# Recent progress in shell-model calculations for pf and pfg-shell nuclei

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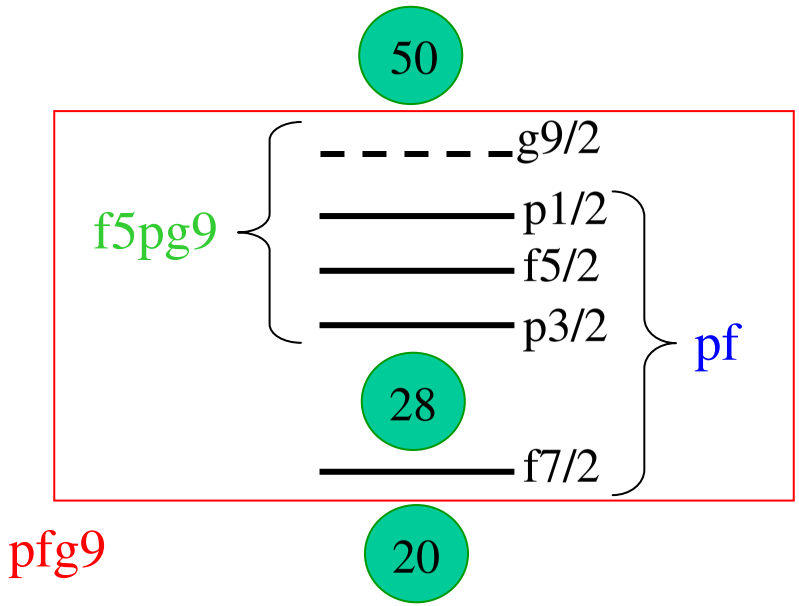
M. Honma (Univ. of Aizu)

T. Otsuka (Univ. of Tokyo/CNS/RIKEN)
T. Mizusaki (Senshu Univ./CNS)
B. A. Brown (MSU)
M. Hjorth-Jensen (Univ. of Oslo)

# Outline

- Introduction
- pf-shell
  - GXPF1 interaction
  - Shell evolution
  - N=32, 34 shell gap
- f5pg9-shell
  - JUN45 interaction
  - Systematics
  - Shape coexistence in $^{68}$Se
- pfg9-shell
  - Neutron-rich Cr
- Summary



# Introduction

- Shell model
  - Powerful tool for the study of nuclear structure
  - Small model space (~1 major shell)
  - Diagonalize effective Hamiltonian with a complete basis set

$$H = \sum_a \varepsilon_a n_a + \sum_{a \le b, c \le d, JT} V(abcd; JT) A^+_{JT}(ab) A_{JT}(cd)$$

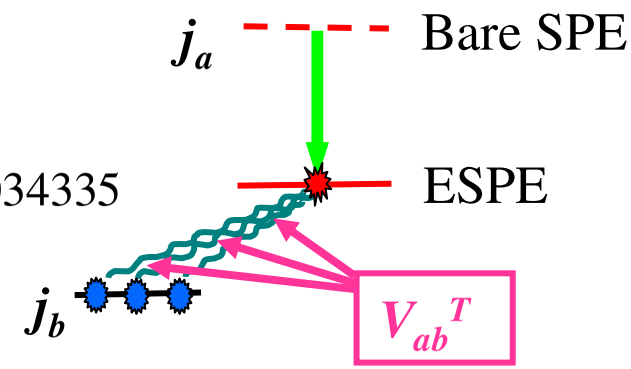
- Large scale shell model
  - Currently, full pf-shell can be treated exactly (~ $10^9$ m-scheme dim.)
  - For larger model space … approximation such as p-h truncation, SMMC, MCSM, extrapolation, …
  - Systematic description of various nuclear properties within a unified framework, covering wide mass range
- Interests
  - Change of shell structure and its relation to the nuclear force
  - Interplay between single-particle and collective degrees of freedom

# Effective interaction

- Realistic interaction
  - Renormalized G-matrix derived from realistic NN potential
  - Difficulties for many valence nucleons ( ex. deformed $^{56}$Ni )
  - Realistic + empirical correction
- Monopole correction
    - KB3 … A. Poves and A. P. Zuker, Phys. Repts. 70 (1981) 235
  - $H = H_m$ (monopole) + $H_M$ (multipole)
  - Monopole part determines average energy of a given configuration
  - Important for B.E., shell gap
  - Centroid .. Angular momentum average → effective SPE

$$V_{ab}^{T} = \frac{\sum_J (2J+1) V_{abab}^{JT}}{\sum_J (2J+1)}$$

- Global fit
    - GXPF1 … M. Honma et al., PRC69 (2004) 034335
  - Fit to experimental energy data
  - Monopole, pairing, QQ, …

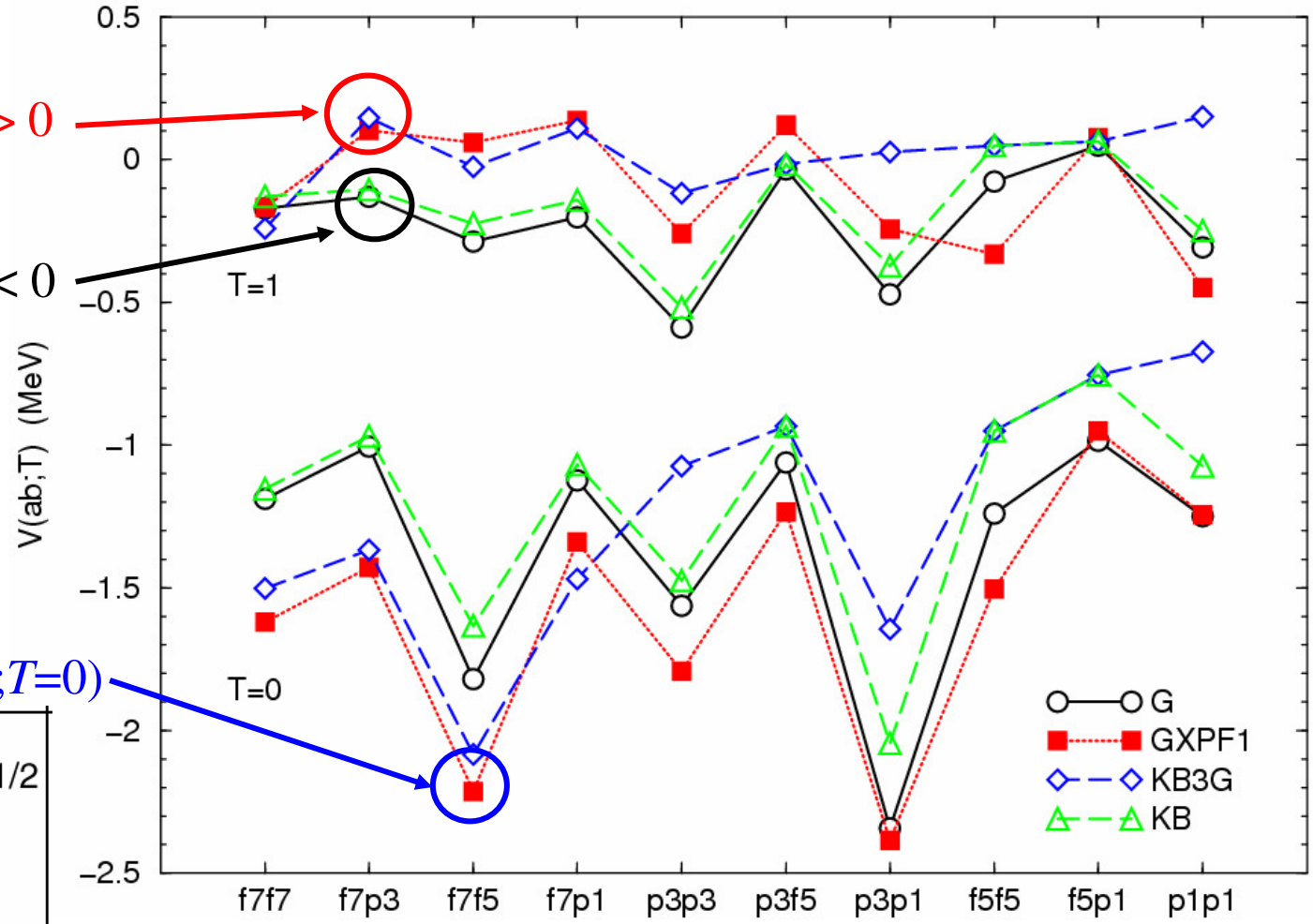


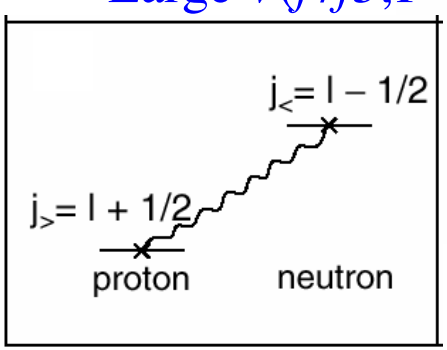
# Monopole centroids

*GXPF1:*
*V*(*f*7*p*3;*T*=1) > 0

*G-matrix:*
*V*(*f*7*p*3;*T*=1) < 0

Large *V*(*f*7*f*5;*T*=0)

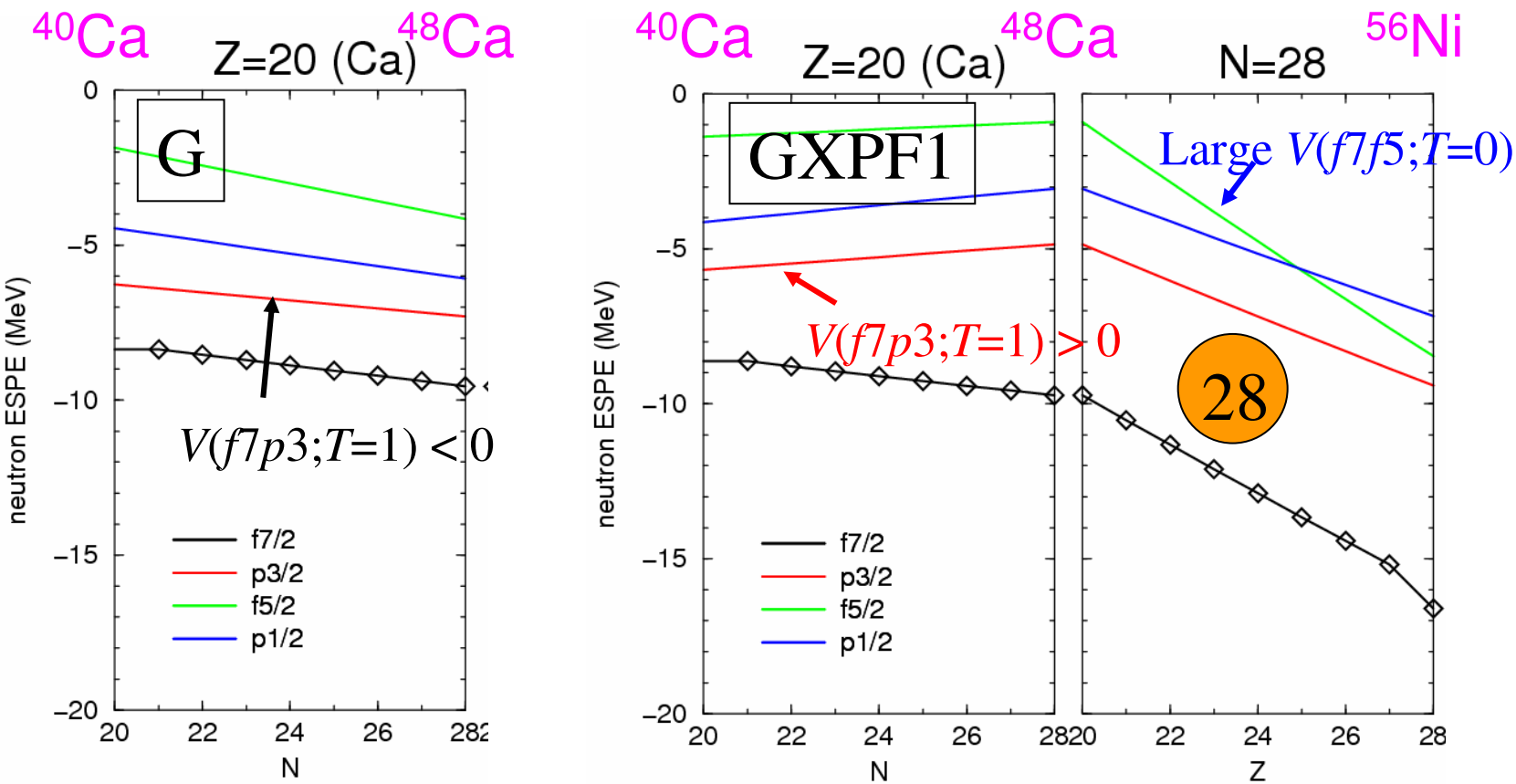



T.Otsuka et al. PRL87 (2001) 082502

# Development of N=28 shell gap

- Monopole centroids affect shell-evolution
- Original G-matrix int. produces no N=28 gap
- Large V(f7f5;T=0) produce inversion of p1/2 and f5/2 (c.f. $^{57}$Ni)

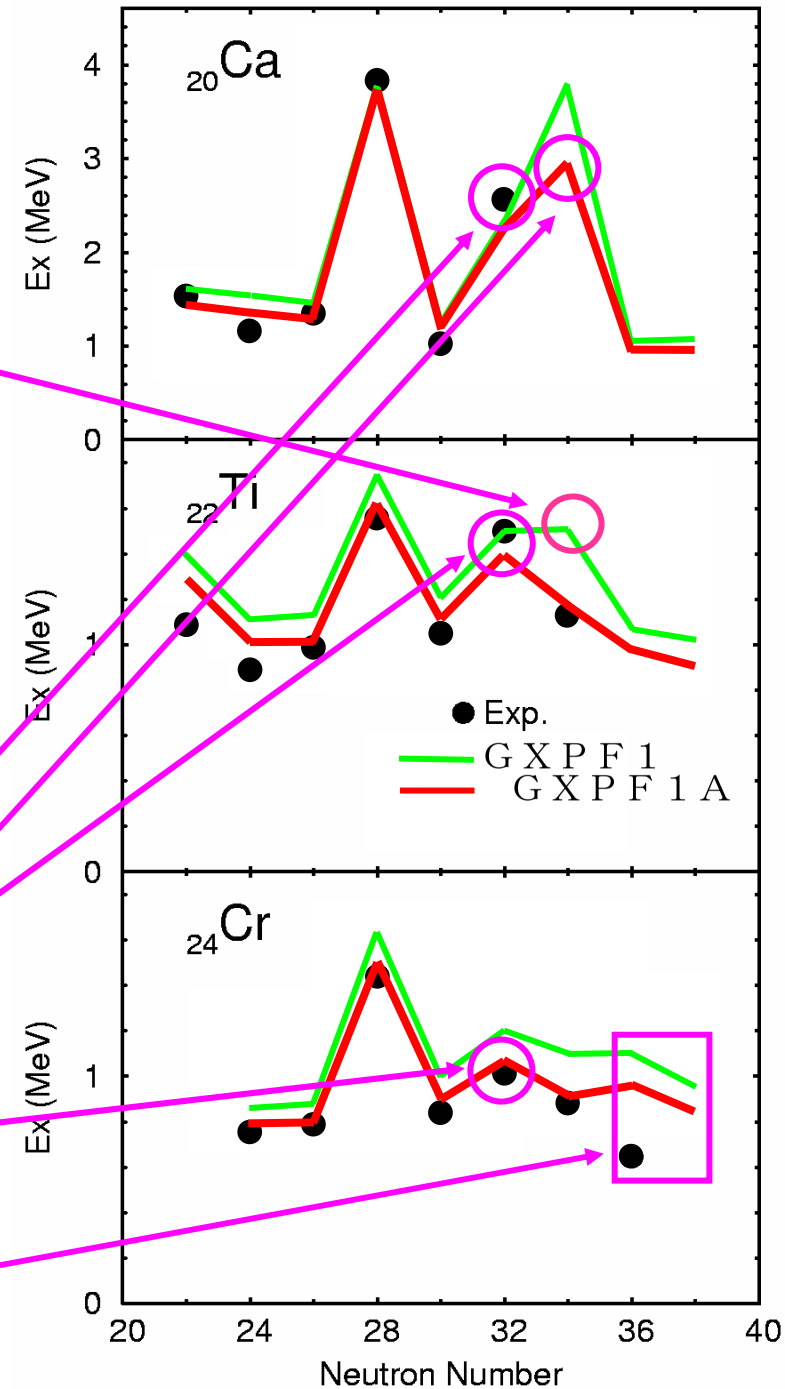


# Improvements

M. Honma et al. EPJA25 Supp.1 (2005) 499

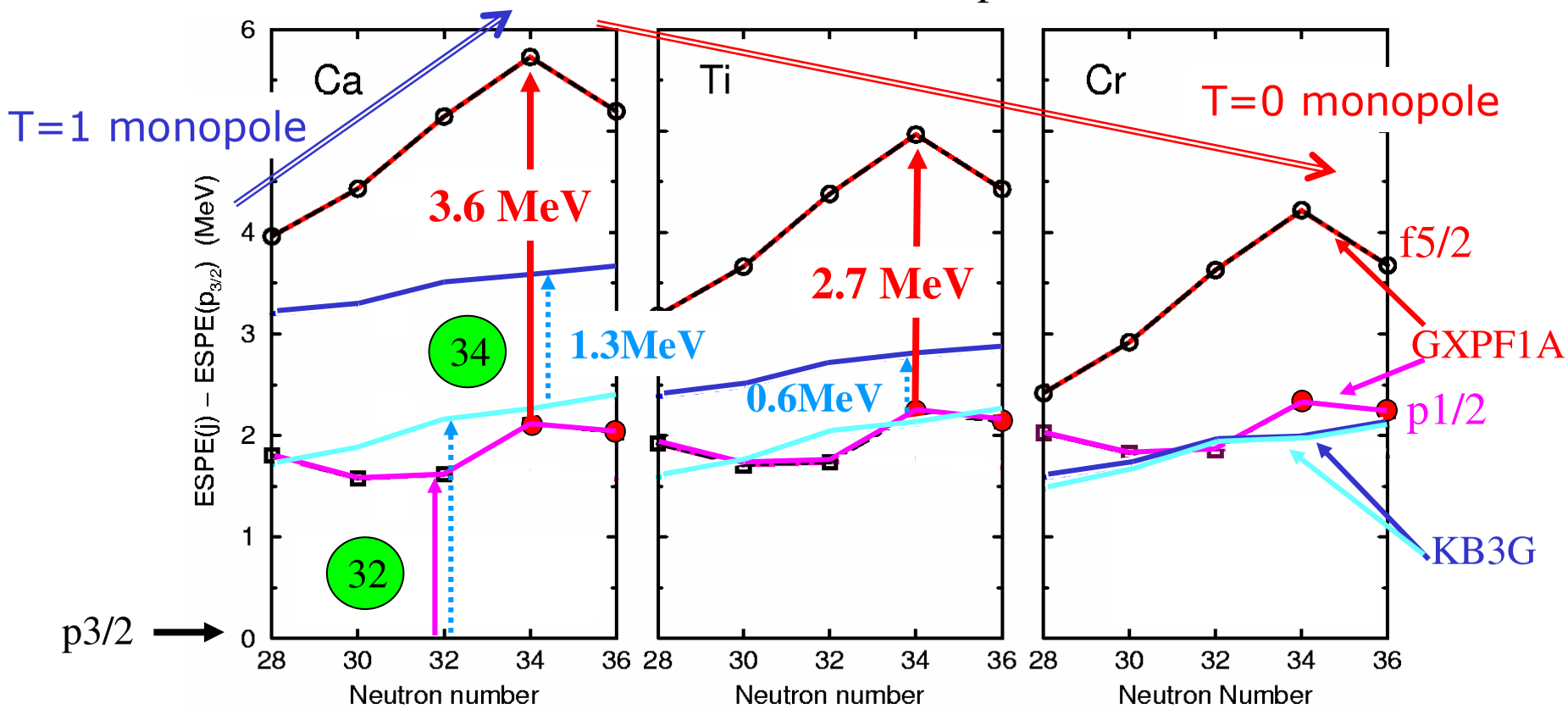
- Measured Ex($2^+$) of $^{56}$Ti is lower than prediction by ~400keV
  S.N.Liddick et al. PRL92 (2004) 072502
- Modify 5 $T$=1 matrix elements
  - f7-f7 papring
  - p1-p1 and p1-f5 pairing
  - p1-f5 QQ strength

    GXPF1⇒ GXPF1A
  - Improved description for most isotopes
- Shell gap
  - N=28
  - N=32 for Ca, Ti, Cr
  - N=34 for Ca ??
- N=36 $^{60}$Cr … g9/2 effect ?



# Evolution of ESPE

Neutron ESPE relative to p3/2

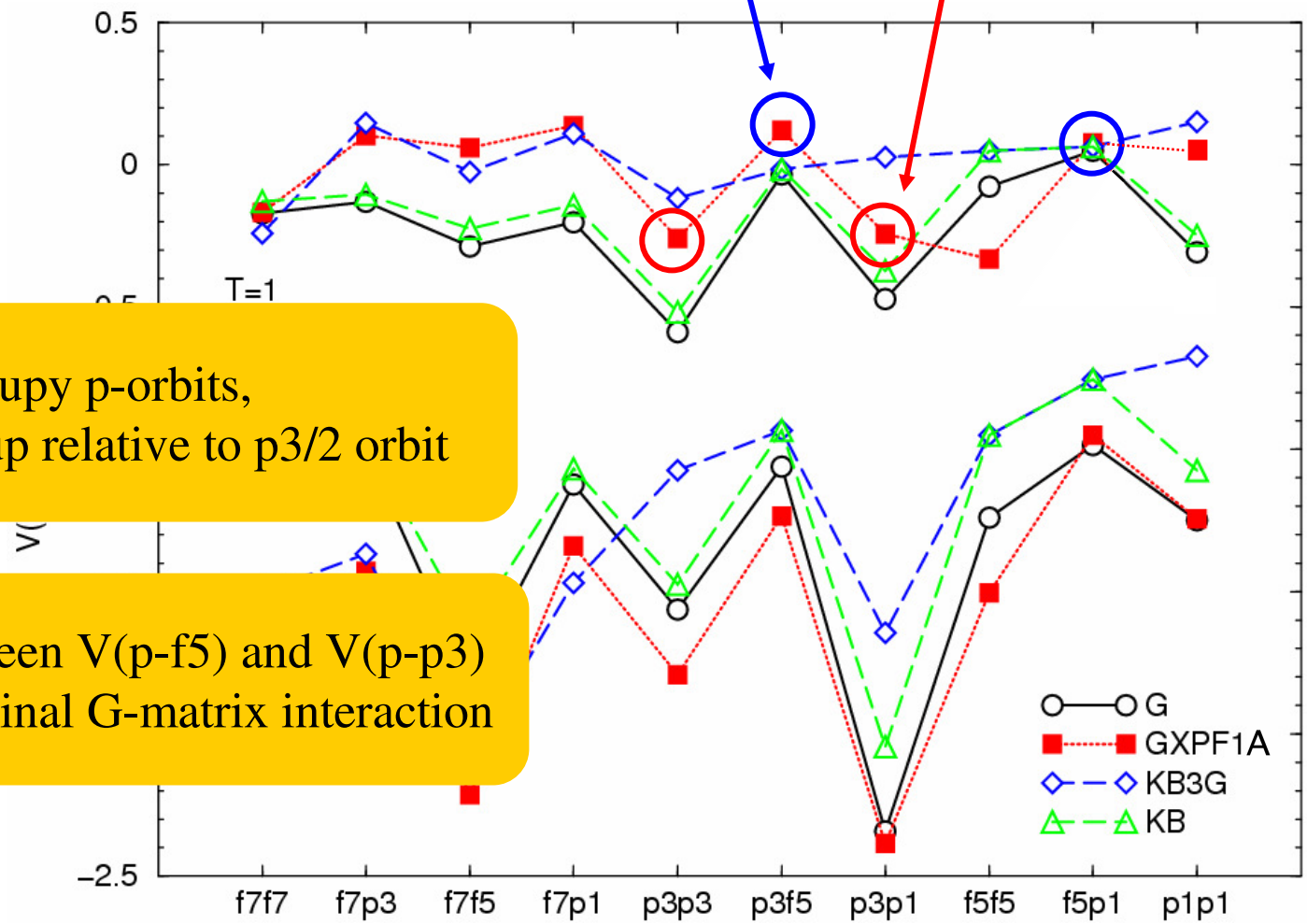



N=32 gap … almost constant

N=34 gap … significant Z dependence ⟵ πf7/2-νf5/2 attraction interaction dependence ( smaller gap by KB3G )

# Monopole centroids

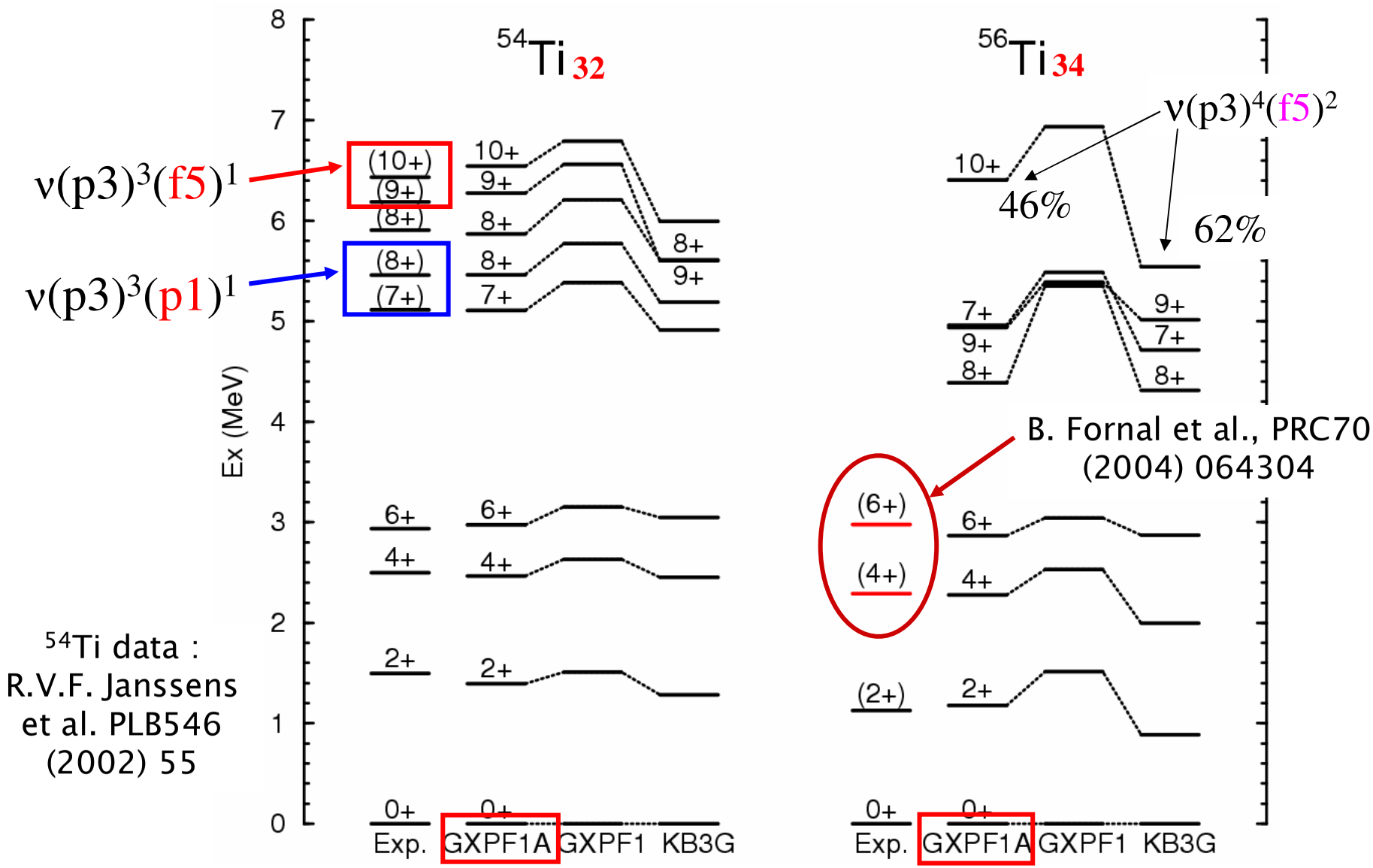
$V$(p-f5; T=1)–$V$(p-p3;T=1) ~ 0.5MeV




As neutrons occupy p-orbits,
f5/2 orbit goes up relative to p3/2 orbit

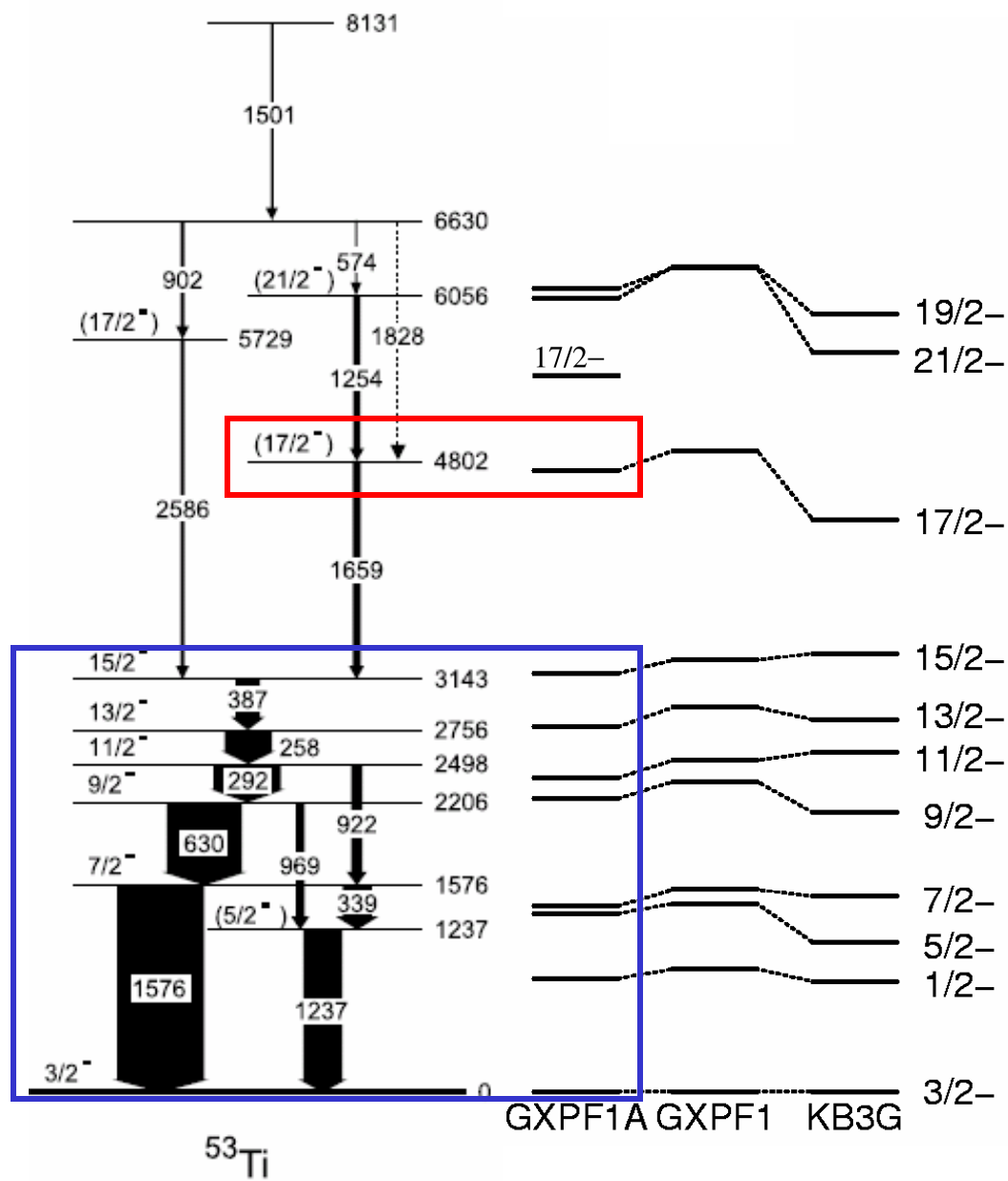
Difference between V(p-f5) and V(p-p3)
follows the original G-matrix interaction

# Even-A Ti


$^{54}Ti_{32}$
$^{56}Ti_{34}$
$\nu(p3)^3(f5)^1$
$\nu(p3)^3(p1)^1$
$\nu(p3)^4(f5)^2$
46%
62%
Ex (MeV)
(10+)
(9+)
(8+)
(8+)
(7+)
10+
9+
8+
8+
7+
6+
4+
2+
0+
(6+)
(4+)
(2+)
Exp.
GXPF1A
GXPF1
KB3G
B. Fornal et al., PRC70 (2004) 064304
$^{54}$Ti data : R.V.F. Janssens et al. PLB546 (2002) 55

# $^{53}Ti_{31}$ yrast structure

- $3/2^-$ to $15/2^-$…$\nu(p3)^3$
- $17/2^-$… $\nu(p3)^2(f5)^1$




B.Fornal et al.,
PRC72 (2005) 044315

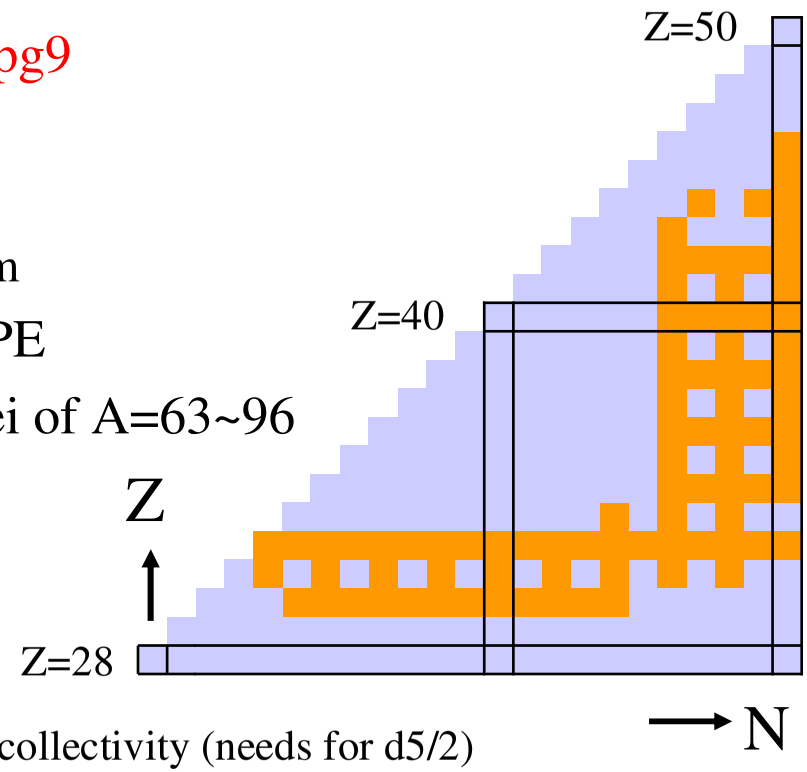
# Global fit for f5pg9-shell

- JUN45 interaction
  - Keep isospin symmetry
  - Modify microscopic interaction G-f5pg9

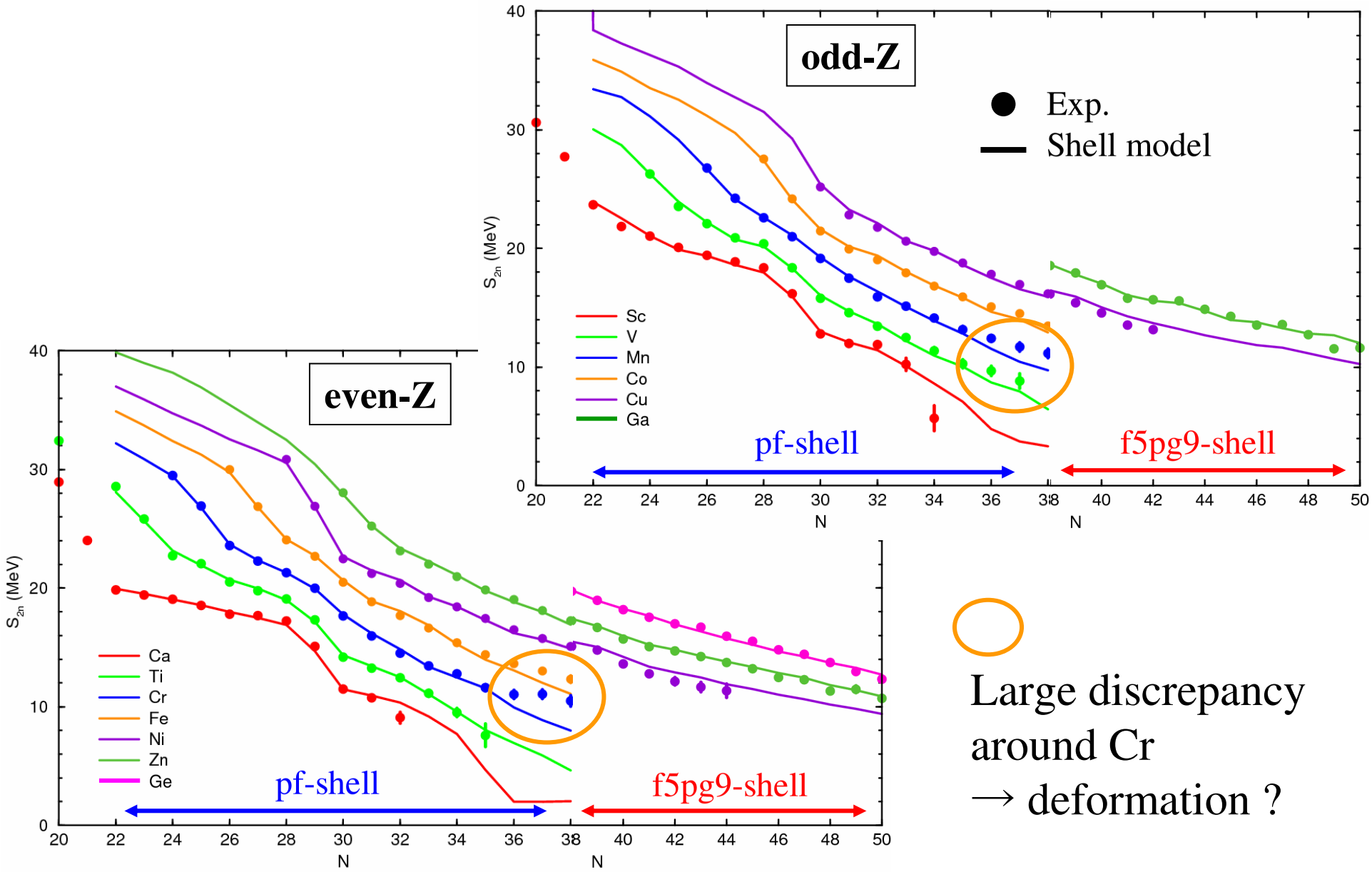
    M. Hjorth-Jensen, unpublished

    Bonn-C potential

    3rd order Q-box and folded diagram
  - Vary 45 LC's of 133 TBME and 4 SPE
  - Fit to 400 energy data out of 87 nuclei of A=63~96
    - Include low-lying states of
      - even-Z nuclei
      - odd-A nuclei
    - Exclude
      - N<46 for Z>33… large quadrupole collectivity (needs for d5/2)
      - Ni, Cu isotopes … large effects of f7/2 core-excitations
  - Assume $A^{-0.3}$ mass dependence
  - Rms error of 185 keV

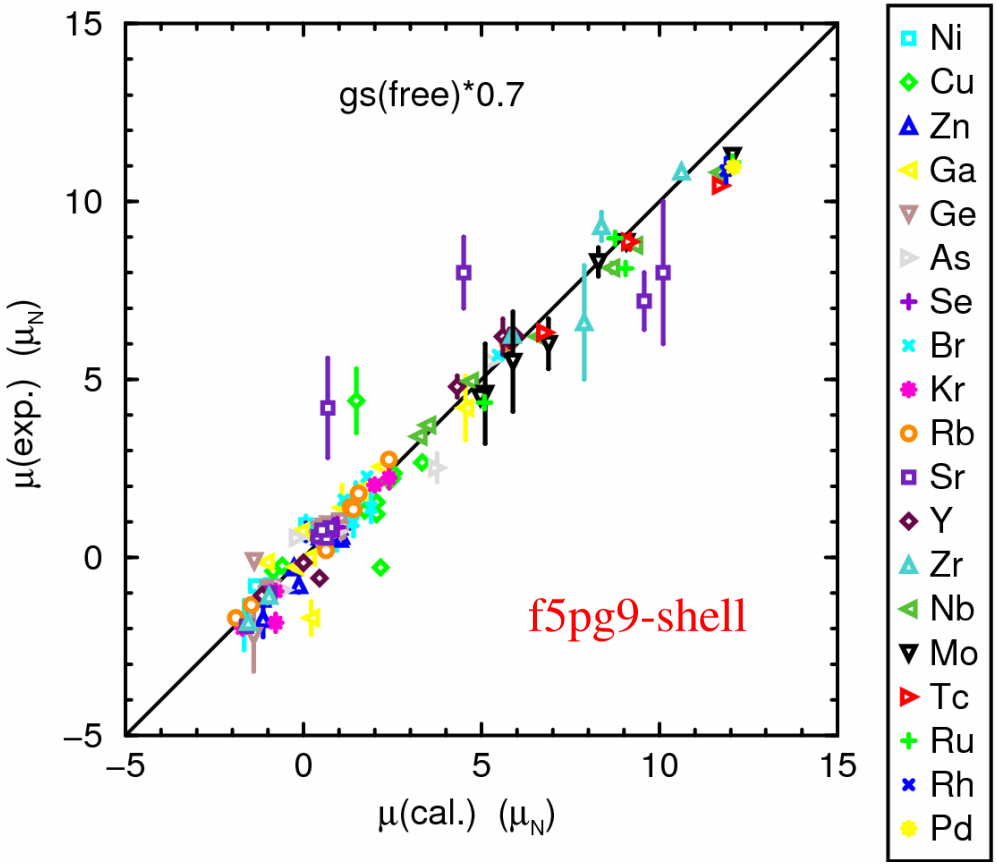


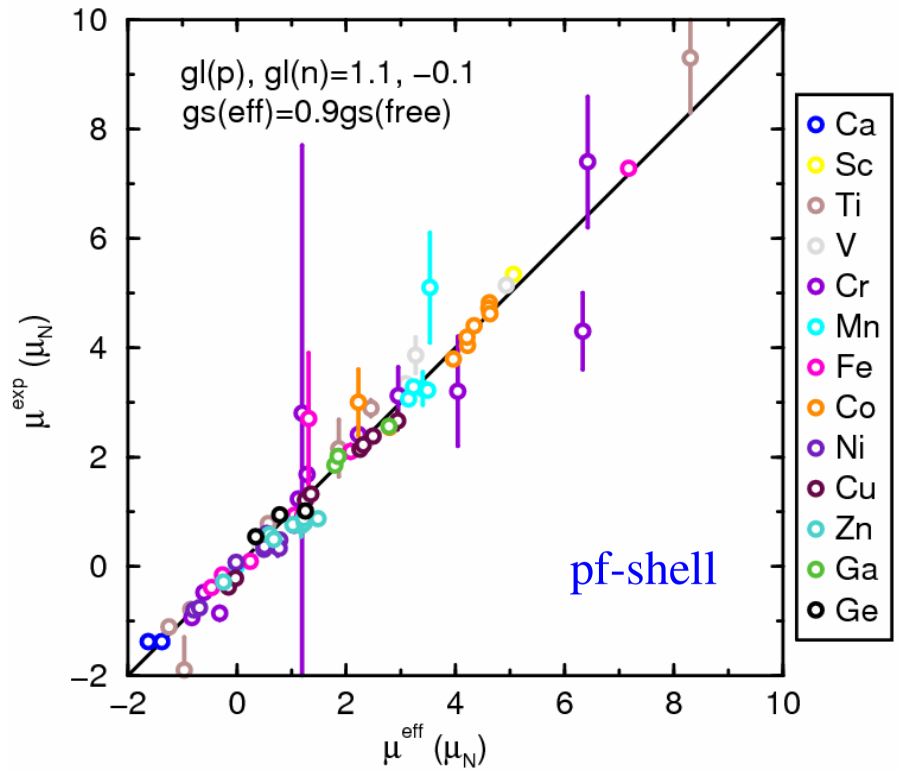
# Two neutron separation energy

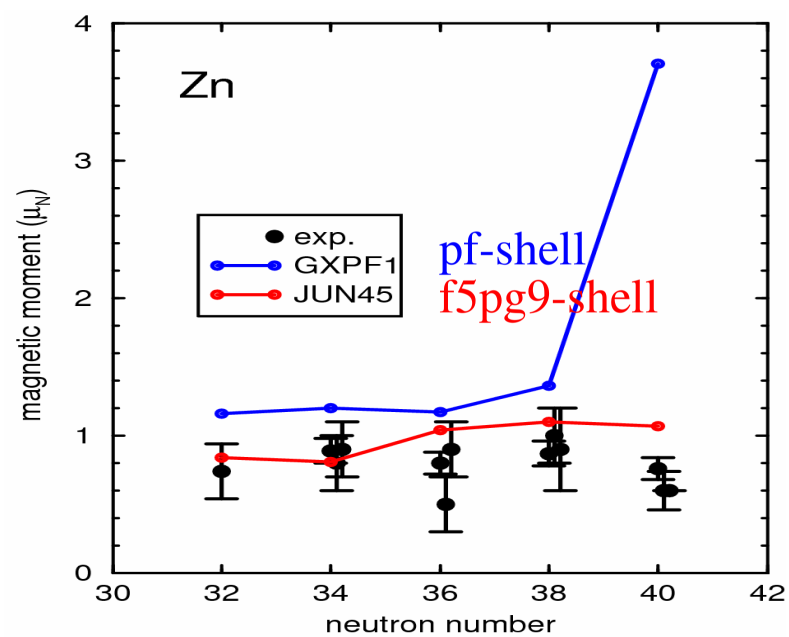



Large discrepancy around Cr
→ deformation ?

# Magnetic moments



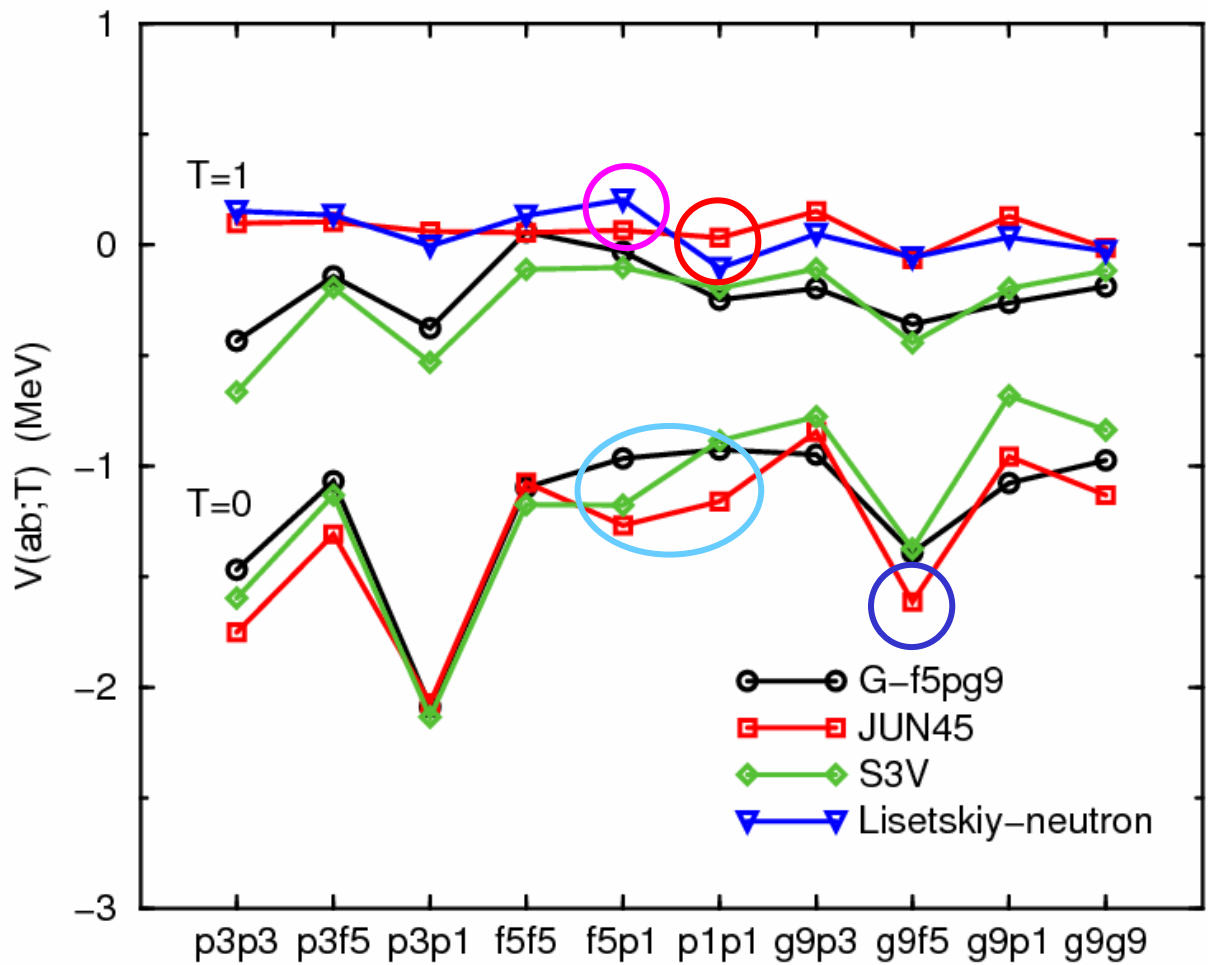




Inclusion of g9/2 improves the description for Zn

# Monopole centroids

- T=0
  - Modifications in p1-p1 and f5-p1 due to missing d5/2 ?
- T=1
  - Similar to Lisetskiy except for f5-p1 and p1-p1
- Similarity between
  - G-f5pg9 and S3V
  - JUN45 and Lisetskiy



# Monopole migration of πf5/2

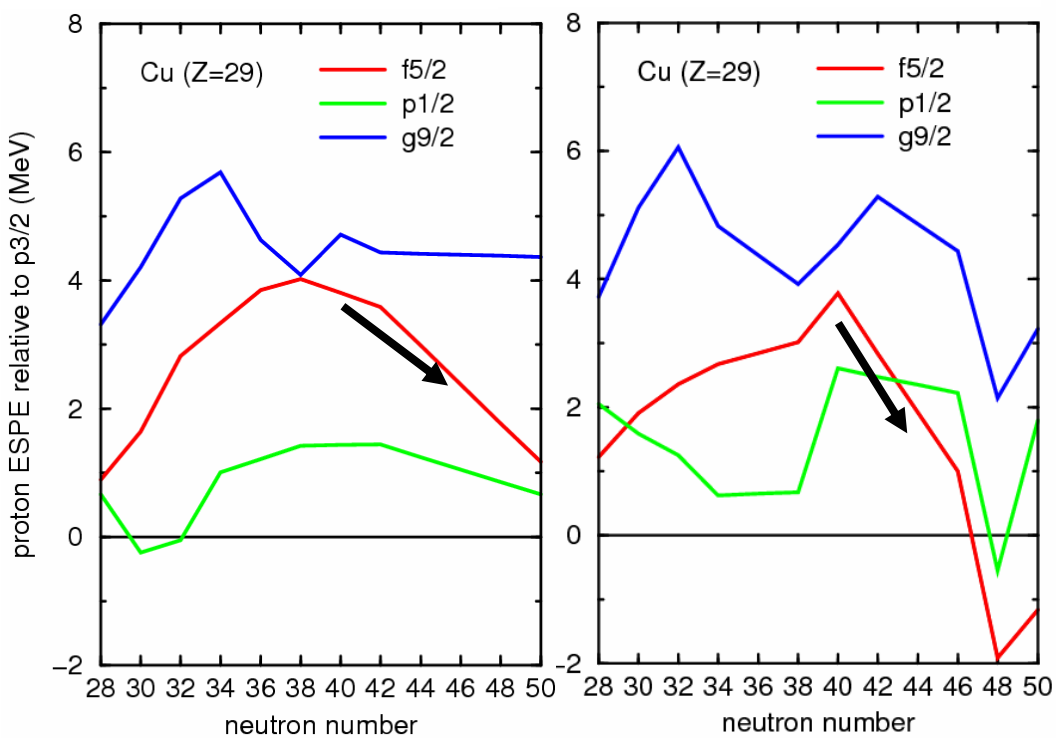
Large difference between

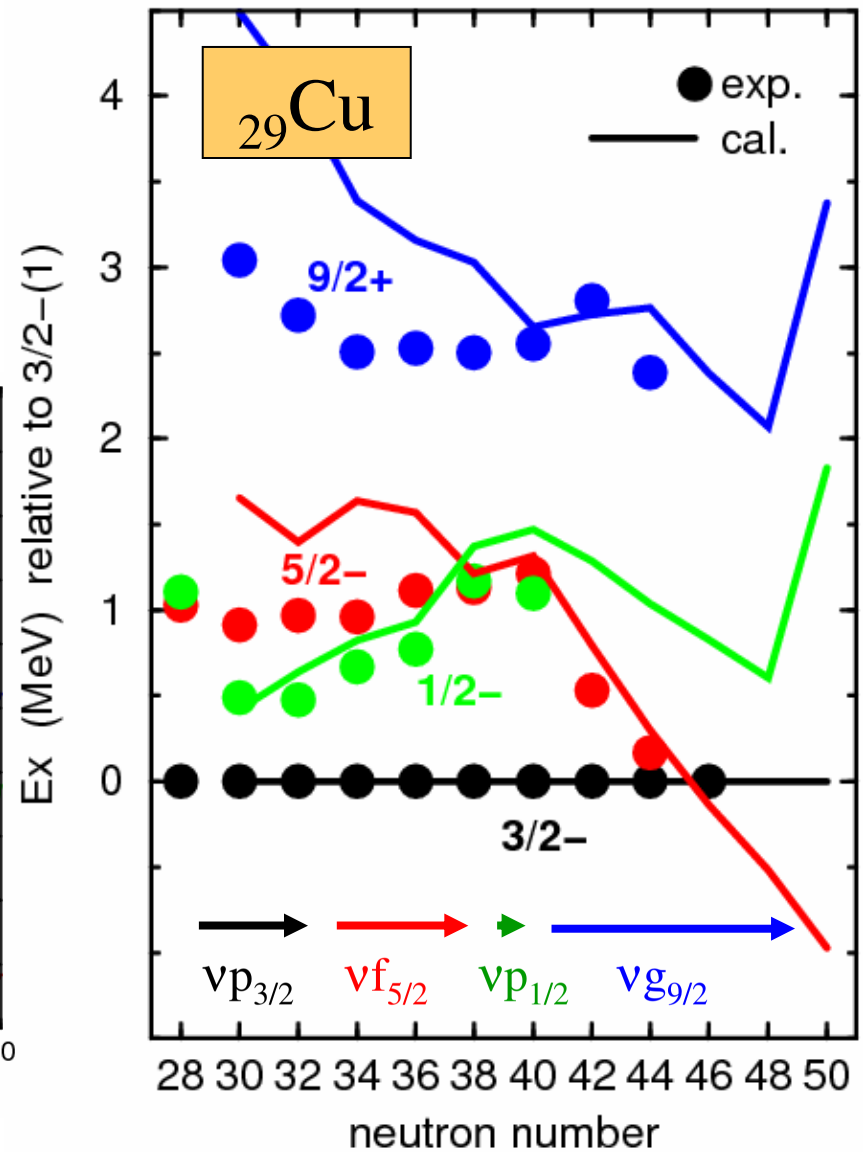
$V^{T=0}$(p-g9) and $V^{T=0}$(f5-g9)

G-f5pg9 ~ 0.5MeV

JUN45 ~ 1.0MeV

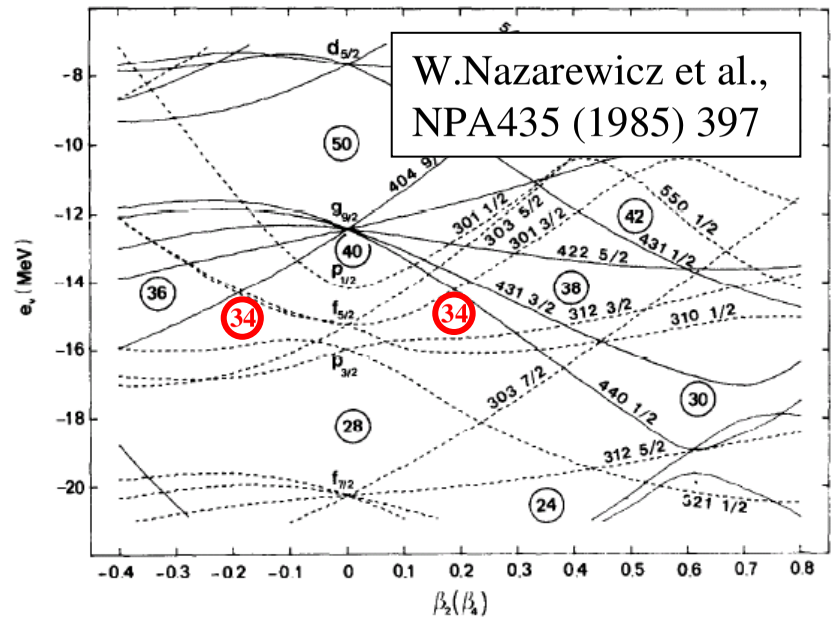
G-f5pg9 JUN45

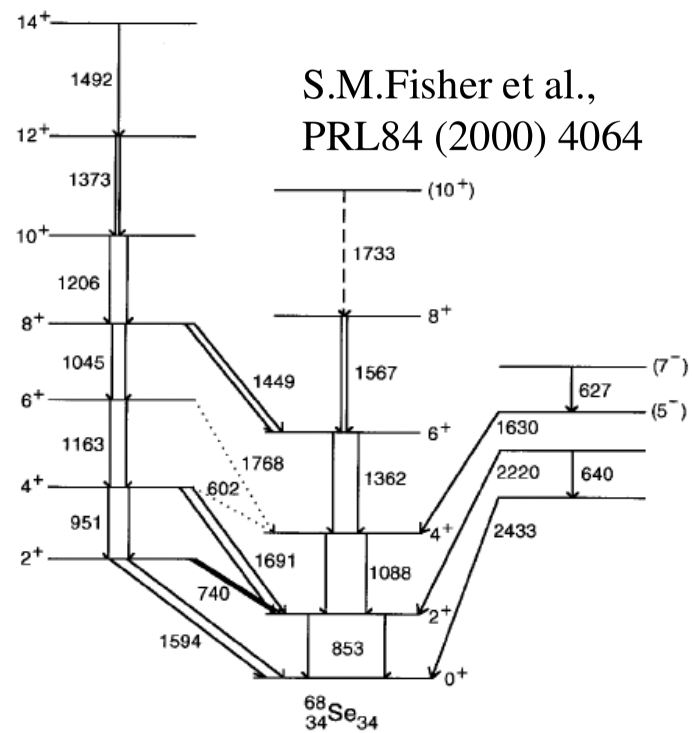


# Shape coexistence in $^{68}$Se

- N=Z=34 proton-rich nuclei
- Prediction by deformed potential
  - Large N=34 gap
  - Oblate gs
  - Prolate minima
- Experimental confirmation
  - Coexistence of two rotational bands
  - Higher-spin band
- Theoretical description
  - Mean Field, PSM, VAMPIR, etc.
- Good challenge for shell model
  - Realistic interaction
  - Description of collective states
  - Extrapolation to unfitted region

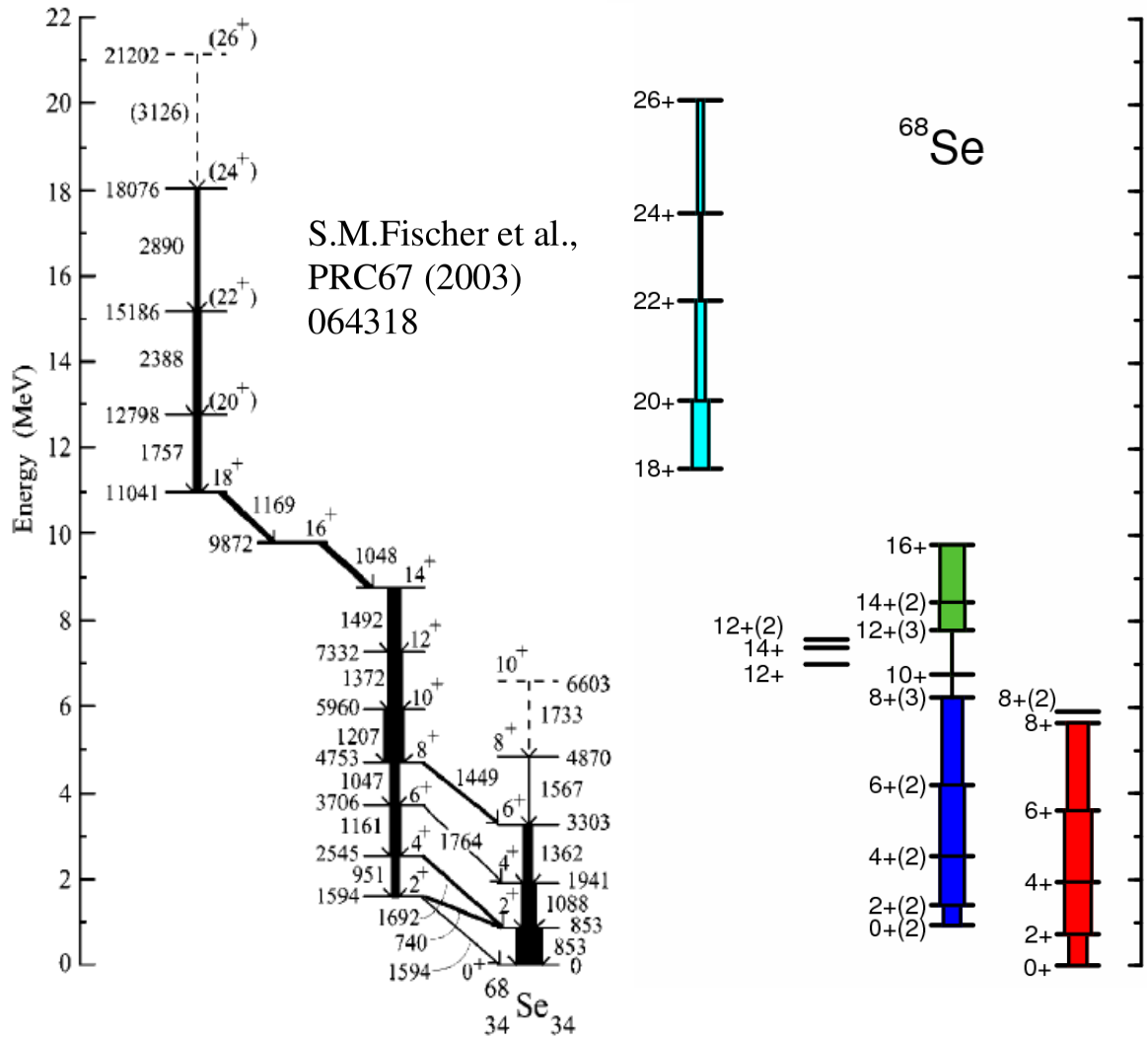


# Band structure

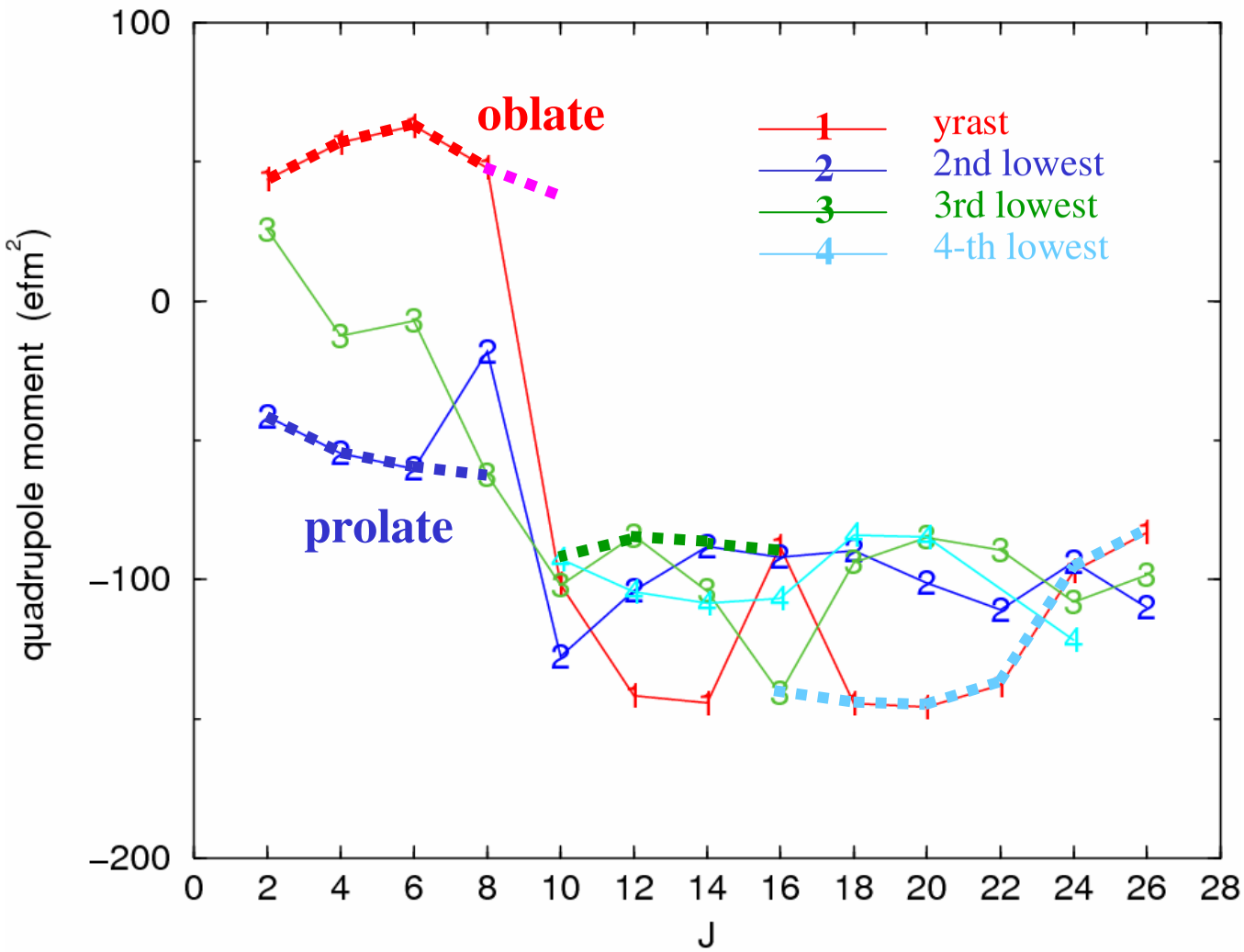
- Connected by relatively large B(E2)
- B(E2; $2^+_1 \rightarrow 0^+_1$) (ep=1.5, en=1.1)

| Ji | Jf | B(E2) $e^2fm^4$ |
|---|---|---|
| $2^+_1$ | $0^+_1$ | 486 (β~0.25) |
| $2^+_2$ | $0^+_1$ | 16 |
| $2^+_2$ | $0^+_2$ | 447 |
| $2^+_2$ | $2^+_1$ | 117 |



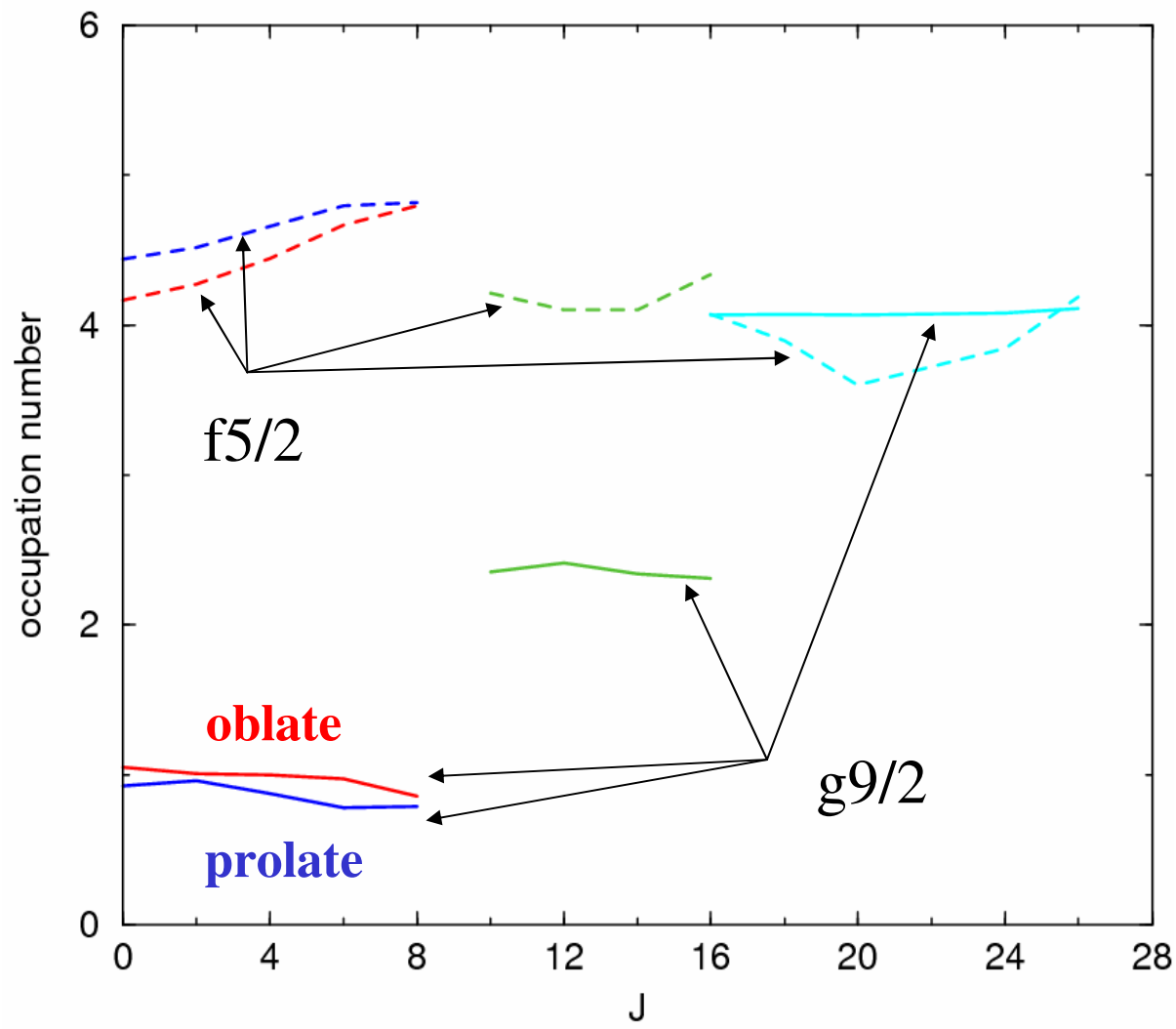
# Quadrupole moment

- Band structure imbedded in complex level scheme
- Ground state band can be extended to 10+(8) state



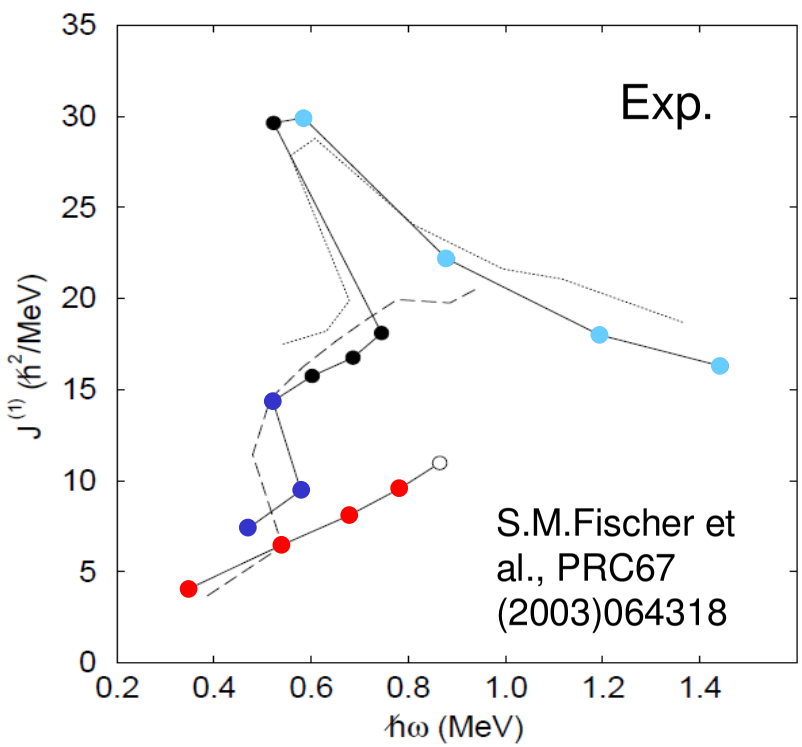
# Occupation number

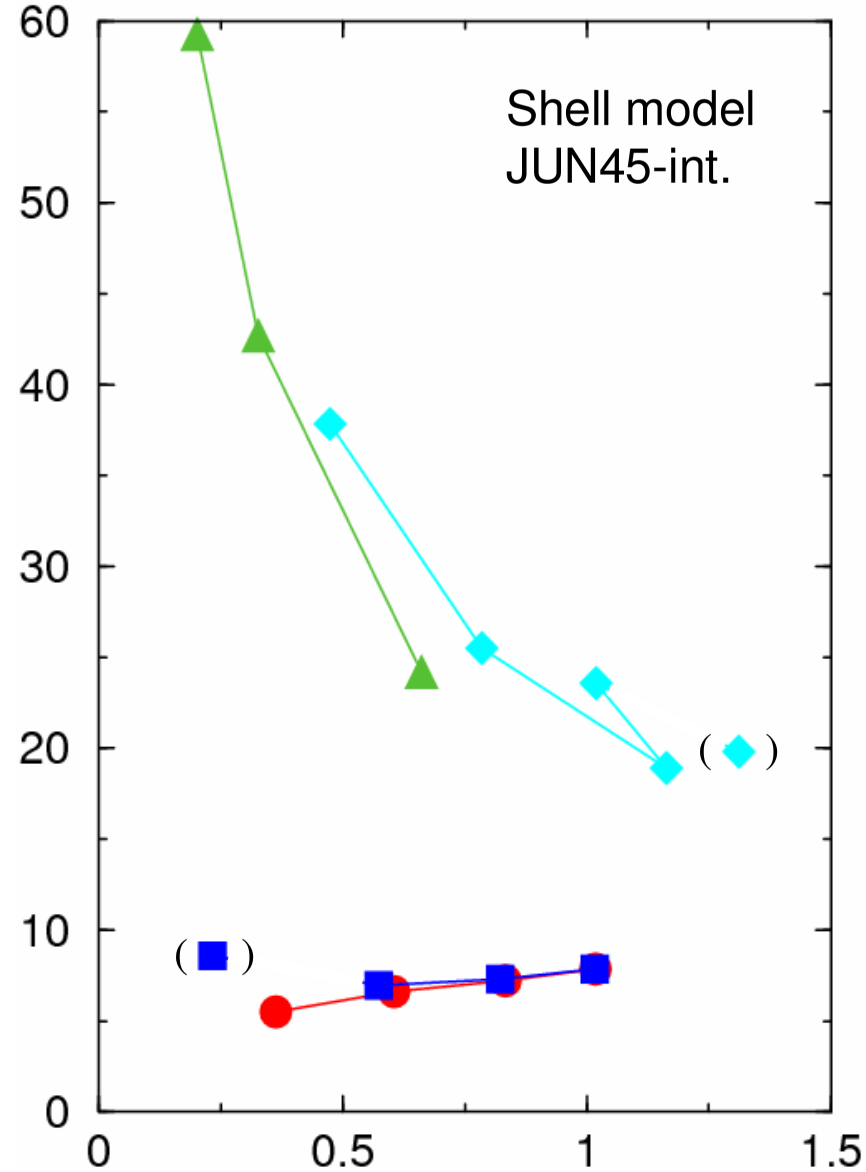
- Stability of intrinsic structure
- Bands are characterized by g9/2 occupation
  - ~ 1.0 … lowest bands
  - ~ 2.3 … middle spin
  - ~ 4.1 … higher spin



# Kinematic moment of inertia

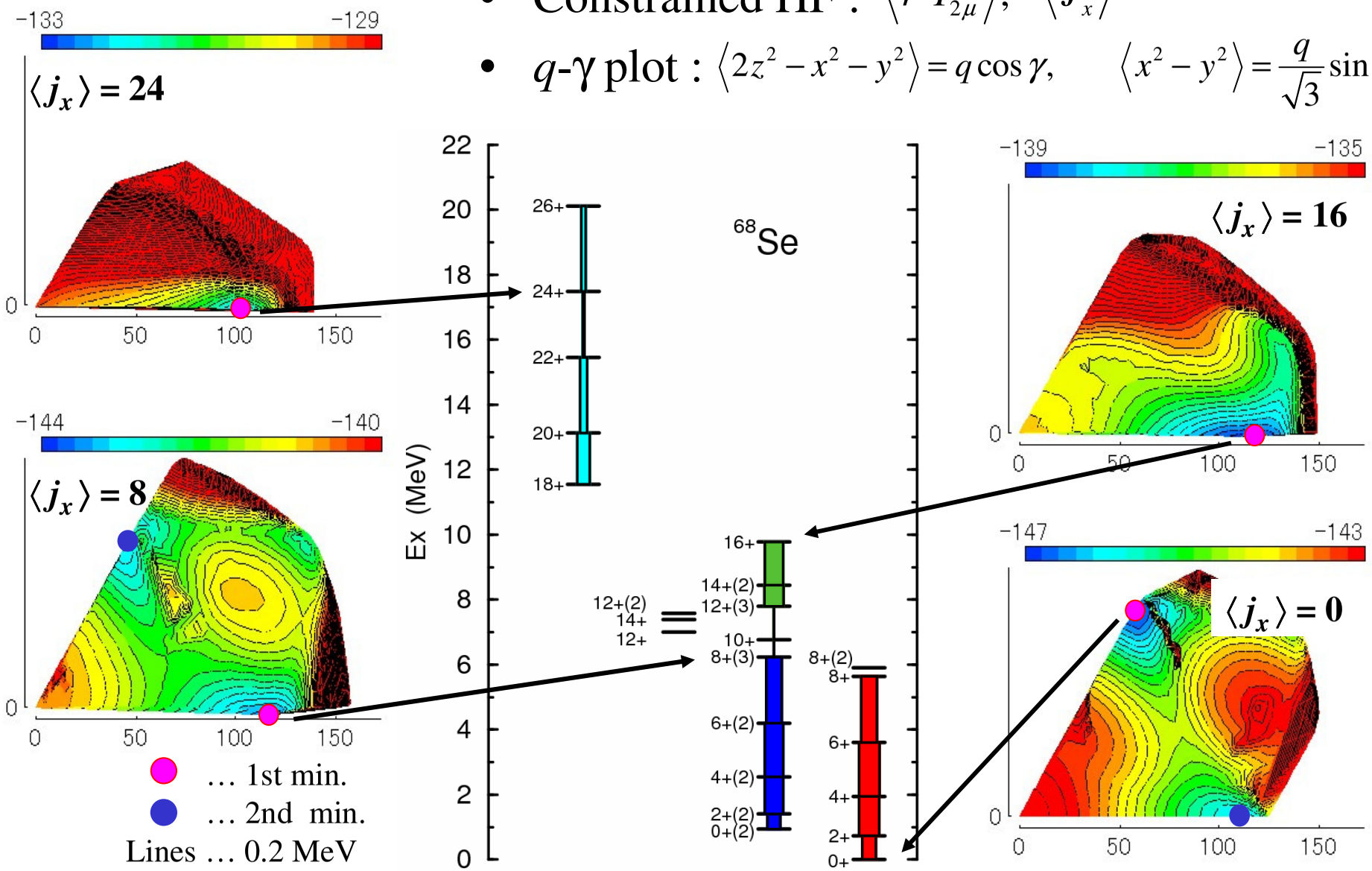
- Low-lying bands
  - Too small collectivity, especially for the prolate band
- Higher energy band
  - New crossing at higher spin



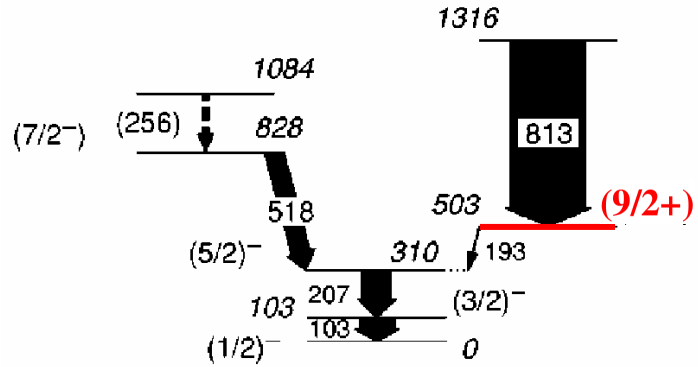
# Energy surface

- Constrained HF : $\langle r^2 Y_{2\mu} \rangle$, $\langle J_x \rangle$
- $q$-γ plot : $\langle 2z^2 - x^2 - y^2 \rangle = q\cos\gamma$, $\langle x^2 - y^2 \rangle = \frac{q}{\sqrt{3}}\sin\gamma$



# g9/2 in $^{55,57,59}Cr$

- Rotational bands in $^{55}Cr_{31}$ and $^{57}Cr_{33}$
  - prolate : [440]1/2+
  - $^{55}Cr_{31}$ at 2087 keV
  - $^{57}Cr_{33}$ at 1507 keV
- Isomer (96(20)μs) in $^{59}Cr_{35}$
  - oblate : [404]9/2+
  - $^{59}Cr_{35}$ at 503 keV

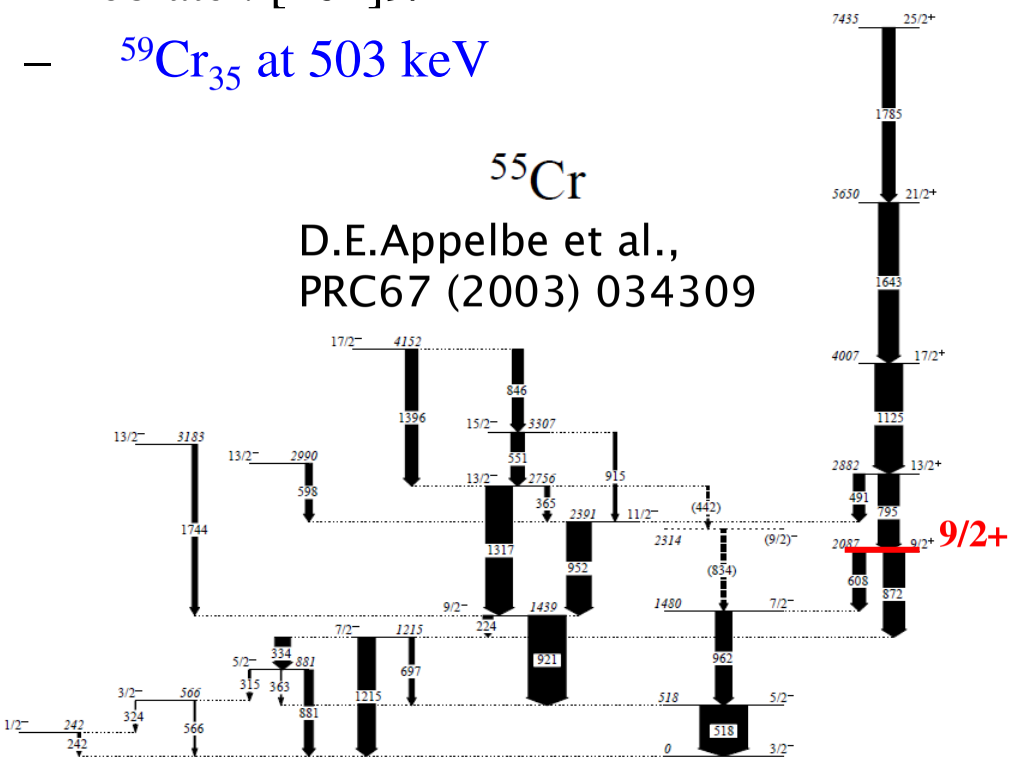



$^{59}Cr$

S.J.Freeman et al., PRC69 (2004) 064301

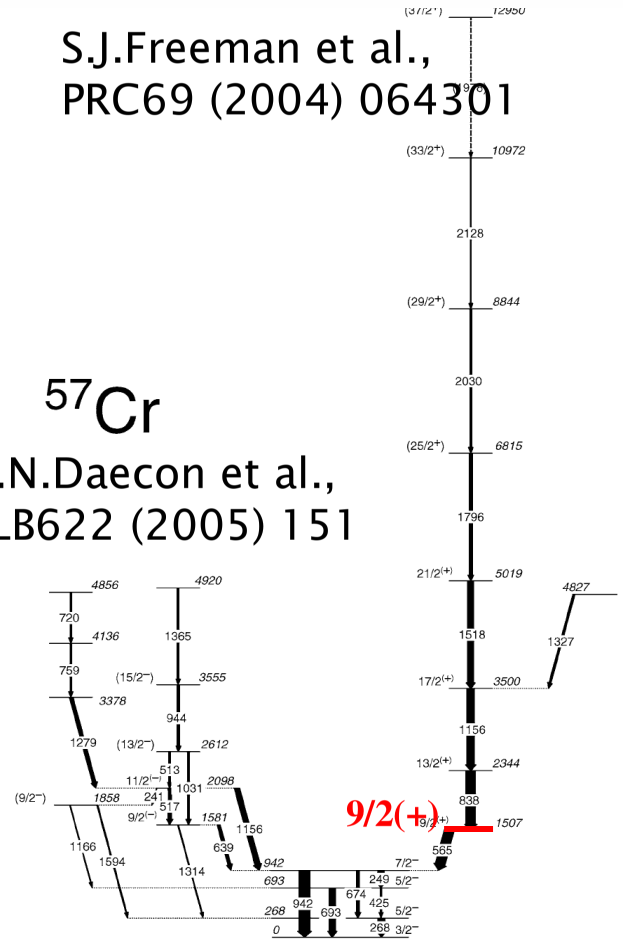
$^{55}Cr$

D.E.Appelbe et al., PRC67 (2003) 034309




$^{57}Cr$

A.N.Daecon et al., PLB622 (2005) 151



# pfg9-shell

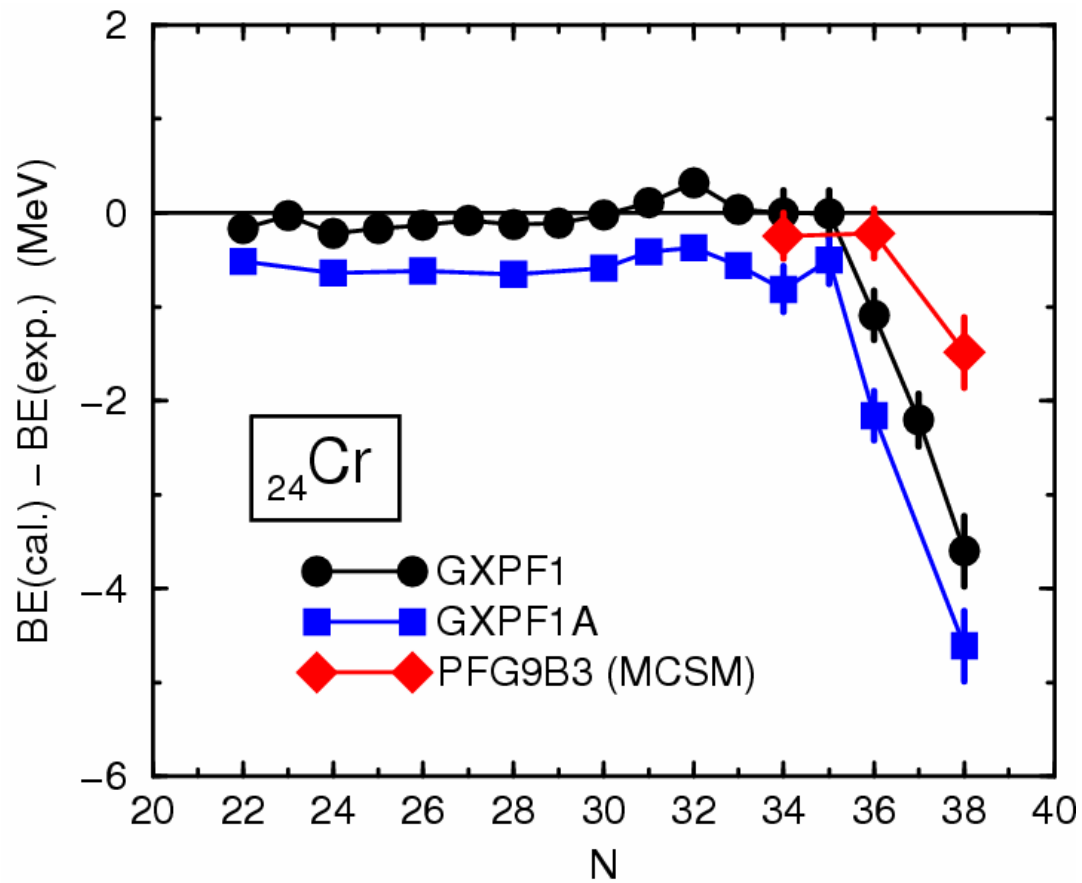
- (f7/2, p3/2, f5/2, p1/2, g9/2)
- 5 SPE + 325 TBME (assume isospin symmetry)
- TBME
  - GXPF1A (pf)
  - JUL32 (other f5pg9) M. Honma et al., J. Phys. Conf. Ser. 20 (2005) 7
    - unrenormalize f7/2 effects
    - mass dependence correction
  - G-pfg9 (f7-g9)
    - microscopic G-matrix int. by M. Hjorth-Jensen
- SPE
  - pf-part GXPF1A
  - ε(g9/2) fit ESPE of $^{57}$Ni to experimental 9/2+ at 3.7MeV

**PFG9B3**

- Shell model calculations
  - Huge dimension … MCSM, FDA
  - Center of mass motion … Lawson's prescription

# Binding energy

- N=36 … good agreement
- N=38 … underbound by ~1.5MeV



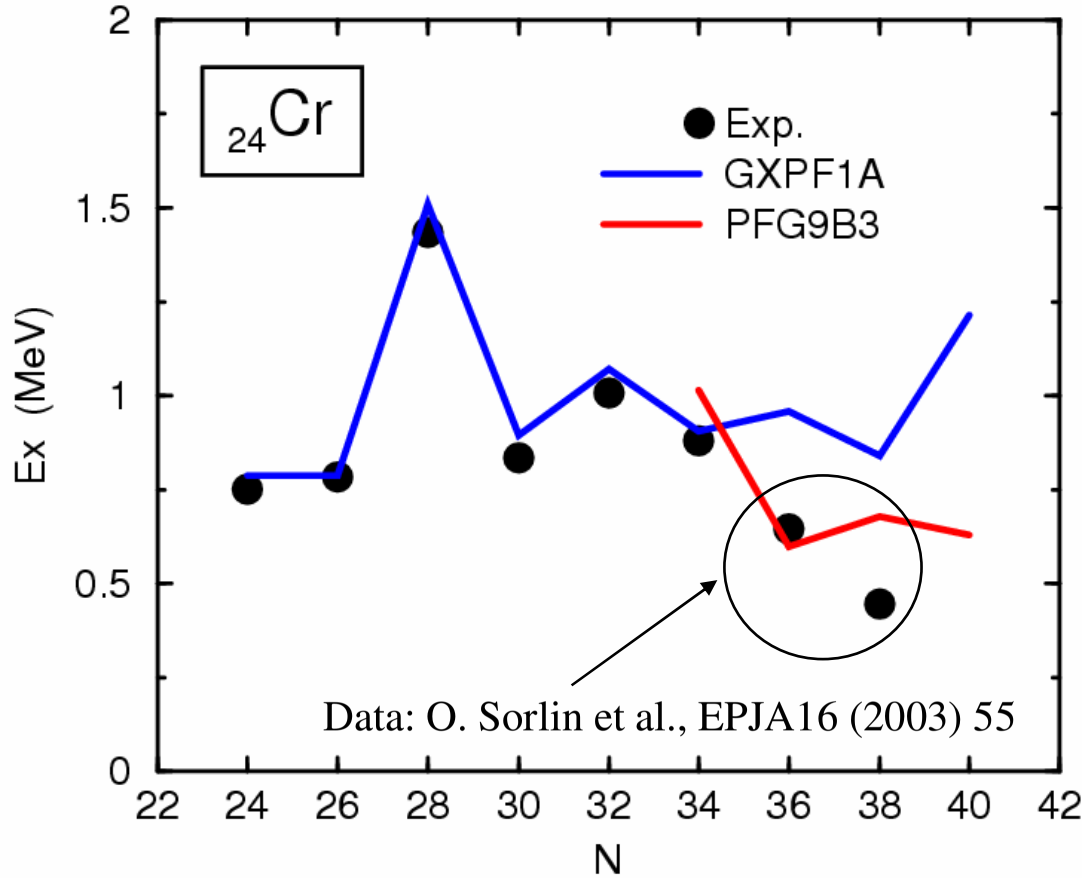
# Ex ($2^+_1$)

- N=36 … good
- N=38 … too high

⇓

d5/2 is needed,

at least for N≥38

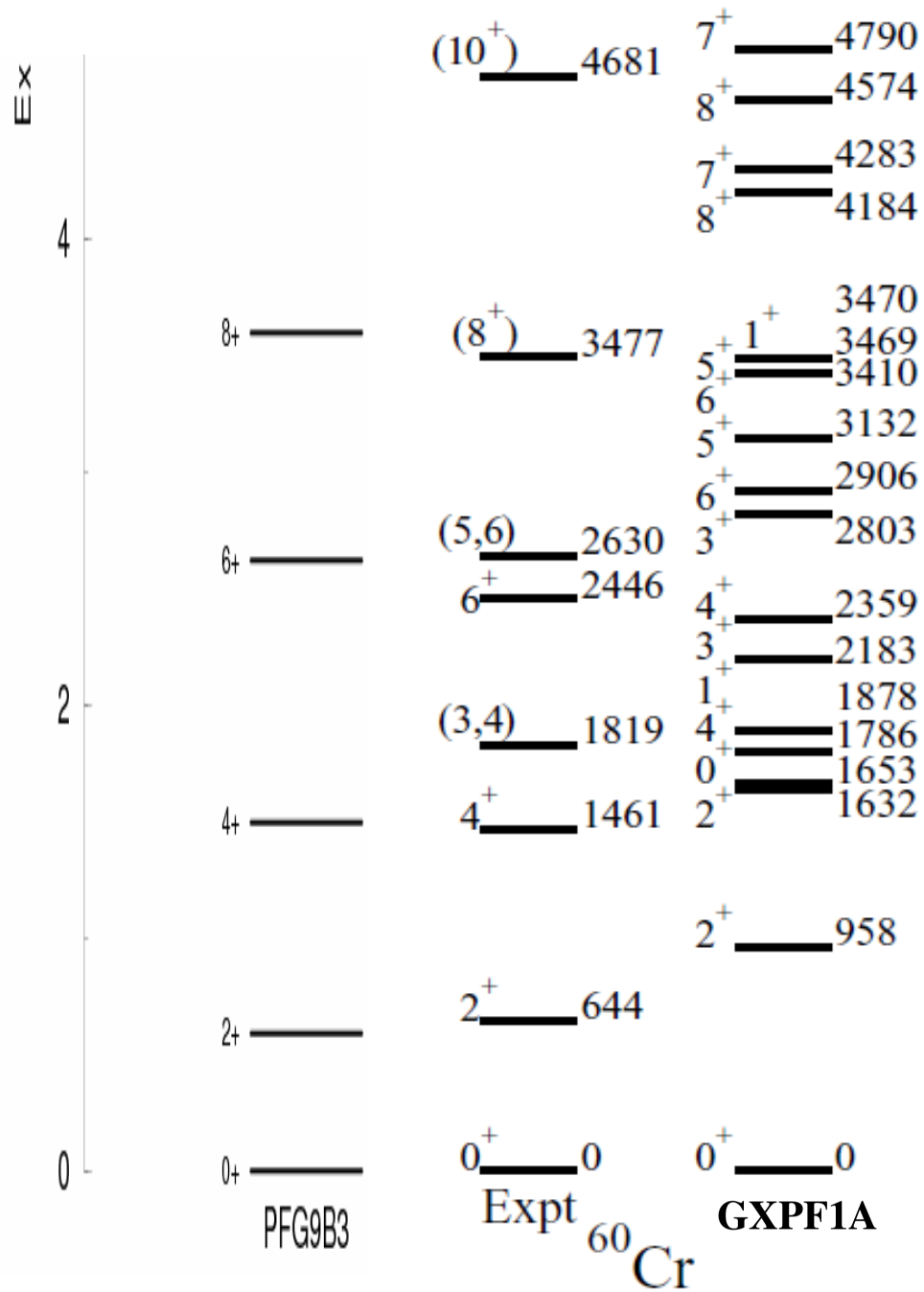



| N | $^{58}Cr_{34}$ | $^{60}Cr_{36}$ | $^{62}Cr_{38}$ | $^{64}Cr_{40}$ |
|---|---|---|---|---|
| Q-mom. ($efm^2$) | –14 | +25 | +17 | –19 |
| ⟨ n(g9/2) ⟩ | 0.3 | 2.0 | 2.5 | 3.8 |
| B(E2;↓) ($e^2fm^4$) ep=1.5,en=0.5 | 195 | 221 | 228 | 265 |
| ep=1.15,en=0.8 | 195 | 281 | 276 | 300 |

Exp. (preliminary, by N.Aoi @HAW05) 430(120) 470(70)

# $^{60}$Cr yrast

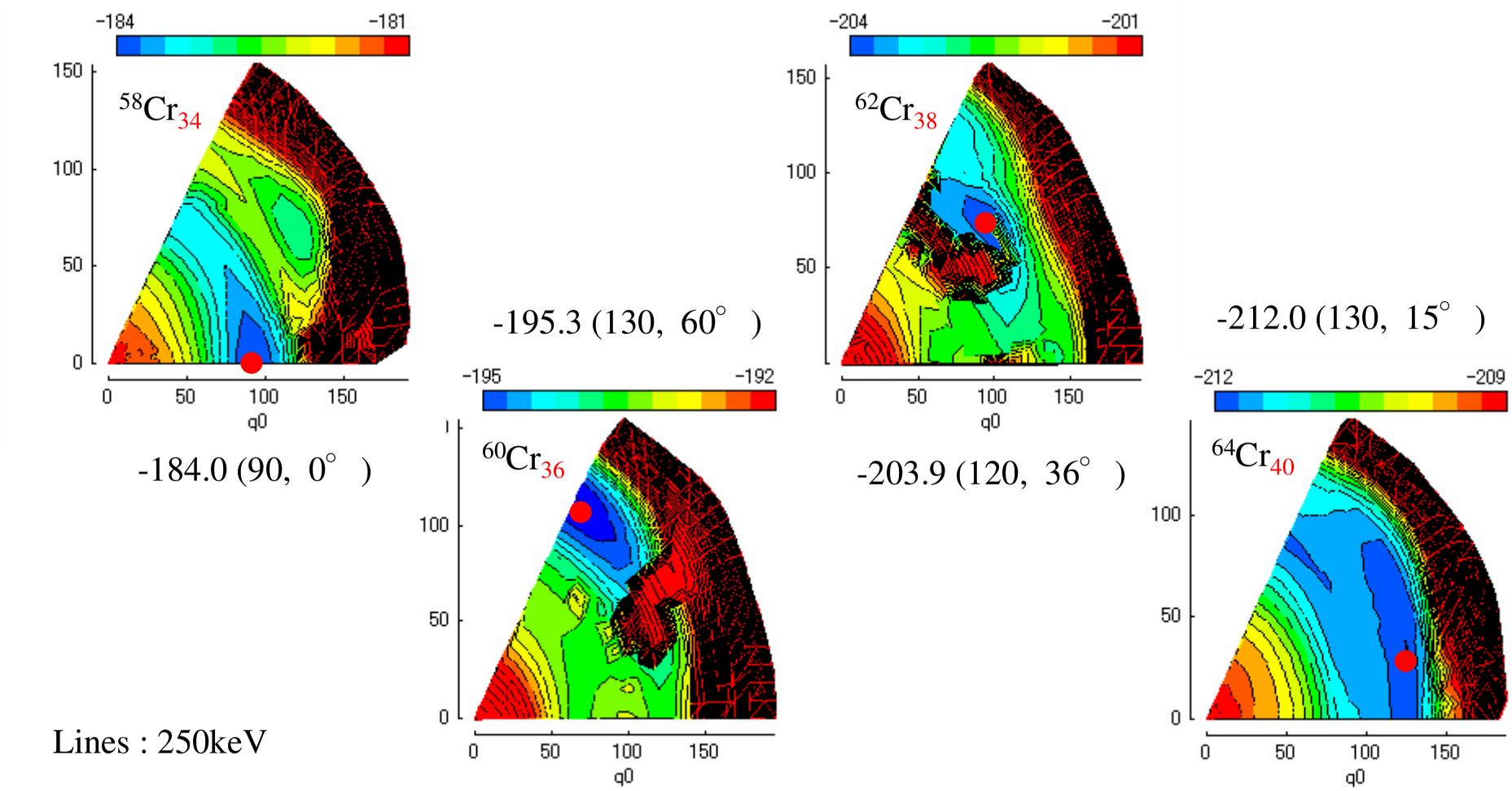
- 5-dim MCSM with PFG9B3 int.




Data: S. Zhu et al., PRC74 (2006) 064315

# Energy surface : pfg9

- Constrained HF : $\langle r^2 Y_{2\mu} \rangle$, $\langle J_x \rangle$
- $q$-$\gamma$ plot : $\langle 2z^2 - x^2 - y^2 \rangle = q\cos\gamma$, $\langle x^2 - y^2 \rangle = \frac{q}{\sqrt{3}}\sin\gamma$




Lines : 250keV

# Summary

- The microscopic effective interaction can be successful if suitable modifications are made, especially in the monopole part which govern the evolution of the shell structure.
- By using the GXPF1A interaction, the new shell closure at N=32 is reasonably described, and also the N=34 shell closure is predicted for Ca.
- New effective interaction JUL45 reasonably describes the shape coexistence in $^{68}$Se. However, insufficiency of the f5pg9-space appears in some collective properties, especially in the prolate side.
- Effect of the g9/2 orbit in neutron-rich Cr was studied by using a combined effective interaction for f5pg9-shell. Binding energy and the yrast energy data is consistent with the oblate $^{60}$Cr, while it is difficult to describe experimental B(E2) values for $^{60}$Cr and $^{62}$Cr.