Finite amplitude method for nuclear response function

Takashi Nakatsukasa (RNC: RIKEN Nishina Center)

Collaborators: Paolo Avogadro (RNC/Milano), Tsunenori Inakura (RNC)

Advances in Nuclear Many-Body Theory, Primosten, June 7-10, 2011

Contents

- Finite amplitude method
  - A feasible approach to the HF+RPA
- Pygmy dipole resonances in light to medium-heavy nuclei
  - Shell effects and magic numbers
  - Neutron-skin effect
- Finite amplitude method for superfluid systems
  - An alternative way to the HFB+QRPA

Time-dependent Hartree-Fock (TDHF)

Time-dependent Hartree-Fock equation

(Time-dependent Kohn-Sham equation)

$$i \frac{\partial}{\partial t} \phi_i(t) = \left\{ h(t) + V_{\mathrm{ext}}(t) \right\} \phi_i(t)$$

$$i \frac{\partial}{\partial t} \rho(t) = \left[h(t) + V_{\mathrm{ext}}(t), \rho(t) \right]$$

$$\rho(\vec{r}, t) = \sum_{i=1}^{N} \left| \phi_i(\vec{r}, t) \right|^2$$

$$h(t) = h\left[\rho(t) \right]$$

Small-amplitude limit (Random-phase approximation)

One-body density operator under a TD external potential

$$i\frac{\partial}{\partial t}\rho(t) = \left[h(t) + V_{\text{ext}}(t), \rho(t)\right]$$

Assuming that the external potential is weak,

$$\rho(t) = \rho_0 + \delta\rho(t) \qquad h(t) = h_0 + \delta h(t) = h_0 + \left.\frac{\delta h}{\delta\rho}\right|_{\rho_0} \cdot \delta\rho(t)$$

$$i\frac{\partial}{\partial t}\delta\rho(t) = \left[h_0, \delta\rho(t)\right] + \left[\delta h(t) + V_{\text{ext}}(t), \rho_0\right]$$

Let us take the external field with a fixed frequency ω,

$$V_{\text{ext}}(t) = V_{\text{ext}}(\omega)e^{-i\omega t} + V_{\text{ext}}^{+}(\omega)e^{+i\omega t}$$

The density and residual field also oscillate with ω,

$$\delta\rho(t) = \delta\rho(\omega)e^{-i\omega t} + \delta\rho^{+}(\omega)e^{+i\omega t}$$

$$\delta h(t) = \delta h(\omega)e^{-i\omega t} + \delta h^{+}(\omega)e^{+i\omega t}$$

The linear response (RPA) equation

$$\omega\delta\rho(\omega) = \left[h_0, \delta\rho(\omega)\right] + \left[\delta h(\omega) + V_{\text{ext}}(\omega), \rho_0\right]$$

Note that all the quantities, except for ρ_0 and h_0, are non-hermitian.

$$\delta\rho(t) = \sum_{i=1}^{A}\left(\left|\delta\psi_i(t)\right\rangle\left\langle\phi_i\right| + \left|\phi_i\right\rangle\left\langle\delta\psi_i(t)\right|\right)$$

$$\Rightarrow \qquad \delta\rho(\omega) = \sum_{i=1}^{A}\left(\left|X_i(\omega)\right\rangle\left\langle\phi_i\right| + \left|\phi_i\right\rangle\left\langle Y_i(\omega)\right|\right)$$

This leads to the following equations for X and Y:

$$\omega\left|X_i(\omega)\right\rangle = \left(h_0 - \varepsilon_i\right)\left|X_i(\omega)\right\rangle + \hat{Q}\left\{\delta h(\omega) + V_{\text{ext}}(\omega)\right\}\left|\phi_i\right\rangle$$

$$\omega\left\langle Y_i(\omega)\right| = -\left\langle Y_i(\omega)\right|\left(h_0 - \varepsilon_i\right) - \left\langle\phi_i\right|\left\{\delta h(\omega) + V_{\text{ext}}(\omega)\right\}\hat{Q}$$

$$\hat{Q} = \sum_{i=1}^{A}\left(1 - \left|\phi_i\right\rangle\left\langle\phi_i\right|\right)$$

These are nothing but the “RPA linear-response equations”.
X and Y are called “forward” and “backward” amplitudes.

Matrix formulation

$$\omega|X_i(\omega)\rangle = (h_0 - \varepsilon_i)|X_i(\omega)\rangle + \hat{Q}\{\delta h(\omega) + V_{\rm ext}(\omega)\}|\phi_i\rangle$$
$$\omega\langle Y_i(\omega)| = -\langle Y_i(\omega)|(h_0 - \varepsilon_i) - \langle\phi_i|\{\delta h(\omega) + V_{\rm ext}(\omega)\}\hat{Q} \qquad (1)$$

$$\hat{Q} = \sum_{i=1}^{A}(1 - |\phi_i\rangle\langle\phi_i|)$$

If we expand the X and Y in *particle orbitals*:

$$|X_i(\omega)\rangle = \sum_{m>A}|\phi_m\rangle X_{mi}(\omega), \quad |Y_i(\omega)\rangle = \sum_{m>A}|\phi_m\rangle Y^*_{mi}(\omega)$$

Taking overlaps of Eq.(1) with particle orbitals

$$\left\{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}\begin{pmatrix} X_{mi}(\omega) \\ Y_{mi}(\omega) \end{pmatrix} = -\begin{pmatrix} (V_{\rm ext})_{mi} \\ (V_{\rm ext})_{im} \end{pmatrix}$$

$$A_{mi,nj} = (\varepsilon_m - \varepsilon)\delta_{mn}\delta_{ij} + \langle\phi_m|\left.\frac{\partial h}{\partial\rho_{nj}}\right|_{\rho_0}|\phi_i\rangle$$

$$B_{mi,nj} = \langle\phi_m|\left.\frac{\partial h}{\partial\rho_{jn}}\right|_{\rho_0}|\phi_i\rangle$$

In many cases, setting $V_{\rm ext}$=0 and solve the normal modes of excitations:
→ Diagonalization of the matrix

Small-amplitude approximation
--- Linear response (RPA) equation ---

$$\left\{ \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \begin{pmatrix} X_{mi}(\omega) \\ Y_{mi}(\omega) \end{pmatrix} = - \begin{pmatrix} (V_{\mathrm{ext}})_{mi} \\ (V_{\mathrm{ext}})_{im} \end{pmatrix}$$

$$A_{mi,nj} = (\varepsilon_m - \varepsilon)\delta_{mn}\delta_{ij} + \left\langle \phi_m \left| \frac{\partial h}{\partial \rho_{nj}} \right|_{\rho_0} \right| \phi_i \rangle$$

$$B_{mi,nj} = \left\langle \phi_m \left| \frac{\partial h}{\partial \rho_{jn}} \right|_{\rho_0} \right| \phi_i \rangle$$

- Tedious calculation of residual interactions
- Computationally very demanding, especially for deformed systems.

However, in principle, the self-consistent single-particle Hamiltonian should contain everything. We can avoid explicit calculation of residual interactions.

Finite Amplitude Method

T.N., Inakura, Yabana, PRC76 (2007) 024318.

Residual fields can be estimated by the finite difference method:

$$\delta h(\omega) = \frac{1}{\eta}\left(h\left[\langle\psi'|,|\psi\rangle\right] - h_0\right)$$

$$|\psi_i\rangle = |\phi_i\rangle + \eta |X_i(\omega)\rangle, \quad \langle\psi_i'| = \langle\phi_i| + \eta\langle Y_i(\omega)|$$

Starting from initial amplitudes $X^{(0)}$ and $Y^{(0)}$, one can use an iterative method to solve the following linear-response equations.

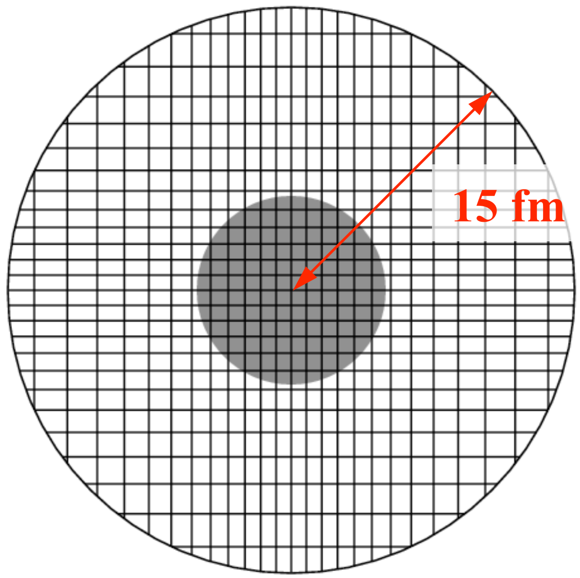
$$\omega |X_i(\omega)\rangle = (h_0 - \varepsilon_i)|X_i(\omega)\rangle + \hat{Q}\{\delta h(\omega) + V_{\text{ext}}(\omega)\}|\phi_i\rangle$$

$$\omega\langle Y_i(\omega)| = -\langle Y_i(\omega)|(h_0 - \varepsilon_i) - \langle\phi_i|\{\delta h(\omega) + V_{\text{ext}}(\omega)\}\hat{Q}$$

Programming of the RPA code becomes very much trivial, because we only need calculation of the single-particle potential, with different bras and kets.

Numerical Details

- SkM* interaction (no pairing)
- 3D mesh in **adaptive coordinate**
- R_{box} = 15 fm
- Complex energy with Γ = 1.0 MeV
- ΔE = 0.3 MeV
  up to E = 38.1 MeV (128 points)
- **Energy-paralleled** calc. on PACS-CS



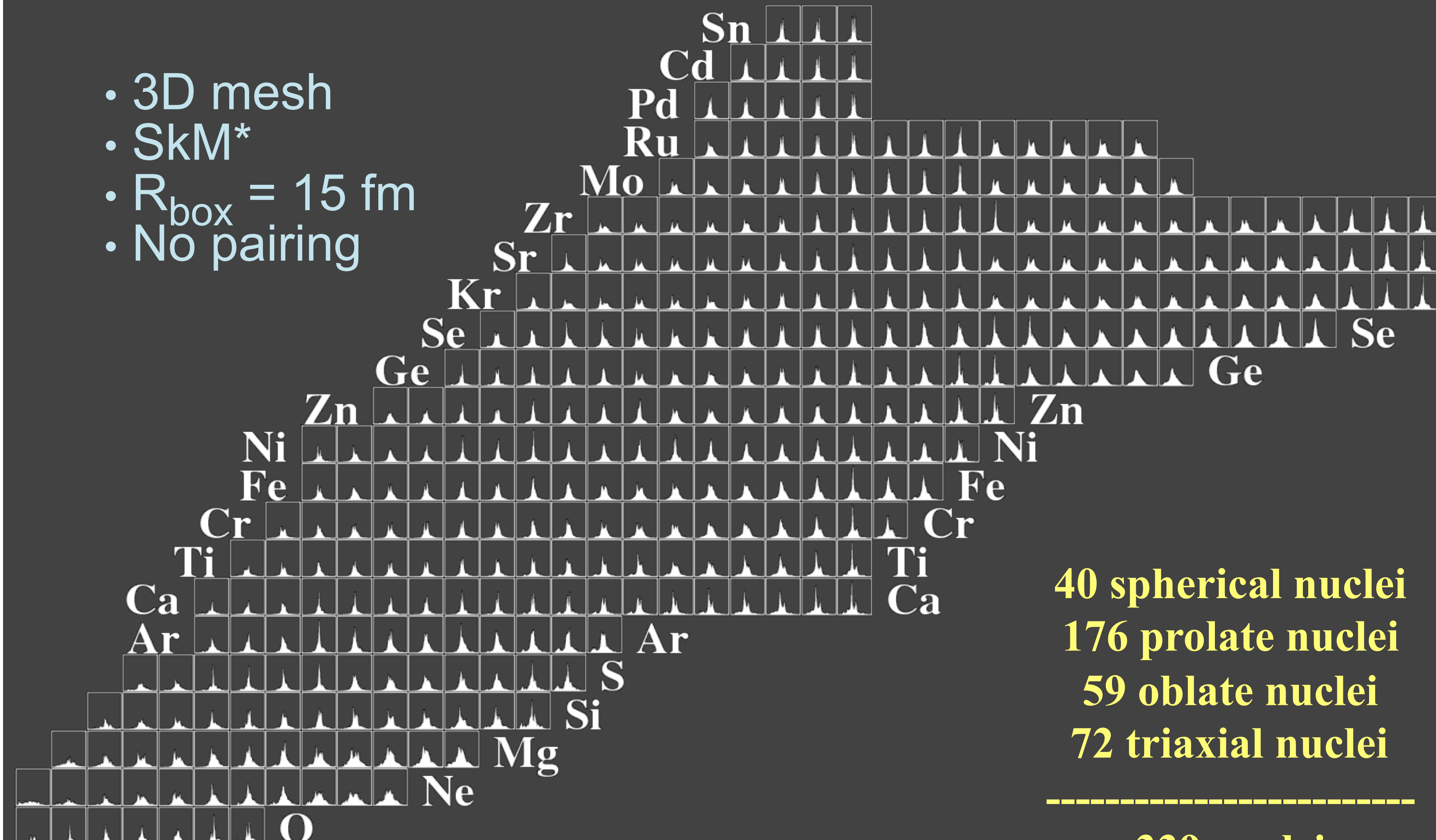
adaptive coordinate
PRC71, 024301

PACS-CS
Parallel Array Computer System
for Computational Sciences

PACS-CS @ Univ. of Tsukuba

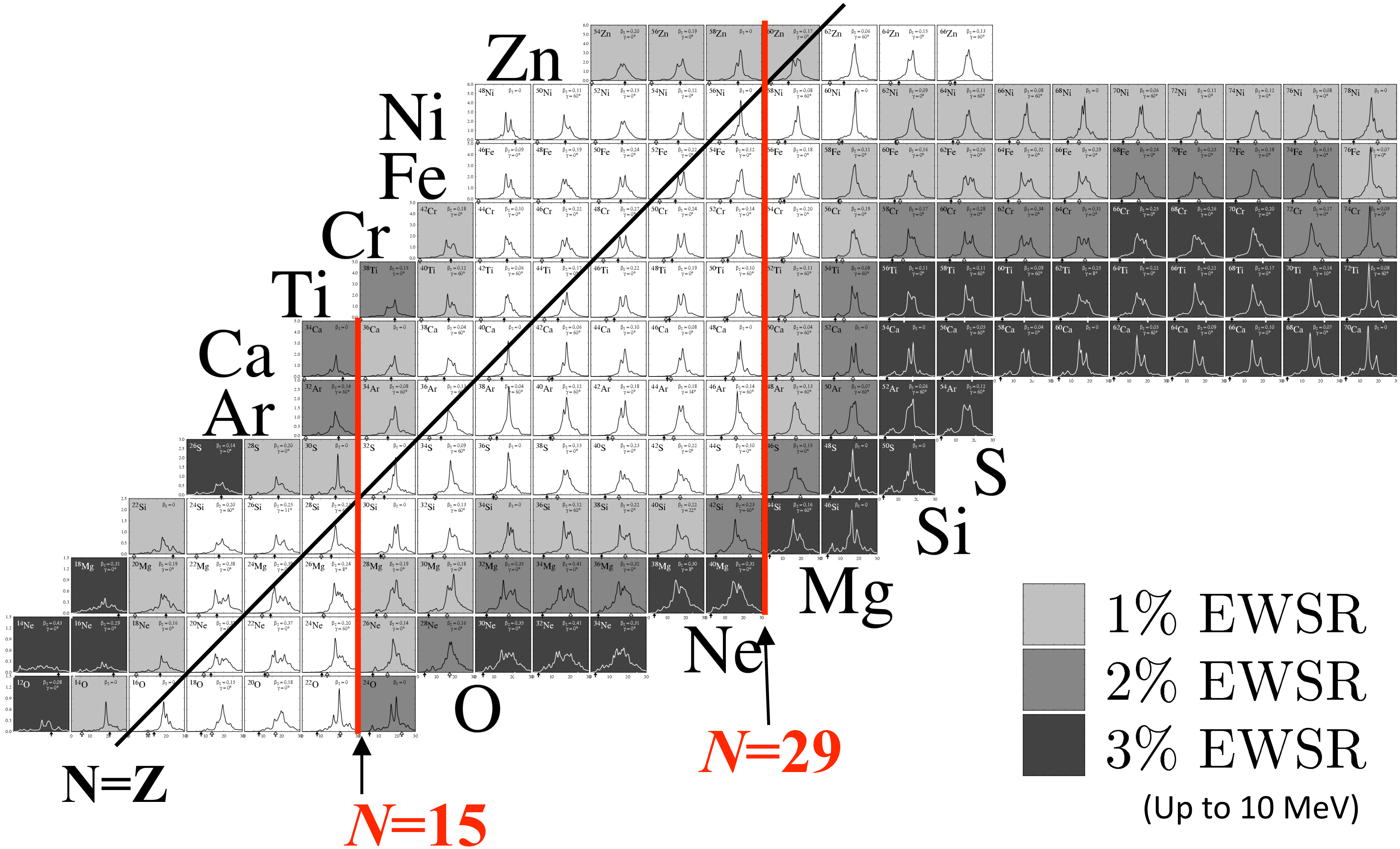
Electric Dipole strength distributions

- 3D mesh
- SkM*
- R_{box} = 15 fm
- No pairing

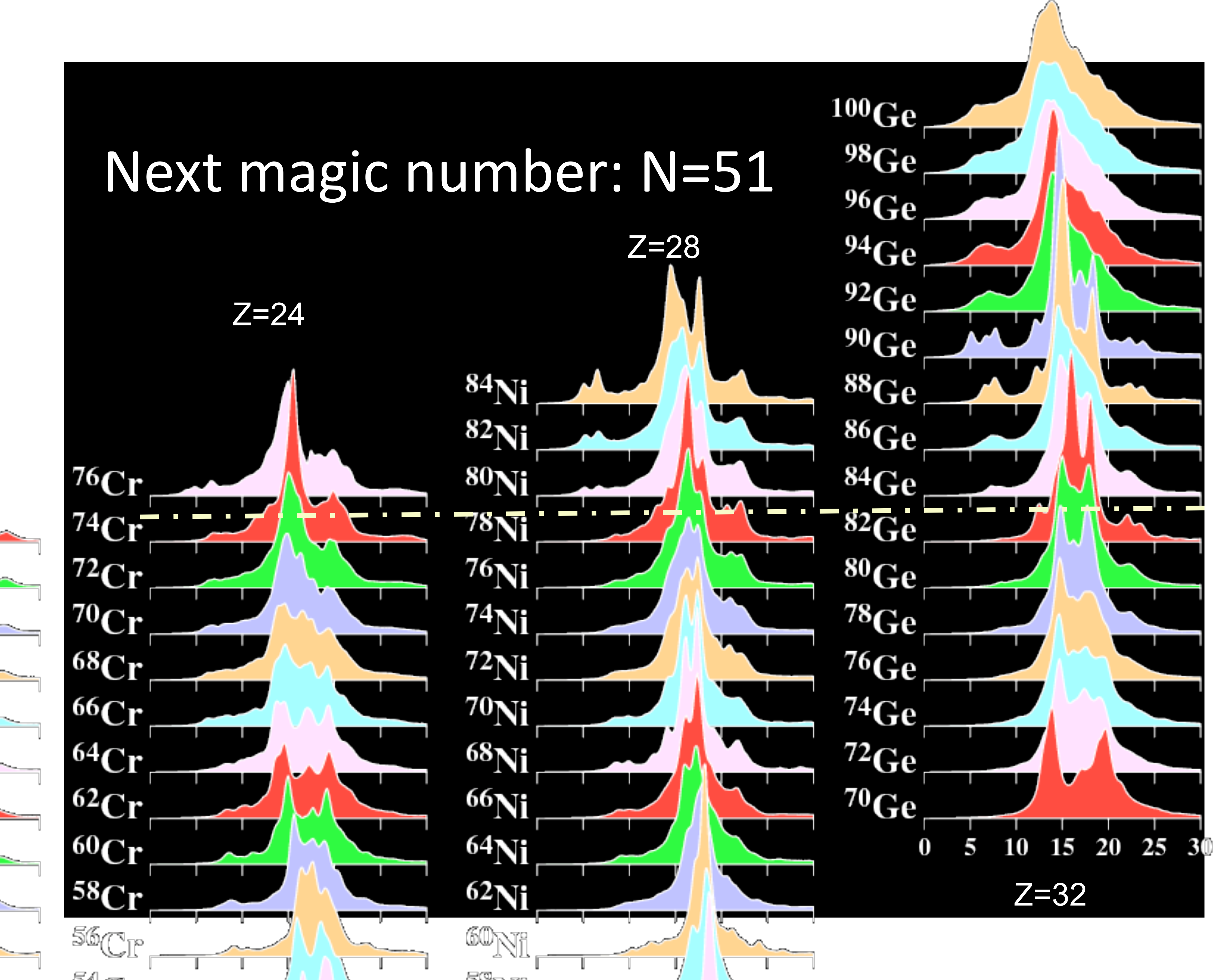


40 spherical nuclei
176 prolate nuclei
59 oblate nuclei
72 triaxial nuclei
----
339 nuclei

Magic numbers for PDR emergence

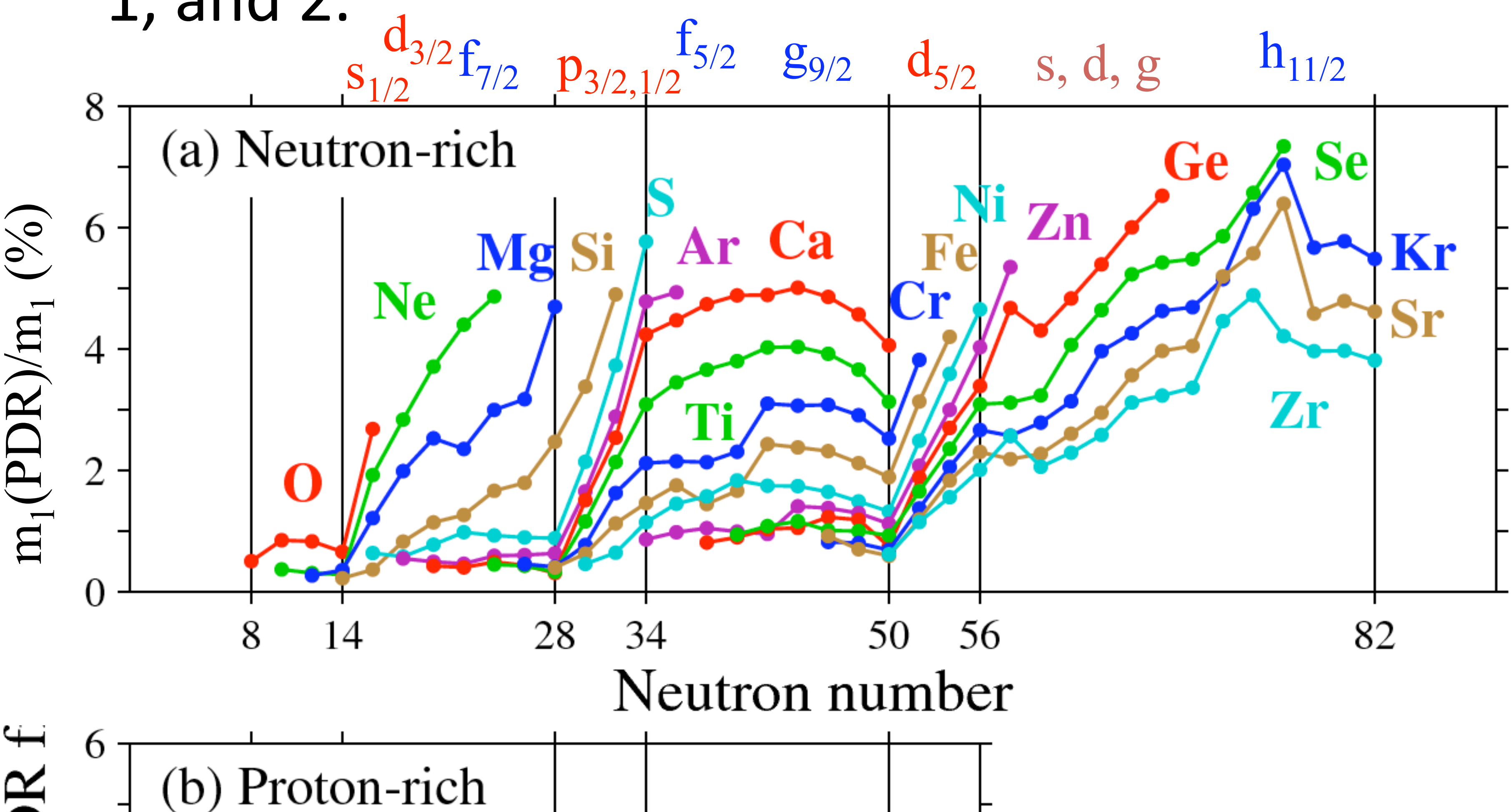


Next magic number: N=51

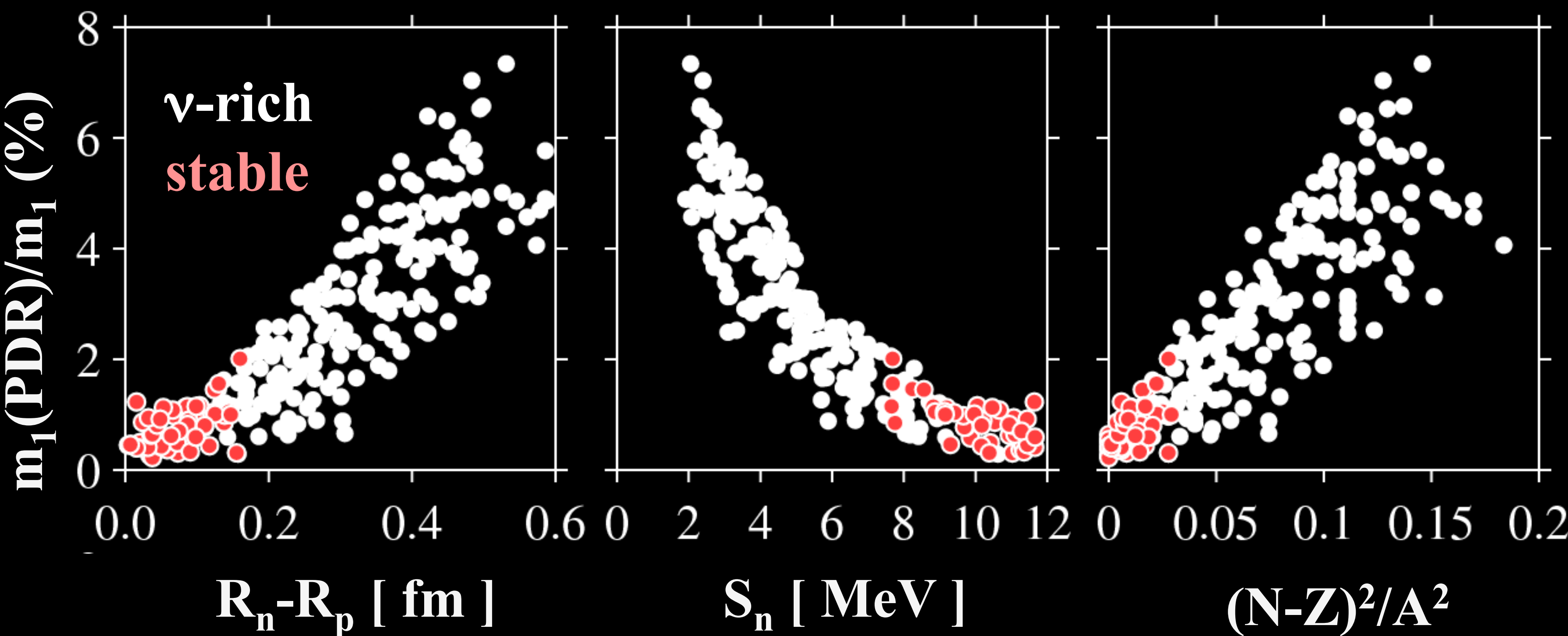


Magic numbers and low-*l* orbits

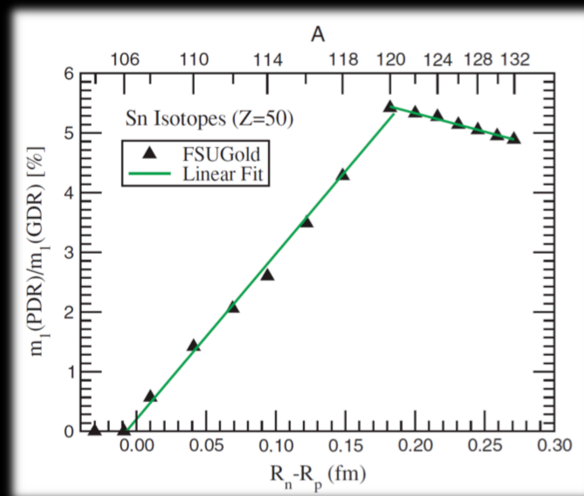
- Magic numbers: N=15, 29, 51, …
- Importance of weakly bound orbits with *l*=0, 1, and 2.



PDR strength is correlated with any quantity?



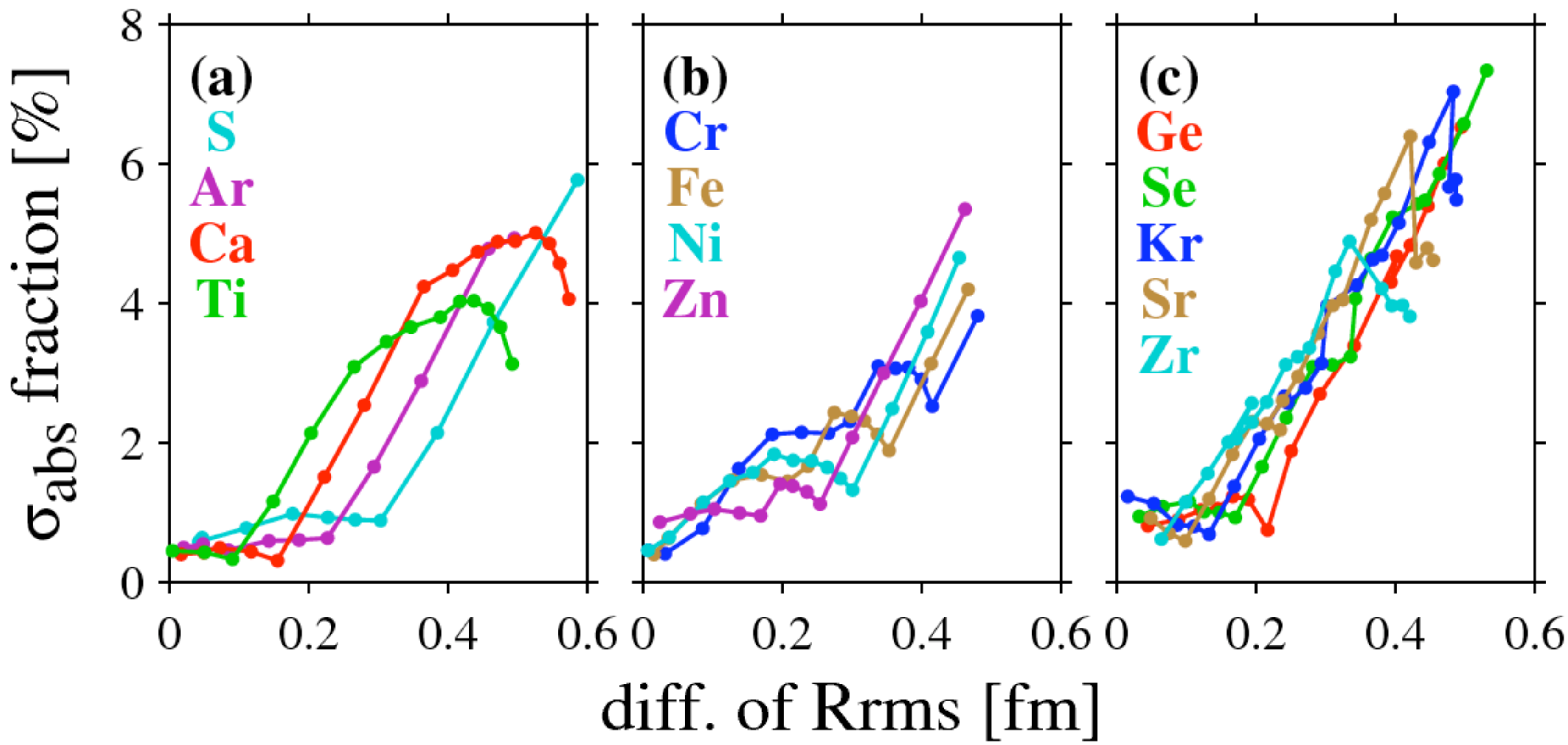
Linear correlation was found for R_n-R_p for neutron-deficient Sn (spherical) isotopes



Piekarewicz, PRC73 (2006) 044325.

Universal correlation with skin thickness

- PDR fraction/ Δ R_{np} shows a universal rate.
- The rate is about 0.2 /fm.



TDHFB for superfluid systems

Time-dependent Hartree-Fock-Bogoliubov equation

$$i\frac{\partial}{\partial t}\Psi_i(t) = \left\{H(t) + V_{\mathrm{ext}}(t)\right\}\Psi_i(t)$$

$$i\frac{\partial}{\partial t}R(t) = \left[H(t) + V_{\mathrm{ext}}(t), R(t)\right]$$

$$\Psi_i = \begin{pmatrix} U_i \\ V_i \end{pmatrix} \qquad H(t) = H\left[R(t)\right] = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$$

$$R(t) = \sum_i \Psi_i \Psi_i^+ = \begin{pmatrix} \rho(t) & \kappa(t) \\ -\kappa^*(t) & 1-\rho^*(t) \end{pmatrix}$$

Finite amplitude method for superfluid systems

Avogadro and TN, PRC in press (arXiv:1104.3692)

Residual fields can be calculated by

$$\delta h(\omega) = \frac{1}{\eta}\left\{ h\left[\overline{V}_\eta^*, V_\eta\right] - h_0 \right\}$$

$$\delta\Delta(\omega) = \frac{1}{\eta}\left\{ \Delta\left[\overline{V}_\eta^*, U_\eta\right] - \Delta_0 \right\}$$

$$V_\eta = V + \eta U^* Y, \quad \overline{V}_\eta^* = V^* + \eta U X$$

$$U_\eta = U + \eta V^* Y$$

QRPA equations are

$$(E_\mu + E_\nu - \omega) X_{\mu\nu} + \delta H_{\mu\nu}^{20} = F_{\mu\nu}^{20}$$

$$(E_\mu + E_\nu + \omega) Y_{\mu\nu} + \delta \widetilde{H}_{\mu\nu}^{02*} = F_{\mu\nu}^{02}$$

$$\begin{pmatrix} & \delta H_{\mu\nu} \\ \delta \widetilde{H}_{\mu\nu} & \end{pmatrix} = W^+ \begin{pmatrix} \delta h & \delta\Delta \\ \delta\widetilde{\Delta}^+ & -\delta h^+ \end{pmatrix} W$$

$$W = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}$$

Finite amplitude method for QRPA

- Numerical implementation to HFBRAD
- Spherical HFB (radial coord.) + FAM
- Time-odd fields are added

FAM-QRPA

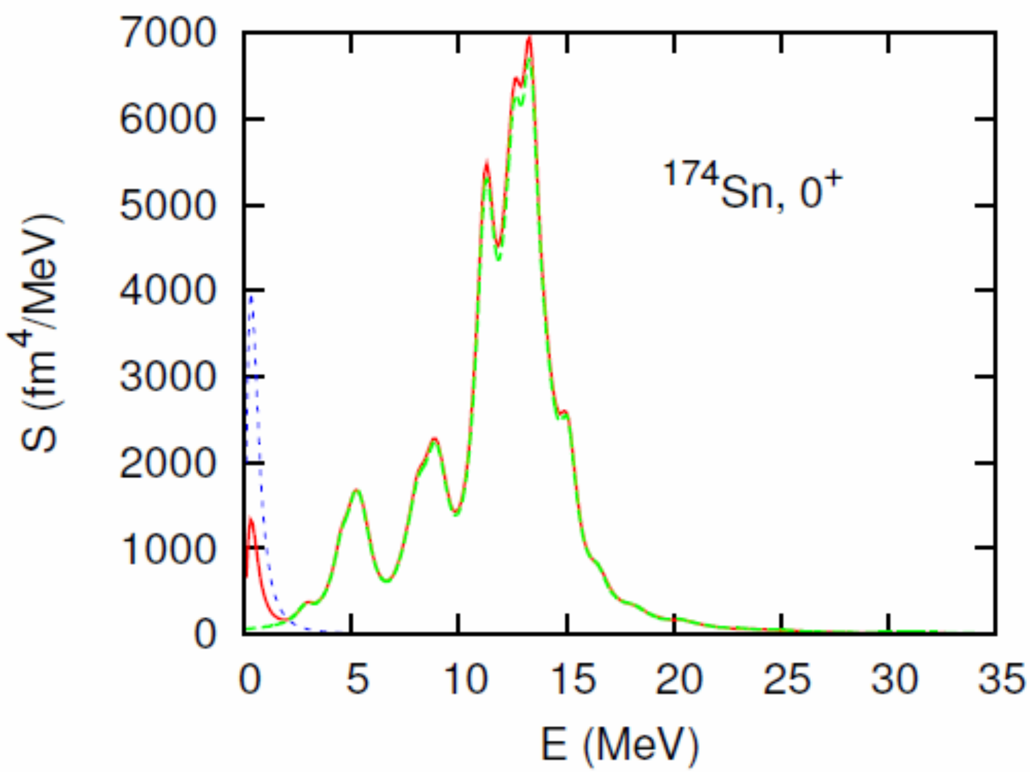
Test calculation: IS monopole

Our result: Red line

qp cut-off at 60 MeV

All 2qp states are included.

Calculation by Terasaki et al. (PRC71, 034310 (2005): Green line



^{174}Sn, 0^+						
	$\omega = 4$ MeV		$\omega = 12$ MeV		$\omega = 20$ MeV	
η	ϵ	$N_{\rm iter}$	ϵ	$N_{\rm iter}$	ϵ	$N_{\rm iter}$
10^{-2}	0.44	1000	$1.63 \cdot 10^{-1}$	1000	$8.84 \cdot 10^{-3}$	1000
10^{-4}	$6.10 \cdot 10^{-5}$	1000	$1.76 \cdot 10^{-5}$	1000	$< 10^{-5}$	469
10^{-5}	$< 10^{-5}$	161	$< 10^{-5}$	439	$< 10^{-5}$	469
10^{-8}	$< 10^{-5}$	161	$< 10^{-5}$	439	$< 10^{-5}$	469
10^{-9}	$< 10^{-5}$	161	$< 10^{-5}$	439	$< 10^{-5}$	469
10^{-10}	$< 10^{-5}$	161	$1.19 \cdot 10^{-5}$	1000	$1.46 \cdot 10^{-5}$	1000

Linearization parameter

$$\eta = 10^{-9} \sim 10^{-5}$$

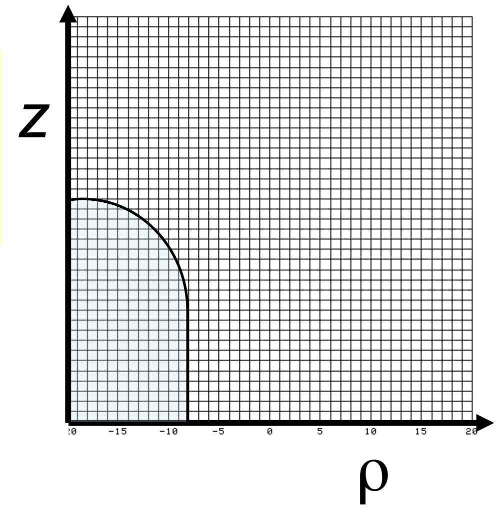
Summary

- Finite amplitude method (PRC76, 024318) provides an alternative approach to (Q)RPA.
  - FAM does not require explicit calculations of residual interactions, thus, fully self-consistent calculations for deformed nuclei can be easily achieved.
- Systematic calculations of photoabsorption cross sections in light to heavy nuclei
  - Reproduce the GDR peak and shape evolution
  - Magic numbers for PDR (N=15, 29, 51, …), which are related to the occupation of low-*l* orbitals (*s, p, d*).
  - Universal correlation between the PDR fraction and the neutron skin thickness; $m_1(\mathrm{PDR})/m_1 \approx (0.2\ /\ \mathrm{fm})\,\Delta R_{np}$.

Axially deformed superfluid nuclei

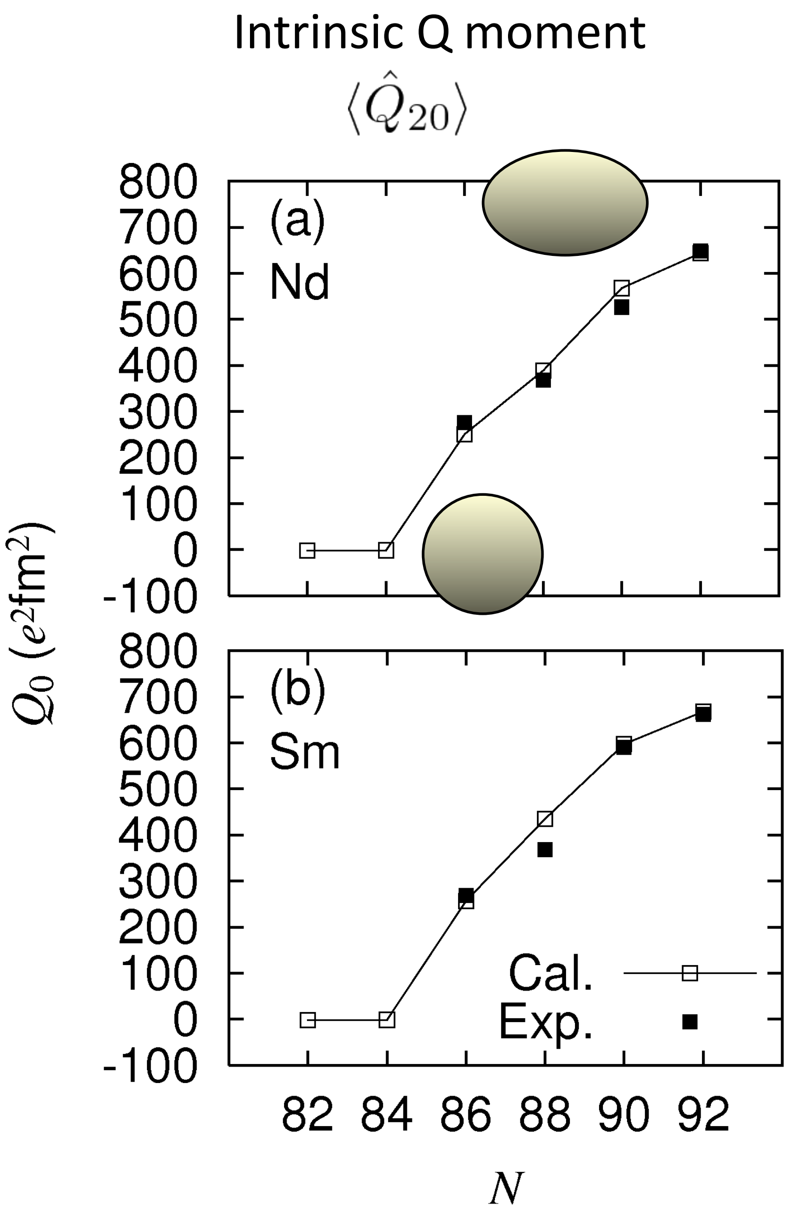
$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -(h-\lambda)^* \end{pmatrix}\begin{pmatrix} U_\mu(\rho,z;\sigma) \\ V_\mu(\rho,z;\sigma) \end{pmatrix} = E_\mu \begin{pmatrix} U_\mu(\rho,z;\sigma) \\ V_\mu(\rho,z;\sigma) \end{pmatrix}$$

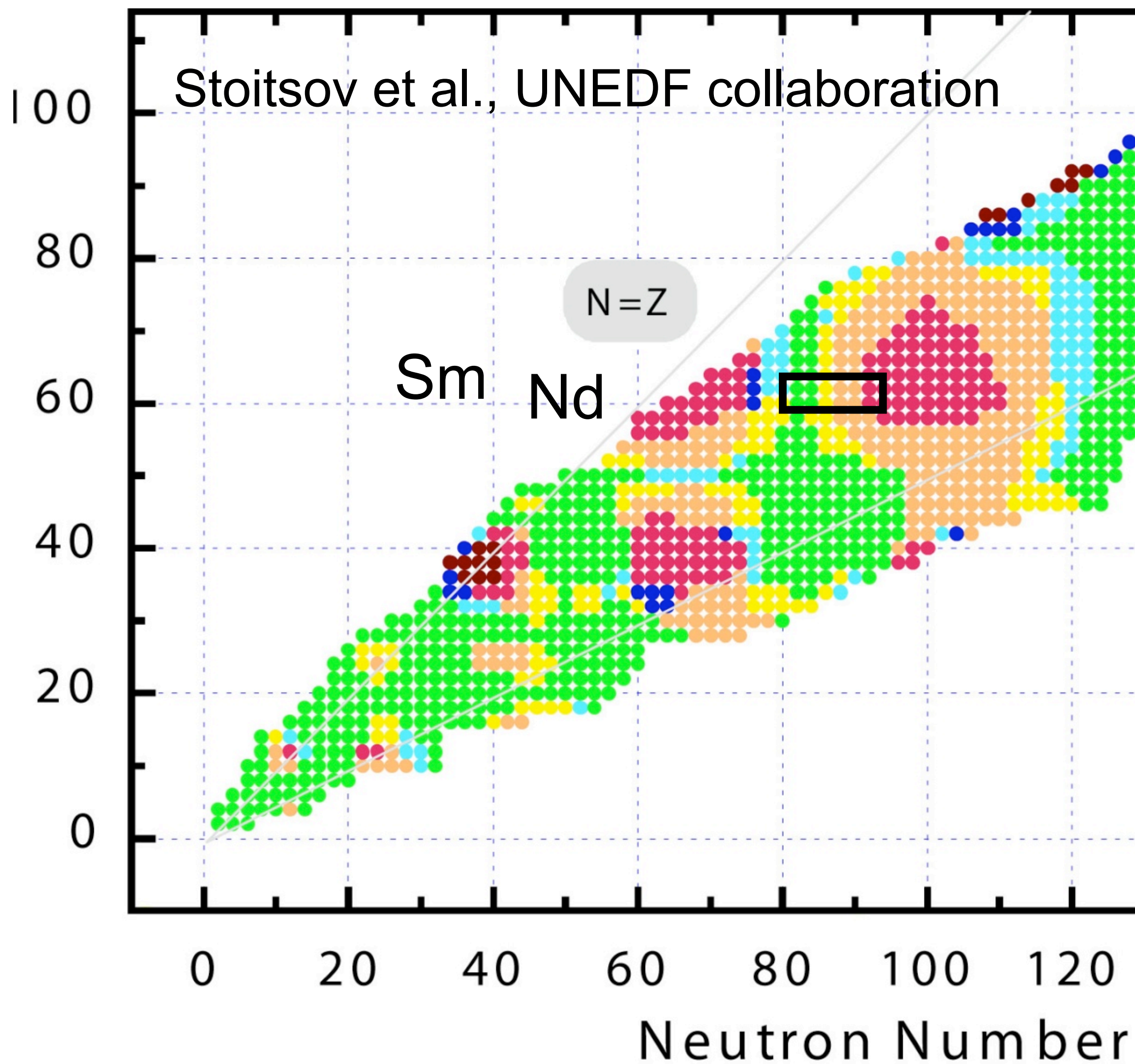
$$\left\{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}\begin{pmatrix} X_{mi}(\omega) \\ Y_{mi}(\omega) \end{pmatrix} = 0$$



- HFB equations are solved in the 2D coordinate space, assuming the axial symmetry for the SkM* functional with the cutoff of $E_{qp} < 60$ MeV.
- The pairing energy functional is the one determined by a global fitting to deformed nuclei (Yamagami, Shimizu, TN, PRC **80**, 064301 (2009))
- QRPA matrix is calculated in the quasiparticle basis ($E_{2qp} < 60$ MeV).
- Neglect the residual Coulomb interaction

Shape phase transition in the EDF approach





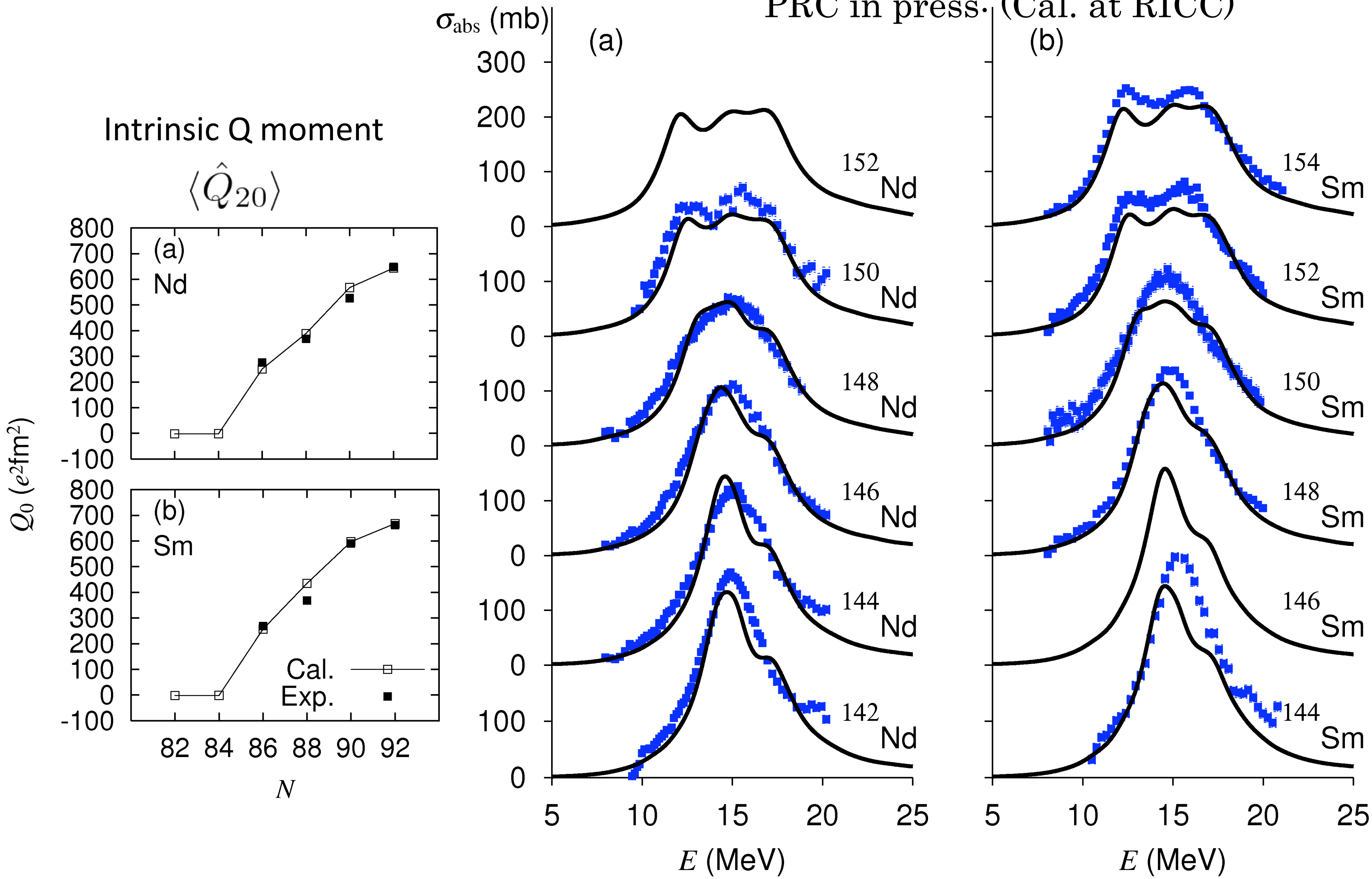
QRPA calculation of photoabsorption cross section

SkM* functional

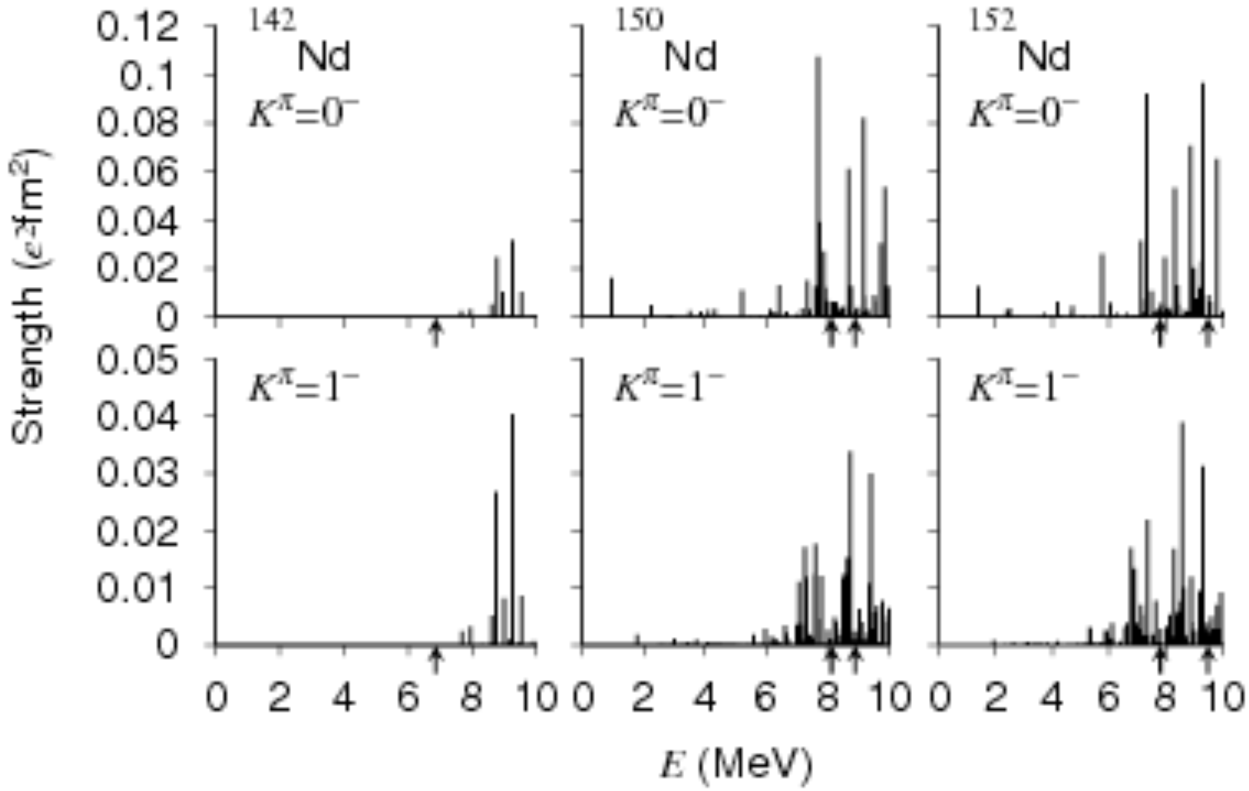
K.Yoshida and TN, arXiv:1008.1520; PRC in press; (Cal. at RICC)

Intrinsic Q moment

$\langle \hat{Q}_{20} \rangle$



PDR in rare-earth nuclei



- Larger PDR strength for deformed nuclei
- Experimental data suggest a concentrated E1 strength in E=5.5-8 MeV.
- Calculation beyond QRPA is necessary.

Finite Amplitude Method

T.N., Inakura, Yabana, PRC76 (2007) 024318.

A method to avoid the explicit calculation of the residual fields (interactions)

$$\delta\rho(t) = \delta\rho(\omega)e^{-i\omega t} + \delta\rho^{+}(\omega)e^{+i\omega t}$$

$$\delta h(t) = \delta h(\omega)e^{-i\omega t} + \delta h^{+}(\omega)e^{+i\omega t}$$

Residual fields are proportional to $\delta\rho(\omega)$

$$\delta h(\omega) = \left.\frac{\delta h}{\delta\rho}\right|_{\rho_0} \cdot \delta\rho(\omega)$$

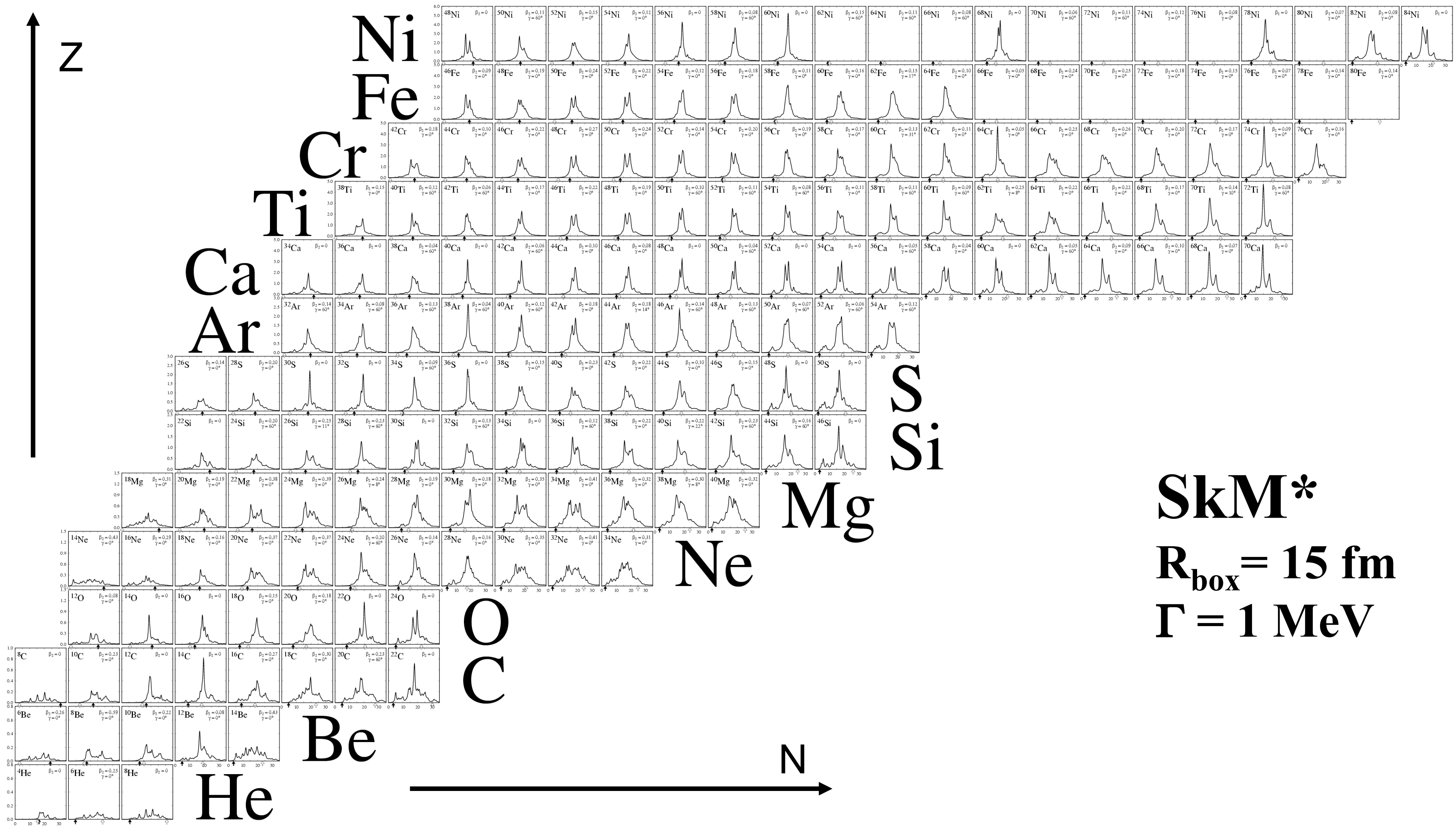
$$\delta\rho(\omega) = \sum_{i=1}^{A} \left(\left| X_i(\omega) \right\rangle \left\langle \phi_i \right| + \left| \phi_i \right\rangle \left\langle Y_i(\omega) \right| \right)$$

Therefore, $\delta h(\omega)$ is a functional of $\left\langle \phi_i \right|, \left| \phi_i \right\rangle, \left| X_i(\omega) \right\rangle, \left\langle Y_i(\omega) \right|$

but, should be independent of $\left| Y_i(\omega) \right\rangle, \left\langle X_i(\omega) \right|$

Fully self-consistent calculation of E1 strength distribution

Inakura, Nakatsukasa, Yabana, in preparation



SkM*

R_{box}= 15 fm

Γ = 1 MeV

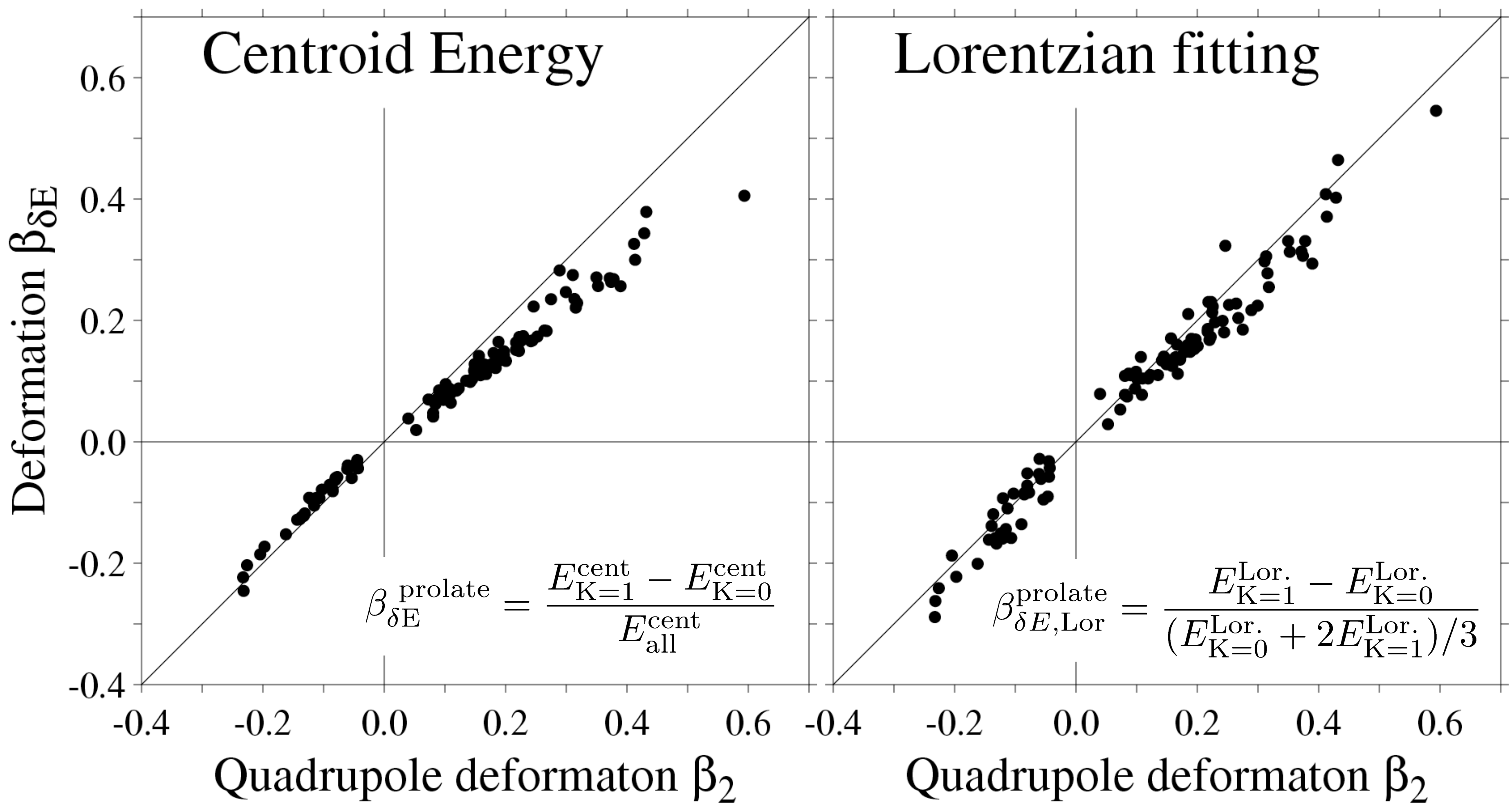
Peak splitting by deformation

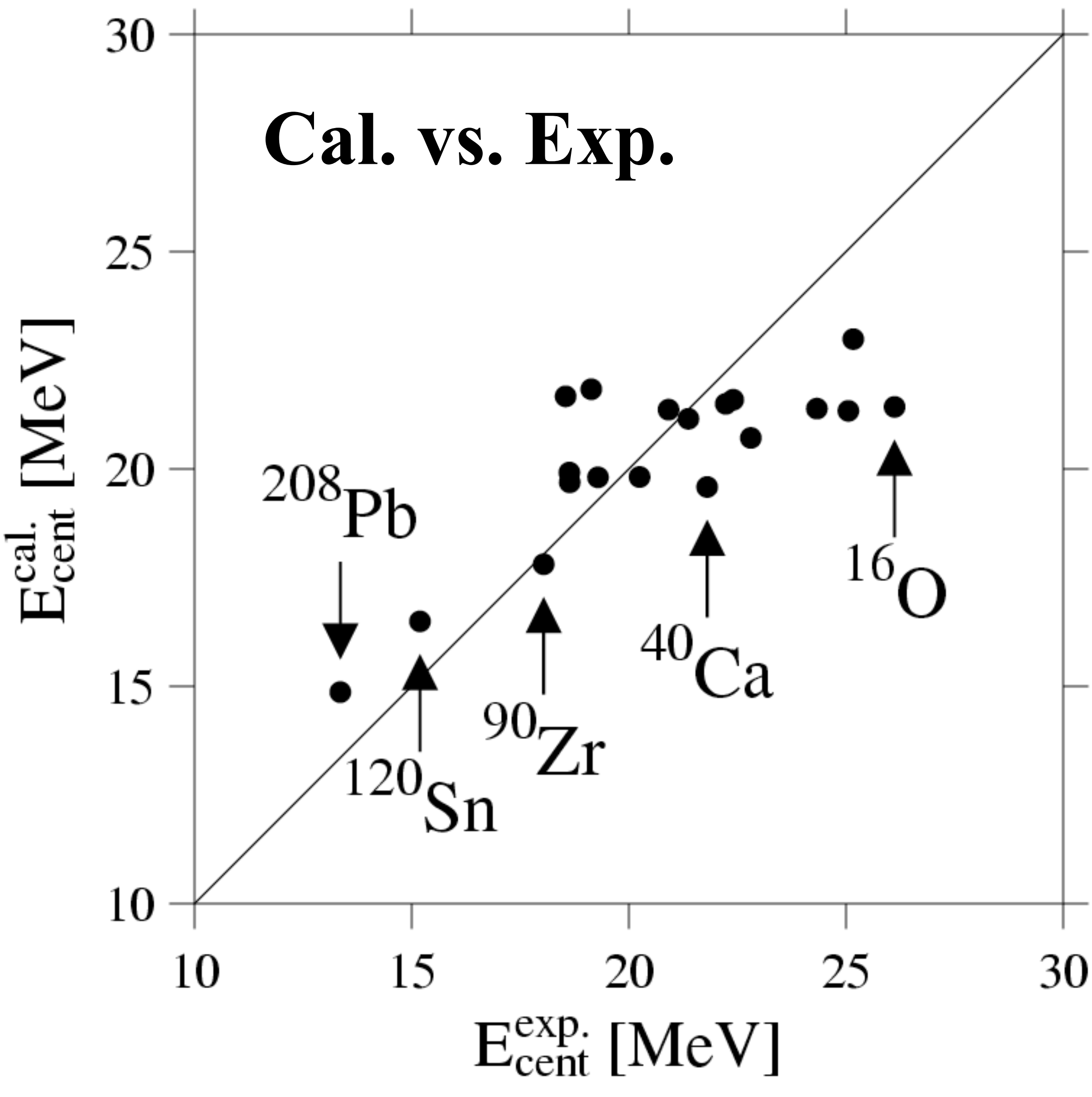
3D H.O. model

$$\beta_{\delta E} \sim \beta_2$$

Bohr-Mottelson, text book.

$$\beta_{2m} = \frac{4\pi}{3} \frac{\langle r^2 Y_{2m} \rangle}{\frac{5}{3}\langle r^2 \rangle}$$





Cal. vs. Exp.
^{208}Pb
^{120}Sn
^{90}Zr
^{40}Ca
^{16}O
$E_{cent}^{cal.}$ [MeV]
$E_{cent}^{exp.}$ [MeV]
10
15
20
25
30

Centroid energy of IVGDR