HPCI project field 5
"The origin of matter and the universe"

Electric dipole (*E1*) transitions in medium-heavy nuclei described with Monte Carlo shell model

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Computational Advances in Nuclear and Hadron Physics (CANHP2015)
1st Oct., 2015, Kyoto

Outline

1. Introduction
2. Framework
   - ✓ Monte Carlo shell model (MCSM)
   - ✓ Collective states described by MCSM
   - ✓ MCSM strength function and
     analogy to Lanczos strength function method
3. Applications
   - ✓ Benchmark test by comparison with Lanczos method
   - ✓ Medium-mass nuclei (Sr and Se isotopes)
4. Summary and Perspective

Introduction

Interests of electric dipole (*E1*) in nuclear structure

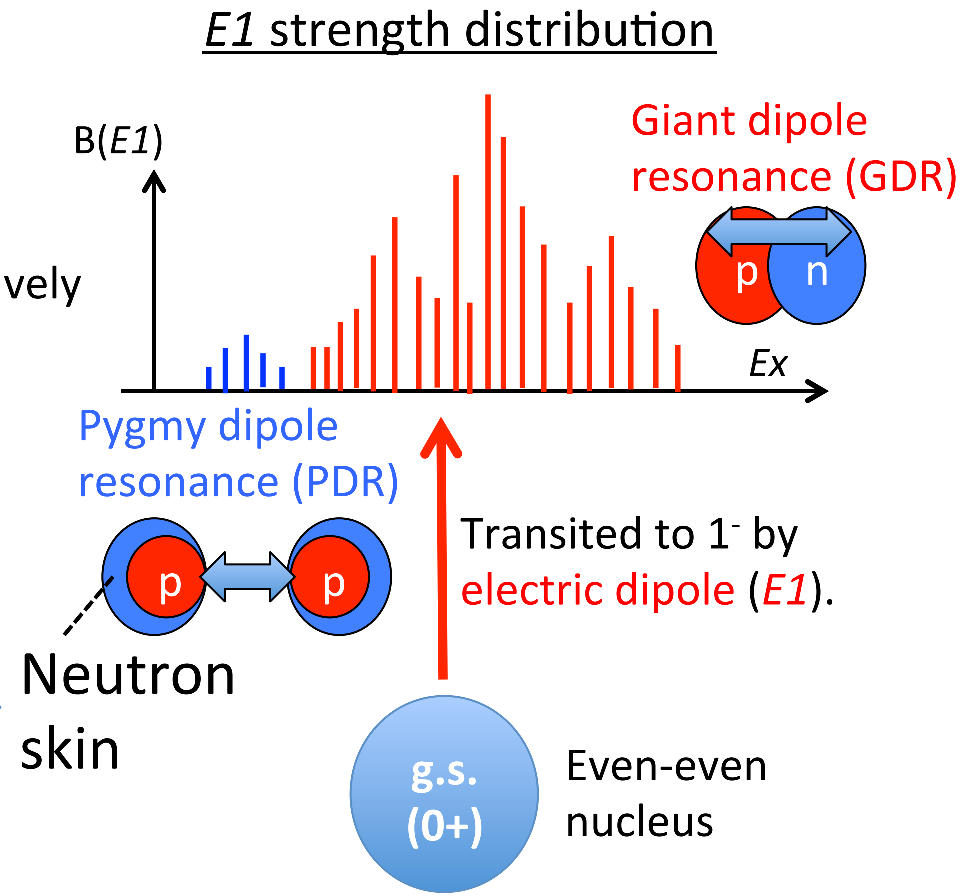
What type of correlations can describe *E1* excited states?

GDR and PDR have been studied intensively by PRA, QPRA, phonon model,… .

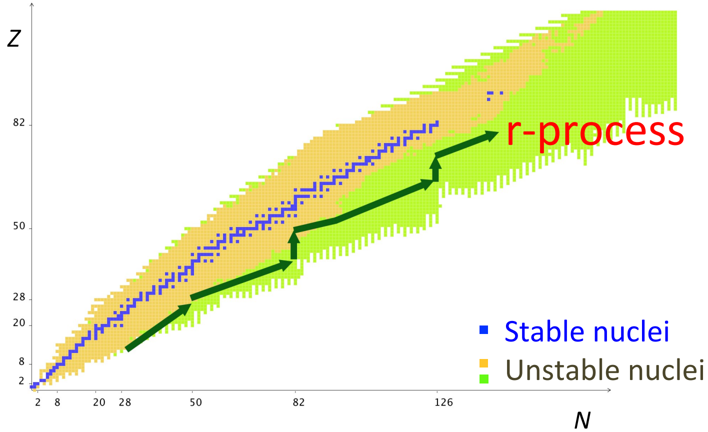
e.g. Inakura (2011), Hartmann *et al*. (2004), …

Symmetry energy in EoS

e.g. Reinhard and Nazarewics (2012), Klimkiewiz *et al.* (2007), Colo (2008), …

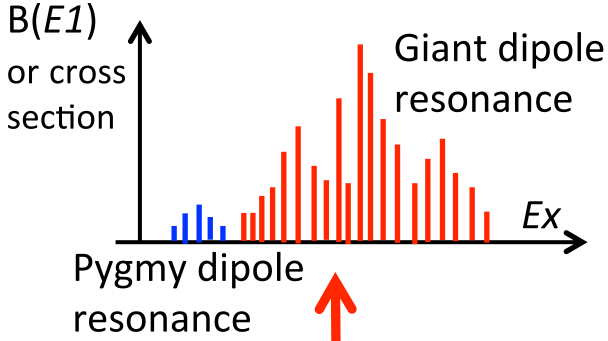


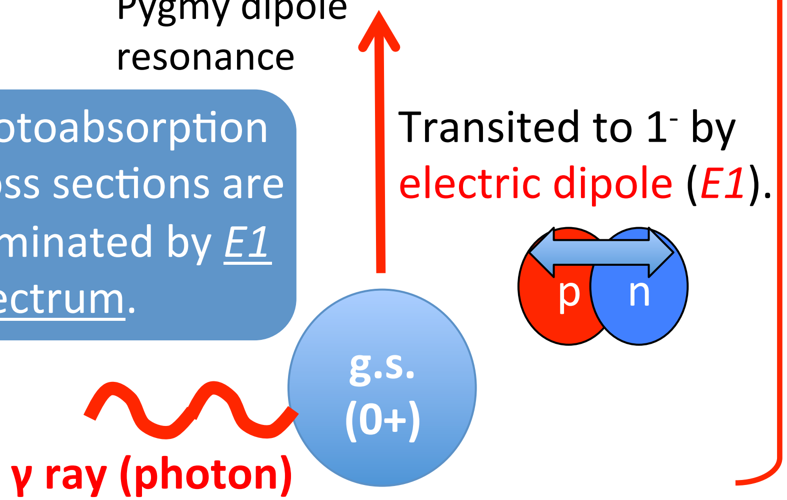
Topics related to electric dipole (*E1*)



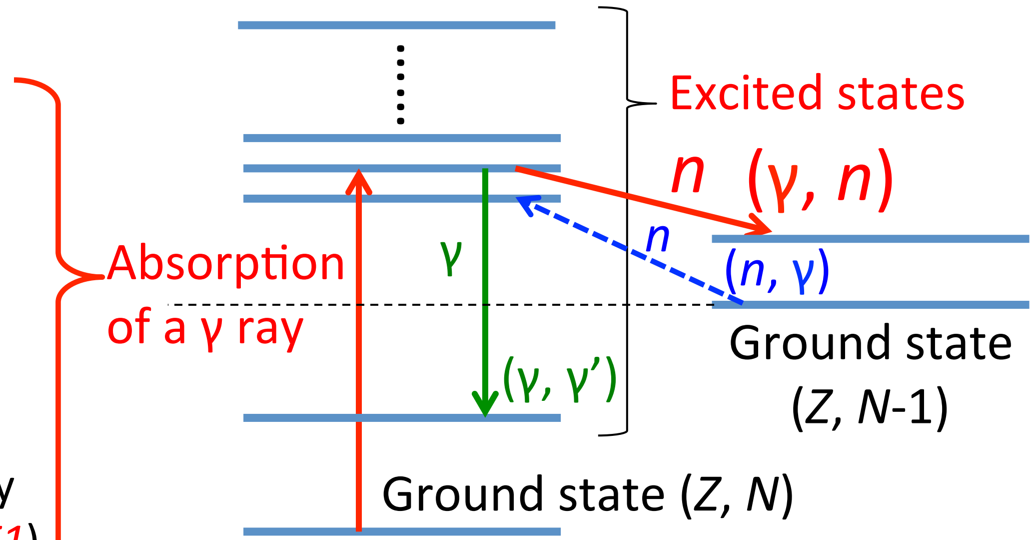
As for astrophysical phenomena, r-process is proceeded by (n,γ) and (γ,n) reactions.

Photoabsorption process need to be understood for a starting point of describing these reactions.





Photoabsorption cross sections are dominated by *E1* spectrum.

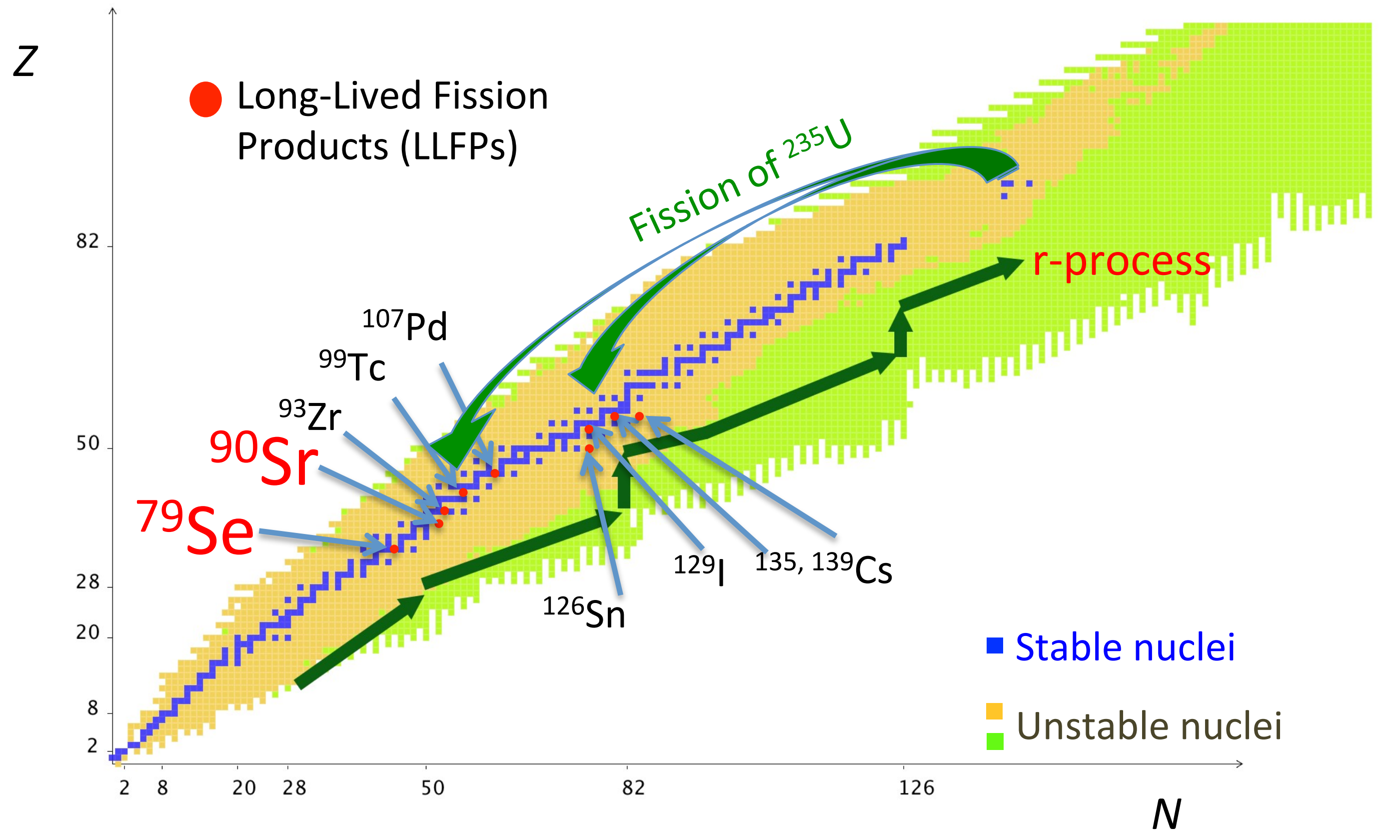


Photoabsorption cross section

$$\sigma_{abs}(E) = \sigma(\gamma, \gamma') + \sigma(\gamma, n) + \sigma(\gamma, n+p) + \sigma(\gamma, p) + \ldots$$

Topics related to electric dipole (*E1*)

(γ,*n*) and (*n*,γ) reactions are the candidates of nuclear transmutation for long-lived fission products (LLFPs).



One of important projects in Strategic Programs for Innovative Research (SPIRE) Field 5.

Shell-model calculations for *E1* spectrum

In shell-model calculation,

- All many-body correlations (pairing, tensor, …) inside the model space can be treated.
- Even- and odd-mass nuclei can be solved on an equal footing.

⇒ *E1* spectrum can be calculated by Lanczos strength function method* in conventional shell-model calculation.

* R.R.Whitehead, "Moment Methods in Many-ferimion Systems", p.235 (1980)

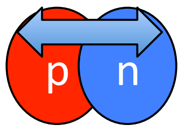
In describing *E1* spectrum in medium-heavy nuclei, the dimension of Hamiltonian matrix increases explosively and the exact diagonlization is not feasible.
(^{90}Sr: 8.2x10^{14} *M*-scheme dim. for 3hw truncation)

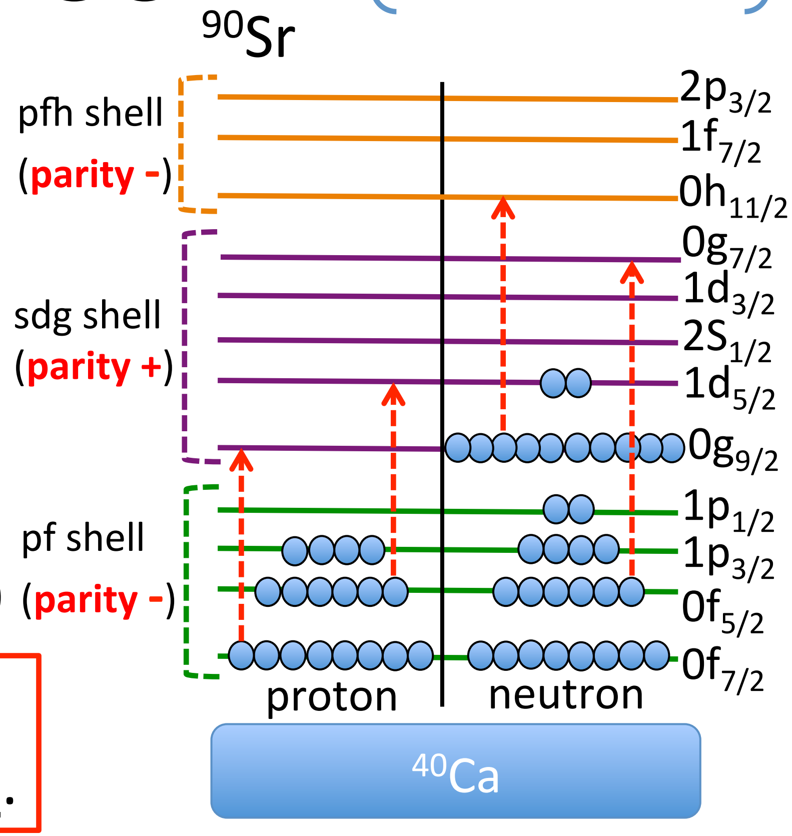
We develop a new function to describe *E1* spectrum for Monte Carlo shell model.

Operator of electric dipole (*E1*)

$$E1 = \sqrt{\frac{3}{4\pi}} \sum_{i=1}^{A} e_i \vec{r}_i$$ => *l* = 1, parity = -1

$$\left(\begin{array}{l} e_i = N/A \text{ (proton)}, \\ \quad -Z/A \text{ (neutron)} \end{array} \right)$$





Framework

Monte Carlo shell model (MCSM)

Wave function:

Number of basis vectors (dimension)

Creation operator of a single-particle orbit (h.o.)

$$|\Psi^m\rangle = \sum_{d=1}^{N_d} f_d^m |\Phi^{J\pi}(q_d)\rangle, \quad |\Phi^{J\pi}(q_d)\rangle = P^{J\pi}|\Phi(q_d)\rangle = P^{J\pi}\prod_j^{N_f}\left(\sum_l^{N_s} D(q_d)_{lj} c_l^\dagger\right)|-\rangle$$

Projection onto J^π

Deformed Slater determinant

Diagonalization of H matrix (~10 x 10 - 100 x 100) ⇔ Conventional shell model (~10^{10} x 10^{10})

$$\sum_d \langle \Phi^{J\pi}(q_p)|H|\Phi^{J\pi}(q_d)\rangle \cdot f_d^m = e_m \sum_d \langle \Phi^{J\pi}(q_p)|\Phi^{J\pi}(q_d)\rangle \cdot f_d^m$$

Basis vectors in low-lying states are chosen by minimizing the average of eigenvalues.
(Variation after projection (VAP) for spin J and parity π)

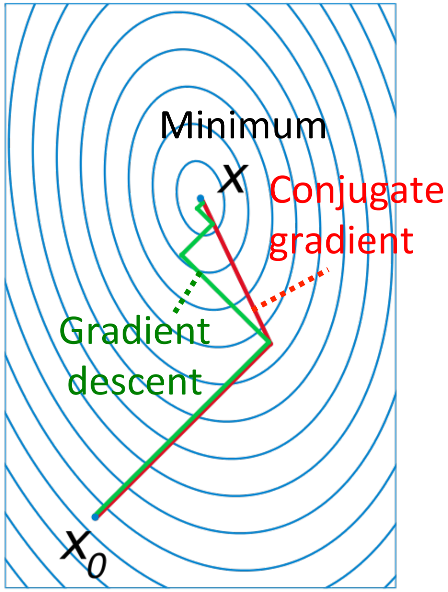
$$E_n = \sum_{m=1}^{n} e_m$$

The m-th eigenvalue

Step 1: The candidate of the basis vector to lower En is chosen by the auxiliary-field Monte Carlo.

$$|\Phi(\sigma)\rangle = \prod e^{\Delta\beta\cdot h(\sigma)}|\Phi^{(0)}\rangle$$

Step 2: En is optimized by conjugate gradient for $D(q)$.



Collective states described by MCSM (1)

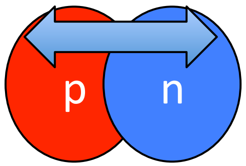
Concept to describe *E1* spectrum with MCSM

(Ref. T. Otsuka, T. Togashi, N. Shimizu *et al*.)

E1 operator

$$E1 = \sqrt{\frac{3}{4\pi}} \sum_{i=1}^{A} e_i \vec{r}_i \quad \left(\begin{array}{l} e_i = N/A \text{ (proton)}, \\ \quad -Z/A \text{ (neutron)} \end{array} \right)$$

=> angular momentum *l* = 1,
parity = -1



We introduce an exponential of one-body operator.

$$\exp(i\varepsilon \cdot E1) \equiv \exp(i\varepsilon \cdot \sum_{i=1}^{A} e_i (x_i + y_i + z_i) \,)$$

corresponding to *E1* operator

※ ε value is determined so as to maximum the sum of *B*(*E1*).

We consider the following type of basis vectors for *E1* spectrum.

$$\left| \Phi_j^{E1} \right\rangle = \exp(i\varepsilon \cdot E1) \left| \Phi_j^{g.s.} \right\rangle$$

The *j* -th basis vector of ground state

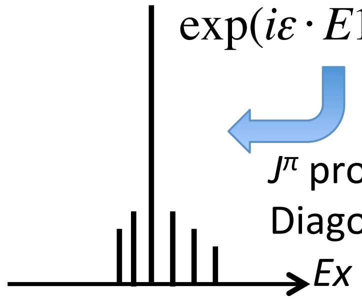
Slater determinant ← Slater determinant

These basis vectors are projected out onto spin-parity states transited by *E1* and the *H* matrix for them is diagonalized.

Collective states described by MCSM (2)

The *E1* operator is decomposed so as to treat transitions between different sets of orbits separately.

$\exp(i\varepsilon \cdot E1)\left|\Phi_j^{g.s.}\right\rangle$



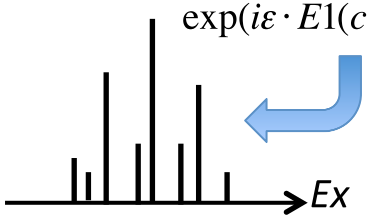
J^π projection + Diagonalization

Strength distribution is too concentrated.

One operator is too naïve to realize spectrum.

$\exp(i\varepsilon \cdot E1(a \to b))\left|\Phi_j^{g.s.}\right\rangle,$

$\exp(i\varepsilon \cdot E1(c \to d))\left|\Phi_j^{g.s.}\right\rangle, \ \ldots$



J^π projection + Diagonalization

Peaks corresponding to different orbital combinations appear.

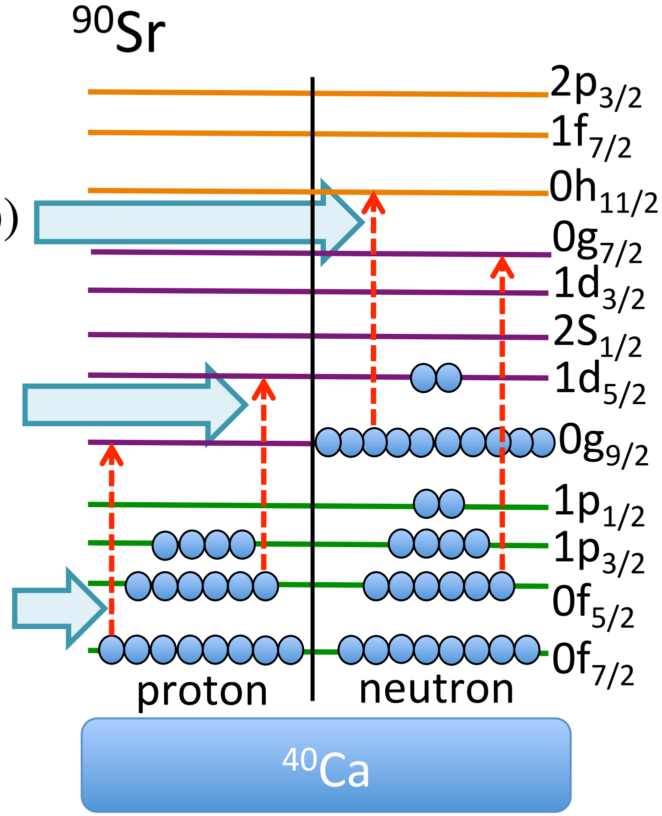
Decomposition of exp(*iε*･*E1*) operator

(Ref. T. Otsuka, T. Togashi, N. Shimizu *et al.*)

$\exp(i\varepsilon \cdot E1(0g_{9/2} \to 0h_{11/2}))$

$\exp(i\varepsilon \cdot E1(0f_{5/2} \to 1d_{5/2}))$

$\exp(i\varepsilon \cdot E1(0f_{7/2} \to 0g_{9/2}))$



*Excluding the transitions not to affect *E1* spectrum, crucial (10) transitions are chosen.

Collective states described by MCSM (3)

Ground state:

$$\sum_{j=1}^{N_d} f_j P^{J^\pi} \left|\Phi_j^{g.s.}\right\rangle$$

Basis vector of the ground state (Slater determinant)

Basis vectors for *E1* spectrum:

$$\left|\varphi_1\right\rangle = \exp(i\varepsilon \cdot E1(a \to b))\left|\Phi_j^{g.s.}\right\rangle,$$
$$\left|\varphi_2\right\rangle = \exp(i\varepsilon \cdot E1(c \to d))\left|\Phi_j^{g.s.}\right\rangle,$$
$$\cdots$$

J^π projection + Diagonalization

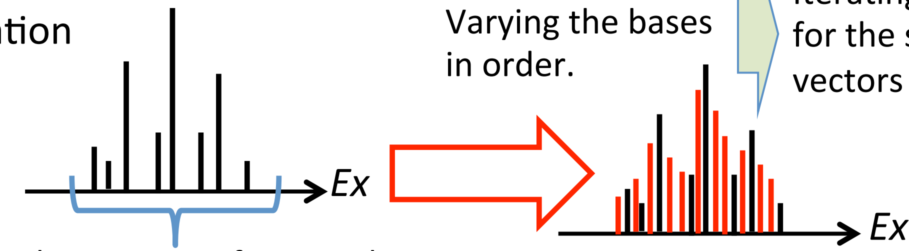
Additional bases for fine structure by variation for energy average *Es*

+ $V_1\left|\varphi_1\right\rangle$, $V_2\left|\varphi_2\right\rangle$, …

$V_k : \left|\varphi_k\right\rangle$ is varied by conjugate gradient keeping the other bases.

Varying the bases in order.

Iterating this operation for the set of basis vectors in several cycles.



Es : the average of eigenvalues corresponding to *Ex* ≤ ~30 MeV

Excitation spectrum up to fine structure

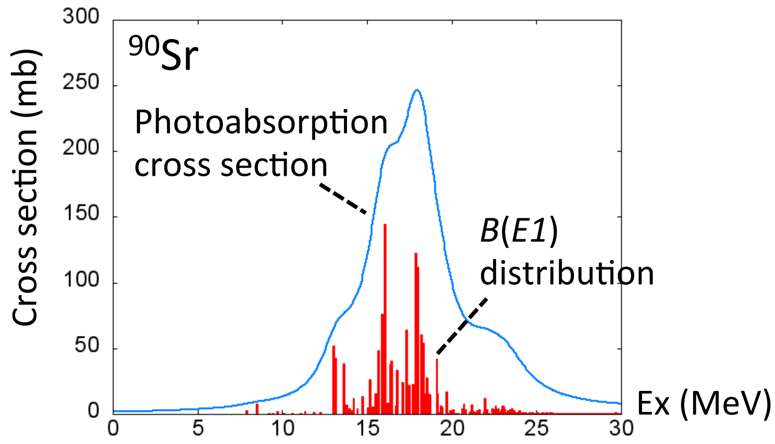
Photoabsorption cross section is calculated by *B*(*E1*) strength from the ground state:

Lorentzian width: γ = Γ/2 (adjusted parameter)

$$\sigma(E)\,[\mathrm{fm}^2] = \frac{16\pi^3}{9}\frac{e^2}{\hbar c}\sum_{J_n^f}\frac{1}{\pi}\frac{\gamma}{(E - Ex(J_n^f))^2 + \gamma^2}\cdot Ex(J_n^f)\cdot B(E1; J^i \to J_n^f).$$

Excitation energy

B(*E1*) strength



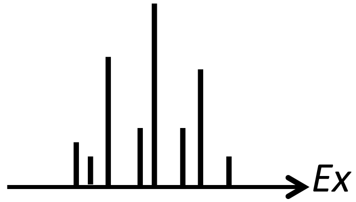
Overview of description of *E1* spectrum with MCSM

Step1. The ground state is solved by MCSM.

$$\left|\Psi(g.s.)\right\rangle = \sum_{j=1}^{N_d} f_j P^{J^\pi} \left|\Phi_j^{g.s.}\right\rangle$$

Step2. Basis vectors for *E1* spectrum are generated by acting exp(*iε*・*E1(a -> b)*), exp(*iε*・*E1(c -> d)*), …on basis vectors of the ground state.

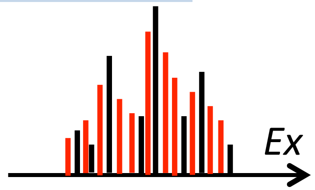
$$\left|\varphi_1\right\rangle = \exp(i\varepsilon \cdot E1(a \to b))\left|\Phi_j^{g.s.}\right\rangle, \quad \left|\varphi_2\right\rangle = \exp(i\varepsilon \cdot E1(c \to d))\left|\Phi_j^{g.s.}\right\rangle, \ \ldots$$



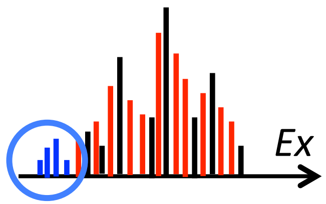
Step3. More basis vectors are generated by the variation for the basis vectors of step2.

$$V_1\left|\varphi_1\right\rangle, \quad V_2\left|\varphi_2\right\rangle, \ \ldots, \ V_1^2\left|\varphi_1\right\rangle, \quad V_2^2\left|\varphi_2\right\rangle, \ \ldots$$

1-cycle variational shift | 2-cycle variational shift

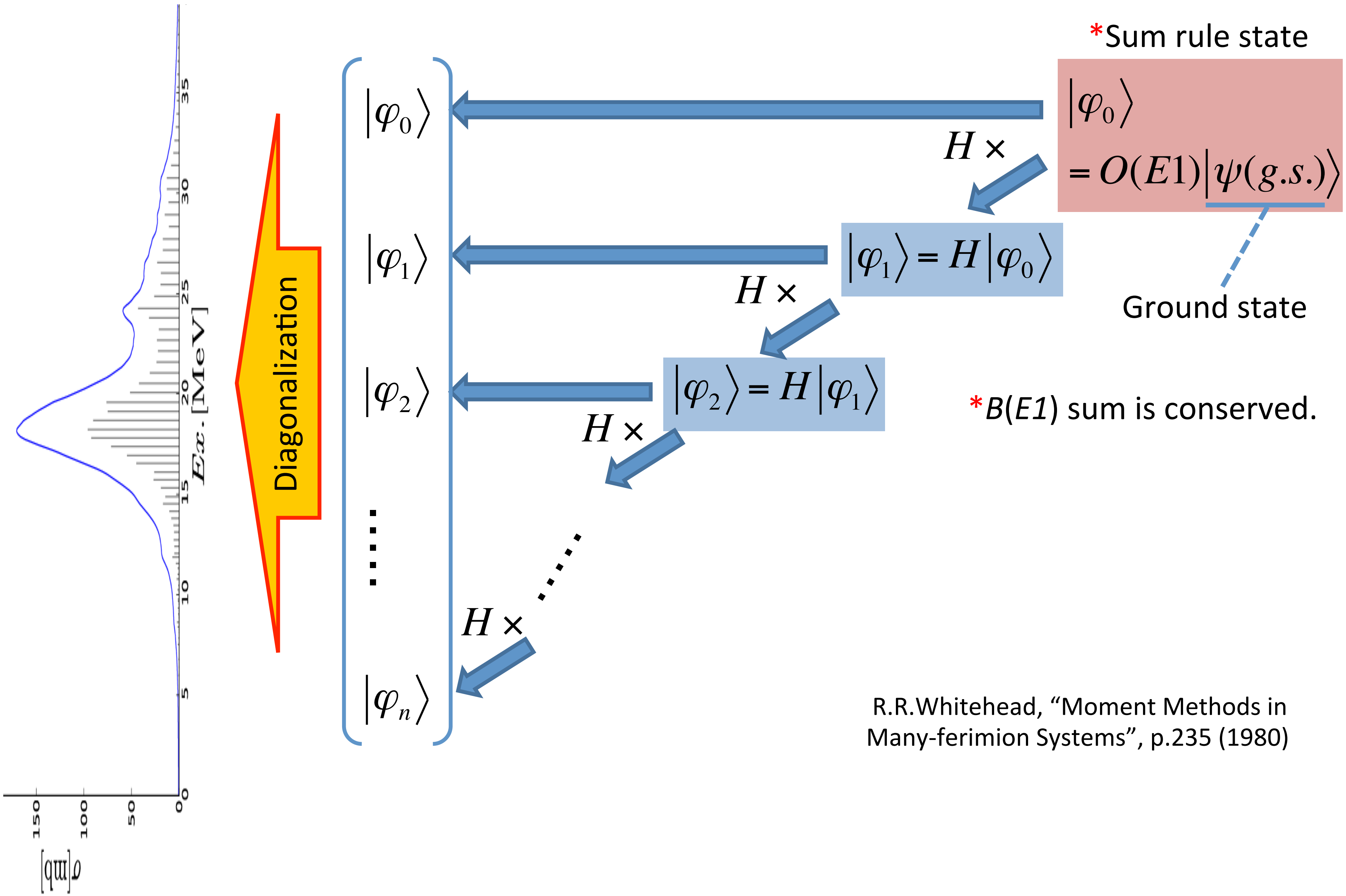


Step4. Low-energy *E1* excited states are solved independently by "normal" MCSM.



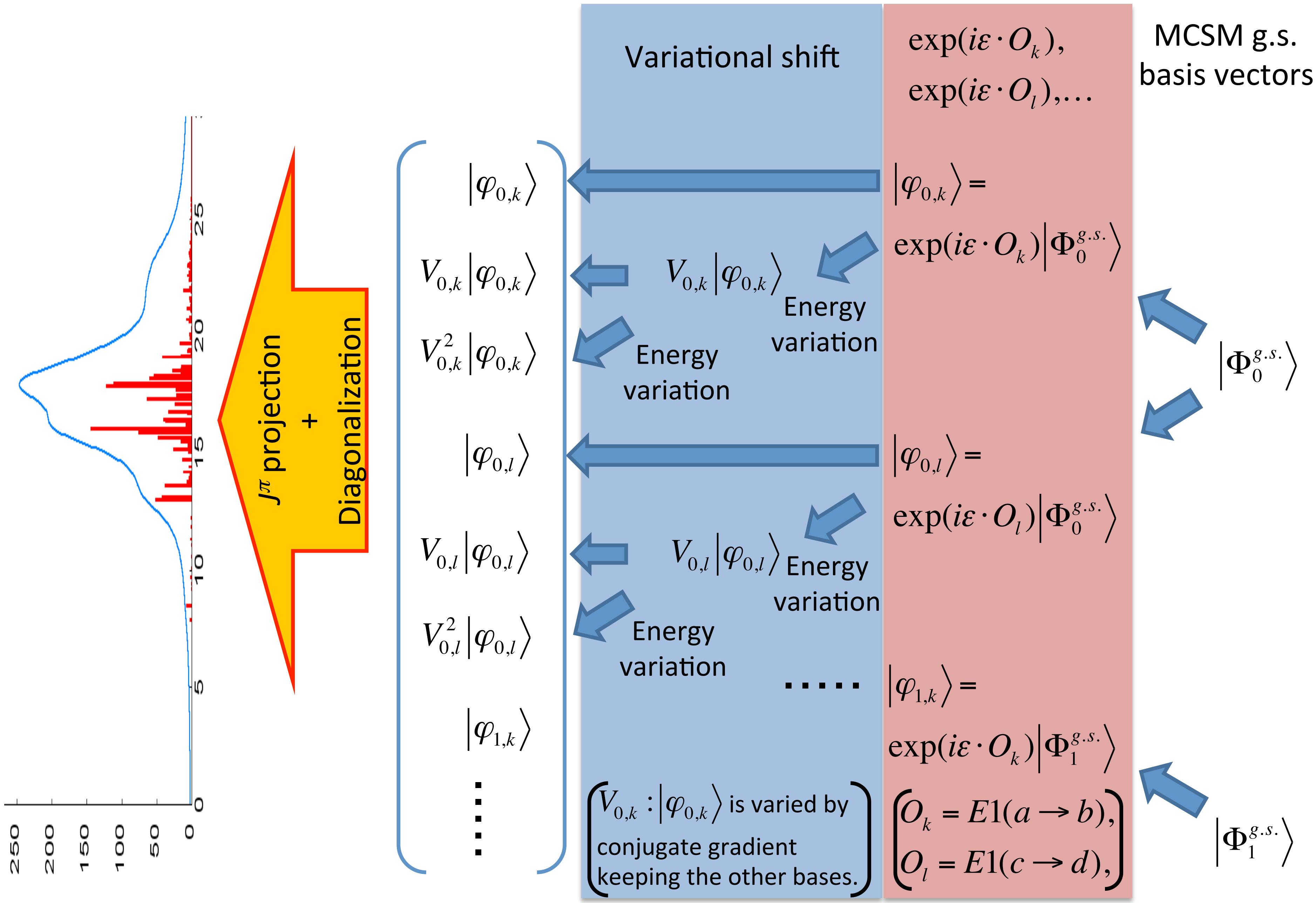
Step5. Diagonalize *H* by the basis vectors of steps.2-4. with J^π projection.

Lanczos strength function method



R.R.Whitehead, "Moment Methods in Many-ferimion Systems", p.235 (1980)

MCSM strength function



Applications

Benchmark test by comparison with Lanczos method

^{18}O with p-sd shell (2 major shell)
psdwbt int.

Lanczos calc. (exact)

M-scheme dimension
40,905,619 (~4 x 10^7)

Iteration of Lanczos strength function method: 500 times

Sum rule : 2.395

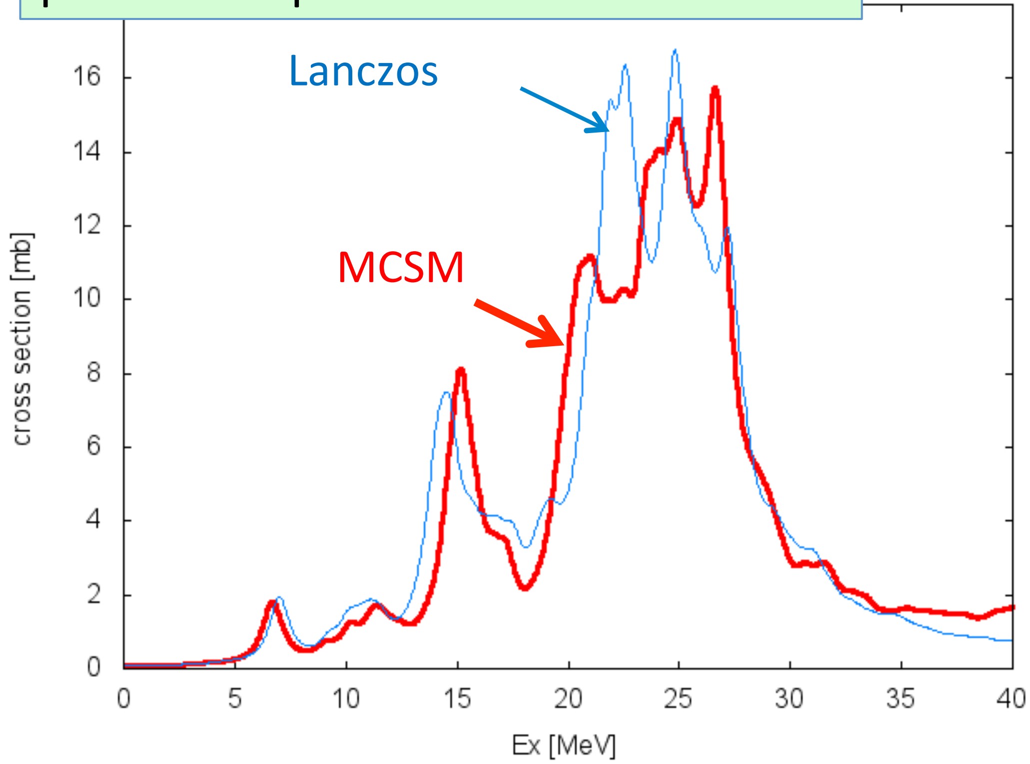
MCSM strength function

600 MCSM basis vectors

B(E1) sum: 2.189
Sum rule : 2.423

Lorentzian width
Γ = 1.0MeV

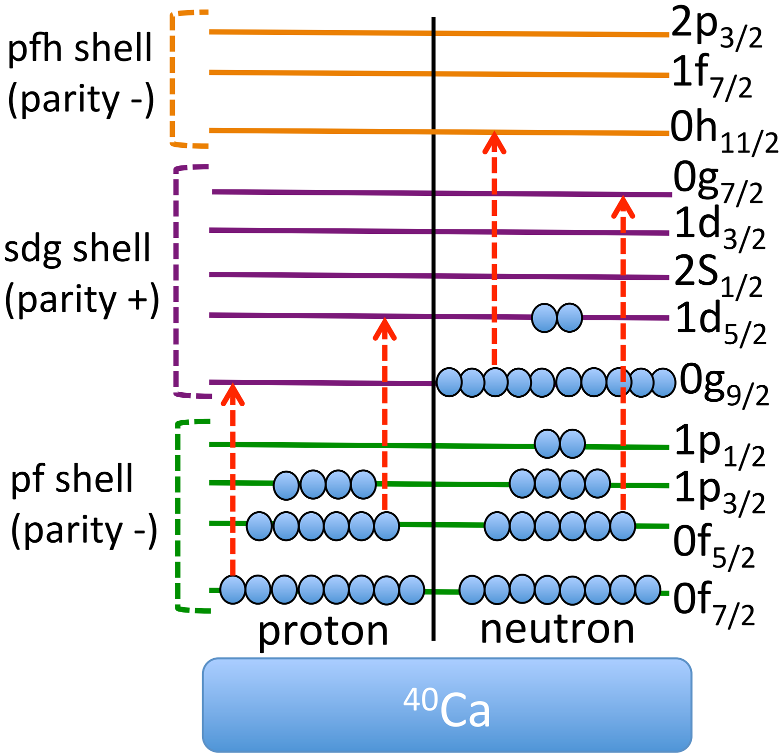
photoabsorption cross section of ^{18}O



Applications to medium-mass nuclei

We apply MCSM strength function to types of large model space (*M*-scheme dim. > ~10^{14}).

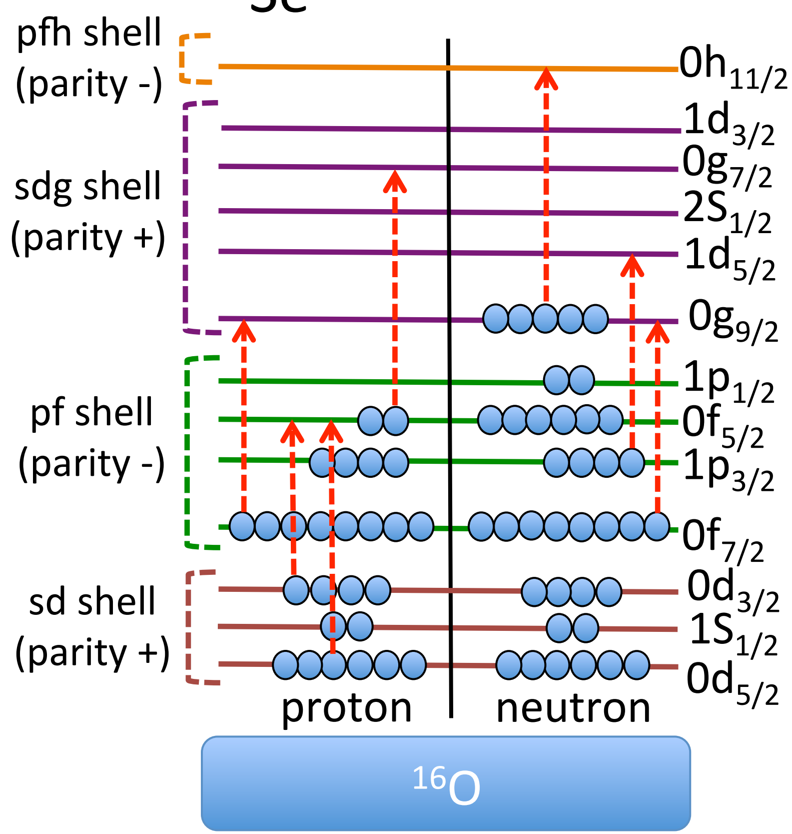
3 major shell ^{90}Sr



[Stable nucleus: ^{88}Sr (Z=38, N=50)
Long-live fission product (LLFP):
^{90}Sr (Z=38, N=52)

Effective int.:
*V_{MU} (central force scaled by 0.55)

4 major shell ^{79}Se

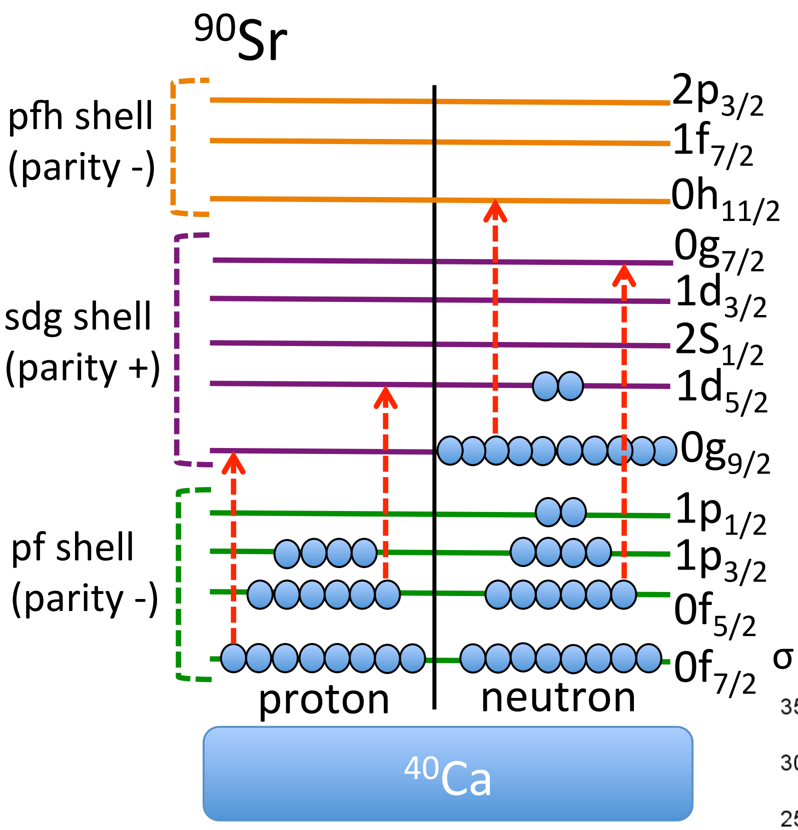


[Stable nuclei: ^{76,78}Se (Z=34, N=42,44)
LLFP: ^{79}Se (Z=34, N=45)

Effective int.: *SDPF-MU (sd-pf) + V_{MU} (others)
(central force scaled by 0.35)

*Y. Utsuno *et.al.*, PRC86, 051301(R) (2012)

Choice of transitional sets of orbits



*18 transitional ways in the above model space

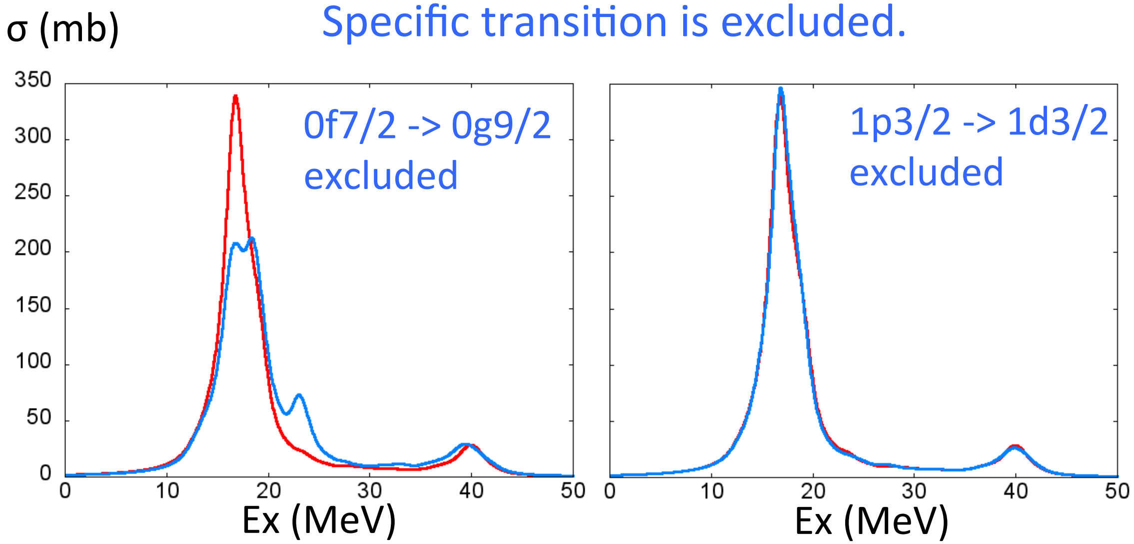
$\exp(i\varepsilon \cdot E1(a \to b))$, $\exp(i\varepsilon \cdot E1(c \to d))$, …

Excluding the transitions not to affect *E1* spectrum, 10 transitions are chosen.

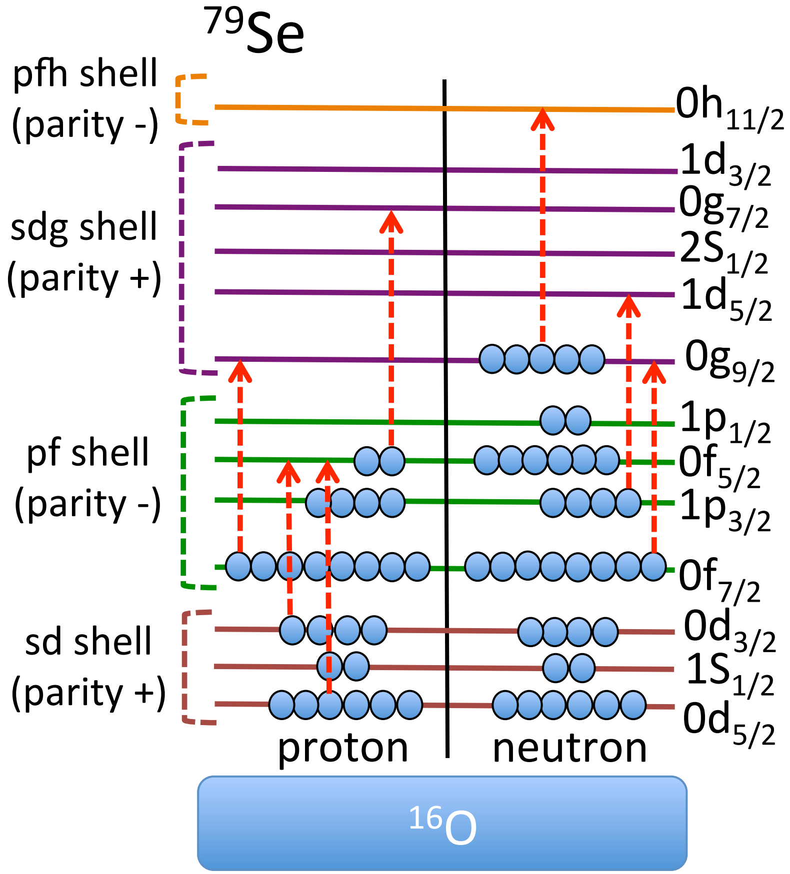
^{88,90}Sr

0f5/2 -> 0g7/2, 0f5/2 -> 1d5/2, 0f7/2 -> 0g7/2, 0f7/2 -> 0g9/2, 1p1/2 -> 1d3/2, 1p1/2 -> 2s1/2, 1p3/2 -> 1d5/2, 0g7/2 -> 1f7/2, 0g9/2 -> 0h11/2, 1d3/2 -> 2p3/2

Ex) ^{90}Sr: All transitional ways are included.
Specific transition is excluded.



Choice of transitional sets of orbits



*20 transitional ways in the above model space

exp($i\varepsilon \cdot E1(a \rightarrow b)$), exp($i\varepsilon \cdot E1(c \rightarrow d)$), …

Excluding the transitions not to affect *E1* spectrum, 10 transitions are chosen.

^{76}Se

0d3/2 -> 0f5/2, 0f5/2 -> 0g7/2, 0f5/2 -> 1d5/2, 0f7/2 -> 0g9/2, 0f7/2 -> 1d5/2, 0f7/2 -> 0g7/2, 1p1/2 -> 1d3/2, 1p3/2 -> 1d5/2, 1p3/2 -> 1d3/2, 0g9/2 -> 0h11/2

^{78,79}Se

0d3/2 -> 0f5/2, 0f5/2 -> 0g7/2, 0f5/2 -> 1d5/2, 0f7/2 -> 0g9/2, 0f7/2 -> 1d5/2, 0f5/2 -> 1d3/2, 1p1/2 -> 1d3/2, 1p3/2 -> 1d5/2, 1p3/2 -> 2s1/2, 0g9/2 -> 0h11/2

Number of basis vectors in MCSM strength function

Ground state:
50 basis vectors → *E1* spectrum: 900 basis vectors

Sr isotopes (^{88,90}Sr)

Initial 20 basis vectors in g.s. x 10 transitional operators
= 200 basis vectors

+

2-cycle variational shifts for the above
=> 200 x 2 = 400 basis vectors

+

Low-lying states solved by 300 basis vectors.

Ground state:
15 basis vectors → *E1* spectrum: 300 basis vectors

Se isotopes (^{76,78,79}Se*)

* 3 spin-parity states of 9/2-, 7/2-, 5/2- transited from g.s. of 7/2+ in ^{79}Se are solved independently.

15 basis vectors in g.s. x 10 transitional operators
= 150 basis vectors

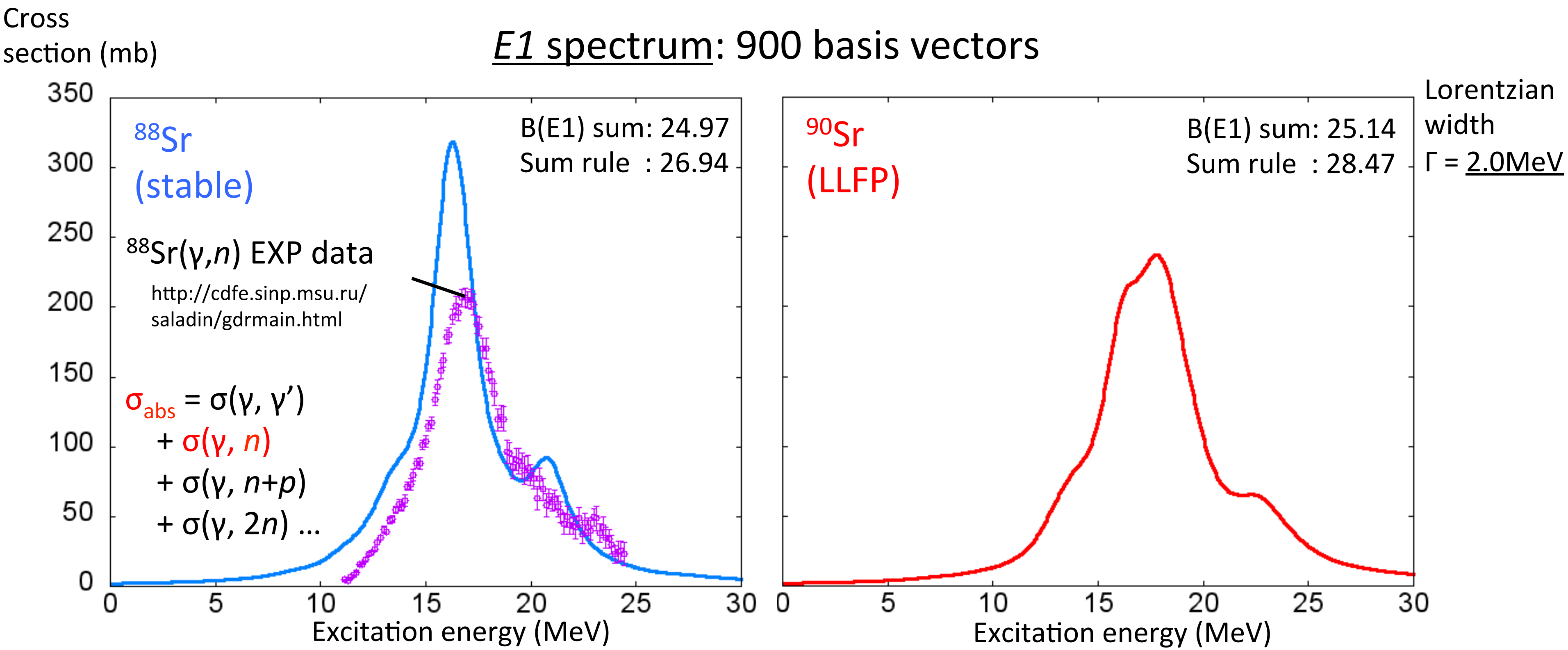
+

1-cycle variational shifts for the above
=> 150 basis vectors

Results of Sr (Z=38) isotopes (preliminary)

Photoabsorption cross section σ_{abs} of ^{88}Sr (N=50), ^{90}Sr (N=52)

E1 spectrum: 900 basis vectors



Thomas-Reiche-Kuhn (TRK) sum rule [MeV barn] : 1.290(^{88}Sr), 1.312(^{90}Sr)

(Ref: P.Ring and P.Schuck, The Nuclear Many-body Problem, p.294)

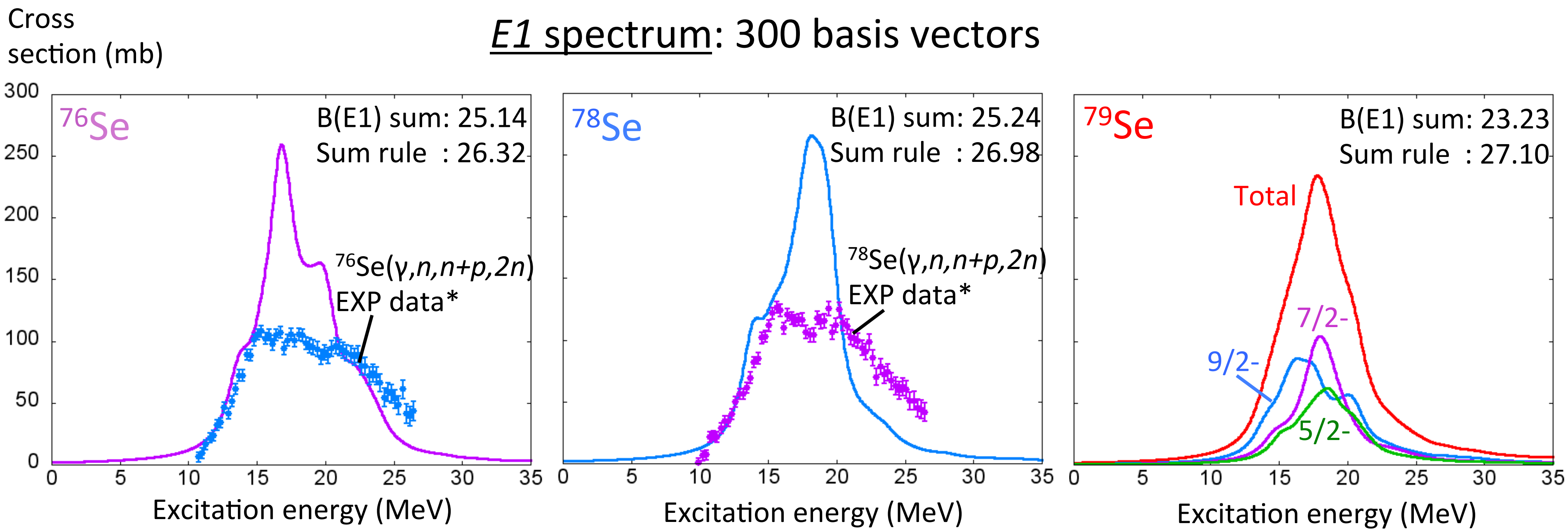
Calculated energy integrated cross section (Ex ≤ 30 MeV) [MeV barn] : 1.536(^{88}Sr), 1.620(^{90}Sr)

(19.1%, 23.5% enhanced)

Results of Se (Z=34) isotopes (very preliminary)

Photoabsorption cross section σ_{abs} of ^{76}Se (N=42), ^{78}Se (N=44), ^{79}Se(N=45)

E1 spectrum: 300 basis vectors



*EXP data: Nucl.Phys.A 258, 365 (1976)

Lorentzian width Γ = 2.0MeV

Thomas-Reiche-Kuhn (TRK) sum rule [MeV barn] : 1.123(^{76}Se), 1.146(^{78}Se), 1.157(^{79}Se)

⇕

Calculated energy integrated cross section (Ex ≤ 30 MeV) [MeV barn] : 1.680(^{76}Se), 1.664(^{78}Se), 1.564(^{79}Se)

(49.7%, 45.2%, 35.2% enhanced)

Summary and Perspectives

We have developed a new function to describe *E1* spectrum for Monte Carlo shell model (MCSM).

MCSM can describe *E1* collective states by

- the basis vectors generated by the exponential operators of *E1* transition between different sets of orbits.
- the basis vectors generated by variational shifts from the above.

Perspective

- Systematic calculations from stable to neutron-rich nuclei.
- Separation between isoscalar and isovector dipole transition.
- Calculation of transition density, and so on.

Acknowledgement

This work is supported by
Strategic Programs for Innovative Research (SPIRE) Field 5
"The origin of matter and the universe" by MEXT in Japan.
This research use computational resources of K computer.

Backup

Formula of photoabsorption cross section

$$\sigma(E)=\frac{4\pi^2 e^2}{\hbar c}(E_f-E_i)\frac{1}{2J^i+1}\sum_{M^i,M^f}\left|\left\langle \Psi_f(J^f,M^f)\middle|D\middle|\Psi_i(J^i,M^i)\right\rangle\right|^2\delta(E-E_f+E_i)$$

$$D=\sqrt{\frac{4\pi}{3}}E1$$

Under the assumption of the photon unpolarized in the z-direction (M=0),

$$\frac{1}{2J^i+1}\sum_{M^i,M^f}\left|\left\langle \Psi_f(J^f,M^f)\middle|D\middle|\Psi_i(J^i,M^i)\right\rangle\right|^2$$

$$=\frac{1}{2J^i+1}\sum_{M^i,M^f}\begin{pmatrix} J^i & J^f & 1 \\ M^i & -M^f & 0 \end{pmatrix}^2\left|\left\langle \Psi^f(J^f)\middle\|D\middle\|\Psi^i(J^i)\right\rangle\right|^2$$

$$=\frac{1}{2J^i+1}\cdot\frac{1}{3}\cdot\frac{4\pi}{3}\left|\left\langle \Psi^f(J^f)\middle\|E1\middle\|\Psi^i(J^i)\right\rangle\right|^2$$

$$=\frac{4\pi}{9}B(E1;J^i\rightarrow J^f)$$

$$\Rightarrow\quad \sigma(E)=\frac{16\pi^3}{9}\frac{e^2}{\hbar c}(E_f-E_i)\cdot B(E1;J^i\rightarrow J^f)\cdot\delta(E-E_f+E_i)$$

Energy levels in low-lying states

^{88}Sr	Ex(MeV)	Exp(MeV)
0^+_1	0.0	0.0
2^+_1	2.95	1.84

^{90}Sr	Ex(MeV)	Exp(MeV)
0^+_1	0.0	0.0
2^+_1	1.03	0.83
4^+_1	1.97	1.65

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^{76}Se	Ex(MeV)	Exp(MeV)
0^+_1	0.0	0.0
2^+_1	0.81	0.56
4^+_1	1.18	1.34

^{78}Se	Ex(MeV)	Exp(MeV)
0^+_1	0.0	0.0
2^+_1	0.76	0.62
4^+_1	1.30	1.51

^{79}Se	Ex(MeV)	Exp(MeV)
$7/2^+_1$	0.0	0.0
$9/2^+_1$	0.30	0.14
$11/2^+_1$	0.49	0.90