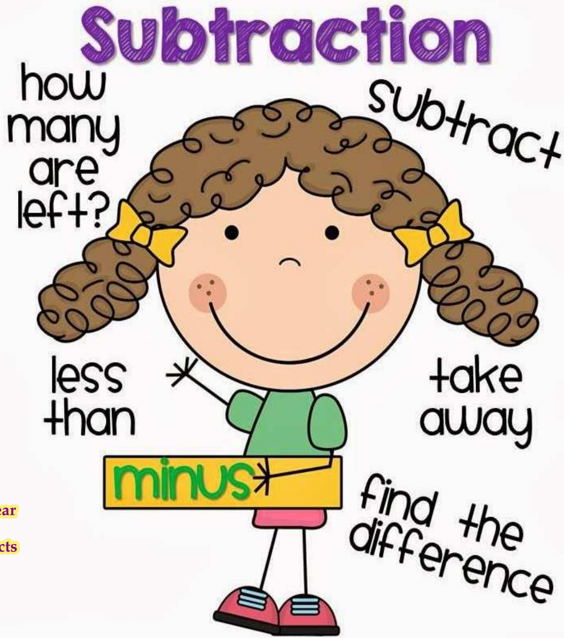
Beyond mean field calculations with Skyrme:



(method)

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ECT* — Unraveling the complexity of nuclear systems: single-particle and collective aspects through the looking glass.

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Going beyond the mean-field

- **Theory should cover and provide reliable predictions** not only in connection to solve existent problems but also on the view of **new experimental challenges in nuclear physics**
- Approaches based on **NN scattering data in the vacuum** are **successful** in their predictions of some properties in **light and medium mass nuclei** but face **computational limitations** in the description of **heavy systems and high-lying excited states**.
- **Nuclear energy density functionals (EDFs)** approaches do not suffer from such a limitation.

Going beyond the mean-field

- **EDFs** are commonly **derived in an approximate way** from a phenomenological interaction solved via the **Hartree (H) or Hartree-Fock (HF)** approximations **[mean field approx.]**
  (Phenomenological, no direct connection with NN or NNN int.!!)
  - **EDFs can** be *safely* applied for the study of **one-body observables (along the whole nuclear chart)** such as **ground state density** and **small fluctuations** around it as well as the associated **total energies**.
  - **EDFs cannot** be applied, e.g., for an accurate study of the **single-particle dynamics** in nuclei
- **Going beyond the mean field (BMF)** is, therefore, **needed** for the study of **any dynamical property** in nuclei such as **fragmentation of single-particle states, resonance widths, half-lifes ...**
- **Particle Vibration Coupling (PVC)** model is one possible realization of a **BMF** threory

Particle Vibration Coupling

⇒One of the most **prominent dynamic property** in nuclear systems is that of **collective excitations**, the main component being a **collective and coherent superposition of particle-hole excitations** (or phonon)

⇒PVC: selects the diagrams associated to collective particle-hole excitations to define a **new degree of freedom, the phonon**, that is then **coupled to HF single-particle** degrees of freedom

Particle Vibration Coupling (in very brief)

⇒ We would like to solve:

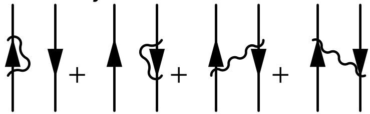
$$(\omega - \mathcal{H} - i\epsilon)\mathcal{G}(\omega) = 1$$

⇒ if our model space is $\mathcal{Q}_1$ contains 1p-1h configurations (build with HF sp) $|ph\rangle$, projecting in $\mathcal{Q}_1$, one obtains **(RPA)**

$$(\omega - \mathcal{Q}_1\mathcal{H}\mathcal{Q}_1 - i\epsilon)\mathcal{Q}_1\mathcal{G}(\omega)\mathcal{Q}_1 = \mathcal{Q}_1$$

⇒ if our model space is now $\mathcal{Q}_1 + \mathcal{Q}_2$ where the latter is made of 1p-1h excitations $|ph\rangle$ coupled to a phonon state$|N\rangle$, projecting in $\mathcal{Q}_1$, one obtains the same eq. corrected by the term **(PVC)**

$$\mathcal{Q}_1\mathcal{H}\mathcal{Q}_2\frac{1}{\mathcal{Q}_2(\omega - \mathcal{H} - i\epsilon)\mathcal{Q}_2}\mathcal{Q}_2\mathcal{H}\mathcal{Q}_1 =$$



⇒ this extra term ($\mathcal{W}$, namely, **spreading** term) accounts for the**coupling of a particle or hole** state with a **phonon**, its propagation on top of the potential, and the **reabsortion** of the phonon into a particle or a hole.

⇒ Specifically, this allows one to describe part of the **width of GR**

Renormalization

⇒ In more detail, $\mathcal{W}$ would correspond to the sum

$$\mathcal{W} = \sum_N \frac{\langle ph|V_{eff}|N\rangle\langle N|V_{eff}|p'h'\rangle}{\omega - \omega_N}$$

⇒ Where V_{eff} **is the effective two-body interaction** adopted.

- Parameters have been **fitted at the MF level** → **renormalization (refit) is complusory** at the new level of approximation
- If V_{eff} is **zero-range**, the sum diverges → **renormalization (cutoff on relative momenta) is complusory**

⇒ **Subtraction method** gives a **recipe** to **(try to) avoid both** a refit of the parameters of the interaction and the use of a cutoff.
⇒ That the **subtraction method formally solve these problems is something that has not been shown yet**. However it does *something* in an effective way as we shall discuss now...

Subtraction method

Subtraction method is based on a simple idea: **modify the theory** so that the **expectation value of any one-body operator** (idealy exact in EDF) **do not change** with respect the EDF prediction.

⇒ One possible **realization** of the avobe definition is to **redefine** $\mathcal{W}$ as follows

$$\mathcal{W}(\omega) - \mathcal{W}(0) = \sum_N \frac{\langle ph|V|N\rangle\langle N|V|p'h'\rangle}{\omega - \omega_N} + \sum_N \frac{\langle ph|V|N\rangle\langle N|V|p'h'\rangle}{\omega_N}$$

⇒ **BMF** contrib. go to **zero in the static (EDF) limit** $(\omega = 0)$

⇒ It **implies** that a fit to **one-body physics** (i.e. at EDF level) **determines** also the **physics beyond** **(*a priory* doubtful)**

⇒ For **zero-range** interactions, the **ultraviolate divergence** $(\omega_N \to \infty)$ is **avoided** **(not formally, yet to be shown)**

⇒ one **possible way** to **extend** the **stability condition** on extended RPA (and RPA-like) theories. **For details see V.I. Tselyaev PRC 88, 054301 (2013).**

Sum Rules

⇒ The expectation value of **one-body observables is now fixed at the static limit** by the subtraction method

⇒ We focus on the study of some properties of **collective excitations** via the **moments of the strength function** that are subject to **fulfill some existing sum rules**. Some of these sum rules, should be also **conserved in beyond EDF** approaches as we should discuss.

⇒ The **strength function** is defined as proportional to the immaginary part of the **polarization propagator** $\Pi(\omega)$
⇒ The $k-$moment of the strength function is defined as

$$m_k = \int_0^\infty \omega^k \mathcal{S}(\omega) d\omega$$

m_0 Non Energy Weighted Sum Rule (NEWSR)
m_1 Energy Weighted Sum Rule (EWSR)
m_{-1} Inverse Energy Weighted Sum Rule (IEWSR)

Inverse energy weighted sum rule

⇒ The **observed spectrum of a nucleus excited by an external field** $\mathcal{F}$ is described by the nuclear **polarization propagator or dynamic polarizability**. In general, it follows the equation

$$\Pi(\omega) = \Pi_0(\omega) + \Pi_0(\omega)\mathcal{W}(\omega)\Pi(\omega)$$

where $\Pi_0(\omega)$ is the dynamic polarizability at the level of approximation that one wants to improve.

⇒ Using the **redefinition of $\mathcal{W}(\omega)$ given by the subtraction method**

$$\Pi(\omega) = \Pi_0(\omega) + \Pi_0(\omega)\left[\mathcal{W}(\omega) - \mathcal{W}(0)\right]\Pi(\omega)$$

it is clear that $\Pi(0) = \Pi_0(0)$ or, equivalently, being $\Pi(\omega = 0) = -2m_{-1}$ proportional to the static limit of the dynamic polarizability **m_{-1}(EDF)=m_{-1}(BEDF)**

⇒ **Static polarizabilities are fixed at the EDF level no matter the excitation type (dipole is being studied experimentally at GSI and RCNP in various nuclei)**

Energy weighted sum rule

⇒ **Thouless theorem**: **EWSR** calculated within the **RPA** approach is **equal** to the **HF expectation value of the double commutator** $\frac{1}{2}[\mathcal{F}, [\mathcal{H}, \mathcal{F}^\dagger]]$ where $\mathcal{F}$ represents the external field.

⇒ **EWSR in second RPA (SRPA)** is also **equal** to the **double commutator (subtraction method was not considered)**

⇒ Both **proofs** based on the quasiboson approximation: **expectation value of the operators** are calculated within the uncorrelated **HF gs instead** of the more consistent treatment that would consider the **correlated RPA (or SRPA) gs**. Is this assuming that for the calculation of the D.C.?

$$\Psi_{\mathrm{HF}}^{\mathrm{GS}} \approx \Psi_{\mathrm{RPA}}^{\mathrm{GS}} \approx \Psi_{\mathrm{SRPA}}^{\mathrm{GS}}$$

If the subtraction is keeping this one would expect, if $[\mathcal{F}, [\mathcal{H}, \mathcal{F}^\dagger]]$ **is a one-body operator**, the **EWSR** calculated within the **SRPA (also BEDF)** method **with and without subtraction should not differ** (much in practice) with the **RPA**.

IEWSR and EWSR: From a different perspective

Consider that the **ground state** density is **perturbed** by an external (one-body) field $\lambda\mathcal{F}$. **Changes in the expectation value** of the Hamiltonian $\mathcal{H}$ can be written as,

$$\delta\langle\mathcal{H}\rangle_{\mathcal{F}} = \lambda^2 \sum_{n\neq 0} \frac{|\langle n|\mathcal{F}|0\rangle|^2}{E_n} + \mathcal{O}(\lambda^3) = \lambda^2 m_{-1} + \mathcal{O}(\lambda^3)$$

where standard perturbation theory has been applied (i.e. $|n\rangle$ and E_n represents an excited state and corresponding energy of the system). In other terms,

$$m_{-1} = \frac{1}{2} \frac{\partial^2 \langle\mathcal{H}\rangle_{\mathcal{F}}}{\partial\lambda^2}\Big|_{\lambda=0}$$

which is nothing but the **dielectric theorem**. So, **for small perturbations, gs state information determines the static polarizability and should be conserved when going BEDF.**

IEWSR and EWSR: From a different perspective

Consider now the case in which $\mathcal{F}$ **is an isoscalar and velocity independent operator** and define the operator $\tilde{\mathcal{F}} \equiv i[\mathcal{H}, \mathcal{F}] = i[T, \mathcal{F}]$ where T is the kinetic energy. Now, the **expectation value of the Hamiltonian** when perturbed by $\tilde{\mathcal{F}}$ is

$$\delta\langle\mathcal{H}\rangle_{\tilde{\mathcal{F}}} = \lambda^2 \sum_{n\neq 0} E_n |\langle n|\mathcal{F}|0\rangle|^2 + \mathcal{O}(\lambda^3) = \lambda^2 m_1 + \mathcal{O}(\lambda^3)$$

$\Rightarrow$ **for some specific operators (excitation modes)** *the Thouless theorem for $\mathcal{F}$ is equivalent to the dielectric theorem applied to $\tilde{\mathcal{F}}$*,

$$m_1 = \frac{1}{2}\frac{\partial^2\langle\mathcal{H}\rangle_{\tilde{\mathcal{F}}}}{\partial\lambda^2}\Big|_{\lambda=0} = \frac{1}{2}\langle 0|[\mathcal{F}, [\mathcal{H}, \mathcal{F}]]|0\rangle$$

provided that the corresponding quantities are calculated consistently within the same approximation.

$\Rightarrow$ Hence, for small perturbations, **gs state information determines the EWSR of some special excitation modes and should be conserved when going BEDF** ($\langle 0|[\mathcal{F}, [\mathcal{H}, \mathcal{F}]]|0\rangle_{\mathrm{BEDF}} \approx \langle 0|[\mathcal{F}, [\mathcal{H}, \mathcal{F}]]|0\rangle_{\mathrm{HF}}$).

Results: some preliminary considerations

⇒ **Study:** m_1 and m_{-1} for the **IS monopole and IS quadrupole** nuclear responses since the external field can be modelized by a **one-body, isoscalar and velocity independent operator**.

⇒ V_{eff}: **SAMi, SLy5, SkM*** to identify **systematics**, if any.

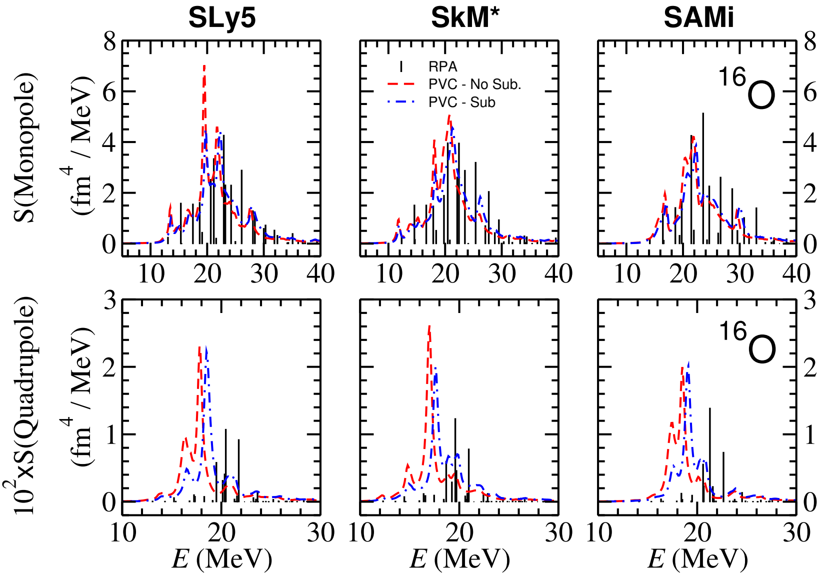
⇒ **Nucleus:** ^{16}**O**

⇒ **Operators:** monopole $\mathcal{F}_0^{IS} = \sum_{i=1}^{A} r_i^2 Y_{00}(\hat{r}_i)$

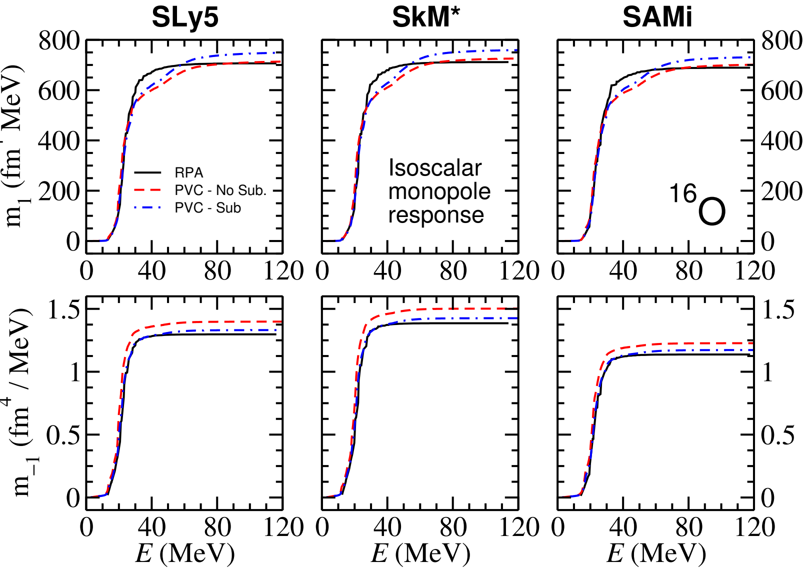
and quadrupole $\mathcal{F}_2^{IS} = \sum_{M} \sum_{i=1}^{A} r_i^2 Y_{2M}(\hat{r}_i)$

⇒ **Model space:** radial mesh of **20 fm in steps of 0.1 fm**; maximum particle energy of **80 MeV**; **doorway phonons** up to multipolarity equal to **5** with energy less than **30 MeV** and absorbing a fraction of the NEWSR larger than **2%**; smearing parameter of 250 keV; and full **effective interaction kept at all levels of approximation**

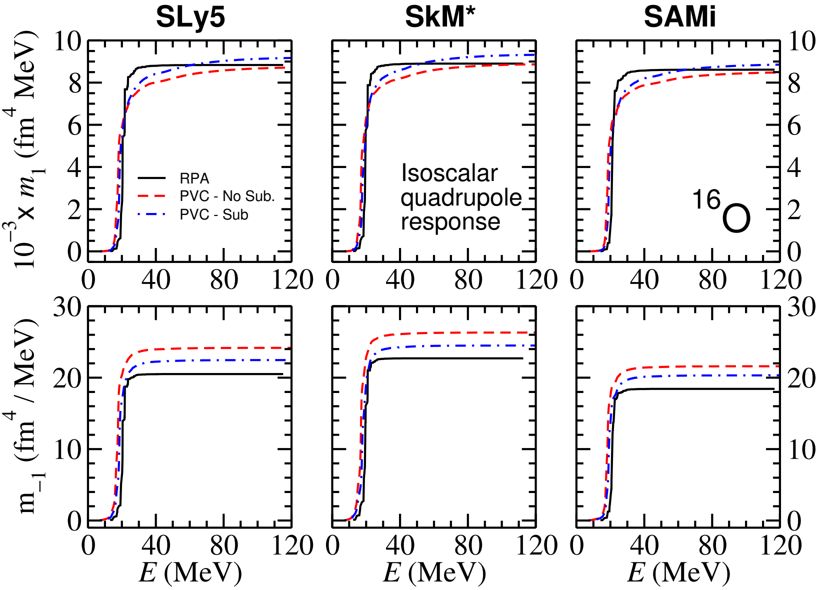
IS monopole and quadrupole resonances in ^{16}O



IS monopole resonance in ^{16}O



IS quadrupole resonance in ^{16}O



Conclusions

⇒ Our **results are not conclusive yet** although the *subtraction method* gives reasonable results –within 10% accuracy– for the studied sum rules.

⇒ The **discrepancy is actually a measure of the accuracy of the adopted approximations** which are essentially two:

i) the $\mathcal{Q}_2$ is assumed to be made of **non-interacting states**

ii) we do **not correct** for the small –but present– contributions to $\mathcal{W}$ that violate the **Pauli** exclusion principle.

Future:

⇒ **To formally and practically address the renormalization problem**. **Already studied** the renormalization of total energy assuming a simplified PVC model in:

* **infinite matter** (C. J. Yang, K. Moghrabi, M. Grasso, G. Colò).

* **finite nuclei** (M. Brenna and G. Colò).

⇒ **To improve our PVC approach** in points i) and ii)

⇒ **To go beyond the spectroscopic properties of PVC** (Hybrid configuration mixing model, G. Colò, P. F. Bortignon, G. Bocchi)

Collaborators

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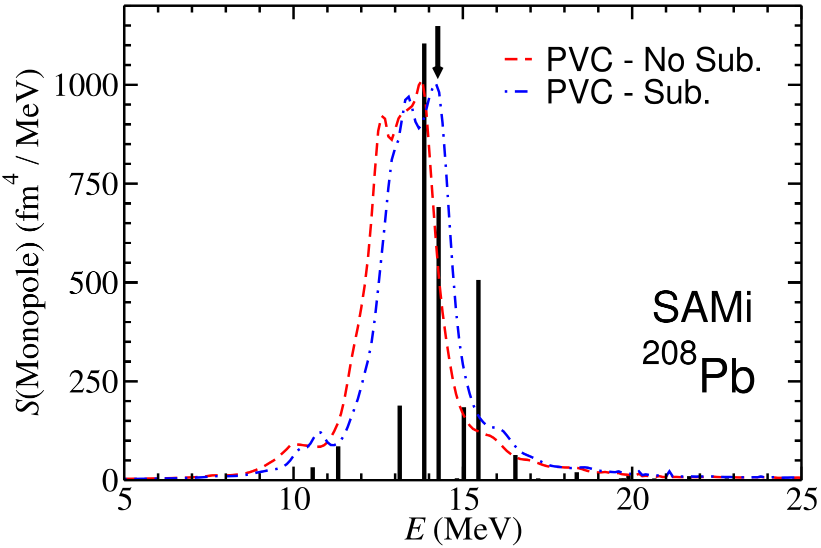
- **G. Colò** and **P. F. Bortignon** from **Università degli Studi di Milano and INFN**, Milan, **Italy**
- **K. Moghrabi** from **Lebanese University**, Beirut, **Lebanon**
- **C. J. Yang** and **M. Grasso** from **Institut de Physique Nucléaire**, Orsay, **France**

Thank you for your attention

Extra material

IS monopole resonances in ^{208}Pb



IS quadrupole resonances in ^{208}Pb