The Hybrid Configuration Mixing (HCM) model

(MR calculations in the particle-vibration coupling scheme)

February 27th - March 2nd, 2017

Gianluca Colò

Università degli Studi and INFN, MIlano

ESNT Workshop on "Pertinent ingredients for MR EDF calculations"

Very short outline

- Motivation/context.
- The model and its first applications to ^{49}Ca and ^{133}Sb.

GC, G. Bocchi, and P.F. Bortignon, Phys. Rev. C (in press, 2017);

thanks also due to: S. Bottoni, P. Casati, B. Fornal, S. Leoni, D. Montanari.

We kindly encourage you to […] you discuss explicitly

a) which degrees of freedom you consider.

b) at which level of modeling they enter (SR, MR, diagrammatic expansion, any combination thereof).

c) which phenomena these can be expected to be (particularly) relevant for.

d) if their treatment as discussed can be (easily) combined with the one of other degrees of freedom (from a technical and computational point of view).

e) if they can be expected to be independent/orthogonal to other degrees of freedom discussed during the workshop.

Motivation: go towards spectroscopy of odd nuclei based on DFT

- *Answer to question c) of our "list": which phenomena do we consider ?*

- In the low-lying part of the spectra of odd-nuclei some states are "particle" states (large cross section in transfer reactions).

- They co-exist with typical "particle plus core vibration" states (gamma decay similar to that of the core vibration) …

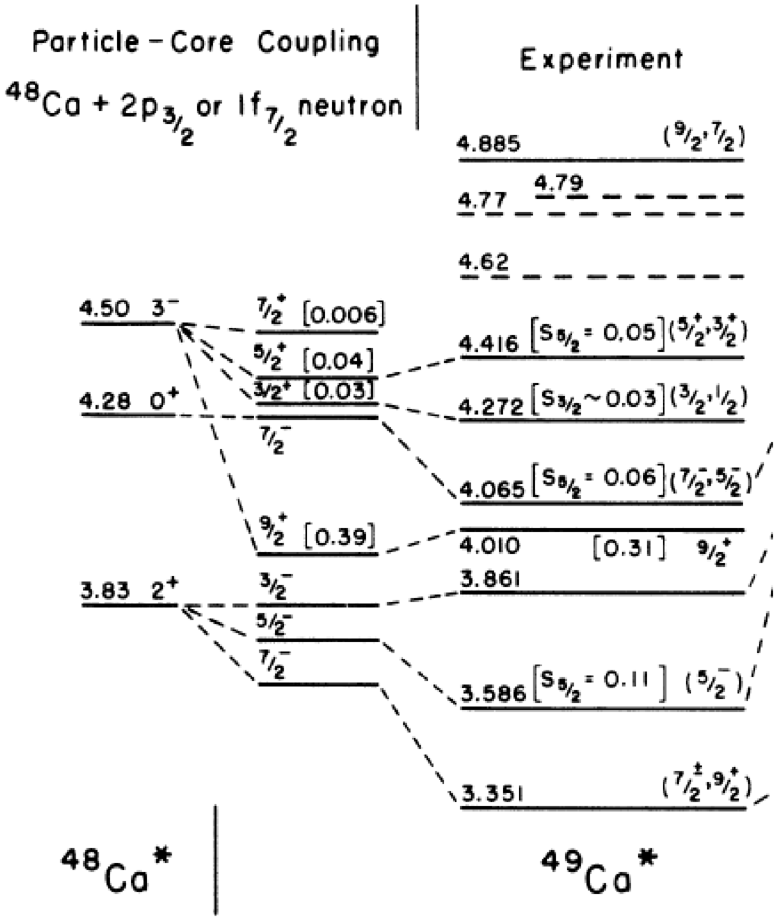
$$B(E\lambda, [j' \otimes \lambda]_j \rightarrow j') = B(E\lambda, \lambda \rightarrow 0)$$

- … and with 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)

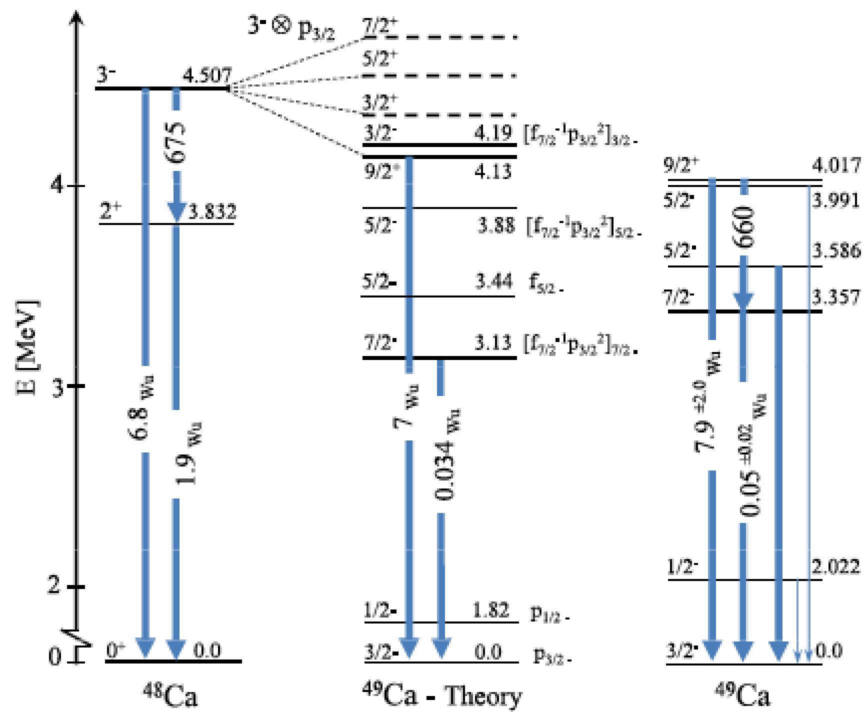
Neutrons plus a ^{48}Ca vibration ?



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

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

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



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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.

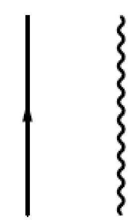
Note that for practical reasons we extract core excitations from RPA.

Nonetheless, we consider both collective solutions (genuine ”vibrations” or “phonons”) and pure 1p-1h.

Answer to a), d), e) about d.o.f.’s.

$$|jm\rangle = a^\dagger_{jm}|0\rangle$$

$$|[j' \otimes NJ]_{jm}\rangle = \left\{ \sum_{ph} \sum_{m'Mm_pm_h} \langle j'm'JM|jm\rangle X^{(NJ)}_{ph} (-1)^{j_h-m_h} \langle j_pm_pj_h - m_h|JM\rangle a^\dagger_{j'm'} a^\dagger_{j_pm_p} a_{j_hm_h}|0\rangle + \right.$$
$$\left. - \sum_{ph} \sum_{m'Mm_pm_h} \langle j'm'JM|jm\rangle Y^{(NJ)}_{ph} (-1)^{j_h-m_h+J+M} \langle j_pm_pj_h - m_h|J - M\rangle a^\dagger_{j'm'} a^\dagger_{j_hm_h} a_{j_pm_p}|0\rangle \right\}$$



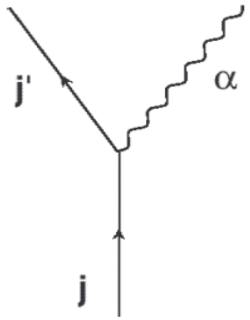
Hybrid Configuration Mixing (HCM) model - II

On this basis we **diagonalize the Hamiltonian:**

$$H = H_0 + V,$$

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

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



At the moment we use a Skyrme-type V_{eff}.

The method is of course more general.

Hybrid Configuration Mixing (HCM) model - III

- 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.

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

Answer to b).

Basic equation (cf. SM and/or GCM)

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

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

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

Electromagnetic transition probabilities

$$
\begin{aligned}
\langle \alpha_f j_f || \hat{O}(X\lambda) || \alpha_i j_i \rangle \; = \; & \sum_{if} \xi_i^{\alpha_i} \xi_f^{\alpha_f} \langle j_f || \hat{O}(X\lambda) || j_i \rangle \\
& + \sum_{if} \xi_i^{\alpha_i} \xi_f^{\alpha_f} \delta(J'_f, \lambda) \delta(j'_f, j_i) \frac{\hat{j}_f}{\hat{\lambda}} \langle J'_f || \hat{O}_{\rm ph} || 0 \rangle \\
& + \sum_{if} \xi_i^{\alpha_i} \xi_f^{\alpha_f} \delta(J'_i, \lambda) \delta(j'_i, j_f) \frac{\hat{j}_i}{\hat{\lambda}} \langle J'_i || \hat{O}_{\rm ph} || 0 \rangle (-)^{j_i - j_f + \lambda + \left({+1 \atop +0} \; {\text{for M} \atop \text{for E}} \right)} \\
& + \sum_{if} \xi_i^{\alpha_i} \xi_f^{\alpha_f} \hat{j}_f \hat{j}_i \Bigg\{ (-)^{j_f + J'_i + \lambda + j'_i} \left\{ \begin{array}{ccc} j_i & j_f & \lambda \\ J'_f & J'_i & j'_f \end{array} \right\} \delta(j'_f, j'_i) \\
& \times \sum_{ph, p'h'} \left[X^f_{ph} X^i_{p'h'} + (-)^{J'_f - J'_i + \lambda} Y^f_{ph} Y^i_{p'h'} \right] \\
& \quad \times \Bigg(\delta(h, h') \hat{J}'_f \hat{J}'_i (-)^{j_h + j_p + J'_i + \lambda} \left\{ \begin{array}{ccc} j_h & J'_i & j_{p'} \\ \lambda & j_p & J'_f \end{array} \right\} \langle j_p || \hat{O}_{sp} || j_{p'} \rangle \\
& \quad - \delta(p, p') \hat{J}'_f \hat{J}'_i (-)^{j_h + j_p + J'_f} \left\{ \begin{array}{ccc} j_p & J'_i & j_{h'} \\ \lambda & j_h & J'_f \end{array} \right\} \langle j_{h'} || \hat{O}_{sp} || j_h \rangle \Bigg) \\
& + (-)^{j_i + j'_f + \lambda + J'_f} \left\{ \begin{array}{ccc} j_f & j_i & \lambda \\ j'_i & j'_f & J'_f \end{array} \right\} \delta(J'_f, J'_i) \langle j'_f || \hat{O}_{sp} || j'_i \rangle \Bigg\} .
\end{aligned}
$$

The different terms correspond to the action of the e.m. operator on the different components of the wave function (odd particle or p/h component of the core excitations).

Shell model

Accurate
Sound physical picture
Strong limitations (related to mass region and/or excitation energy)
No link with MBPT / DFT

OUR HCM

Rooted in DFT (no *ad hoc* parameter from phenomenology)
Includes different types of correlations
Provides link between spectroscopy and physics at high E (giant resonances)
Approximations

MR-DFT

Well rooted in many-body theory and DFT
At present, **limitations in the degrees of freedom**

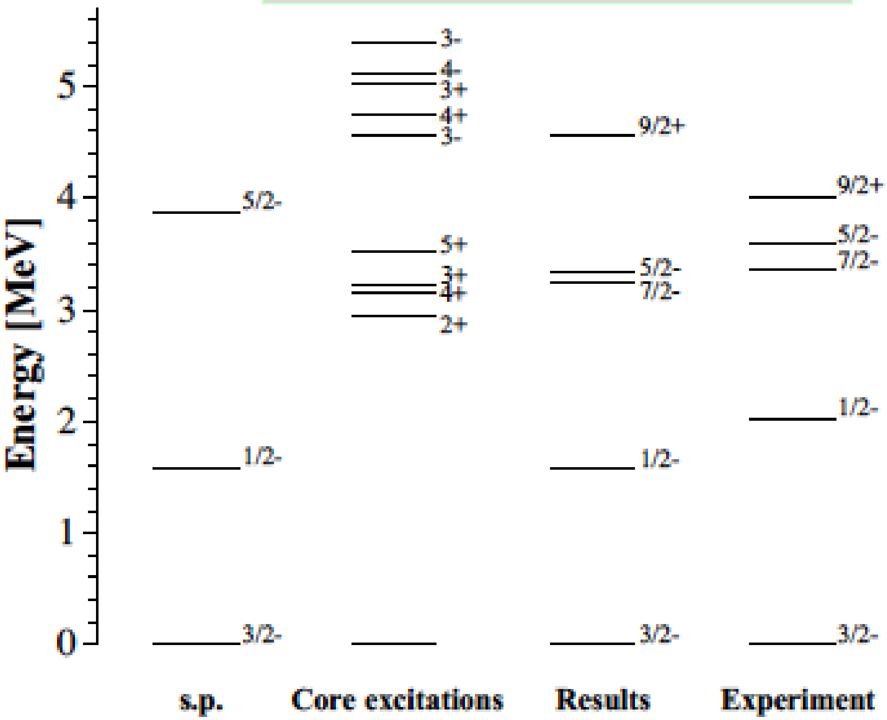
HF-RPA

Cf. talk by N. Pillet

Results for ^{49}Ca

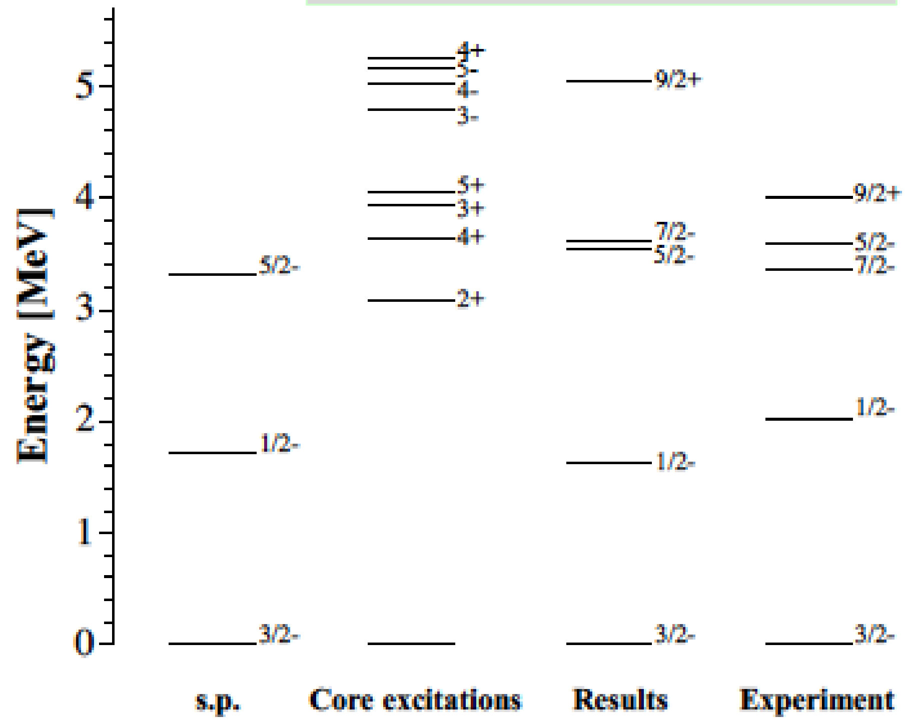
SkX

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



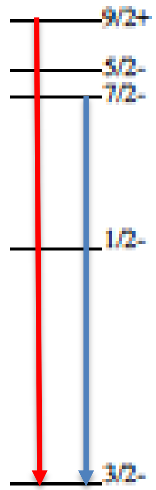
SLy5

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 states ($5/2^-$ mixed).

^{49}Ca: only few γ transitions are known and with a significant experimental error



E.m. transitions in ^{49}Ca

	Theory SkX	Theory SLy5	Exp.
$B(E3, 9/2^+ \to 3/2^-)$	6.4	5.7	7.9 ± 2.0 W.u.
$B(E2, 7/2^- \to 3/2^-)$	1.4	1.0	0.05 ± 0.02 W.u.

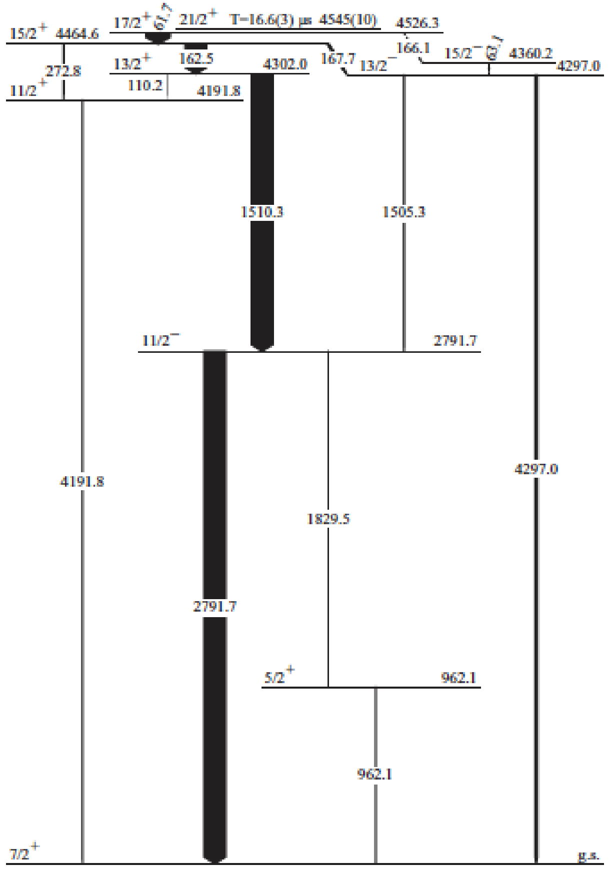
Core excitations of ^{48}Ca

J^π	Energy [MeV] Exp.	Energy [MeV] Theory (SkX)	Energy [MeV] Theory (SLy5)	B(E/Mλ) [W.u.] Exp.	B(E/Mλ) [W.u.] Theory (SkX)	B(E/Mλ) [W.u.] Theory (SLy5)
2_1^+	3.83	2.87	3.02	1.71	1.31	1.12
4_1^+	4.50	3.12	3.60		0.43	0.70
3_1^-	4.51	4.43	4.75	5.0	6.77	6.12
3_1^+	4.61	3.22	3.92		$6.6 \cdot 10^{-4}$	$6.6 \cdot 10^{-3}$
4_1^-	5.26	5.11	5.01		0.07	1.80
3_2^-	5.37	5.37			0.05	
3_2^+		5.02			$7.6 \cdot 10^{-4}$	
4_2^+		4.70	5.20		1.02	0.86
5_1^+		3.51	3.90		$5.0 \cdot 10^{-3}$	0.01

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 $25/2^+$).
  $B(M1, 15/2^+ \rightarrow 13/2^+) = 0.24$ W.u.
  $B(M1, 13/2^+ \rightarrow 11/2^+) = 0.004$ 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.

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.

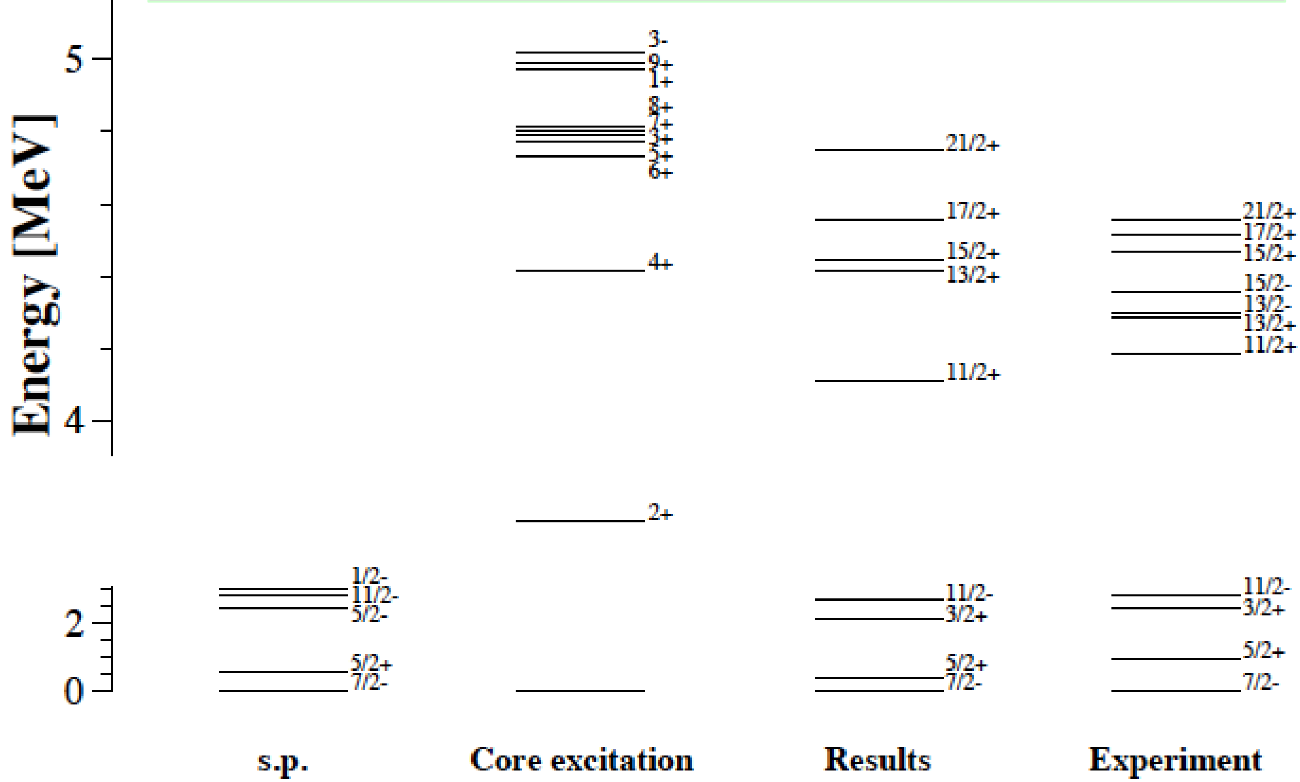
Results for ^{133}Sb

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.

<u>The spectrum includes particle-phonon states as well as 2p-1h states.</u>

- 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.



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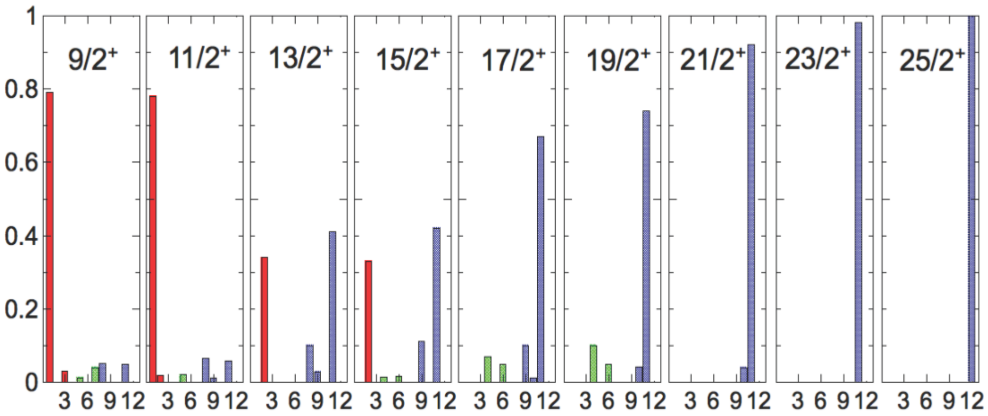
Microscopic content of the states

	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		$5.11\ [\pi g_{7/2} \nu h^{-1}_{11/2} \nu f_{7/2}\ (1.00)]$

Electromagnetic transitions and the mutable nature of the wave function



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 $13/2^+ \rightarrow 11/2^+$, 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.

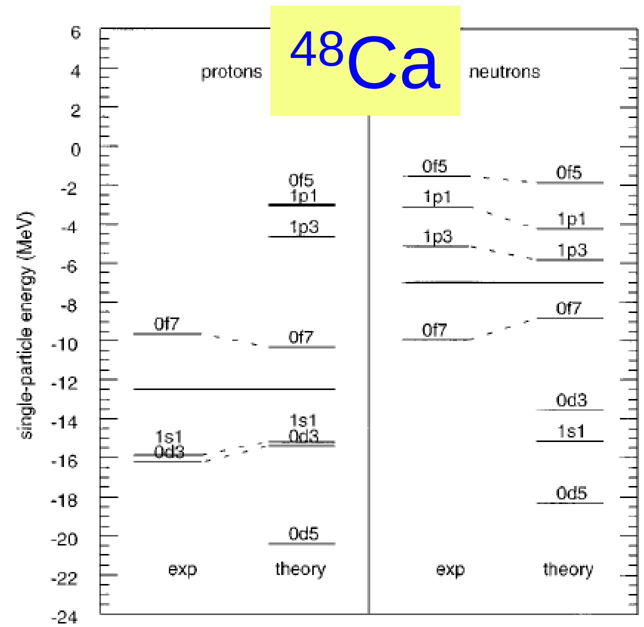
PHYSICAL REVIEW C VOLUME 58, NUMBER 1 JULY 1998

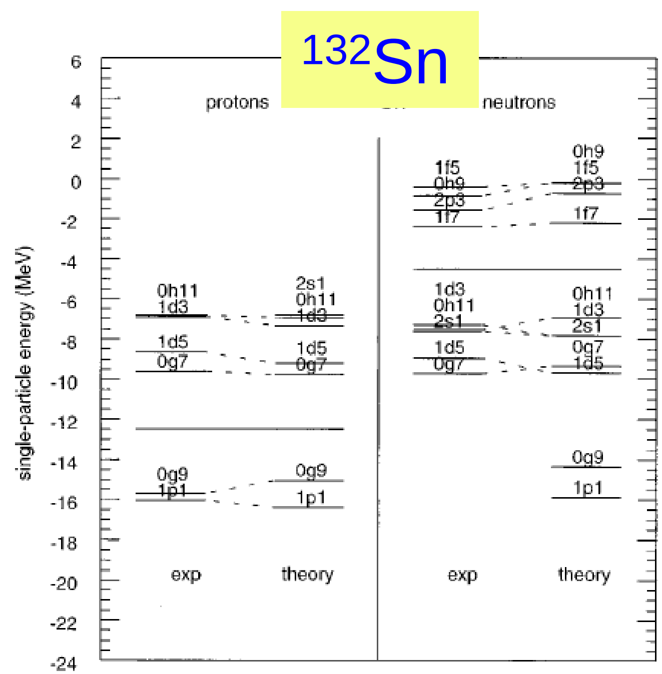
New Skyrme interaction for normal and exotic nuclei

B. Alex Brown
Department of Physics and Astronomy and National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, Michigan 48824-1321
and Department of Physics, University of Stellenbosch, Stellenbosch 7600, South Africa
(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-





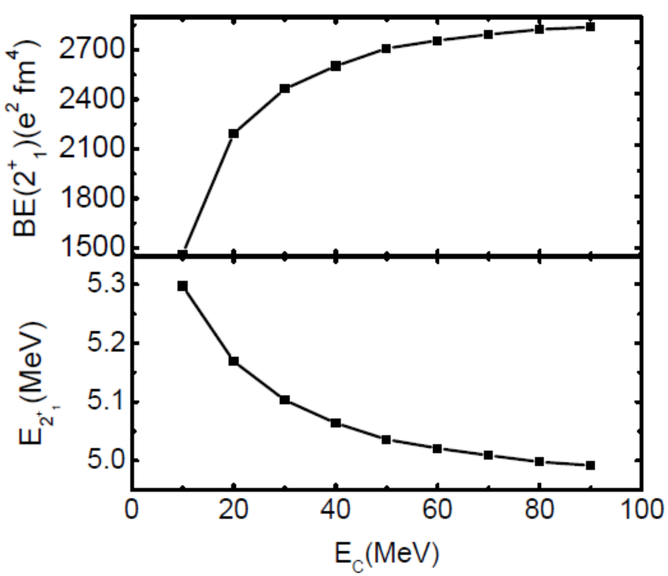
Our RPA implementation

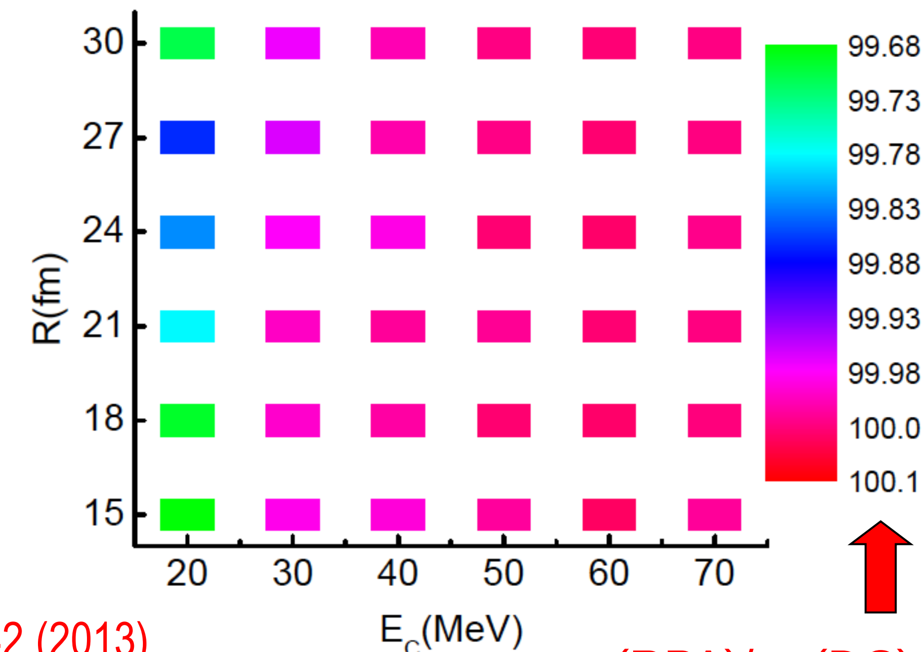
The continuum is discretized. We define a p-h basis and then the RPA matrix on this basis is diagonalized. Parameters: R, E_C.

The energy-weighted sum rule should be equal to the double-commutator value: well fulfilled !

$$m_1(\hat{O}) = \sum_\nu E_\nu |\langle \nu|\hat{O}|\tilde{0}\rangle|^2 = \frac{1}{2}\langle 0|[\hat{O},[H,\hat{O}]]|0\rangle$$

^{208}Pb - SGII





G.C. *et al.*, Computer Physics Commun. 184, 142 (2013)

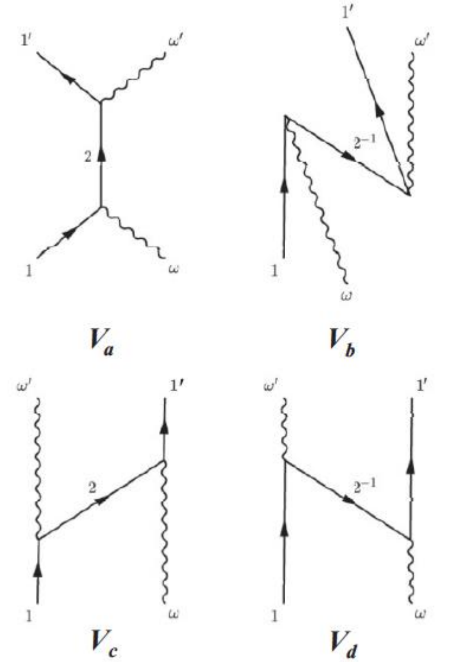
m_1(RPA)/m_1(DC) [%]

Progress with respect to “traditional” PVC

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

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

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

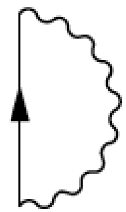


- **We go beyond perturbation theory.**
- **We include non-collective states.**
- **We formulate the problem based on a given H_{eff}.**

Fragmentation of s.p. strength

Dyson equation in coordinate space.

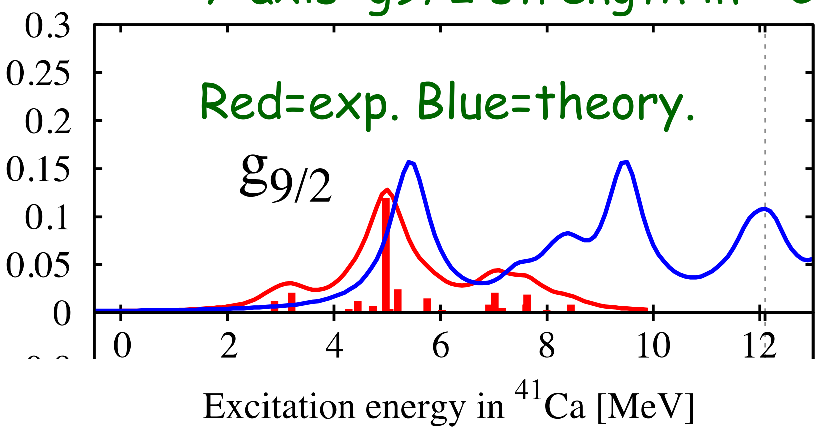
$$\Sigma =$$



$$G = G^0 + G^0 \Sigma G$$

$$S = -\frac{1}{\pi}\int d^3r\ G(\vec{r},\vec{r};\omega)$$

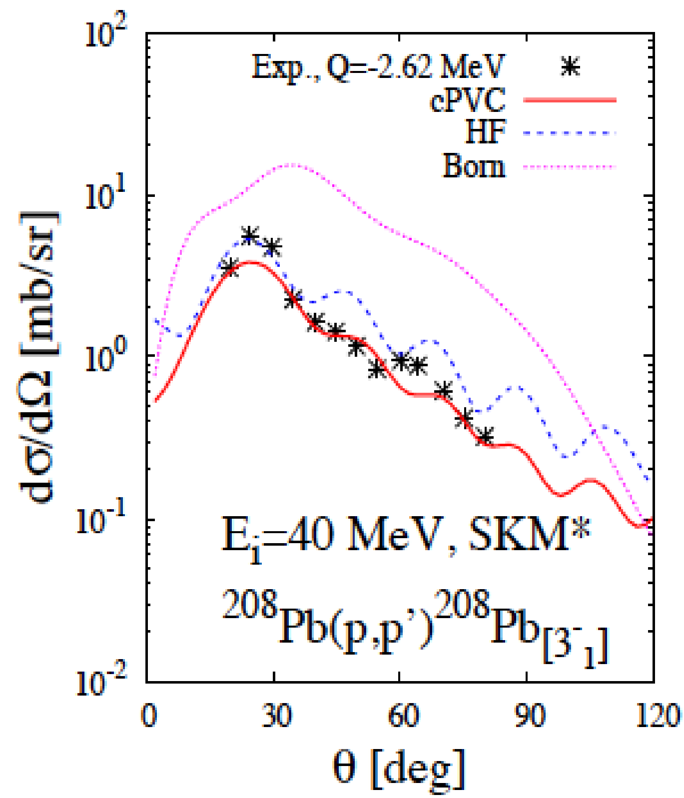
Y-axis: g9/2 strength in ^{41}Ca



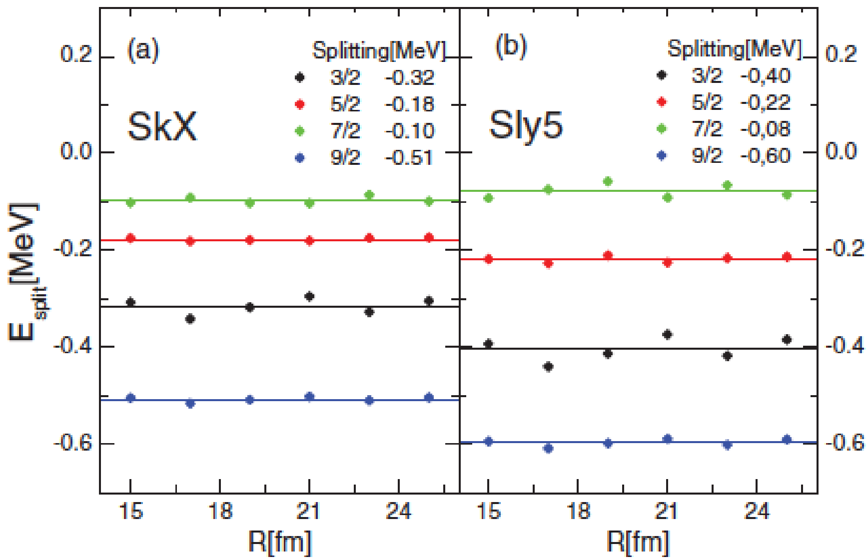
K. Mizuyama, GC, and E. Vigezzi, PRC 86, 034318 (2012).

APPLICATION TO SCATTERING

Courtesy: K. Mizuyama



Dependence on the box size



Case of ^{49}Ca

The insensitivity with respect to the box size can be qualitatively understood.

As the box size increases, more states are coupled but the coupling matrix elements decrease because of reduced overlaps.

Within PT the stability of the results can be seen analitically.

Università degli Studi and INFN, MIlano

Conclusions

- This work fits the general philosophy of choosing an effective interaction and using it within a many-body model.
- In this case, we wish to use a class of interactions that are well tailored for study of giant resonances, EoS etc. and use them for spectroscopy.
- Approximations are involved but with respect to “traditional” PVC we have a clear view of how to systematically enlarge the model space.

Perspectives

- Solution of schematic H.
- Comparison with MR-DFT when core excitations becomes very low.

- Extension to open-shell systems.
- Convergence with respect to model space.

- Interaction fitted at the spectroscopic level.