Systematic calculation of electric dipole responses

Advances and perspectives in computational nuclear physics
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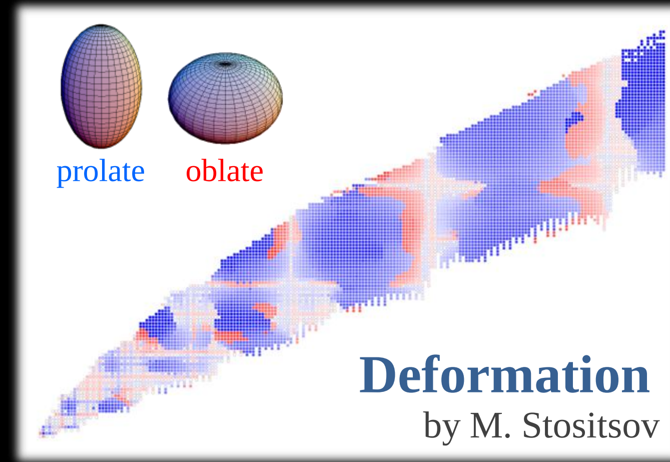
Ground state is calculated systematically.

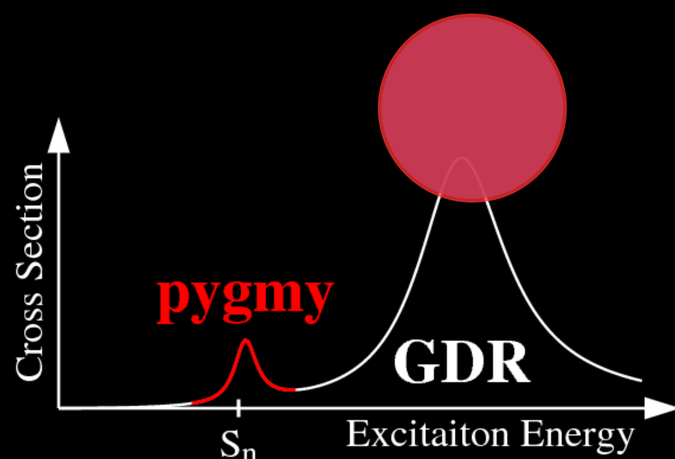
But excited state is less known.

Systematic calc. is now undertaking.

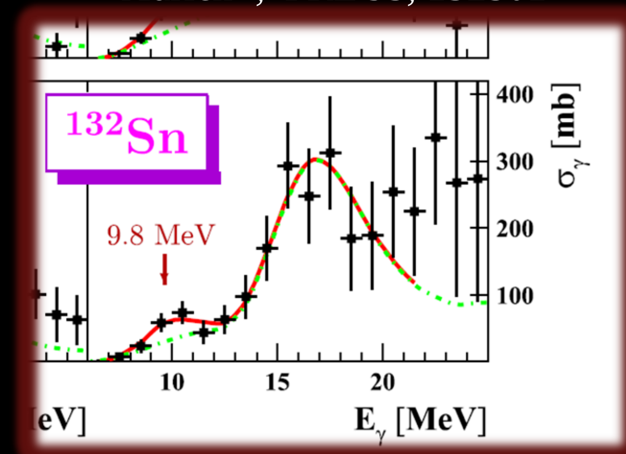


Electric dipole (E1) mode

- Giant Dipole Resonance is simplest collective vibration mode.
- Experimental data in stable region have been accumulated.
- Pygmy Dipole Resonance

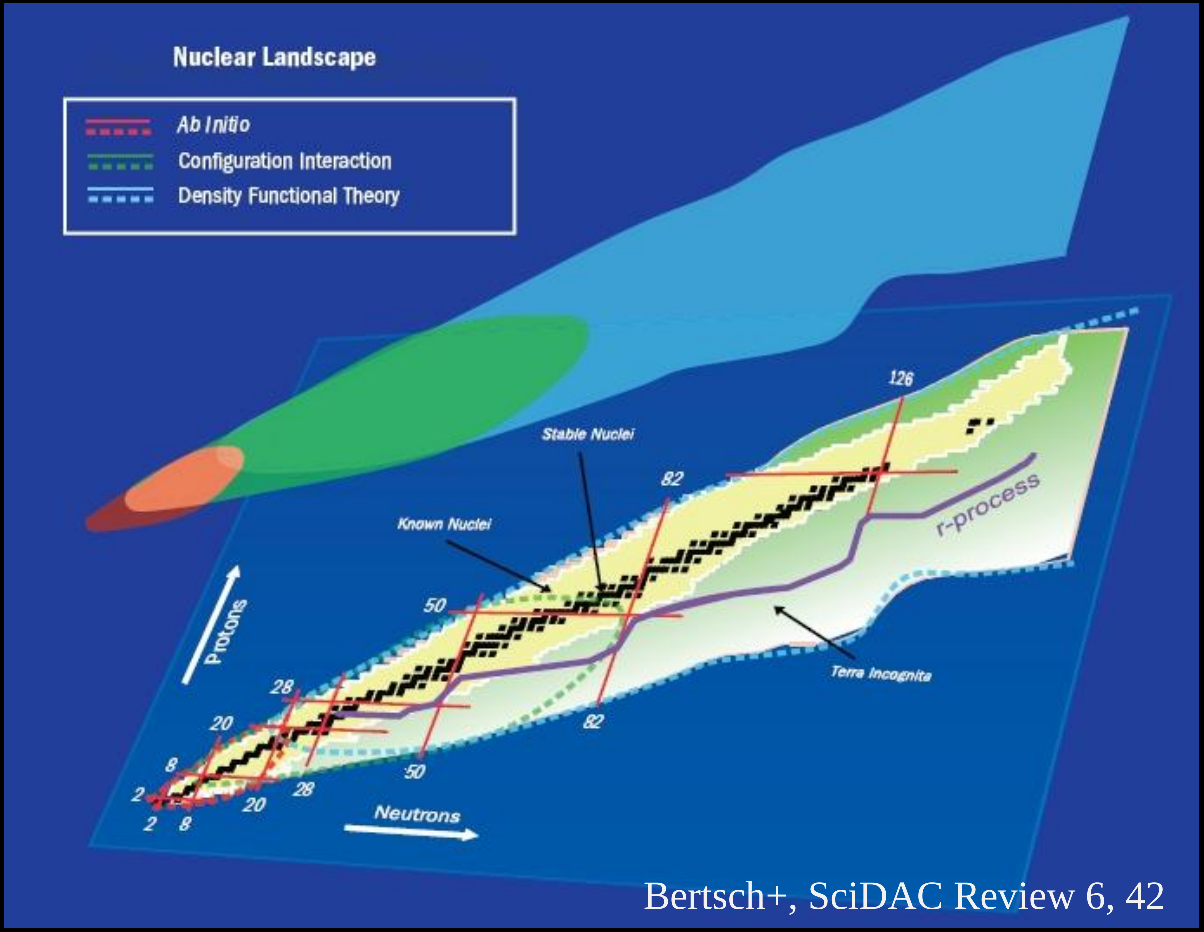


Adrich+, PRL 95, 132501



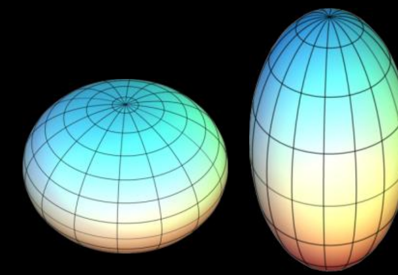
You cannot see the forest for the trees.

Nuclear landscape and theoretical model



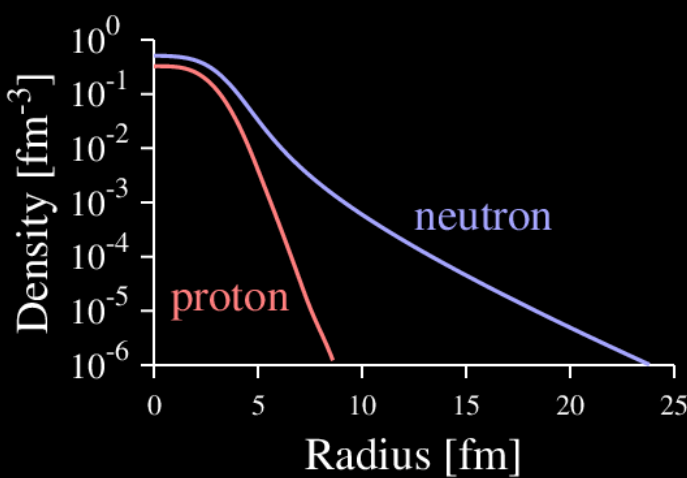
Bertsch+, SciDAC Review 6, 42

- Ab-initio no-core shell model calculations : light nuclei.
- Configuration interaction (i.e. shell model) : reaches to medium mass.
- Coupled cluster : the vicinity of doubly magic nuclei.
- Density functional theory (**DFT**) : the whole nuclear chart except for light nuclei

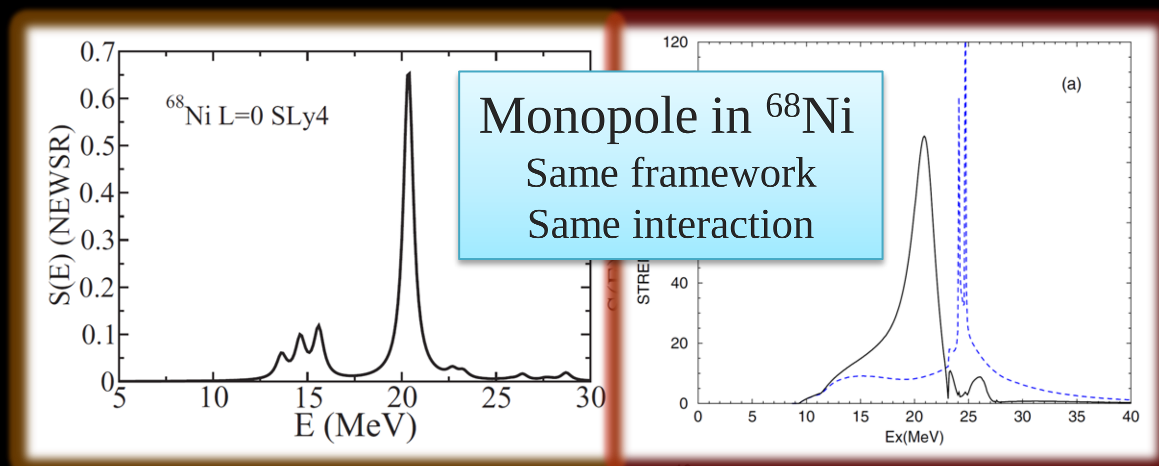


Key ingredients

- **Coordinate representation** [for describing unstable nuclei having skin (or halo)]
- **Continuum states** [for describing excitation beyond particle threshold energy]
- **Deformation** [Nuclei are mostly deformed.]
- **Pairing correlation** [Superfluidity plays essential role for several modes.]



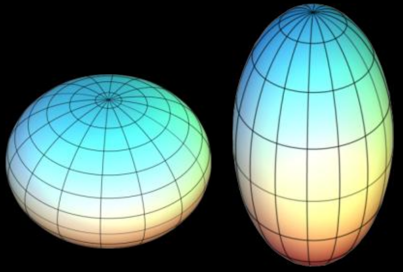
Density distribution of halo nuclei



Harmonic oscillator basis
Discretized continuum
Khan+, PRC84, 051301

Coordinate space
proper treatment of continuum
Hamamoto+, PRC90, 031302

Key ingredients



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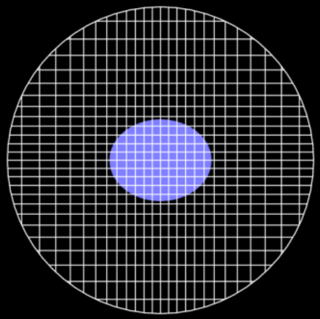
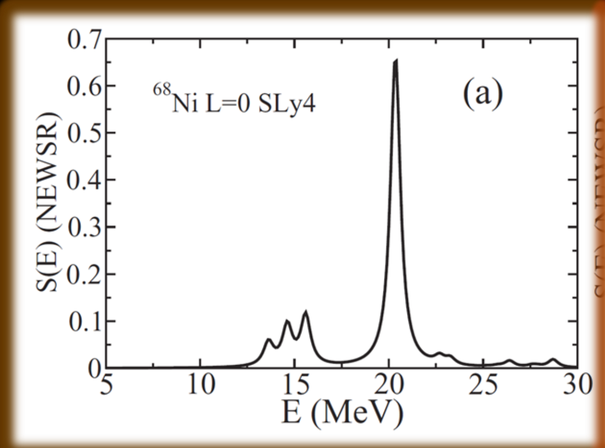
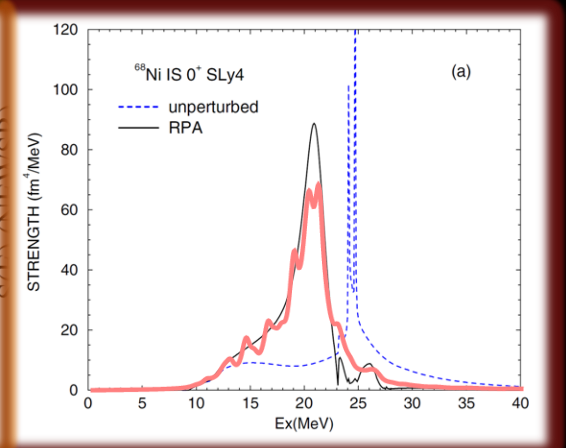




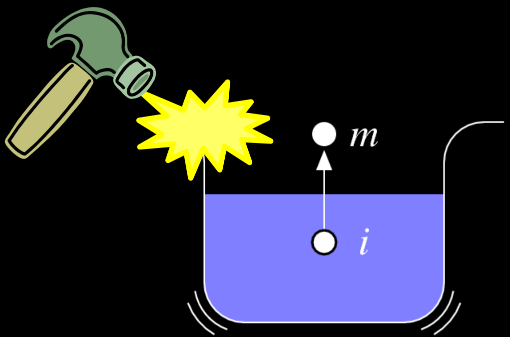


3D lattice representation

- applicable to **deformed** nuclei
- good approximation for **continuum state**

NO pairing correlation which has minor impact on E1 mode.

Linear-Response (RPA) equation



Response External field

$$\left\{ \begin{bmatrix} A & B \\ B^* & A^* \end{bmatrix} - \begin{bmatrix} \hbar\omega & 0 \\ 0 & -\hbar\omega^* \end{bmatrix} \right\} \begin{bmatrix} X \\ Y \end{bmatrix} = - \begin{bmatrix} V_{\mathrm{ext}} \\ V_{\mathrm{ext}}^{\dagger} \end{bmatrix}$$

$$|\mathrm{vib.}\rangle = \sum_{mi} f_{mi} |1\mathrm{p}{-}1\mathrm{h}\rangle$$

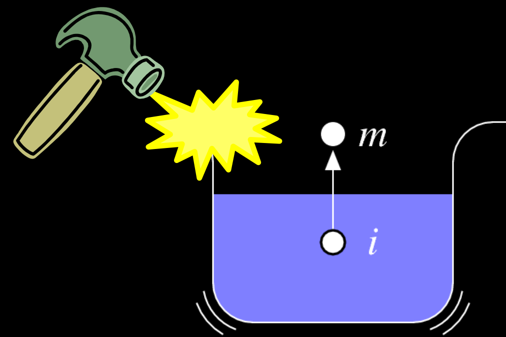
$$A_{(ph),(p'h')} = (\varepsilon_p - \varepsilon_h)\, \delta_{pp'}\delta_{hh'} + \left.\frac{\delta h_{(ph)}}{\delta \rho_{(p'h')}}\right|_{\rho=\rho_0}$$

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

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

- Taking **3D coordinate representation** makes A, B matrices enormous.
- Dimension of matrices A, B is # of particle-hole combination (*mi*), ~ $\boldsymbol{O(10^{6\text{-}7})}$.
- The matrix elements change in solving iteratively.

Linear-Response (RPA) equation



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$$|\text{vib.}\rangle = \sum_{mi} f_{mi} |\text{1p}-\text{1h}\rangle$$

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We avoid explicit calculation of induced field δ*h*/δρ by use of Finite Amplitude Method and Krylov subspace method.

Krylov subspace method

Iterative method for solving linear matrix equation, ***Ax*=*b***.

In n^{th} step, ***x*** is optimized in the subspace spanned by

$$K_n(A, b) = \mathrm{span}\{b, Ab, A^2b, \cdots, A^{n-1}b\}$$

The well-known solvers are the Conjugate Gradient (CG), Lanczos, Arnoldi.

But, nobody knows **which solver works well**.

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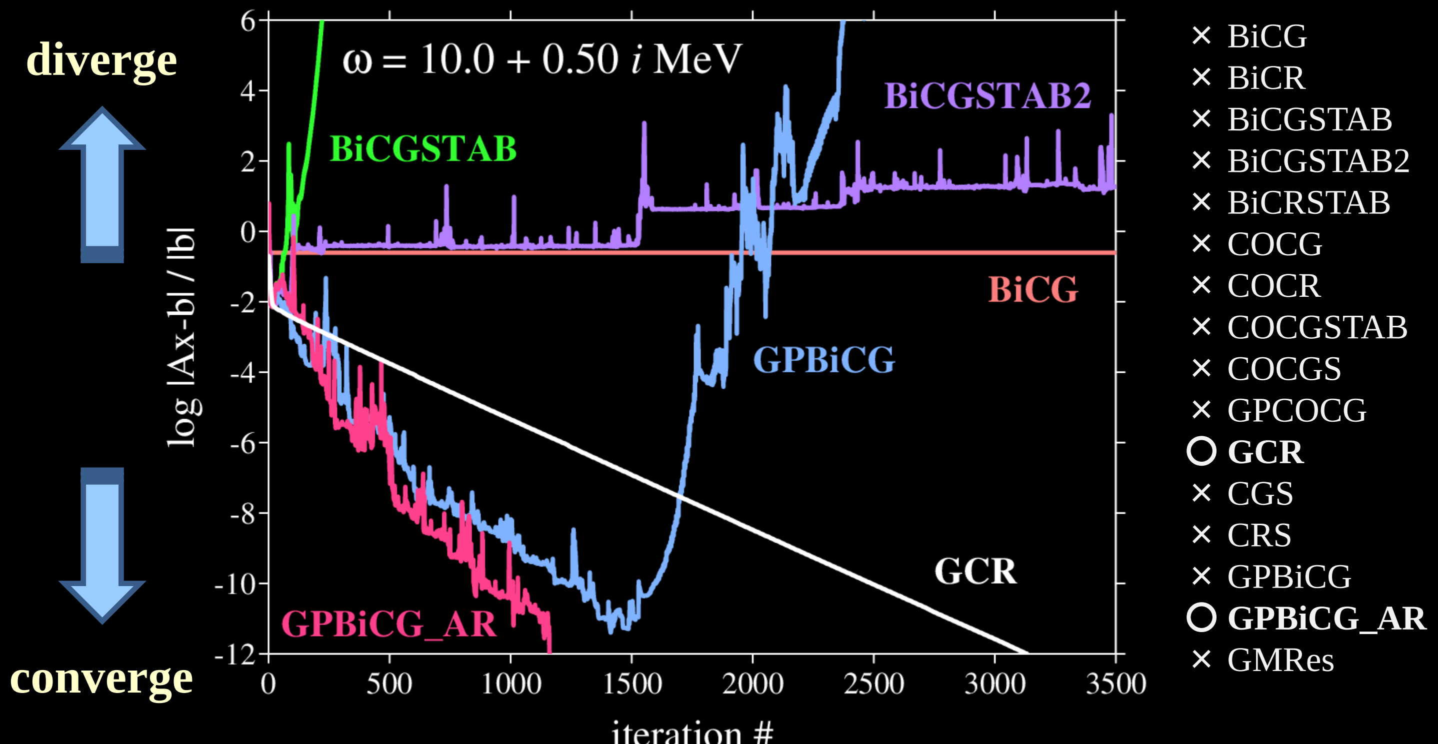

Krylov subspace method for ***Ax*****=*****b*** optimizes the solution ***x*** in subspace

$\boldsymbol{K_n(A,b)} = \mathbf{span}\{\boldsymbol{b}, \boldsymbol{Ab}, \boldsymbol{A^2b}, \ldots, \boldsymbol{A^{n\text{-}1}b}\}$, therefore ***A*** itself is not required.

$\Rightarrow$ If we can appropriately estimate $\delta h_{(ph)} = \sum_{(p'h')} \left.\frac{\partial h_{(ph)}}{\partial \rho_{(p'h')}}\right|_{\rho_0} \delta\rho_{(p'h')}$,

we do not have to calculate the induced filed $\frac{\partial h_{(ph)}}{\partial \rho_{(p'h')}}$.

Linear-Response (RPA) equation

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Krylov subspace method for $\boldsymbol{Ax=b}$ optimizes the solution $\boldsymbol{x}$ in subspace $\boldsymbol{K_n(A,b)} = \mathbf{span}\{\boldsymbol{b, Ab, A^2b, \ldots, A^{n-1}b}\}$, therefore $\boldsymbol{A}$ itself is not required.

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Finite Amplitude Method (FAM)

Nakatsukasa, TI, Yabana, PRC76, 024318

δh can be estimated by the finite difference method:

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

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

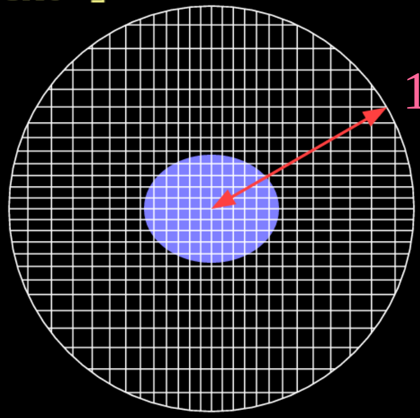
FAM reduces calculation costs : $O(N^2) \Rightarrow O(N)$

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

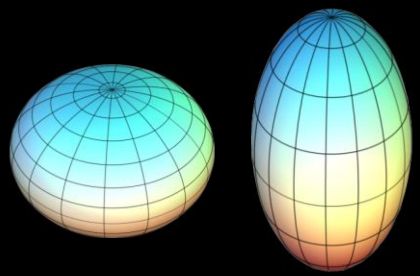
Numerical Detail

$$\left\{\begin{bmatrix} A & B \\ B^* & A^* \end{bmatrix} - \begin{bmatrix} \hbar\omega & 0 \\ 0 & -\hbar\omega^* \end{bmatrix}\right\}\begin{bmatrix} X \\ Y \end{bmatrix} = -\begin{bmatrix} V_{\mathrm{ext}} \\ V_{\mathrm{ext}}^{\dagger} \end{bmatrix}$$

- Energy Density Functional: SkM* (Skyrme-EDF)
- **Fully self-consistent calculation**.
- **No pairing correlation.**
- **3D lattice** without any spatial symmetry.
- R_{box} = 15 fm.
- Complex excitation energy with $\Gamma = 1.0$ MeV.
- ΔE = 0.30 MeV
  up to 38.1 MeV (128 points)
- **Energy-paralleled calc.**

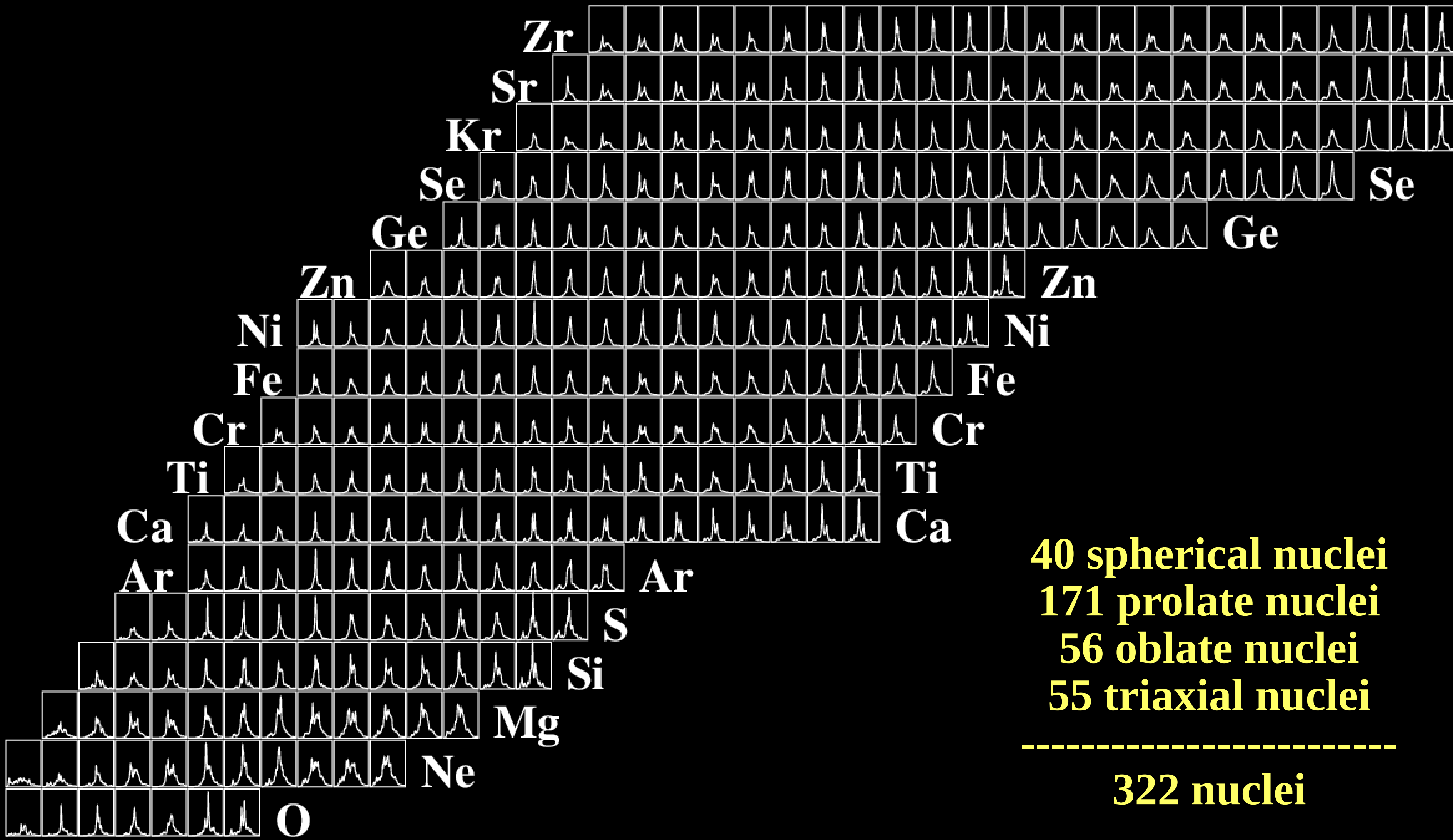


adaptive coordinate
PRC71, 024301



Electric Dipole strength distributions

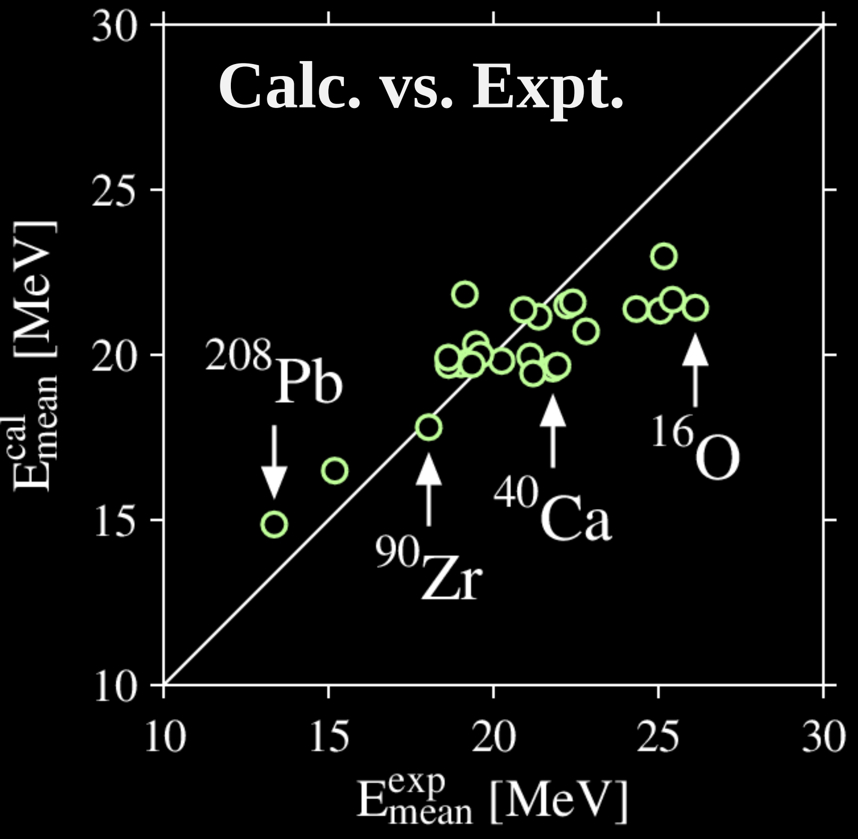
Inkaura+, PRC84, 021302



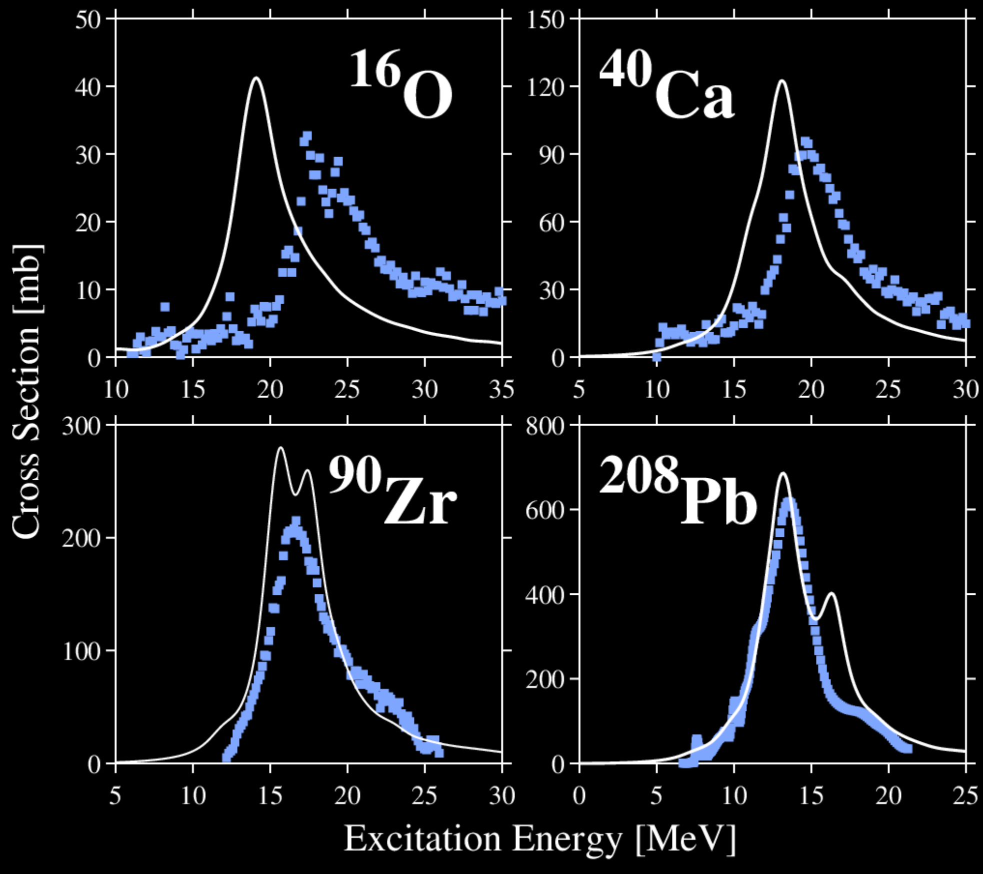
40 spherical nuclei
171 prolate nuclei
56 oblate nuclei
55 triaxial nuclei
----
322 nuclei

GDR: comparison with experiment

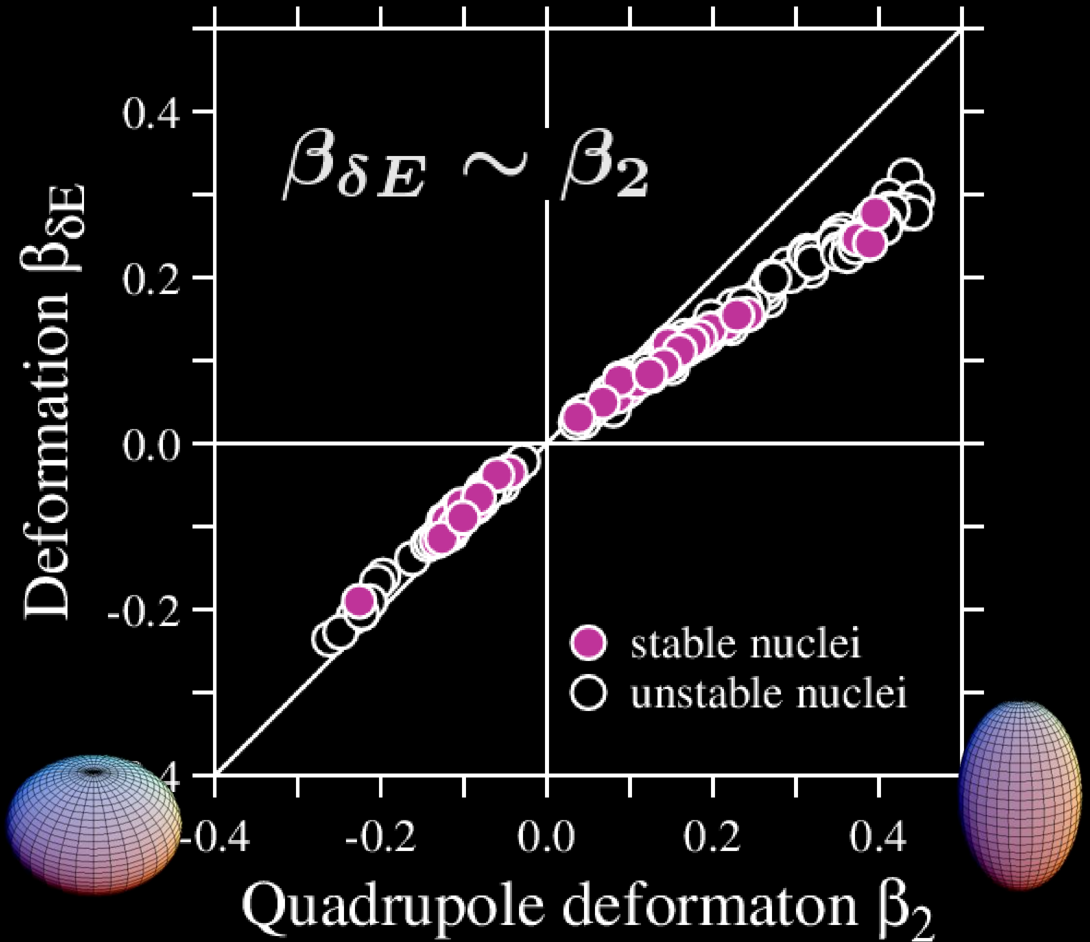
$$E_{\mathrm{mean}} = \frac{\int dE\, \sigma_{\mathrm{abs}}(E)\, E}{\int dE\, \sigma_{\mathrm{abs}}(E)}$$

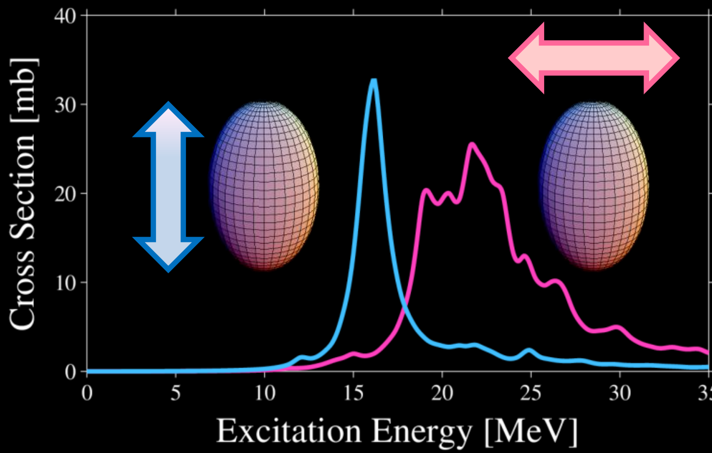


R_{box} = 25 fm.
Γ = 2.0 MeV.



GDR splitting by deformation



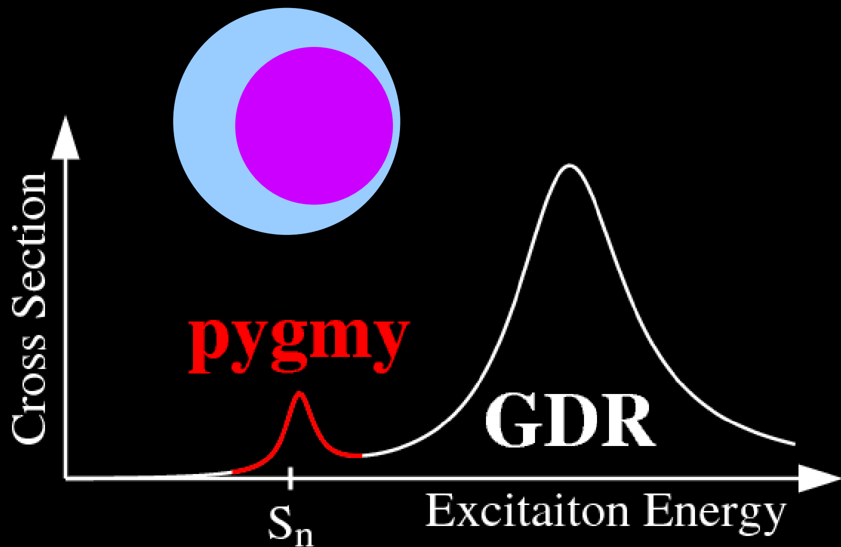


$$\beta_{\delta E} = \frac{E_{\text{mean}}^{K=1} - E_{\text{mean}}^{K=0}}{E_{\text{mean}}^{\text{all}}}$$

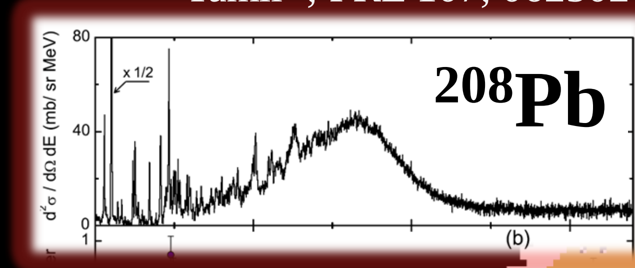
$$\beta_2 \propto \frac{\langle 2z^2 - x^2 - y^2 \rangle}{\langle r^2 \rangle}$$

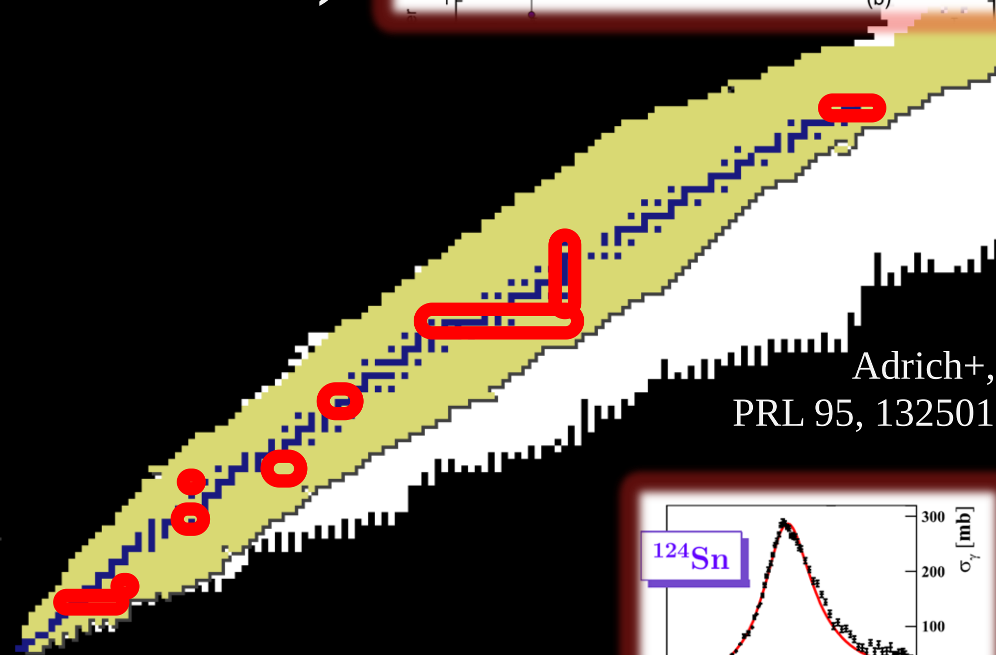
Pygmy Dipole Resonance (PDR)

(or low-energy E1 mode)

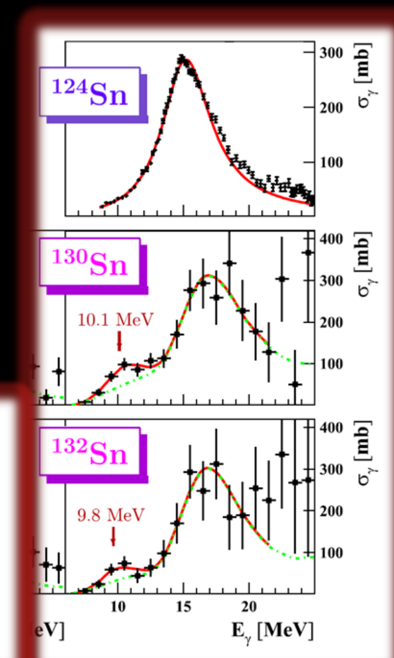


Tamii+, PRL 107, 062502

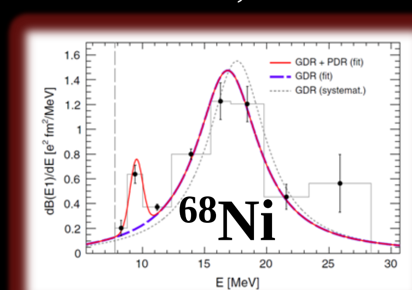




Adrich+, PRL 95, 132501

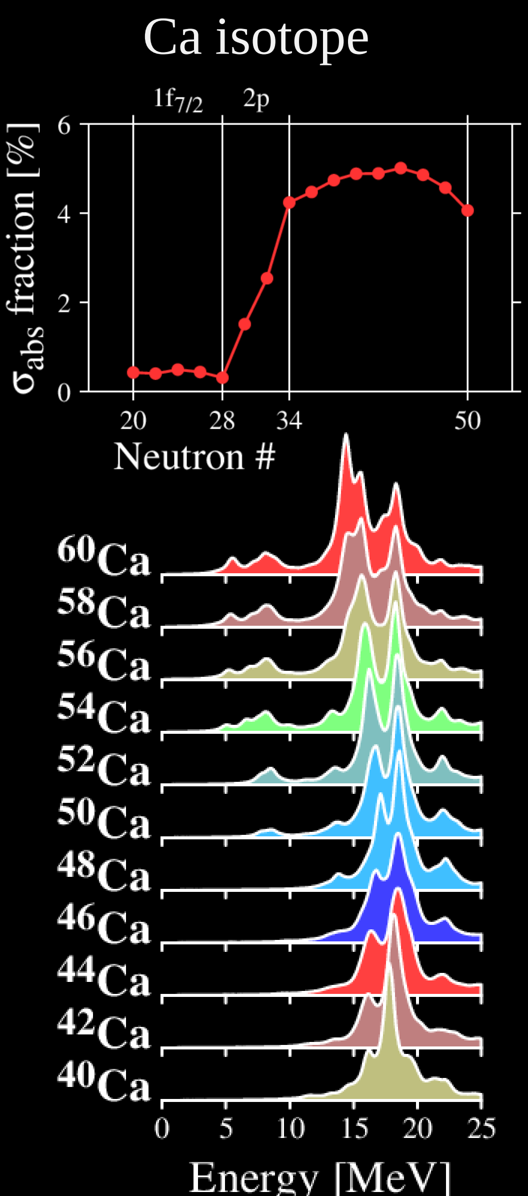


Rossi+, PRL 111, 242503

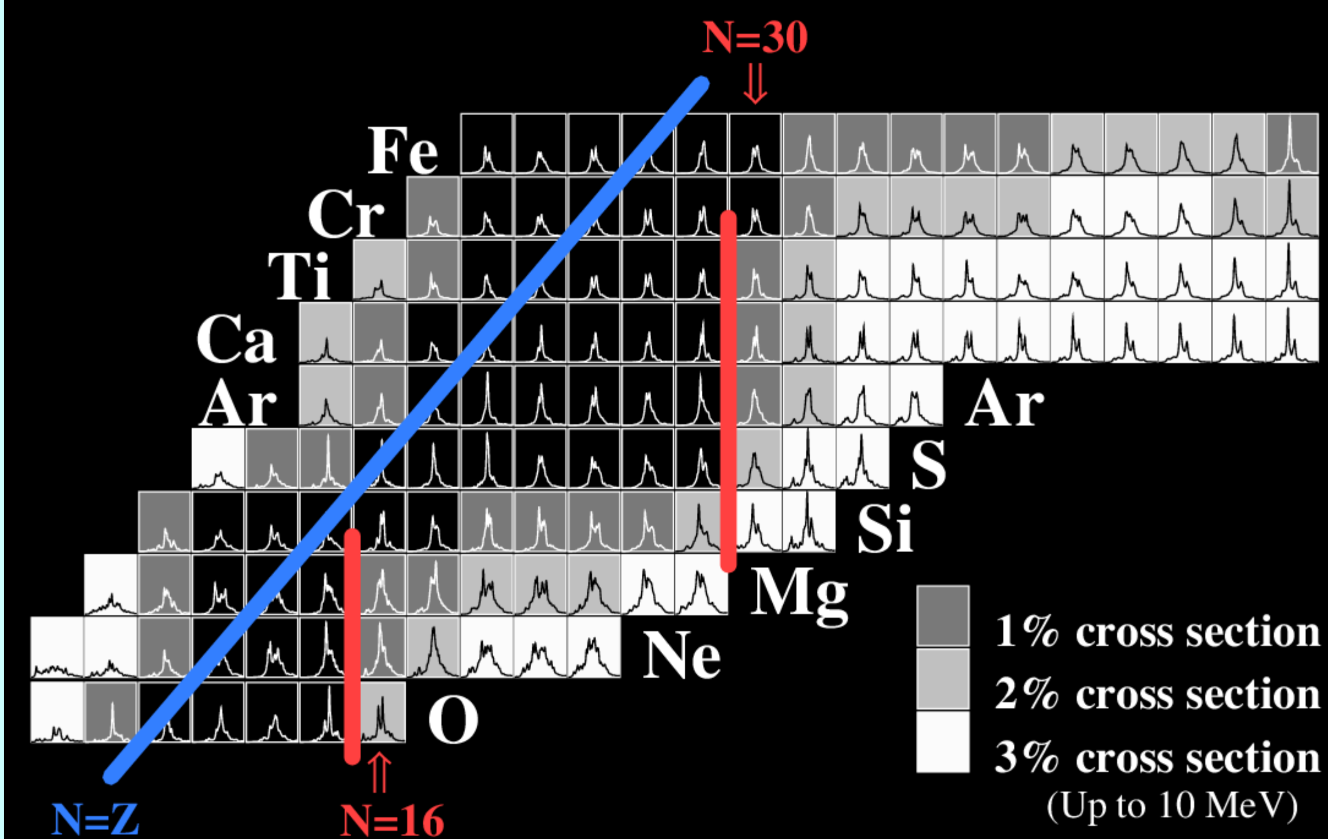


- New collective mode unique in n-rich nuclei such as oscillation between skin and core?
- What is emergence condition?
- Alternative observation of neutron skin thickness and/or neutron matter EoS?

Magic numbers for PDR emergence



PDR emerges and develops beyond *N* = 14, 28.



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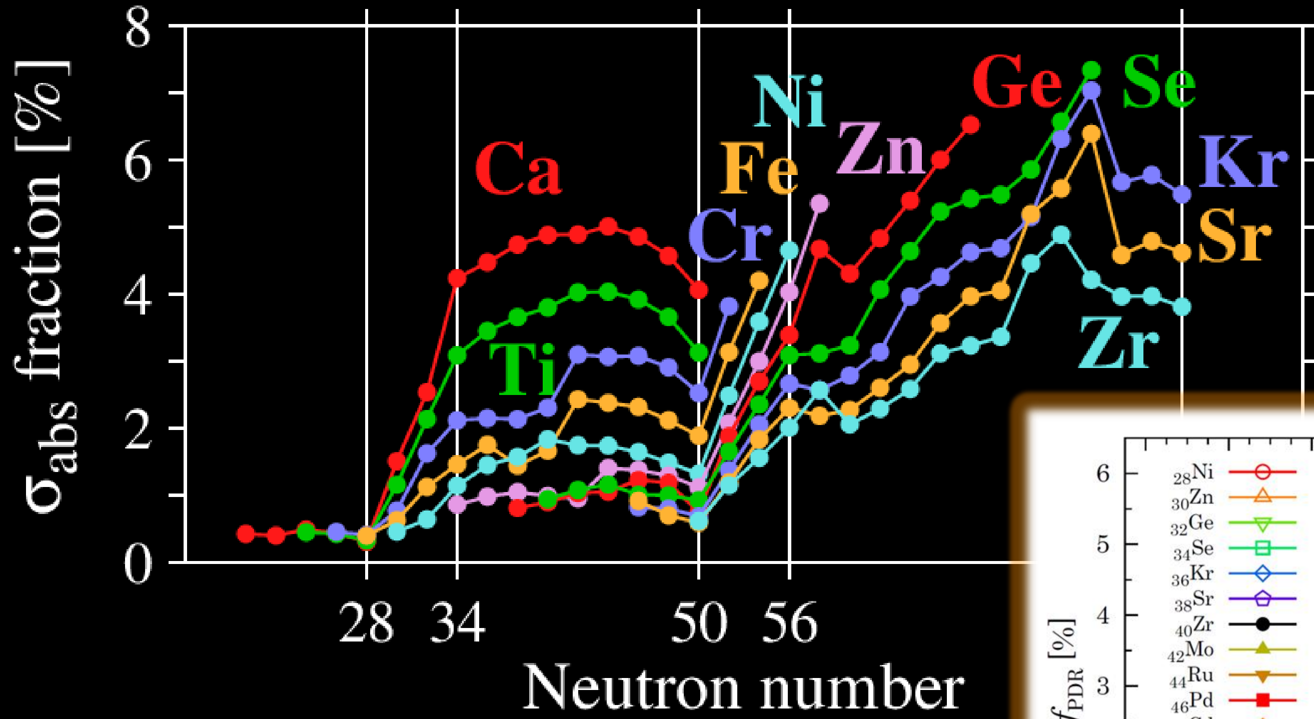
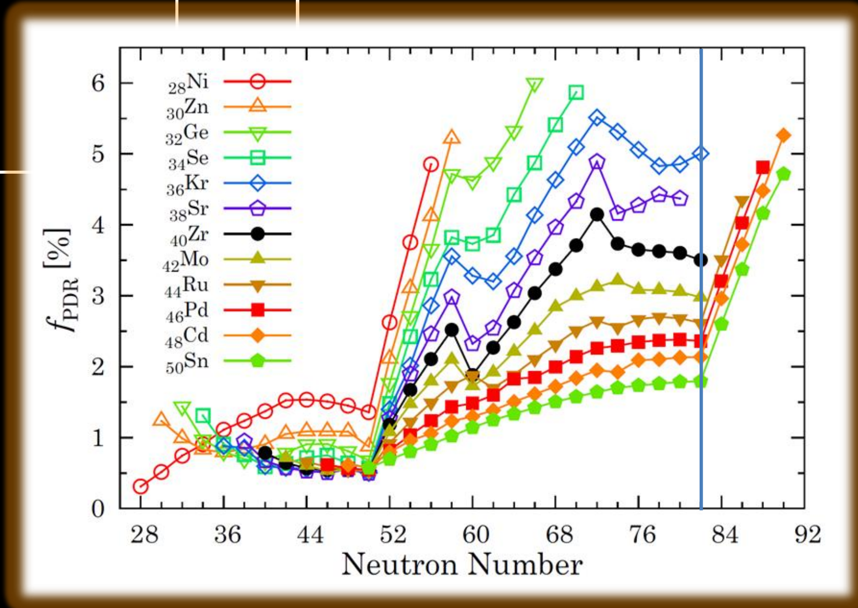


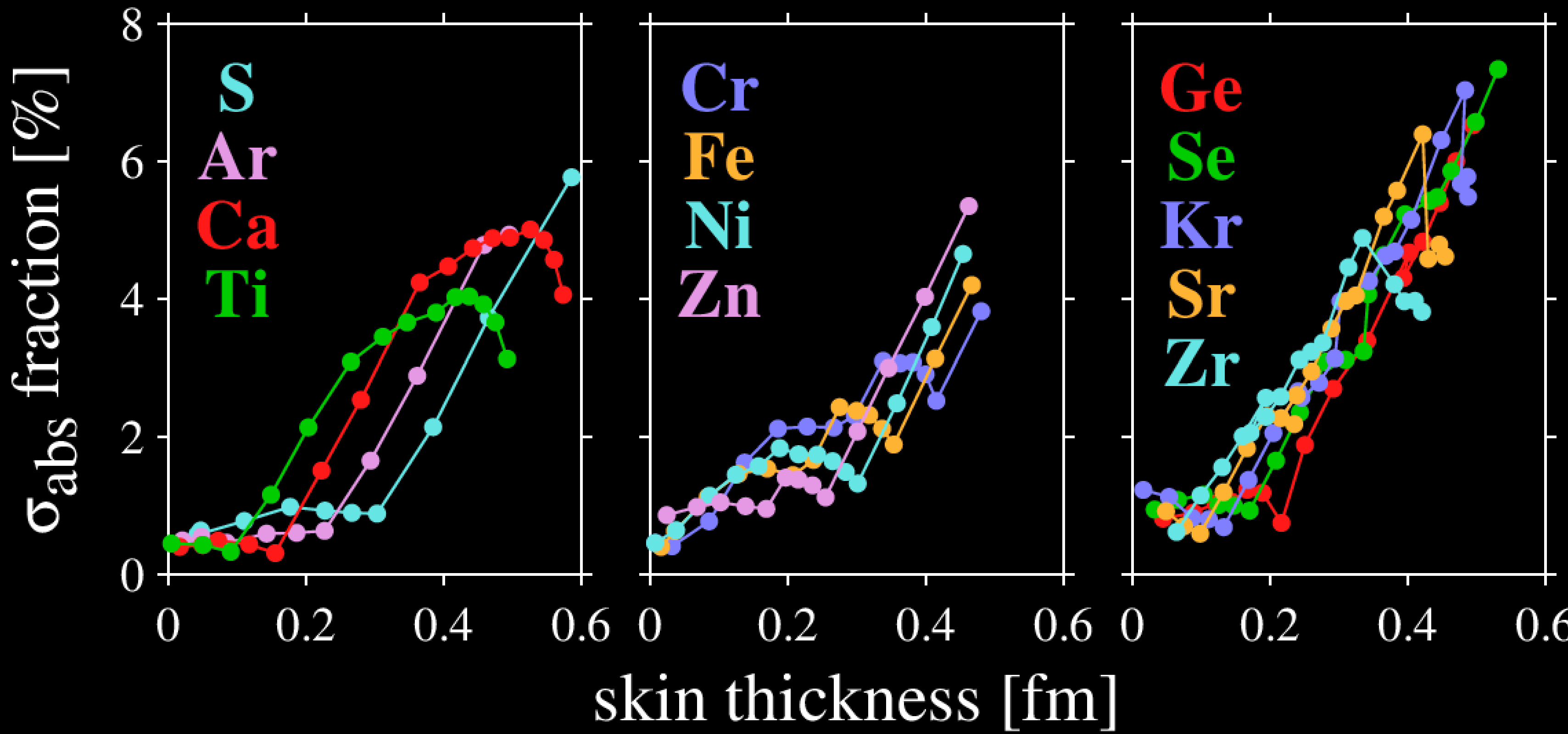
Inakura+,
PRC84, 021302



Canonical-basis TDHFB
Ebata, Nakatsukasa, TI, PRC90, 024303

Universal correlation with skin thickness

- PDR fraction - skin thickness shows a universal rate ~ 0.2 fm^{-1}.
- PDR could be an alternative observation of skin thickness.

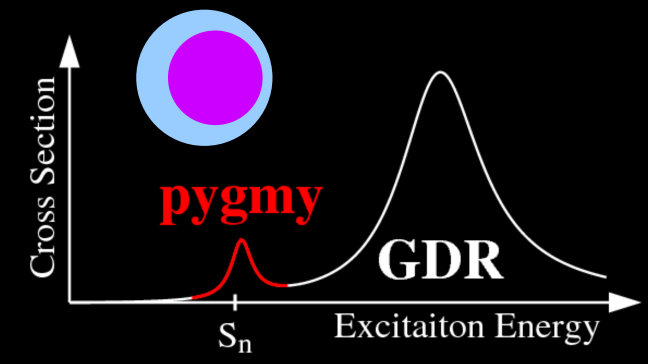


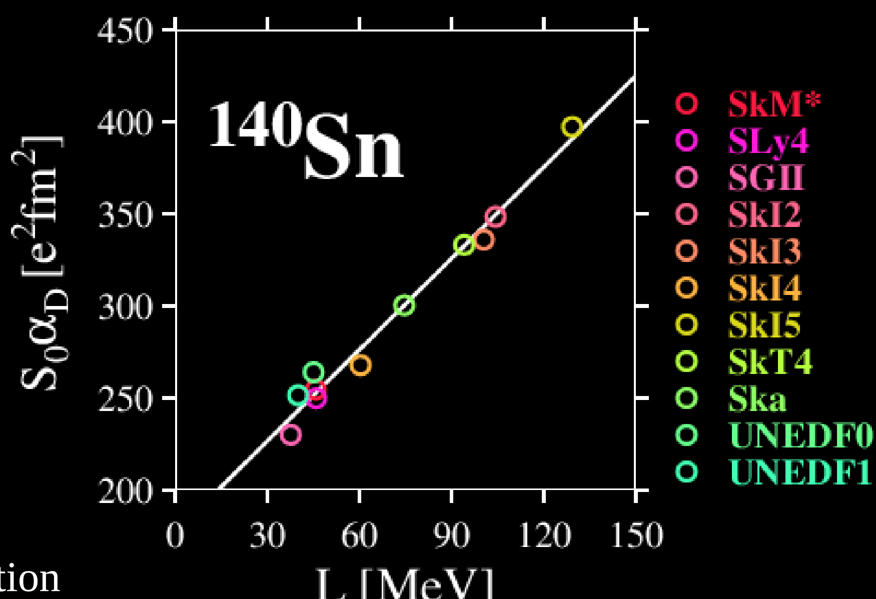
Inakura+, PRC84, 021302

PDR constraints neutron matter EoS.

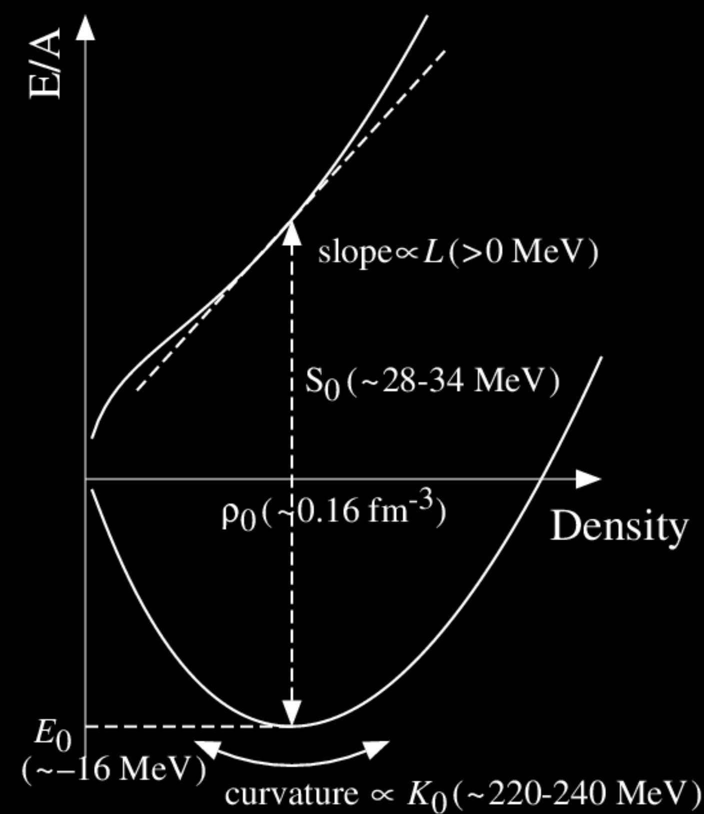
PDR may have some information on neutron matter equation of state.

- Dipole polarizability $\alpha_D \propto \int \mathrm{d}E \, \frac{S(E1;E)}{E}$ is promising for constraint on NM EoS.
- Well-developed PDR in spherical n-rich nuclei is better.





Inakura+,
in preparation



Summary

We performed systematic calculation of E1 responses using DFT and studied properties of PDR.

- There are magic numbers for PDR emergence and development.
- PDR could be an alternative observation of skin thickness.
- PDR could constraint on neutron matter equation of state.

Perspective

Pairing correlation : RPA ⇒ quasi-particle RPA (QPRA)

Dimension of matrix becomes huge.

RPA : particle # x coordinate # ~ O(10^{6-7})

QRPA : coordinate # x coordinate # ~ O(10^{8-9})

⇒ systematic calculation of quadrupole (E2) responses