Towards the improvement of spin-isospin properties in nuclear energy density functionals

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- Propose a new fitting protocol: Example with a Skyrme interaction
Spin and Isospin excitations in Nuclei

- **Nucleons** are fermions characterized by their spin and isospin.
- **Nucleons** with spin (isospin) may **change their state** in **phase**: spin-scalar $S=0$ modes (isospin-scalar $T=0$ modes); or **out of phase**: spin-vector $S=1$ modes (isospin-vector $T=1$ modes).
- They can be **excited by strong probes** (charge-exchange reactions) and they can **decay via the weak interaction** (axial-vector current couples to the spin and induces $\beta$—decay processes).

One of the most important nuclear excitation modes is the 

- **Gamow Teller Resonance** which is a pure **spin-isospin mode** (i.e., from a theoretical picture, it is excited by an operator $\hat{O} \sim \sigma \tau$).

**Spin-isospin modes** of excitation (such as the **GTR**) give **direct information** on the spin-isospin channel of the **effective interaction** (or generator of our EDF).
Example: $\beta$–decay transition

Transitions from $^{42}\text{Ti}$: $\beta$ decay

proton: $f_{7/2} \rightarrow$ neutron $f_{7/2}$
proton: $f_{7/2} \rightarrow$ neutron $f_{5/2}$

Courtesy of Y. Fujita; taken from his lectures [http://www.mi.infn.it/~colo/lectures/lectures.html](http://www.mi.infn.it/~colo/lectures/lectures.html)
Example: Gamow Teller transition

Transitions from $^{42}\text{Ca} : CE$ Reaction

β decay and CE reaction make Isospin Analogous transitions (mirror transitions in proton and neutron)

neutron: $f_{7/2} \rightarrow$ proton $f_{7/2}$
neutron: $f_{7/2} \rightarrow$ proton $f_{5/2}$

Courtesy of Y. Fujita; taken from his lectures [http://www.mi.infn.it/~colo/lectures/lectures.html](http://www.mi.infn.it/~colo/lectures/lectures.html)
GT and β-decay transitions give the same/similar information.

Therefore, (as we already know ... )

- allowed GT transitions mainly determine β-decay half-lives
- GT transitions determine weak interaction rates essential role in the core-collapse dynamics of massive stars leading to supernova explosion
- In neutron-rich environment, neutrino-induced nucleosynthesis may take place via GT processes
- GT matrix elements are necessary for the study of double-β-decay
- may be useful in the calibration of detectors used to measure neutrinos that reach the Earth
- ... (see N. Paar’s Talk)
Some comments on the nuclear many-body problem:

▶ **Many-body** calculations based on **NN scattering data** in the vacuum are **not conclusive** yet:
  ▶ **different predictions** are found **depending** on the approach
  ▶ **EoS** and (only very recently) **few groups** in the world are able to perform extensive calculations for **light and medium mass nuclei**

▶ Based on effective interactions (generators), **Nuclear Energy Density Functionals** are **successful** (but still not perfect) in the description of **masses, nuclear sizes, deformations, Giant Resonances,**...
Nuclear Energy Density Functionals:

(remenber G. Colò’s Talk)

Kohn-Sham iterative scheme (static approximation)

- Determine a good $E[\rho]$
- Initial guess $\rho_0$
- Calculate potential $V_{\text{eff}}$ from $\rho_0$
- Solve single particle (Schrödinger) equation and find single particle wave functions $\phi_i$
- Use $\phi_i$ for calculating new $\rho_1 = \sum_i^A |\phi_i|^2$
- Repeat until convergence

Runge-Gross Theorem: dynamic generalization of the static EDFs.

$$\int dt \{ \langle \Phi(t) | i \partial_t | \Phi(t) \rangle - E[\rho(t), t] \} = 0$$

Giant Resonances well described within the small amplitude limit (known as RPA approach)
Nuclear Energy Density Functionals:
Main types of successful EDFs derived from the mean-field approximation

- **Relativistic H o HF models**, based on Lagrangians where effective (heavy) mesons carry the interaction.

\[
\mathcal{L}_{\text{int}} = \bar{\Psi} \Gamma_\sigma (\bar{\Psi}, \Psi) \Psi \Phi_\sigma + \bar{\Psi} \Gamma_\delta (\bar{\Psi}, \Psi) \tau \Psi \Phi_\delta \\
- \bar{\Psi} \Gamma_\omega (\bar{\Psi}, \Psi) \gamma_\mu \Psi A^{(\omega)}_\mu - \bar{\Psi} \Gamma_\rho (\bar{\Psi}, \Psi) \gamma_\mu \tau \Psi A^{(\rho)}_\mu \\
- e \bar{\Psi} \hat{Q} \gamma_\mu \Psi A^{(\gamma)}_\mu
\]

- **Non-relativistic HF models**, based on Hamiltonians where effective interactions are proposed and tested:

\[
V_{\text{eff}}^{\text{Nucl}} = V_{\text{long-range}}^{\text{attractive}} + V_{\text{short-range}}^{\text{repulsive}} + V_{\text{SO}}
\]

- Fitted parameters contain (important) correlations beyond the mean-field

- Nuclear energy functionals are **phenomenological → not directly connected to any NN (or NNN) interaction**
On the one side,

- we expect that the $H(F)+\text{RPA}$ method based on nuclear effective interactions of the Skyrme, Gogny or Relativistic (can be understood as an approximate realization of an EDF) ⇒ reasonable description of g.s. energy and density of the system

On the other side,

- there are still some open problems ... but we will concentrate here on how to improve the spin-isospin properties of our EDF
Motivation: Gamow Teller Resonance

The $E_x$ is not properly described in $H(F) + \text{RPA}$

- **SGII**: earliest attempt to give a quantitative description of the GTR
- **SkO'**: accurate in ground state finite nuclear properties and improves the GTR
- **PKO1**: relativistic HF, reasonable GTR still not perfect
- **Relativistic H**: residual interaction modified $ad$-$hoc$

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\[ a \text{ PLB 106, 379 (1981), } b \text{ PRC 60, 014316 (1999), } c \text{ PRL 101, 122502 (2008), } d \text{ PRC 69, 054303} \]
Motivation: Gamow Teller Resonance

Exchange (Fock) effects on GTR in relativistic models

Effect of Migdal term $\rightarrow$ fitted to $^{208}\text{Pb}$ in RH
Motivation: which gs properties are important for describing the $E_{\chi}^{\text{GTR}}$?

The study\textsuperscript{a} of the GTR and the spin-isospin Landau-Migdal parameter $G'_0$ using several Skyrme sets,

- concluded that $G'_0$ is not the only important quantity in determining the excitation energy of the GTR
- spin-orbit splittings also influences the GTR

Empirical indications\textsuperscript{b}

suggest that $G'_0 > G_0 > 0$

Not a very common feature within available Skyrme forces\textsuperscript{c}

Why spin-orbit splittings are important in $E_{\chi}^{\text{GTR}}$?

Schematic picture of single-particle transitions involved in the Gamow Teller Resonance of $^{90}\text{Zr}$. Transitions excited by $\sigma \tau_-$ operator.

\[
E_{\chi}^1 \approx \epsilon_{\pi 1g_{7/2}} - \epsilon_{\nu 1g_{9/2}} + \epsilon_{\text{ph}}^1 \quad E_{\chi}^2 \approx \epsilon_{\pi 1g_{9/2}} - \epsilon_{\nu 1g_{9/2}} + \epsilon_{\text{ph}}^2
\]

\[
\Delta E_{\chi} \approx \Delta \epsilon_{\pi 1g} + \Delta \epsilon_{\text{ph}}
\]

F. Osterfeld, Rev. Mod. Phys. 64, 491 (1992)
We propose a new fitting protocol that help improving spin-isospin properties...

Example with a Skyrme interaction
(Standard) Skyrme Model

[ ... have a quick look!]
Includes central tensor terms ($J^2$ terms) due to the coupling of tensor and spin and gradients terms and two spin-orbit parameters (same as SkO and some SkI forces)

\[ \mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{\text{eff}} + \mathcal{H}_{\text{fin}} + \mathcal{H}_{\text{SO}} + \mathcal{H}_{\text{sg}} + \mathcal{H}_{\text{Coul}} \]

\[ \mathcal{K} = \hbar^2 \tau/2m \]

\[ \mathcal{H}_0 = (1/4)t_0[(2 + x_0)\rho^2 - (2x_0 + 1)(\rho_n^2 + \rho_p^2)] \quad \text{(CENTRAL)} \]

\[ \mathcal{H}_3 = (1/24)t_3 \rho^\alpha[(2 + x_3)\rho^2 - (2x_3 + 1)(\rho_n^2 + \rho_p^2)] \quad \text{(DENSITY DEP.)} \]

\[ \mathcal{H}_{\text{eff}} = (1/8)[t_1(2 + x_1) + t_2(2 + x_2)]\tau \rho \]
\[ + (1/8)[t_2(2x_2 + 1) - t_1(2x_1 + 1)](\tau_n \rho_n + \tau_p \rho_p) \quad \text{(EFF. MASS)} \]

\[ \mathcal{H}_{\text{fin}} = (1/32)[3t_1(2 + x_1) - t_2(2 + x_2)](\nabla \rho)^2 \]
\[ - (1/32)[3t_1(2x_1 + 1) + t_2(2x_2 + 1)][(\nabla \rho_n)^2 + (\nabla \rho_p)^2] \quad \text{(FIN RANGE)} \]

\[ \mathcal{H}_{\text{SO}} = (1/2)W_0 \mathbf{J} \cdot \nabla \rho + (1/2)W'_0(\mathbf{J} \cdot n \nabla \rho_n + \mathbf{J}_p \cdot \nabla \rho_p) \]

\[ \mathcal{H}_{\text{sg}} = -(1/16)(t_1 x_1 + t_2 x_2)\mathbf{J}^2 + (1/16)(t_1 - t_2)(\mathbf{J}_n^2 + \mathbf{J}_p^2) \]
Fitting Protocol: Inspired on SLy5

$\chi^2$ definition: $\chi^2 = \frac{1}{N_{\text{data}}} \sum_{i}^{N_{\text{data}}} \frac{(\mathcal{O}_{i}^{\text{theo}} - \mathcal{O}_{i}^{\text{data}})^2}{(\Delta \mathcal{O}_{i}^{\text{data}})^2}$

Landau-Migdal parameters in infinite nuclear matter $G_0$ and $G'_0$ fixed to 0.15 and 0.35, respectively, at $\rho_0$.

Table: Data and pseudo-data $\mathcal{O}_i$, adopted errors for the fit $\Delta \mathcal{O}_i$ and selected finite nuclei and EoS.

<table>
<thead>
<tr>
<th>$\mathcal{O}_i$</th>
<th>$\Delta \mathcal{O}_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B$ 1.00 MeV</td>
<td>$^{40,48}<em>{\text{Ca}}, ^{90}</em>{\text{Zr}}, ^{132}<em>{\text{Sn}}$ and $^{208}</em>{\text{Pb}}$</td>
</tr>
<tr>
<td>$r_c$ 0.01 fm</td>
<td>$^{40,48}<em>{\text{Ca}}, ^{90}</em>{\text{Zr}}$ and $^{208}_{\text{Pb}}$</td>
</tr>
<tr>
<td>$\Delta E_{SO}$</td>
<td>0.04$\times \mathcal{O}<em>i$ $\pi 1g$ in $^{90}</em>{\text{Zr}}$ and $\pi 2f$ in $^{208}_{\text{Pb}}$</td>
</tr>
<tr>
<td>$e_n(\rho)$</td>
<td>0.20$\times \mathcal{O}_i$ R. B. Wiringa et al., PRC 38, 1010 (1988)</td>
</tr>
</tbody>
</table>

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Skyrme Aizu Milano interaction: SAMi

Parameter set:

<table>
<thead>
<tr>
<th>value(σ)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_0$</td>
<td>$-1877.75(75)$ MeV fm$^3$</td>
</tr>
<tr>
<td>$t_1$</td>
<td>$475.6(1.4)$ MeV fm$^5$</td>
</tr>
<tr>
<td>$t_2$</td>
<td>$-85.2(1.0)$ MeV fm$^5$</td>
</tr>
<tr>
<td>$t_3$</td>
<td>$10219.6(7.6)$ MeV fm$^{3+3\alpha}$</td>
</tr>
<tr>
<td>$x_0$</td>
<td>$0.320(16)$</td>
</tr>
<tr>
<td>$x_1$</td>
<td>$-0.532(70)$</td>
</tr>
<tr>
<td>$x_2$</td>
<td>$-0.014(15)$</td>
</tr>
<tr>
<td>$x_3$</td>
<td>$0.688(30)$</td>
</tr>
<tr>
<td>$W_0'$</td>
<td>$137(11)$</td>
</tr>
<tr>
<td>$W_0'$</td>
<td>$42(22)$</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>$0.25614(37)$</td>
</tr>
</tbody>
</table>

$\sigma$ is the one standard deviation $\Delta p$ defined as $\chi^2(p_0 + \Delta p) - \chi^2(p_0) = 1$
Skyrme Aizu Milano interaction: SAMi

But those, where not the actual fitted parameters

- we found **convenient** to use as parameters **nuclear matter** saturation properties instead.
- provides a more **transparent control on the parameter space** you would like to explore
- the **conversion** from nuclear matter parameters to the Skyrme interaction parameters is **one to one**

(Note: we convert all parameters of the interaction contributing to NM)

<table>
<thead>
<tr>
<th>Prop.</th>
<th>value(σ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_\infty$</td>
<td>0.159(1) fm$^{-3}$</td>
</tr>
<tr>
<td>$e_\infty$</td>
<td>$-15.93(9)$ MeV</td>
</tr>
<tr>
<td>$m^*_\text{IS}$</td>
<td>0.6752(3)</td>
</tr>
<tr>
<td>$m^*_\text{IV}$</td>
<td>0.664(13)</td>
</tr>
<tr>
<td>$J$</td>
<td>28(1) MeV</td>
</tr>
<tr>
<td>$L$</td>
<td>44(7) MeV</td>
</tr>
<tr>
<td>$K_\infty$</td>
<td>245(1) MeV</td>
</tr>
<tr>
<td>$G_0$</td>
<td>0.15 (fixed)</td>
</tr>
<tr>
<td>$G'_0$</td>
<td>0.35 (fixed)</td>
</tr>
</tbody>
</table>
SAMi: spin and spin-isospin instabilities

Imposing that spin and isospin d.o.f. at the Fermi surface are stable under generalized deformations [Bäckman et al., Nucl. Phys. A 321, 10 (1979)]

\[ 1 + G_0 > 0 \quad 1 + G'_0 > 0 \]
Results

Equation of State: SAMi vs ab-initio calculations

Results

Finite Nuclei: spherical double-magic nuclei

Figure: Finite nuclei properties as predicted by the HF SAMi (black circles) and some predictions (blue circles) for spherical double-magic nuclei. Experimental data taken from Refs. G. Audi et al., NPA 729, 337 (2003), I. Angeli, ADNDT 87, 185 (2004), M. Zalewski et al., PRC 77, 024316 (2008)
Results

Giant Monopole and Dipole Resonances in $^{208}\text{Pb}$

Figure: Strength function at the relevant excitation energies in $^{208}\text{Pb}$ as predicted by SLy5 and the SAMi interaction for GMR and GDR. A Lorentzian smearing parameter equal to 1 MeV is used. Experimental data for the centroid energies are also shown: $E_c (\text{GMR}) = 14.24 \pm 0.11$ MeV [D. H. Youngblood, et al., Phys. Rev. Lett. 82, 691 (1999)] and $E_c (\text{GDR}) = 13.25 \pm 0.10$ MeV [N. Ryezayeva et al., Phys. Rev. Lett. 89, 272502 (2002)].
Results

Gamow Teller
Resonance in $^{48}$Ca, $^{90}$Zr and $^{208}$Pb

$$\sum_{i=1}^{A} \sigma(i) \tau_{\pm}(i)$$

Results

Spin Dipole Resonances in $^{90}$Zr and $^{208}$Pb

Operator:
\[ \sum_{i=1}^{A} \sum_{M} \tau_{\pm}^i (r_{L}^i) \left[ Y_{L} (\hat{r}_{i}) \otimes \sigma(i) \right] J_{M} \]

Sum Rule:
\[ \int [R_{SD-}(E) - R_{SD+}(E)] dE = \frac{9}{4\pi} \left( N\langle r_{n}^2 \rangle - Z\langle r_{p}^2 \rangle \right) \]


Conclusions:

- We have remained some of the problems in the spin-isospin channels in Skyrme and RH models (as compared to RHF) using as an example the GTR.
- We have briefly presented:
  - the benefits of the new proposed fitting protocol that cure part of the previous problems
  - test the new protocol and show some results when applied with a Skyrme interaction.
Conclusions:

▶ And for the future....

▶ Include tensor to better describe spin-isospin resonances such as the SDR.

▶ Improve the isospin-nuclear channel by fixing first the Coulomb channel [models may differ in the Coulomb energy contribution more than expected → may influence the isospin channel]

▶ Since RHF depends on non-local potentials (more complicated) and implies a non-negligible computational cost when improving the calculations and/or going beyond the mean-field: we will propose a new method (see H. Liang’s talk) to determine a localized RHF model ...
Thank you!

Work in collaboration with:
G. Colò, H. Sagawa, H. Liang, J. Meng, P. Ring and P. Zhao
Extra Material
We propose a new fitting protocol that help improving spin-isospin properties...

Minimization method used
Algorithm: variable metric method (MINUIT)

- In analogy with differential geometry it is convenient to consider the properties of a function ($\chi^2(p)$) as being properties of the space in the variables $p$.
- The fundamental invariant in non-Euclidean space is $\Delta s^2 = \Delta p^T A \Delta p$ ($A$ covariant metric tensor ⇒ determines properties of the space).
- The Hessian matrix ($M$) behave as a covariant tensor under coordinate transformations ⇒ will be our metric.
- $\Delta s^2$: square of the generalized distance produced by $\Delta p$.
- $\Delta s$: the number of standard deviations $\Delta p$ away from $p_0$ (optimal set of parameters).
Algorithm: variable metric method (MINUIT)

- **Vertical distance** $\Delta d^2$: the other invariant quantity build with the contravariant tensor $\mathcal{M}^{-1}$ (named covariant matrix, $\Delta d^2 = g^T \mathcal{M}^{-1} g$)
- $\Delta d^2$: scale $\Delta \mathbf{p}$ so that it has physical (statistical) meaning and become an invariant quantity (instead of being expressed in arbitrary units).
- The latter provides a **scale-free convergence criterion**
- If $\chi^2(\mathbf{p})$ is not quadratic in $\mathbf{p}$, but more complex, $\mathcal{M}$ is non-constant with variations of $\mathbf{p}$: **Variable Metric Method**
- One does a kind of Newton-Raphson $\mathbf{p}_{i+1} = \mathbf{p}_i - \mathcal{M}_{i}^{-1} g_i$
  where $g_i$ is the gradient vector evaluated at $\mathbf{p}_i$ and $\mathcal{M}_{i+1}^{-1}$ is usually corrected by using information on the previous step (that is, not fully re-evaluated) each time.
SAMi-J and SAMi-m families: AGDR and IAS
Empirical constraints on $G_0$ and $G'_0$


- In our fit, we do not use the obtained values as pseudodata because our theoretical framework is different and the results are associated to different $m^*$ (our sp energies are based on HF calculations instead of a Wood-Saxon potential).

- We use the empirical result in which an **hierarchy** between spin and spin-isospin parameters is suggested: $G'_0 > G_0 > 0$
Motivation: Gamow Teller Resonance
Quenching of the strength

- **Experimentally**, the GTR exhausts 60–70% of the Ikeda sum rule: \( \int [R_{\text{GT}^-(E)} - R_{\text{GT}^+(E)}] \, dE = 3(N - Z) \)
- To explain the problem, two possibilities that go beyond (1p – 1h) RPA correlations have been drawn:
  - the effects of the second-order configuration mixing: 2p-2h correlations
  - within the quark model, a n(p) can become a p(n) or a \( \Delta^+(\Delta^{++}) \) under the action of the GT\(^-\) operator and since there is no Pauli blocking for \( \Delta-\)h excitations ⇒ it may contribute to the GTR.
- The experimental analysis of \(^{90}\text{Zr} \Rightarrow \text{quenching} \) (2/3) has to be mainly attributed to 2p-2h coupling and not to \( \Delta-\)isobar effects much smaller [T. Wakasa et. al., Phys. Rev. C 55, 2909 (1997)].
- \( E_x \) GTR in nuclei mainly in the region of several tens of MeV and the \( \Delta-\)h states are hundreds of MeV above the GT ⇒ hard to excite the \( \Delta \) in the nuclear medium.