Division of Astrophysics and Nuclear Physics: Nuclear Physics Group (Parallel session #1)

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Members of Nuclear Theory Group

- Staff members
  - Kazuhiro Yabana (3-alpha reaction, TDDFT)
  - Yukio Hashimoto (TDHFB)
  - Jun Terasaki (Double beta decay)
  - Takashi Nakatsukasa [from April 2014]
- PD
  - Yasutaka Taniguchi*
- Graduate students
  - Yuta Fukuoka* (Config. mixing cal.) → T.N.
  - Kazuyuki Sekizawa (Transfer reaction)
  - Others (??)

*Absent

Nuclear response and dynamics in TDDFT [TDHF(B)]

– Yukio Hashimoto (TDHFB)
– Jun Terasaki (Double beta decay)
– Kazuhiro Yabana (TDDFT in Cond. Matt. Phys.)
– Kazuyuki Sekizawa (TDHF: Transfer reaction)

Saturation properties of nuclear matter

- Constant binding energy per nucleon

$$B/A \approx S_{n(p)} \approx 16\ \mathrm{MeV}$$

- Saturation density

$$\rho \approx 0.16\ \mathrm{fm}^{-3} \quad \Rightarrow \quad k_F \approx 1.35\ \mathrm{fm}^{-1}$$

- Naïve mean-field picture breaks down
  - State-dependent effective interaction
    - Density dependent interction
  - Energy density functional

$$E[\rho] \Rightarrow \quad h[\rho]|\varphi_i\rangle = \varepsilon_i|\varphi_i\rangle \qquad\qquad h[\rho] \equiv \frac{\delta E}{\delta \rho}$$

Basic equation

- TDHF eq. (TDKS eq.)

$$i\frac{\partial}{\partial t}\varphi_i(t)=\left\{-\frac{\hbar^2}{2m}\nabla^2+V_{\mathrm{KS}}\left[\rho(t)\right]\right\}\varphi_i(t)$$

- TDHFB eq. (TDBdGKS eq.)

$$i\frac{\partial}{\partial t}\begin{pmatrix}U_\mu(t)\\ V_\mu(t)\end{pmatrix}=\begin{pmatrix}h(t)-\lambda & \Delta(t)\\ -\Delta^*(t) & -\left(h(t)-\lambda\right)^*\end{pmatrix}\begin{pmatrix}U_\mu(t)\\ V_\mu(t)\end{pmatrix}$$

Time-dependent DFT (TDDFT)

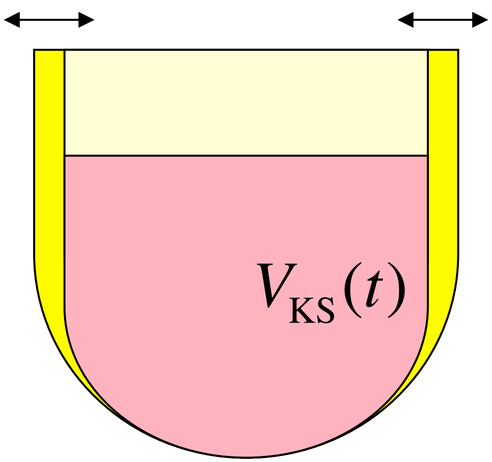
Time-dependent Kohn-Sham equation (1984)

$$i\frac{\partial}{\partial t}\varphi_i(t) = \left\{-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{KS}}\left[\rho(t)\right] - \varepsilon_i\right\}\varphi_i(t)$$

$$V_{\mathrm{KS}}\left[\rho(t)\right] = V_0 + \delta V_{\mathrm{KS}}(t)$$

Induced (screening) field

$$\delta V_{\mathrm{KS}}(t) = \frac{\delta V_{\mathrm{KS}}}{\delta\rho}\delta\rho(t)$$



The collective motion is induced by the motion of the potential.

Complete analogue of the unified model by Bohr and Mottelson

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

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

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

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

- 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:

$$\delta h(\omega) = \frac{1}{\eta}\left(h\left[\rho_\eta\right] - h\left[\rho_0\right]\right)$$

$$\rho_\eta \equiv \sum \left|\psi_i\right\rangle\left\langle\psi_i^{'}\right|$$

$$\left|\psi_i\right\rangle = \left|\varphi_i\right\rangle + \eta\left|X_i(\omega)\right\rangle, \quad \left\langle\psi_i^{'}\right| = \left\langle\varphi_i\right| + \eta\left\langle Y_i(\omega)\right|$$

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

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

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

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

Step-by-step numerical procedure

1. Set the initial amplitudes $X^{(0)}$ and $Y^{(0)}$
2. Calculate the residual fields δh by the FAM formula

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

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

3. Now, we can calculate the l.h.s. of the following equations:

$$\left.\begin{array}{l} (\omega - h_0 + \varepsilon_i)|X_i(\omega)\rangle - \delta h(\omega)|\phi_i\rangle = V_{\mathrm{ext}}(\omega)|\phi_i\rangle \\ \langle Y_i(\omega)|(\omega + h_0 - \varepsilon_i) + \langle\phi_i|\delta h(\omega) = -\langle\phi_i|V_{\mathrm{ext}}(\omega) \end{array}\right\} \Rightarrow A\vec{x} = \vec{b}$$

$$\vec{x} = \begin{pmatrix} |X_i(\omega)\rangle \\ \langle Y_i(\omega)| \end{pmatrix}, \qquad \vec{b} = \begin{pmatrix} V_{\mathrm{ext}}(\omega)|\phi_i\rangle \\ -\langle\phi_i|V_{\mathrm{ext}}(\omega) \end{pmatrix}$$

4. Update the amplitude to $(X^{(1)},Y^{(1)})$ by an iterative algorithm, such as the conjugate gradient method and its derivatives

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Iterative approaches to strength functions:
Johnson et al., CPC 120, 155 (1999)
Toivanen et al., PRC 81, 034312 (2010); Carlsson et al., PRC 86, 014307 (2012)

Finite amplitude method for superfluid systems

Avogadro and TN, PRC **84**, 014314 (2011)

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

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

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

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

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

FAM meets HFBRAD

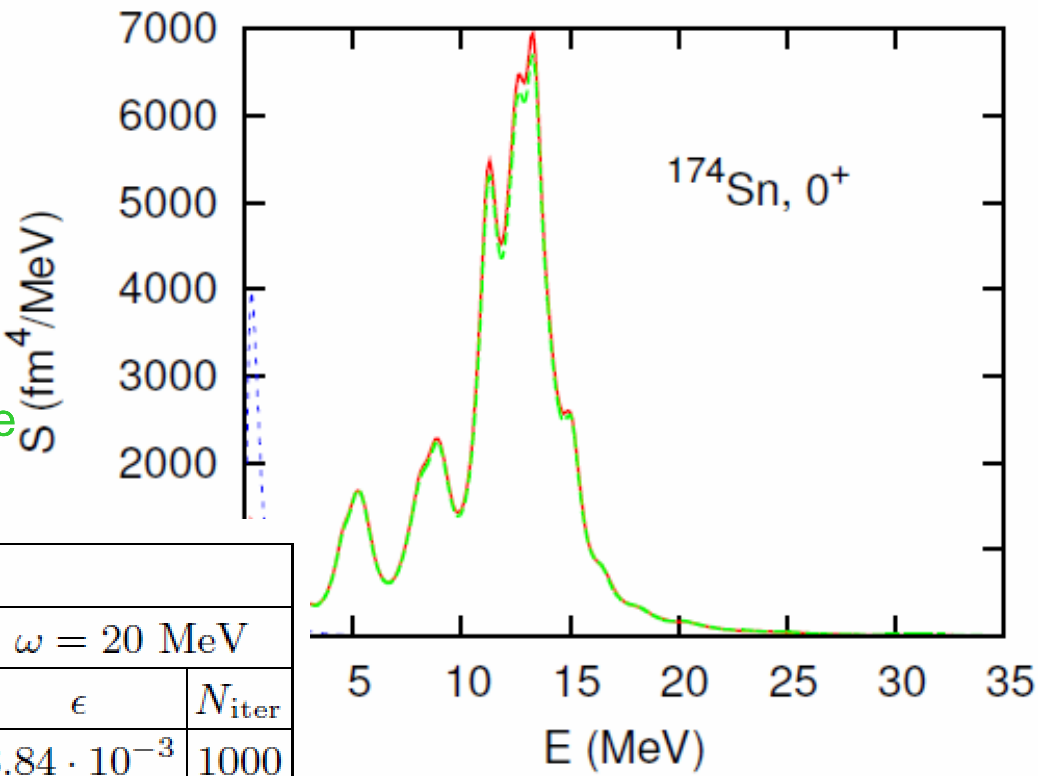
Test calculation: IS monopole

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

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

FAM meets HFBTHO

- I discussed with Mario about the possibility of HFBTHO+FAM
  - UNEDF Annual Meeting at Pack Forest, WA, USA (2009)

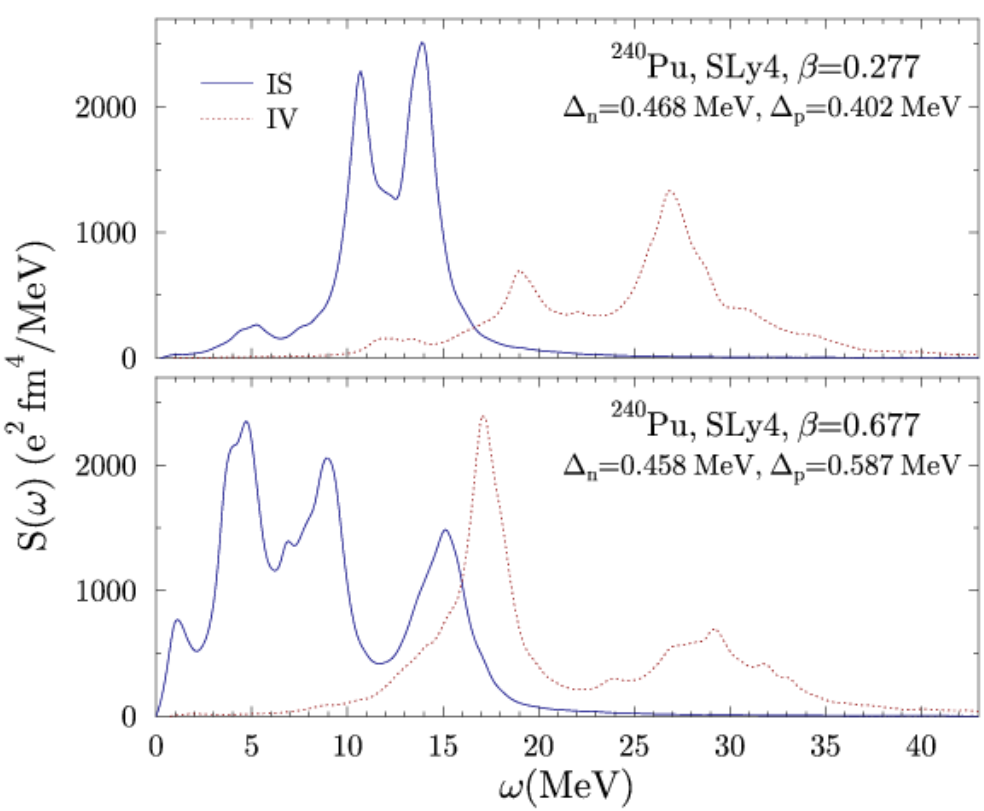
- A symposium in November, 2010
  - Mario visited us at RIKEN after the symposium.
  - Mario and Markus started working on HFBTHO+FAM.
  - The first-shot result before Christmas, 2010
  - The paper was published in July, 2011

Computational advantage in FAM

M. Stoitsov, et al., PRC **84**, 041305 (2011)

GMR in ^{240}Pu (g.s. & f. i)

(Space: 20 major shells)



QRPA			FAM
v_{crit}	Size of A, B matrices	Memory (in GB)	Memory (in GB)
^{40}Mg			
10^{-3}	32039×32039	16.4	
10^{-4}	53386×53386	45.6	
10^{-5}	53823×53823	46.35	
10^{-10}	130936×130936	274.31	
10^{-15}	189271×189271	473.18	
10^{-20}	211159×211159	713.41	0.572
^{100}Zr			
10^{-3}	83970×83970	112.81	
10^{-4}	140229×140229	314.63	
10^{-5}	160633×160633	412.85	
10^{-10}	189500×189500	574.56	
10^{-15}	230274×230274	848.41	
10^{-20}	230304×230304	848.64	0.572

Explicit construction of (Q)RPA matrix with FAM

- An advantageous feature in the iterative solver with FAM (i-FAM)
  - No need to calculate the (Q)RPA matrix explicitly
  - Computationally fast and simple
- Disadvantage in i-FAM
  - Normal-mode eigenstates are missing
- (Q)RPA matrix construction with FAM (m-FAM)
  - Again, it is very easy and computationally efficient!

RPA matrix (revisited)

$$\left\{ \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega^{(n)} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \begin{pmatrix} X^{(n)} \\ Y^{(n)} \end{pmatrix} = 0$$

$$A_{ph,p'h'} = (\varepsilon_m - \varepsilon)\delta_{pp'}\delta_{hh'} + \left. \frac{\partial h_{ph}}{\partial \rho_{p'h'}} \right|_{\rho_0}$$

$$B_{ph,p'h'} = \left. \frac{\partial h_{ph}}{\partial \rho_{h'p'}} \right|_{\rho_0}$$

FAM can provide the following quantities for a given vector $\begin{pmatrix} X_{ph} \\ Y_{ph} \end{pmatrix}$

$$\delta h_{ph} = \sum_{p'h'} \left(\left. \frac{\partial h_{ph}}{\partial \rho_{p'h'}} \right|_{\rho_0} \delta\rho_{p'h'} + \left. \frac{\partial h_{ph}}{\partial \rho_{h'p'}} \right|_{\rho_0} \delta\rho_{h'p'} \right)$$

m-FAM

Avogadro and TN, PRC**87**, 014331 (2013)

$$\rho_\eta \equiv \rho_0 + \eta\delta\rho = \sum_{i\in h} |\psi_i\rangle\langle\psi_i^{'}|$$

$$|\psi_i\rangle = |\varphi_i\rangle + \eta|X_i\rangle, \quad \langle\psi_i^{'}| = \langle\varphi_i| + \eta\langle Y_i|$$

$$\Rightarrow \quad \begin{aligned} \delta\rho_{ph} &= (\rho_\eta)_{ph}/\eta = X_{ph} \\ \delta\rho_{hp} &= (\rho_\eta)_{hp}/\eta = Y_{ph} \end{aligned}$$

$$|X_i\rangle = \sum_{m>A} |\varphi_m\rangle X_{mi}, \quad |Y_i\rangle = \sum_{m>A} |\varphi_m\rangle Y_{mi}^{*}$$

Adopting the following vector leads to "A" matrix $A_{ph,mi}$

$$\begin{aligned} X_{p'h'} &= \delta_{p'm}\delta_{h'i} \\ Y_{p'h'} &= 0 \end{aligned} \quad \Rightarrow \quad \delta h_{ph} = \sum_{p'h'} \left(\left.\frac{\partial h_{ph}}{\partial \rho_{p'h'}}\right|_{\rho_0} \delta\rho_{p'h'} + \left.\frac{\partial h_{ph}}{\partial \rho_{h'p'}}\right|_{\rho_0} \delta\rho_{h'p'} \right) = \left.\frac{\partial h_{ph}}{\partial \rho_{mi}}\right|_{\rho_0}$$

Adopting the following vector leads to "B" matrix $B_{ph,mi}$

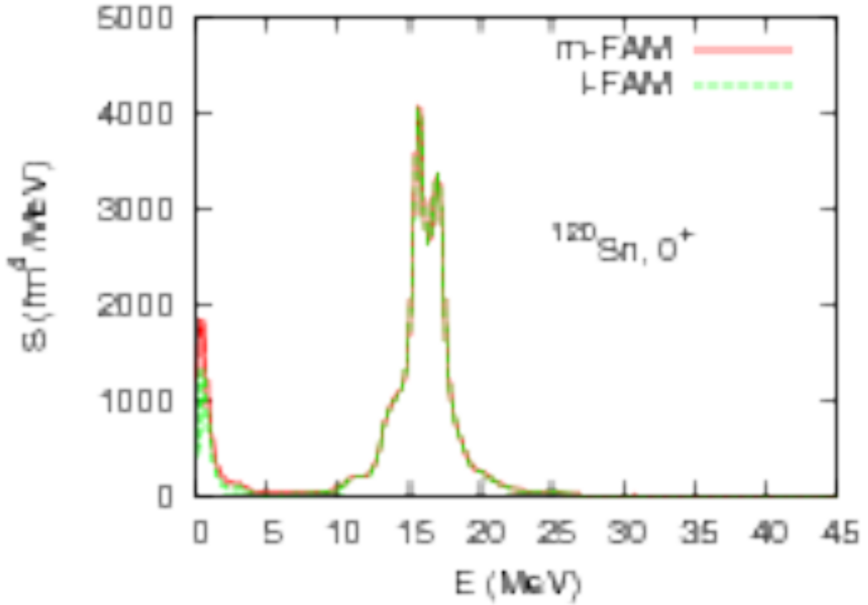
$$\begin{aligned} X_{p'h'} &= 0 \\ Y_{p'h'} &= \delta_{p'm}\delta_{h'i} \end{aligned} \quad \Rightarrow \quad \delta h_{ph} = \sum_{p'h'} \left(\left.\frac{\partial h_{ph}}{\partial \rho_{p'h'}}\right|_{\rho_0} \delta\rho_{p'h'} + \left.\frac{\partial h_{ph}}{\partial \rho_{h'p'}}\right|_{\rho_0} \delta\rho_{h'p'} \right) = \left.\frac{\partial h_{ph}}{\partial \rho_{im}}\right|_{\rho_0}$$

Repeat the calculation with all possible (m,i)-pairs.
Then, all the RPA matrix elements are explicitly calculated.

Test numerical calculation

HFBRAD+FAM (QRPA)

- m-FAM is efficient for small matrix.
- Computational time for the m-FAM scales like $N^2 \sim N^3$
- i-FAM scales like N



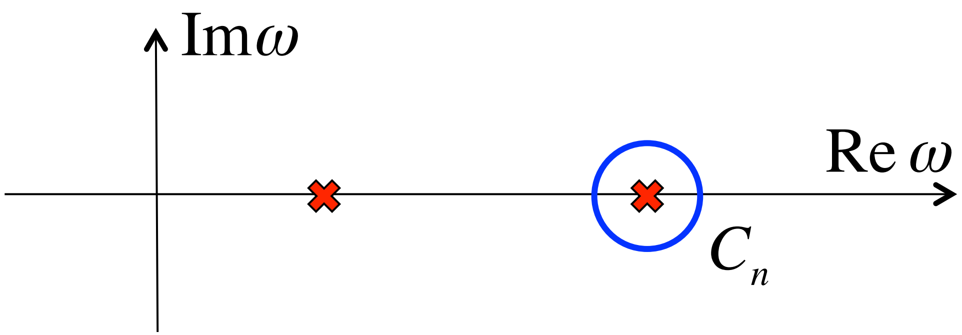
E(qp) cut off	2 x N(2qp)	i-FAM	m-FAM
60 MeV	3482	1	0.16
80 MeV	4656	1.43	0.38
100 MeV	5842	1.93	0.60
160 MeV	9528	4.08	2.56

FAM-(Q)RPA

N. Hinohara, M. Kortelainen, W. Nazarewicz, Phys. Rev. C **87**, 064309 (2013)

- QRPA eigenmodes by contour integration in the complex frequency plane

$$X^n_{\mu\nu} \propto \frac{1}{2\pi i}\oint_{C_n} X_{\mu\nu}(\omega)\,d\omega, \quad Y^n_{\mu\nu} \propto \frac{1}{2\pi i}\oint_{C_n} Y_{\mu\nu}(\omega)\,d\omega$$

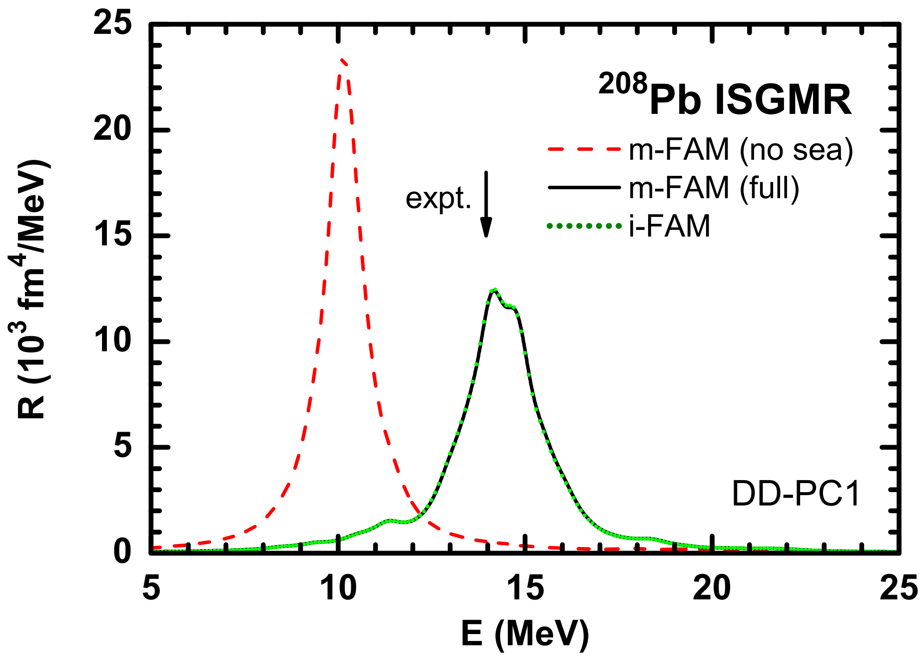


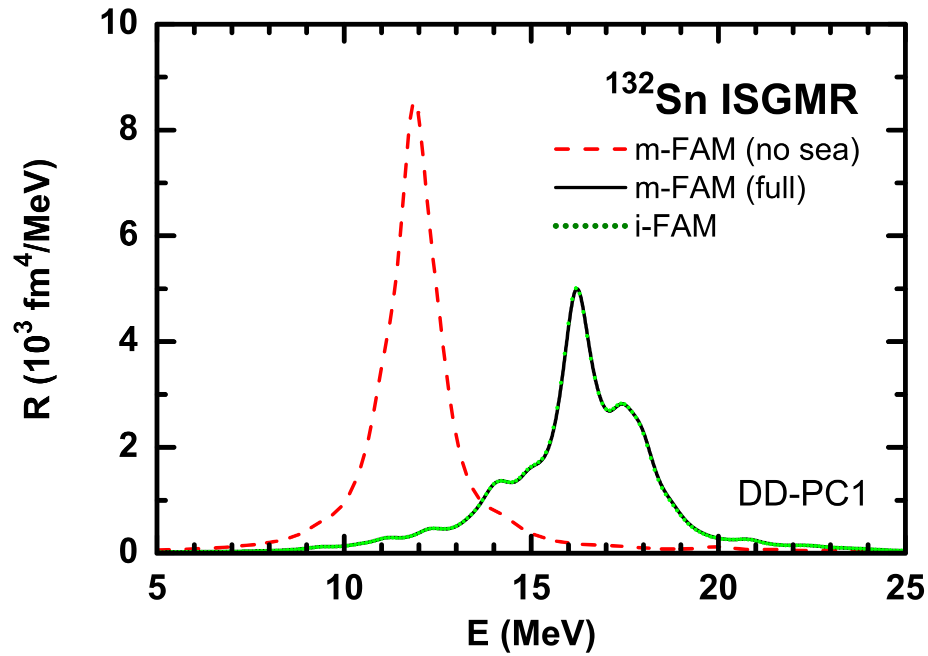
  – Test application with the HFBTHO code

Relativistic TDMF (Covariant TDDFT)

Liang, Nakatsukasa, Niu, Meng, Phys. Rev. C 87, 054310 (2013)

- Dirac sea effects are automatically included.
- Minor extra computational cost for rearrangement terms.

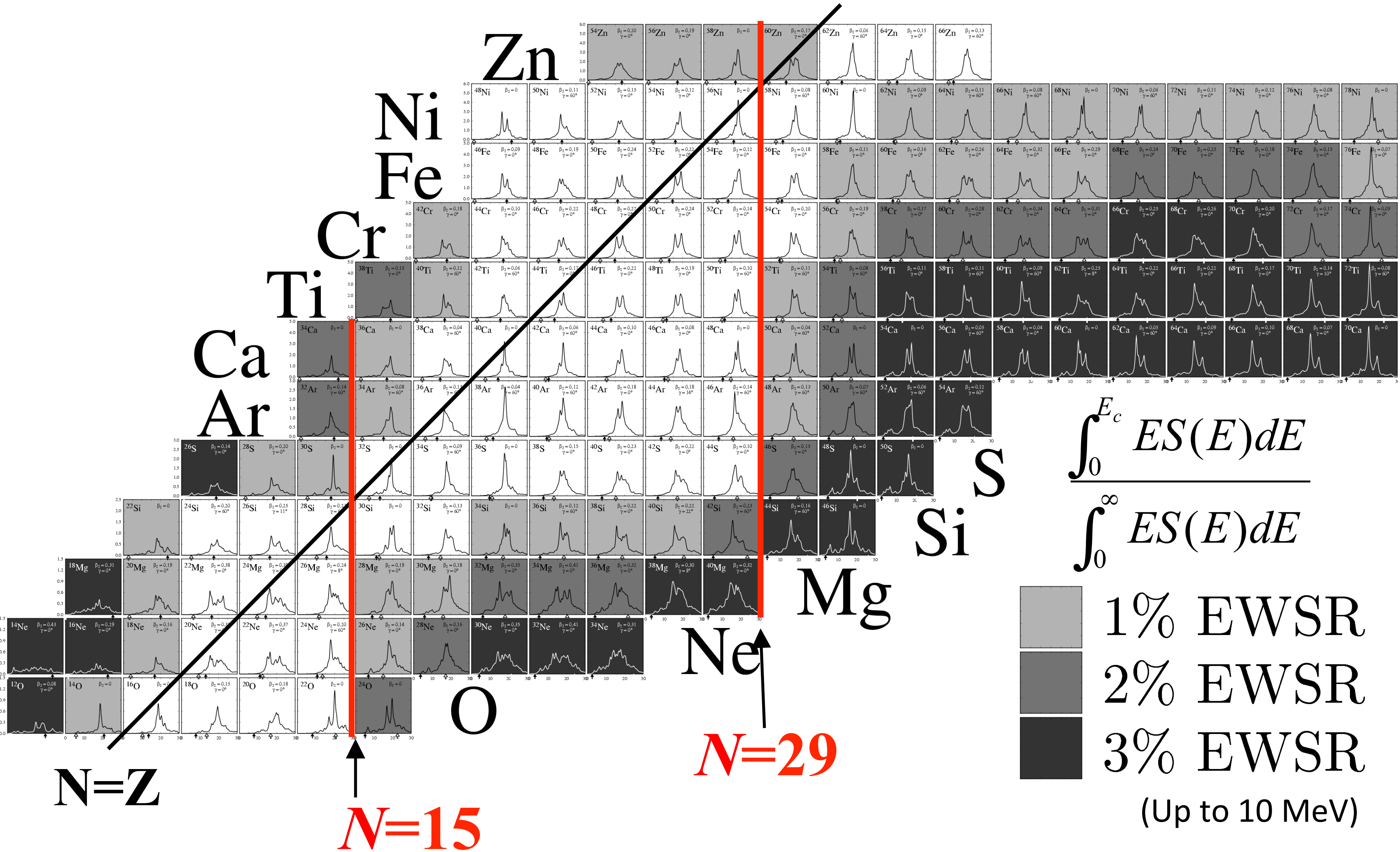




Magic numbers for low-energy E1 strength

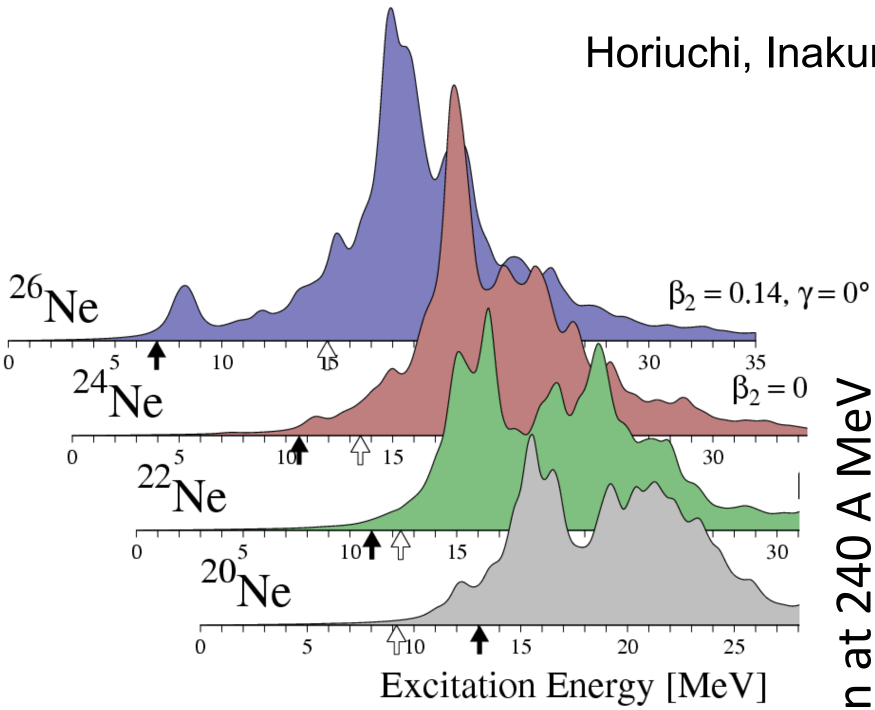
Inakura, et al

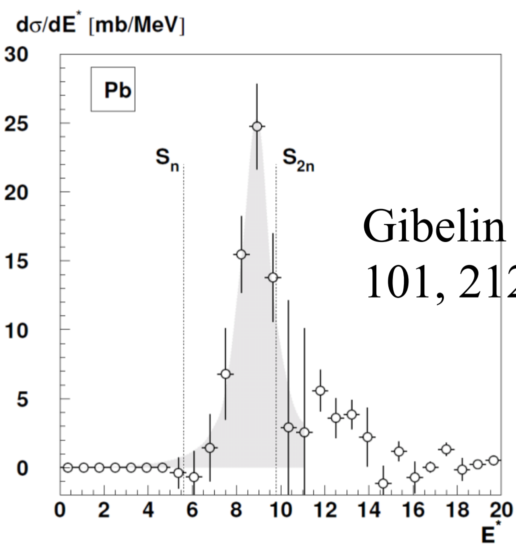
Pygmy dipole resonance (PDR)



Development of neutron radius

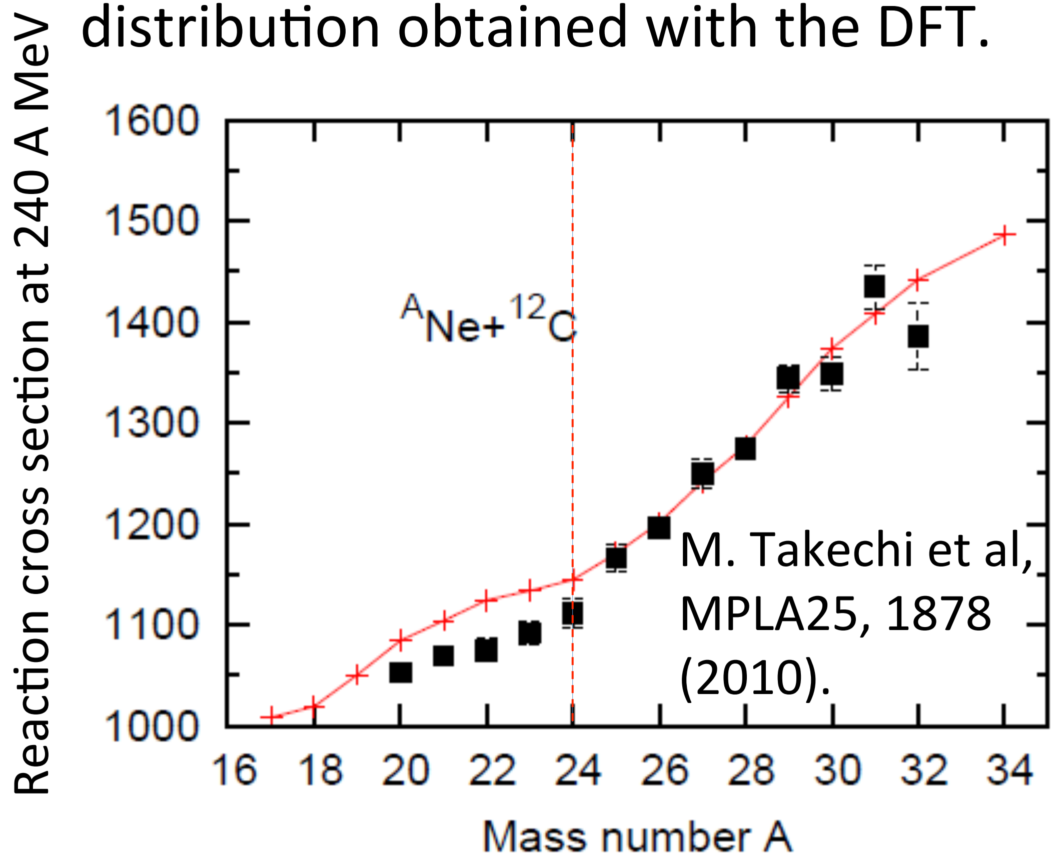
Horiuchi, Inakura, Nakatsukasa, Suzuki, PRC 86, 024614 (2012)





Gibelin et al, PRL 101, 212503 (2008)

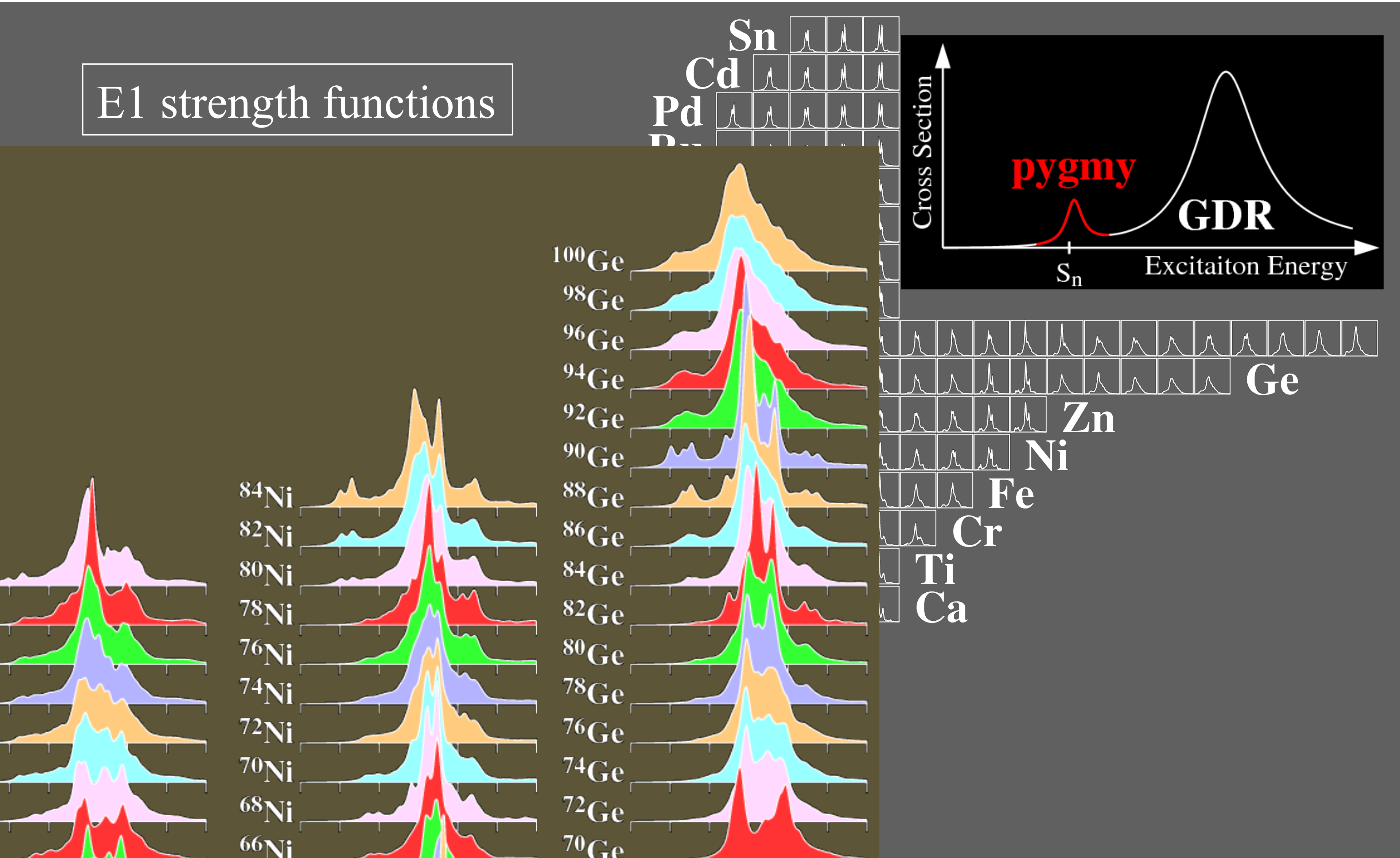
Glauber calculation using the density distribution obtained with the DFT.



M. Takechi et al, MPLA25, 1878 (2010).

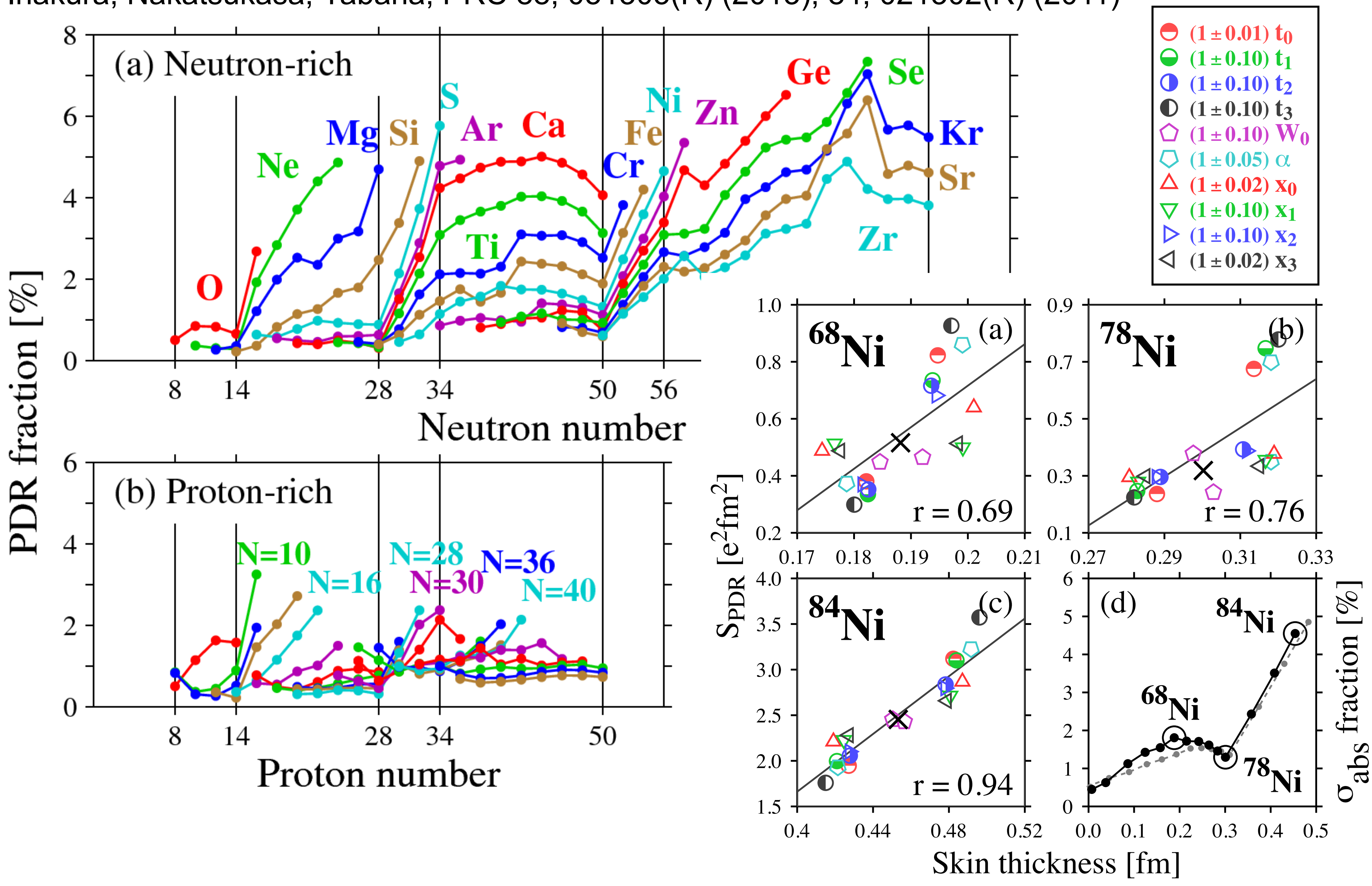
Photoabsorption cross sections

Inakura, T.N., Yabana, PRC 84, 021302 (R) (2011); PRC 88, 051305(R) (2013)



Pygmy dipoles & neutron skins

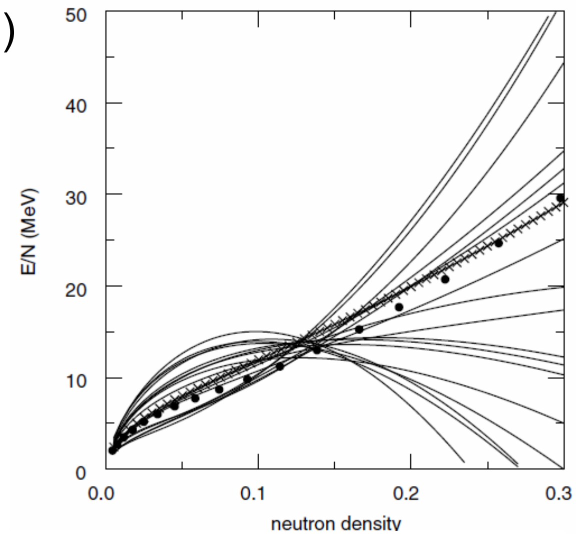
Inakura, Nakatsukasa, Yabana, PRC 88, 051305(R) (2013); 84, 021302(R) (2011)



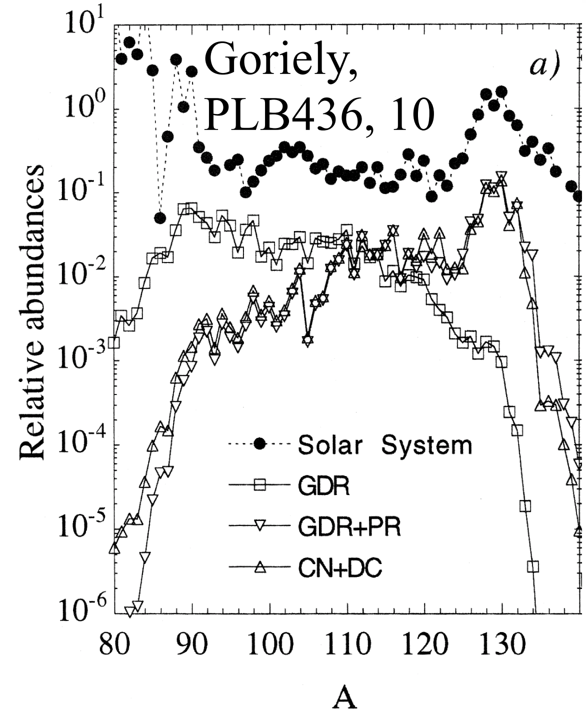
Low-energy *E1* strength in exotic nuclei

Inakura, Nakatsukasa, Yabana, PRC 84, PRC 88, 051305(R) (2013)

Ebata, Nakatsukasa, Inakura, in preparation.



- Constrain the neutron skin thickness and the NM EOS?
  - Yes, but better in very neutron rich!
  - Data on ^{84}Ni are better than ^{68}Ni



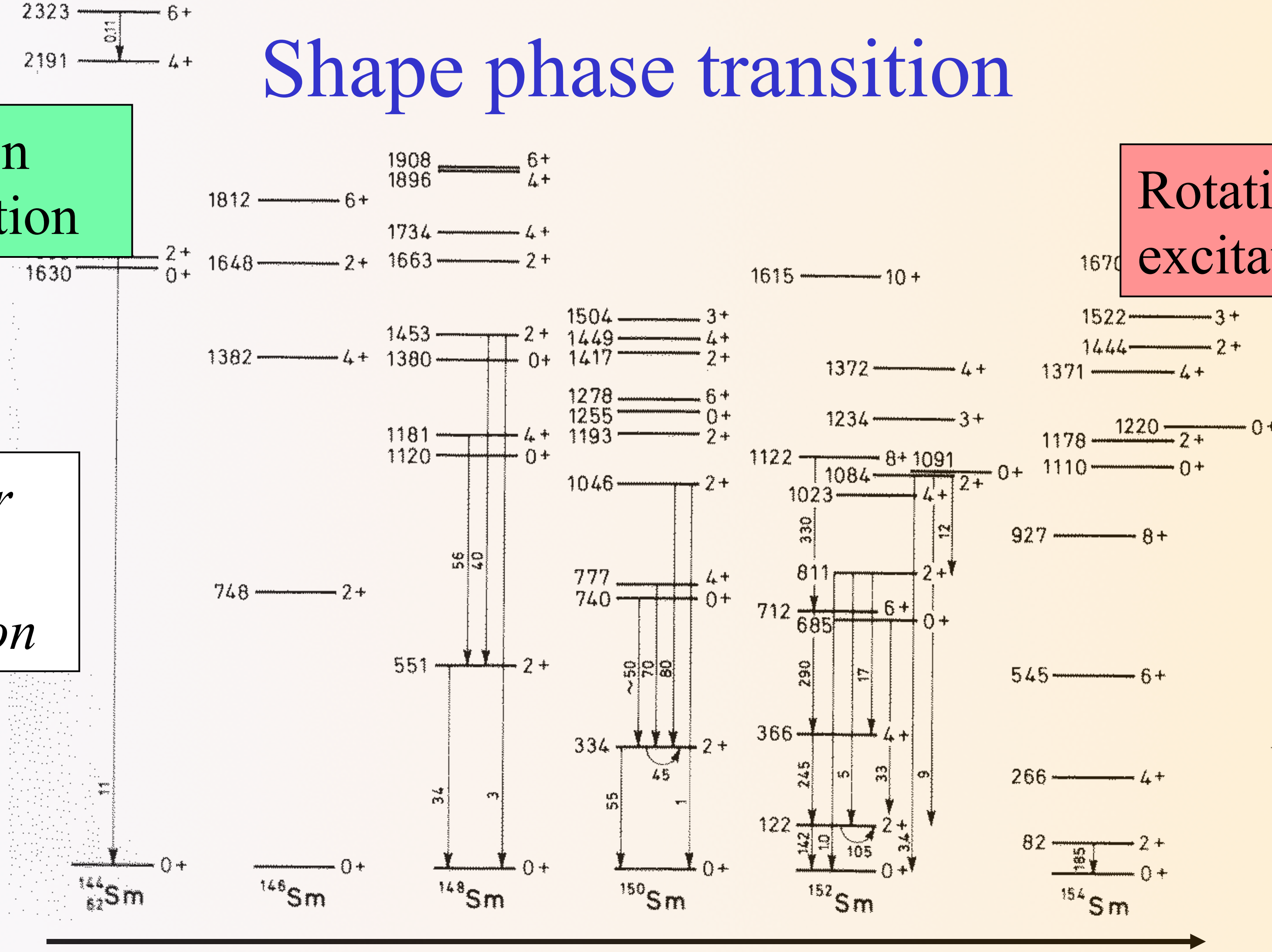
- Influence the r-process?
  - Significantly influence the direct neutron capture process near the neutron drip line
  - We need calculation with a proper treatment of the continuum.

Shape phase transition

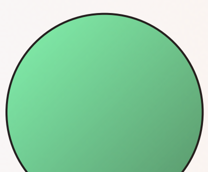
Phonon excitation

Rotational excitation

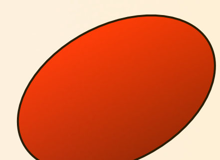
Nuclear surface vibration



Increasing neutrons



spherical



deformed

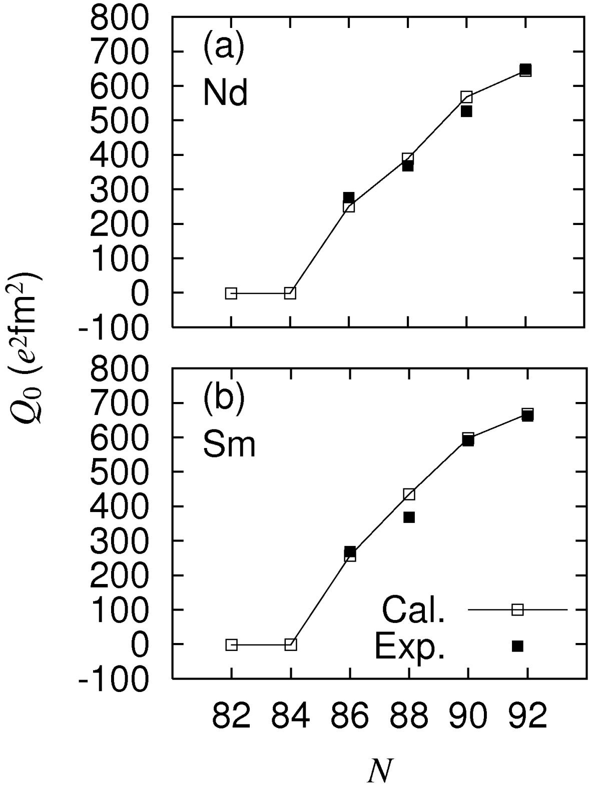
Linear response and photoabsorption cross section

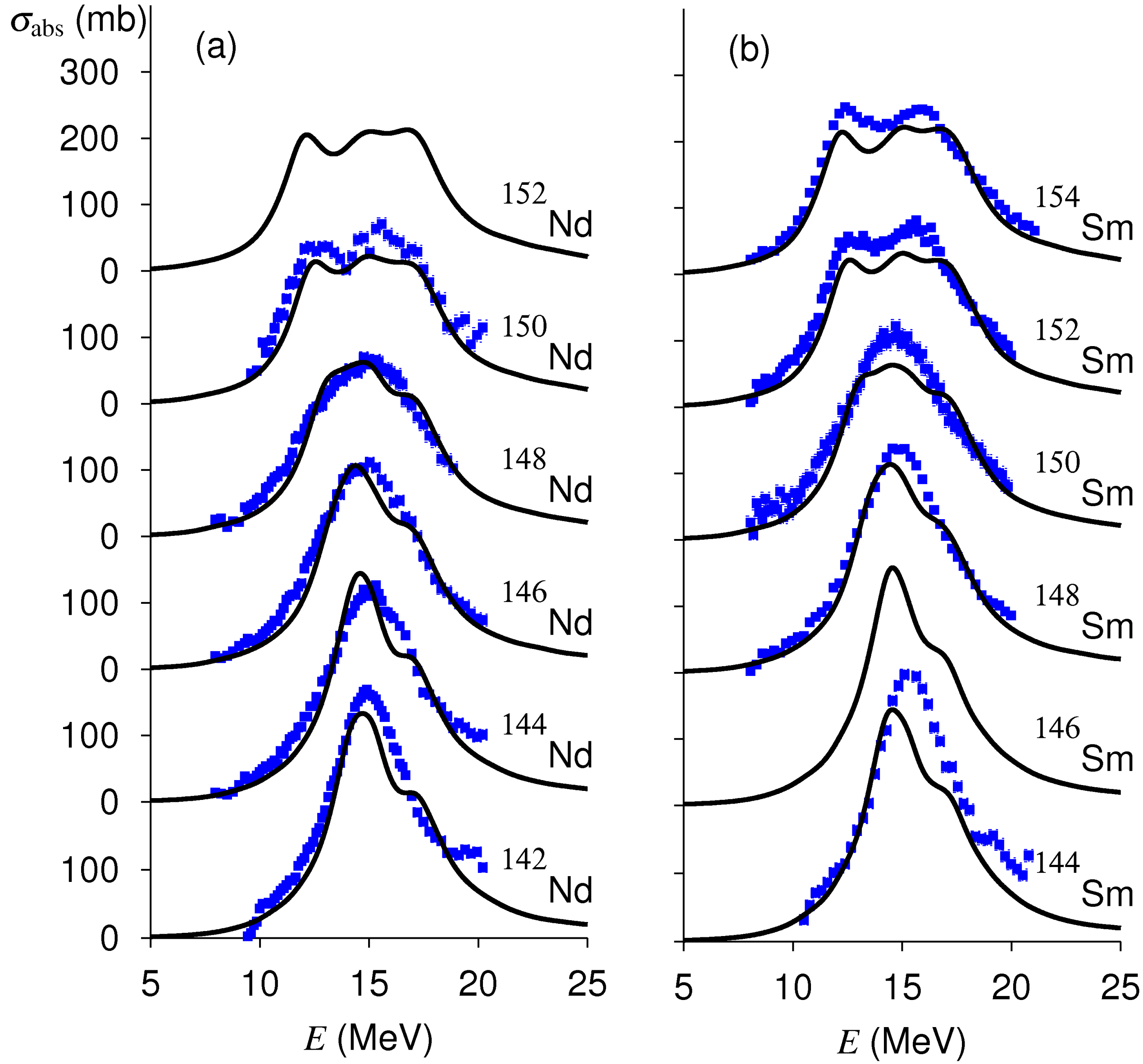
Yoshida, Nakatsukasa, PRC 83, 021304(R) (2011)

SkM* functional

Intrinsic Q moment

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

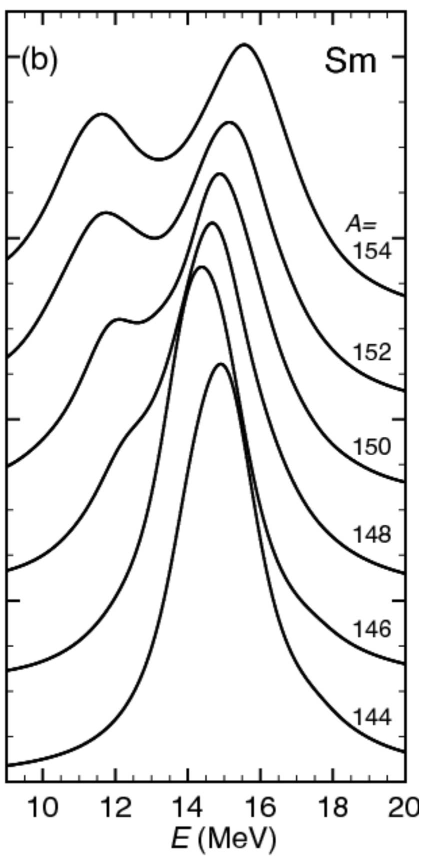


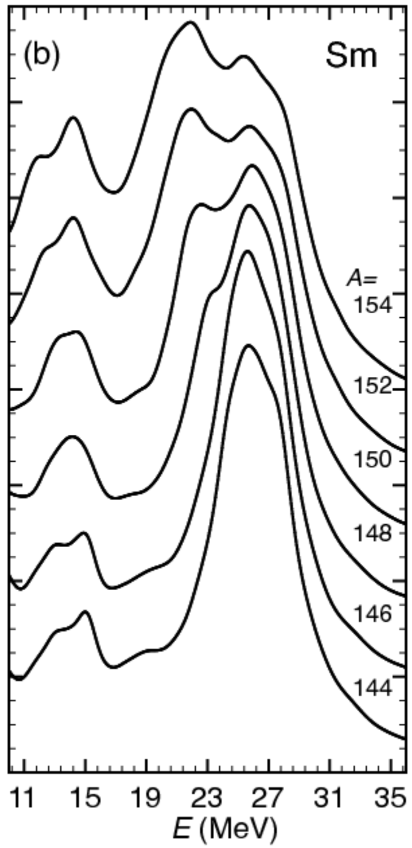


核変形と巨大共鳴(IS,IV; L=0~3)

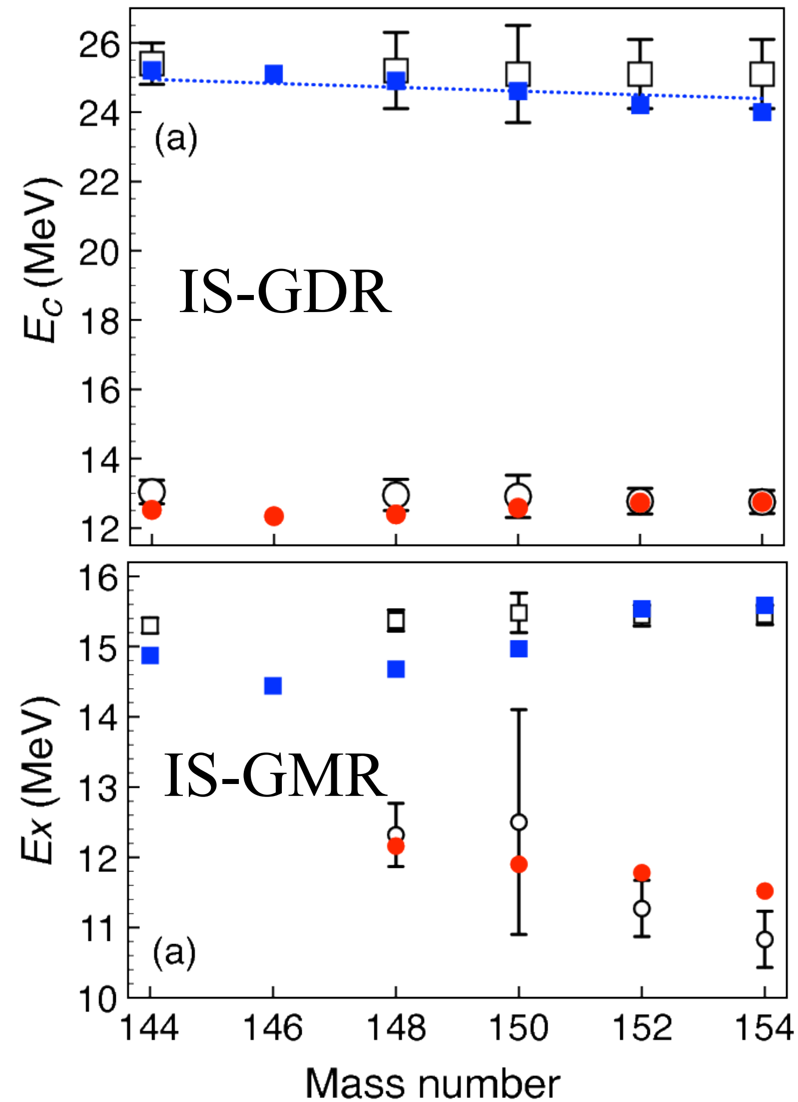
Yoshida, Nakatsukasa, PRC 88, 034309 (2013)

IS-GMR





IS-GDR

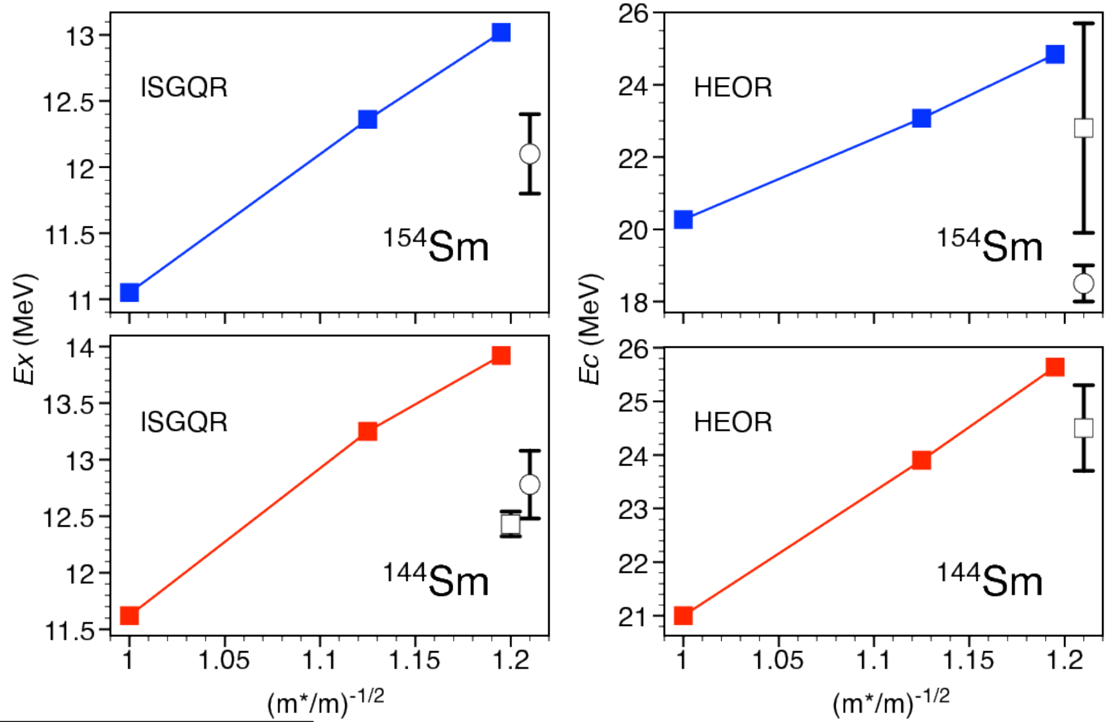


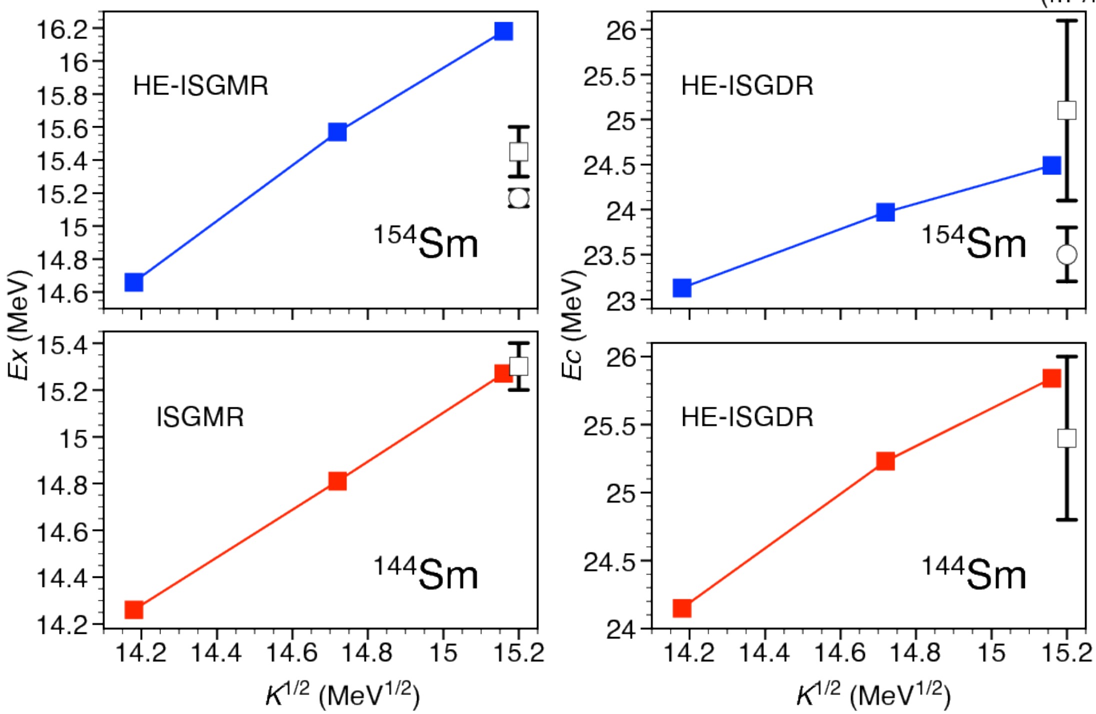
Sm isotopes: experiment at RCNP (2003)

密度汎関数の比較

核子有効質量

$$m^*/m = 0.8 \sim 0.9$$





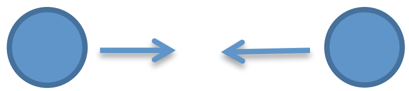
非圧縮率

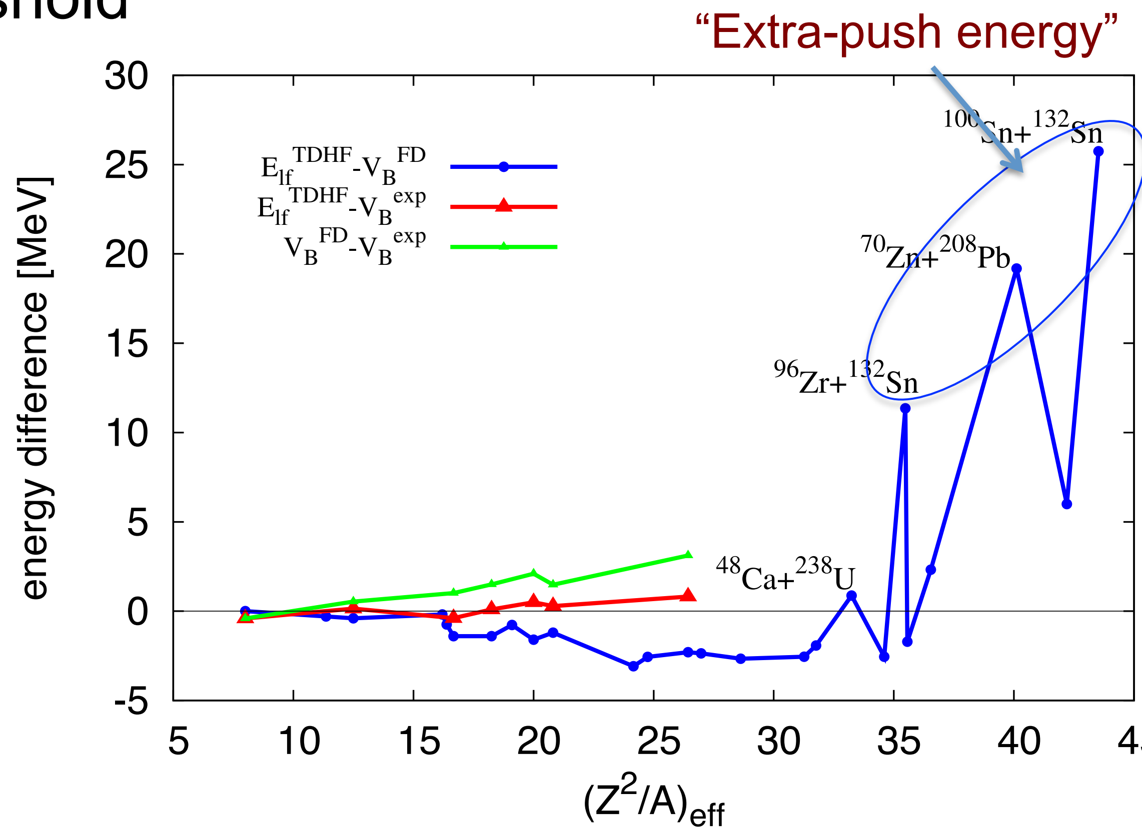
$$K = 210 \sim 230 \text{ MeV}$$

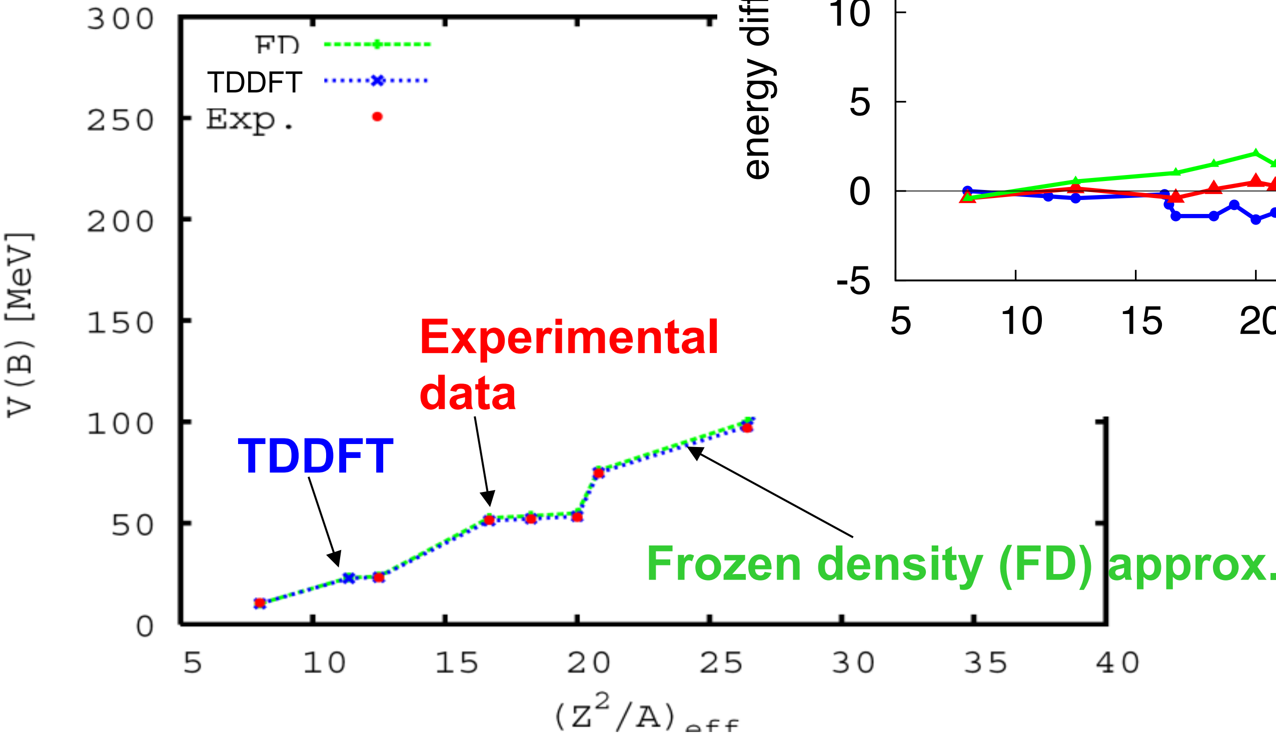
TDDFT simulation of nuclear fusion reaction

Guo, Nakatsukasa, EPJWC 38, 09003 (2012)

Fusion barrier threshold







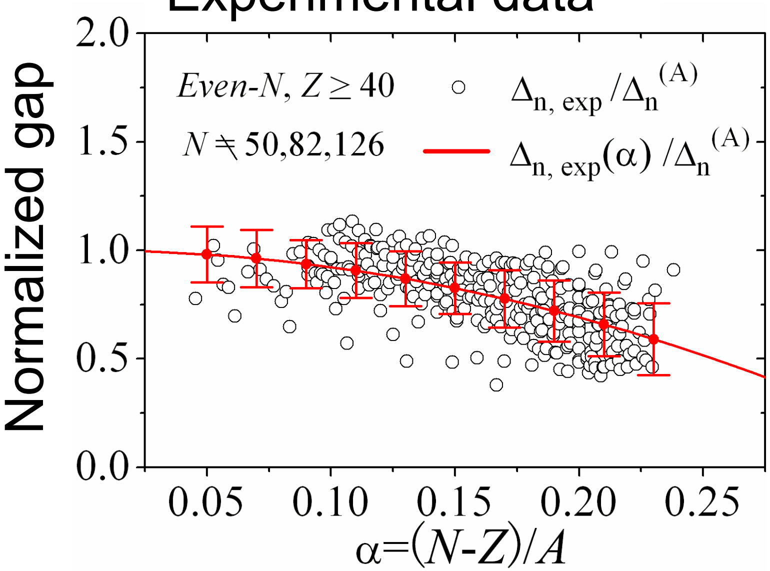
Toward a universal Energy Density Functional (EDF)

- Improvement of the EDF is essential for accurate description of nuclear properties
- Pairing energy functional
- Correlations beyond the Kohn-Sham scheme

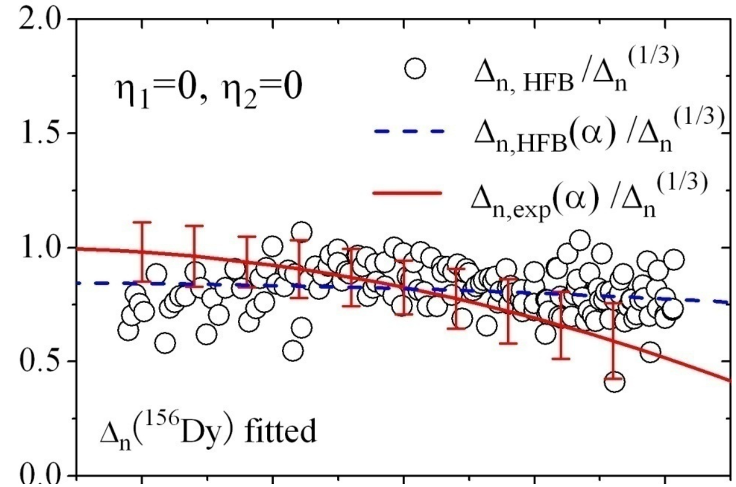
Pairing energy functional

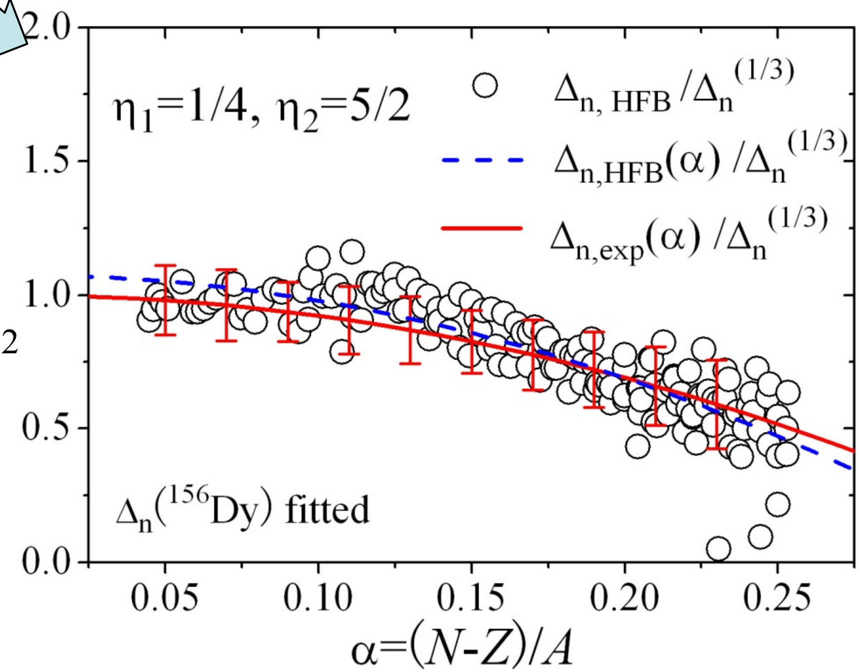
Yamagami, Shimizu, Nakatsukasa, PRC 80, 064301 (2009)

Experimental data



Δ_n





$$H_{pair}\left(\vec{r}\right)=\frac{V_0}{4}\sum_{\tau=n,p} g_\tau\left[\rho,\tau_3\rho_1\right]\left\{\tilde{\rho}_\tau\left(\vec{r}\right)\right\}^2$$

$$g_\tau\left[\rho,\rho_1\right]=1-\eta_0\frac{\rho}{\rho_0}-\eta_1\frac{\tau_3\rho_1}{\rho_0}-\eta_2\left(\frac{\rho_1}{\rho_0}\right)^2$$

DFT with proton-neutron mixing

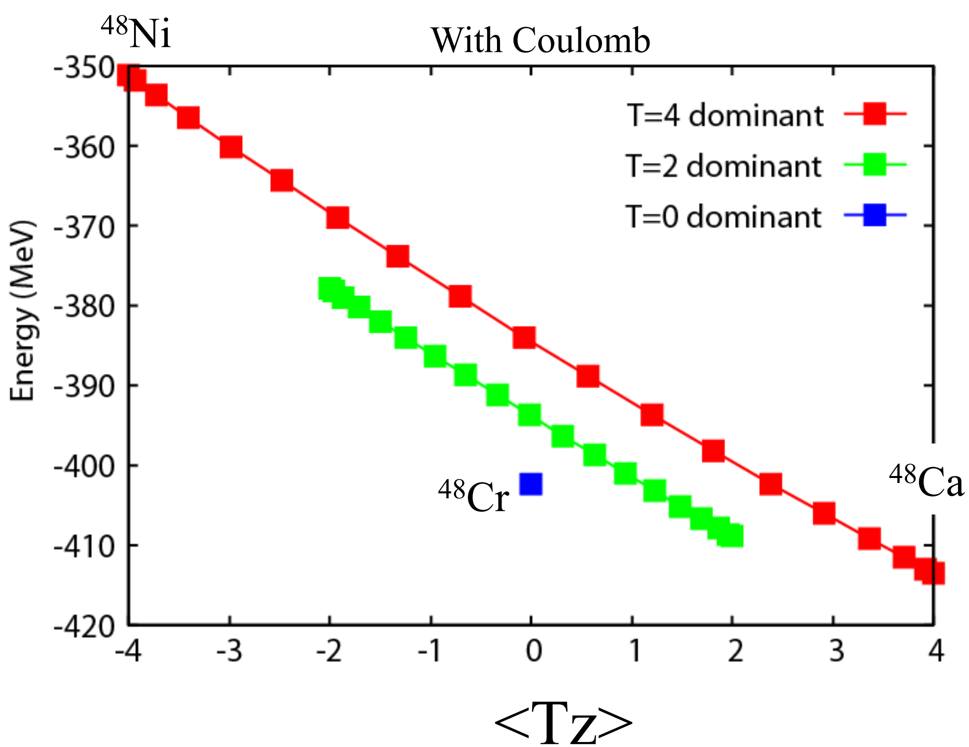
Sato, Dobaczewski, Nakatsukasa, Satula, PRC 88, 061301(R) (2013)

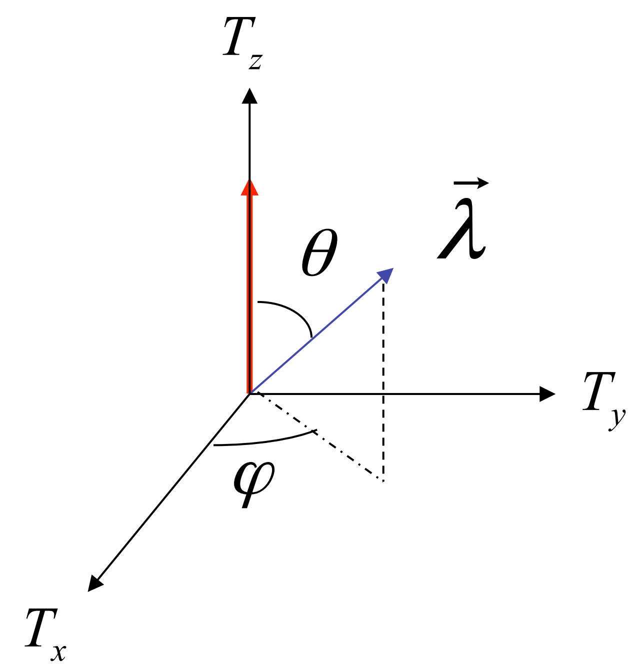
pn-mixing DFT code has been developed with a collaboration with a Warsaw group.

$$\boxed{E\left[\rho_n,\rho_p\right] \;\Rightarrow\; E\left[\rho_0,\vec{\rho}_1\right]}$$

Future subjects:
- Properties of T=0 and T=1 pairing
- Charge-exchange reaction

$$\hat{H}' = \hat{H} - \vec{\lambda}\cdot\vec{T}$$





Related presentation

- Time-dependent density functional theory
  - Yukio Hashimoto (TDHFB)
  - Jun Terasaki (Double beta decay)
  - Kazuhiro Yabana (TDDFT in Cond. Matt. Phys.)
  - Kazuyuki Sekizawa (Transfer reaction)
- Multi-reference DFT
  - Yukio Hashimoto (GCM with TAC)
  - Yuta Fukuoka* (Stochastic config. mixing cal.)

    → T.N.

*Absent

- Triple-alpha reaction
  - Kazuhiro Yabana (Imaginary-time approach)