Towards an Extended SU(3) Shell Model for Upper-fp (and beyond) Shell Nuclei

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OUTLINE

- Motivation

- Part 1: Calculations in upper-fp ($f_{5/2}, p_{3/2}, p_{1/2}$) + $g_{9/2}$ shell model space using fixed realistic interaction
  - SU(3) symmetry in lower-lying (upper-fp) states
  - Energy spectra & B(E2) strengths in N=Z nuclei
  - Track occupancy in the intruder $g_{9/2}$ level

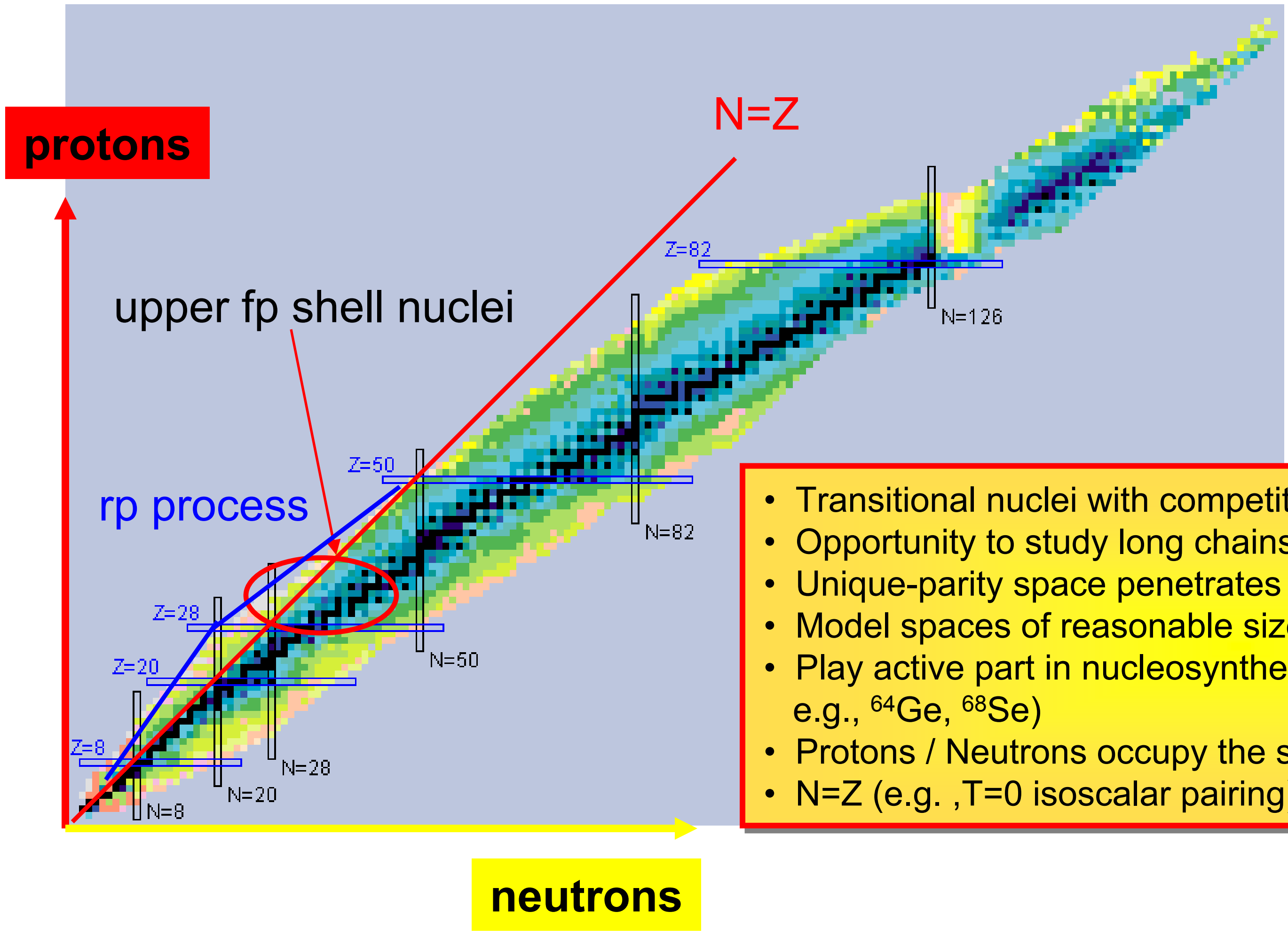
$$(f_{5/2}p)^m(g_{9/2})^n$$

- Part 2: Extended shell model calculations with particles in the upper-fp ($f_{5/2}, p_{3/2}, p_{1/2}$) + gds (full space, just $g_{9/2}$) with results for ^{64}Ge and ^{68}Se
  - SU(3) symmetry in upper and lower spaces
  - Energy spectra & B(E2) transition strengths
  - Track occupancy in the intruder gds shell

$$(f_{5/2}p)^m(gds)^n$$

- Conclusion

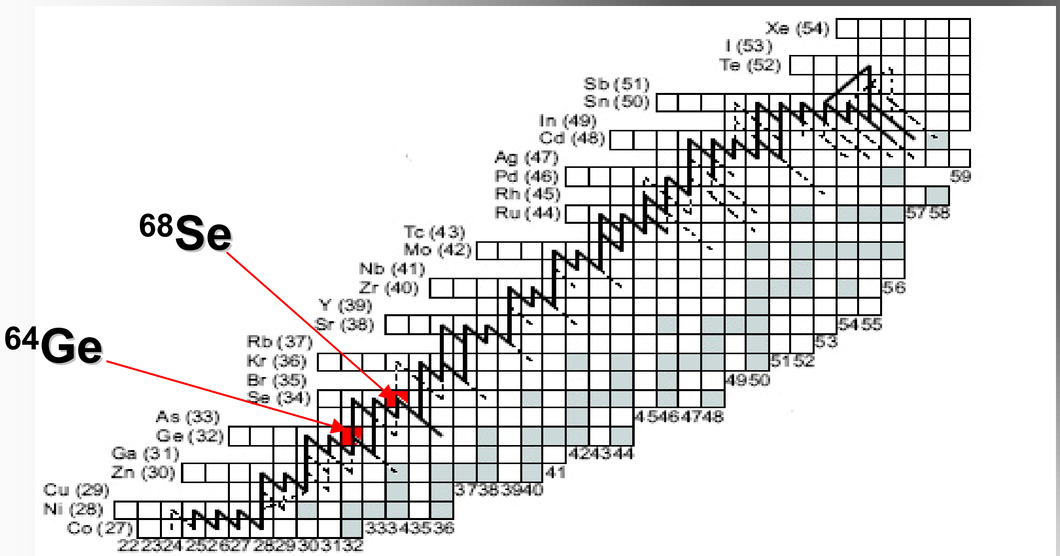
Motivation: Why study upper-fp shell nuclei?



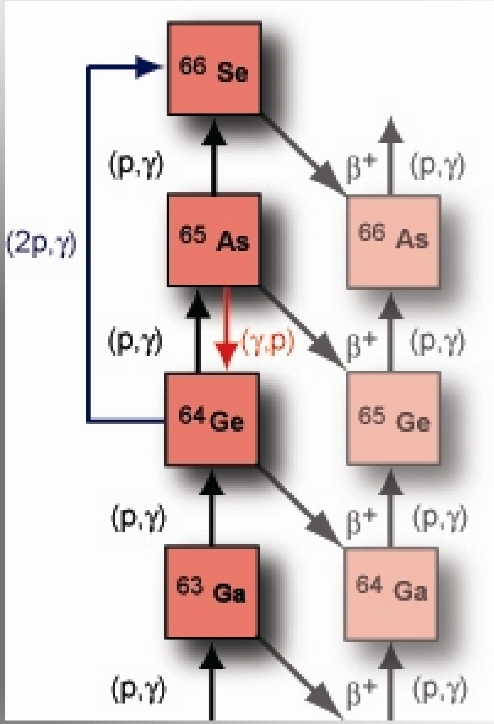
- Transitional nuclei with competitive P & Q.Q modes
- Opportunity to study long chains of isotopes (isotones)
- Unique-parity space penetrates into normal-parity space
- Model spaces of reasonable size so calculations feasible
- Play active part in nucleosynthesis (waiting-point nuclei – e.g., ^{64}Ge, ^{68}Se)
- Protons / Neutrons occupy the same shell
- N=Z (e.g. ,T=0 isoscalar pairing) effects

Motivation: Role of $^{64}_{32}Ge_{32}$ and $^{68}_{34}Se_{34}$

Astrophysical implications – waiting-point nuclei



Schatz et al., Phys. Rep. 294 (1998) 167



- (p,γ) ↔ (γ,p) equilibrium
- waiting for β+ decay
- 2p capture possible

Part 1: SMC with realistic interaction: $(f_{5/2}p)^m(g_{9/2})^n$

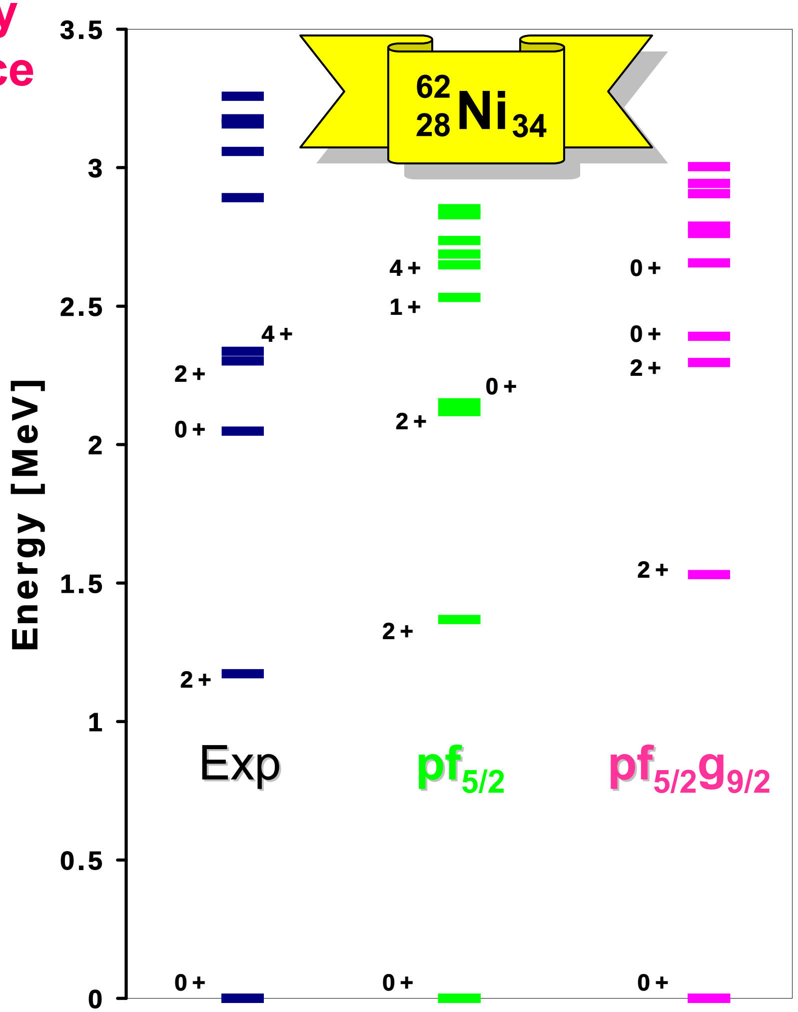
Realistic G-matrix with phenomenologically adjusted monopole part in the $pf_{5/2}g_{9/2}$ space

Renormalized G-matrix counterpart for the $pf_{5/2}$ space only (excluding the $g_{9/2}$ orbital)

[Interactions provided by P. Van Isacker, see e.g.:
E. Caurier, F. Nowacki, A. Poves, & J. Retamosa,
Phys. Rev. Lett. 77, 1954 (1996)]

➡ **Reasonable results for the low-lying energy spectra of ^{58,60,62,64,66}Ni, ^{58}Cu, ^{60,62,64}Zn, ^{62}Ga, ^{64}Ge, ^{68}Se in both cases**

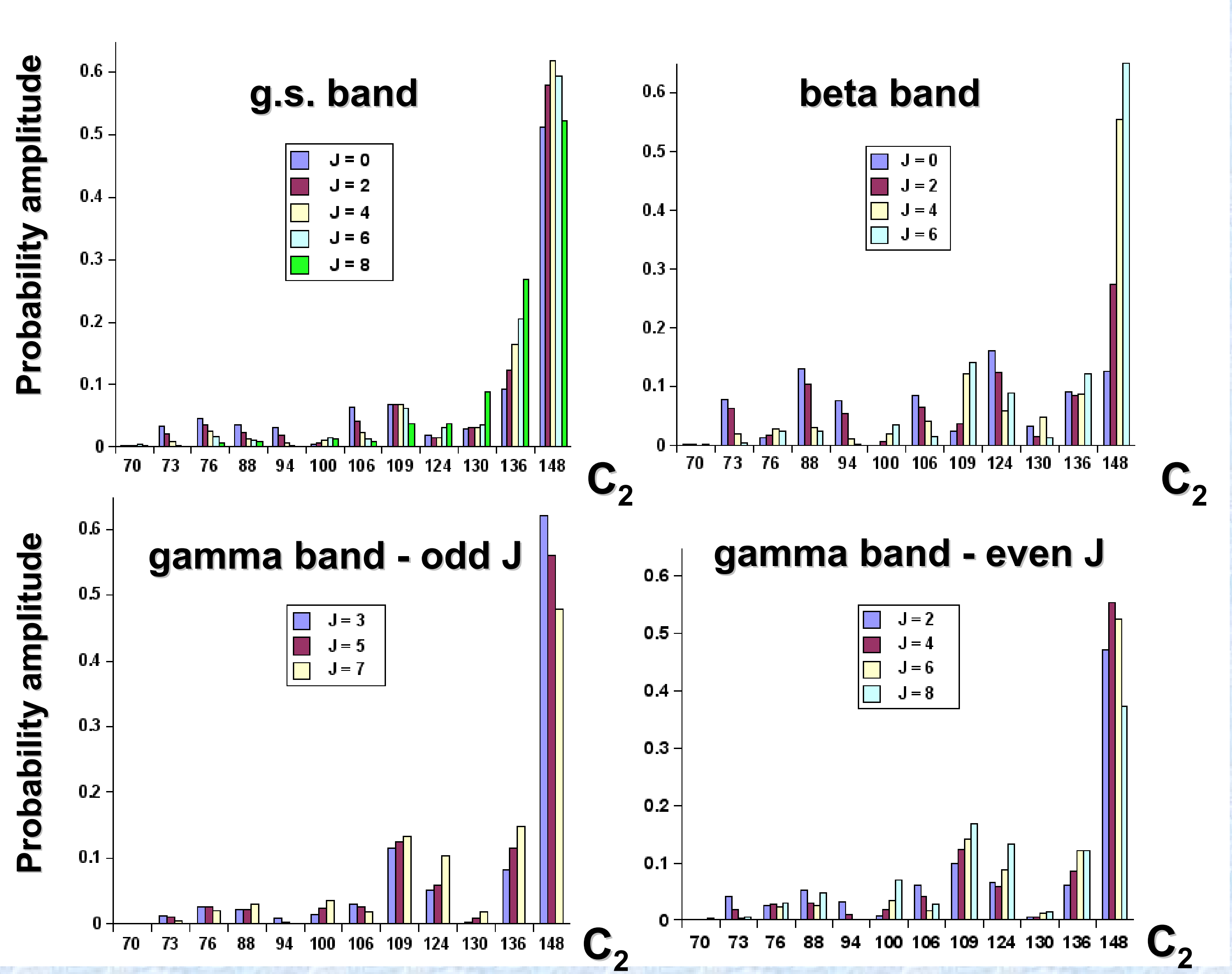
➡ **Demonstrates quality of pseudo-SU(3) symmetry for upper-fp shell for these nuclei**



Other results (^{58}Cu, ^{60}Zn, ^{60}Ni, ^{62}Ga)

[P. Van Isacker, O. Juillet and F. Nowacki,
Phys. Rev. Lett. 80, (1999) 2060
S. M. Vincent et al., Phys. Lett. B 437, 264 (1998)]

Pseudo-SU(3) symmetry in $^{64}_{32}Ge_{32}$



Pseudo-SU(3) symmetry in low-lying states: N=Z nuclei

J	$^{58}_{29}Cu_{29}$	J	$^{60}_{30}Zn_{30}$	J	$^{62}_{31}Ga_{31}$	J	$^{64}_{32}Ge_{32}$	J	$^{68}_{34}Se_{34}$
1_1	81.42	0_1	54.93 $(93.67)_3$	0_1	54.53 $(73.54)_3$ $(92.35)_6$	0_1	51.13 $(63.33)_3$ $(90.41)_{10}$	0_1	40.89 $(72.59)_3$ $(90.38)_6$
0_1	72.65	2_1	59.03 $(95.41)_3$	1_1	46.56 $(73.62)_3$	2_1	57.92 $(73.37)_3$	2_1	43.6 $(76.53)_3$
3_1	89.6	4_1	73.99 $(98.83)_3$	1_2	40.18 $(61.27)_3$	2_2	47.01 $(53.75)_3$	0_2	11.03 $(20.47)_3$
1_2	71.99	0_2	16.43 $(78.32)_3$	3_1	66.02 $(86.23)_3$	0_2	12.7 $(25.02)_3$	4_1	45.99 $(79.2)_3$
2_1	92.55	2_2	20.06 $(78.34)_3$	2_1	57.5 $(79.68)_3$	3_1	62.03 $(70.56)_3$	2_2	30.3 $(48.24)_3$
2_2	69.07	1_1	0 $(87.38)_3$	2_2	41.66 $(66.38)_3$	4_1	61.81 $(81.45)_3$	0_3	63.67 $(69.96)_3$
3_2	83.96	2_3	0.21 $(64.89)_3$	1_3	72.63 $(80.03)_3$	2_3	27.42 $(37.48)_3$	3_1	0 $(35.25)_3$
4_1	100	6_1	83.91 $(99.75)_3$	2_3	79.63 $(85.33)_3$	4_2	55.4 $(64.49)_3$	2_3	17.27 $(46.1)_3$
5_1	100	1_2	0 $(81.75)_3$	3_2	31.55 $(59.75)_3$	1_1	0 $(52.25)_3$	4_2	0 $(11.75)_3$
2_3	0.02	3_1	0 $(86.2)_3$	5_1	69.54 $(85.38)_3$	2_4	7.16 $(16.07)_3$	1_1	0 $(44.75)_3$

Leading SU(3) irrep

First three distinct SU(3) irreps

First n distinct SU(3) irreps needed for 90% overlap with the realistic eigenstate

B(E2) transition strengths [e^2fm^4]: $^{58}_{29}Cu_{29}$ and $^{62}_{31}Ga_{31}$

$^{58}_{29}Cu_{29}$

$e_{eff} = 0.5$

$^{62}_{31}Ga_{31}$

J_i, T_i	J_f, T_f	B(E2; J_i -> J_f) Exp	$pf_{5/2}$	$pf_{5/2}g_{9/2}$	J_i, T_i	J_f, T_f	B(E2; J_i -> J_f) Exp	$pf_{5/2}$	$pf_{5/2}g_{9/2}$
3_1, 0	1_1, 0	101(18)	39.63	39.60	1_2, 0	3_1, 0	-	1.59	1.58
1_2, 0	1_1, 0	-	48.39	48.90	2_1, 0	3_1, 0	-	19.12	19.02
2_1, 0	1_1, 0	-	34.36	33.62	2_2, 1	3_1, 0	2^{+9}_{-2}	2.16	2.21
2_2, 1	1_1, 0	< 60	5.64	5.77	2_1, 0	1_2, 0	-	31.58	30.83
2_1, 0	0_1, 1	-	0.46	0.56	2_2, 1	1_2, 0	27(22)	2.18	2.31
2_2, 1	0_1, 1	122(47)	39.94	38.74	2_2, 1	2_1, 0	-	1.96	1.94

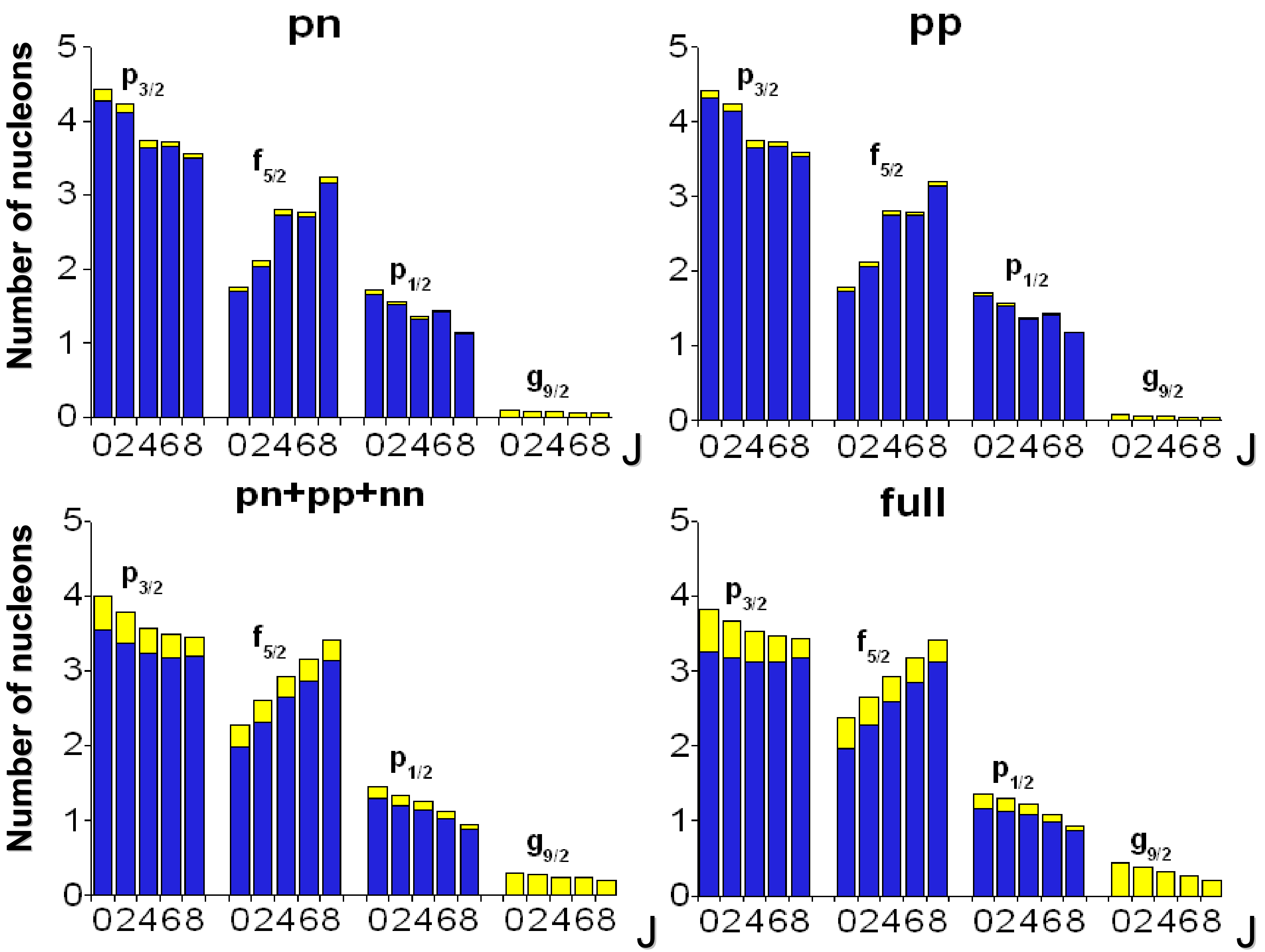
core excitations (e.g., $f_{7/2}$) missing but other effects enter as well …

the overall degree of collectivity too small

J_i, T_i	J_f, T_f	B(E2; J_i -> J_f) Exp	$pf_{5/2}$	$pf_{5/2}g_{9/2}$	J_i, T_i	J_f, T_f	B(E2; J_i -> J_f) Exp	$pf_{5/2}$	$pf_{5/2}g_{9/2}$
2_1, 1	0_1, 1	-	195.39	188.79	3_1, 0	1_1, 0	-	32.7	24.75
2_2, 0	0_1, 1	-	0.04	0.02	2_1, 1	1_2, 0	-	0.46	0.36
3_1, 0	1_1, 0	197(69)	141.14	141.18	2_2, 0	1_2, 0	-	182.89	175.79
2_1, 1	1_1, 0	-	0.09	0.04	2_1, 1	3_1, 0	-	0.71	0.75
2_2, 0	1_1, 0	-	4.61	8.74	2_2, 0	3_1, 0	-	12.86	13.02

A. Lisetskiy et al., Phys. Rev. C **68**, 034316 (2003); A. Costin et al., Phys. Rev. C **72**, 054305 (2005); S. M. Vincent et al., Phys. Lett. B 437, 264 (1998)

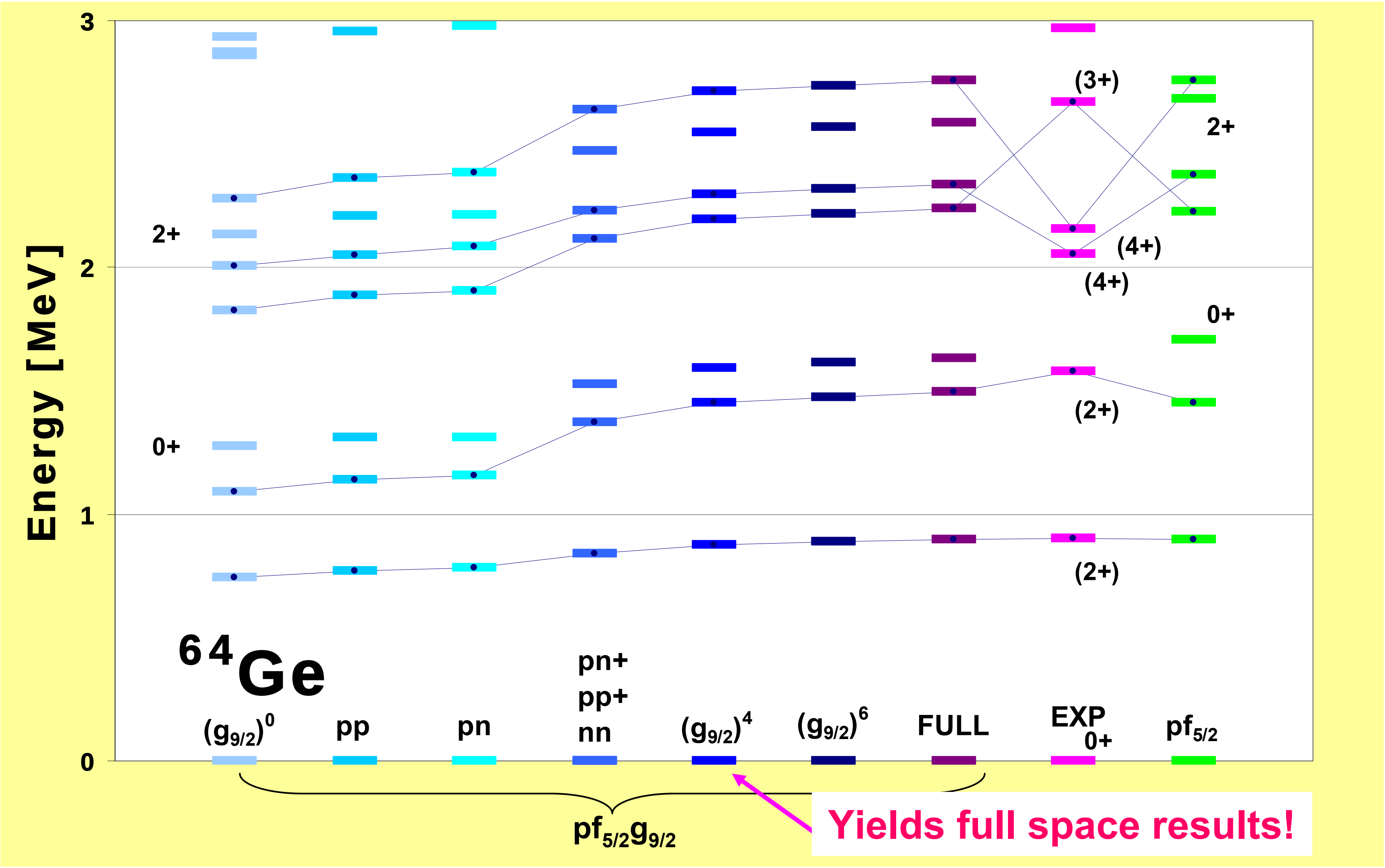
Occupancy in $^{64}_{32}Ge_{32}$



Contribution from basis states with empty $g_{9/2}$ intruder.

Contribution from basis states with occupied $g_{9/2}$ intruder.

Energy spectrum for $^{64}_{32}Ge_{32}$ in different model spaces



B(E2) transition strengths: $^{64}_{32}Ge_{32}$ [e^2fm^4]

transition	$pf_{5/2}$	pn	pp/nn	pn+pp+nn	$(g_{9/2})^4$	full
2_1->0	257.22	236.96	238.22	252.75	254.09	253.94
2_2->0	1.99	1.09	1.07	1.17	1.27	1.42
2_2->2_1	251.68	337.37	336.79	255.26	248.21	241.41
0_2->2_1	52.92	53.87	51.24	50.22	43.6	38.95
0_2->2_2	161	254.18	259.62	171.08	163.69	157.49
3_1->2_1	4.21	1.18	1.05	2.75	3.05	3.40
3_1->2_2	371.15	334.37	332.24	354.63	356.75	357.79
4_1->2_1	332.54	276.6	273.04	338.09	341.47	342.51
4_1->2_2	9.81	49.96	51.84	5.96	3.91	2.73
4_1->3_1	45.47	37.79	65.32	69.88	75.77	79.57

Yields ~full space results !

Part 2: SMC in deformed SU(3) basis: $(f_{5/2}p)^m(gds)^n$

A model space which consists of configurations with at most 4 particles in the abnormal space is enough to describe the energies and the B(E2) transition strengths obtained in the full space calculations

Pseudo-SU(3) symmetry is reasonably good (especially for N=Z nuclei)

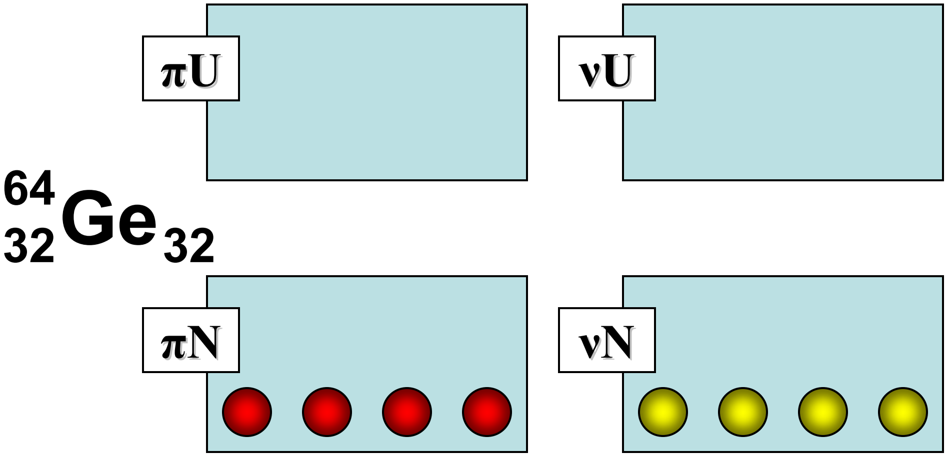
It is possible to build SU(3) symmetry-adapted truncated basis for performing calculations in two (upper-fp + gds) shells!

The shell model with actively included particles from the abnormal space will:

- open the **whole** gds shell (not only the $g_{9/2}$ level) for calculations of properties in nuclei of great importance in the processes of nucleosynthesis
- provide a tool for **description of the shape coexistence in nuclei** based on the dominance of various deformed configurations in different energy intervals
- allow description of B(E2) strengths with a significantly reduced value for the effective charge used

Extended SU(3) Shell Model: Model Space

FOUR SPACES (abnormal spaces explicitly included)



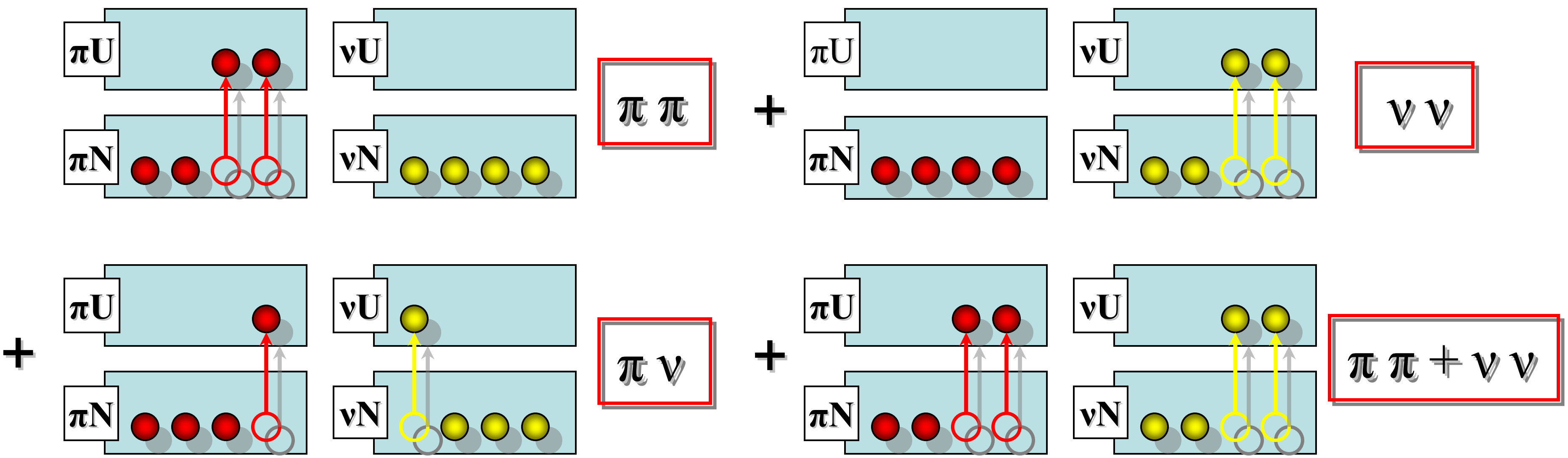
gds

Dominant configuration (empty abnormal spaces)

upper-fp → pseudo-ds

($f_{5/2}p$) → ($\tilde{d}\tilde{s}$)

…mixed with …



Extended SU(3) Shell Model: Basis States

$$\left| \{\alpha_{\pi N}\alpha_{\pi U}\}\rho_\pi(\lambda_\pi,\mu_\pi),S_\pi;\{\alpha_{\nu N}\alpha_{\nu U}\}\rho_\nu(\lambda_\nu,\mu_\nu),S_\nu\}\rho(\lambda,\mu)kL,S;JM \right\rangle$$

$$\alpha_\sigma \equiv \left\{N_\sigma[f_\sigma](\lambda_\sigma,\mu_\sigma),S_\sigma\right\}$$

- Well-defined particle number and total angular momentum
- Include S = 0,1/2 & 1 states in both the normal and unique spaces
- For each S the states with the maximum value of the second order Casimir operator $C_2 = \frac{1}{4}\left(Q.Q + 3\hat{L}^2\right)$ in the coupled proton-neutron space are selected

Extended SU(3) Shell model: Model Hamiltonian

$$H = H_{sp}^{\pi N} + H_{sp}^{\pi U} + H_{sp}^{\nu N} + H_{sp}^{\nu U}$$ single-particle energies

$$- G^{\pi N} H_{pair}^{\pi N} - G^{\pi U} H_{pair}^{\pi U} - G^{\nu N} H_{pair}^{\nu N} - G^{\nu U} H_{pair}^{\nu U}$$ pp and nn pairing

$$- G^{\pi N,\nu N} H_{pair}^{\pi N,\nu N} - G^{\pi U,\nu U} H_{pair}^{\pi U,\nu U}$$ pn pairing

$$- G^{\pi N,\pi U} H_{psc}^{\pi N,\pi U} + h.c.$$ pp pair-scattering

$$- G^{\nu N,\nu U} H_{psc}^{\nu N,\nu U} + h.c.$$ nn pair-scattering

$$- G^{NU} H_{psc}^{NU} + h.c.$$ pn pair-scattering

$$- \frac{1}{2}\chi :Q.Q: + aK_J^2 + bJ^2$$ ← SU(3) symmetry preserving interaction

$$H_{sp} = \hbar\omega_0(\eta + \frac{3}{2}) - k\hbar\omega_0\{2\vec{l}.\vec{s} + \mu \vec{l}^2\}$$

mixes configurations with a specific distribution of particles over the shells

mixes configurations with different distributions of particles over the shells

Interaction strength parameters

$$\hbar\omega_0 = 41A^{-1/3}[MeV]$$

Experimental single-particle energies of ^{57}Ni for the normal space and systematic estimates for the unique space

$$G_{\pi N} = G_{\pi U} = G_{\nu N} = G_{\nu U} \approx \frac{18}{A}[MeV]$$

Invariant under the pseudo-spin transformation

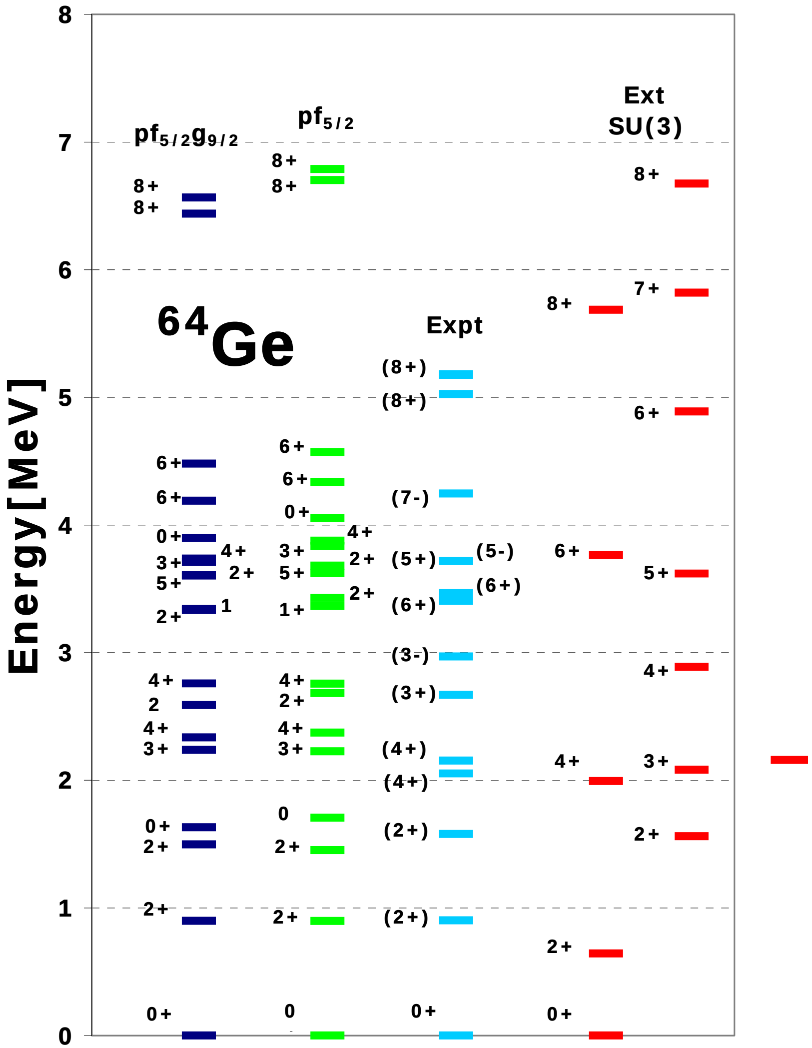
$$\chi = \frac{18}{A^{5/3}}[MeV]$$

Not invariant under the pseudo-spin transformation !

$$Q_\mu \approx \frac{\tilde{\eta}+1}{\tilde{\eta}}\tilde{Q}_\mu$$

P. Ring, P. Schuck, The Nuclear Many-Body Problem, Springer, Berlin, 1979
K. Kaneko, M. Hasegawa, T. Mizusaki, Phys. Rev. C 66, 051306(R) (2002)
M. Dufour, A. Zuker, Phys. Rev. C 54, 1641 (1996)

Energy spectrum for $^{64}_{32}Ge_{32}$



Are comparable to the realistic result obtained in a much larger space

2nd 0^+ at ~2.15 MeV …

Moment of inertia large

B(E2) transition strengths [e^2fm^4]: $^{64}_{32}Ge_{32}$ and $^{68}_{34}Se_{34}$

$^{64}_{32}Ge_{32}$

$$Q \approx e_\pi \left(\frac{\tilde{\eta}_\pi + 1}{\tilde{\eta}_\pi} \tilde{Q}_{\pi N} + Q_{\pi U} \right) + e_\nu \left(\frac{\tilde{\eta}_\nu + 1}{\tilde{\eta}_\nu} \tilde{Q}_{\nu N} + Q_{\nu U} \right)$$

$(J+2)^+ \to J^+$	$pf_{5/2}$	$pf_{5/2}g_{9/2}$	Ext. SU(3)
$2_{g.s.}^+ \to 0_{g.s.}^+$	257.22	253.91	288.3
$4_{g.s.}^+ \to 2_{g.s.}^+$	332.54	342.51	357.0
$6_{g.s.}^+ \to 4_{g.s.}^+$	340.51	356.92	391.2
$8_{g.s.}^+ \to 6_{g.s.}^+$	303.31	320.14	269.2
$4_\gamma^+ \to 2_\gamma^+$	89.26	93.13	88.7
$6_\gamma^+ \to 4_\gamma^+$	164.23	144.19	180.1
$8_\gamma^+ \to 6_\gamma^+$	92.12	84.38	172.6
$(J+1)^+ \to J^+$			
$3_\gamma^+ \to 2_\gamma^+$	371.15	357.79	513.0
$5_\gamma^+ \to 4_\gamma^+$	238.48	240.4	154.2
$7_\gamma^+ \to 6_\gamma^+$	159.44	161.24	121.3
$J_\alpha^+ \to J_\beta^+$			
$2_\gamma^+ \to 0_{g.s.}^+$	1.98	1.42	5.7
$2_\gamma^+ \to 2_{g.s.}^+$	251.68	241.41	196.1
$3_\gamma^+ \to 2_{g.s.}^+$	4.21	3.4	9.8
$4_\gamma^+ \to 4_{g.s.}^+$	72.1	74.69	55.2
$4_\gamma^+ \to 2_{g.s.}^+$	18.86	19.31	7.1

$e_{eff} = 0.5$

$^{68}_{34}Se_{34}$

$(J+2)^+ \to J^+$	$pf_{5/2}$	Ext. SU(3)
$2_{g.s.}^+ \to 0_{g.s.}^+$	322.71	373.7
$4_{g.s.}^+ \to 2_{g.s.}^+$	448.07	506.0
$6_{g.s.}^+ \to 4_{g.s.}^+$	441.58	496.2
$4_\gamma^+ \to 2_\gamma^+$	216.57	477.1
$6_\gamma^+ \to 4_\gamma^+$	183.35	470.5
$(J+1)^+ \to J^+$		
$3_\gamma^+ \to 2_\gamma^+$	1.94	1.1
$5_\gamma^+ \to 4_\gamma^+$	0.05	0.3
$J_\alpha^+ \to J_\beta^+$		
$2_\gamma^+ \to 0_{g.s.}^+$	4.8	5.8
$2_\gamma^+ \to 2_{g.s.}^+$	16.79	24.9
$3_\gamma^+ \to 2_{g.s.}^+$	0.35	0.2
$4_\gamma^+ \to 4_{g.s.}^+$	6.72	5.5
$4_\gamma^+ \to 2_{g.s.}^+$	0.11	1.5

Wave function decomposition: g.s. band

$^{64}_{32}Ge_{32}$

4 + 4 = 8

$\{(\lambda_\pi,\mu_\pi)S_\pi;(\lambda_\nu,\mu_\nu)S_\nu\}(\lambda,\mu)S$	$0^+_{g.s.}$	$2^+_{g.s.}$	$4^+_{g.s.}$	$6^+_{g.s.}$	$8^+_{g.s.}$
{ (4,2)0 ; (4,2)0 } (8,4)0	80.81	80.19	76.88	60.26	15.11
(10,0)0	10.91	9.65	5.59	1.52	-
{ (4,2)0 ; (5,0)1 } (9,2)1	4.56	6.11	12.32	28.39	35.63
{ (4,2)0 ; (2,3)1 } (6,5)1	1.61	1.69	2.31	3.45	2.39
{ (5,0)1 ; (5,0)1 } (10,0)2	-	-	-	3.77	44.1

$^{68}_{34}Se_{34}$

6 + 6 = 12

$\{(\lambda_\pi,\mu_\pi)S_\pi;(\lambda_\nu,\mu_\nu)S_\nu\}(\lambda,\mu)S$	$0^+_{g.s.}$	$2^+_{g.s.}$	$4^+_{g.s.}$	$6^+_{g.s.}$
{ (6,0)0 ; (6,0)0 } (12,0)0	81.76	86.51	88.11	87.08
{ (0,6)0 ; (0,6)0 } (0,12)0	3.04	-	-	-
{ (6,0)0 ; (3,3)0 } (9,3)0	-	-	1.10	2.47
(6,6)0	9.37	6.29	3.62	1.34
{ (6,0)0 ; (4,1)2 } (10,1)1	3.47	3.87	4.32	5.03

The most deformed SU(3) configurations dominate !

Model space dimensions

Realistic calculations in m-scheme basis (m=0)

	$pf_{5/2}g_{9/2}$					$pf_{5/2}$
	pp/nn	pn	pn+pp+nn	$(g_{9/2})^4$	FULL	
^{64}Ge	144,423	393,909	625,749	1,193,337	1,831,531	28,503
^{68}Se	819,636	1,156,433	1,929,014	-	-	93,710

Calculations in the Extended SU(3) model

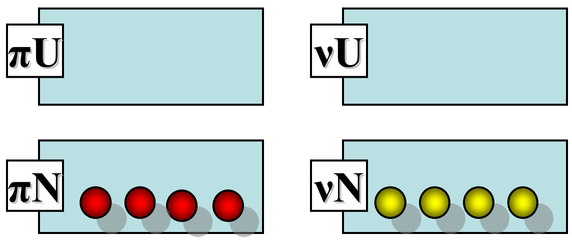
	4 irreps	5 irreps
^{64}Ge	148 (J=0) to 700 (J=8)	322 (J=0) to 2208 (J=8)

	7 irreps
^{68}Se	337 (J=0) to 2532 (J=6)

Dominant configurations for low-energy spectra

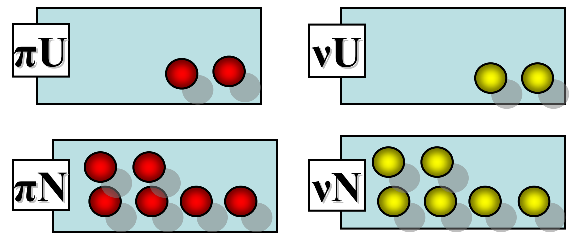
Upper-fp shell nuclei

$^{64}_{32}\mathrm{Ge}_{32}$, $^{68}_{34}\mathrm{Se}_{34}$ . . .



Empty abnormal space

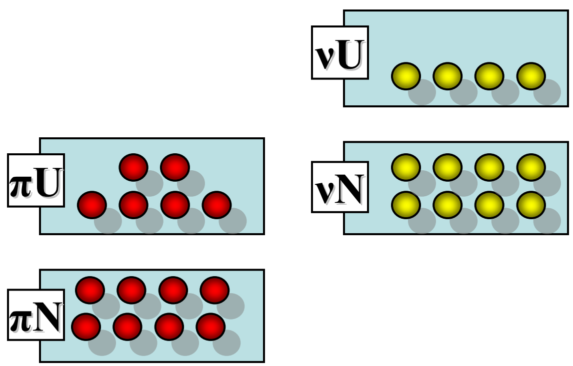
$^{72}_{36}\mathrm{Kr}_{36}$, $^{69}_{35}\mathrm{Br}_{34}$ . . .



Couple of particles in the abnormal space

Rare-earth nuclei

$^{158}_{64}\mathrm{Gd}_{94}$, $^{160}_{66}\mathrm{Dy}_{94}$ . . .



Many particles in the abnormal space

results in reduction of the required effective charge!

Conclusion: Summary of Findings

Part 1: SMC in $(f_{5/2}p)^m(g_{9/2})^n$ [Goodness of pseudo-SU(3)]

- Calculations using a realistic interaction for the N=Z isotopes of ^{58}Cu, ^{60}Zn, ^{62}Ga, ^{64}Ge and ^{68}Se as well as for isotopes away from the N=Z line were performed.
- Pseudo-SU(3) symmetry shown to be reasonably good for the even-even and odd-odd N=Z nuclei studied → use of symmetry-adapted basis beneficial.

Part 2: SMC in $(f_{5/2}p)^m(gds)^n$ [Extended SU(3) shell model]

- Introduced an extended SU(3) model that includes active nucleons (protons and neutrons) in the full unique-parity space.
- Results for ^{64}Ge and ^{68}Se suggest that this model can provide a reasonable mean for truncating the full space to a few SU(3) representations:
  - reasonable description of the energy spectra
  - leading irrep dominates for both ^{64}Ge and ^{68}Se
  - well-described B(E2) strengths, but still needs e_{eff}
  - single-particle occupancy - expected behavior observed
  - proof of principle complete - need to construct a “robust” code

Conclusion: Future Work

- Application of the extended SU(3) model to additional upper-fp + gds shell nuclei (Br and Kr isotopes of particular interest)
- Application of the theory to heavier deformed (rare-earth / actinide) nuclei
  - Origin and multiplicity of 0^+ states
  - B(E2) & B(M1) transition strengths
  - Vertical mixing and cluster modes
- Role of truncations [e.g., (λ,μ) & S] in the symmetry-adapted basis
- Search for new and improved interactions (parameter optimization)
- Evolution of key parameters from the theory of effective interactions