JICFuS

Priority Issue 9
to be Tackled by Using Post K Computer
"Elucidation of the Fundamental Laws
and Evolution of the Universe"
KAKENHI grant 17K05433, 25870168

CNS Summer school 2019
2019/08/21-27, Hongo, The University of Tokyo

Nuclear shell model calculations
– basics and practices –

1. shell model

CENTER for NUCLEAR STUDY

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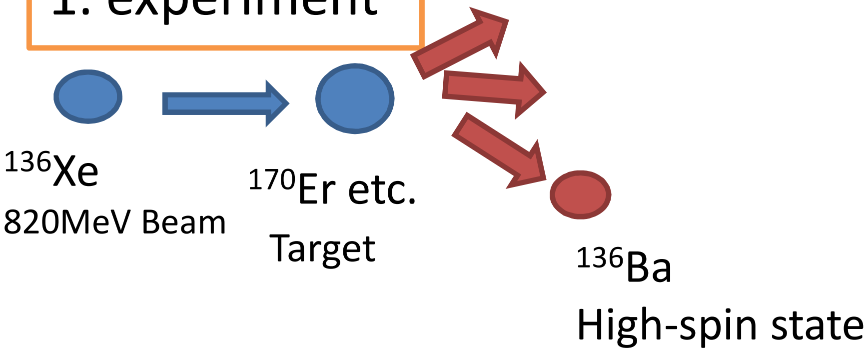
Outline

- What is shell-model calculations?
  - Configuration mixing
  - M-scheme and J-scheme
  - Effective interaction
- Shell-model code “KSHELL”
  - Performance
  - demonstration of the code
  - homework for Sunday
- Inside “KSHELL”
  - Truncation
  - Massively parallel computation and its performance
  - Algorithm and thick-restart block Lanczos method
  - Recent progress of shell-model studies

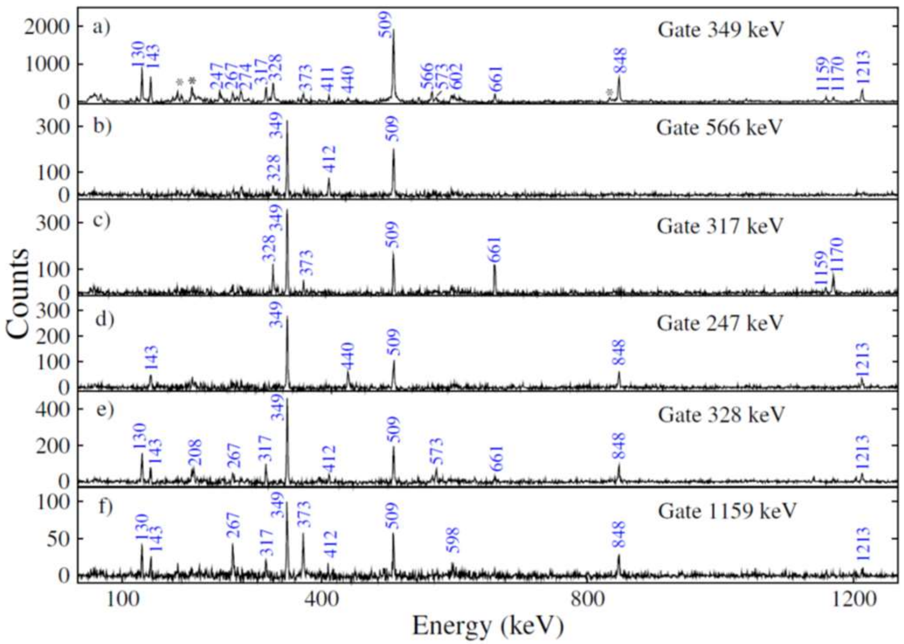
C. Petrache *et al.*, in prep.

Example of gamma-ray spectroscopy

1. experiment

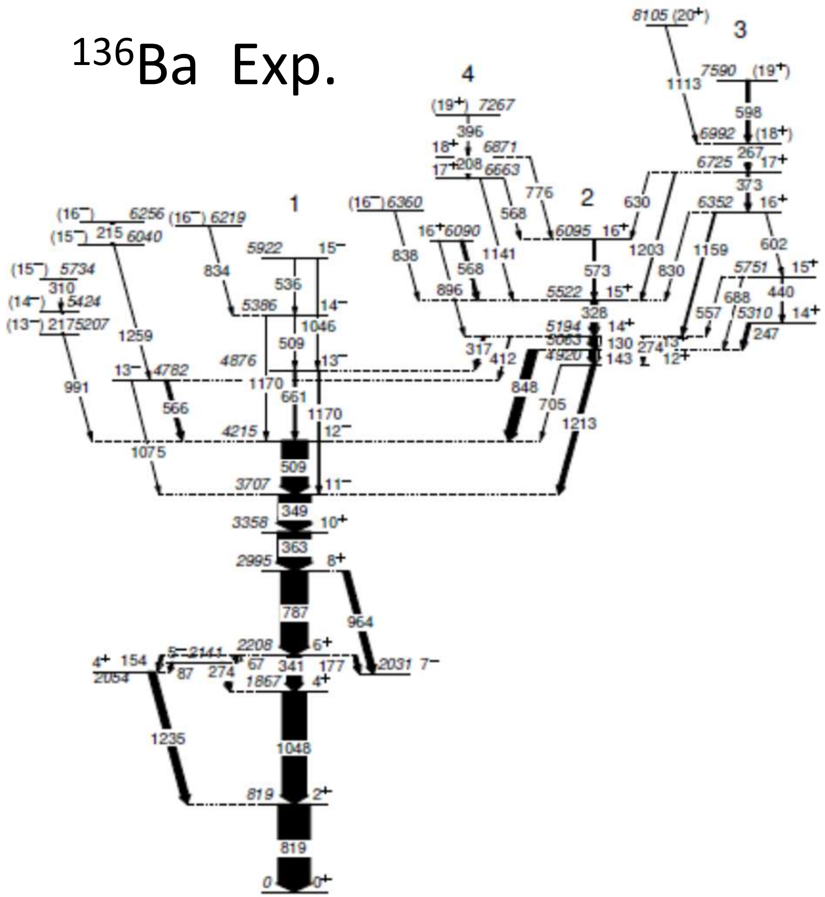


2. Measure deexcitation gamma rays



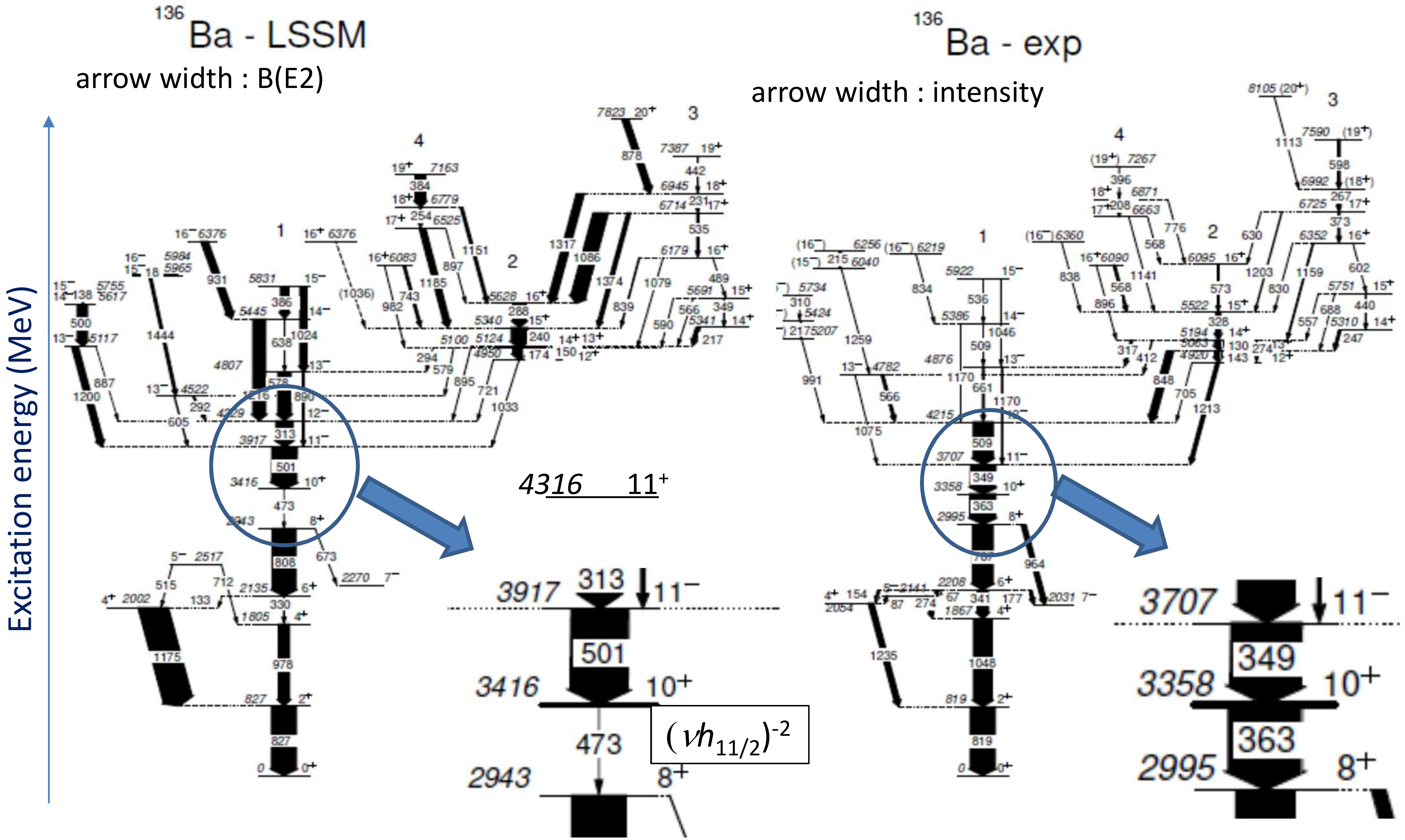
3. identify and discuss levels

^{136}Ba Exp.



Shell-model calculation is the first choice to be compared.

$^{136}_{56}Ba_{80}$: shell-model calc. vs. Exp.



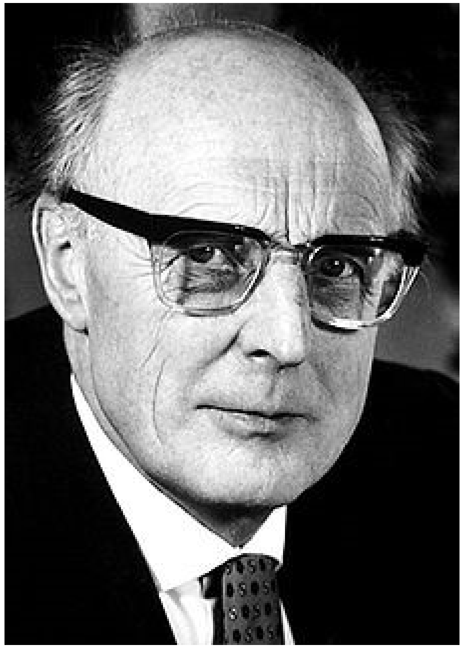
Magic number and “single-particle” shell model

Z, N=2, 8, 20, 28, 50, 82, 126

Nobel prize (1963)

M. G.-Mayer

J.H. D. Jensen



Magic number of nuclei is described by the independent particle model in the mean-field potential with strong spin-orbit coupling.

(3) An odd number of identical nucleons in a state j will couple to give a total spin j and a magnetic moment equal to that of a single particle in that state.

(4) For a given nucleus the "pairing energy" of the nucleons in the same orbit is greater for orbits with larger j.

The last assumption leads to the prediction that the higher j value appears less often as the spin of odd nuclei than the energy order of Table II predicts. For instance, if the $3s_{1/2}$ level has slightly lower energy than $h_{11/2}$, but if the pairing energy of $h_{11/2}$ exceeds that of $s_{1/2}$ by more than this difference, the spin 11/2 would not occur in odd nuclei, but 1/2 would be observed instead.

There is some theoretical justification for assumptions 2, 3, and 4, and this will be discussed in the next paper.

Assumption 2 has the consequence that all even-even nuclei have spin zero. The main testing ground for the level assignment consists then in the spins and magnetic moments of the nuclei of odd A. According to the assumptions we will adopt for these nuclei the extreme one-particle picture, ascribing both spin and magnetic moments to the last odd proton or neutron.

III. MAGNETIC MOMENTS OF ODD A NUCLEI

If assumption 3 were exactly correct, the magnetic moments of all odd nuclei could be computed by the vector model from the known gyromagnetic ratios of proton and neutron. The two possible cases, $l=j-\frac{1}{2}$ and $l=j+\frac{1}{2}$ for given j value lead to two computed lines in a plot of magnetic moment μ against j for nuclei with odd neutron number and two (different) lines for nuclei with odd proton number. These theoretical lines will be referred to as "Schmidt lines."[5] The experimental values lie in between the Schmidt lines, but do not coincide with them. For each j value the magnetic moments seem to fall into two groups, one reasonably close to the line corresponding to $l=j+\frac{1}{2}$, the other scattered from near the line corresponding to $l=j-\frac{1}{2}$ to about halfway. It turns out that the assignment of levels made attributes to the first group an odd nucleon in a state $l=j+\frac{1}{2}$, to the second one $l=j-\frac{1}{2}$. In the later discussion l-values as derived from magnetic moments will be quoted only if the magnetic moment of the nucleus is rather close to one of the two Schmidt lines.

The deviation of the magnetic moments from the Schmidt lines may be taken as an indication of the crudity of the single particle model. However, there is no indication that the magnetic moments for nuclei with one particle more or less than a closed shell fit the Schmidt lines any better than others, which might have been expected, since one would be inclined to expect greater validity of the single particle model in these cases.

For a given value of j, the different possible l-values

[5] T. Schmidt, Zeits. f. Physik **106**, 358 (1937); H. H. Goldsmith and D. R. Inglis, Brookhaven Publications.

TABLE I. Classification of nuclear states.

1	2	3	4	5	6	7	8
Oscillator-quantum number r	Multiplicity	Sum of all multiplicities	Orbital momentum l	Total angular momentum j	l_j-symbol	Multiplicities	Magic numbers
1	2	2	0	1/2	$s_{1/2}$	2	
2			1	3/2	$p_{3/2}$	4	
	6	8		1/2	$p_{1/2}$	2	
3			2	5/2	$d_{5/2}$	6	14
				3/2	$d_{3/2}$	4	
	12	20	0	1/2	$s_{1/2}$	2	
4			3	7/2	$f_{7/2}$	8	28
				5/2	$f_{5/2}$	6	
			1	3/2	$p_{3/2}$	4	
	20	40		1/2	$p_{1/2}$	2	
5			4	9/2	$g_{9/2}$	10	50
				7/2	$g_{7/2}$	8	
			2	5/2	$d_{5/2}$	6	
				3/2	$d_{3/2}$	4	
	30	70	0	1/2	$s_{1/2}$	2	
6			5	11/2	$h_{11/2}$	12	82
				9/2	$h_{9/2}$	10	
			3	7/2	$f_{7/2}$	8	
				5/2	$f_{5/2}$	6	
			1	3/2	$p_{3/2}$	4	
	42	112		1/2	$p_{1/2}$	2	
7			6	13/2	$i_{13/2}$	14	126
				11/2	$i_{11/2}$	12	
			4	9/2	$g_{9/2}$	10	

M. G.-Mayer, Phys. Rev. 78, 16 (1950)

ev **75**, 1766 (1949)

Spin-orbit term in mean-field potential

Mayer Jensen introduced

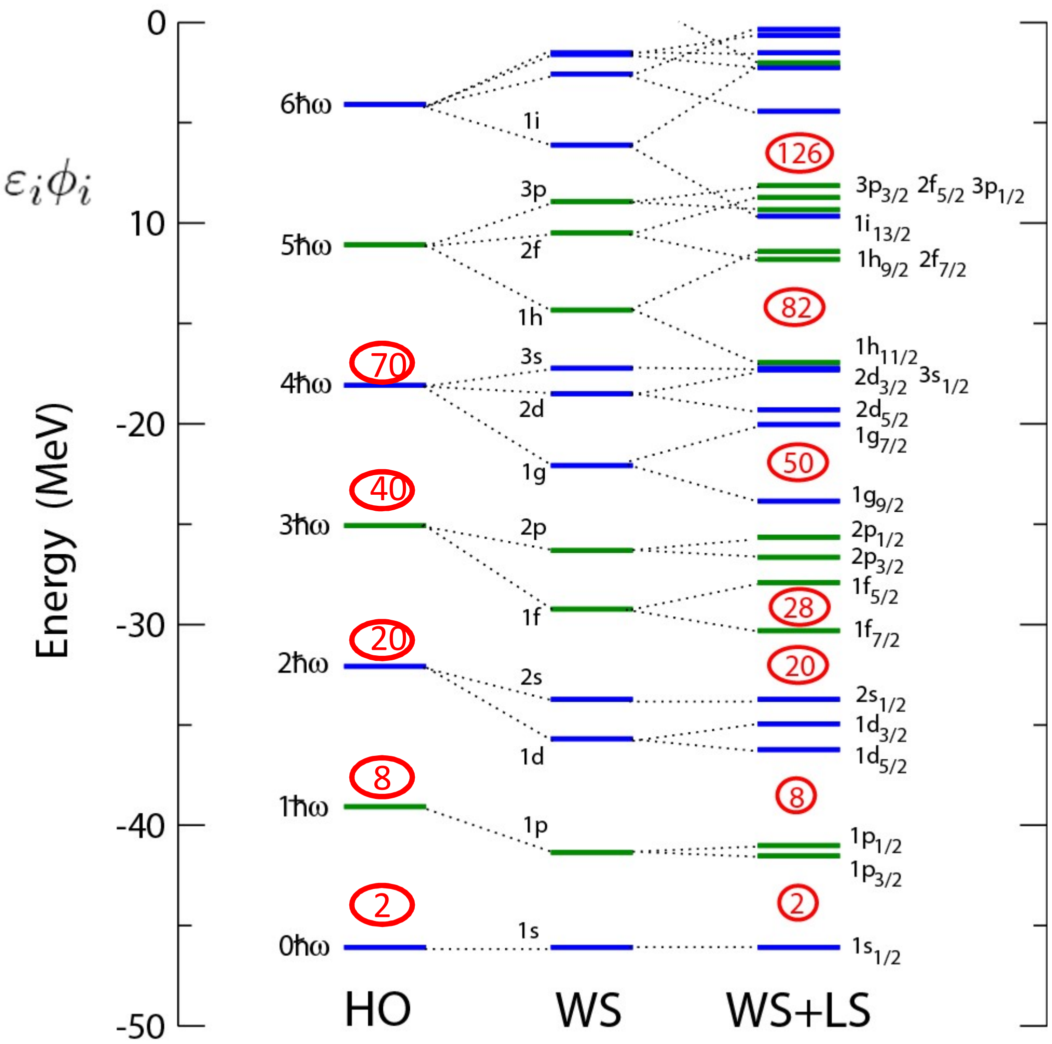
$$[T + U_{\mathrm{C}}(r) + U_{\mathrm{LS}}(r)\,\boldsymbol{\ell}\cdot\boldsymbol{s}]\,\phi_i = \varepsilon_i\phi_i$$

harmonic oscillator

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

Woods-Saxon potential

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

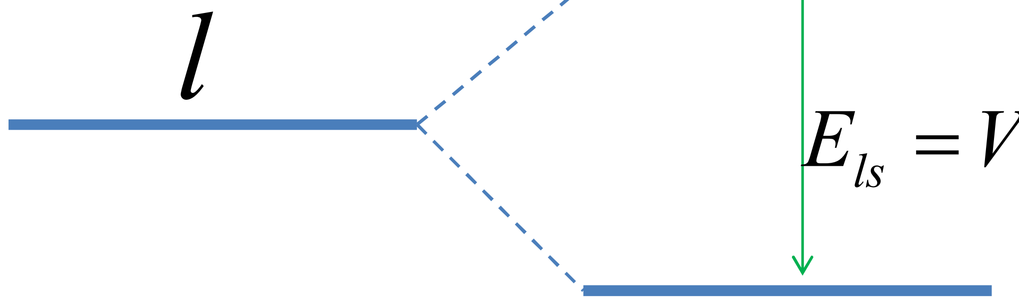


spin-orbit interaction

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

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

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



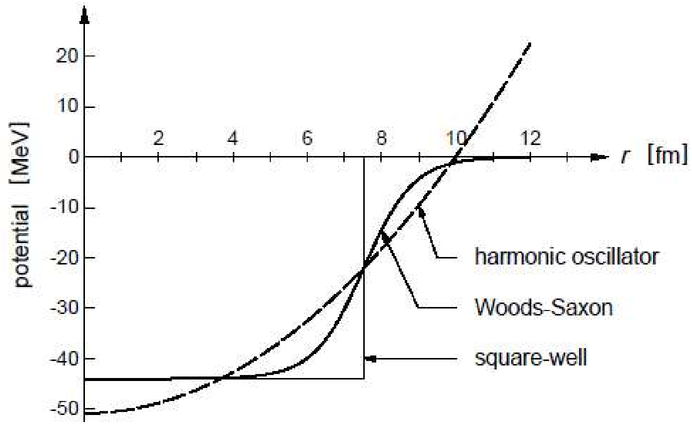
$$j_{<} = l - \frac{1}{2}$$

$$E_{ls} = V_{ls}(l + 1/2)$$

$$j_{>} = l + \frac{1}{2}$$

single-particle wave function

- Mean-field potential



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

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

$s = 1/2$ $\quad$ $j = l + s$ $\quad$ *jj*-coupling scheme symbol $s, p, d, f, g, h, i, \ldots$

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

$$1d_{5/2}$$

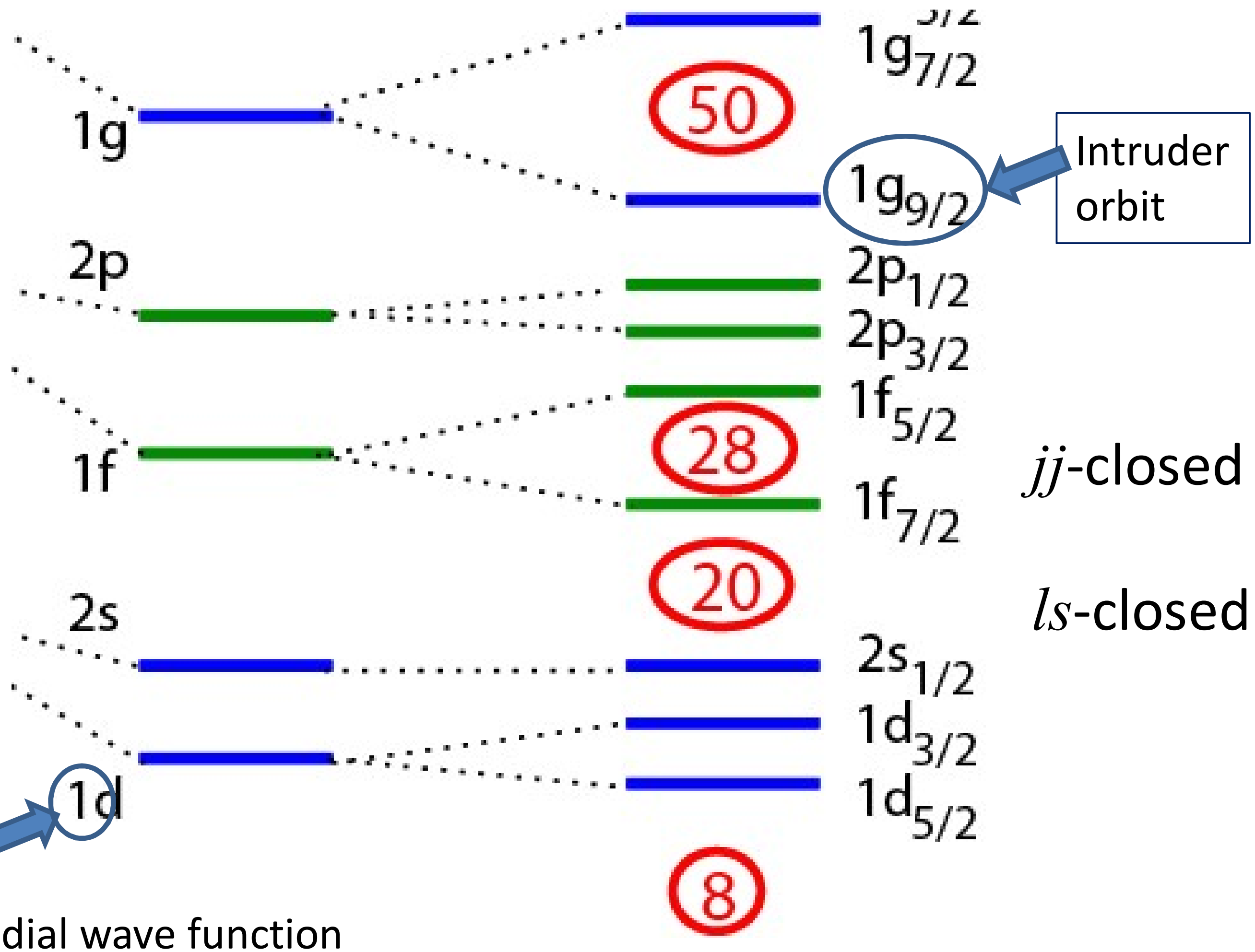
$n = 1$ (or 0)

$l = 2$

$j = 5/2$

$N = 2n + l$

$\Pi = (-1)^l$



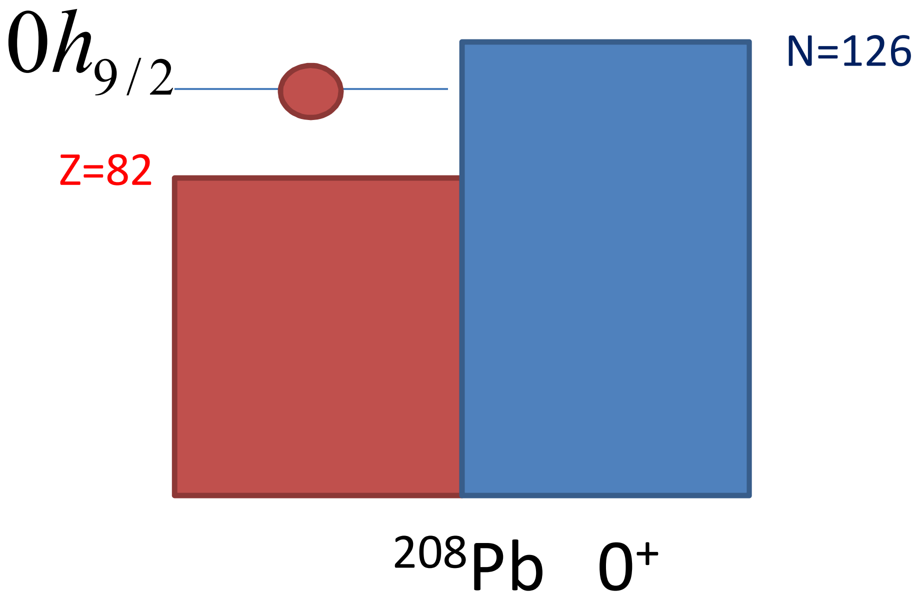
Number of nodes in radial wave function

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

Doubly closed ± 1 particle

^{209}Bi, Z=83, N=126

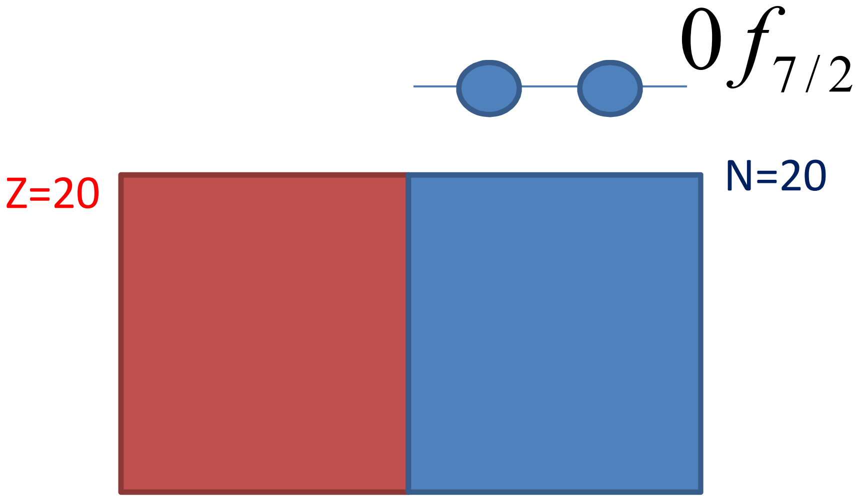
What is the spin and parity of the ground state?



$$J^{\pi} = \frac{9}{2}^{-}$$

Doubly closed core + 2 active nucleons

42Ca

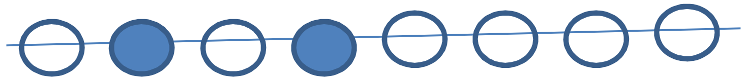


^{40}Ca 0^+

What kind of state is allowed?

$$j = 7/2$$

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

$01010000 \Rightarrow 6$

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		

J-scheme dimension

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

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

J-coupled two-body state

- 2 particles in f7/2

$$|JM\rangle = \frac{1}{2}\sum_{m_1,m_2}\left\langle\frac{7}{2},m_1,\frac{7}{2}m_2\middle|JM\right\rangle c^\dagger_{m_1}c^\dagger_{m_2}\,|-\rangle$$

Only J=0, 2, 4, 6 are allowed.
Why odd J is prohibited?

Antisymmtrization of Fermi particles

$$\langle j_1 m_1, j_2 m_2 | JM\rangle = (-1)^{j_1+j_2-J}\langle j_2 m_2, j_1 m_1 | JM\rangle$$

- multi-j orbits:

$$|a,b,JM\rangle = \frac{1}{\sqrt{1+\delta_{ab}}}\sum_{m_a,m_b}\langle j_a,m_a,j_b,m_b|JM\rangle c^\dagger_{m_a}c^\dagger_{m_b}\,|-\rangle$$

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 $a = (n_a, l_a, j_a, m_a)$
- 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

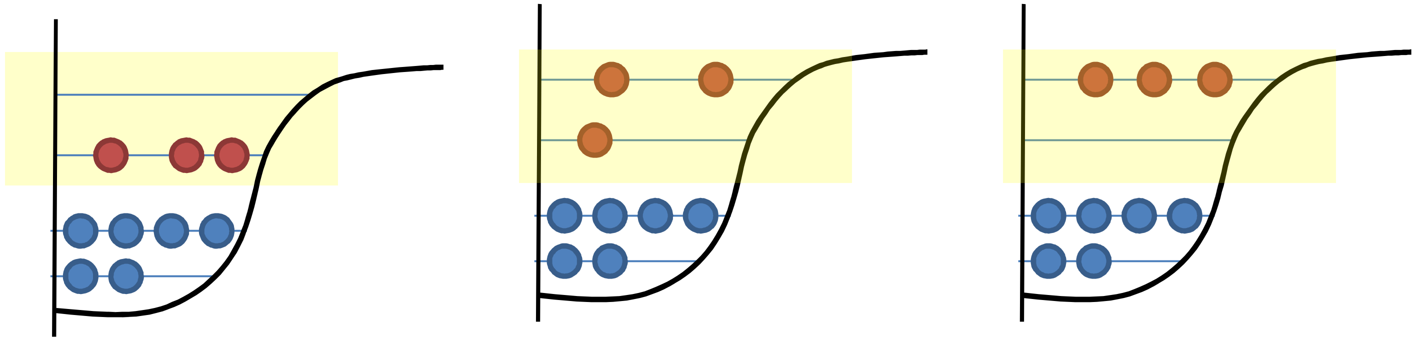
J-scheme basis state

- It is an eigenstate of J^2
- The number of the basis states are reduced by $O(10^{-2})$, but the operations are complicated
- $D_J = D_{M=J} - D_{M=J+1}$

$$\left|\psi\right\rangle = \frac{1}{\sqrt{N}} \left[\left[\left[c^{\dagger}_{j_1} \otimes c^{\dagger}_{j_2}\right]^{(J_1, \nu_1, a)} \otimes c^{\dagger}_{j_3}\right] \ldots \otimes c^{\dagger}_{j_n}\right]^{(J, \nu_n, , k)} \left|-\right\rangle$$

Large-scale shell model calculation (LSSM)

- Configuration interaction (CI) method
- Nuclear wave function is expressed as a linear combination of M-scheme basis states



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

- How many basis states are required?

$$D = \quad {}_{N_{sps}}C_Z \times {}_{N_{sps}}C_Z$$

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

$$D = \quad {}_{20}C_8 \times {}_{20}C_8 = 2.5 \times 10^{19}$$

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

Nuclear chart

Ab initio:

without empirical correction

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

Configuration Interaction:

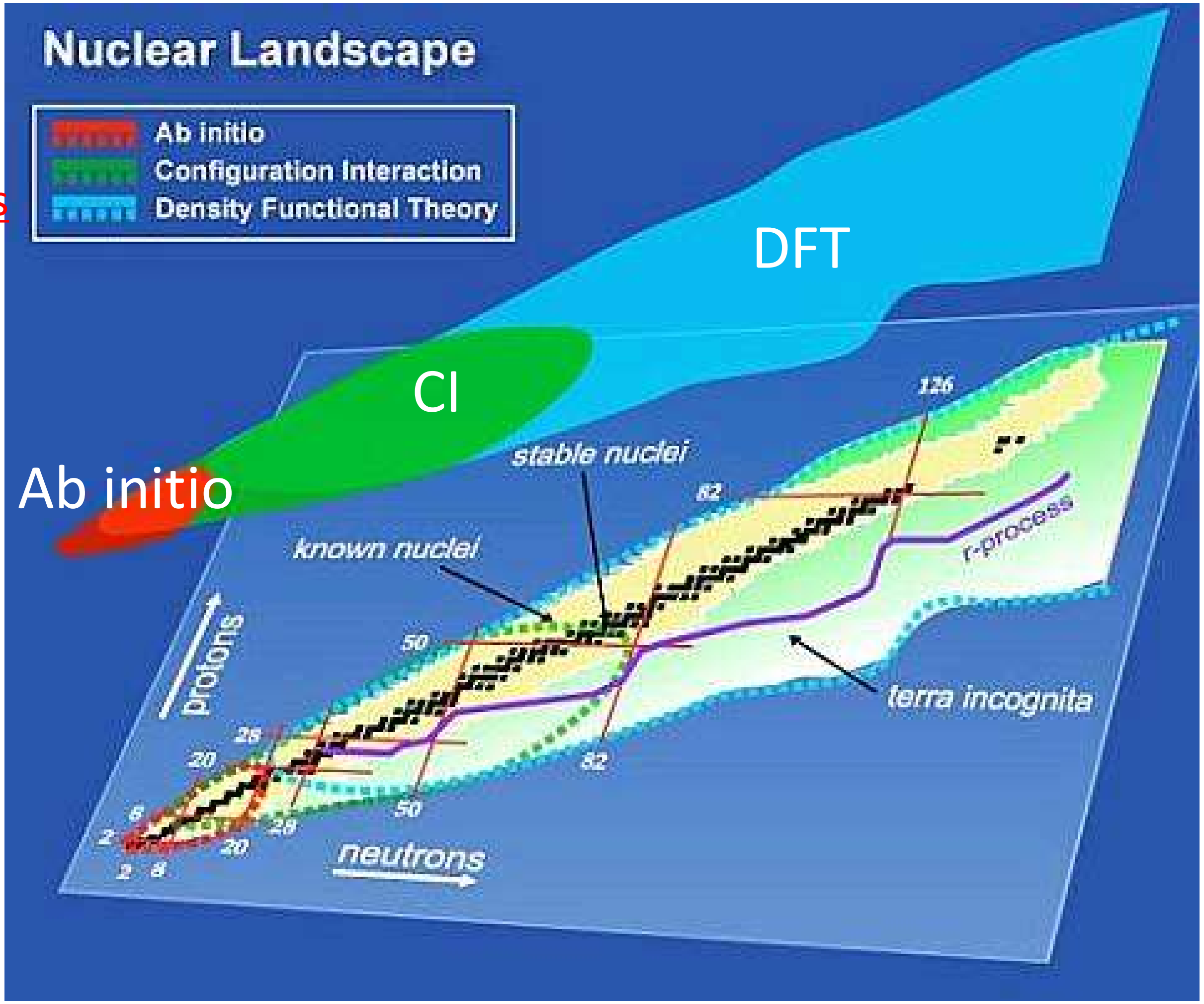
- Large-scale shell model calc.

with an inert core.

Effective interaction corrected by the medium effect and phenomenology

Density Functional Theory:

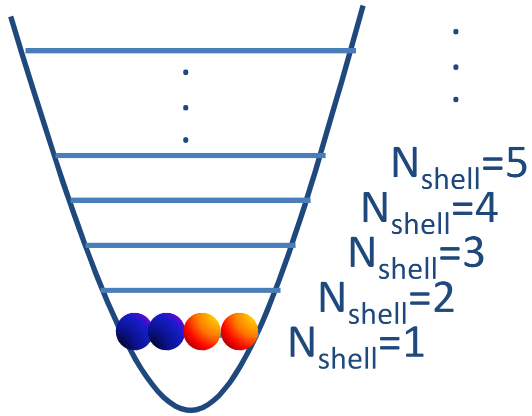
- Functional is determined by phenomenology



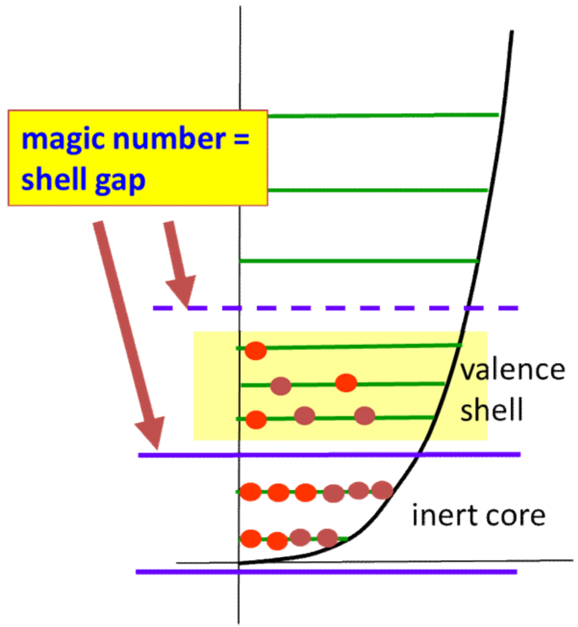
Taken from: http://unedf.org/

Two kinds of "shell model calculations"

- No-core shell-model approach
  - All nucleons are active and do not assume the inert core
  - "ab initio" calculation
  - Only for light nuclei up to ^{16}O



- Large-scale shell-model calculations
  - Assume inert core and model space
  - Solve the motion of active particles in the model space
  - Medium-heavy nuclei



Large-scale shell model calculation (LSSM)

More generally, let us consider many valence particles

Solve Schrodinger's Equation

$$H\left|\Psi\right\rangle = E\left|\Psi\right\rangle$$

The wave function is expanded by simple many-body basis states defined in mean-field potential
（e.g. Harmonic oscillator or Hartree-Fock basis)

$$\left|\Psi\right\rangle = \sum_m u_m \left|m\right\rangle$$

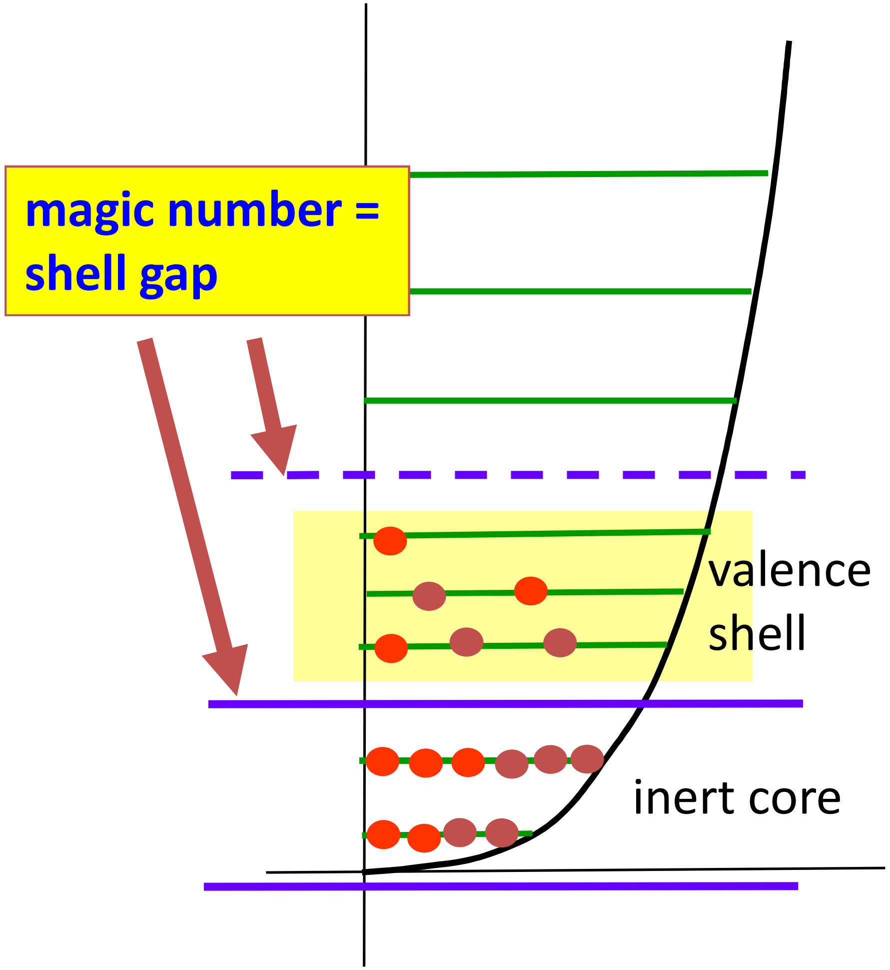
$$\left\langle m\right| H \sum_{m'} \left|m'\right\rangle\left\langle m'\right|\Psi\right\rangle = E\left\langle m\middle|\Psi\right\rangle$$

$$\sum_{M'} H_{MM'} u_M = E u_M$$

Now, we solve the eigenvalue problem of the Hamiltonian matrix

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)

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

$a = (n_a, l_a, j_a)$ to specify a single-particle orbit

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

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

Shell model Hamiltonian cont'd

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

proton-neutron formalism

- Rotation symmetry : Rank-0 spherical tensor
- Parity : $V(abcd;J)=0$ if (-1)$^{la+lb+lc+ld}$ = -1
- Isospin invariance : isospin formalism (OXBASH / Nushell)

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

isospin formalism

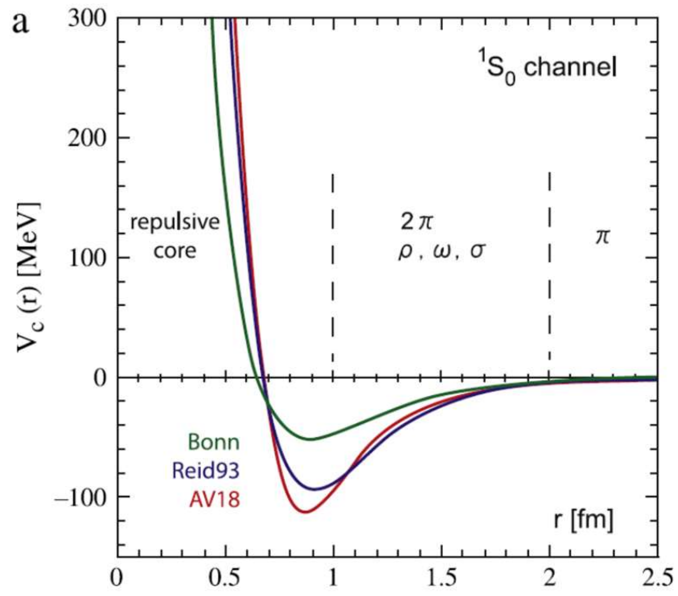
How to construct a realistic shell-model Hamiltonian

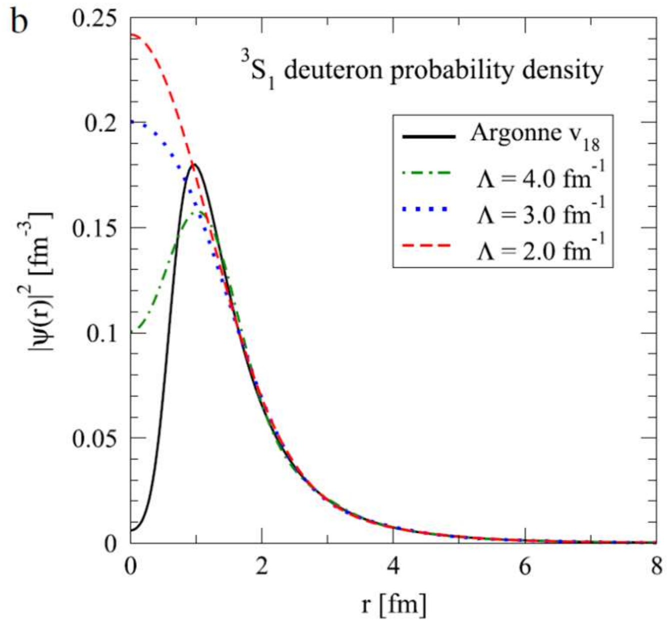
- Some successful interactions (USD, GXPF1A, JUN45, …) are derived by the following procedure.

- SPE is determined by the experimental levels of the core + 1 nucleus.
  - E.g. 41Ca for SPE of *pf* shell

- TBME is derived by :
  1. Prepare NN interaction (CD-Bonn, AV18, chiral N3LO, …)
  2. Soften short-range replustion (G-matrix, Vlow-k, SRG, …)
  3. Include the effect outside the model by many-body perturubation 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 caluclations

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

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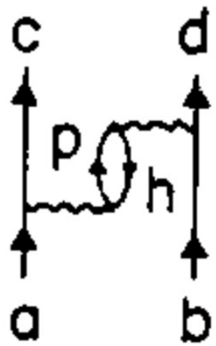
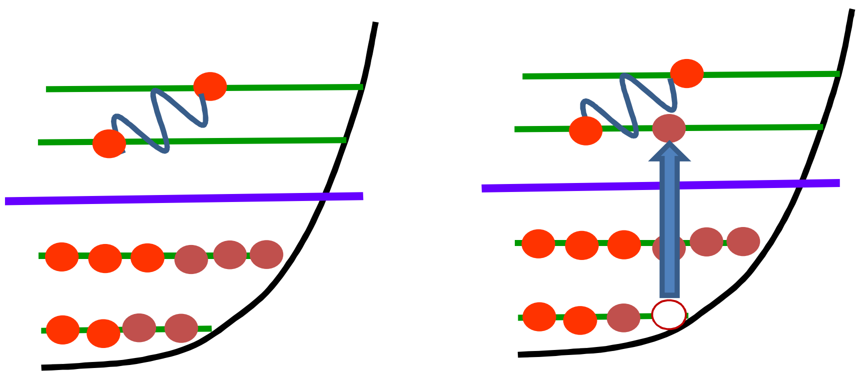
Core polarization

- 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





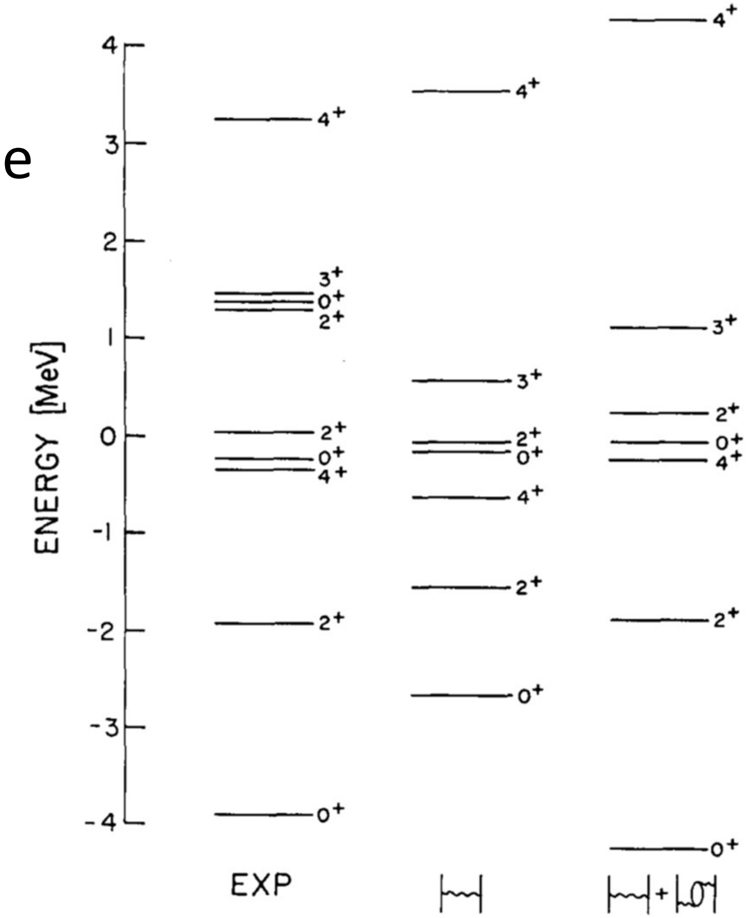


Fig. 13. The spectra of ^{18}O.

T. T. S. Kuo and B. A. Brown, Nucl. Phys. 85, 40 (1960)

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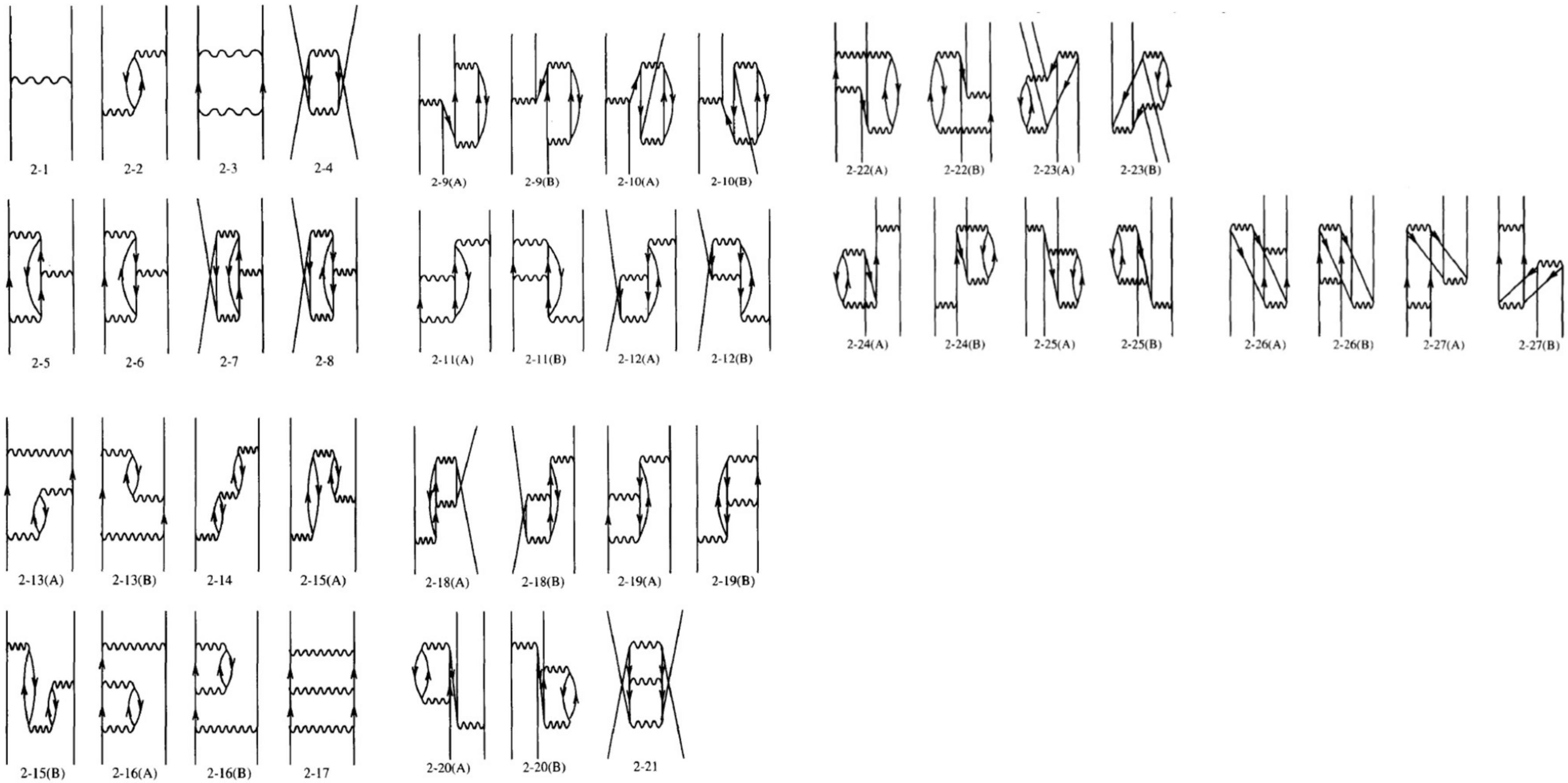
Many-body perturbation theory

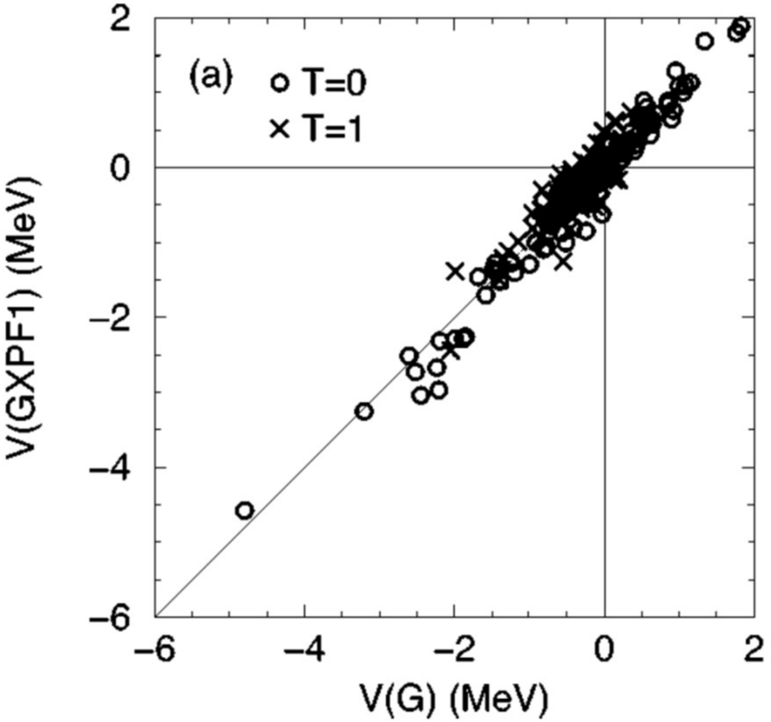


M.H-Jensen, T.T.S. Kuo, and E Osnes, Phys. Rev. 2611 125 (1995)

Phenomenological correction

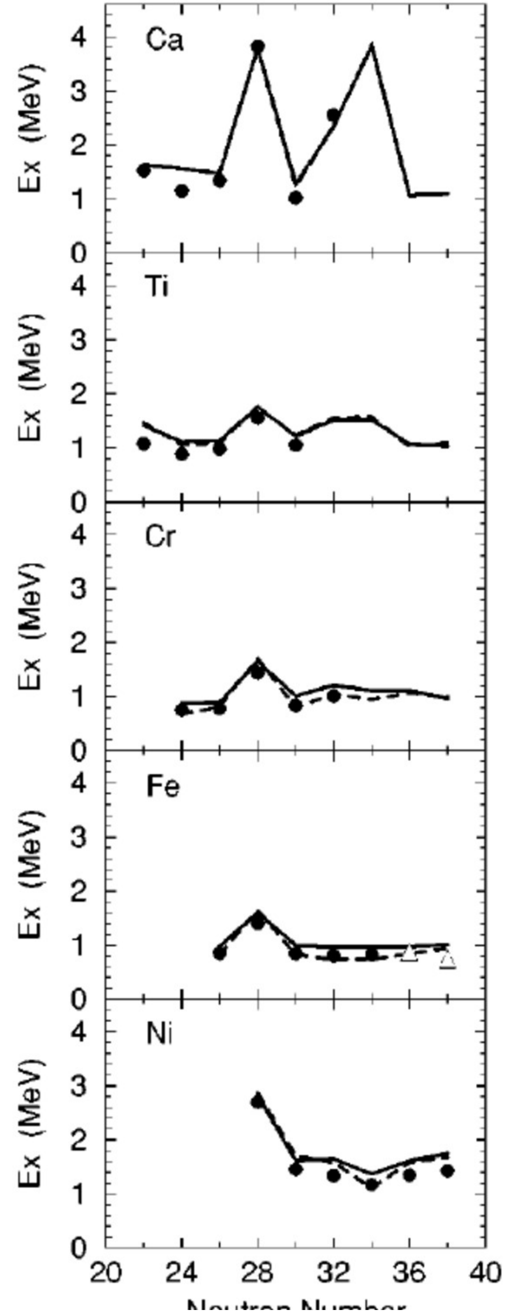
The GXPF1 interaction

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.

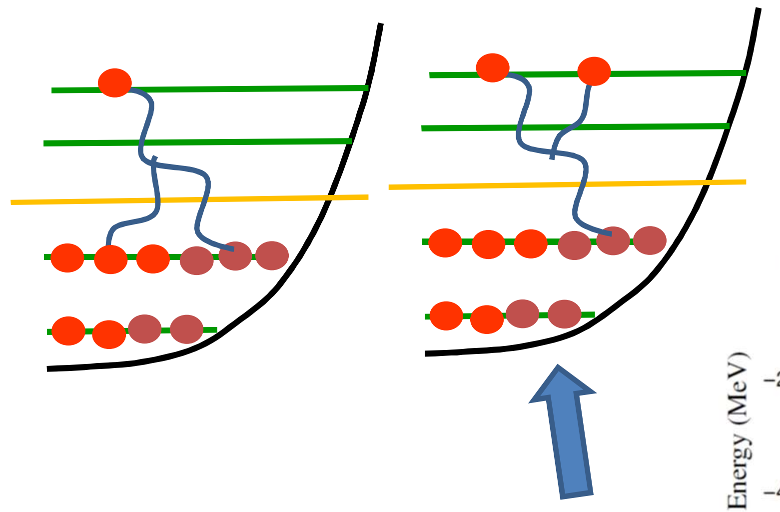


Ref. M. Honma, T. Otsuka, B. A. Brown, and T. Mizusaki, Phys. Rev. C 65, 061301(R) (2002)

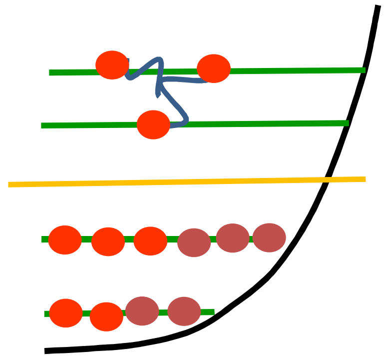
Contribution of the three-body force

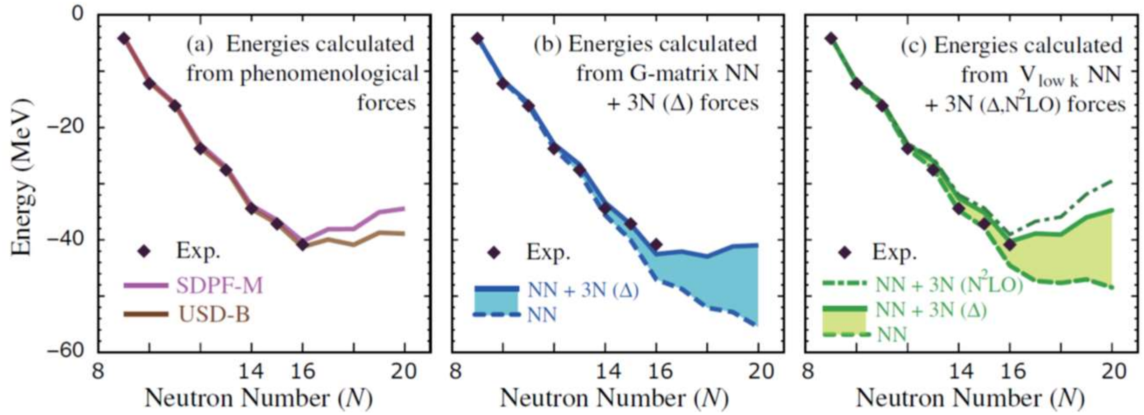
Is the phenomenological correction explained
by the three-body force?

Normal ordering with the inert core



Correction to
two-body force



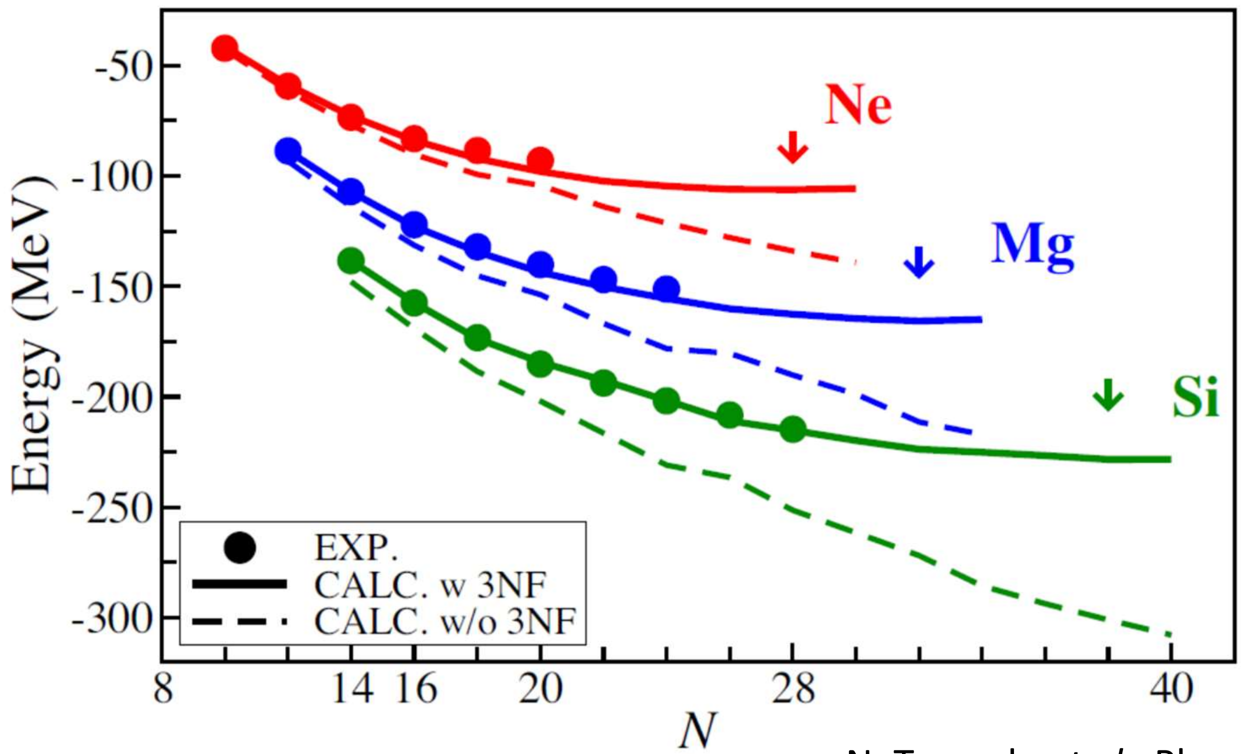


T. Otsuka, T. Suzuki, J. D. Holt, A. Schwenk, and Y. Akaishi,
Phys. Rev. Lett. 105, 032501 (2010).

Three-body force contribution

TBME without phenomenological correction with normal-ordered three-body force

Ground-state energies of Ne, Mg, Si isotope
(EEdf1 interaction, model space : *sd+pf* shells)

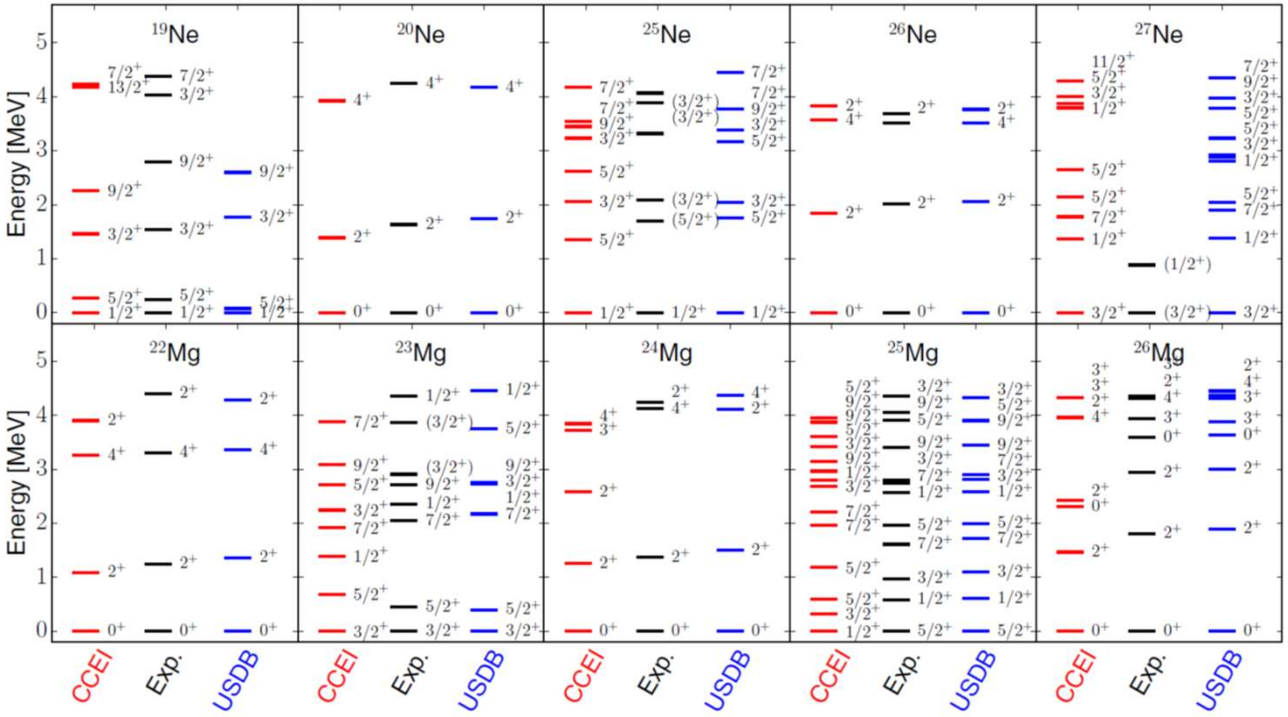


Neutron number

N. Tsunoda *et al.,* Phys. Rev. C 95, 021304 (2017)

Challenge : Shell model calculations in "ab initio" way

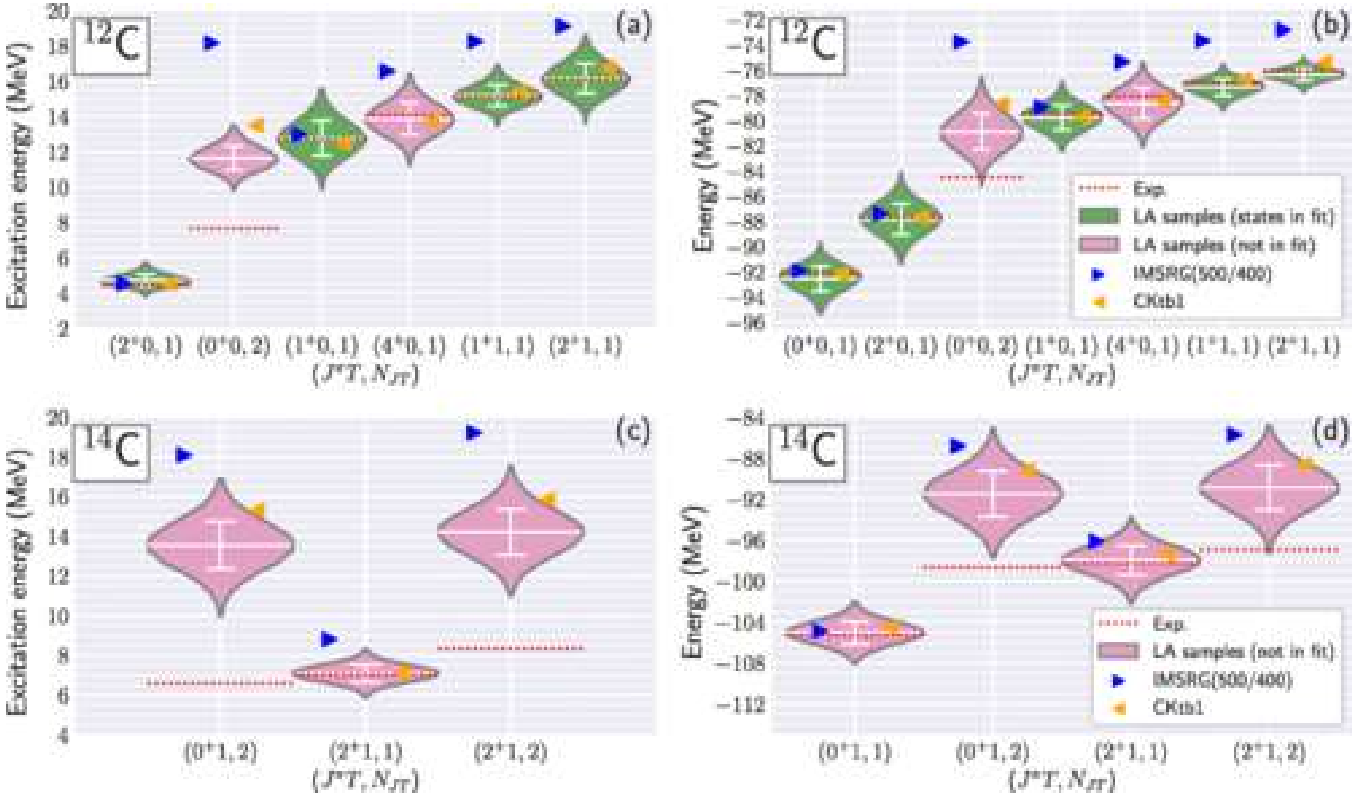
- Shell-model effective interaction is obtained without phenomenological corrections by ab initio methods, such as the coupled-cluster method and in-medium similarity renormalization group method.



Ref. G.R. Jansen, M. D. Schuster, A. Signoracci, G. Hagen and P. Navratgil, Phys. Rev. C 94 011301(R) (2016)

Uncertainty estimation of the shell-model Hamiltonian

- Bayesian analysis to quantify the uncertainty from the parameters of the Hamiltonian.



S. Yoshida, N. Shimizu, T. Togashi and T. Otsuka, Phys. Rev. C 98, 061301(R) (2018)

Summary

- shell model and LSSM
  - shell-model Hamiltonian
- *M*-scheme basis state vs. *J*-scheme
- Realistic effective interaction
  - Conventional way and recent challenges

Before the next lecture ...

- https://sites.google.com/a/cns.s.u-tokyo.ac.jp/shimizu/cns-summer-school-2019

Linux:

- Install gfortran, BLAS, LAPACK, and python

  (Ubuntu: apt-get install python gfortran liblapack-dev libblas-dev)

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

- MS-Windows : install "Windows subsystem for Linux" or Cygwin
- Mac OS X : install Xcode