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

2015/09/15 COMEX5 at Krakow

Large-scale shell model calculations on E1 spectra of medium-heavy nuclei

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Introduction

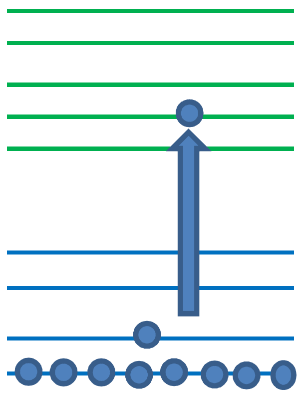
- Giant Dipole Resonance (GDR) and Pygmy Dipole Resonance (PDR) have been studied intensively by RPA, QRPA, phonon model, …

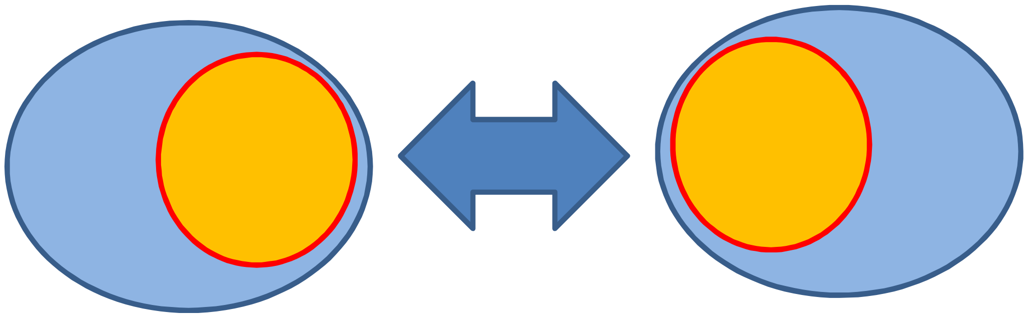
  e.g. Inakura (2011), Hartmann *et al.* (2004), ...

- Neutron skin, EoS, symmetry energy

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

- PDR: single-particle excitation vs. collective excitation?





- A few studies by shell model (SM) calc. in medium-heavy nuclei

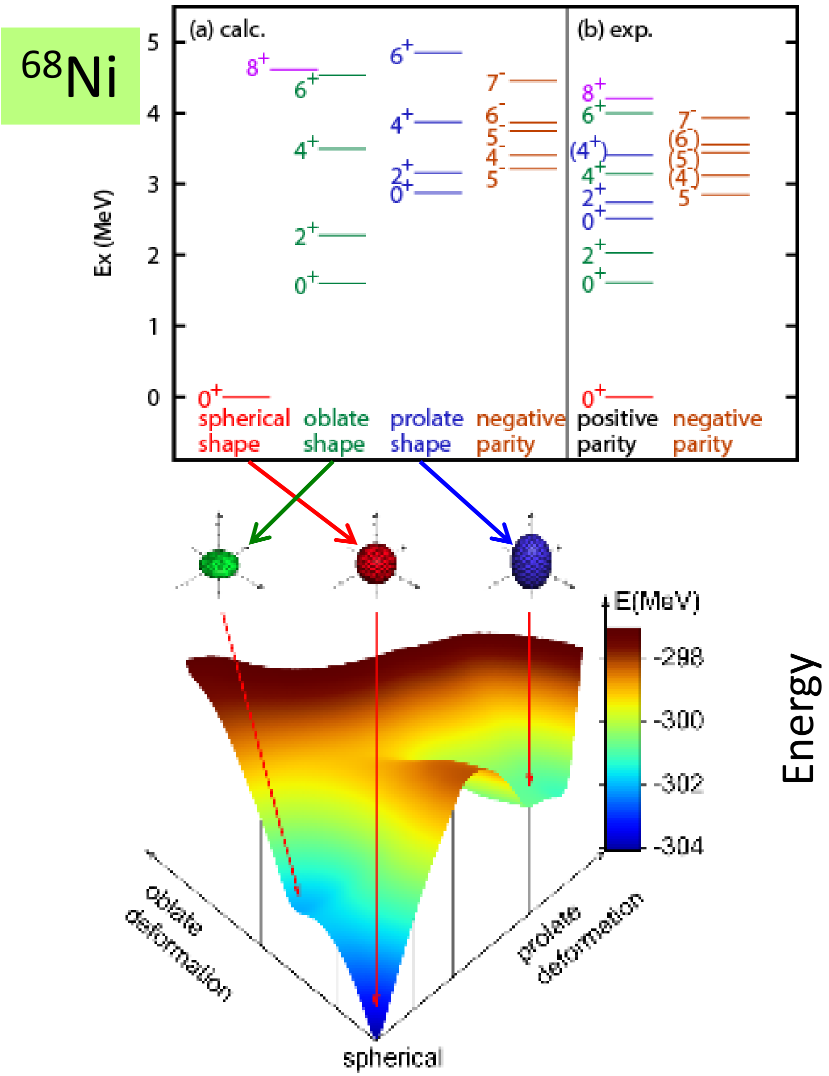
  Schwengner Brown (2010) , Sagawa Suzuki (1999), K. Sieja (2013), ...

purpose

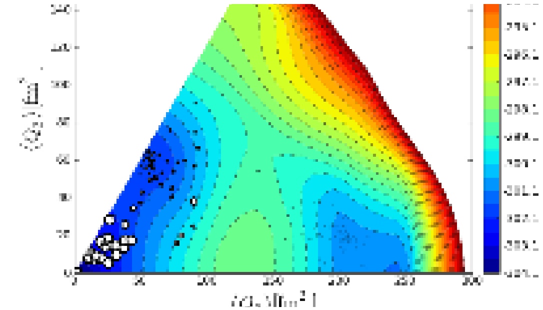
Large-scale shell model (LSSM) calculations and Monte Carlo shell model (MCSM) for GDR/PDR in medium-heavy nuclei with including various many-body correlations

A successful example of shell-model calc. (MCSM): Neutron-rich Ni isotopes and shell evolution

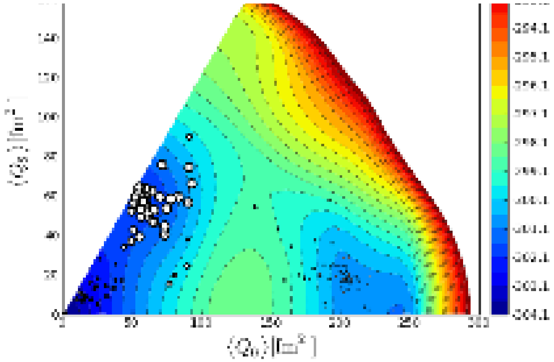
Y. Tsunoda, T. Otsuka, N. Shimizu, M. Honma and Y. Utsuno,
PRC 89, 031301(R) (2014)



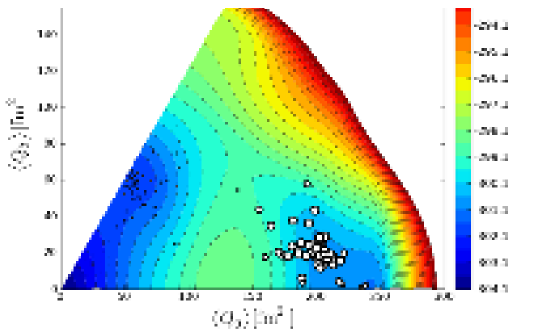
0^+_1 : spherical $\beta \sim 0$



0^+_2 : oblate $\beta \sim -0.2$



0^+_3 : prolate $\beta \sim +0.4$



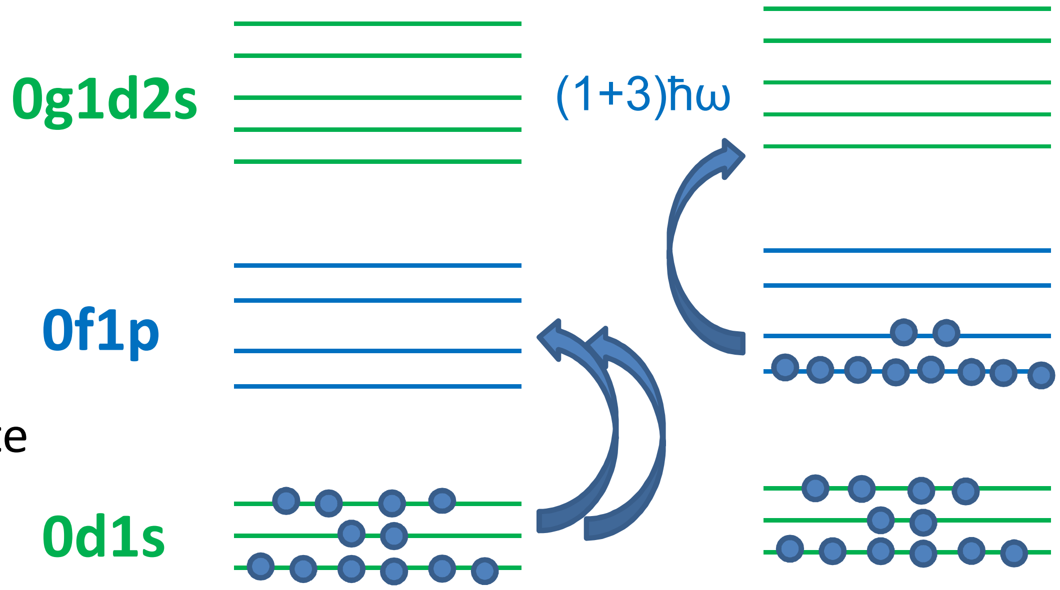
Strength function in shell model

- In principle, the shell model is quite useful for describing high excited states.
- *E*1 excitation causes parity change. 3-major-shell model space ($1\hbar\omega$) is required unlike *M*1 and Gamow-Teller transitions ($0\hbar\omega$ SM).
- In practice, direct diagonalization with the Lanczos method or MCSM cannot be applicable to high excited states because of high level density.
- Methods
  - Lanczos strength function method
    - E1 excitation of Ca isotopes
  - New extension of Monte Carlo shell model for strength function

Model space and effective int. for Ca isotopes

- Model space
  - full *sd-pf-sdg* shell
- 1ħω truncation
  - 0ħω for natural parity state
  - 1ħω for unnatural parity state

  ☆ Full correlation inside pf-shell



- (1+3)ħω truncation
  - (0+2)ħω for natural parity state
  - (1+3)ħω for unnatural parity state

1ħω : 4.1x10^6 M-scheme dim. for ^{48}Ca at PC

(1+3)ħω : 1.2x10^{10} M-scheme dim.

parallel code (KSHELL) + supercomputer

- effective interaction

USD+GXPF1B+VMU Utsuno *et al.*, PTPS 196, 304 (2012)

shell gaps and 3$^-$ states of Ca isotopes

smeared by Lorentzian $\Gamma = 1\mathrm{MeV}$

bare effective charge subtracting CoM

$$(e_\pi, e_\nu) = \left(\frac{N}{A}e, -\frac{Z}{A}e\right)$$

Lanczos strength-function method for E1 excitation spectrum

often used for Gamow-Teller transitions

Ref. R.R.Whitehead Phys. Lett. B 89, 313 (1980)

$$|\varphi_0(1^-)\rangle = O(\mathrm{E1})|0^+_1\rangle$$

ground state

Lanczos iteration using $|\varphi_0(1^-)\rangle$ as an initial state. (doorway state)

diagonalize the matrix in the Krylov subspace, $\left\{H^n|\varphi_0\rangle, H^{n-1}|\varphi_0\rangle, \ldots., H^1|\varphi_0\rangle, |\varphi_0\rangle\right\}$

to obtain approximated states $\left\{|\phi_0\rangle, |\phi_1\rangle, |\phi_2\rangle, \ldots., |\phi_{n+1}\rangle\right\}$ in the same way as Lanczos method.

Smoothing with Lorentz distribution

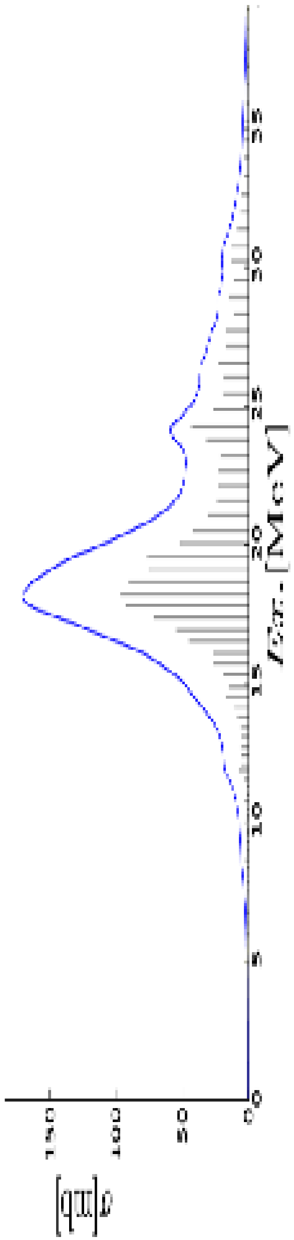
$$L(x, x_0, \Gamma) = \frac{1}{\pi}\frac{\gamma}{(x-x_0)^2+\gamma^2}$$

$$\text{with } \gamma = \Gamma/2. \qquad \Gamma = 1.0\,\mathrm{MeV}$$

Good distribution obtained in a few hundred Lanczos iterations

Lawson method is used for the removal of contamination of spurious mass motion

Concept of Lanczos strength function method



Diagonalization

"Sum rule" state

$|\varphi_0\rangle$ ⟵ $|\varphi_0(1^-)\rangle$ $= O(\mathrm{E1})\,|0^+{}_1\rangle$

$|\varphi_1\rangle$ ⟵ $|\varphi_1\rangle = H|\varphi_0\rangle$

$|\varphi_2\rangle$ ⟵ $|\varphi_2\rangle = H|\varphi_1\rangle$

$\vdots$

$|\varphi_n\rangle$

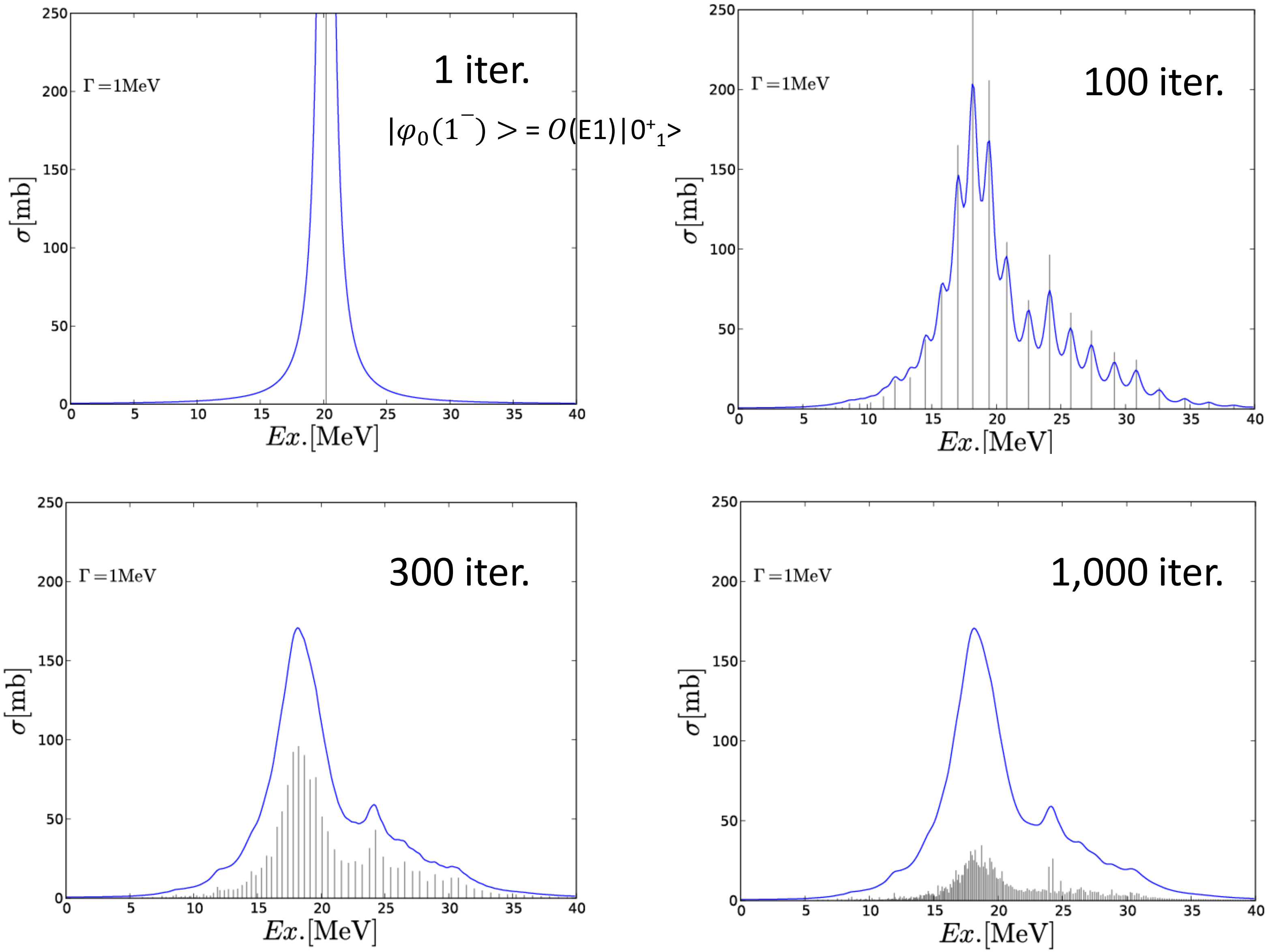
$|\varphi_k\rangle$: basis vectors

huge in M-scheme

10^{10} dim. ⇒ 80GB / a vector

$1 \le k \le n,\ \ n \sim 300$

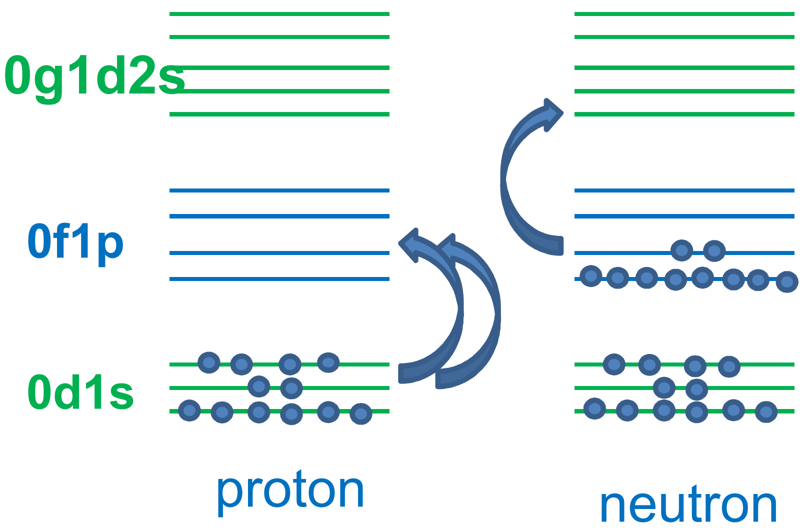
Convergence of strength distribution

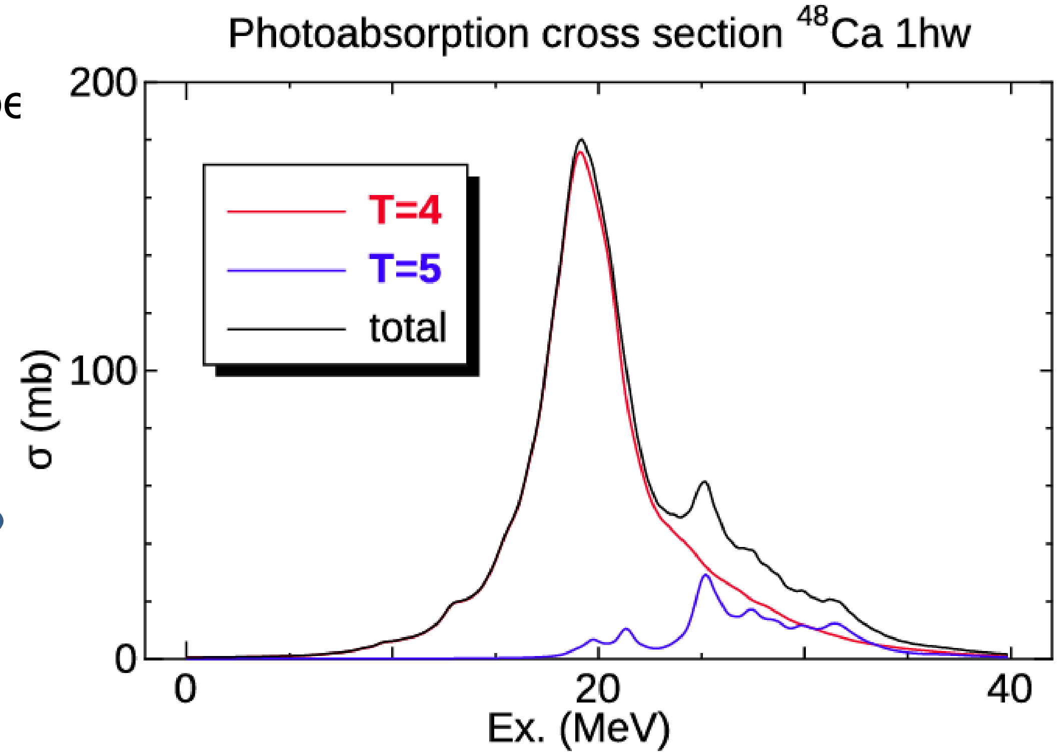


E1 excitation of Ca isotopes in LSSM

NS, Y. Utsuno, S. Ebata, T. Otsuka, M. Honma and T. Mizusaki, in preparation

1hw/3hw sd-pf-sdg shell calculations
for negative-parity states of Ca isotope
to describe E1 excitations





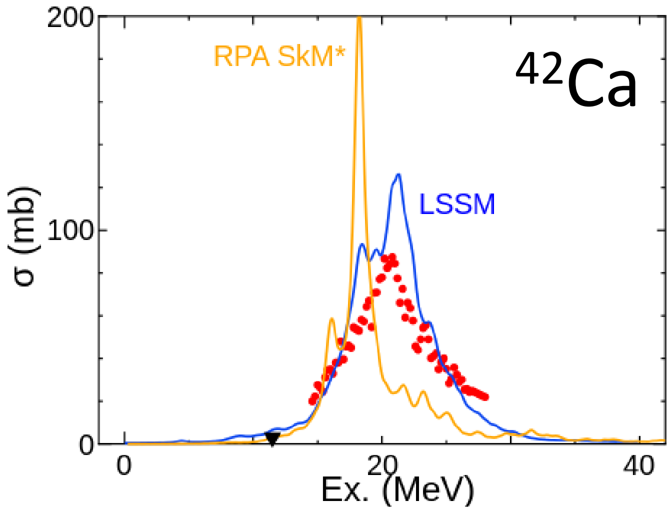
SM calc. well reproduce exp.
GDP peak position and width

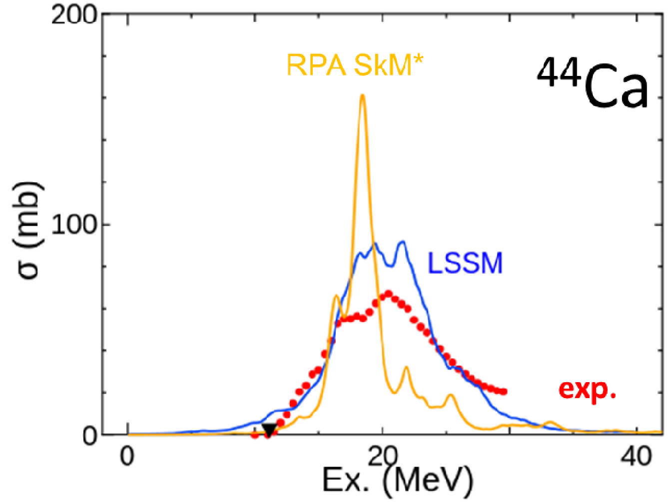
- GDR (1+3)ħω essential
- Ex. < 15MeV 1ħω enough

"Lanczos strength function method"

1hw : upto 1hw excitation in sd-pf-sdg shell
4.1×10^{6} M-scheme dim. at PC

(1+3)hw: up to 3hw excitation in sd-pf-sdg shell
1.2×10^{10} M-scheme dim.
at supercomputer





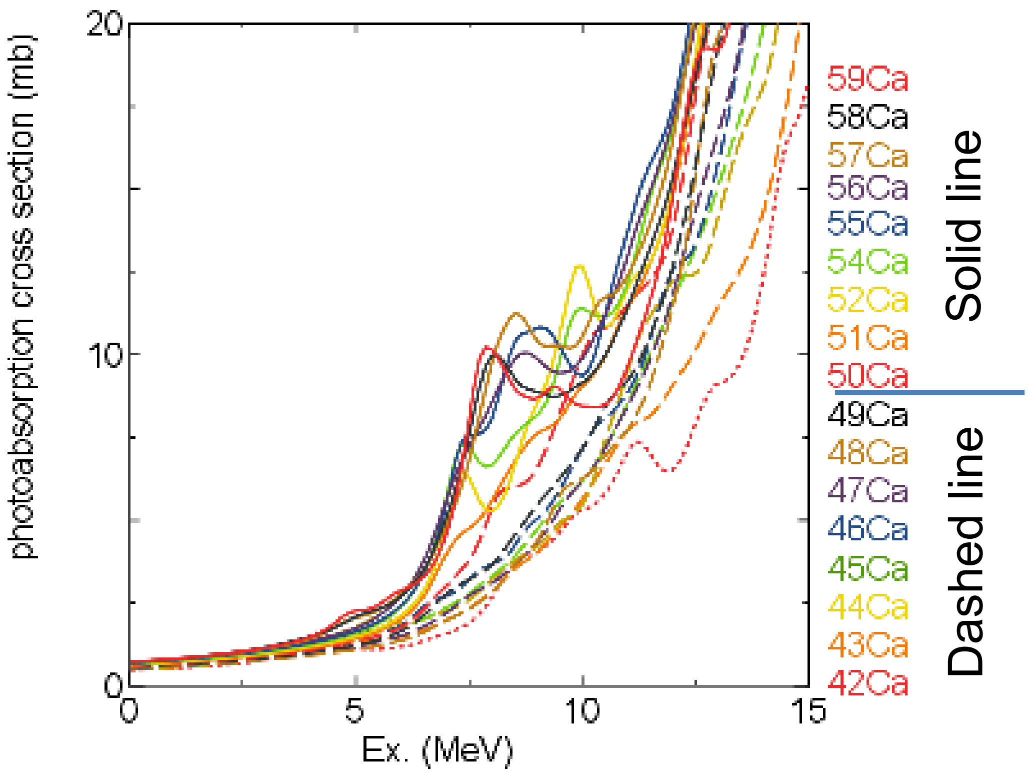
SM calc. well reproduce exp.
GDP peak position and width

- GDR (1+3)ħω essential
- Ex. < 15MeV 1ħω enough

RPA: Cb-TDHFB by S. Ebata, 5fm 3D sphere, 1fm mesh

photoabsorption cross section of Ca isotopes including odd nuclei

Low-energy region (1ħω)

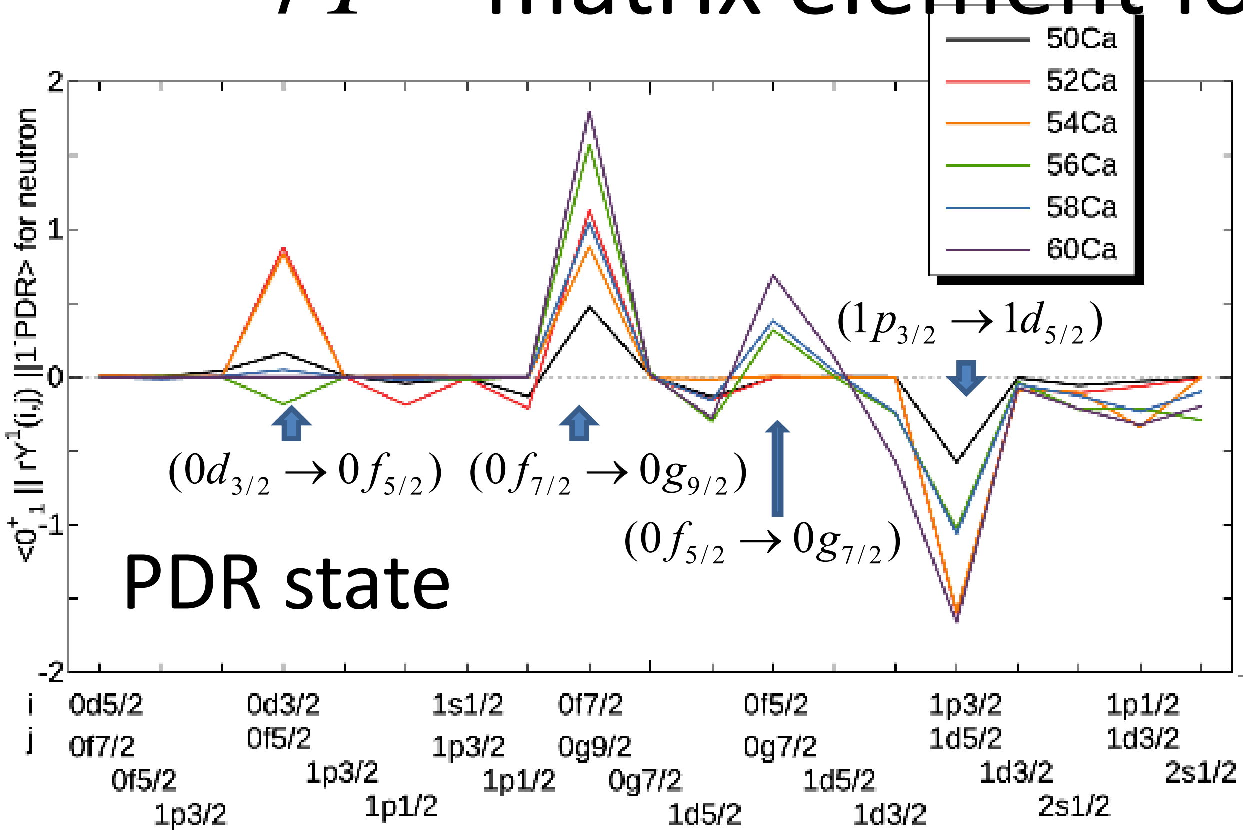


Dashed lines : 42Ca – 49Ca
Solid lines : 50Ca – 59Ca

$rY^{(1)}$ matrix element for neutron

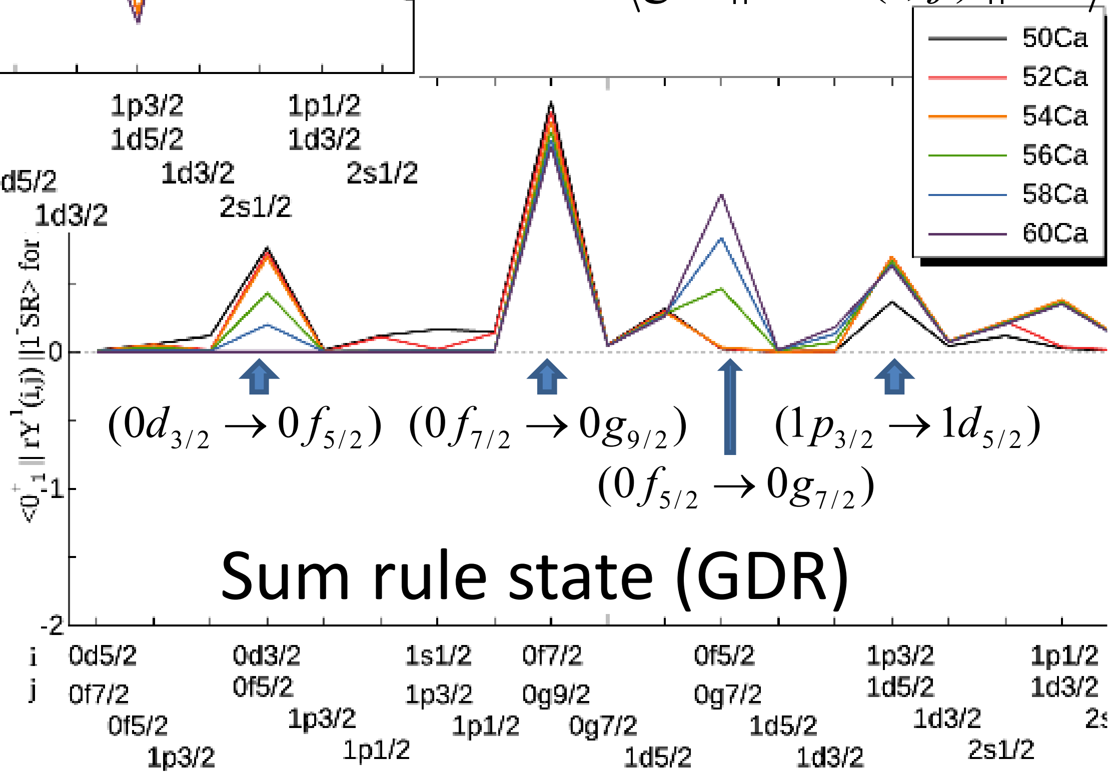
$|\mathrm{PDR}\rangle$ … large B(E1) state in low energy

$\langle \mathrm{g.s.} \| rY^{(1)}(i,j) \| \mathrm{PDR} \rangle$



$$|\mathrm{SR}\rangle = \frac{1}{N} rY^{(1)} |\mathrm{g.s.}\rangle$$

$$\langle \mathrm{g.s.} \| rY^{(1)}(i,j) \| \mathrm{SR} \rangle$$



$$B(E1) = \left(e_{tz} \sum_{i,j} \langle \mathrm{g.s.} \| rY^{(1)}(i,j,tz) \| 1^- \rangle \right)^2$$

stretched orbital pairs contribute
GDR: constructive
PDR: destructive

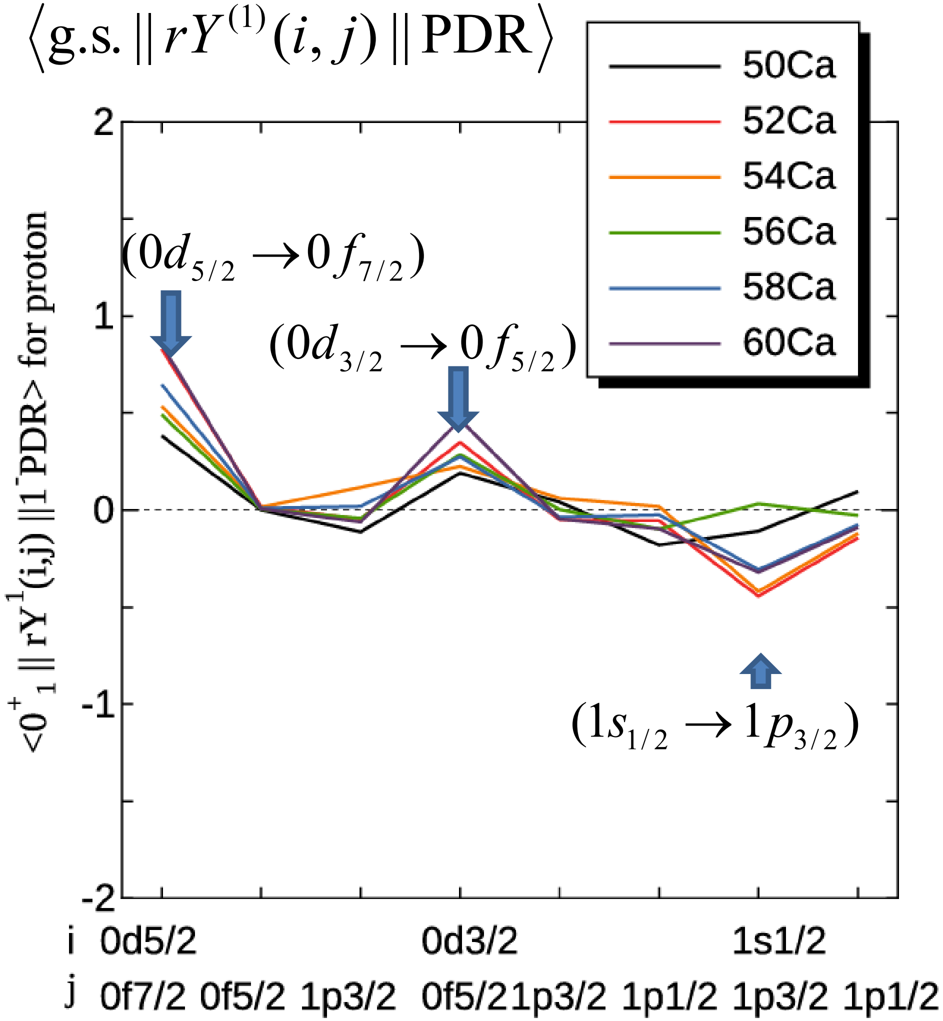
$rY^{(1)}$ matrix element for proton

$$B(E1) = \left(e_{tz} \sum_{i,j} \langle \text{g.s.} \| rY^{(1)}(i,j,tz) \| 1^- \rangle \right)^2$$

PDR state

$|\text{PDR}\rangle$ … large B(E1) state in low energy

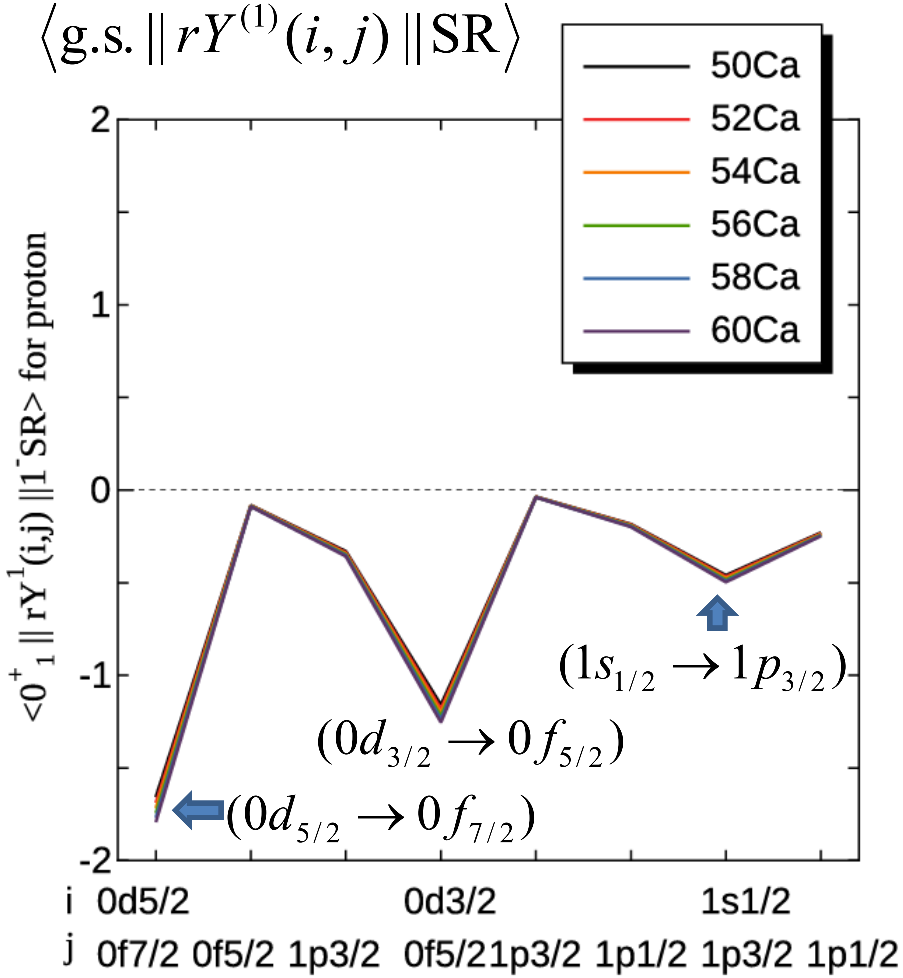
$\langle \text{g.s.} \| rY^{(1)}(i,j) \| \text{PDR} \rangle$



Sum rule state (GDR)

$$|\text{SR}\rangle = \frac{1}{N} rY^{(1)} |\text{g.s.}\rangle$$

$\langle \text{g.s.} \| rY^{(1)}(i,j) \| \text{SR} \rangle$



Beyond $3\hbar\omega$ truncation
and
toward heavier region
by Monte Carlo shell model
(MCSM)

Very brief outline of MCSM

- Efficient description of nuclear many-body states based on the basic picture of nuclear structure
  = intrinsic state + rotation + superposition

$$\left|\varphi(D^{(d)})\right\rangle = \prod_{\alpha=1}^{N}\left(\sum_{i=1}^{N_{sp}} c_i^{\dagger} D_{i\alpha}^{(d)}\right)\left|-\right\rangle$$

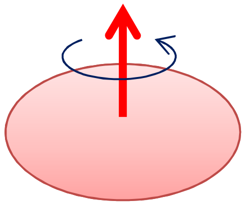
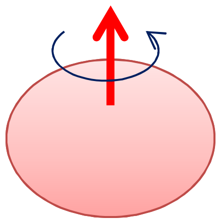
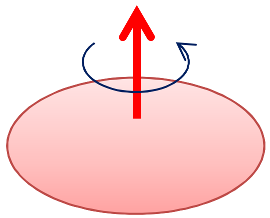
$$|\Psi^{IM\pi}(N_b)\rangle = \underbrace{\sum_{d=1}^{N_b} f^{(d)}}_{\text{superposition}} \underbrace{\sum_{K=-I}^{I} g_K^{(d)}\ \hat{P}^{\pi}\ \hat{P}_{MK}^{I}}_{\text{projection onto good quantum numbers}} \underbrace{|\varphi(D^{(d)})\rangle}_{\text{optimized Slater determinant}}$$

MCSM basis dimension ≈ 100

superposition → mixing with different shapes

projection onto good quantum numbers → rotation

optimized Slater determinant → deformed intrinsic state

Wave function = $f^{(1)}$  + $f^{(2)}$  + $f^{(3)}$  + ...

$D^{(d)}$: determined stochastically and variationally

Nħω configuration with N>3 ?

B(E1) sum rule
by Monte Carlo shell model

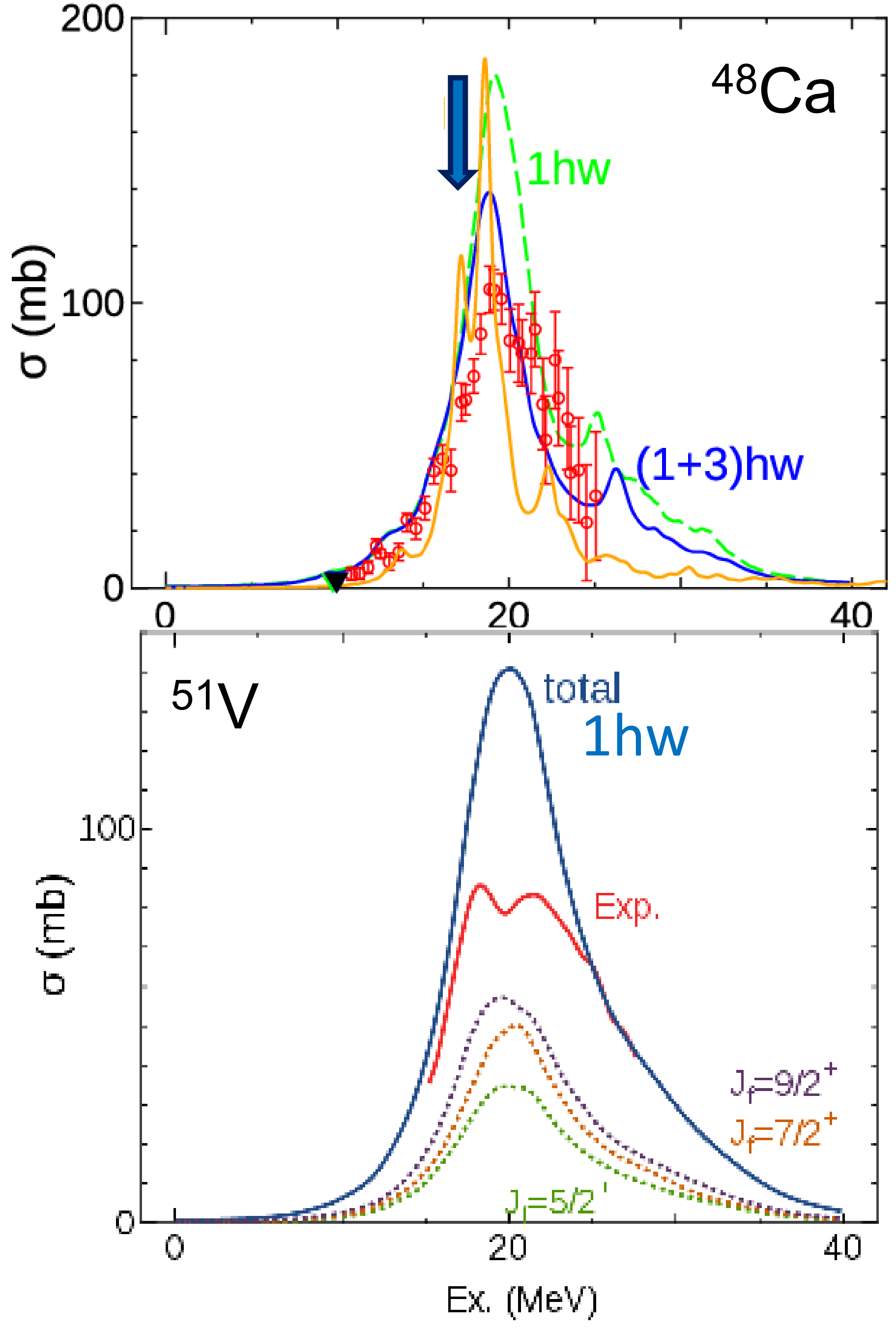
- ^{48}Ca B(E1) sum rule (e^2fm^2)
  - 1ħω ... **16.5**
  - (1+3)ħω ... **13.6**
  - MCSM 50dim. ... **10.1**

-18%

-38%

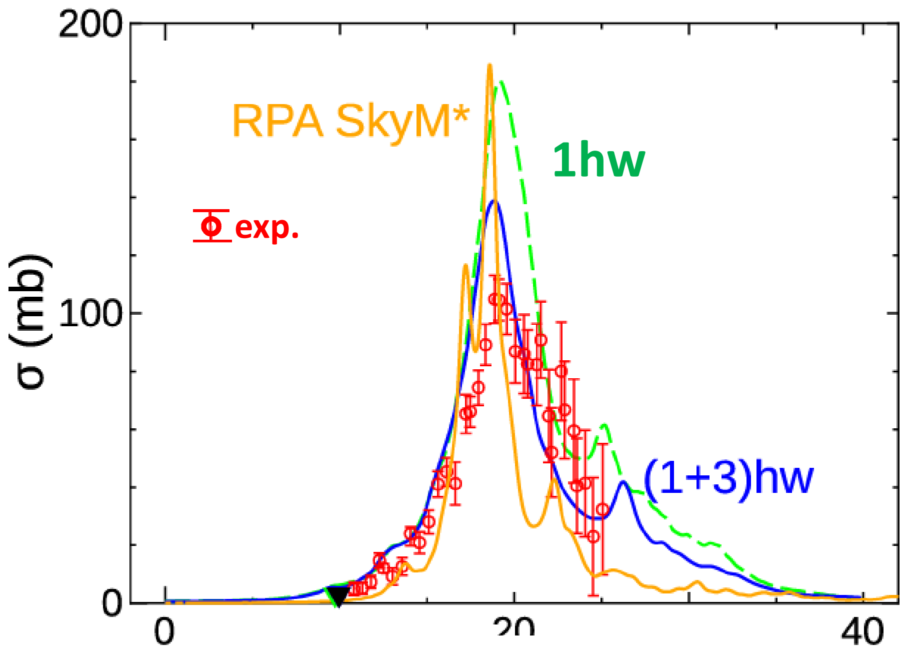
- ^{51}V B(E1) sum rule
  - 1ħω ... **18.1**
  - (1+3)ħω ... **NA**
  - MCSM 50dim ... **12.4**

-32%

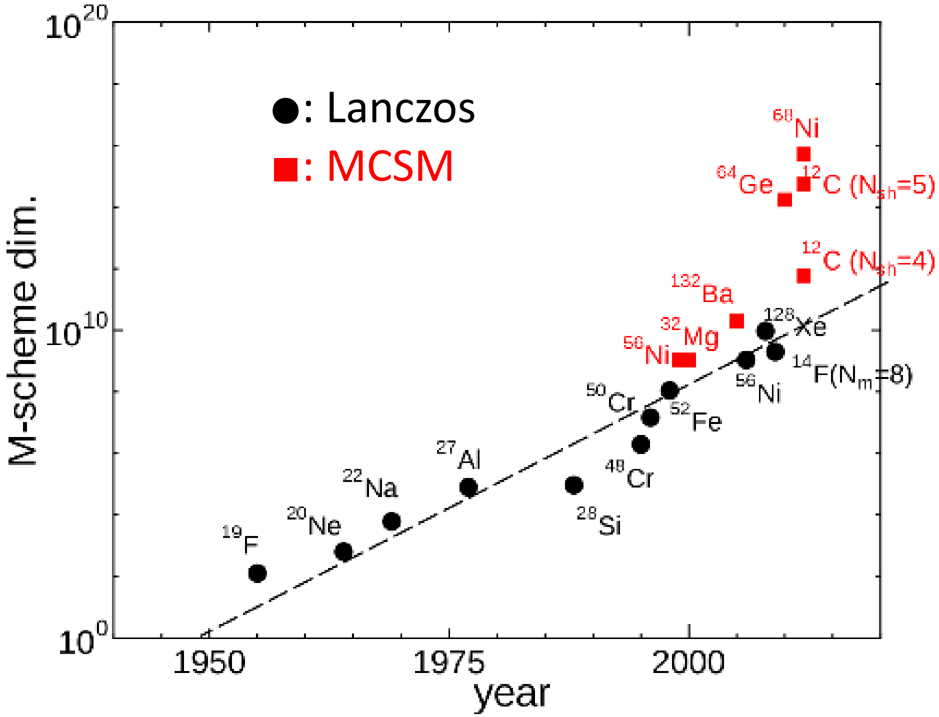


Many-body correlations suppress B(E1) rule

Photo-absorption cross section of ^{48}Ca



Progress of SM calc : Lancos vs MCSM



1hw : upto 1ħω excitation in sd-pf-sdg shell
4.1×10^{6} M-scheme dim. at PC

(1+3)hw: up to 3ħω excitation in sd-pf-sdg shell
1.2×10^{10} M-scheme dim. at supercomputer

^{79}Se (1+3) ħω : 1.2×10^{14} dim.
far beyond the current capability of Lanczos method

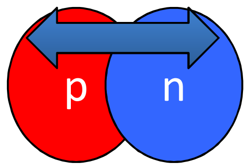
Monte Carlo shell model for E1 spectrum

Ref. T. Otsuka, T. Togashi, N. Shimizu et al.

Concept to describe *E1* spectrum with MCSM

E1 operator

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



We introduce an exponential of one-body operator.

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

We consider the following type of states:

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

basis vectors to represent
E1 excited states (i, ε)

Slater determinant ← Slater determinant

Although this was a good idea, it is still too naïve
to use this kind of states as the basis vectors for E1 spectrum.

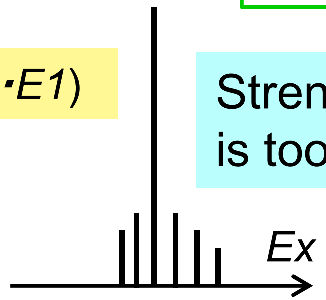
Ref. T. Otsuka, T. Togashi, N. Shimizu et al.

Decomposition of exp($i\varepsilon \cdot E1$) operator

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

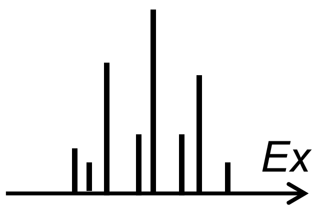
$$\boxed{\exp(i\varepsilon \cdot E1(0f_{7/2} \rightarrow 0g_{9/2}))}, \ldots \boxed{\exp(i\varepsilon \cdot E1(0g_{9/2} \rightarrow 0h_{11/2}))}, \ldots$$

exp($i\varepsilon \cdot E1$)

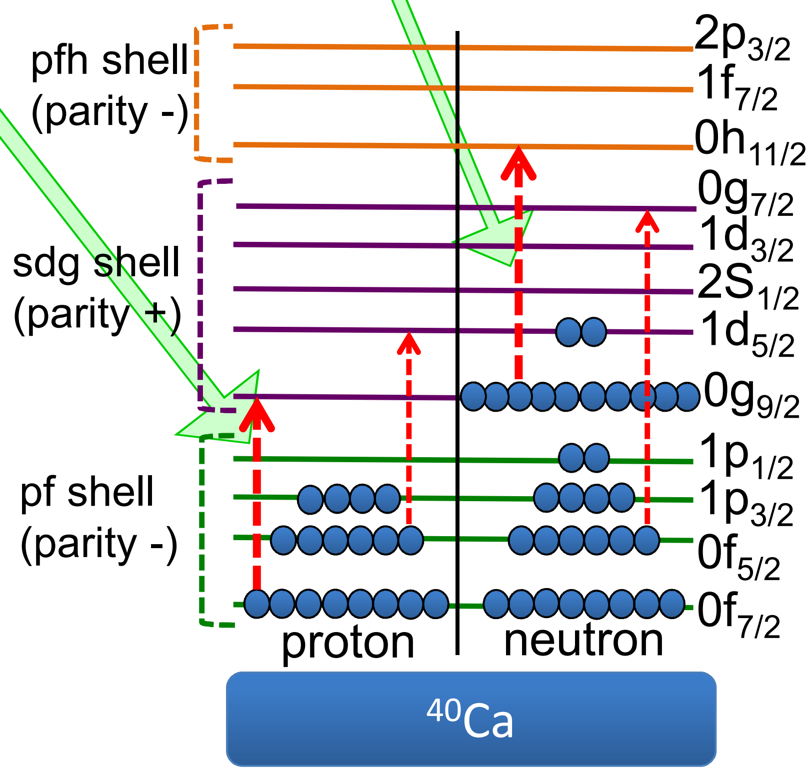


Strength distribution is too concentrated.

exp($i\varepsilon \cdot E1(a \to b)$)
exp($i\varepsilon \cdot E1(c \to d)$) …
separate basis vectors



Peaks corresponding to different orbital combinations appear.



E1 excitation spectrum can be calculated by MCSM

Ground state:

$$|\Psi\rangle = \sum_{k=1}^{N_{MCSM}} f_k P^{J,\pi} \boxed{|\varphi_k\rangle}$$

Basis vector of the ground state (Slater determinant)

Basis vectors for *E1* spectrum (*a,b,c,d,* … : orbits)

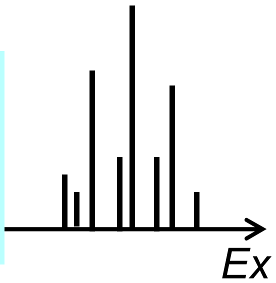
$$\boxed{\exp(i\varepsilon \cdot E1(a \to b))|\varphi_k\rangle, \exp(i\varepsilon \cdot E1(c \to d))|\varphi_k\rangle, \ldots (k = 1,2, \ldots)}$$

+

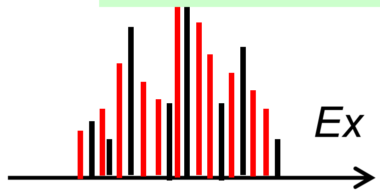
Additional bases for fine tuning :
variation for energy average by the conjugate gradient

$$|\varphi_k(E1(a \to b))^{Var}\rangle, |\varphi_k(E1(c \to d))^{Var}\rangle, \cdots$$

Diagonalization with these basis vectors after projection to 1⁻



Excitation spectrum up to certain fine structure



E1 spectrum with ~3000 levels connected somehow to the g.s. (confirmed by E1 sum rule)

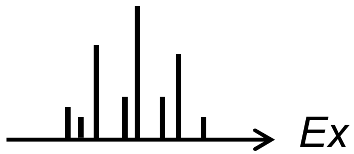
Overview of description of *E1* spectrum with MCSM

Step1. The ground state is solved by MCSM.

$$\left|\Psi(g.s.)\right\rangle = \sum_i f_i \left|\varphi_i^{g.s.}\right\rangle$$

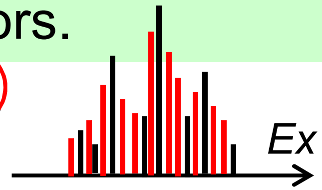
Step2. Basis vectors for *E1* spectrum are generated by acting exp(*iε*･*E1(a -> b)*), exp(*iε*･*E1(c -> d)*), …on basis vectors of the ground state.

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



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

$$\exp(i\varepsilon \cdot E1(a \to b))\left|\varphi_i^{g.s.}\right\rangle \xrightarrow{\text{Variational shift by conjugate gradient}} \left|\varphi_i(E1(a \to b))^{Var}\right\rangle$$



Step4. Low-energy *E1* excited states are solved independently by “normal” MCSM and are added to the spectrum.

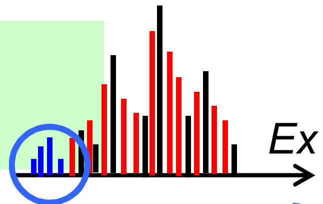
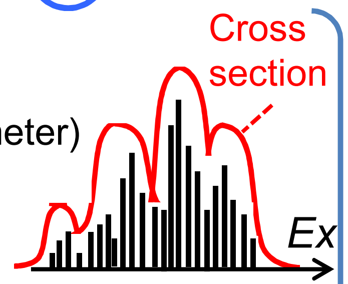


Photo absorption cross section is calculated

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

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

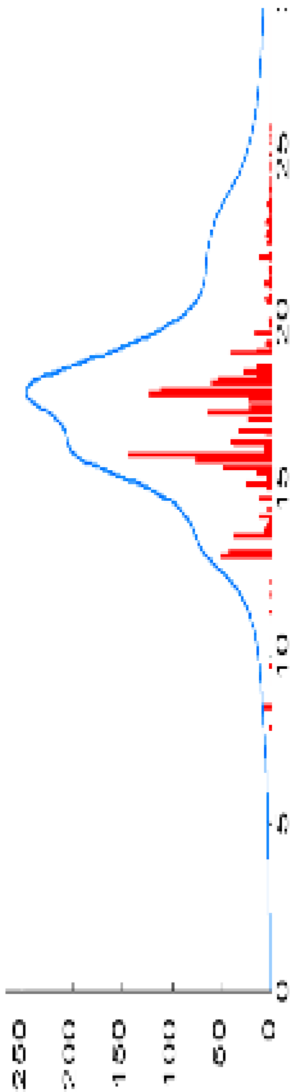
Excitation energy of n-th *E1* excited state



Concept of MCSM strength function

with keeping Slater-det. form

$$|\Phi_{g.s.}\rangle = \Sigma_i f_i P^{J\pi}|\varphi_i\rangle$$



J^π-Projection
+
Diagonalization

Variational shift

$|\varphi_{0,k}\rangle$

$|\varphi_{0,k}{}^{Var}\rangle$ $\leftarrow$ $|\varphi_{0,k}{}^{Var}\rangle$

$|\varphi_{0,k}{}^{VarVar}\rangle$

$|\varphi_{0,l}\rangle$

$|\varphi_{0,l}{}^{Var}\rangle$ $\leftarrow$ $|\varphi_{0,l}{}^{Var}\rangle$

$|\varphi_{0,l}{}^{VarVar}\rangle$

Var: variation by 2-step conjugate gradient

E1 $e^{i\varepsilon O_k}$

MCSM g.s. basis vectors

$|\varphi_{0,k}\rangle = e^{i\varepsilon O_k}|\varphi_0\rangle$

$|\varphi_0\rangle$

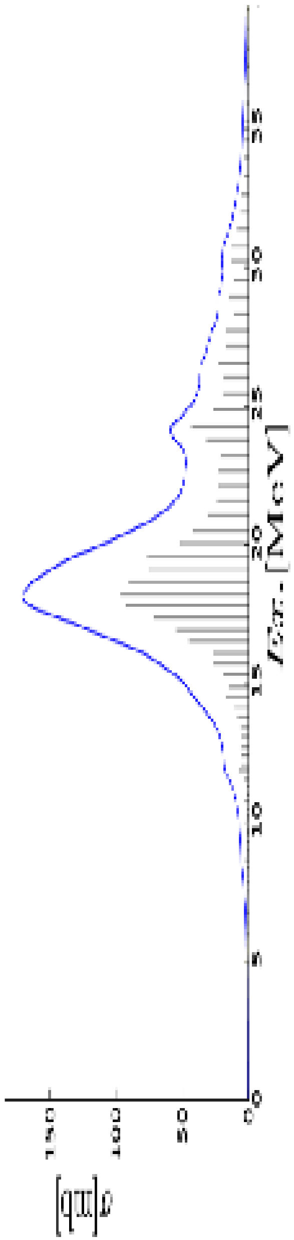
$|\varphi_{0,l}\rangle = e^{i\varepsilon O_l}|\varphi_0\rangle$

..... $|\varphi_{1,k}\rangle = e^{i\varepsilon O_k}|\varphi_1\rangle$

$O_k = E1(a \rightarrow b)$

$|\varphi_1\rangle$

Concept of Lanczos strength function method



Diagonalization

"Sum rule" state

$|\varphi_0(1^-)\rangle$
$= O(\mathrm{E1})\ |0^+{}_1\rangle$

$|\varphi_0\rangle$

$|\varphi_1\rangle$ $\qquad |\varphi_1\rangle = H|\varphi_0\rangle$

$|\varphi_2\rangle$ $\qquad |\varphi_2\rangle = H|\varphi_1\rangle$

⋮

$|\varphi_n\rangle$

$|\varphi_k\rangle$: basis vectors
huge in M-scheme
10^{10} dim. ⇒ 80GB
$1 \le k \le n,\ \ n{\sim}300$

E1 excitation described by Monte Carlo shell model

Benchmark test

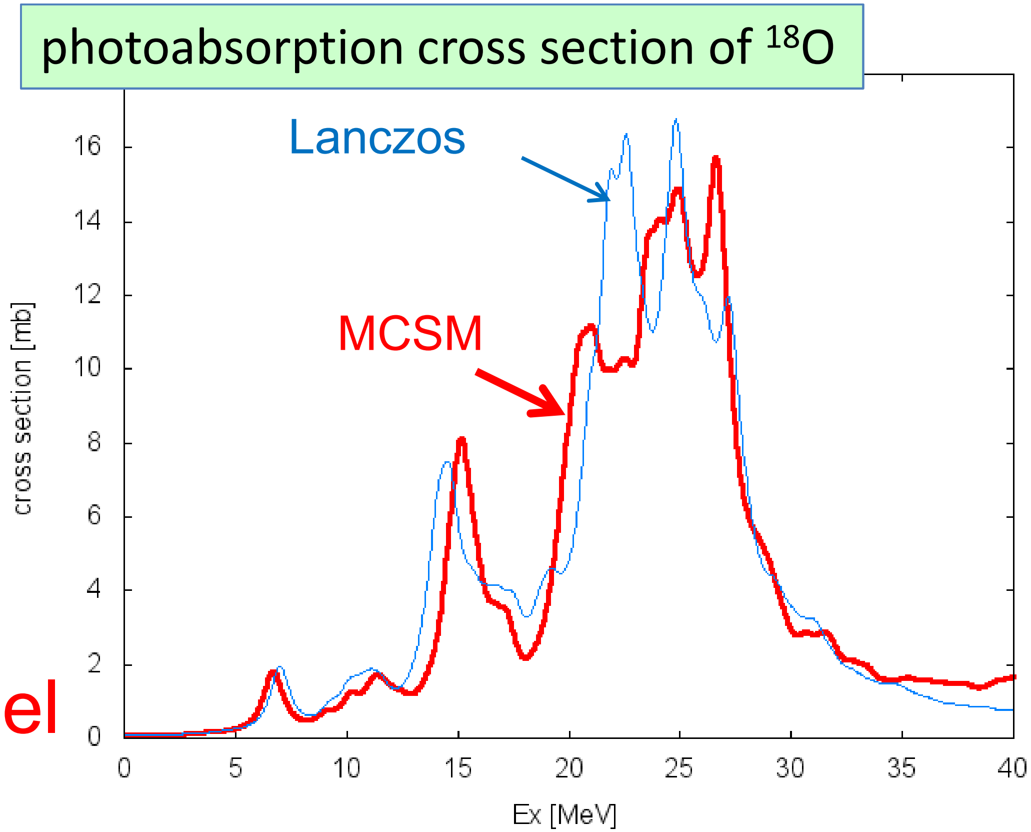
Lanczos calc. (exact)

M-scheme dimension
<u>3,844,499</u>

↓

Monte Carlo shell model (MCSM)

<u>600</u> MCSM basis vectors



^{18}O with p-sd shell
psdwbt int.

$$\left|\Psi\right\rangle = \sum_{k=1}^{N_{MCSM}} f_k P^{J,\pi} \left|\varphi_k\right\rangle \qquad \left|\varphi_k\right\rangle = \prod_{\alpha=1}^{N} \left(\sum_{i=1}^{N_{sp}} c_i^\dagger D_{i\alpha}^{(k)} \right) \left|-\right\rangle$$

Photoabsorption cross section of ^{88}Sr, ^{90}Sr

T. Togashi, T. Otsuka *et al.*

- Model space:
  pf - sdg - pfh($0h_{11/2}$, $1f_{7/2}$, $2p_{3/2}$) shell
  (3 major shell)

- Effective Hamiltonian: *V_{MU}(+ M3Y LS)
  (central force scaled by 0.55)

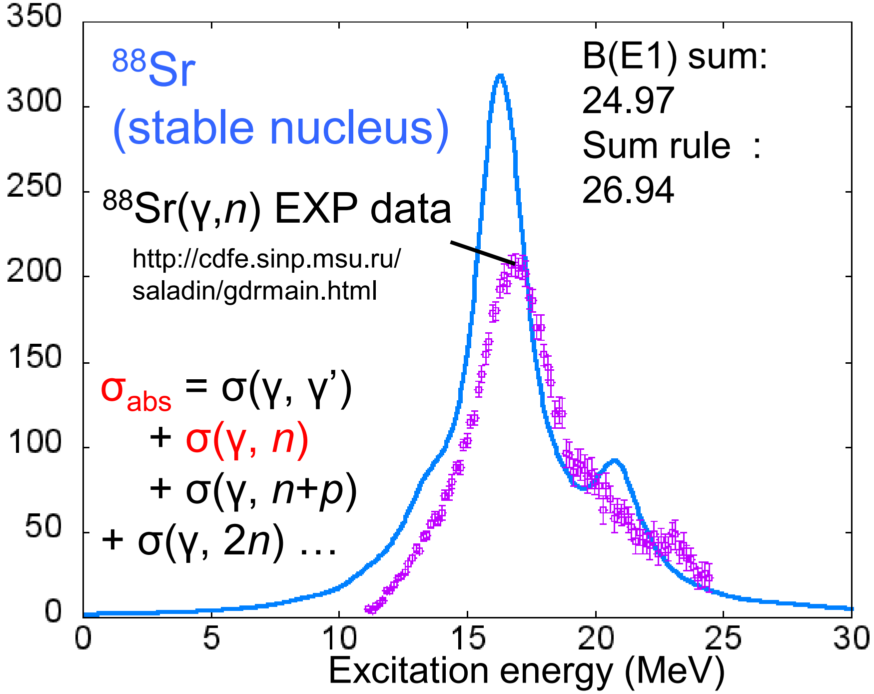
  *Y.Utsuno *et.al.*, PRC86, 051301(R) (2012)

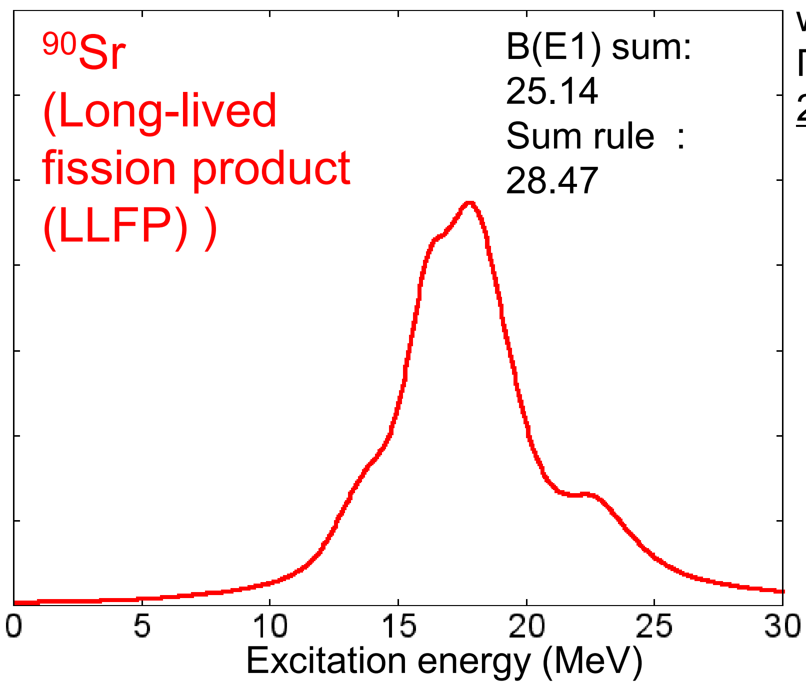
- The number of basis:
  1000 basis vectors are used to describe *E1* spectrum.

M-scheme dimension of Hamiltonian matrix for ^{90}Sr is 8.2×10^{14} with truncation of 3hw excitation.

Photoabsorption cross section σ_{abs} of ^{88}Sr (Z=38, N=50),^{90}Sr (Z=38,N=52)

Cross section (mb)





Lorentzian width
Γ =
2.0MeV

Results of Se (Z=34) isotopes

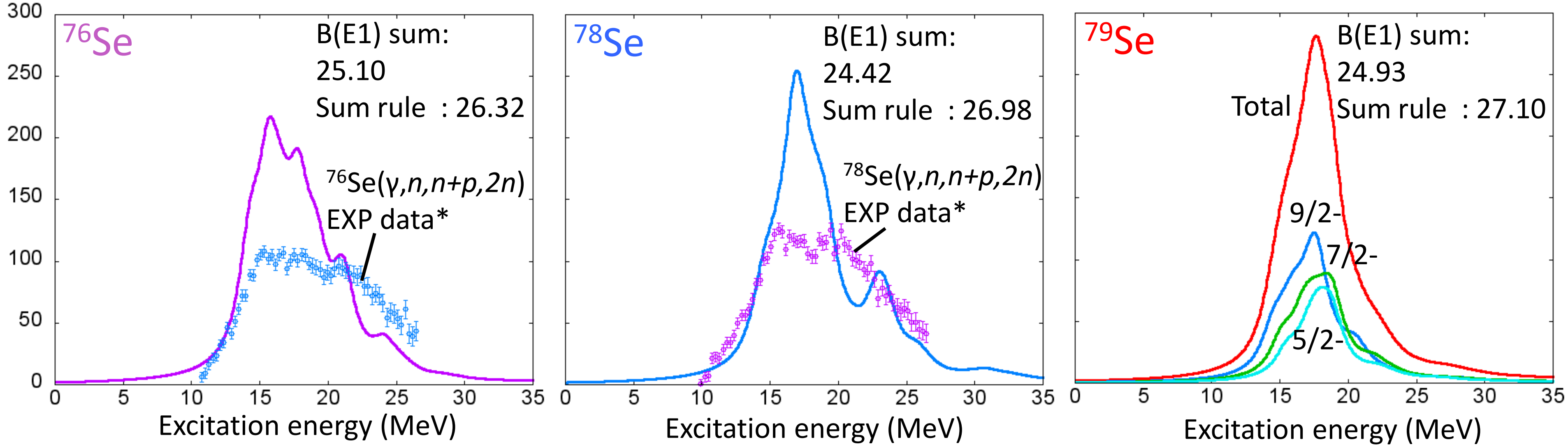
- Model space:
  sd - pf - sdg - $0h_{11/2}$
  (4 major shell)

- Effective Hamiltonian: *SDPF-MU (sd-pf) + V_{MU} (others)
  (central force scaled by 0.35)
  *Y. Utsuno *et.al.*, PRC86, 051301(R) (2012)

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

Cross section (mb)

Lorentzian width
Γ = 2.0MeV



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

300 bases are used to describe *E1* spectrum as preliminary calculation.

Summary

- Lanczos strength function in LSSM
  - E1 of Ca isotopes with LSSM
    - GDR (1+3)ħω essential, higher ħω configuration
    - PDR 1ħω enough
    - odd nuclei are feasible : Ca isotopes, ^{51}V
  - PDR enhancement in ^{52}Ca-^{60}Ca
    - PDR is on the tail of GDR
    - $rY^{(1)}$ reduced matrix elements

- Monte Carlo shell model for strength function
  - construct J^{π}-projected subspace spanned by $E1$-excited Slater determinants
  - feasibility tested, odd nuclei are feasible
  - undergoing application to systematic studies and LLFP nuclides