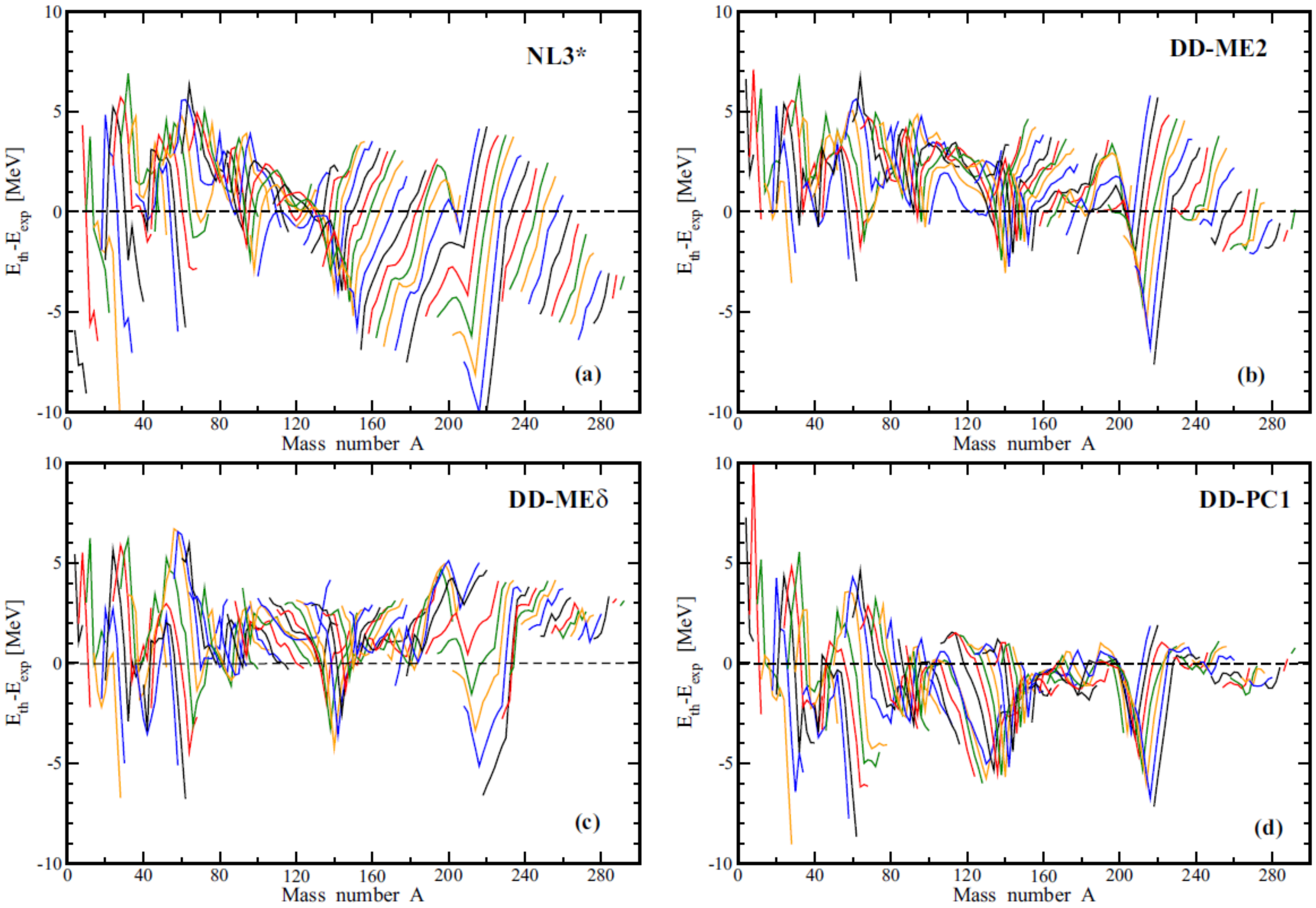
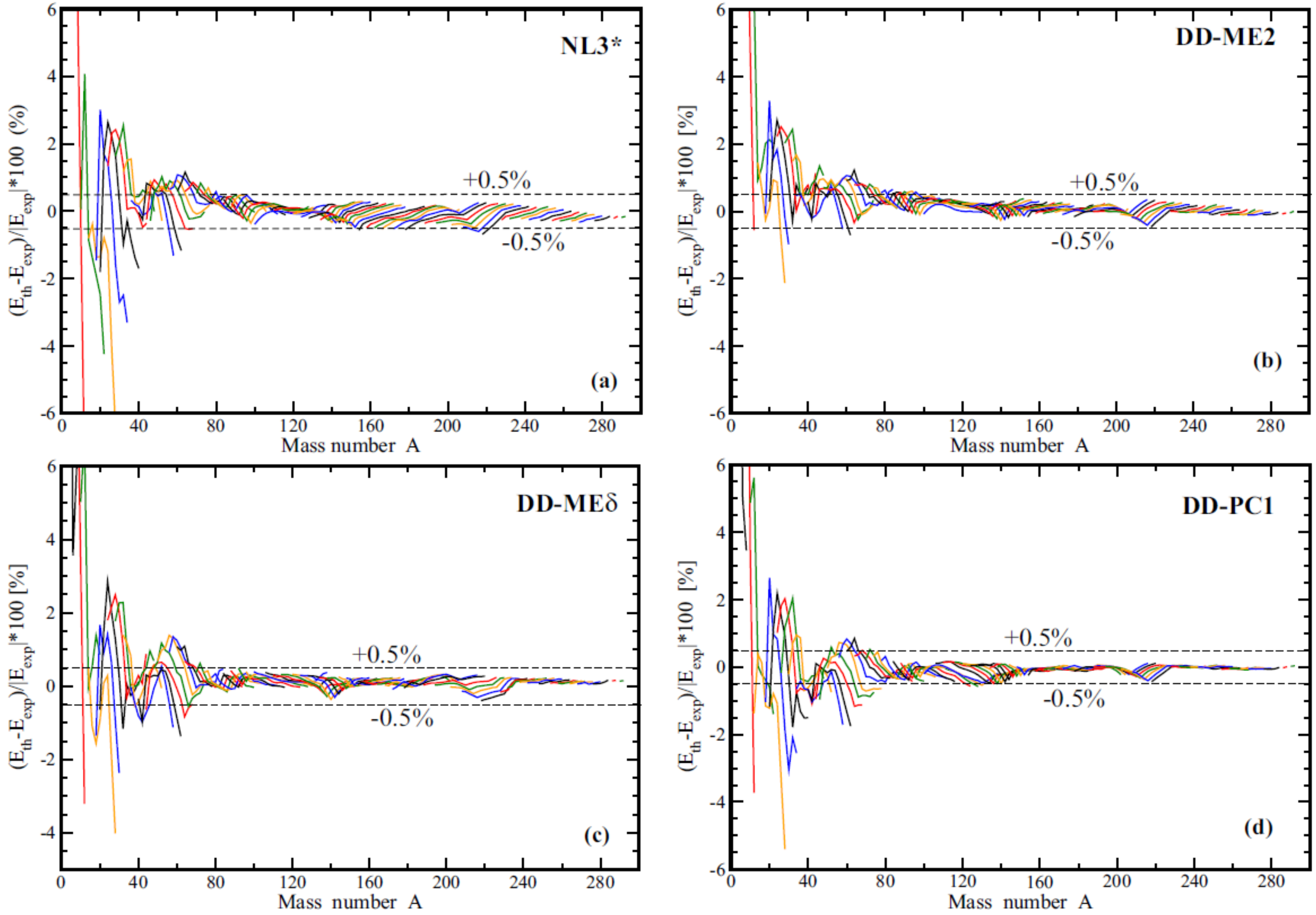
Open problems on the mean field level

- How to optimize the functionals?
- Time-odd terms ?
- Single particles levels?
- Tensor forces?
- Fock-terms?
- pn-pairing
- Ab-initio derivation?
- Symmetry violation !
- Shape coexistence ?
- Correlations beyond mean field?
- zero-point vibrations ?
- contributions of Goldstone modes ?

Absolute masses for 4 Covariant Density Functionals



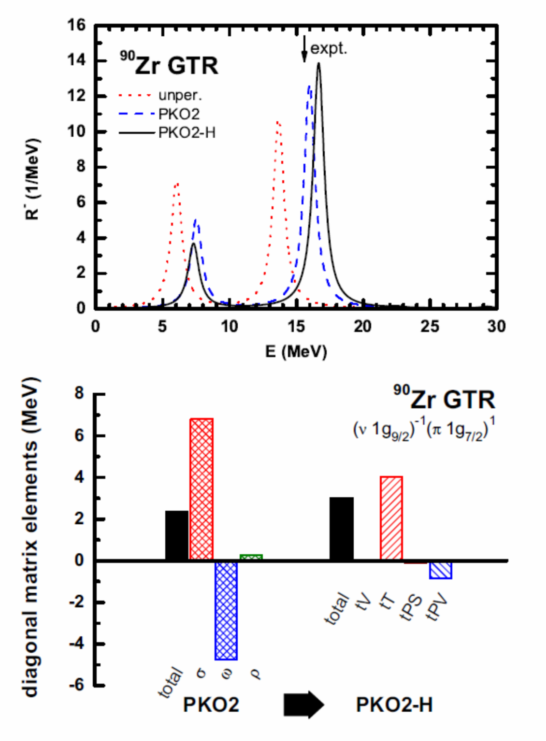
Absolute masses for 4 Covariant Density Functionals



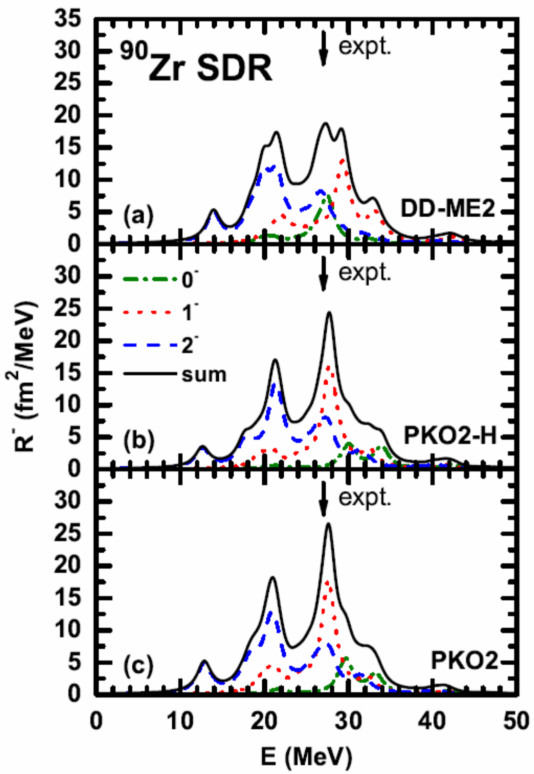
Exchange terms in spin-isospin exitations: (RHF)

Gamov Teller resonance

Spin-dipole resonance



no pion !

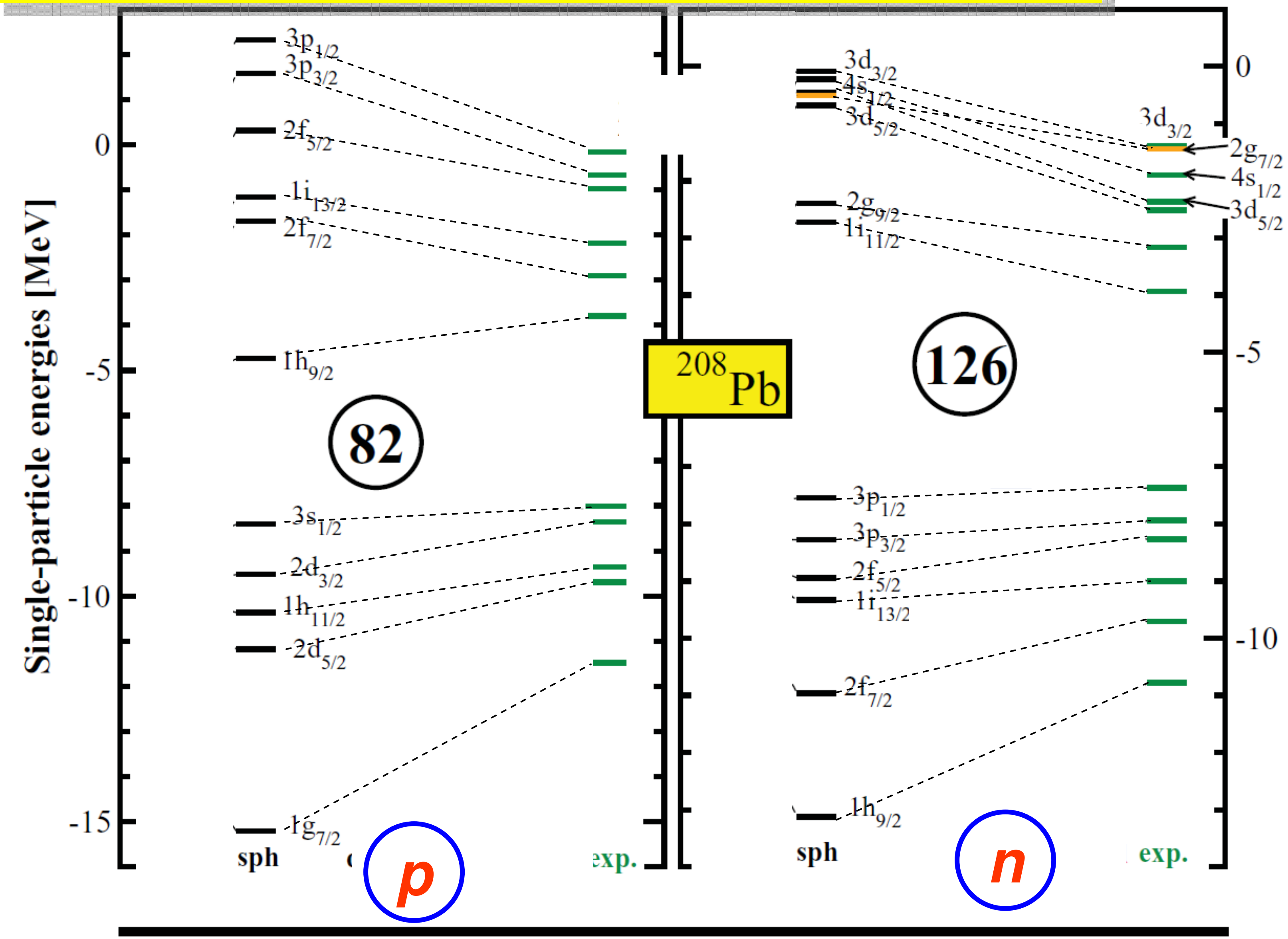


Haozhao Liang to be published

DFT for excited states:

- Time-dependent density functional theory
- Energy dependence of the self energy $V_{KS}(\omega)$
- Particle-vibrational coupling (Second RPA ???)
- a) numerical complexity in deformed nuclei
- b) divergent terms in perturbation theory ?
- c) particle vibrational coupling to spurious modes ?
- Limitation to small amplitudes

Problem: single particle spectra



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):

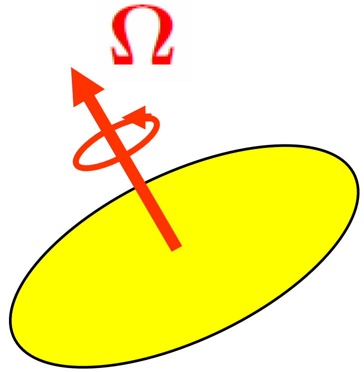
One-to-one correspondence: $\rho(\mathbf{r}, t) \iff f_{\text{ext}}(\mathbf{r}, t)$ and there exists a fictitious system of non-interacting particles with the wave functions $\varphi_i(\mathbf{r}, t)$ satisfying

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

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

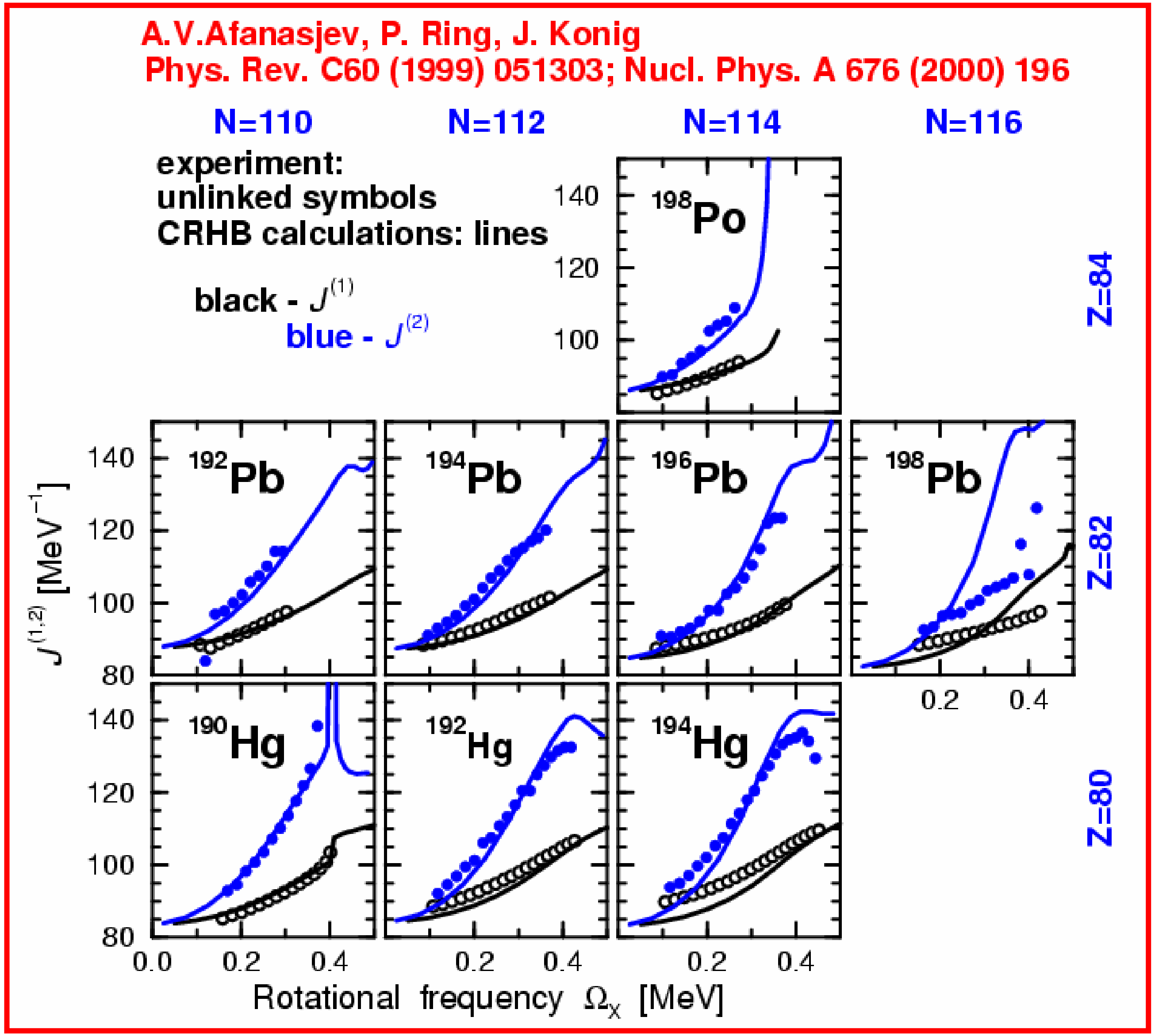
Cranking model: Inglis (1956):

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

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")

Superdeformed band in the Hg-Pb region:



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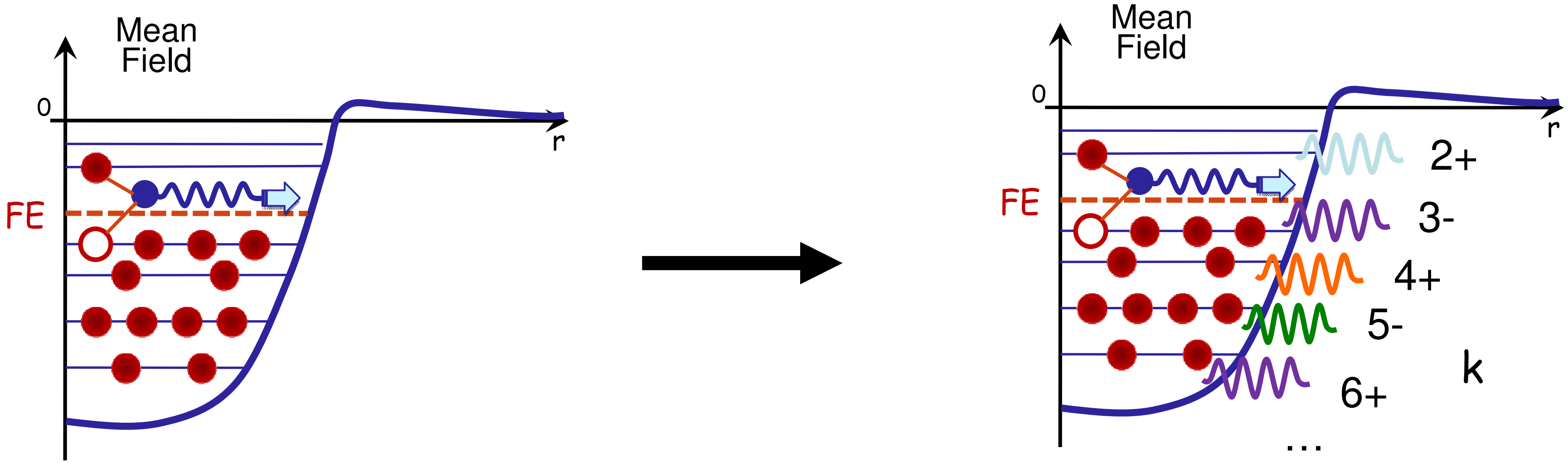
Inclusion of many-body correlations:



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)

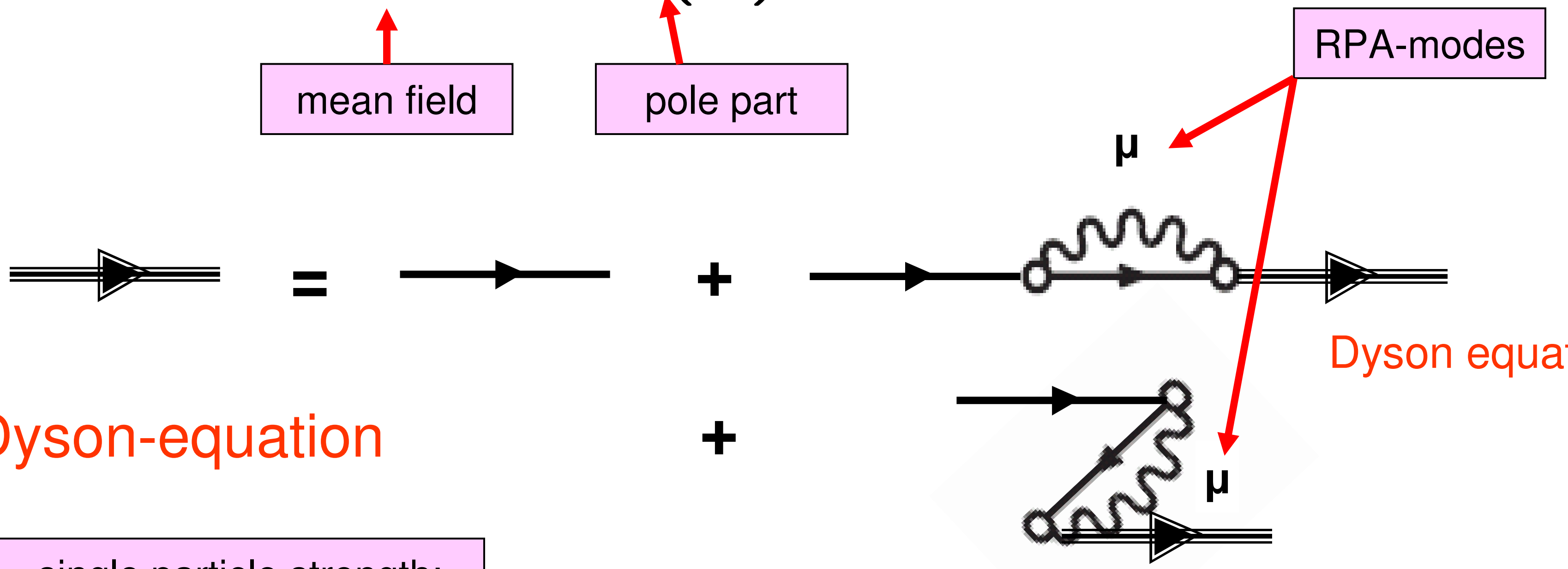
Particle-vibrational coupling (PVC) energy dependent self-energy

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

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

mean field → $S + V$

pole part → $\Sigma(\omega)$

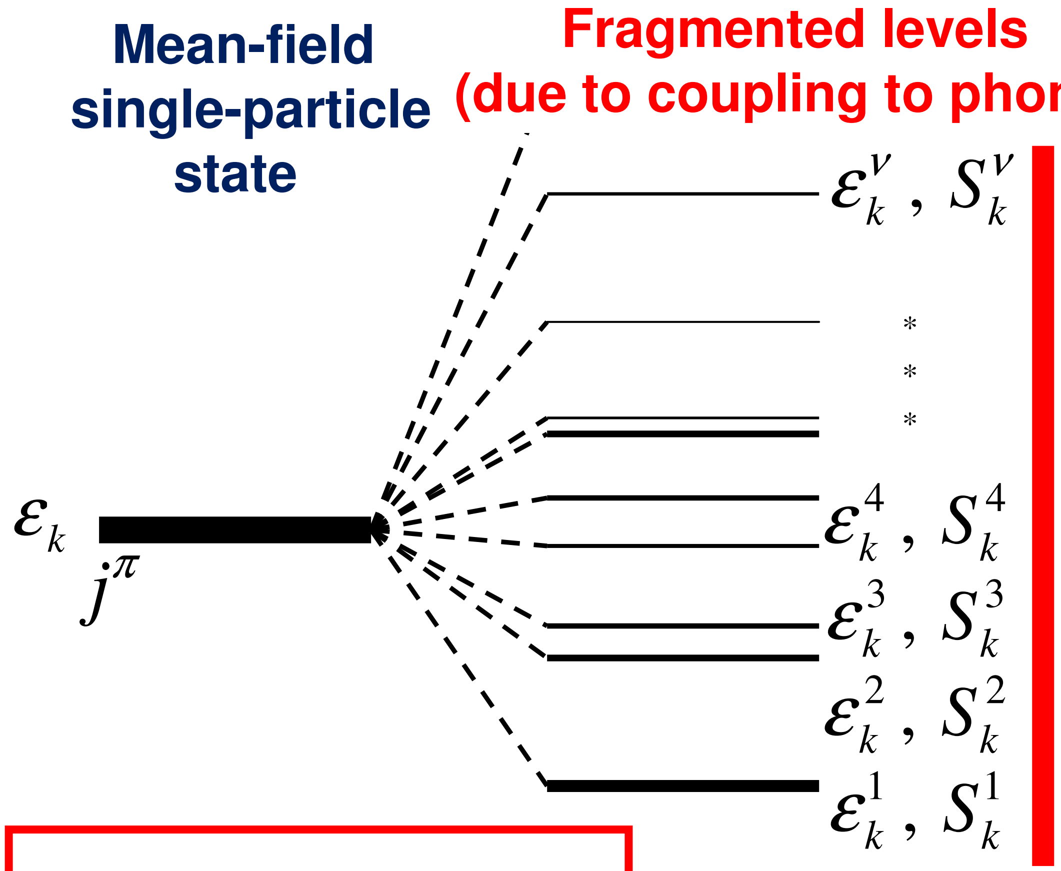


Dyson-equation

single particle strength:

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

The single particle energies are fragmented:



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

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

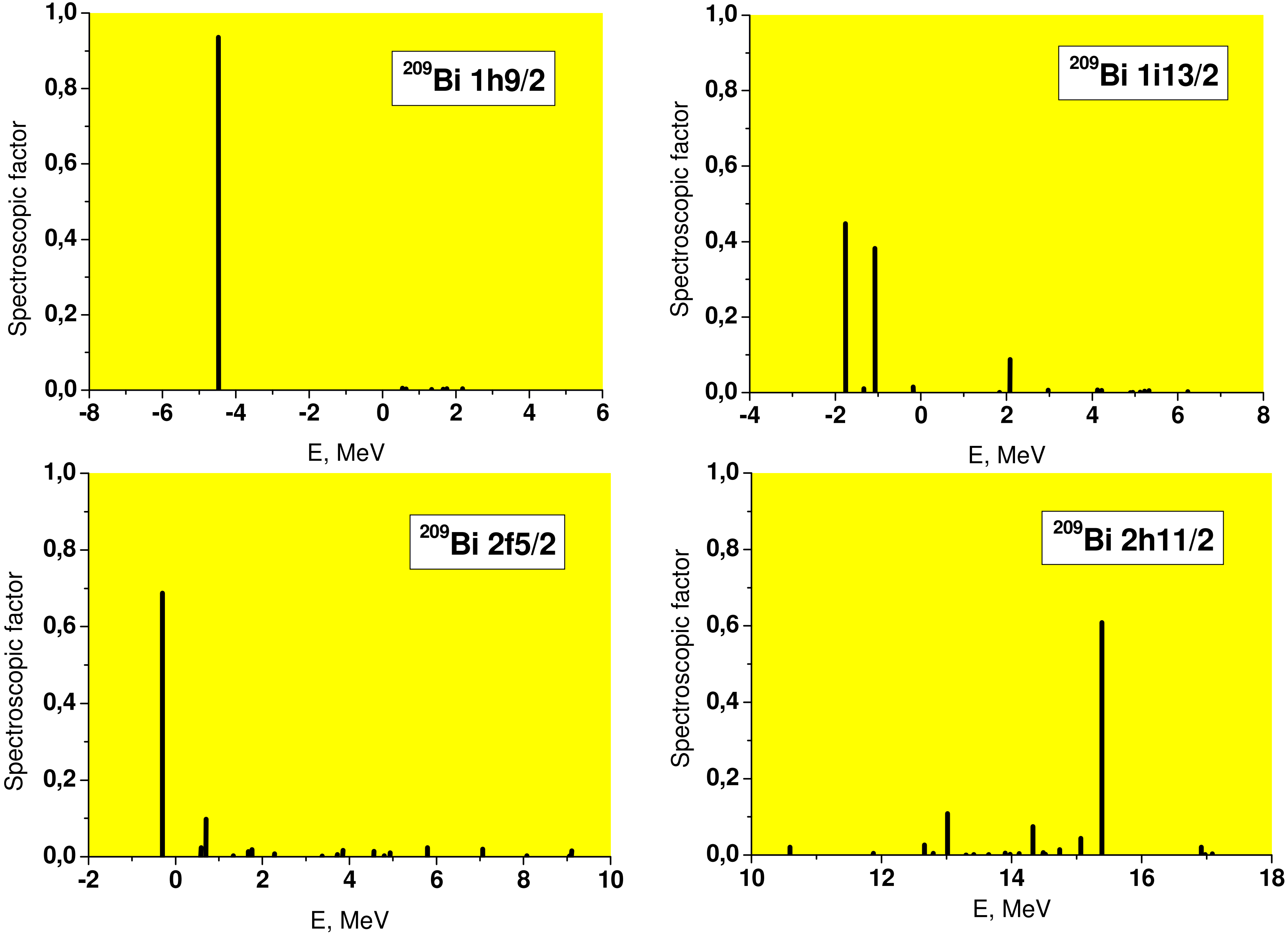
	(³He,d)	(α,t) reactions
$1h_{9/2}$	1.17	0.80
$2f_{7/2}$	0.78	0.76
$1i_{13/2}$	0.56	0.74
$2f_{5/2}$	0.88	0.57
$3p_{3/2}$	0.67	0.44
$3p_{1/2}$	0.49	0.20

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

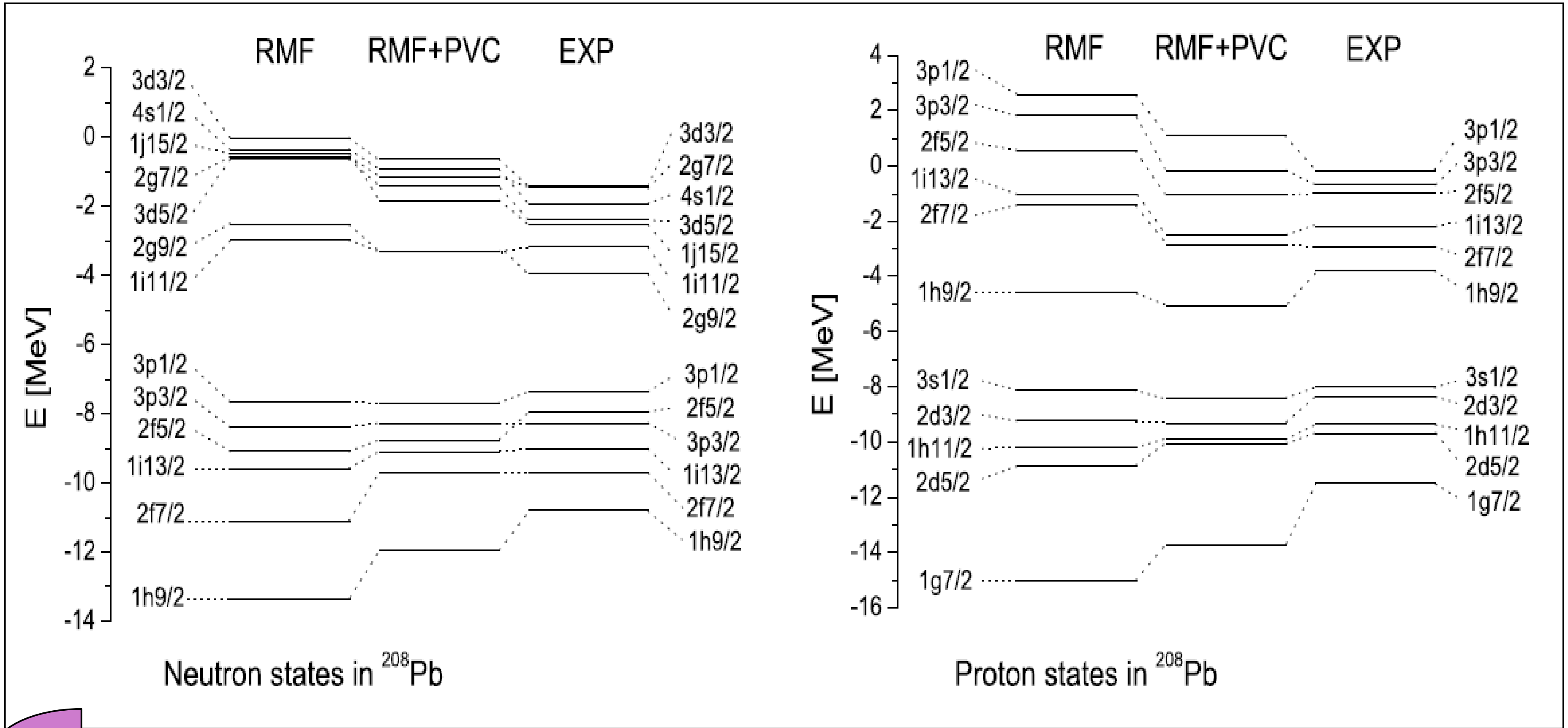
is frequently violated.

E. Litvinova

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:

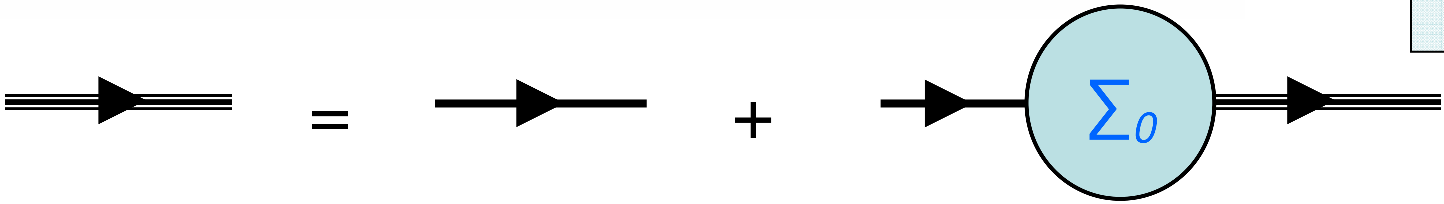
Nucleus	State	S_{theor}	S_{expt}
^{133}Sn	$2f_{7/2}$	0.89	0.86 ± 0.16
	$3p_{3/2}$	0.91	0.92 ± 0.18
	$1h_{9/2}$	0.88	
	$3p_{1/2}$	0.91	1.1 ± 0.3
	$2f_{5/2}$	0.89	1.1 ± 0.2

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

Dirac equation: propagation of one particle

$$G(\omega) = G_0(\omega) + G_0(\omega)\,\Sigma_0\,G(\omega)$$

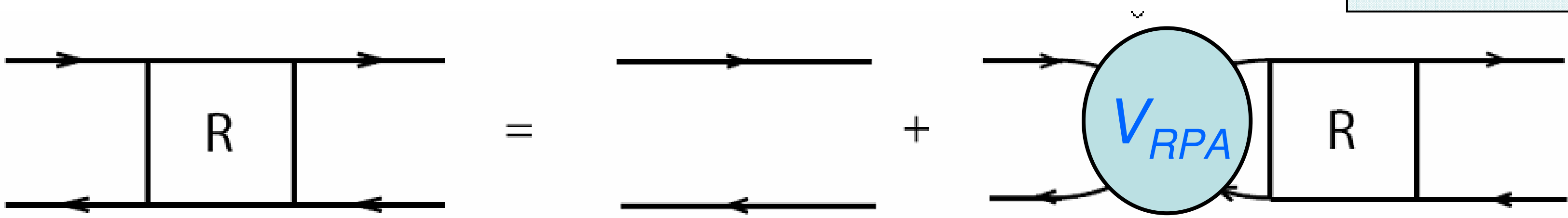
$$\Sigma_0 = \frac{\delta E}{\delta \rho}$$



Response equation: propagation of a phonon

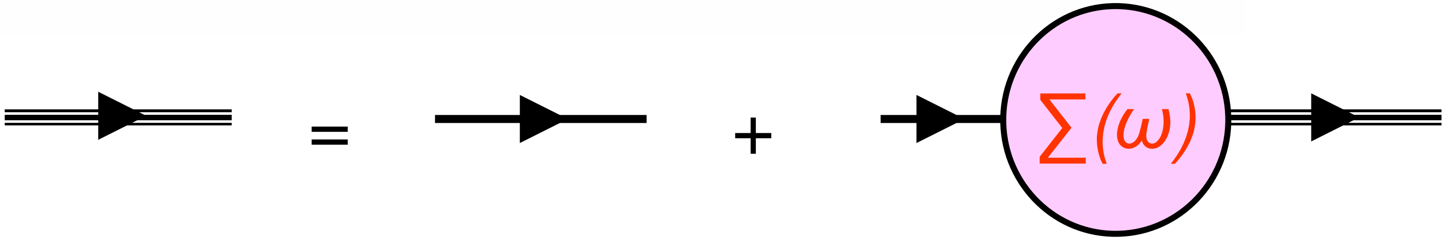
$$R(\omega) = R_0(\omega) + R_0(\omega)\,V_{RPA}\,R(\omega)$$

$$V_{RPA} = \frac{\delta \Sigma_0}{\delta \rho}$$



Dyson equation: propagation of one quasi-particle

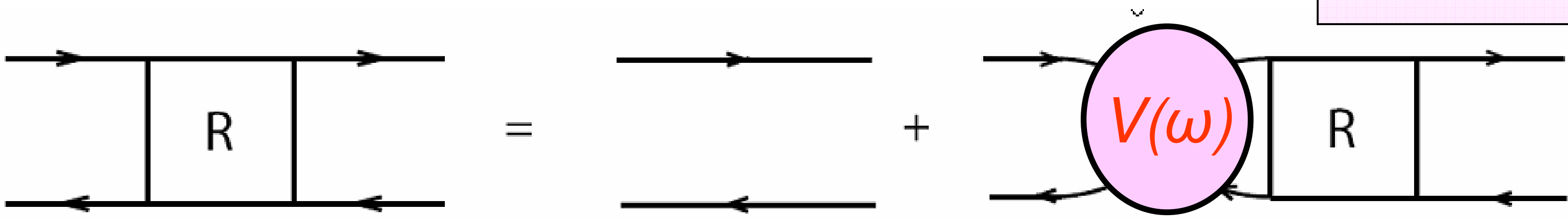
$$G(\omega) = G_0(\omega) + G_0(\omega)\Sigma(\omega)G(\omega)$$



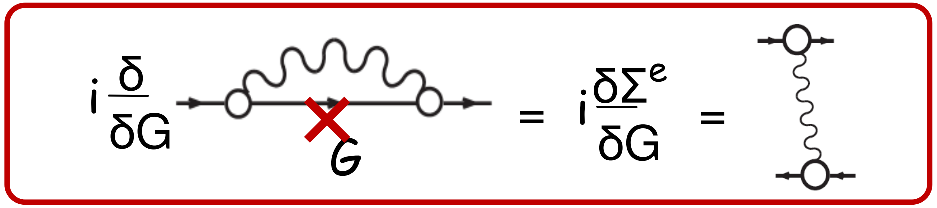
Response equation: propagation of a phonon

$$R(\omega) = R_0(\omega) + R_0(\omega)\, V(\omega)\, R(\omega)$$

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



Energy dependent self energy: $\Sigma(\omega) = \Sigma_0 + \Sigma^e(\omega)$

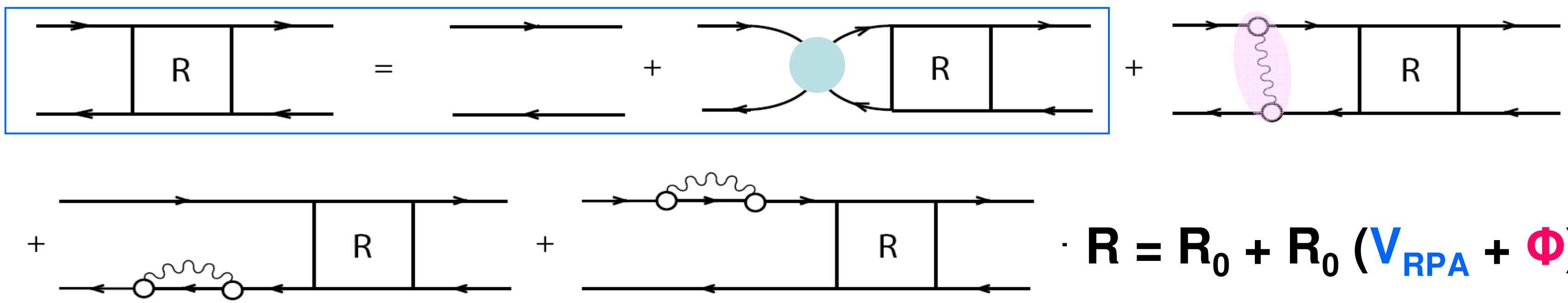


Problem of divergengies:

Renormalization of the interaction:

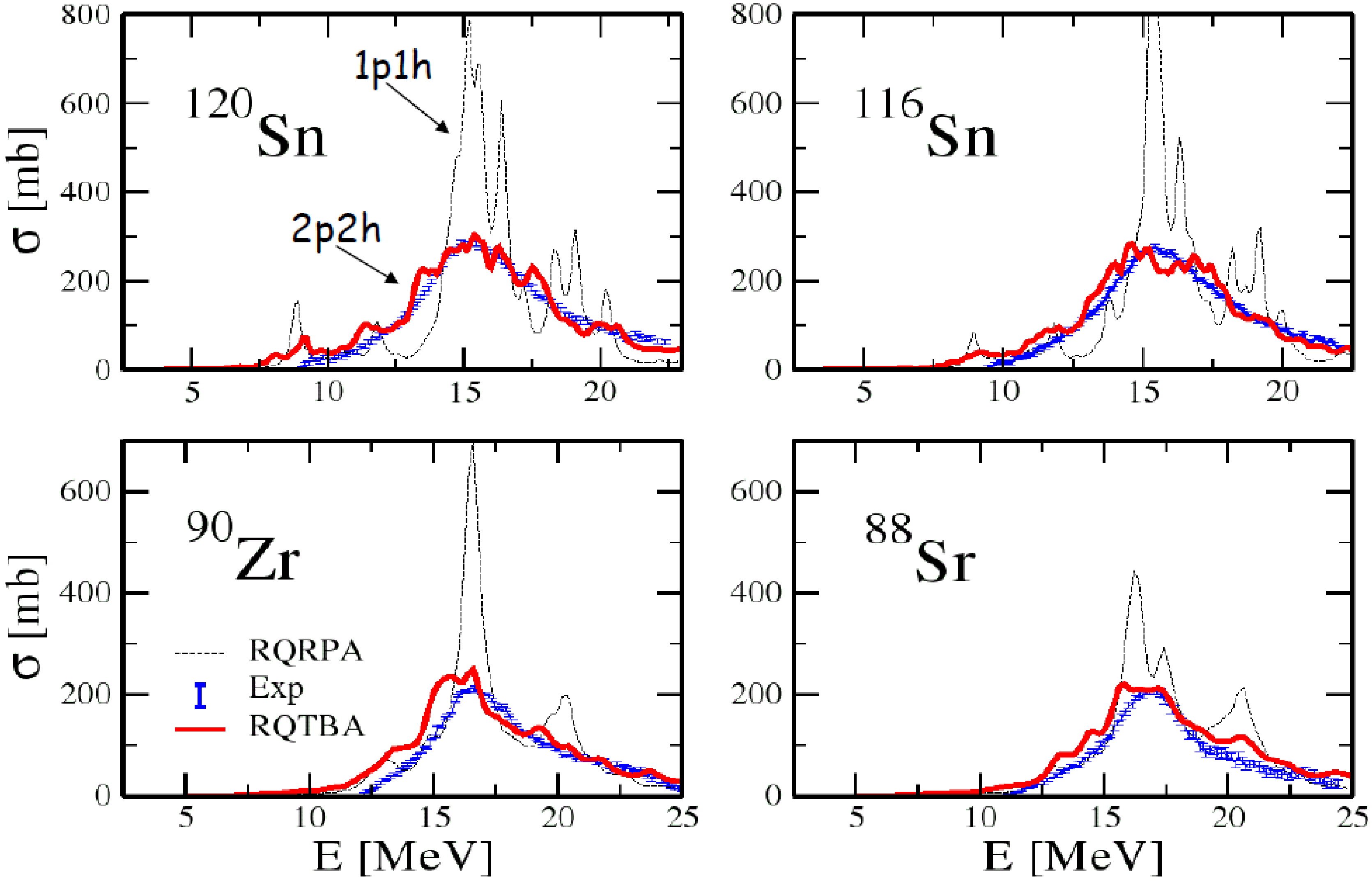
$V(\omega) \;\rightarrow V_{RPA} + \Phi(\omega) - \Phi(0)$

Time Blocking Approximation TBA



$R = R_0 + R_0\,(V_{RPA} + \Phi)\,R$

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

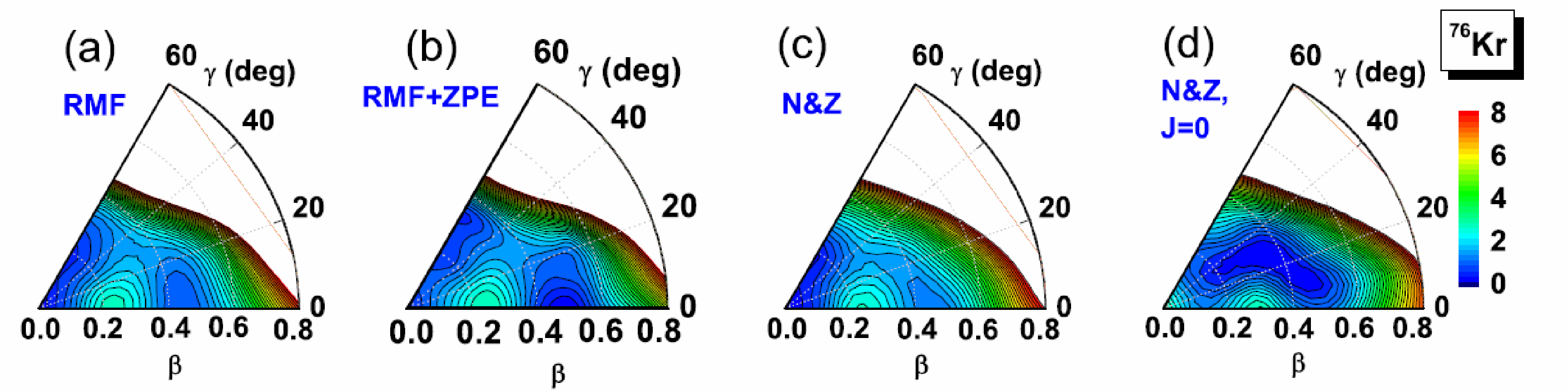


Litvinova, P.R., Tselyaev, PRC 78, 014312 (2008)

Beyond mean field: GCM

- Projection !
- Isospin projection! (seven-dimensional integrals)
- Variation after projection !
- Egido poles
- Choice of collective degrees of freedom?
- Coupling to single-particle 1ph, 2ph configurations
- Collective Hamiltonian (Bohr-Hamiltonian)
- Inertia parameters (level crossings)

Transitional nuclei: DFT beyond mean field:



Generator-Coordinates: q = (β,γ)

Projection on J and N:

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

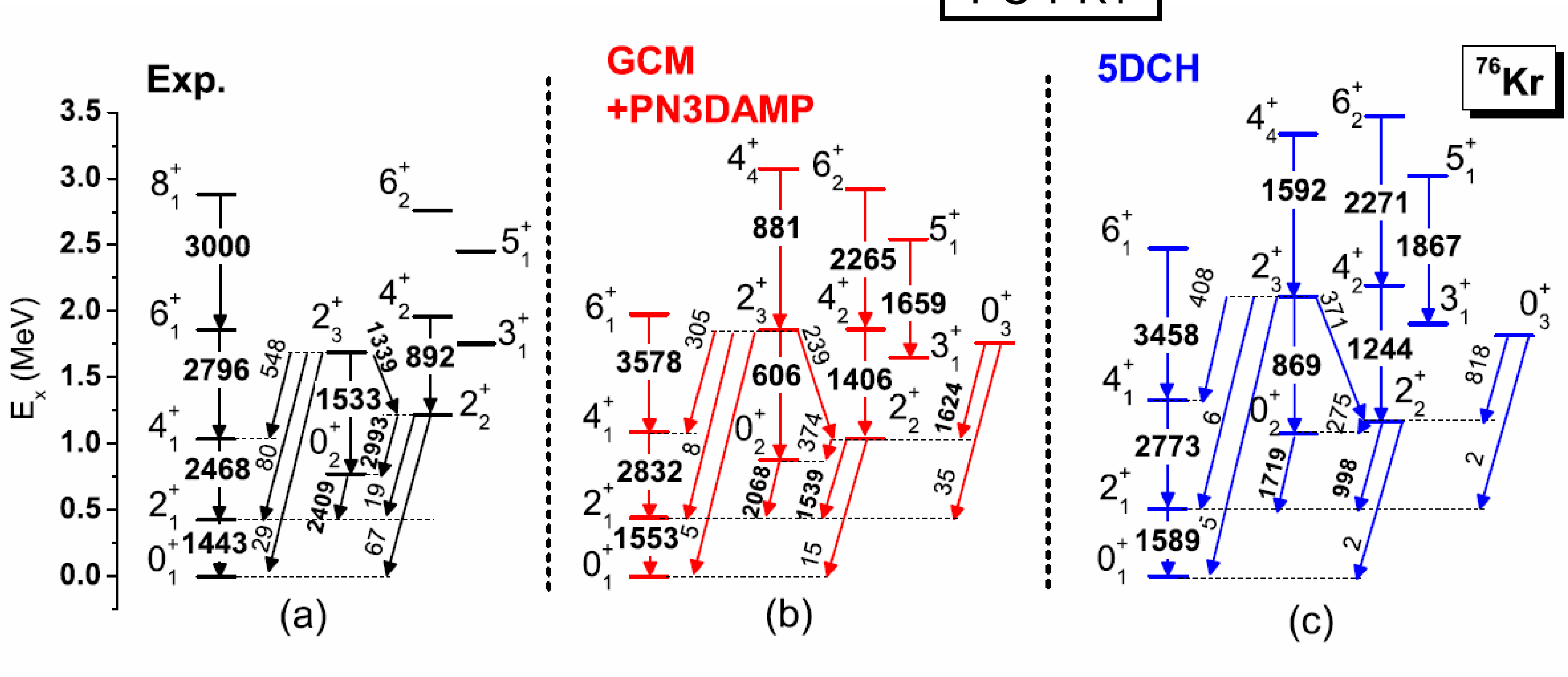
Bohr Hamiltonian: $H = -\frac{\partial}{dq}\frac{1}{2B(q)}\frac{\partial}{dq} + V(q) + V_{corr}(q)$

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

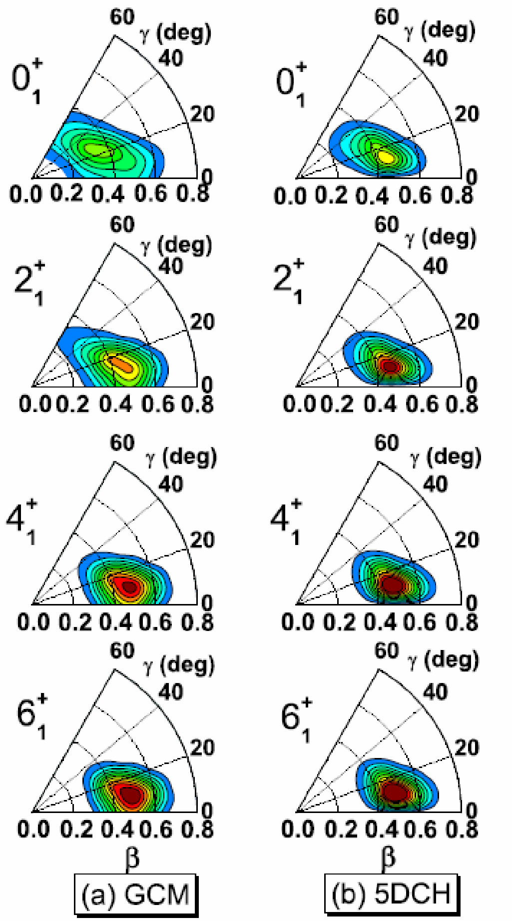
Spectra: GCM (7D)

Bohr Hamiltonian (5DCH)

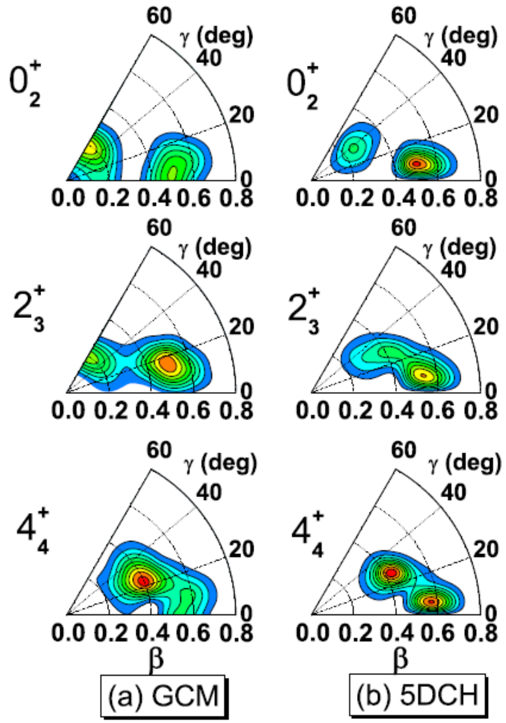
PC-PK1



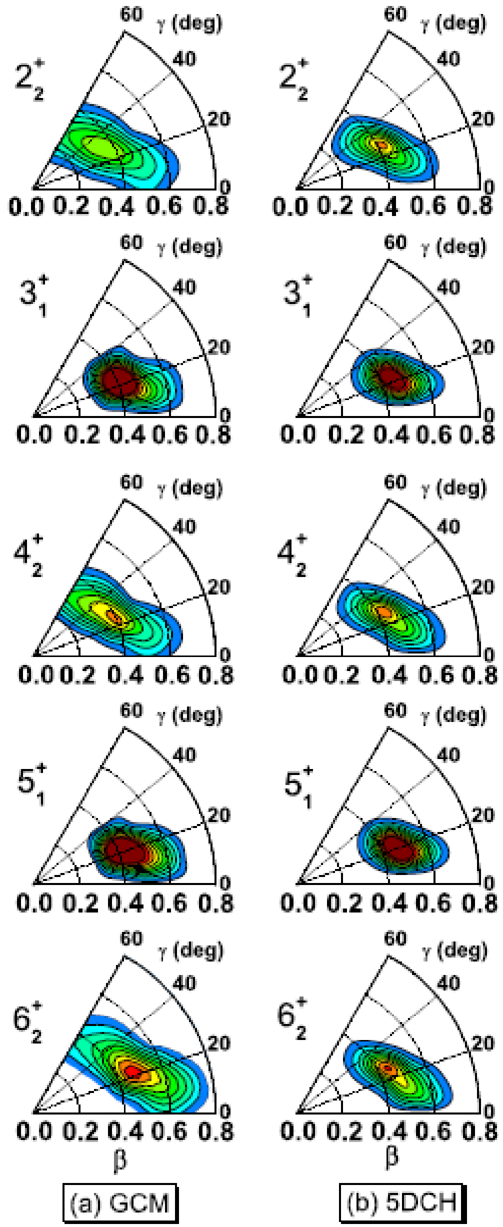
J.M. Yao et al, PRC (2014)



0_1^+
2_1^+
4_1^+
6_1^+
γ (deg)
β
(a) GCM
(b) 5DCH



0_2^+
2_3^+
4_4^+
γ (deg)
β
(a) GCM
(b) 5DCH



2_2^+
3_1^+
4_2^+
5_1^+
6_2^+
γ (deg)
β
(a) GCM
(b) 5DCH

- Structure of the functionals
  - relevant data are limited
  - simple answer: relativistic (neglect Dirac sea!)
  - better answer: ab-initio
- Symmetry violations
  - simple answer: projection (neglect Egido poles)
  - better answer: projection before variation
- Correlations (configuration mixing)
  - answer: generator coordinates (GCM)
  - simpler answer: Collective Hamiltonian (5DCH)
  - better answer: Selfconsistent collective path ???
- Energy dependence of the self energy
  - answer: particle-vibrational coupling
  - better answer: vibrational-vibrational coupling