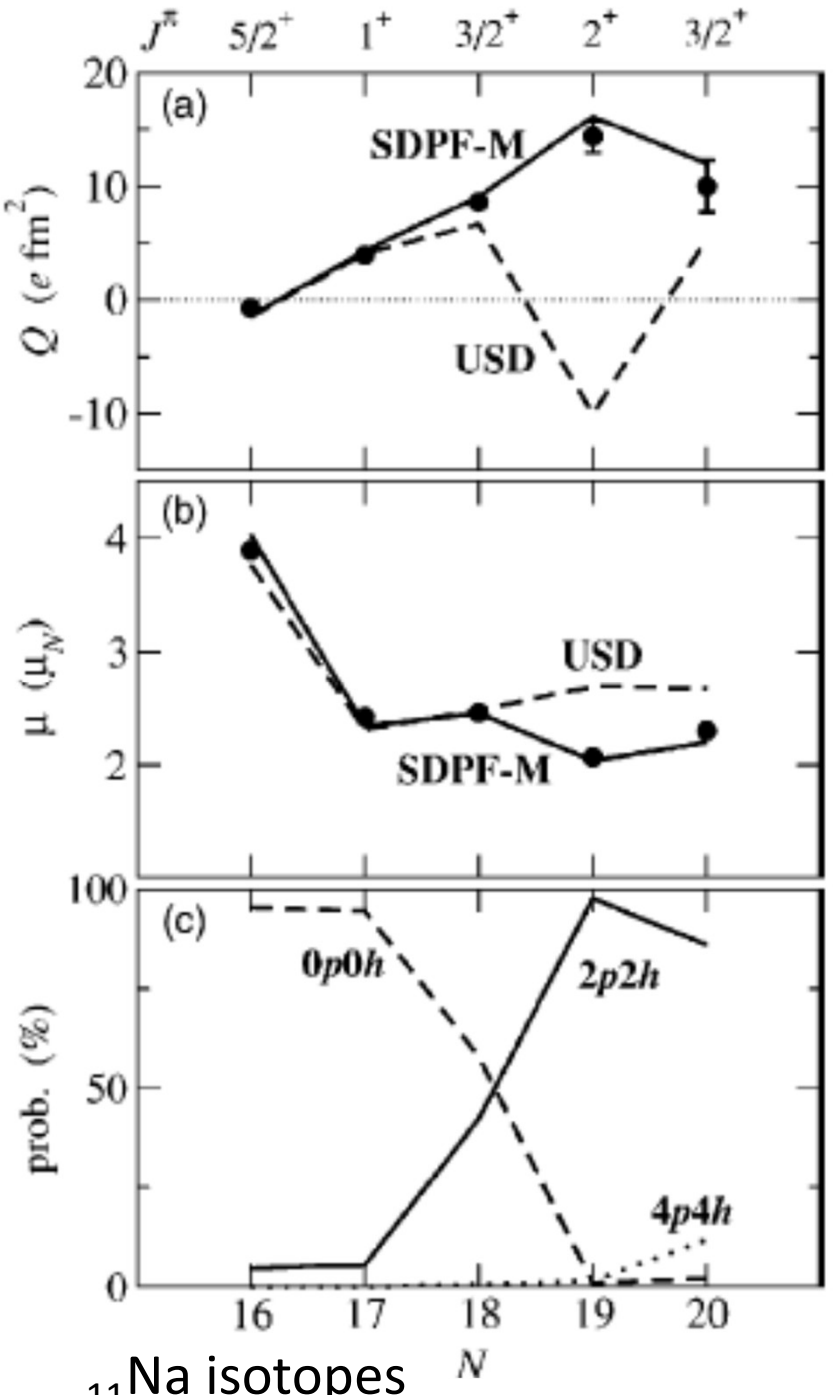
model space: sd-shell + 0f7/2 + 1p3/2

isospin symmetric

USD + Millner-Kurath + Kuo-Brown

good description for island of inversion

Note: care for contamination of center-of-mass motion



$_{11}$Na isotopes

SDPF-MU interaction

Y. Utsuno *et al.*, Phys. Rev. C 86, 051301(R) (2012).

file: sdpf-mu.snt

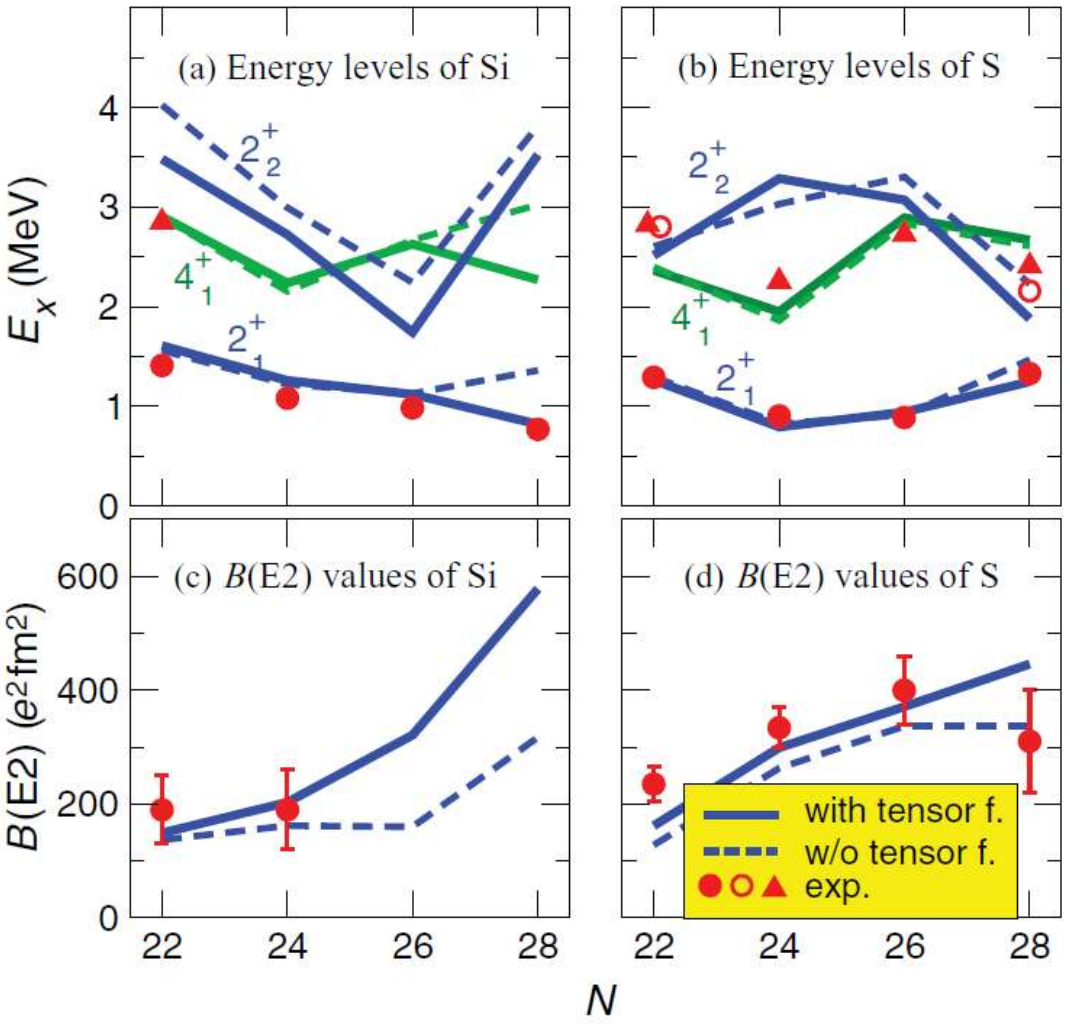
model space: sd +pf shell

isospin conserved

USD + GXPF1B + V_{MU}

good description for island of inversion

Note: $0\hbar\omega/1\hbar\omega$ truncation is assumed



Cohen-Kurath interaction

S. Cohen and D. Kurath, Nucl. Phys. 73, 1 (1965)

file : ckpot.snt

model space : p-shell

(0p3/2, 0p1/2 with ^{4}He core)

max. 84 M-scheme dim.

T-conserved

all 15 TBME fitted

phenomenologically

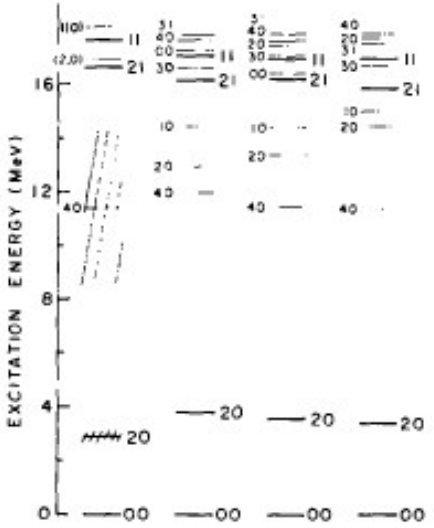


Fig. 3. The level scheme of Be^8. See caption of fig. 1 for details.

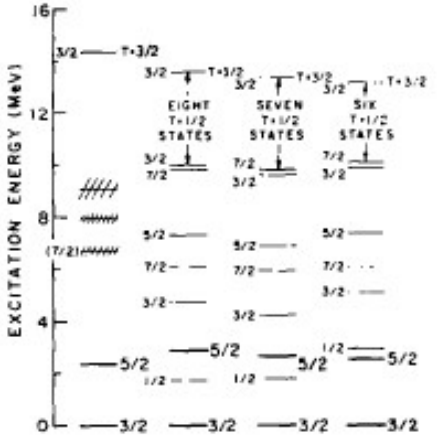


Fig. 4. The level scheme of Be^9. See caption of fig. 2 for details.

exp. ckpot

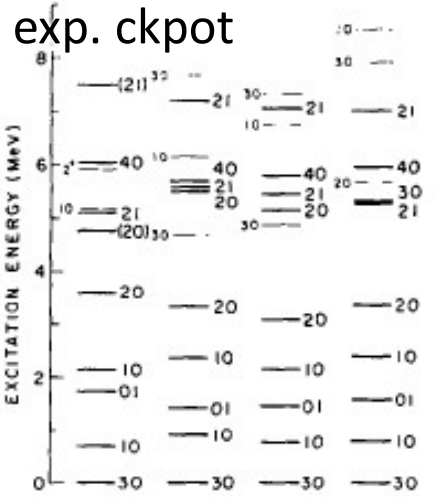


Fig. 5. The level scheme of B^{10}. See caption of fig. 1 for details.

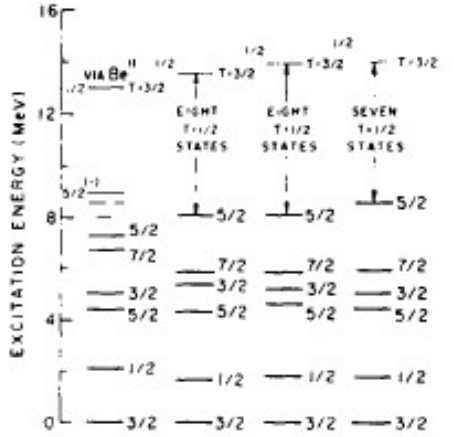


Fig. 6. The level scheme of B^{11}. See caption of fig. 2 for details.

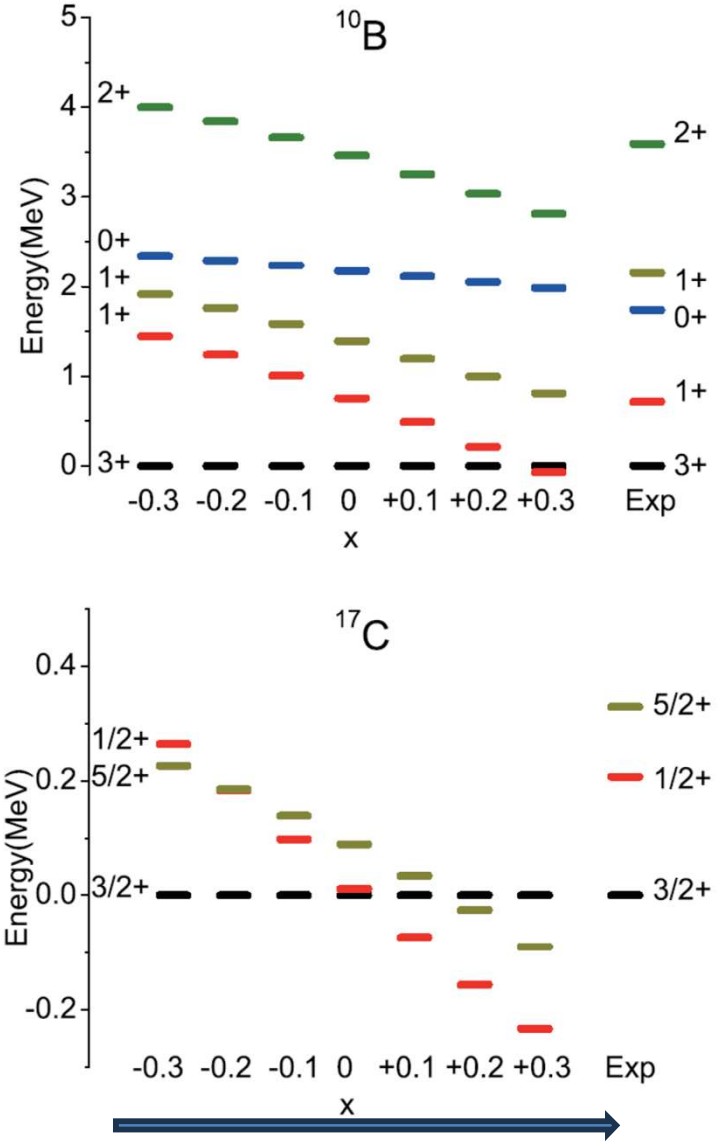
YSOX interaction

C. Yuan, T. Suzuki, T. Otsuka, F. Xu, and N. Tsunoda, Phys. Rev. C 85, 064324 (2012)

file: ysox.snt

model space: p-sd shell with 0-3$\hbar\omega$ excitations

based on Monopole-based Universal Interaction



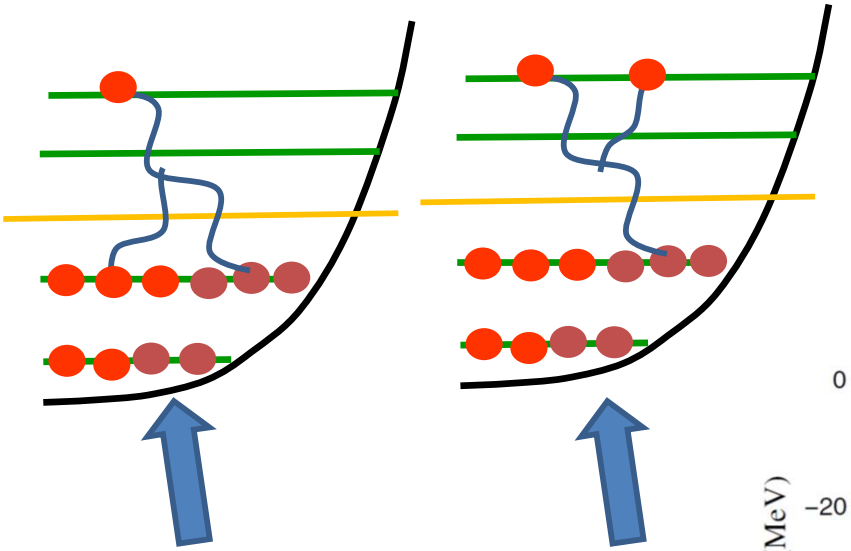
appropriate $2\hbar\omega$ configuration is necessary

What is the microscopic origin of the phenomenological correction?

Contribution of the three-body force

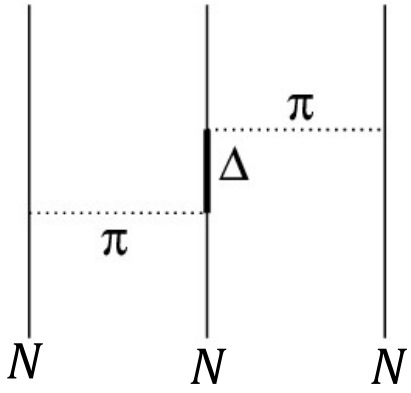
Is this phenomenological correction explained by the three-body force?

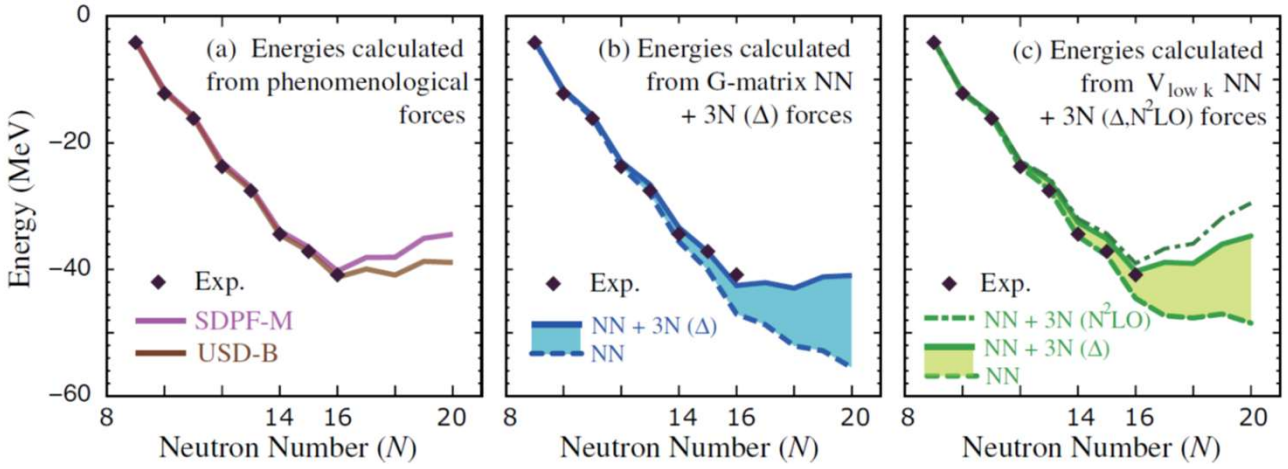
Normal ordering with the inert core



Correction to SPEs

Correction to TBMEs





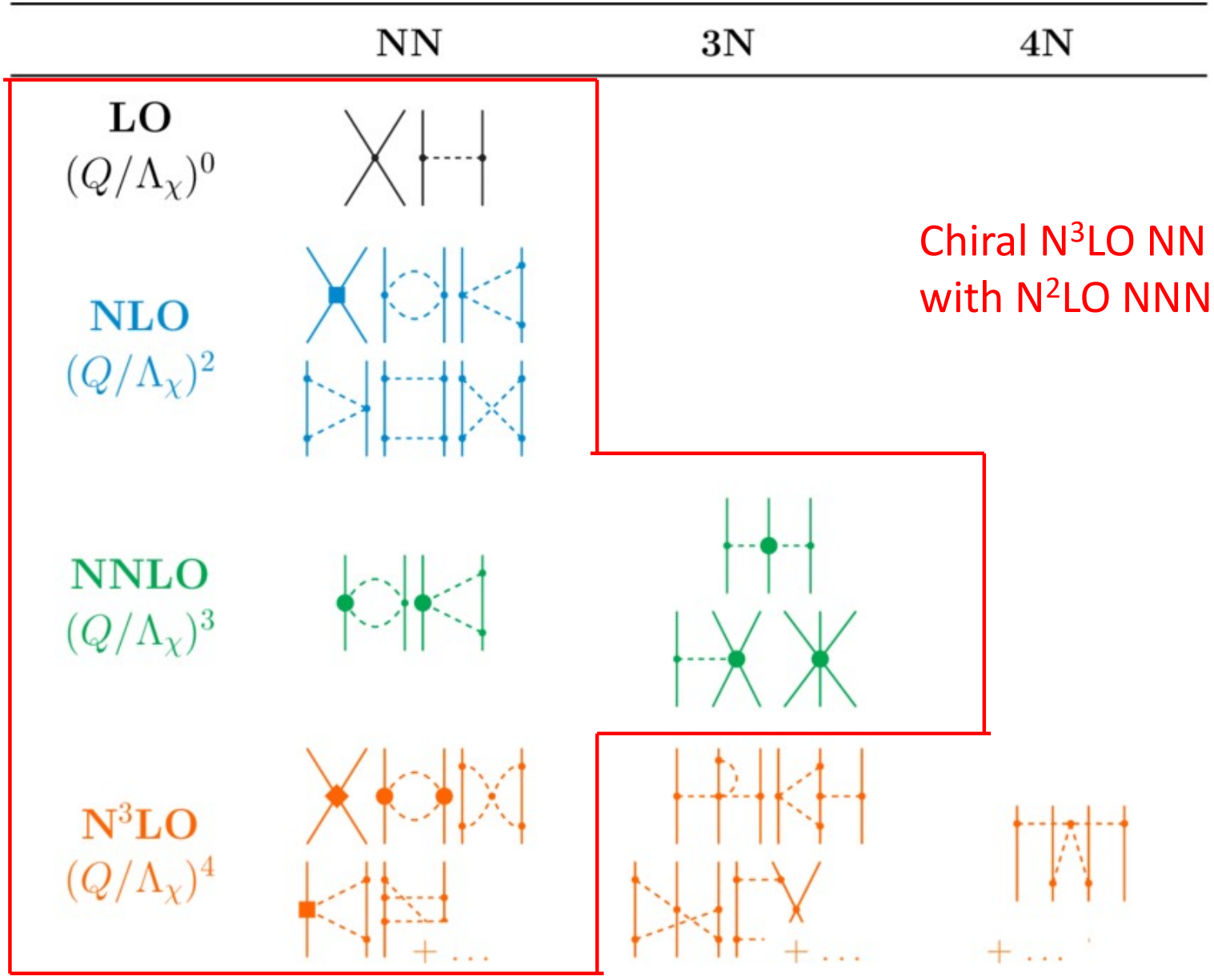
T. Otsuka, T. Suzuki, J. D. Holt, A. Schwenk, and Y. Akaishi, Phys. Rev. Lett. 105, 032501 (2010).

Ab initio construction of the shell-model Hamiltonian using the chiral EFT NN+NNN force

- Many-body perturbation theory (Realistic shell model, L. Corragio et al.)
- Valence-space In-medium Similarity Renormalization group method (S. K. Bogner, H. Hergert, J. D. Holt, T. Miyagi, A. Schwenk, S. R. Stroberg et al.)
- Coupled cluster theory (G. Hagen et al.)
- No-core shell model with core (B. R. Barrett, I. J. Shin, N. A. Smironova et al.)

Chiral effective field theory

Low-energy approach to QCD, nuclear structure energies
Approximate chiral symmetry, Systematic expansion

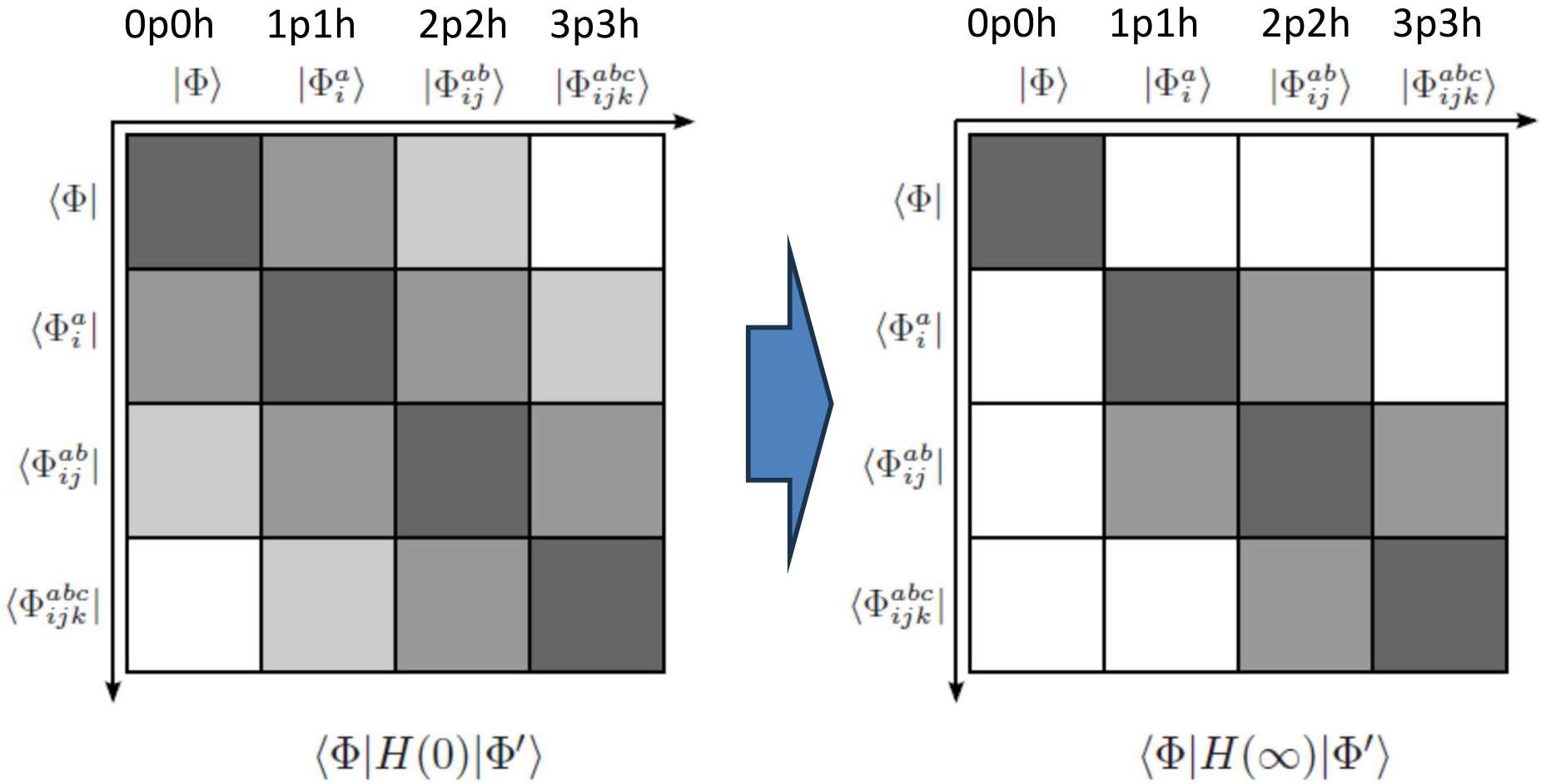


Chiral N^{3}LO NN force
with N^{2}LO NNN force

In-medium Similarity Renormalization Group (IMSRG) method

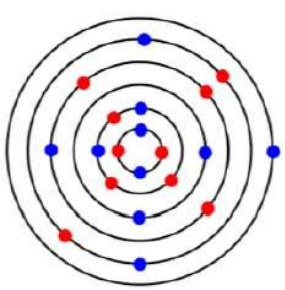
Unitary transformation to force the non-diagonal matrix elements zero.

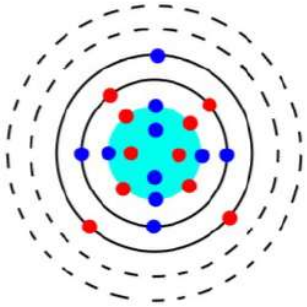
$$H(s) = U(s)HU^{\dagger}(s)$$

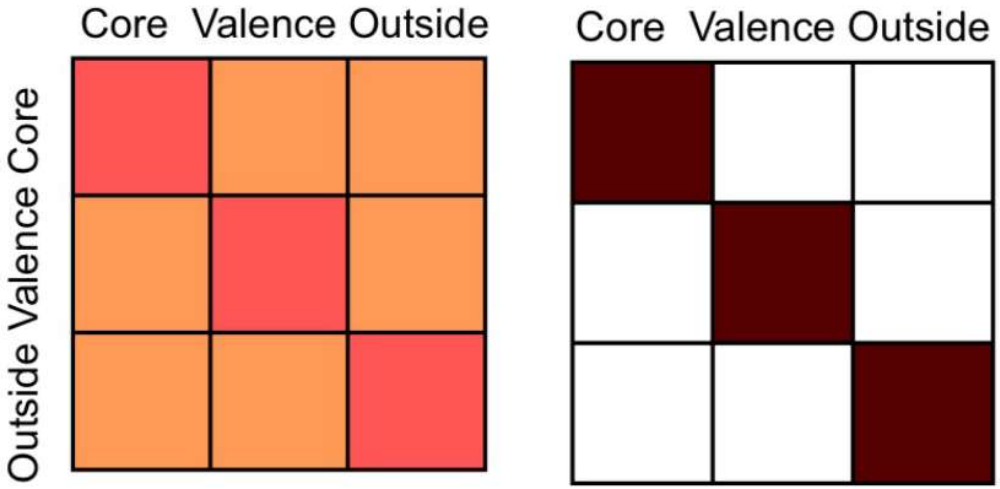


Solve “flow equation” to construct this unitary transformation (with 2-body approximation).
Effective operator has to be constructed in the same “unitary transformation”.

Valence-space IMSRG (VS-IMSRG)



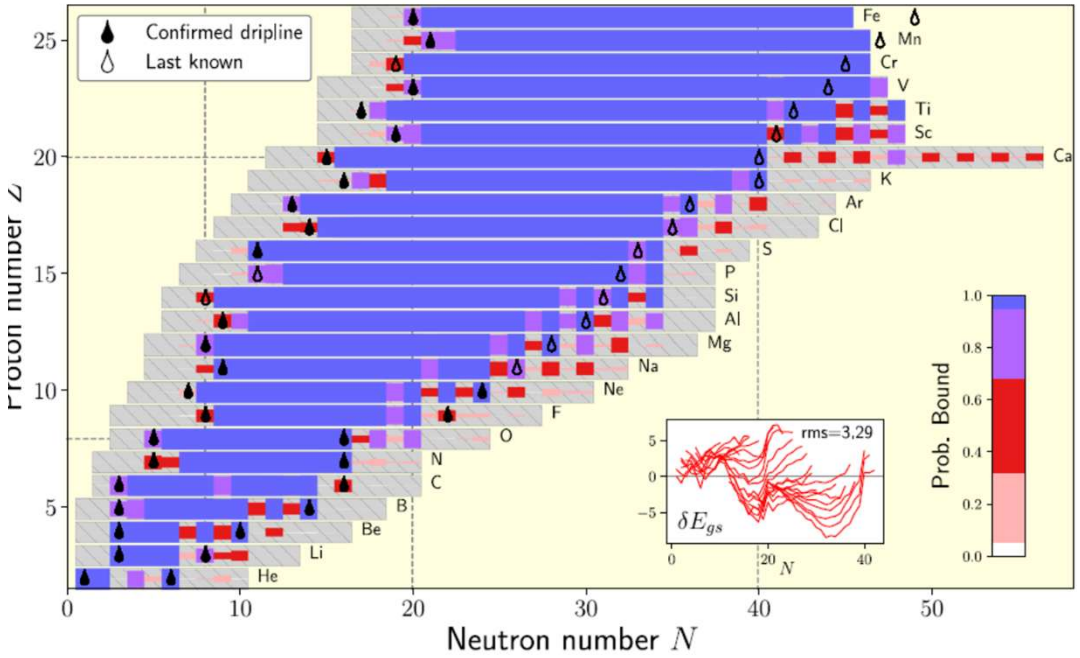




$$\langle i|H_0|j\rangle \qquad \langle i|H(s)|j\rangle$$

Unitary transformation

$$H(s) = U(s)H_0U^\dagger(s)$$



S. R. Stroberg, J. D. Holt, A. Schwenk, and J. Simons, Phys. Rev. Lett. 126, 022501 (2021)

A workflow for “ab initio” shell model calc. (VS-IMSRG)

- NuHamil: T. Miyagi, Eur. Phys. J. A 59, 150 (2023).
  - https://github.com/Takayuki-Miyagi/NuHamil-public
  - Chiral EFT NN+NNN force (EMN, N^3LO_{lnl}, EM500, ΔN^2LO_{GO}, …)
  - SRG evolution in momentum space

HO matrix elements

- imsrg++: R. Stroberg *et al.,* Ann. Rev. Nucl. Part. Sci. 69, 307 (2019).
  - https://github.com/ragnarstroberg/imsrg
  - VS-IMSRG evolution to construct the operators in “model space”

snt file, effective operator

- KSHELL: N. Shimizu *et al.*, Comp. Phys. Comm. 244, 372 (2019).
  - https://sites.google.com/alumni.tsukuba.ac.jp/kshell-nuclear/
  - Many-body solver (shell-model calc.)

Summary

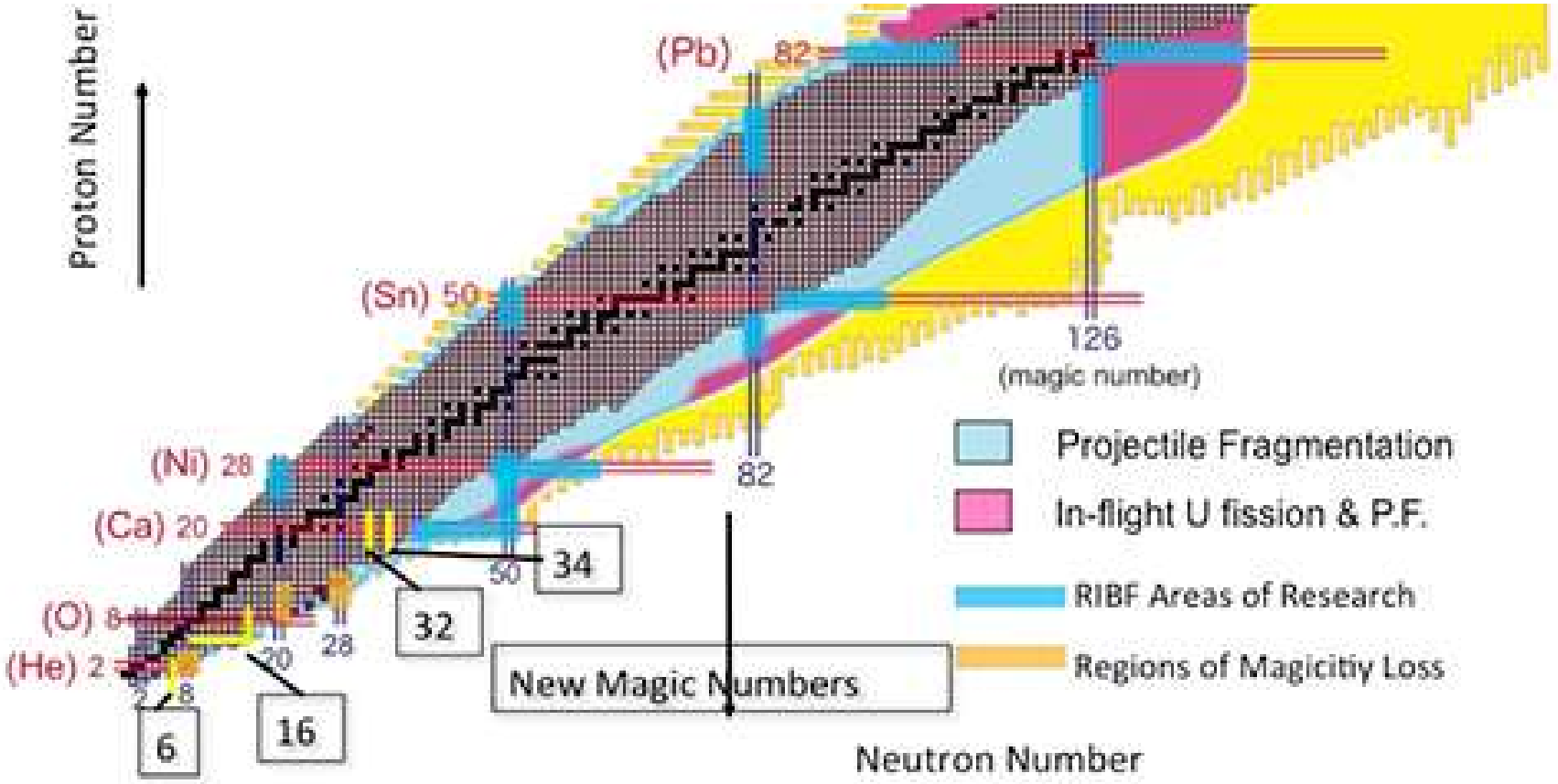
- Conventional shell-model Hamiltonian in 1980s - 2000s
  - NN-force + G-matrix + MBPT + empirical fit for exp. data in the model-space
  - You can easily perform shell-model calculations using the prepared interactions. It is a first choice for the comparison with the experimental data.

- NNN-force is essential to construct the SM Hamiltonian nonempirically
  - Modern ab initio theories to treat NN+NNN force were proposed in 2010s
  - Enthusiastically developed and successful, but quadrupole collectivity is challenge.
  - Many source codes are in public while expertise are required.

Monopole interaction, effective single particle energies, and shell evolution

Magic numbers are not constants

The gaps at 8, 20, 28 were established on nuclei near stability. Moving to large neutron excess, some of them close and new ones open.



From RIKEN Nishina Center

Anatomy of realistic shell-model interaction

M. Dufour, A. P. Zuker Phys. Rev. C 54, 1641 (1996)

$$H = H_m + H_M$$

H (full)

Every TBME, all J and T.

A complete but unreadable specification of the physics.

=

H_mono

Monopole interaction:
The angular-momentum averaged part.

- bulk binding energies
- effective single-particle energies and shell gaps

+

H_multi

Everything left over.

- pairing (J = 0)
- quadrupole (Q · Q)
- collectivity, deformation

Pairing and QQ scales with $A^{-1/3}$

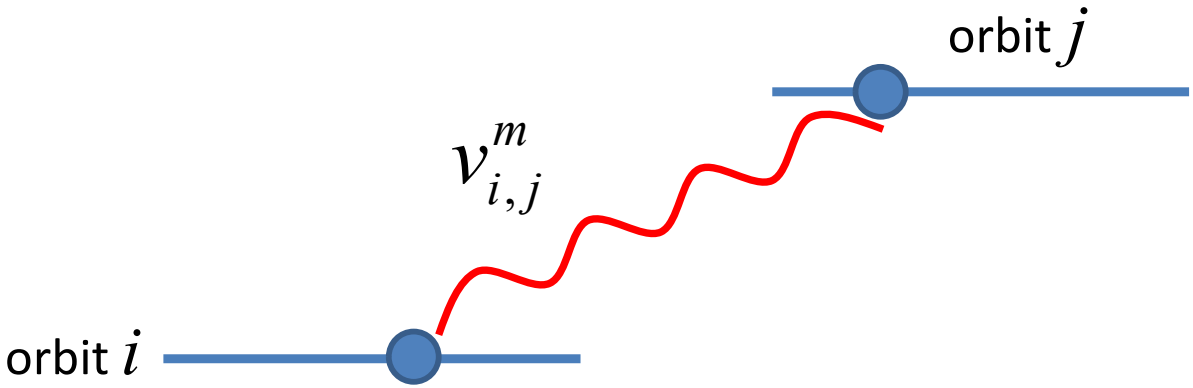
The two parts act on different things: the monopole term is diagonal in the occupation numbers and moves whole orbits, while the multipole term mixes configurations and builds collective states.

Multipole-part is rather universal. Fine tuning is often required for the monopole part.

Monopole interaction

$$v^m_{i,j} = \frac{\sum_J (2J+1)\langle ij\,J|V|ij\,J\rangle}{\sum_J (2J+1)}$$

sum matrix elements concerning any allowed J.



"average" potential between orbit i and orbit j.

"Effective single-particle energies" and its variation are discussed using this monopole interaction.
Pairing ($J = 0$) matrix element contributes weakly.

R. K. Bansal and J. B. French, Phys. Lett. **11**, 145 (1964)

What the monopole part controls

$$H_{\text{mono}} = \sum_a \varepsilon_a n_a + \sum_{a<b} V_{ab} n_a n_b + \sum_a V_{aa} \frac{n_a(n_a - 1)}{2}$$

It does

- Bulk binding energy of closed shells
- Saturation along an isotopic chain
- Effective single-particle energies
- Position and size of shell gaps
- Where the drip line falls

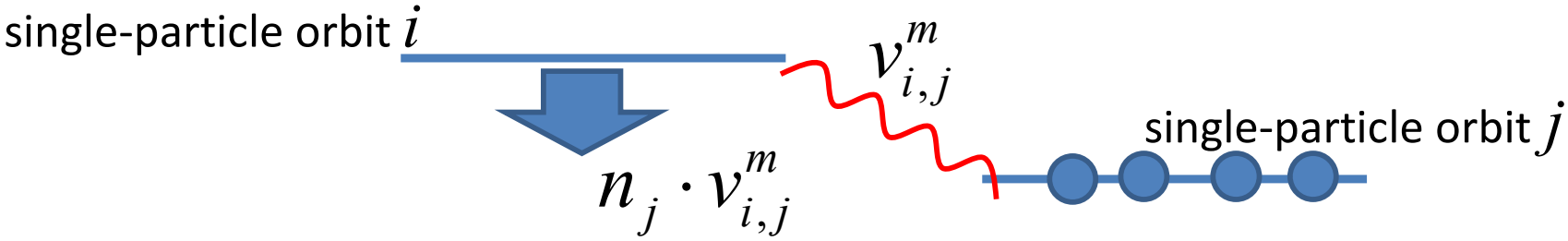
It does not

- Pairing gaps and odd-even staggering
- B(E2) strengths
- Deformation and rotational bands
- Configuration mixing
- Level ordering within a multiplet

Effective single-particle energy (ESPE)

configuration (occupancy in the valence space) can change the single-particle energies

$$H_{mono} = \sum_i \varepsilon_i \hat{n}_i + \frac{1}{2}\sum_{i,j} v^m_{i,j} : \hat{n}_i \hat{n}_j :$$



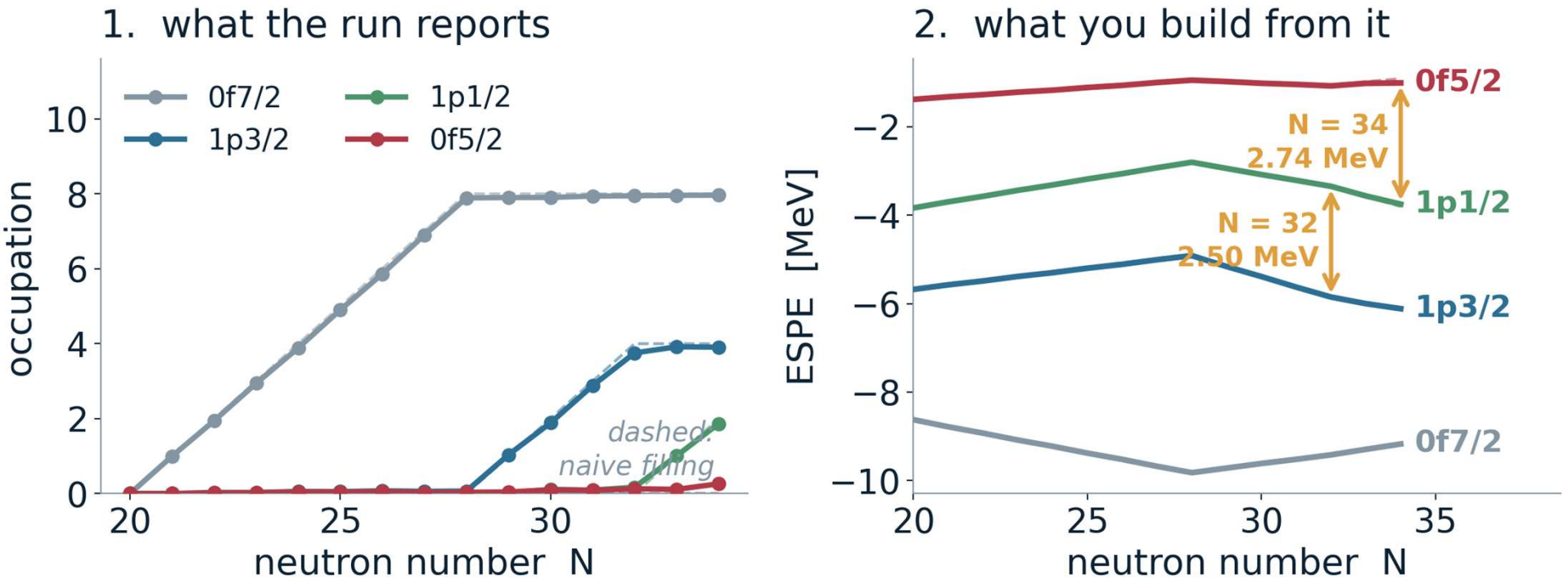
Summation of the contributions from all orbits

$$\varepsilon_i(\{n_j\}) \approx \varepsilon_i^{(0)} + \sum_j n_j \cdot v^m_{i,j}$$

Y. Utsuno T. Otsuka, T. Mizusaki and M. Honma, Phys. Rev. C **60**, 054315 (1999).

Occupations plus monopoles gives the ESPE

$$\mathrm{ESPE}(a) = \varepsilon_a + \sum_b V_{ab}\langle n_b \rangle$$



Ca isotopes, GXPF1Br2, full pf shell; occupations from the ground state of each diagonalisation

Natural filling configuration (particles occupy the lowest unoccupied orbit) is used for $\langle n_b \rangle$.
In heavier nuclei, $\langle n_b \rangle$ of the shell-model results is adopted.

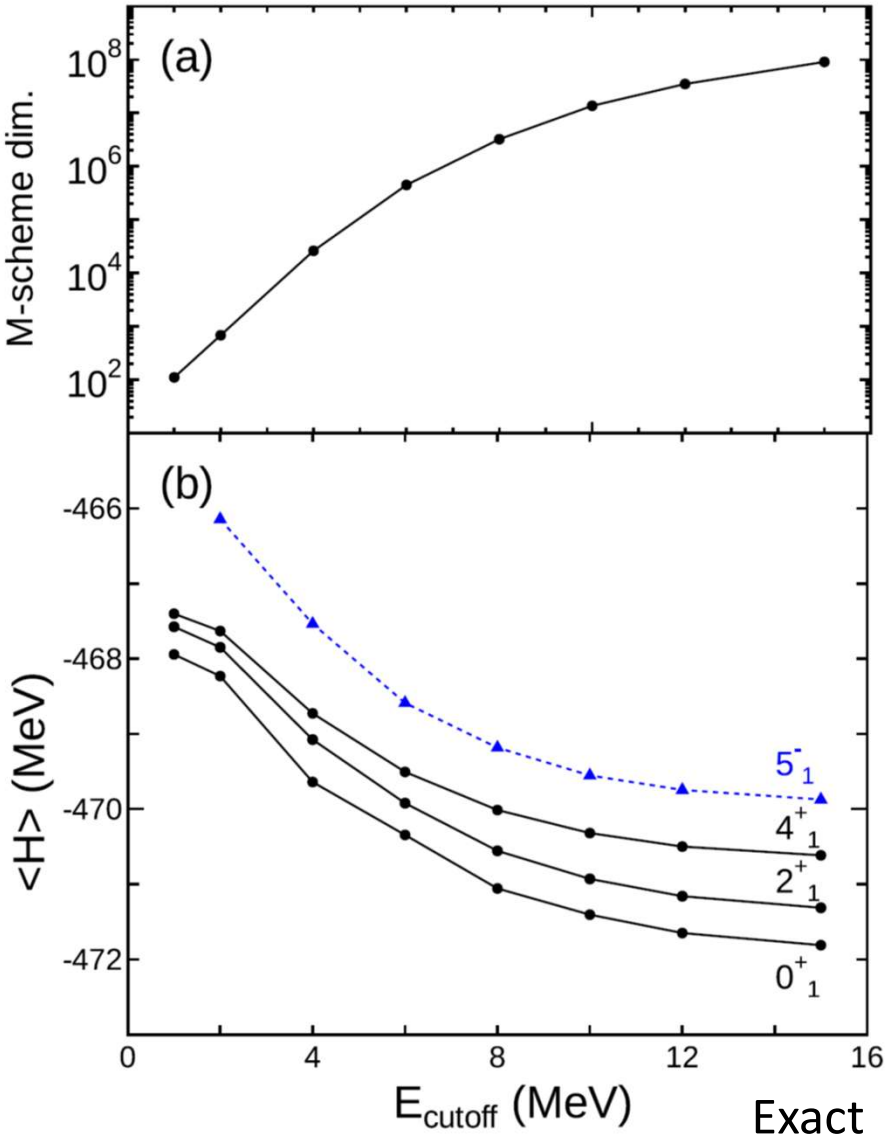
Monopole-based truncation

```
truncation for "+" parity state in  Mg20_w_p.ptn
truncation scheme ?
      0 : No truncation (default)
      1 : particle-hole truncation for orbit(s)
      2 : hw truncation
      3 : Both (1) and (2)
      4 : Monopole-based partition truncation
```

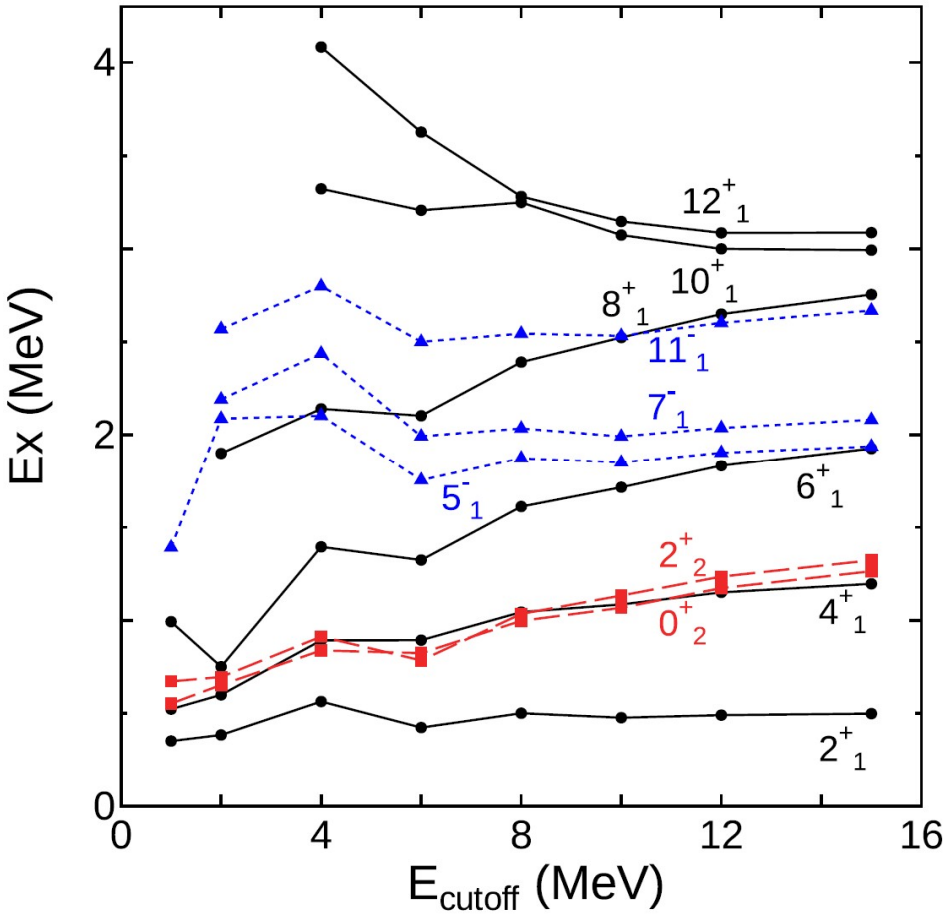
- Full model space is split into “partitions”, which is labeled a set of occupation numbers of each orbit : $(n_1, n_2, \cdots, n_a)$.
- Compute monopole energy of each partition and include it into the model space if the energy is below a certain threshold.

$$\text{any } |M\rangle \quad \text{for} \quad \langle M|H_{mono}|M\rangle < E_{\min} + E_{\text{cutoff}}$$

Monopole truncation ^{200}Hg



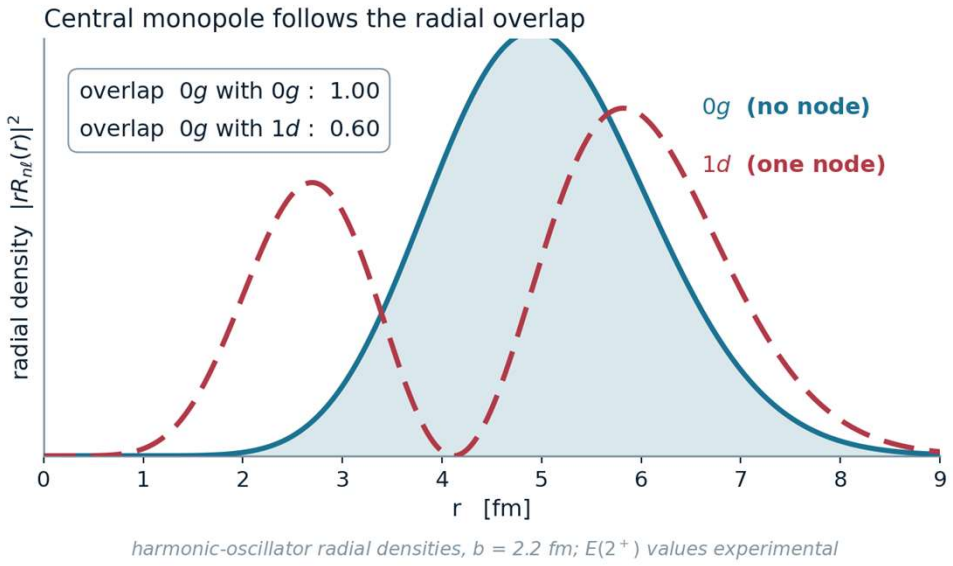
Exact

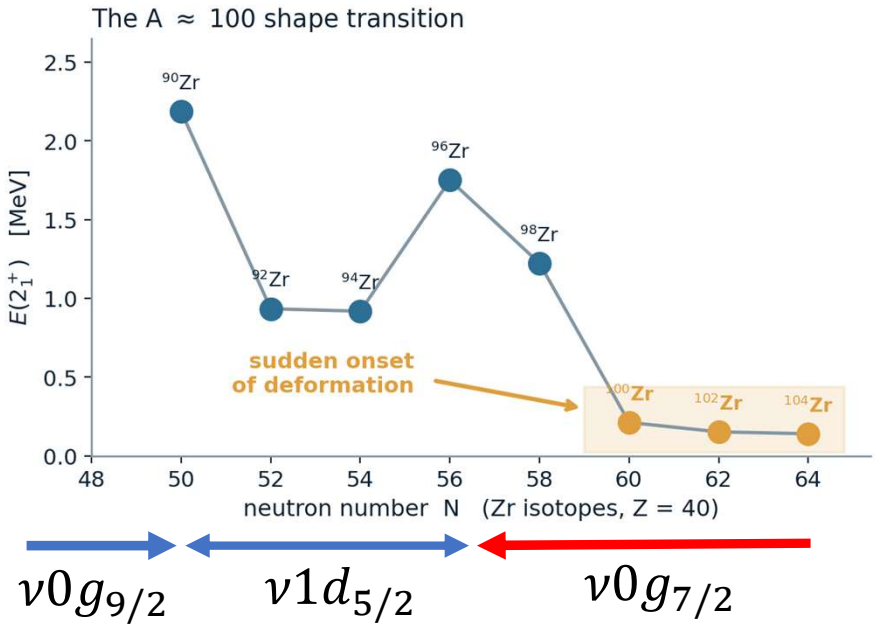


The central-force monopole: Federman and Pittel

Federman and Pittel, Phys. Lett. B 69 (1977) 385; Phys. Rev. C 20 (1979) 820

$Ex(2^+)$ of Zr isotopes





Overlap, not alignment

The central monopole tracks the spatial overlap of the two radial wave functions — largest between orbits sharing a node number and a similar orbital angular momentum. Spin-orbit partners are the extreme case.

$$n_\pi = n_\nu$$
$$l_\pi = l_\nu, or\ l_\nu \pm 1$$

The mechanism

The strongly attractive **π 0g9/2 – ν 0g7/2** monopole lowers the proton g9/2 orbit as neutrons fill g7/2, eroding the Z = 40 subshell and releasing quadrupole correlations.

The signature

E(2+) in Zr collapses from 1223 keV at N = 58 to 212 keV at N = 60 — one of the sharpest shape transitions on the chart.

Z=40 subshell gap locates between pf shell and $\pi 0g_{9/2}$

Tensor force monopole: Otsuka *et al.*

- Monopole part of the tensor force satisfies:

$$(2j_> + 1)V^T_{j_>,j'} + (2j_< + 1)V^T_{j_<,j'} = 0,$$

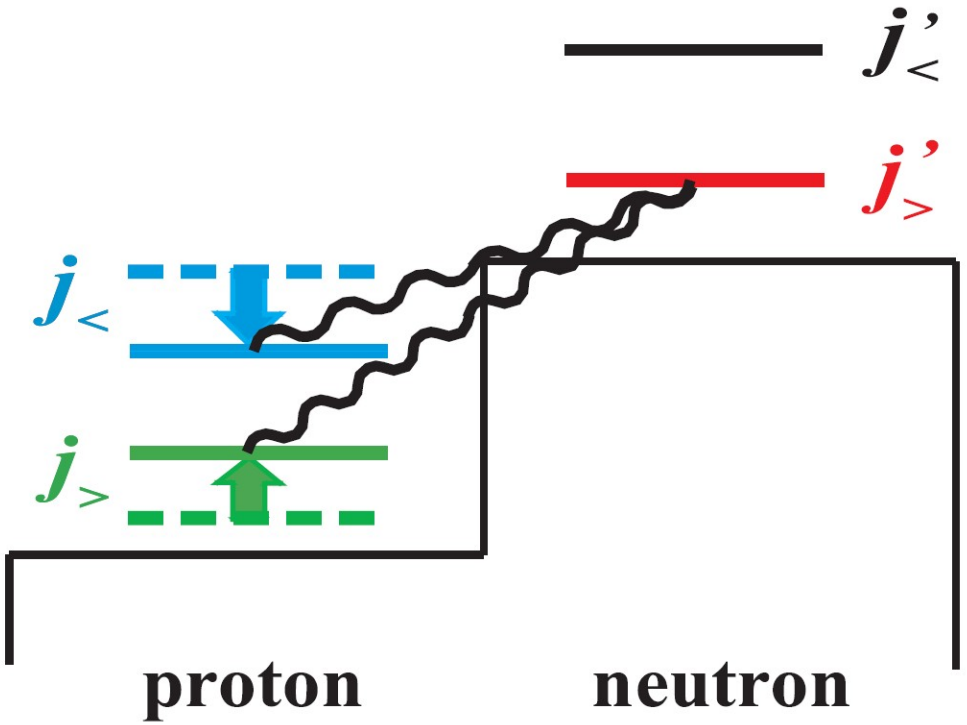
$j_> = l + 1/2$
$j_< = l - 1/2$
e.g. $(j_>, j_<) = (f_{7/2}, f_{5/2})$

repulsive : $j_< \sim j'_<$, $j_> \sim j'_>$
attractive : $j_< \sim j'_>$, $j_> \sim j'_<$

That of the proton-neutron interaction strongly affects the spin-orbit splitting.

Filling j> shrinks ls splitting.

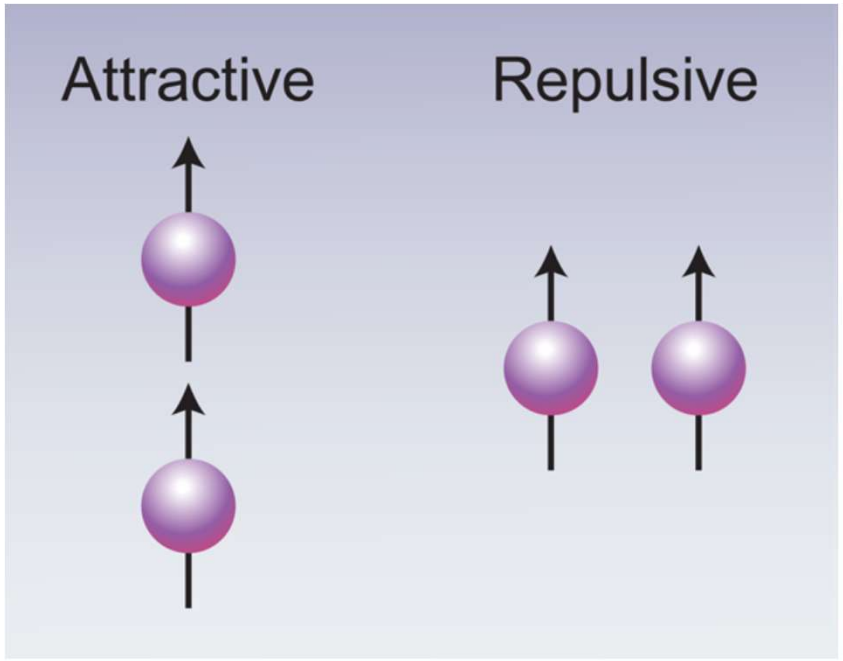
Filling j< restores it.

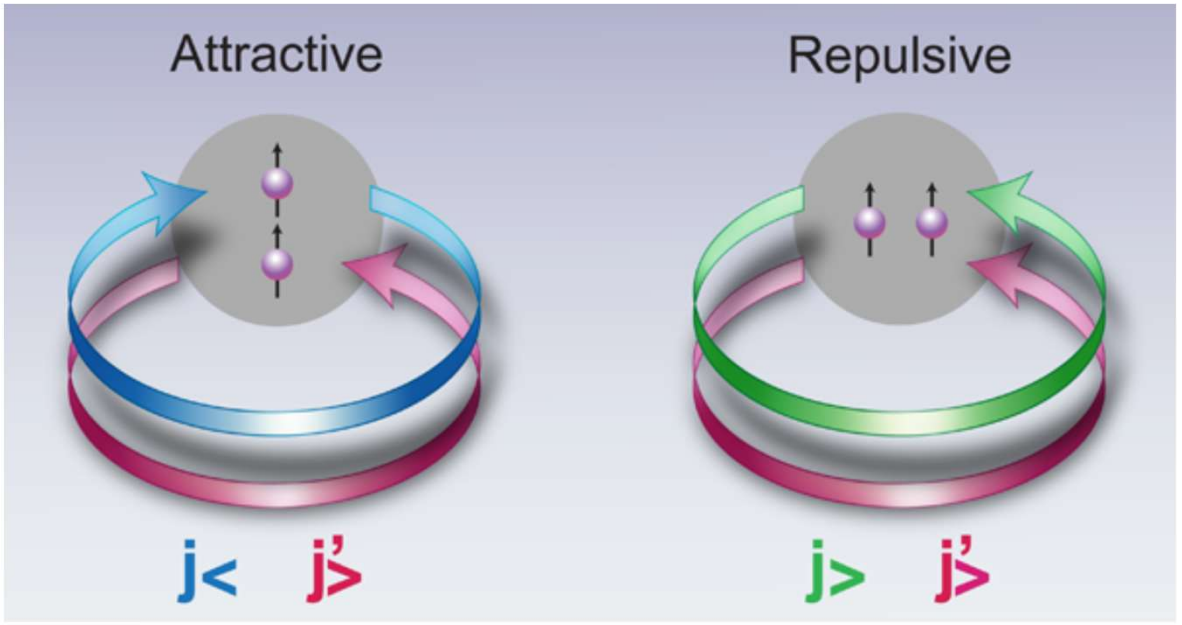


Ref. T. Otsuka *et al.,* Phys. Rev. Lett. 95, 232502 (2005)

Tensor force

$$V_T = (\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2) f(r) S_{12}, \qquad S_{12} = 3(\boldsymbol{\sigma}_1 \cdot \hat{\boldsymbol{r}})(\boldsymbol{\sigma}_2 \cdot \hat{\boldsymbol{r}}) - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$



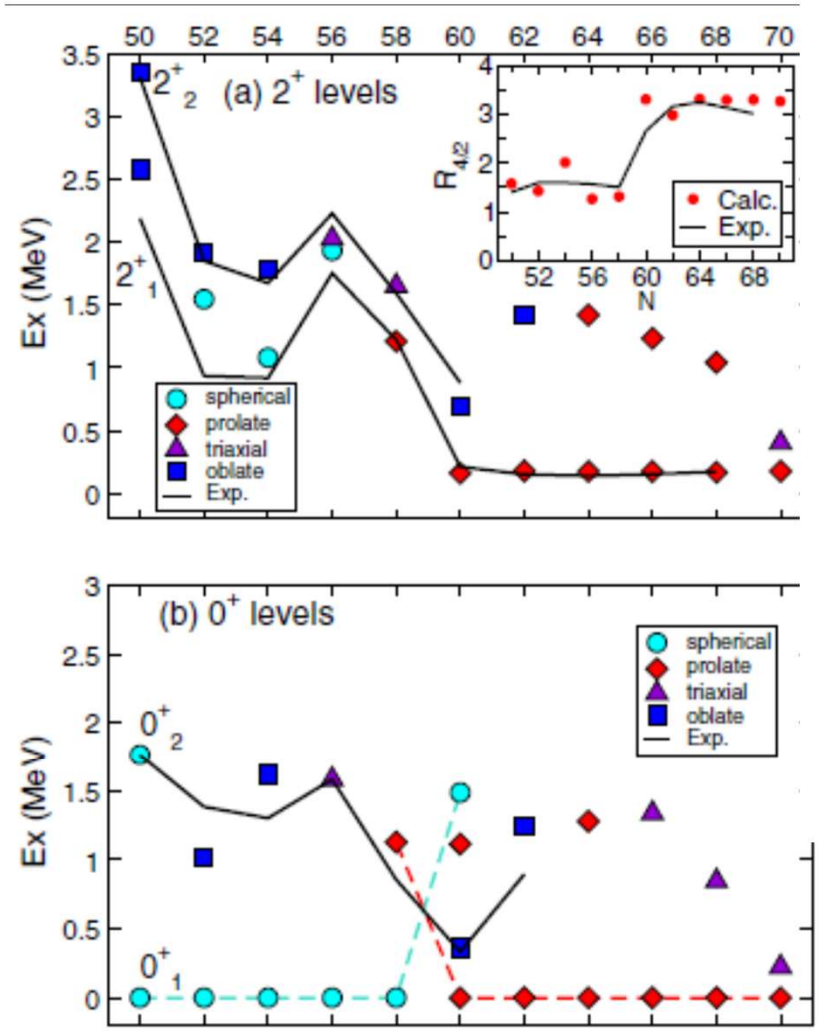


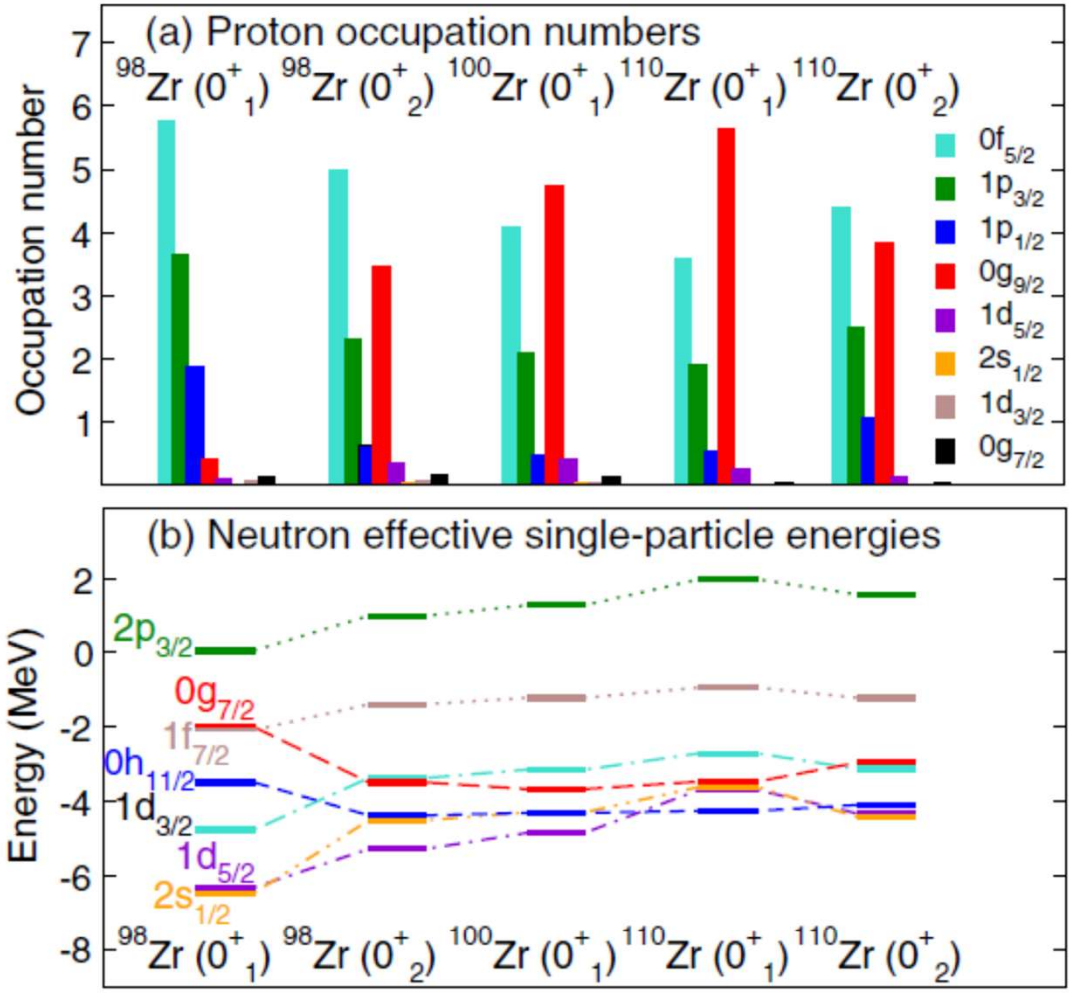
$$(2j_> + 1)V^T_{j_>,j'} + (2j_< + 1)V^T_{j_<,j'} = 0,$$

J. P. Schiffer, Viewpoint, Physics 3, 2 (2010)

Zr isotopes again

proton g9/2 occupied in deformed states



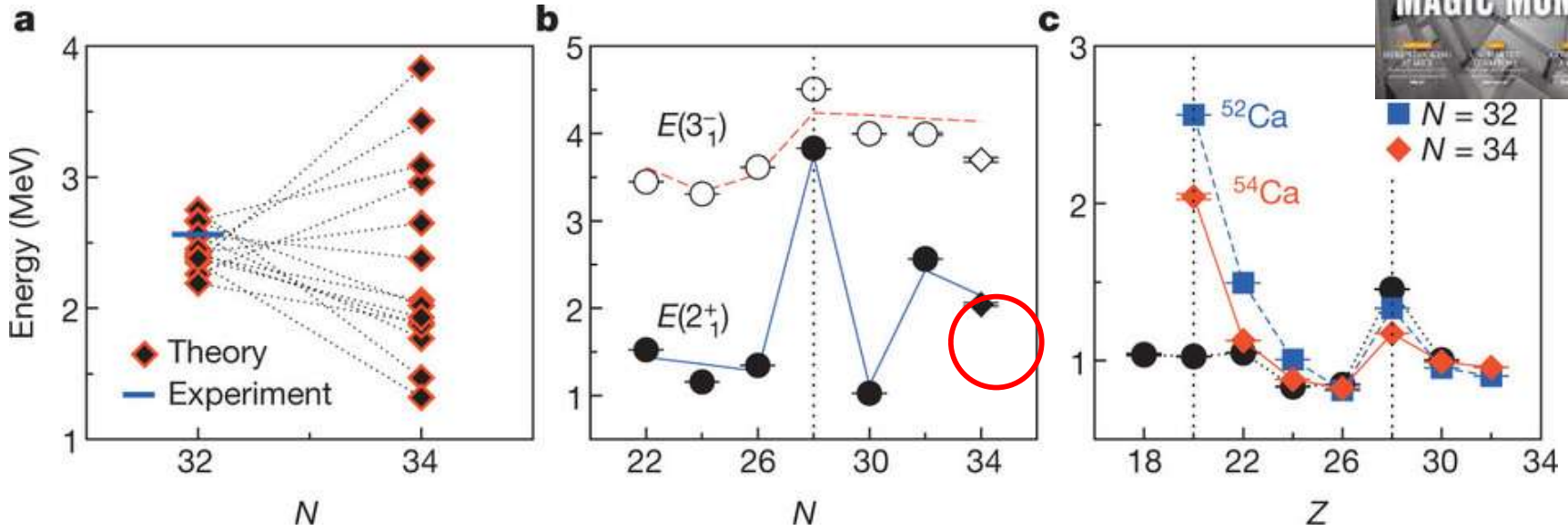


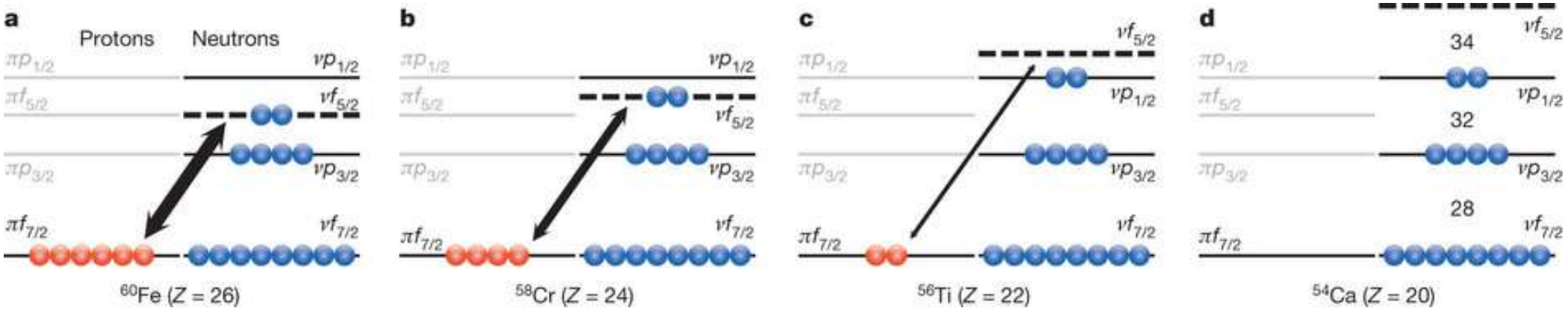
neutron g7/2 drops down by the occupation of proton g9/2 with the central and tensor monopoles coherently.

Togashi et al., PRL 117, 172502 (2016)

^{54}Ca and N=34 magicity

2^+ Excitation energies of Ca isotopes

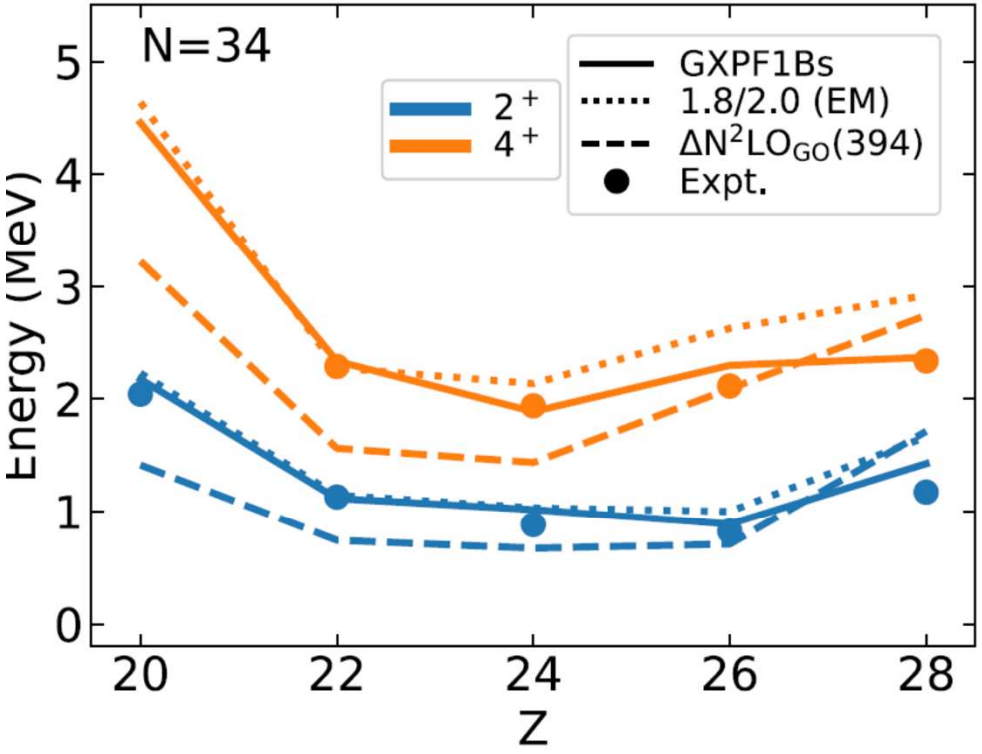


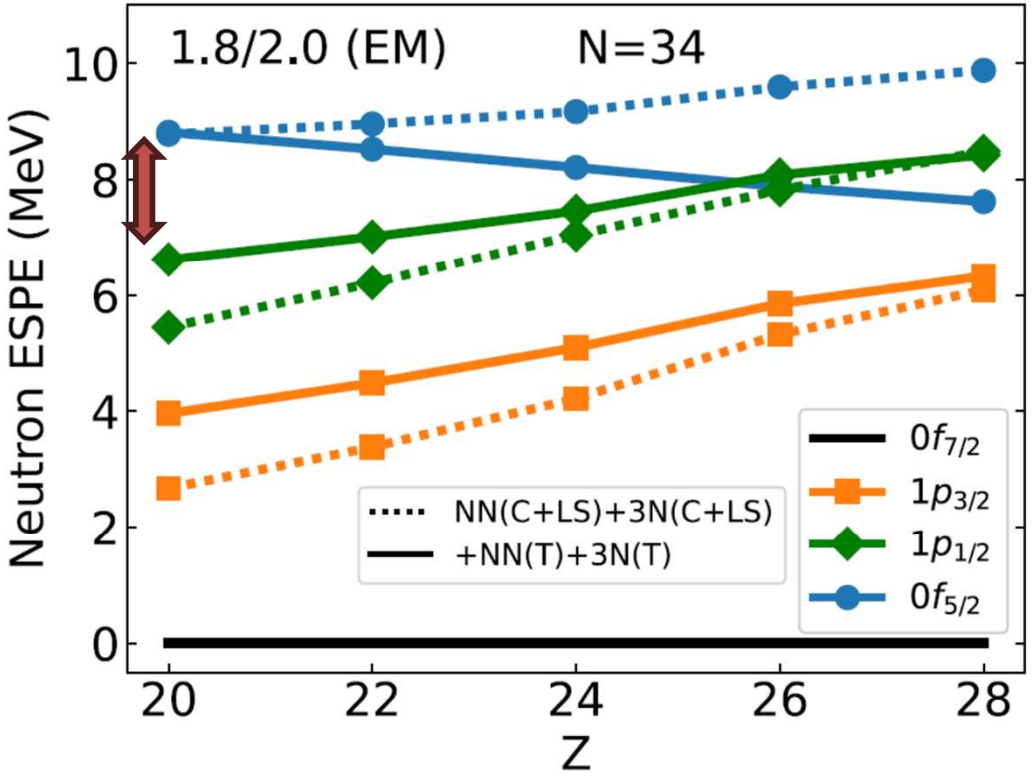


tensor monpole gives strong attraction between $\pi f_{7/2}$ and $\nu f_{5/2}$ orbits

D Steppenbeck *et al. Nature* **502**, 207-210 (2013) doi:10.1038/nature12522

shell evolution of N=34 isotones by “ab initio” VS-IMSRG





- Tensor monopole reduces the N=34 gap as Z increases.
- NNN force enhances the tensor monopole by 17%.

A. Kumar, T. Miyagi, and N. Shimizu, Phys. Lett. B 880 140801 (2026)

Summary

- Shell-model Hamiltonian
  - Monopole interaction
    - Central monopole is strong for $\Delta n = 0, \Delta l = 0$ pn-pair orbits
    - tensor monopole: $j_> - j_>$, $j_< - j_<$ repulsive, $j_> - j_<$ attractive
    - ESPE, shell gap, shell evolution
  - Multipole interaction
    - pairing and QQ interactions dominate collectivity

- Effective single-particle energies and shell evolution
  - Monopole interaction causes the change of effective single-particle energies by filling orbits
  - It affects shell gap, magic number, and deformation

Collaborators

- Kazunari Kaneko (Kyusyu Tech)
- Anil Kumar (Tsukuba)
- Takayuki Miyagi (Tsukuba)
- Takahiro Mizusaki (Senshu)
- Takaharu Otsuka (RIKEN/Tokyo)
- Yang Sun (SJTU)
- Naofumi Tsunoda (Tokyo)
- Yusuke Tsunoda (Tsukuba)
- Tomoaki Togashi (Tokyo)
- Yutaka Utsuno (JAEA/CNS Tokyo)

- and many others.