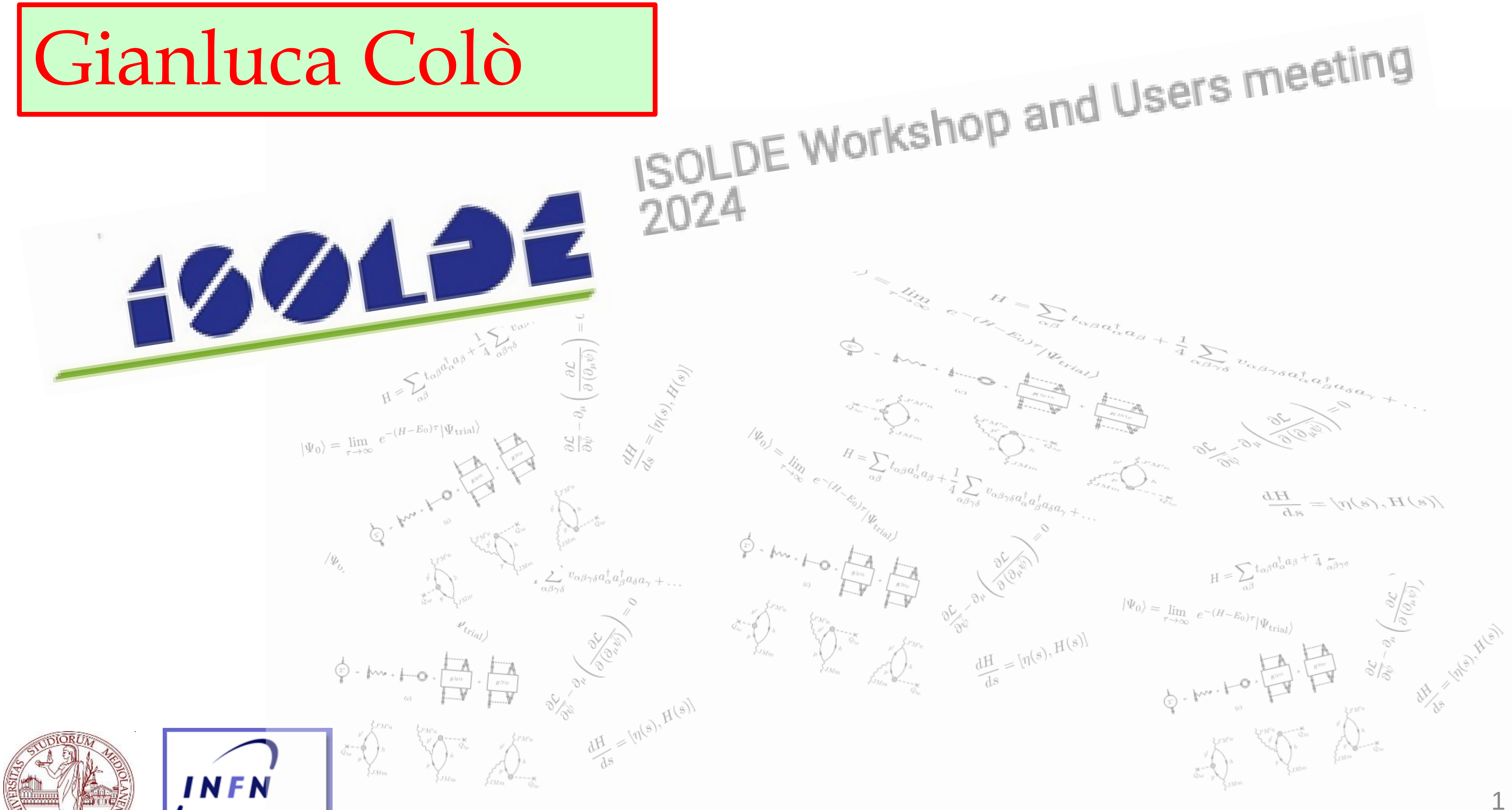
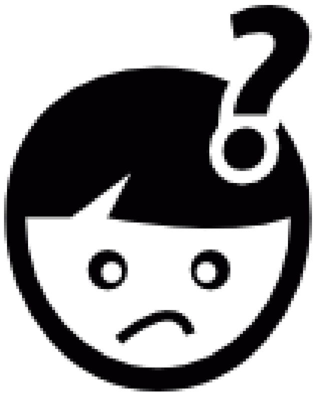
Nuclear Density Functional Theory: general aspects and interpretation of recent experiments

Gianluca Colò



There are several combinations of **nuclear Hamiltonians and many-body methods** to solve the nuclear problem.



Ab initio approaches

Configuration interaction/Shell model

Mean-field and DFT

Ab initio: realistic *H* together with many-body methods having controlled uncertainties – agreement with experiment depend on *H*

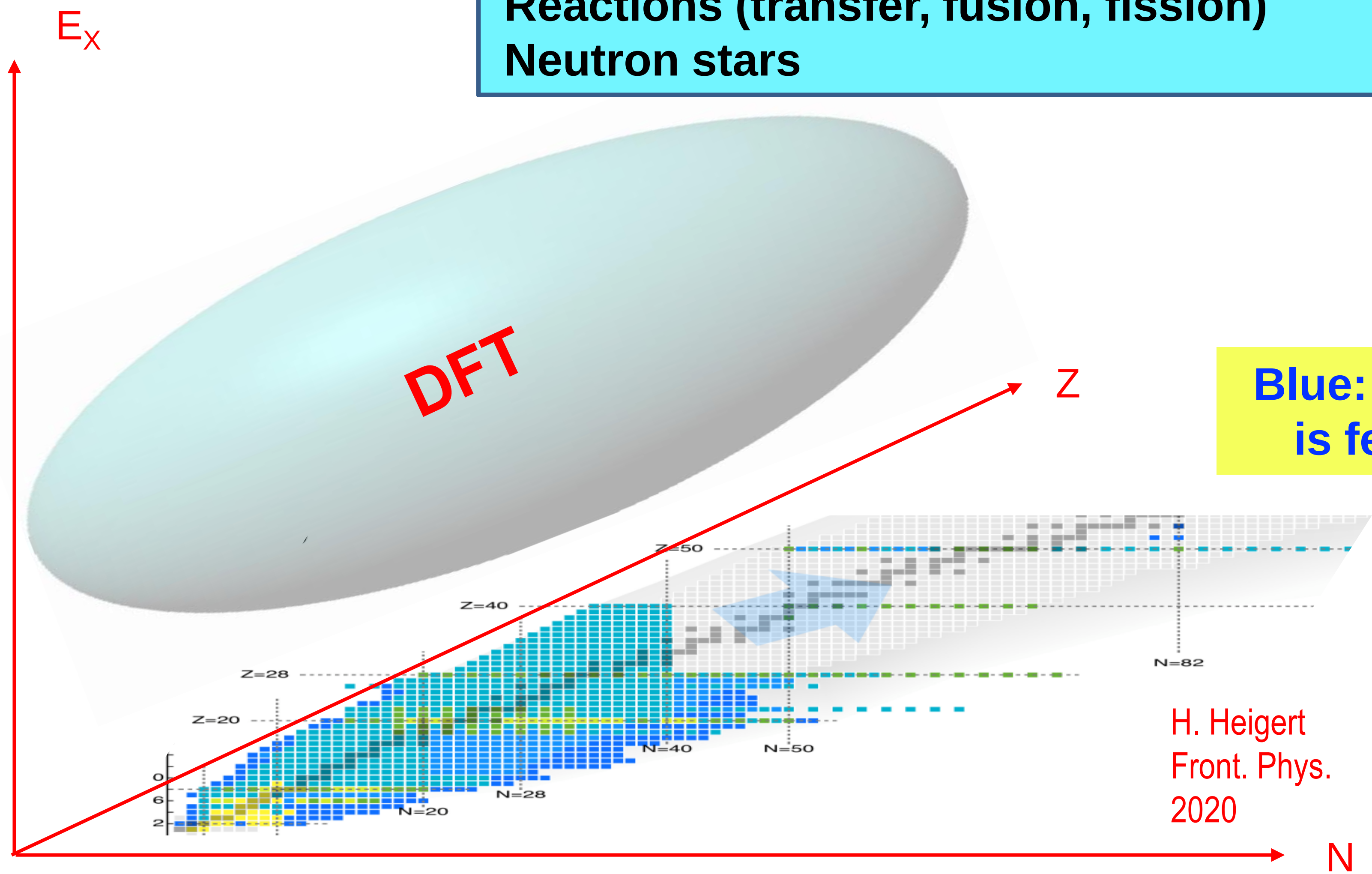
Shell model: H_{eff} diagonalized in a large model space – difficulties with heavy nuclei/high excitation energy

DFT: wide range of applicability – based on a phenomenological ansatz

$$H\Psi = E\Psi$$

$$H = T + V = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} V_2(i,j) + \sum_{i<j<k} V_3(i,j,k)$$

Giant Resonances and highly excited states
Spectroscopy of heavy and superheavy nuclei
Reactions (transfer, fusion, fission)
Neutron stars



Blue: *ab initio* is feasible

H. Heigert
Front. Phys.
2020

Shell model: precision spectroscopy

(Nuclear) Density Functional Theory

$$E = \int \mathcal{E}[\rho]\; d^3r$$

Energy density = $\mathcal{E}$

E is a functional called **EDF**

$$E_{\text{ground state}} = \min_\rho E[\rho]$$

The **exact** functional has a **minimum** at the exact ground-state density, where it assumes the exact *E* as a value.

- Existence is guaranteed by the **Hohenberg-Kohn theorem**.
- It gives access, in principle, to all properties of the system.

- The theorem does **not** tell what the EDF looks like.
- Starting from current EDFs, the road for improvement is not fully clear.

$$\rho \;\rightarrow\; E[\rho]$$

Skyrme, Gogny or covariant craftsman

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):

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

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

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

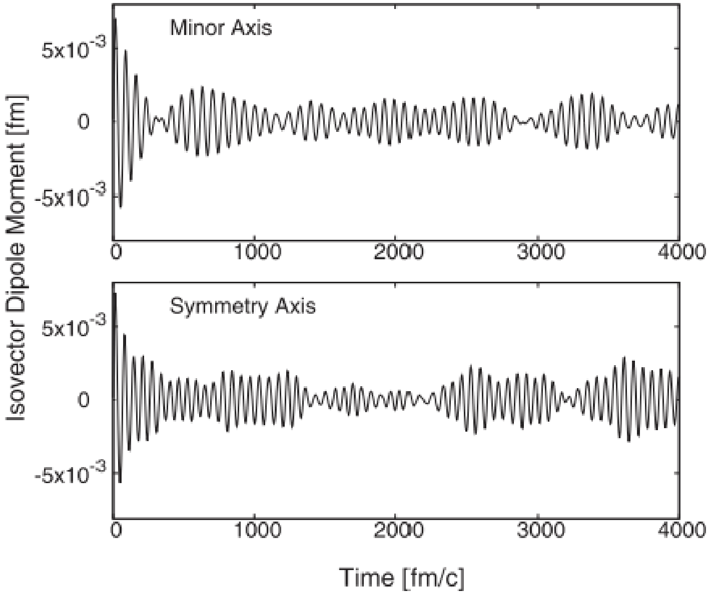
$$h\phi_i = \varepsilon_i \phi_i$$

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

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:

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

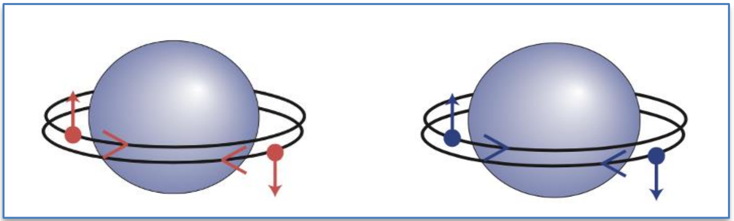
$$\rho(t=0) \neq \rho_{\text{g.s.}}$$

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

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

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

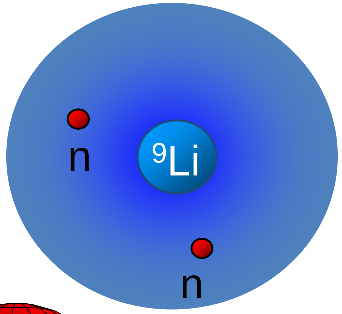
G.C. *et al.*, Computer Physics Commun. 184, 142 (2013).

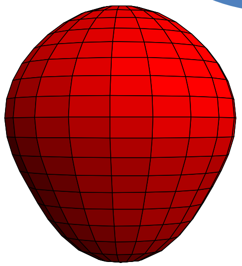


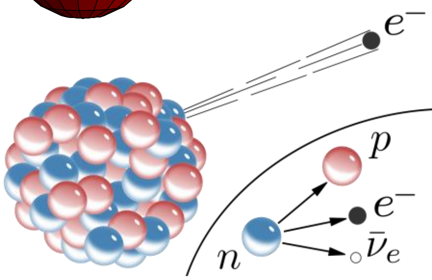
In RPA the excited states are 1p-1h superpositions

Status of nuclear DFT (short...)

- Error on **masses** of the order of 1 MeV.
- (Controlled) predictions of **drip lines** and **super heavy** nuclei.
- Trends of **charge radii and deformations** fairly well reproduced.
- **Extrapolation to neutron matter and neutron stars.**
- Techniques based on **symmetry restoration** are available.
- **Giant resonances, charge-exchange transitions** are studied**.**
- Interest in **reactions, large amplitude phenomena like fission**.







Skyrme, Gogny, covariant EDFs exist

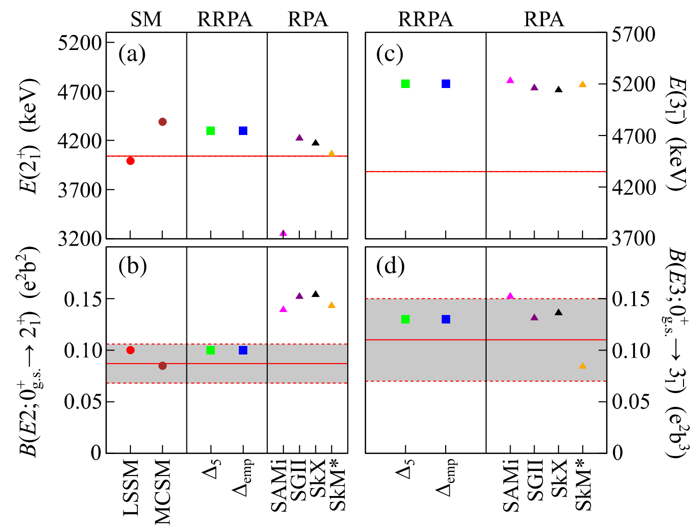
RPA and the nuclear Shell Model (SM)

PHYSICAL REVIEW LETTERS **121,** 252501 (2018)

Enhanced Quadrupole and Octupole Strength in Doubly Magic ^{132}Sn

D. Rosiak,[1] M. Seidlitz,[1,*] P. Reiter,[1] H. Naïdja,[2,3,4] Y. Tsunoda,[5] T. Togashi,[5] F. Nowacki,[2,3] T. Otsuka,[6,5,7,8,9] G. Colò,[10,11] K. Arnswald,[1] T. Berry,[12] A. Blazhev,[1] M. J. G. Borge,[13,†] J. Cederkäll,[14] D. M. Cox,[15,16] H. De Witte,[8] L. P. Gaffney,[13] C. Henrich,[17] R. Hirsch,[1] M. Huyse,[8] A. Illana,[8] K. Johnston,[13] L. Kaya,[1] Th. Kröll,[17] M. L. Lozano Benito,[13] J. Ojala,[15,16] J. Pakarinen,[15,16] M. Queiser,[1] G. Rainovski,[18] J. A. Rodriguez,[13] B. Siebeck,[1] E. Siesling,[13] J. Snäll,[14] P. Van Duppen,[8] A. Vogt,[1] M. von Schmid,[17] N. Warr,[1] F. Wenander,[13] and K. O. Zell[1]

(MINIBALL and HIE-ISOLDE Collaborations)



theory [11,12]. Because of the computational limits of the valence space, the SM approaches do not provide information on the 3_1^- state. The RPA and RRPA calculations

In addition, the shell model cannot provide response at high energy (cross sections for high-E neutrinos, just to make an example, are doable within RPA and QRPA but not SM).

Possible improvements

- Changing the form of the functional (more parameters, more terms, different form...)

- Advanced statistical methods (Bayesian inference, ML...)

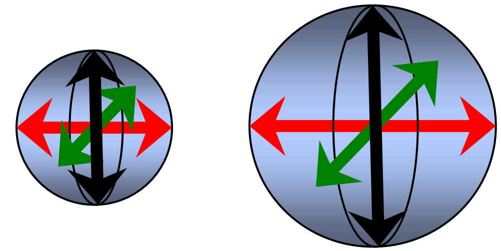
- Adding specific many-body correlations

- Building the EDFs from *ab initio*

Physics case #1:
the monopole resonance
and the nuclear incompressibility

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)

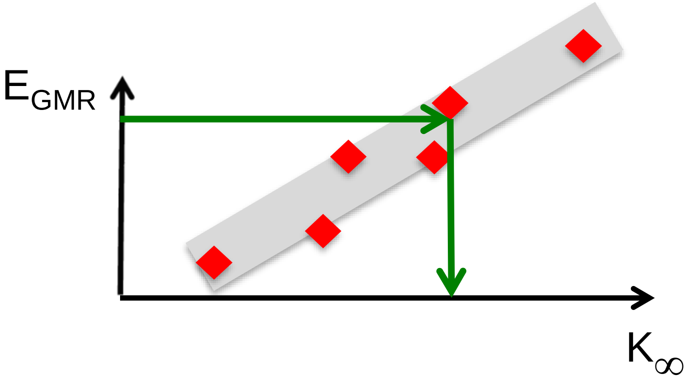
Probing the Incompressibility of Nuclear Matter at Ultrahigh Density through the Prompt Collapse of Asymmetric Neutron Star Binaries

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]

Why is tin so fluffy?

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.

This happens using (Q)RPA calculations.



Only models 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.

QRPA → QPVC

(Q)RPA + (Q)PVC

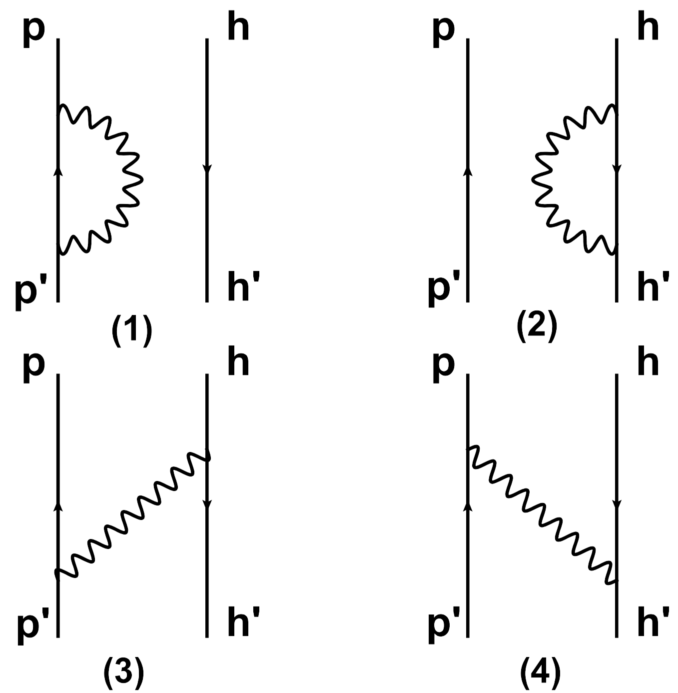
$$\begin{pmatrix} A+\Sigma(E) & B \\ -B & -A-\Sigma^*(-E) \end{pmatrix} \quad \Sigma_{\mathrm{php'h'}}(E) = \sum_\alpha \frac{\langle ph|V|\alpha\rangle\langle\alpha|V|p'h'\rangle}{E-E_\alpha+i\eta}$$

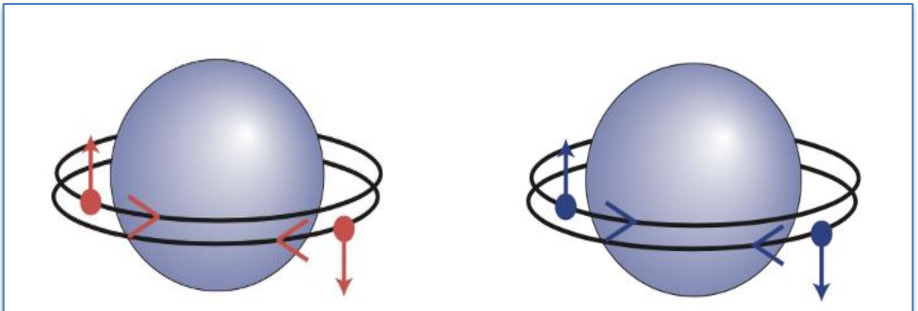
The state α is 1p-1h plus one phonon.

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

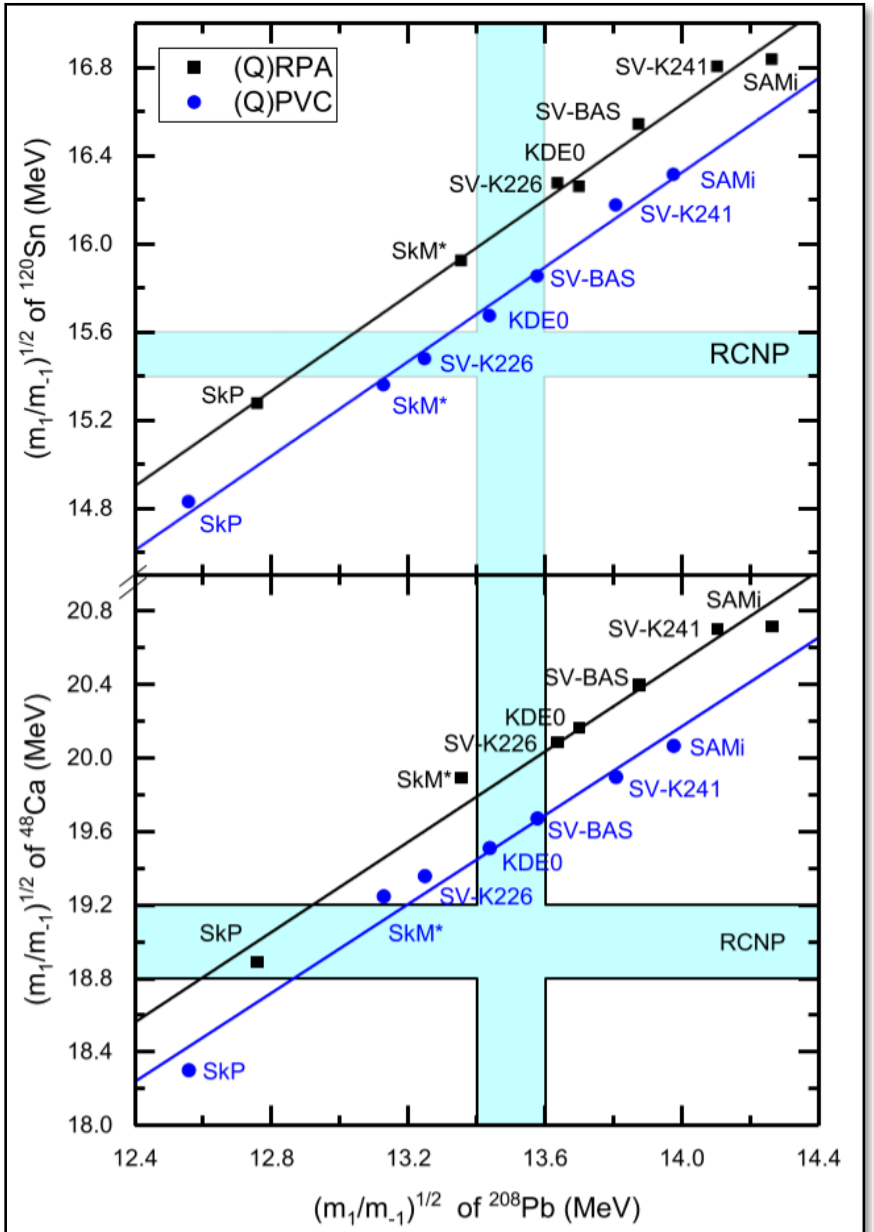
$$\Sigma(E) \approx \int dE' \, \frac{V^2}{E-E'+i\epsilon}$$

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





WE HAVE A SCHEME INCLUDING PAIRING for all GRs



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.

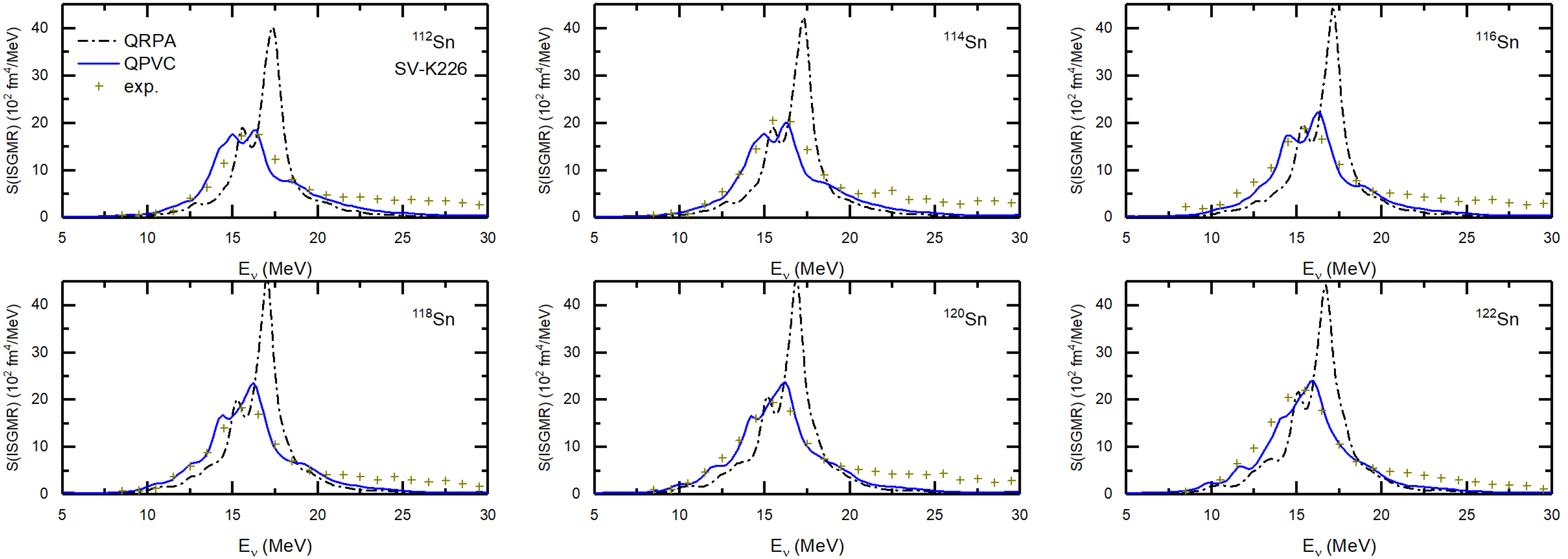
We have used many Skyrme EDFs.

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

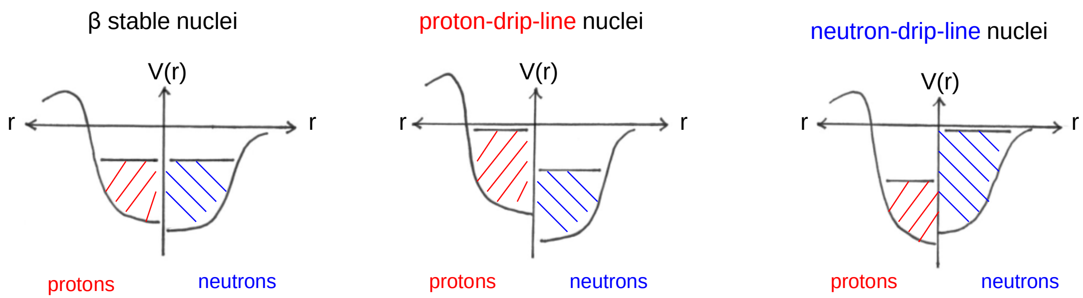


- Exp. data from D. Patel *et al*., Phys. Lett. B726, 178 (2013)
- QPVC reproduces the experimental data quite well.
- The best description is obtained with the Skyrme EDF SV-K226.

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

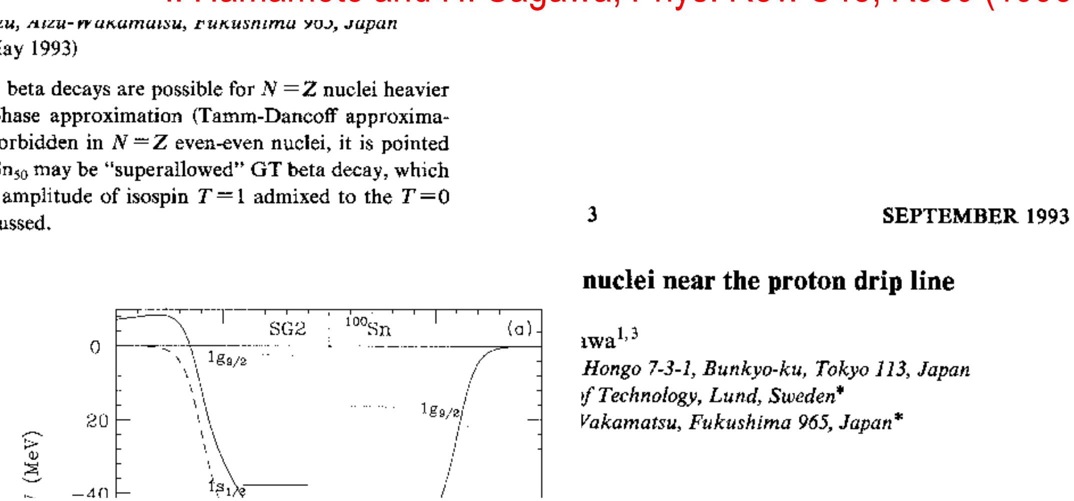
Physics case #2:
evolution of single-particle states

Single-particle spectroscopy: neutron-rich and neutron-deficient nuclei

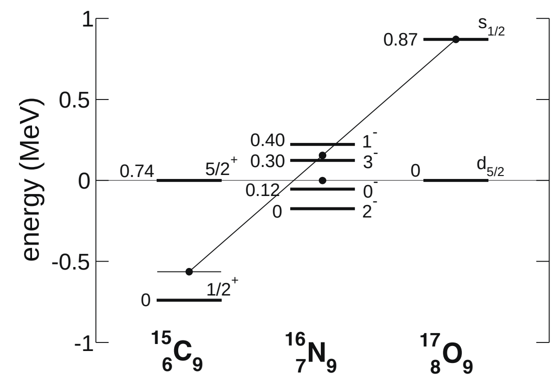


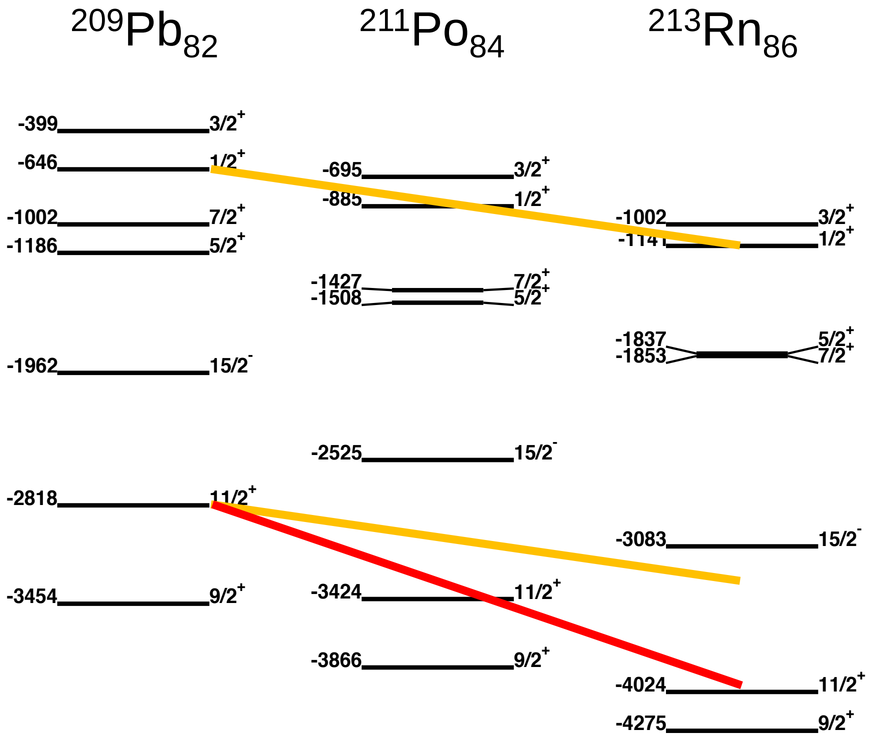
If the <u>neutron number increases</u>, neutrons occupies higher levels – protons become more bound due to the dominance of the p-n interaction.

I. Hamamoto and H. Sagawa, Phys. Rev. C48, R960 (1993)



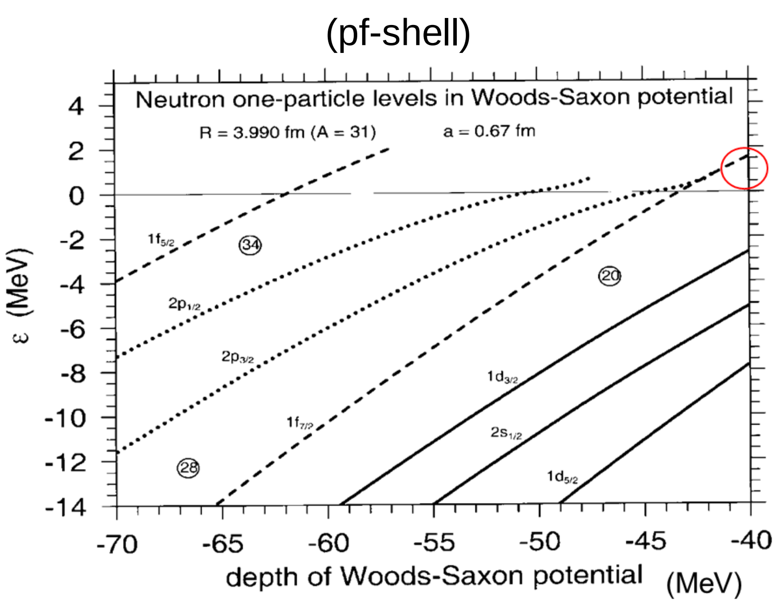
I. Talmi and I. Unna, Phys. Rev. Lett. 4, 469 (1960)





Changes of orbitals (either upward or downward) are LARGER for HIGHER angular momenta.

In fact, orbitals with smaller values of angular momenta are less constrained by the centrifugal barrier and overlap less with the other states.



In particular, the trend of s- and p-orbitals becomes almost flat when their energies approach zero.

We expect changes in the shell structure when going far from the stability valley

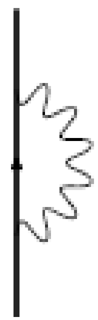
Particle-vibration coupling

So far, Kohn-Sham eigenstates correspond to **single-particle states.**

We have seen that RPA eigenvalues correspond to **vibrational states**.

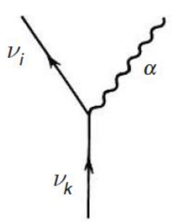
As already discussed, we can take into account the coupling between them (**Particle-Vibration Coupling or PVC**, on top of DFT).

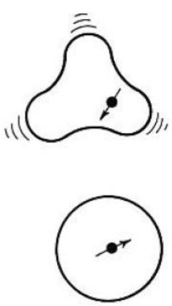
$$\Sigma =$$



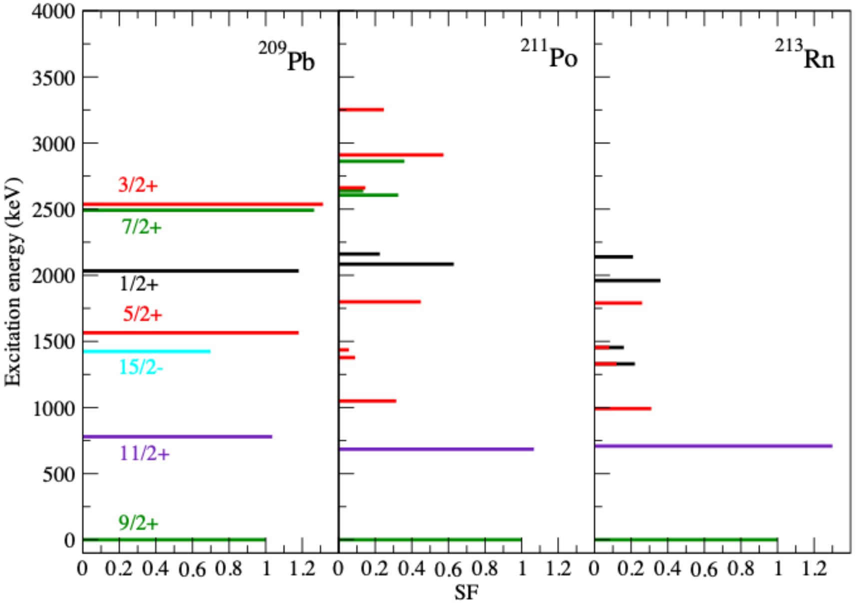
Odd nuclei: core + 1 particle + **1 particle plus phonon …**

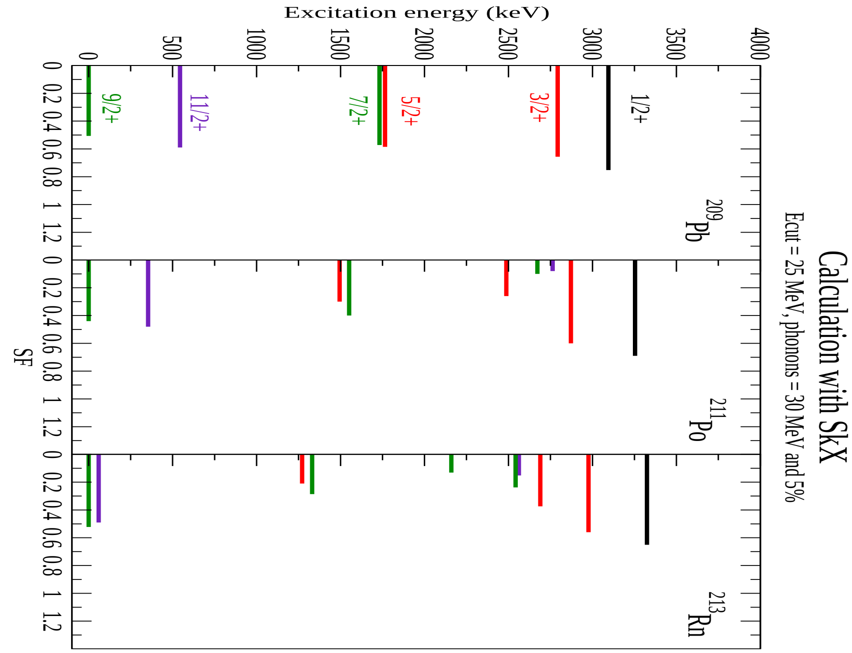
$$G = G_0 + G_0 \Sigma G$$





Applied to:
^{49}Ca - D. Montanari *et al*., Phys. Lett. B697, 288 (2011);
^{133}Sb - G. Bocchi *et al*., Phys. Lett. B760, 273 (2016);
^{41,47,49}Ca - S. Bottoni *et al*., Phys. Rev. C103, 014320 (2021).





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

Comparison with DFT+QPVC

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

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

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

- <u>We are currently working on new EDFs, either based on *ab initio* or on Bayesian inference from experimental data</u>

- 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

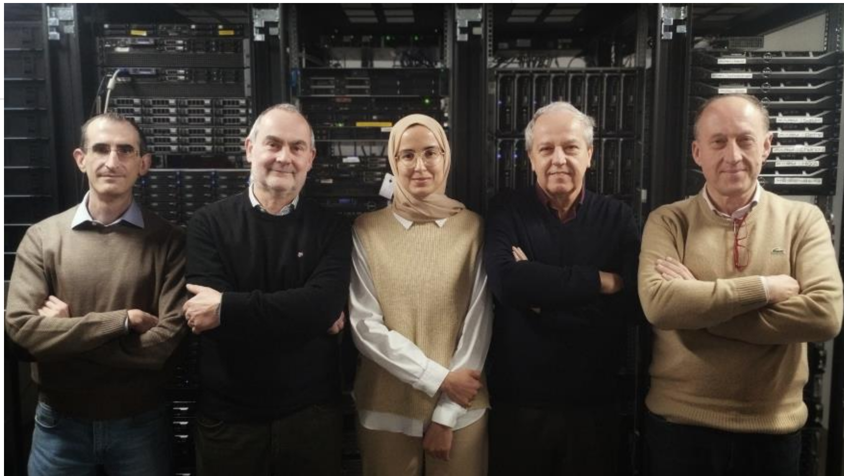
The Structure4exp virtual access (VA) facility, at ns4exp.mi.infn.it, is a part of the Theo4Exp VA infrastructure and, as such, is intended to provide theoretical tools for the EURO-LABS project as well as for the wider nuclear physics community. The key nuclear structure codes available are now either 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

EURO-LABS
EUROPEAN LABORATORIES FOR ACCELERATOR BASED SCIENCES



Backup slides

Skyrme EDFs (even-even nuclei)

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

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

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

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

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

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

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

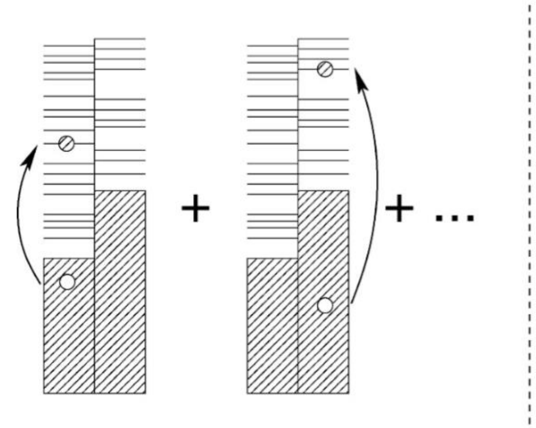
$$C^{\rho\rho}[\rho] = A + B\rho^\gamma$$

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

Simple interpretation

- RPA or QRPA based on EDFs includes only 1p-1h excitations.

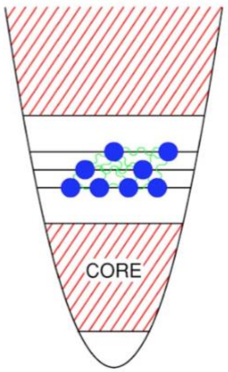
  (GC *et al*., Comp. Phys. Comm. 184, 142, 2013; N. Paar *et al*., Rep. Prog. Phys. 70, 691, 2007)



RPA

- One would like to aim at calculations in which many nucleons are excited. But SM calculations can be performed only in light nuclei.

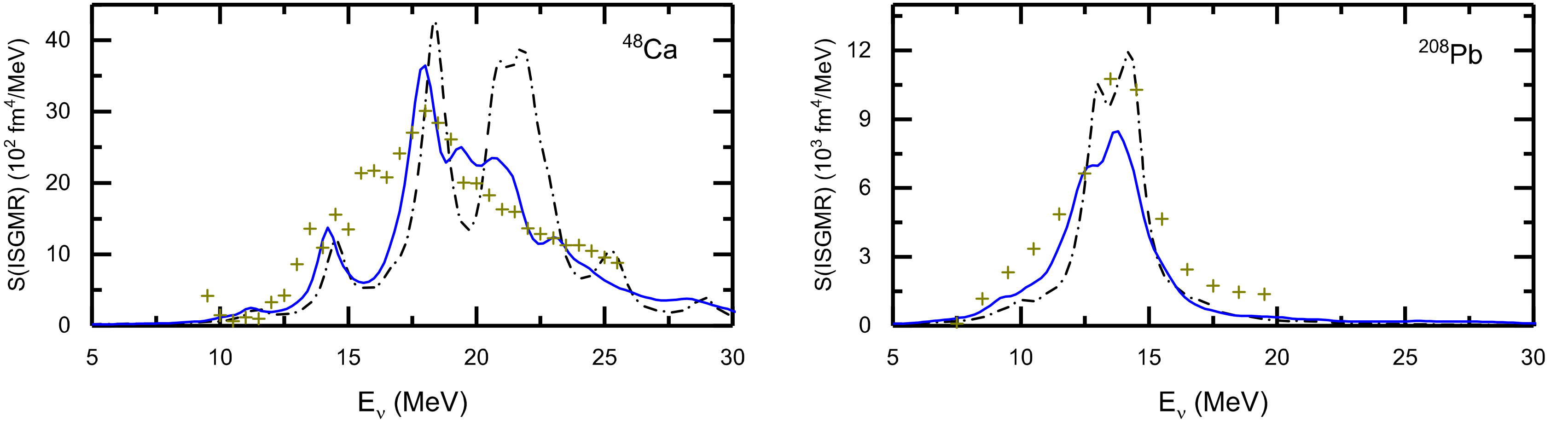
  (S.E. Koonin *et al*., Phys. Rep. 278, 1, 1997; E. Caurier *et al*., Rev. Mod. Phys. 77, 427, 2005)



SM

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

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



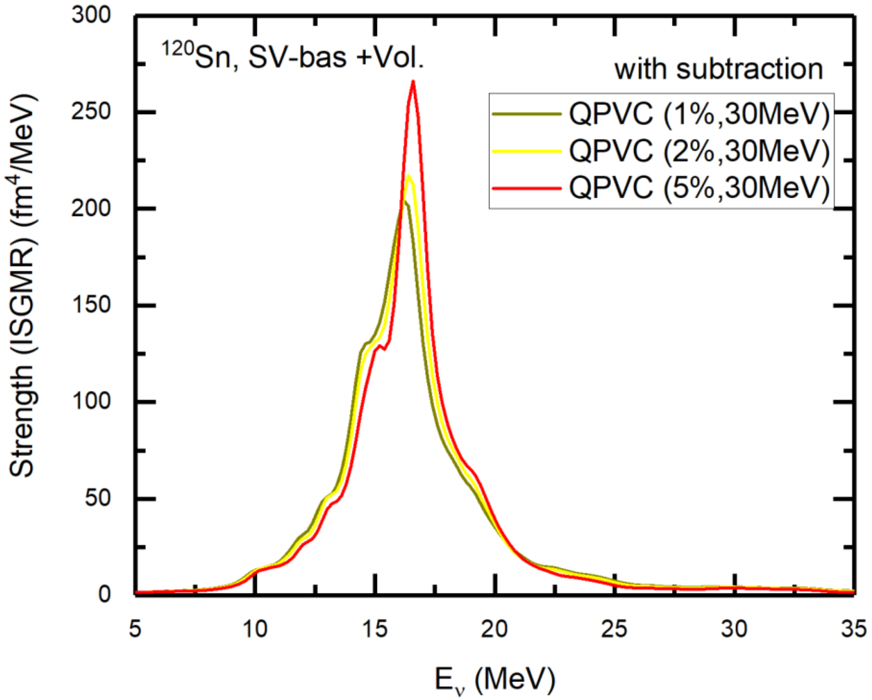
- Exp. data from T. Li *et al*., Phys. Rev. Lett. 99, 162503 (2007) and S.D. Olorunfunmi, Phys. Rev. C 105, 054319 (2022).
- In these two cases there is no pairing.

Some detail + the subtraction scheme

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

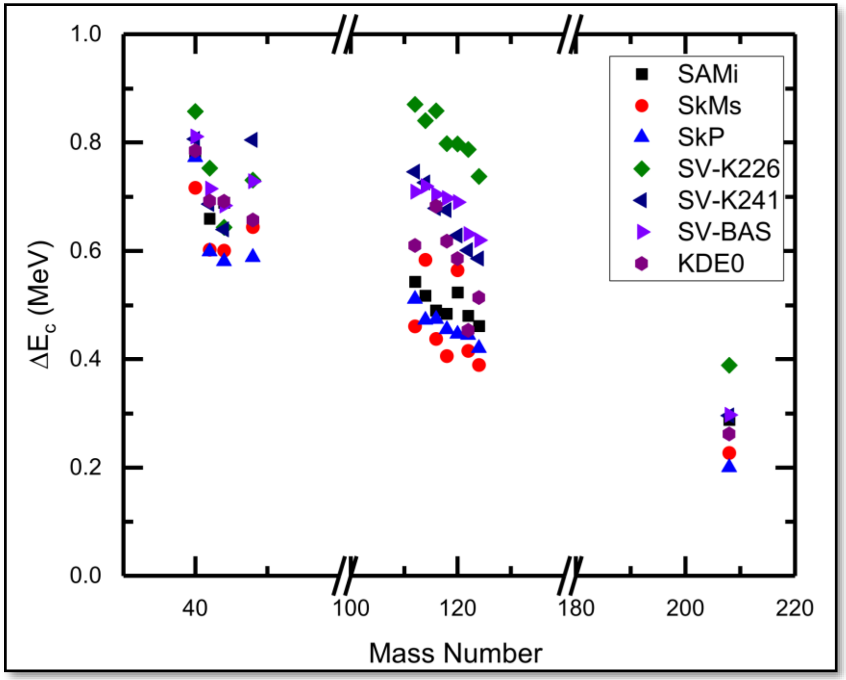
We calculate natural-parity phonons with 0^+, 1^-, 2^+ ... 5^- and select those having energy less than 30 MeV and strength larger than 2% of the total strength.

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



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

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

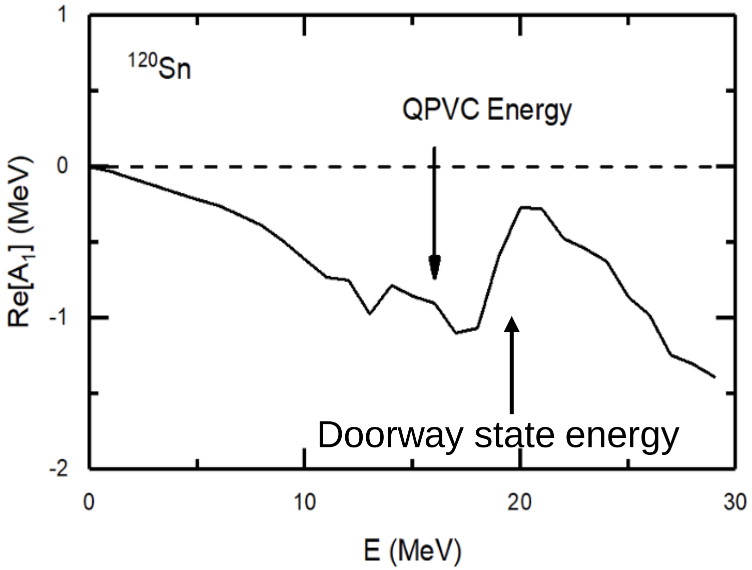
$$\Sigma(E) \approx \int dE' \, \frac{V^2}{E - E' + i\epsilon}$$

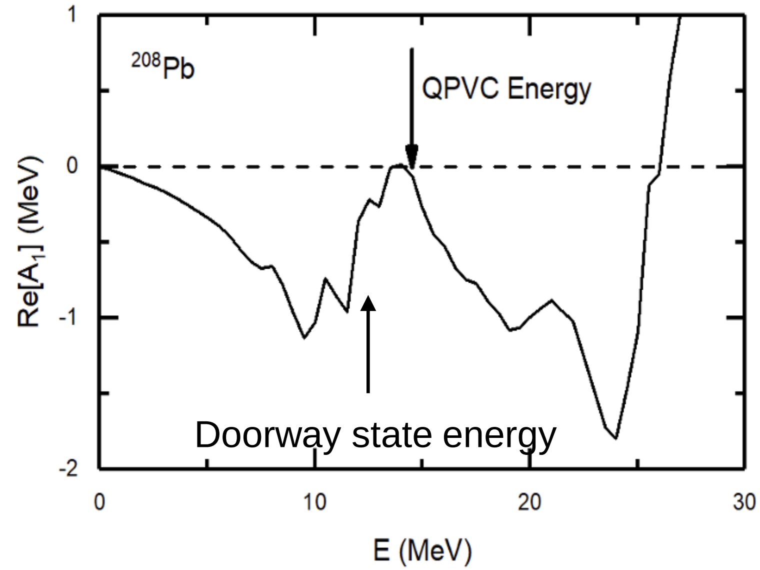
$$\frac{1}{E - E' + i\epsilon} \rightarrow \frac{1}{E - E'} - i\pi\delta(E - E')$$

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

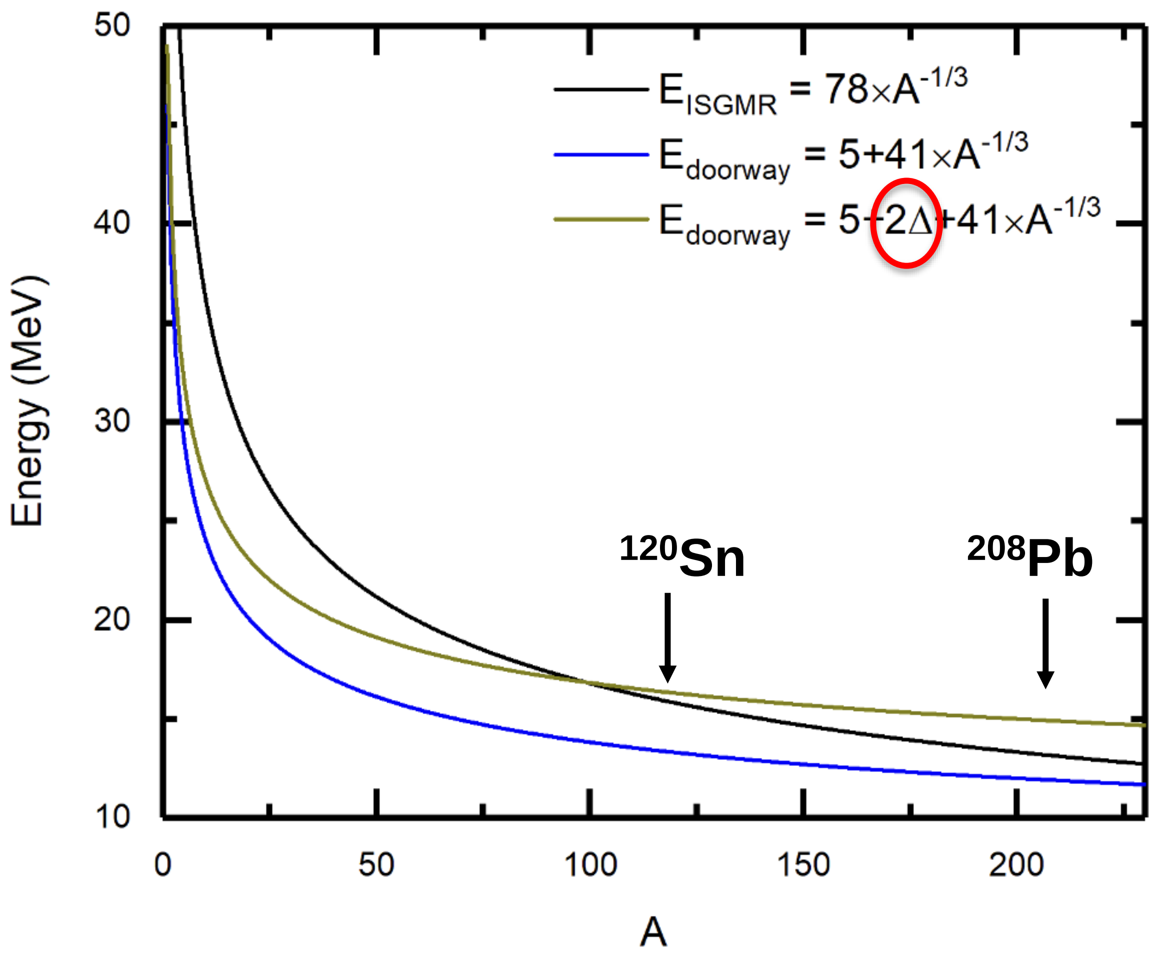
E = **QPVC** energy of the GMR
E' = energy of the **doorway states**

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





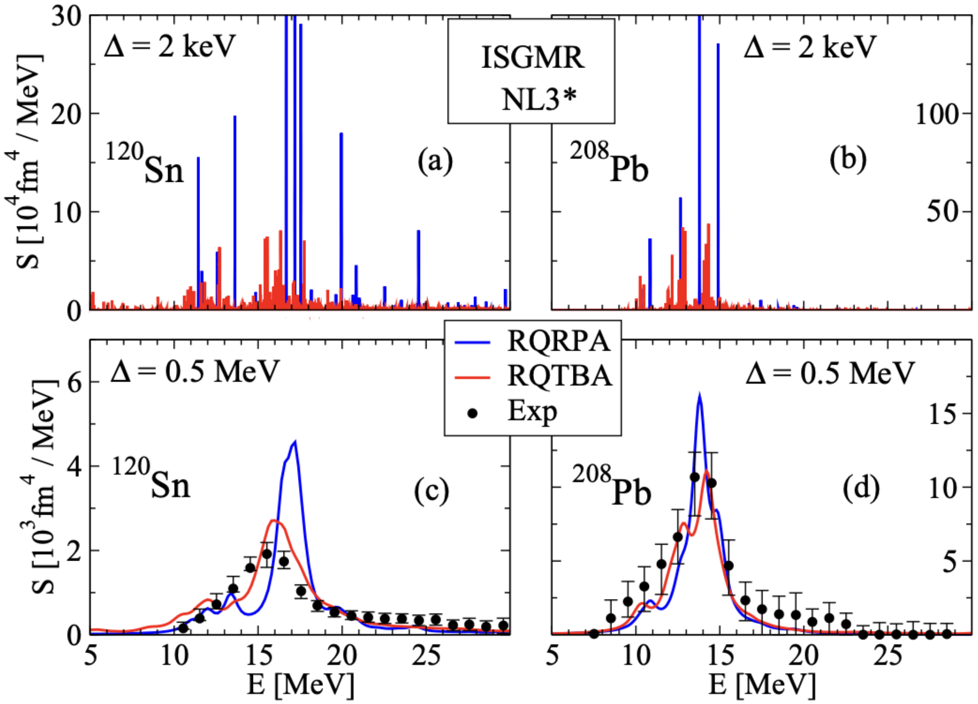
The QPVC energy is not very different in the two nuclei, but doorway state energies are higher in Sn than in Pb



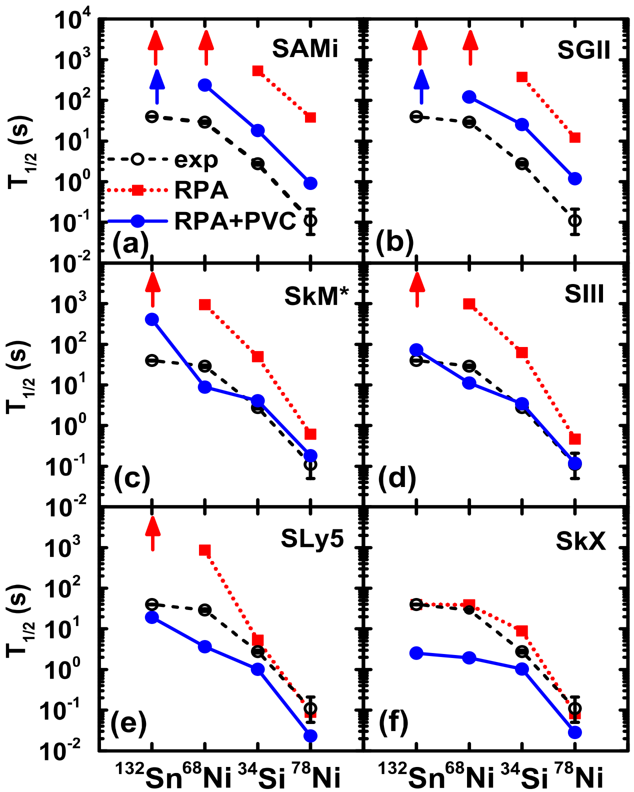
The pairing gap Δ makes the relative energy position of the ISGMR and of the doorway states different!

- Calculations performed by E. Litvinova, based on covariant DFT, confirm the importance of PVC correlations [cf. PRC 107, L041302 (2023)].

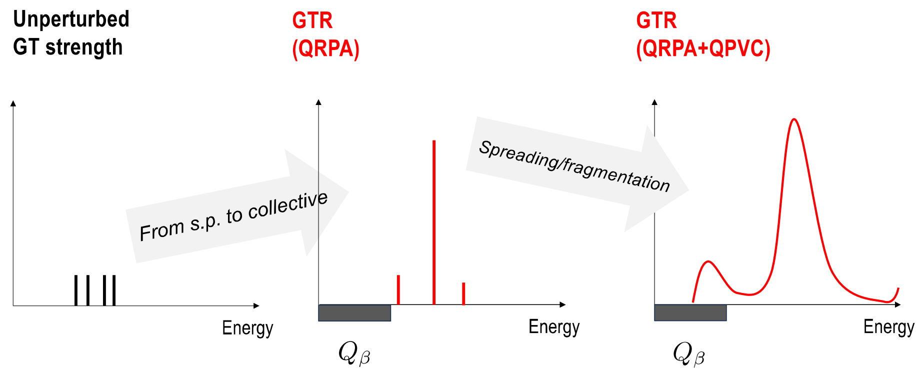
- However: only one specific EDF.



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.