Time-dependent density functional calculation of nuclear response functions

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Collaborators

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Basic equation

- TDHF eq. (TDKS eq.)

$$i\frac{\partial}{\partial t}\varphi_i(t) = h\left[\rho(t)\right]\varphi_i(t), \qquad h\left[\rho\right] \equiv \frac{\delta E\left[\rho\right]}{\delta \rho}$$

- TDHFB eq. (TDBdGKS eq.)

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

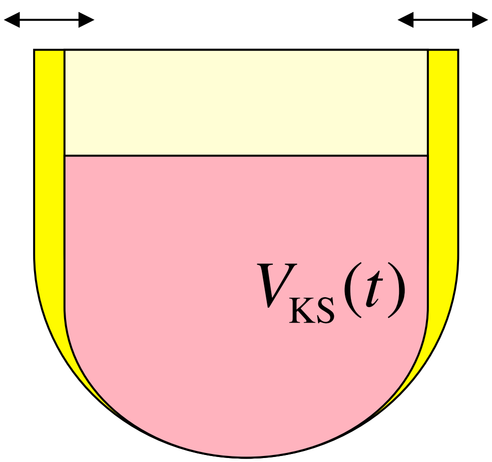
$$h\left[\rho,\kappa,\kappa^*\right] \equiv \frac{\delta E\left[\rho,\kappa,\kappa^*\right]}{\delta \rho}, \quad \Delta\left[\rho,\kappa,\kappa^*\right] \equiv \frac{\delta E\left[\rho,\kappa,\kappa^*\right]}{\delta \kappa^*}$$

Time-dependent DFT (TDDFT)

Time-dependent Kohn-Sham equation (1984)

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

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

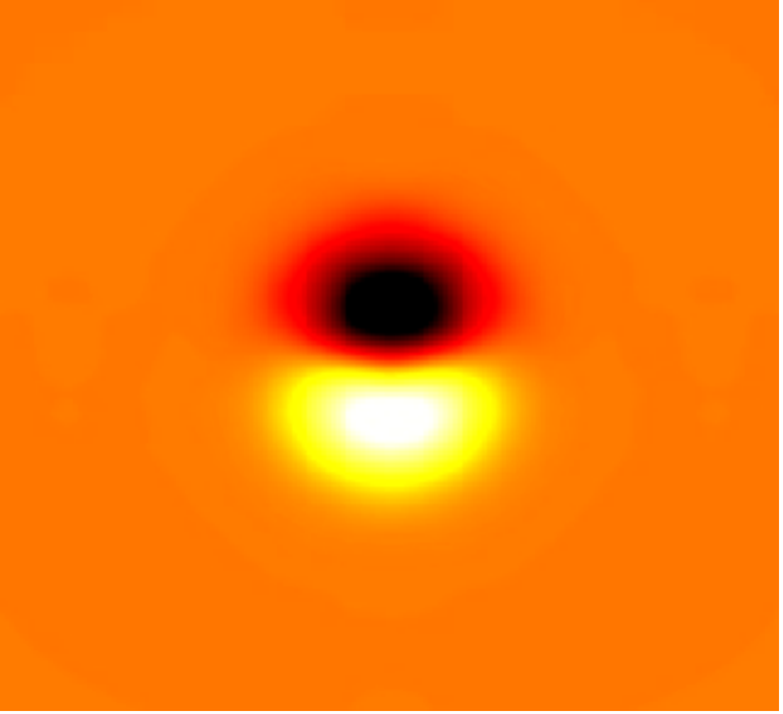


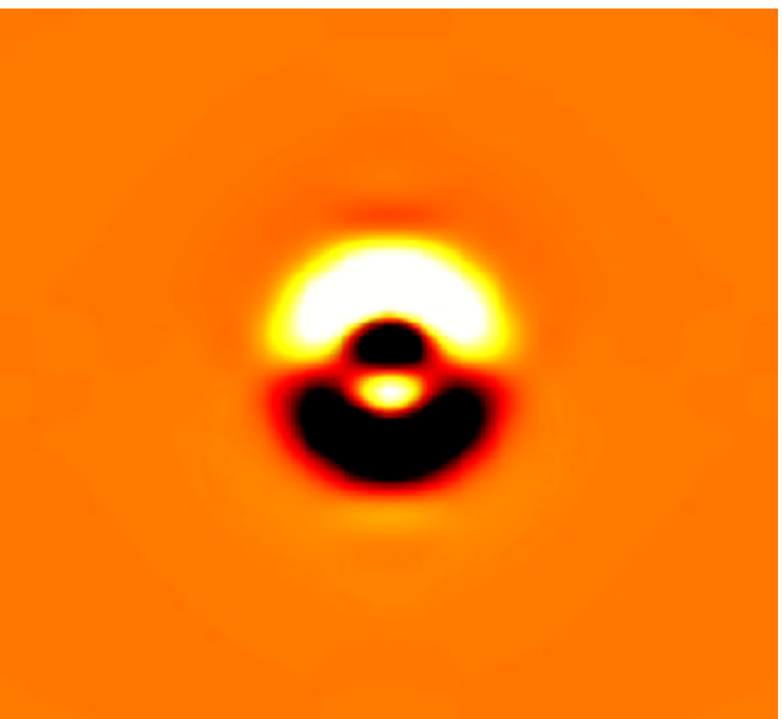
Induced (screening) field

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

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

Complete analogue of the unified model by Bohr and Mottelson





Neutrons

^{16}O

$$\delta\rho_n(t) = \rho_n(t) - \left(\rho_0\right)_n$$

Time-dep. transition density

Instantaneous weak E1 field

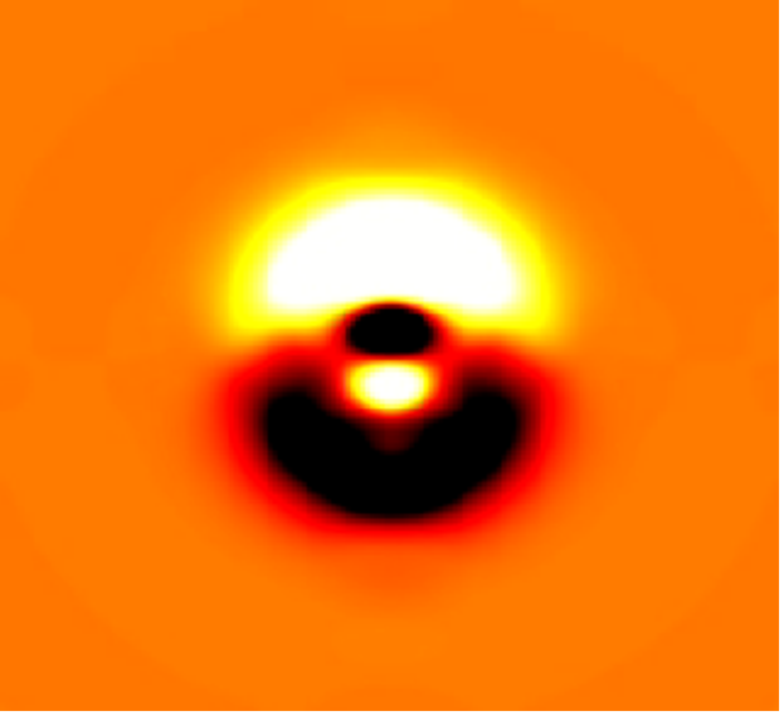
δρ> 0

δρ< 0

$$V_{\mathrm{ext}}(t) = \eta M(E1)\delta(t)$$

$$\delta\rho_p(t) = \rho_p(t) - \left(\rho_0\right)_p$$

Protons



Neutrons

^{22}O

$$\delta\rho_n(t) = \rho_n(t) - \left(\rho_0\right)_n$$

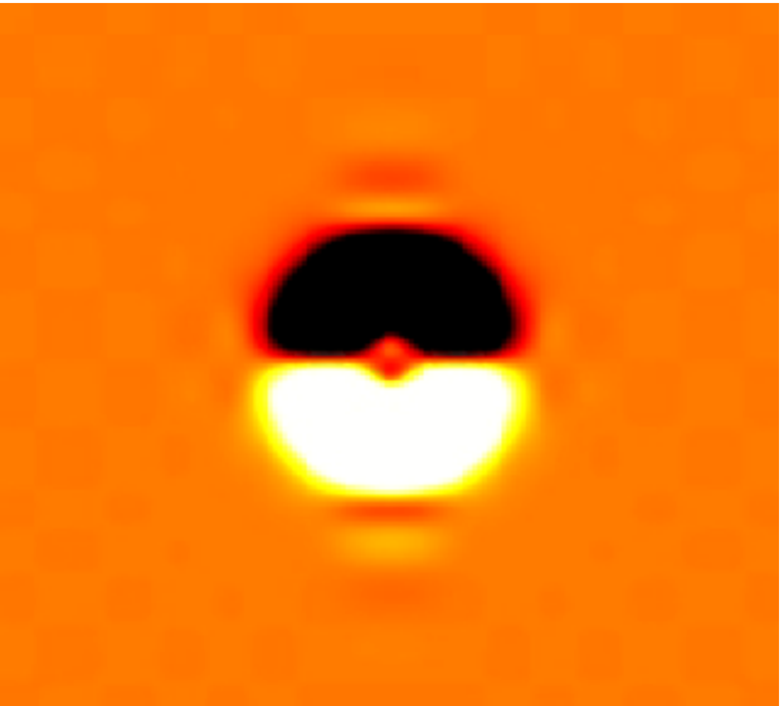
Time-dep. transition density

Instantaneous weak E1 field

δρ> 0

δρ< 0

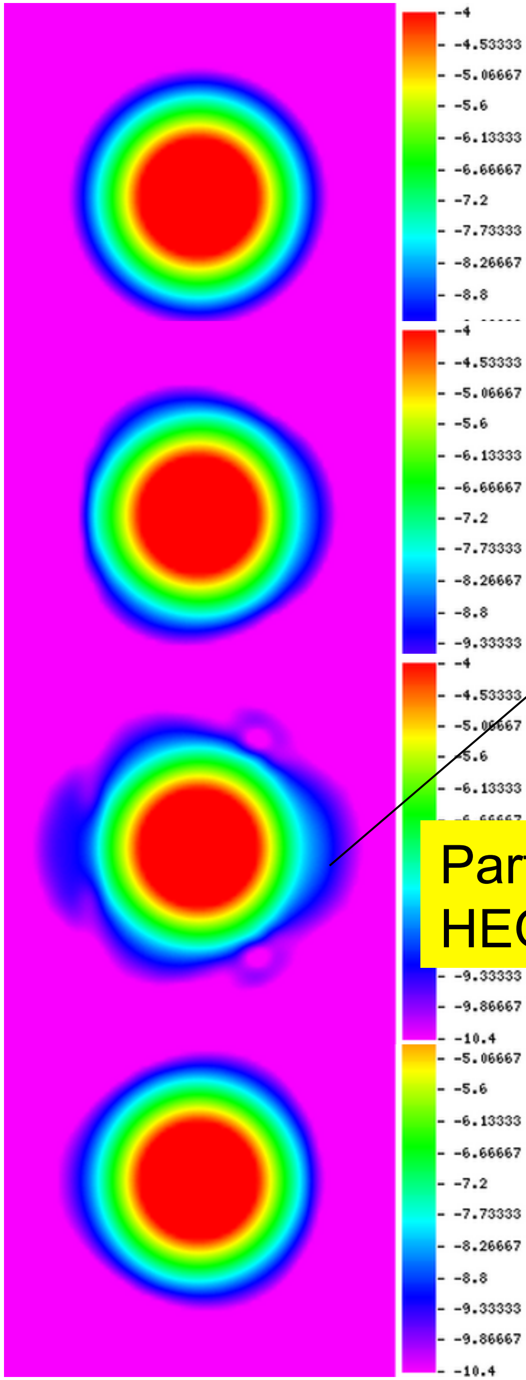
$$V_{\rm ext}(t) = \eta M(E1)\delta(t)$$



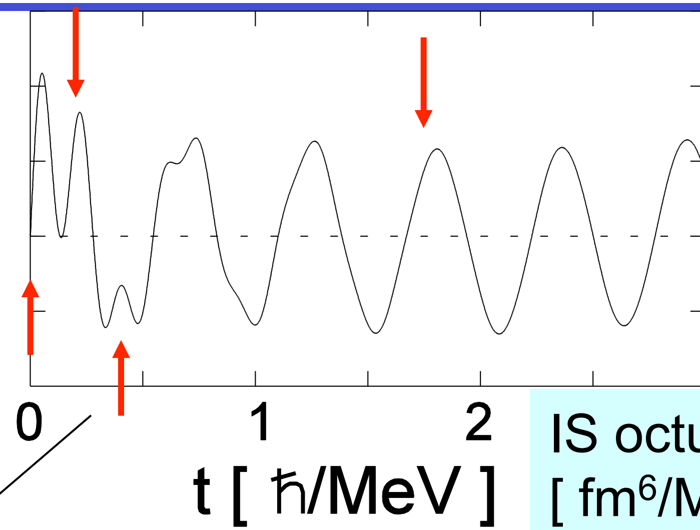
$$\delta\rho_p(t) = \rho_p(t) - \left(\rho_0\right)_p$$

Protons

IS octupole resonances in ^{16}O

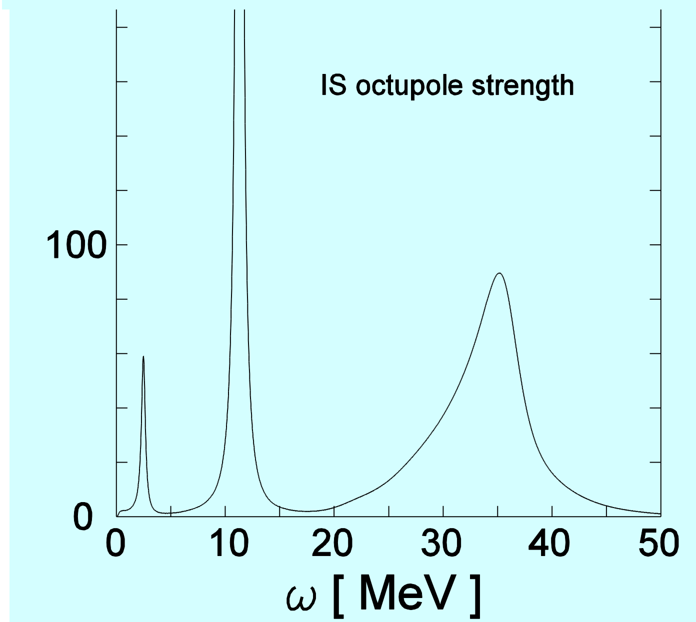


Particle decay of HEOR



Time evolution of IS octupole moment

IS octupole strength function [fm^6/MeV]



Canonical-basis TDHFB

Ebata, TN, Inakura, Yoshida, Hashimoto, Yabana, PRC 82 (2010) 034306

$$i\frac{\partial}{\partial t}\left|k(t)\right\rangle = \left(h(t)-\eta_k(t)\right)\left|k(t)\right\rangle$$

$$i\frac{\partial}{\partial t}\rho_k(t) = \Delta_k^*(t)K_k(t) - \text{c.c.}$$

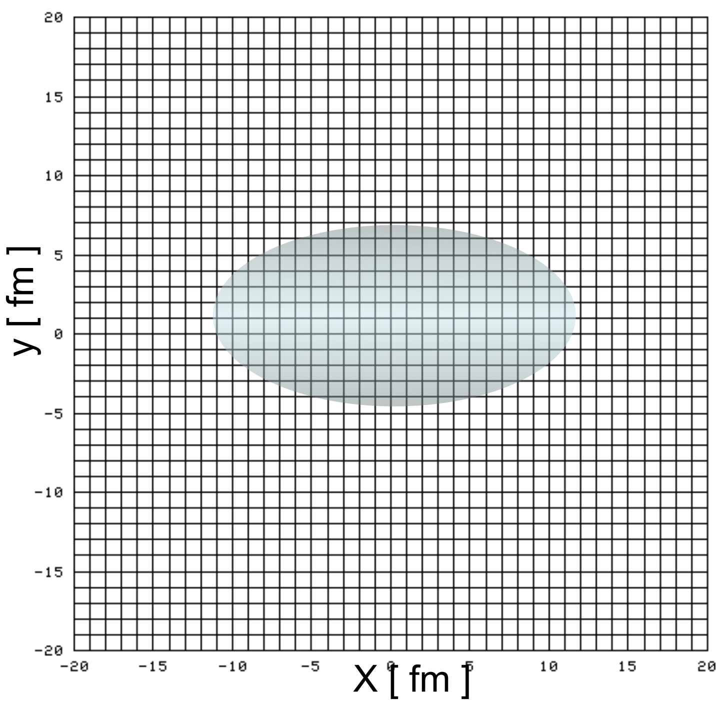
$$i\frac{\partial}{\partial t}K_k(t) = \left(\eta_k(t)+\eta_{\bar{k}}(t)\right)K_k(t) + \Delta_k(t)\left(2\rho_k(t)-1\right)$$

- Time-dependent canonical states “k”
- Time-dependent (u,v)-factors

Skyrme Cb-TDHFB in real space & real time

Time evolution is calculated by the predictor-corrector method.

3D mesh representation for canonical states



$$\langle \mathbf{r},\sigma;t\,|\,k\rangle = \left\{\langle \mathbf{r}_i,\sigma;t_n\,|\,k\rangle\right\}_{i=1,\cdots Mr}^{n=1,\cdots Mt}, \quad k=1,\cdots,M \geq N$$

$$u_k(t), v_k(t) \quad k=1,\cdots,M$$

Spatial size is a spherical box of radius of 12 - 15 fm.

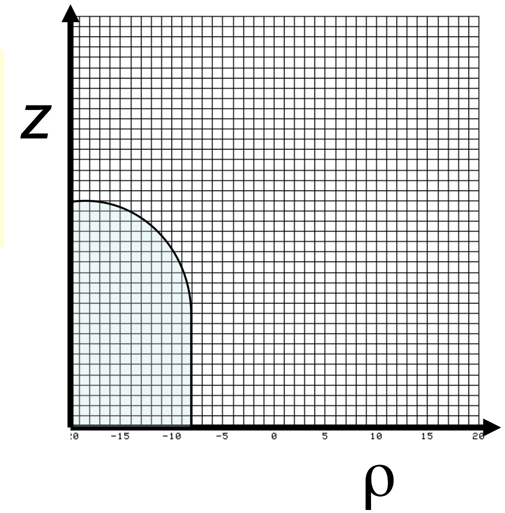
Spatial mesh size is 0.8 fm.

Time step is about 0.2 fm/c

HFB+QRPA for axially deformed nuclei

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

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



- 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).
- All the residual interactions are taken into account, except for the residual Coulomb interaction.

Finite Amplitude Method

T.N., Inakura, Yabana, PRC **76** (2007) 024318
Avogadro and T.N., PRC **84**, 014314 (2011)

To avoid the calculation of "two-body"-like residual interaction

$$\left\{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}\begin{pmatrix} X_{\mu\nu}(\omega) \\ Y_{\mu\nu}(\omega) \end{pmatrix} = \begin{pmatrix} F^{20}_{\mu\nu} \\ F^{02}_{\mu\nu} \end{pmatrix} \quad \Rightarrow \quad \begin{aligned} (E_\mu + E_\nu - \omega) X_{\mu\nu}(\omega) + \delta H^{20}_{\mu\nu}(\omega) &= F^{20}_{\mu\nu}(\omega) \\ (E_\mu + E_\nu + \omega) Y_{\mu\nu}(\omega) + \delta H^{02}_{\mu\nu}(\omega) &= F^{02}_{\mu\nu}(\omega) \end{aligned}$$

Residual fields can be calculated with small parameter η

$$\delta H(\omega) = \frac{1}{\eta}\left\{ H\left[\overline{V}^*_\eta, \overline{U}^*_\eta; V_\eta, U_\eta\right] - H_0 \right\}$$

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

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

Trivial programming of the (Q)RPA code
Only need the single-particle potential, with different bras and kets.

- 3D real-space FAM without pairing
  - Inakura, T.N., Yabana, PRC **80**, 044301 (2009); PRC 84, 021302 (2011)
- 2D HO-basis FAM with pairing
  - Stoitsov et al, PRC 84, 041305 (2011)

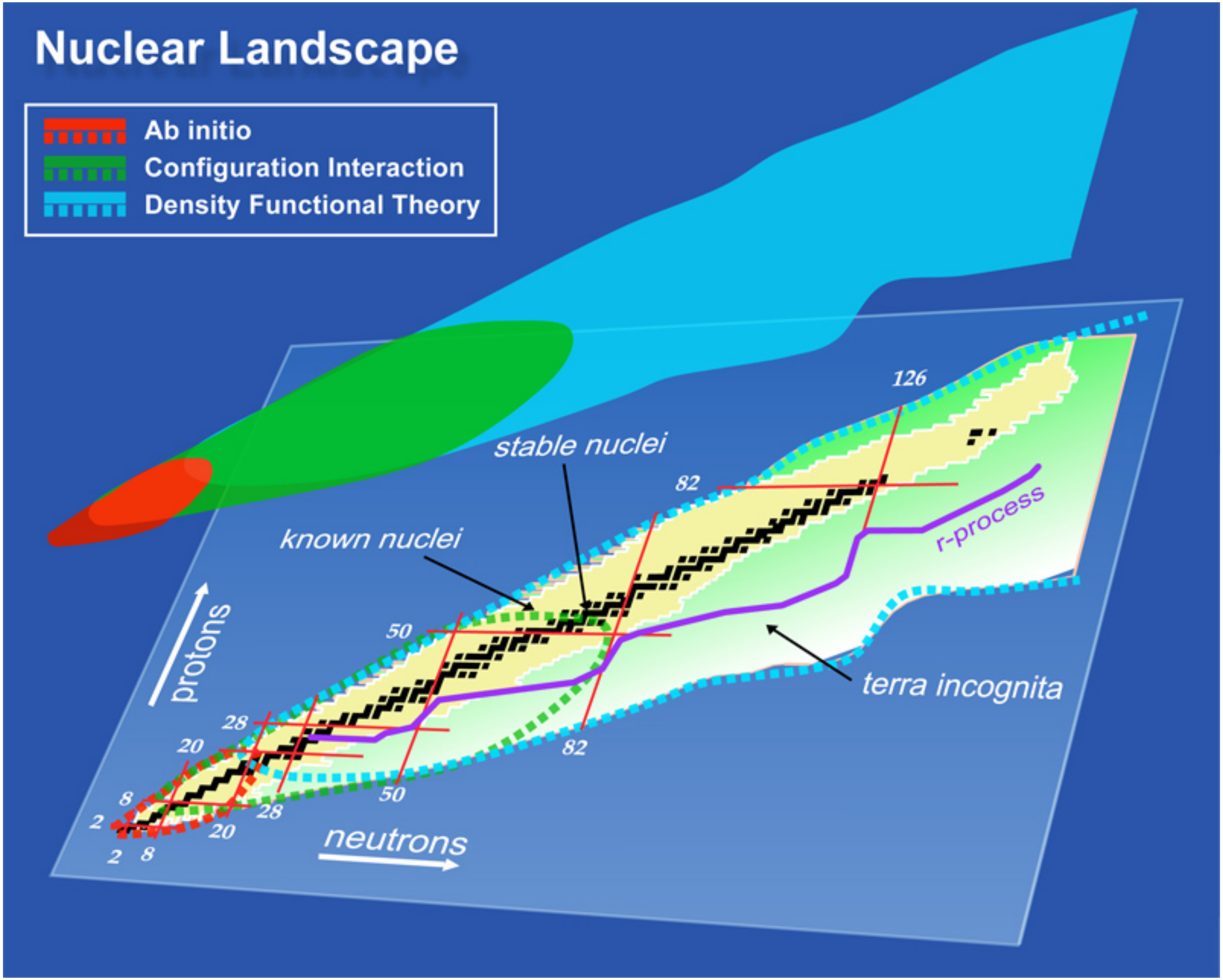


Figure from UNEDF Web Site

Skyrme energy density functional

$$E\left[\rho_q, \tau_q, \overleftrightarrow{J}_q; \kappa_q\right]$$

kinetic

pair density

spin-current

- Kohn-Sham scheme (BdG-KS, HFB)

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

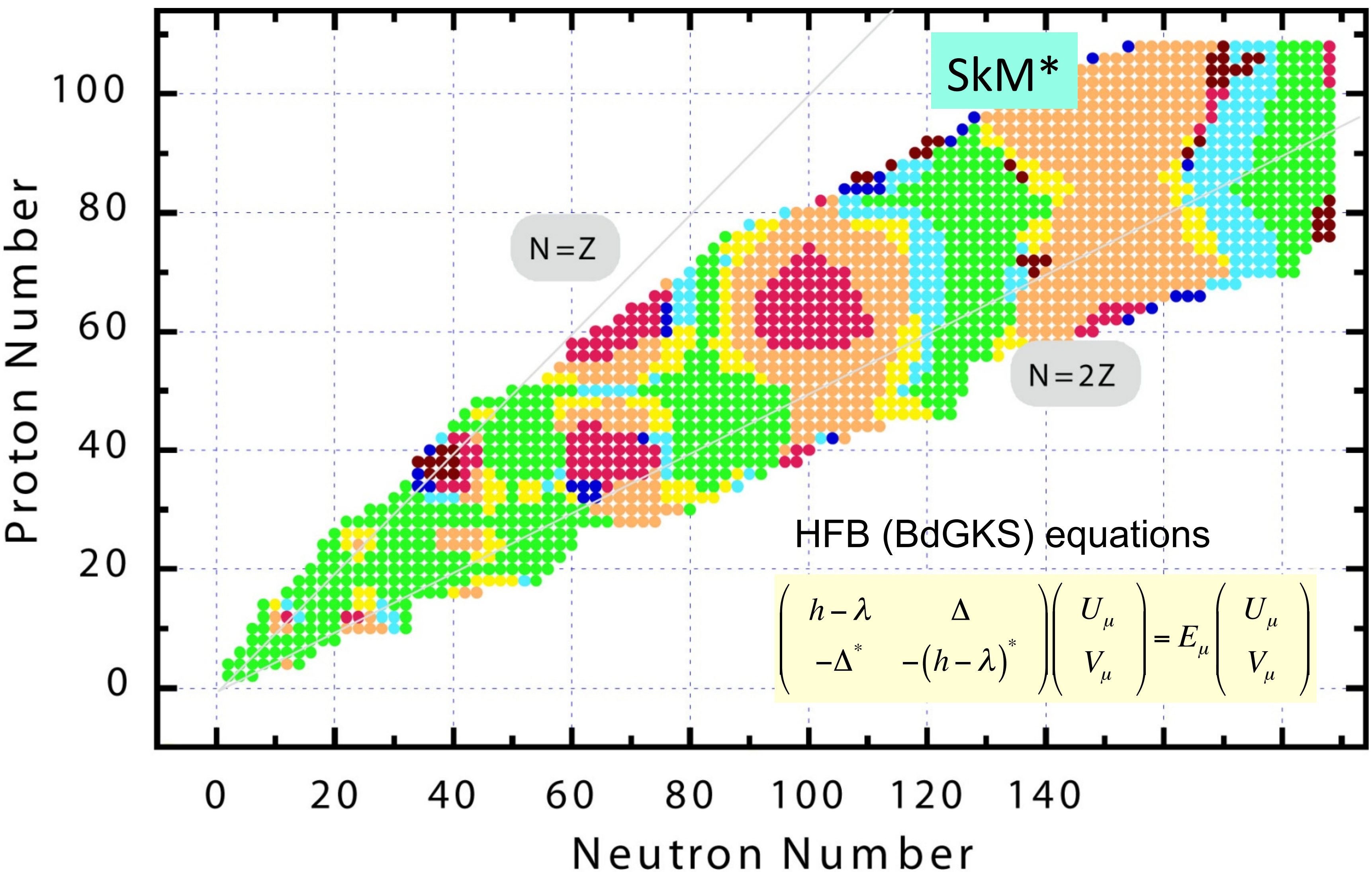
$$\rho = VV^+, \quad \kappa = UV^T$$

$$h[\rho] \equiv \frac{\delta E}{\delta \rho} = -\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{KS}}[\rho](\vec{r}), \quad \Delta[\kappa] \equiv \frac{\delta E}{\delta \kappa^*}$$

- Spontaneous symmetry breaking
  - nuclear deformation, pair condensation

In this talk, I present results with the SkM* functional.

Nuclear deformation predicted by Energy Density Functional Theory (EDFT)



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

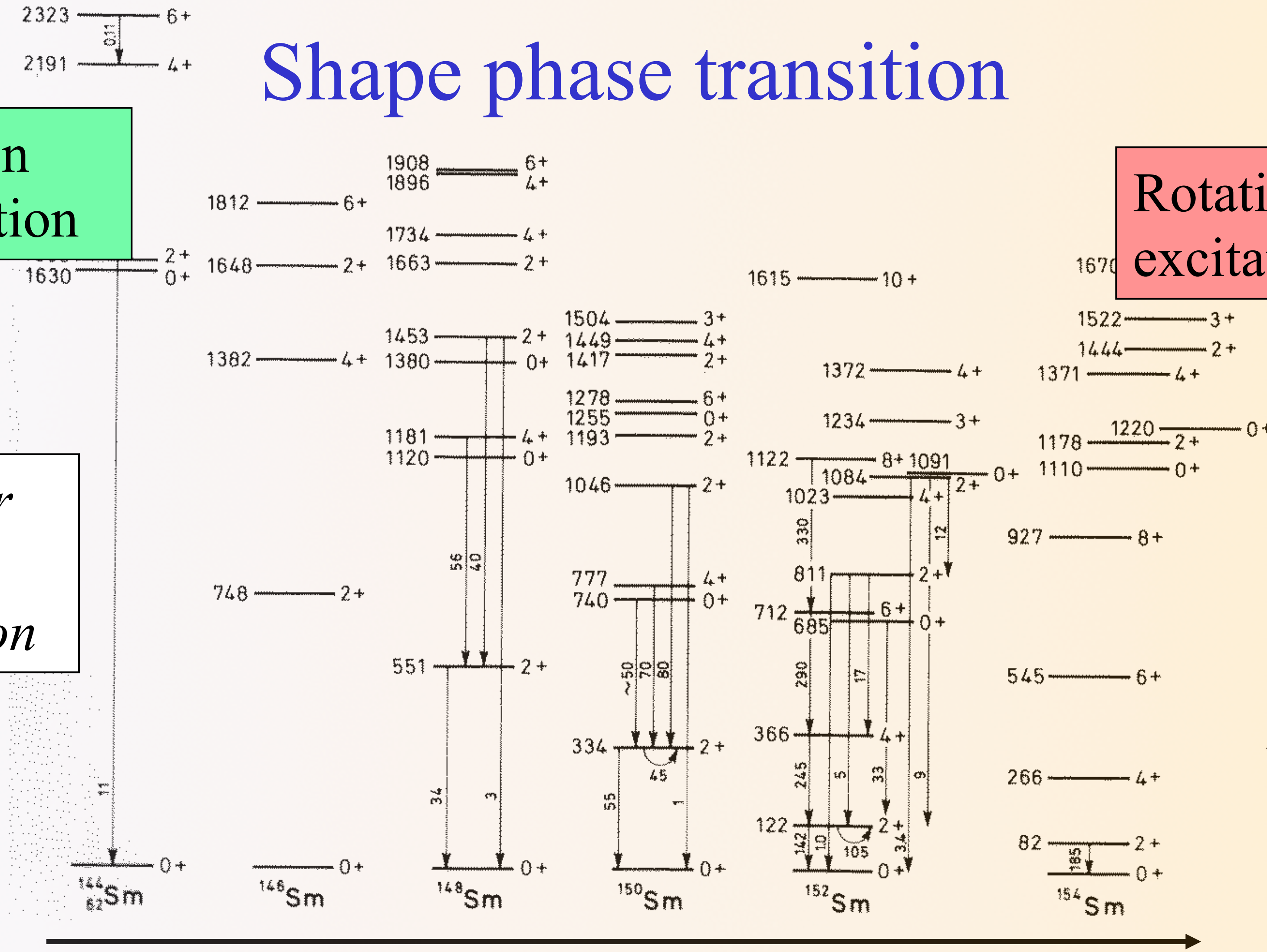
M.V. Stoitsov *et al.*, Phys. Rev. C68(2003) 054312

Shape phase transition

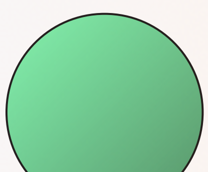
Phonon excitation

Rotational excitation

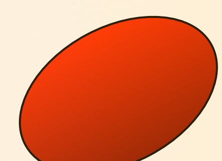
Nuclear surface vibration



Increasing neutrons



spherical



deformed

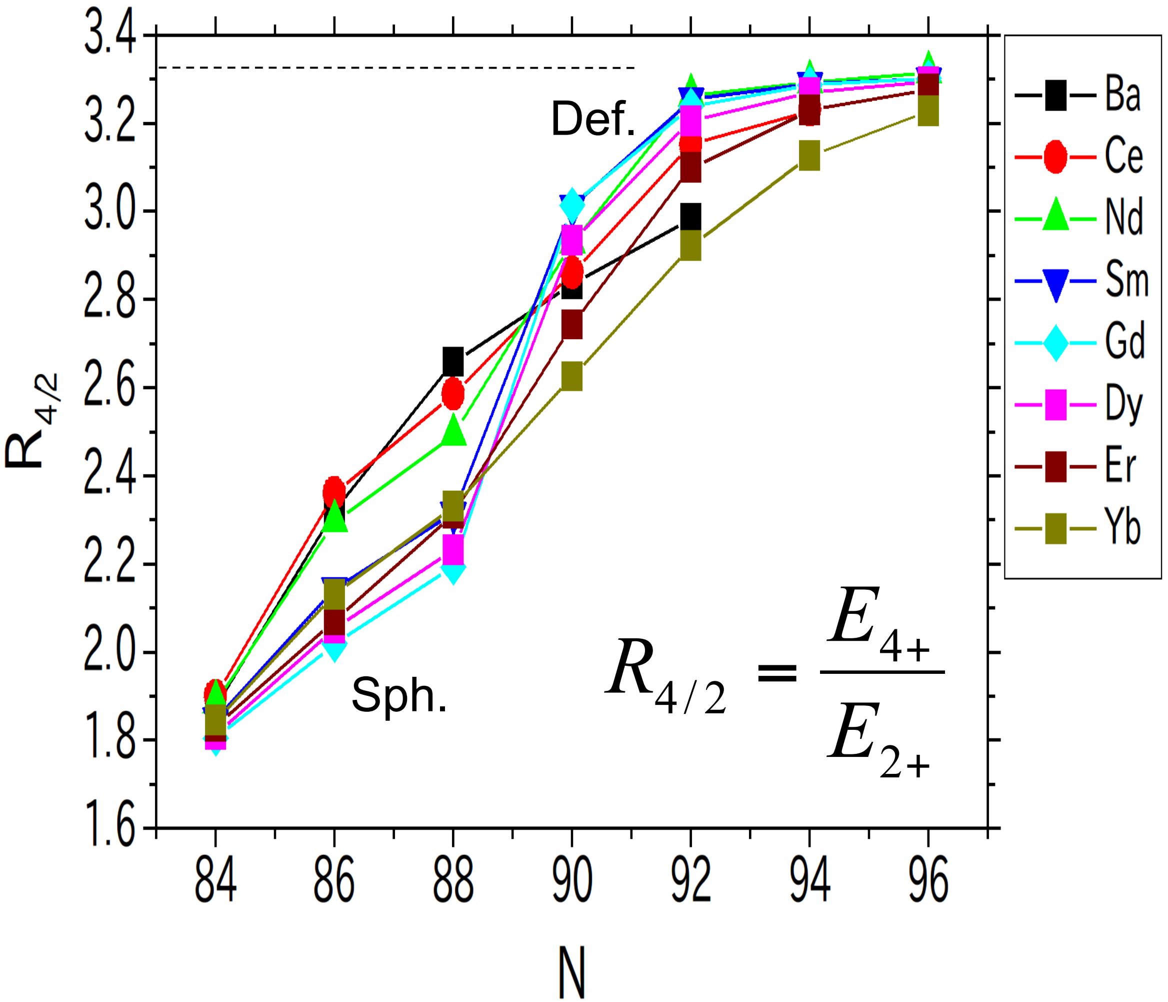
Evolution of nuclear shapes: $R_{4/2}$

$$E_I = \frac{I(I+1)}{2\mathfrak{I}}$$

$$\Downarrow$$

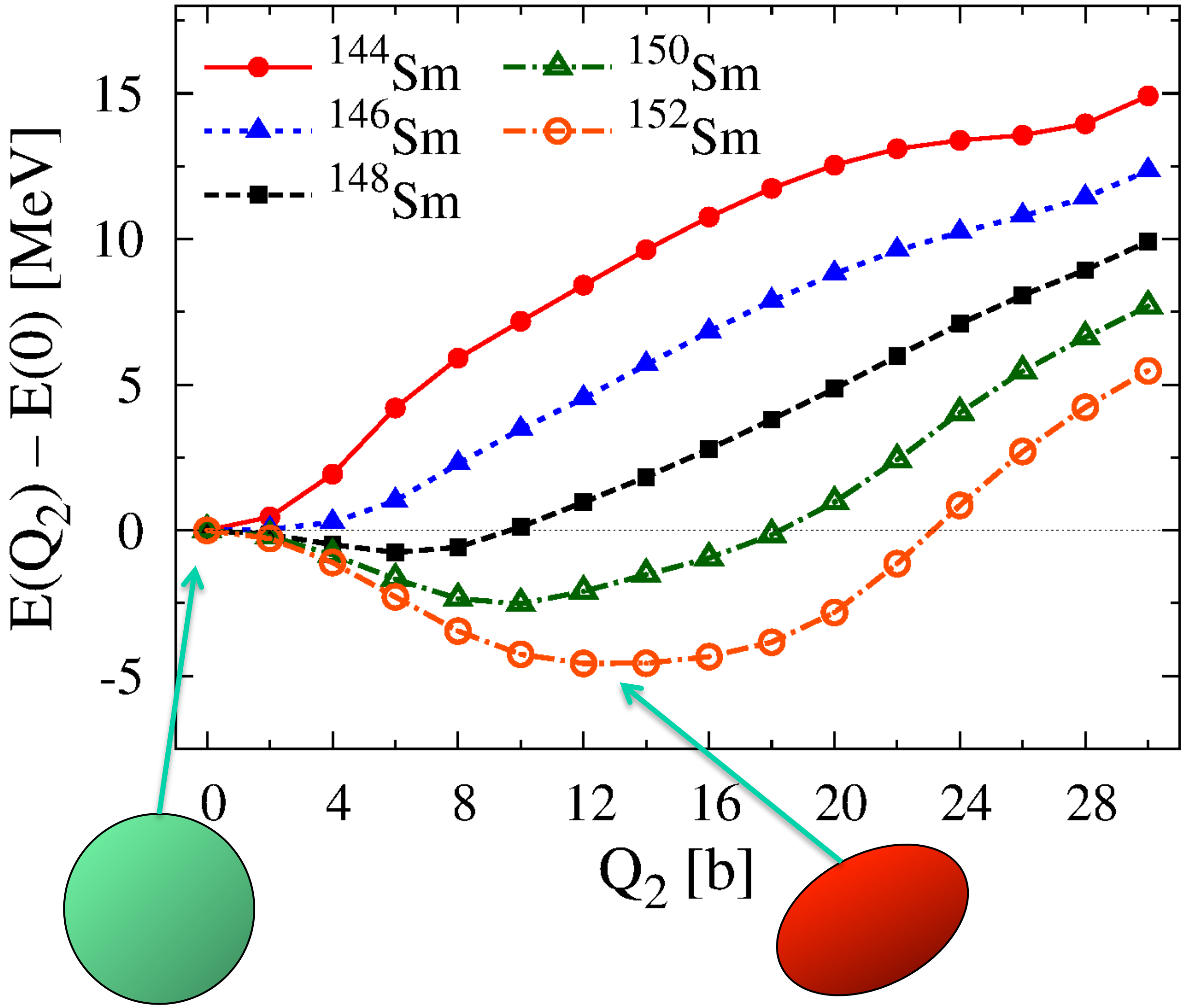
$$R_{4/2} \equiv \frac{E_4}{E_2} = \frac{20}{6} = 3.33\cdots$$

R. Casten



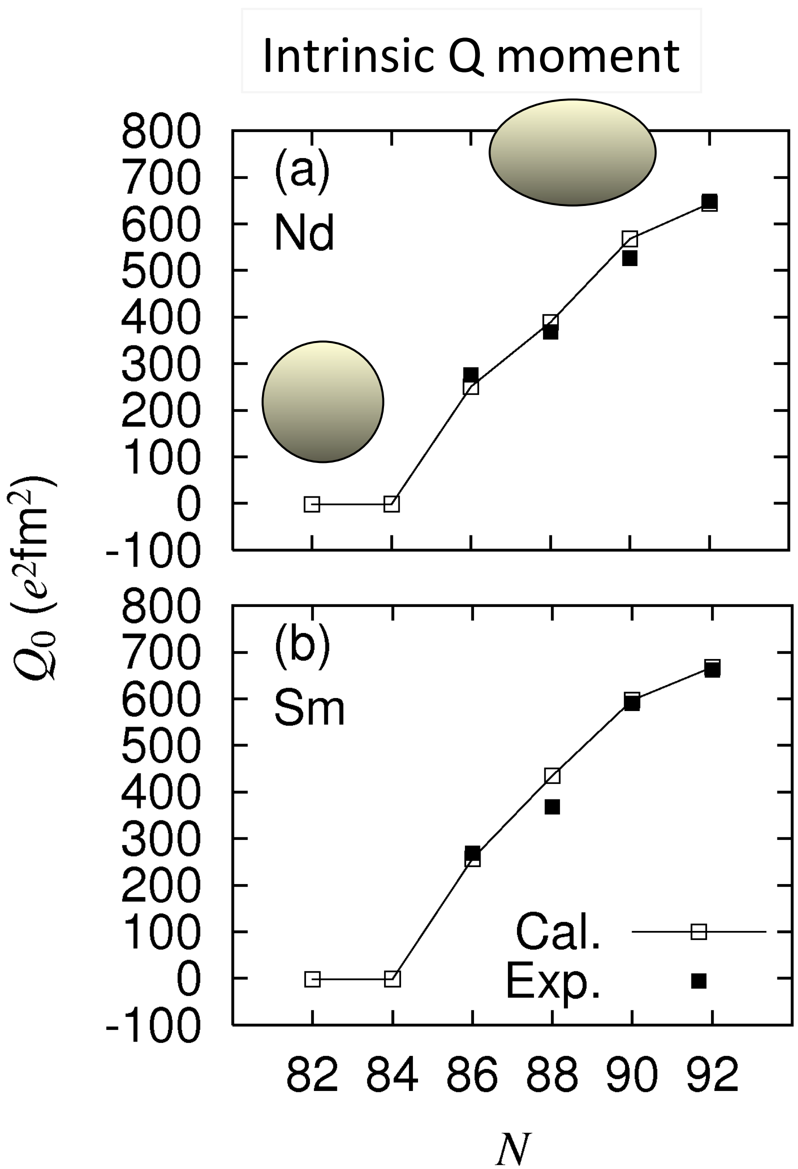
Onset of deformation →

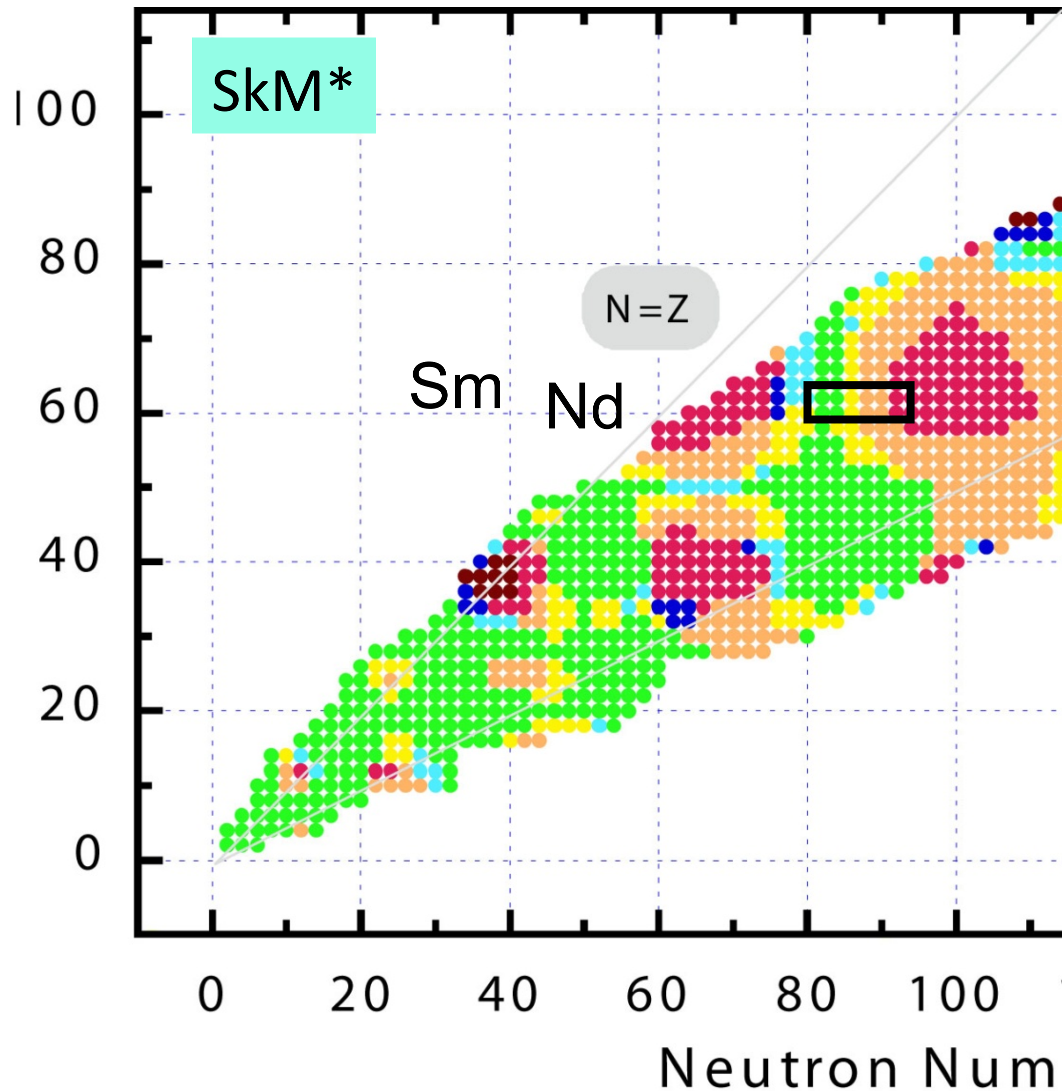
Calculated effective potential



Shape transition produced by EDFT

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





Time-dependent density-functional theory with Skyrme energy density functionals

- Time-odd densities (current density, spin density, etc.)

$$E\left[\rho_q(t),\underbrace{\tau_q(t)}_{\text{kinetic}},\underbrace{\overleftrightarrow{J}_q(t)}_{\text{spin-current}},\underbrace{\vec{j}_q(t)}_{\text{current}},\underbrace{\vec{s}_q(t)}_{\text{spin}},\underbrace{\vec{T}_q(t)}_{\text{spin-kinetic}};\underbrace{\kappa_q(t)}_{\text{pair density}}\right]$$

- Time-dependent BdGKS (HFB) eq.

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

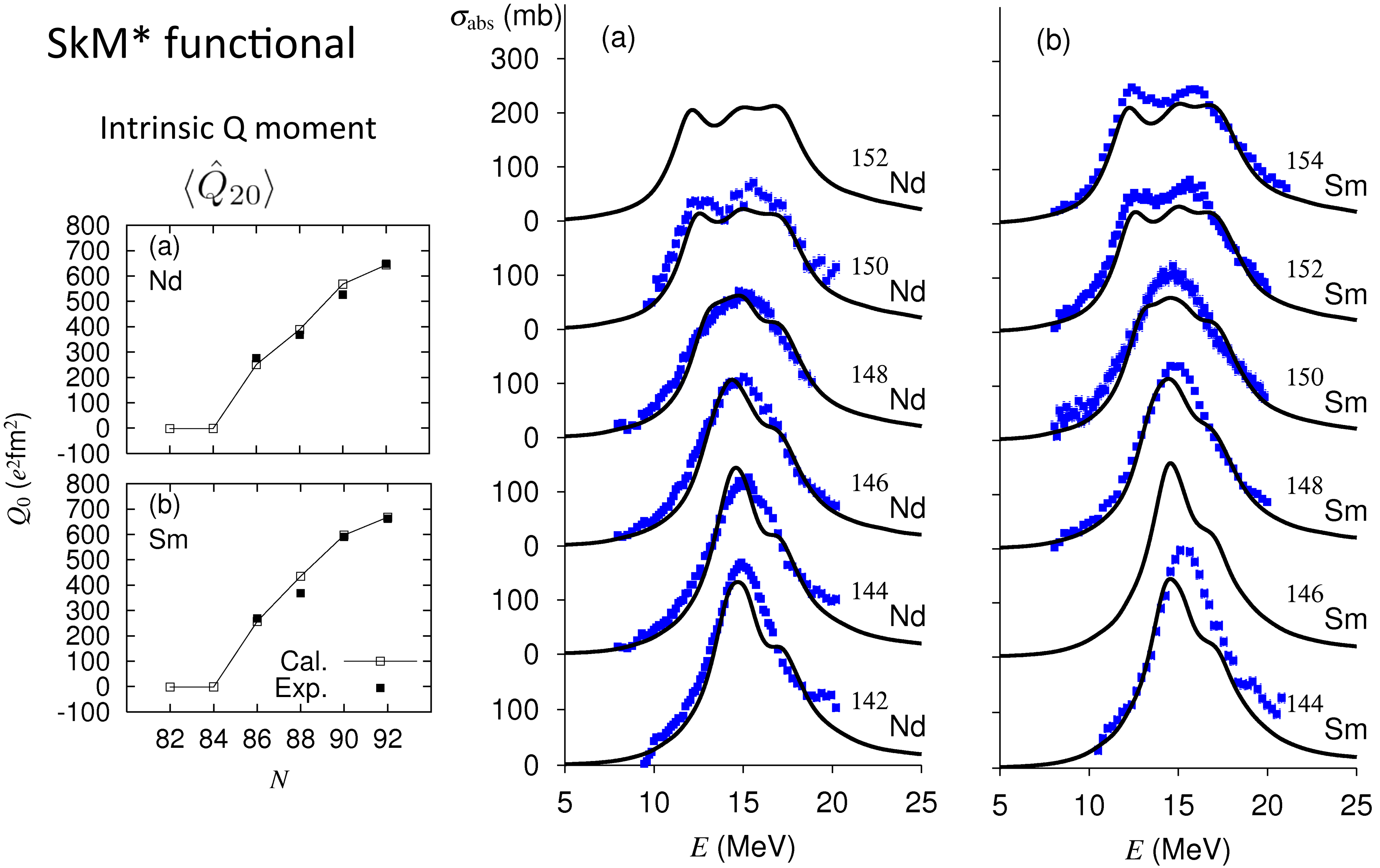
Linear response and photoabsorption cross section

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

SkM* functional

Intrinsic Q moment

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



Giant resonances in Sm isotopes (IS, L=0~3)

SkM* functional

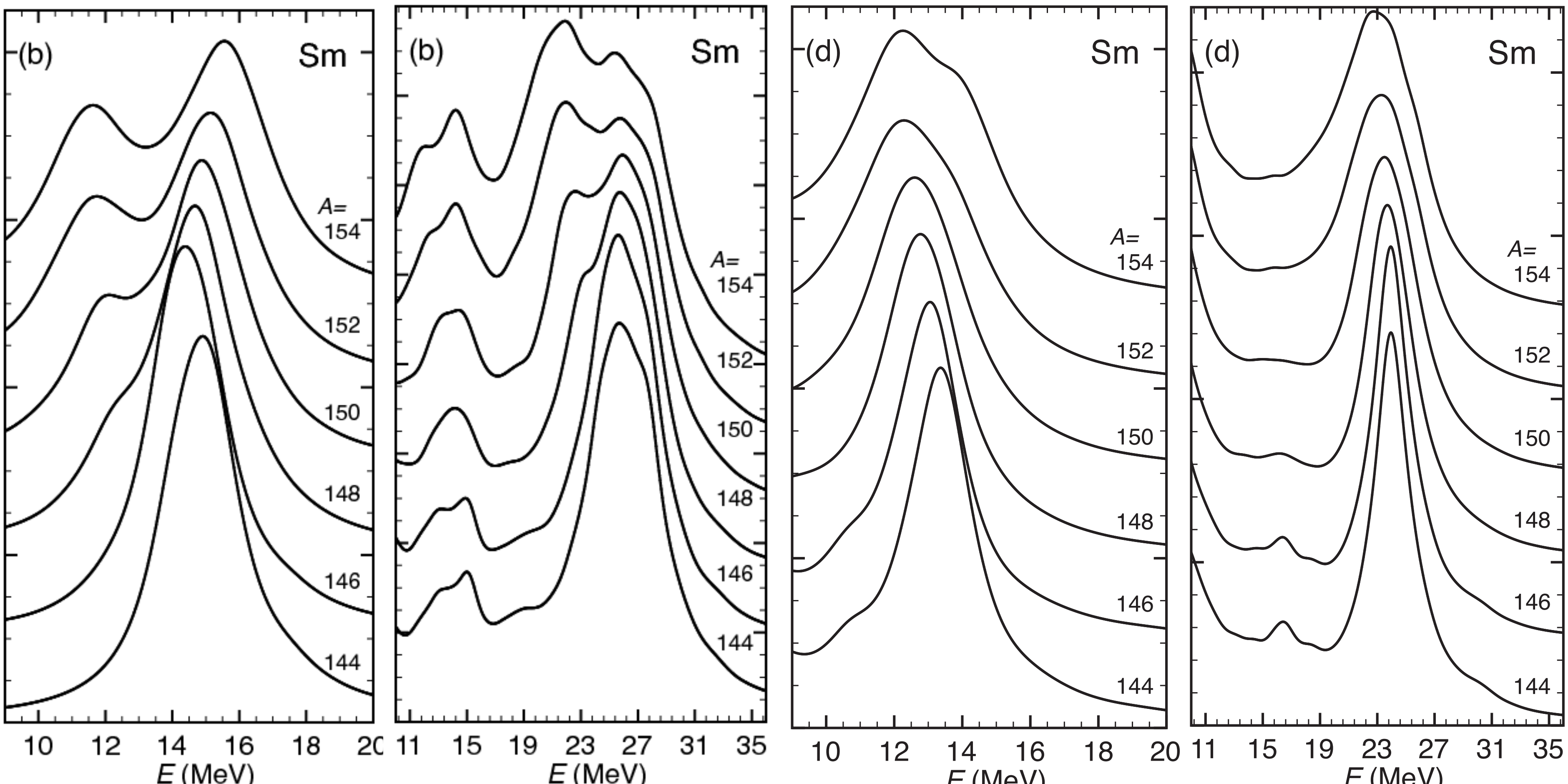
K.Yoshida and TN, PRC 88 034309 (2013)

IS-GMR

IS-GDR

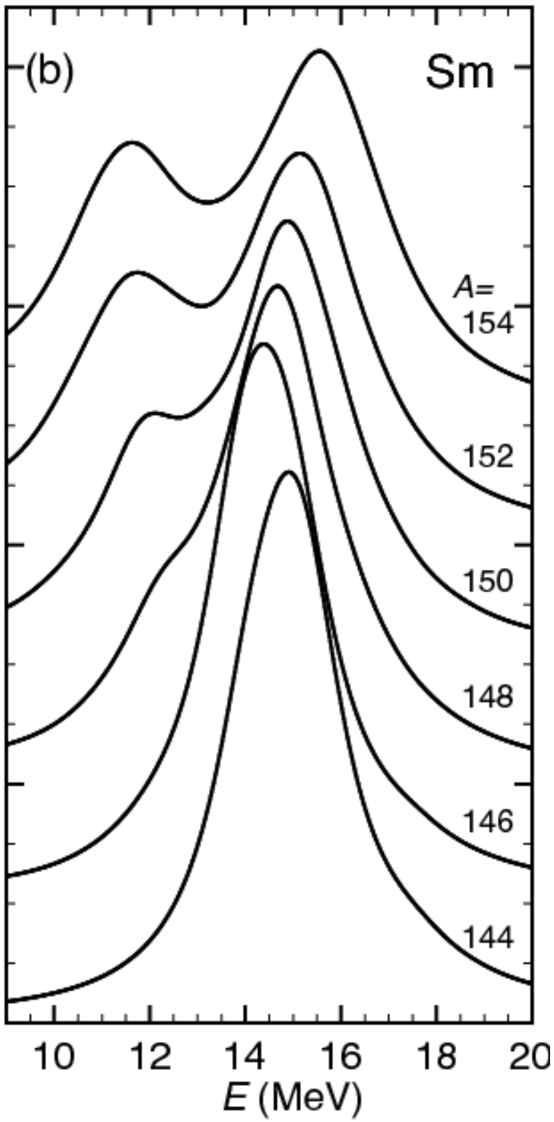
IS-GQR

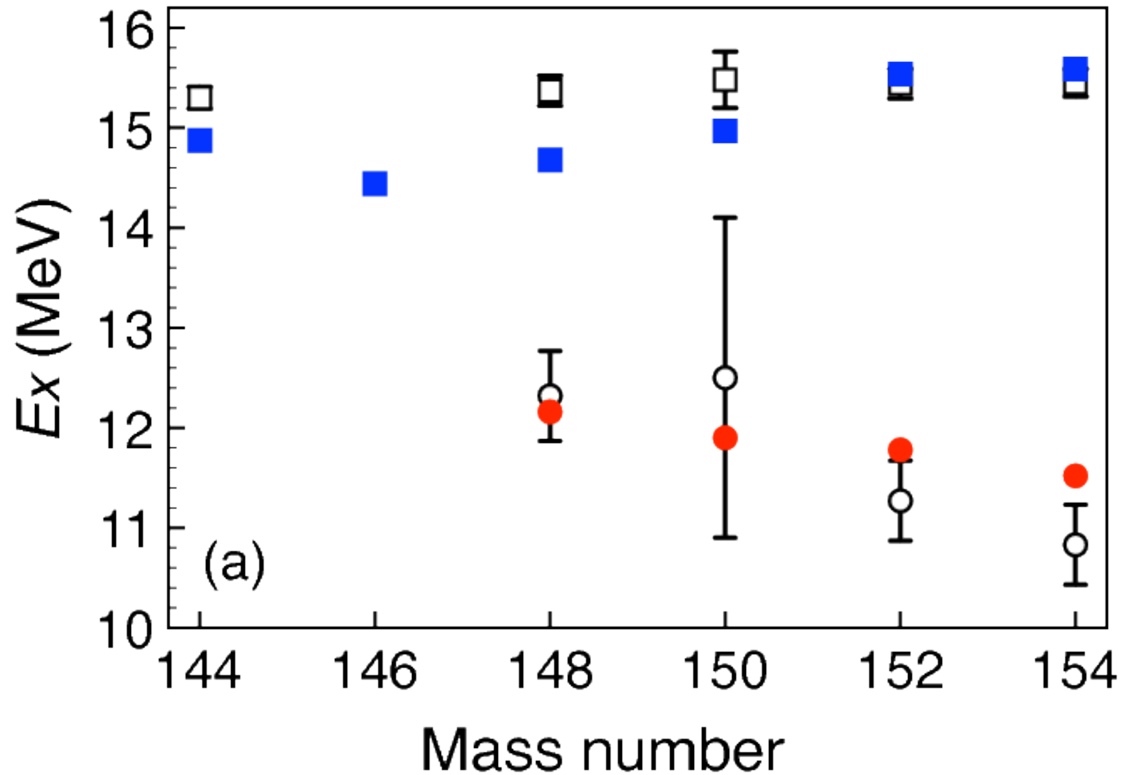
IS-GOR (HEOR)



Isoscalar giant monopole resonances

SkM* functional

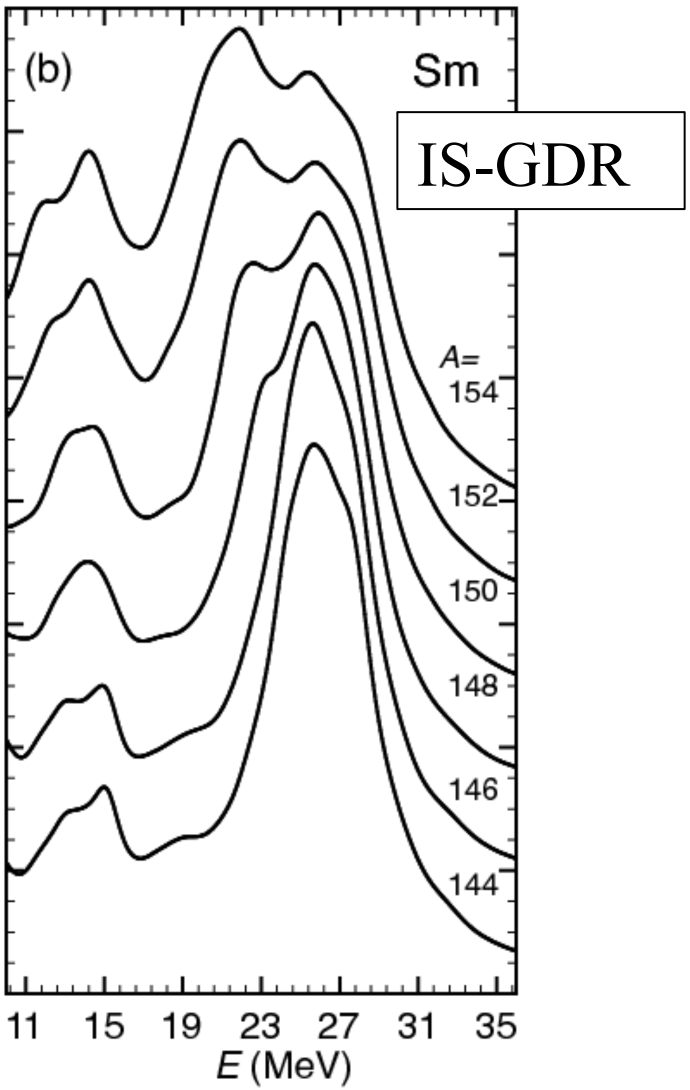


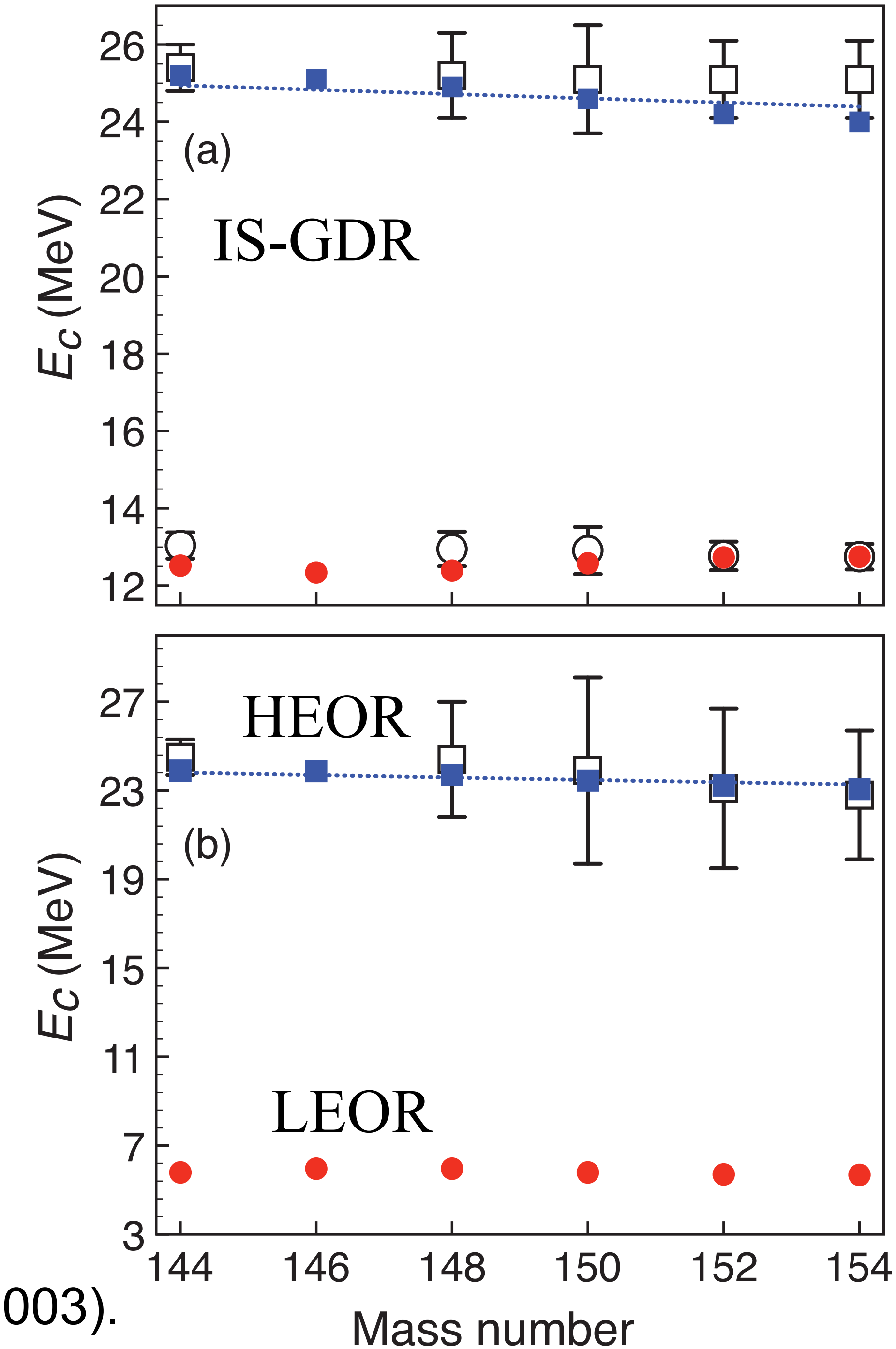


Exp: M. Itoh et al., PRC 68, 064602 (2003).

Peak splitting is properly described.
Coupling to IS-GQR due to deformation

IS-GDR and IS-GOR





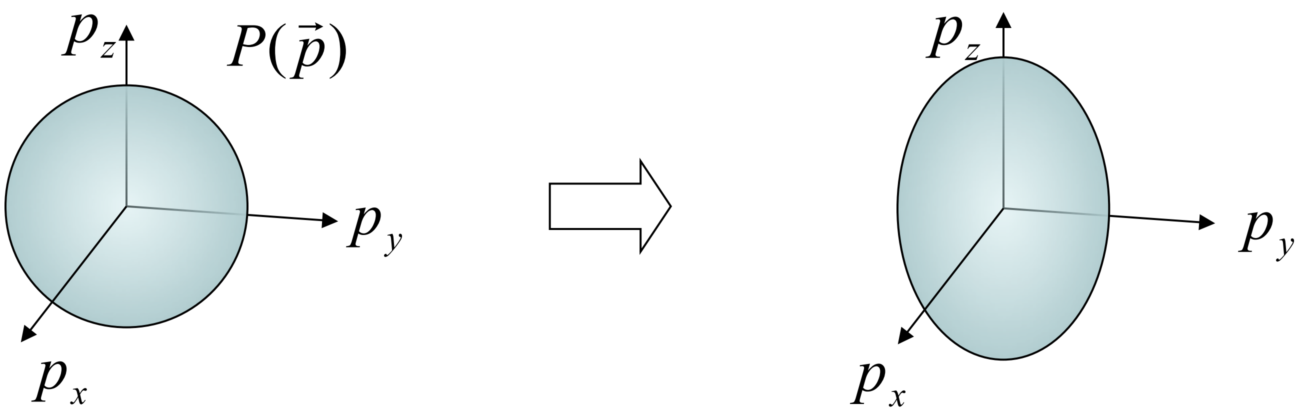
Exp: M. Itoh et al., PRC 68, 064602 (2003).

Fermi Liquid Properties

Sum-rule analysis for nuclear IS Giant Quadrupole Resonance

$$m_3 \propto \frac{1}{2}\frac{\partial^2}{\partial\eta^2}E(\eta)\bigg|_{\eta=0} \propto \langle T \rangle$$

The restoring force originates from the kinetic energy.



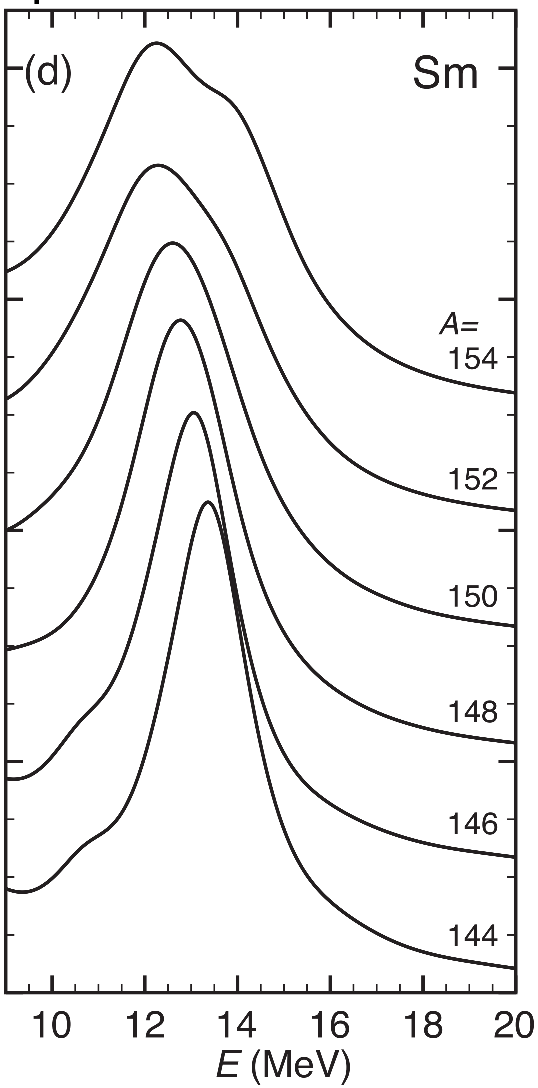
The spatial deformation leads to the deformation of the Fermi sphere.

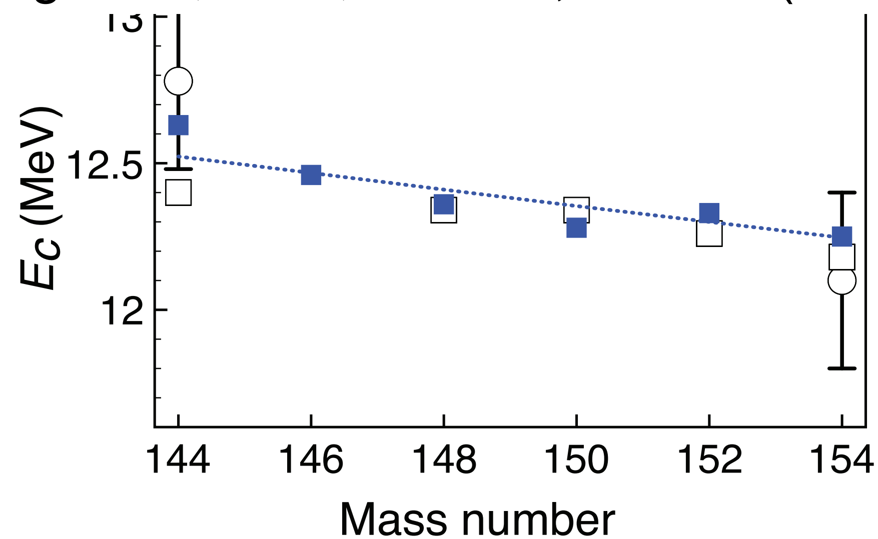
This is different from the classical (incompressible) liquid model.

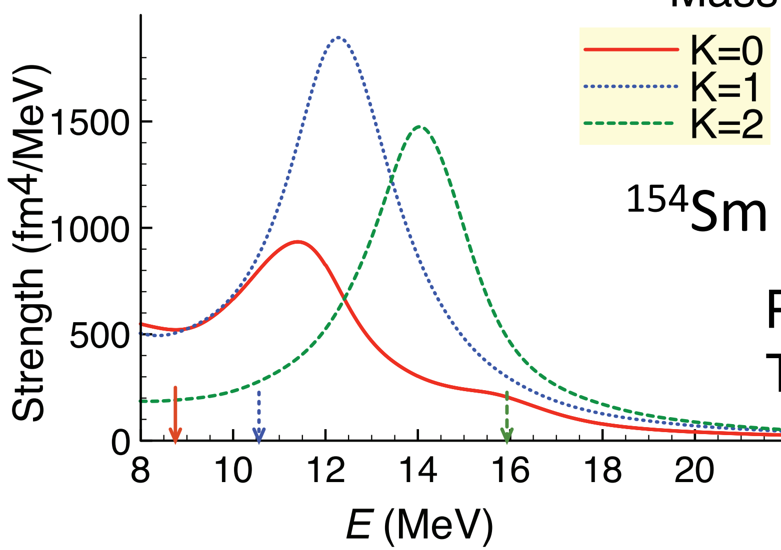
Isoscalar giant quadrupole resonances

Exp: Youngblood, et al., PRC **69,** 034315 (2004)

No prominent deformation splitting







^{154}Sm

	$E_{K=2} - E_{K=0}$
P+Q	7 MeV
TDDFT	2.8 MeV

Self-consistency between potential and density

Nuclear matter properties

$$\omega_{ISGMR} = \Omega\sqrt{5K \big/ 3m\langle r^2\rangle}$$

$$\omega_{ISGDR} = \Omega\sqrt{\frac{7}{3}\left[\frac{5K}{3m\langle r^2\rangle} + \frac{8}{5}\left(\frac{m}{m^*}\right)\right]}$$

$$\Omega = 41A^{-1/3}\ \mathrm{MeV}$$

$$\omega_{ISGQR} = \Omega\sqrt{2m \big/ 3m^*}$$

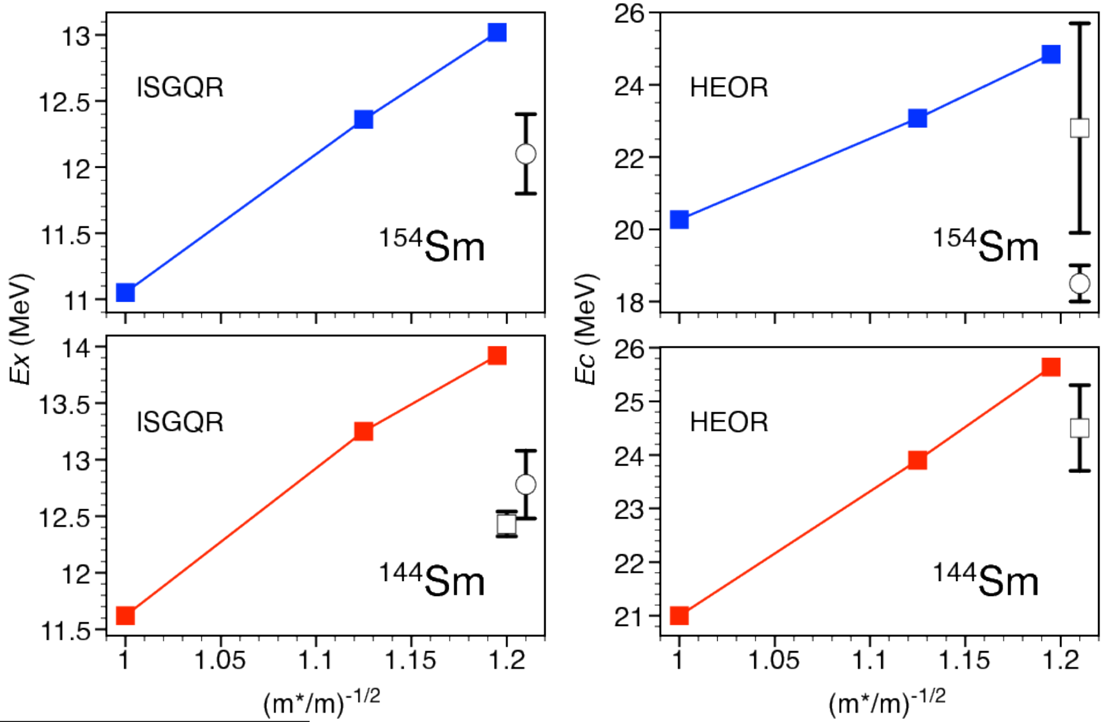
$$\omega_{HEQR} = \Omega\sqrt{28m \big/ 5m^*}$$

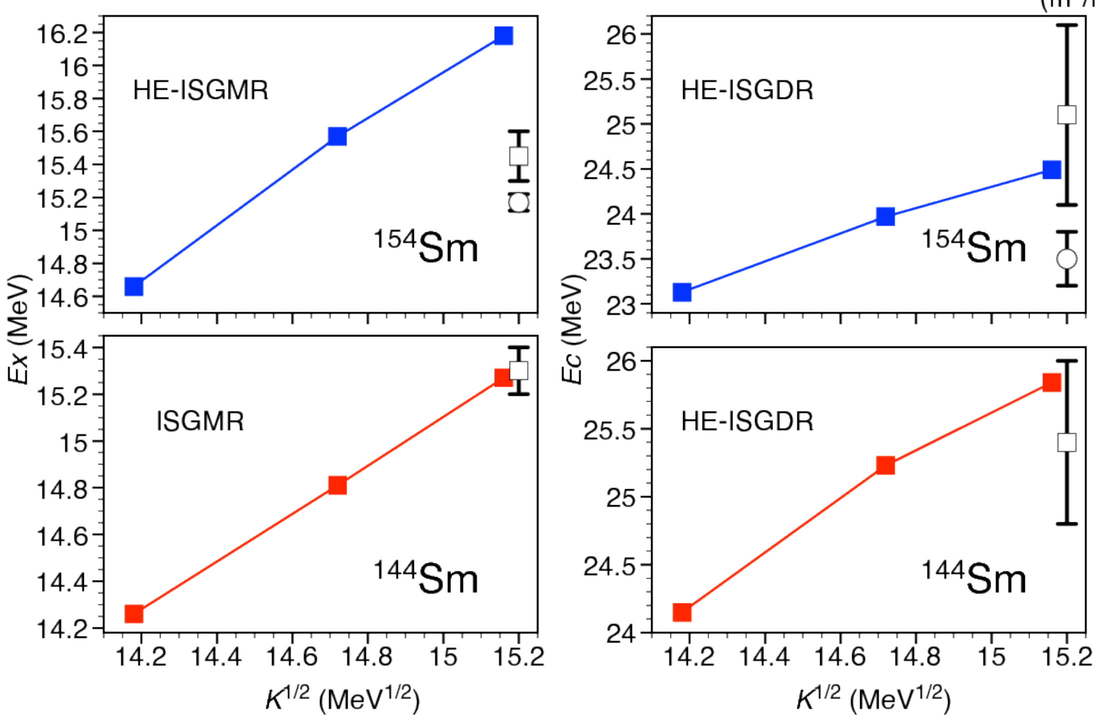
Effective mass
and
Incompressibility

SkM*, SLy4, SkP

Effective mass

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



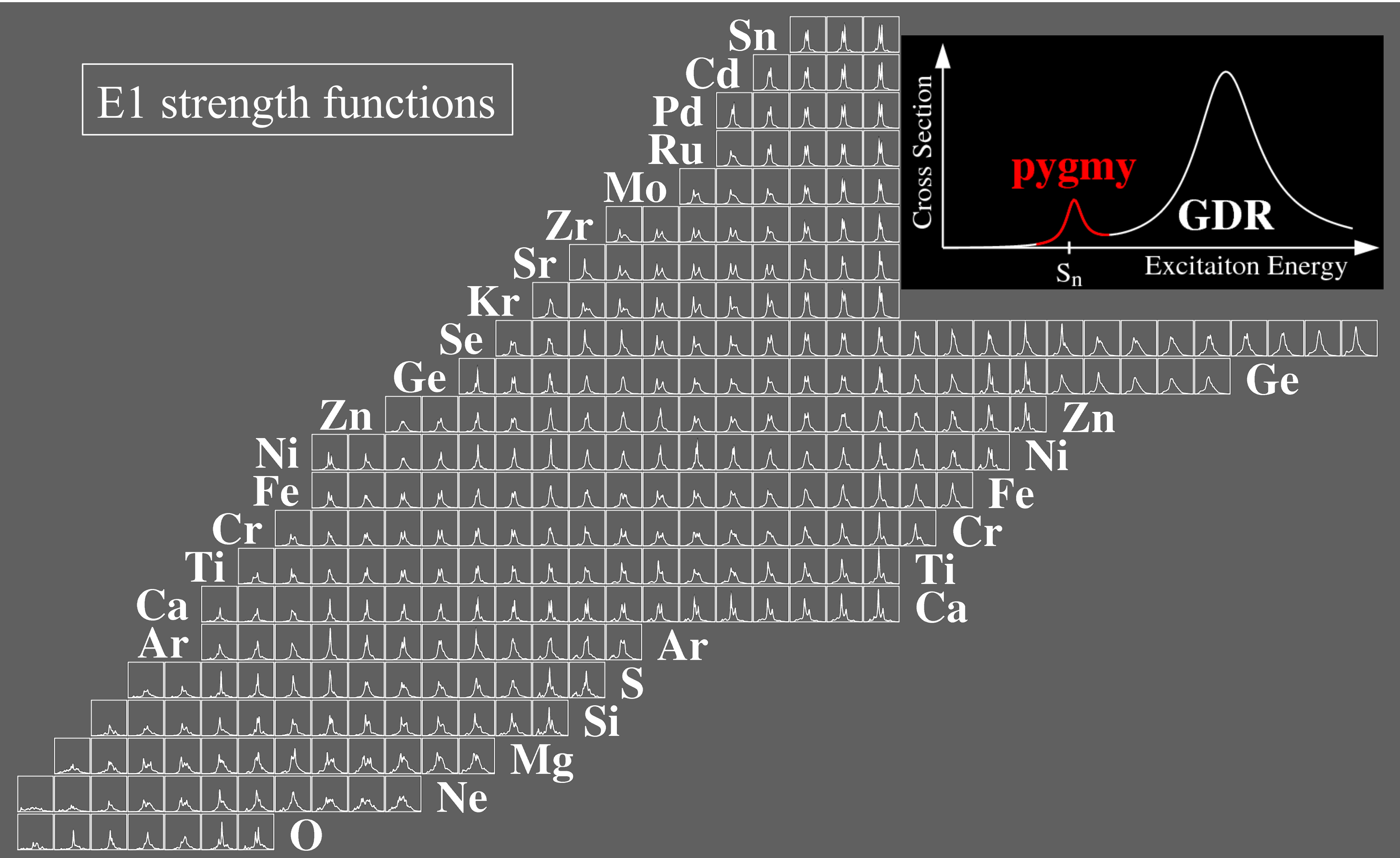


Incompressibility

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

Photoabsorption cross sections

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

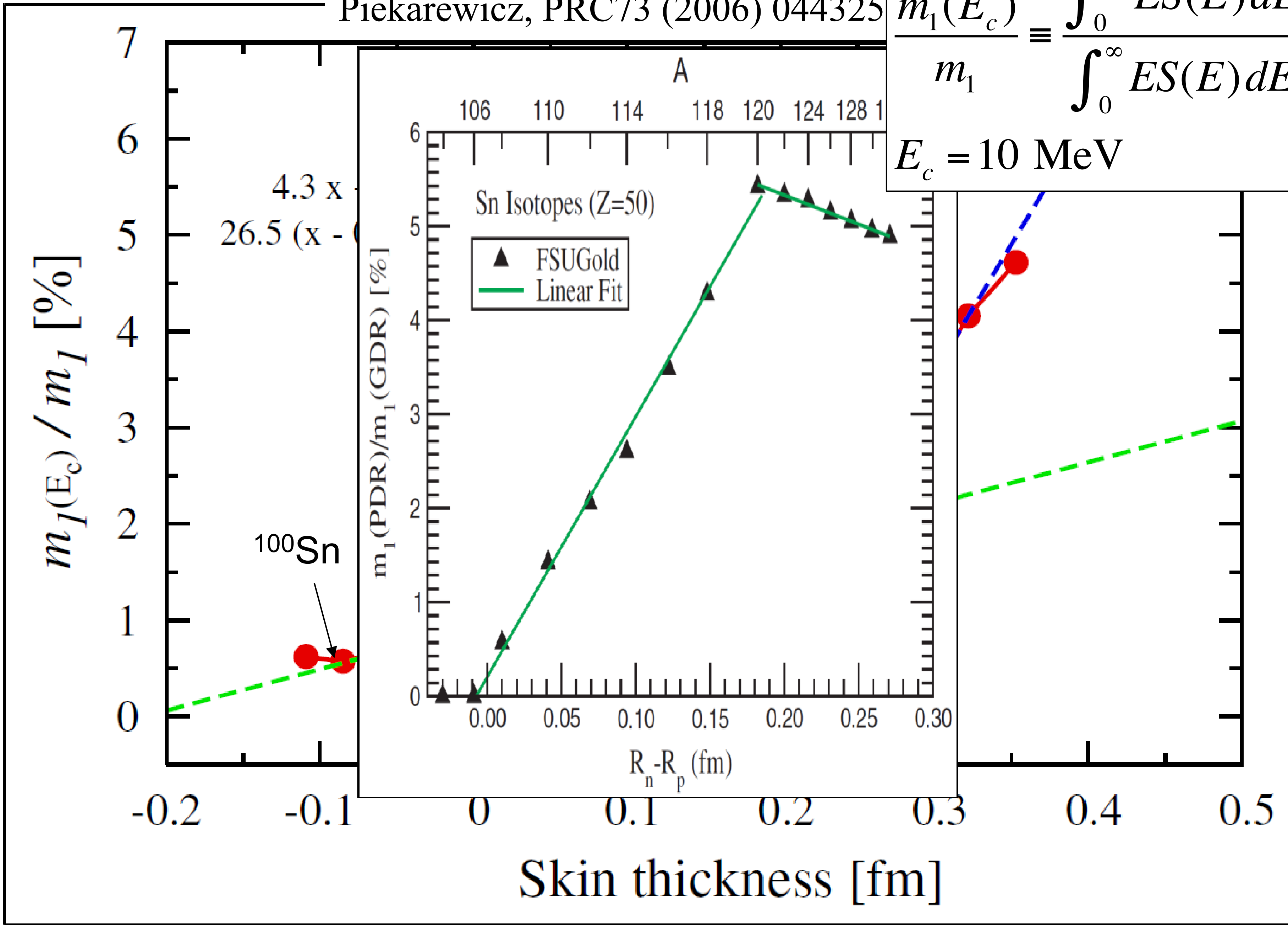


Pygmy dipole states

- Robust features
  - Strong shell effects for *E1* strengths *S(E1)*
  - "Magic numbers"
  - Correlation between *S(E1)* and the skin thickness [*L* parameter] in select nuclei
- Model dependent features
  - Absolute values of *S(E1)*
  - Collective nature
  - Correlation between *S(E1)* and skin thickness in general

Ebata, Nakatsukasa, Inakura, arXiv:1403.7336

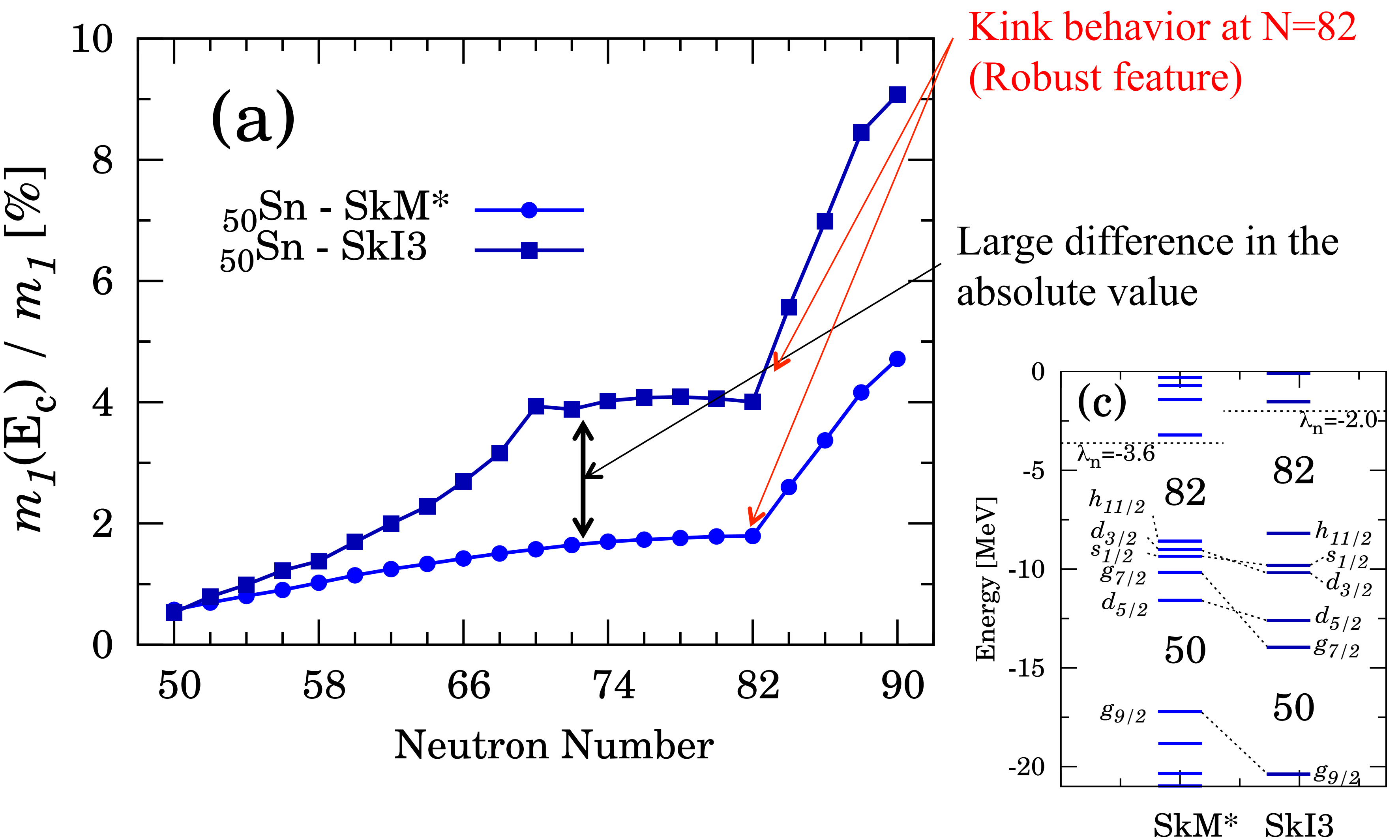
Piekarewicz, PRC73 (2006) 044325



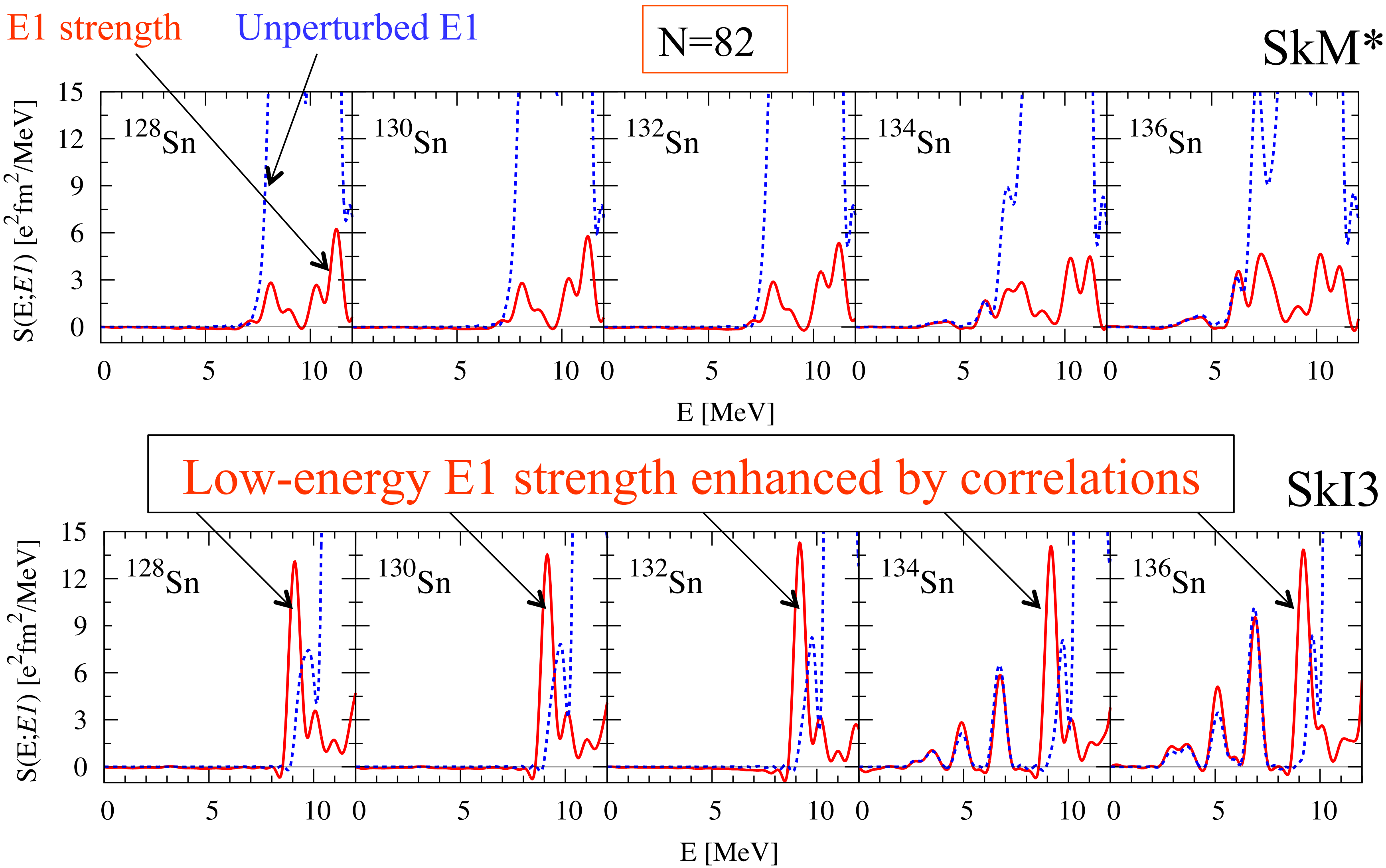
$$\frac{m_1(E_c)}{m_1} \equiv \frac{\int_0^{E_c} ES(E)\,dE}{\int_0^{\infty} ES(E)\,dE}$$

$$E_c = 10\ \text{MeV}$$

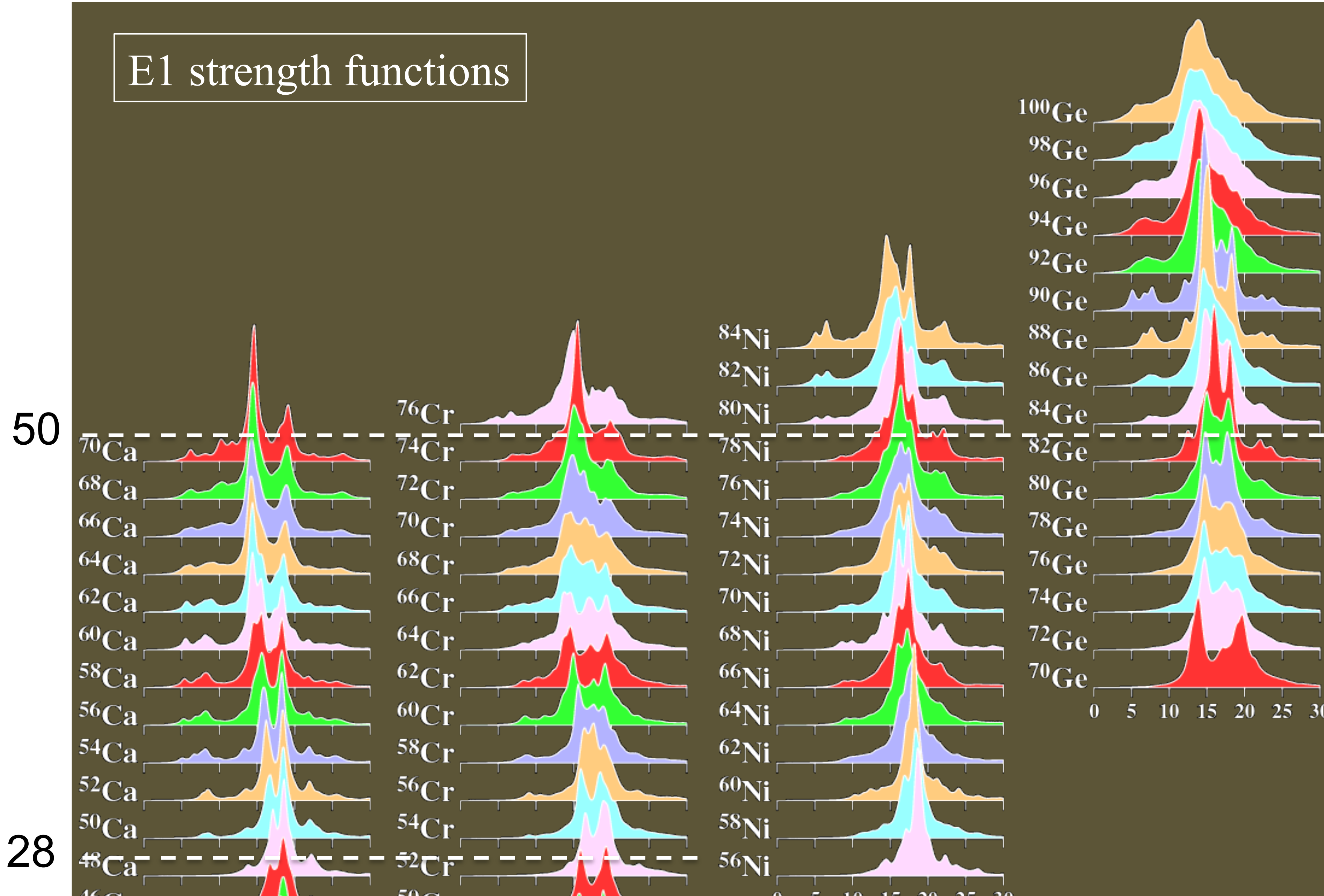
Model dependence & independence



E1 hindrance or enhancement?



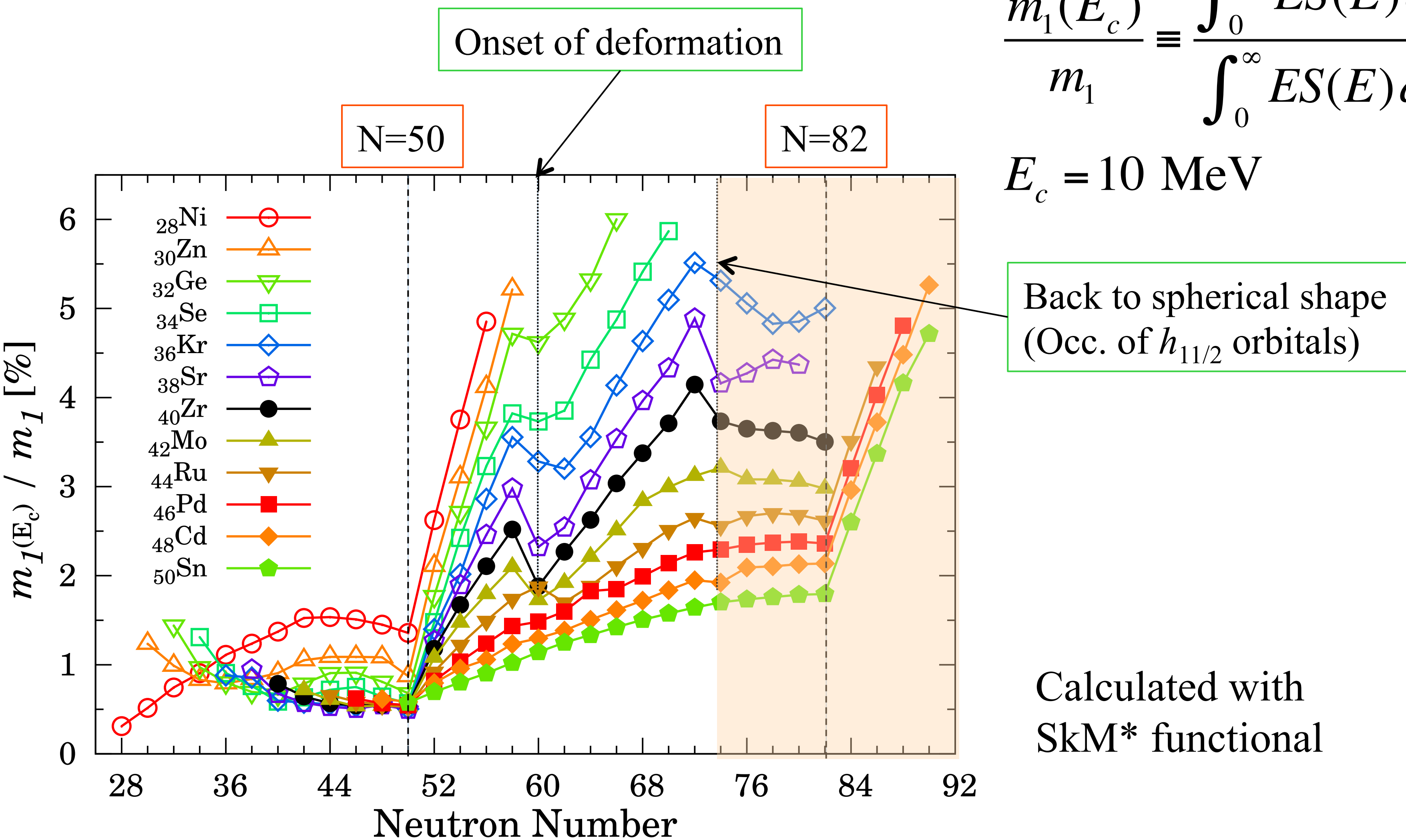
"Magic" numbers



Shell effect

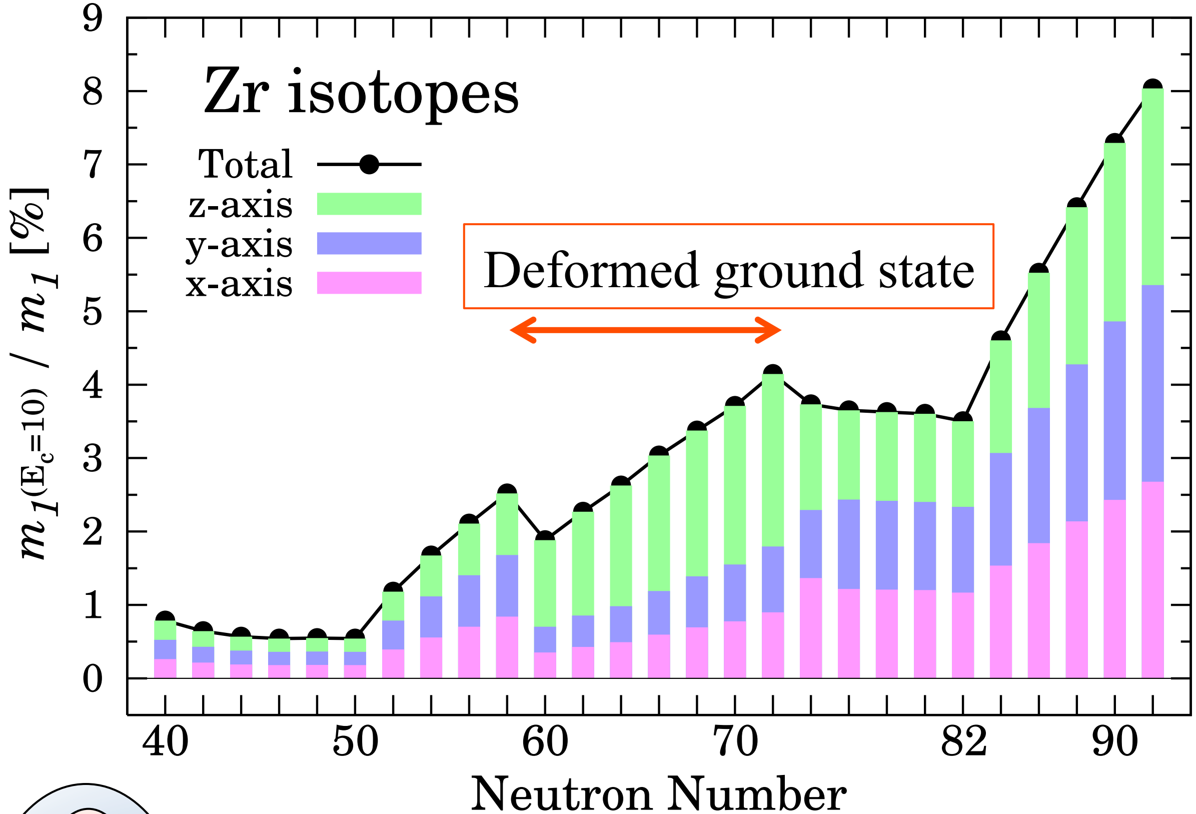
$$\frac{m_1(E_c)}{m_1} \equiv \frac{\int_0^{E_c} ES(E)dE}{\int_0^{\infty} ES(E)dE}$$

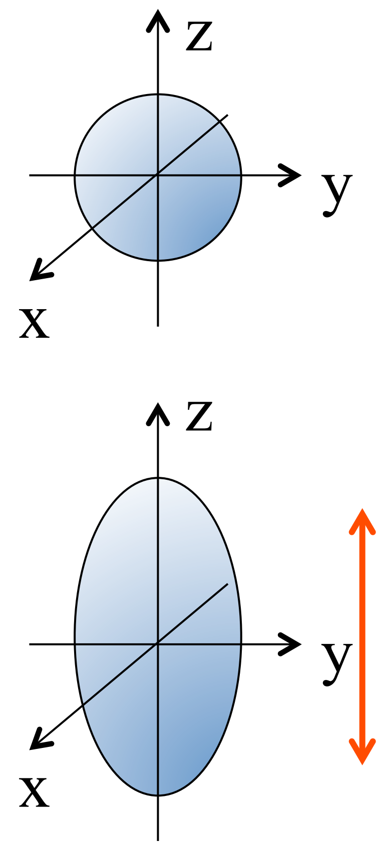
$E_c = 10$ MeV

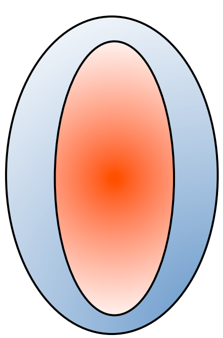


Calculated with SkM* functional

Deformation effect



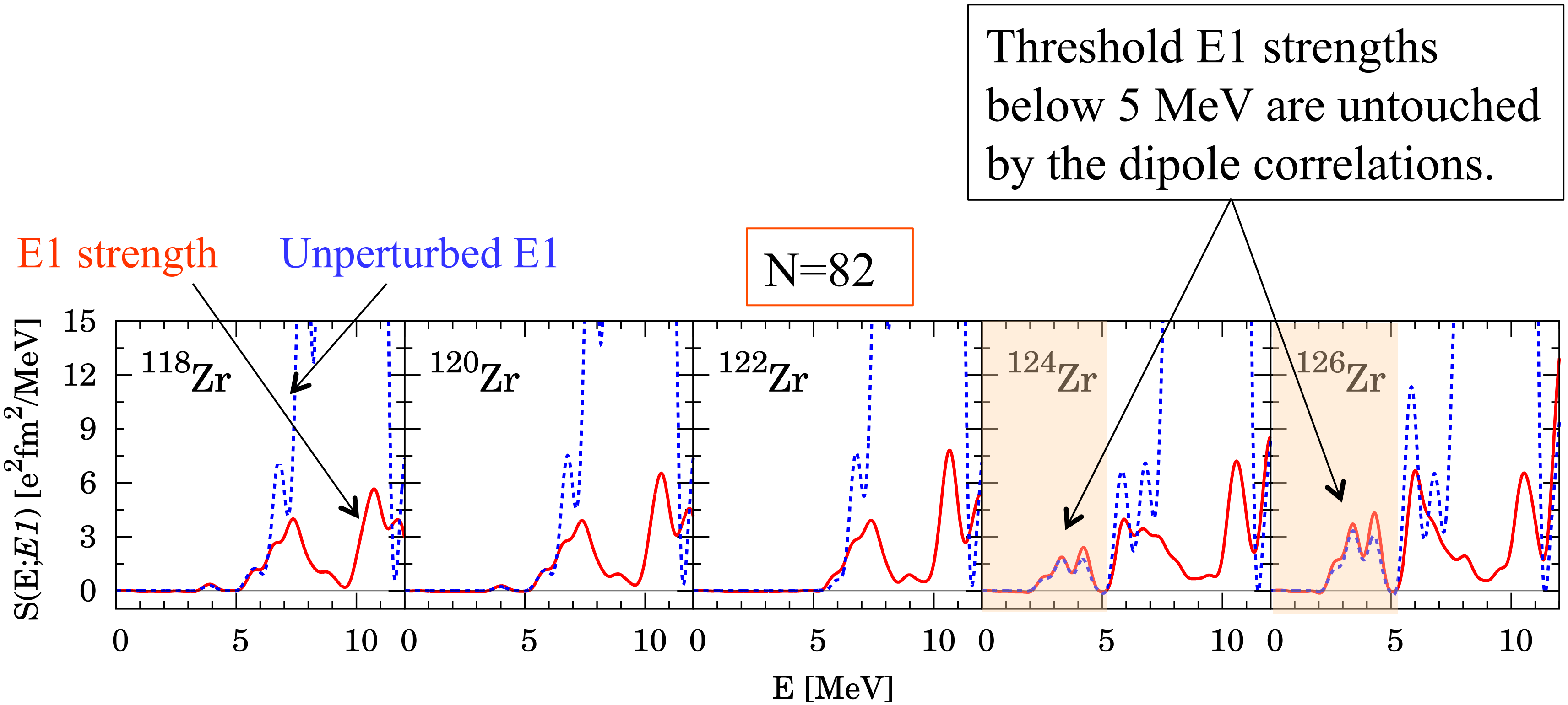




The skin thickness is larger for (x,y) directions than z direction.
Inconsistent with the skin-mode picture?

Enhancement of the low-energy E1 strength along z axis

E1 Hindrance and decoupling



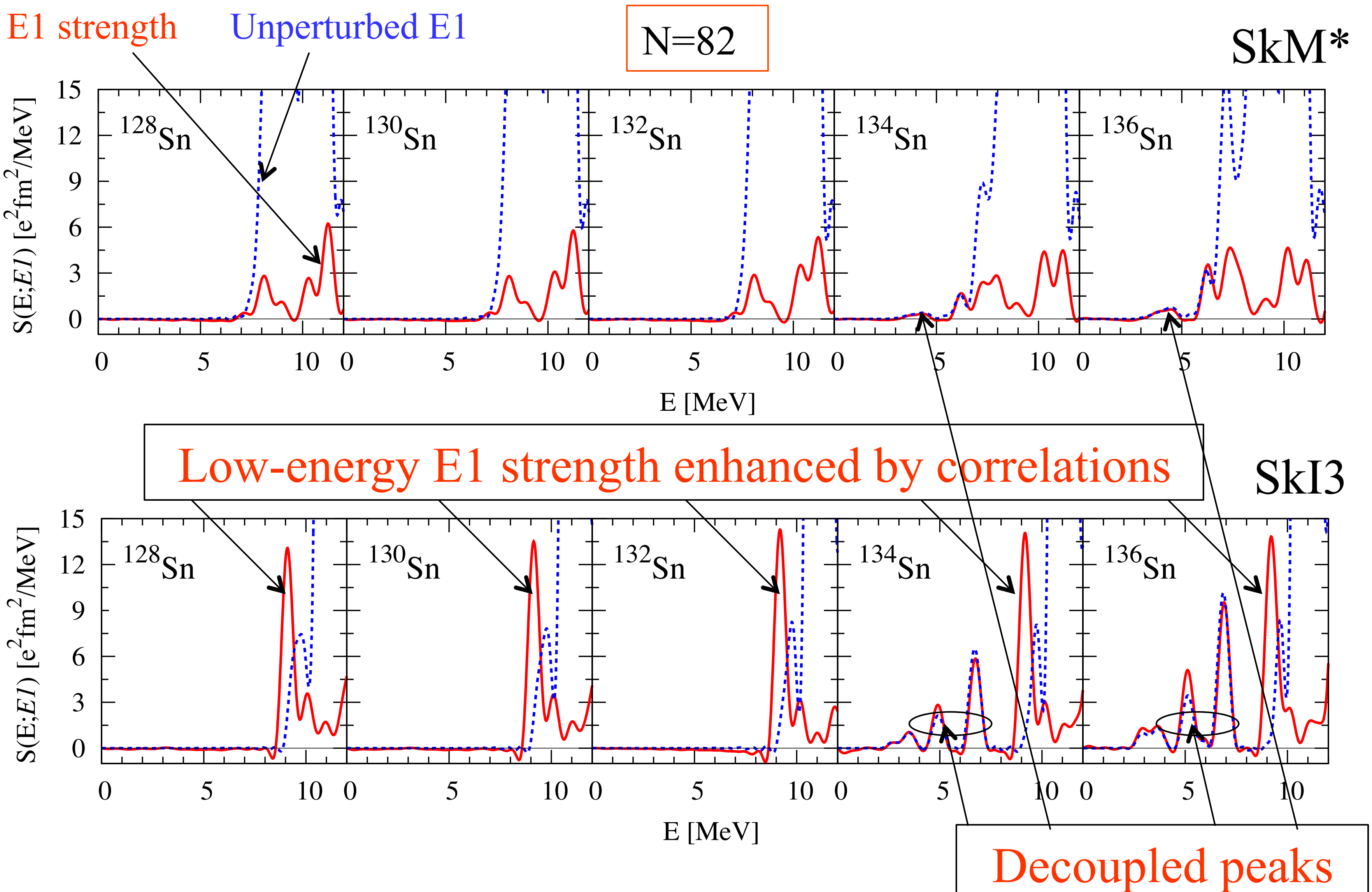
$\lambda_n \approx 4$ MeV

- Hindrance of low-energy E1
- "Destructive coherence"
- Strength goes to GDR

$\lambda_n \approx 2$ MeV

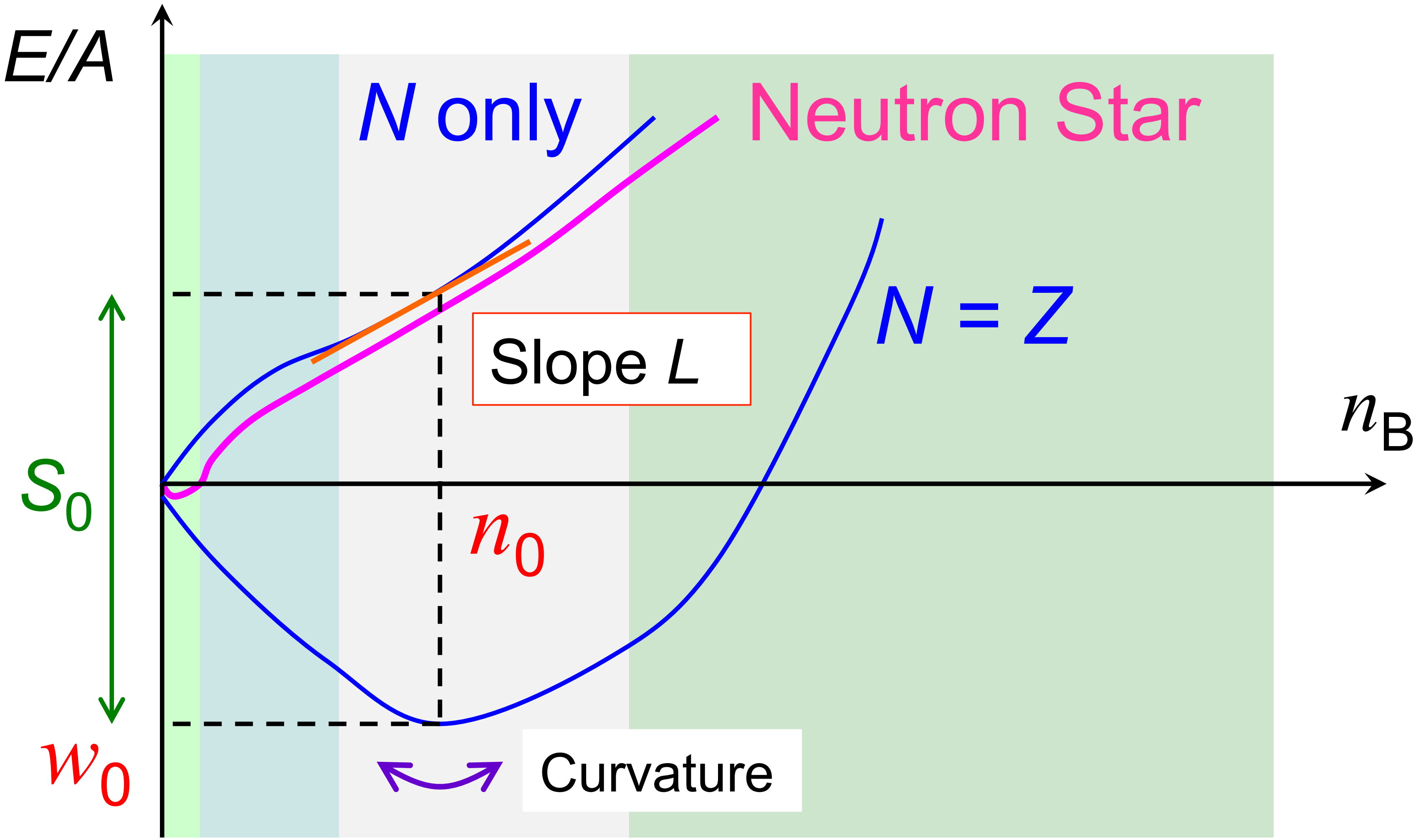
- Decoupling of low-lying dipole modes
- "Single-particle" excitations

Decoupling of low-E *E1*



Slope parameter of symmetry energy

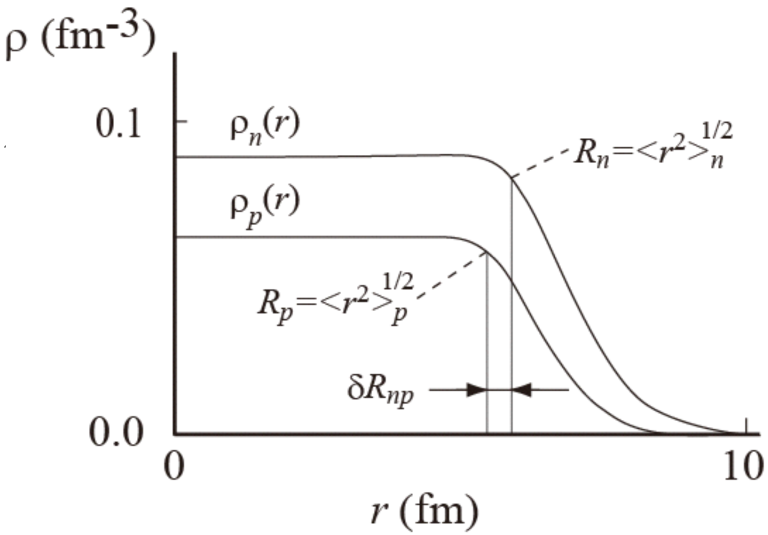
- Symmetry energy

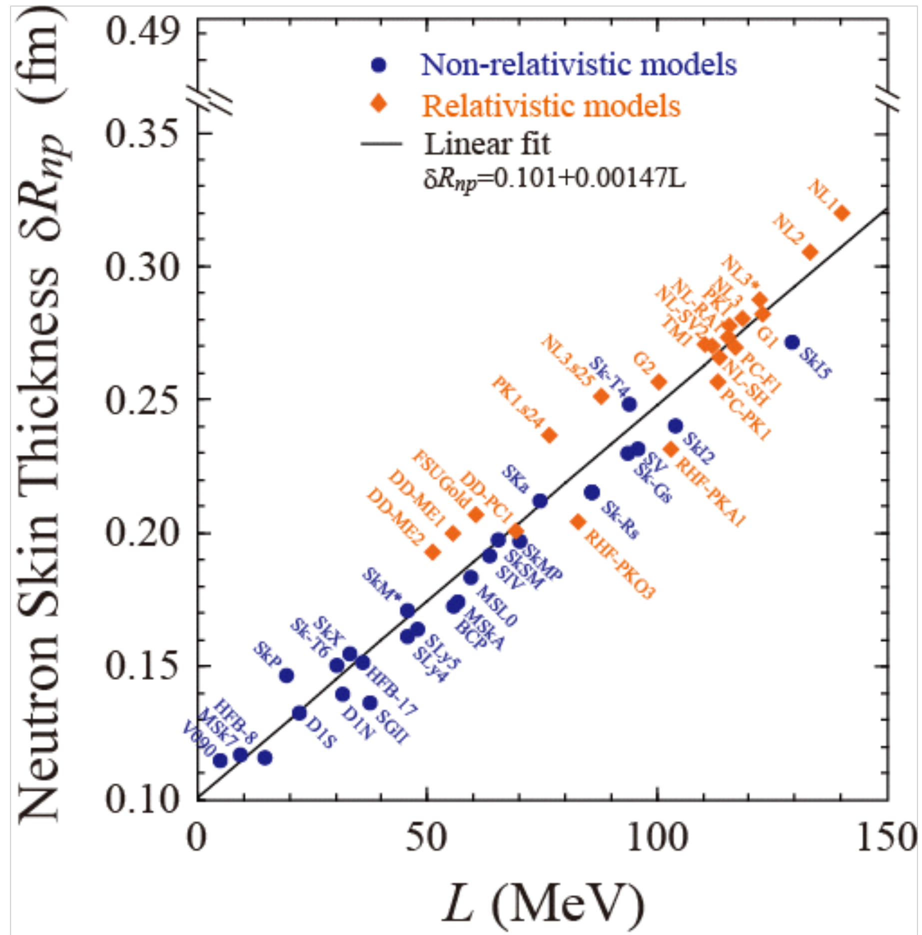


Neutron skin thickness

Roca-Maza et al., PRL106, 252501 (2011)

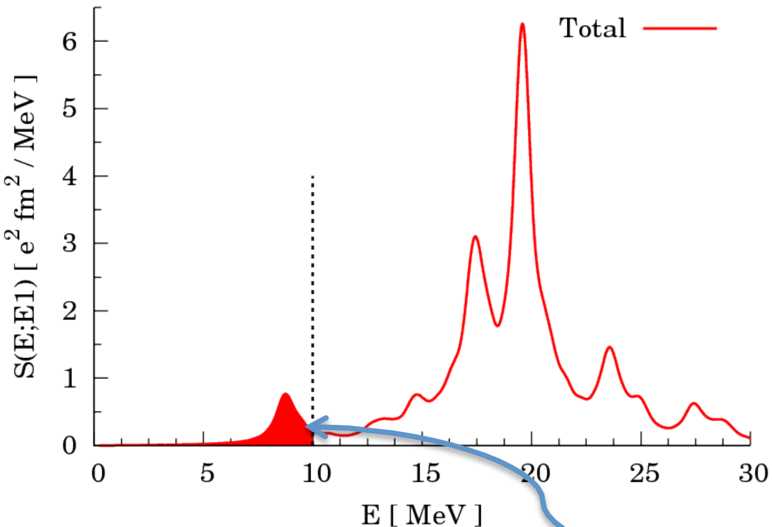
Neutron skin thickness
(Difference in radius between neutrons and protons)

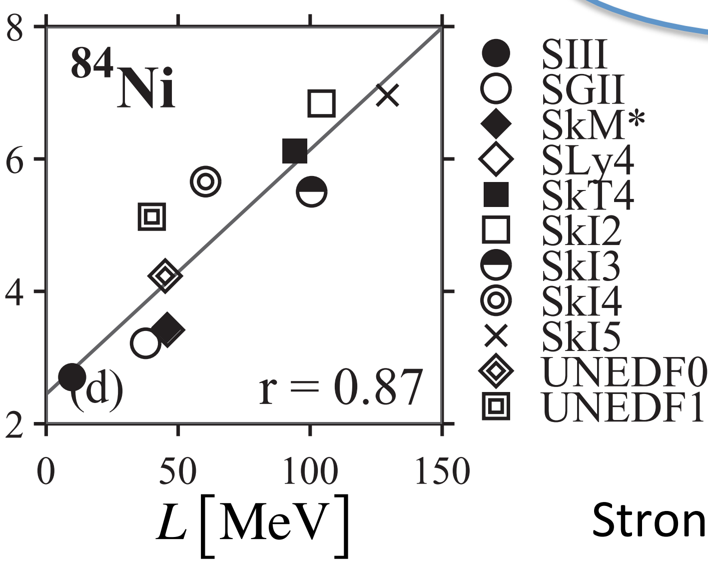


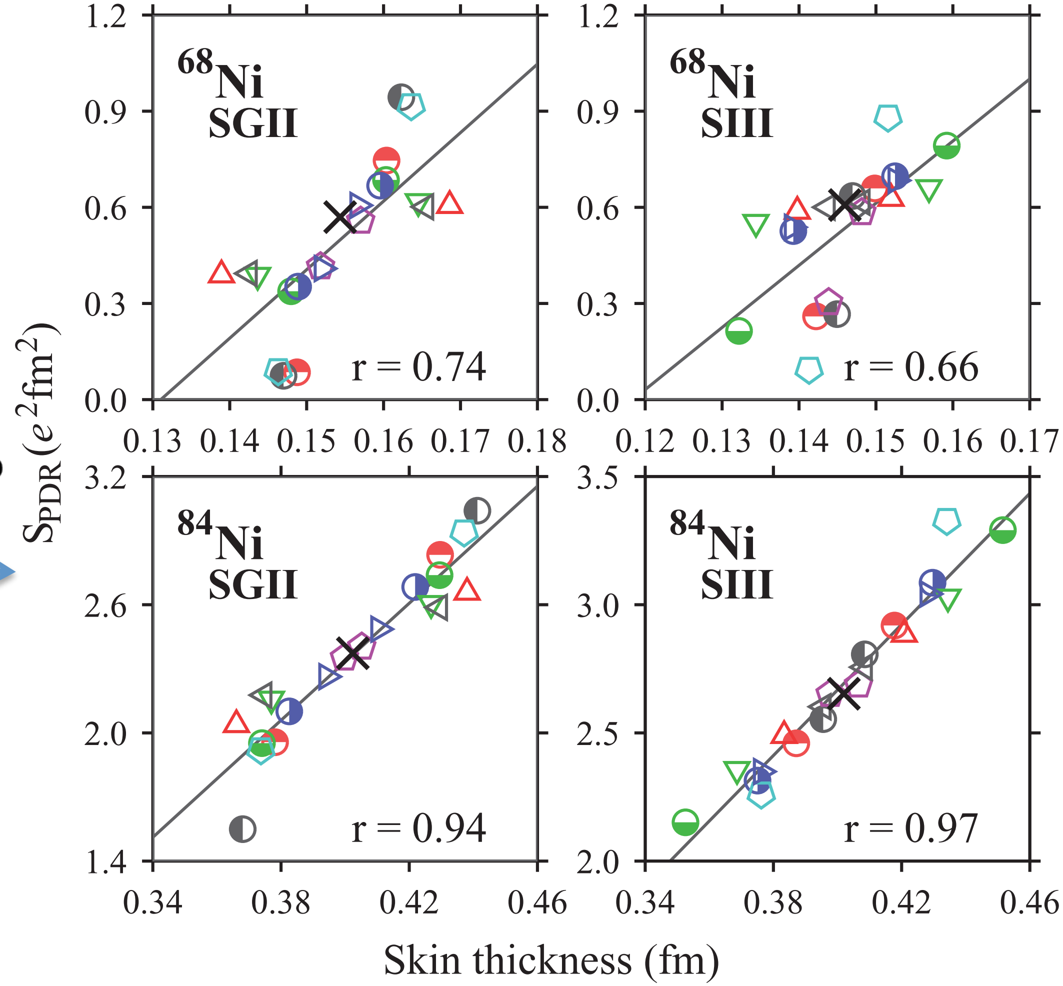


Selected isotopes

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







Strong correlation between low-energy E1 strength and skin thickness (slope parameter L) in selected nuclei

Summary

- Nuclear TDDFT
  - Calculation of response functions
  - Parallel computing
    - Orbital parallelization (real-time cal.)
    - Matrix element parallelization (QRPA cal.)
- Evolution of IS giant resonances
  - Peak splitting due to deformation
    - Prominent in GMR, “invisible” in GQR/GOR
  - m^*/m = 0.8 ~ 0.9; K = 210 ~ 230 MeV
- Pygmy dipole states in neutron-rich nuclei
  - Strong neutron shell effects
  - Decoupling from GDR
  - Skin thickness (L parameter) in select nuclei

Phonon condensation

$$\left|\Phi_0\right\rangle$$ Ground state

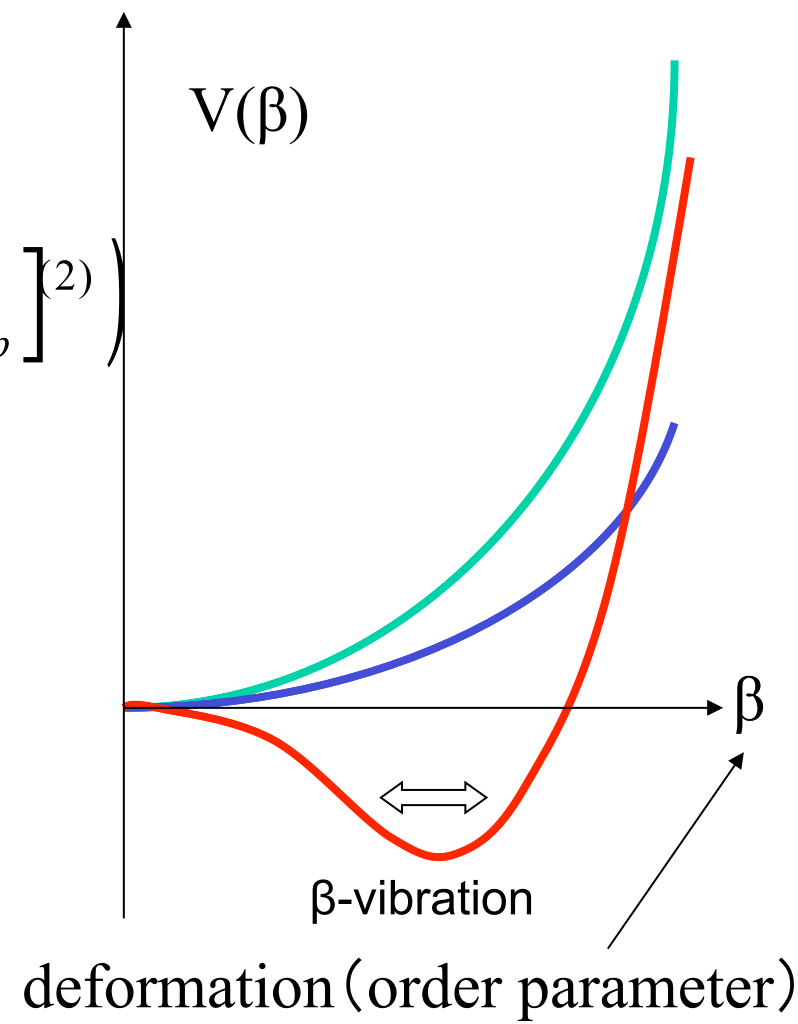
$$B^{+}_{2^+}\left|\Phi_0\right\rangle$$ Excited state (2^+)

$$B^{+}_{2^+} \approx \sum_{p,h}\left(X_{ph}\left[c_p^{+}c_h\right]^{(2)} + Y_{ph}\left[c_h^{+}c_p\right]^{(2)}\right)$$

Away from the closed-shell

$$\left|\Phi_{\mathrm{def}}\right\rangle \approx \exp(cB^{+}_{2^+})\left|\Phi_0\right\rangle$$

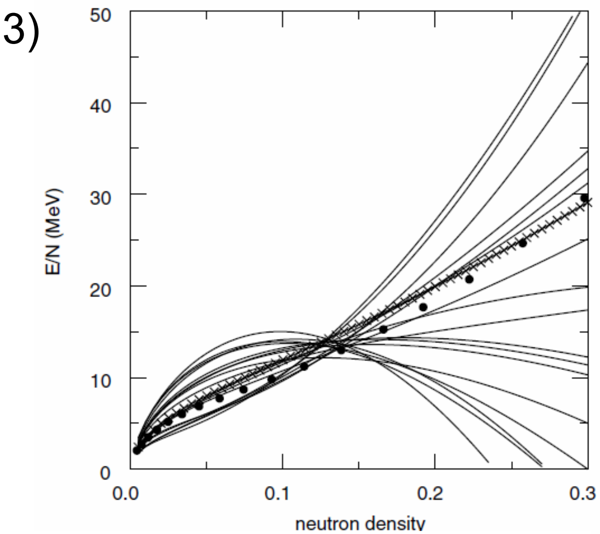
$$\beta \propto \left\langle\Phi_{\mathrm{def}}\left|r^2 Y_{20}(\hat{r})\right|\Phi_{\mathrm{def}}\right\rangle$$



Low-energy *E1* strength in exotic nuclei

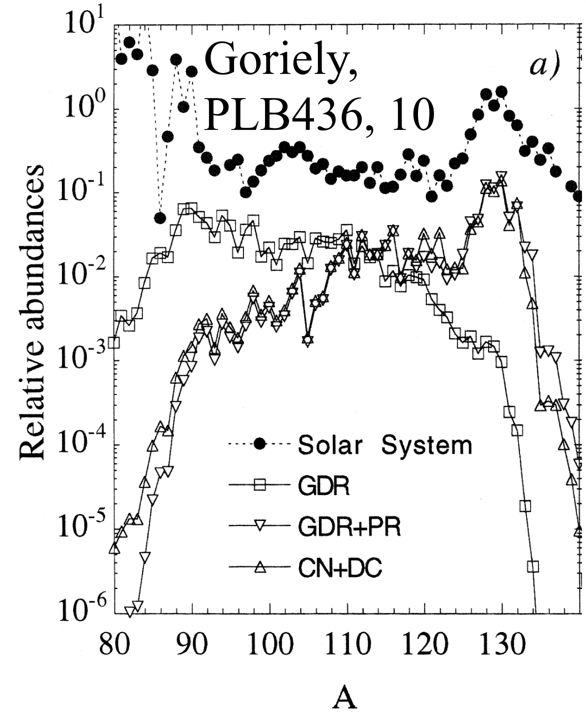
Inakura, Nakatsukasa, Yabana, PRC 84, PRC 88, 051305(R) (2013)

Ebata, Nakatsukasa, Inakura, in preparation.



- Constrain the neutron skin thickness and the neutron matter 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.



Beyond the linear regime
Future subjects

- Nuclear reaction involving a large shape change, such as fission, fusion, etc.
- Problems
  - Numerical cost for solution of TDHFB eq.

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

  - How to obtain quantum spectra?

Time-dependent Hartree-Fock-Bogoliubov (TDHFB) calculations with Gogny interaction (Y. Hashimoto)

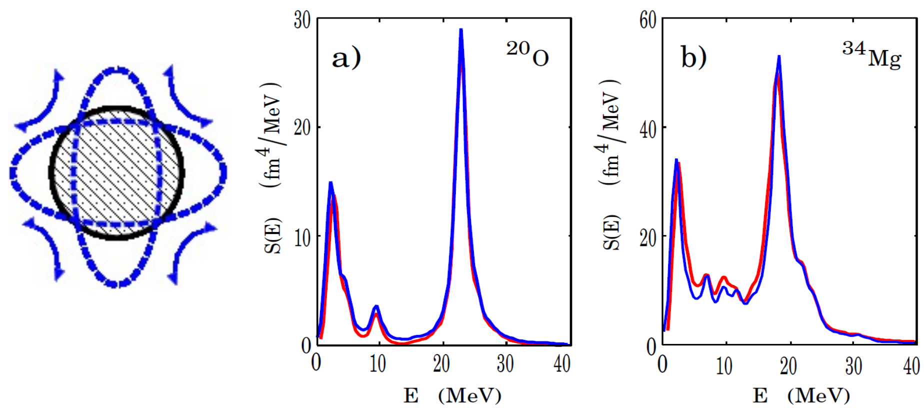
1. Aim:

The aim of the TDHFB calculations is to understand the dynamical role of the pairing correlation in the large-amplitude collective motions including the reaction processes.

2. Method :

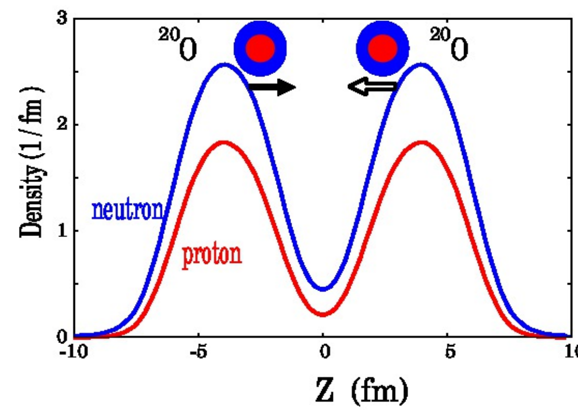
i) A new method of carrying out the Gogny-TDHFB calculations was proposed with the three-dimensional harmonic oscillator basis (3DHO).

ii) The program codes were extended to make use of the **spatial grids** (Lagrange mesh) instead of the 3DHO . At present, two-dimensional harmonic oscillator + one-dimensional Lagrange mesh (2DHO+LM) is used.



Strength functions of quadrupole vibrations in superconducting nuclei ^{20}O and ^{34}Mg.

EPJ A48:55 (2012) PRC88, 034307 (2013)



Colliding superconducting nuclei $^{20}O + ^{20}O$.

(calculations are in progress on a computer)

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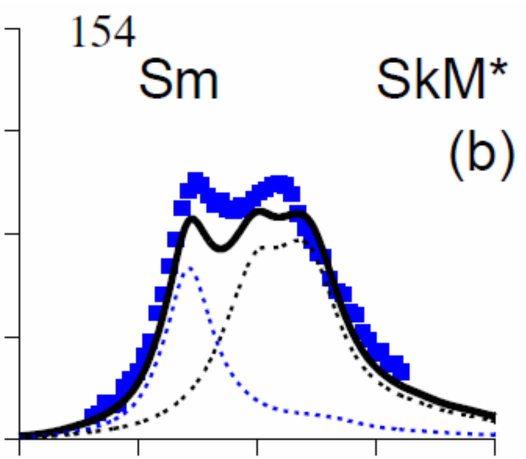
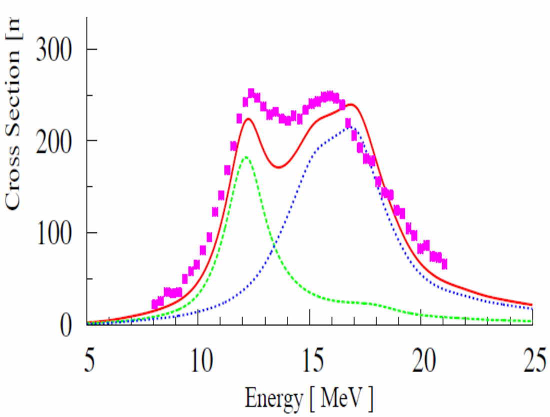
$$i\frac{\partial}{\partial t}\left|k(t)\right\rangle = \left(h(t)-\eta_k(t)\right)\left|k(t)\right\rangle$$

$$i\frac{\partial}{\partial t}\rho_k(t) = \Delta_k^*(t)K_k(t) - \text{c.c.}$$

$$i\frac{\partial}{\partial t}K_k(t) = \left(\eta_k(t)+\eta_{\bar{k}}(t)\right)K_k(t) + \Delta_k(t)\left(2\rho_k(t)-1\right)$$

Synopsis: Time-saving steps





Canonical-basis time-dependent Hartree-Fock-Bogoliubov theory and linear-response calculations

Shuichiro Ebata, Takashi Nakatsukasa, Tsunenori Inakura, Kenichi Yoshida, Yukio Hashimoto, and Kazuhiro Yabana

Phys. Rev. C **82**, 034306 (2010)

Published September 9, 2010

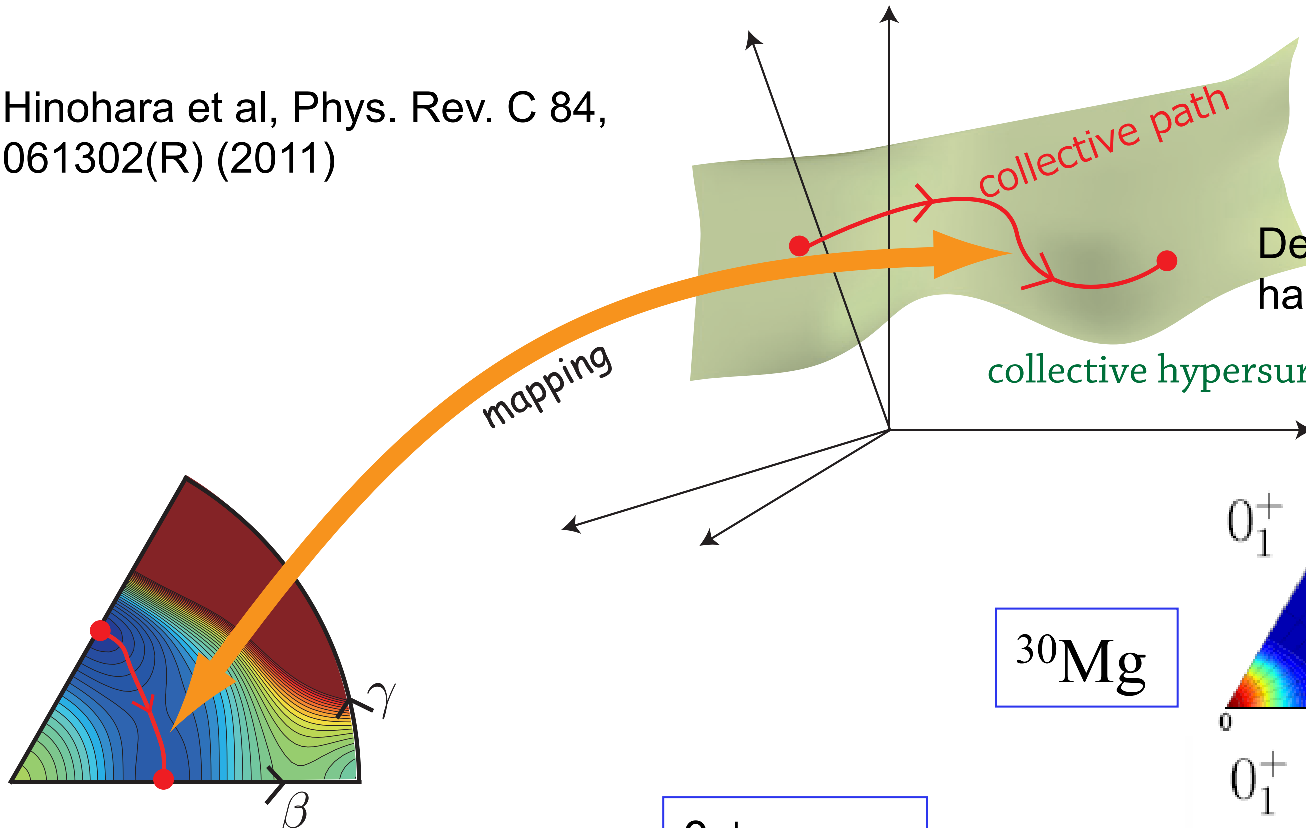
2D cal. w/o Coulomb	→	3D cal. w Coulomb
~1000 CPU h		~ 20 CPU hours

Canonical-basis real-time method may significantly reduces computational task.

Applicable to nuclear dynamics beyond the liner regime: fusion and fission reactions.

Collective subspace

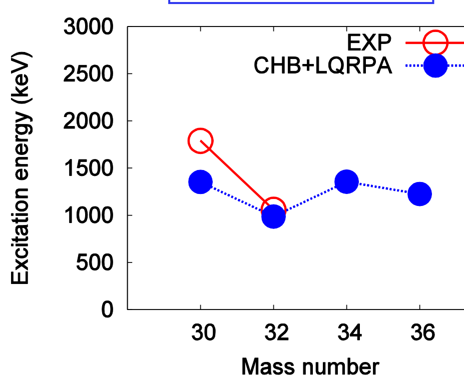
Hinohara et al, Phys. Rev. C 84, 061302(R) (2011)



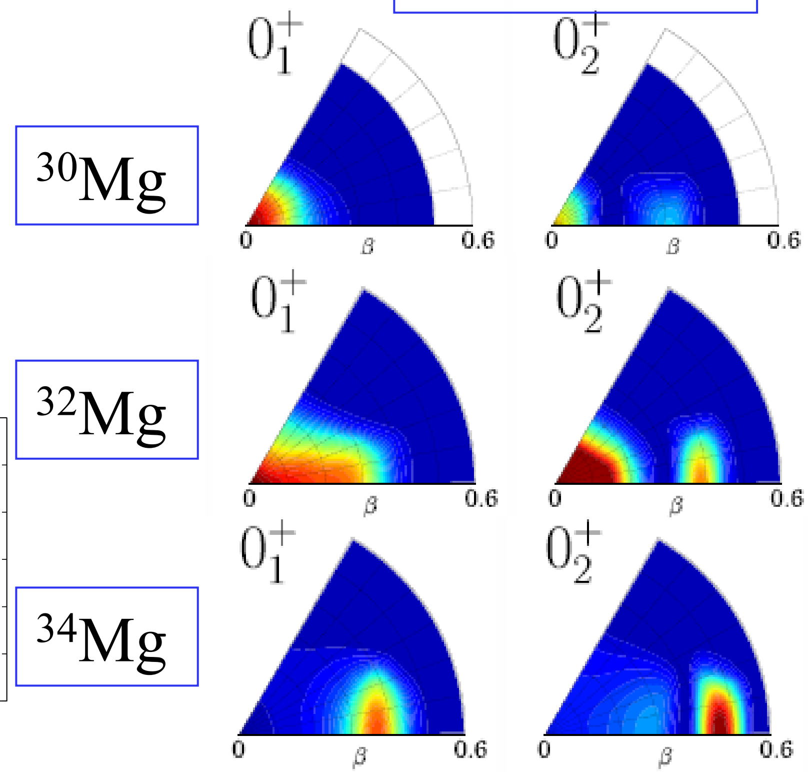
Determined by the local harmonic equation (LHE)

collective potential energy map in the (β, γ) plane

0_2^+ energy



wave functions



Next stage: Applications to fission problems

- Constrained Hamiltonian

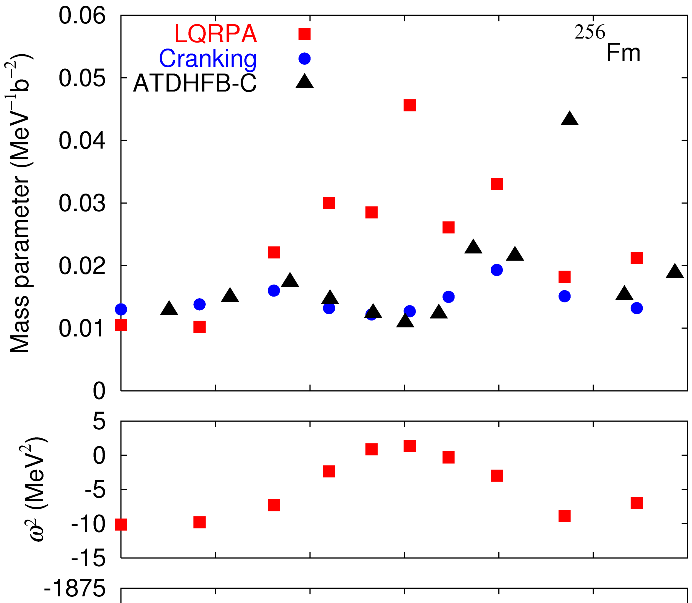
$$H = H - \lambda q$$

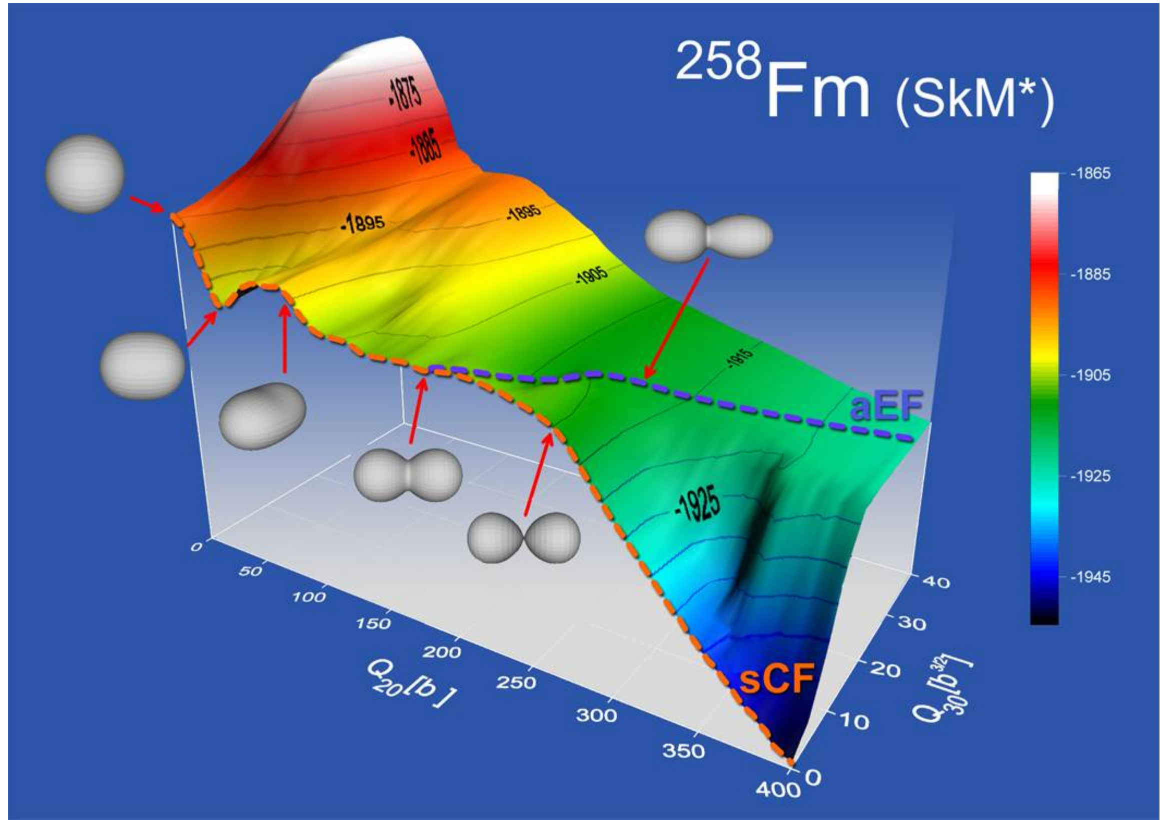
- Constrained operator

q Solution of LHE

- Collective mass parameters

Test calculation



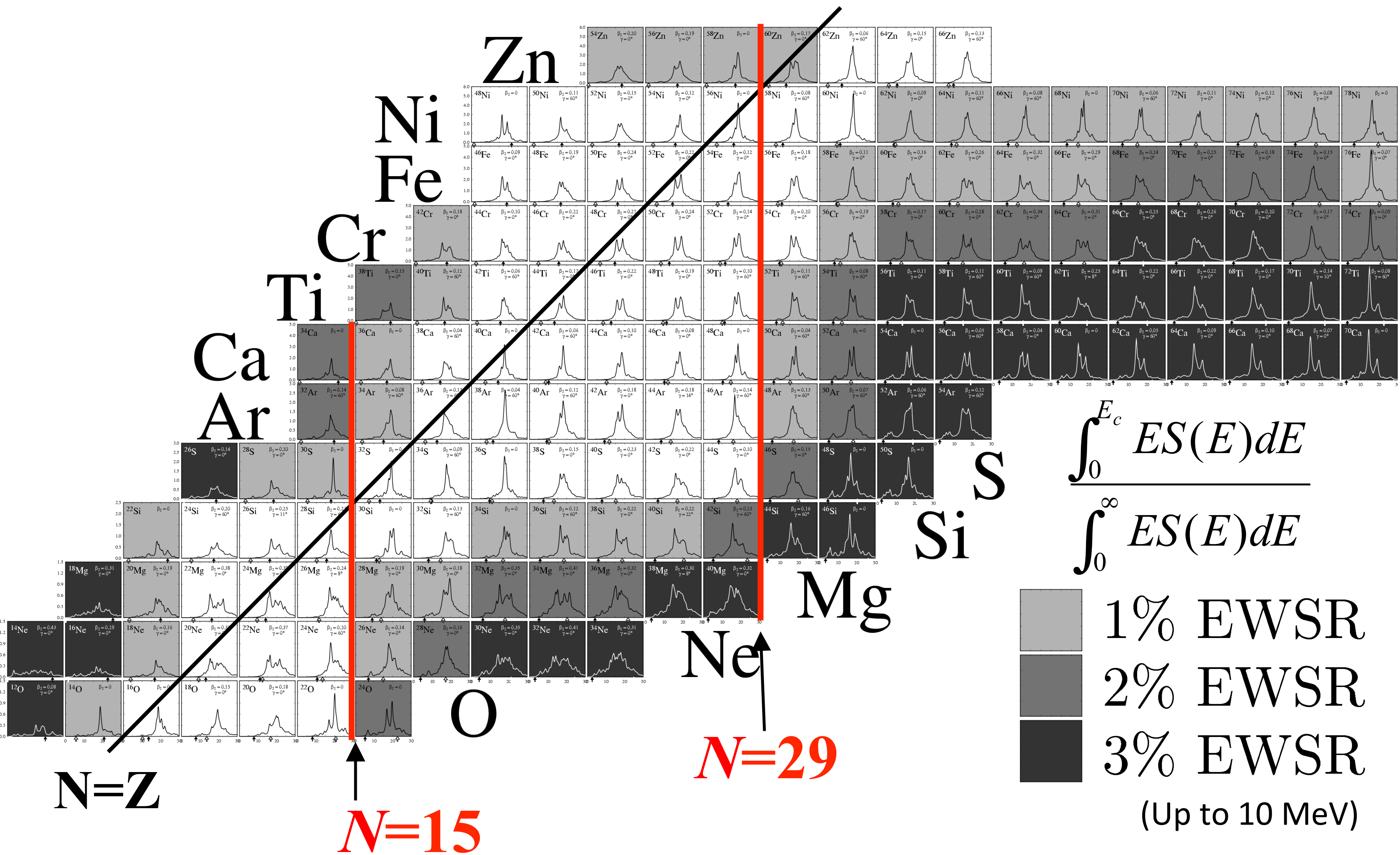


Local Harmonic Equation (LHE) is able to calculate the collective mass parameters including dynamical effect by the time-odd mean fields.

Magic numbers for low-energy E1 strength

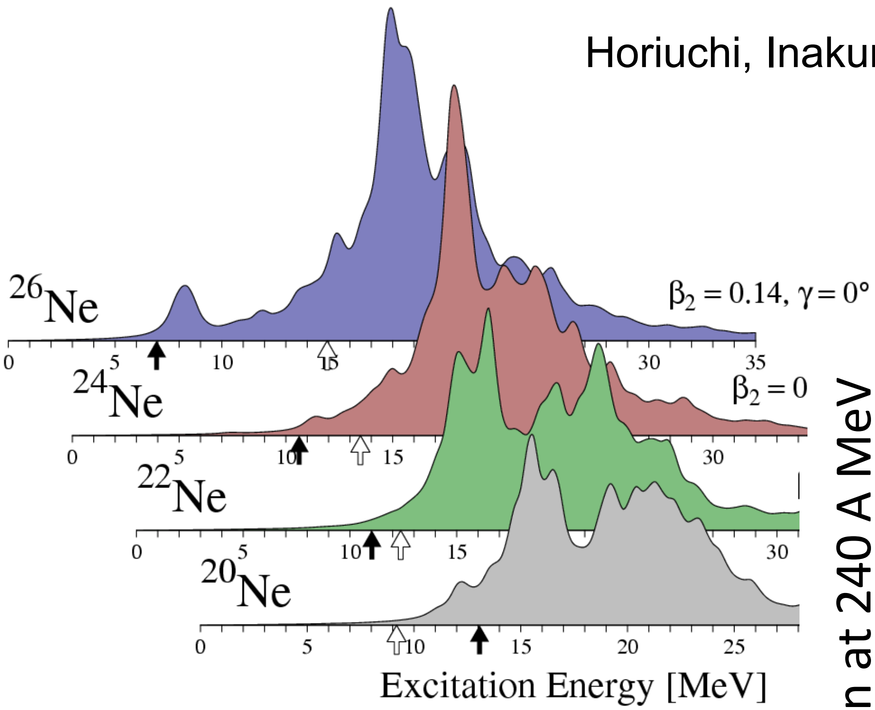
Pygmy dipole resonance (PDR)

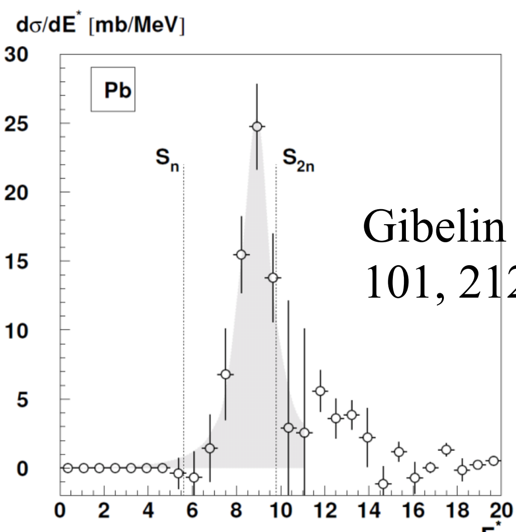
Cal. by Inakura



Development of neutron radius

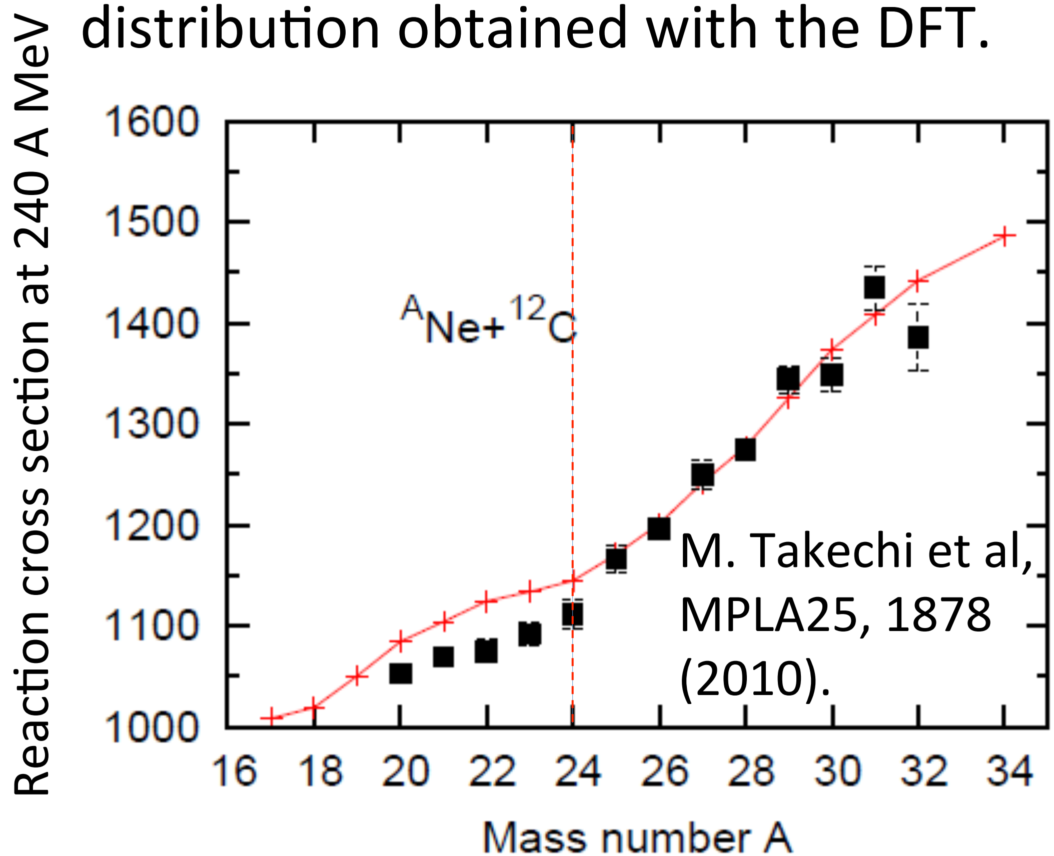
Horiuchi, Inakura, Nakatsukasa, Suzuki, PRC 86, 024614 (2012)





Gibelin et al, PRL 101, 212503 (2008)

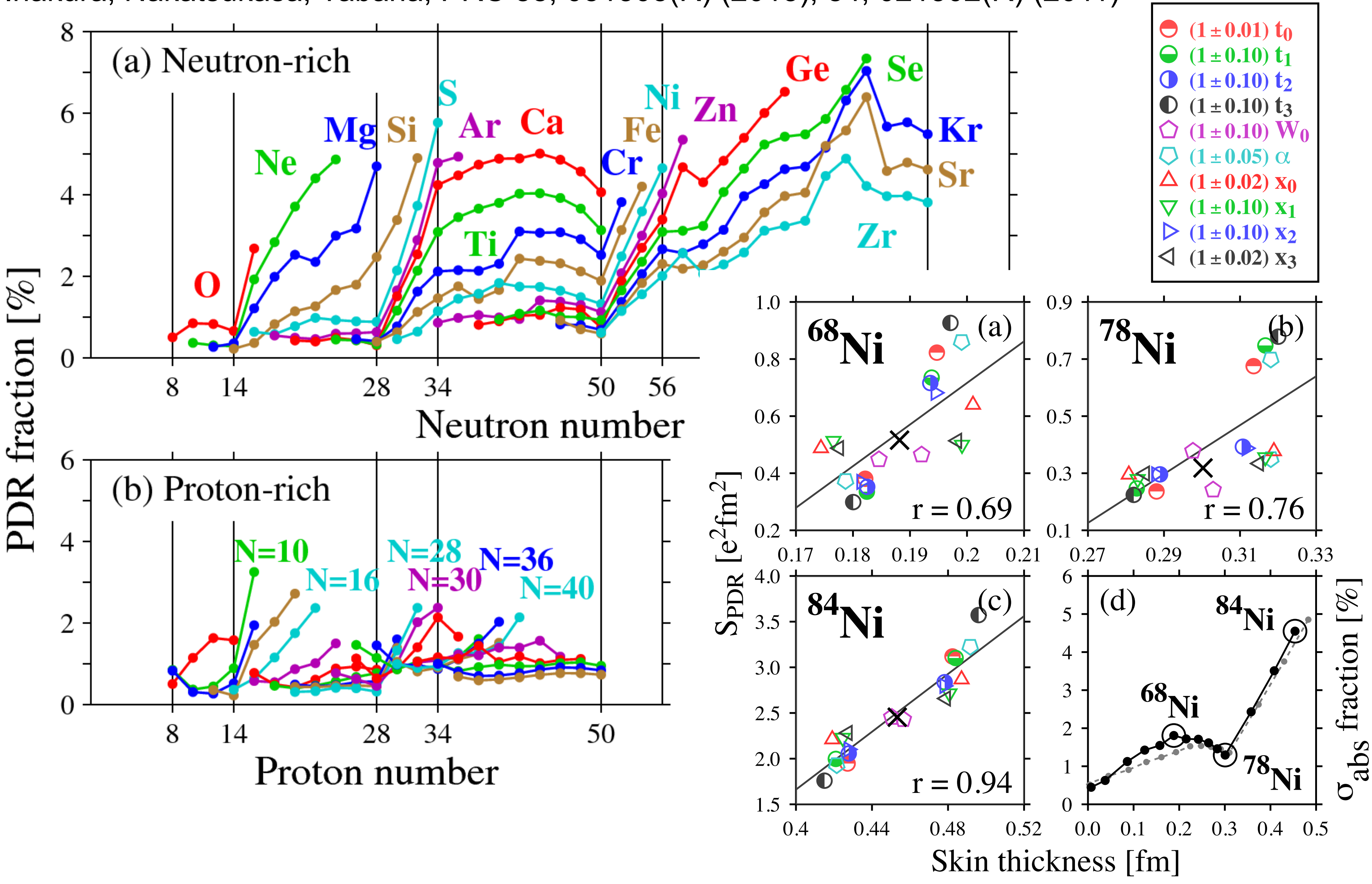
Glauber calculation using the density distribution obtained with the DFT.



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

Pygmy dipoles & neutron skins

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



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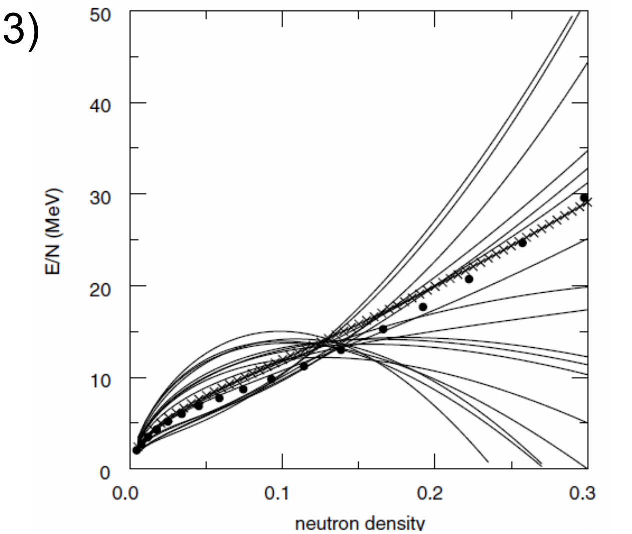
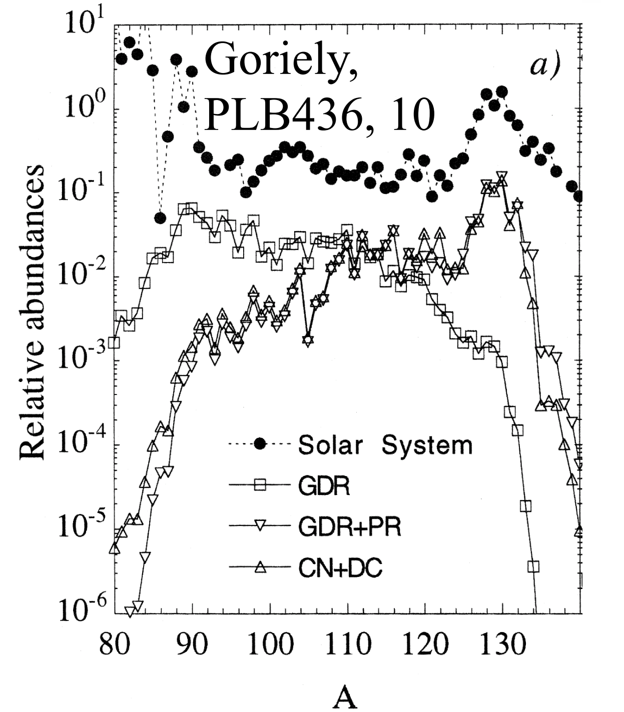
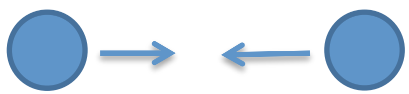


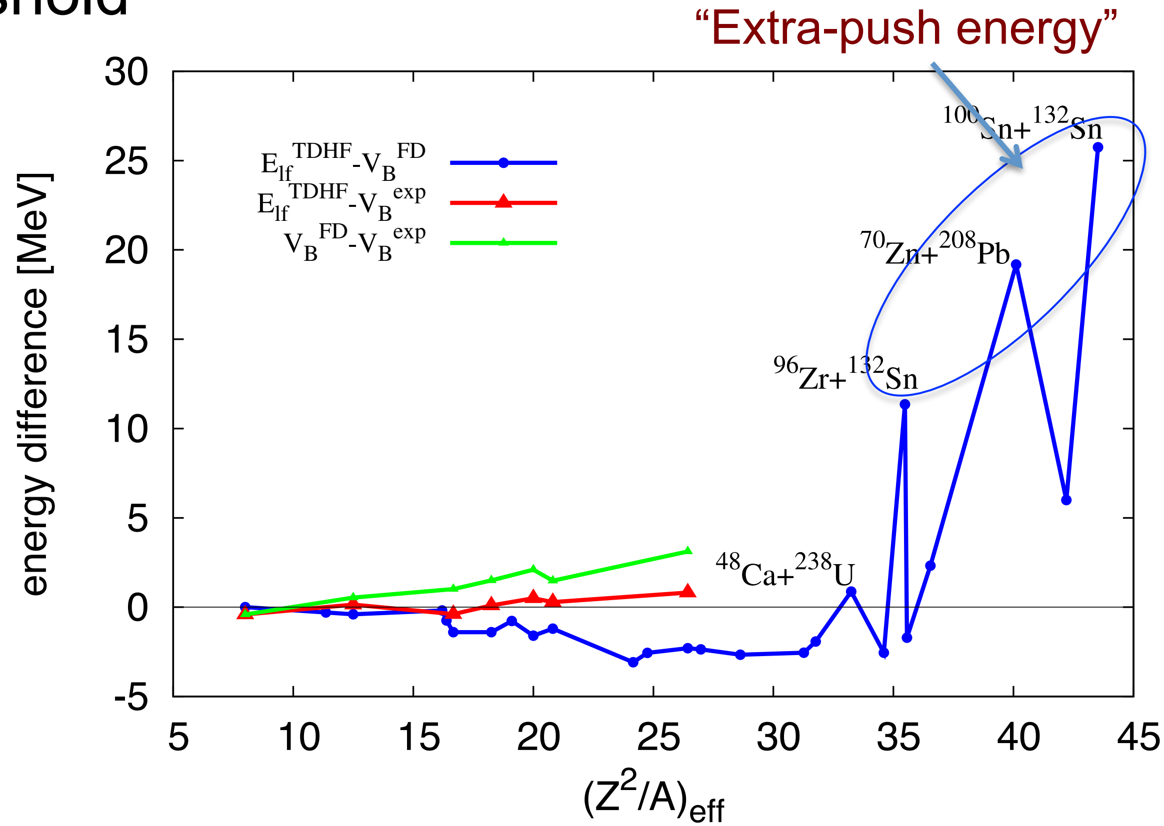


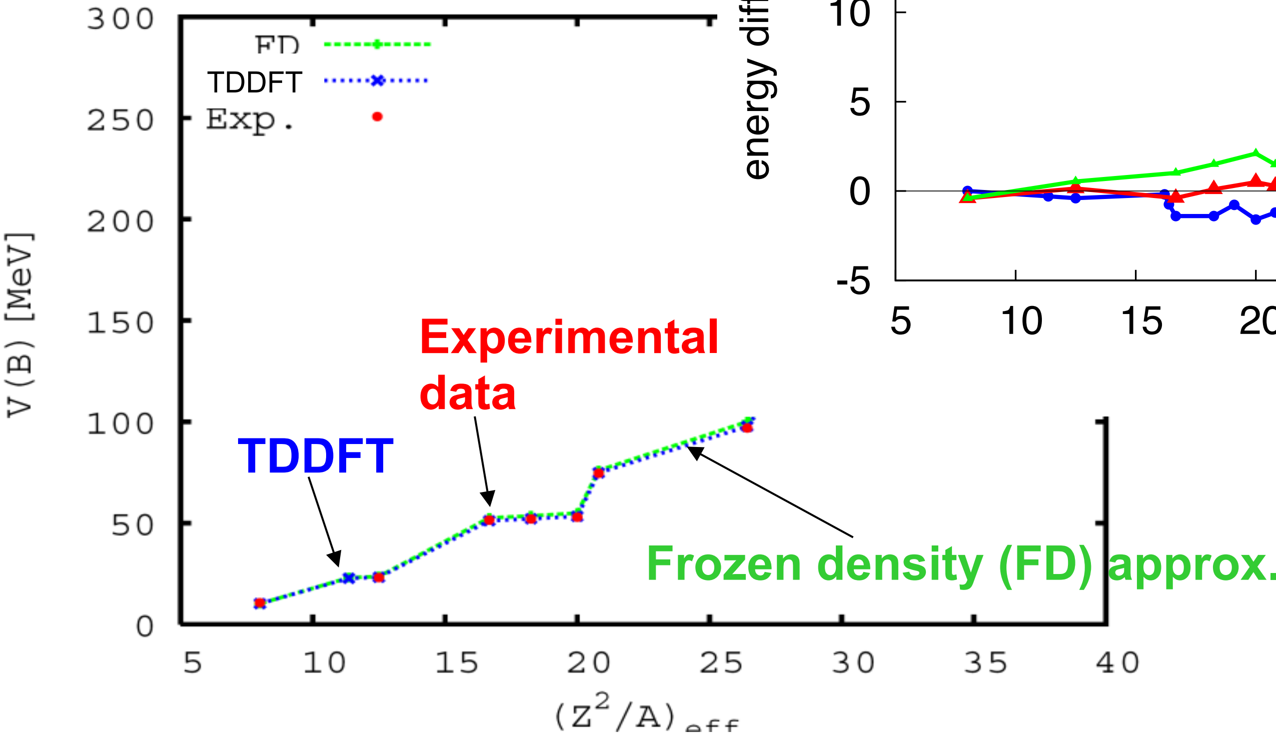
TDDFT simulation of nuclear fusion reaction

Guo, Nakatsukasa, EPJWC 38, 09003 (2012)

Fusion barrier threshold







Computational efforts

- Ground state: 2D solution of BdGKS equations
  - Use of 64 processors in parallel (MPI)
- Linear response and E1 strength functions

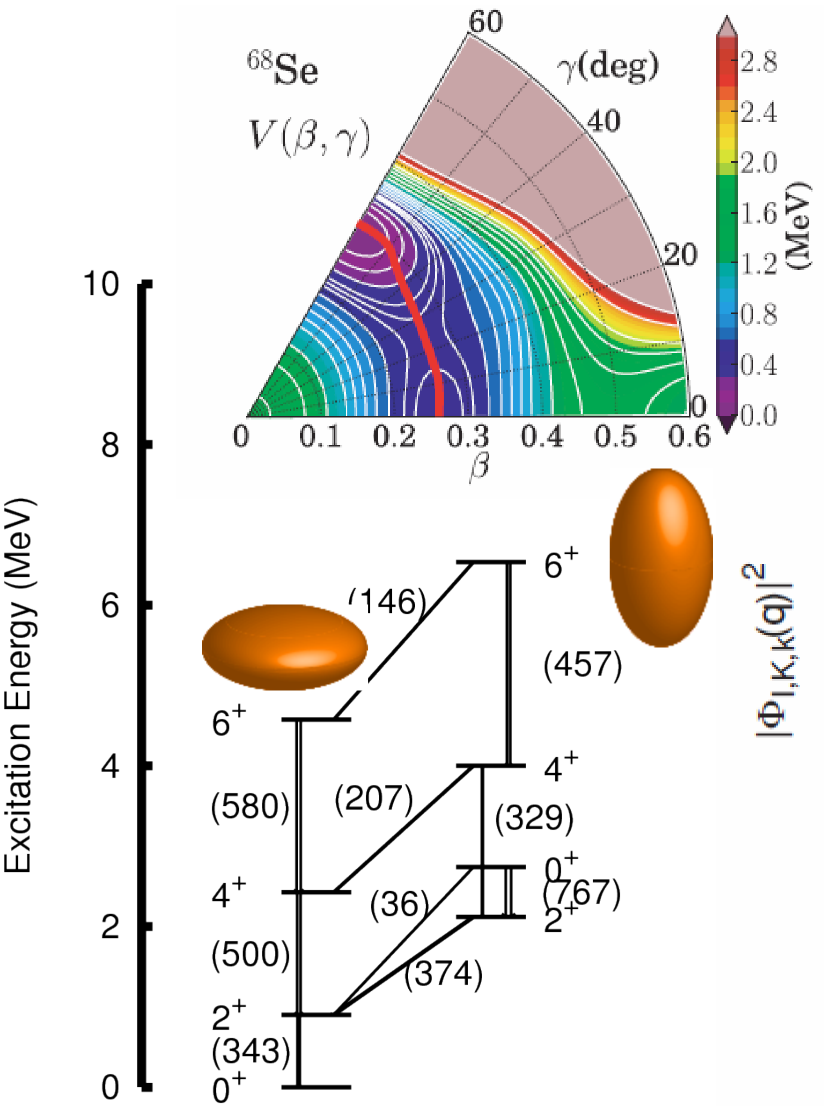
$$\left\{ \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\} \begin{pmatrix} X_{mi}(\omega) \\ Y_{mi}(\omega) \end{pmatrix} = 0$$

  - Use of 500-1000 processors in parallel (MPI)
  - Use of BLACS (Basic Linear Algebra Communication Subprograms) for load balancing and ScaLAPACK for matrix diagonalization
  - Truncate the space into about 50,000 2qp excitations
  - Neglect the residual Coulomb terms
  - Several hours to obtain the total strengths

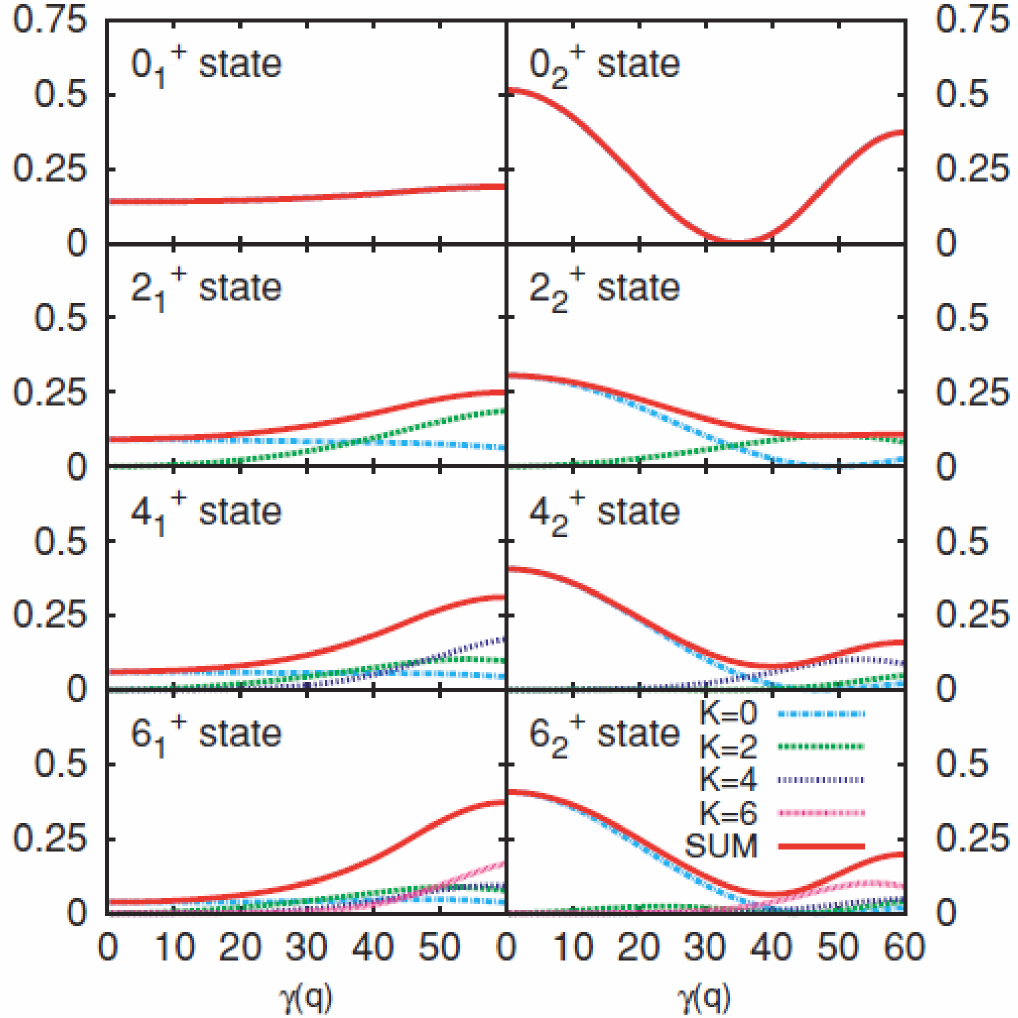
Including residual Coulomb in a larger model space (canonical basis), the project is currently running on use of "K" computer. [4.4 M node*h]

Low-lying spectra in ^{68}Se

Hinohara, et al



Rotation-induced localization



Strong shape mixing

EXP：Fischer et al., Phys.Rev.**C67** (2003) 064318.