The description of stable and neutron-rich nuclei: correlations within and beyond Density Functional Theory

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Motivation and outline

- Self-consistent mean-field or DFT calculations provide, if calibrated, good results for bulk properties (masses, radii). Problems with spectroscopy.

- Time-dependent calculations (RPA) are also standard tools.

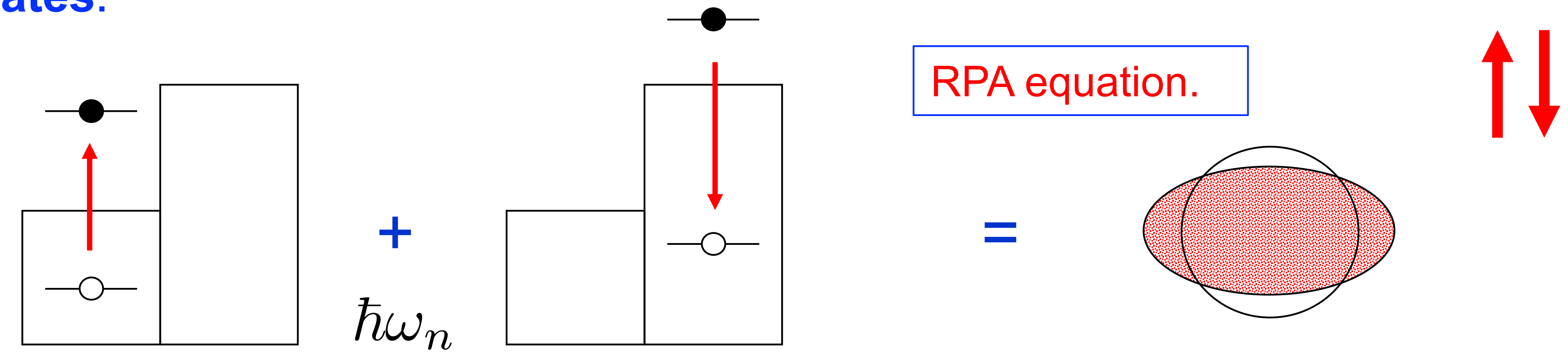
- It is possible to introduce more correlations if necessary.

- Description of β-decay: problems with RPA and how to reproduce experimental findings.

- A model to describe low-lying states in odd-nuclei.

Hartree-Fock ground-state and RPA

We use V_{Skyrme}. The g.s. of closed-shell nuclei is obtained by Hartree-Fock. The excitations can be described by superposition of **1 particle-1 hole states**.

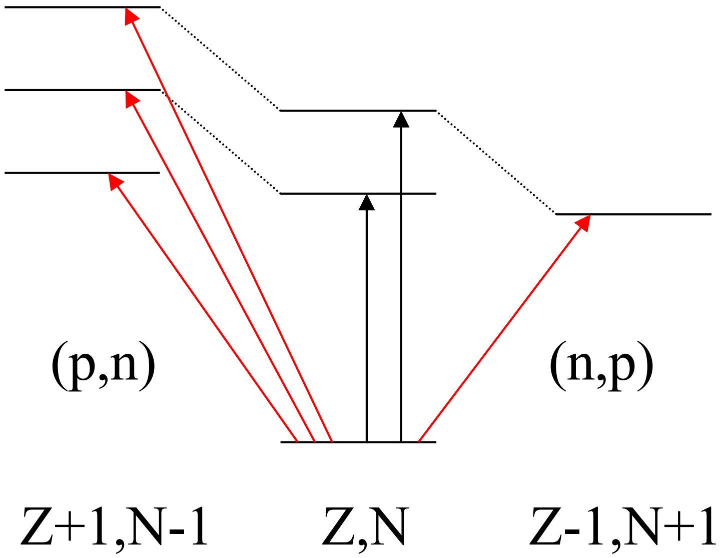


RPA equation.

$$|n\rangle = \sum_{ph} X_{ph}|ph^{-1}\rangle + Y_{ph}|hp^{-1}\rangle$$

RPA can be applied to charge-exchange transitions.

Some require external energy from (p,n) or $(^3$He,t), others are inside the β-decay window.



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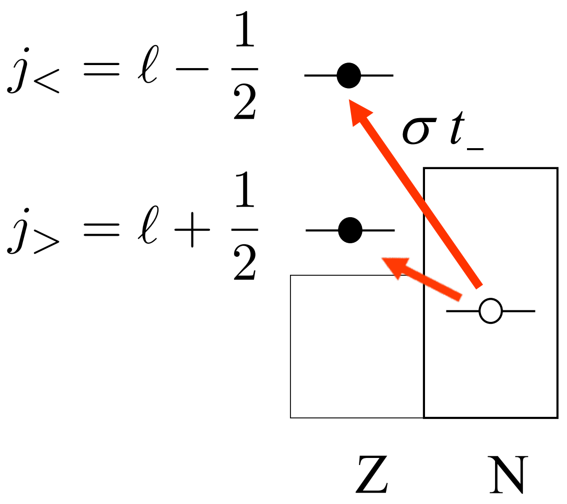
The Gamow-Teller (GT) resonance



$$\varepsilon_{\rm ph}^{(II)}, \varepsilon_{\rm ph}^{(I)}$$

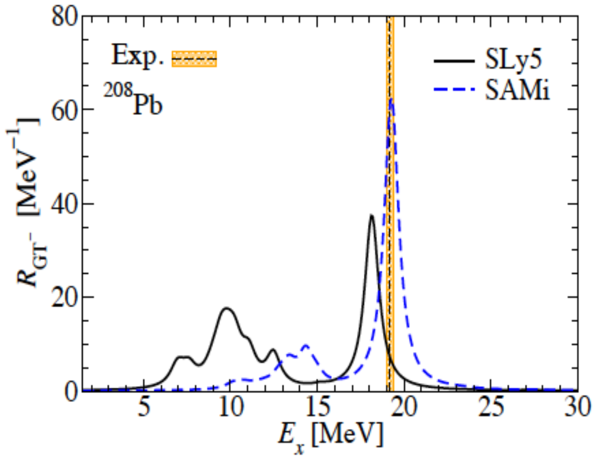
Highest and lowest particle-hole transitions in the picture

$$\varepsilon_{\rm ph}^{(II)} - \varepsilon_{\rm ph}^{(I)} = \varepsilon_{j_<} - \varepsilon_{j_>}$$

$j_>$

Unperturbed GT energy related to the spin-orbit splitting

$$\hbar\omega \approx \varepsilon_{\rm ph} + \langle V_{\rm res} \rangle$$



RPA GT energy related also to V in στ channel

We are able now to perform self-consistent calculations of the GTR – with a given Skyrme force we reproduce its integral properties.

X. Roca-Maza, G.C., H. Sagawa, PRC 86, 031306(R) (2012)

β-decay

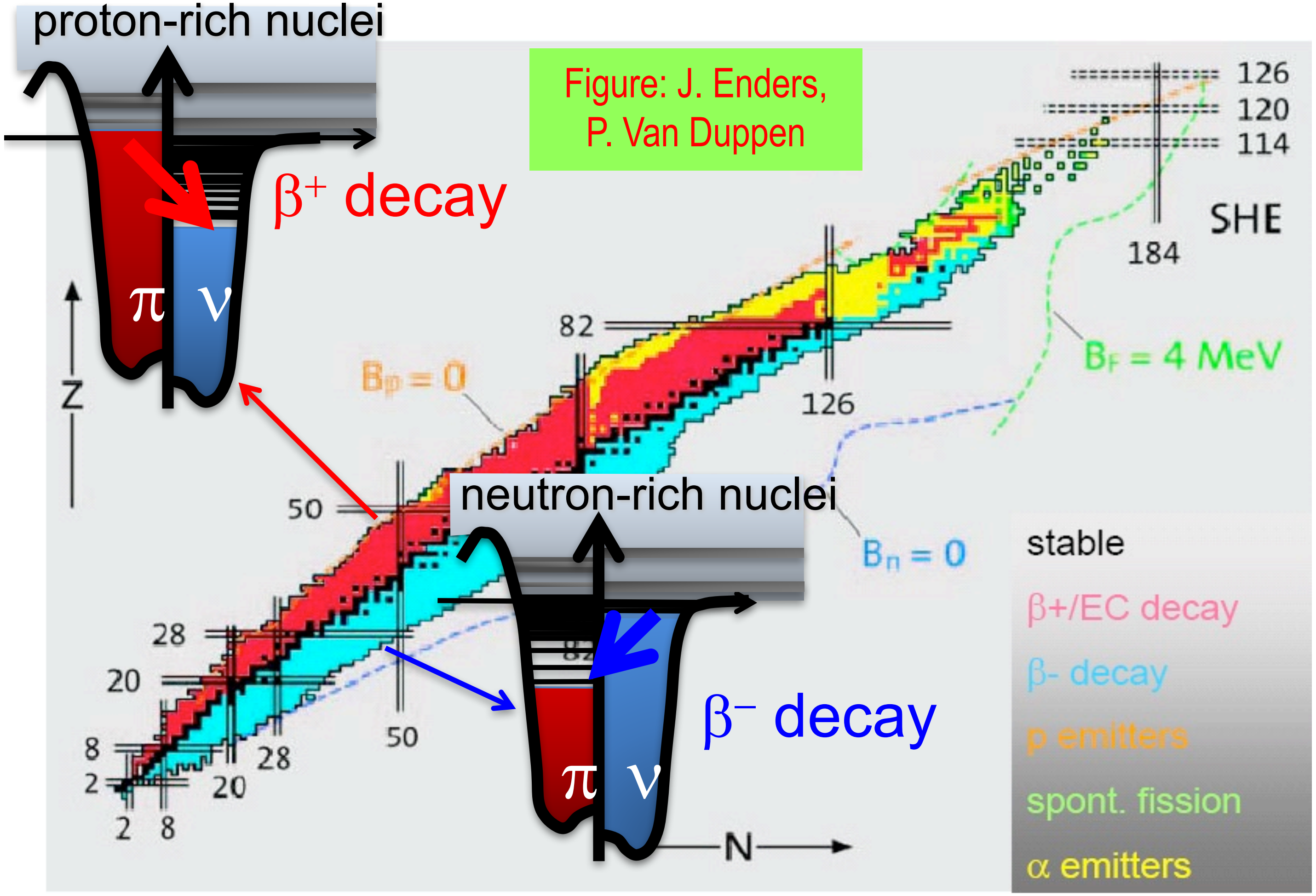
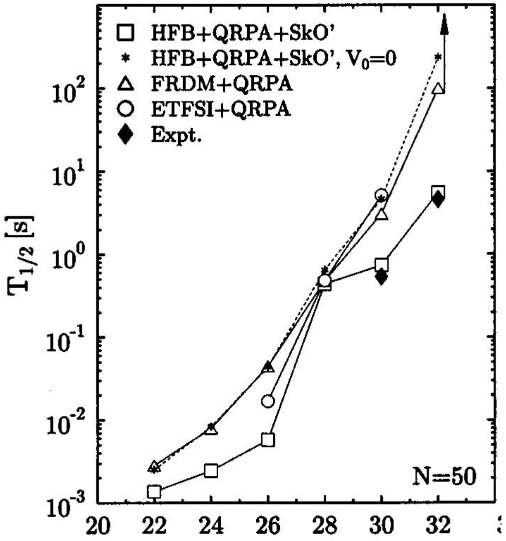


Figure: J. Enders, P. Van Duppen

It is one of the main nuclear decays and **RPA is often unable to reproduce it.**



Engel, et al., PRC 60, 014302 (1999)

(unless one adds *ad hoc* parameters that must be tuned).

Particle-vibration coupling (PVC): general philosophy

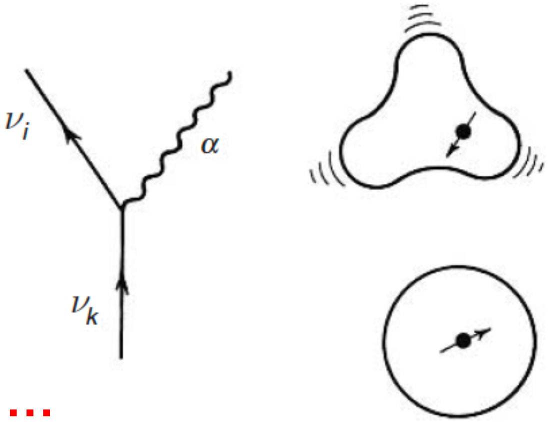
- The basic idea is that in spherical nuclei there are **single-particle states** and (mainly surface) **collective vibrations**. The spectra result from their **interplay.** (Deformed nuclei: particle-rotation coupling)

- **Vibrations = phonons.**

- **Adiabatic approximation in general not valid**.

- Even nuclei: core + 1p-1h + **1p-1h plus phonon …**

- Odd nuclei: core + 1 particle + **1 particle plus phonon …**



- In the past, phenomenological models based on the experimental properties of the phonons have been introduced: Nuclear Field Theory or NFT (Copenhagen), Quasiparticle-phonon model or QPM (Dubna).

- NOW WE PERFORM **FULLY MICROSCOPIC CALCULATIONS**.

RPA plus particle-vibration coupling (PVC)

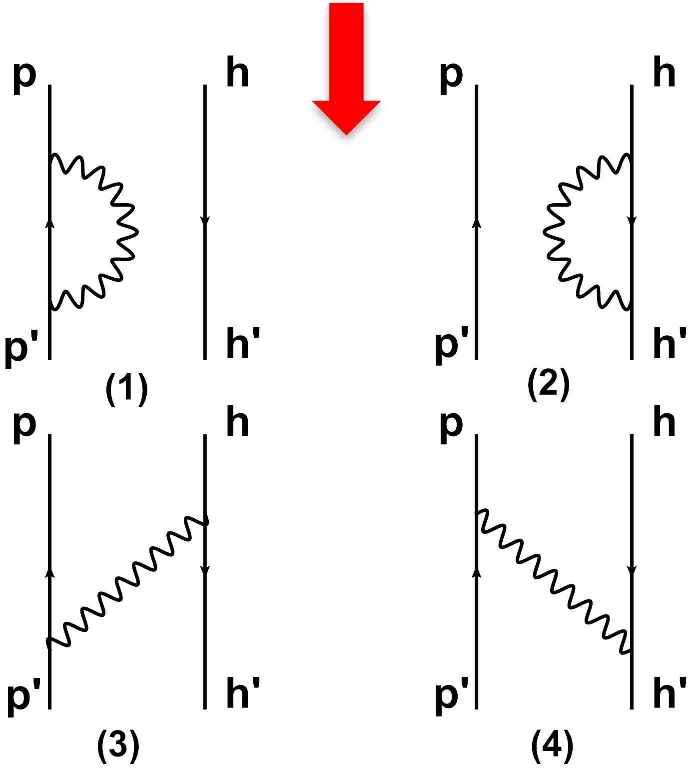
$$\begin{pmatrix} A+\Sigma(E) & B \\ -B & -A-\Sigma^*(-E) \end{pmatrix} \qquad \Sigma_{\mathrm{php'h'}}(E) = \sum_\alpha \frac{\langle ph|V|\alpha\rangle\langle\alpha|V|p'h'\rangle}{E-E_\alpha+i\eta}$$

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

One adds the self-energy contribution (the state α is 1p-1h plus one phonon).

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

Y.F. Niu et *al.*, PRC 85, 034314 (2012);
Y. F. Niu, G.C., and E. Vigezzi, Phys. Rev. C 90, 054328 (2014).



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β-decay from RPA and RPA+PVC

In RPA often the half-life are **infinite**, because no GT strength is found in the β-decay window.

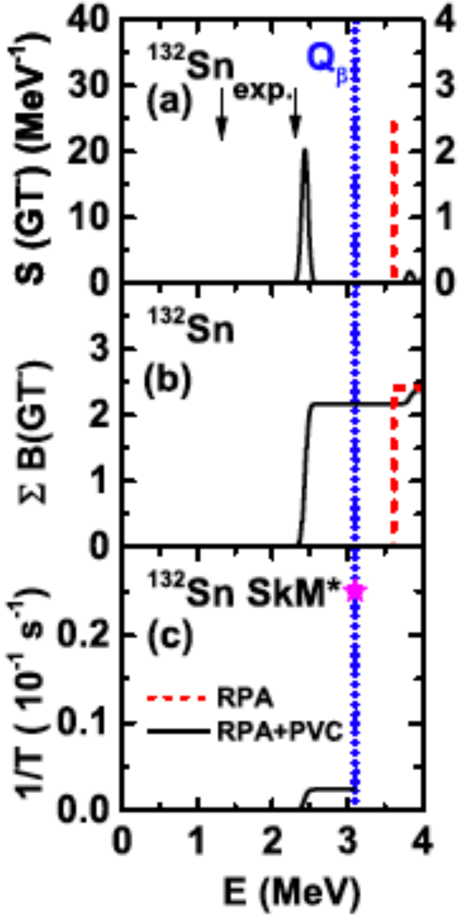
PVC can strongly affect the half-lives: its effect is fragment and shift down the RPA peaks, so that there more strength in the decay window.

The effect is **enhanced by the phase-space factor**.

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

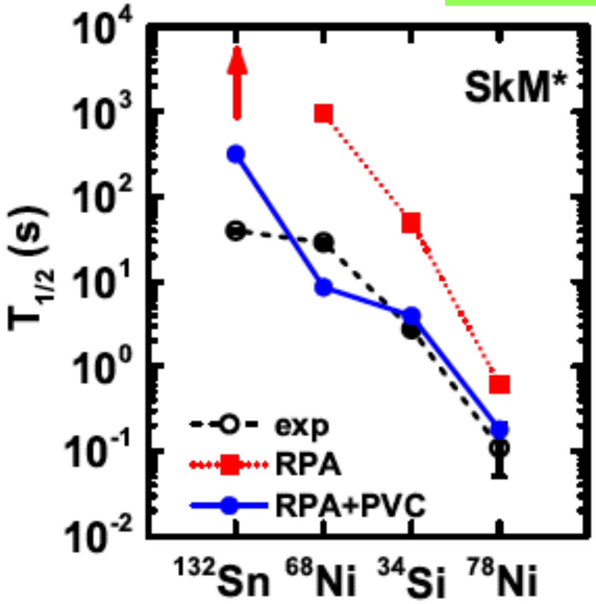
$$f(Z,\omega) = \int_{m_e c^2}^{\omega} p_e E_e (\omega - E_e)^2 F_0(Z+1, E_e) dE_e$$

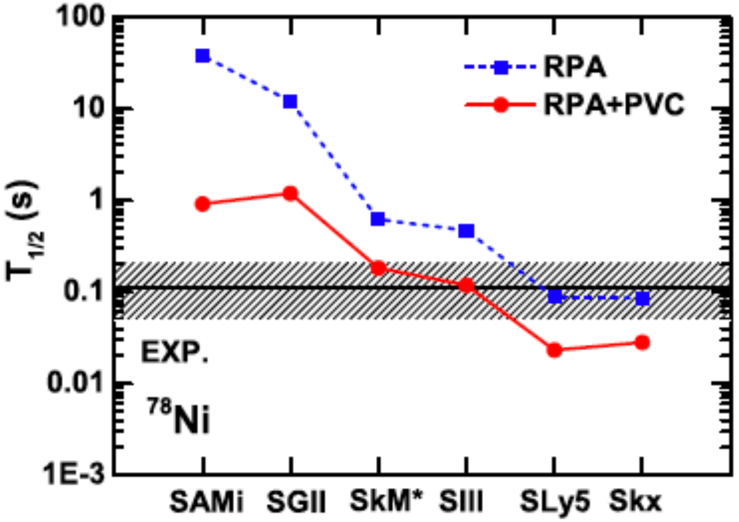
$$\omega = Q_\beta + m_e c^2 - E = \Delta_{np} - E_M$$



Results from RPA+PVC

Y.F. Niu, Z.M. Niu, G.C., and E. Vigezzi, Phys. Rev. Lett. 114, 142501 (2015).





We definitely improve agreement with experiment.

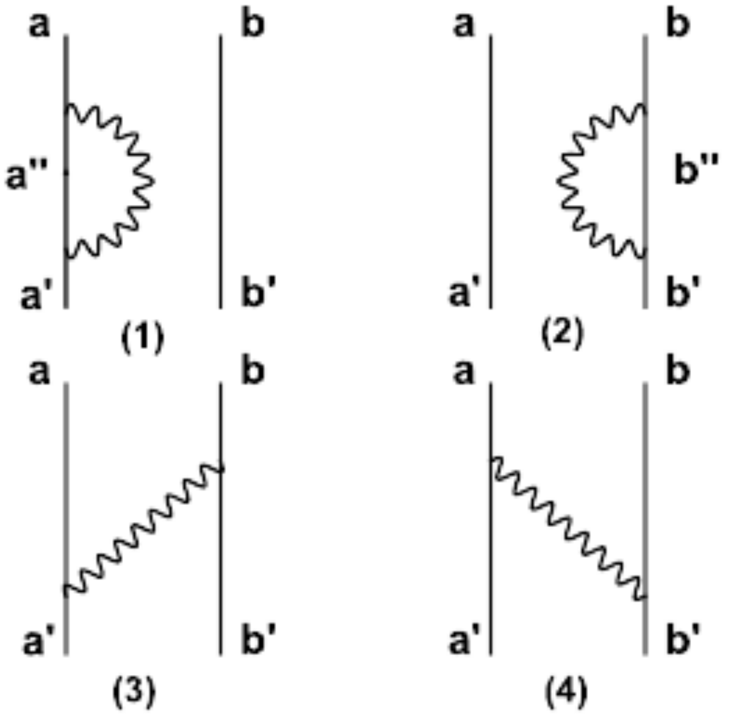
We do not introduce **any free parameter** (at variance with the case in which one tunes *ad hoc* terms in the Hamiltonian).

Dependence on V_{Skyrme}: there are forces (SkM*) with which **we reproduce also the GT widths in the same mass region.**

Extension to the case of open-shell nuclei

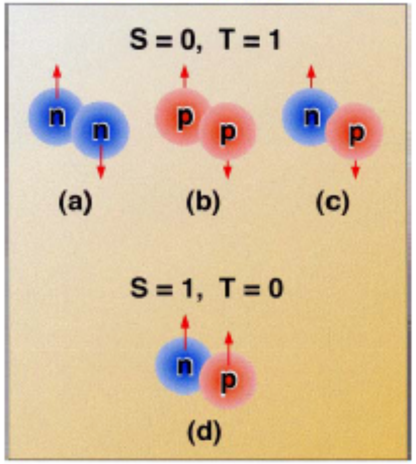
The basis is made up with states from **full HFB**. In the case of zero-range interactions, at a given cut-off for E_{qp} the pairing gap is fitted.

Phonons are from **quasi-particle RPA** (QRPA). We select the collective ones.



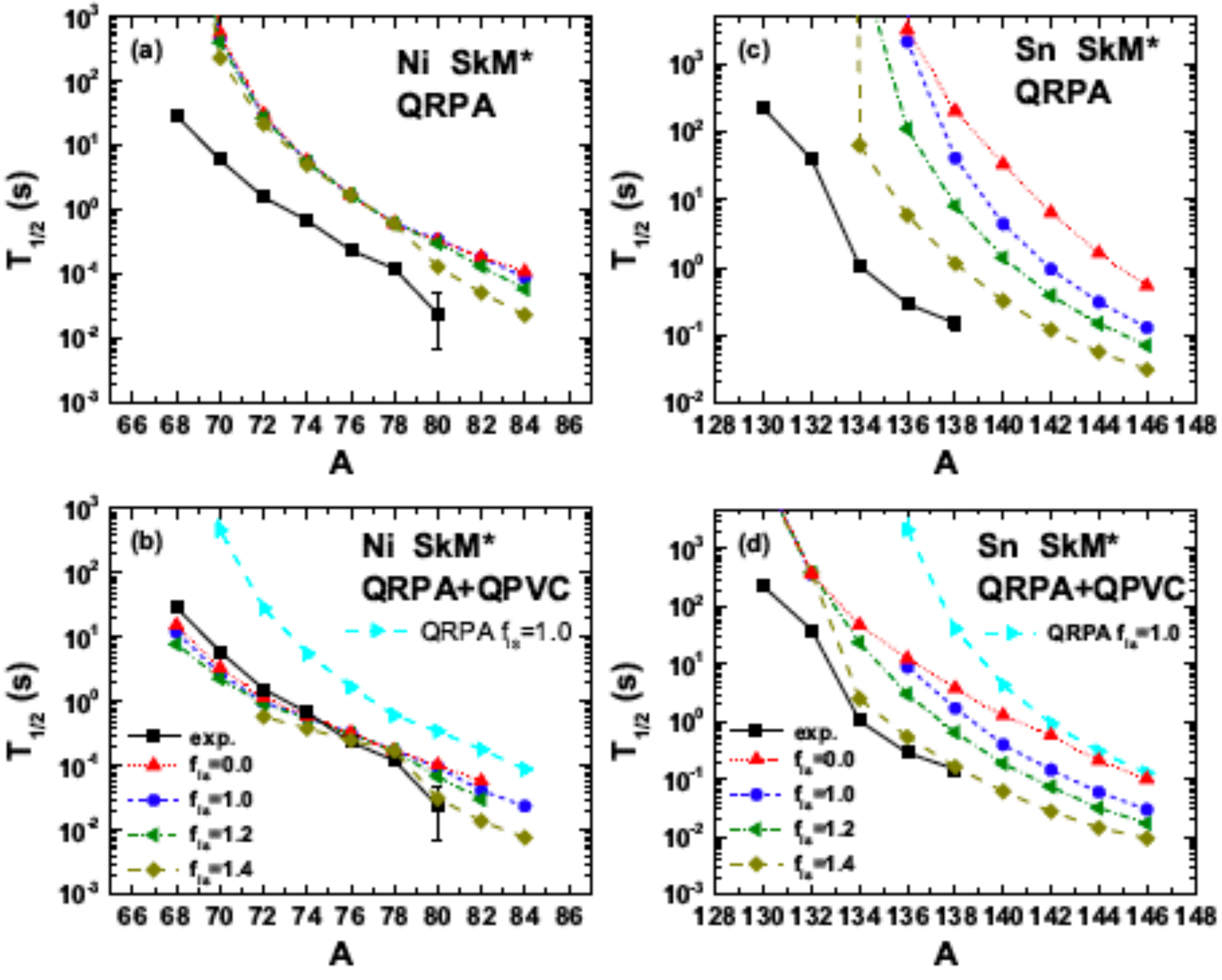
The scheme is fully self-consistent also in the pairing channel.

We are sensitive to T=1 and T=0 pairing.



Y.F. Niu, G.C., E. Vigezzi, C.L. Bai, H. Sagawa, Phys. Rev. C 94, 064328 (2016).

Effect of PVC and pairing on β-decay



PVC plays a more important role.

T=0 pairing is relevant for those nuclei which are not (too) near to the shell closure.

f_{IS} is the ratio between T=0 and T=1 pairing strength.

Values of f_{IS} around 1.5 acceptable.

H. Sagawa, C.L. Bai, and G.C., Physica Scripta 91, 083011 (2016).

Motivation: go towards spectroscopy of odd nuclei based on DFT

- 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).

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

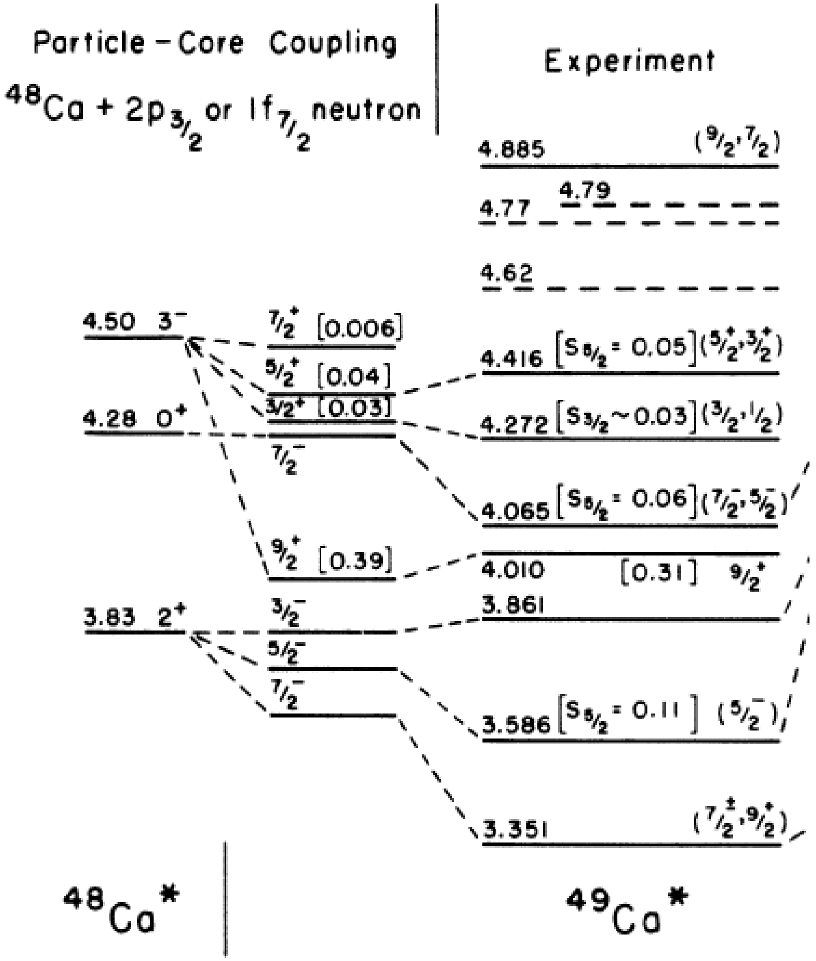
- Could be a good playground for particle-vibration coupling models …

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

States from (d,p) on ^{48}Ca.

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

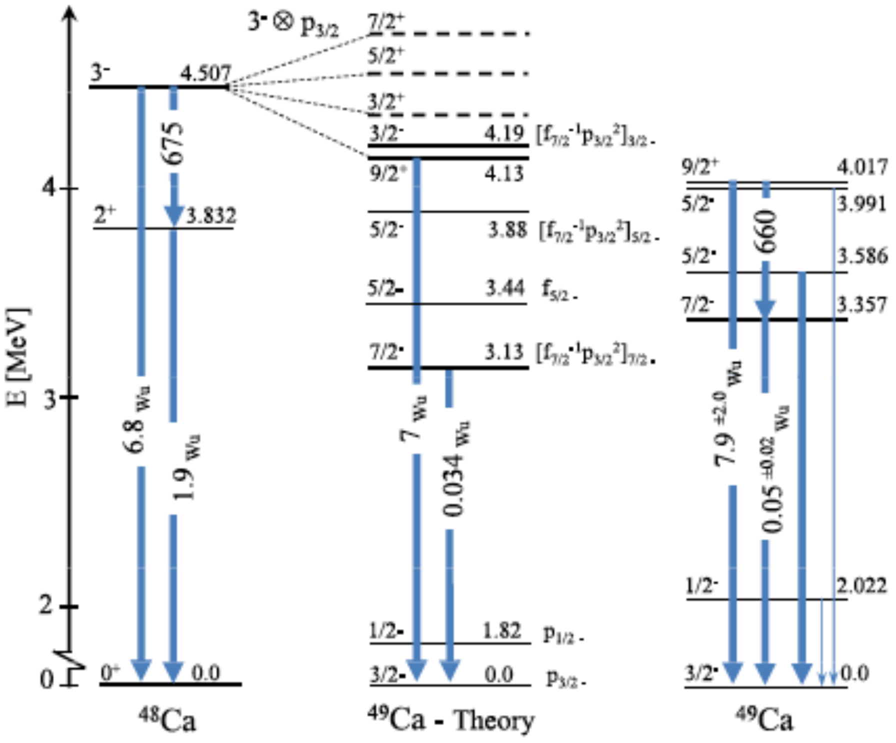
Neutrons plus a ^{48}Ca vibration ?



^{64}Ni+^{48}Ca (5.7 MeV/u) performed at LNL, Italy.

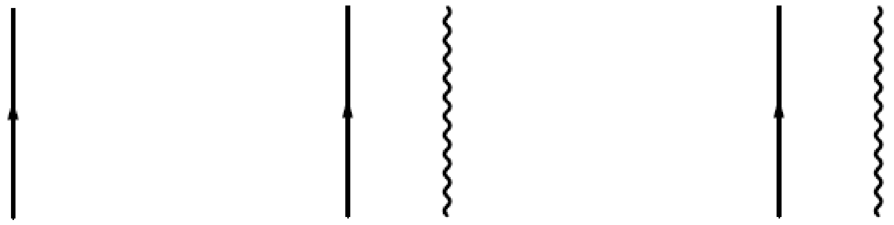
The angular momenta have been found to be aligned perpendicular to the reaction plane. Spin and lifetimes extracted.

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



Hybrid Configuration Mixing (HCM) model - I

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

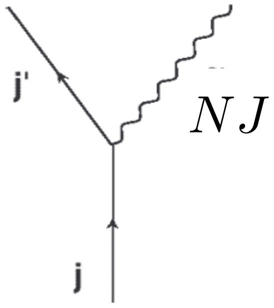


On this basis we **diagonalize the Hamiltonian** $H = H_0 + V,$

V_{Skyrme}

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

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



Hybrid Configuration Mixing (HCM) model - II

- As already stressed, some of the RPA solutions 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.**

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

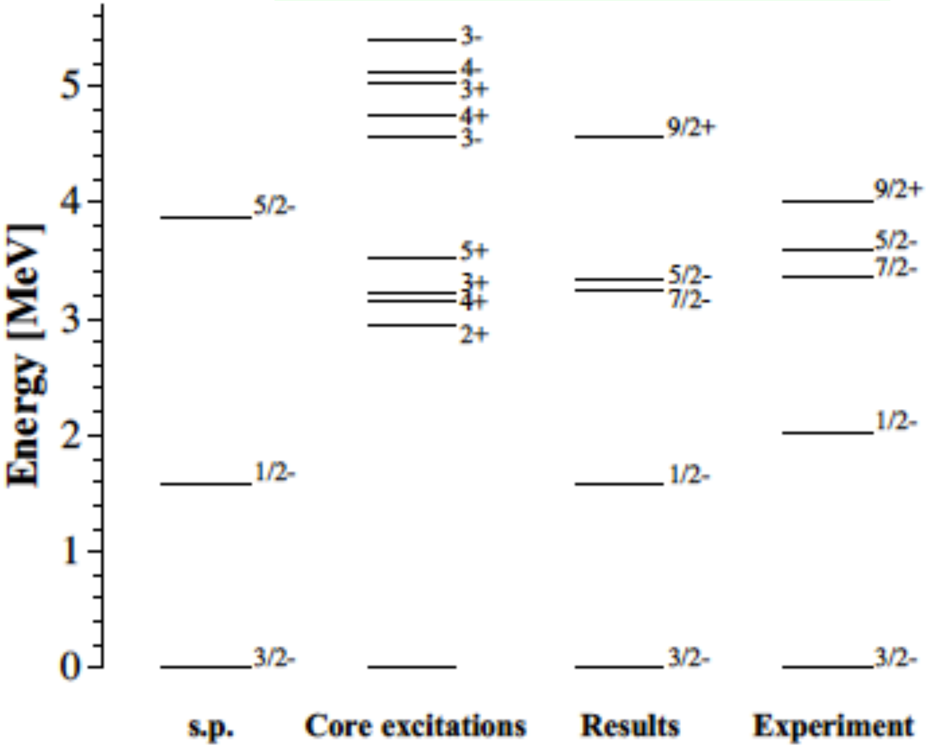
This is the overlap between 1p-1 “phonon” states. The diagonal part reduces to 1 – $(2j+1)^{-1}$ in simple cases.

$$\boxed{\left(\mathcal{H} - E\mathcal{N}\right)\Psi = 0}$$

Results for ^{49}Ca

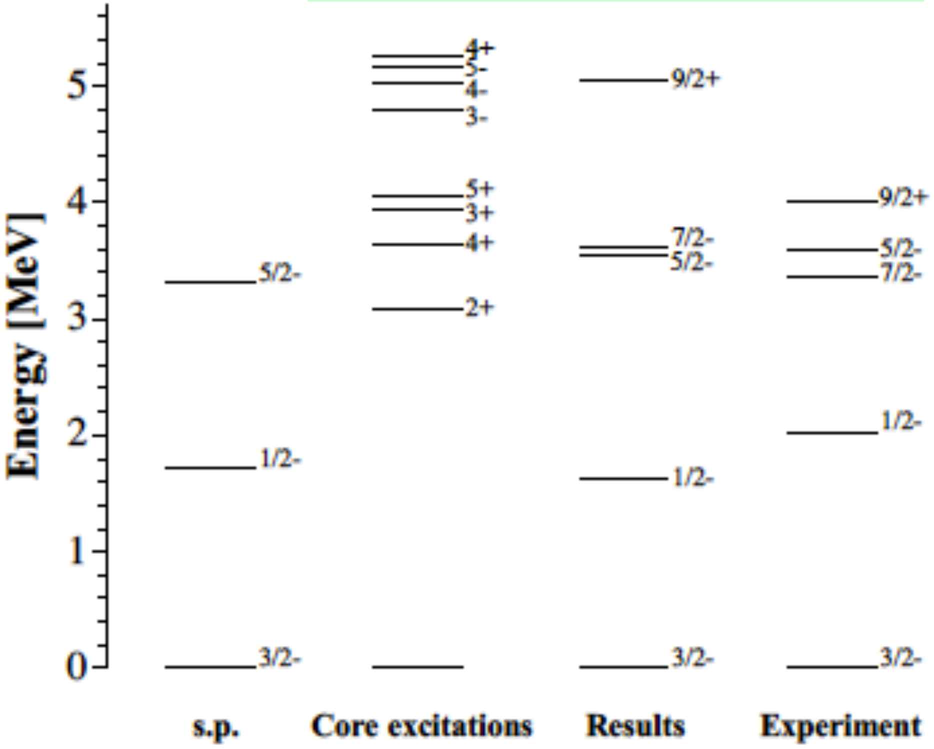
SkX

R.m.s. deviation th.-exp.:
0.429 MeV



SLy5

R.m.s. deviation th.-exp.:
0.661 MeV



The spectrum is **more stretched** in theory than in experiment; nonetheless, the **agreement is good**. Different kind of states.

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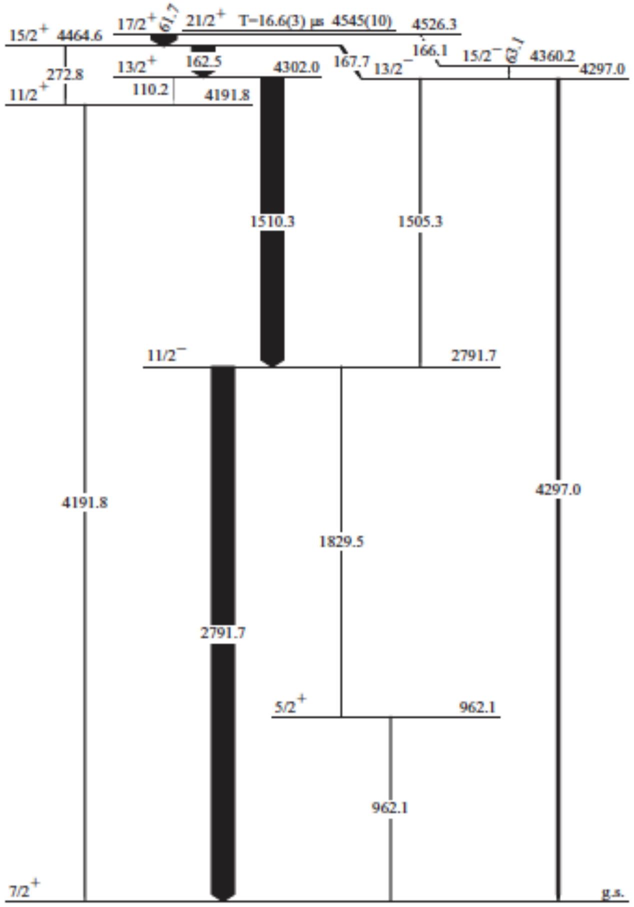
Spectroscopy of ^{133}Sb (^{132}Sn + p)

- 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$^+$).
  B(M1, 15/2$^+$→13/2$^+$) = 0.24 W.u.
  B(M1, 13/2$^+$→11/2$^+$) = 0.004 W.u.
  (ratio = 60).

- 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.

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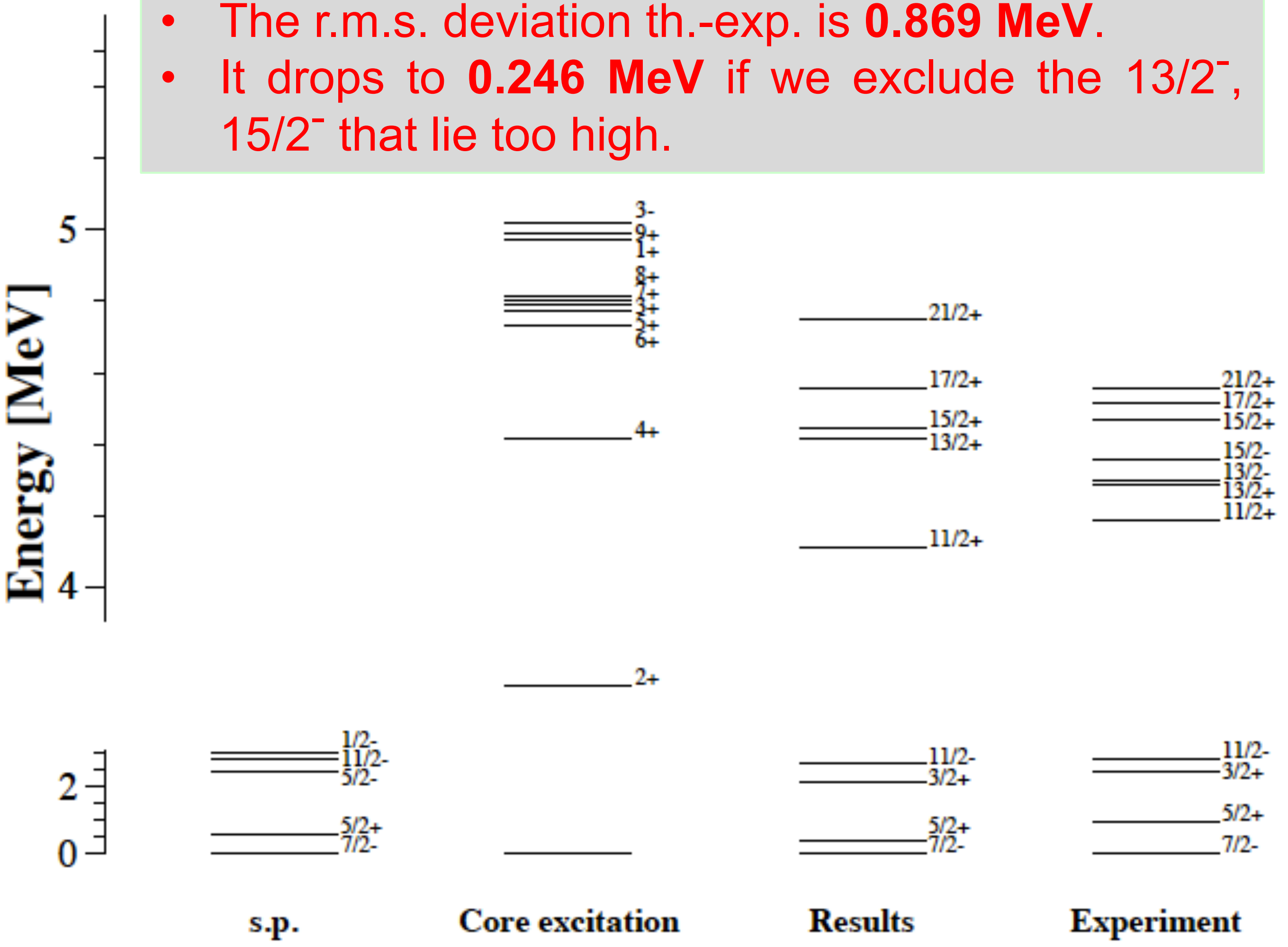
Results for ^{133}Sb

SkX

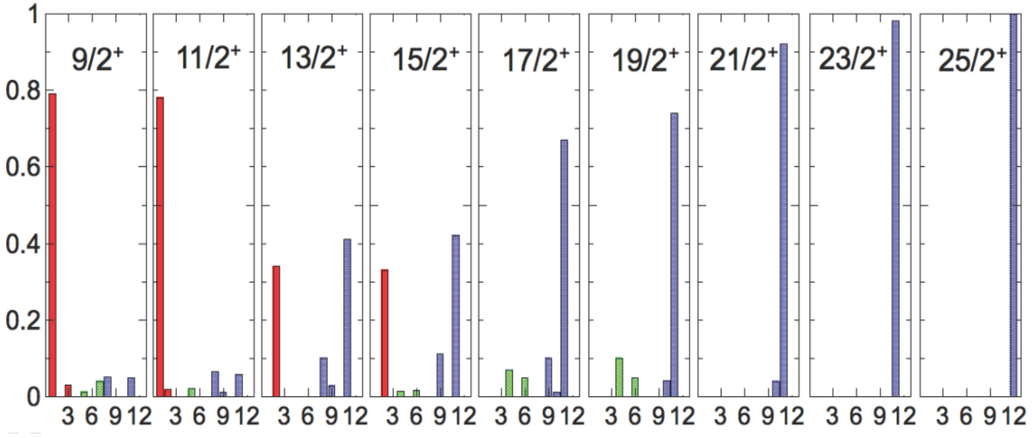
Only 2^+, 3^- and 4^+ core excitations are genuine “phonons”. There are more core excitations in the model space, and they are 1p-1h (mainly $h_{11/2}^{-1}$-$f_{7/2}$). 6+ has 2-3 components.

The spectrum includes particle-phonon states as well as 2p-1h states.

- The r.m.s. deviation th.-exp. is **0.869 MeV**.
- It drops to **0.246 MeV** if we exclude the $13/2^-$, $15/2^-$ that lie too high.



Electromagnetic transitions and the mutable nature of the wavefunction



red: $\pi g_{9/2} \otimes 2^+, 4^+$

blue: $\pi g_{9/2}\ \nu h_{11/2}^{-1}\ \nu f_{7/2}$

This nature is reflected in the M1 transition probabilities.

The wave functions of 15/2$^+$ and 13/2$^+$ are dominated by $g_{9/2}$, $h_{11/2}^{-1}$ $f_{7/2}$, so the B(M1) transition is made up with s.p. amplitudes. $B(M1)_{th}$ = 0.021 W.u.

In the case of the transition 13/2$^+$ → 11/2$^+$, the final state has phonon component so there is a mismatch in the components and B(M1) is quenched, $B(M1)_{th}$ = 0.001 W.u. Ratio = 20.

Conclusions

- Skyrme forces are used to describe **ground-state bulk properties of nuclei, but also giant resonances, the Equation of State**…

- We want to **establish a bridge with spectroscopy**, by keeping the same Hamiltonian and introducing more correlations.

- **PVC correlations and further ones** have been considered.

- Even-even to odd-odd transitions (β-decay) and spectra of odd nuclei have been described, finding good agreement with experiment.

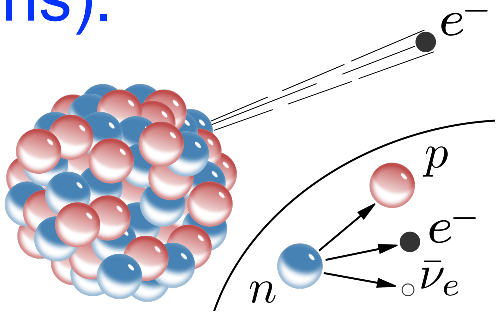
Backup slides

What would we like to explain theoretically ?

- Masses $M(N,Z) = Zm_pc^2 + Nm_nc^2 - BE(N,Z)$
- Radii
- Deformations

From: P. Flip

- Excited states: single-particle states, vibrations, rotations.
- Decays (for instance, β and ββ transitions).
- Large amplitude motion (fission).



…

The Skyrme force

attraction

$$\hat{v}_{\mathrm{Sk}}(\mathbf{r}_{12}) = \underline{t_0(1+x_0\hat{P}_\sigma)\delta(\mathbf{r}_{12})} + \frac{1}{2}\underline{t_1(1+x_1\hat{P}_\sigma)(\hat{k}^{\dagger 2}\delta(\mathbf{r}_{12}) + \delta(\mathbf{r}_{12})\hat{k}^2)}$$

$$+ \underline{t_2(1+x_2\hat{P}_\sigma)\hat{k}^\dagger \cdot \delta(\mathbf{r}_{12})\hat{k}} + \underline{\frac{1}{6}t_3(1+x_3\hat{P}_\sigma)\delta(\mathbf{r}_{12})\rho^\alpha\left(\frac{\mathbf{r}_1+\mathbf{r}_2}{2}\right)}$$

$$+ \mathrm{i}W_0(\hat{\sigma}_1+\hat{\sigma}_2)\cdot\hat{k}^\dagger \times \delta(\mathbf{r}_{12})\hat{k}.$$

short-range repulsion

$$k = \frac{i}{2}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right)$$

- There are velocity-dependent terms which mimick the finite-range. They are related to m*.

- The last term is a zero-range spin-orbit.

- In total: 10 free parameters to be fitted (typically).

β-decay of ^{100}Sn

Superallowed Gamow–Teller decay of the doubly magic nucleus ^{100}Sn

Nature 486, 341 (2012)

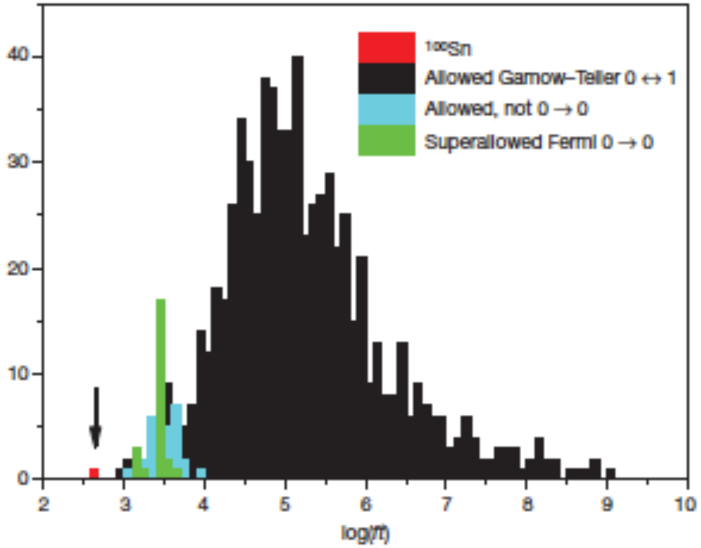


Figure 6 | Log(ft) values of allowed nuclear β-decays. Number distribution of log(ft) values for allowed β-transitions (obeying the selection rules). The data are from ref. 26. The values are for generally allowed Gamow–Teller transitions between 0^+ and 1^+ states (black), mixed Fermi/Gamow–Teller transitions (blue) and the well-established pure, superallowed Fermi transitions from 0^+ to 0^+ states (green). The decay of ^{100}Sn is unique because it has the smallest known log(ft) value (red) of any nuclear β-decay.

$t_{1/2}$

RPA	17.41 s
RPA+PVC	4.18 s
Exp.	1.11 s

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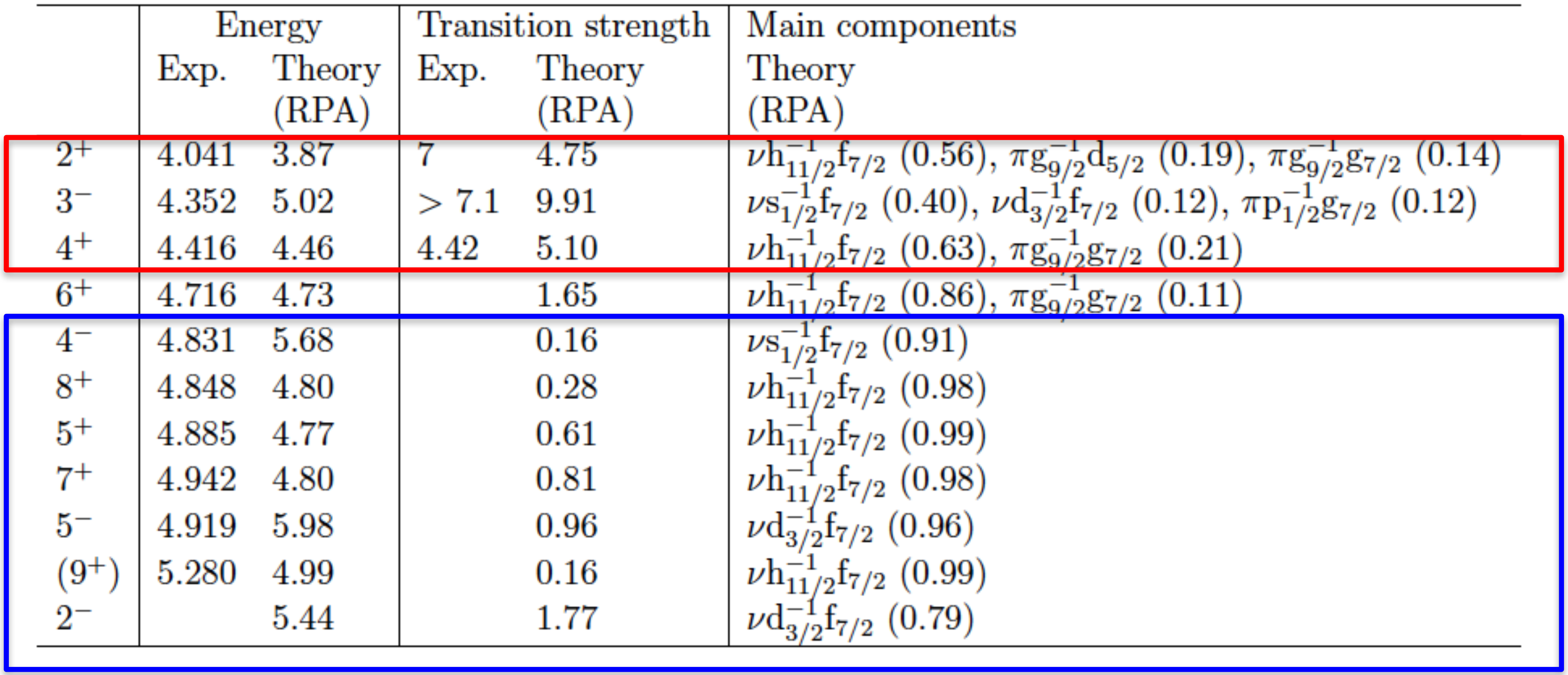
Different kinds of excitations in ^{132}Sn



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

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