Nuclear single-particle and collective spectroscopy

Gianluca Colò

Fifth Gogny Conference
Paris, 10th-13th Dec. 2024

Outline

- Quasi-particle states: particle-vibration coupling on top of EDFs
- The same model applied to collective states
- How to improve EDFs (short)

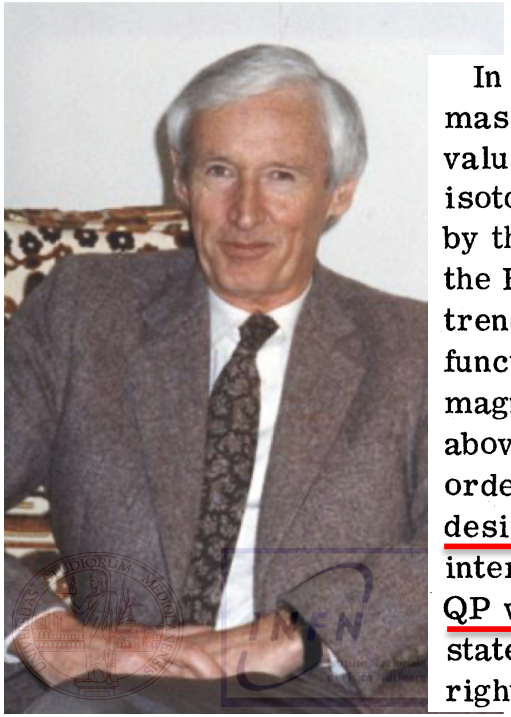
Single-particle states (I)

Given an effective Hamiltonian H_{eff}, the single-particle (or quasi-particle) states can be calculated using HF (or HFB)

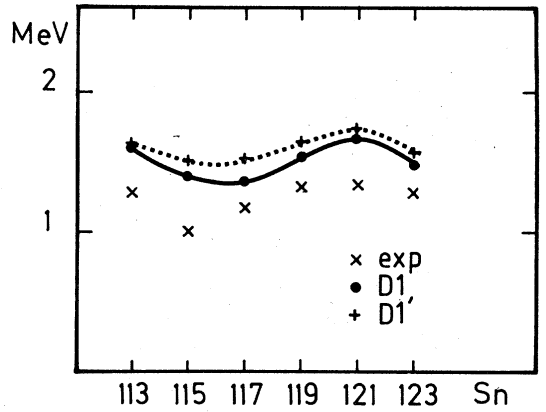
PHYSICAL REVIEW C VOLUME 21, NUMBER 4 APRIL 1980

Hartree-Fock-Bogolyubov calculations with the *D*1 effective interaction on spherical nuclei

J. Dechargé and D. Gogny
Service de Physique Neutronique et Nucléaire, Centre d'Etudes de Bruyères-le-Châtel, Boîte Postale No. 561, 92542 Montrouge Cedex, France
(Received 3 August 1979)

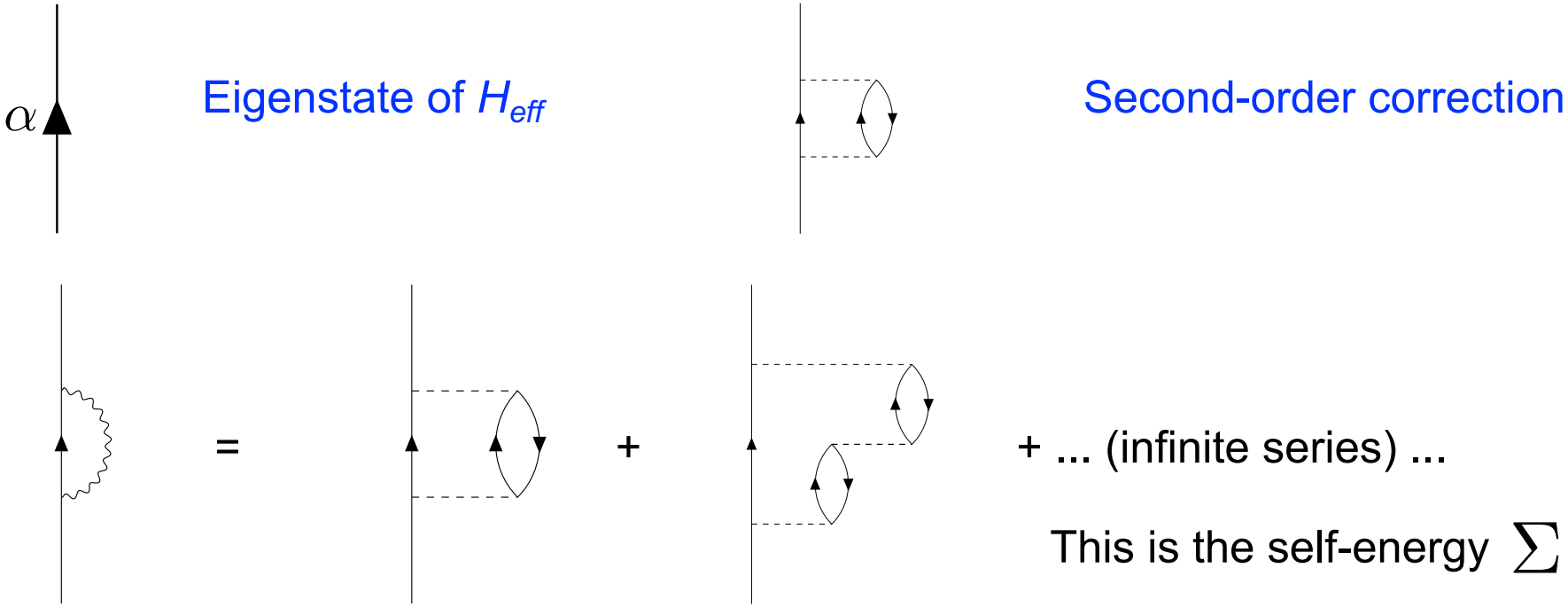


In Fig. 3 we have reported the HFB odd-even mass differences along with the experimental values and we also give in Table V for each isotope the spin of its ground state as predicted by the HFB calculations. First we notice that the HFB calculations reproduce the oscillating trends which are observed experimentally as a function of the neutron number. Concerning the magnitude of our predictions, they are all shifted above the experimental value by amount of the order of 300 keV. Somehow such deviation is desirable since one expects that the residual interaction between the three QP states (or the QP vibration coupling) would lower the ground state energy of the odd nuclei which goes in the right sense. Referring to the work of Kuo *et al.*[31]



Having no idea of the higher-order corrections we have no idea of which accuracy one should request

Single-particle states (II)



- We actually diagonalize H_{eff} in a basis made with 1p states plus 1p-1 phonon (RPA) states
- This has been generalised to 1 qp plus 1qp states-1 QRPA phonon states

Skyrme EDFs (even-even nuclei)

They are **local** functionals depending on various densities.

Here, proton/neutron labels are omitted for the sake of simplicity.

$$E = \int d^3r \ \left[\mathcal{E}^{\rm kin} + \mathcal{E}^{\rm Skyrme} + \mathcal{E}^{\rm pairing} + \mathcal{E}^{\rm Coulomb}\right]$$

$$\mathcal{E}^{\rm Skyrme} = C^{\rho\rho}[\rho]\rho^2 + C^{\rho\tau}\rho\tau + C^{J^2}\vec{J}^{\,2} + C^{(\nabla\rho)^2}\left(\vec{\nabla}\rho\right)^2 + C^{\rho\vec{\nabla}\cdot\vec{J}}\rho\vec{\nabla}\cdot\vec{J}$$

$$\rho(\vec{r}) = \rho(\vec{r},\vec{r}')|_{\vec{r}'=\vec{r}}$$

$$\tau(\vec{r}) = \nabla\cdot\nabla'\rho(\vec{r},\vec{r}')|_{\vec{r}'=\vec{r}}$$

$$\vec{J}(\vec{r}) \ \ \text{spin}-\text{orbit density}$$

$$C^{\rho\rho}[\rho] = A + B\rho^{\gamma}$$

Parameters are determined by a **fit to data** (or pseudo-data).

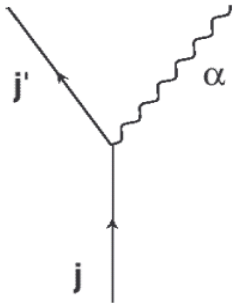
(Quasi)particle-vibration coupling (I)

- The model is self-consistent (no empirical input). We employ H_{Skyrme} but one can think of using it with any Hamiltonian

$$H = H_0 + V,$$

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

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



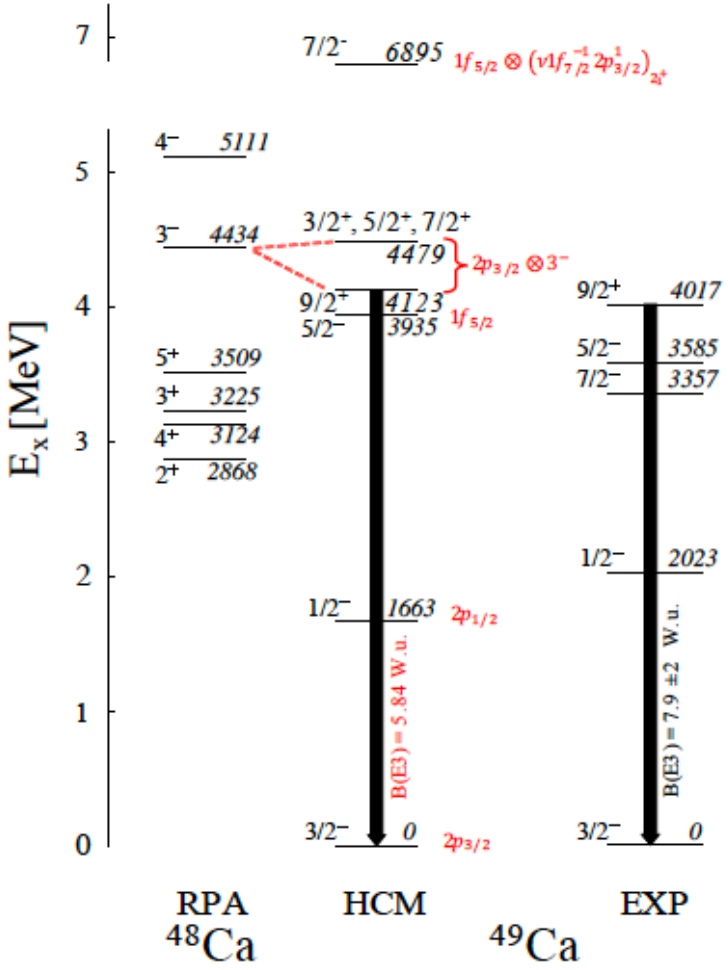
- We correct for the non-orthonormality and overcompleteness of the basis by introducing the NORM matrix

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

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

^{49}Ca

Energies and γ transitions



Spectroscopic factors of ^{49}Ca

Results obtained with SkX

J^π	ℓ	C^2S (exp[a])	ξ^2(s.p.) (HCM)
$3/2^-$	1	0.84(12)	0.98
$1/2^-$	1	0.91(15)	0.99
$5/2^-$	3	0.84	0.97
$9/2^+$	4	0.14	0.11

[a]The authors report the errors on C^2S for the $5/2^-$ and $9/2^+$ states as "a few percent".

TABLE X. Experimental and theoretical (see [8] and references therein) C^2S spectroscopic factors for the $9/2^+$ at 4296 keV in ^{49}Ca.

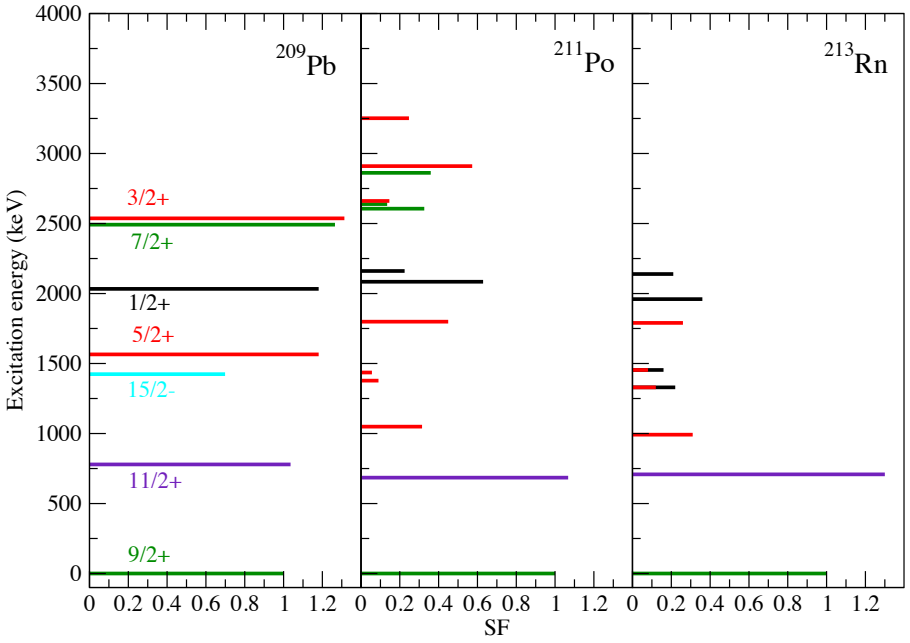
Experiment	C^2S
(d, p) [72]	0.14
$^{12}C + ^{48}Ca$ [8]	0.27(1)
Theory	C^2S
HCM	0.11
GXPF1 [8]	0.42

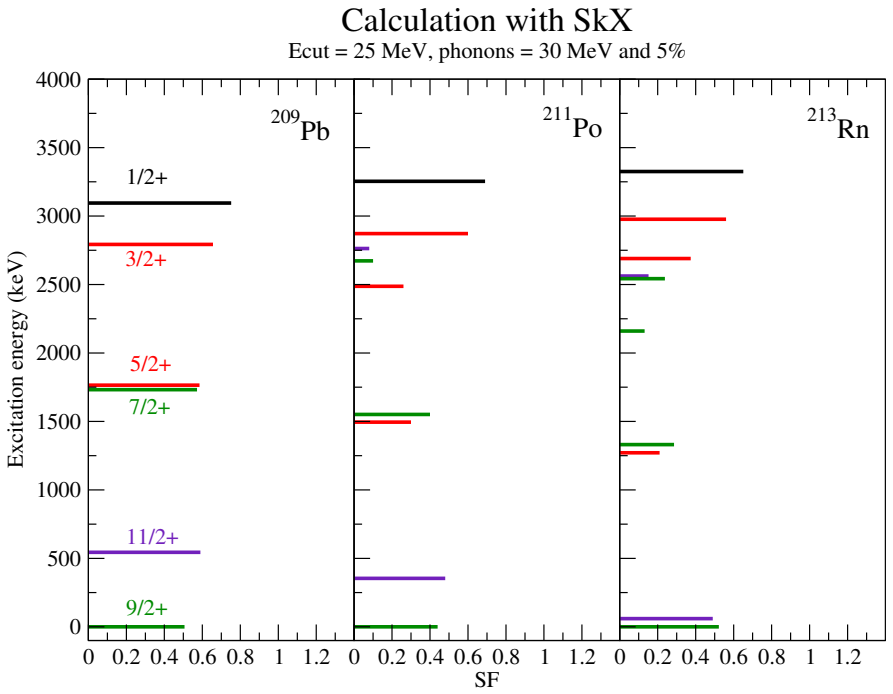
S. Bottoni et al., Phys. Rev. C103, 014320 (2021)

The subtraction scheme

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

- This prescription has been introduced in the context of the theories beyond RPA for the collective excitations, when based on EDFs
- The goal is to avoid the double-counting of static correlations
- It also avoids undesired divergences (“renormalization”)
- It can be implemented with the same aim(s) when considering single-particle spectroscopy
- Note: working with pairing sets a zero-energy for quasi-particles





IS689: Single-particle structure along N=127: ^{212}Rn(d,p)^{213}Rn

VERY PRELIMINARY RESULTS
courtesy of D. Clarke, D.K. Sharp (University of Manchester)

Comparison with DFT+QPVC

Note: theory reports the absolute S_F, while in experiment the values are normalized to the g.s. S_F

ISOLDE Solenoidal Spectrometer

- Quasi-particle states: particle-vibration coupling on top of EDFs

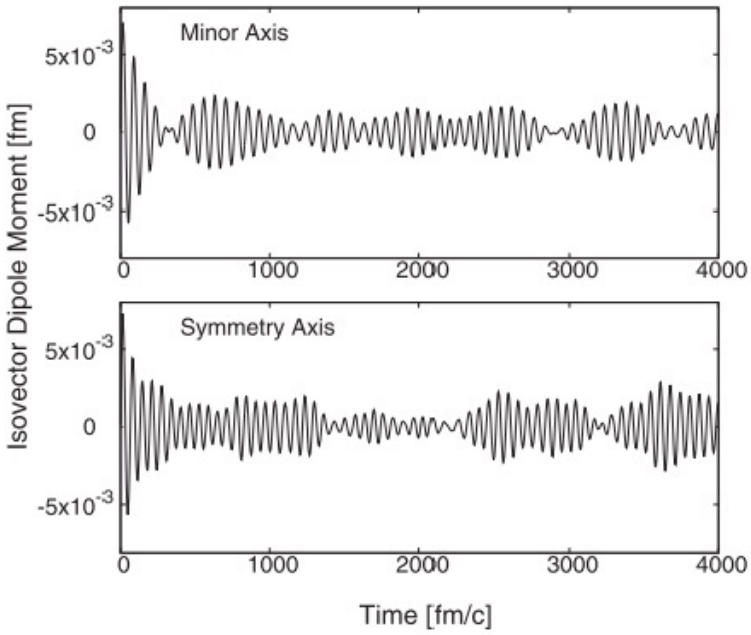
- The same model applied to collective states

- How to improve EDFs (short)

Random Phase Approximation

$$h\phi_i = \varepsilon_i \phi_i$$

From: P. Stevenson (U. Surrey)



In the time-dependent case, one can solve the evolution equation for the density directly:

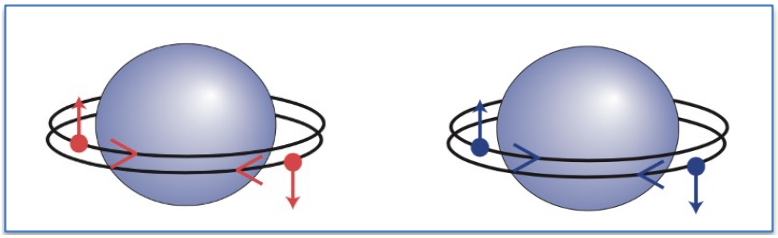
$$h(t) = h + f(t) \qquad [h(t), \rho(t)] = i\hbar\, \dot{\rho}(t)$$

$$\rho(t = 0) \neq \rho_{\text{g.s.}}$$

$$\rho(t = \Delta t) = U(t = 0, t = \Delta t)\rho(t = 0) \qquad U = e^{-i\frac{\Delta t}{\hbar}\cdot h}$$

If the equation for the density is linearized and solved on a basis: **Random Phase Approximation or RPA.**

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



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

In RPA the excited states are 1p-1h superpositions

(Q)RPA + (Q)PVC

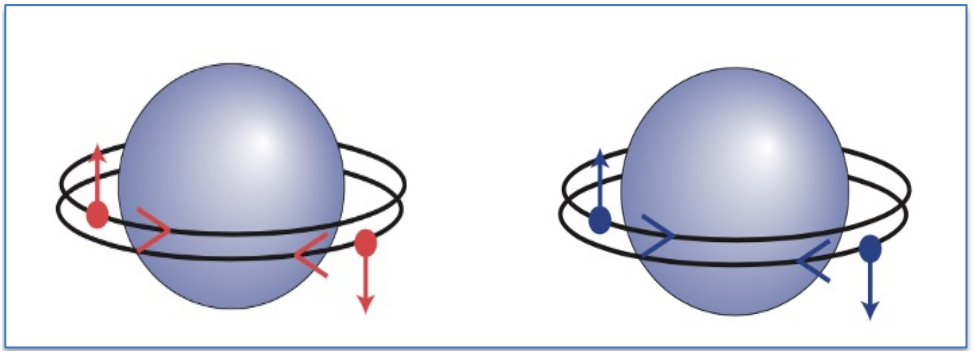
$$\begin{pmatrix} A+\Sigma(E) & B \\ -B & -A-\Sigma^*(-E) \end{pmatrix} \qquad \Sigma_{\mathrm{php'h'}}(E) = \sum_\alpha \frac{\langle ph|V|\alpha\rangle\langle\alpha|V|p'h'\rangle}{E-E_\alpha+i\eta}$$

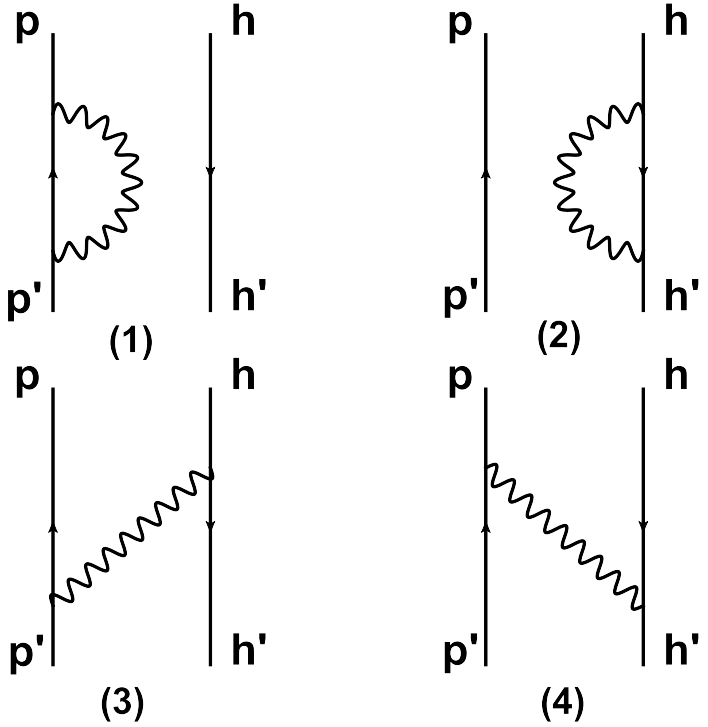
The state α is 1p-1h plus one phonon.

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

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

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

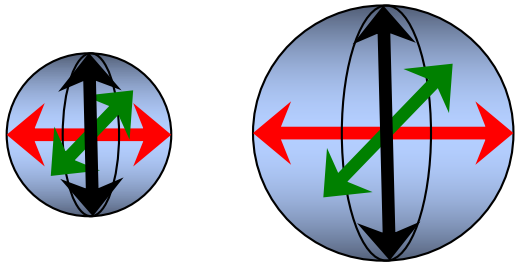




WE HAVE A SCHEME INCLUDING PAIRING for all GRs

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

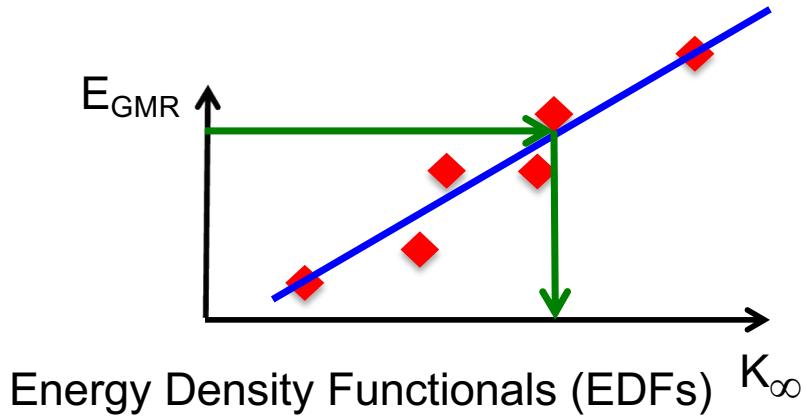
SN1987a

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

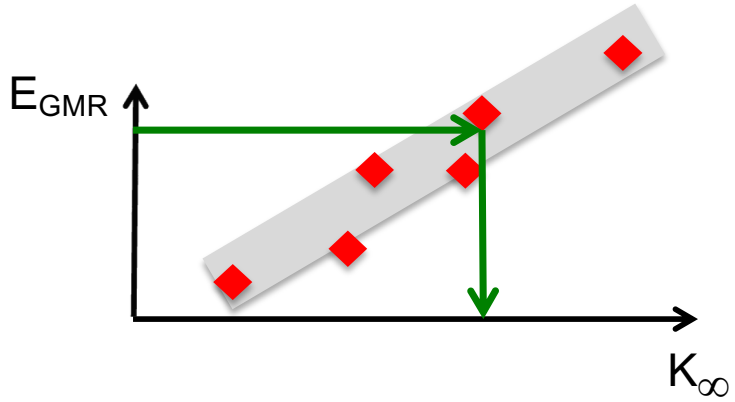
Probing the Incompressibility of Nuclear Matter at Ultrahigh Density through the Prompt Collapse of Asymmetric Neutron Star Binaries

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]

How correlated are E_{ISGMR} and K_∞?



Energy Density Functionals (EDFs)



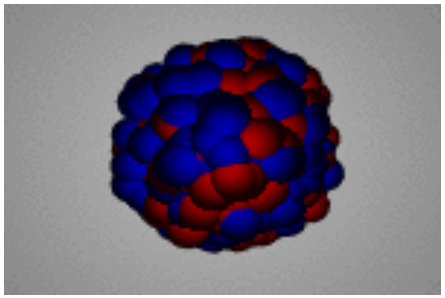
Only self-consistent DFT calculations that treat **uniform matter and the response of finite nuclei on equal footing** allow extracting K_∞

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.

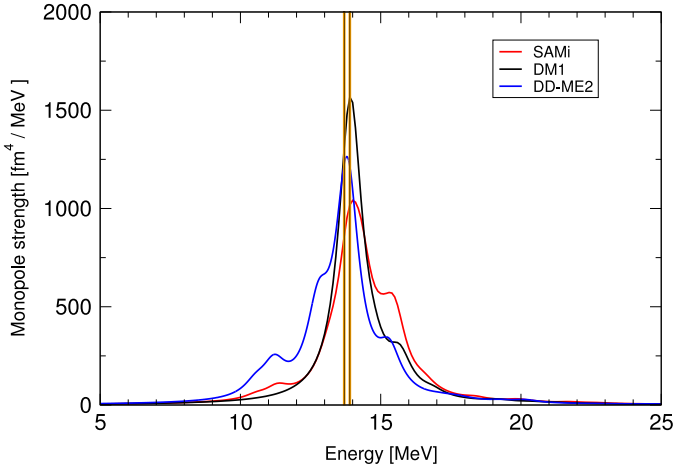


- **Sensitivity to the choice of the nucleus??**

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

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

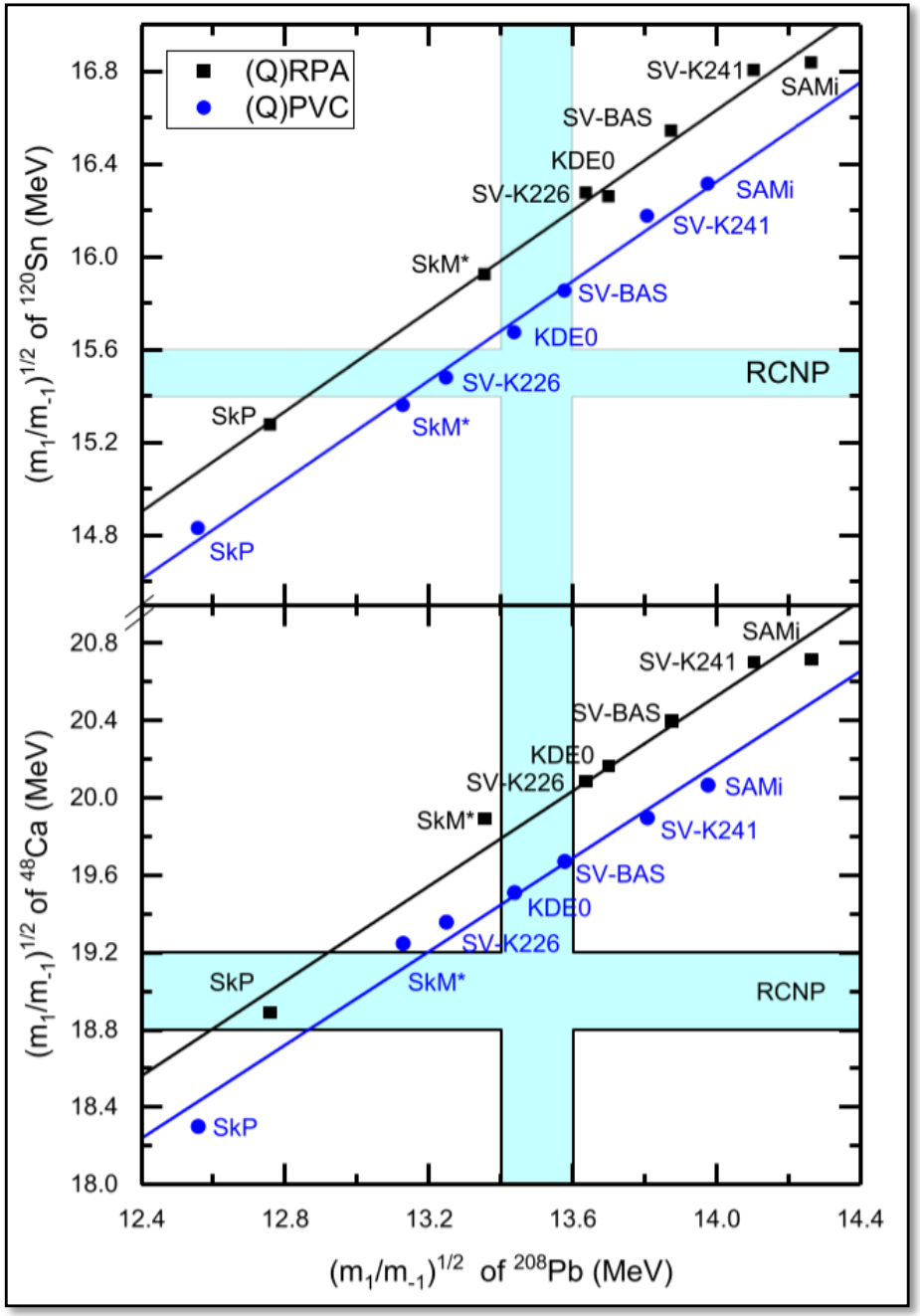
U. Garg, GC, PPNP 101 (2018) 55



However, in even-even $^{112\text{-}124}$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?

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



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.

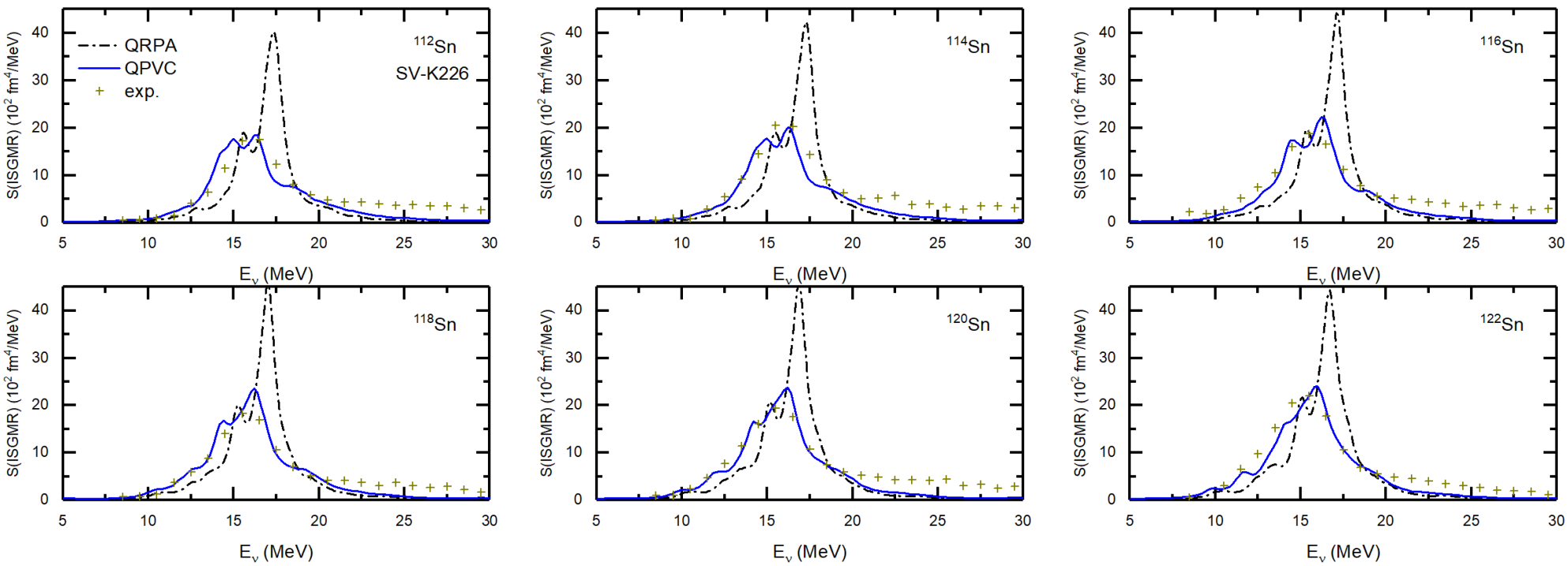
We have used many Skyrme EDFs.

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, Phys. Rev. Lett. 131, 082501 (2023)

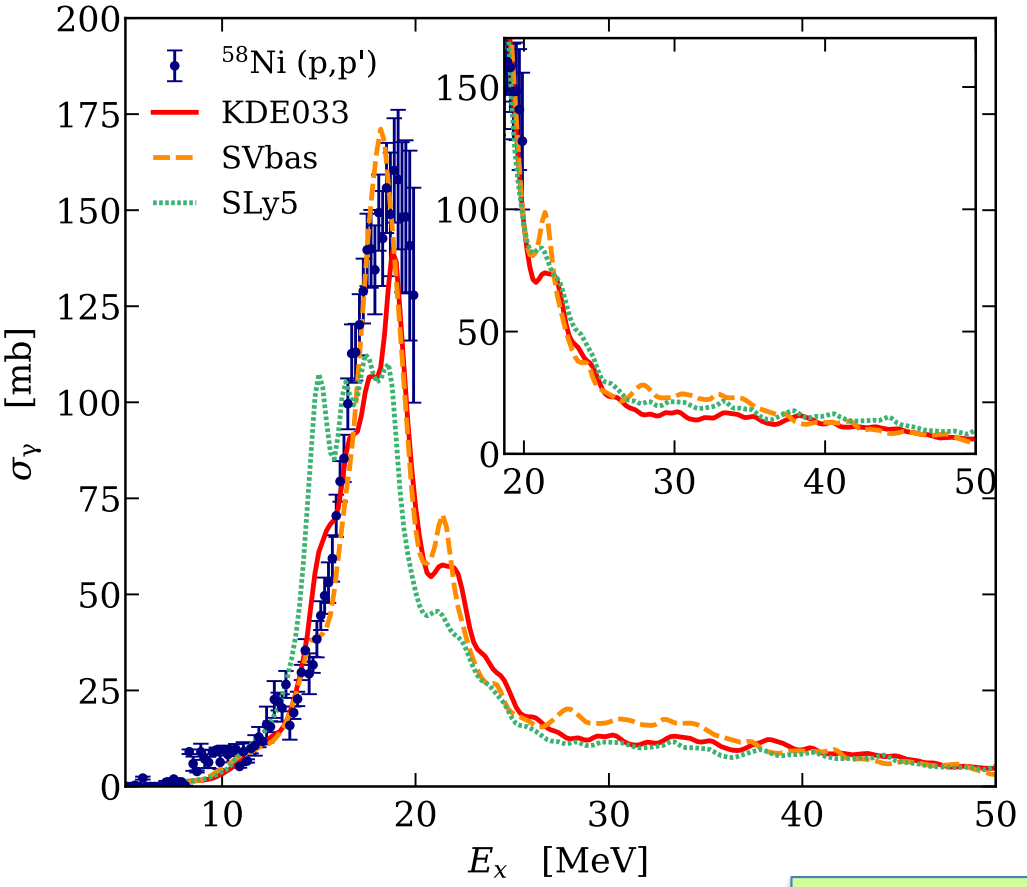
ISGMR in Sn isotopes



- 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)

Other applications of QPVC



Comparison with very recent data from (p,p') measured at RCNP, Osaka.

Exp. data from I. Brandherm *et al.*

Theory reproduces very well the dipole polarizabilty and can be used to estimate the high-energy dipole tail.

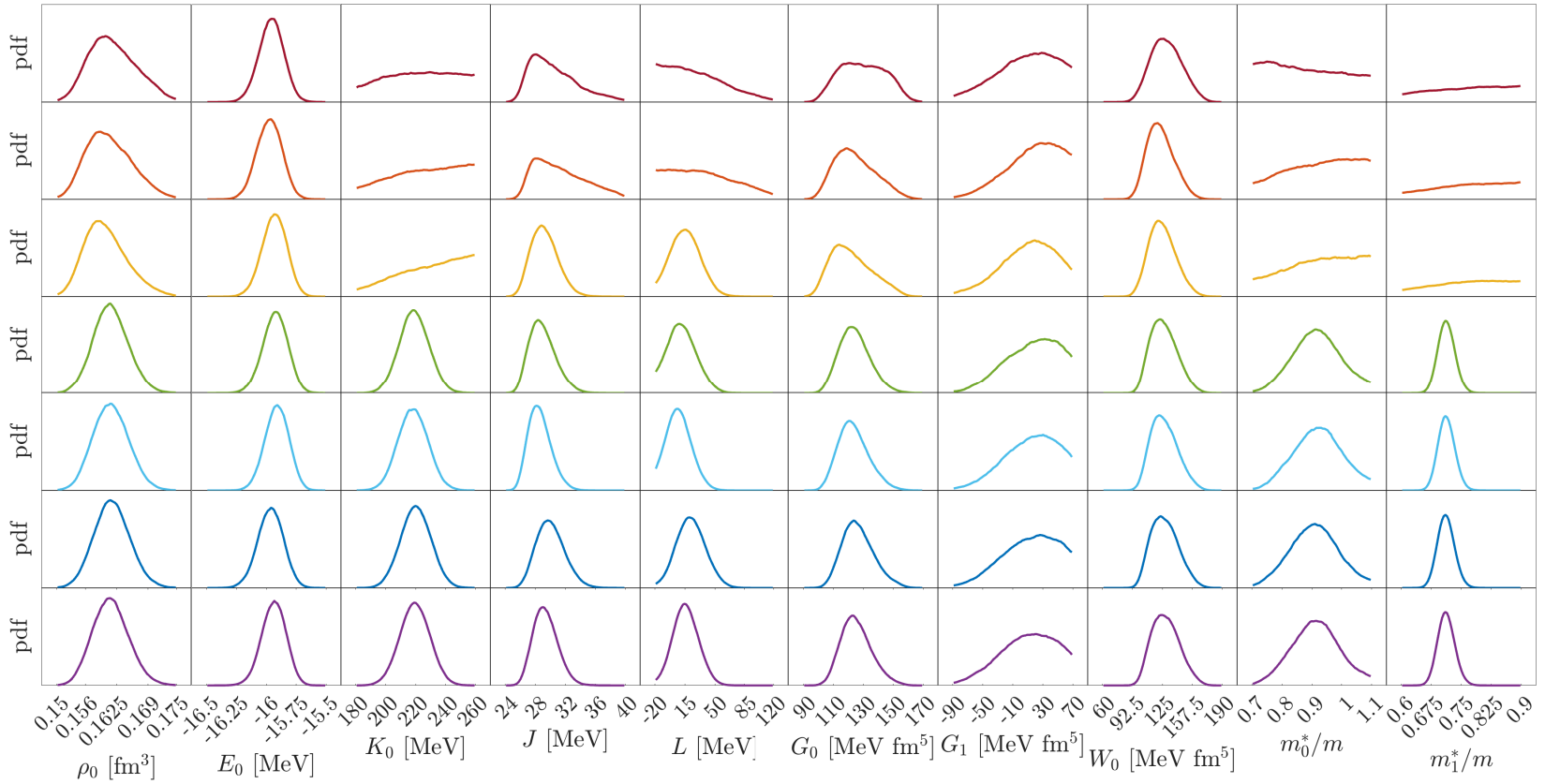
arXiv:2410.00610v1 [nucl-ex] 1 Oct 2024

- Quasi-particle states: particle-vibration coupling on top of EDFs

- The same model applied to collective states

- How to improve EDFs (short)

Bayesian inference of a Skyrme EDF



Basic BE, radii

+ ΔE_{so}

+ α_D

+ E(GRs)

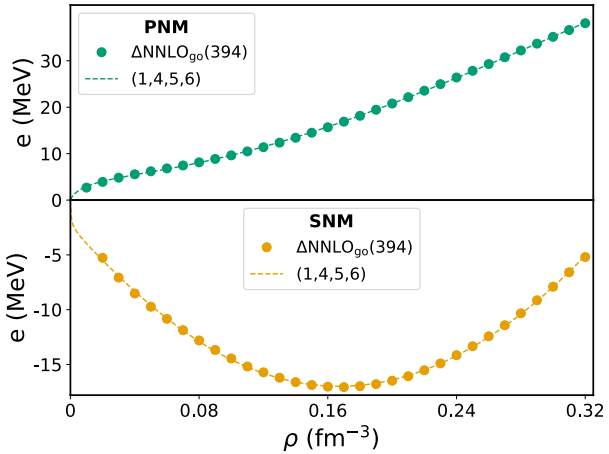
+ CREX only

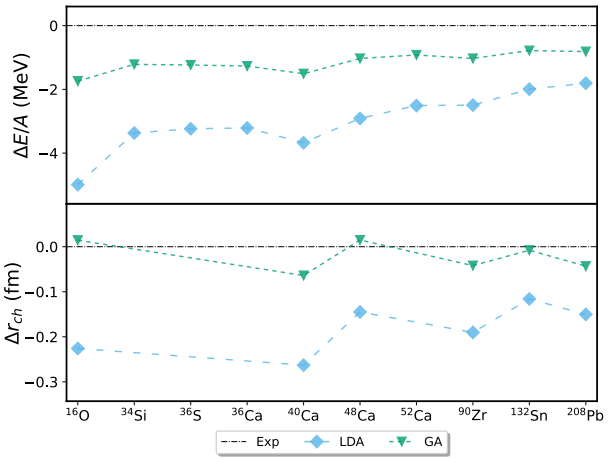
+ PREX only

all observables

- Results are in line with other types of analysis, except for a tendency towards low J and L
- Tension associated with $A_{PV}(^{208}Pb)$
- Still not possible at the level beyond EDF (e.g. including QPVC)

Ab initio-based EDFs





Local Density Approximation (LDA):

Starting from *ab initio* EoS, we fix the (bulk) density dependence of the EDF. No gradient terms.

$$v(\rho,\beta) = \sum_{\gamma} \left(c_{\gamma,0} + \beta^2 c_{\gamma,1}\right) \rho^{\gamma}$$

$$\rho = \rho_n + \rho_p$$

$$\beta = \frac{\rho_n - \rho_p}{\rho}$$

Work in progress on *ab initio* GA (gradient approximation) EDFs.

GC *et al.*, QNP24 conference proceedings

Conclusions

- Not only DFT is the only theory for heavy nuclei, but also the only theory for highly excited states
- The dynamical correlations associated with the **quasiparticle-vibration coupling (QPVC) approach** have been introduced on top of DFT and shown to be essential for solving the problem of the nuclear incompressibility
- Our method also allows studying the fragmentation of the single-particle strength and its evolution
- We are currently working on new EDFs, either based on *ab initio* or on Bayesian inference from experimental data

- C. Barbieri, E.Vigezzi (Univ. of Milano and INFN, Italy)
- F. Pederiva (Univ. of Trento and INFN, Italy)
- P. Klausner, M. Antonelli, F. Gulminelli (LPC Caen, France)
- F. Marino (Mainz University, Germany)
- X. Roca-Maza (Univ. of Barcelona, Spain)
- A. Lovato (ANL, USA)
- Z.Z. Li, Y. Niu (Lanzhou University)

Thanks to collaborators

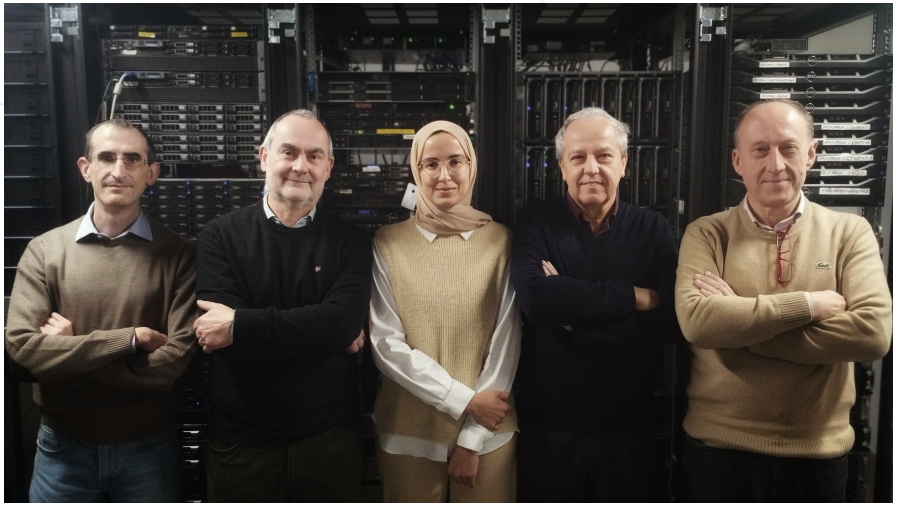
https://ns4exp.mi.infn.it

The Structure4exp virtual access (VA) facility, at ns4exp.mi.infn.it, is a part of the Theo4Exp VA infrastructure and, as such, is intended to provide theoretical tools for the EURO-LABS project as well as for the wider nuclear physics community. The key nuclear structure codes available are now either HF plus RPA and HFBCS plus QRPA for spherical nuclei, or a shell model code. All, in different ways, produce output for basic observable quantities that are the subject of current experimental activity:

i. Binding energies, density distributions and mean square radii
ii. Energies and wave functions/transition densities of the excited states
iii. Electromagnetic transition probabilities to the ground state.

This facility includes three codes:

Random Phase Approximation (RPA) plus Hartree Fock (HF)
HF_Bardeen_Cooper_Schrieffer-Quasiparticle RPA (HFBCS-QRPA)
KSHELL code



Backup slides

The Kohn-Sham scheme

We assume that the density can be expressed in terms of **single-particle orbitals**, and that the kinetic energy has the simple form:

$$\rho(\vec{r}) = \sum_i \phi_i^*(\vec{r})\phi_i(\vec{r}) \qquad T = \sum_i \int d^3r\ \phi_i^*(\vec{r}) \left(-\frac{\hbar^2 \nabla_i^2}{2m} \right) \phi_i(\vec{r})$$

We have said that the energy must be minimized, but we add a constraint associated with the fact that we want **orbitals that form an orthonormal set** (Lagrange multiplier):

$$E - \sum_i \varepsilon_i \int d^3r\ \phi_i^*(\vec{r})\phi_i(\vec{r}) = T + F[\rho] + \int d^3r\ V_{\text{ext}}(\vec{r})\rho(\vec{r}) - \sum_i \varepsilon_i \int d^3r\ \phi_i^*(\vec{r})\phi_i(\vec{r})$$

The variation of this quantity, $(\delta/\delta\phi^*)\ldots = 0$ produces a Schrödinger-like equation:

$$\left(-\frac{\hbar^2 \nabla_i^2}{2m} + \frac{\delta F}{\delta \rho} + V_{\text{ext}} \right) \phi_i(\vec{r}) = \varepsilon_i \phi_i(\vec{r})$$

$$h\phi_i = \varepsilon_i \phi_i$$

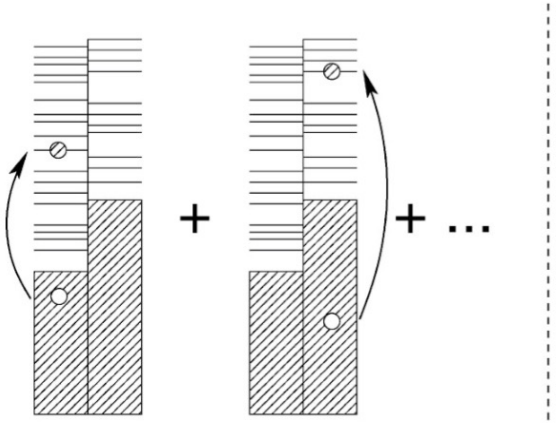
"DFT is an exactification of Hartree-Fock" (W. Kohn).

Simple interpretation

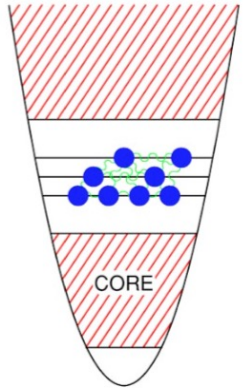
- RPA or QRPA based on EDFs includes only 1p-1h excitations.
  (GC *et al.*, Comp. Phys. Comm. 184, 142, 2013; N. Paar *et al.*, Rep. Prog. Phys. 70, 691, 2007)

- One would like to aim at calculations in which many nucleons are excited. But SM calculations can be performed only in light nuclei.
  (S.E. Koonin *et al.*, Phys. Rep. 278, 1, 1997; E. Caurier *et al.*, Rev. Mod. Phys. 77, 427, 2005)

- QPVC stays somehow in between. 2p-2h excitations are included, and the ring diagrams are summed in the intermediate states.



RPA



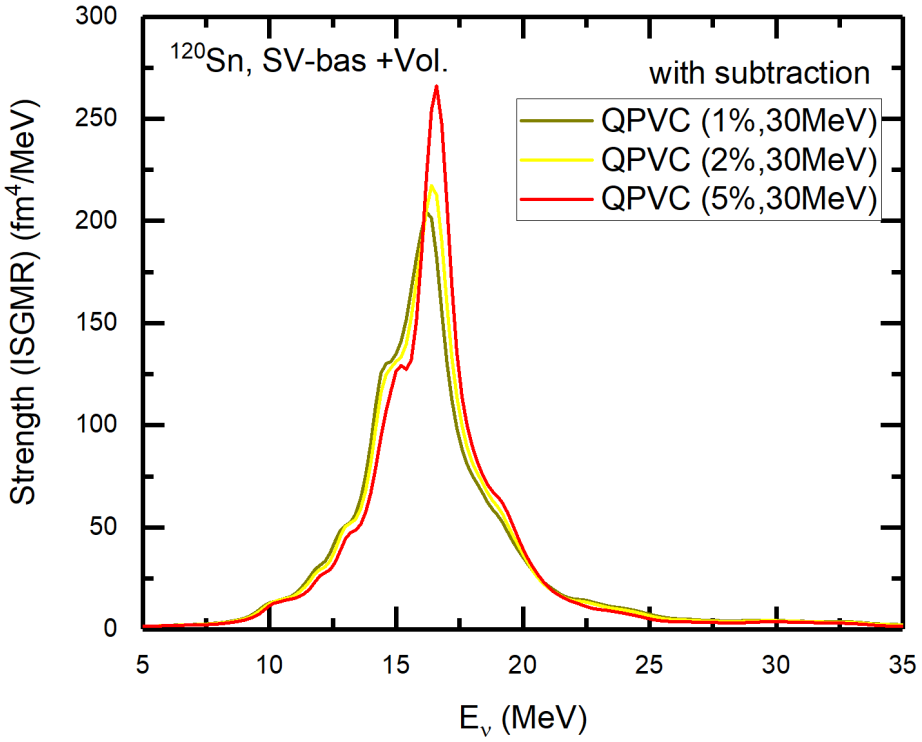
SM

Some detail + the subtraction scheme

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

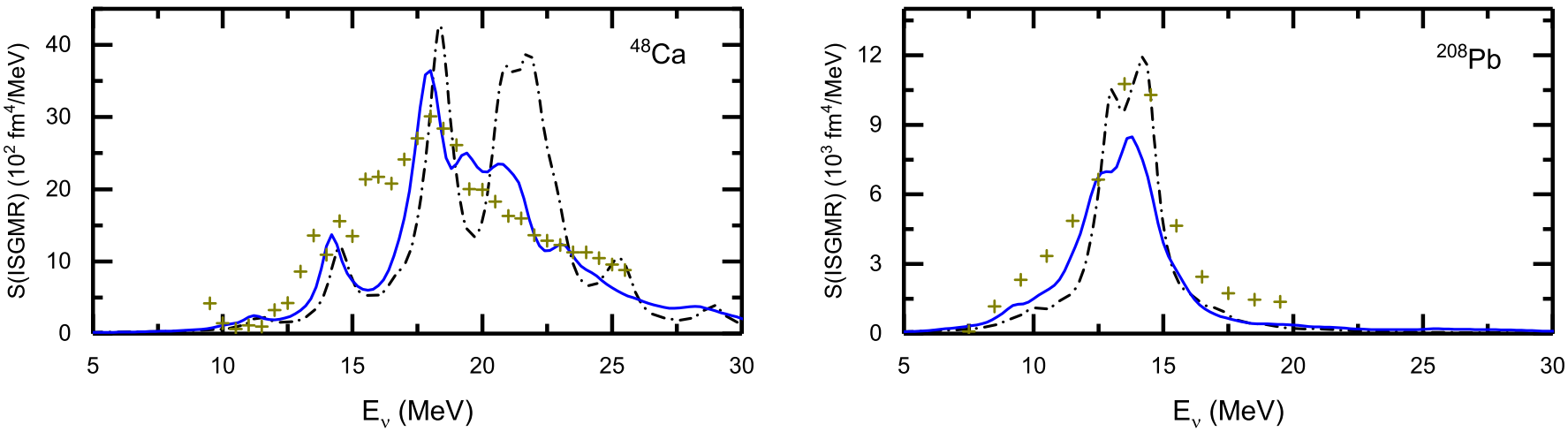
We calculate natural-parity phonons with 0^+, 1^-, 2^+ ... 5^- and select those having energy less than 30 MeV and strength larger than 2% of the total strength.

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



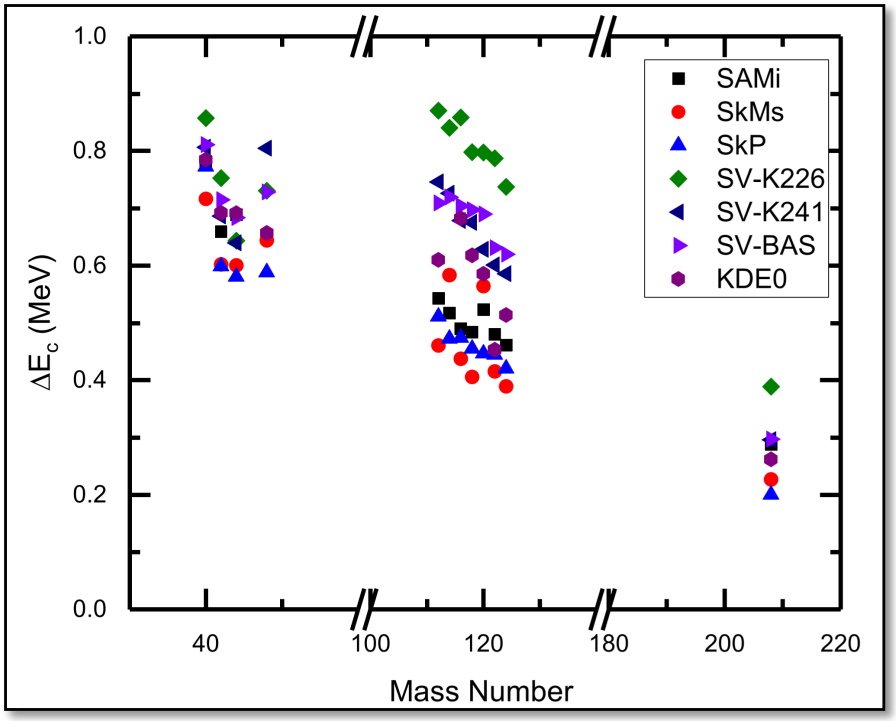
Subtraction: $\Sigma(E) \rightarrow \Sigma(E) - \Sigma(E=0)$

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.

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

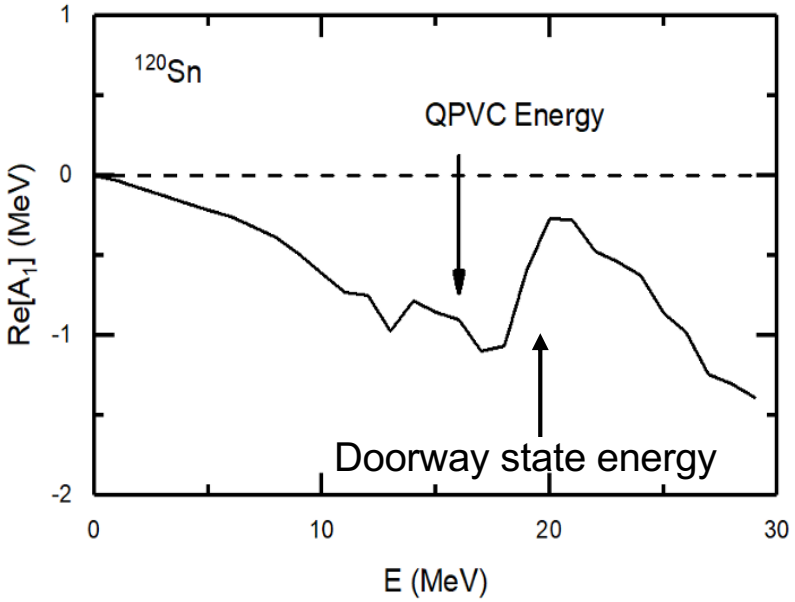
$$\Sigma(E) \approx \int dE' \; \frac{V^2}{E - E' + i\epsilon}$$

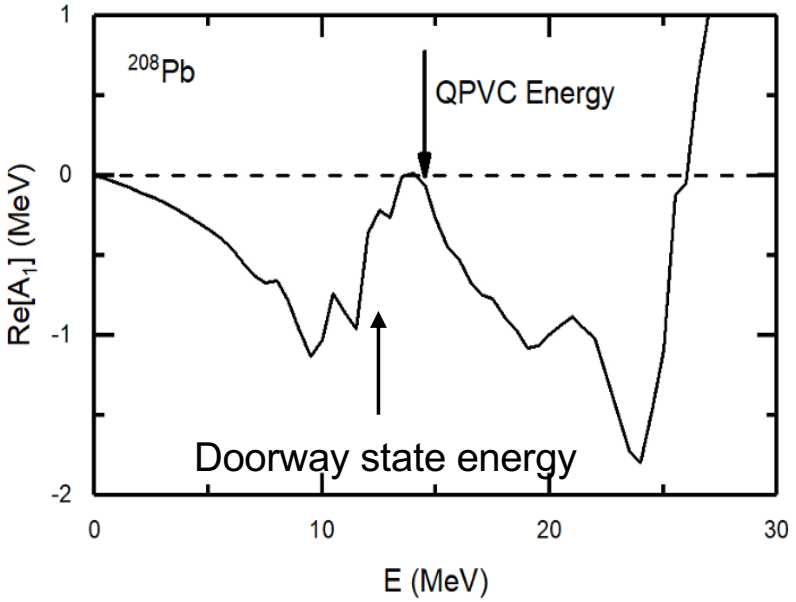
$$\frac{1}{E - E' + i\epsilon} \rightarrow \frac{1}{E - E'} - i\pi\delta(E - E')$$

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

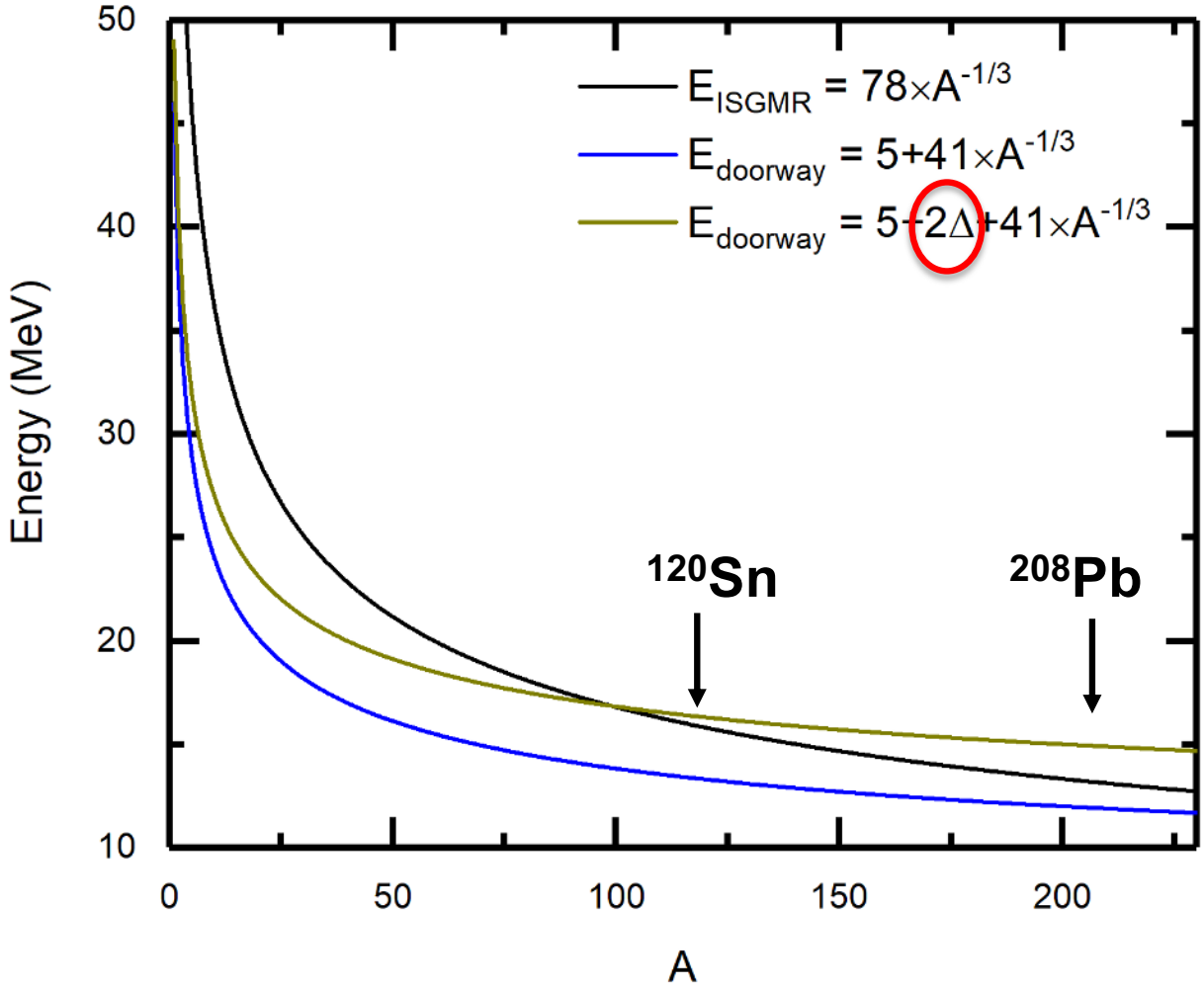
E = **QPVC** energy of the GMR
E' = energy of the **doorway states**

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



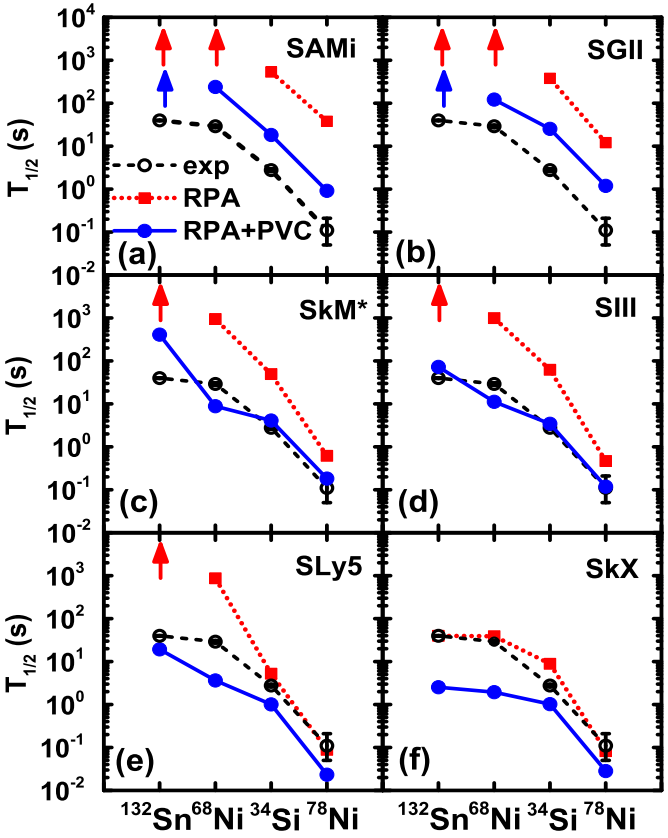


The QPVC energy is not very different in the two nuclei, but doorway state energies are higher in Sn than in Pb

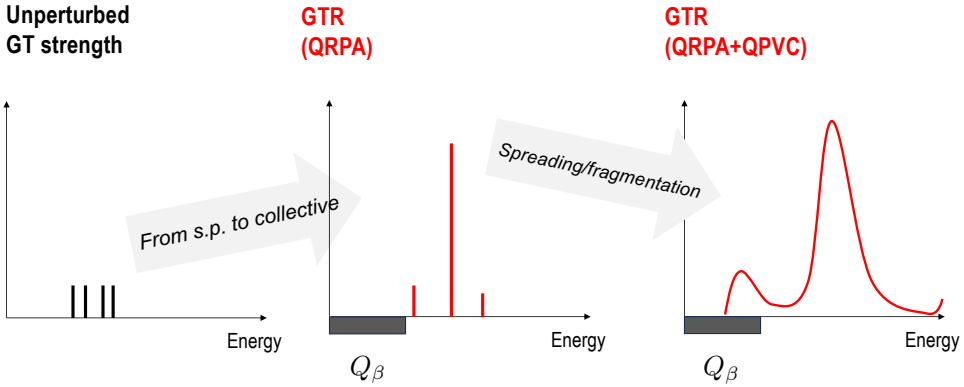


The pairing gap Δ makes the relative energy position of the ISGMR and of the doorway states different!

More applications of QPVC: β-decay



Y. F. Niu *et al.*, Phys. Rev. Lett. 114, 142501



While QRPA collects the simple two-quasiparticle excitation in a main peak, it does not account for spread and fragmentation of the strength. QPVC remedies to this shortcoming.

In the case of β-decay, this is particularly important because of the phase-space factor.

Towards the gradient approximation

$$\mathcal{E}^{\text{Skyrme}} = C^{\rho\rho}[\rho]\rho^2 + C^{\rho\tau}\rho\tau + C^{J^2}\vec{J}^{\,2} + C^{(\nabla\rho)^2}\left(\vec{\nabla}\rho\right)^2 + C^{\rho\vec{\nabla}\cdot\vec{J}}\rho\vec{\nabla}\cdot\vec{J}$$

LDA

Nuclei are finite systems and the dependence of the EDF on $\nabla\varrho$, τ and J is mandatory. These quantities vanish in uniform matter.

How can *ab initio* inform us about this dependence?

Uniform matter perturbed by a (weak) periodic potential