Correlations beyond mean field based on covariant density functional theory

Sofia, Oct. 3, 2019

Peter Ring

Technical University Munich
Excellence Cluster "Origins"
Peking University

Correlations ?

- all effects going beyond independent particle motion
- Configuration mixing
- Pauli correlations: Slater determinants
- mean field theory: correlations by symmetry breaking

- short range correlations:
  - Jastrow factors, correlators: $|\psi) = e^{C}\,|\Phi)$
  - Brueckner theory
  - renormalized effective force (V_low-k, SRG …)

- Correlations beyond mean field:
  - mixing of Slater determinants

Content:

Applications of CDFT beyond mean field:

- Generator Coordinate Method (GCM)
- α-clustering in light nuclei
- Collective Hamiltonian (5DCH)
- benchmark calculations (full GCM ↔ 5DCH)
- Configuration Interaction Projected DFT (CI-PDFT)
- Neutrino-less double beta decay
- Complex Configurations in time-dependent mean field theory
- particle-vibrational coupling

Conclusions and outlook

Density functional theory is a mapping
of the complicated many-body problem
→ to a simple one-body problem
which preserves the local density ρ (r)
and therefore the energy E(ρ),
and quantities depending on ρ (r),
e.g. rms-radii

Starting point: $E = E[\rho]$

Mean field: $h = \frac{\delta E[\rho]}{\delta \rho}$

Interaction: $V = \frac{\delta^2 E[\rho]}{\delta \rho^2}$

DFT has many advantages:

- universal
- provides an easy understanding (e.g. deformation)
- technically simple

DFT fails in many respects:

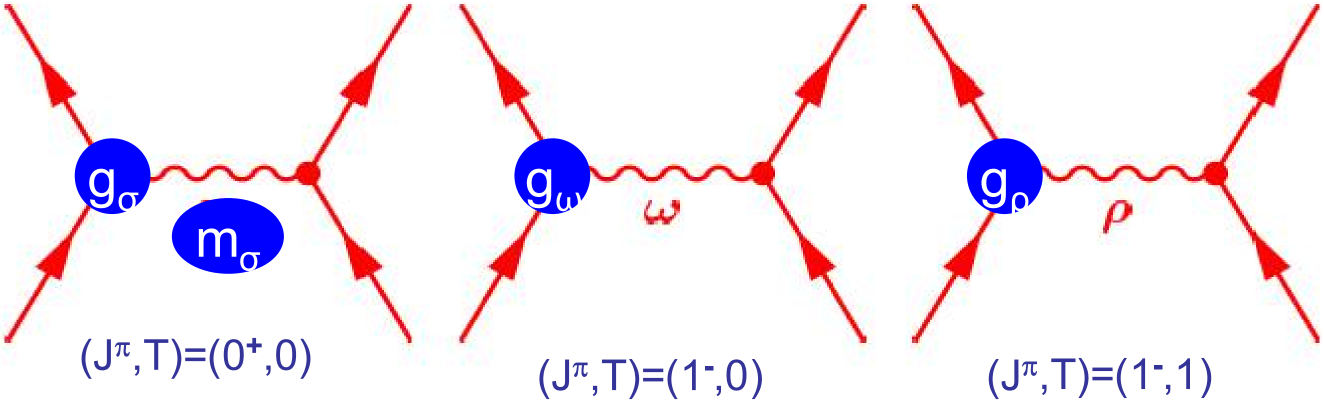
- no spectroscopic properties
- low level density at Fermi surface
- no shape coexistence
- no width of giant resonances
- …..

DFT is phenomenological

Covariant DFT is based on the Walecka model

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

This model has only four parameters:



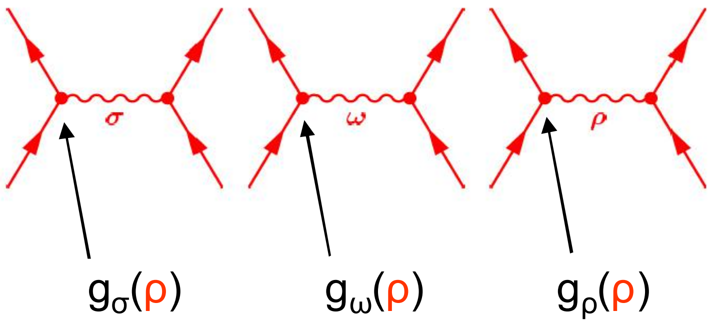
$$S(r) = g_\sigma \sigma(r) \quad V(r) = g_\omega \omega(r) + g_\rho \rho(r) + eA(r)$$

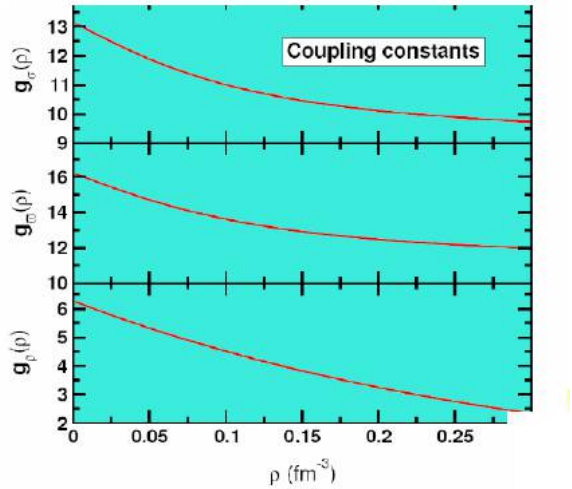
Effective density dependence:

The basic idea comes from ab initio calculations
density dependencd includes Brueckner correlations and threebody forces

a) non-linear meson couplings: **NL3, FSU, PK1 ….**

b) density dependent couplings: **DD-ME1, DD-ME2, DD-MEδ ….**





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**
Roca-Maza, Vinas, Centelles, PR, Schuck, PRC 84, 54309 (2011) **DD-MEδ**

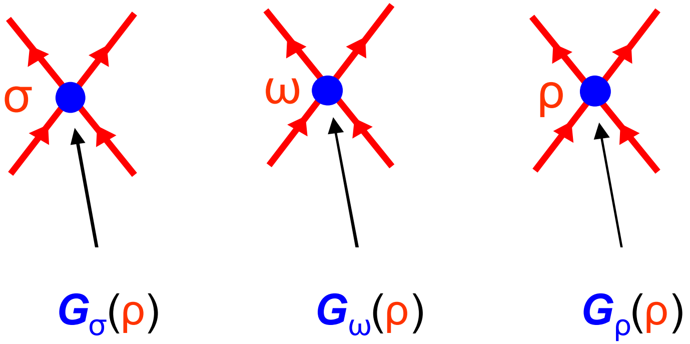
Effective density dependence:

The basic idea comes from ab initio calculations
density dependencd includes Brueckner correlations and threebody forces

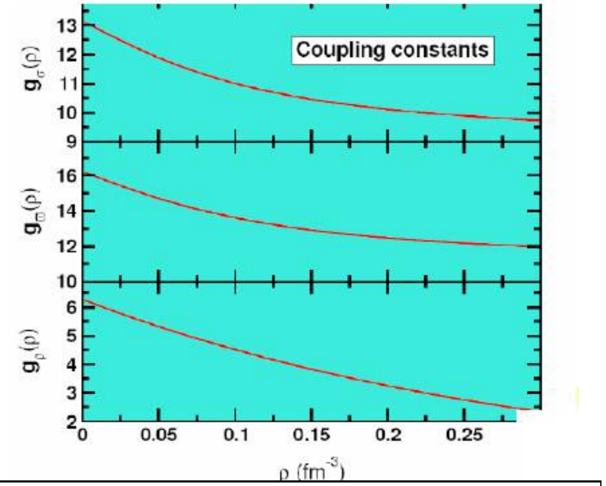
a) non-linear meson couplings: **NL3, FSU, PK1 …**

b) density dependent couplings: **DD-ME1, DD-ME2 ….**

c) Point coupling models: **PC-F1, DD-PC1, PC-PK1 …**



$$D\ (\bar\psi\psi)\Delta(\bar\psi\psi)$$



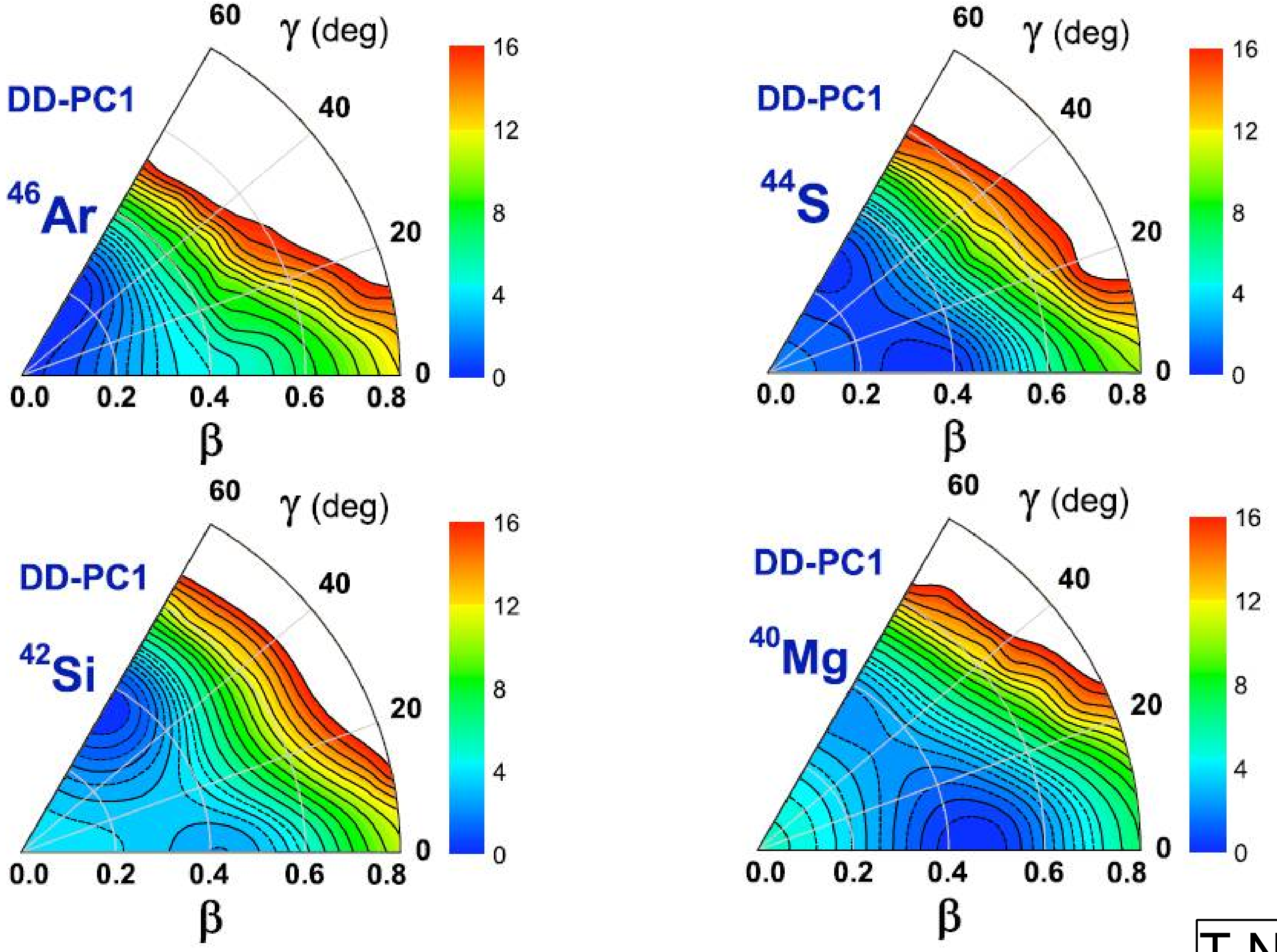
adjusted to ground state properties of finite nuclei

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, J. Meng, PRC, 82, 054319 (2010) **PC-PK1**

Transitional nuclei
and
changes of deformation
in isotonic and isotopic chains

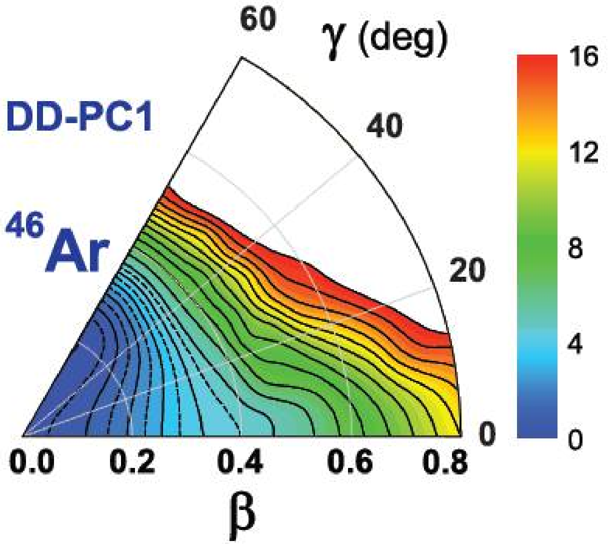
Applications: $N = 28$ isotones

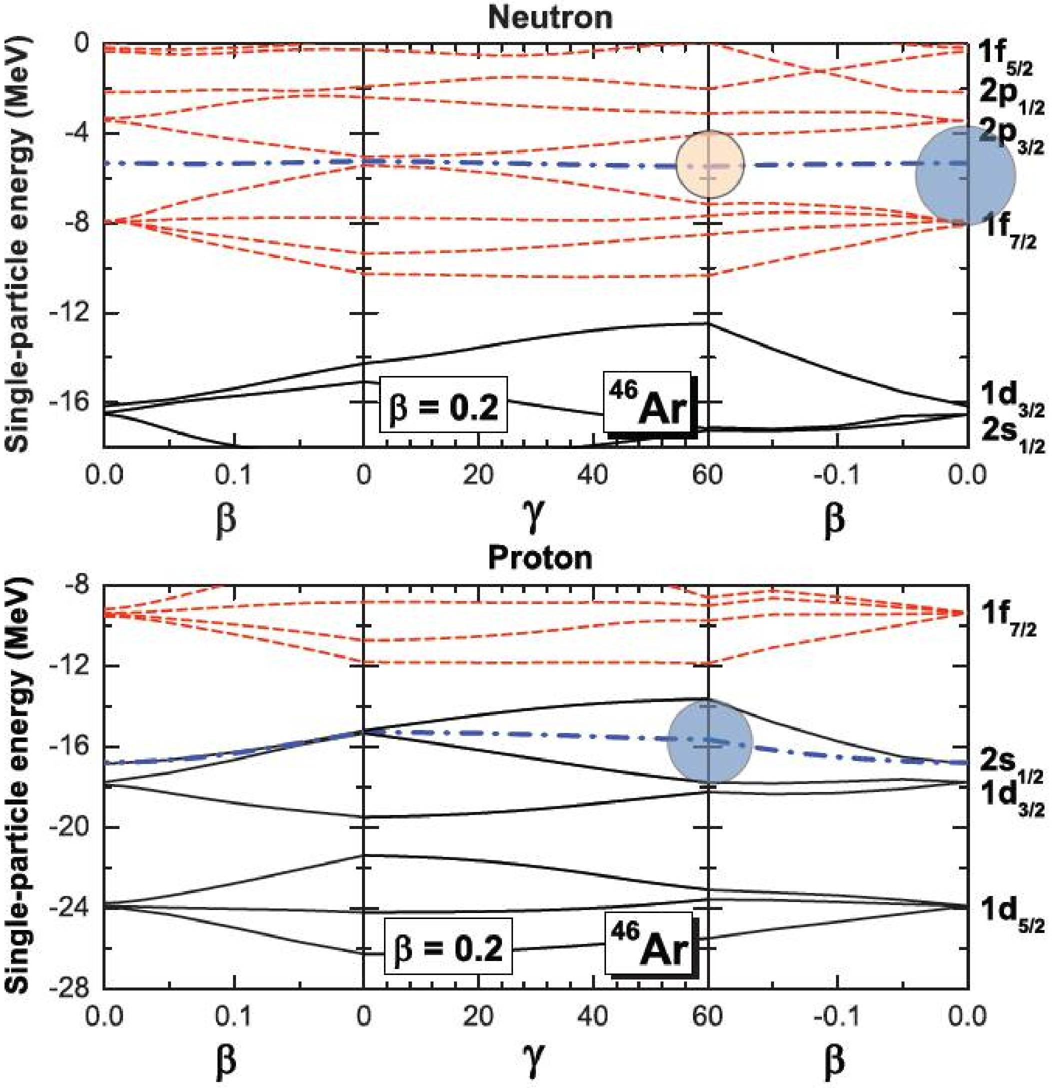
The variation of the mean-field shapes is governed by the evolution of the underlying shell structure of single-nucleon orbitals.



T.Niksic (2011)

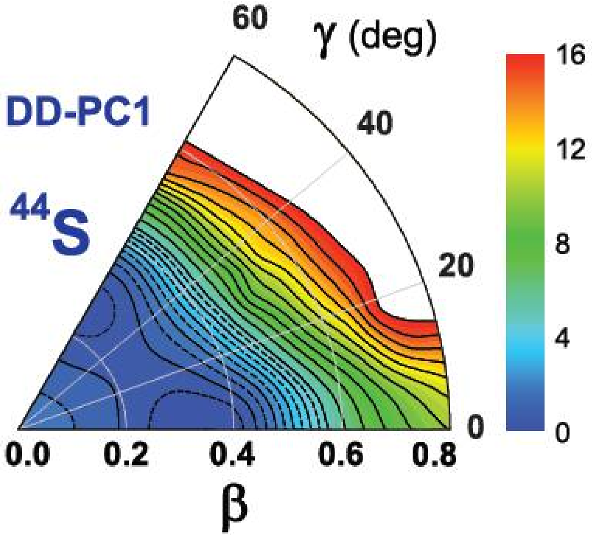
^{46}Ar isotope: single-particle levels

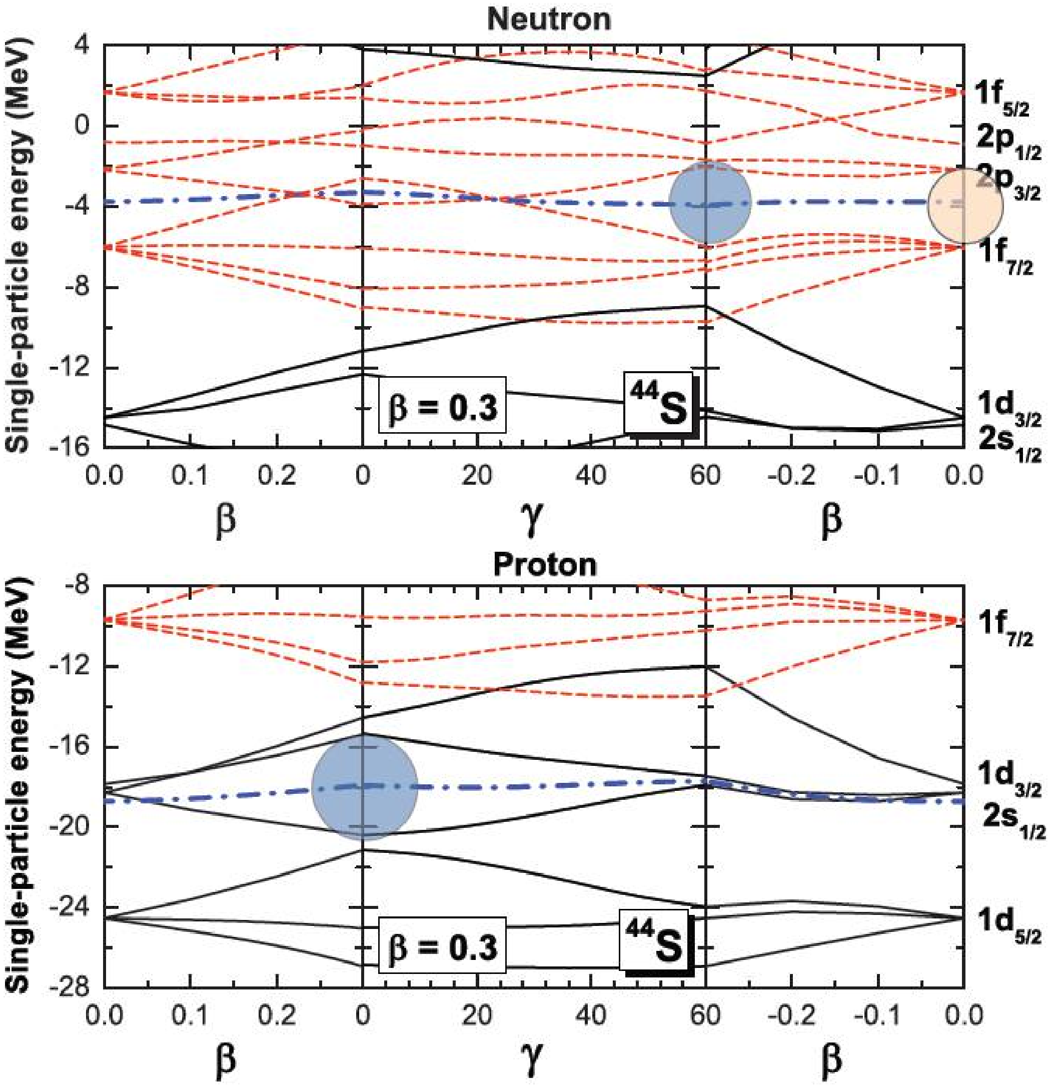




T.Niksic (2011)

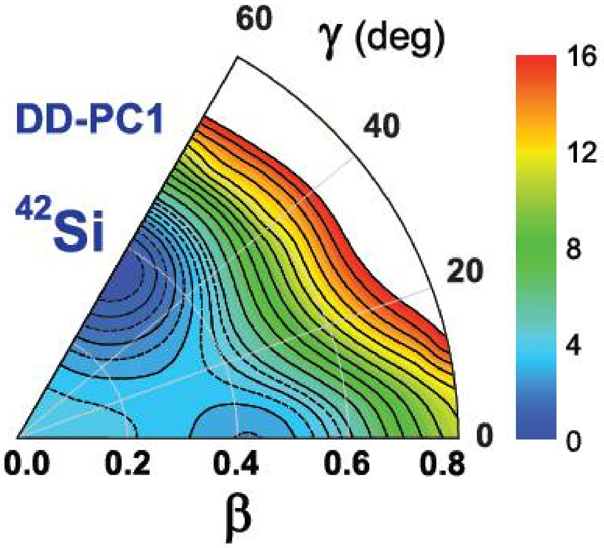
^{44}S isotope: single-particle levels

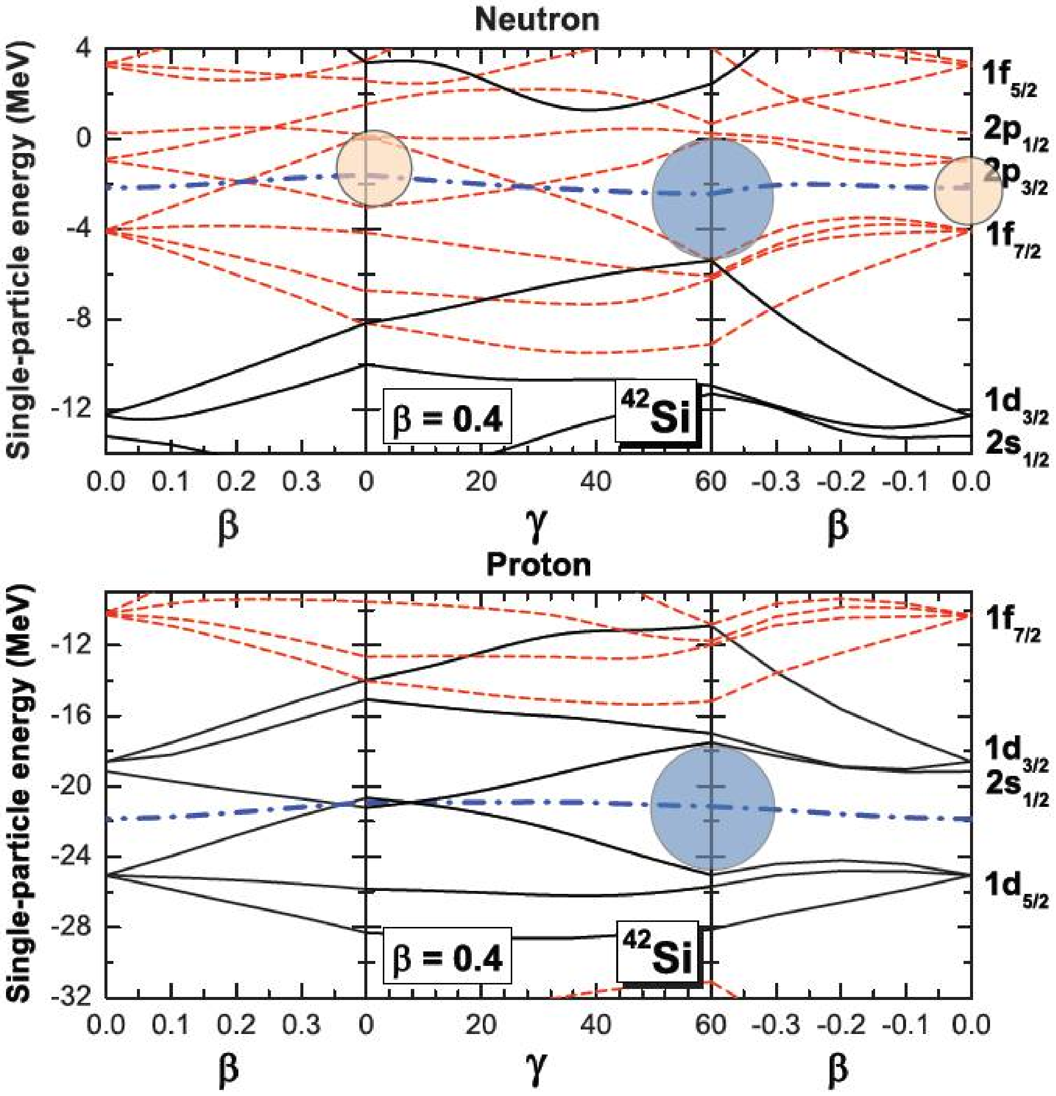




T.Niksic (2011)

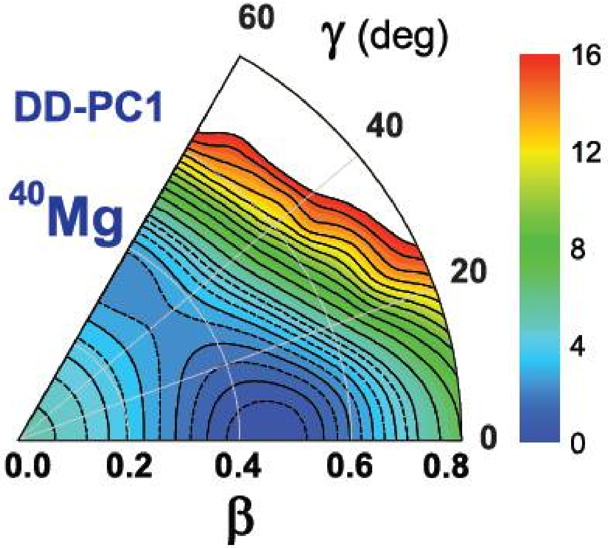
^{42}Si isotope: single-particle levels

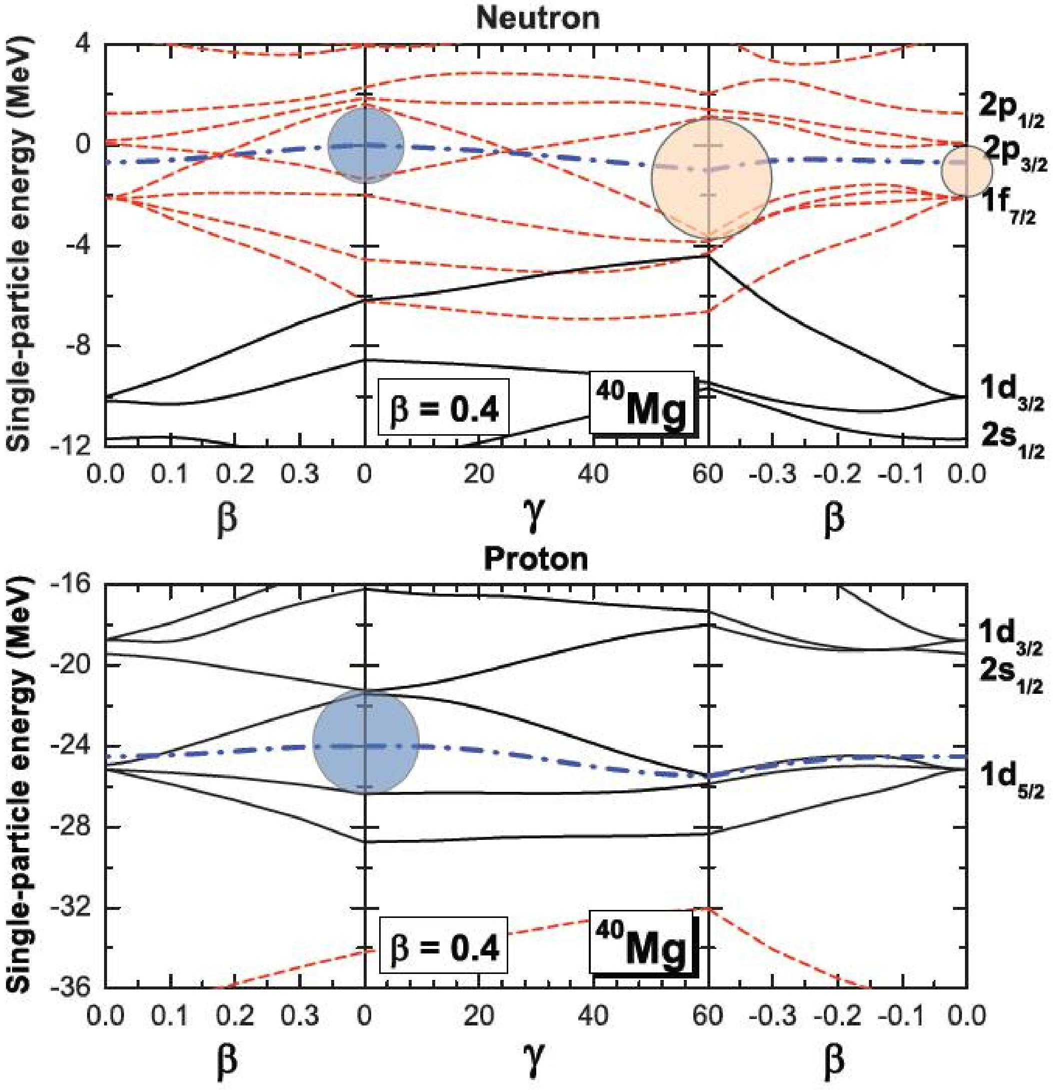




T.Niksic (2011)

^{40}Mg isotope: single-particle levels





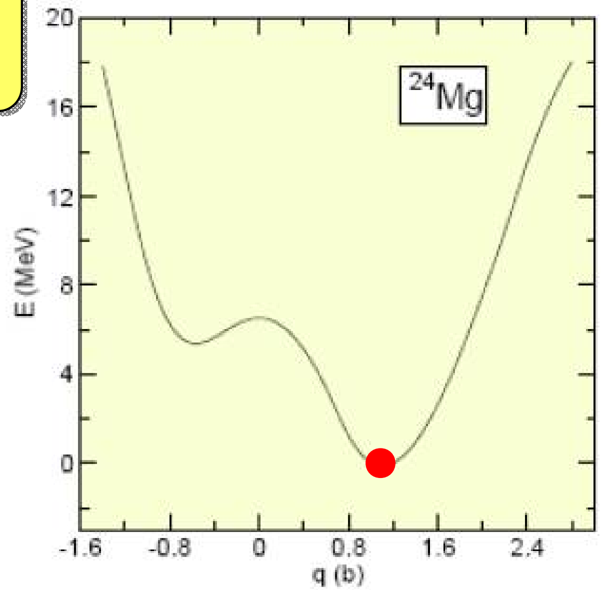
T.Niksic (2011)

Density functional theory
beyond mean field
The Generator Coordinate Method

DFT beyond mean field: GCM-method

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

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



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

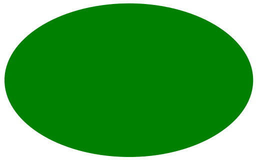
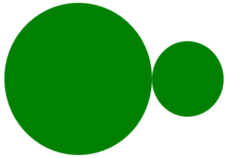
Hill-Wheeler equation:

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

with projection:

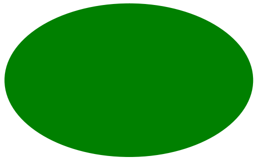
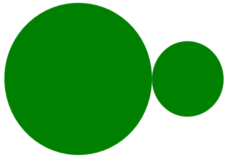
$$| \Psi \rangle = \int dq\, f(q) \hat{P}^N \hat{P}^I | q \rangle$$

alpha-clustering in nuclei:

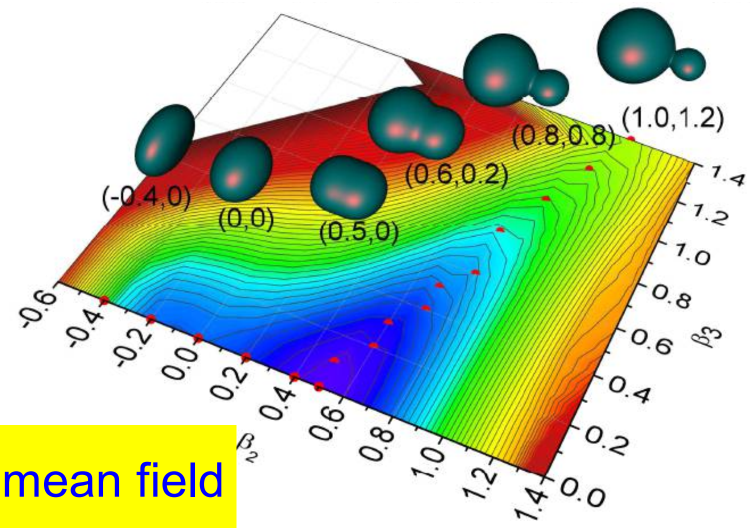
^{20}Ne:  or  ?

Relativistic GCM provides a tool for a quantitative assessment

alpha-clustering in nuclei:

^{20}Ne:  or  ?

Relativistic GCM provides a tool for a quantitative assessment

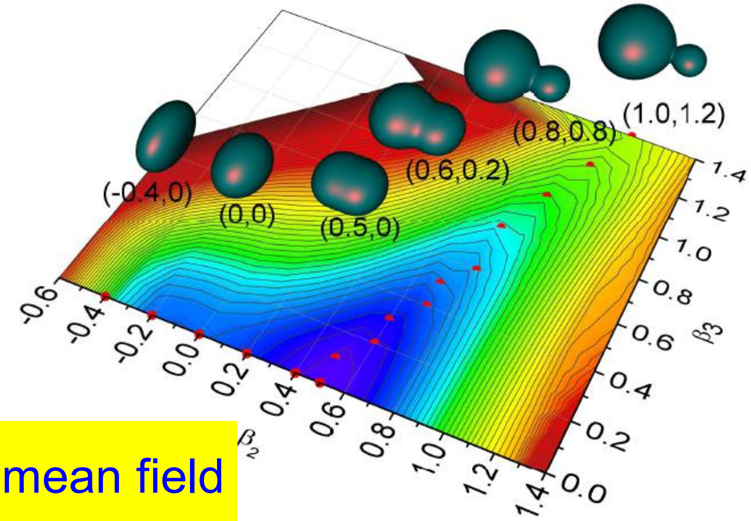


mean field

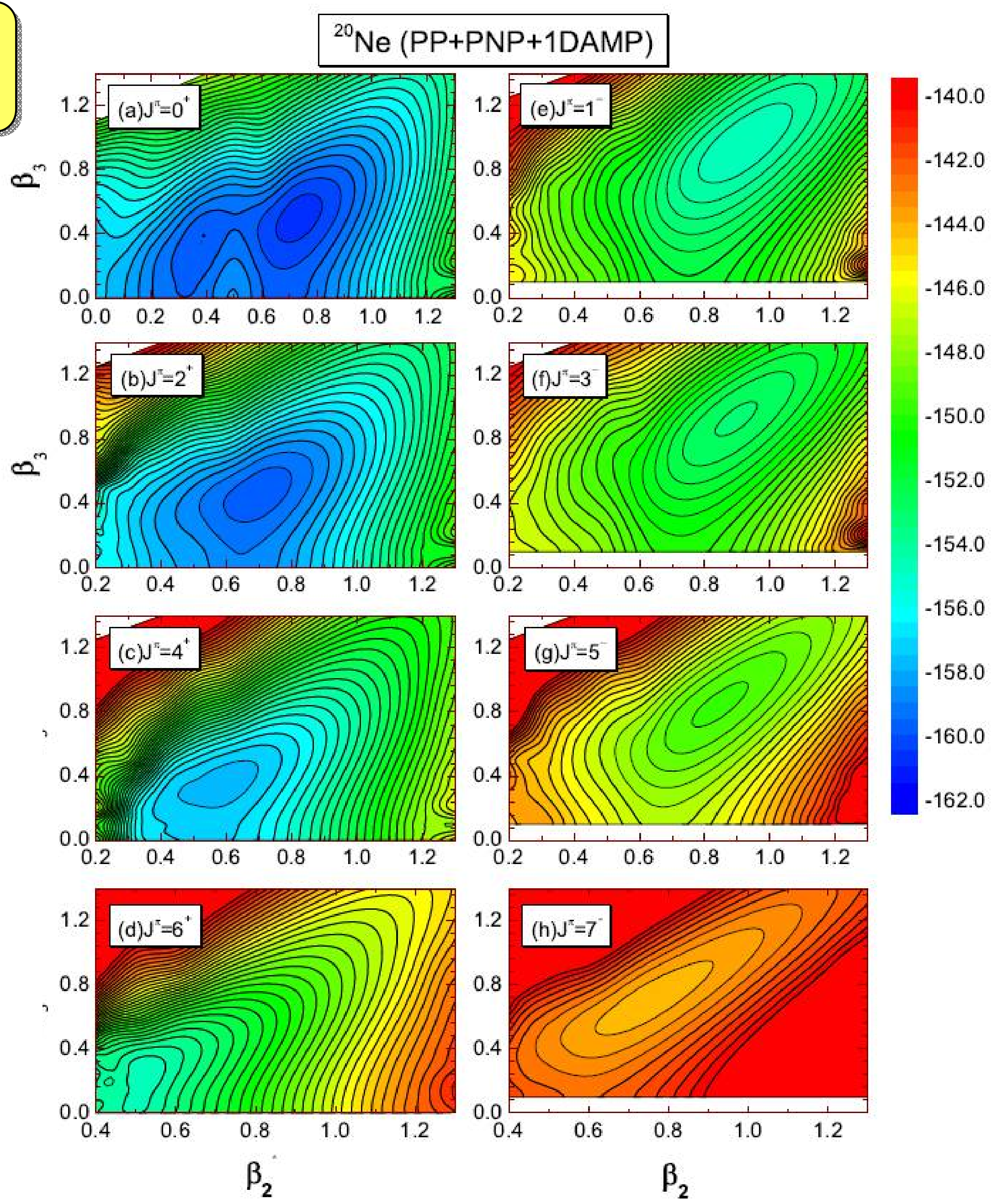
$$|J^\pi NZ;\alpha\rangle = \sum_{\kappa\in\{q,K\}} f_\kappa^{J\pi\alpha} \hat{P}_{MK}^J \hat{P}^N \hat{P}^Z \hat{P}^\pi |q\rangle,$$

Enfu Zhou et al.   PLB 2016

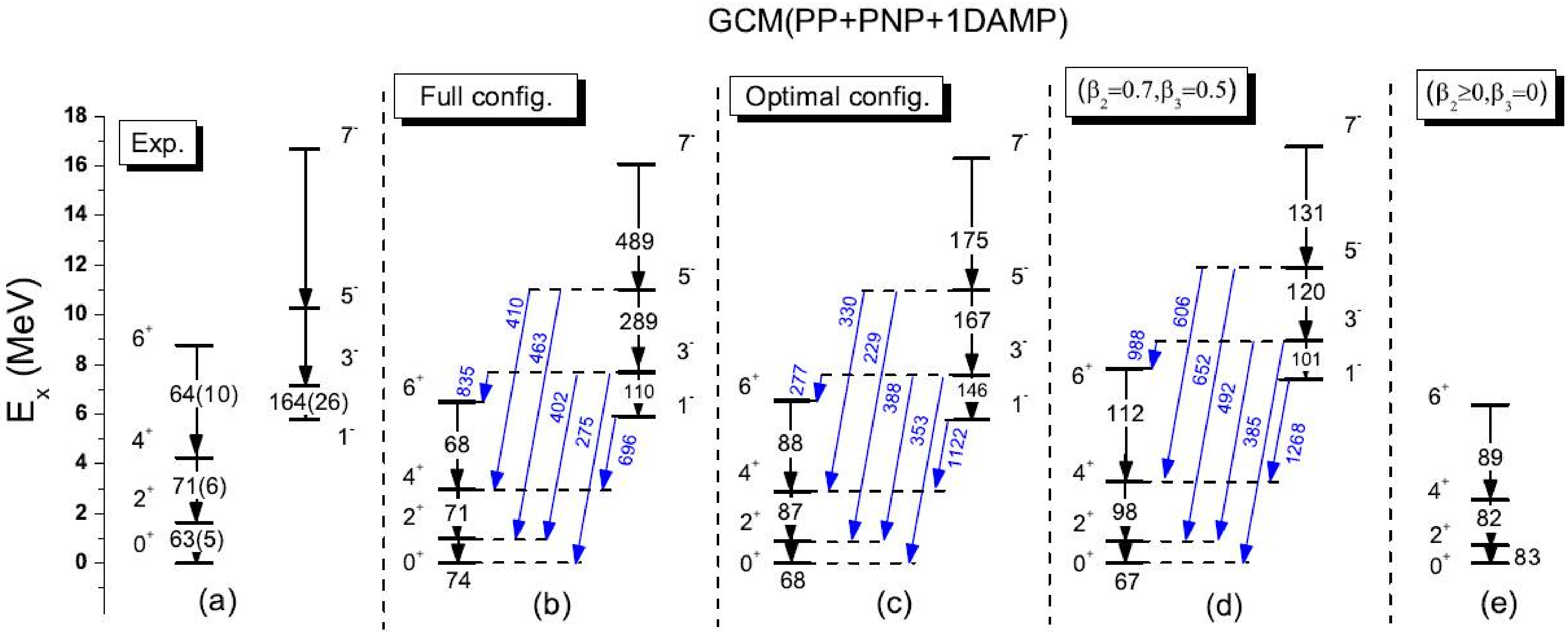
Projected energy surfaces:



mean field



Low-lying spectra:

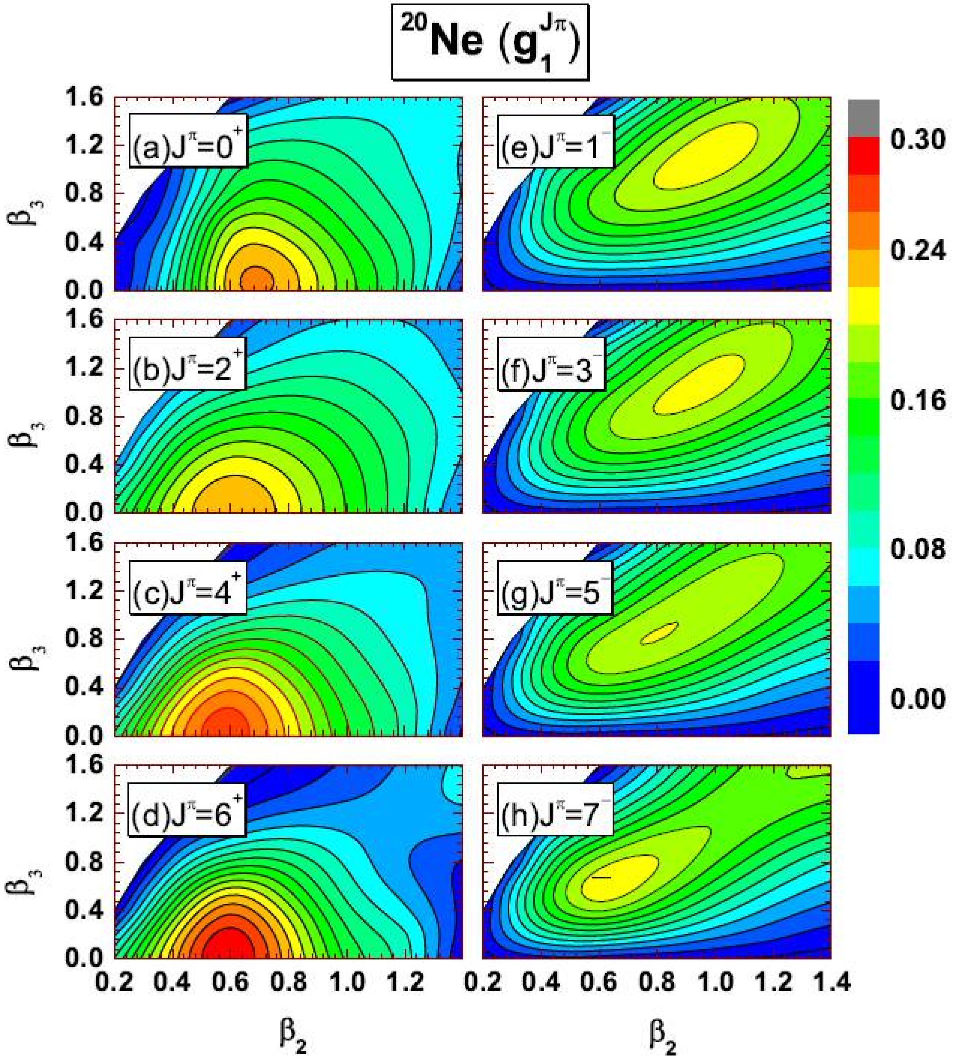


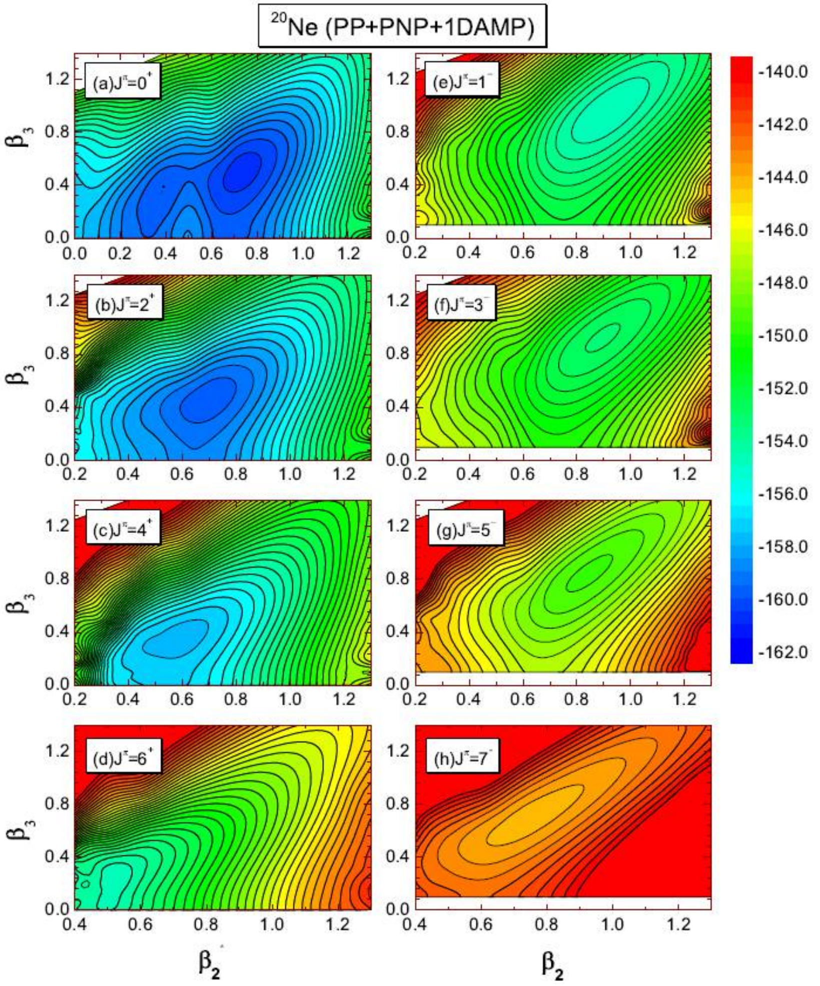
↓ B(E2)

↓ B(E3)

Weights: $g^{J\pi}$

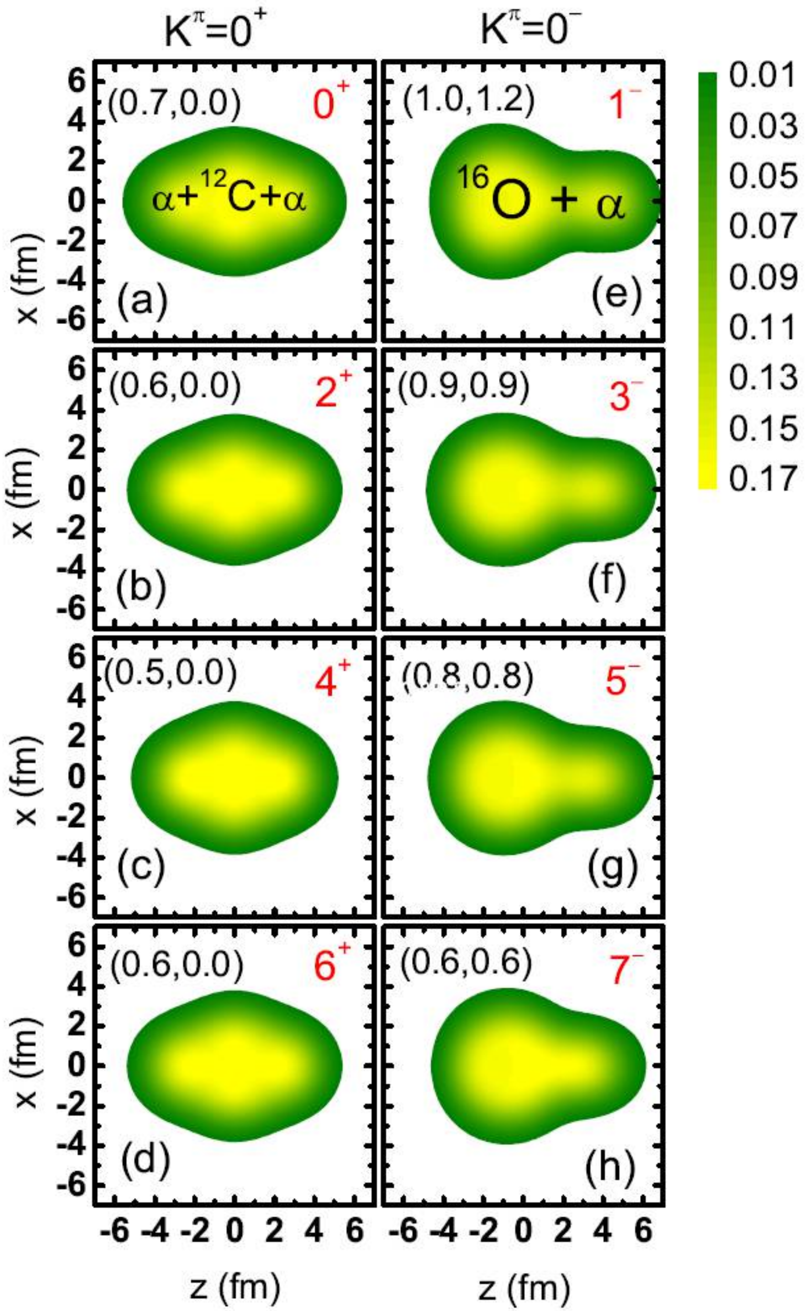
projected energy:





Enfu Zhou et al. 2016

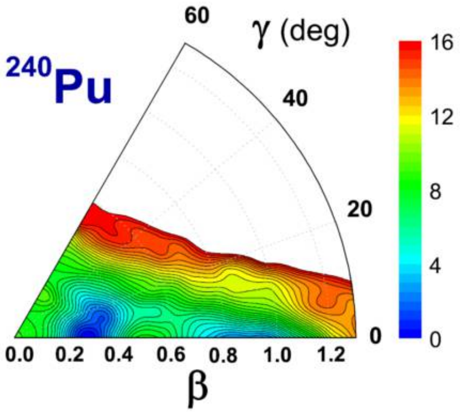
Intrinsic density of the dominand configuration for each J^{π}-value



Enfu Zhou et al. 2016

Derivation of a Collective Hamiltonian

Five dimensional collective Hamiltonian (5DCH)



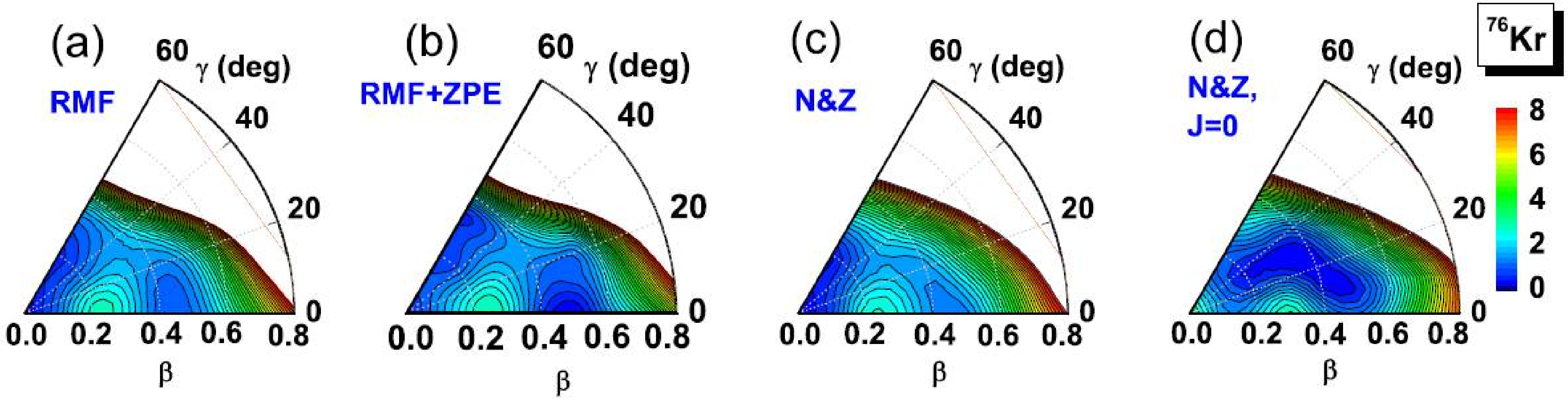
The entire dynamics of the collective Hamiltonian is governed by seven functions of the intrinsic deformations β and γ: The collective potential energy, the three mass parameters $B_{\beta\beta}$, $B_{\beta\gamma}$, $B_{\gamma\gamma}$ and the three moment of inertia I_k

$$H_{\text{coll}} = \mathcal{T}_{\text{vib}}(\beta,\gamma) + \mathcal{T}_{\text{rot}}(\beta,\gamma,\Omega) + \mathcal{V}_{\text{coll}}(\beta,\gamma)$$

$$\mathcal{T}_{\text{vib}} = \frac{1}{2}B_{\beta\beta}\dot{\beta}^2 + \beta B_{\beta\gamma}\dot{\beta}\dot{\gamma} + \frac{1}{2}\beta^2 B_{\gamma\gamma}\dot{\gamma}^2$$

$$\mathcal{T}_{\text{rot}} = \frac{1}{2}\sum_{k=1}^{3}\mathcal{I}_k\omega_k^2$$

Benchmark calculation: GCM ↔ 5DCH



Generator-Coordinates: q = (β,γ)
Projection on J: (3 angles)

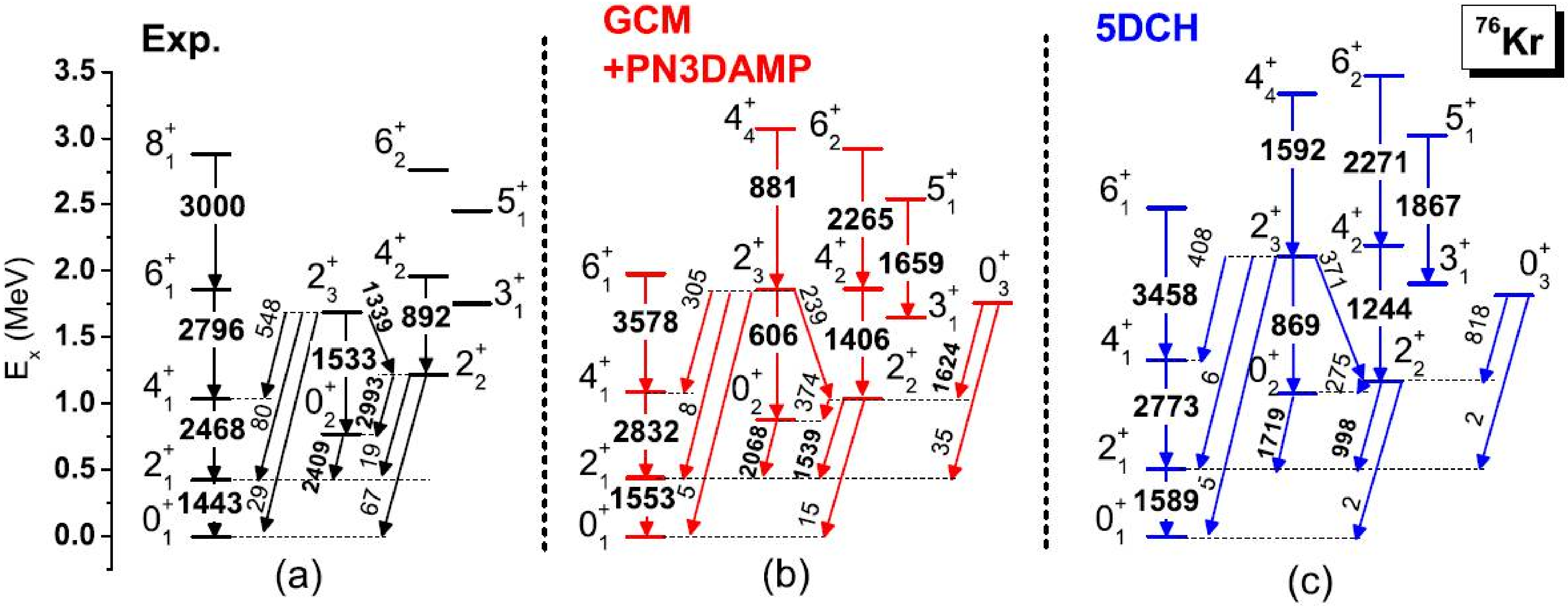
$$|JNZ;\alpha\rangle = \sum_{q,K} f_\alpha^{JK}(q)\hat{P}^J_{MK}\hat{P}^N\hat{P}^Z|q\rangle,$$

Bohr Hamiltonian: $H = -\frac{\partial}{dq}\frac{1}{2B(q)}\frac{\partial}{dq} + V(q) + V_{corr}(q)$

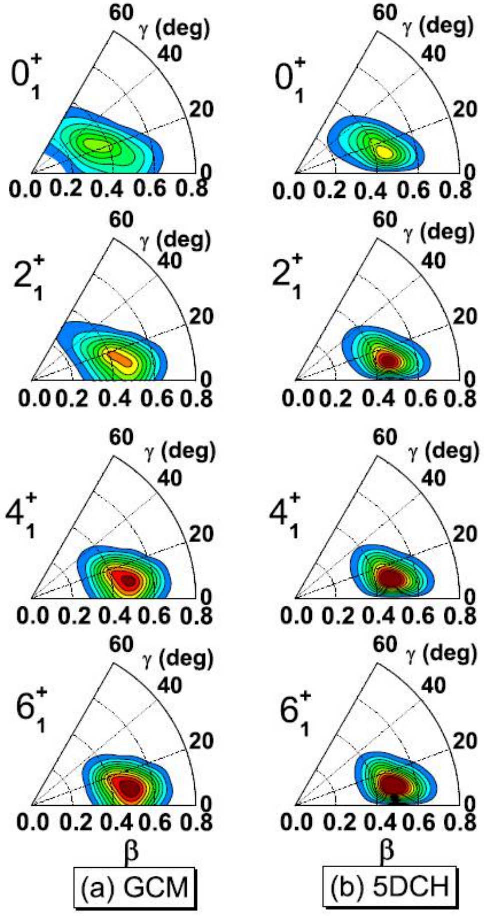
J.M. Yao, K. Hagino, Z.P. Li, P.R. , J. Meng PRC (2014)

Spectra: GCM (7D)
Bohr Hamiltonian (5DCH)

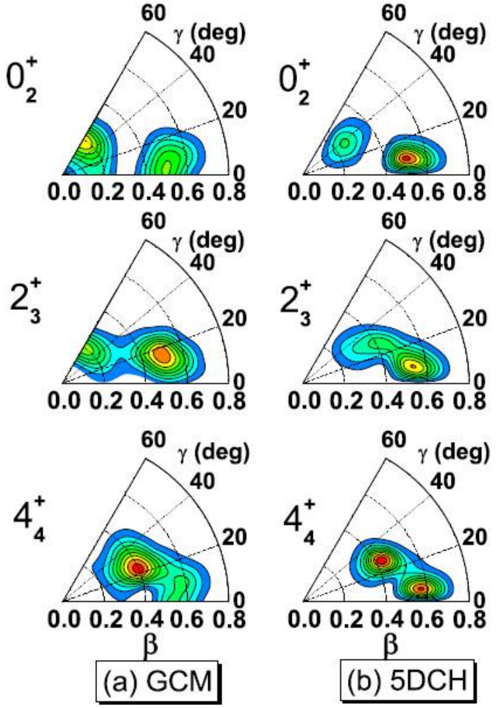
PC-PK1



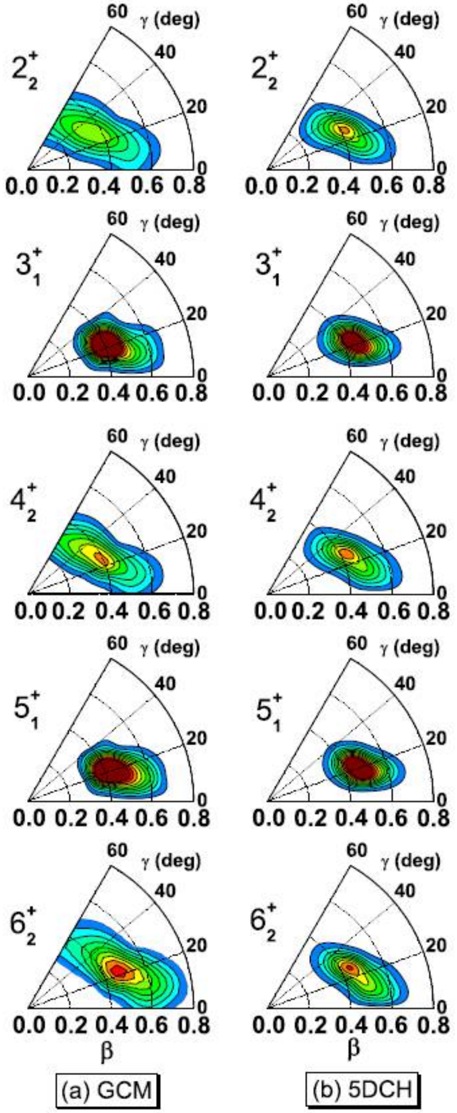
J.M. Yao et al, PRC (2014)



ground state band



quasi-β band



quasi-γ band

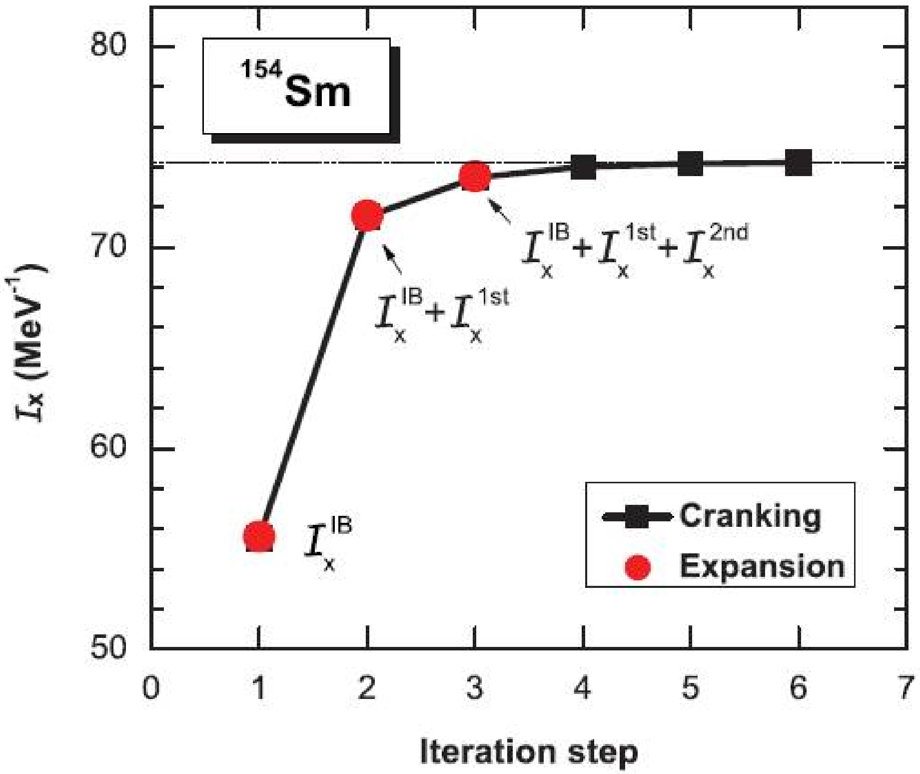
wave functions

J.M. Yao et al, PRC (2014)

Full moment of inertia expressed by phonons:

$$\mathcal{J}_{TV} = 2\sum_{\mu} \frac{\langle\mu|j_x|0\rangle}{\Omega_\mu - \Omega_0}$$

Thouless, Valatin Nucl. Phys. 31, 211 (1962)



Solution
in different orders

Z.P. Li et al, PRC. 86, 34334 (2012)

(C)DFT and the Shell Model

(C)DFT

✓ Universal density functionals

Symmetry broken
Single config. fruitful physics
No Configuration mixing

✓ Applicable for almost all nuclei
✗ No spectroscopic properties

Shell Model

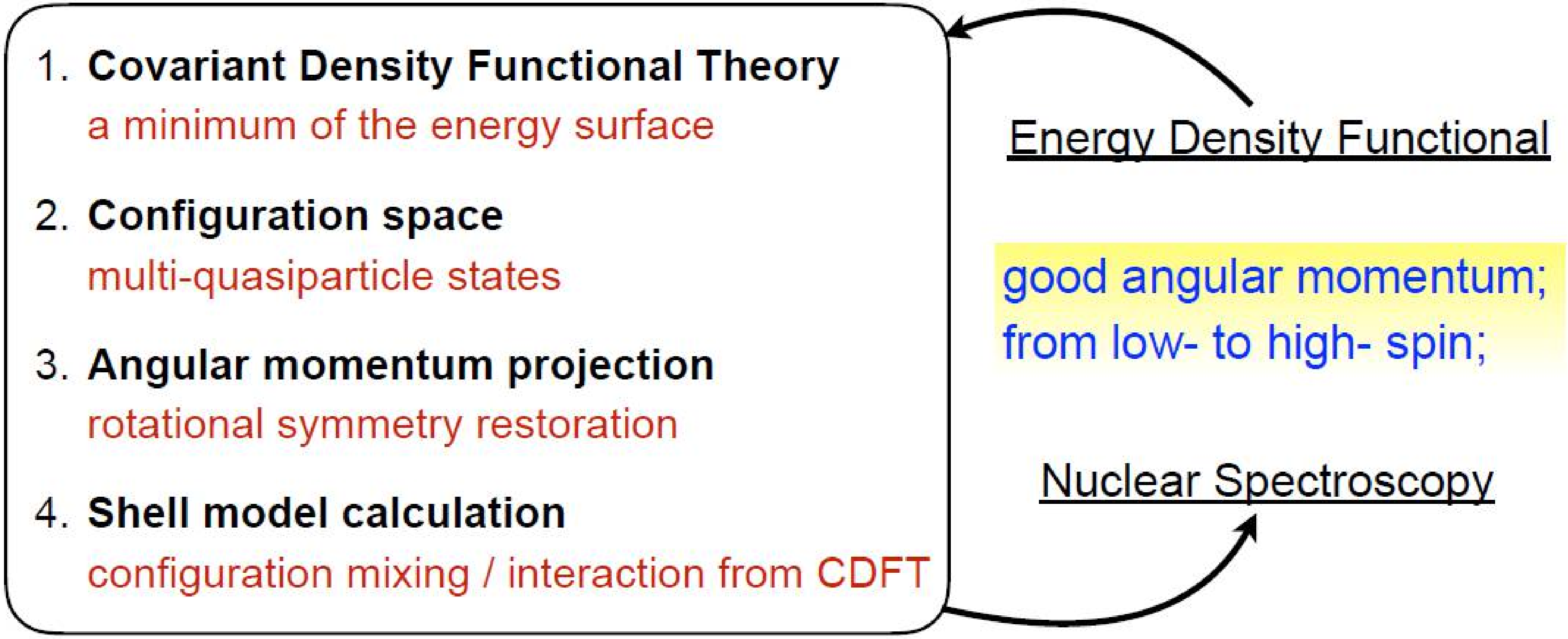
✗ Non-universal effective interactions

No symmetry broken
Single config. little physics
Configuration mixing

✗ intractable for deformed heavy nuclei
✓ spectroscopy from multi config.

a theory combining the advantages from both approaches ?

Pengwei Zhao, Jie Meng, P.R., PRC 94, 041301 (2016)



1. **Covariant Density Functional Theory**
   a minimum of the energy surface
2. **Configuration space**
   multi-quasiparticle states
3. **Angular momentum projection**
   rotational symmetry restoration
4. **Shell model calculation**
   configuration mixing / interaction from CDFT

Energy Density Functional

good angular momentum;
from low- to high- spin;

Nuclear Spectroscopy

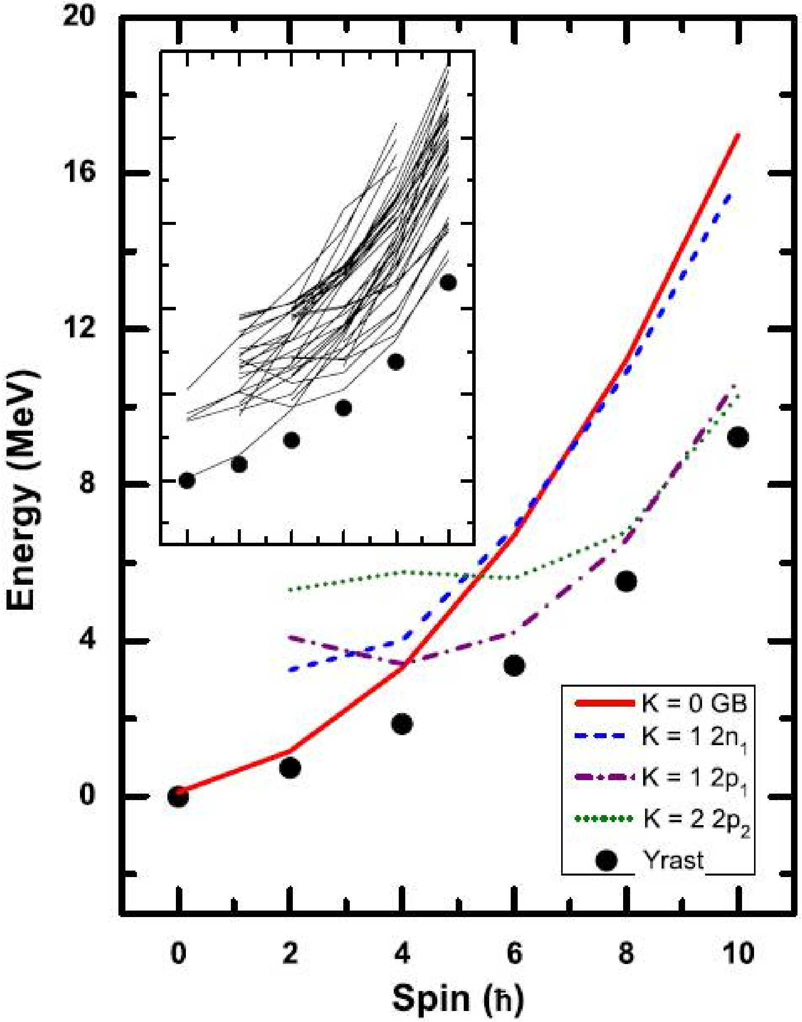
Configuration Interaction Projected DFT (CI-PDFT)

$$|\Psi^I\rangle = C_0 P^I |q\rangle + \sum_{\mu\nu} C_{\mu\nu} P^I \alpha^\dagger_\mu \alpha^\dagger_\nu |q\rangle + \ldots$$

Pengwei Zhao, Jie Meng, P.R., PRC 94, 041301 (2016)

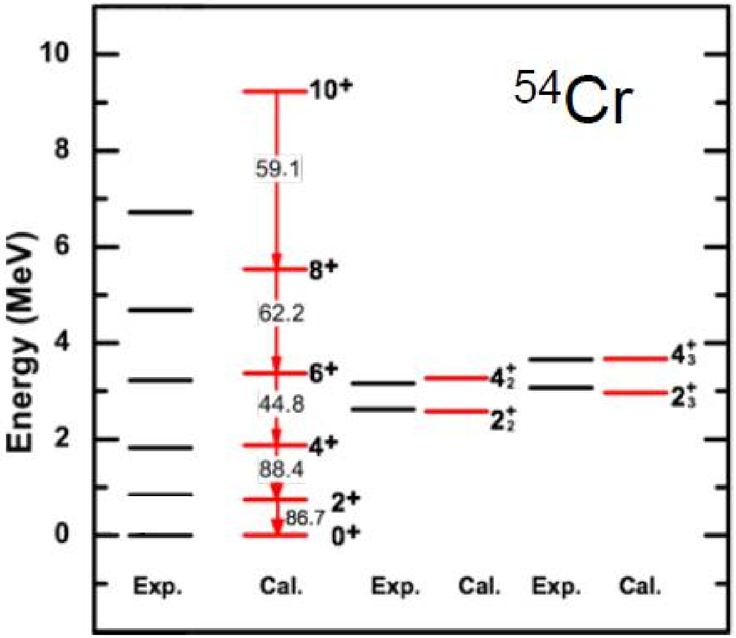
Level scheme for ^{54}Cr

Pengwei Zhao, Jie Meng, P.R., PRC (2016) in print



time-odd interaction;

beyond 2-qp configurations;

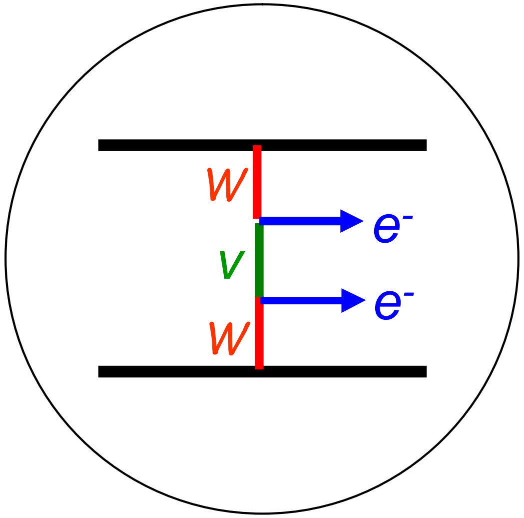


Towards neutron-rich nuclei

Half live of 0νββ decay

Assuming the light neutrino decay mechanism, we find the decay rate:

$$\left[T_{1/2}^{0\nu}\right]^{-1} = G_{0\nu}\, g_A^4 \frac{\langle m_\nu \rangle^2}{m_e^2} |M^{0\nu}|^2$$



g_A : axial vector coupling constant

m_e : electron mass

$G_{0\nu}$: kinematic phase space factor

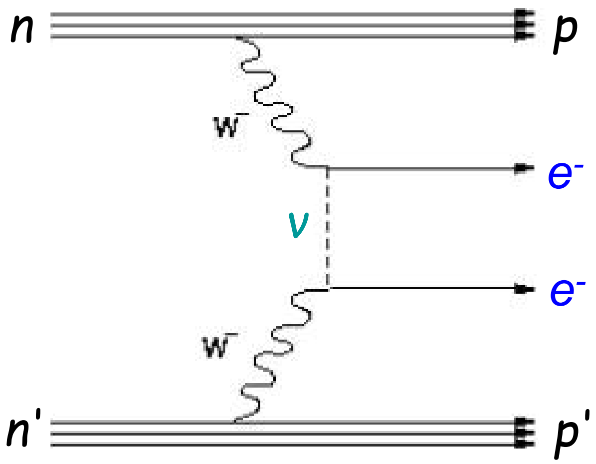
$\langle m_\nu \rangle$: effective neutrino mass: $\langle m_\nu \rangle = \sum_k U_{ek}^2 m_k \xi_k$

$M^{0\nu}$: nuclear matrix element (NME)

Kotila 2012: PRC 85, 034016
Bilenky 1987: RMP 59, 671

The observation of 0νββ-decay
would teach us the nature of the neutrino.
and the neutrino mass (provided that the NME is known)

0νßß - matrix elements:



weak interaction:

$$\mathcal{H}_{\text{weak}}(x) = \frac{G_F \cos\theta_C}{\sqrt{2}} j^\mu(x) J_\mu^\dagger(x) + h.c.$$

leptonic current (V-A):

$$j^\mu(x) = \bar{e}(x)\gamma^\mu(1-\gamma_5)\nu_e(x)$$

hadronic current:

$$J_\mu^\dagger(x) = \bar{\psi}_p(x)\left[g_V(q^2)\gamma_\mu - i g_M(q^2)\frac{\sigma_{\mu\nu}}{2m_p}q^\nu - g_A(q^2)\gamma_\mu\gamma_5 + g_P(q^2)\gamma_5 q_\mu\right]\tau_-\psi_n(x)$$

Second order perturbation theory and integration over leptonic sector:

$$\mathcal{O}^{0\nu} = \frac{4\pi R}{g_A^2}\int \frac{d^3q}{(2\pi)^2}\frac{e^{i\mathbf{q}(\mathbf{x}_1-\mathbf{x}_2)}}{q}\sum_m \frac{J_\mu^\dagger(\mathbf{x}_1)|m\rangle\langle m|J^{\mu\dagger}(\mathbf{x}_2)}{q+E_m-E_0-Q_{\beta\beta}/2}$$

$E_m - E_0 - Q_{\beta\beta}/2 \to E_d$ and closure approximation: $\sum_m |m\rangle\langle m| \to 1$

Nuclear wave functions:

- Intrinsic state:

  self-consistent constained RMF+BCS calculations: $|\beta\rangle = |\Phi(\beta)\rangle$

- Projected state: $|JZN,\beta\rangle = \hat{P}^J\hat{P}^Z\hat{P}^N|\beta\rangle$

- Generator coordinate method (GCM): shape mixing

$$|\Psi^{JZN}\rangle \ = \int d\beta f(\beta)|JZN,\beta\rangle$$

- Transition matrix element:

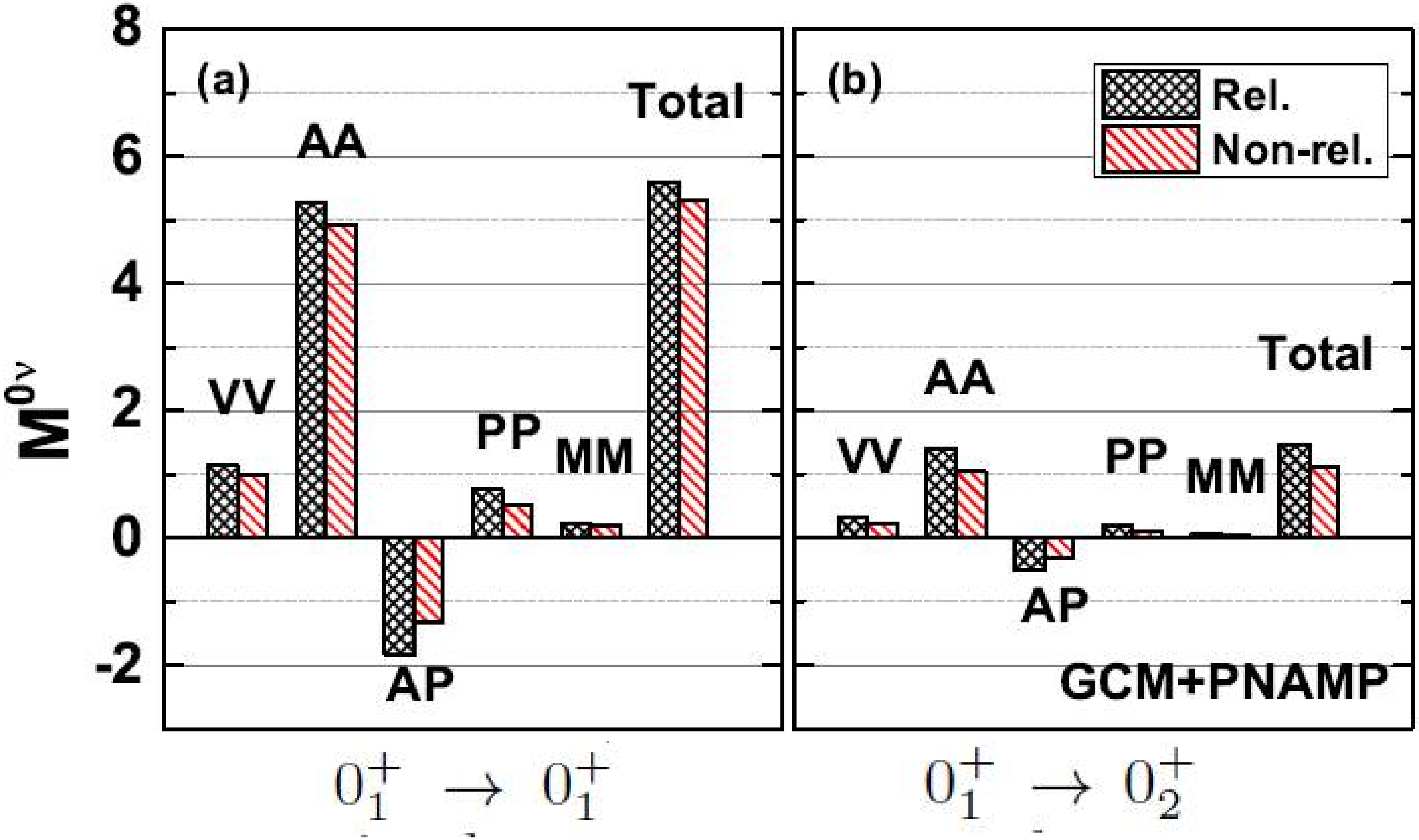
$$M^{0\nu} = \int\int d\beta_F d\beta_I \, f^*(\beta_F)f(\beta_I)\, M^{0\nu}(\beta_F,\beta_I)$$

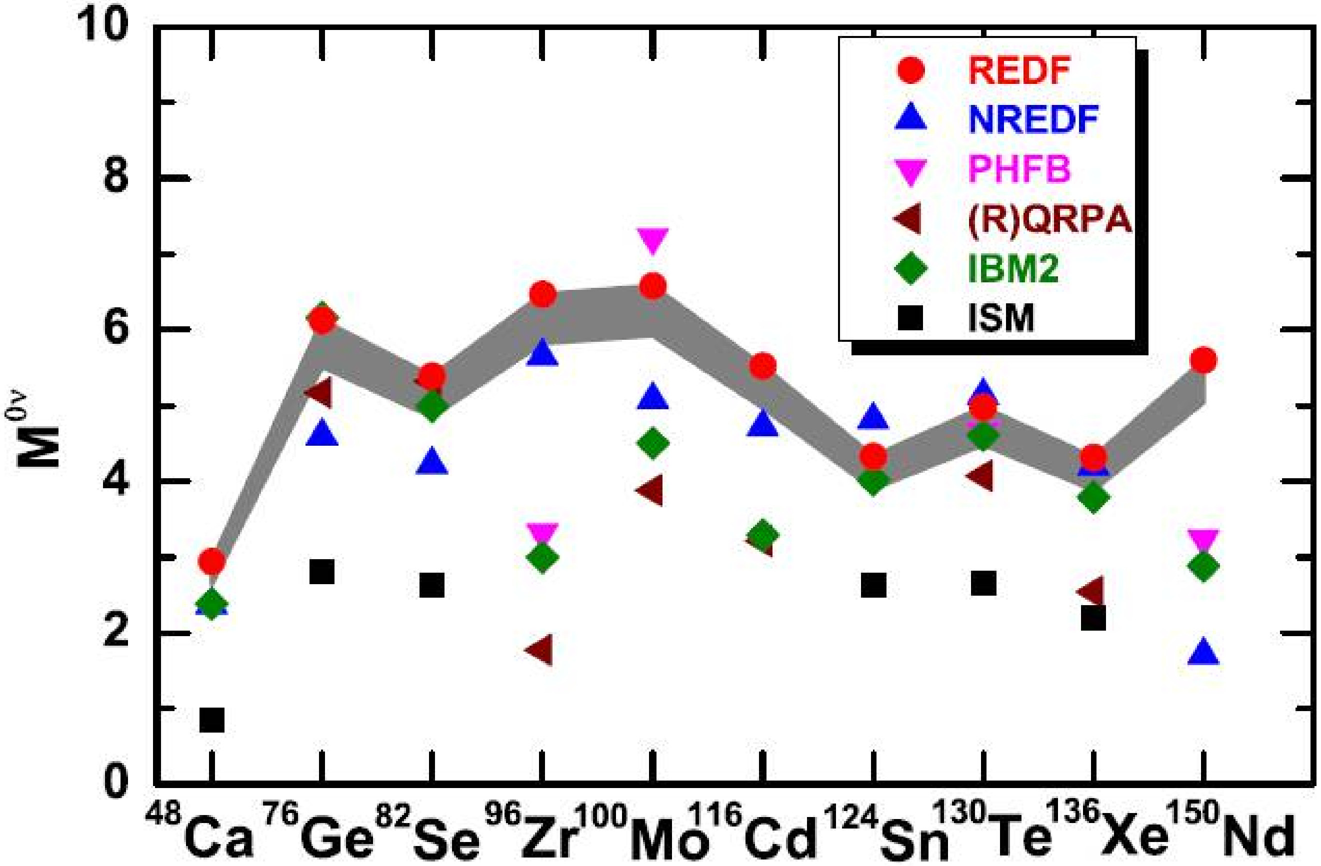
$$M^{0\nu}(\beta_F,\beta_I) = \sum_{pp'nn'} \langle pp'|\mathcal{O}|nn'\rangle\langle\beta_F|c_p^\dagger c_p^\dagger c_n c_n|IZN,\beta_I\rangle$$

Basic assumptions:

- Closure approximation
- Higher order currents are fully incorporated
- The tensorial part is included automatically
- Finite nuclear size corrections are taken into accout by form factors $g(q^2)$ (from Simkovic et al, PRC 2008)
- Short range correlations are neglected
- $g_A(0) = 1.254$ (no renormalization)

Transition ^{150}Nd → ^{150}Sm:
Matrix element of 0νββ decay and its contributions:

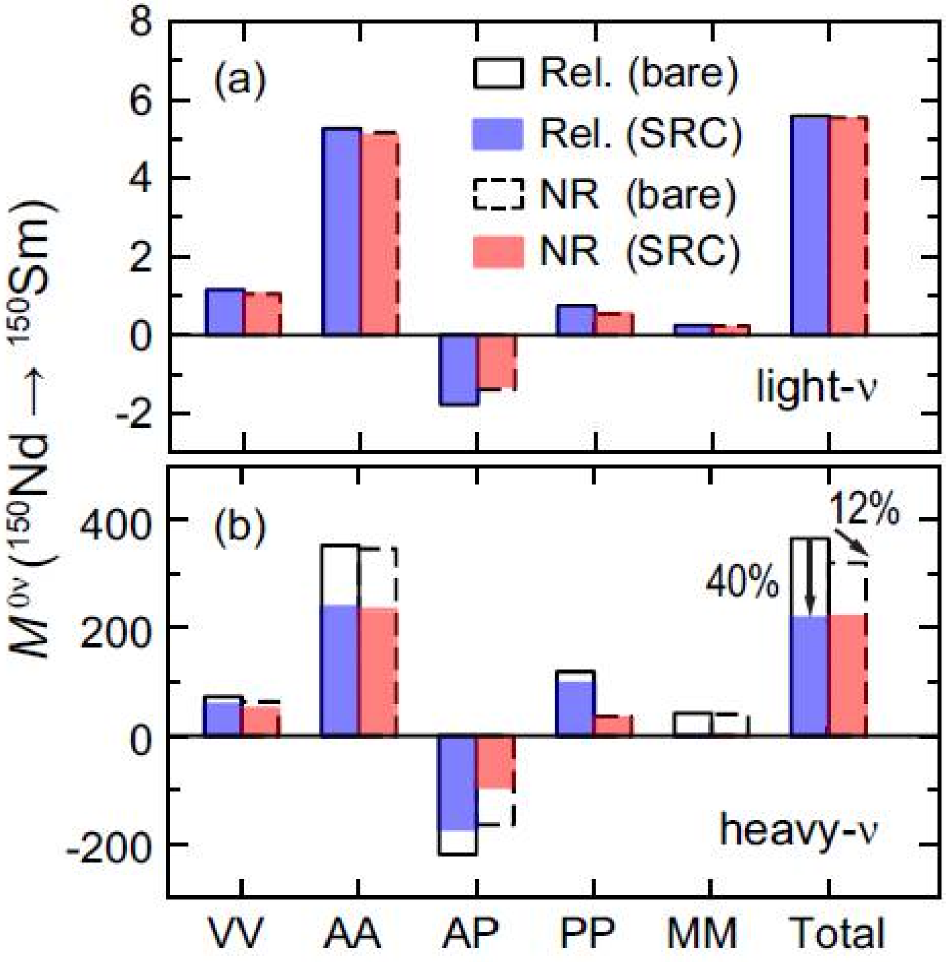




- The matrix elements differ by a factor 2 to 3
- Density functionals are at the upper end
- Not much sensitivity to the EDF (except for ^{150}Nd)
- Relativistic effects and tensor terms are with 10 %

J.M. Yao, L.S. Song, K.Hagino, P.R., J.Meng, PRC 91, 24316 (2015)

The influence of short range correlations



Jastrow factor: $F(r) = 1 - ce^{-ar^2}(1 - br^2),$

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

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

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 $\rho(\mathbf{r},t)$.

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.

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

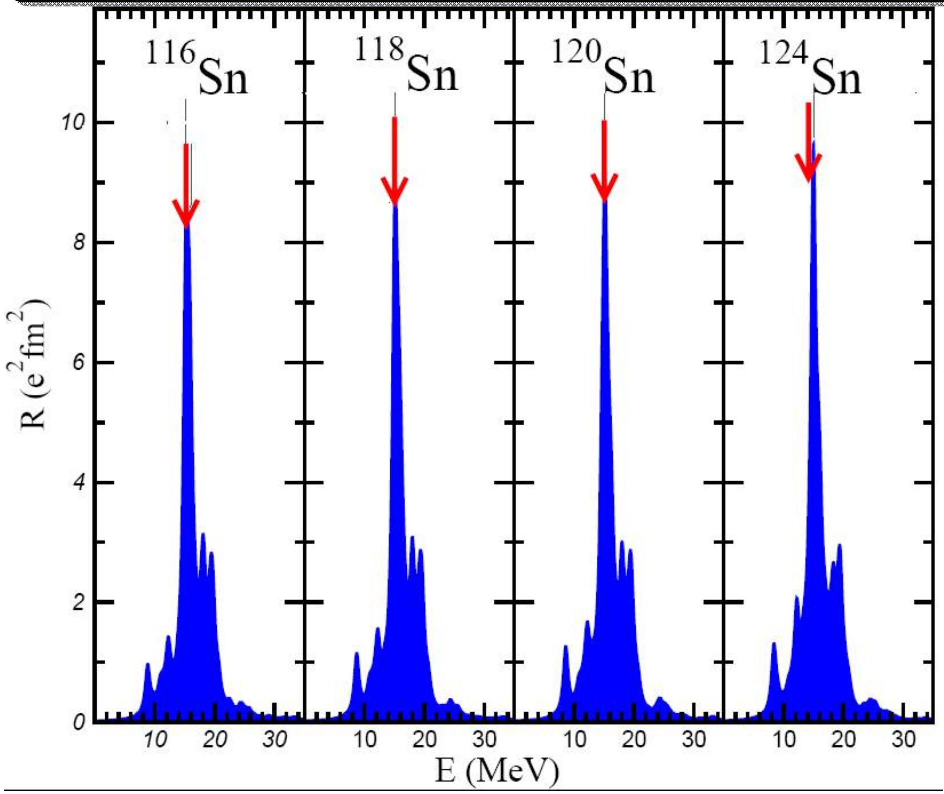
In this approximation $v[\rho]$ is no longer depending on the function $\rho(\mathbf{r},t)$ of 4 variables, but rather on the function $\rho_s(\mathbf{r}) = \rho(\mathbf{r},t)$ depending only 3 variables. The time is just a parameter. We obtain for the effective interaction in the adiabatic approximation

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

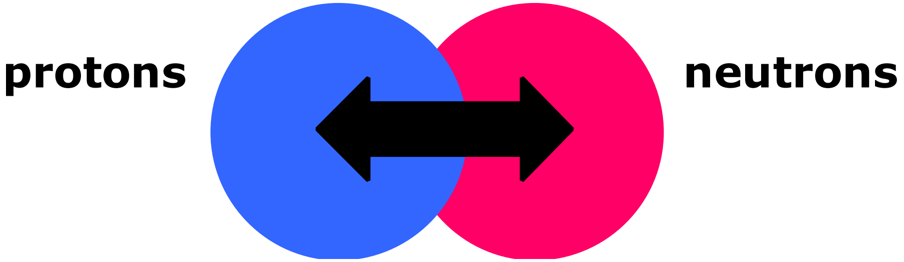
This approximation is well known. It corresponds to the small amplitude limit of the time-dependent mean field equations, i.e. to $\boxed{\text{RPA}}$ or in superfluid systems to $\boxed{\text{QRPA}}$ and it is extensively used in nuclear physics.

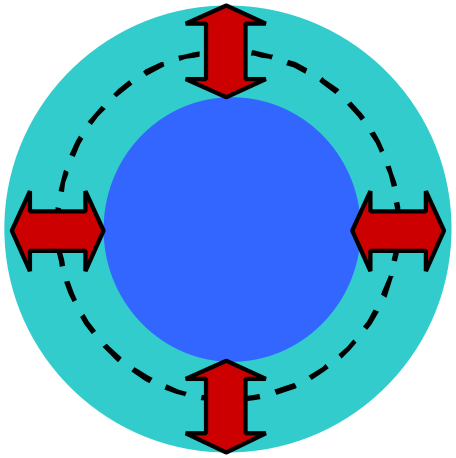
Relativistic (Q)RPA calculations of giant resonances:

Sn isotopes: DD-ME2 effective interaction + Gogny pairing

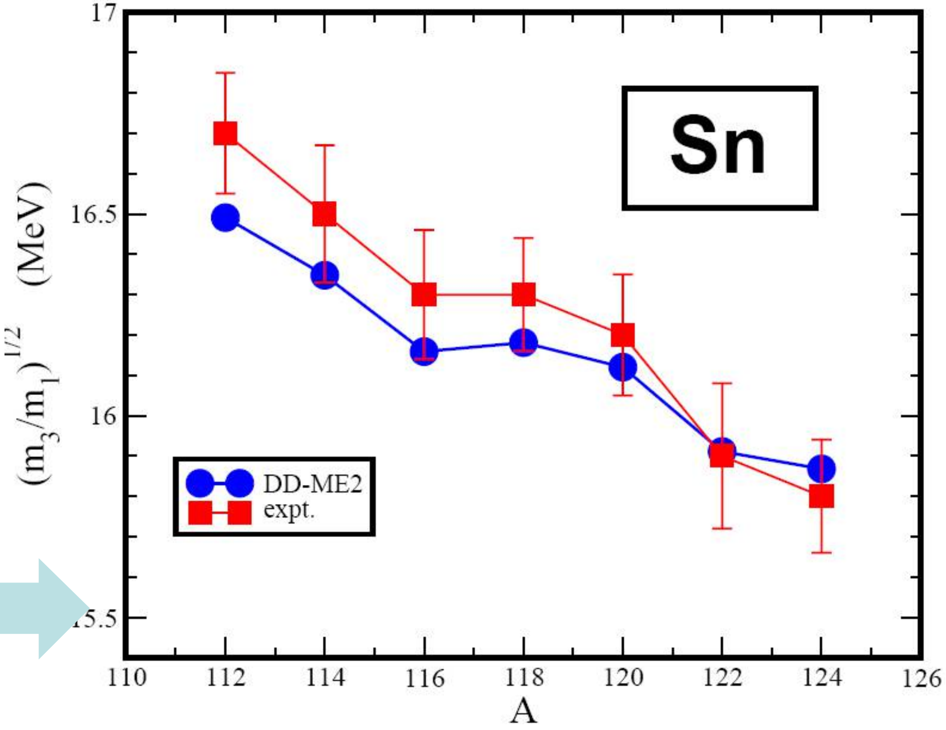


Isovector dipole response

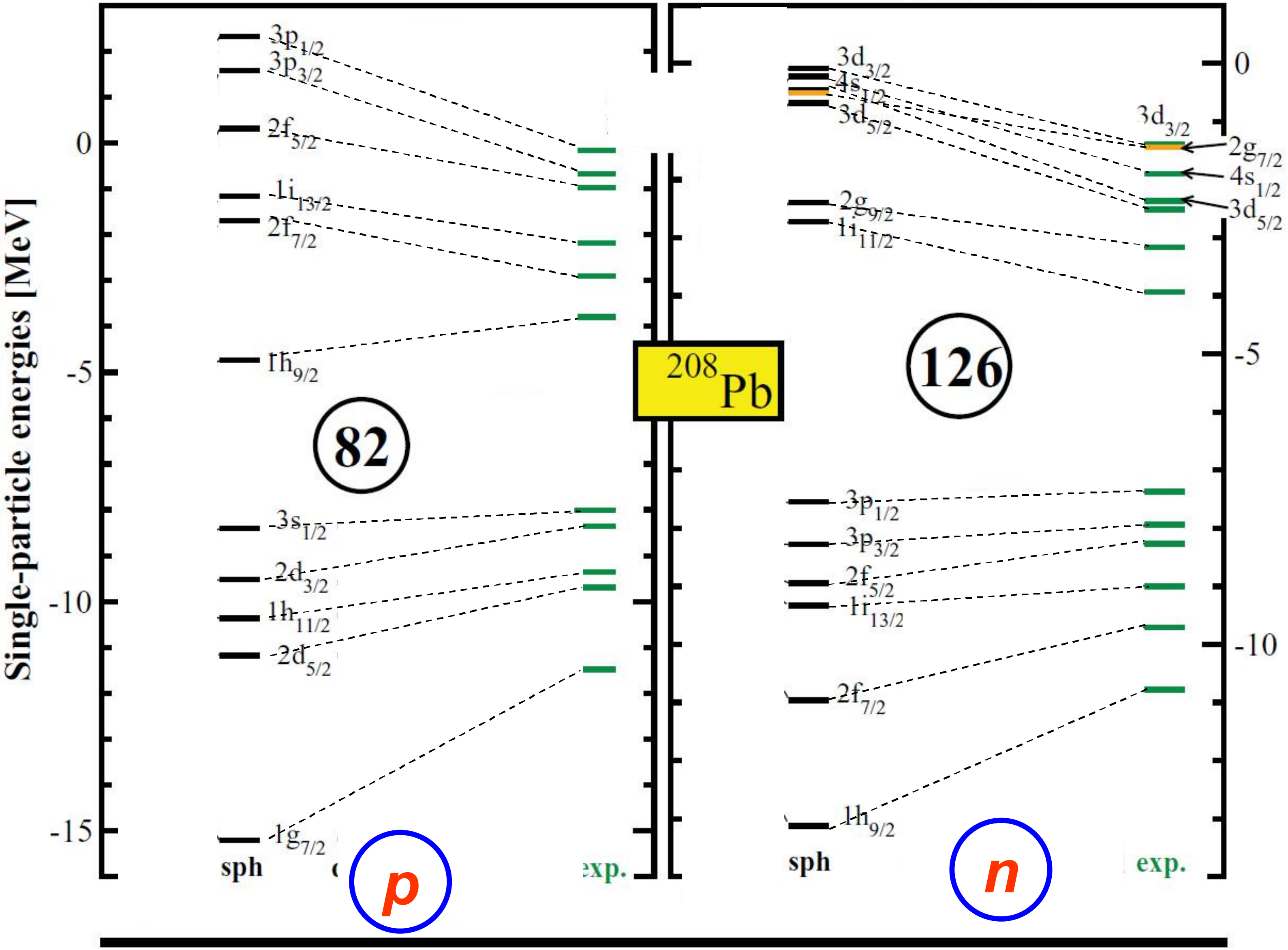




Isoscalar monopole response



Problem: single particle spectra



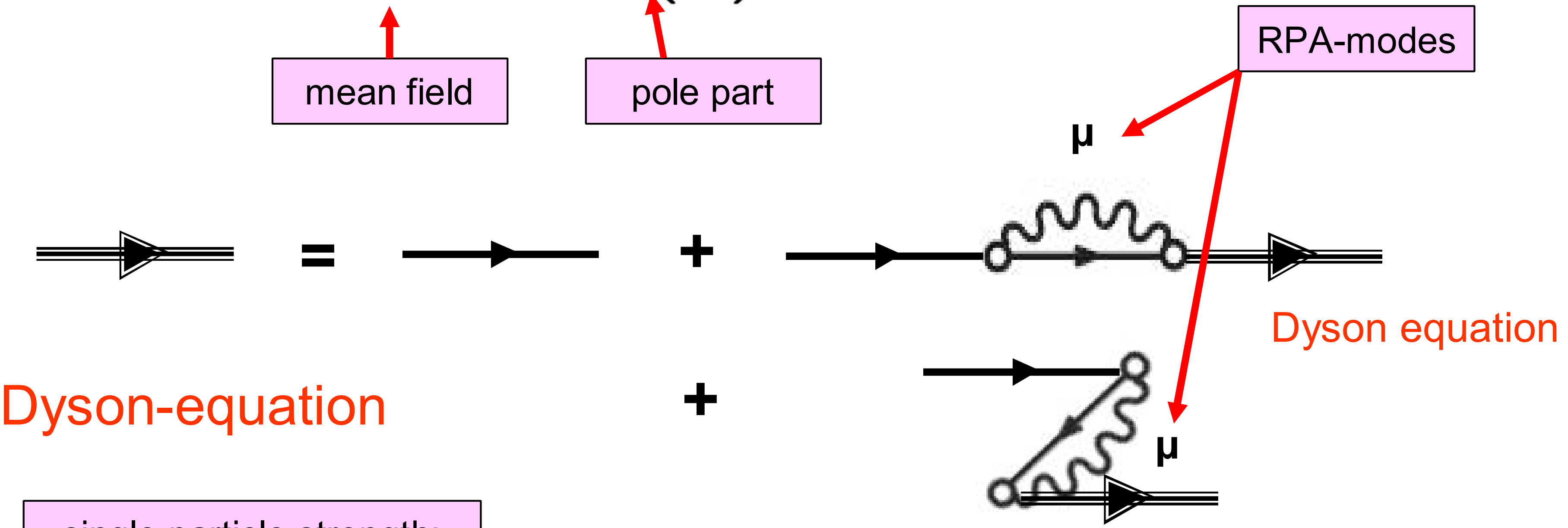
Particle-vibrational coupling (PVC) energy dependent self-energy

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

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

mean field

pole part



Dyson-equation

single particle strength:

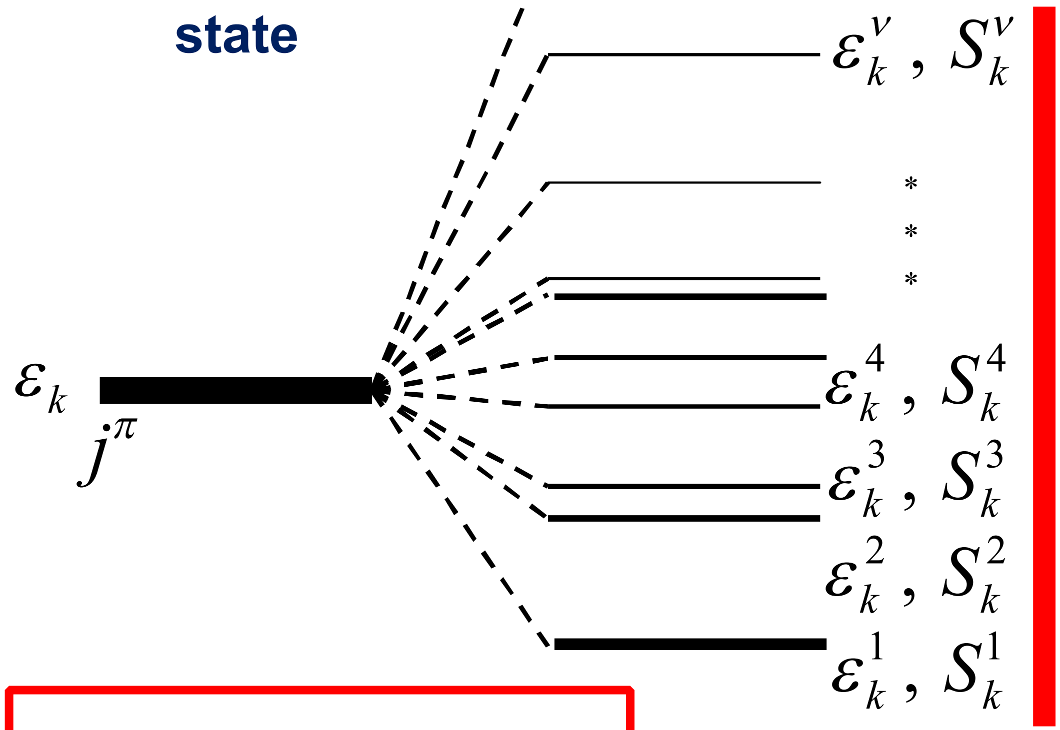
$$S_\nu = \left[1 - \frac{d\Sigma_{\nu\nu}}{d\omega}\Big|_{\omega=\epsilon_\nu}\right]^{-1}$$

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)

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.

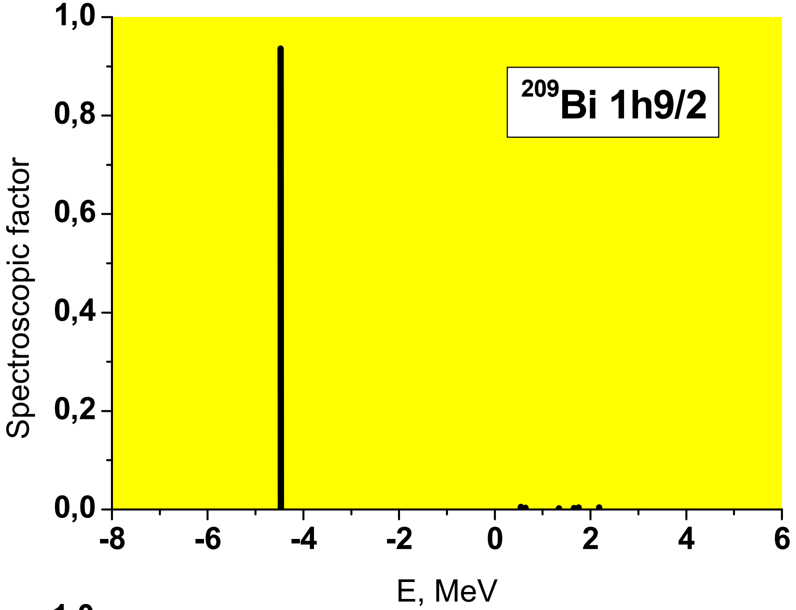
Spectroscopic factors depend on reaction and method of extraction: example of spectroscopic factors in ^{209}Bi

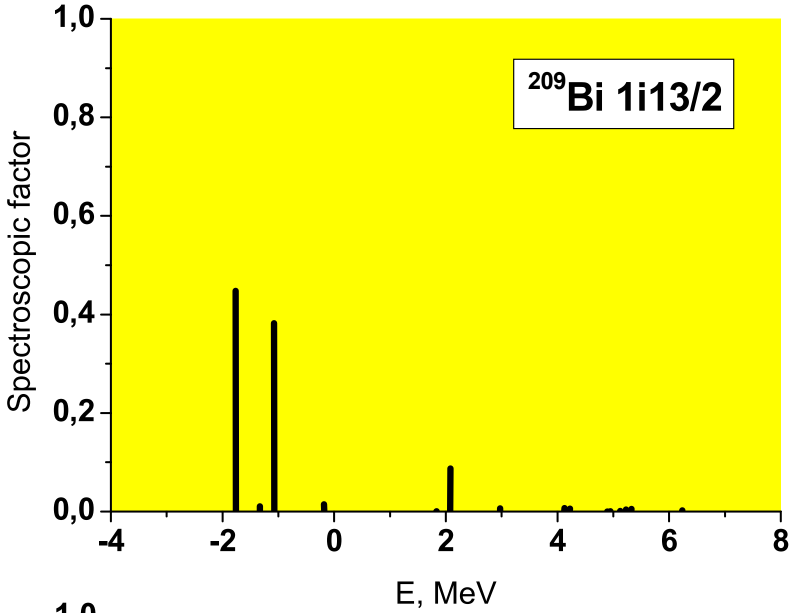
$1h_{9/2}$	1.17	0.80
$2f_{7/2}$	0.78	0.76
$1i_{13/2}$	0.56	0.74
$2f_{5/2}$	0.88	0.57
$3p_{3/2}$	0.67	0.44
$3p_{1/2}$	0.49	0.20
	(^{3}He,d)	(α,t) reactions

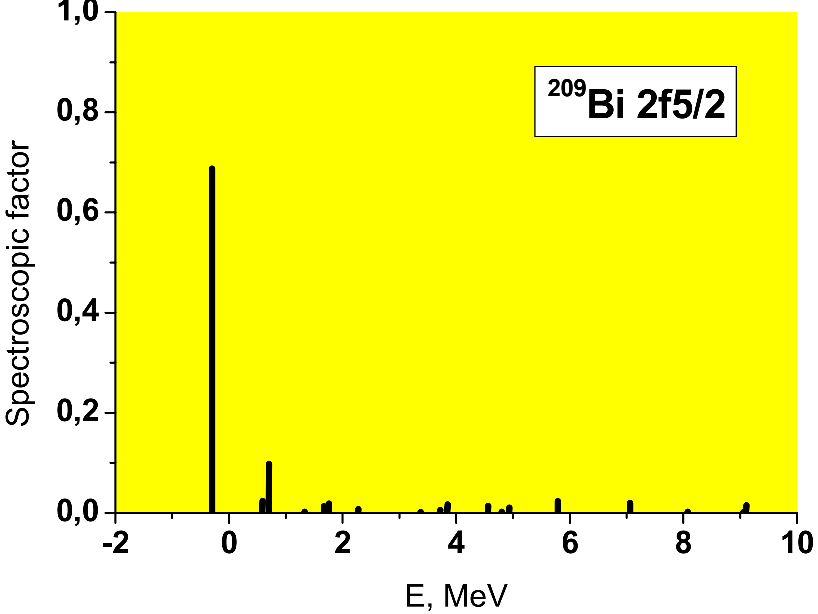
sum rule: $\sum_\nu S_k^\nu = 1$

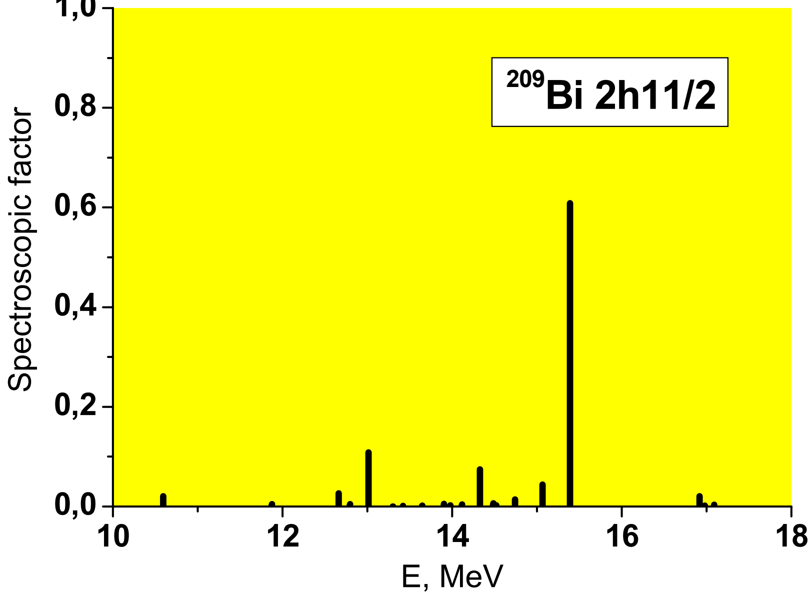
is frequently violated.

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

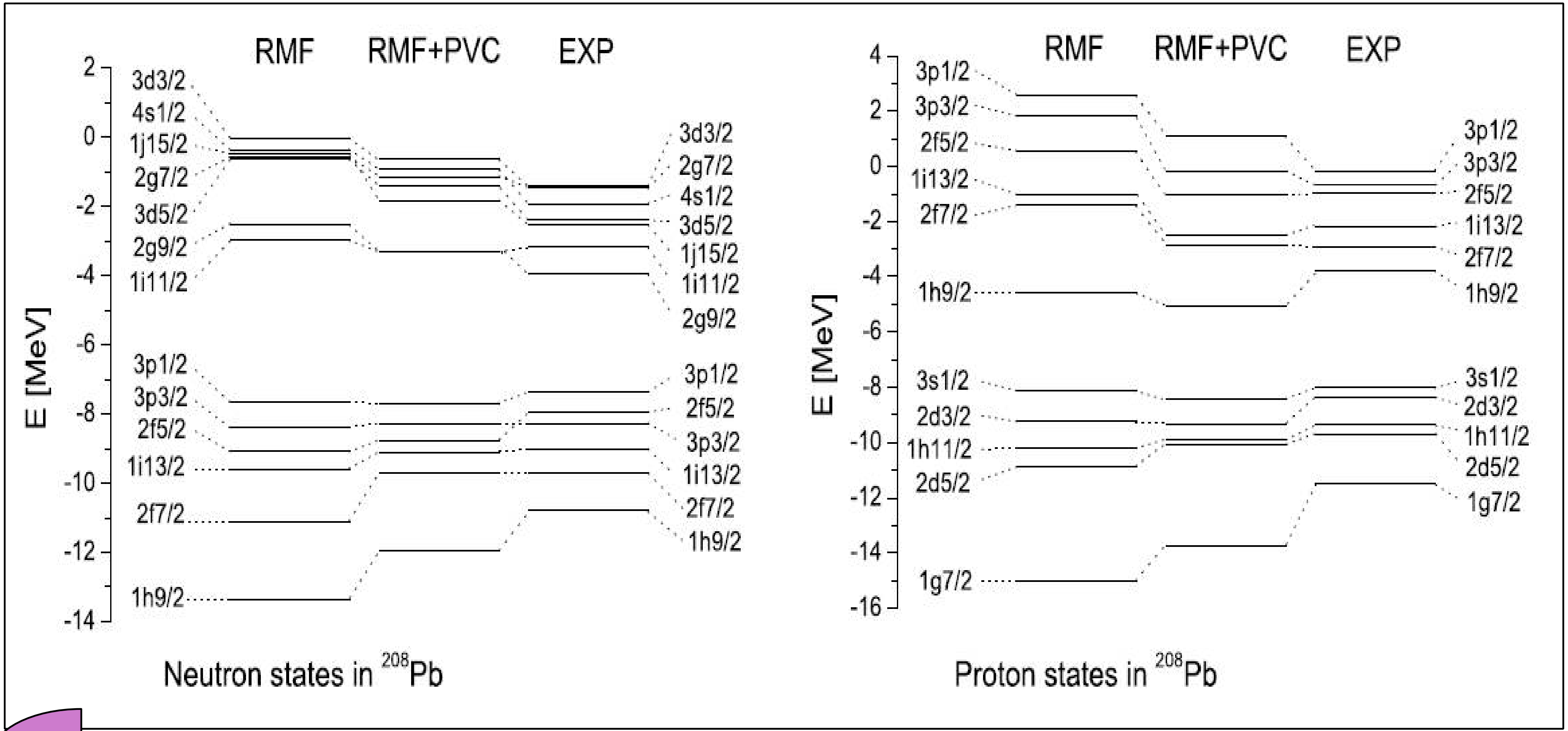








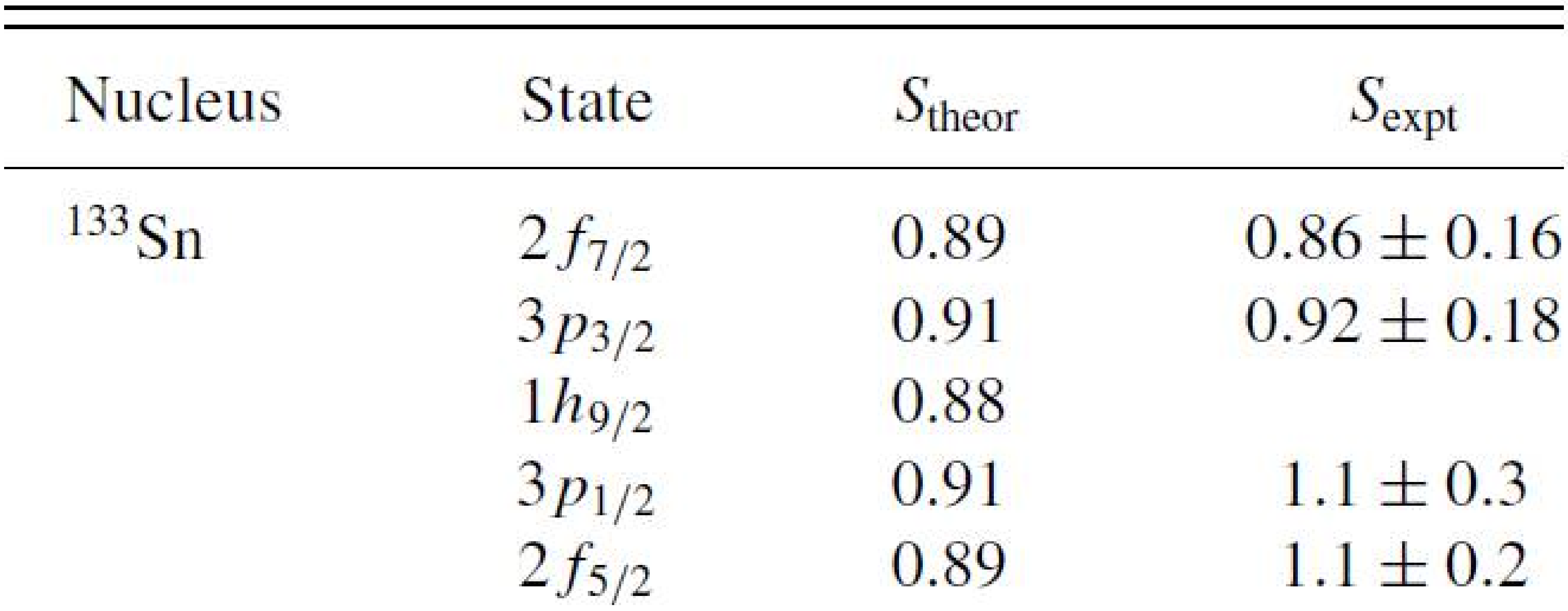
Single particle spectrum in the Pb-region:



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:



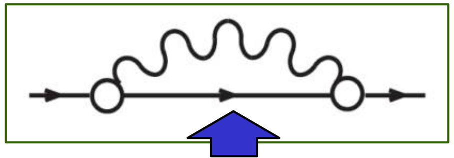
Nucleus	State	S_{theor}	S_{expt}
^{133}Sn	$2f_{7/2}$	0.89	0.86 ± 0.16
	$3p_{3/2}$	0.91	0.92 ± 0.18
	$1h_{9/2}$	0.88	
	$3p_{1/2}$	0.91	1.1 ± 0.3
	$2f_{5/2}$	0.89	1.1 ± 0.2

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

Width of giant resonances:

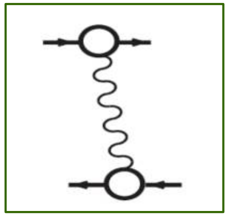
The full response contains energy dependent parts coming from vibrational couplings.

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

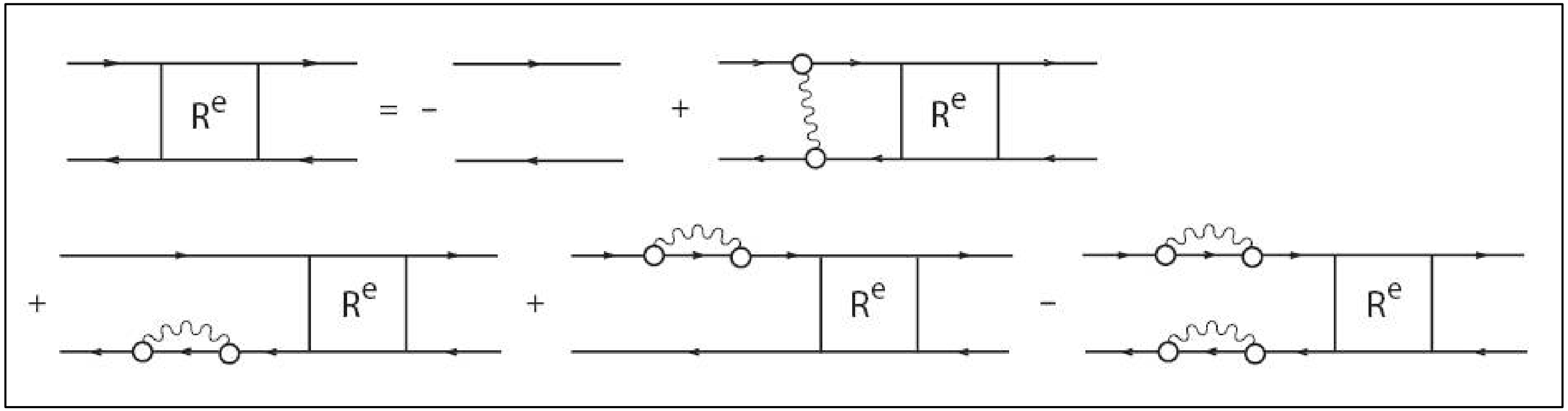


Self energy

ph-phonon vertices (QRPA)



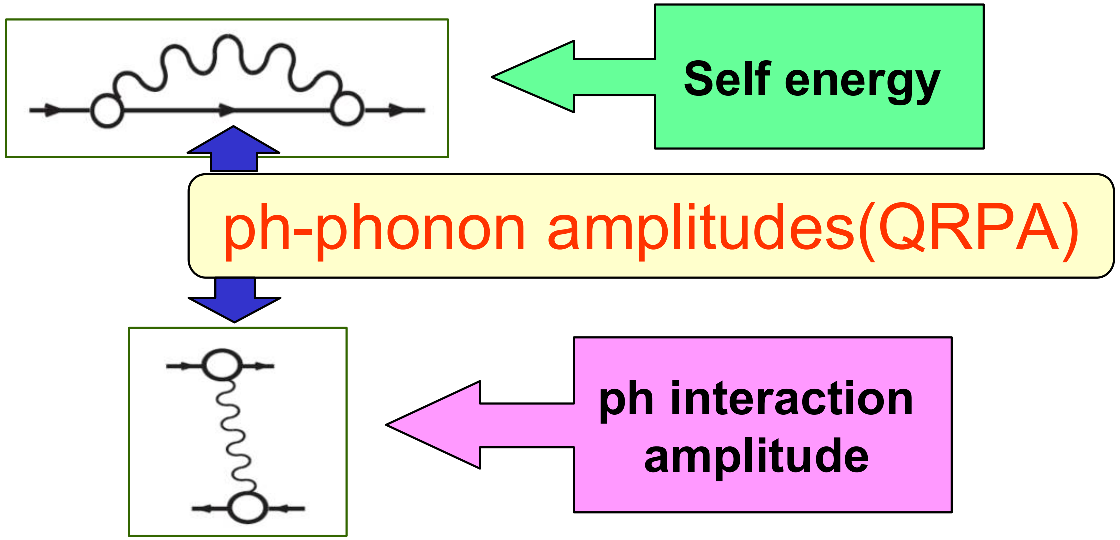
ph interaction amplitude



Width of giant resonances:

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

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



Self energy

ph-phonon amplitudes(QRPA)

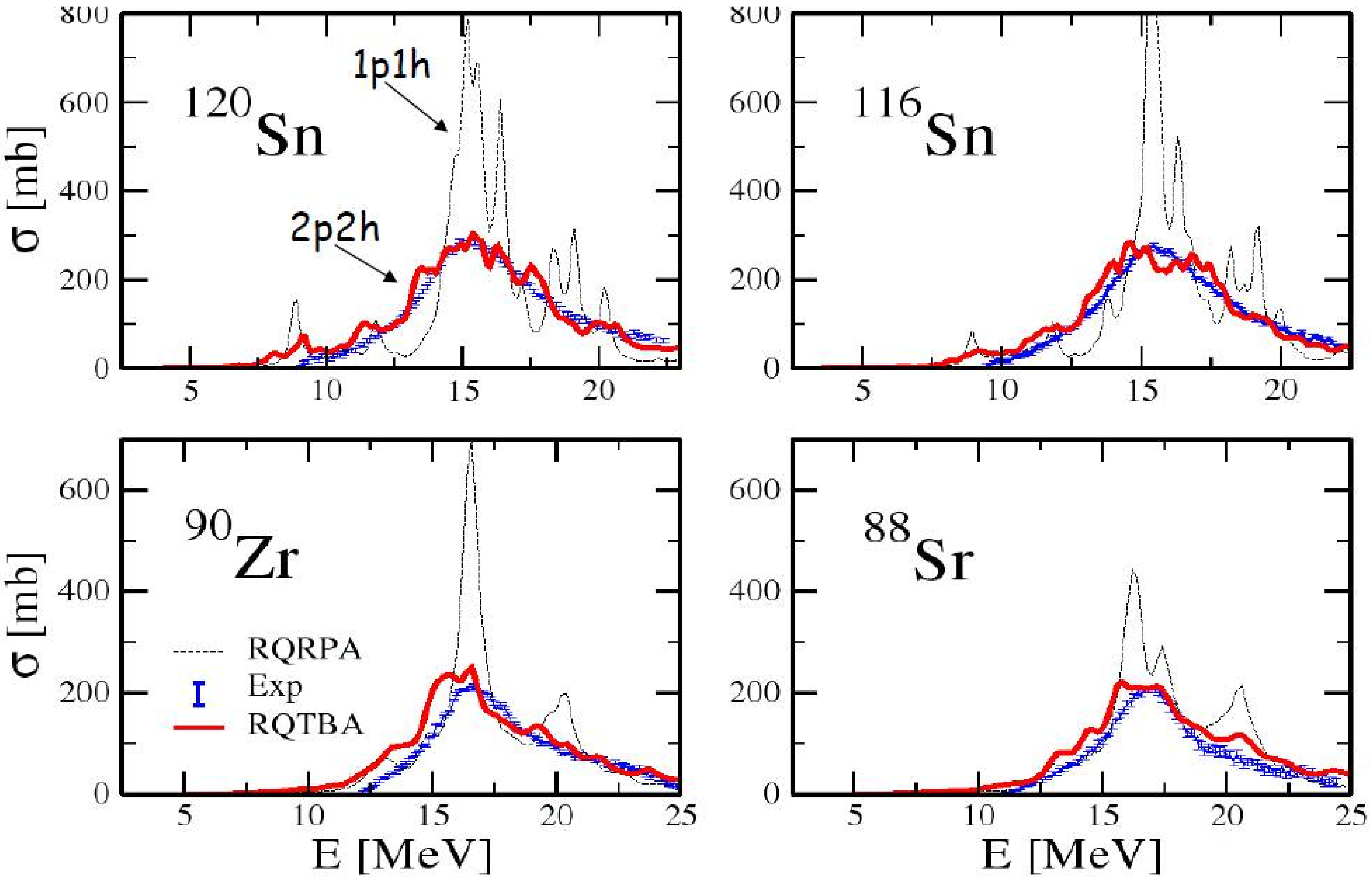
ph interaction amplitude

Problem of divergengies:

Renormalization of the interaction:

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

Coupling to surface vibrations (2p2h): IVGD:



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

Conclusions:

- Density functional theory in nuclei is very successful:
- technically simple
  easy to visualize
  universal

- At present there is no microscopic derivation
- Covariant density functionals have many advantages
- DFT is deeply connected with symmetry violation

- Extensions beyond-mean field:
- GCM for various deformations
- 5D-collective Hamiltonian is a good approximation
- Configuration Interaction Projected DFT (CI-PDFT)
- Particle-Vibrational Coupling in time-dependent mean field theory

Outlook

- Better understanding of single particle structure
  - tensor force
  - particle-vibrational coupling
- Microscopic derivation of density functionals
- relativistic Brueckner-Hartree-Fock theory
- …

Thanks to my collaborators:

J. Meng	(Beijing)
P. W. Zhao	(Beijing)
L. S. Song	(Beijing)
Jiangming Yao	(Michigan State Univ.).
Zhipan Li	(Chongqing)
E.F. Zhou	(Chongqing)
G. Lalazissis	(Thessaloniki)
E. Litvinova	(Western Michigan Univ.)
D. Vretenar	(Zagreb)
T. Niksic	(Zagreb)