Approaches for configuration mixing based on mean-field extensions

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Outline

- Fermi systems: many-body theory vs. density functional theory (DFT).
- Specific approaches: shell-model, many particle-many hole (p-h) models, multi-reference DFT, particle-vibration coupling (PVC) models …
- An implementation of **PVC based on Skyrme functionals.**
- Application to **Giant Resonances and to β-decay.**
- A generalization **from PVC to Hybrid Configuration Mixing (HCM) model.**
- First results for **odd nuclei: ^{49}Ca, ^{133}Sb …**

DFT and time-dependent DFT

- Many groups are active in developing new energy density functionals (EDFs). The Hohenberg-Kohn theorem guarantees a functional exists that provides the exact g.s. solution:

$$H = T + V + V_{\rm ext} \qquad \min_\Psi \langle \Psi | H | \Psi \rangle = \min_\rho E[\rho]$$

- No clue how to build the exact functional. Start from the mean-field idea of working in a space of Slater determinants and improve on it ?

$$E[\rho] = \langle \Phi | H_{\rm eff} | \Phi \rangle \qquad \Phi = \text{Slater det.}$$

- One big problem is the time-dependent case. Runge-Gross theorem guarantees an exact functional …

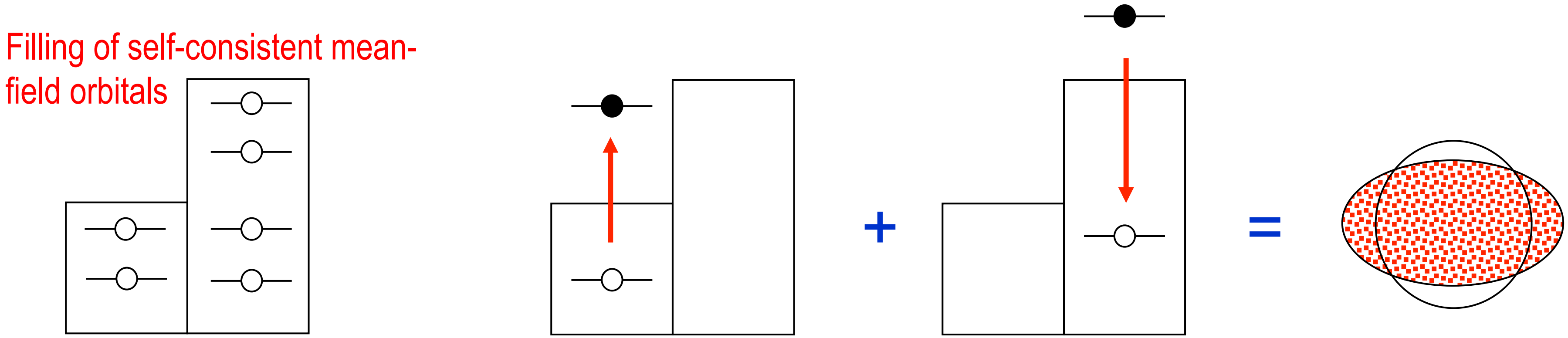
$$H' = H + V_{\rm pert}(t) \quad \Rightarrow \quad E[\rho(\vec{r}, t)]$$

- … but the exact functional should bear memory of the system's history !

$$\boxed{E_{\rm xc} = E_{xc}[\rho(\vec{r}, t')] \quad t' < t}$$

Many-body approaches

- In the many-body language, one starts from the **static mean-field** (Hartree-Fock, HF) or **time-dependent mean-field** (Random Phase Approximation, RPA) as the simplest approximations to describe ground-state (or excited states).



- Correlations can be associated with new degrees of freedom that are **explicitly** put in the model space …

- … or they can be associated with self-energy terms (new degrees of freedom are **“implicitly”** taken into account).

Approaches to the electron-electron interaction

- *Density-functional theory* (for ground-state properties only):

$$\left[-\tfrac{1}{2}\nabla^2 + V_{\text{ext}}(\mathbf{r}) + V_{\text{Hartree}}(\mathbf{r}) + V_{\text{xc}}(\mathbf{r}) - \varepsilon_i\right]\psi_i(\mathbf{r}) = 0$$

- *Many-body perturbation theory* based on Green's functions:

$$\left[-\tfrac{1}{2}\nabla^2 + V_{\text{ext}} + V_{\text{Hartree}} + \Sigma_{\text{xc}}(\omega) - \omega\right]G(\mathbf{r},\mathbf{r}',\omega) = \delta(\mathbf{r}-\mathbf{r}')$$

(which, *inter alia*, leads to the quasiparticle equation

$$\left[-\tfrac{1}{2}\nabla^2 + V_{\text{ext}} + V_{\text{Hartree}} + \Sigma_{\text{xc}}(\varepsilon) - \varepsilon\right]\psi(\mathbf{r}) = 0)$$

Note the two ways of describing exchange and correlation:

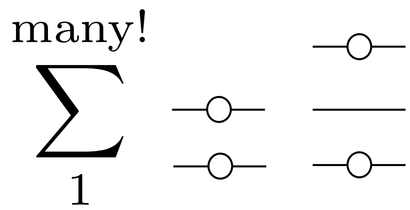
In DFT: $V_{\text{xc}}(\mathbf{r})$ (local, energy-independent potential)

In many-body theory: $\Sigma_{\text{xc}}(\mathbf{r},\mathbf{r}',\omega)$ (non-local, energy-dependent potential)

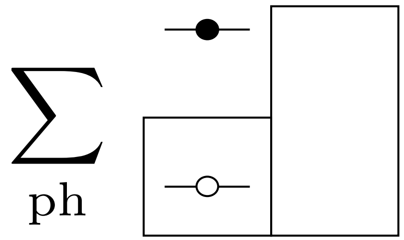
Courtesy: R. Godby

Examples

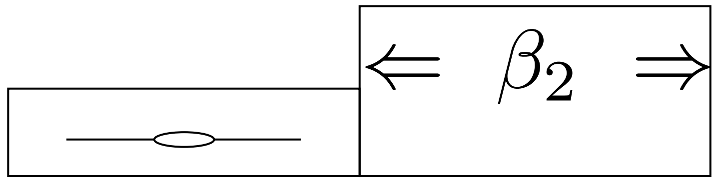
- Shell model: H is diagonalized on a basis of different Slater determinants



- "Many p-h" models (cf N. Pillet, P. Schuck, *et al.*, PRC)

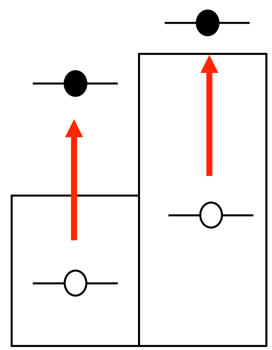


- Multi-reference DFT: basis that spans shapes (e.g. quadrupole deformations)



- Second-RPA: RPA plus 2p-2h

PVC : particles/core vibrations

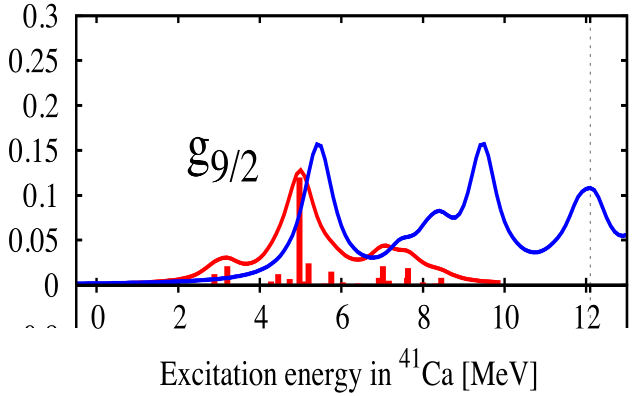


Aim: calculate strength fragmentation

We want to do PVC calculations because this is the most effective way, if not the only one, to explain **fragmentation and widths** of single-particle and giant resonances in a consistent fashion.

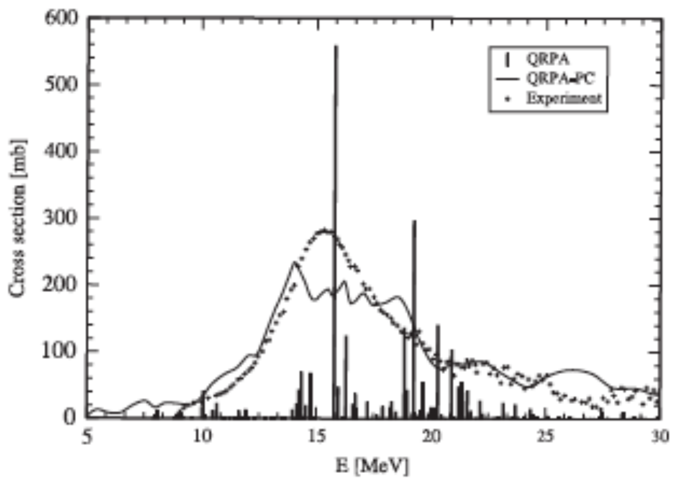
Single-particle strength

$9/2^+$ strength in ^{41}Ca (^{40}Ca core)



Multipole strength

Photoabsorbtion (dipole) cross section in ^{120}Sn



(Q)RPA plus PVC implementation

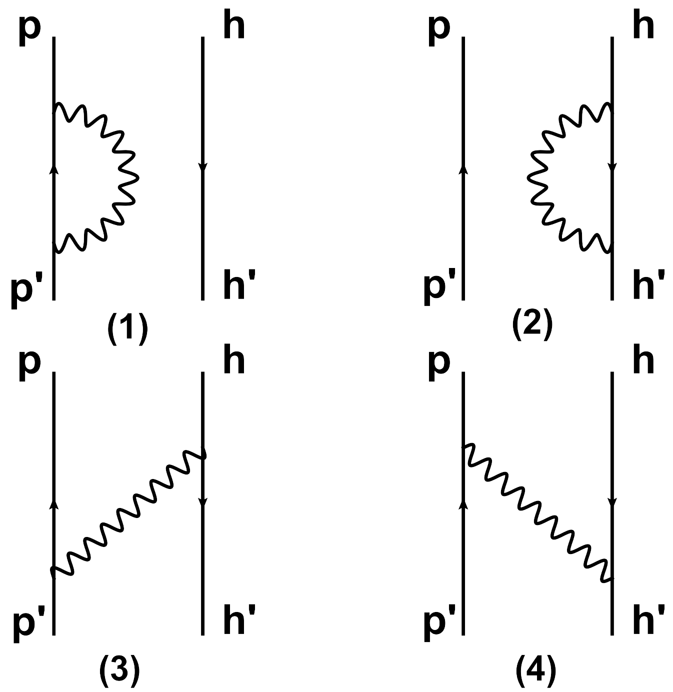
$$\begin{pmatrix} A+\Sigma(E) & B \\ -B & -A-\Sigma^*(-E) \end{pmatrix} \qquad \Sigma_{\mathrm{php'h'}}(E) = \sum_\alpha \frac{\langle ph|V|\alpha\rangle\langle\alpha|V|p'h'\rangle}{E-E_\alpha+i\eta}$$

One first solves the self-consistent Hartree-Fock plus Random Phase Approximation (HF-RPA) with Skyrme forces.

Then, the self-energy contribution is added (the state α is 1p-1h plus one phonon).

The scheme is known to be effective to produce the spreading width of GRs.

It is also possible to include the coupling of 1p-1h to continuum and calculate the particle decay.



Details, status and open problems

- The effective Hamiltonian is used consistently to build HF states, to solve RPA both for the states of interest and for the intermediate "phonons", and to calculate the interaction vertices.

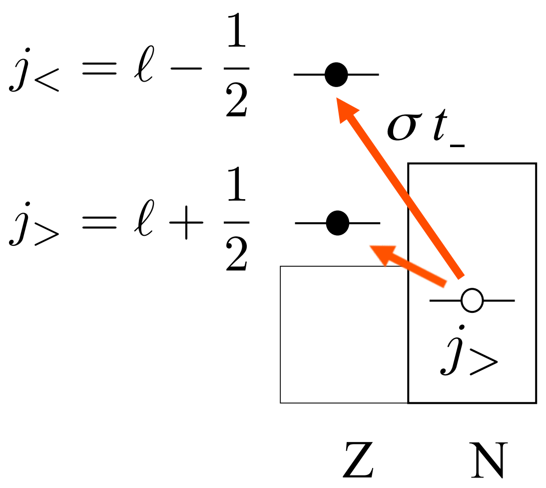
- All terms, including spin-orbit and tensor, are taken care of.

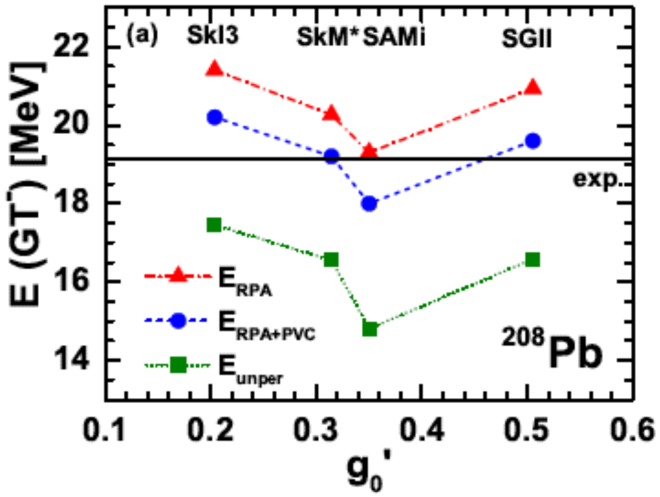
- The "cutoff" of the theory is provided by the fact that only collective phonons (usually those with fraction of strength larger than ≈2-5%) are retained.

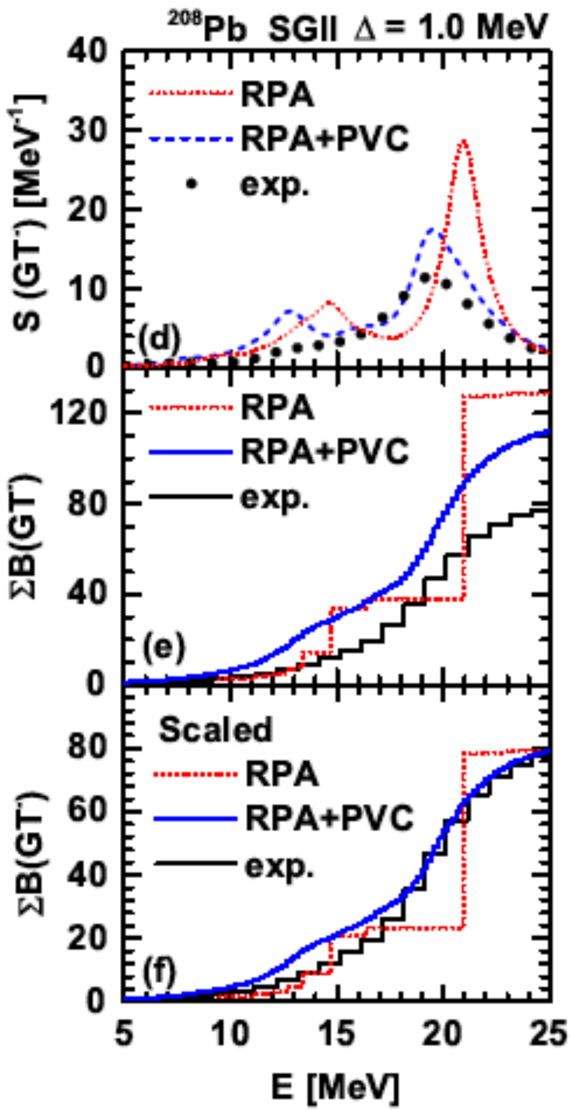
- Non-collective phonons: work in progress (see later).

- Still not much discussed: the parameters of the theory should, in principle, be refitted at the PVC level.

PVC model for Gamow-Teller Resonances







- The energy shift induced by PVC is very weakly interaction-dependent.
- The PVC calculations reproduce the lineshape of the GT response quite well.

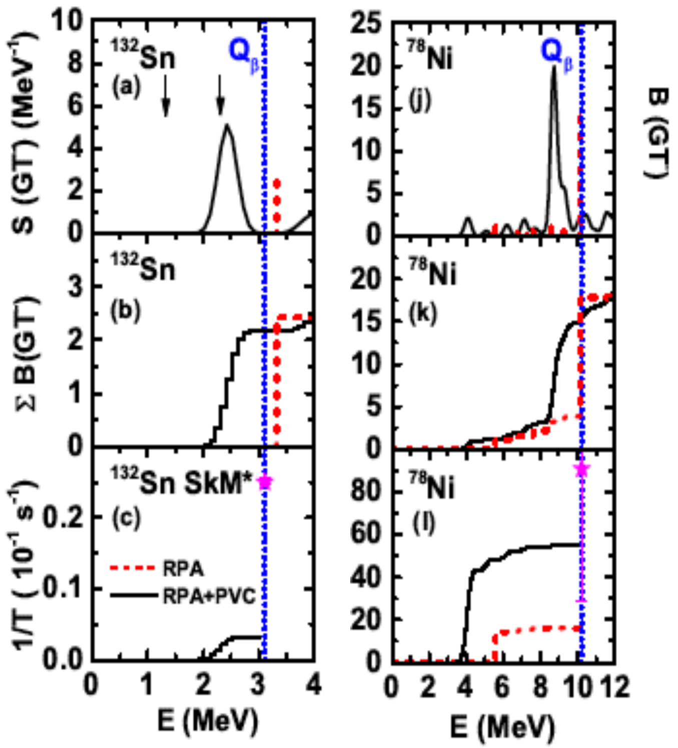
Y. Niu *et al.*, PRC 90, 054328 (2014).

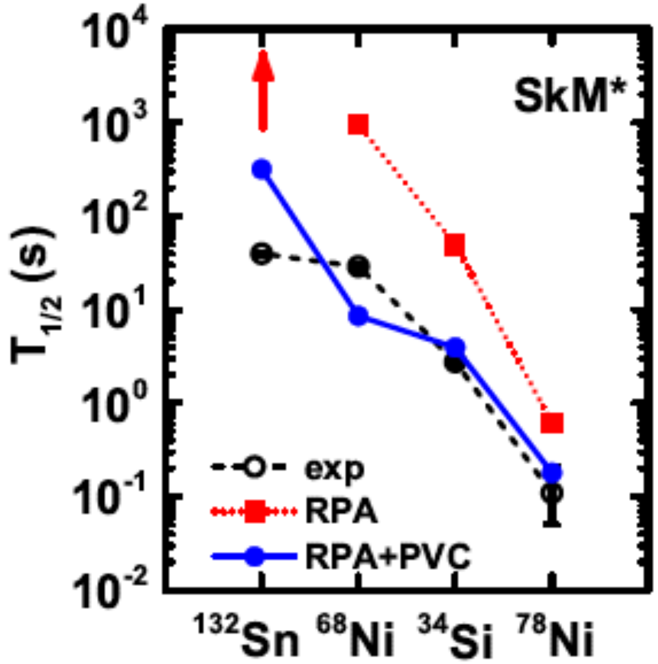
Application of PVC to β-decay

PVC can strongly affect the half-lives:

$$T_{1/2} = \frac{D}{g_A^2 \int_{E_c}^{Q_\beta} S(E) f(Z,E) dE}$$

Its effect is mainly of fragmenting and shifting down the RPA peaks, so that there is more strength in the decay window. The effect is enhanced by the phase-space factor. We definitely improve agreement with experiment.



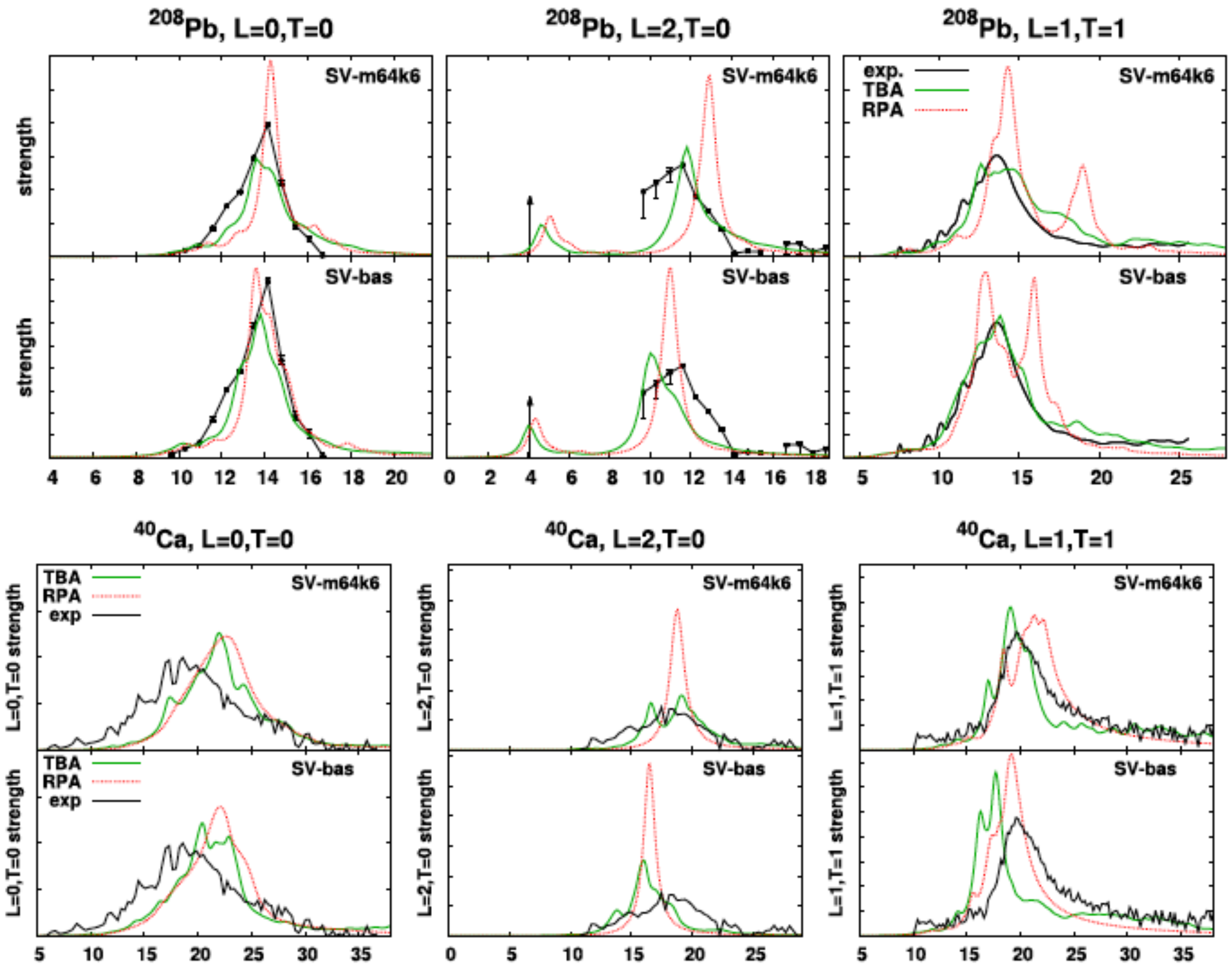


Y. Niu *et al.*, PRL 114, 142501 (2015).

TBA for non charge-exchange states

- TBA = Time-blocking approximation. Same diagrams as shown above.
- **Continuum included**

N. Lyutorovich *et al.*, PLB 749, 292 (2015)



Black = experiment
Red = RPA (width put by hand)
Green = full calculation

Relativistic TBA calculations

E. Litvinova *et al.*

- Results available for both non charge-exchange and charge-exchange excitations.
- **Upper panel: photobsorbtion cross section** [50 Years of Nuclear BCS, World Scientific, 2013];
- **Lower panel**: **spin-dipole strength** [PLB 706, 477 (2012)].

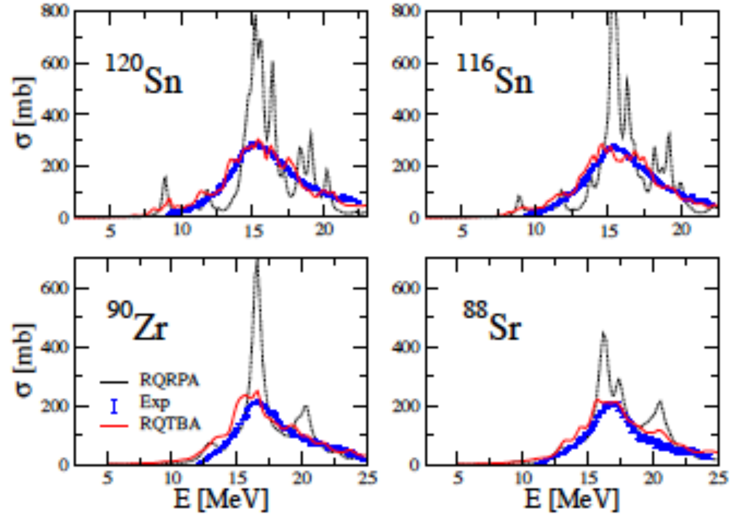
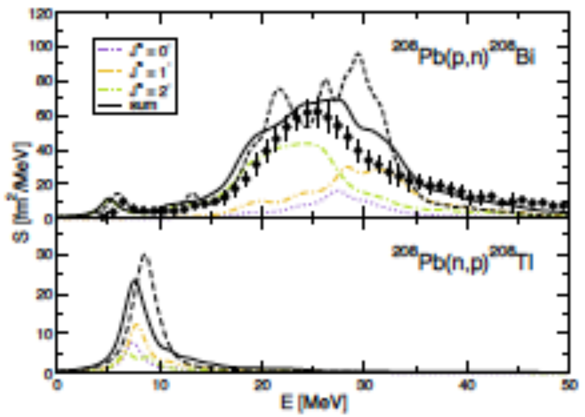


Fig. 1. Total dipole photoabsorption cross section in stable medium-mass nuclei.

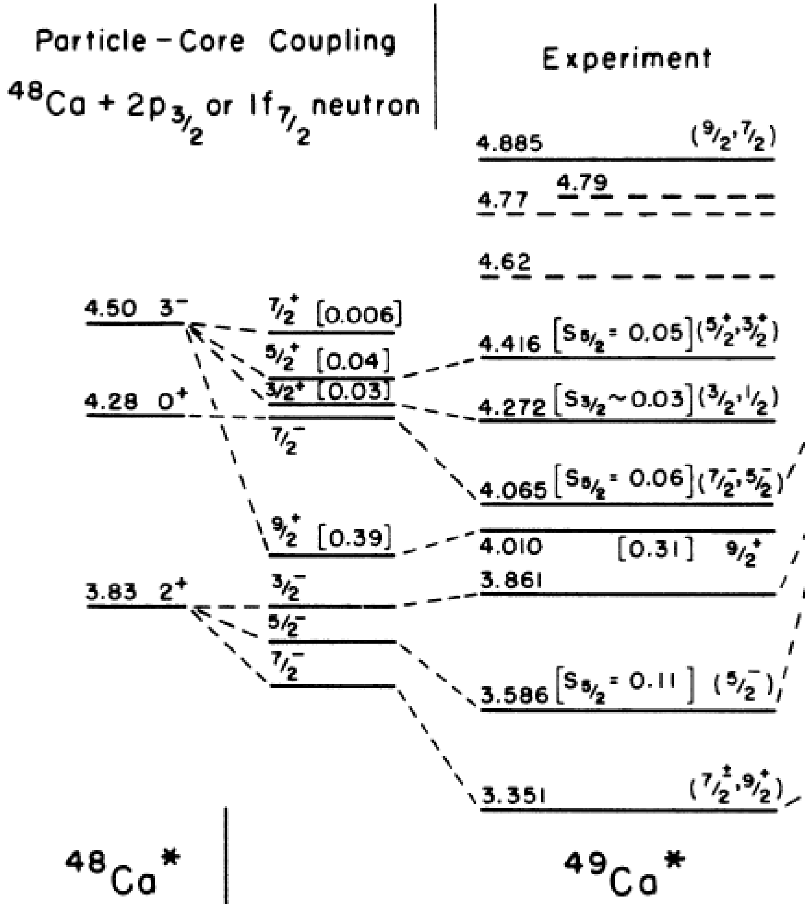
- RMF Lagrangians employed.
- Pairing included in the case of open-shell systems.
- Extension beyond TBA in progress: Phys. Rev. C 91, 034332 (2015). Cf. also: M. Baldo *et al.*, J. Phys. G 42 (2015) 085109.



MOVING TO ODD NUCLEI ...

Example: states from an old (d,p) experiment on ^{48}Ca.

Interpreted as neutrons coupled with a ^{48}Ca phonon.

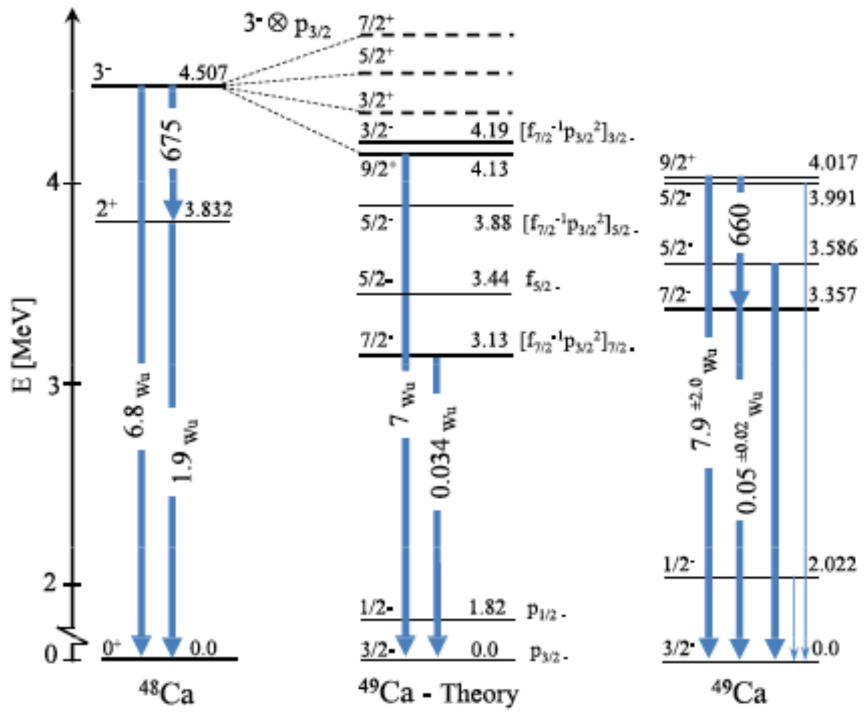


T.R. Canada *et al.*, Phys. Rev. C4, 471 (1971)

$^{64}Ni+^{48}Ca$ (5.7 MeV/u) performed at LNL recently. Analysis for ^{49}Ca.

The angular momenta have been found to be aligned perpendicular to the reaction plane.

Spin / lifetimes extracted.



D. Montanari *et al.*, Phys. Lett. B 697, 288 (2011)

Physics case: spectroscopy of odd nuclei close to a magic core

- There are several examples of spectra in which "particle" states (large spectroscopic factor in transfer reactions) co-exist with states made up with "particle plus core vibration" states (gamma decay similar to that of the core vibration).

$$B(E\lambda, [j' \otimes \lambda]_j \to j') = B(E\lambda, \lambda \to 0)$$

- Could be a good playground for particle-vibration coupling models …

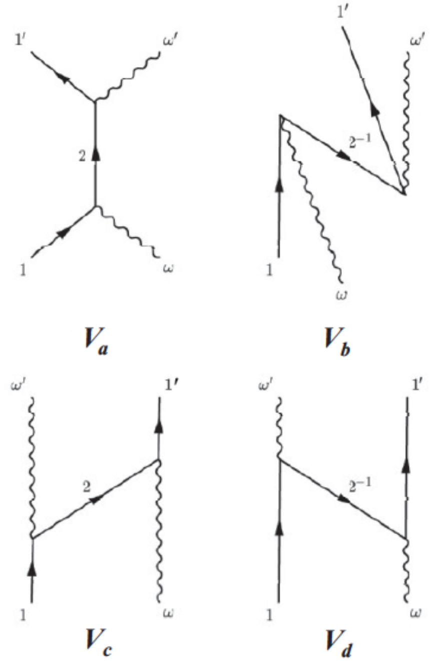
- … but in some cases particle-phonon states are instead 2p-1h, or 3p-2h states ("shell model-like" states).

Perturbative particle-vibration coupling

- Formulas for the perturbative coupling between a **particle-phonon state** and **other states** are well-known.

$$\langle [j' \otimes J]_j \, | V_a + V_b | \, [j' \otimes J]_j \rangle = \sum_{j_1} \frac{1}{2j_1+1} \frac{\langle j_1 || V || j', J \rangle^2}{\varepsilon(j') - \varepsilon(j_1) + \hbar\omega_J}$$

$$\langle [j' \otimes J]_j \, | V_c + V_d | \, [j' \otimes J]_j \rangle = \sum_{j_1} \frac{2j'+1}{2j_1+1} \left\{ \begin{array}{ccc} J & j' & j_1 \\ J & j' & j \end{array} \right\} \frac{\langle j_1 || V || j', J \rangle^2}{\varepsilon(j_1) - \varepsilon(j') + \hbar\omega_J}$$



- **Novelty: we use now Skyrme consistently.**

Single-particle energies from HF, phonons from RPA and the same V at the vertex (no phenomenological parameter).

D. Montanari *et al.*, Phys. Lett. B 697, 288 (2011); PRC 85, 044301 (2012).

PHYSICAL REVIEW C VOLUME 58, NUMBER 1 JULY 1998

New Skyrme interaction for normal and exotic nuclei

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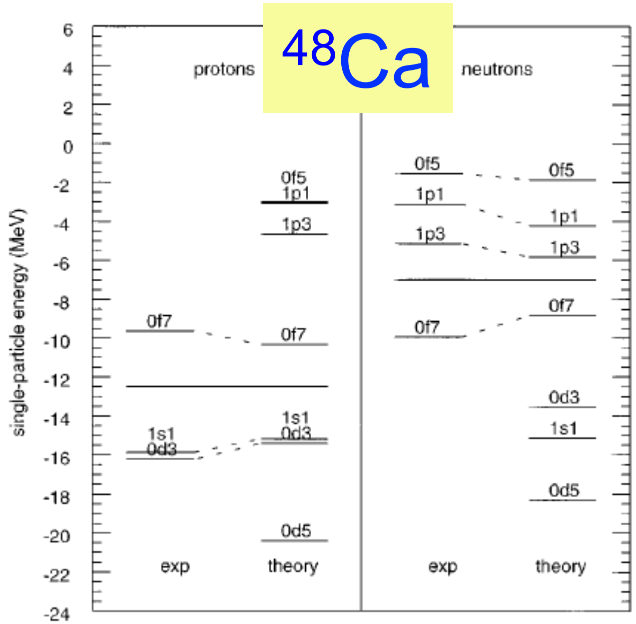
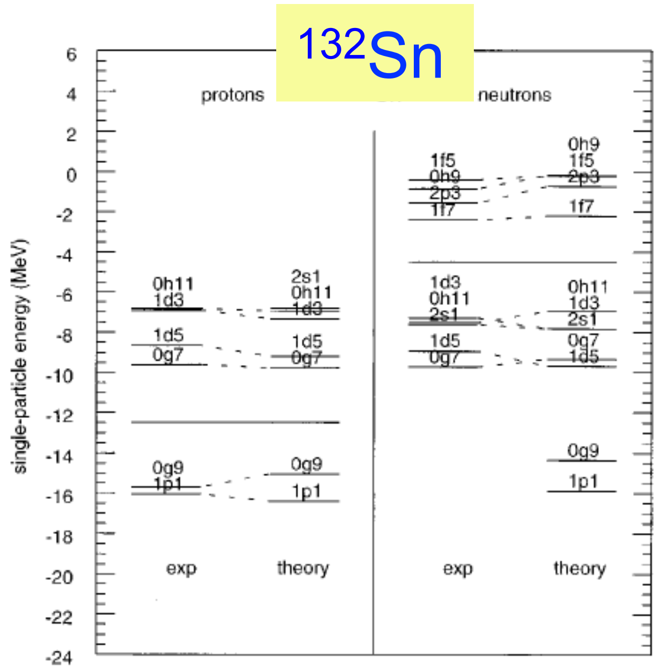
(Received 5 May 1997)

SkX : fitted to s.p. energies as well.
Because of that reason, produces also reasonable low-lying vibrational states.

gies. A complete microscopic model of nuclear structure might be based upon starting with the SKX mean field (or a similar suitable Skyrme interaction) and then adding the correlation energy due to the valence interactions, which includes the deformation driving proton-neutron interaction and the like-nucleon interactions (mainly pairing). It is interesting to try to derive the valence interactions from the Skyrme interactions [46,58], however, they may not be adequate since the valence spectra are sensitive to the higher multipole components of the interaction which are not determined from the closed shell data. At the most microscopic level the valence correlations can be treated by the large-basis shell-model methods for light nuclei [17] which are being extended to heavy nuclei with the Monte-Carlo meth-





Results (slide by S. Leoni)

Particle-Vibration Coupling

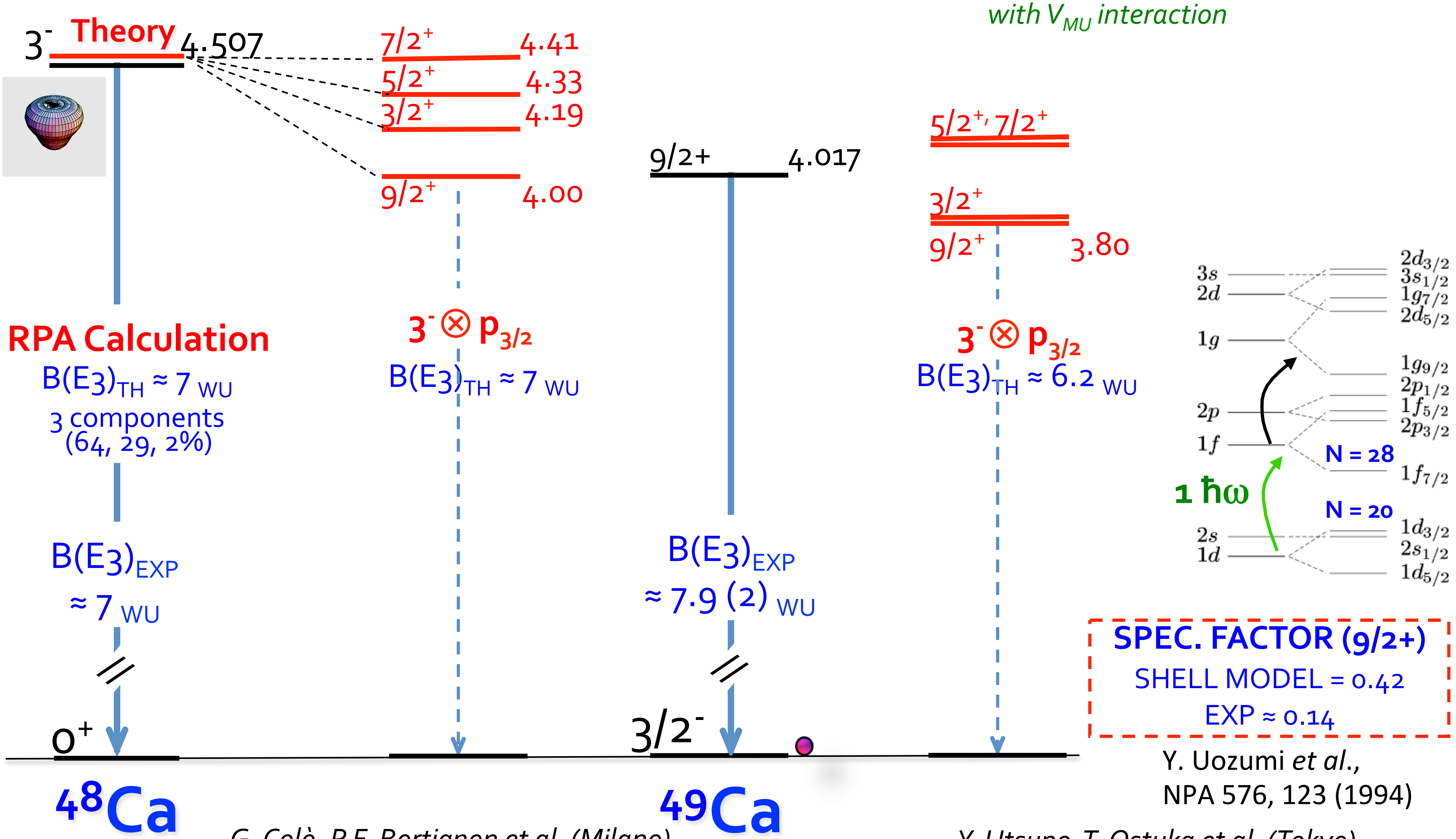
Weak coupling

Large Scale SHELL Model

FULL sd-pf-sdg shell still NOT possible

Truncation scheme sd+pf+sdg (2.515.437 conf)

with V_{MU} interaction



G. Colò, P.F. Bortignon et al. (Milano)

Y. Utsuno, T. Ostuka et al. (Tokyo)

Shell model calculations

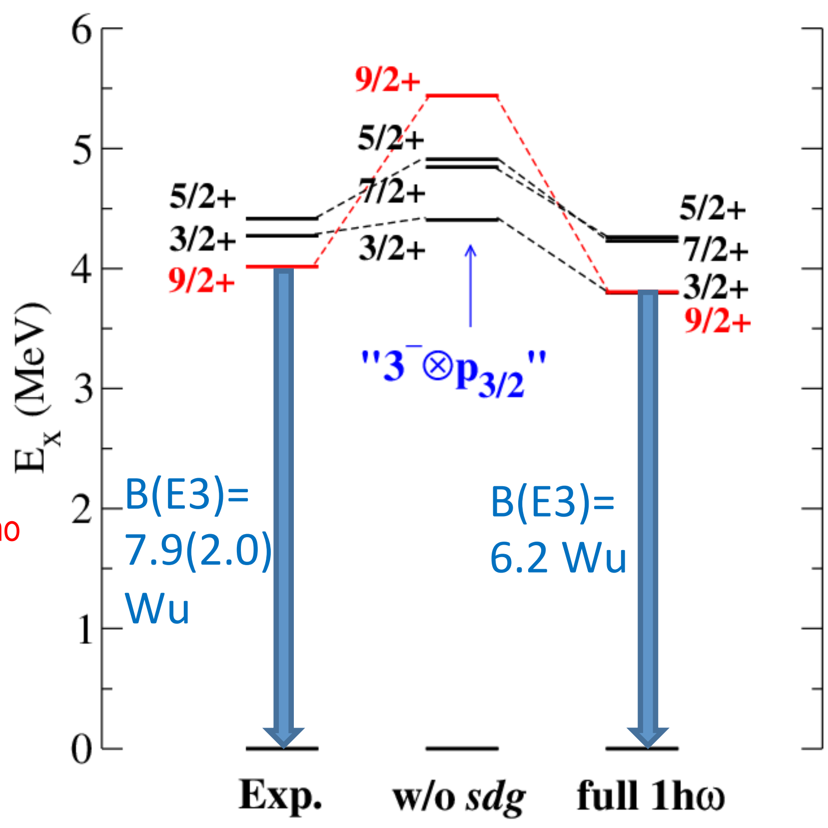
- Ca region may lie at the **limits for SM.**

- Need to mix different effective interactions and adjust pf-sdg gap.

Y. Utsuno *et al.*, Phys. Rev. C86, 051301(R) (2012)

- The 9/2$^+$ state in ^{49}Ca is predicted to be quite mixed: $p_{3/2} \times 3^- + g_{9/2}$

Spec. factor (0.42) larger than exp. (0.14);
B(E3) smaller than exp.

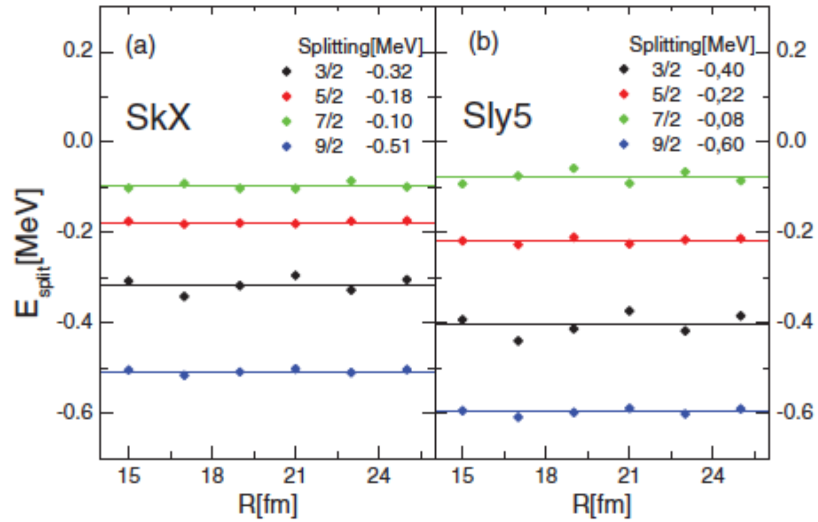


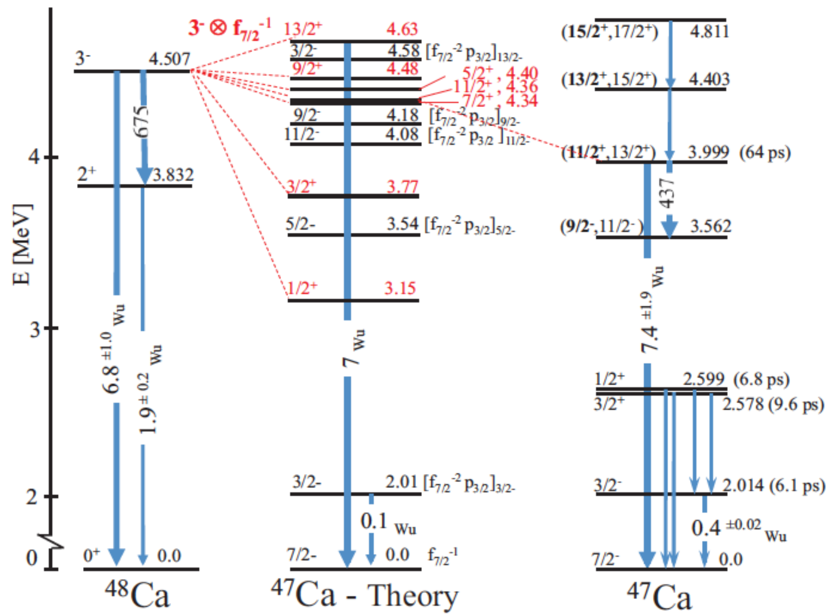
Courtesy: Y. Utsuno

- **^{132}Sn region unfeasible !**

More results from the Ca region

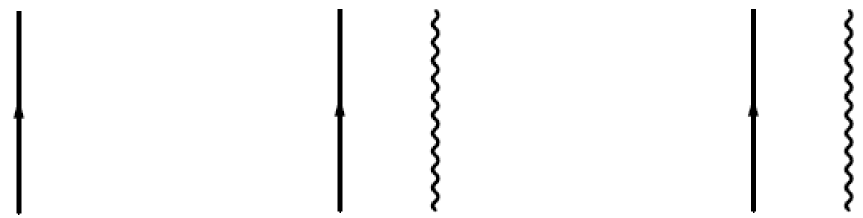
- We have included **quasi-bound and continuum states**.
- **Sensitivity to the interaction** has been studied. Not too strong but is there.
- In ^{47}Ca we see situations in which the coupling is **not perturbative**, and also states that seem, from shell-model calculations, to be of **2h-1p type**.





Configuration mixing (CM) model

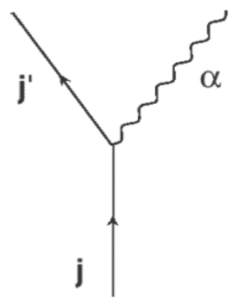
We start from a **basis** made up with **particles** (or holes) around a core, and with **excitations** of the same core (RPA "phonons").



On this basis we **diagonalize the Hamiltonian** $H = H_0 + V$,

$$H_0 = \sum_{jm} \varepsilon_j a^\dagger_{jm} a_{jm} + \sum_{NJM} \hbar\omega_{NJ} \Gamma^\dagger_{NJM} \Gamma_{NJM},$$

$$V = \sum_{jmj'm'} \sum_{NJM} \frac{\langle j || V || j', NJ \rangle}{\hat{j}} a_{jm} \left[a^\dagger_{j'} \otimes \Gamma^\dagger_{NJ} \right]_j$$



"Hybrid" configuration mixing

- Some of the RPA phonons might be actually pure p-h states. Then, the states of our basis are 2p-1h**. In this sense they are not "vibrations" and the model cannot be considered "PVC".**

- In this case Pauli principle violations can be important. **We correct for the non-orthonormality and overcompleteness of the basis by introducing the NORM matrix.**

$$n(j_1' n_1 J_1, j_2' n_2 J_2) = \delta(j_1', j_2')\delta(n_1, n_2)\delta(J_1, J_2) - \sum_{h_1} (-)^{J_1+J_2+j_1'+j_2'} \hat{J}_1 \hat{J}_2 \left\{ \begin{array}{ccc} j_2' & j_{h_1} & J_1 \\ j_1' & j & J_2 \end{array} \right\} X^{(n_1 J_1)}_{j_2' h_1} X^{(n_2 J_2)}_{j_1' h_1}$$

This is the overlap between 1p-1 "phonon" states.

The diagonal part reduces to 1 – $(2j+1)^{-1}$ in simple cases.
In those cases, the interpretation is simple.

Cf. S. Mishev and V.V. Voronov, PRC 78, 024310 (2008)

Basic equation (cf. SM/MR-DFT)

$$\boxed{\mathcal{H} - E\mathcal{N} = 0}$$

$$\mathcal{H} = \begin{pmatrix} \varepsilon_{n_1 lj} & 0 & \frac{\langle n_1 lj||V||n_1' l_1' j_1' N_1 J_1\rangle}{\hat{j}} & \frac{\langle n_1 lj||V||n_2' l_2' j_2' N_2 J_2\rangle}{\hat{j}} \\ 0 & \varepsilon_{n_2 lj} & \frac{\langle n_2 lj||V||n_1' l_1' j_1' N_1 J_1\rangle}{\hat{j}} & \frac{\langle n_2 lj||V||n_2' l_2' j_2' N_2 J_2\rangle}{\hat{j}} \\ \frac{\langle n_1 lj||V||n_1' l' j_1' N_1 J_1\rangle}{\hat{j}} & \frac{\langle n_2 lj||V||n_1' l' j_1' N_1 J_1\rangle}{\hat{j}} & \varepsilon_{n_1' l_1' j_1'} + \hbar\omega_{N_1 J_1} & 0 \\ \frac{\langle n_1 lj||V||n_2' j_2' N_2 J_2\rangle}{\hat{j}} & \frac{\langle n_2 lj||V||n_2' l' j_2' N_2 J_2\rangle}{\hat{j}} & 0 & \varepsilon_{n_2' l_2' j_2'} + \hbar\omega_{N_2 J_2} \end{pmatrix}.$$

$$\mathcal{N} = \begin{pmatrix} 1 & 0 & \ldots & 0 & 0 & \ldots \\ 0 & 1 & \ldots & 0 & 0 & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & n(j_1' n_1 J_1, j_1' n_1 J_1) & n(j_1' n_1 J_1, j_2' n_2 J_2) & \ldots \\ 0 & 0 & \ldots & n(j_2' n_2 J_2, j_1' n_1 J_1) & n(j_2' n_2 J_2, j_1' n_1 J_1) & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix}.$$

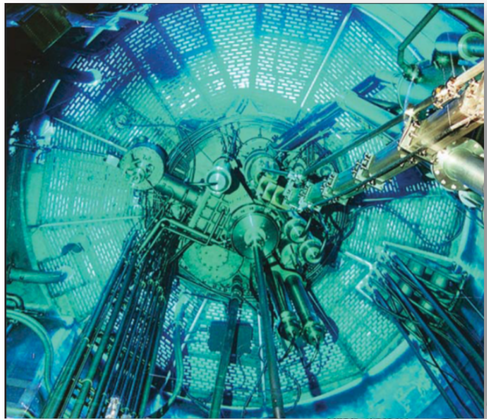
Spurious states !

The γ-Spectroscopy Campaign @ ILL-reactor (Grenoble)

2012-2013: 2 Reactor Cycles (100 days)

Induced fission of ^{235}U and ^{241}Pu – for the first time HPGe installed around n

58 MW REACTOR



World Brightest Continuum neutron source

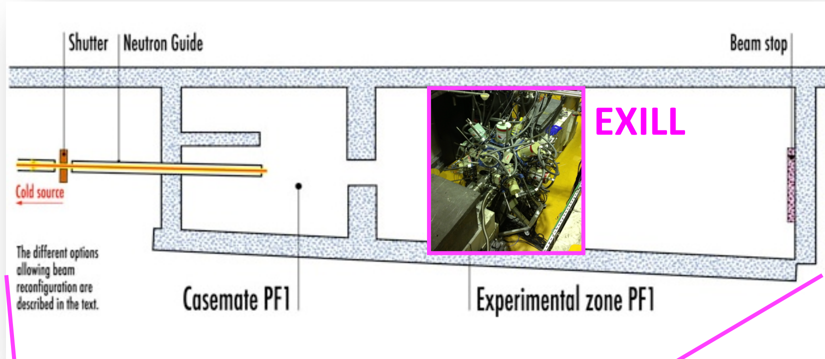
In pile

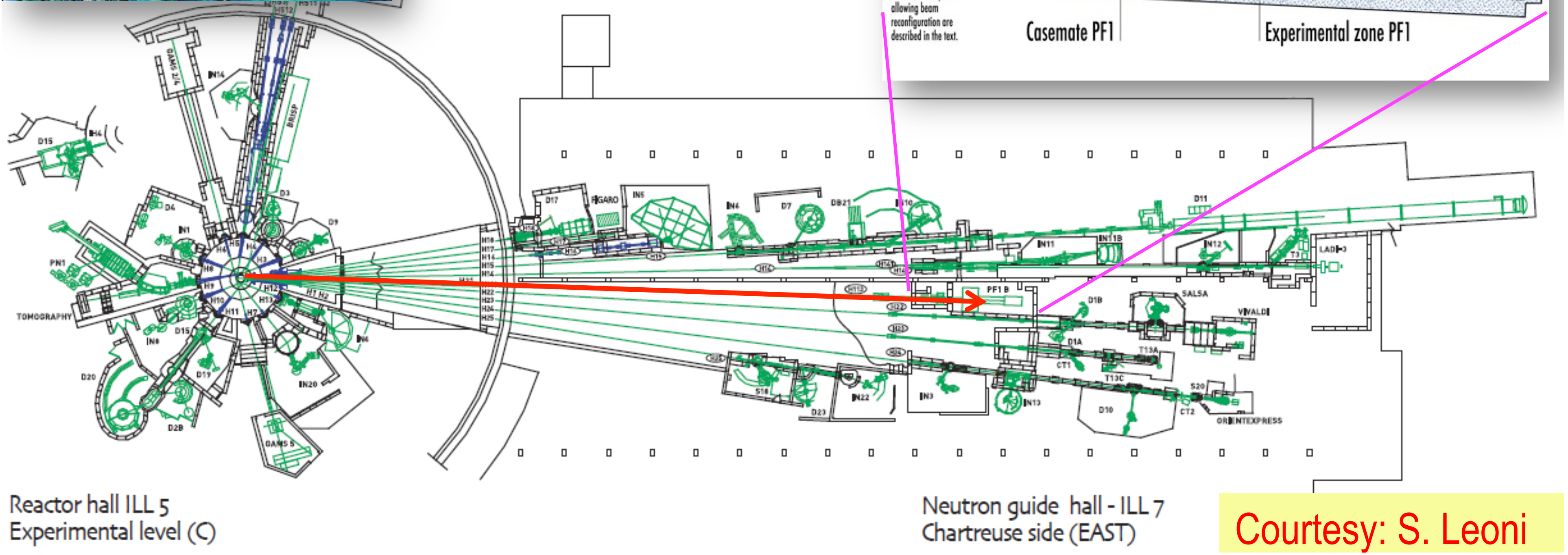
$\Phi_n = 5\times10^{14}\ n\ cm^{-2}\ s^{-1}$

Dedicated ballistic neutron guide

Highly collimated beam (1 cm²)
Cold neutrons (meV)

$\Phi_n = 2\times10^{8}\ n\ cm^{-2}\ s^{-1}$

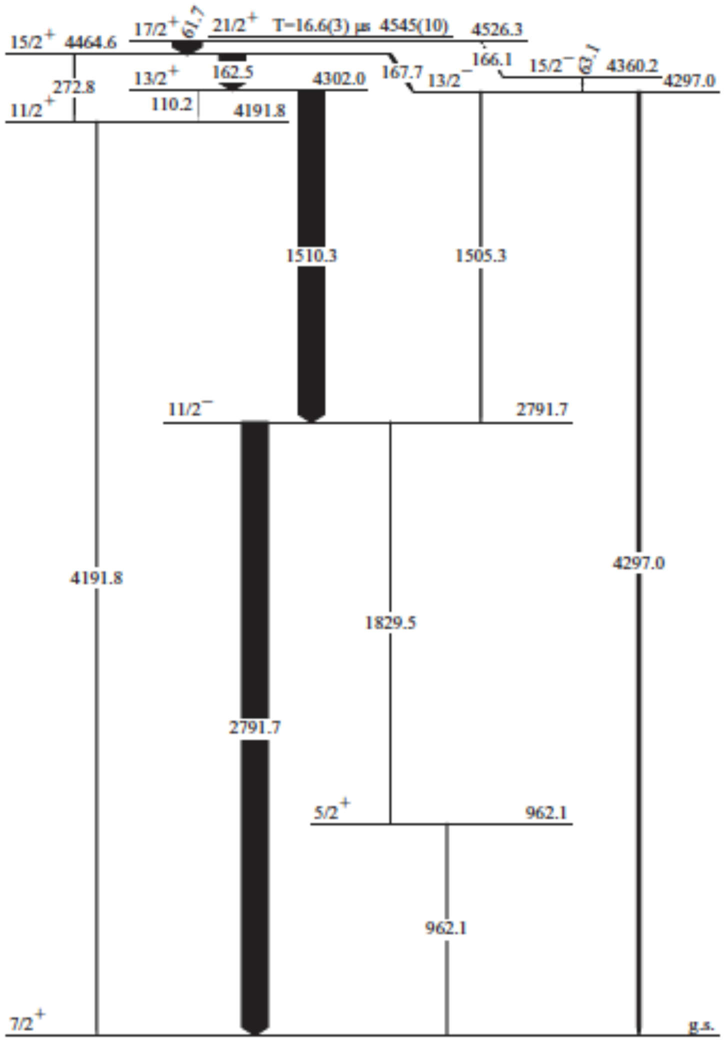




Courtesy: S. Leoni

Spectroscopy of ^{133}Sb (^{132}Sn + p)

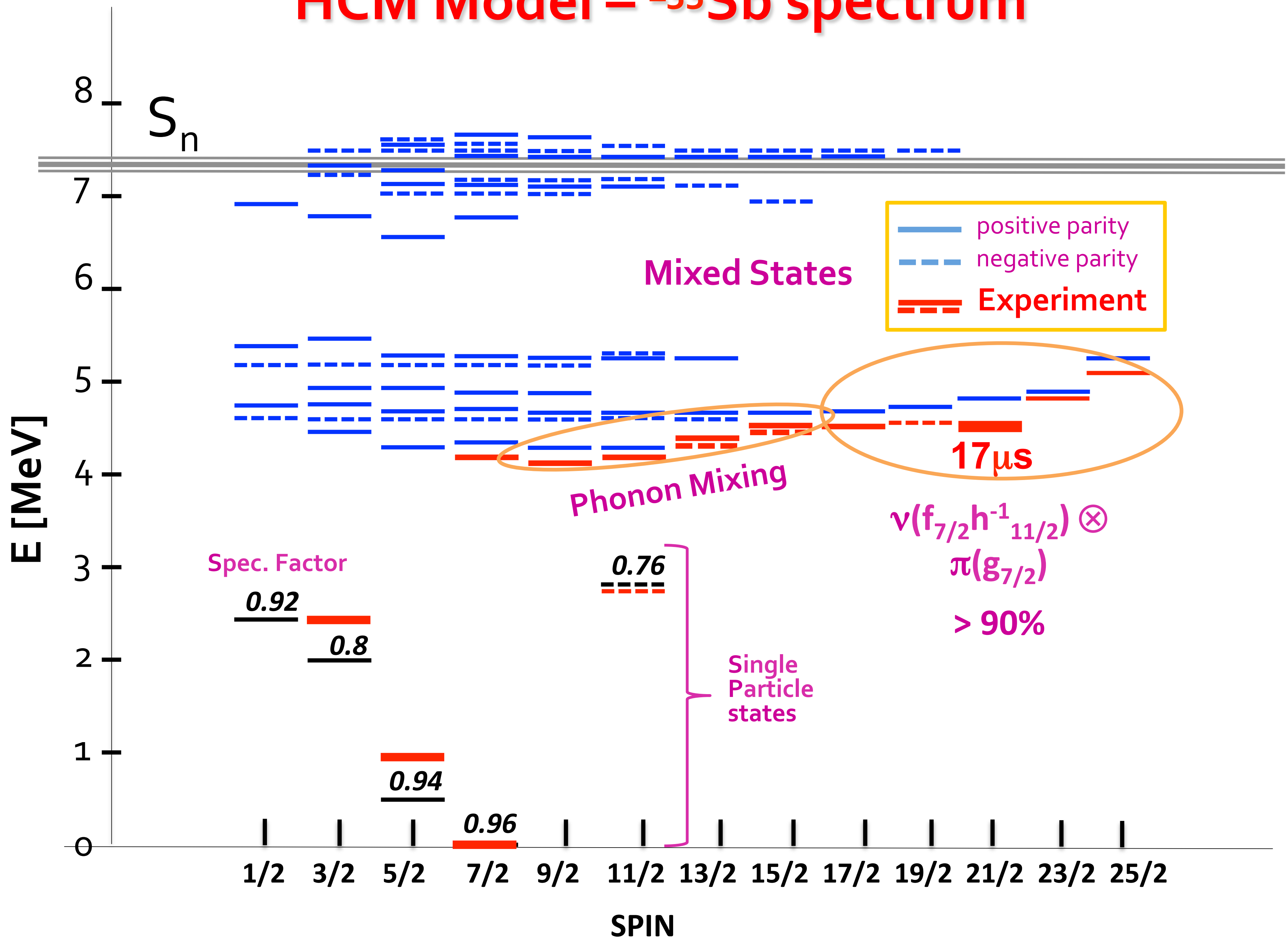
- Despite the importance of the region around ^{132}Sn, the information about **low-lying states of neighbouring nuclei** need still be completed.



W. Urban *et al.*, PRC 79, 037304 (2009)

- Recently new measurements (G. Bocchi *et al.*) have shed light on some **HIGHER SPIN** states (up tp $25/2^{+}$).
- The odd proton is $g_{7/2}$.
- Low spin states may come from coupling to 2^{+}, 3^{-}, 4^{+} phonons.
- High spin states can only come from $g_{7/2}$ coupled to $h_{11/2}^{-1}\ f_{7/2}$ neutron p-h states.
- **Lifetimes** have been measured.

HCM Model – ^{133}Sb spectrum



Microscopic content of the states

	EXP.	Calculation with 2^+, 3^-, 4^+	All excitations below 5.5 MeV included
$9/2^+$	4.027	3.84 $[\pi g_{7/2} \otimes 2^+ \ (0.82)]$	4.08 $[\pi g_{7/2} \otimes 2^+ \ (0.80)]$
$11/2^+$	4.192	3.82 $[\pi g_{7/2} \otimes 2^+ \ (0.74)]$	4.11 $[\pi g_{7/2} \otimes 2^+ \ (0.78)]$
$13/2^+$	4.302	4.66 $[\pi g_{7/2} \otimes 4^+ \ (1.00)]$	4.44 $[\pi g_{7/2} \nu h^{-1}_{11/2} \nu f_{7/2} \ (0.40)]$
$15/2^+$	4.464	4.37 $[\pi g_{7/2} \otimes 4^+ \ (0.98)]$	4.45 $[\pi g_{7/2} \nu h^{-1}_{11/2} \nu f_{7/2} \ (0.40)]$
$17/2^+$	4.526		4.58 $[\pi g_{7/2} \nu h^{-1}_{11/2} \nu f_{7/2} \ (0.66)]$
$19/2^+$	4.539		4.64 $[\pi g_{7/2} \nu h^{-1}_{11/2} \nu f_{7/2} \ (0.73)]$
$21/2^+$	4.545		4.76 $[\pi g_{7/2} \nu h^{-1}_{11/2} \nu f_{7/2} \ (0.92)]$
$23/2^+$	4.753		4.83 $[\pi g_{7/2} \nu h^{-1}_{11/2} \nu f_{7/2} \ (0.98)]$
$25/2^+$	4.844		5.11 $[\pi g_{7/2} \nu h^{-1}_{11/2} \nu f_{7/2} \ (1.00)]$

Different kinds of excitations in ^{132}Sn

	Energy		Transition strength		Main components
	Exp.	Theory (RPA)	Exp.	Theory (RPA)	Theory (RPA)
2^+	4.041	3.87	7	4.75	$\nu h^{-1}_{11/2} f_{7/2}$ (0.56), $\pi g^{-1}_{9/2} d_{5/2}$ (0.19), $\pi g^{-1}_{9/2} g_{7/2}$ (0.14)
3^-	4.352	5.02	> 7.1	9.91	$\nu s^{-1}_{1/2} f_{7/2}$ (0.40), $\nu d^{-1}_{3/2} f_{7/2}$ (0.12), $\pi p^{-1}_{1/2} g_{7/2}$ (0.12)
4^+	4.416	4.46	4.42	5.10	$\nu h^{-1}_{11/2} f_{7/2}$ (0.63), $\pi g^{-1}_{9/2} g_{7/2}$ (0.21)
6^+	4.716	4.73		1.65	$\nu h^{-1}_{11/2} f_{7/2}$ (0.86), $\pi g^{-1}_{9/2} g_{7/2}$ (0.11)
4^-	4.831	5.68		0.16	$\nu s^{-1}_{1/2} f_{7/2}$ (0.91)
8^+	4.848	4.80		0.28	$\nu h^{-1}_{11/2} f_{7/2}$ (0.98)
5^+	4.885	4.77		0.61	$\nu h^{-1}_{11/2} f_{7/2}$ (0.99)
7^+	4.942	4.80		0.81	$\nu h^{-1}_{11/2} f_{7/2}$ (0.98)
5^-	4.919	5.98		0.96	$\nu d^{-1}_{3/2} f_{7/2}$ (0.96)
(9^+)	5.280	4.99		0.16	$\nu h^{-1}_{11/2} f_{7/2}$ (0.99)
2^-		5.44		1.77	$\nu d^{-1}_{3/2} f_{7/2}$ (0.79)

One should contrast real phonons with pure p-h states.

Co-workers

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Conclusions

- Among/confronted with other many-body methods, particle-vibration coupling can be put on a firm basis, and treated with modern effective interactions without approximations.

- Agreement with data for the giant resonance or β-decay lineshape.

- We wish now to treat the spectra of odd nuclei, in which **states have mixed character**, namely they can be also 2p-1h, … We thus extend PVC, by taking into account **norm overlaps.**

- Conceptual problem: the **interaction** should be refitted.