# Covariant density functional theory in finite nuclei: microscopic theory of quantum phase transistions

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# Content:

- **New density functionals**
  - \- point coupling models
  - \- δ-meson
  - \- tensor forces
  - \- separable-pairing forces
- **Static applications**
  - \- Fission barriers
- **time-dependent density functional theory**
  - \- continuum RPA
  - \- GMR in superfluid nuclei
  - \- pygmy modes
- **energy dependent kernels:**
  - \- level densities
  - \- width of giant resonances
- **spectroscopy with density functionals**
  - \- projection and configuration mixing
  - \- quantum phase transitions

# Density functional theory in nuclei:

- In nuclei DFT has been introduced by **effective Hamiltonians**:

$$E = \langle\Psi|H|\Psi\rangle \approx \langle\Phi|\hat{H}_{eff}(\hat{\rho})|\Phi\rangle = E[\hat{\rho}]$$

Skyrme
Gogny
Rel. MF

- More degrees of freedom: **spin, isospin, relativistic, pairing**

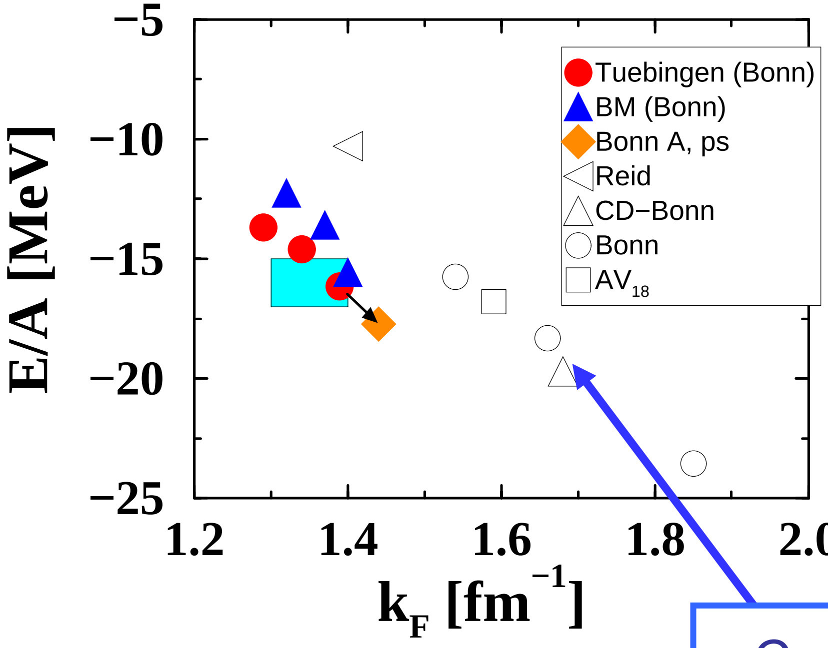
- Nuclei are **self-bound systems**.
  The exact density is a constant. $\rho(r) = \text{const}$
  Hohenberg-Kohn theorem is true, but useless
  $\rho(r)$ has to be replaced by the intrinsic density:

$$\rho_I(\vec{r}) = \rho(\vec{r} + \vec{R}_{CM}) \quad \text{with} \quad \vec{R}_{CM} = \frac{1}{A}\sum_i \vec{r}_i$$

- Density functional theory in nuclei is probably **not exact**,
  but a very good approximation.

## Why covariant:

1) Large spin-orbit splitting in nuclei
2) Large fields V≈350 MeV , S≈-400 MeV
3) Success of Relativistic Brueckner
4) Success of intermediate energy proton scattering
5) relativistic saturation mechanism
6) consistent treatment of time-odd fields
7) Pseudo-spin Symmetry
8) Connection to underlying theories ?
9) **As many symmetries as possible**



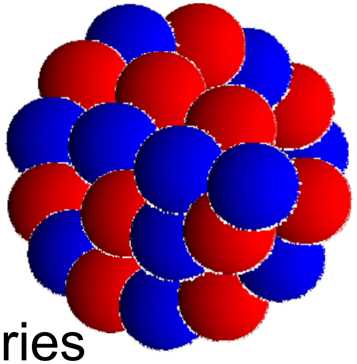
Coester-line

**time-odd fields:**

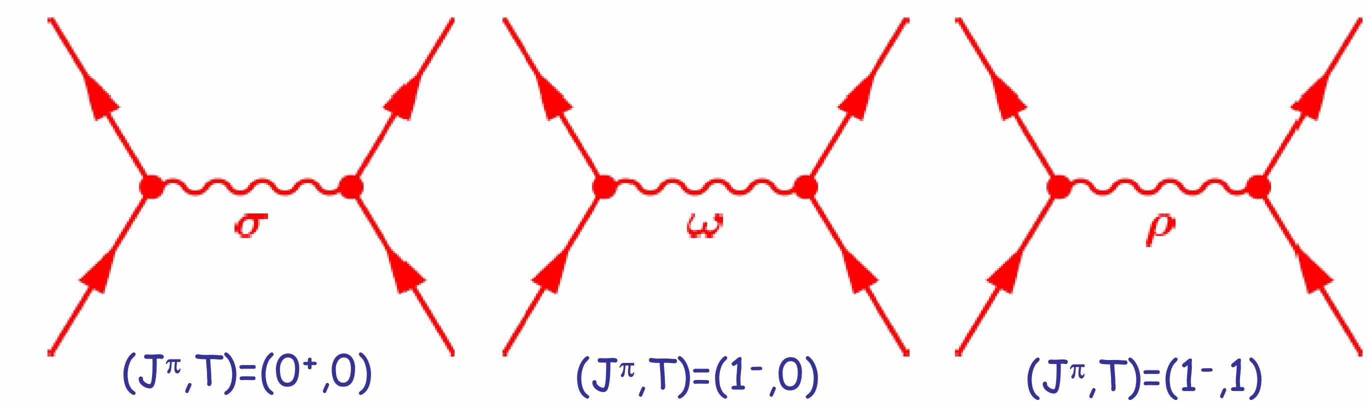
- rotations
  SD bands, magnetic rotation
- odd-mass nuclei
  magnetic moments
- magnetars:
  see poster by Pena et al

$\boxed{E[\rho]}$

# Walecka model:



- the basis is an effective Lagrangian with all relativistic symmetries
- it is used in a mean field concept (Hartree-level)
- with the no-sea approximation



$$S(\mathbf{r}) = g_{\sigma}\sigma(\mathbf{r}) \qquad V(\mathbf{r}) = g_{\omega}\omega(\mathbf{r}) + g_{\rho}\vec{\tau}\vec{\rho}(\mathbf{r}) + eA(\mathbf{r})$$

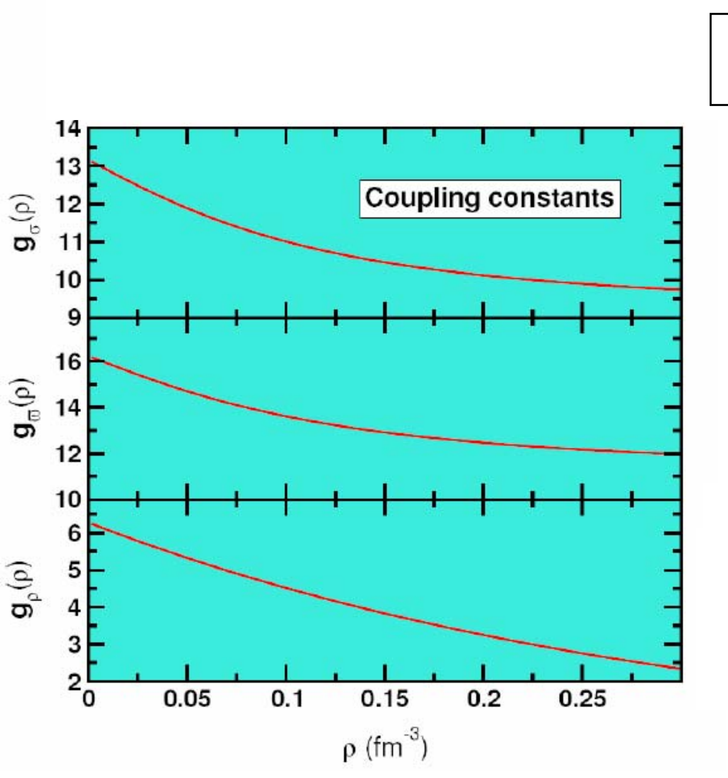
Sigma-meson:
attractive scalar field

Omega-meson:
short-range repulsive

Rho-meson:
isovector field

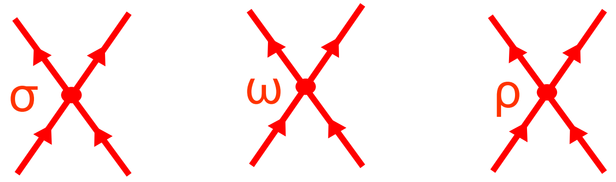
# Effective density dependence:

The basic idea comes from ab initio calculations
density dependent coupling constants include Brueckner correlations
and threebody forces



non-linear meson coupling: **NL3**

Point-coupling models
with derivative terms:

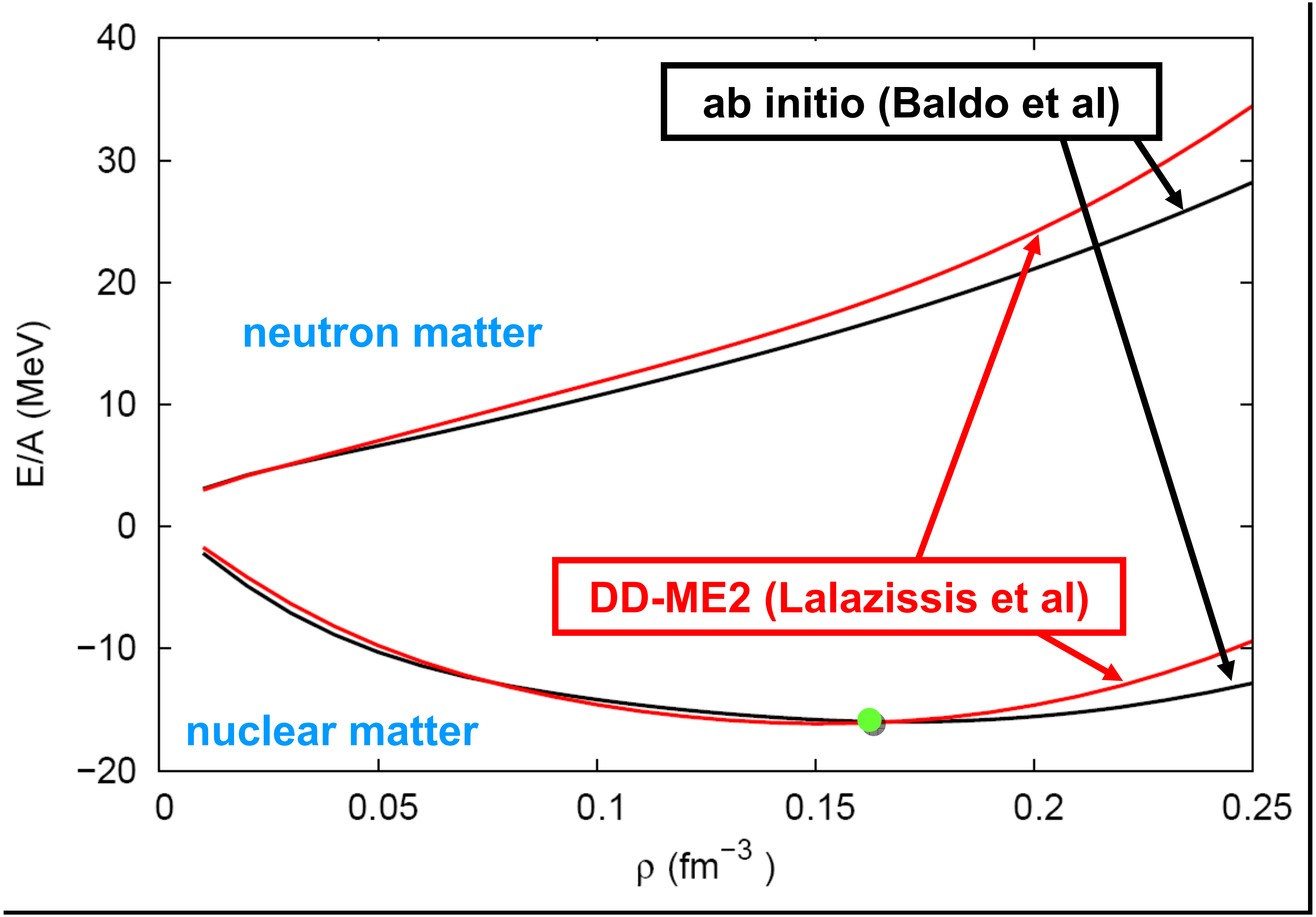


$g_\sigma(\rho)$ $g_\omega(\rho)$ $g_\rho(\rho)$

adjusted to ground state properties of finite nuclei

Manakos and Mannel, Z.Phys. **330**, 223 (1988)
Bürvenich, Madland, Maruhn, Reinhard, PRC **65**, 044308 (2002): **PC-F1,** **PC-PK1**
Niksic, Vretenar, P.R., PRC 78, 034318 (2008): **DD-PC1**

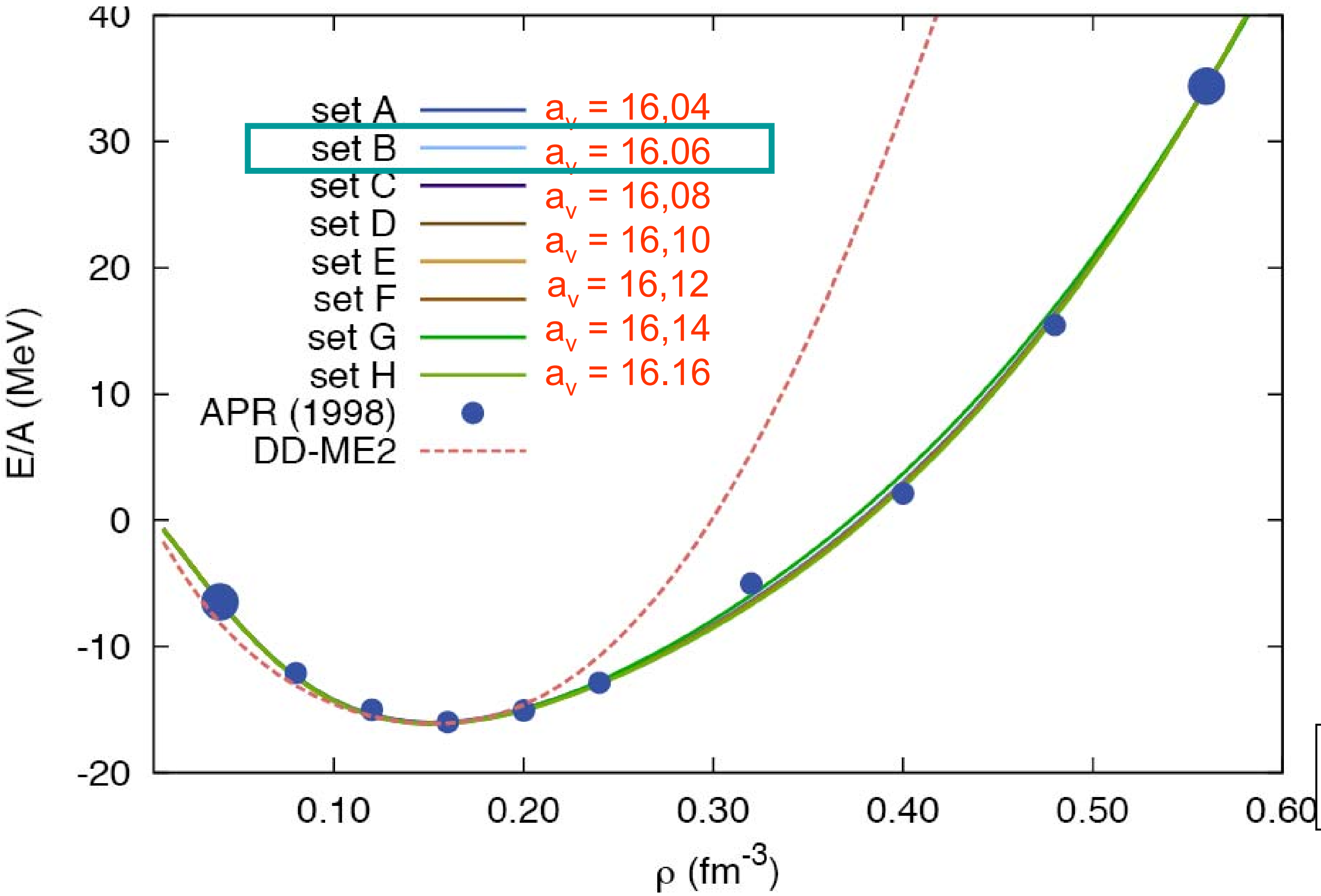
# Comparision with ab initio calculations:



# Fit to ab-initio results and to finite nuclei:

DD-PC1

point coupling model is fitted to microscopic nuclear matter:



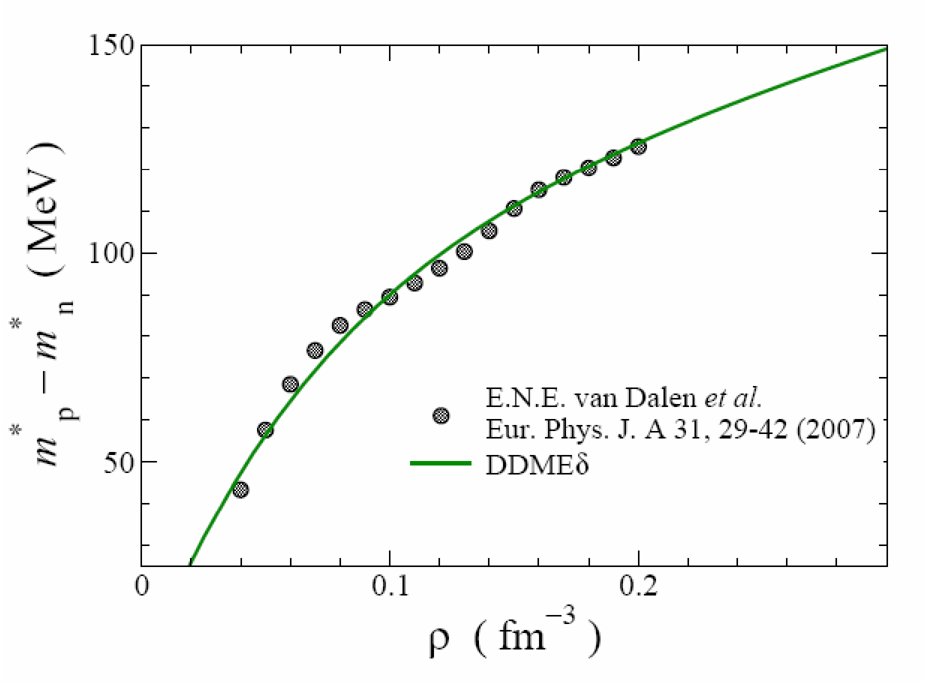
$a_v = 16{,}04$
$a_v = 16.06$
$a_v = 16{,}08$
$a_v = 16{,}10$
$a_v = 16{,}12$
$a_v = 16{,}14$
$a_v = 16.16$

$\rho_{sat} = 0.152\ \mathrm{fm}^{-3}$
$m^* = 0.58m$
$K_{nm} = 230$ MeV

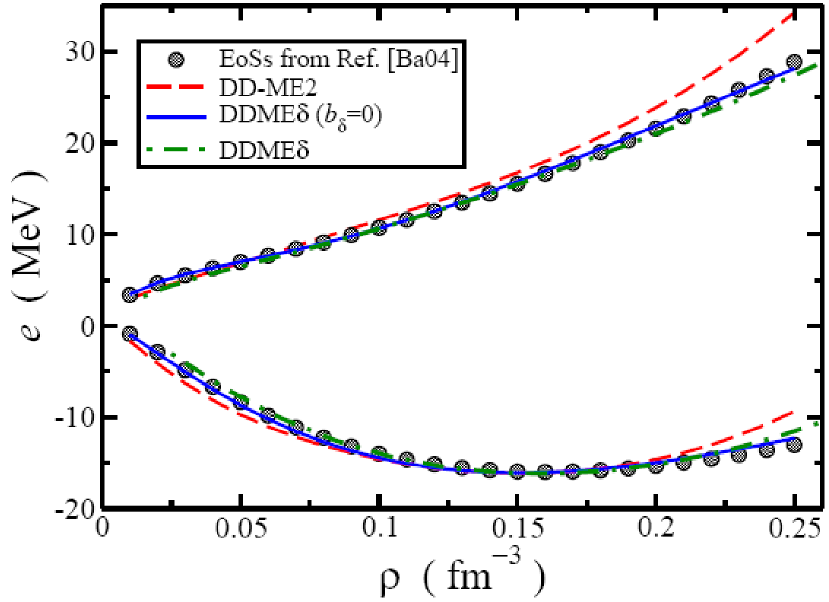
see talk of T. Niksik

● A. Akmal, V.R. Pandharipande, and D.G. Ravenhall, PRC. 58, 1804 (1998).

# Inclusion of the $\delta$ -meson (J=0, T=1) by fit to Rel. Brueckner Calculations:



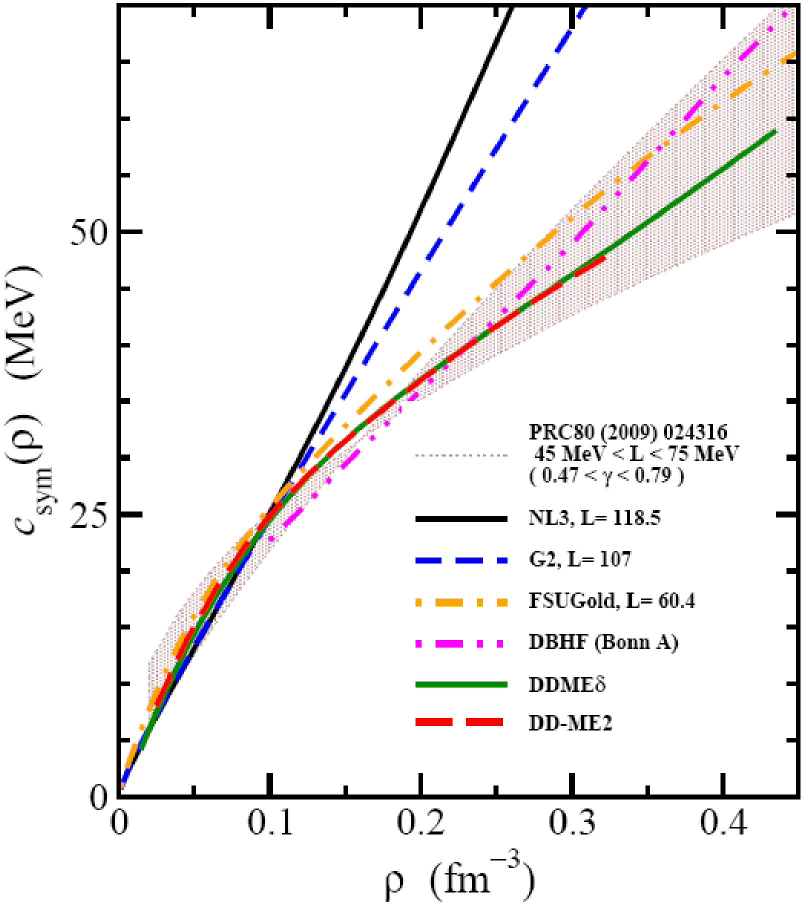
iso-vector effective mass

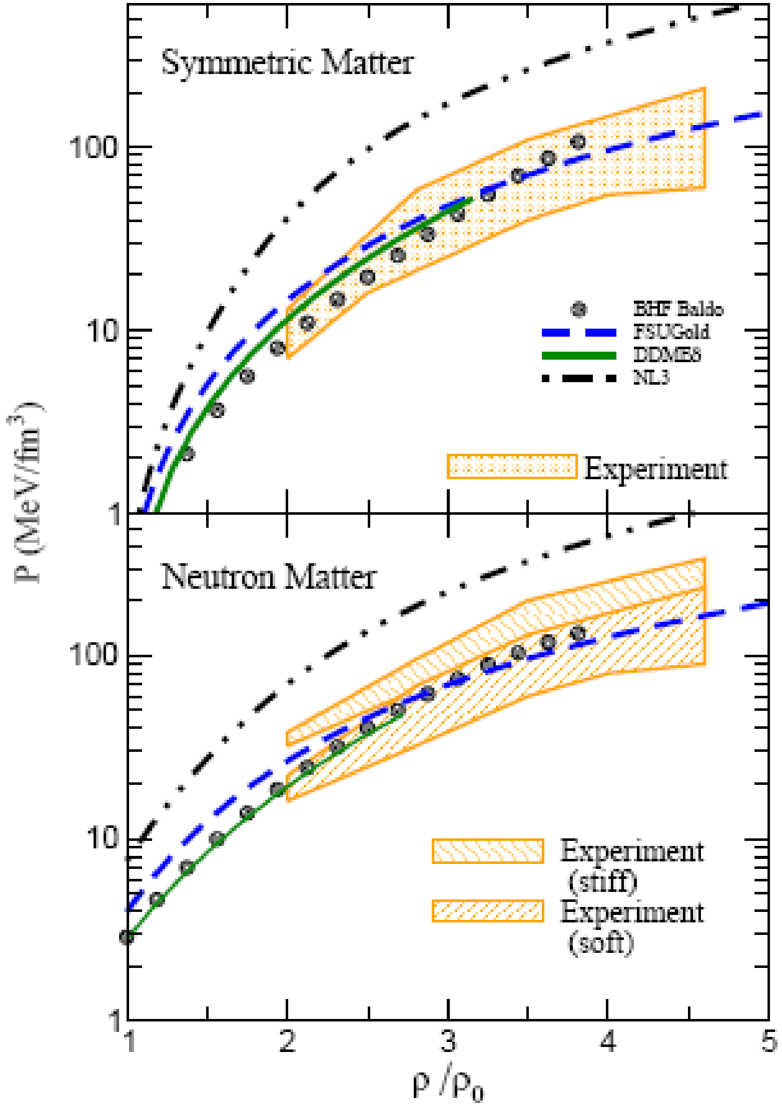


equation of state

Roca-Maza, Centelles, Vinas, P.R., Schuck (2010)

# Symmetry energy:

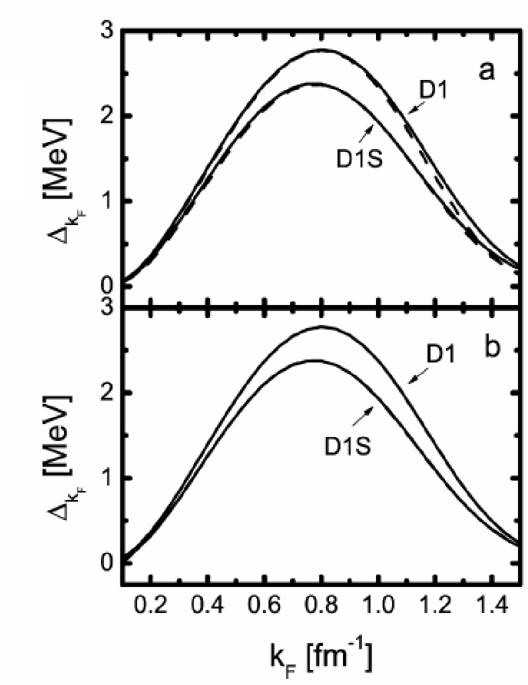




pressure at high densities

# effective pairing forces:

nucl. matter:



seniority force: constant G
zero range; δ-force

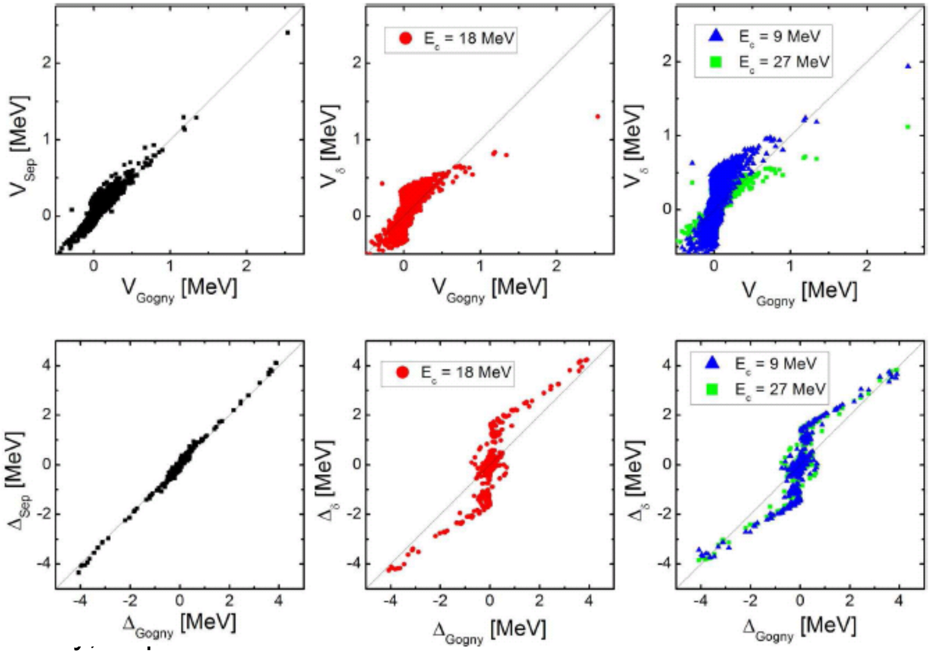
pairing part of Gogny D1S

Gonzales-Llarena et al, PLB 379, 13 (1996)

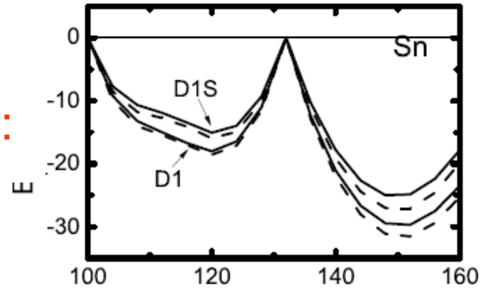
Gogny equivalent separable force:

Tian, Ma, P.R. PLB 676, 44 (2009)

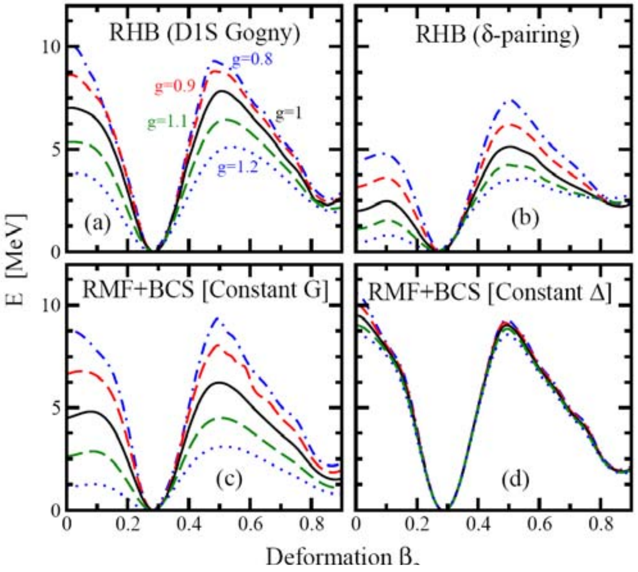
$$V^{0}_{121'2'} = -\,G\sum_{N} V^{N}_{12}V^{N}_{1'2'}$$

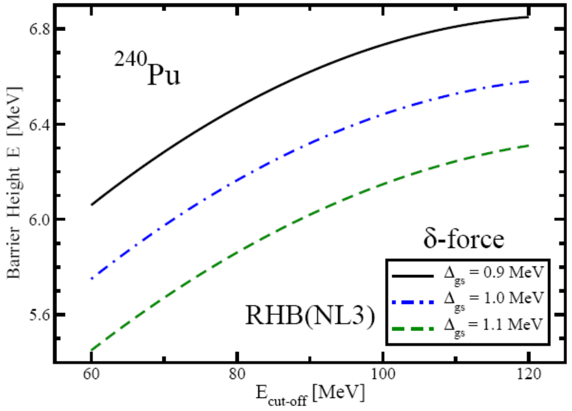


finite nuclei:



# Influence of pairing on the fission barriers:



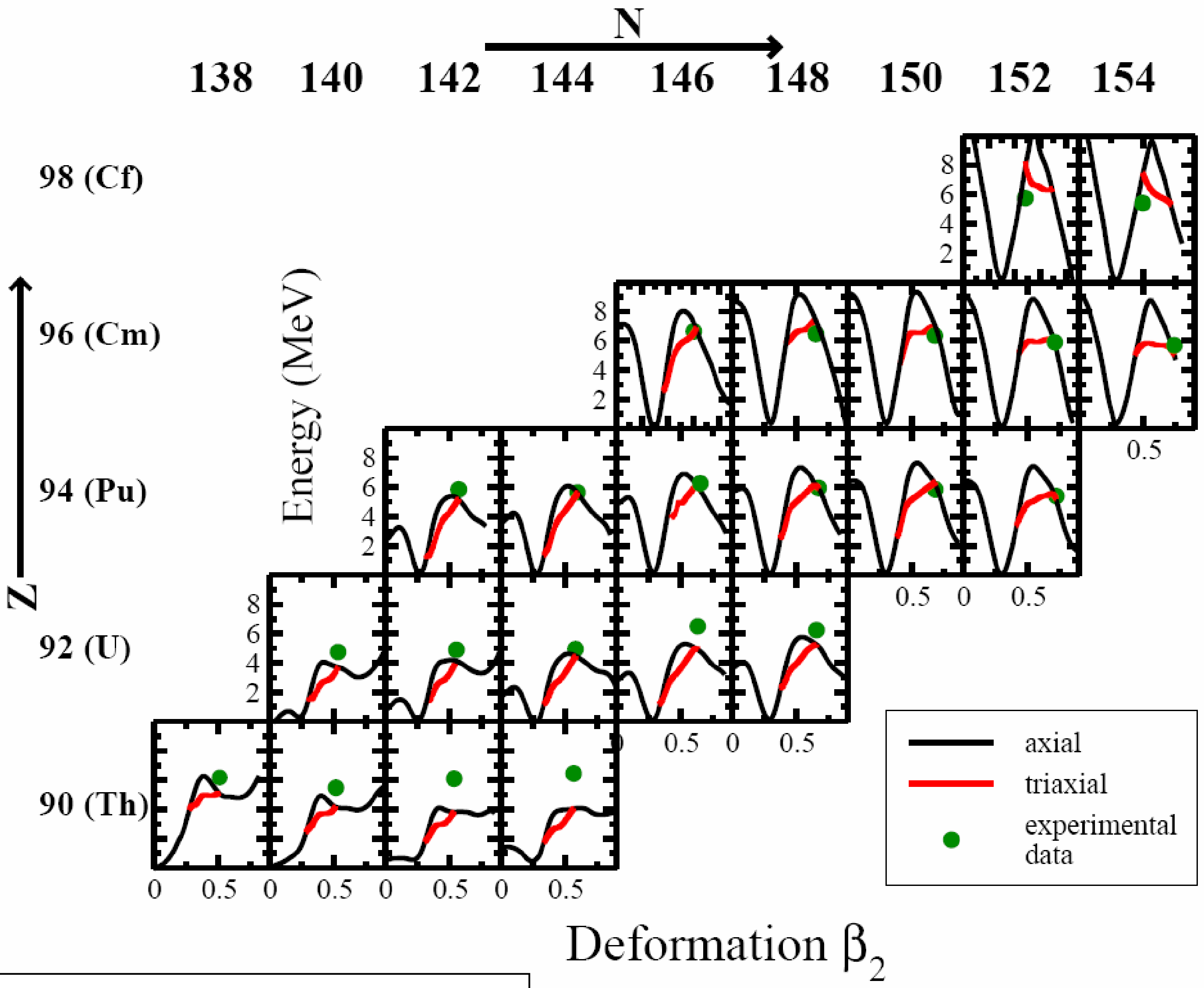


- fission barriers depend senitively on the strength of the pairing force

- for δ-pairing with identical ground state gap the barrier height depends on the cut-off energy

(Karatzikos et al, PLB 689, 72 (2010)

# Fission barriers for triaxially deformed shapes:



Abusara, Afanasjev,P.R. PRC, in print

# Time dependent density functional theory:

$$\int dt\,\{\langle\Phi(t)|i\partial_t|\Phi(t)\rangle - E_t[\rho(t)]\} = 0$$

Runge-Gross theorem
PRL 52, 997 (1984)

$$i\partial_t\hat{\rho} = \left[\hat{h}(\hat{\rho}) + \hat{f}, \hat{\rho}\right]$$

$$\boxed{i\partial_t\psi(t) = [(\vec{\alpha}(\vec{p} - \vec{V}(t)) + V(t) + \beta(m - S(t))]\psi(t)}$$

We neglect retardation
and find for the fields
at each time-step:

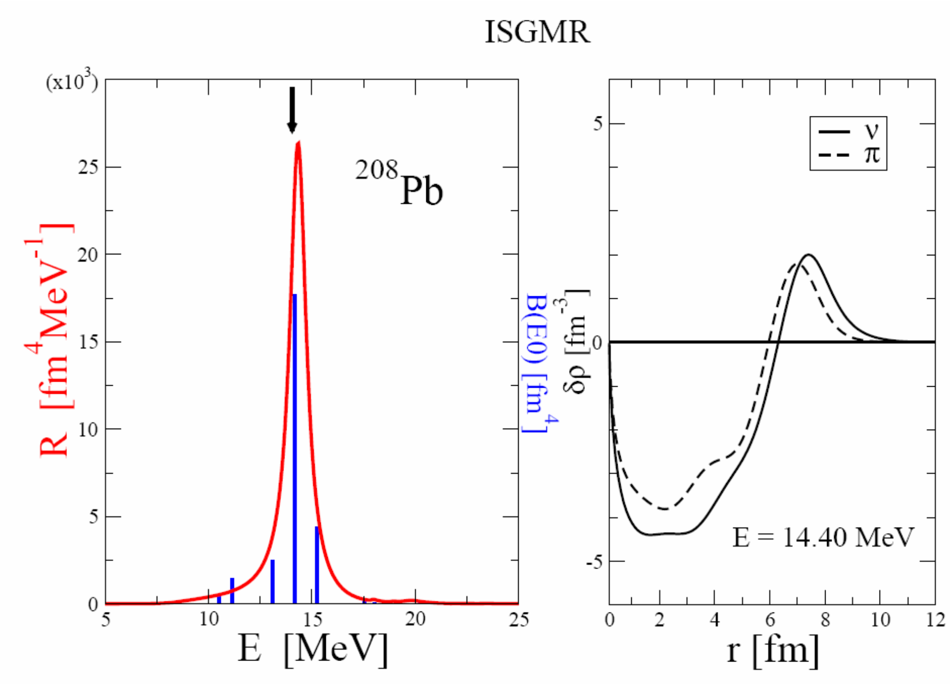
$$S(t) = G_\sigma \rho_s(t)$$

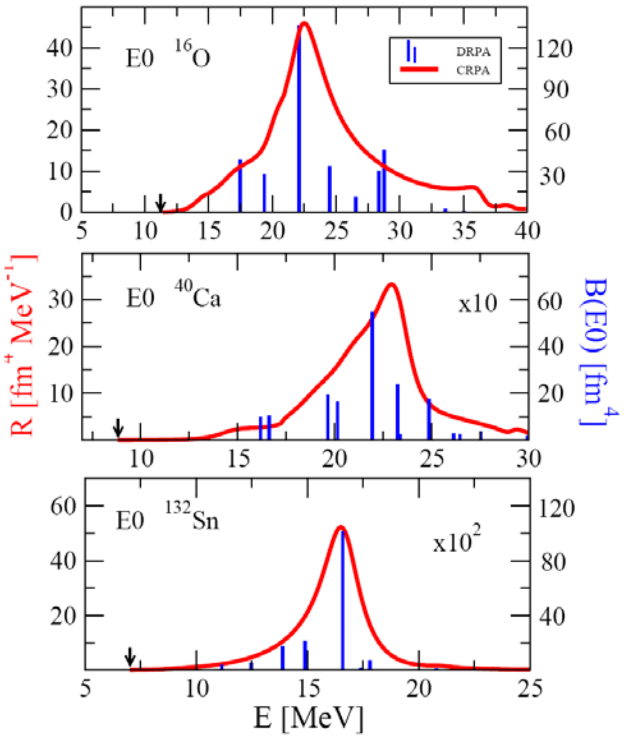
$$V(t) = G_\omega \rho(t)$$

$$\vec{V}(t) = G_\omega \vec{j}(t)$$

and similar equations for the isovector and electromagnetic-fields

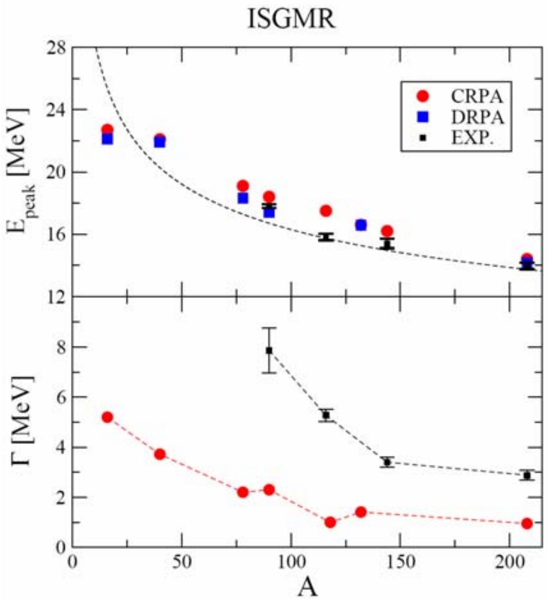
# Rel. Continuum RPA: E0:





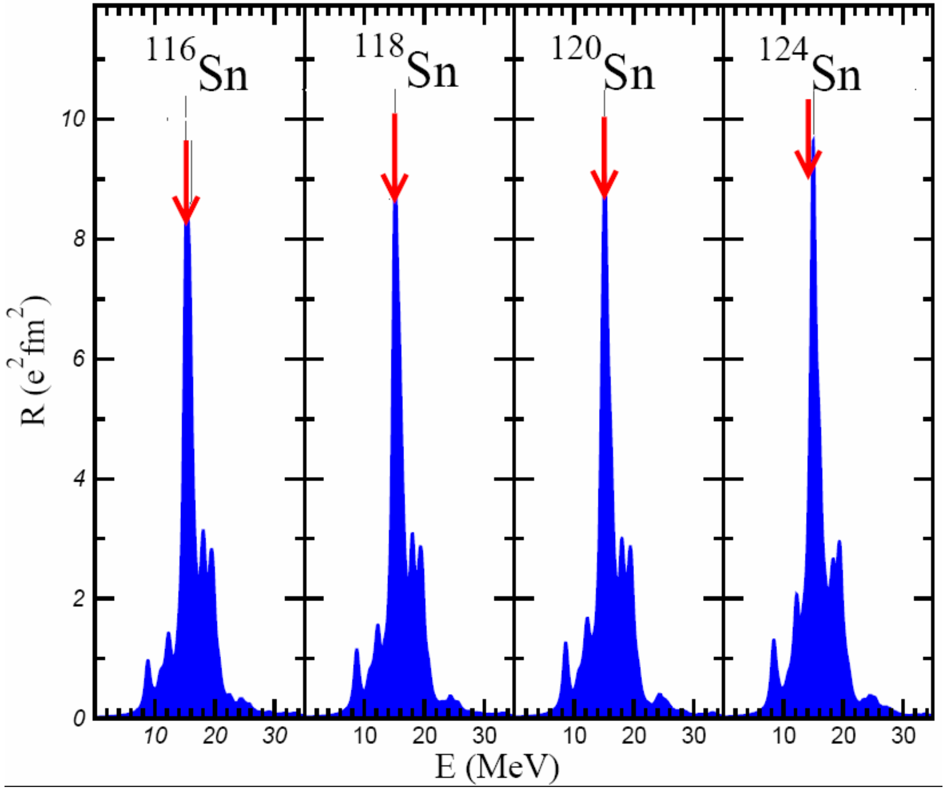
peak energy:

escape width:



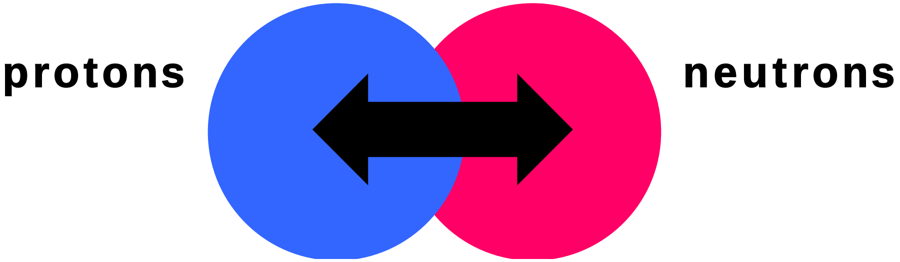
I. Daoutidis, P.R. PRC 80, 024309 (2009)

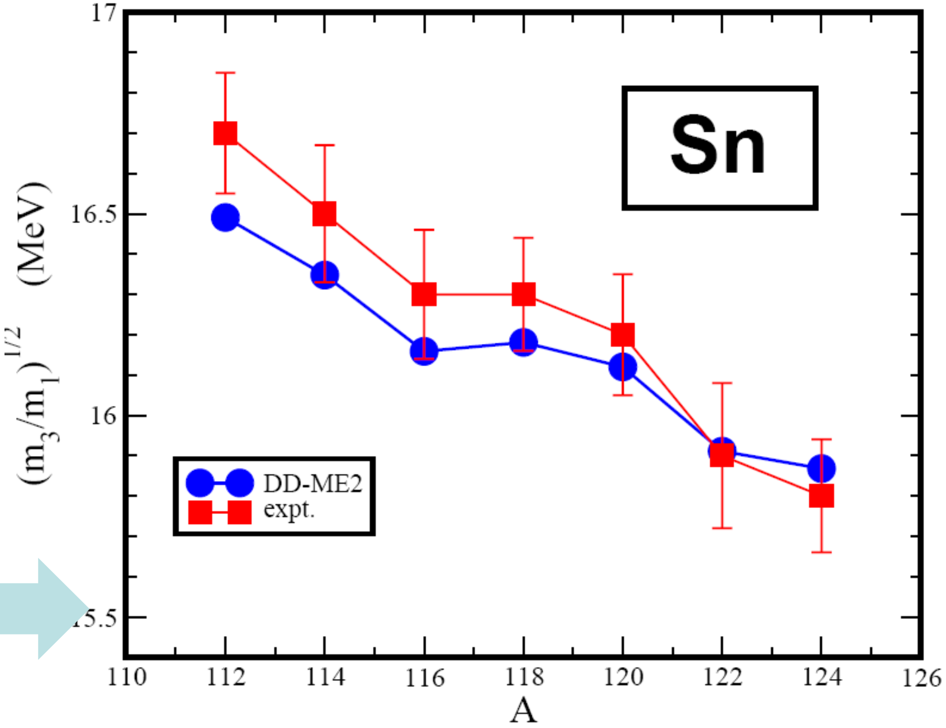
# Relativistic (Q)RPA calculations of giant resonances

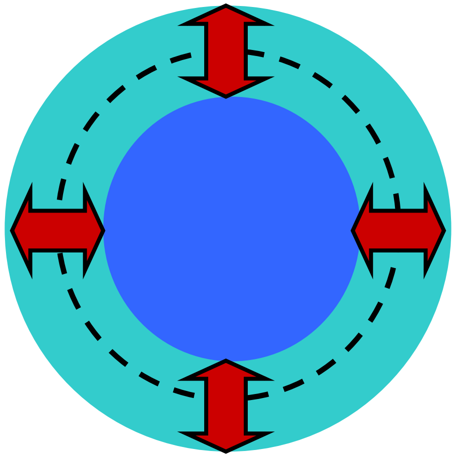


Sn isotopes: DD-ME2 effective interaction + Gogny pairing

Isovector dipole response







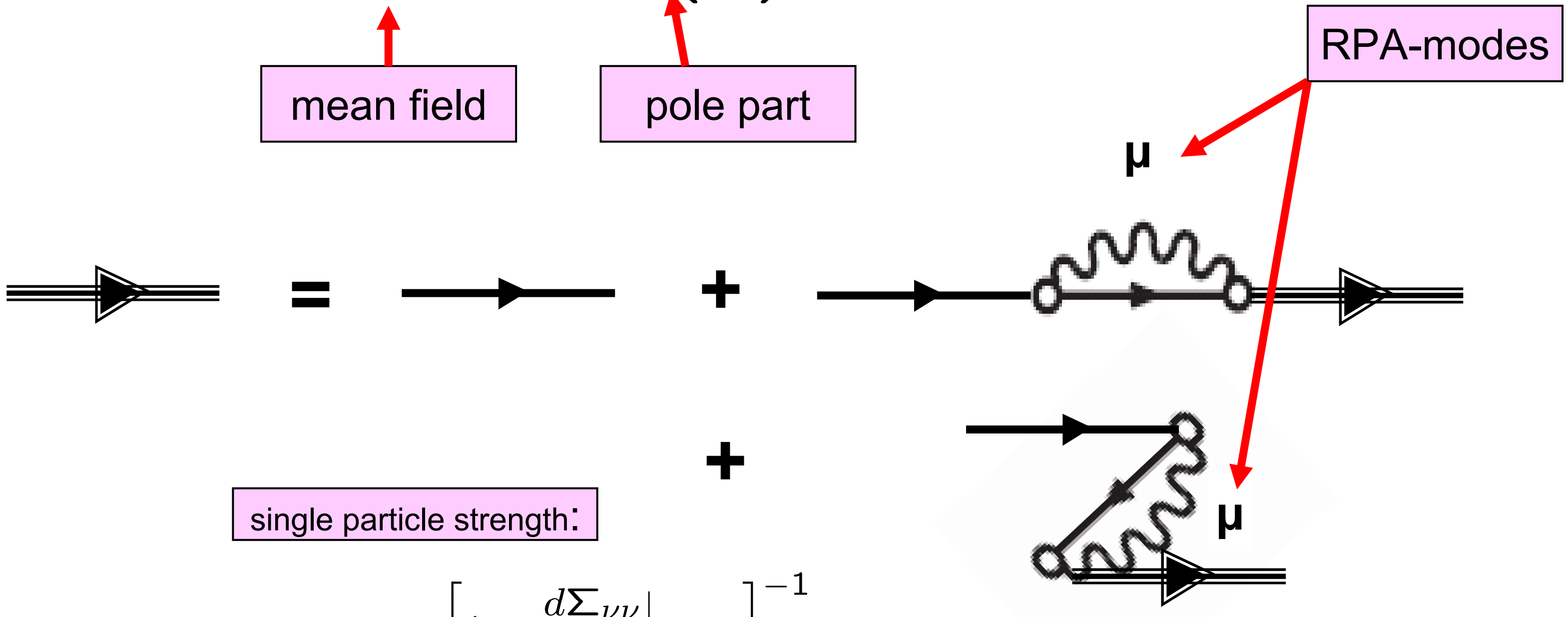
Isoscalar monopole response

# Energy dependent kernel: particle-vibr. coupling

$$\Sigma = S + V + \Sigma(\omega)$$

mean field

pole part

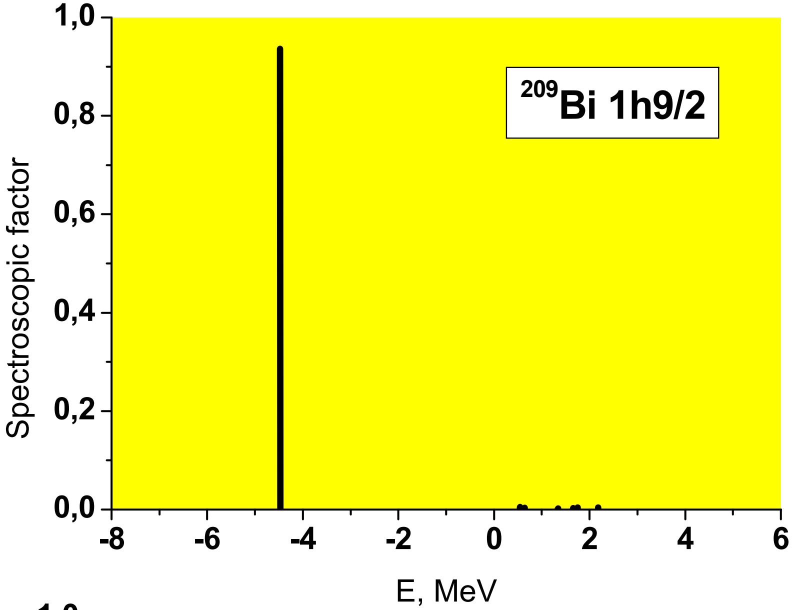


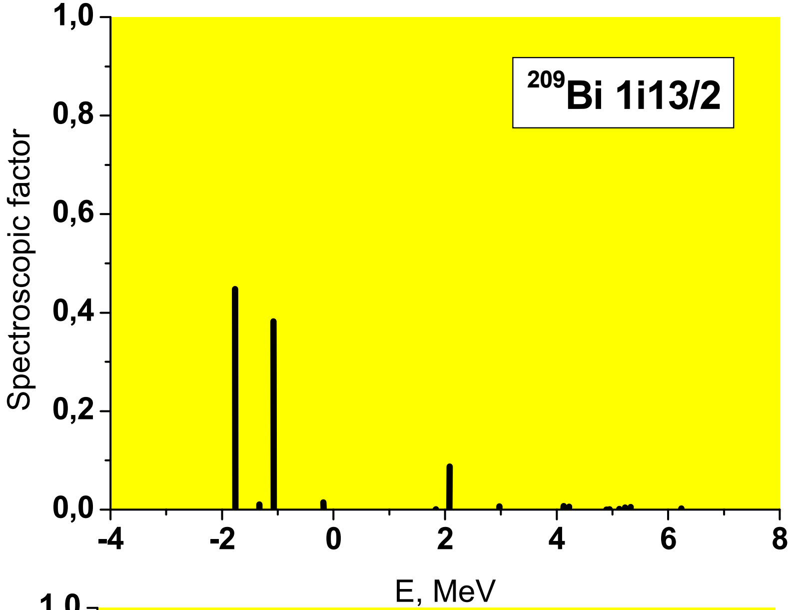
single particle strength:

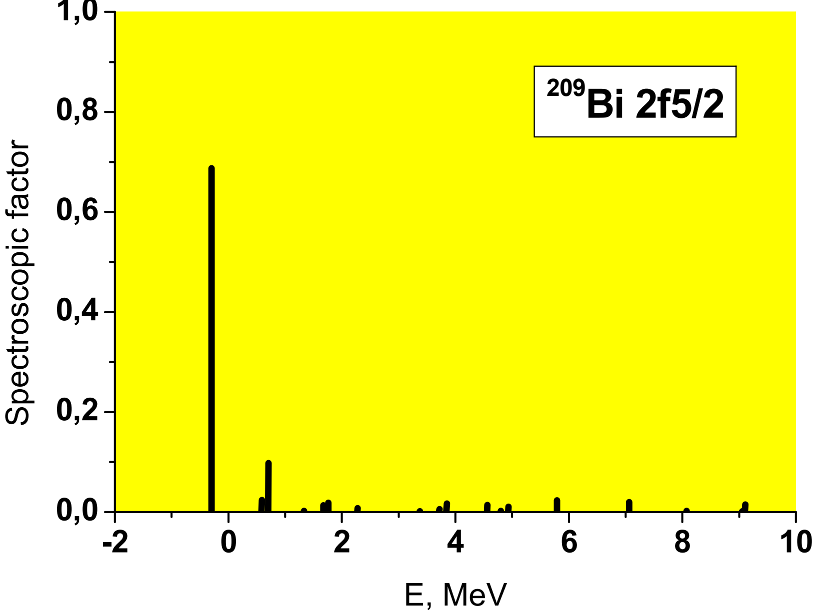
$$z_\nu = \left[ 1 - \frac{d\Sigma_{\nu\nu}}{d\omega}\bigg|_{\omega=\epsilon_\nu} \right]^{-1}$$

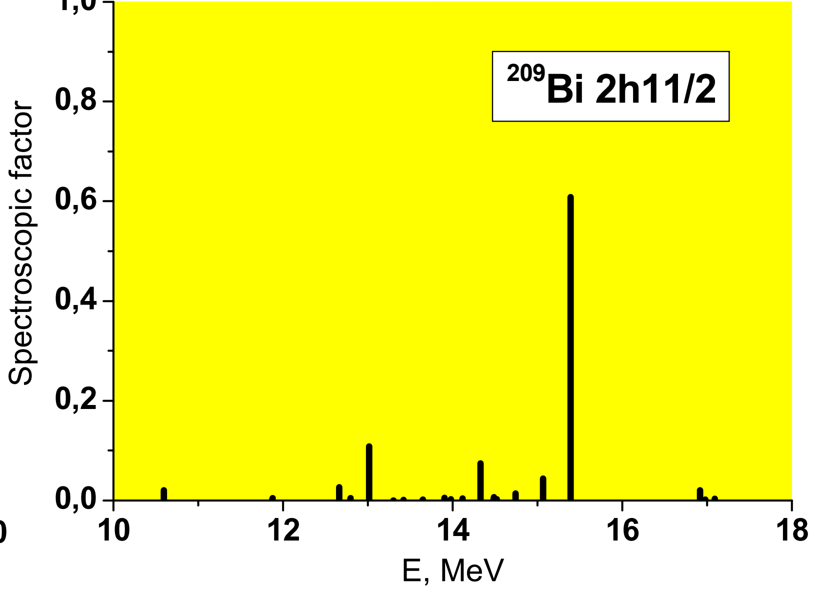
**Density functional theory - Landau-Migdal theory**

# Distribution of single-particle strength in $^{209}$Bi

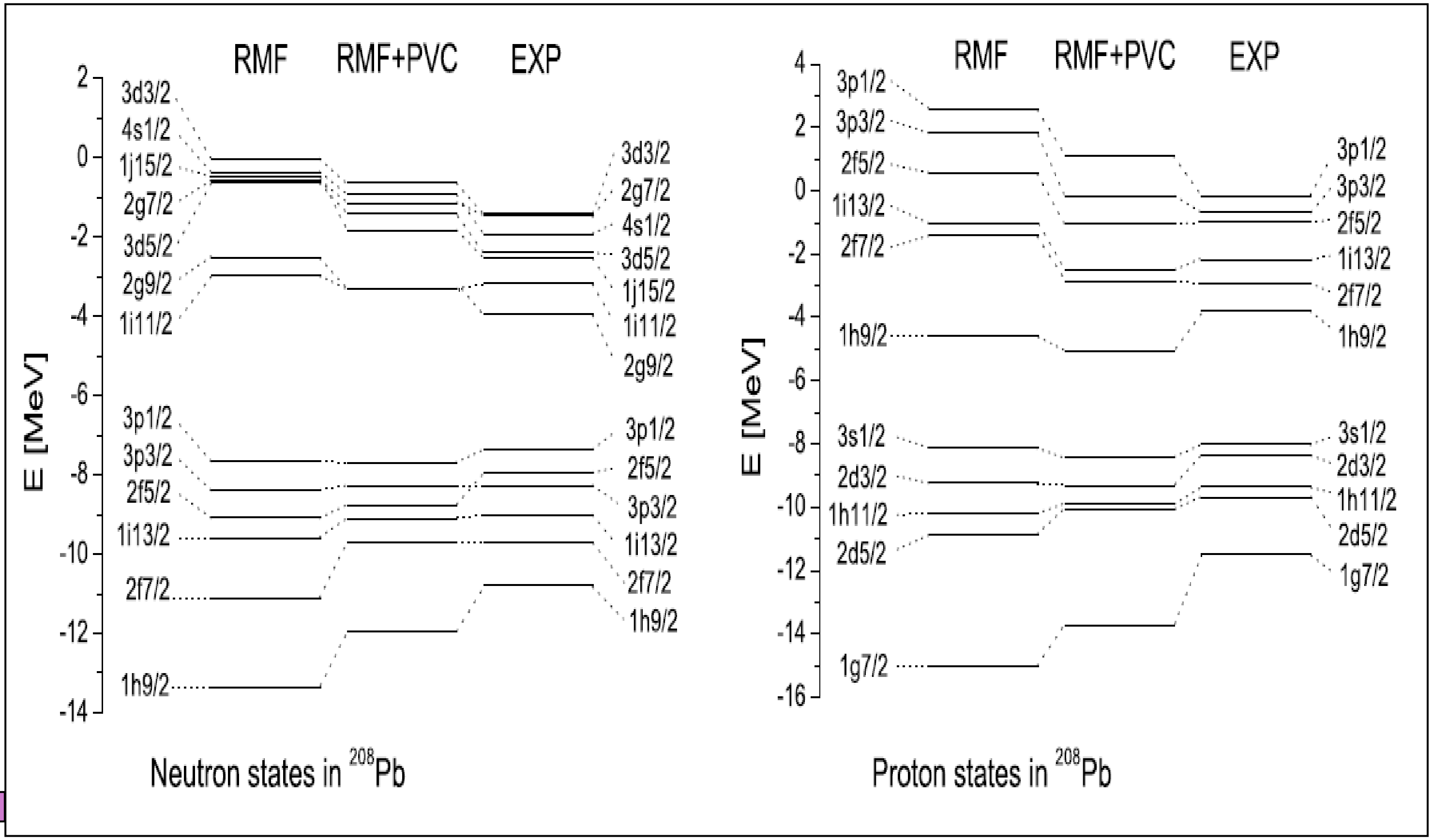








# Single particle spectrum in the Pb region:



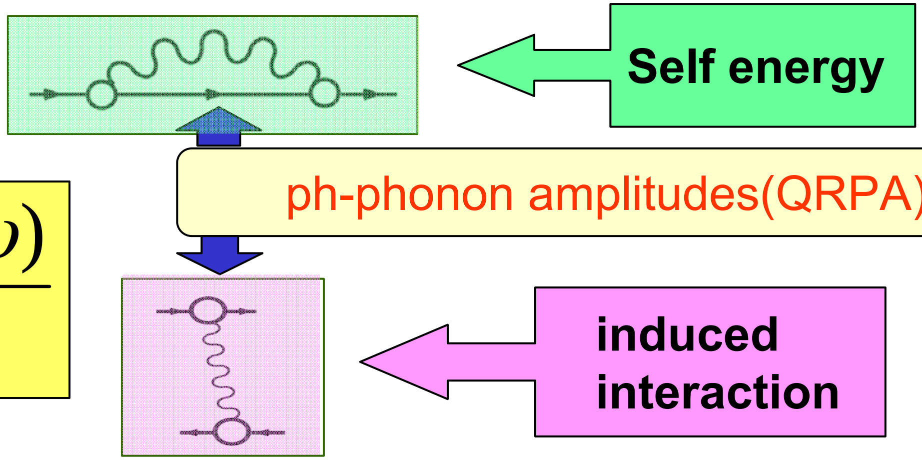
$m_{eff}$ **0.76** **0.92** **1.0** **0.71** **0.85** **1.0**

E. Litvinova, P.R., PRC 73, 44328 (2006)

# Width of Giant Resonances:

The full response contains energy dependent parts coming from vibrational couplings.

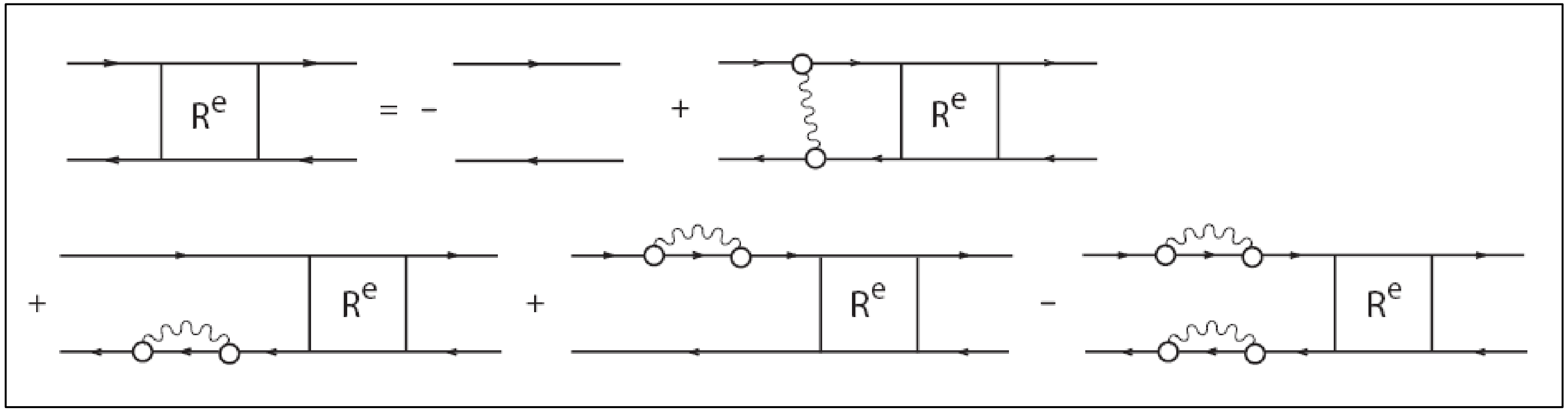
$$V(\omega)=\frac{\delta\Sigma(\omega)}{\delta\rho}$$



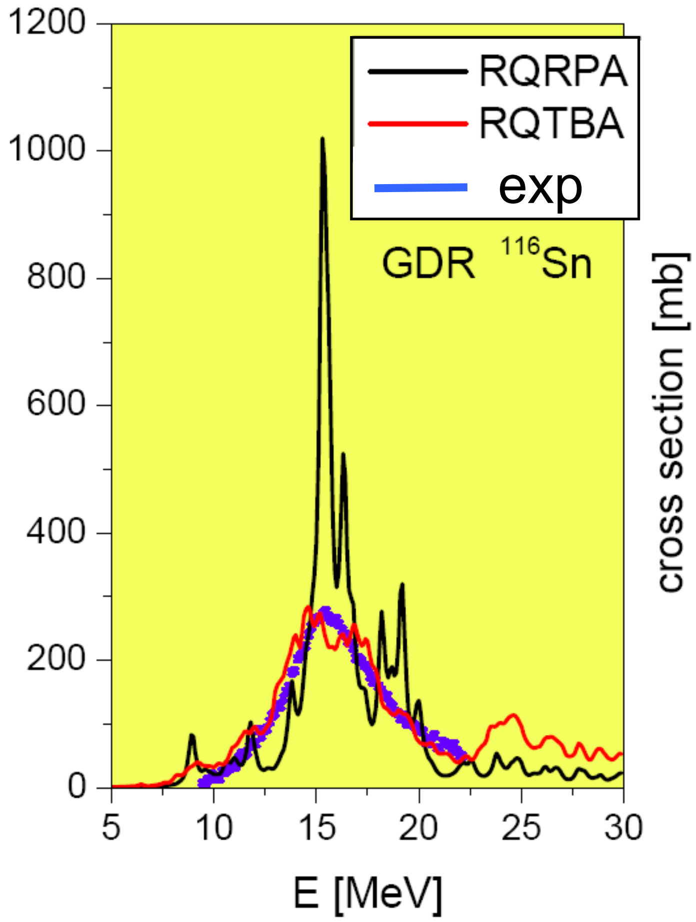
**Self energy**

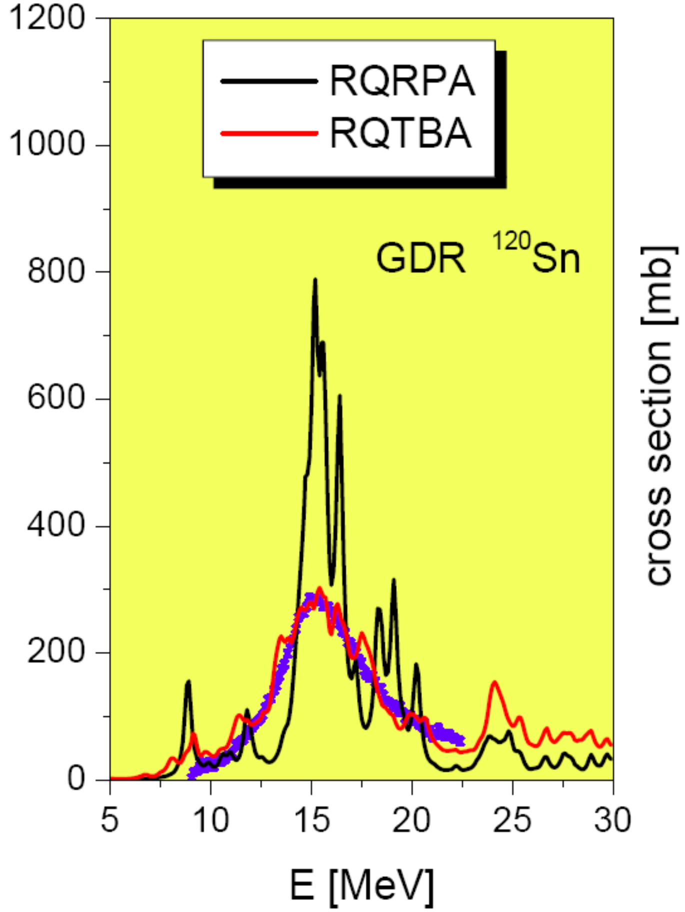
ph-phonon amplitudes(QRPA)

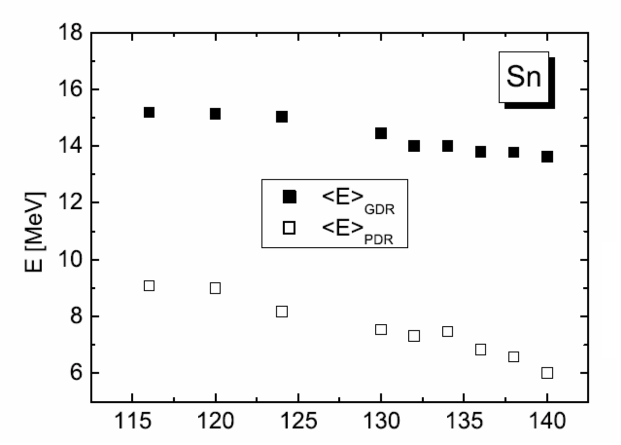
**induced interaction**



Litvinova, P.R. Tselyaev, PRC 75, 64308 (2007)







centroid energies for
GDR and PDR

Litvinova, P.R. Tselyaev, PRC 78, 14312 (2008)
Litvinova, P.R. Tselyaev, Langanke, PRC 79, 054312 (2009)

# Parameters of Lorentz distribution* (GDR)

| | | <E> (MeV) | Γ (MeV) | EWSR (%) |
|---|---|---|---|---|
| $^{208}$Pb | RRPA | 12.9 | 2.0 | 128 |
| | RRPA-PC | 13.7 | 4.3 | 134 |
| | Exp. [1] | 13.4 | 4.1 | |
| $^{132}$Sn | RRPA | 14.5 | 2.6 | 126 |
| | RRPA-PC | 15.1 | 4.4 | 131 |
| | Exp. [2] | 16.1(7) | 4.7(2.1) | |
| $^{48}$Ni | RRPA | 17.9 | 3.1 | 119 |
| | RRPA-PC | 18.6 | 5.1 | 125 |
| $^{46}$Fe | RRPA | 17.9 | 3.2 | 122 |
| | RRPA-PC | 18.7 | 5.5 | 128 |

*Averaging interval: 0-30 MeV

[1] Reference Input Parameter Library, Version 2

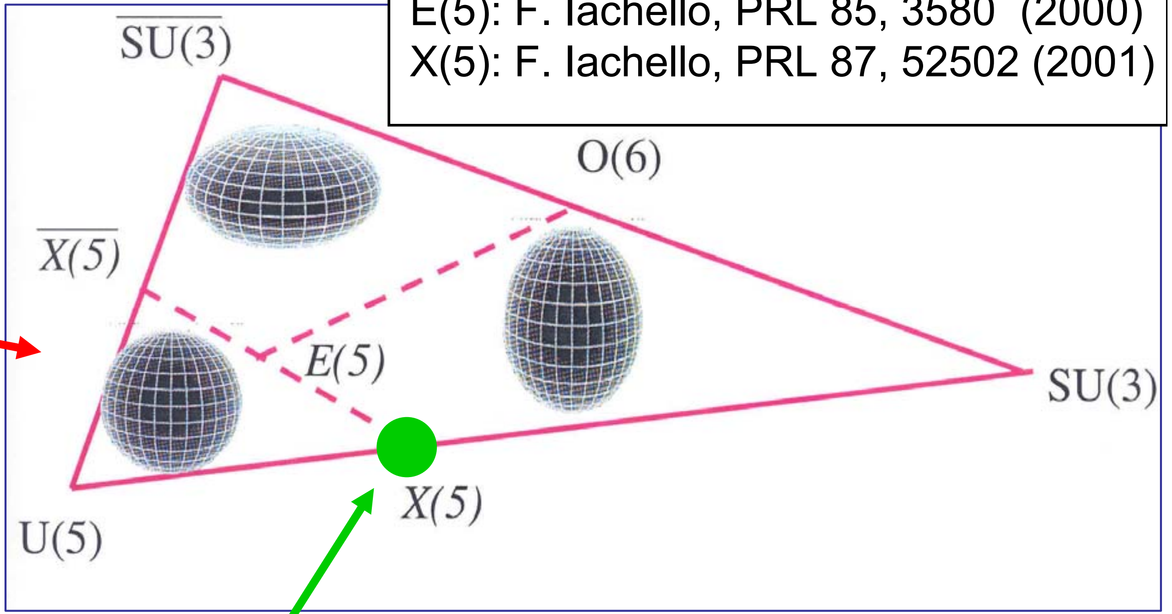
[2] Adrich et al., PRL **95**, 132501 (2005).

# Quantum phase transitions and critical symmetries:

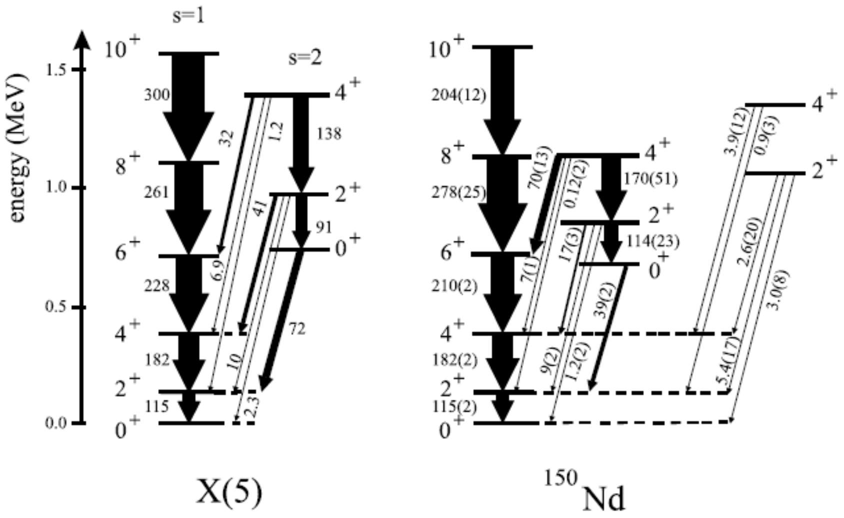
**Interacting Boson Model**

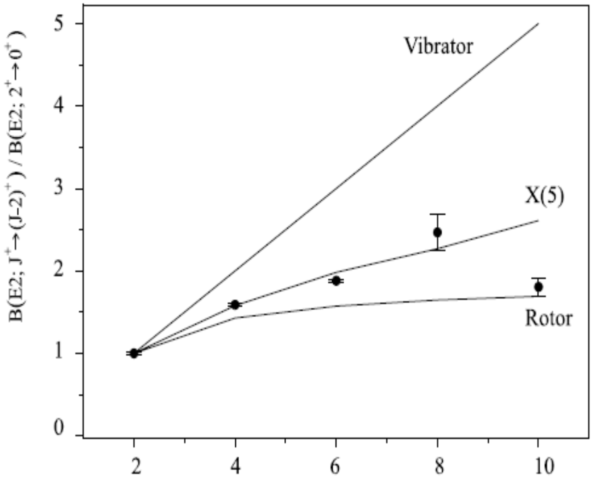
**Casten Triangle**

E(5): F. Iachello, PRL 85, 3580  (2000)
X(5): F. Iachello, PRL 87, 52502 (2001)



R. Krücken *et al*, PRL 88, 232501  (2002)

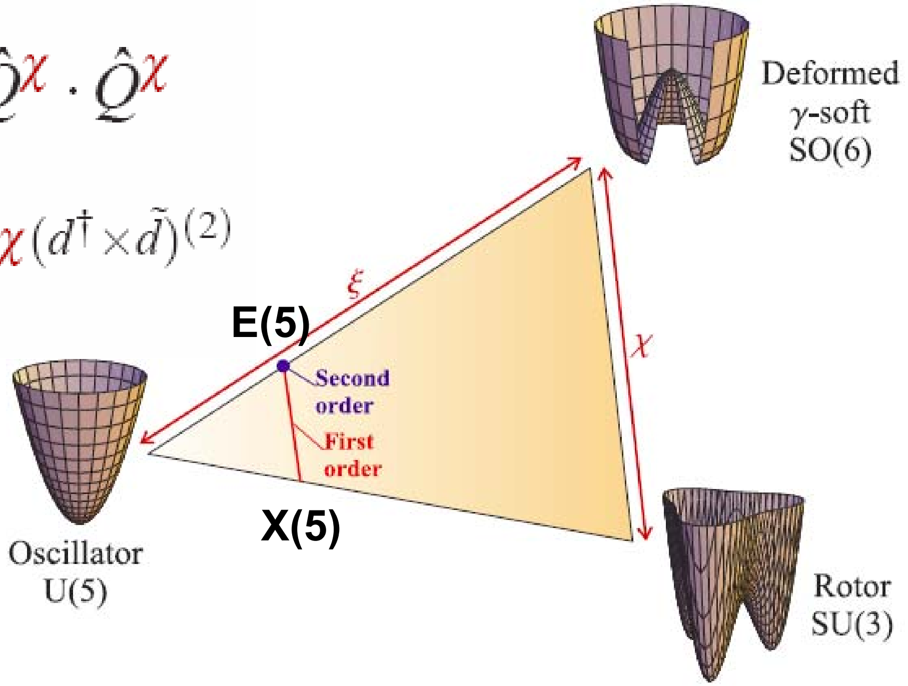




# Quantum phase transitions in the Interacting boson model:

$$H_{\mathrm{IBM}} = \frac{(1-\xi)}{N}\hat{n}_d - \frac{\xi}{N^2}\hat{Q}^{\chi}\cdot\hat{Q}^{\chi}$$

$$\hat{n}_d = d^{\dagger}\cdot\tilde{d} \qquad \hat{Q}^{\chi} = (s^{\dagger}\times\tilde{d} + d^{\dagger}\times\tilde{s})^{(2)} + \chi(d^{\dagger}\times\tilde{d})^{(2)}$$



$$|\beta,\gamma;N\rangle \quad = \quad (N!)^{-1/2}(b_c^{\dagger})^{N}\,|0\rangle\ ,$$

$$b_c^{\dagger} = (1+\beta^2)^{-1/2}[\beta\cos\gamma\, d_0^{\dagger} + \beta\sin\gamma\,(d_2^{\dagger} + d_{-2}^{\dagger})/\sqrt{2} + s^{\dagger}]$$

E(5): F. Iachello, PRL 85, 3580 (2000)
X(5): F. Iachello, PRL 87, 52502 (2001)

Can a universal density functional, adjusted to ground state properties, at the same time reproduce critical phenomena in spectra ?

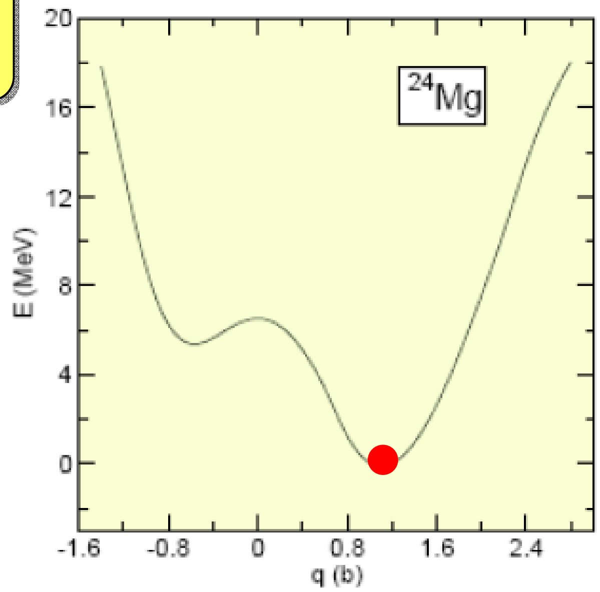
We need a method to derive spectra: GCM, ATDRMF

We consider the chain of Ne-isotopes with a phase transition from spherical (U(5)) to axially deformed (SU(3))

# Generator Coordinate Method (GCM):

$$\langle \delta\Phi | \hat{H} - q\hat{Q} | \Phi \rangle = 0$$

$$| q \rangle = | \Phi(q) \rangle$$



Constraint Hartree Fock produces
wave functions depending on a generator coordinate q

$$|\Psi\rangle = \int dq\ f(q) | q \rangle$$

GCM wave function is a
superposition of Slater determinants

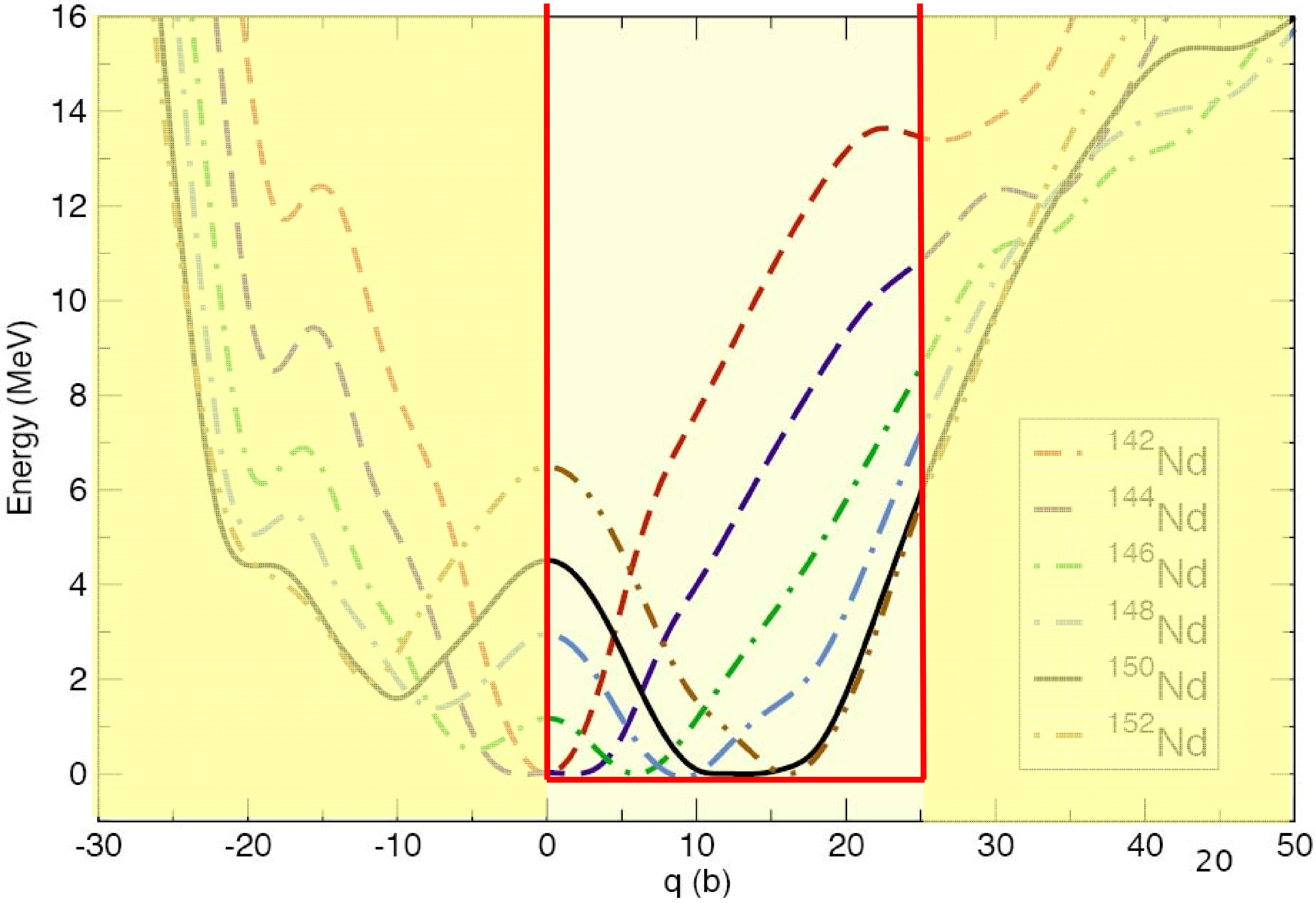
Hill-Wheeler equation:

$$\int dq' \left[ \langle q | H | q' \rangle - E \langle q | q' \rangle \right] f(q') = 0$$

with projection:

$$|\Psi\rangle = \int dq\ f(q) \hat{P}^N \hat{P}^I \, | q \rangle$$

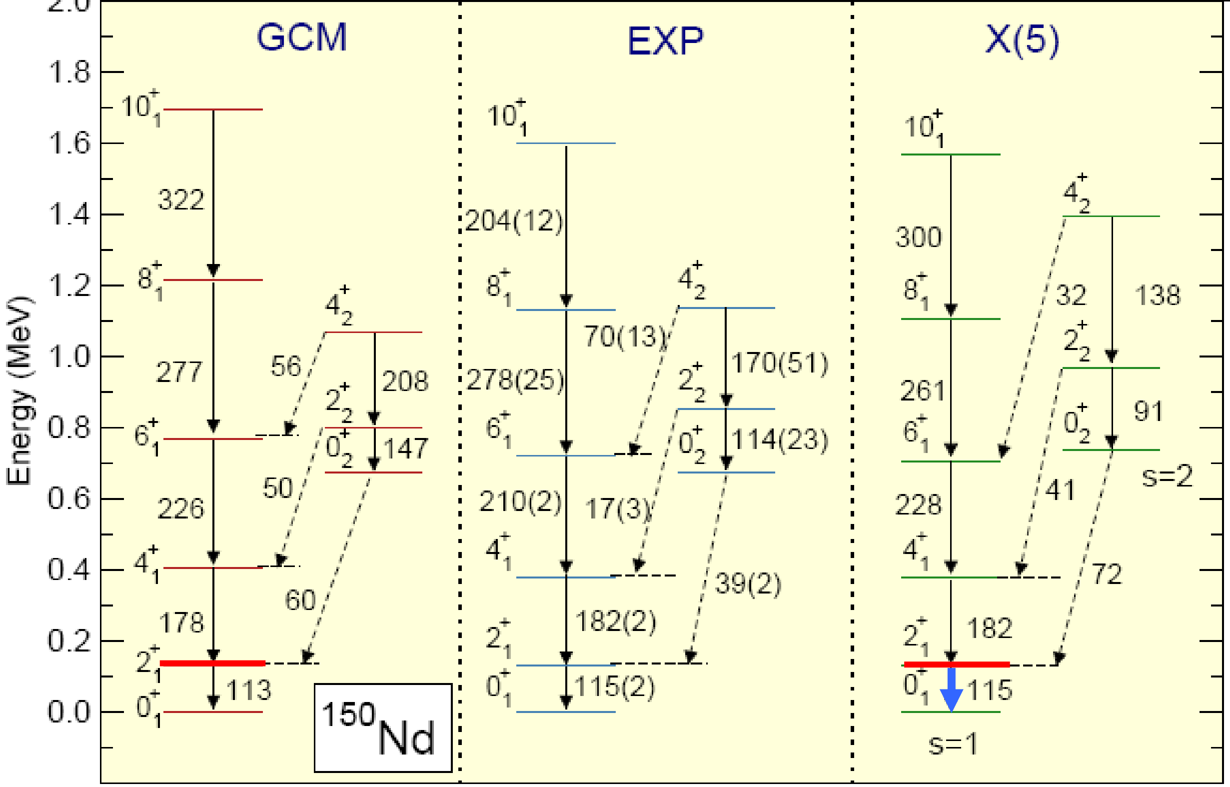
# Self-consistent RMF plus Lipkin-Nogami BCS binding energy curves of $^{142-152}$Nd, as functions of the mass quadrupole moment.



Niksic *et al* PRL 99, 92502 (2007)

R. Krücken *et al*, PRL 88, 232501 (2002)

F. Iachello, PRL 87, 52502 (2001)

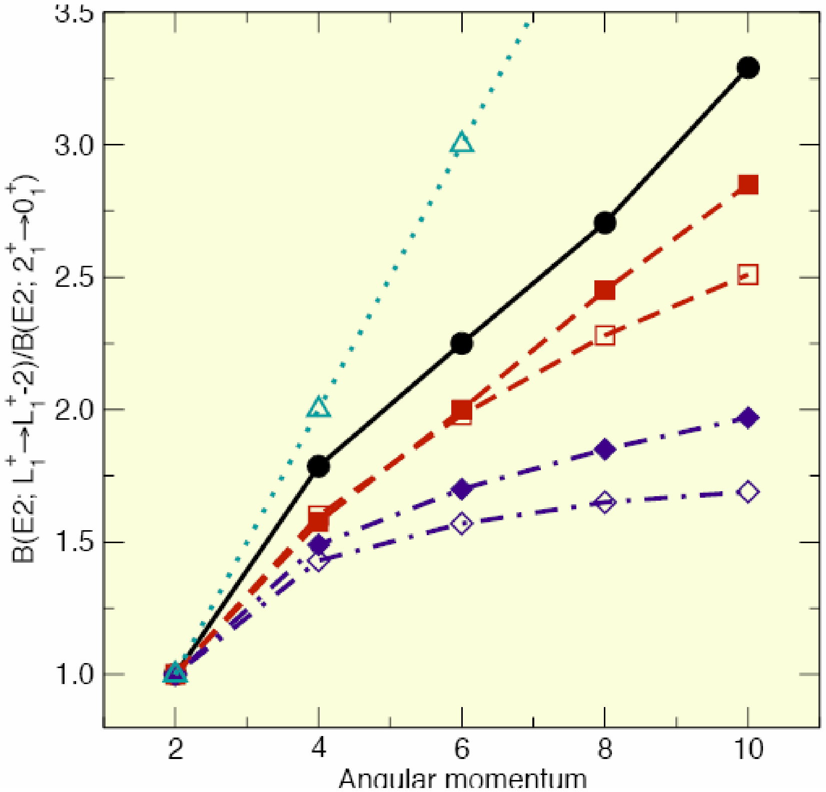


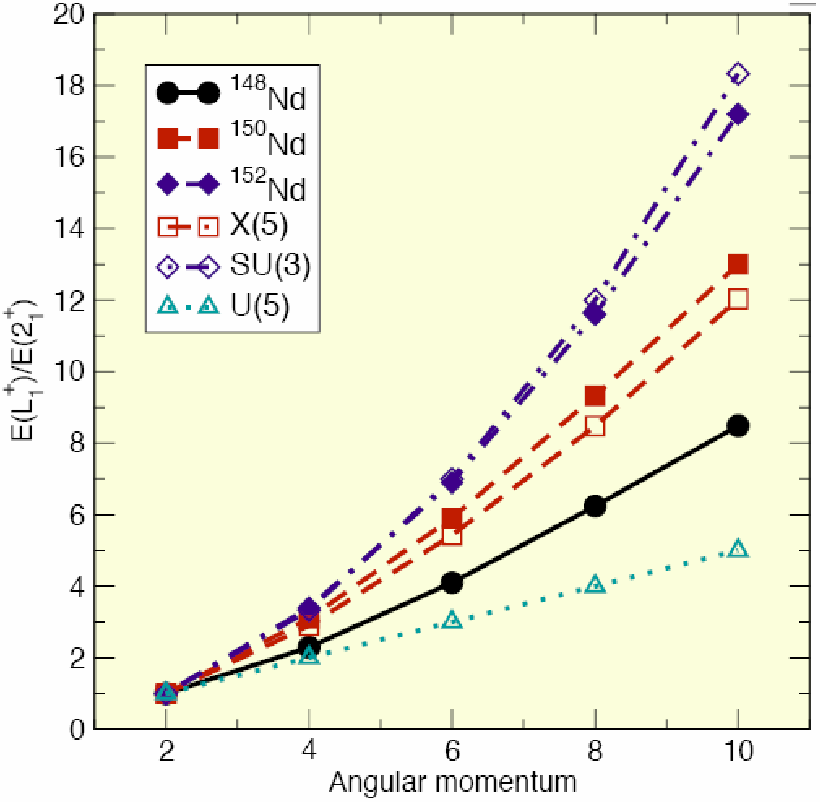
**GCM: only one scale parameter:** **$E(2_1)$**

**X(5): two scale parameters:** **$E(2_1)$, $BE2(2_2 \rightarrow 0_1)$**

**Problem of GCM at this level:** **restricted to γ=0**

B(E2; L → L-2) values and excitation energies for the yrast states: **$^{148}$Nd**, **$^{150}$Nd**, and **$^{152}$Nd**, calculated with the GCM and compared with those predicted by the **X(5)**, **SU(3)** and **U(5)** symmetries.





# Extensions:

1) triaxial degrees of freedom with three-dimensional projection:

see talk of J.-M. Yao (Saturday)

2) derivation of a Bohr Hamiltonian in 5 dimensions:

see talk of Z.-P. Li (Saturday)

3) Variation after projection (time odd components)

4) pairing as a collective degree of freedom ($0^+$)

# Summary and Conclusions:

**New functionals**

- less phenomenological,
- better pairing

**For excited states we need energy dependent kernel**

- higher level density
- quantitative description of the width of Giant Resonances

**GCM calculations for spectra in transitional nuclei**

- J+N projection is important,
- triaxial calculations so only for very light nuclei possible
- microscopic theory of quantum phase transitions

**Derivation of a collective Hamiltonian**

- allows triaxial calculations
- nuclear spectroscopy based on density functionals
- open question of inertia parameters

**The microscopic framework** based on universal density functionals provides a consistent and (nearly) parameter free description of quantum phase transitions

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