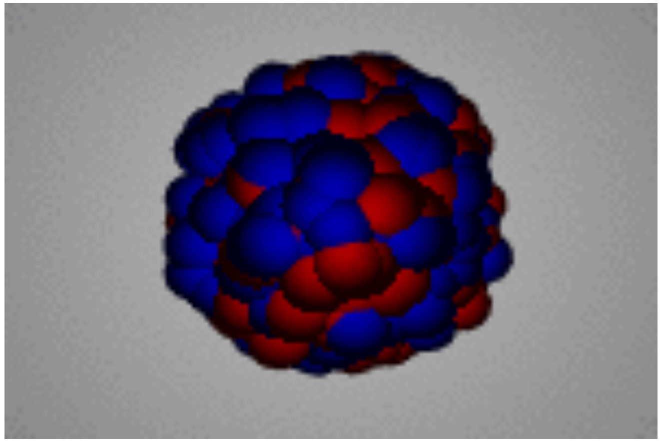
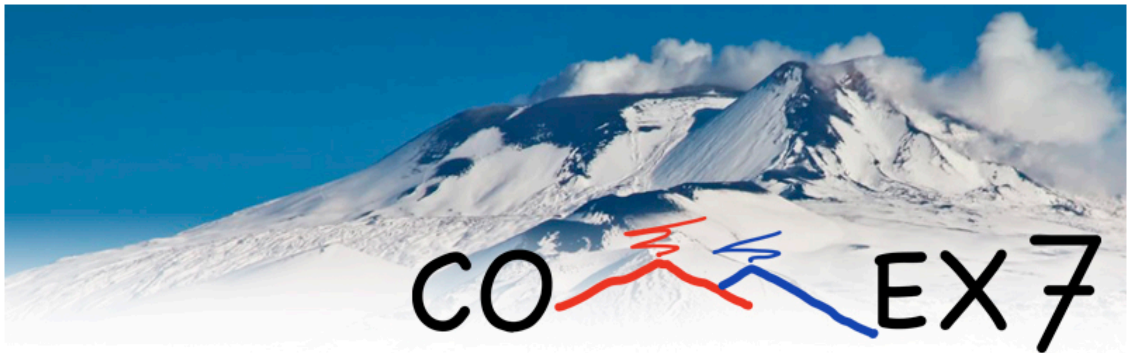
DFT calculations for collective states and application to the monopole resonances

Gianluca Colò
U. Milano and INFN

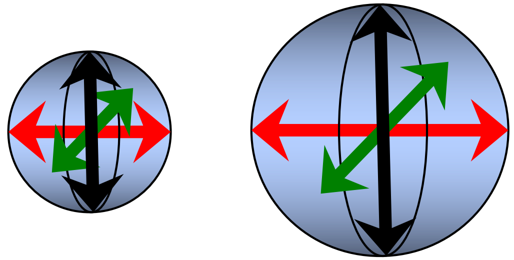




COMEX 7, Catania, 12-16 June 2023

Nuclear incompressibility and the ISGMR

Isoscalar Giant Monopole Resonance or "breathing mode": its energy should be correlated with the incompressibility of nuclear matter.



$$K_\infty = 9\rho_0^2 \frac{d^2}{d\rho^2}\left(\frac{E}{A}\right)_{\rho=\rho_0}$$

$$\chi \equiv -\frac{1}{\Omega}\left(\frac{\partial P}{\partial \Omega}\right)^{-1}$$

$$\chi^{-1} = \rho^3 \frac{d^2}{d\rho^2}\left(\frac{E}{A}\right)$$

Impact on astrophysics: supernova explosion, neutron star merging

SN1987a

PHYSICAL REVIEW LETTERS **129,** 032701 (2022)

Probing the Incompressibility of Nuclear Matter at Ultrahigh Density through the Prompt Collapse of Asymmetric Neutron Star Binaries

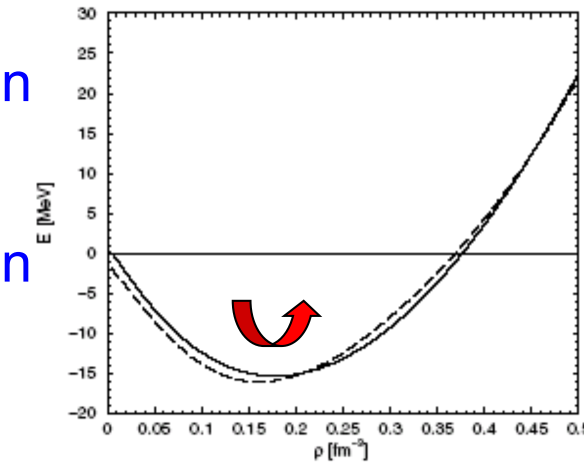
Albino Perego,[1,2,*] Domenico Logoteta,[3,4] David Radice,[5,6,7] Sebastiano Bernuzzi,[8] Rahul Kashyap,[5,6] Abhishek Das,[5,6] Surendra Padamata,[5,6] and Aviral Prakash[5,6]

(Q)RPA using EDFs in a nutshell

$$E = \langle \Psi | \hat{H} | \Psi \rangle = \langle \Phi | \hat{H}_{eff} | \Phi \rangle = E[\hat{\rho}]$$

$|\Phi\rangle$ **Slater determinant** $\Leftrightarrow$ $\hat{\rho}$ **1-body density matrix**

If V_{eff} is well designed, the g.s. (minimum) energy can match experiment at best. Hartree-Fock or Kohn-Sham.



- Within a time-dependent theory (TDHF), one can describe oscillations around the minimum.

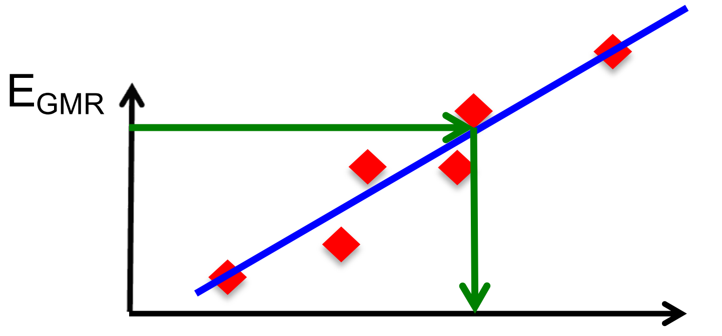
- The restoring force is: $v \equiv \frac{\delta^2 E}{\delta \rho^2}$

$$X_{\rm ph}|ph^{-1}\rangle - Y_{\rm ph}|hp^{-1}\rangle$$

- The linearization of the equation of the motion leads to RPA[1]. [1]Random Phase Approximation.

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \hbar\omega \begin{pmatrix} X \\ Y \end{pmatrix}$$

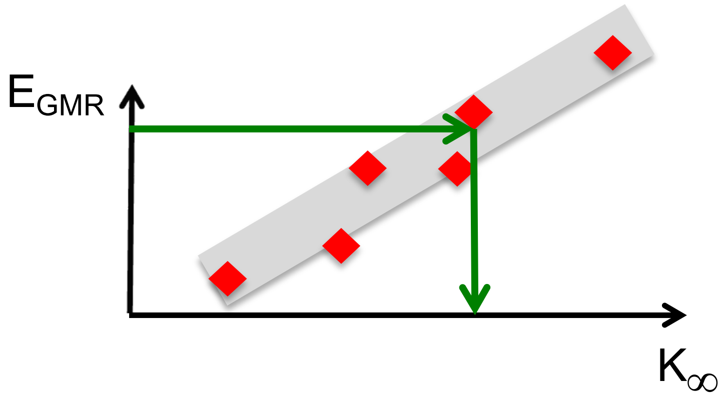
How much correlated are E_{GMR} and K_∞?



Energy Density Functionals (EDFs)

Only self-consistent DFT calculations that treat **uniform matter and the response of finite nuclei on equal footing** allow extracting K_∞

J.P. Blaizot, Phys. Rep. 64, 171 (1980)



There are different sources of model dependence in this procedure.

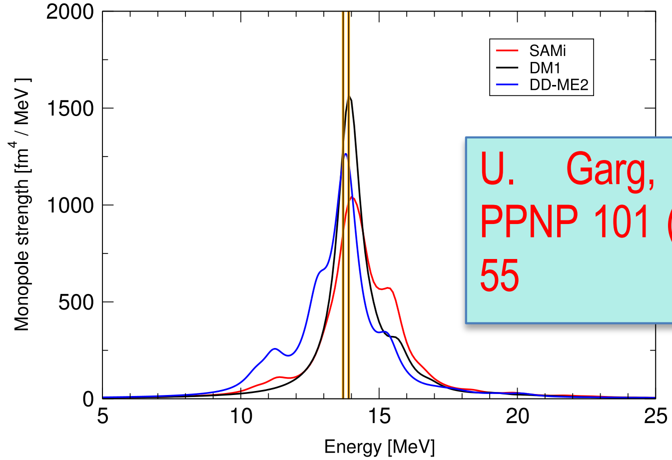
One **key point** is that different EDFs have different assumptions for the density dependence.

GC *et al.*, Phys. Rev. C70 (2004) 024307.

- **Sensitivity to the choice of the nucleus?**

From the ISGMR measured in ^{208}Pb one extracts:

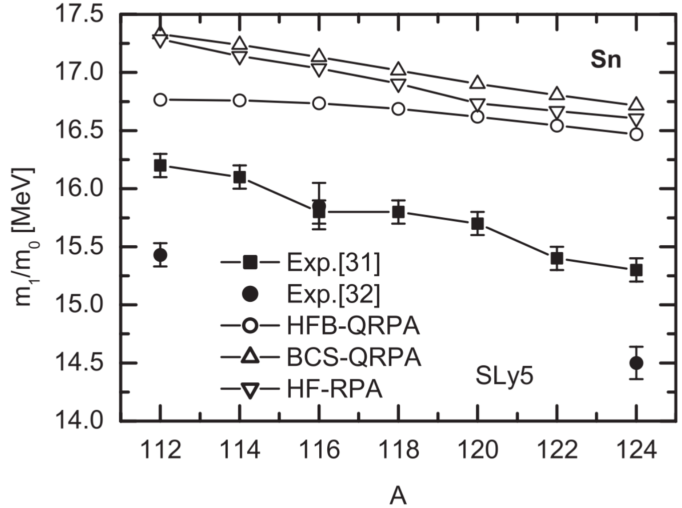
$$K_\infty = 240 \pm 20 \text{ MeV}$$



U. Garg, GC, PPNP 101 (2018) 55

However, in even-even $^{112-124}$Sn, the ISGMR centroid energy is overestimated by about 1 MeV by the same models, which reproduce the ISGMR energy well in ^{208}Pb.

Why is Tin so soft?



J. Li et al., PRC 78, 064304 (2008)

Pairing can partly explain the problem but with some remaining ambiguity.

- Our solution to the “softness” puzzle

(Q)RPA + (Q)PVC

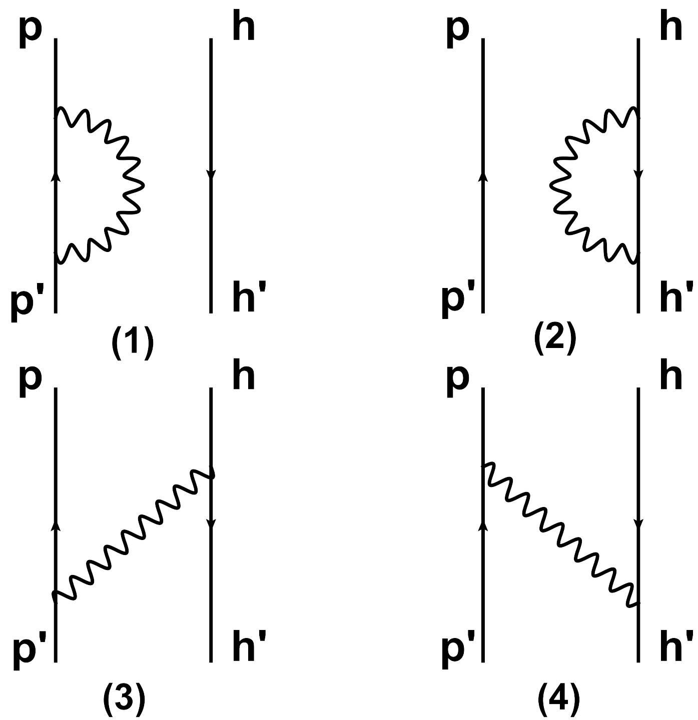
$$\begin{pmatrix} A+\Sigma(E) & B \\ -B & -A-\Sigma^*(-E) \end{pmatrix} \qquad \Sigma_{\mathrm{php'h'}}(E) = \sum_\alpha \frac{\langle ph|V|\alpha\rangle\langle\alpha|V|p'h'\rangle}{E-E_\alpha+i\eta}$$

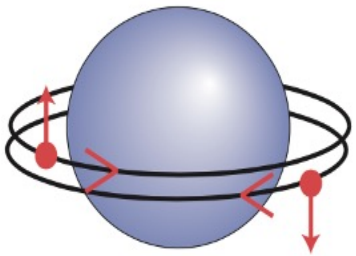
The state α is 1p-1h plus one phonon.

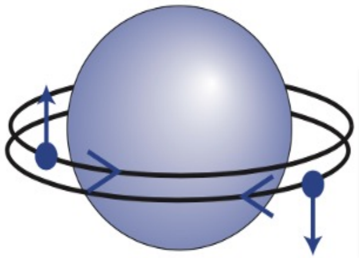
The scheme is very effective to produce GR widths. It also produces a downward shift of the GRs.

$$\Sigma(E) \approx \int dE' \, \frac{V^2}{E-E'+i\epsilon}$$

$$\frac{1}{E-E'+i\epsilon} \rightarrow \frac{1}{E-E'} - i\pi\delta(E-E')$$







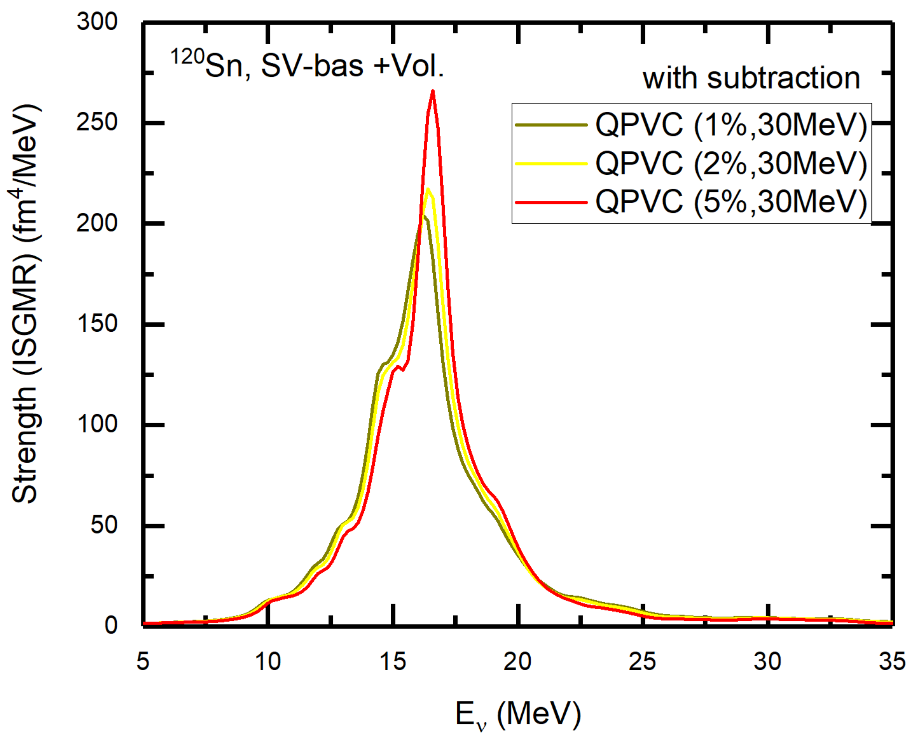
WE HAVE BUILT A NEW SCHEME INCLUDING PAIRING

Some detail + the subtraction scheme

All QRPA calculations are performed in a model space which is large enough so that the EWSR is satisfied.

We calculate natural-parity phonons with 0^+, 1^-, 2^+ ... 5^- and select those having energy less than 30 MeV and strength larger than 2% of the total strength.

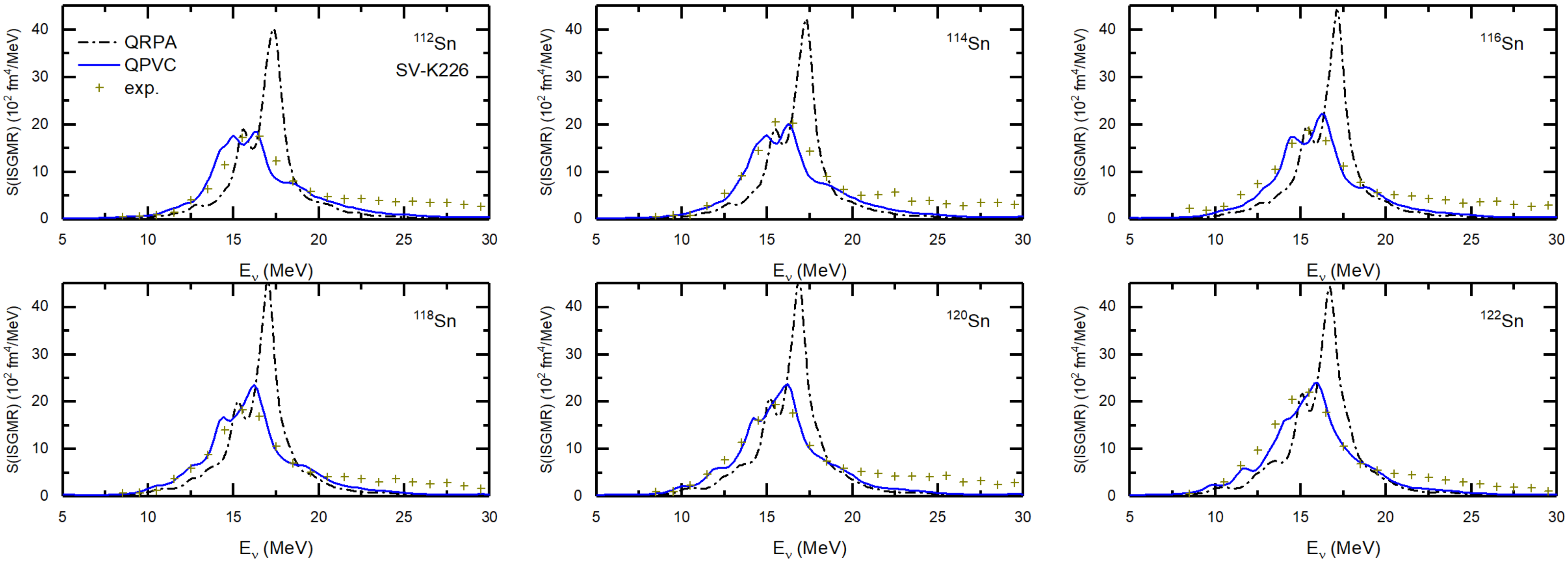
The convergence of the results with respect to the choice of the model space has been carefully assessed.



Subtraction: $$\Sigma(E) \quad \rightarrow \quad \Sigma(E) - \Sigma(E=0)$$

THIS PRESCRIPTION KEEPS THE VALUE OF THE m_{-1} SUM RULE AS IN QRPA

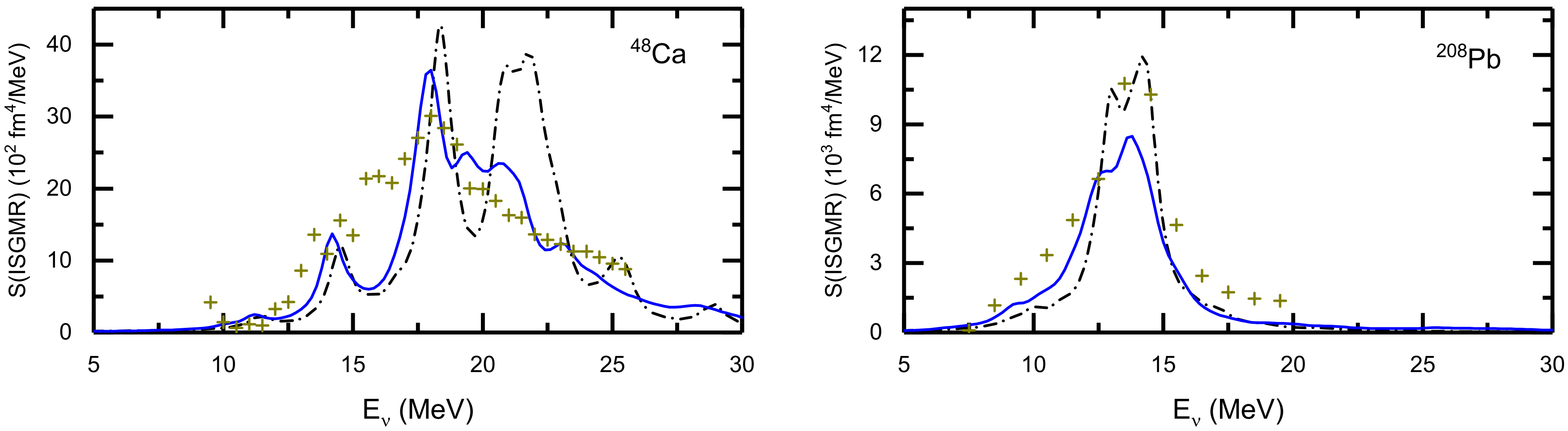
ISGMR in Sn isotopes



- Exp. data from D. Patel *et al*., Phys. Lett. B726, 178 (2013)
- QPVC reproduces the experimental data quite well.
- The best description is obtained with the Skyrme EDF SV-K226.

Klüpfel, Reinhard, *et al.*, PRC 79, 034310 (2009)

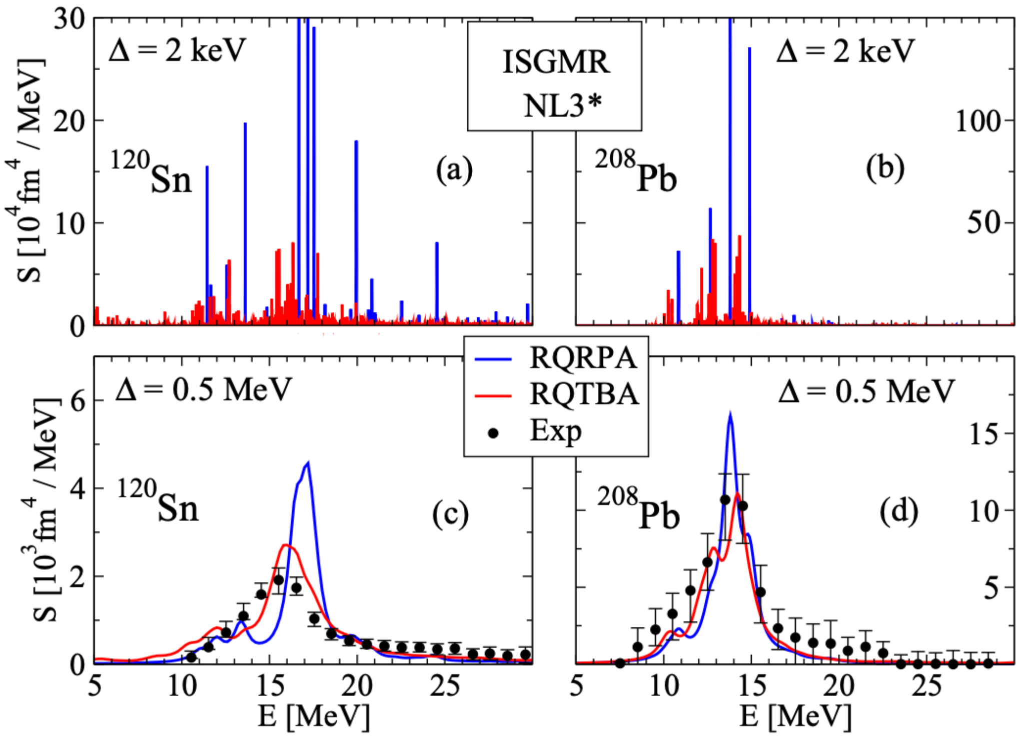
ISGMR in ^{48}Ca and ^{208}Pb

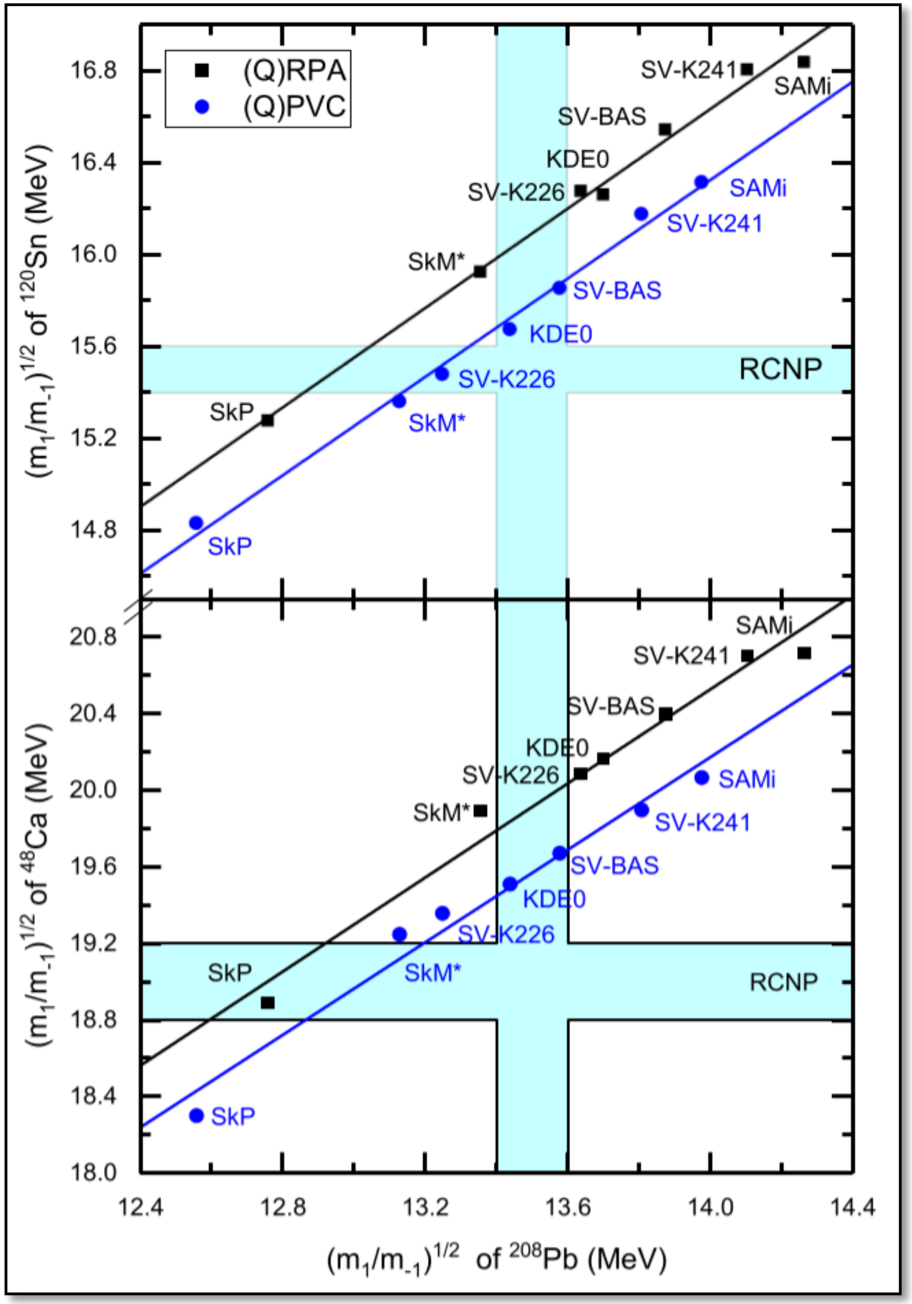


- Exp. data from T. Li *et al.*, Phys. Rev. Lett. 99, 162503 (2007) and S.D. Olorunfunmi, Phys. Rev. C 105, 054319 (2022).
- In these two cases there is no pairing.

- More details can be found in
  Z.Z. Li, Y.F. Niu, GC, arXiV:2211.01264 [nucl-th]
  submitted on 2 Nov 2022

- A later work by E. Litvinova confirms the importance of PVC correlations
  arXiv:2212.14766 [nucl-th], submitted on 30 Dec 2022





In our work, we have been able, for the first time, to analyse **in a systematic manner** the consistency between ISGMR energies in different nuclei.

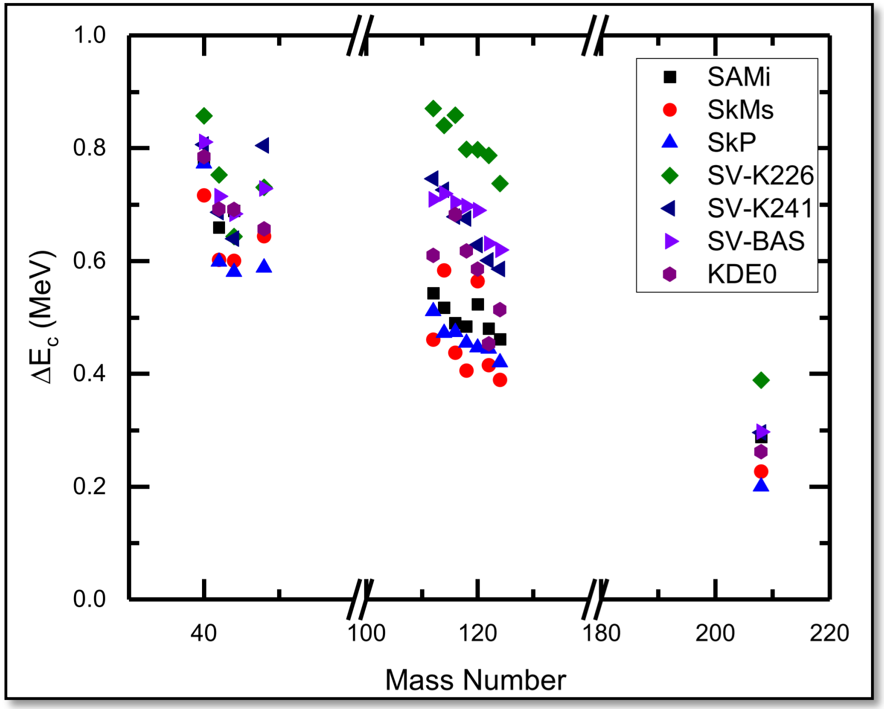
We have used many Skyrme EDFs.

With the inclusion of QPVC effects, a big improvement is achieved.

Within QPVC, the ISGMR energy in ^{208}Pb is consistent with ^{120}Sn.

Z.Z. Li, Y.F. Niu, GC, arXiv:2211.01264

The energy shift from QRPA to QPVC



In general, the coupling with the vibrations shifts the mean energies downward.

$$\Delta E_c = E_c(\mathrm{QRPA}) - E_c(\mathrm{QPVC})$$

$$E_c = \sqrt{m_1/m_{-1}}$$

For monopole, the shift is not large (less than 1 MeV).

Still, the shift in ^{208}Pb is smaller than for Sn and Ca isotopes.

The mechanism behind the energy shift

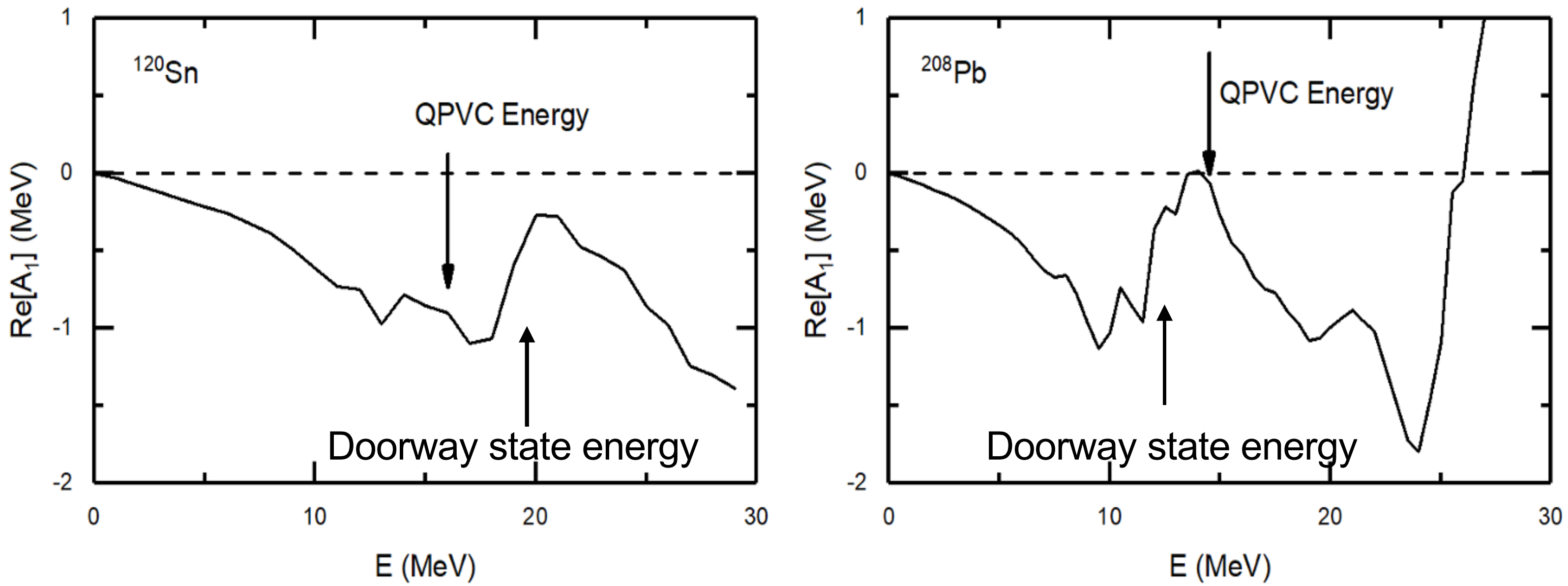
$$\Sigma(E) \approx \int dE' \, \frac{V^2}{E - E' + i\epsilon}$$

$$\frac{1}{E - E' + i\epsilon} \to \frac{1}{E - E'} - i\pi\delta(E - E')$$

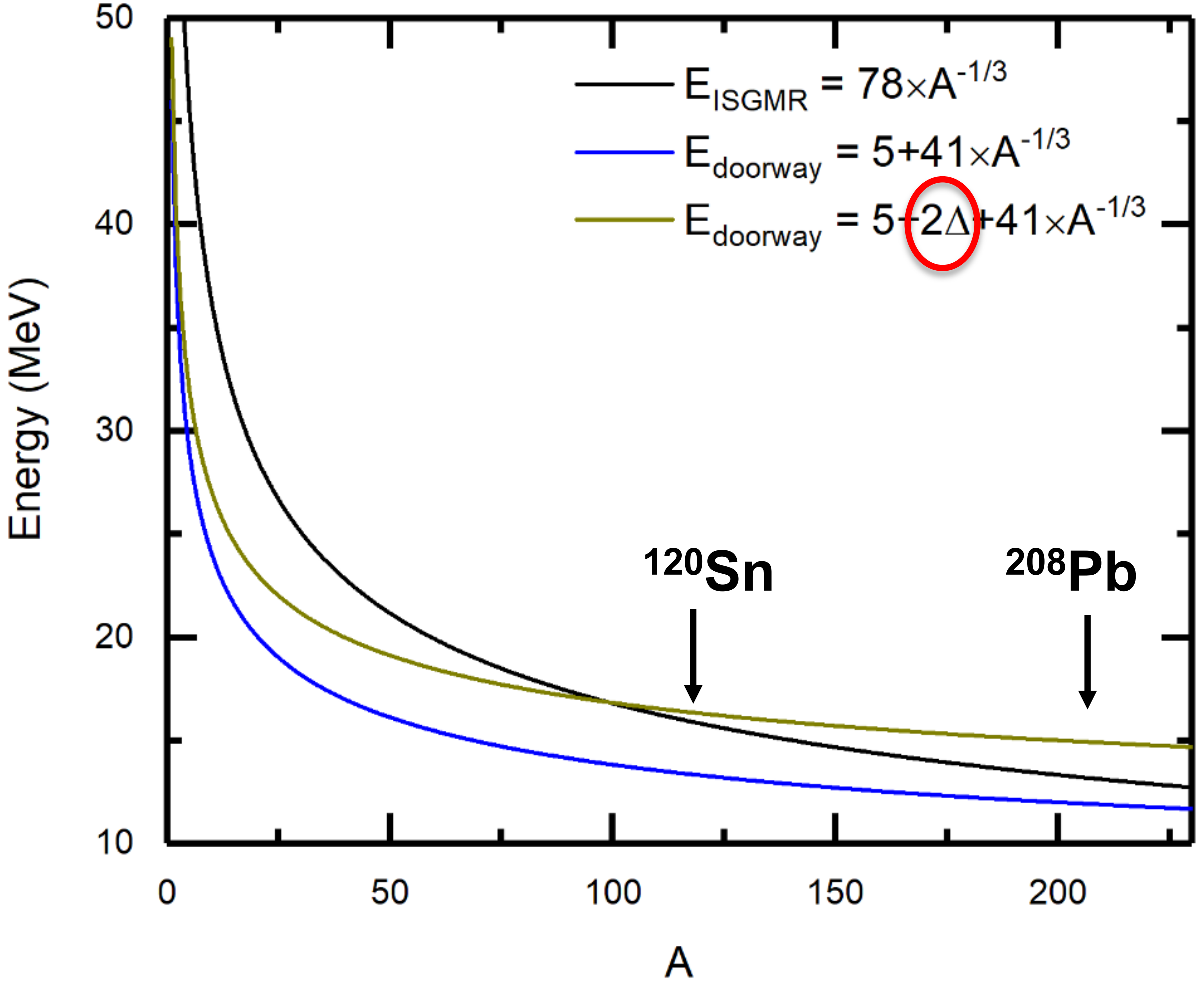
The **real part of the self-energy** produces the energy shift

E = **QPVC** energy of the GMR
E' = energy of the **doorway states**

$$2 \text{ q.p.} \otimes 1 \text{ phonon}$$



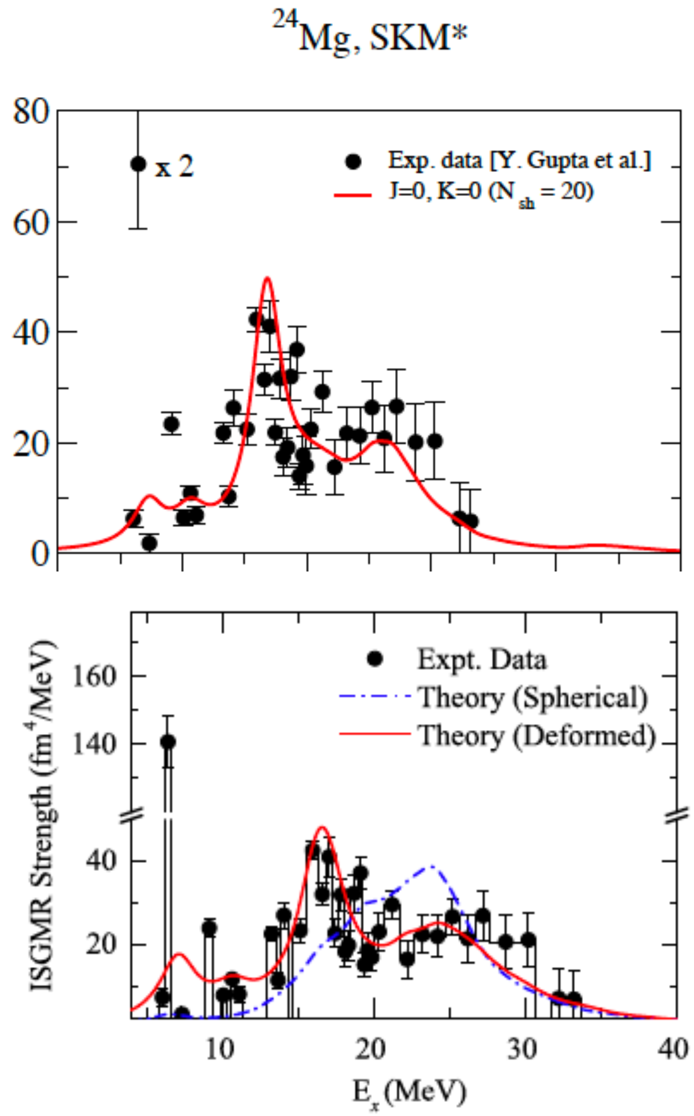
The QPVC energy is not very different in the two nuclei but doorway state energies are higher in Sn than in Pb



The pairing gap Δ makes the relative energy position of the ISGMR and of the doorway states different!

- Deformed nuclei

Well-deformed nuclei



We compare with RCNP data from Y. Gupta *et al.*, PRC 93, 044324 (2016).

The two-peak structure is evident.

Thanks to K. Howard.

Calculations by K. Yoshida were used to show that the double peak is related to deformation.

Other deformed QRPA schemes

- Either **HFB or HF-BCS equations** with a Skyrme force and a pairing force are solved (HFBTHO / SKYAX).

M. Stoitsov *et al.*, Comp. Phys. Comm. 184 (2013) 1592;
P.G. Reinhard *et al.*, Comp. Phys. Comm. 258 (2021) 107603

- This allows to study the potential energy surfaces (PESs).

$$E = E(\beta)$$

- The **QRPA equations** are solved at β_{min} on a basis with **good** $\mathbf{K}^{\pi}$.

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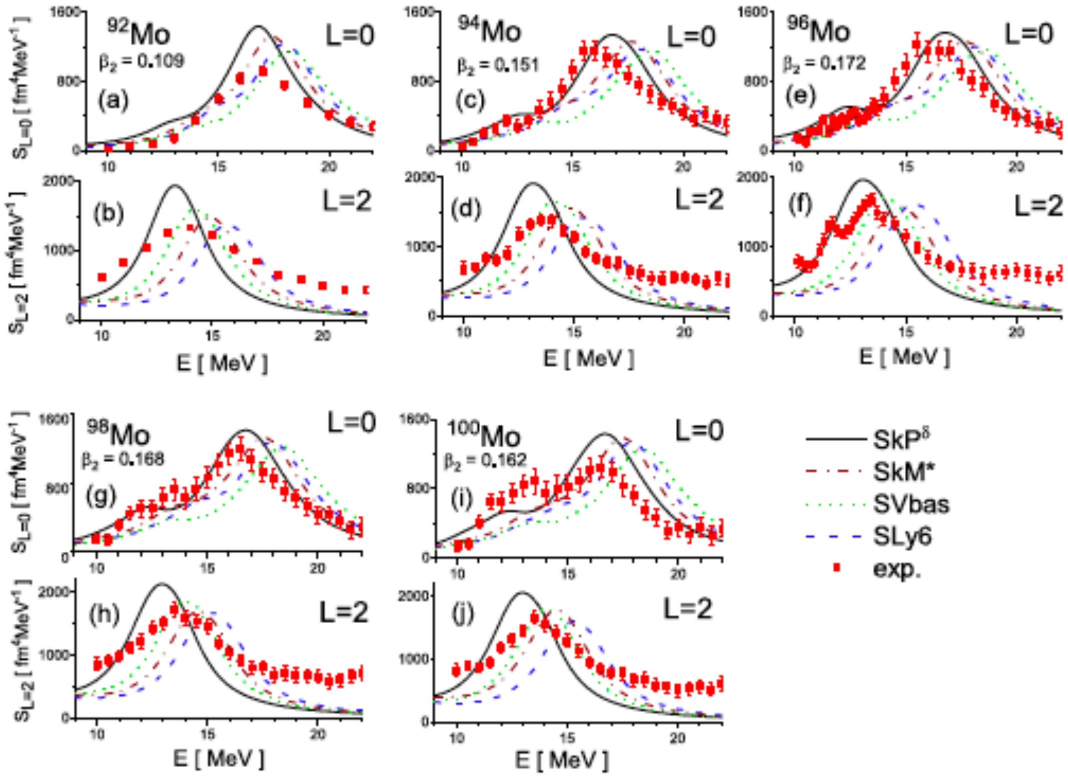
Isoscalar monopole and quadrupole modes in Mo isotopes: Microscopic analysis

Gianluca Colò[a,b,*], Danilo Gambacurta[c,d], Wolfgang Kleinig[e], Jan Kvasil[f], Valentin O. Nesterenko[e,g,h], Alessandro Pastore[i]

Monopole and quadrupole strength in ^{A}Mo



The "shoulder" is due to the monopole-quadrupole coupling.

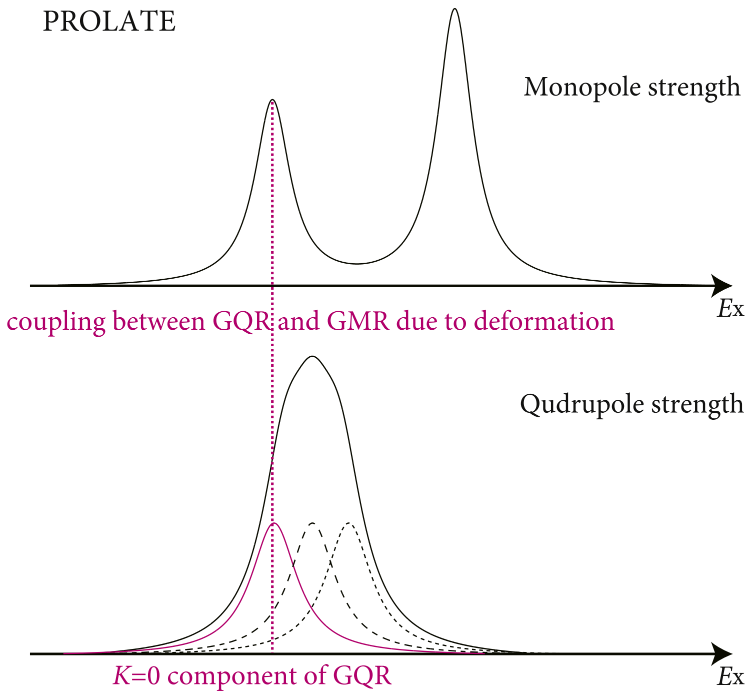
The Skyrme EDF that better reproduces the GMR (GQR) results is SkP$^\delta$ (SVbas).

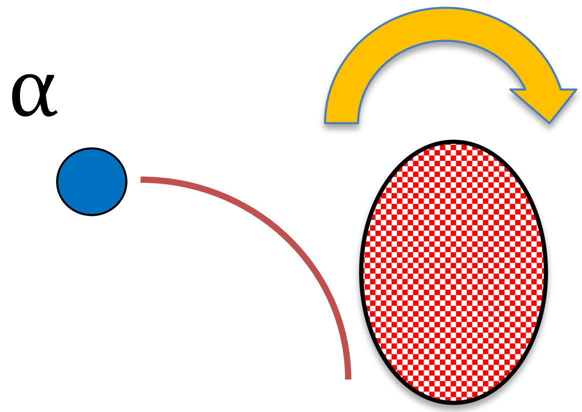
Warning, warning ...

Incompressibility K_∞ and isoscalar effective mass m^*/m for the Skyrme forces SVbas, SLy6, SkM*, and SkP$^\delta$.

	SVbas	SLy6	SkM*	SkP$^\delta$
K_∞ [MeV]	234	230	217	202
m^*/m	0.9	0.69	0.79	1

Need of angular momentum projected QRPA





In axially deformed nuclei, K is the good quantum number in the intrinsic frame and there is monopole-quadrupole coupling.

Nevertheless, the external monopole field in the lab must be transformed into the intrinsic frame.

Or, analogously, we should **project the intrinsic states into states with good J.**

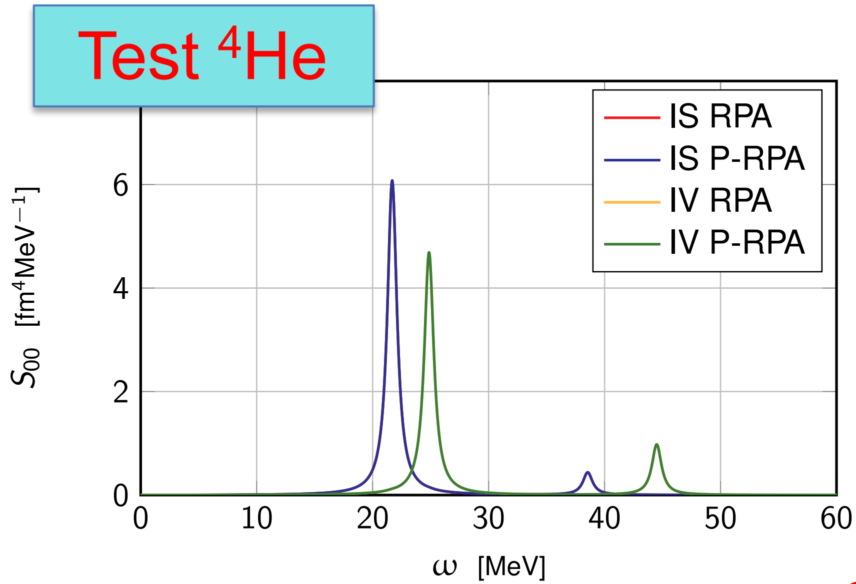
$$|KM\rangle \;\; \rightarrow \;\; |JKM\rangle = P^J_{KM}|KM\rangle = \int d\Omega \; \mathcal{D}^{\dagger J}_{KM}(\Omega) R(\Omega) \; |KM\rangle$$

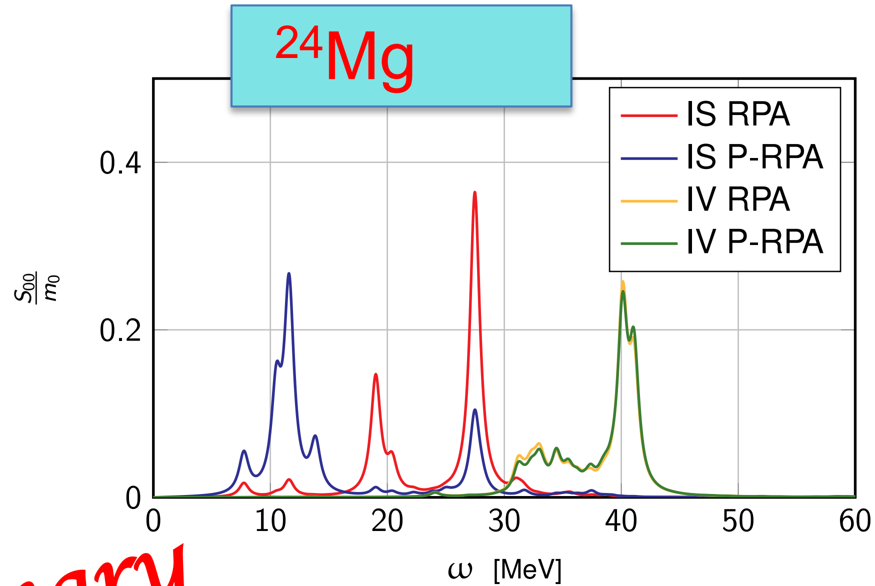
$$\langle \mathrm{RPA} \| T_\lambda \| \omega \rangle = N_0 N_\omega (2J_0+1)(-1)^{J_0-K_0} \sum_{ph} \sum_{\mu=-\lambda}^{+\lambda} \left\{ X_{ph}^{\omega} + (-1)^{\mu} Y_{ph}^{\omega} \right\} \begin{pmatrix} J_0 & \lambda & J_\omega \\ -K_0 & \mu & K_0-\mu \end{pmatrix} \langle \mathrm{HF} | T_{\lambda\mu} P^{J_\omega}_{K_0-\mu, K_{ph}} c_p^\dagger c_h | \mathrm{HF} \rangle$$

$$N_i^{-1} = \sqrt{\langle \Phi_i | P^{J_i}_{K_i K_i} | \Phi_i \rangle}$$

$$P^J_{MK} = \frac{2J+1}{2} \int_{-1}^{+1} \mathrm{d}(\cos\beta)\, d^J_{MK}(\beta) e^{-i\beta J_y}$$

In the J=0 case d^0_{00} =1: we are superimposing configurations that are simply rotated.





Preliminary

Conclusions

- Since the 1980s, there has been big progress in our understanding of the ISGMR (e.g., regarding model dependence, relativistic vs. nonrelativistic etc.)

- We have developed a fully self-consistent QRPA+QPVC model in which the "puzzle" of Sn vs. Pb appears to be solved.

- The EDFs that reproduce the ISMGR energies in Ca, Zr, Sn and Pb have K_∞ equal to 226 MeV and 229 MeV.

- We are dealing with deformed nuclei by implementing projection on top of QRPA.

- Danilo Gambacurta (LNS, Catania, Italy)
- Andrea Porro (CEA, Saclay, France)
- Yifei Niu, **Z.Z. Li** (Lanzhou University, China)

Thanks to Collaborators

Backup slides

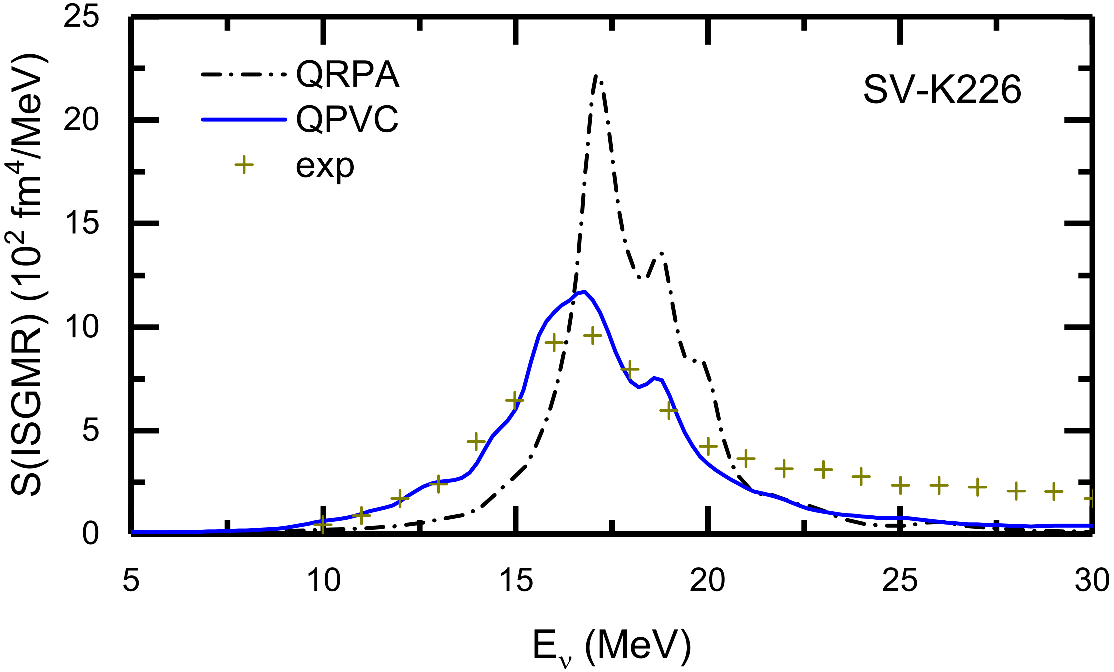


FIG. 5. (Color online) ISGMR strength functions in ^{90}Zr calculated either by (Q)RPA using a smoothing with Lorentzian functions having a width of 1 MeV (dash dot [black] line), or in (Q)RPA+(Q)PVC (solid [blue] line). The SV-K226 Skyrme force is used. The experimental data are given by green crosses [4].