Developments of effective interactions for shell-model calculations

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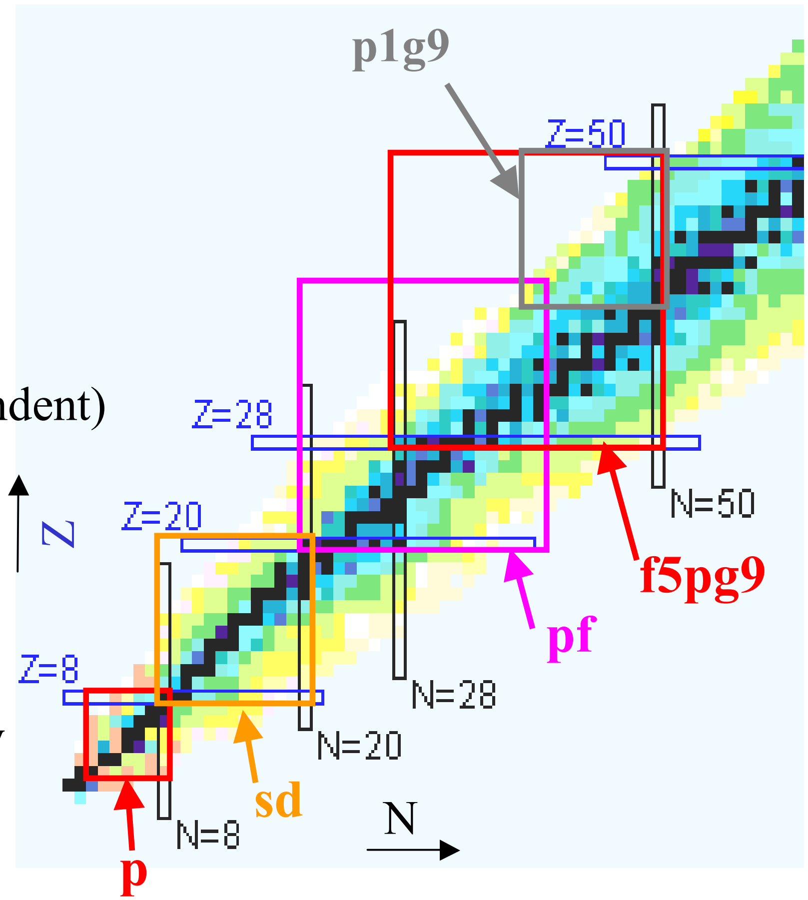
Outline

- Development of effective interaction
  - Direct fitting
  - Microscopic interaction
  - Modifications
- Current frontier … f5pg9-shell
  - JUN45 interaction
  - Application to 2ν-ββ-decay

Shell-model

- Model space
  - Inert core + valence-shell
- Effective interaction
  - Empirical
    - Fit to experimental data (model independent)
    - Potential model (model dependent)
  - Microscopic (realistic)
    - Derived from NN-interaction
  - Semi-empirical
    - Modify microscopic TBME empirically
- Hamiltonian
  - Single particle energy （SPE)
  - Two-body interaction （TBME)

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



p-shell

- ^{4}He core + (p3/2, p1/2) $2 \leq N, Z \leq 8$
- 15 TBME + 2 SPE
- CK-interaction
  - S. Cohen and D. Kurath, Nucl. Phys. 73 (1965) 1
  - Fit to experimental energy data
    - Binding energies relative to 4He core
    - Excitation energies
  - 2BME … General fit with 17 parameters
  - POT … Potential with 13 parameters
    - A=8-16… 35 data, rms error : 2BME 400 keV, POT 430 keV
    - A=6-16… 44 data, rms error : 2BME 570 keV, POT 650 keV
  - Tests: Magnetic moments, M1 transitions, GT beta-decay

p1g9-shell

- ^{88}Sr (Z=38, N=50) core + (p1/2, g9/2) $38 \leq Z, N \leq 50$
  - Proton particle & neutron hole
- 18 TBME + 2 SPE(π) + 2 SPE(ν)
- SLG, SLGT
  - For protons … fit to N=50 (45 data) D.H.Gloekner, F.J.D.Serduke, NPA220 (1974) 477
  - For pn … fit to N=49 (63 data) F.J.D.Serduke, R.D.Lawson, D.H.Gloekner, NPA256 (1976) 45
  - Isospin formalism … H.Herndl and B.A.Brown, NPA627 (1997) 35
- GF
  - R.Gross, A.Frenkel, NPA267 (1976) 85
  - 33 parameters : 4(SPE) + 9(pp) + 20(pn)
  - Ft to 95 data of N=50,49,48(^{86}Sr)
- JS
  - I.P.Johnstone and L.D.Skouras, Eur.Phys.J.A11 (2001) 125
  - Fit to 477 data of $38 \leq Z \leq 50$, $47 \leq N \leq 50$ with rms error 128 keV

Microscopic effective interaction

- Derived from NN-potential
  - Renormalized G-matrix
- Examples (pf-shell)
  - KB … T.T.S.Kuo and G.E.Brown Nucl. Phys. A114 (1968) 241
    - Hamada-Johnston potential
    - Renormalization due to core-polalization
  - G … M. Hjorth-Jensen, et al., Phys. Repts. 261 (1995) 125
    - Bonn-C potential
    - 3rd order Q-box + folded diagram
- Reasonable near the closed shell
- Problems for cases with many valence nucleon

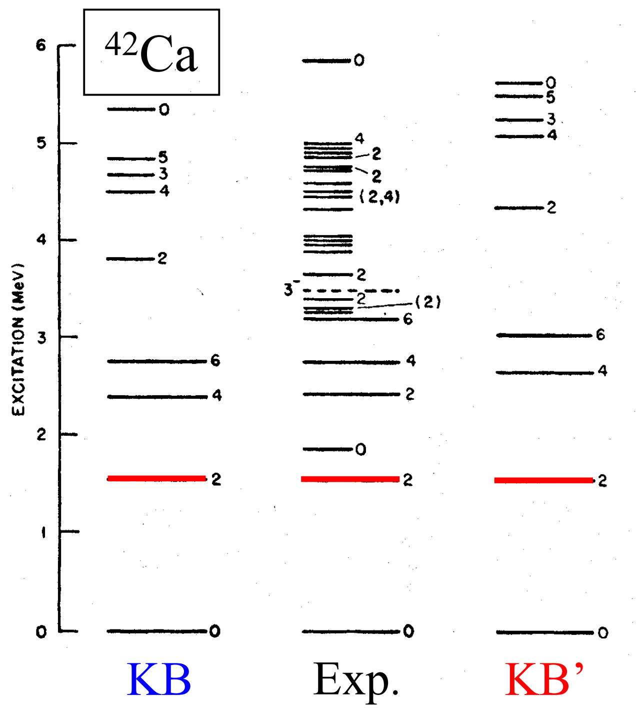
  ⇨ Empirical modification is necessary for practical use
    - Fitting
    - Monopole corrections

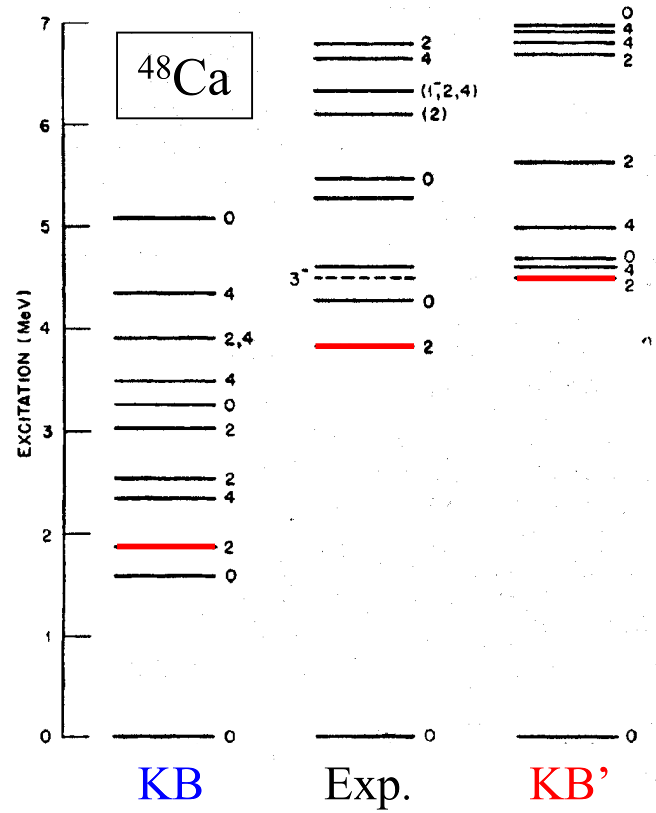
Problems in microscopic interaction

J. B. McGrory et al., PRC2 (1970) 186

- Example: KB
  - ^{42}Ca … OK, but ^{48}Ca … too small gap
- Modification … KB'

$$\left\langle f_{7/2}^2 J \middle| V \middle| f_{7/2}^2 J \right\rangle \quad \Rightarrow \quad -300\text{keV for } J = 0, 2$$
$$\left\langle f_{7/2} p_{3/2} J \middle| V \middle| f_{7/2} p_{3/2} J \right\rangle \quad \Rightarrow \quad +300\text{keV}$$





Model independent fit

Shell-model Hamiltonian

$$H = \sum_a \varepsilon_a n_a + \sum_{a\le b, c\le d, JT} V(abcd;JT) A^{+}_{JT}(ab) A_{JT}(cd) = \sum_{l=1}^{p} x_l O_l \quad (l = 1, 2, \dots, p)$$

p: number of parameters

1. Starting Hamiltonian : $\mathbf{x}=(x_1, x_2, \dots, x_p)$
2. Shell-model calculation ⇒ eigenvalues λ^k, eigenstates $|\psi^k\rangle$

$$\lambda^k = \Sigma_l x_l \langle \psi^k | O_l | \psi^k \rangle = \Sigma_l x_l \beta_l^k \quad (k = 1, 2, \dots, n) \quad n: \text{ number of data}$$

3. Minimize $\chi^2 = \Sigma_{k=1}^n (E_{\exp}^k - \lambda^k)^2$

$$\frac{\partial \chi^2}{\partial x_m} = 0 \quad \rightarrow \quad \Sigma_{k=1}^n (E_{\exp}^k - \lambda^k) \frac{\partial(\Sigma_l x_l \beta_l^k)}{\partial x_m} = 0$$

Assumption : dependence of β_l^k on x_m is weak ($\partial \beta_l^k / \partial x_m \approx 0$)

$$\rightarrow \quad \Sigma_{k=1}^n (E_{\exp}^k - \Sigma_l x_l \beta_l^k) \beta_m^k = 0 \quad \rightarrow \quad \Sigma_l \gamma_{ml} x_l = \xi_m \quad \begin{pmatrix} \Sigma_{k=1}^n E_{\exp}^k \beta_m^k \equiv \xi_m \\ \Sigma_{k=1}^n \beta_l^k \beta_m^k \equiv \gamma_{lm} \end{pmatrix}$$

$$(\gamma_{lm}) \equiv G, \quad (\xi_m) \equiv \xi \quad \rightarrow \quad G\mathbf{x} = \xi \quad \rightarrow \quad \mathbf{x}' = G^{-1}\xi$$

x' : New interaction

4. Repeat 2~3 until convergence

Linear combination (LC) method

- Linear equation for determining new parameters $\mathbf{x}$

  $G\mathbf{x} = \xi \ldots(1)$ G : real, symmetric $p \times p$ matrix
- Diagonalize G by orthogonal matrix A

  $D = \mathrm{diag}(1/d_1, 1/d_2, \ldots, 1/d_p) = AGA^{\mathrm{T}}$

  $$(1) \Leftrightarrow \underbrace{(AGA^{\mathrm{T}})}_{D} \underbrace{(A\mathbf{x})}_{\mathbf{y}} = \underbrace{(A\,\xi)}_{\mathbf{c}}$$

  $$\Leftrightarrow D\mathbf{y} = \mathbf{c}$$

  $\therefore \mathbf{y} = D^{-1}\mathbf{c}$ i.e. $y_i = d_i c_i$: independent LC

For large d_i, small variation of the "data" c_i gives large change of $y_i \Rightarrow$ not well-determined

- Procedure:

  $\mathbf{x}^{\mathrm{s}}$: starting Hamiltonian (ex. G-matrix)

  $\rightarrow \lambda^k, \beta_l^k \rightarrow G, \xi \rightarrow D, A, \mathbf{c}$

  $\rightarrow \mathbf{y}^{\mathrm{S}} \equiv A\mathbf{x}^{\mathrm{S}}$: starting LC

  new LC: $\mathbf{y}' = \begin{cases} \mathbf{y} & (d_i \le \delta) \\ \mathbf{y}^{\mathrm{S}} & (d_i > \delta) \end{cases}$ δ : criterion

Only well-determined LC's are modified

Remaining LC's are taken from original Hamiltonian

sd-sell

- ^{16}O core + (d5/2, s1/2, d3/2) $8 \leq Z, N \leq 20$
- 63 TBME + 3 SPE
- W-interaction (USD)
  - B.H.Wildenthal, Prog.Part.Nucl.Phys.11 (1984) 5
  - Fit to 447 experimental energy data (j-dim. Less than 1000)
  - Start from renormalized G-matrix (KB)

    T.T.S.Kuo, NPA103 (1967) 71
  - Vary 47 best-determined linear combinations of parameters
  - Mass dependence $(A/18)^{-0.3}$
  - Rms error 185 keV
  - Applications:
    - M1/E2 transitions and moments … effective operators
    - GT quenching $(0.77)^2=0.6$
    - Spectroscopic factors
    - Masses, separation energies, etc.

pf-sell

- ^{40}Ca core + (f7/2, p3/2, f5/2, p1/2) $20 \leq Z, N \leq 40$
- 195 TBME + 4 SPE
- KB3-interaction
  - A. Poves and A. P. Zuker, Phys. Repts. 70 (1981) 235
  - Modify renormalized G-matrix (KB)
    T.T.S.Kuo and G.E.Brown Nucl. Phys. A114 (1968) 241
  - Monopole corrections
  - Excellent for A≦52
  - Problems in cross-shell excitation over *N*, *Z*=28 shell gap
  - Latest version : KB3G …A.Poves et al., NPA694 (2001) 157
- FPD6-interaction
  - W.A.Richter et al., NPA523 (1991) 325
  - Empirical potential (6 parameters + 4 SPE)
  - Parameters are fitted to 61 energy data of A=41~49 nuclei
  - Good description of ^{56}Ni, but too low f7/2 orbit

Global fit for pf-shell

- GXPF1 interaction

  M. Honma et al., PRC65 (2002) 061301(R); PRC69 (2004) 034335

  - Modify microscopic G interaction

    M. Hjorth-Jensen, et al., Phys. Repts. 261 (1995) 125

    - Bonn-C potential
    - 3rd order Q-box + folded diagram
  - Vary 70 well-determined LC's of 195 TBME and 4 SPE
  - Fit to 699 experimental energy data of 87 nuclei
  - Mass dependence : $A^{-0.3}$
  - Data selection to avoid intruder: $47 \leq A, \quad Z \leq 32$
  - Energy evaluation by FDA* $\Rightarrow$ 168keV rms error

    $\Uparrow$

    Few-dimensional-bases approximation with empirical corrections

    QMCD basis dimension ~ 3

- Successful description of $(f_{7/2})^{16}$ core excitations
  - ^{56}Ni, ^{55}Co, ^{57}Ni … key nuclei

Monopole properties

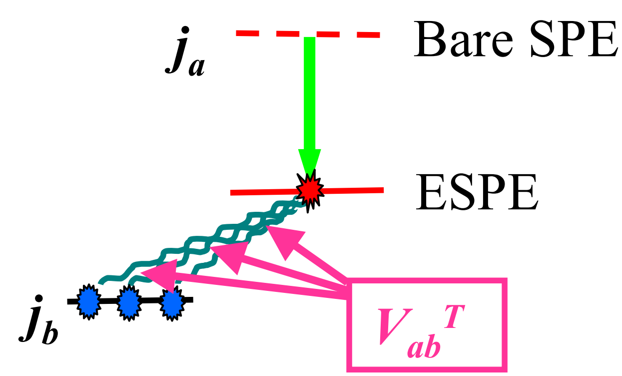
- $H = H_m$ (monopole) + H_M (multipole)
- Monopole part
  - Average energy of a given configuration → B.E., shell gap

$$H_m = \sum_a \varepsilon_a n_a + \sum_{a \le b} \frac{1}{1+\delta_{ab}} \left[\frac{3V_{ab}^1 + V_{ab}^0}{4} n_a (n_a - \delta_{ab}) + (V_{ab}^1 - V_{ab}^0)(T_a \cdot T_b - \frac{3}{4} n_a \delta_{ab}) \right]$$

n_a, T_a … number, isospin operators of orbit a

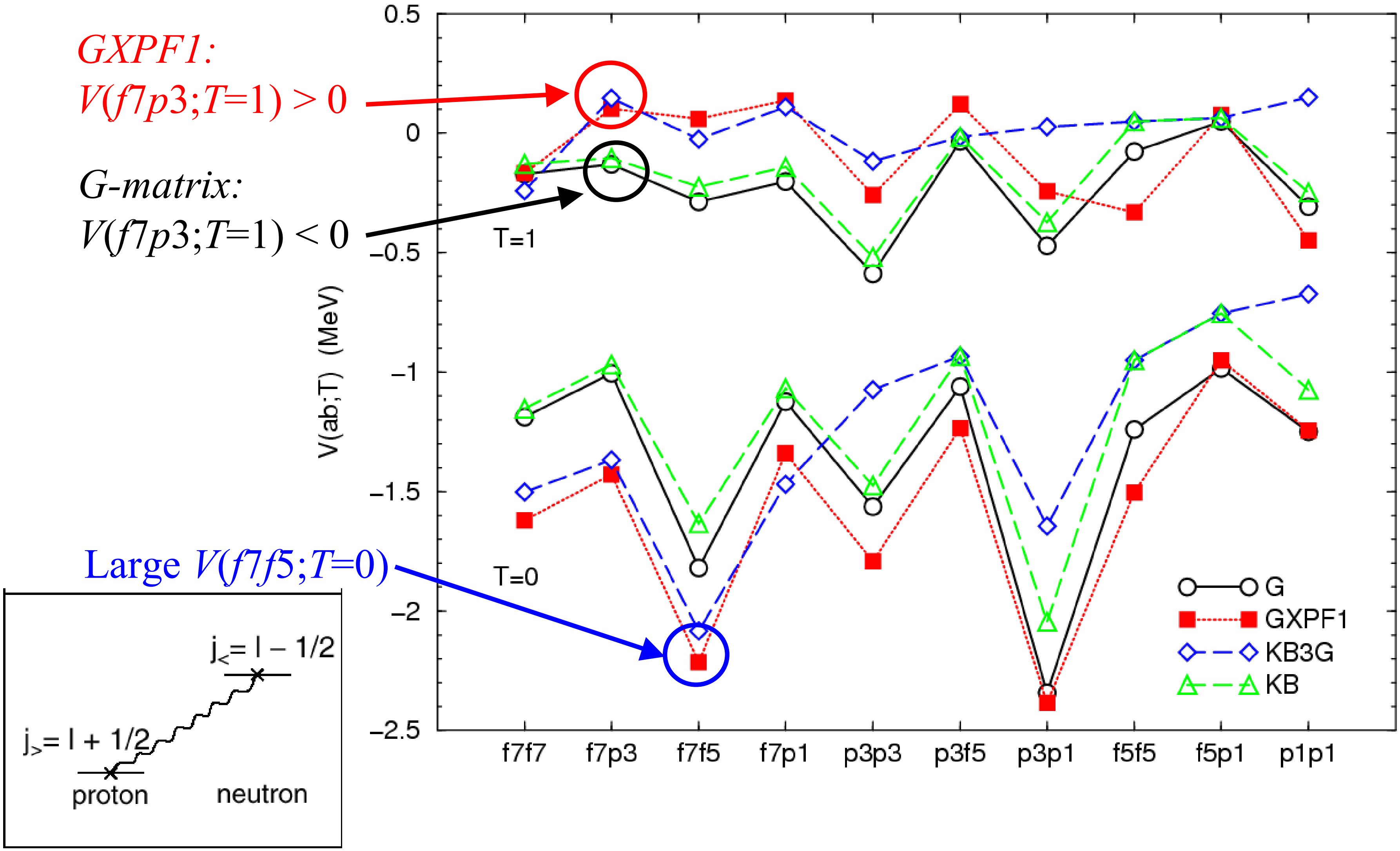
  - Centroid

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



- Effective single-particle energy (ESPE)
  - Assume the lowest filling configuration
  - Evaluate energy difference by H_m due to
  - Bare SPE + averaged effects of two-body interaction

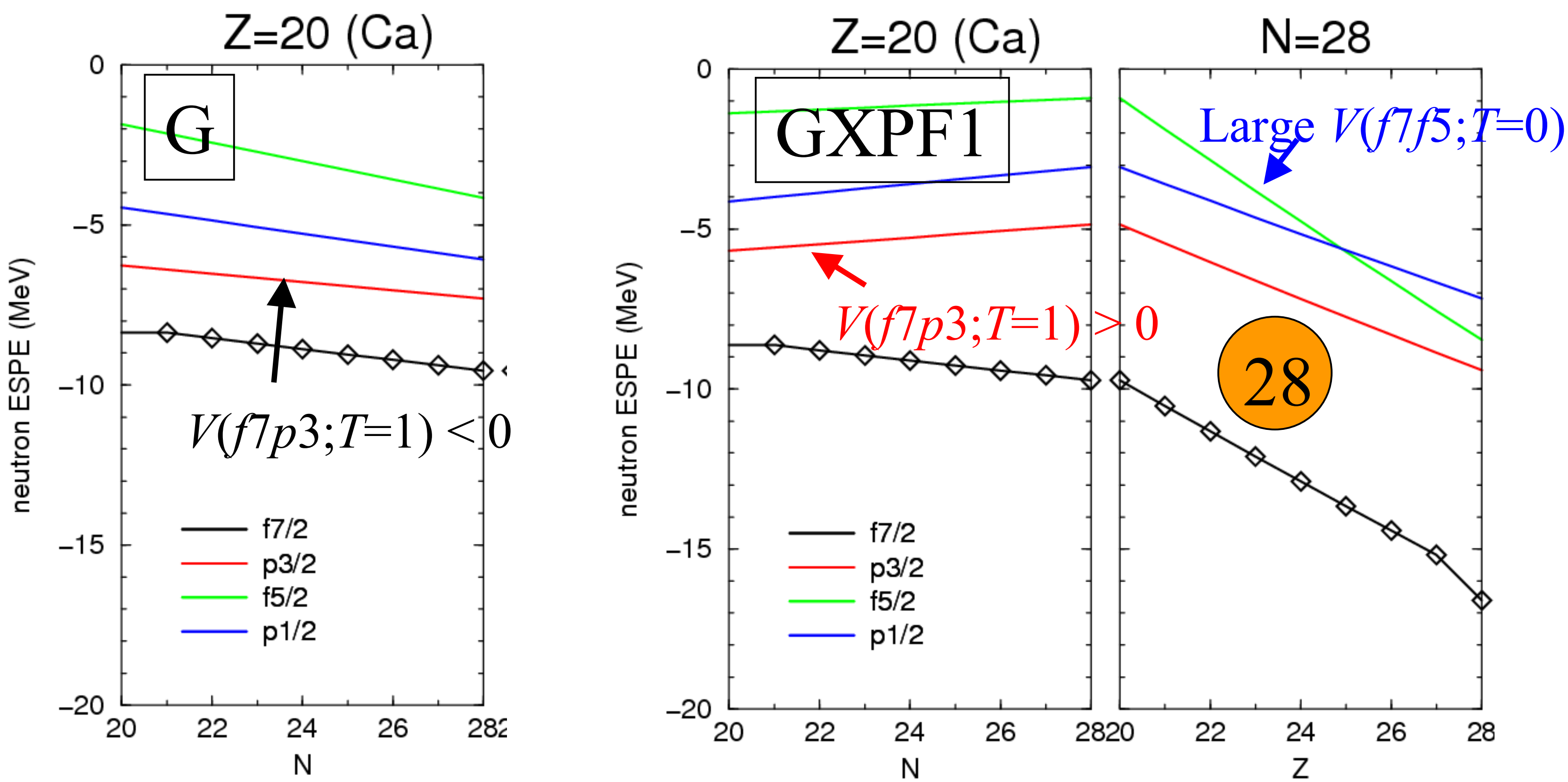
Monopole centroids



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)



How to fix monopole ?

- Core + 1 particle
  - Example: pf-shell (40Ca core)

    ESPE(^{48}Ca; νf7/2) = ε(f7/2) + 7*V*(f7f7;T=1)

    ESPE(^{48}Ca; νp3/2) = ε(p3/2) + 8*V*(f7p3;T=1)

    ESPE(^{48}Sc; πp3/2) = ε(p3/2) + (7/2)*V*(f7p3;T=1)+(9/2)*V*(f7p3;T=0)

    … etc.

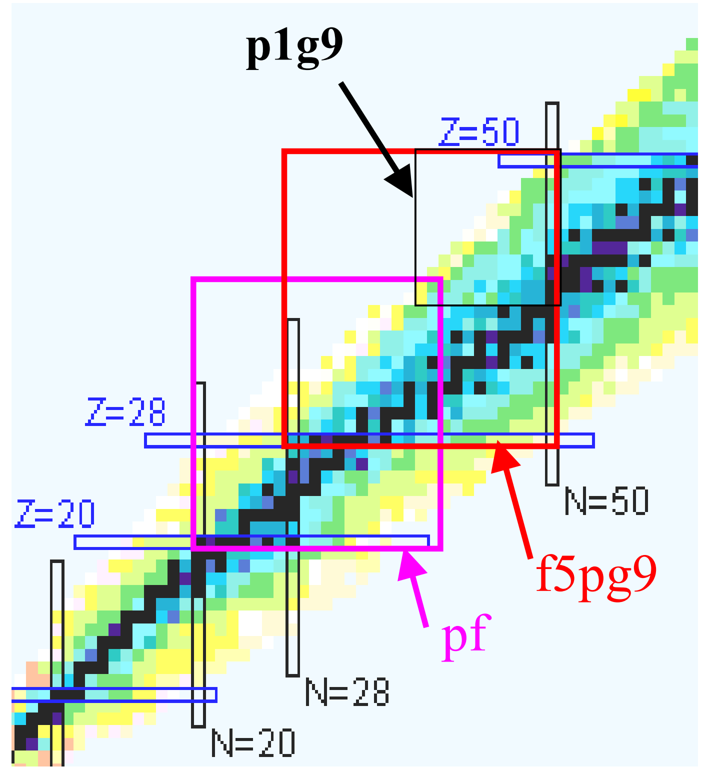
		KB3			KB			Exp.
r	ε	*V*(fr;1)	ESPE	rel.	*V*(fr;1)	ESPE	rel.	Ex / Δ
νf5/2	6.5	0.075	7.10	3.53	–0.225	4.70	3.53	3.59
νp1/2	4.0	0.159	5.27	1.70	–0.141	2.87	1.70	2.02
νp3/2	2.0	0.196	3.57	0	–0.104	1.17	0	0
νf7/2	0.0	–0.241	–1.69	–5.26	–0.128	–0.90	–2.07	–4.81

^{41}Ca

$$\Delta(^{48}\mathrm{Ca}) = 2BE(^{48}\mathrm{Ca}) - BE(^{49}\mathrm{Ca}) - BE(^{47}\mathrm{Ca})$$

f5pg9-shell

- f5pg9-shell
  - ^{56}Ni inert core
  - Valence orbits : $p_{3/2}$, $f_{5/2}$, $p_{1/2}$, $g_{9/2}$
  - No spurious center-of-mass motion
- Interests
  - Neutron-rich
  - Isomer
  - Shape-coexistence
  - Astorophysics
- Recent shell-model studies
  - S3V… J.Sinatkas, et al., J. Phys. G18, 1377; 1401 (1992)
    - Second order correction to the Sussex matrix elements
    - N=50,49,48 with severe truncation (weak coupling assumption)
  - Lisetskiy… A.F.Lisetskiy et al., PRC70, 044314 (2004)
    - Modify G-matrix interaction by least squares fit
    - T=1 part for proton and neutron (Ni isotopes and N=50 isotones)



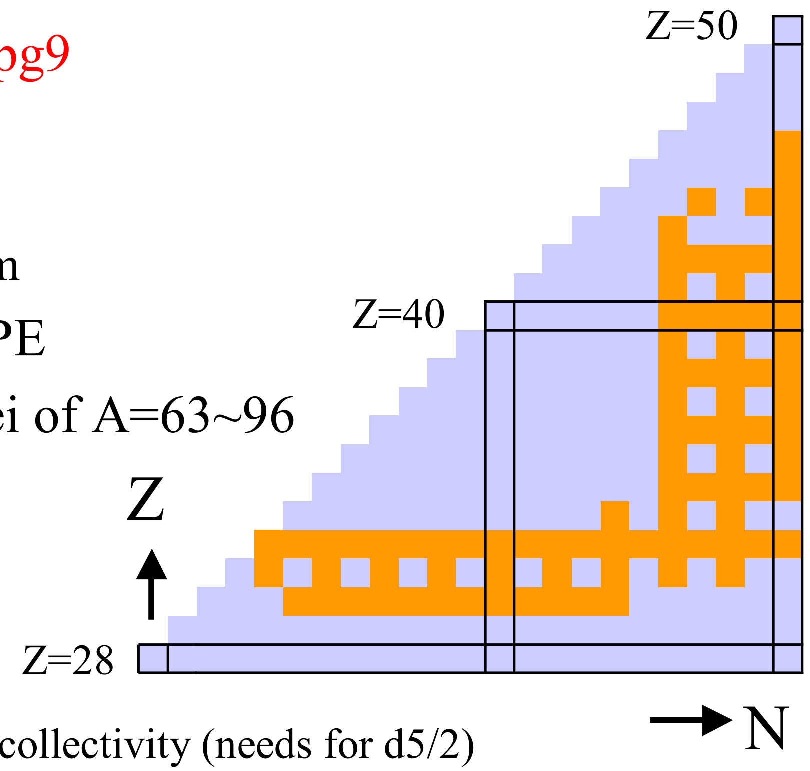
Global fit for f5pg9-shell

- 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

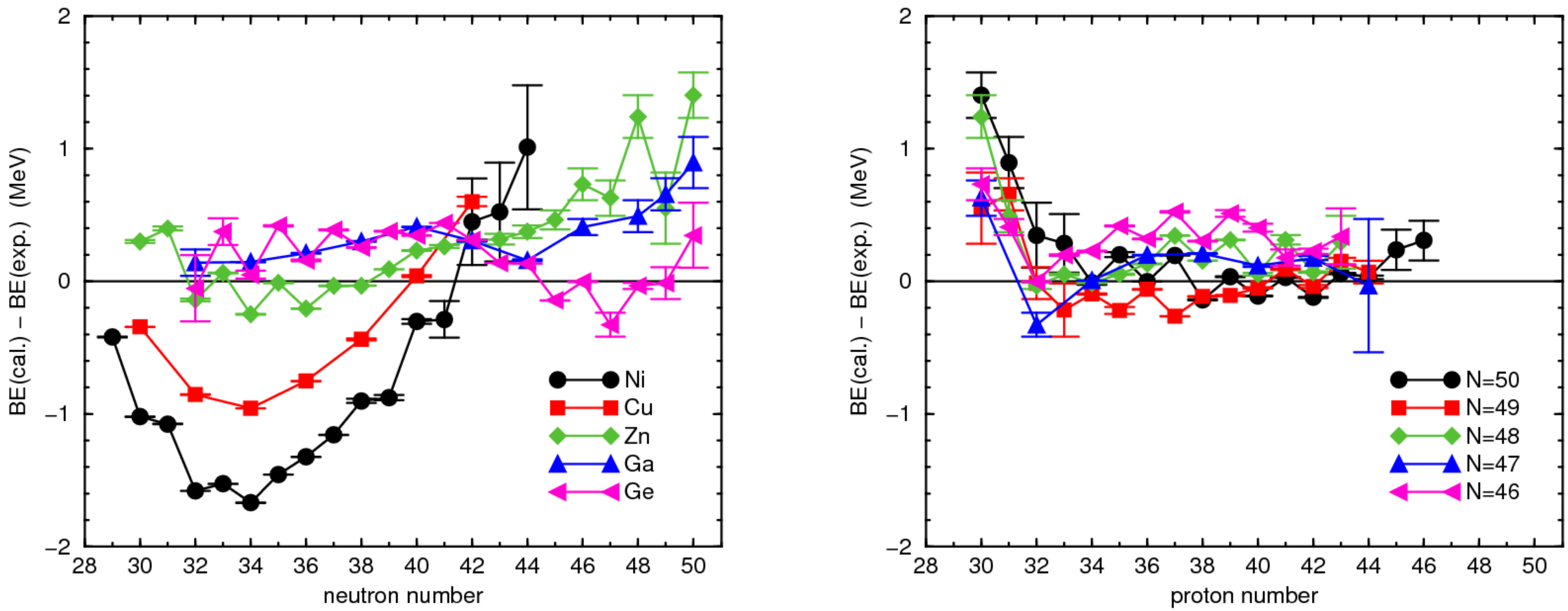


Binding energy

- Empirical Coulomb energy   B.J.Cole, PRC59(1999)726

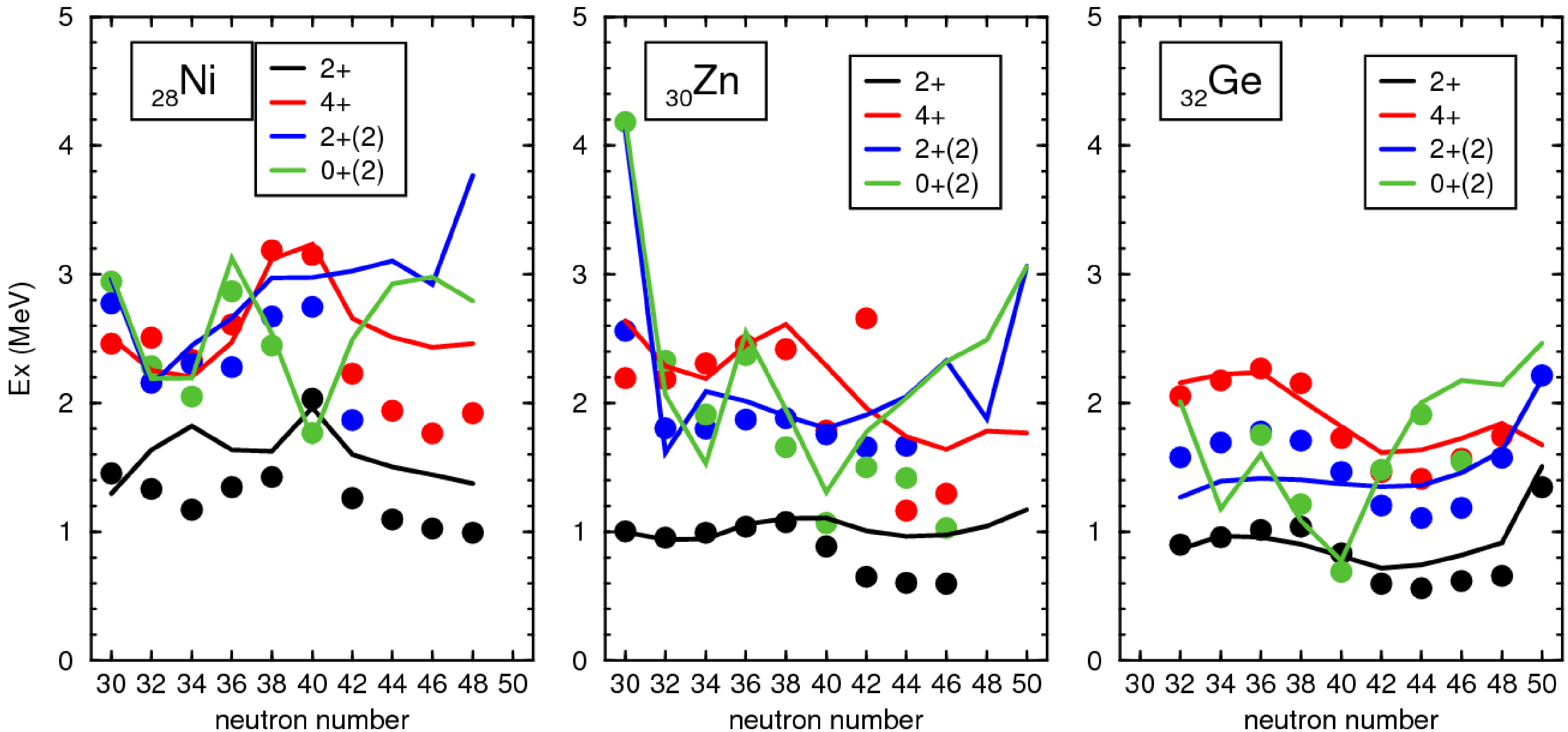
$$E_C(\pi,\nu) = \varepsilon_C \pi + V_C \frac{\pi(\pi-1)}{2} + b_C[\frac{1}{2}\pi] - \Delta_{\pi\nu}\pi\nu \qquad \pi,\nu \cdots \text{valence nucleon \#}$$

- f7/2 effects ? … due to the weight on Ge in the fit
  - Underbinding in Ni, Cu with N<40
  - Overbinding in neutron-rich Ni, Cu, Zn, Ga



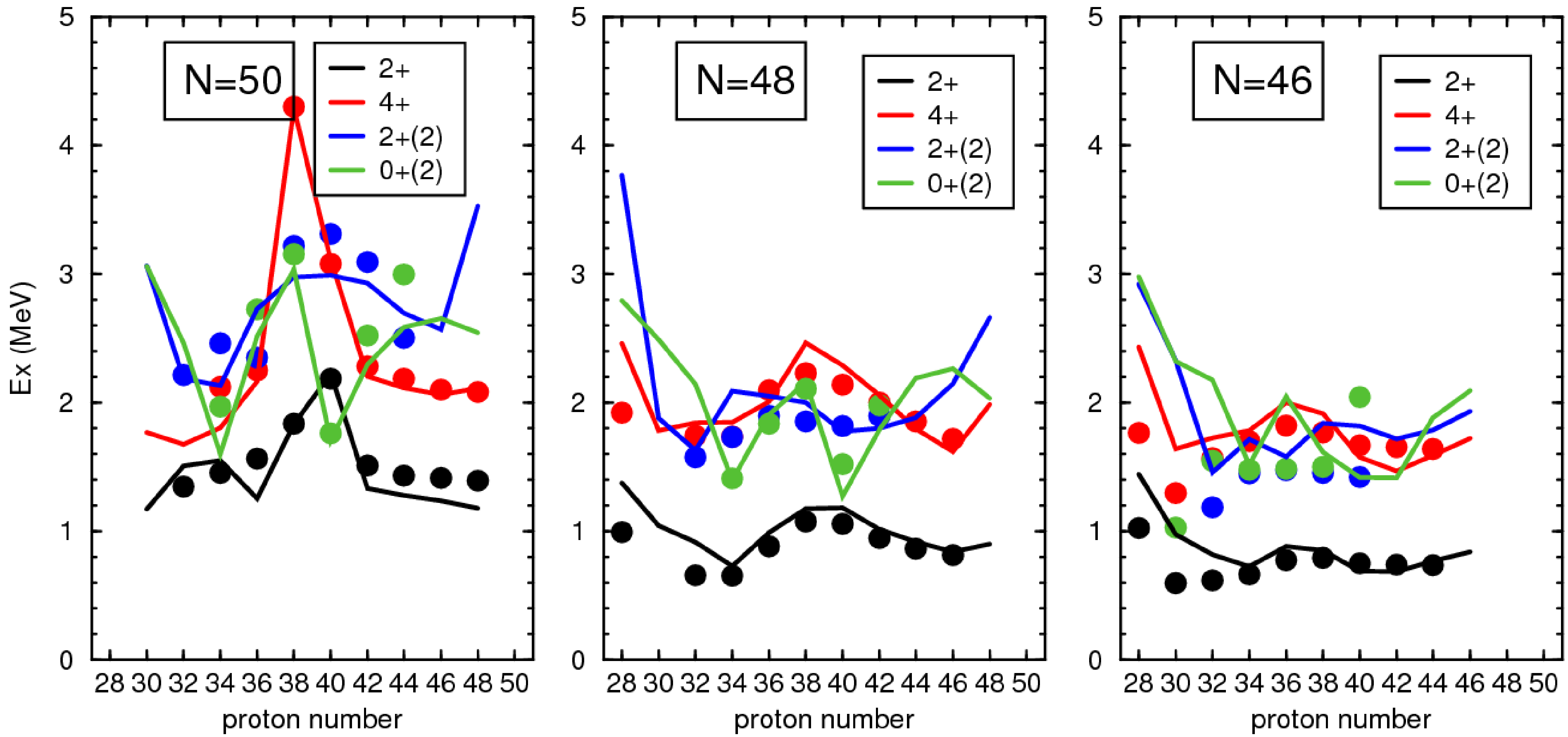
Low-lying states (Z=28,30,32)

- General behavior is OK for N<40
- Relatively large deviations for N>40 … f7/2 effect ?



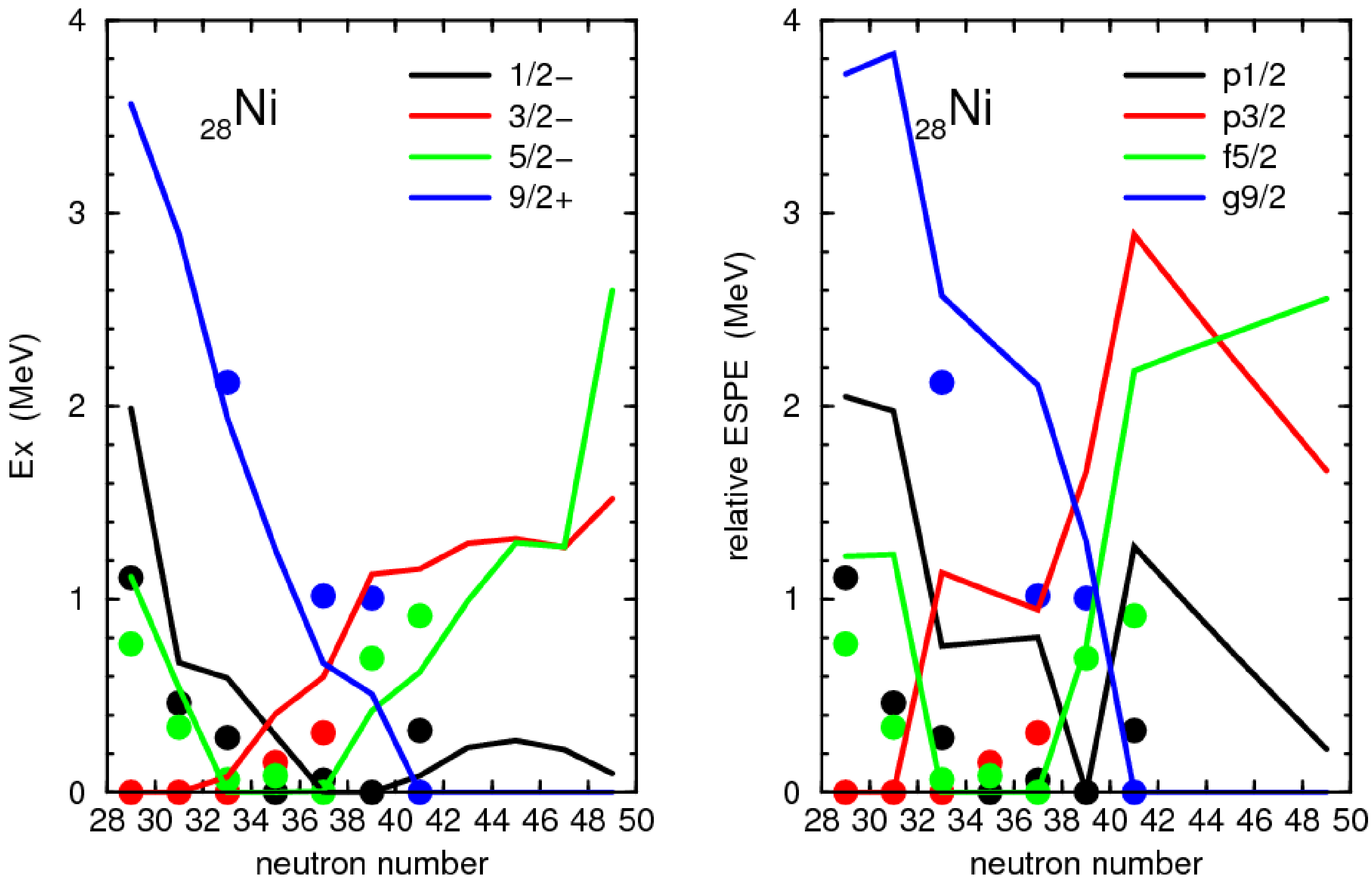
Low-lying states (N=46,48,50)

- Successful for almost all yrast states



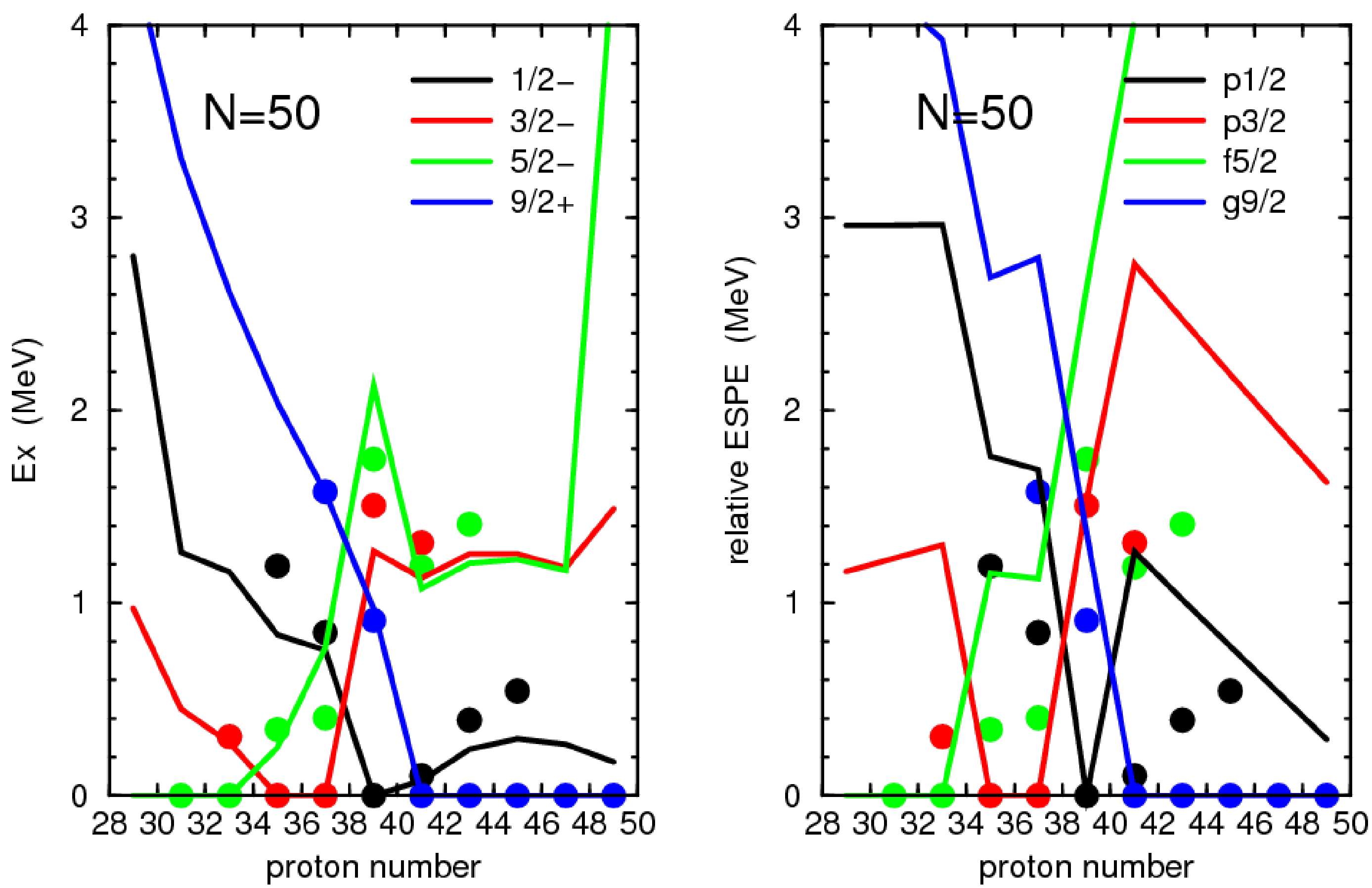
Odd-N (Z=28,30,32)

- ESPE for neutron (T=1 effects)



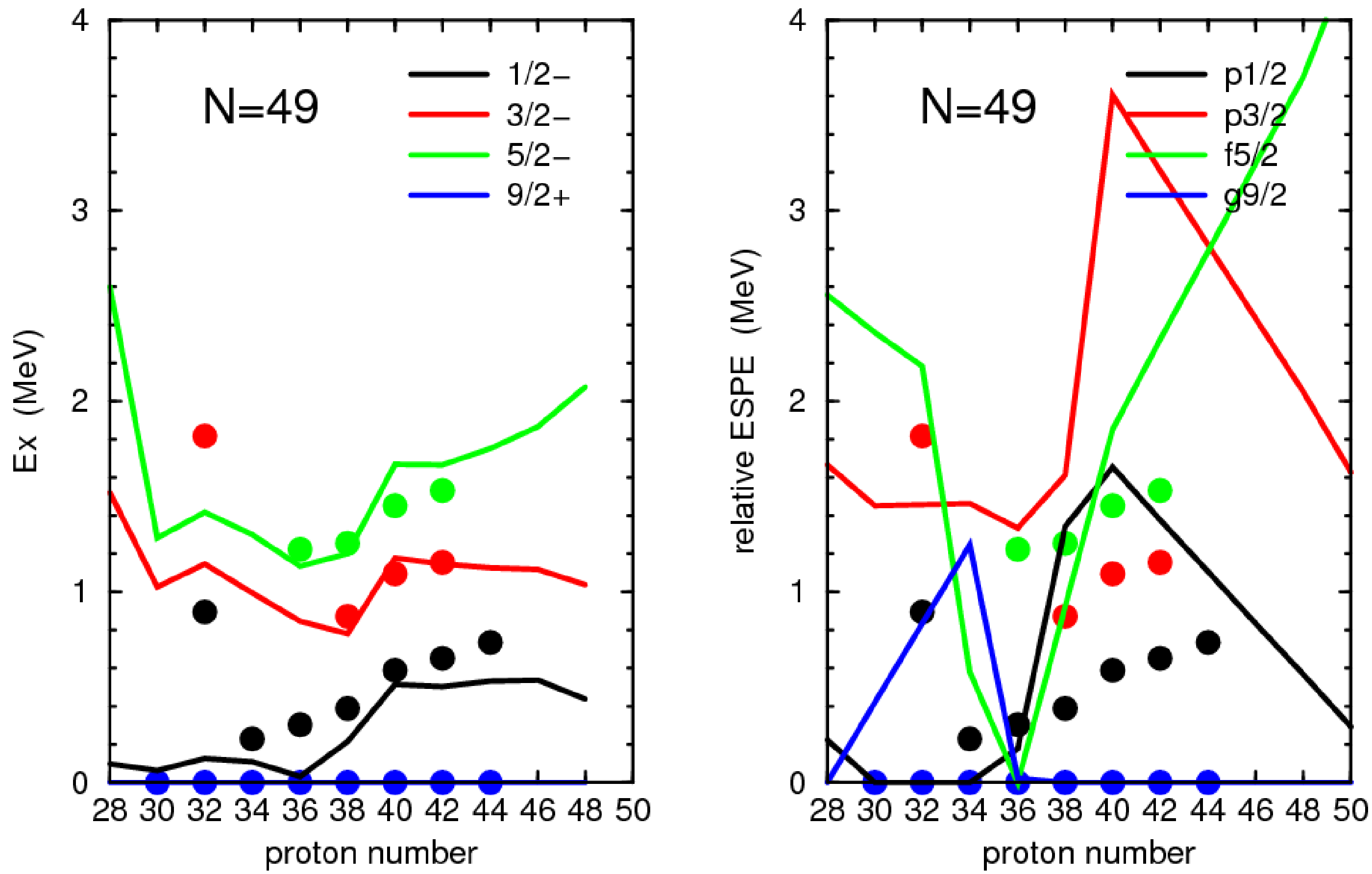
Odd-Z (N=46,48,50)

- ESPE for protons (T=1 effects)



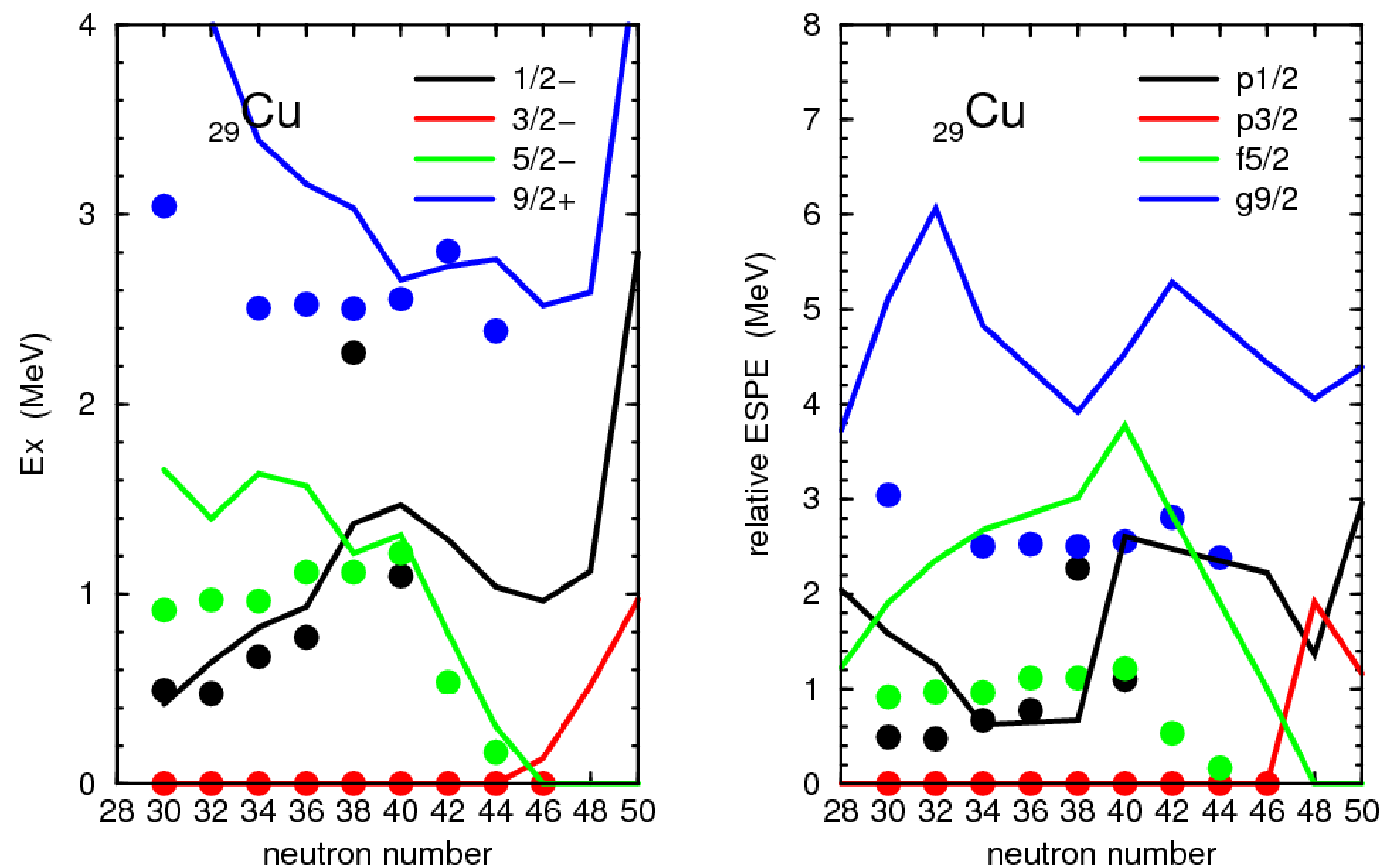
Odd-N (N=45,47,49)

- ESPE for neutrons (T=1 & T=0 effects)



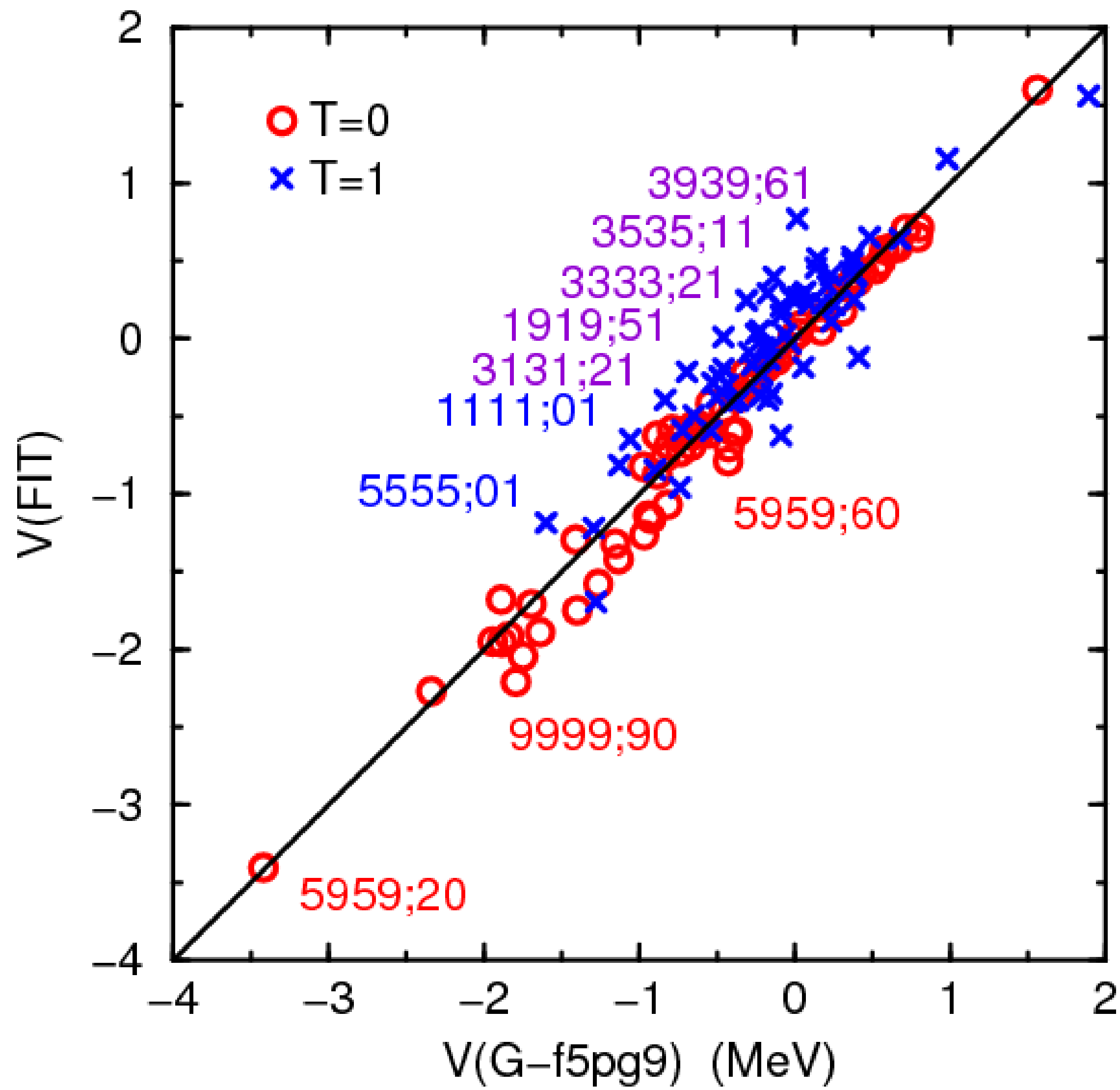
Odd-Z (Z=29,31,33)

- ESPE for protons (T=1 & T=0 effects)
- Large deviations for $9/2^{+}$

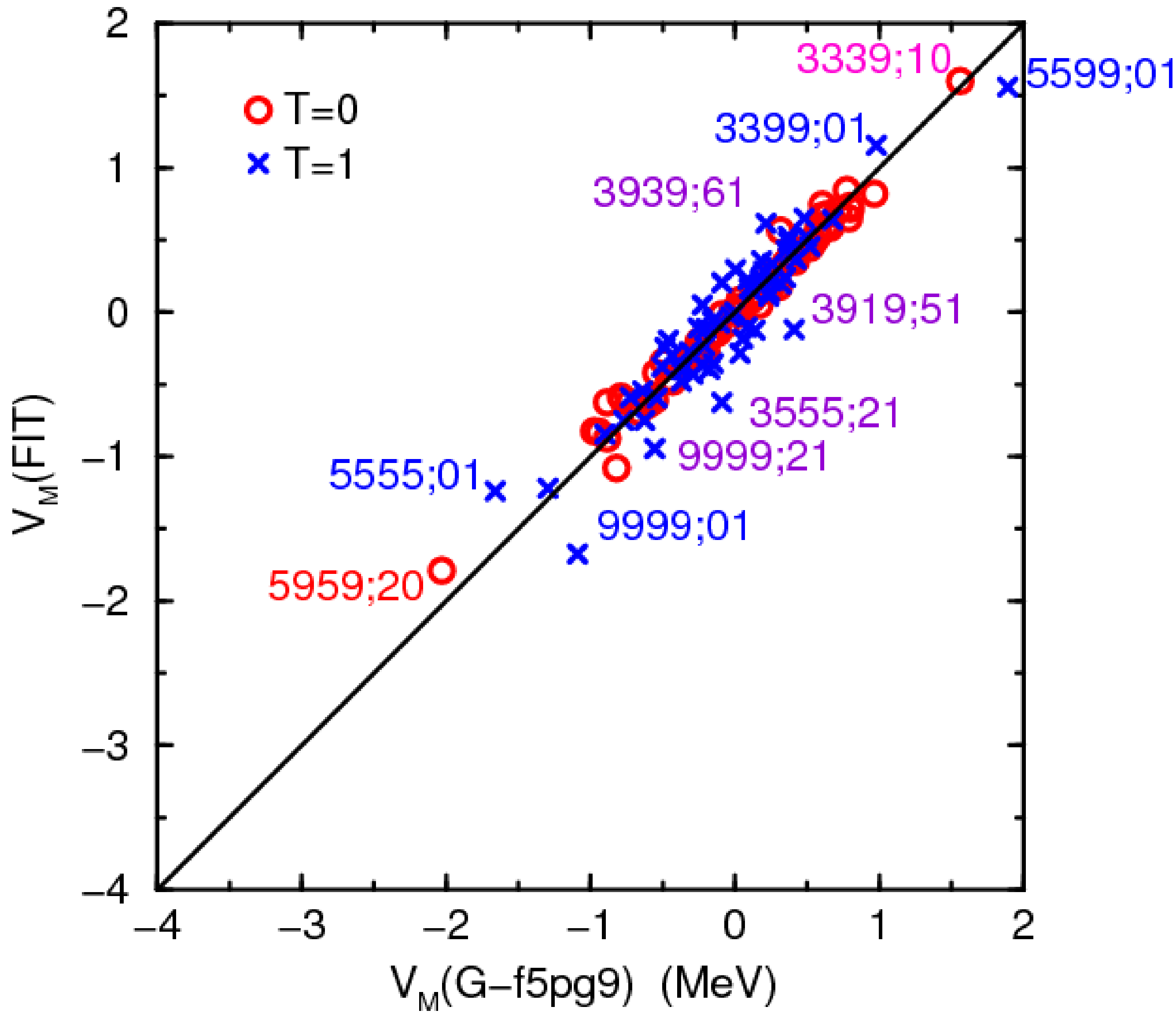


G vs. FIT(JUN45)

- TBME
  $V(abcd;JT) \Rightarrow abcd;JT$
  - 3= $p_{3/2}$
  - 5= $f_{5/2}$
  - 1= $p_{1/2}$
  - 9= $g_{9/2}$
- Modification by the fit
  - T=0 … attractive
  - T=1 … repulsive
  - Large in
    $V(abab\ ;JT\ )$
    diagonal, large J
    $V(aabb\ ;01\ )$
    monopole pairing

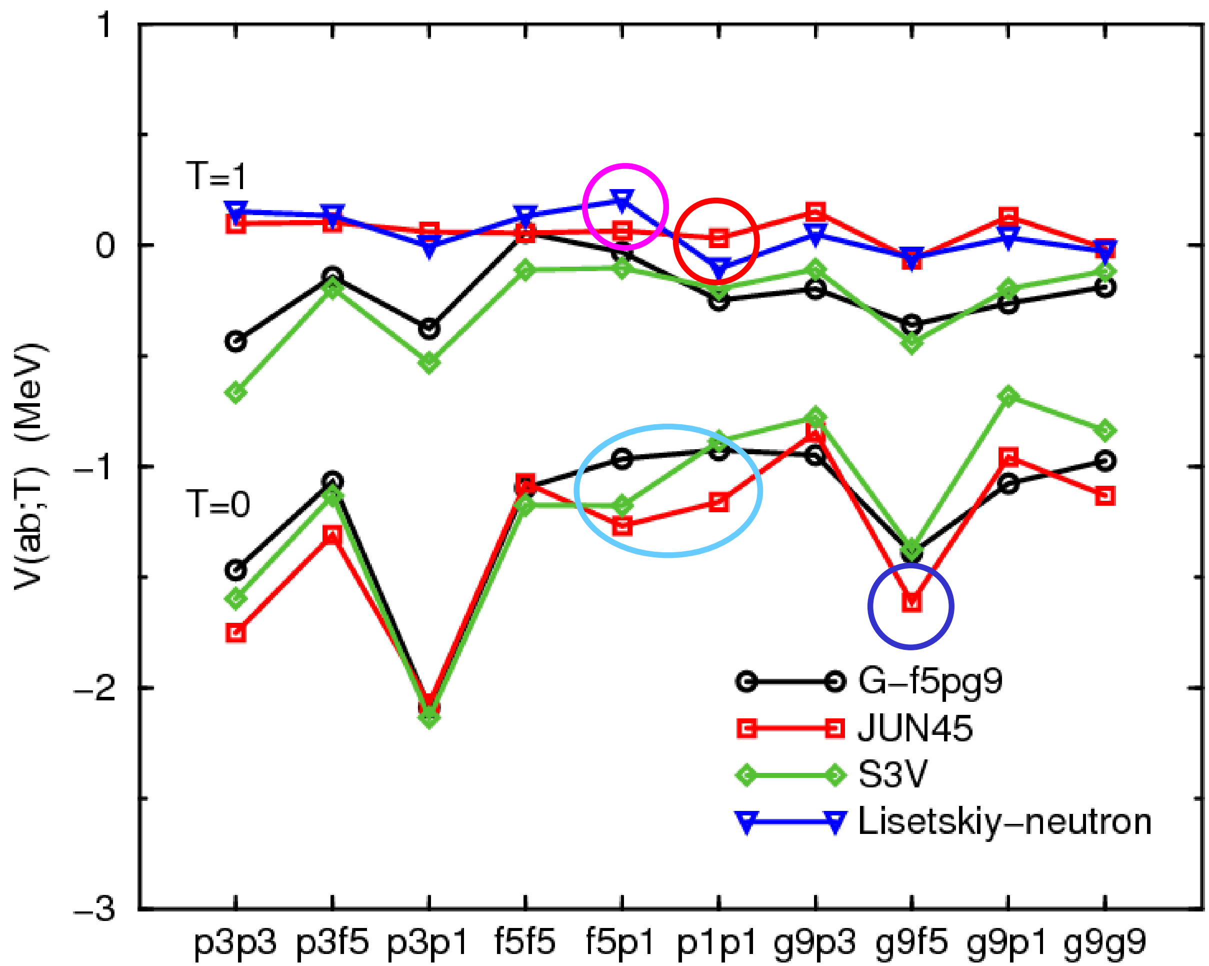


G vs. FIT(JUN45 multipole part)



Monopole centroids

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



Monopole migration of πf5/2

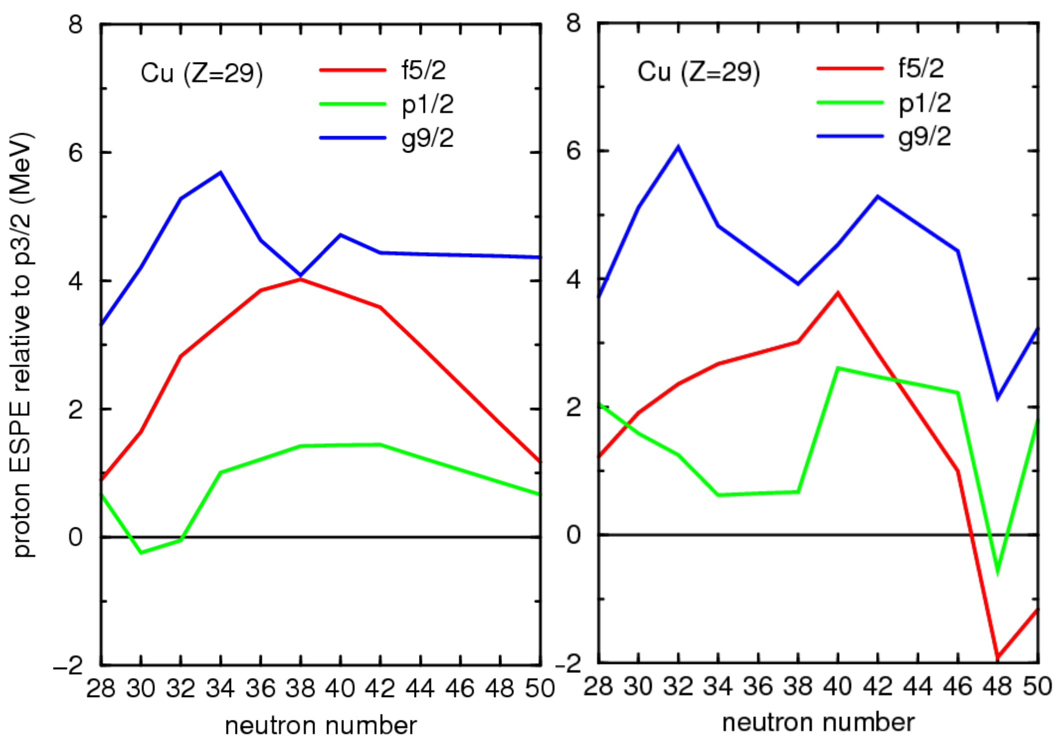
Large difference between

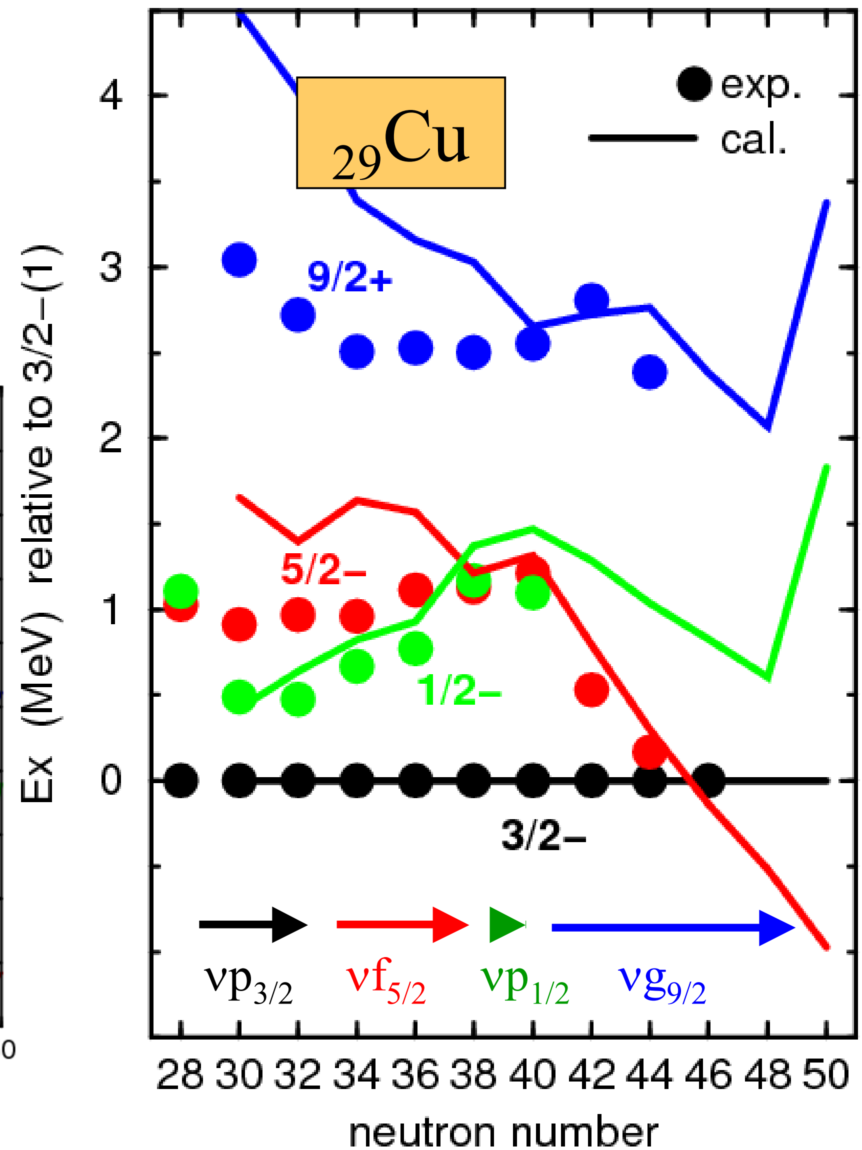
$V^{T=0}$(p-g9) and $V^{T=0}$(f5-g9)

G-f5pg9 ~ 0.9MeV

JUN45 ~ 1.6MeV

G-f5pg9 JUN45





2ν ββ-decay of ^{76}Ge, ^{82}Se

- 0ν-mode … lepton number violation
  - Majorana neutrino
  - Absolute mass scale, mass hierarchies of three neutrinos
- 2ν-mode … lepton number conservation
  - Test of the nuclear structure model
- Nuclear matrix elements
  - pn-QRPA … large single-particle space, but limited correlations
  - Shell model … restricted space, but full correlations

$$\left[T_{1/2}^{(2\nu)}(0^+ \rightarrow 0^+)\right]^{-1} = G\left|M_{GT}^{(2\nu)}\right|^2$$

G … phase-space factor including the weak-coupling constant

$$M_{GT}^{(2\nu)} = \sum_m \frac{\left\langle 0_f^+ \left\| \sum_k \sigma_k \tau_k^- \right\| 1_m^+ \right\rangle \left\langle 1_m^+ \left\| \sum_k \sigma_k \tau_k^- \right\| 0_i^+ \right\rangle}{\frac{1}{2} Q_{\beta\beta} + E_x(1_m^+) - E_0}$$

E_0 … mass difference $M_i - M_m$

GT quenching for f5pg9-shell

- Quenching of GT operator : $O_{\mathrm{GT}} \to qO_{\mathrm{GT}}$
  – Take into account the configurations outside the model space
  – p-shell … $q = 0.82$ W.T.Chou et al, PRC47 (1993) 163
  – sd-shell … $q = 0.77$ B.H.Wildenthal et al., PRC28 (1983) 1343
  – pf-shell … $q = 0.74$ G.Martinez-Pinedo et al., PRC53 (1996) R2602
- f5pg9-shell
  – Violate Ikeda sum-rule : $S_- - S_+ = 3(N-Z)$
  – Low-lying transitions … spin-flip contribution may be minor
- Fitting to β-decay data
  – Effective GT matrix element $M_{\mathrm{eff}} = \sqrt{(2J_i+1)B(GT)}$
  – Sum over final states relative to the sum-rule

$$T = \sqrt{\Sigma_i \left(M_{\mathrm{eff}\,i}\right)^2} \Big/ W \qquad W = \begin{cases} \left|g_A/g_V\right| \sqrt{(2J_i+1)3\left|N_i - Z_i\right|} & (\text{if} \quad N_i \neq Z_i) \\ \left|g_A/g_V\right| \sqrt{(2J_f+1)3\left|N_f - Z_f\right|} & (\text{if} \quad N_i = Z_i) \end{cases}$$

Effective M_{GT}

- Exp. Data

  setA … all data

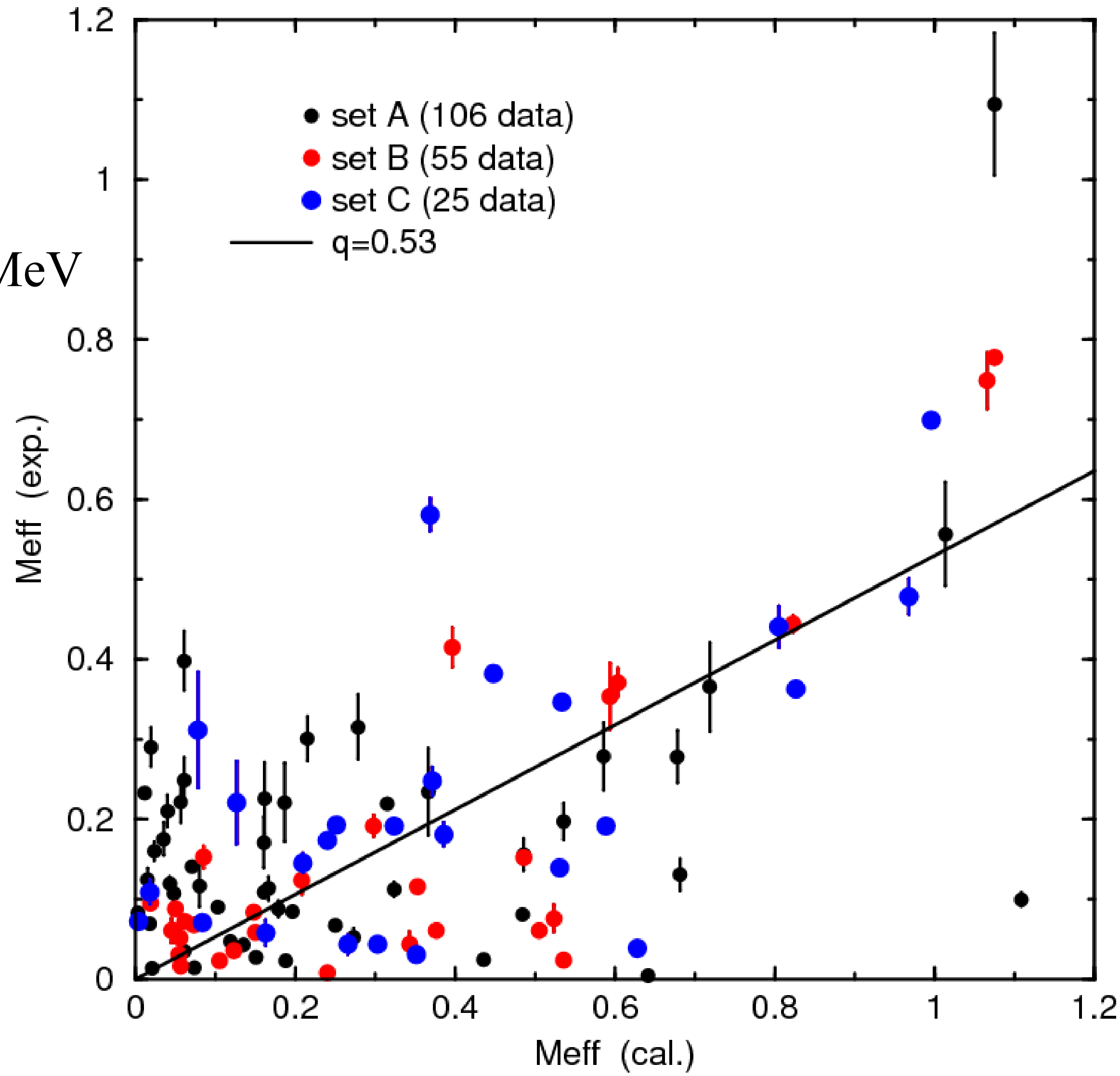
  setB … spin assigned

  setC … error in Ex < 0.1MeV

- Fit to setC

  $\Rightarrow q \sim 0.53$

  (large uncertainty)



Summed relative strength

- Fit to setC

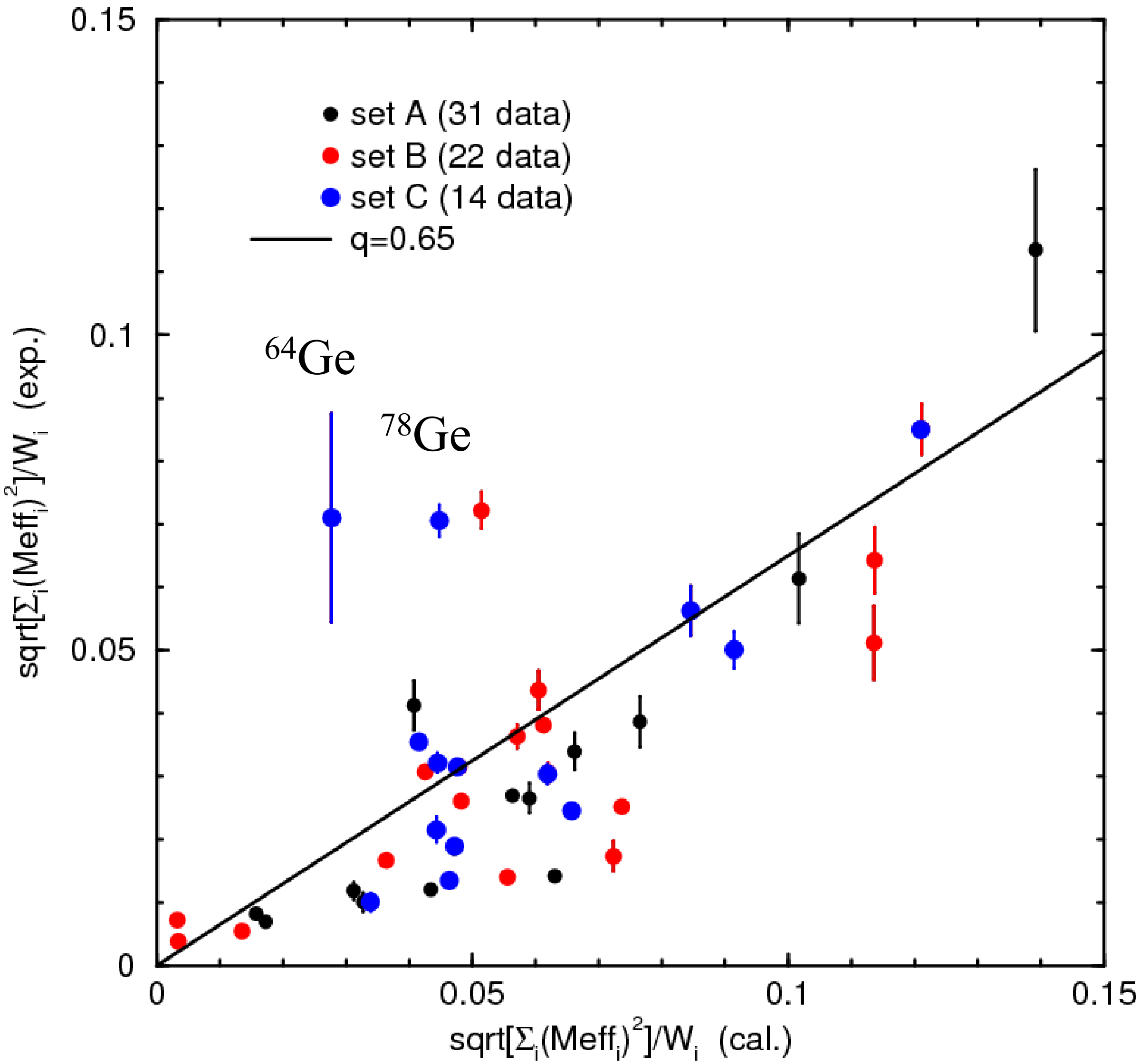
  $\Rightarrow q \sim 0.65$

  (with ^{64}Ge, ^{78}Ge)

  $\Rightarrow q \sim 0.59$

  (without ^{64}Ge, ^{78}Ge)

Adopt
$q = 0.6$



Lanczos iteration

J.Engel, W.C.Haxton, P.Vogel, PRC46 (1992) R2153

- Initial vector : $|v_1\rangle = O_{GT}\,|0^+{}_i\rangle$
- Lanczos step

$$
\begin{aligned}
Hv_1 &= \alpha_1 v_1 + \beta_1 v_2 \\
Hv_2 &= \beta_1 v_1 + \alpha_2 v_2 + \beta_2 v_3 \\
Hv_3 &= \qquad\quad \beta_2 v_2 + \alpha_3 v_3 + \beta_3 v_4 \\
&\dots
\end{aligned}
$$

$$
J_i = \begin{bmatrix} \alpha_1 & \beta_1 & & \\ \beta_1 & \alpha_2 & \beta_2 & \\ & \beta_2 & \ddots & \\ & & & \end{bmatrix}
$$

- Action of Green's function

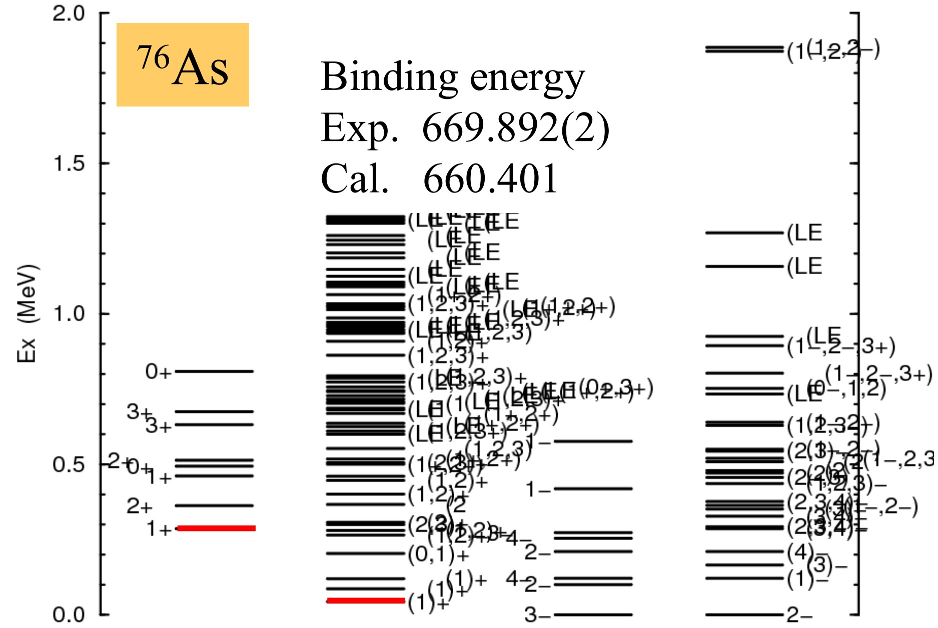
$$
\frac{1}{E_0 - H}|v_1\rangle = g_1(E_0)|v_1\rangle + g_2(E_0)|v_2\rangle + \cdots
$$

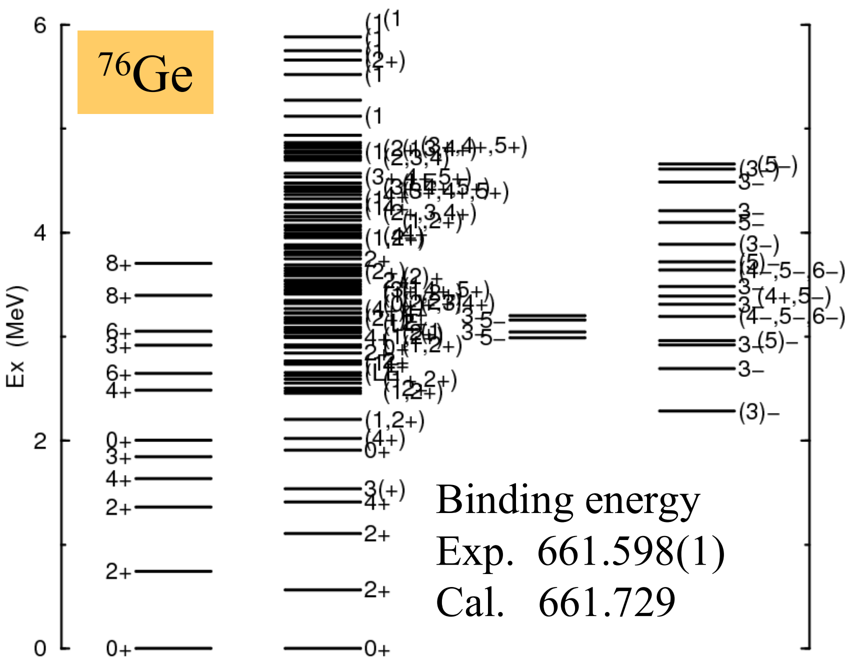
- Continued fractions … convergence is very rapid ~20 iterations

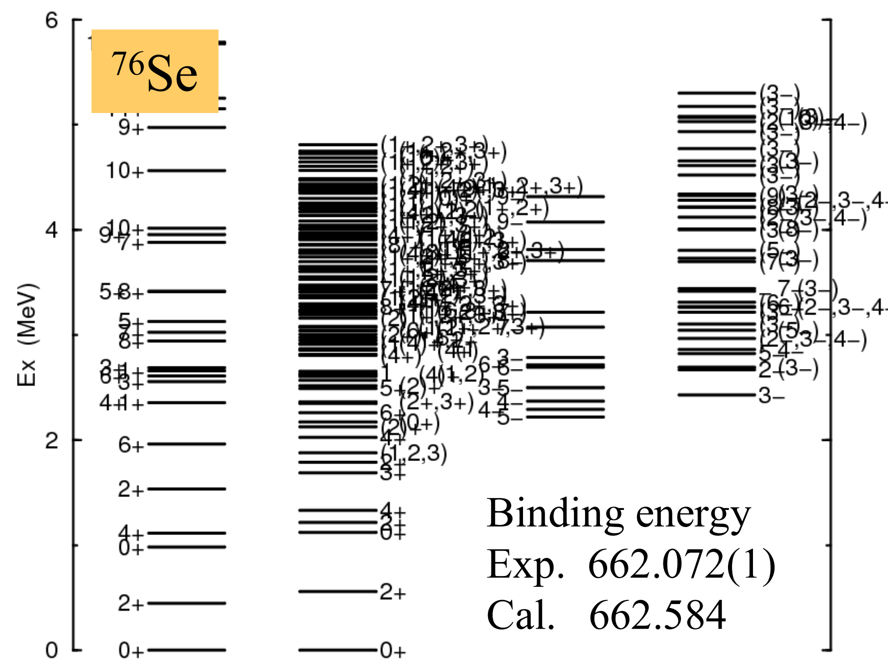
$$
g_1(E_0) = \cfrac{1}{E_0 - \alpha_1 - \cfrac{\beta_1^2}{E_0 - \alpha_2 - \cfrac{\beta_2^2}{E_0 - \alpha_3 - \cfrac{\beta_3^2}{\ddots}}}}
$$

^{76}Ge

- $^{76}_{32}Ge_{44} \rightarrow {}^{76}_{33}As_{43} \rightarrow {}^{76}_{34}Se_{42}$
- $Q_{\beta\beta} = 2.039$ MeV
- $Ex(1^+_1)$
  - Exp. 0.044 MeV
  - Cal. 0.286 MeV

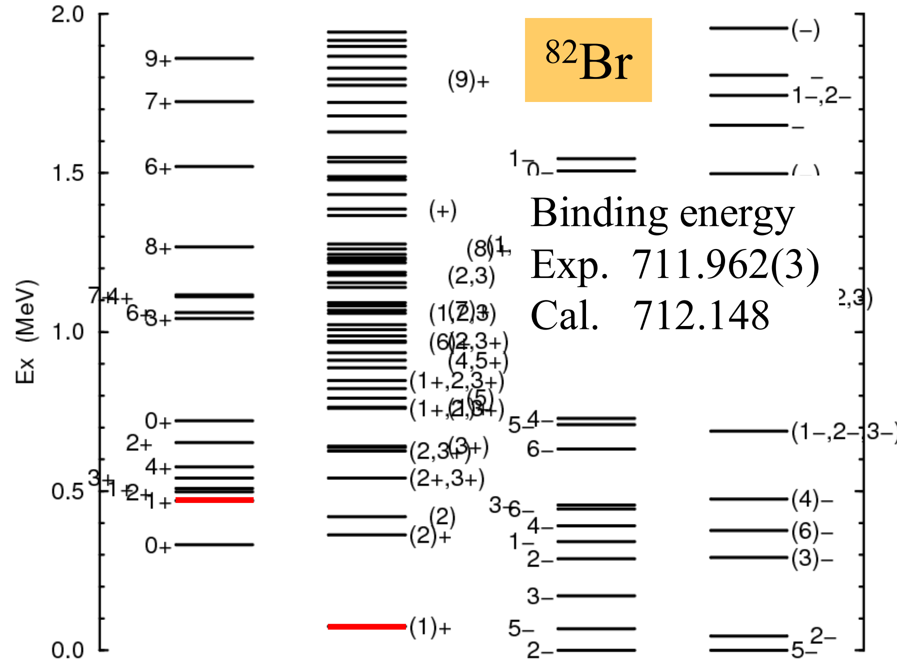


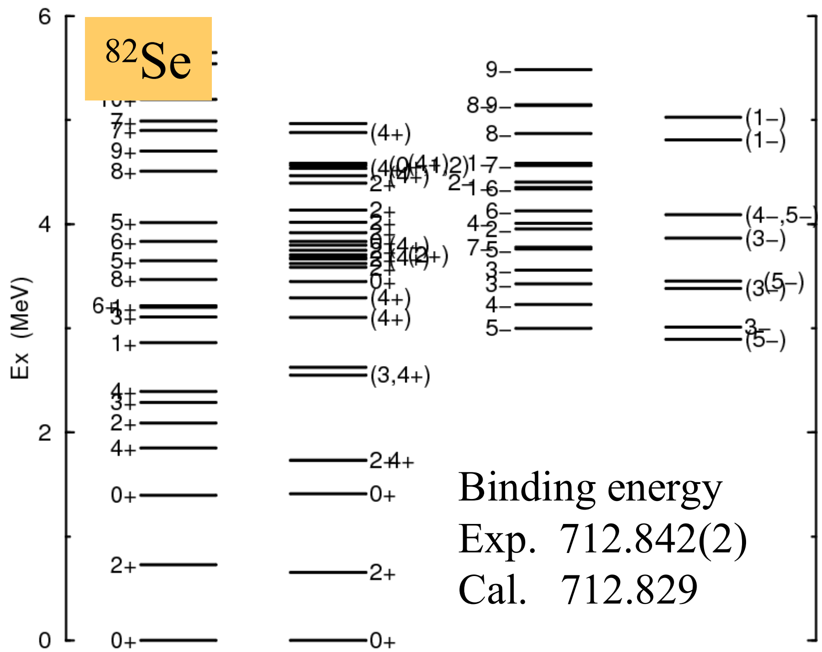


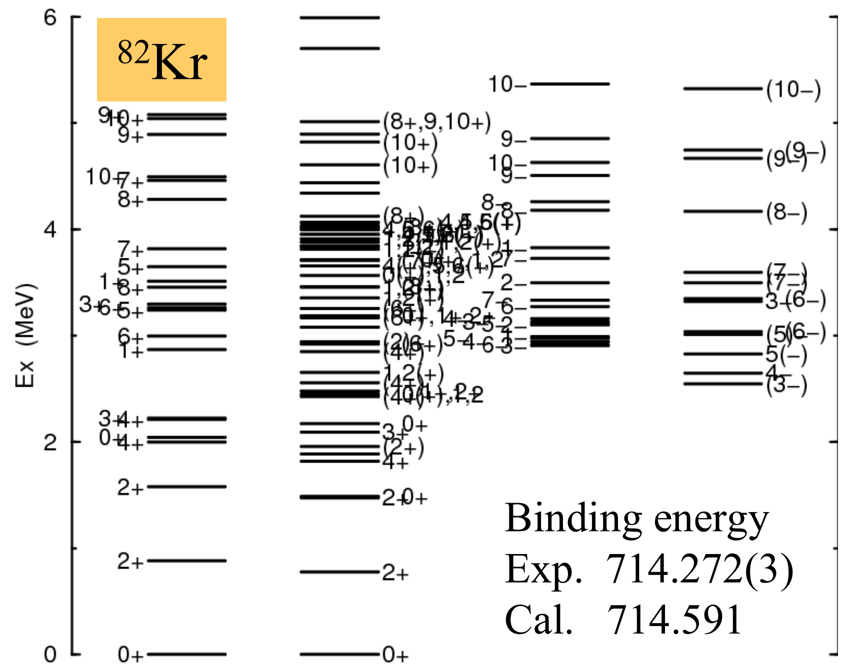


^{82}Se

- ${}^{82}_{34}Se_{48} \rightarrow {}^{82}_{35}Br_{47} \rightarrow {}^{82}_{36}Kr_{46}$
- $Q_{\beta\beta} = 2.992$ MeV
- $Ex(1^+_1)$
  - Exp. 0.075 MeV
  - Cal. 0.470 MeV







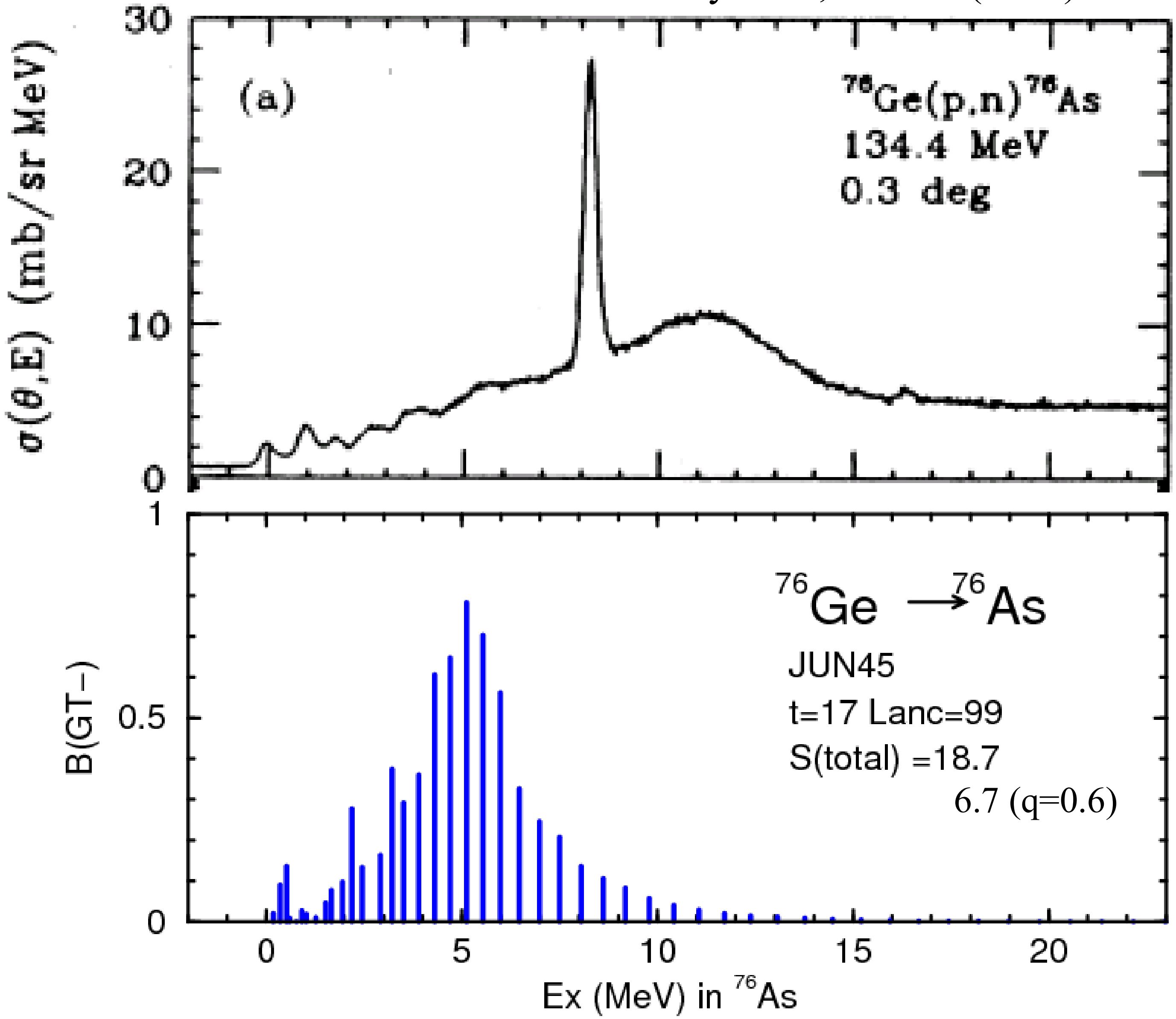
^{76}Ge GT-

R.Madey et al., PRC40 (1989) 540

Low-lying strength (< 6MeV)

Exp. 4.9

Cal. 5.4



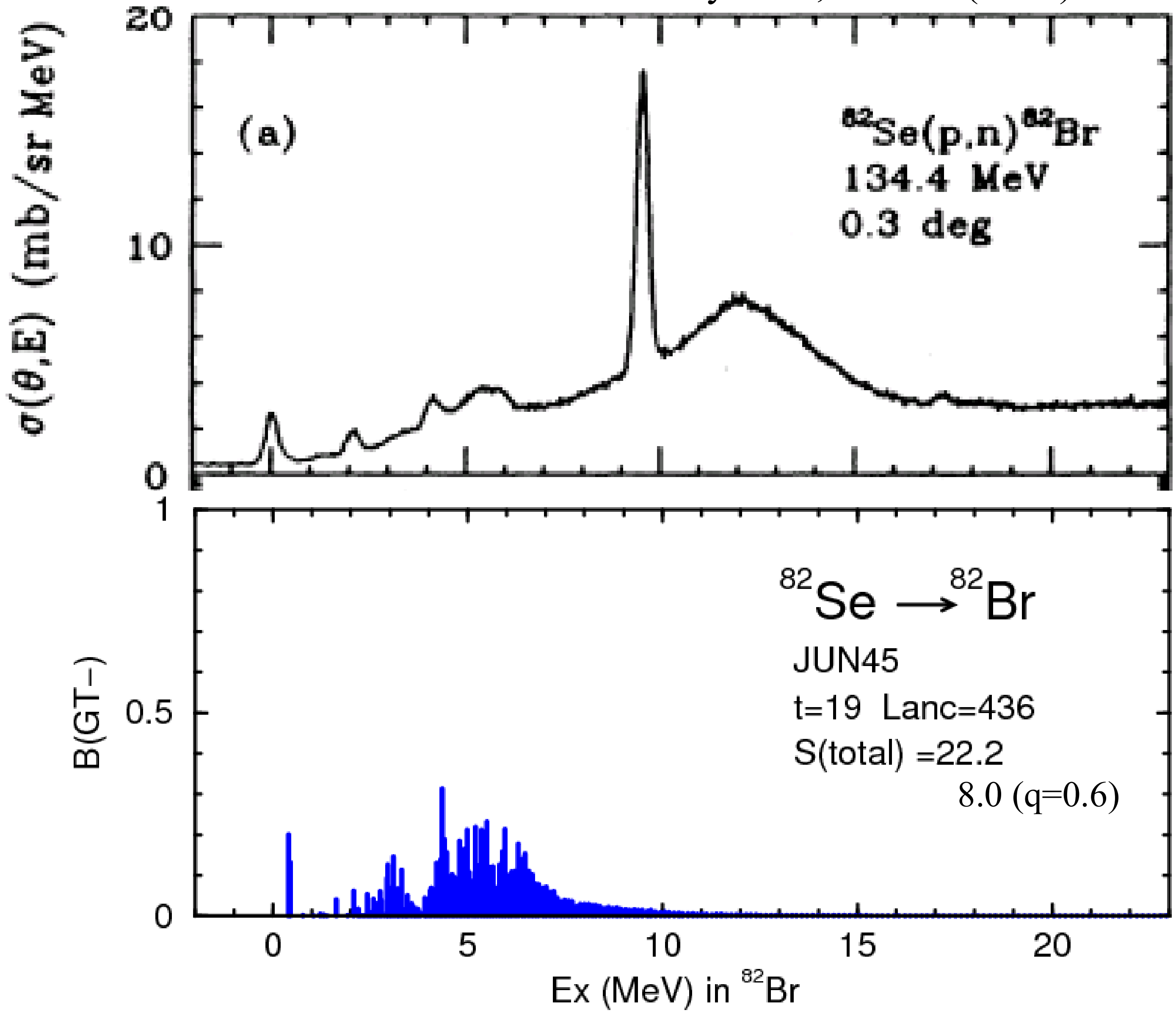
^{82}Se GT-

R.Madey et al., PRC40 (1989) 540

Low-lying strength (< 7MeV)

Exp. 5.0

Cal. 7.1



Results of $M^{(2\nu)}_{GT}$

		$M^{(2\nu)}_{GT}$ (eV^{-1})		$S-$	$S+$
		$E_x(1^+_1)$exp.	$E_x(1^+_1)$cal.		
^{76}Ge	Exp. [a]	$0.127^{+0.006}_{-0.004}$		3(N–Z)=36	
	JUN45(q=1)	0.333	0.308	18.68	0.129
	(q=0.6)	0.120	0.111		
	Caurier [b]	0.180	0.140	17.14	0.258
^{82}Se	Exp. [a]	$0.090^{+0.002}_{-0.010}$		3(N–Z)=42	
	JUN45(q=1)	0.345	0.295	22.18	0.052
	(q=0.6)	0.124	0.106		
	Caurier [b]	0.208	0.164	21.55	0.226

a) Taken from compilations by H.Ejiri, Phys. Repts. 338 (2000) 265

b) E.Caurier et al., PRL77 (1996) 1954

G-matrix by Kuo with monopole corrections determined by fitting to 60 energy data of Ni and N=50 isotone

A=76: t=4 truncation for Ge, Se and t=5 for As

Summary

- Microscopic effective interaction can be successful if suitable modifications are made, especially in the monopole part which govern the evolution of the shell structure.
- Determination of the monopole shift is not straightforward and there remains large uncertainty in the choice of the effective interaction. Empirical fit is one possible method and experimental data of neutron-rich nuclei play a key role.
- Significant quenching (q~0.6) is required for Gamow-Teller operator in the f5pg9-shell with relatively large uncertainty, suggesting the needs for larger model space.
- 2ν-ββ-decay matrix element for ^{76}Ge and ^{82}Se are successfully described. Calculations of the 0ν mode are in preparation.