Systematic calculation of photo-response with the Skyrme functional

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3rd Workshop on Level Density and Gamma Strength, Oslo, May 23-27, 2011

Time-dependent DFT

Time-dependent Kohn-Sham (TDKS) equation

Time-dependent Hartree-Fock (TDHF) equation

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

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

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

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

TDDFT for superfluid systems

Time-dependent Kohn-Sham-Bogoliubov (TDKSB) equation
Time-dependent Hartree-Fock-Bogoliubov (TDHFB) equation

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

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

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

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

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

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

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

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

- 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.

Finite amplitude method for superfluid systems

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

Residual fields can be calculated by

$$\delta h(\omega) = \frac{1}{\eta}\left\{h\left[\tilde{v}^*, v\right] - h_0\right\}$$

$$\delta\Delta(\omega) = \frac{1}{\eta}\left\{\Delta\left[\tilde{v}^*, u\right] - \Delta_0\right\}$$

$$v = V + \eta U X, \quad \tilde{v}^* = V + \eta U^* Y$$

$$u = U + \eta V^* Y, \quad \tilde{v}^* = U^* + \eta V^* X$$

QRPA equations are

$$(E_\mu + E_\nu - \omega) X_{\mu\nu} + \delta H_{\mu\nu} = 0$$

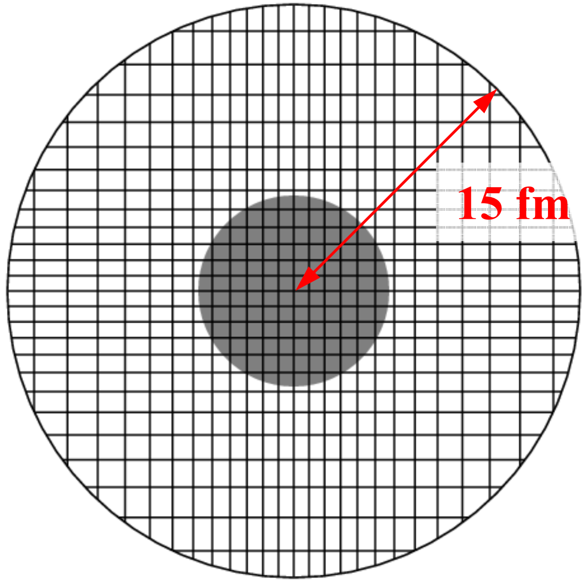
$$(E_\mu + E_\nu + \omega) Y_{\mu\nu} + \delta \tilde{H}^*_{\nu\mu} = 0$$

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

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

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



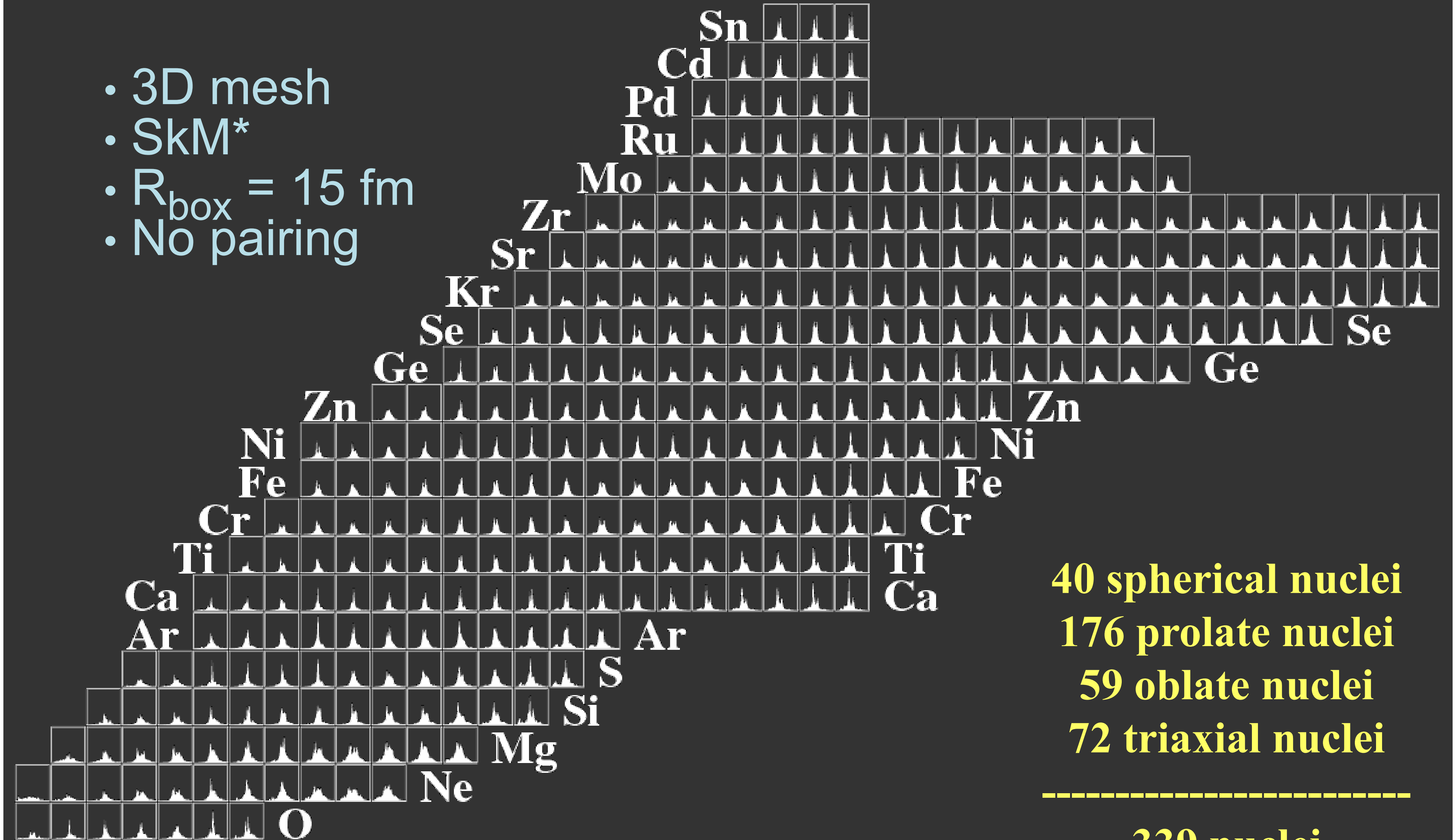
adaptive coordinate
PRC71, 024301

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
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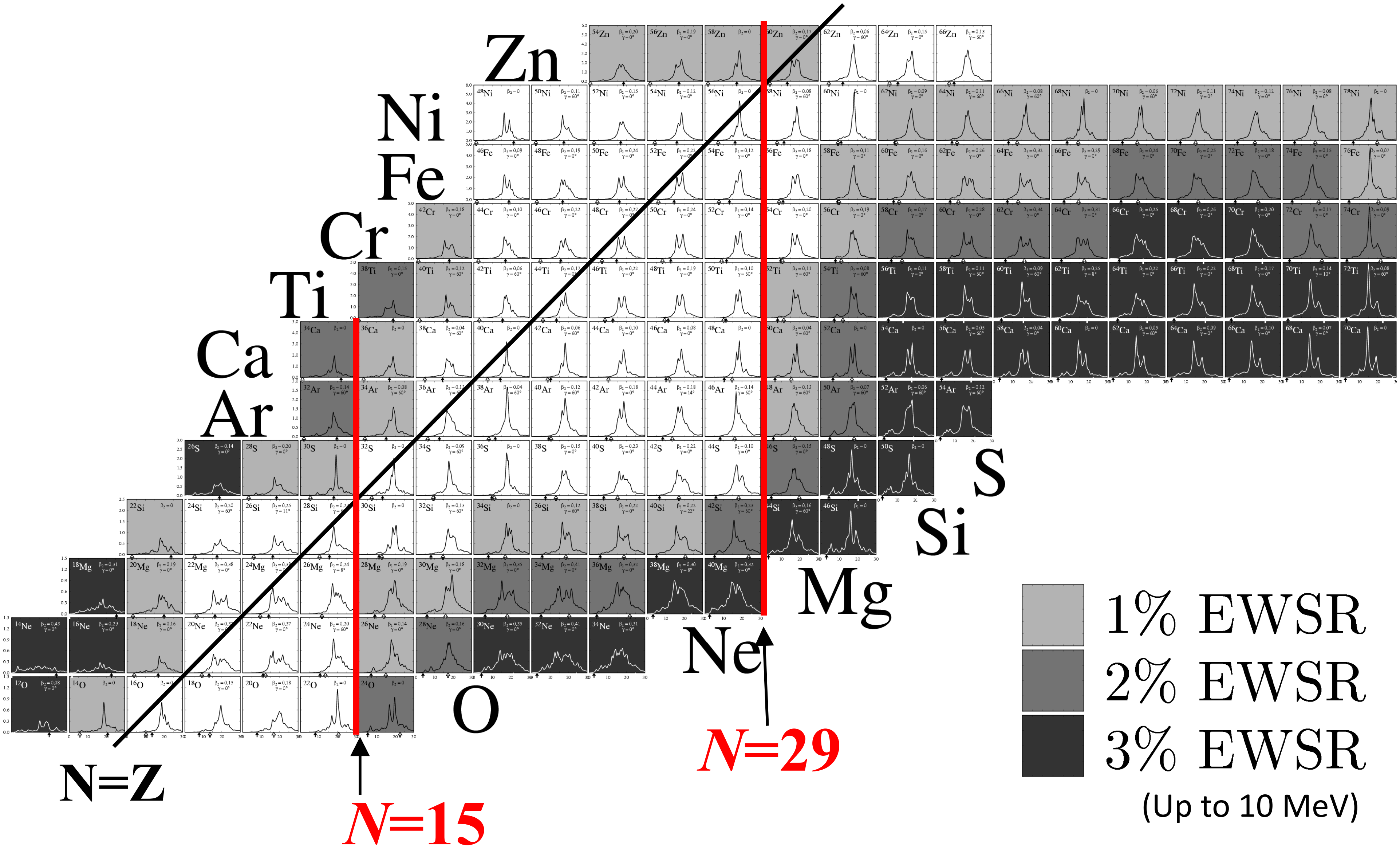
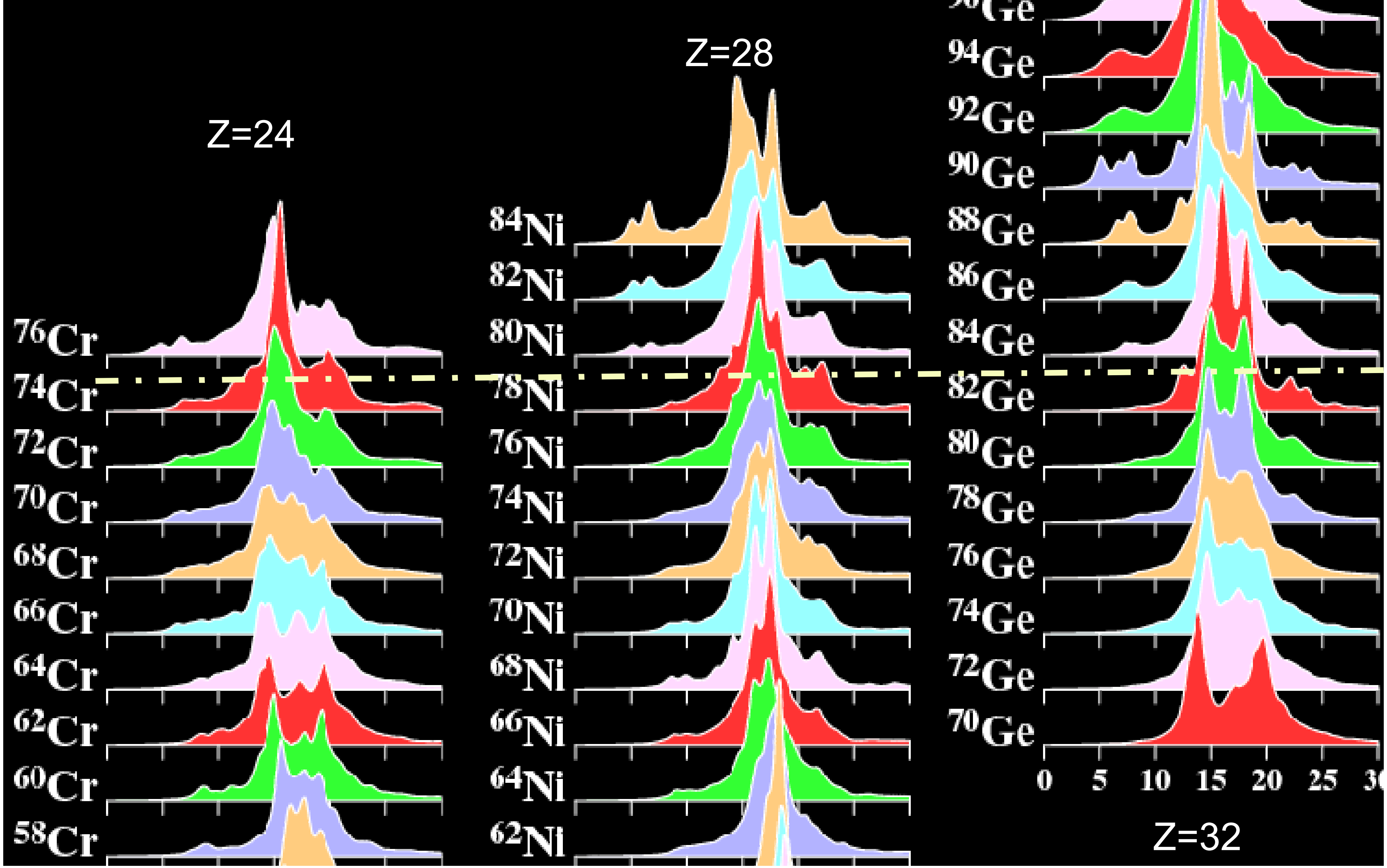
339 nuclei

Magic numbers for PDR emergence

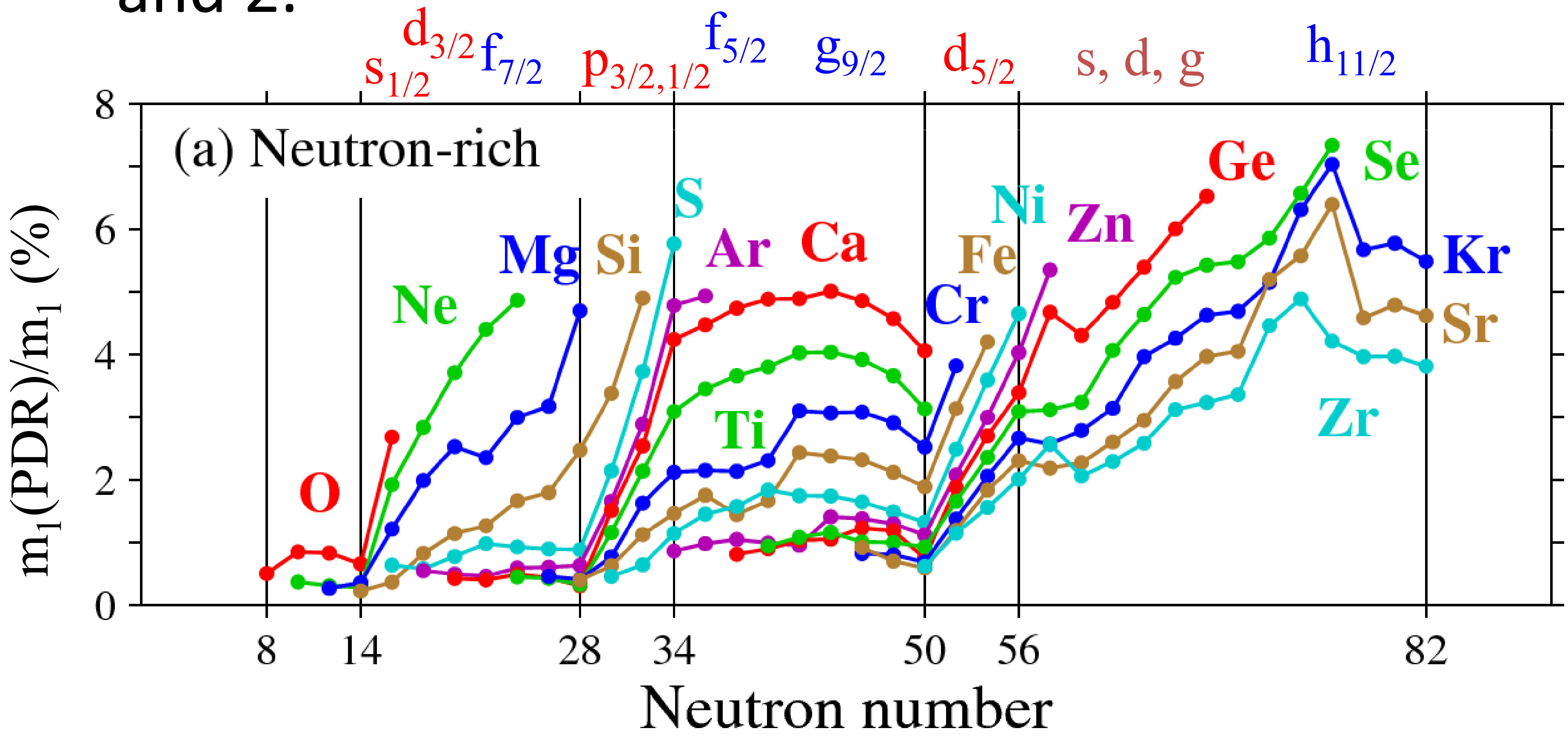


Next magic number: N=51

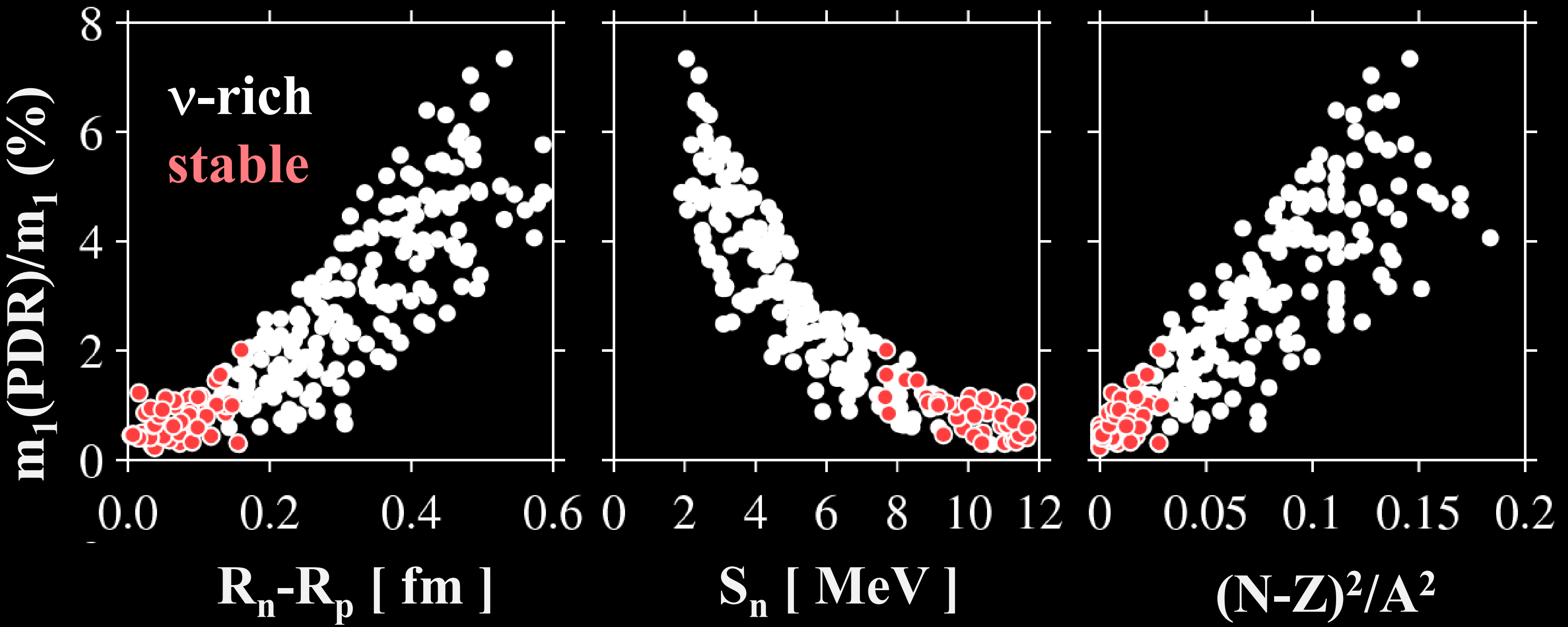


Magic numbers and low-*l* orbits

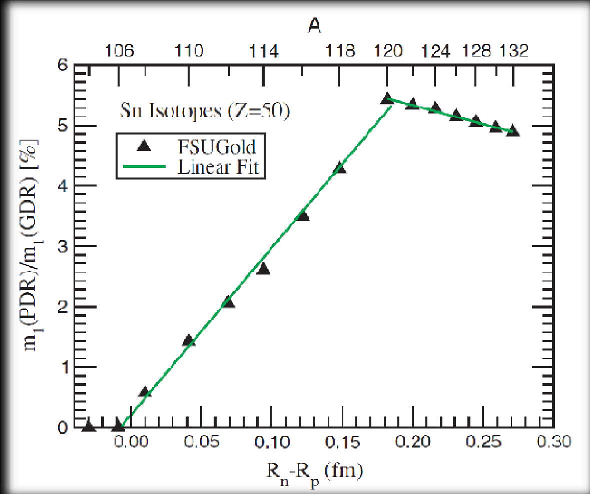
- Magic numbers: N=15, 29, 51, …
- Importance of weakly bound orbits with *l*=0, 1, and 2.



PDR strength is correlated with any quantity?



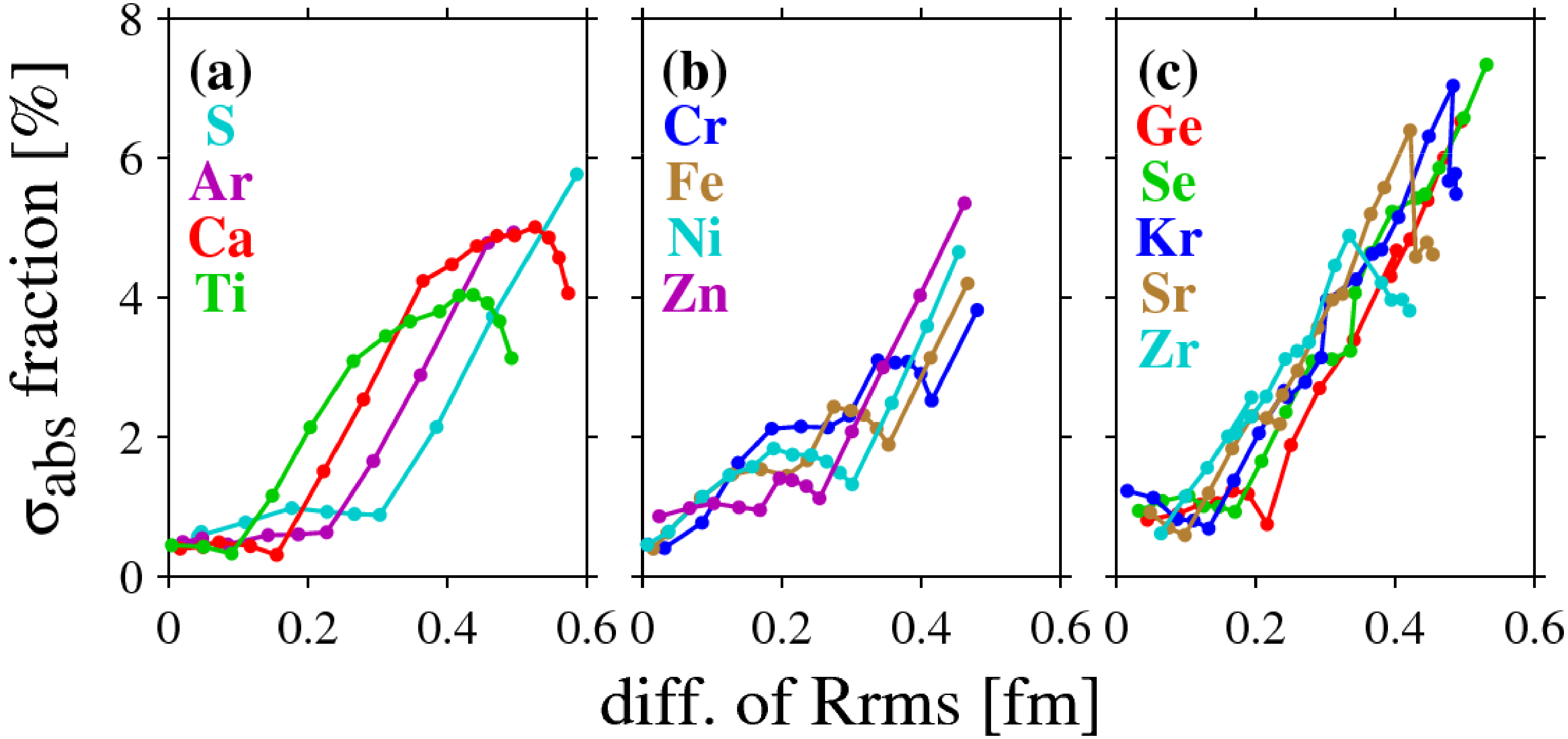
Linear correlation was found for R_n-R_p for neutron-deficient Sn (spherical) isotopes



Piekarewicz, PRC73 (2006) 044325.

Universal correlation with skin thickness

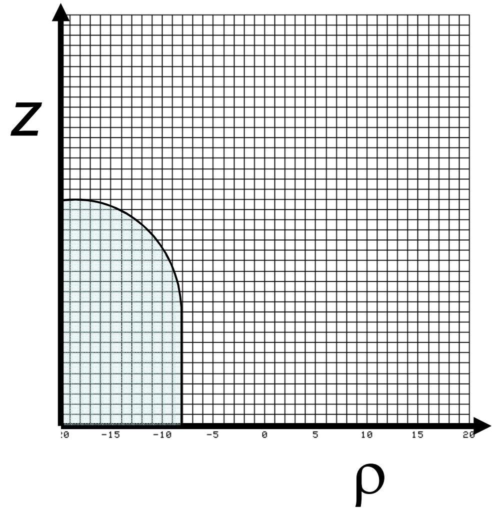
- PDR fraction/ ΔR_{np} shows a universal rate.
- The rate is about 0.2 /fm.



Axially deformed superfluid nuclei

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

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

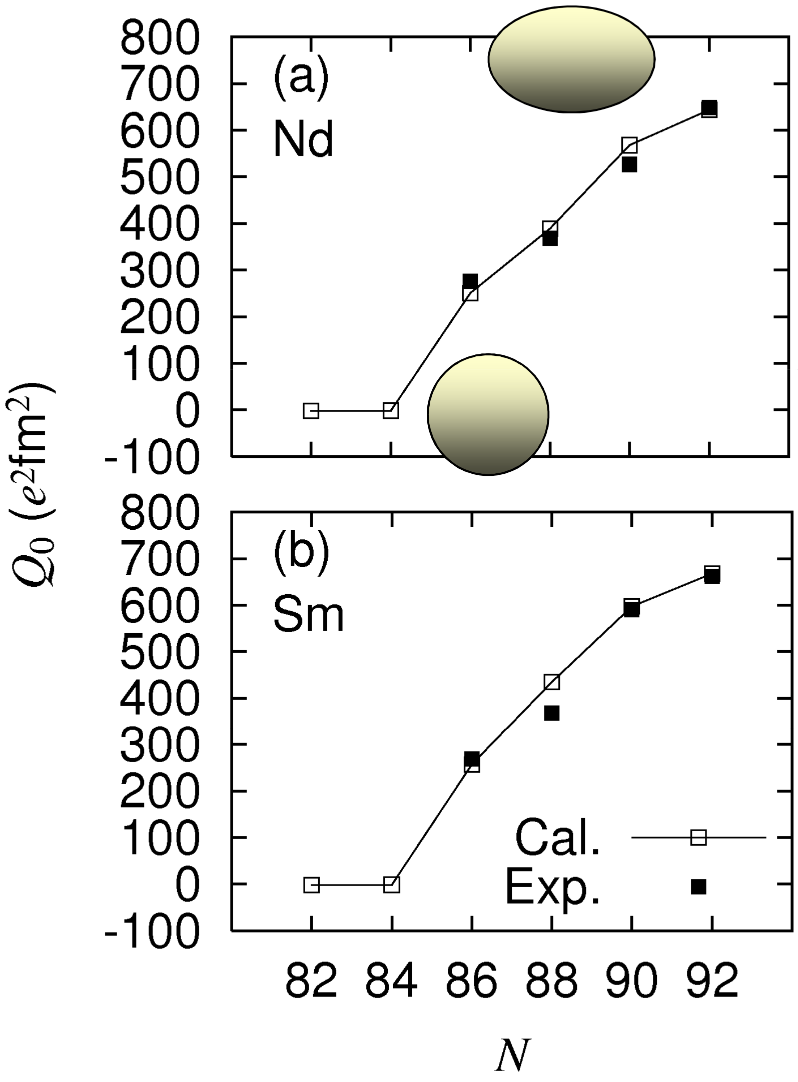


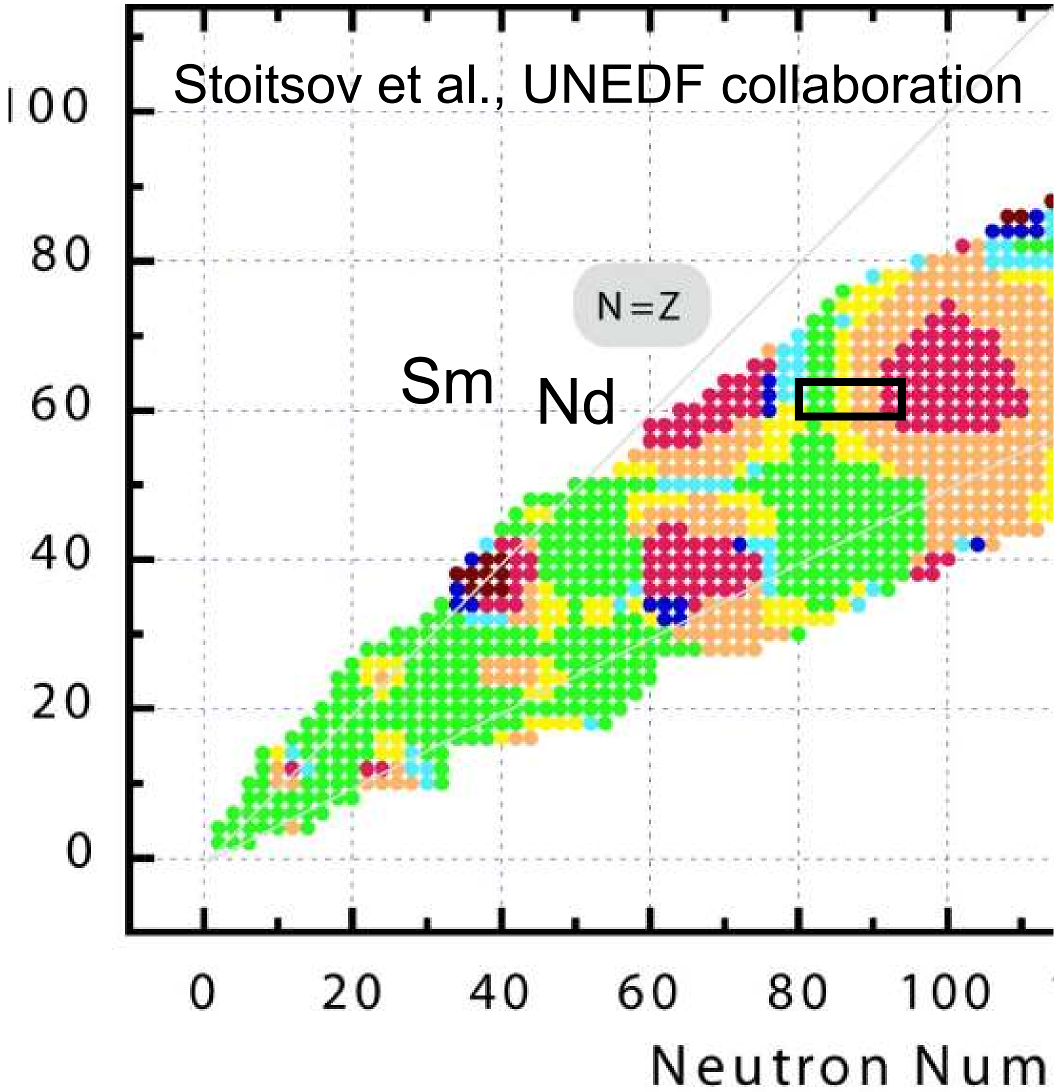
- HFB equations are solved in the 2D coordinate space, assuming the axial symmetry for the SkM* functional with the cutoff of $E_{\mathrm{qp}} < 60$ MeV.
- The pairing energy functional is the one determined by a global fitting to deformed nuclei (Yamagami, Shimizu, TN, PRC **80**, 064301 (2009))
- QRPA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

Shape phase transition in the EDF approach

Intrinsic Q moment

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





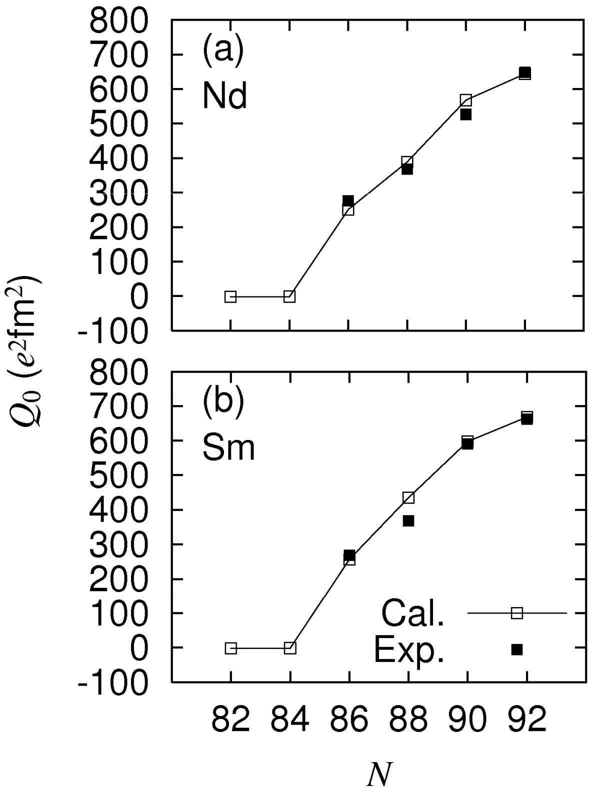
QRPA calculation of photoabsorption cross section

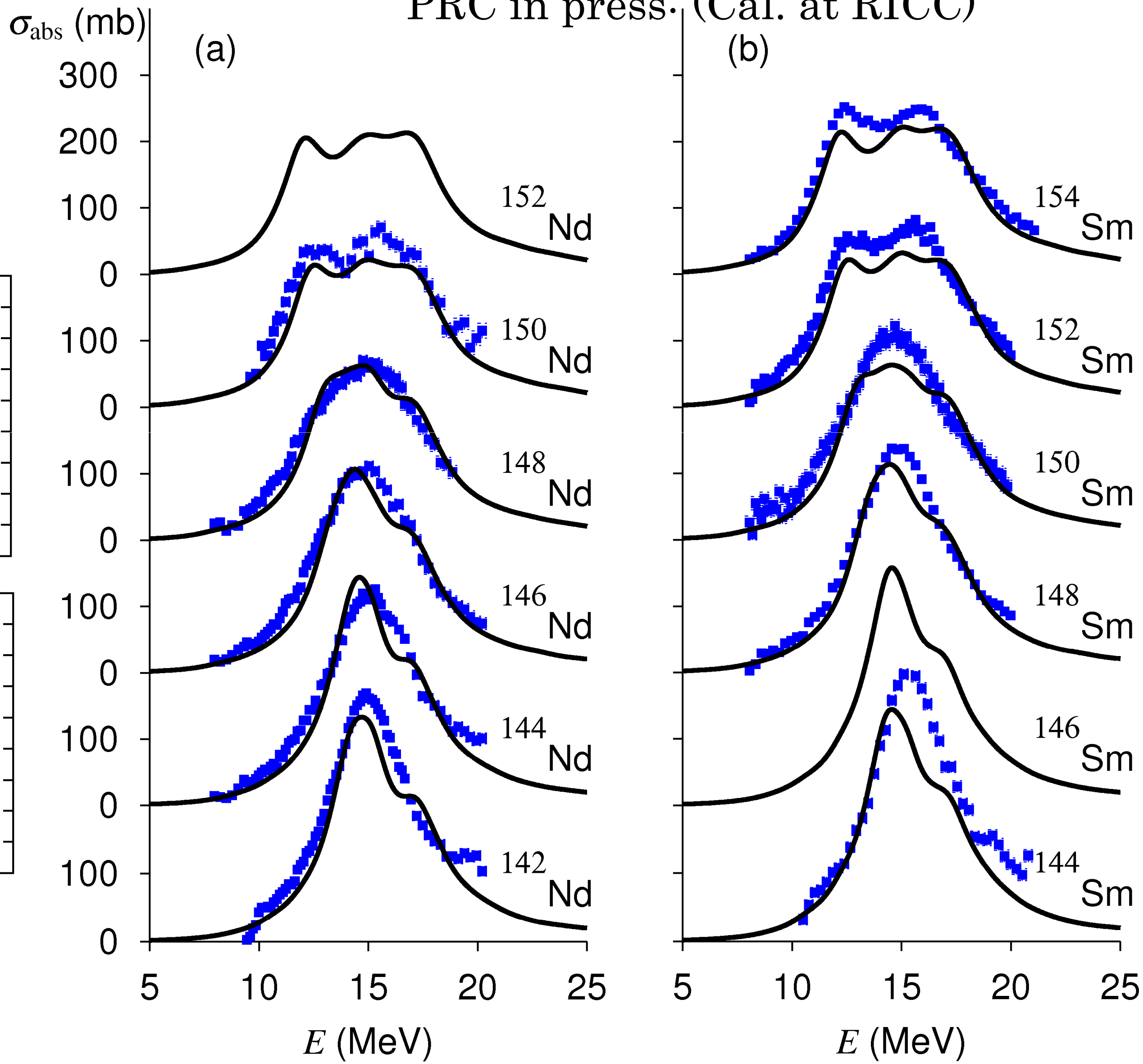
SkM* functional

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

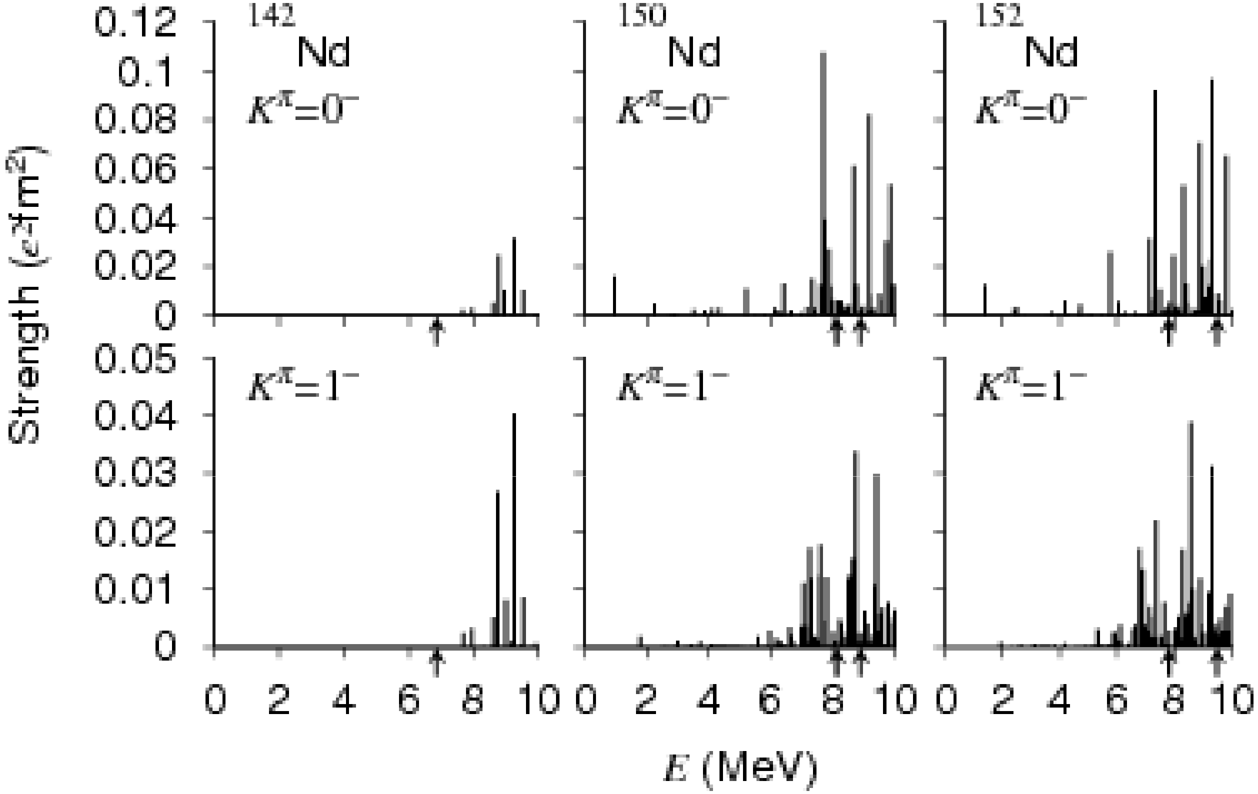
Intrinsic Q moment

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





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.

Summary

- Linearized (small-amplitude) TDDFT can be formulated in several different ways.
  - 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, …)
  - Universal correlation between the PDR fraction and the neutron skin thickness; $m_1(\mathrm{PDR})/m_1 \approx (0.2\ /\ \mathrm{fm})\,\Delta R_{np}$.