Covariant Density Functional Theory for Excited States in Nuclei

Kazimierz Sept. 28, 2011

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“Origin of the Universe”

Content:

- Motivation
- Modern relativisitic density functionals
- Density functional theory for excited states
- Energy dependent self energy
- Single particle excitations
- The width of giant resonances
- Outlook

Density functional theory for quantum manybody systems

Density functional theory starts from the

Hohenberg-Kohn theorem:

> „The exact ground state energy E[ρ] is a universal functional for the local density“

This functional is usually decomposed into three parts:

$$E_{HK}[\rho] = E_{ni}[\rho] + E_{H}[\rho] + E_{xc}[\rho]$$

$$E_H[\rho] = \frac{1}{2}\int \rho(\mathbf{r}) V(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}')d^3r d^3r'$$

Static Kohn-Sham theory:

In order to reproduce shell structure Kohn and Sham introduced a auxiliary single particle potential $v_{\mathrm{eff}}(\mathbf{r})$, defined by the condition, that after the solution of the eigenvalue problem

$$\left\{-\frac{\hbar^2}{2m}\Delta + v_{\mathrm{eff}}(\mathbf{r})\right\}\varphi_i(\mathbf{r}) = \varepsilon_i\varphi_i(\mathbf{r})$$

the exact density is obtained as $\rho(\mathbf{r}) = \sum_i^A |\varphi_i(\mathbf{r})|^2$.

Obviously to each density $\rho(\mathbf{r})$ there exist such a potential $v_{\mathrm{eff}}(\mathbf{r})$ and one finds

$$v_{\mathrm{eff}}(\mathbf{r}) = f_{\mathrm{ext}}(\mathbf{r}) + v_{\mathrm{H}}(\mathbf{r}) + v_{xc}(\mathbf{r})$$

with $\boxed{v_{\mathrm{H}}(\mathbf{r}) = \int V(\mathbf{r},\mathbf{r}')\rho(r')d^3r}$ and $\boxed{v_{\mathrm{xc}}(\mathbf{r}) = \frac{\delta E_{\mathrm{xc}}}{\delta\rho(\mathbf{r})}}$

Covariant DFT is based on the Walecka model

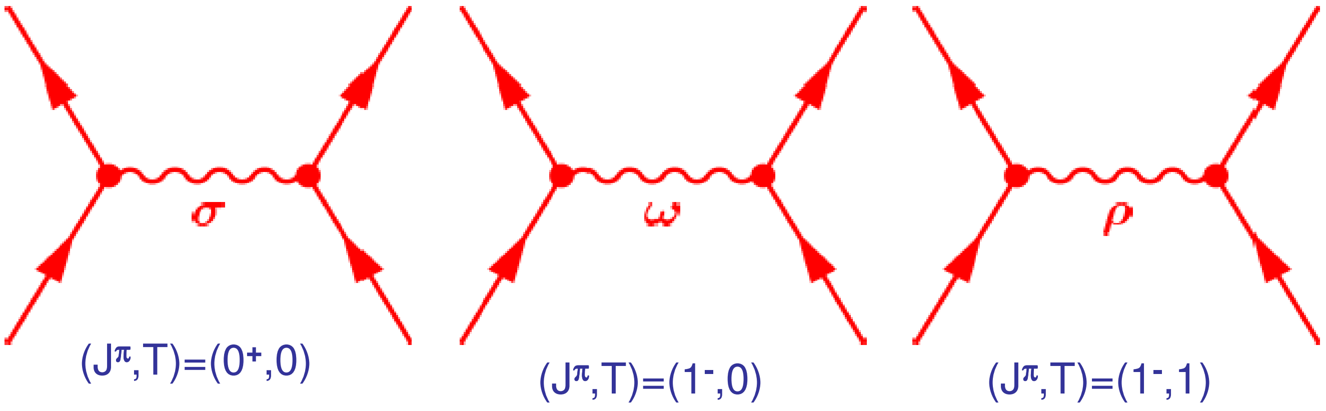
Dürr and Teller, Phys.Rev 101 (1956)

Walecka, Phys.Rev. C83 (1974)

Boguta and Bodmer, Nucl.Phys. A292 (1977)

The nuclear fields are obtained by coupling the nucleons through the exchange of effective mesons through an effective Lagrangian.

$$\boxed{E[\rho]}$$



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

sigma-meson:
attractive scalar field

omega-meson:
short-range repulsive

rho-meson:
isovector field

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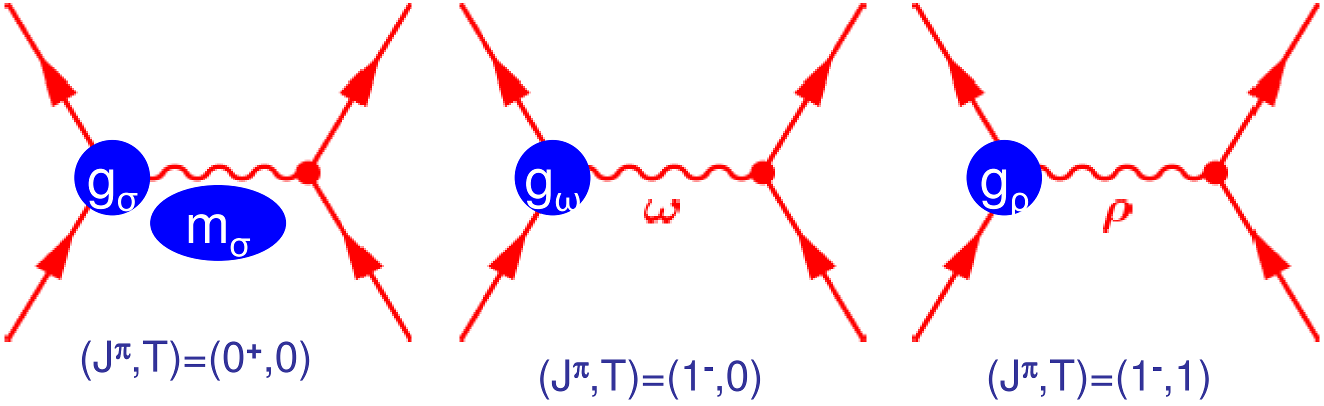
This model has only four parameters:



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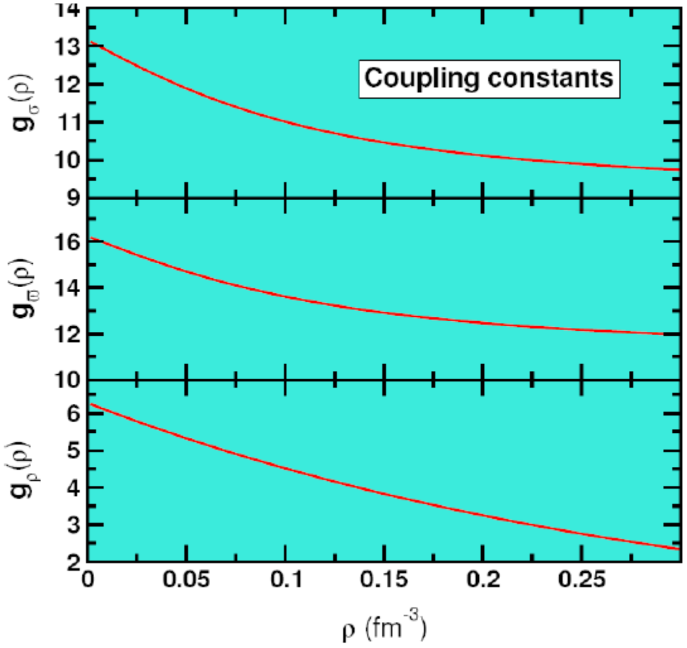
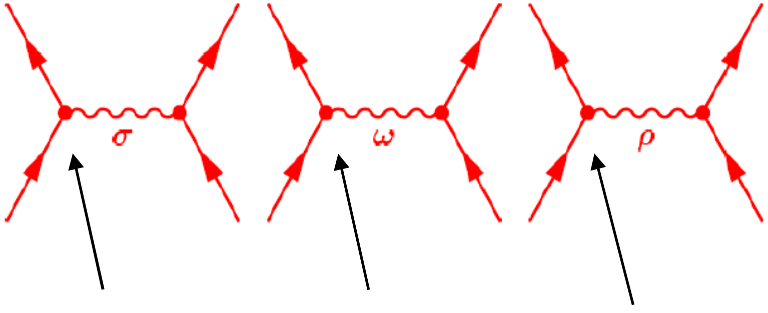
Effective density dependence:

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

non-linear meson coupling: **NL3**



Effective interactions with medium-dependent couplings:



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

adjusted to ground state properties of finite nuclei

Typel, Wolter, NPA **656**, 331 (1999)
Niksic, Vretenar, Finelli, P.R., PRC **66**, 024306 (2002): **DD-ME1**
Lalazissis, Niksic, Vretenar, P.R., PRC 78, 034318 (2008): **DD-ME2**

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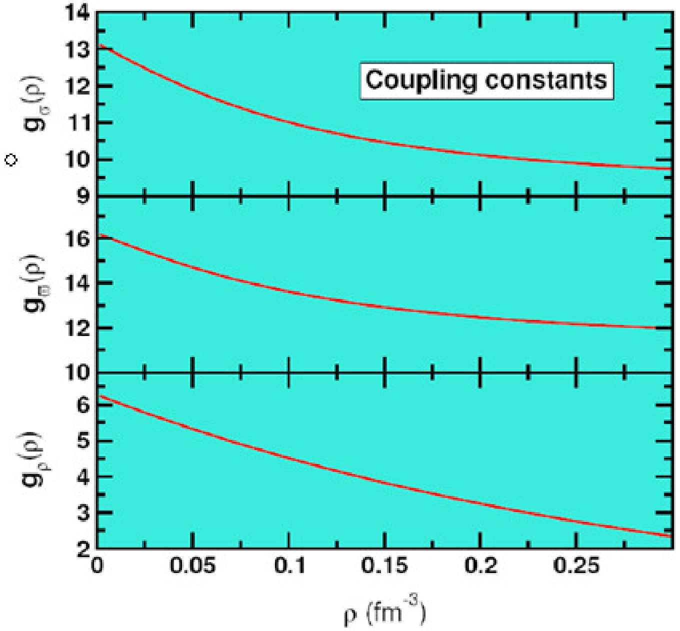
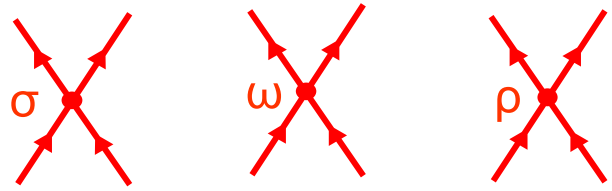


Point-coupling models
with derivative terms:



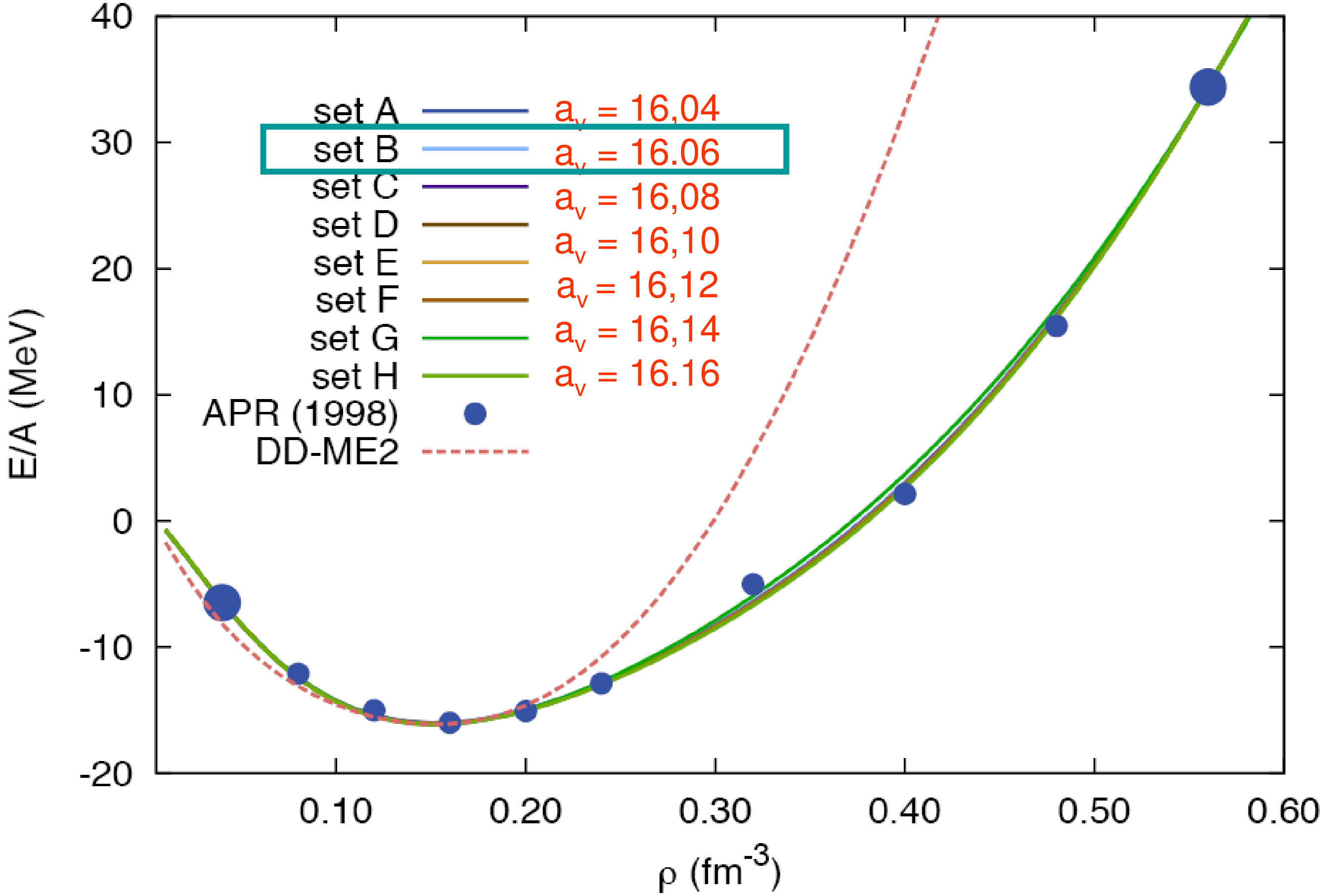
$g_\sigma(\rho)$ $g_\omega(\rho)$ $g_\rho(\rho)$

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**
Niksic, Vretenar, P.R., PRC 78, 034318 (2008): **DD-PC1**
Zhao, Li, Yao, Meng, PRC 82, 054319 (2010): **PK-PC1**

semi-microscopic relativistic functionals

Density dependence is determined from microscopic calculations
Remaining 4 parameters are fitted to masses of deformed nuclei:



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

ρ_{sat} = 0.152 fm^{-3}
m* = 0.58m
K_{nm} = 230 MeV
a_4 = 33 MeV

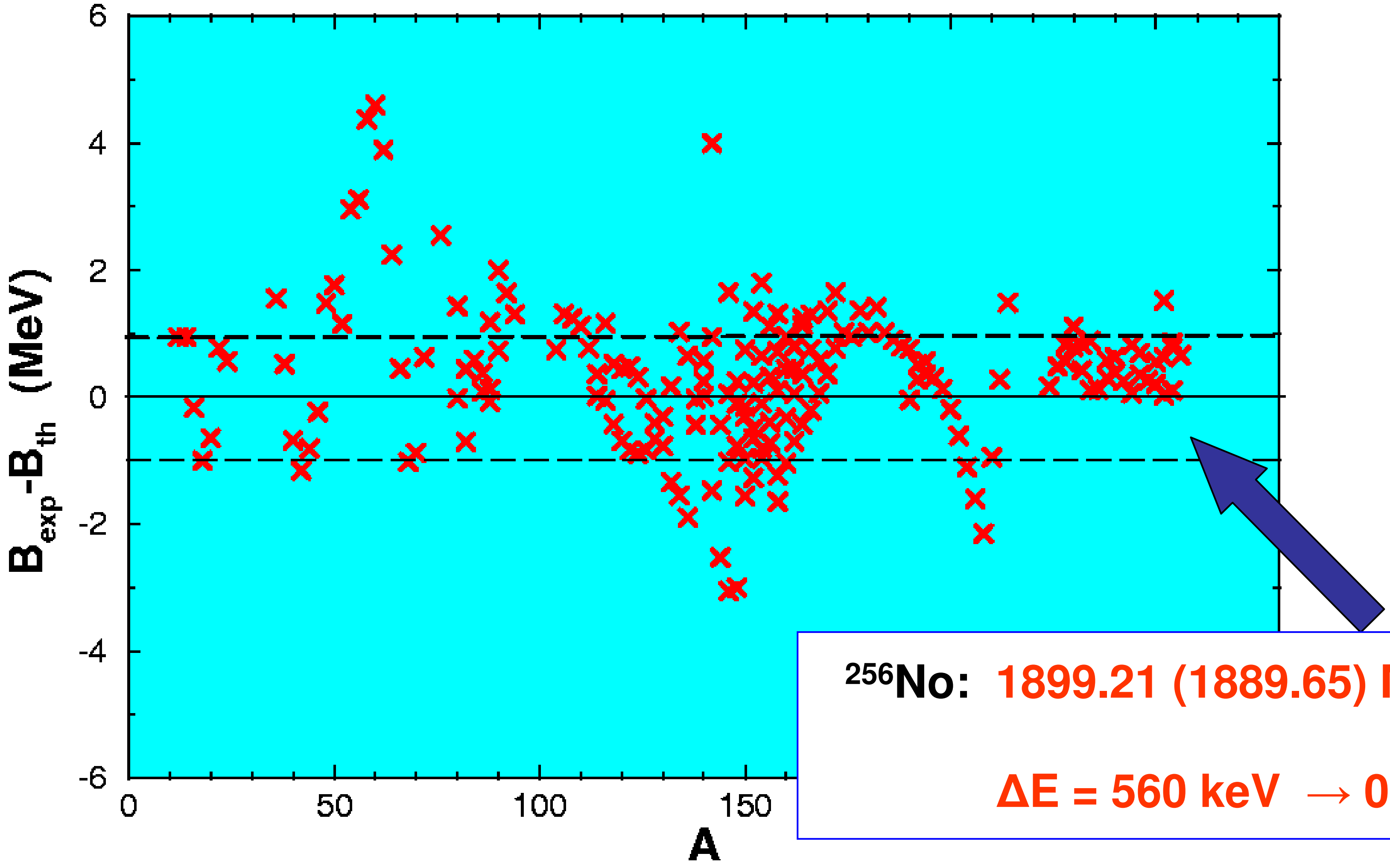
Niksic et al, (2008)

DD-PC1

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

rms-deviations: masses: Δm = 900 keV
radii: Δr = 0.015 fm

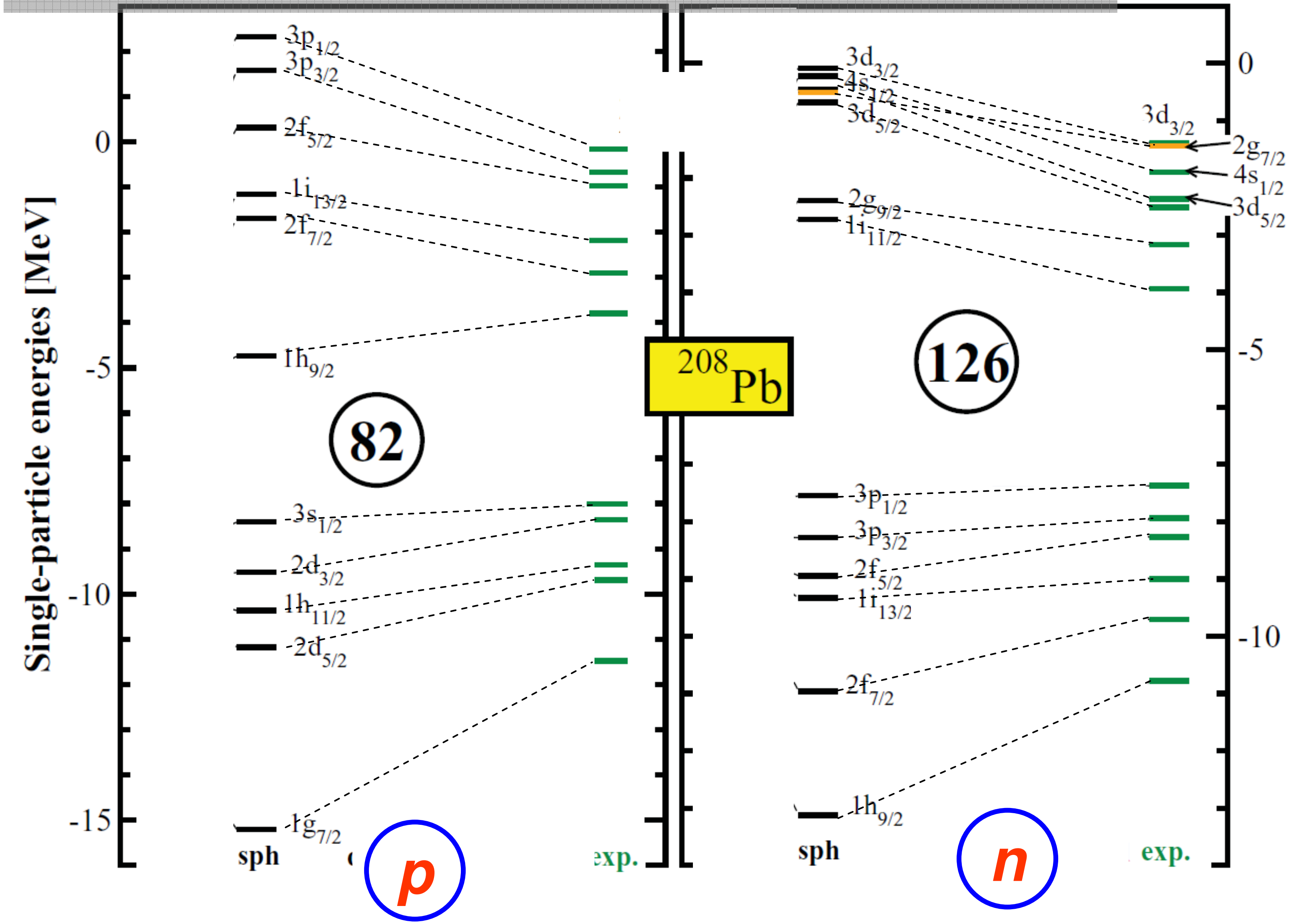
Lalazissis, Niksic, Vretenar, Ring, PRC 71, 024312 (2005)



^{256}No: 1899.21 (1889.65) MeV

ΔE = 560 keV → 0.3 ‰

Problem: single particle spectra



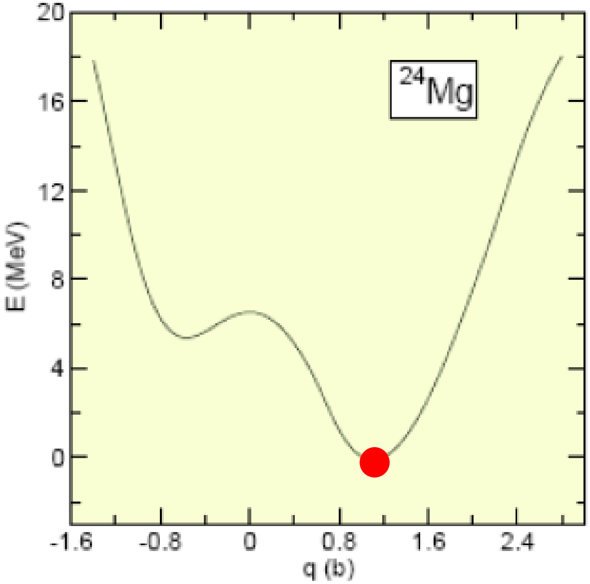
Problems of the mean field approach:

- No energy dependence of the self energy: $\sum(\omega)$

- No fluctuations:

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

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

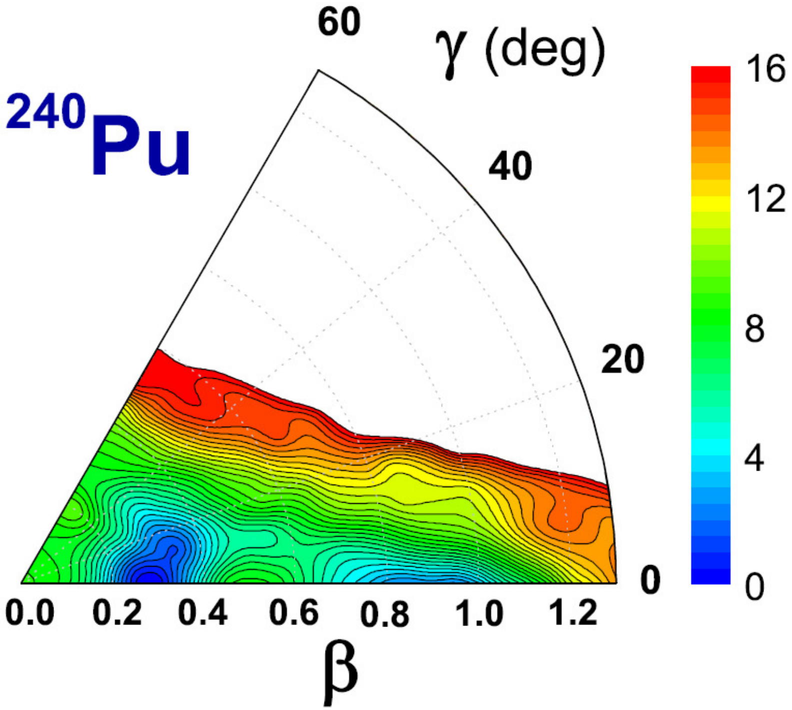


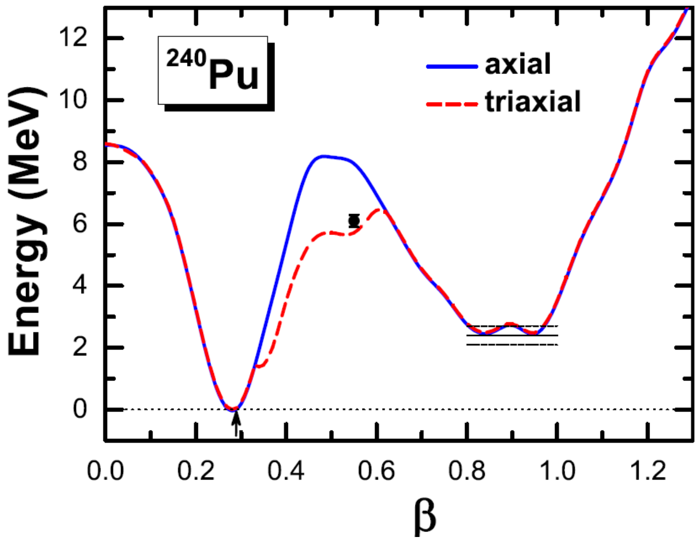
- Violation of symmetries

  projection methods

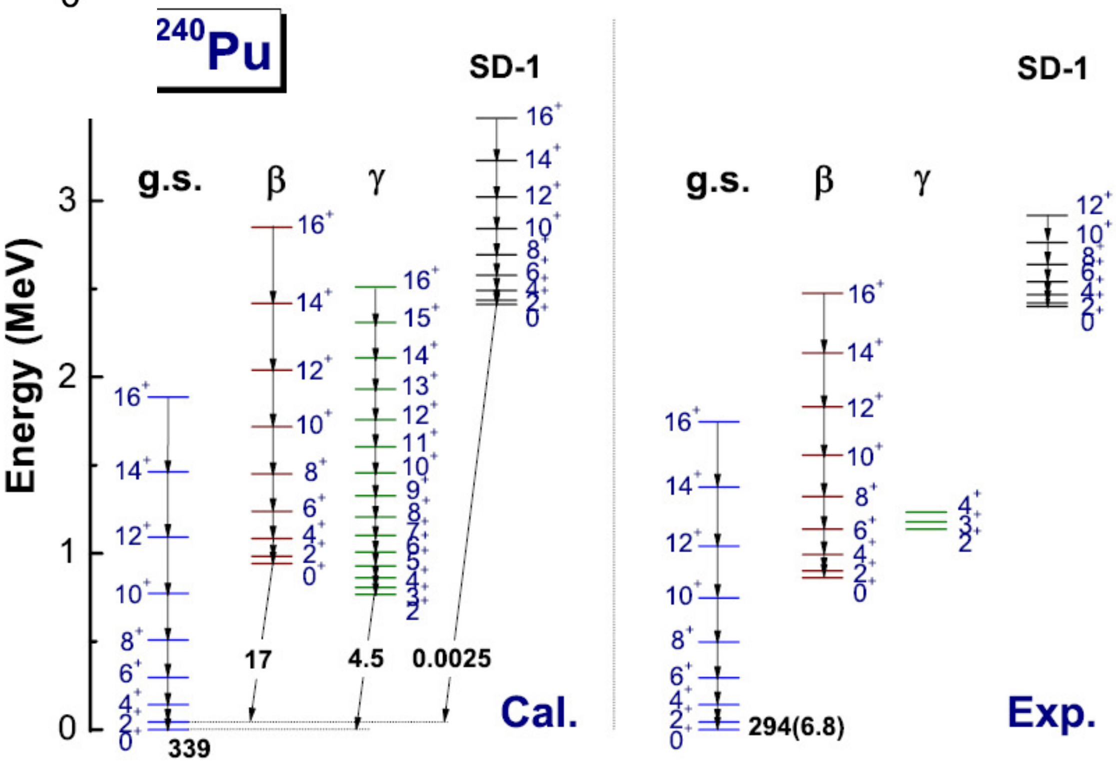
$$| \Psi \rangle = \int dq\, f(q) \hat{P}^N \hat{P}^I | q \rangle$$

Fission barrier and super-deformed bands in ^{240}Pu





DD-PC1



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Timedependent density functional theory:

Exact solution $|\Psi(t)\rangle$ of a time-dependent Schroedinger equation with initial condition $|\Psi(0)\rangle$

$$i\partial_t|\Psi(t)\rangle = (\hat{H} + f_{\text{ext}}(t))|\Psi(t)\rangle$$

Runge-Gross theorem (1984):

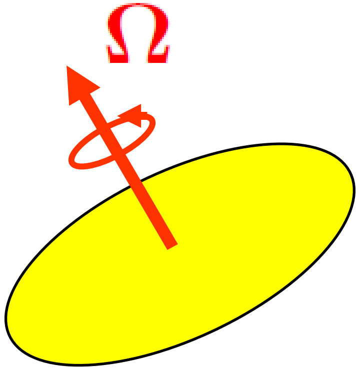
One-to-one correspondence: $\rho(\mathbf{r},t) \iff f_{\text{ext}}(\mathbf{r},t)$ and there exists a fictitious system of non-interacting particles with the wave functions $\varphi_i(\mathbf{r},t)$ satisfying

$$i\partial_t\varphi_i(\mathbf{r},t) = \left[-\nabla^2/2m + v_{\text{eff}}[\rho](\mathbf{r},t)\right]\varphi_i(\mathbf{r},t).$$

for a $v_{\text{eff}}[\rho](\mathbf{r},t)$ and $\rho(\mathbf{r},t) = \sum_i^A |\varphi_i(\mathbf{r},t)|^2$ is the exact density of the interacting many-body system. $v_{\text{eff}}[\rho](\mathbf{r},t)$ is a function of $\mathbf{r}$ and t, but it is in addition a unique functional of the time-dependent density $\rho(\mathbf{r},t)$.

Rotational excitations:

We assume that the time-dependence is given by a rotation with constant velocity $\boldsymbol{\Omega}$



$$\rho(\boldsymbol{r},t) = e^{-i\boldsymbol{\Omega}\boldsymbol{j}t}\rho(\boldsymbol{r})e^{i\boldsymbol{\Omega}\boldsymbol{j}t}$$

This leads to quasi-static Kohn-Sham equations in the rotations frame

Cranking model: Inglis (1956):

$$\left[-\boldsymbol{\nabla}^2/2m + v[\rho](\boldsymbol{r}) - \boldsymbol{\Omega}\boldsymbol{j}\right]\varphi_i(\boldsymbol{r}) = \varepsilon_i(\boldsymbol{\Omega})\varphi_i(\boldsymbol{r})$$

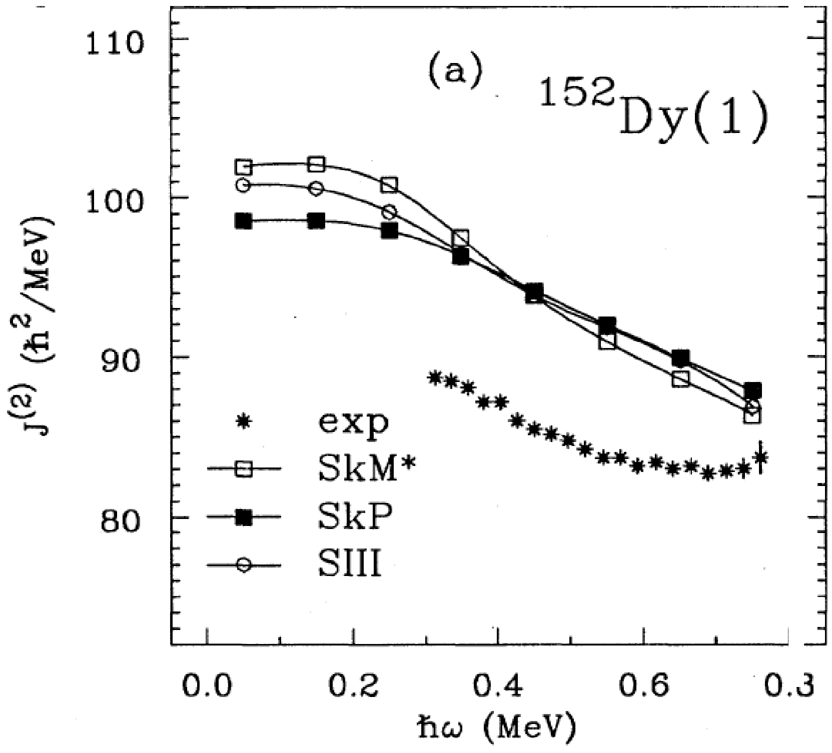
with the exact intrinsic density $\rho(\boldsymbol{r}) = \sum_{i=1}^{A}|\varphi_i(\boldsymbol{r})|^2$

Here we assume, that $v[\rho](\boldsymbol{r})$ is the static Kohn-Sham potential ("adiabatic approximation")

Moments of inertia in rotating nuclei:

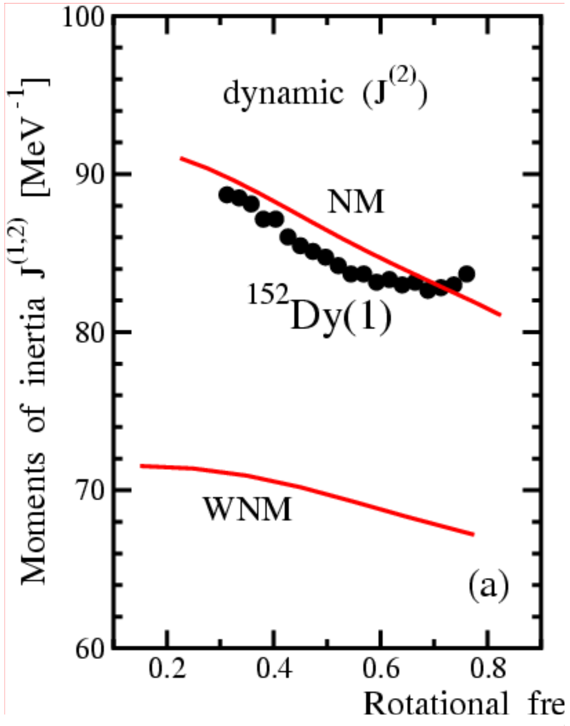
$$\left[\boldsymbol{\alpha}\cdot(-i\boldsymbol{\nabla}-\mathbf{V})+\beta\,(m+S)+V-\boldsymbol{\Omega}\cdot\hat{\mathbf{J}}\right]\psi_i \;=\; \varepsilon_i\psi_i$$

Nuclear magnetism



Skyrme

Dobaczewski, Dudek, PRC (1995)



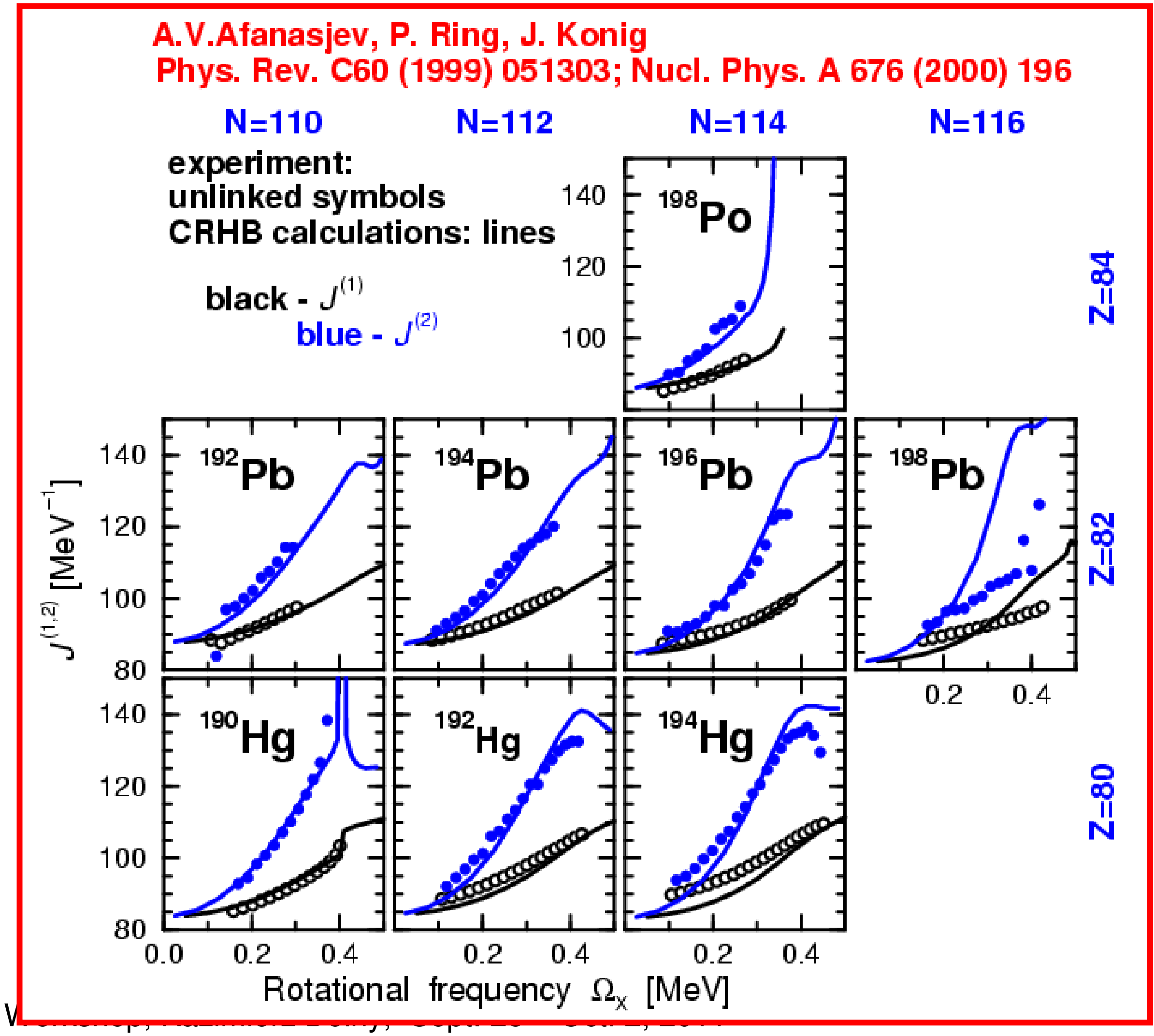
RMF NL1

Afanasjev, P.R. PRC (1996)

Superdeformed bands in the Hg-Pb region:

$$\left[\boldsymbol{\alpha}\cdot\left(-i\boldsymbol{\nabla}-\mathbf{V}\right)+\beta\left(m+S\right)+V-\boldsymbol{\Omega}\cdot\hat{\mathbf{J}}\right]\psi_i \;=\; \varepsilon_i\psi_i$$

Cranked
RHB calculations:



A.V.Afanasjev, P. Ring, J. Konig
Phys. Rev. C60 (1999) 051303; Nucl. Phys. A 676 (2000) 196

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Linear response theory:

If $f_{\text{ext}}(\mathbf{r}, t)$ is **weak** we have: $\rho(\mathbf{r}, t) = \rho_{\text{s}}(\mathbf{r}) + \delta\rho(\mathbf{r}, t)$.

and: $v[\rho](\mathbf{r},t) = v_s(\mathbf{r}) + \int dt' \int d^3r' V(\mathbf{r}, \mathbf{r}', t - t')\delta\rho(\mathbf{r}, t')$.

V is an effective interaction $V(\mathbf{r}, \mathbf{r}', t - t') = \left.\frac{\delta v(\mathbf{r},t)}{\delta\rho(\mathbf{r}',t')}\right|_{\rho=\rho_{\text{s}}}$.

For $\delta\rho(\mathbf{r}, t) = \int d^3r' \int dt' R(\mathbf{r}, \mathbf{r}', t - t') f_{ext}(\mathbf{r}', t')$

we find

$$\boxed{R(\omega) = R_0(\omega) + R_0(\omega)V(\omega)R(\omega)}$$

All these quantities are functionals of the exact ground state density $\rho_{\text{s}}(\mathbf{r})$.

If f_{ext} is weak, these equations are exact, but we do not know the functional $v[\rho(\mathbf{r}, t)]$ nor its functional derivative at $\rho = \rho_{\text{s}}$.

The adiabatic approximation:

Here one neglects the memory and assumes that the density changes only very slowly, such that the potential is given at each time by the static potential v_s corresponding to this density.

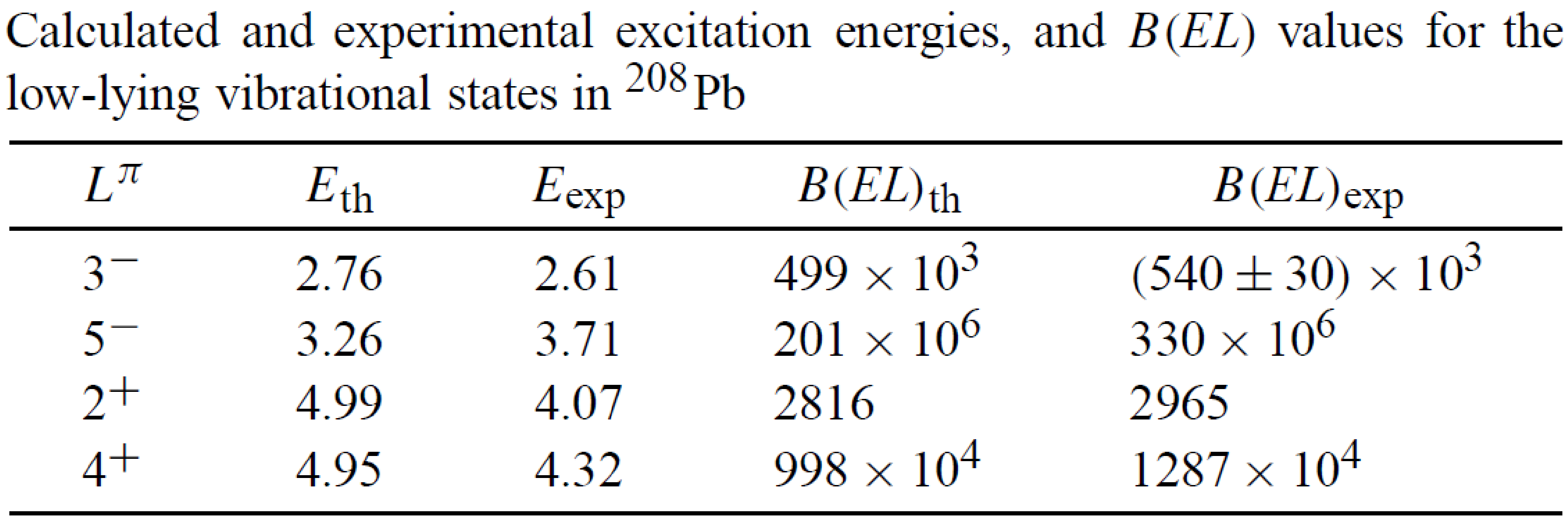
$$v[\rho](\mathbf{r},t) \approx v_s[\rho_s](\mathbf{r},t)$$

In this approximation $v[\rho]$ is no longer depending on the function $\rho(\mathbf{r},t)$ of 4 variables, but rather on the function $\rho_s(\mathbf{r}) = \rho(\mathbf{r},t)$ depending only 3 variables. The time is just a parameter. We obtain for the effective interaction in the adiabatic approximation

$$V_{ad}(\mathbf{r},\mathbf{r}',t-t') = \frac{\delta E[\rho_s]}{\delta\rho_s(\mathbf{r})\delta\rho_s(\mathbf{r}')}\delta(t-t')$$

This approximation is well known. It corresponds to the small amplitude limit of the time-dependent mean field equations, i.e. to RPA or in superfluid systems to QRPA and it is extensively used in nuclear physics.

Low lying collective states in ^{208}Pb:

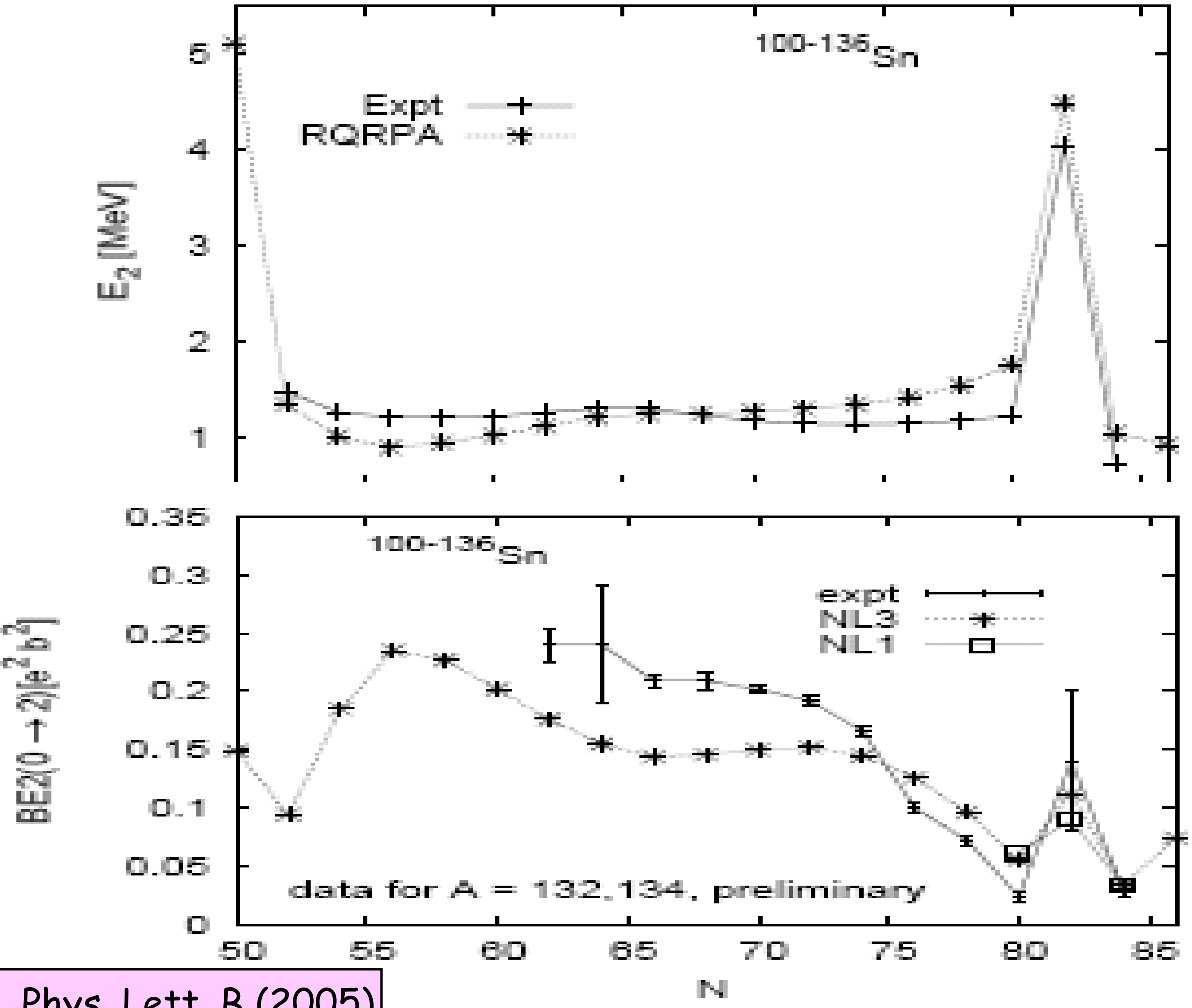


Calculated and experimental excitation energies, and $B(EL)$ values for the low-lying vibrational states in ^{208}Pb

L^π	E_{th}	E_{exp}	$B(EL)_{\mathrm{th}}$	$B(EL)_{\mathrm{exp}}$
3^-	2.76	2.61	499×10^3	$(540 \pm 30) \times 10^3$
5^-	3.26	3.71	201×10^6	330×10^6
2^+	4.99	4.07	2816	2965
4^+	4.95	4.32	998×10^4	1287×10^4

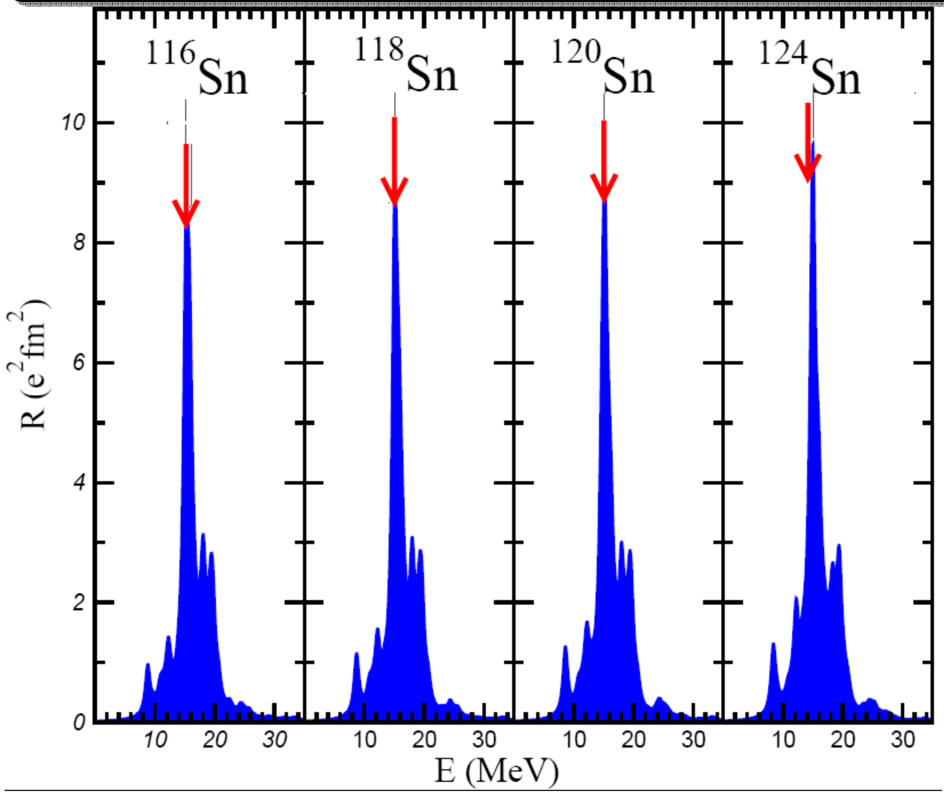
Ma, Wandelt et al, Nucl. Phys. (2002)

QRPA: 2^+-excitation in Sn-isotopes:



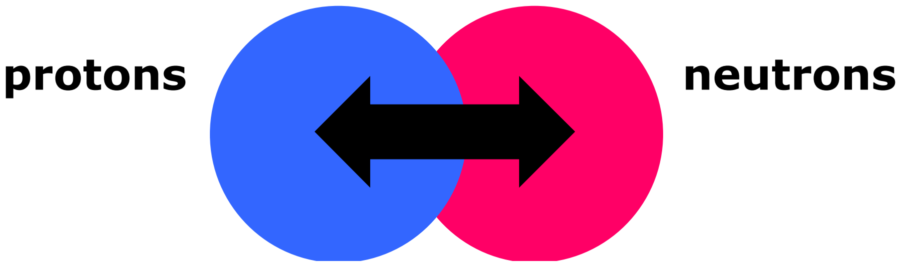
A. Ansari, Phys. Lett. B (2005)

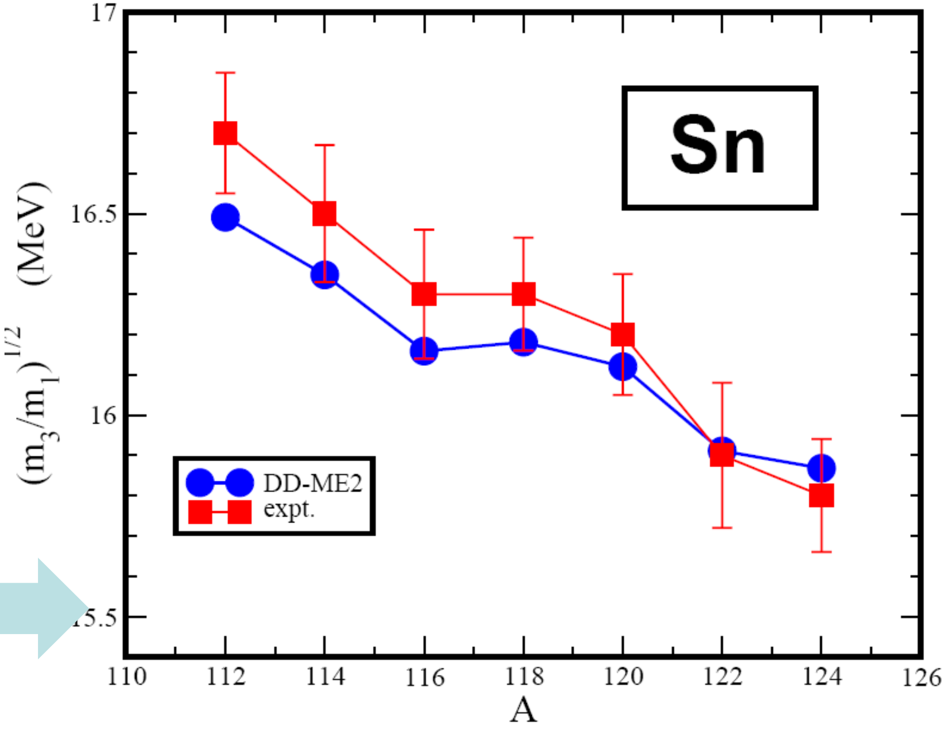
Relativistic (Q)RPA calculations of giant resonances:

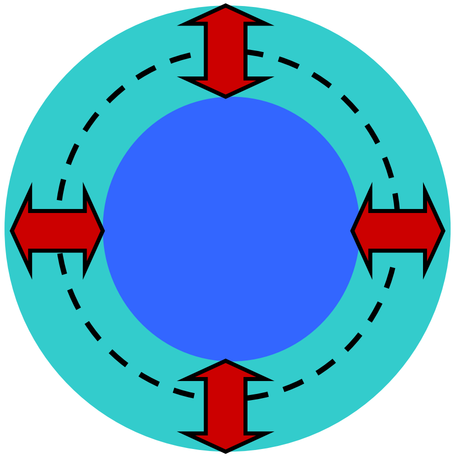


Sn isotopes: DD-ME2 effective interaction + Gogny pairing

Isovector dipole response



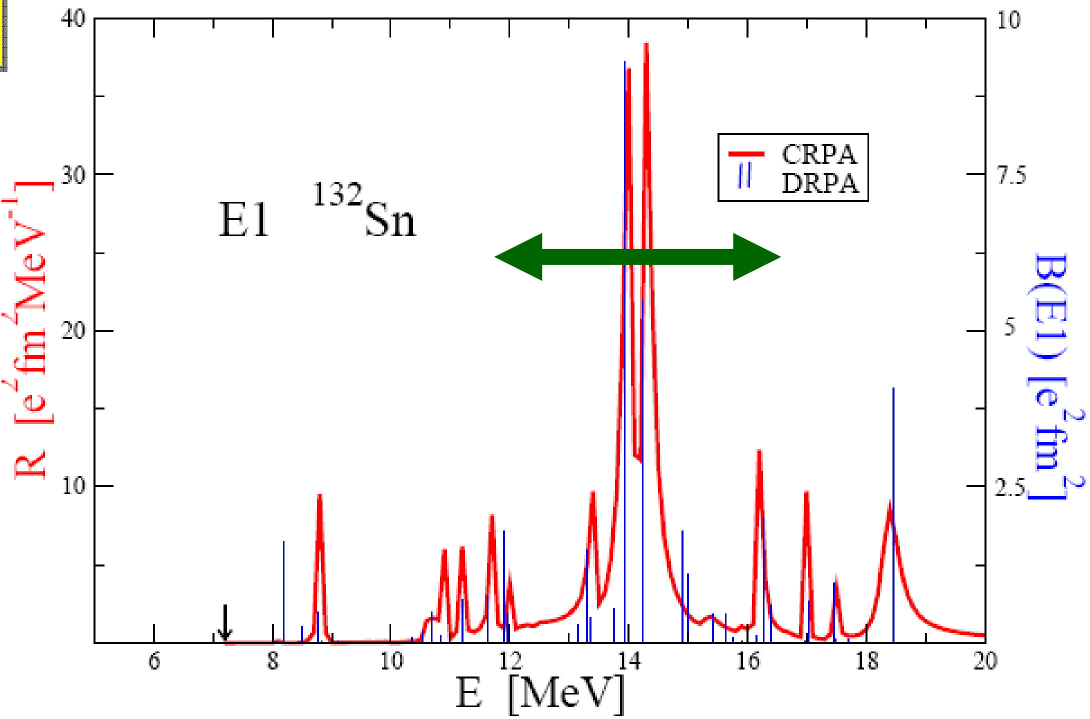




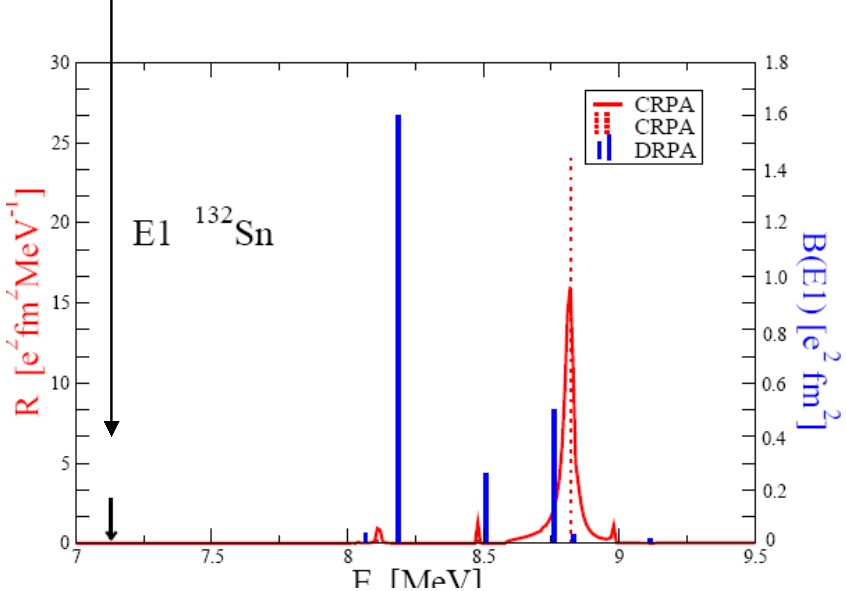
Isoscalar monopole response

E1-continuum RPA

^{132}Sn



neutron threshold:



	CRPA		DRPA	
No.	E	B(E1)	E	B(E1)
1	8.11	0.03	8.067	0.037
2	8.48	0.02	8.186	1.601
3	8.82	1.44	8.511	0.260
Σ		1.490		1.898

2.4 % 3.4 % of EWSR

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

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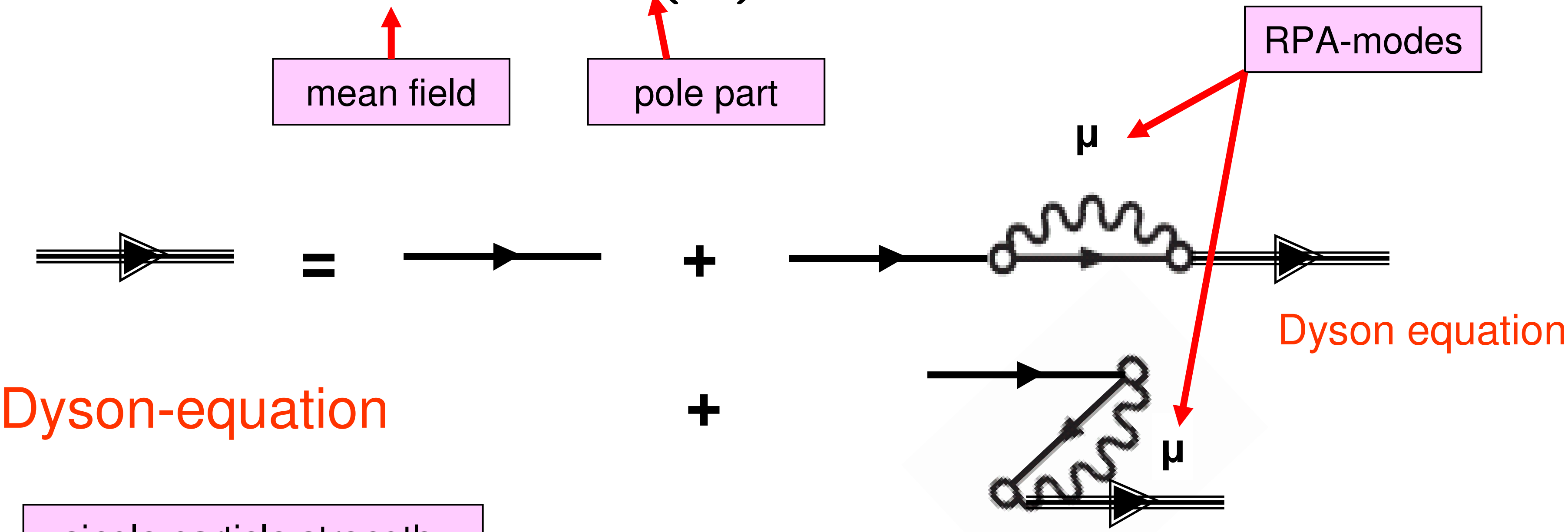
Particle-vibrational coupling (PVC) energy dependent self-energy

eff. Potential v_{eff}
→ self-energy Σ

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

mean field

pole part



RPA-modes

μ

μ

Dyson equation

Dyson-equation

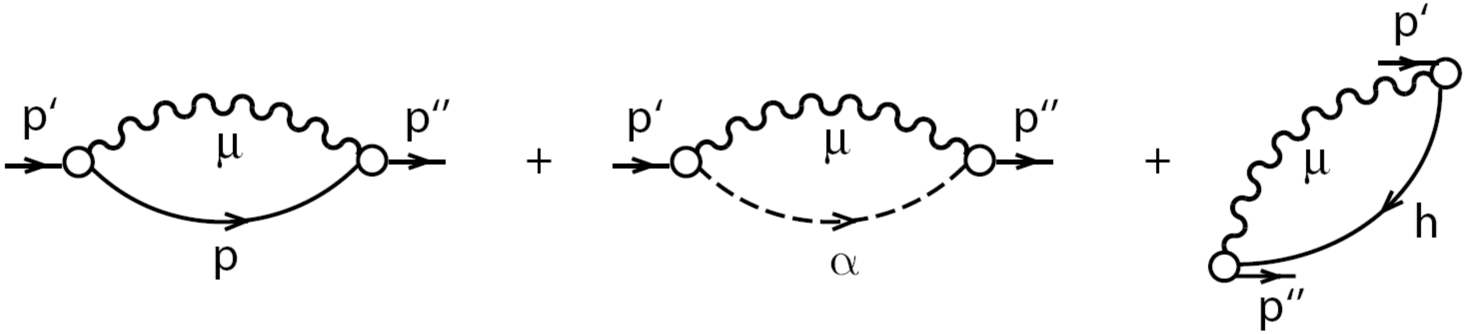
single particle strength:

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

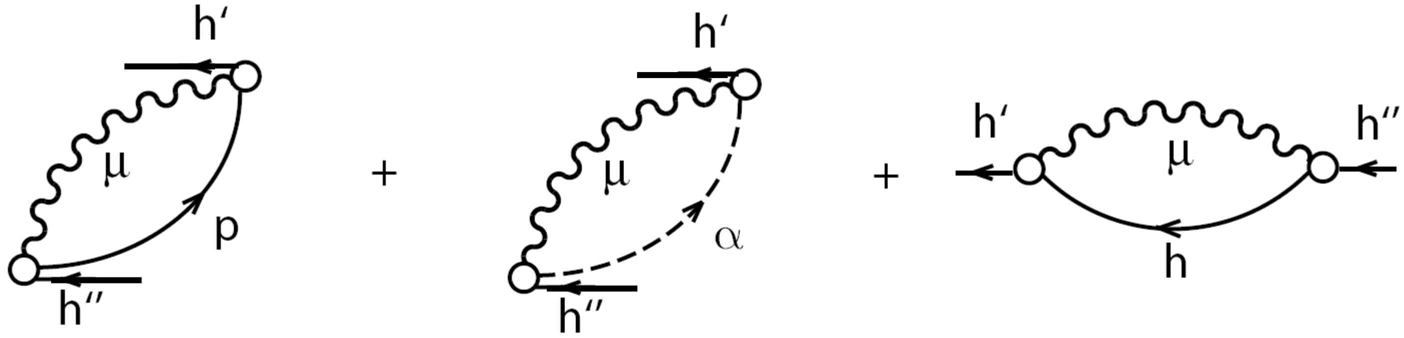
non-relativistic investigations:
Ring, Werner (1973)
Hamamoto, Siemens (1976)
Perazzo, Reich, Sofia (1980)
Bortignon et al (1980)
Bernard, Giai (1980)
Platonov (1981)
Kamerdzhiev, Tselyaev (1986)

Contributions to Σ(ω) in the relativistic case:

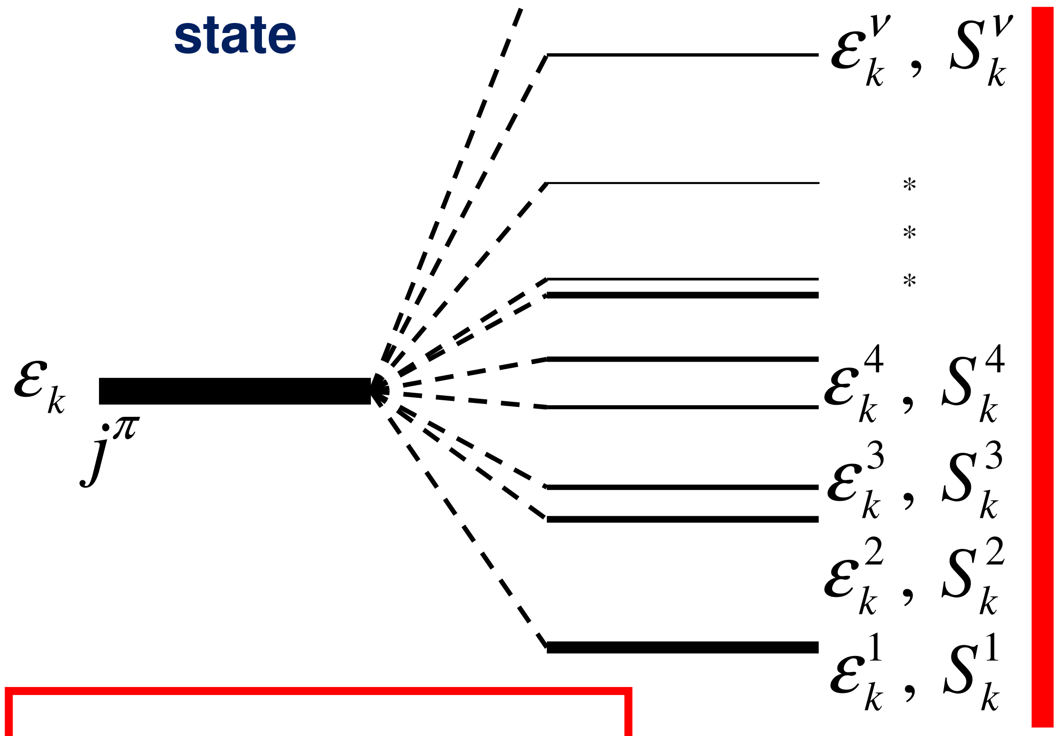
$$\Sigma^{e}_{p'p''} =$$



$$\Sigma^{e}_{h'h''} =$$



The single particle energies are fragmented:



Mean-field single-particle state

Fragmented levels (due to coupling to phonons)

$$\varepsilon_k^{grav} = \left[\sum_\nu S_k^\nu \cdot \varepsilon_k^\nu\right] / \left[\sum_\nu S_k^\nu\right]$$

This energy is associated with a "bare" single-particle energy.

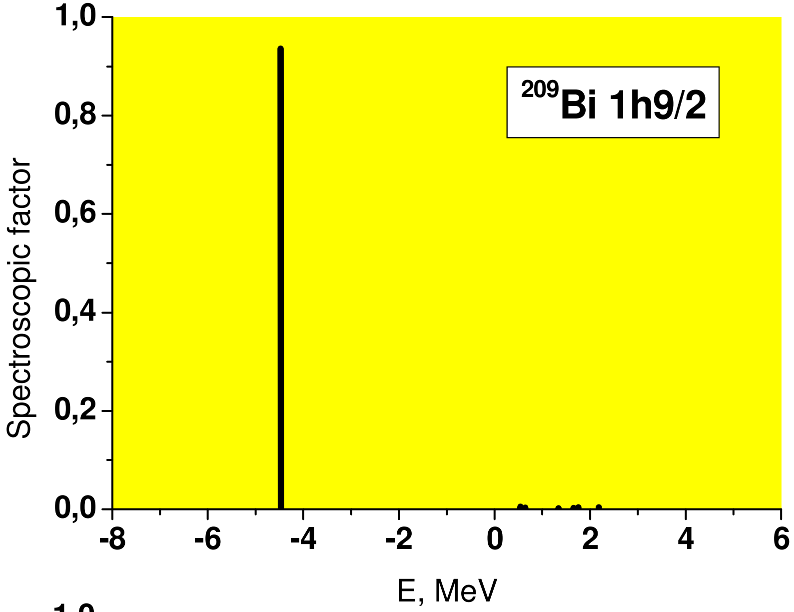
Spectroscopic factors depend on reaction and method of extraction: example of spectroscopic factors in ^{209}Bi

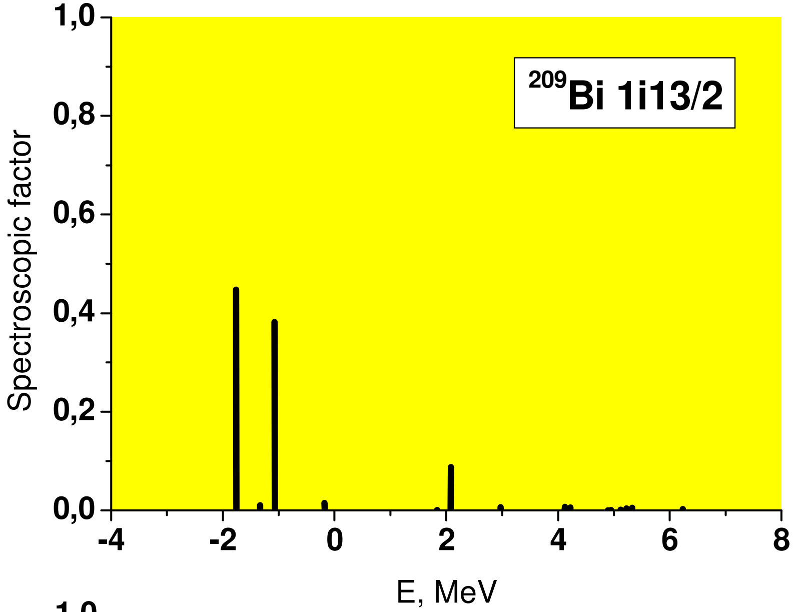
	(^{3}He,d)	(α,t) reactions
$1h_{9/2}$	1.17	0.80
$2f_{7/2}$	0.78	0.76
$1i_{13/2}$	0.56	0.74
$2f_{5/2}$	0.88	0.57
$3p_{3/2}$	0.67	0.44
$3p_{1/2}$	0.49	0.20

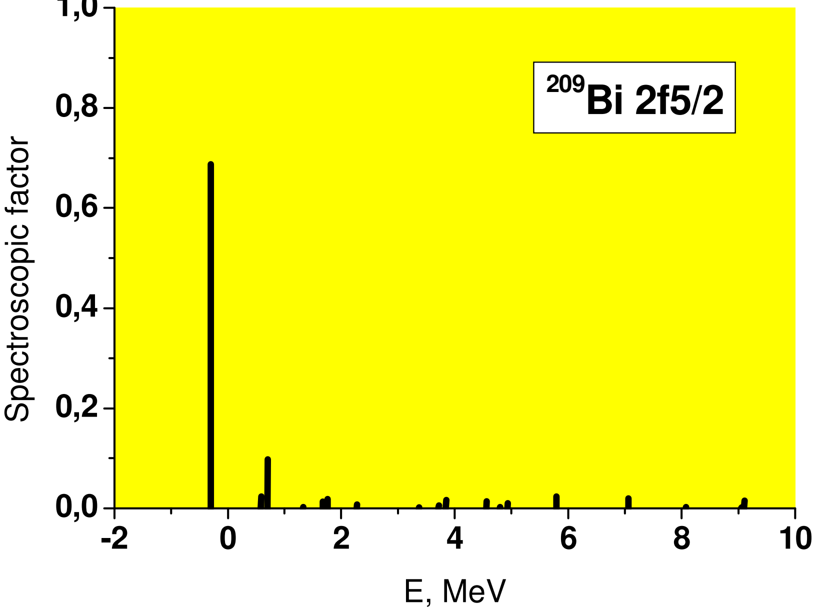
sum rule: $\sum_\nu S_k^\nu = 1$

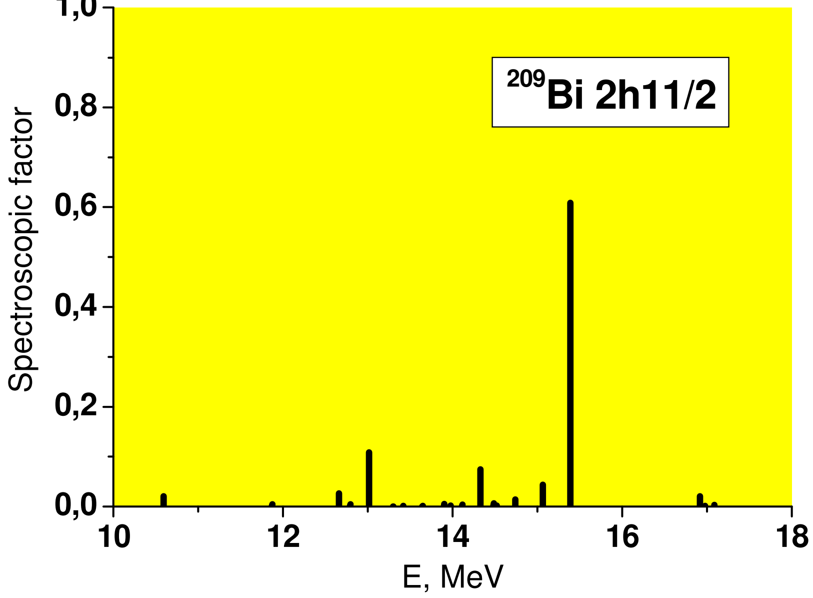
is frequently violated.

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

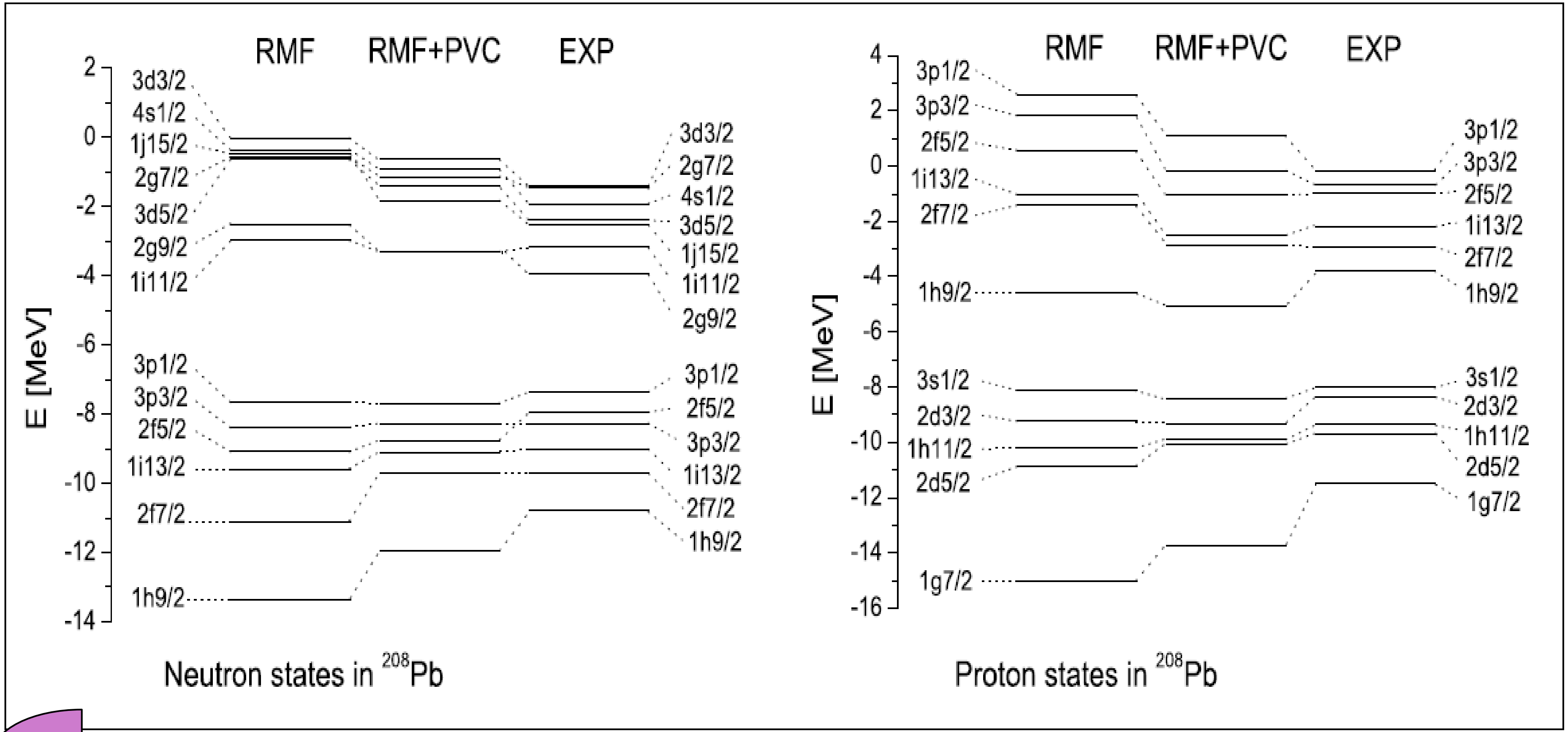








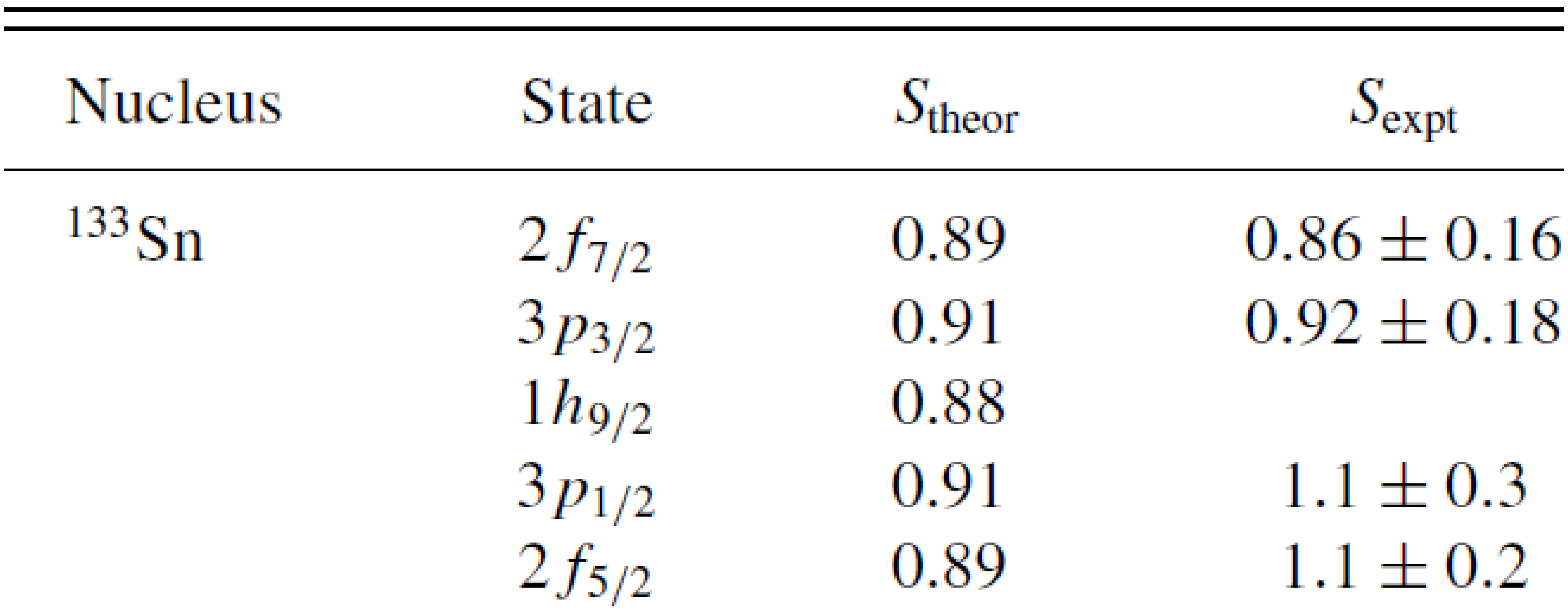
Single particle spectrum in the Pb-region:



m_{eff} 0.76 0.92 1.0 0.71 0.85 1.0

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

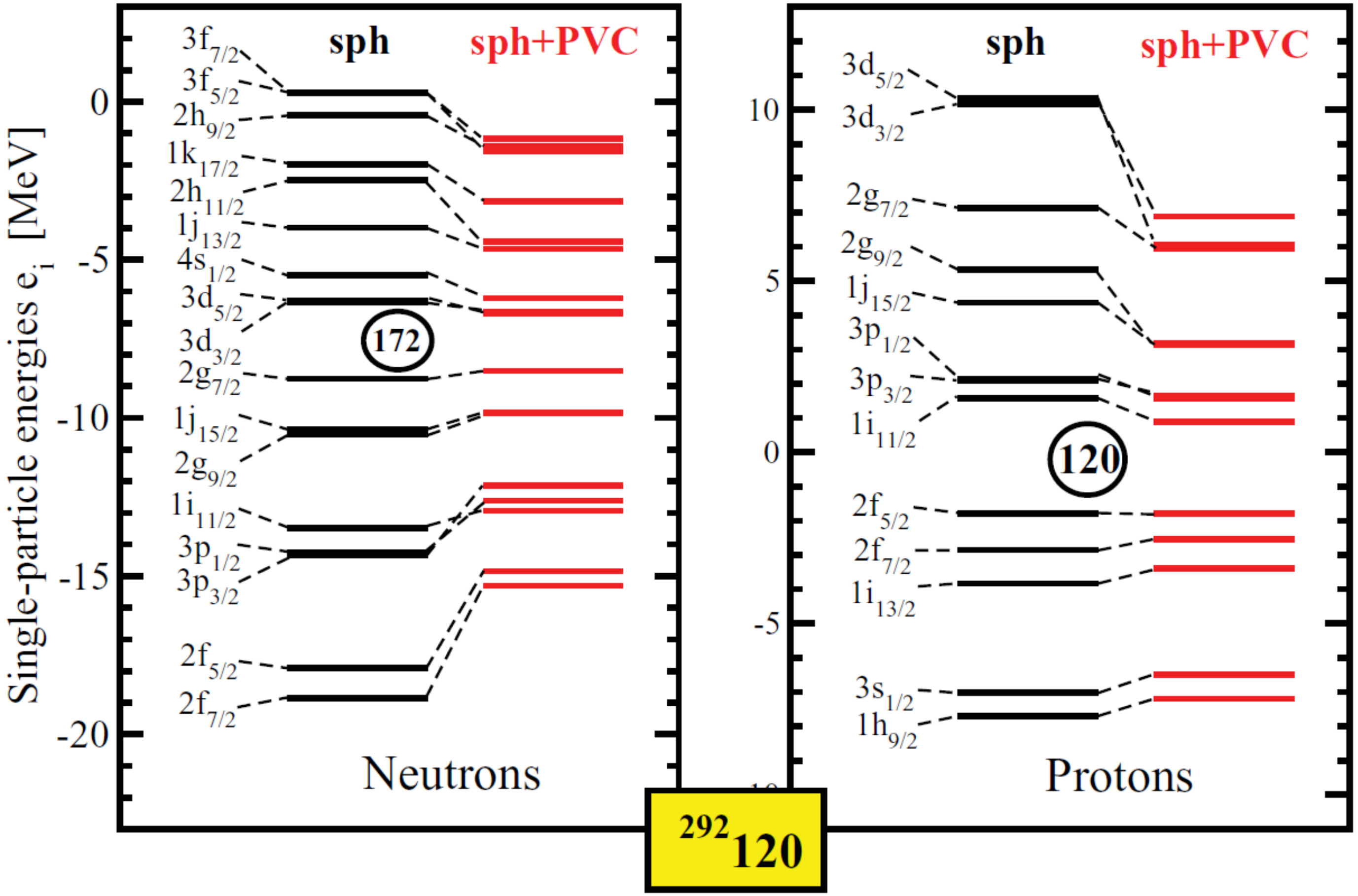
Spectroscopic factors in ^{133}Sn:



Nucleus	State	S_{theor}	S_{expt}
^{133}Sn	$2f_{7/2}$	0.89	0.86 ± 0.16
	$3p_{3/2}$	0.91	0.92 ± 0.18
	$1h_{9/2}$	0.88	
	$3p_{1/2}$	0.91	1.1 ± 0.3
	$2f_{5/2}$	0.89	1.1 ± 0.2

E. Litvinova and A. Afanasjev, PRC 84 (2011)

Particle vibration coupling in superheavy elements:

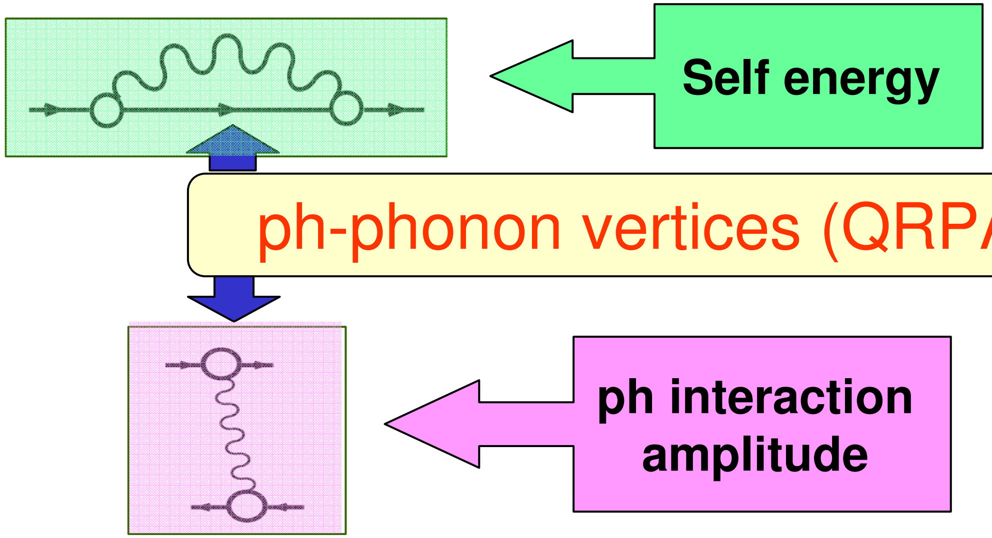


Litvinova, Afanasjev, PRC 84, 014305 (2011).

Width of giant resonances:

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

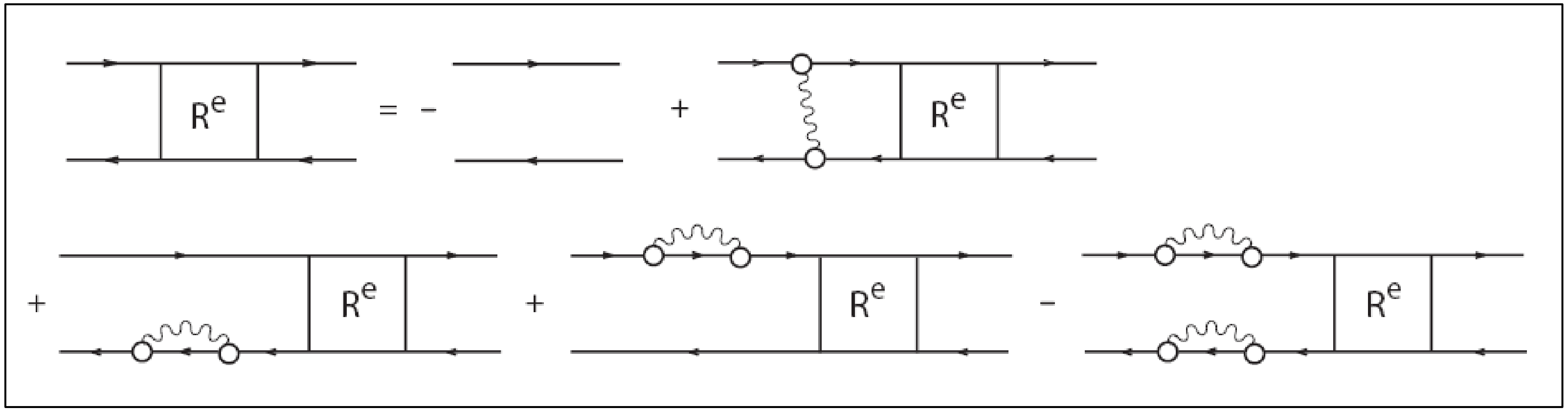
$$V(\omega) = \frac{\delta\Sigma(\omega)}{\delta\rho}$$



Self energy

ph-phonon vertices (QRPA)

ph interaction amplitude



Width of giant resonances:

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

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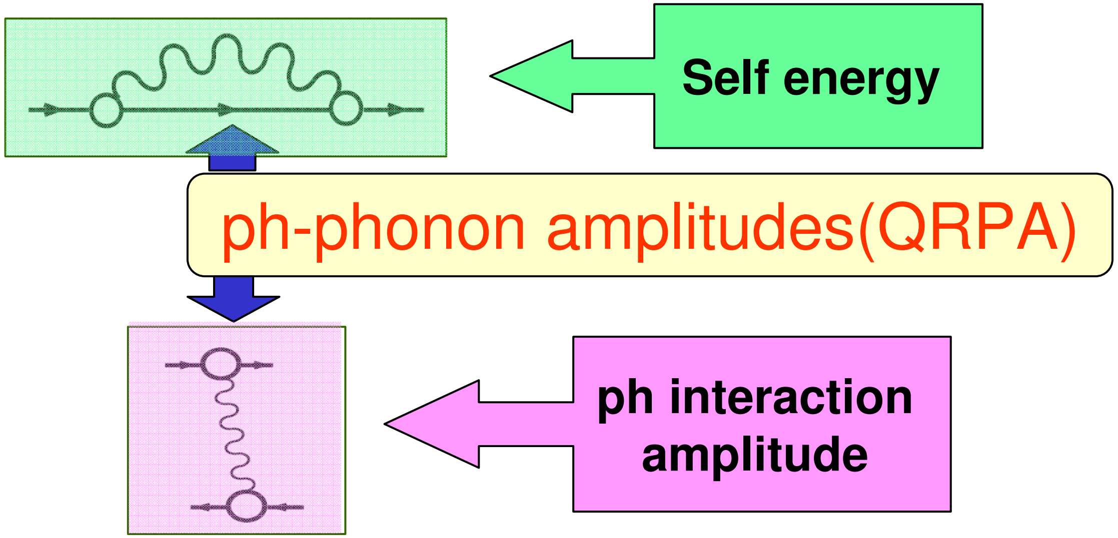


Self energy

ph-phonon amplitudes(QRPA)

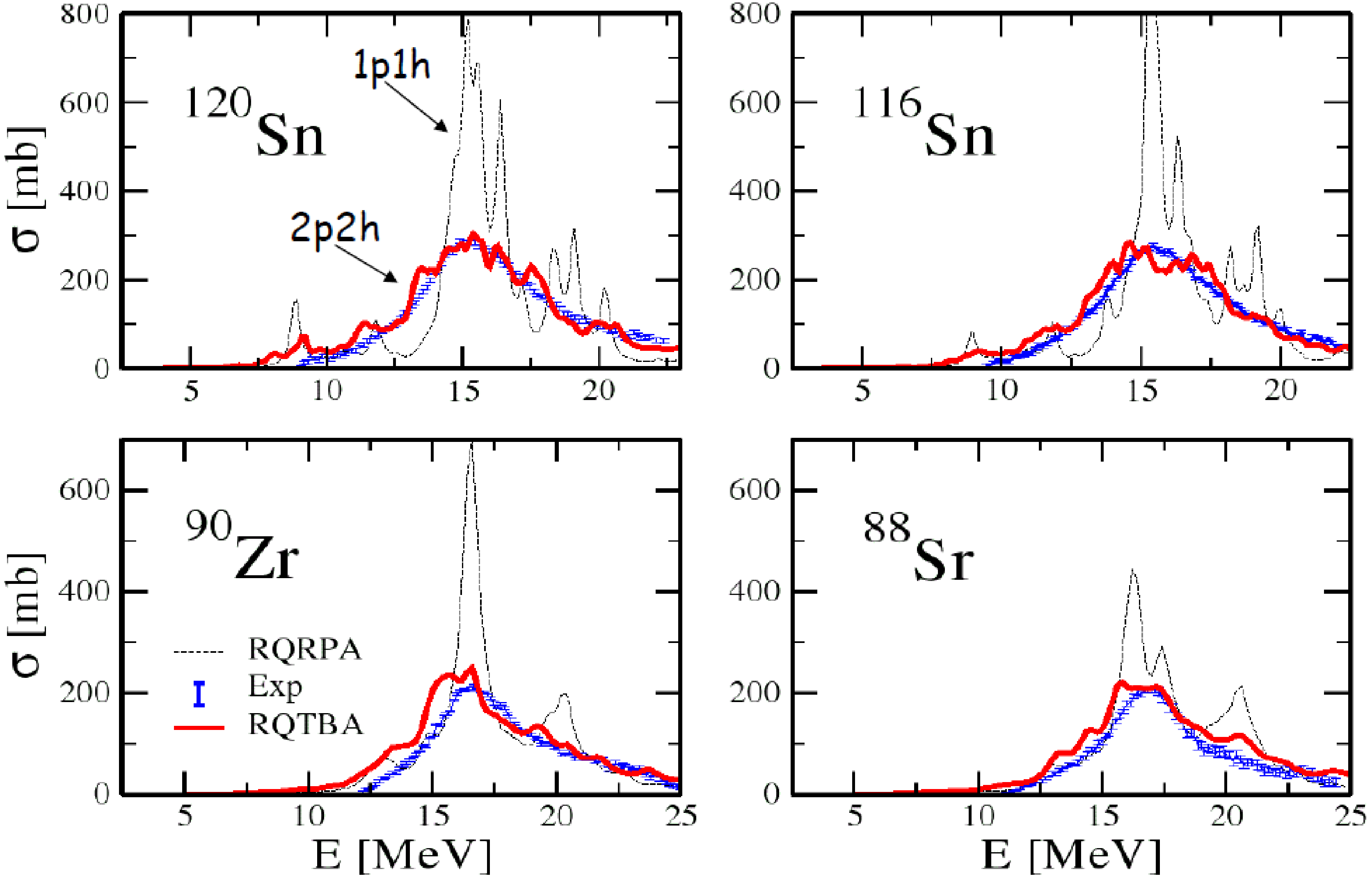
ph interaction amplitude

Problem of divergengies:

Renormalization of the interaction:

$$V(\omega) \rightarrow V_{RPA} + V(\omega) - V(0)$$

Giant Dipole Resonance within Relativistic Quasiparticle Time Blocking Approximation (RQTBA)



Litvinova, P.R., Tselyaev, PRC 78, 014312 (2008)

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).

Dipole vibration of neutron excess: ^{132}Sn

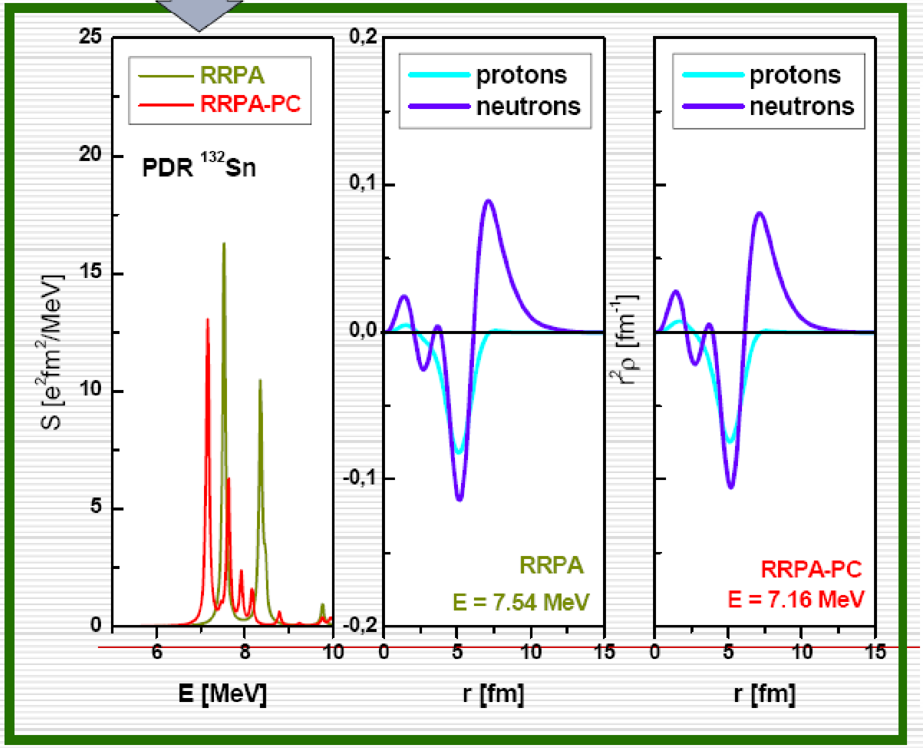
Strength function

Transition density, RRPA

Transition density, RRPA-PC

Distribution of neutron p-h configurations

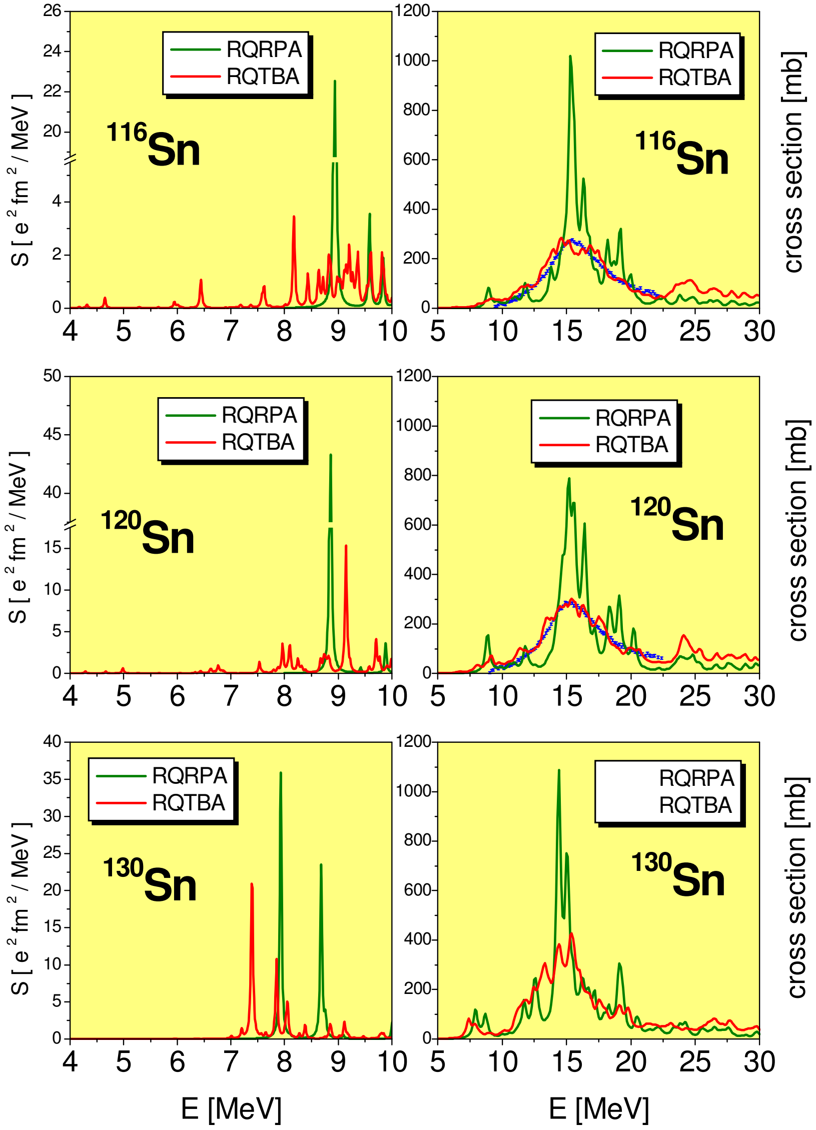
$$\left(|\rho^n_{ph}|^2 - |\rho^n_{hp}|^2\right)$$



RRPA, 7.54 MeV	RRPA-PC, 7.16 MeV
53.6 % (3s1/2 → 3p3/2)	49.5 % (3s1/2 → 3p3/2)
16.5 % (3s1/2 → 3p1/2)	21.5 % (3s1/2 → 3p1/2)
9.7 % (2d3/2 → 3p1/2)	6.4 % (2d3/2 → 3p1/2)
7.3 % (2d3/2 → 3p3/2)	4.1 % (1h11/2 → 1i13/2)
4.7 % (1h11/2 → 1i13/2)	3.9 % (2d3/2 → 3p3/2)
0.9 % (1g7/2 → 1h9/2)	0.7 % (1g7/2 → 1h9/2)
0.3 % (2d5/2 → 3p3/2)	0.1 % (1g7/2 → 2f5/2)
0.2 % (1g7/2 → 2f5/2)	0.1 % (2d5/2 → 3p3/2)
0.1 % (1g7/2 → 2f7/2)	0.1 % (2d3/2 → 4p1/2*)
0.1 % (2d3/2 → 4p1/2*)	0.1 % (1g7/2 → 2f7/2)
	0.1 % (3s1/2 → 4p1/2*)
	0.1 % (3s1/2 → 4p3/2*)
93.4 %	86.7 %

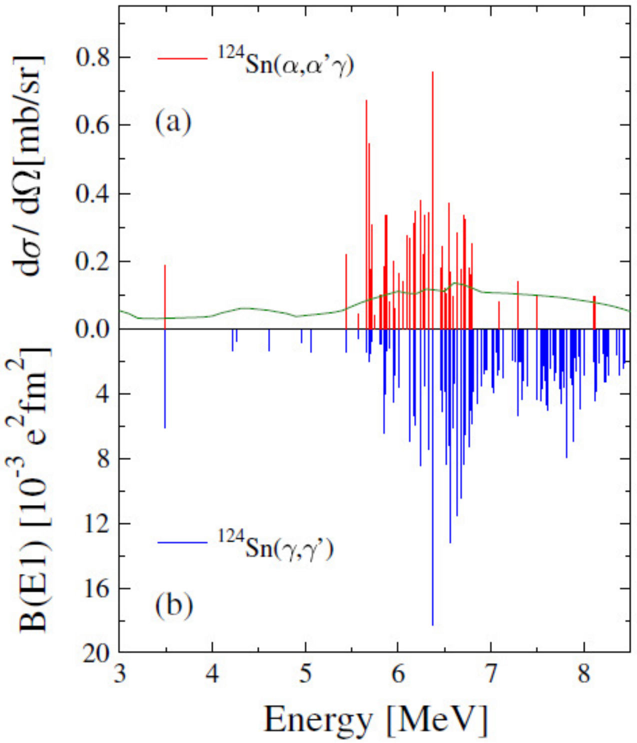
Litvinova, P.R., Vretenar, PLB 647, 111 (2007)

Dipole strength in Sn isotopes

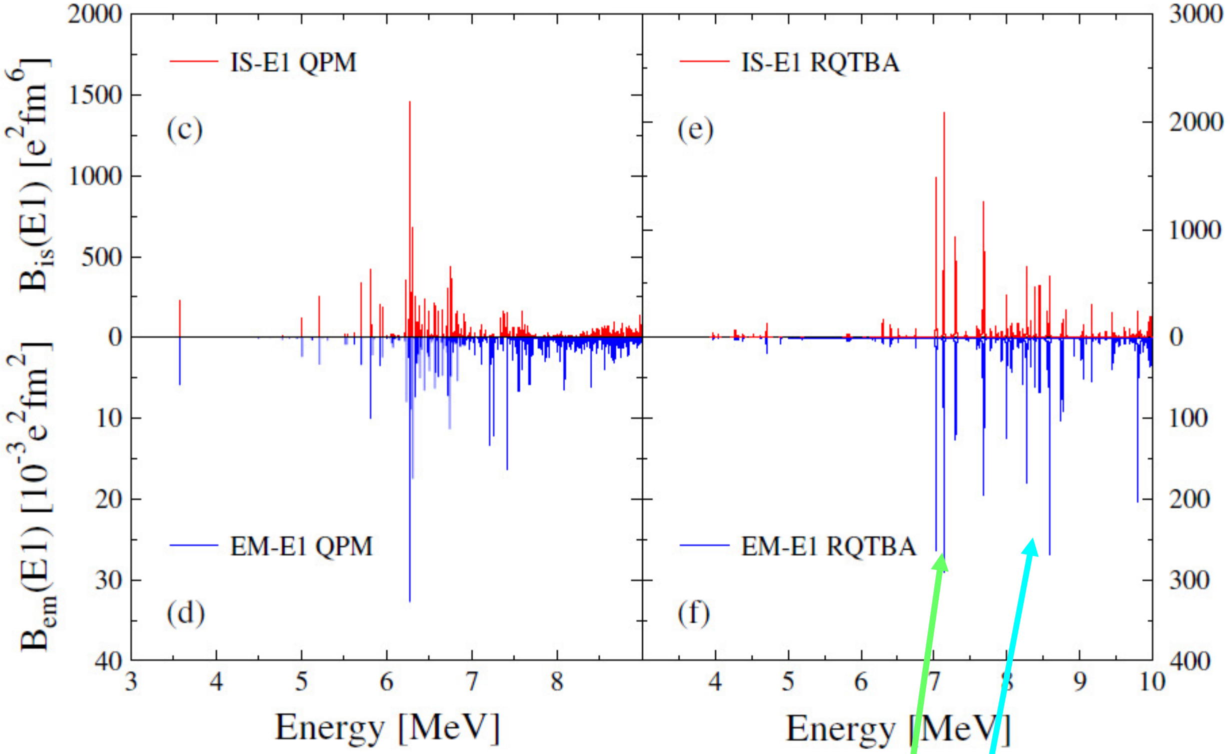


Litvinova, P.R. Tselyaev, PRC 78, 14312 (2008)

EXP. (Endres et al)

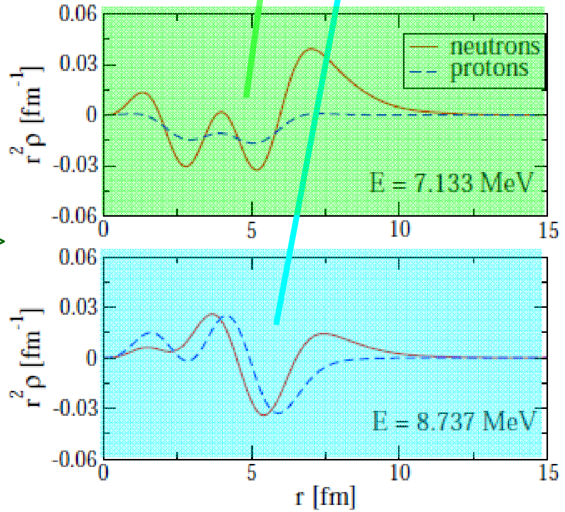


QPM (Ponomarev) QRTBA



Hadron vs Coulomb excitation

Transition densities



Enders et al, PRL 105, 212503 (2010)

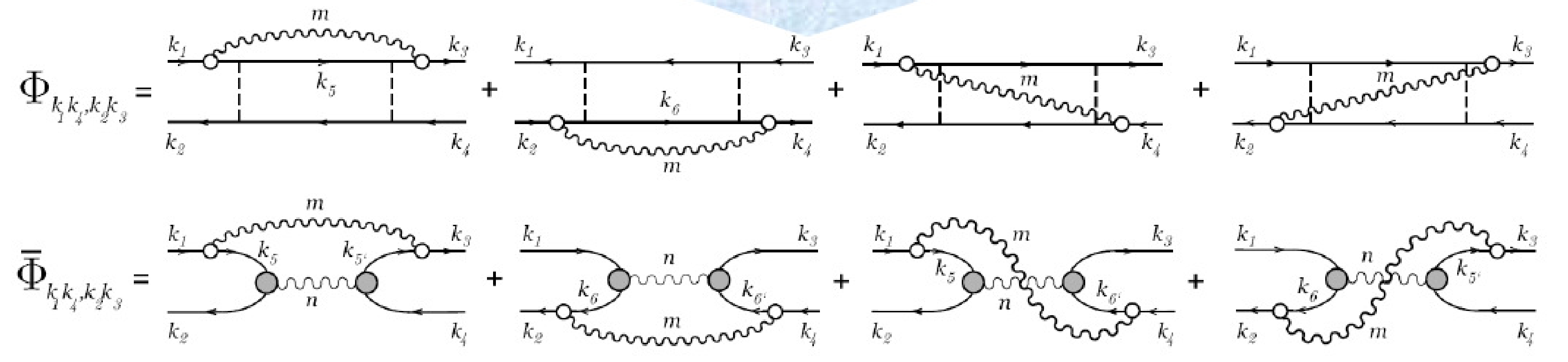
From "2q+phonon" to "2 phonons"

P. Schuck, Z. Phys. A 279, 31 (1976)
V.I. Tselyaev, PRC 75, 024306 (2007)

&

Mode Coupling Theory
Time Blocking Approximation

Replacement of the uncorrelated propagator inside the Φ amplitude by QRPA response



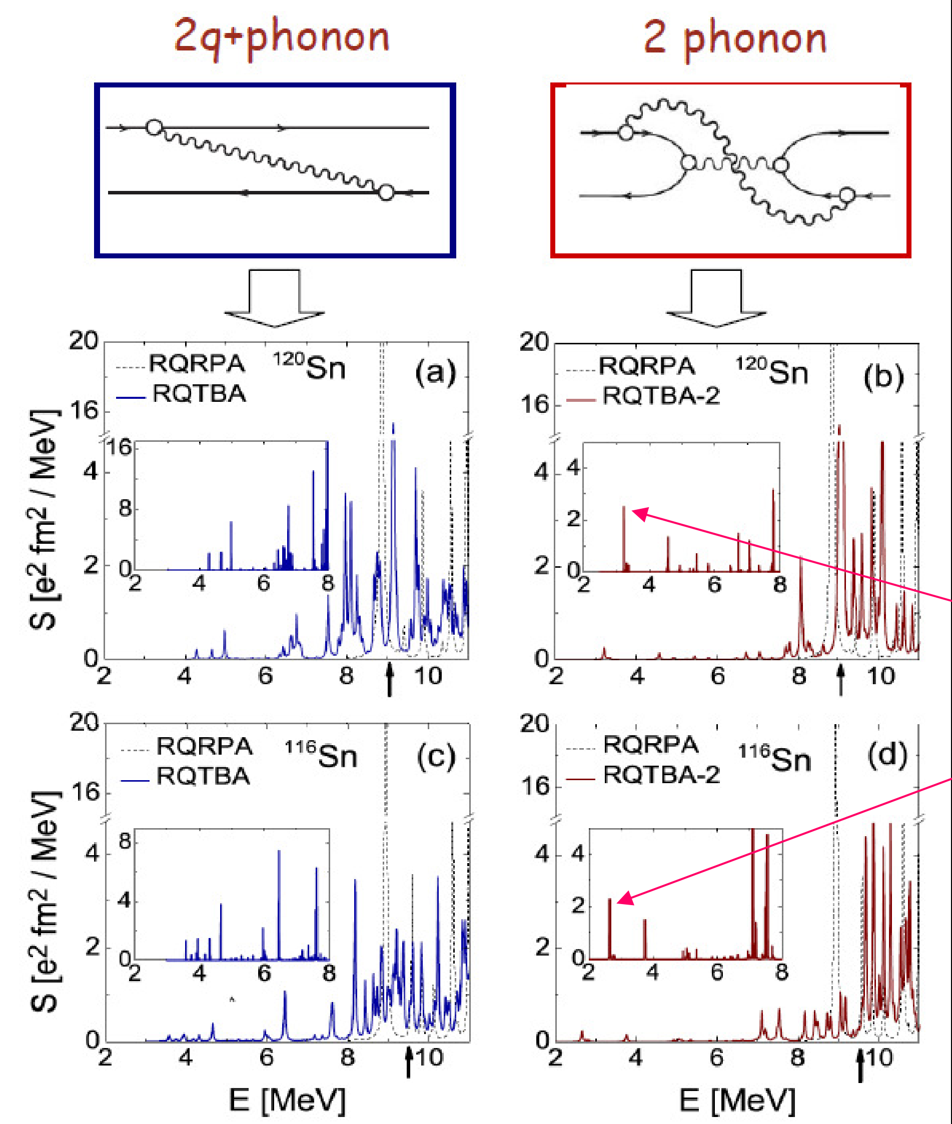
Nuclear response: $R = A + A\,(V + \bar{\Phi})\,R$

Poles may appear at lower energies:

'2q+phonon' response:
$\Phi_{iji'j'}(\omega) \sim \Sigma_{\mu k}\, \alpha_{ijk\mu}/(\omega - E_{i'} - E_k - \Omega_\mu)$

'2 phonon' response:
$\Phi_{iji'j'}(\omega) \sim \Sigma_{\mu\nu}\, \alpha_{iji'j'}/(\omega - \Omega_\nu - \Omega_\mu)$

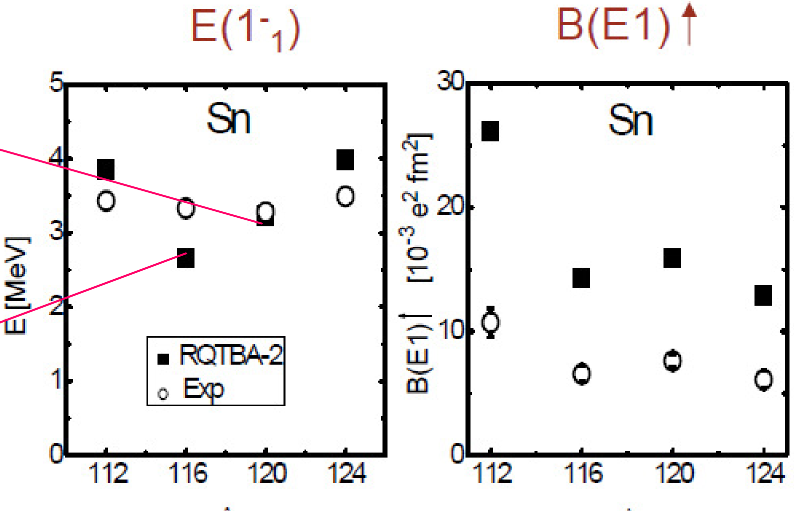
Phonon-phonon coupling:



First two-phonon state 1^-_1

$$3^- \otimes 2^+$$

$$E(1^-_1) \approx E(2^+_1) + E(3^-_1)$$



Litvinova, Ring, Tselyaev, PRL 105, 022502 (2010)
Exp: Pysmenetska et al, PRC 73, 017302 (2006)

Summary and outlook:

- Present status

  density functional theory has been extended for excited states
  by a consistent treatment of manybody correlations using
  Greensfunction techniques to include particle-vibrational coupling

  2qp-phonon and 2phonon coupling schemes have been studied

  giant resonances position and width, low energy dipole modes, two-phonon states
  in heavy spherical nuclei are reproduced within a fully consistent scheme

- Open problems and perspectives

  static part: we are far from a microscopic derivation
  we have to improve the functionals in the ph and the pp-channel
  dynamic part: inclusion of pairing vibrations
  explicite single particle continuum
  inclusion of deformation
  how does the energy dependent kernel behave at large amplitudes?
  ……..

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A. Afanasjev (Mississippi)

E. Litvinova (GSI), V. Tselyaev (St. Petersburg)

Z.-Y. Ma (CIAE, Beijing)