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

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Spin and Isospin excitations in Nuclei

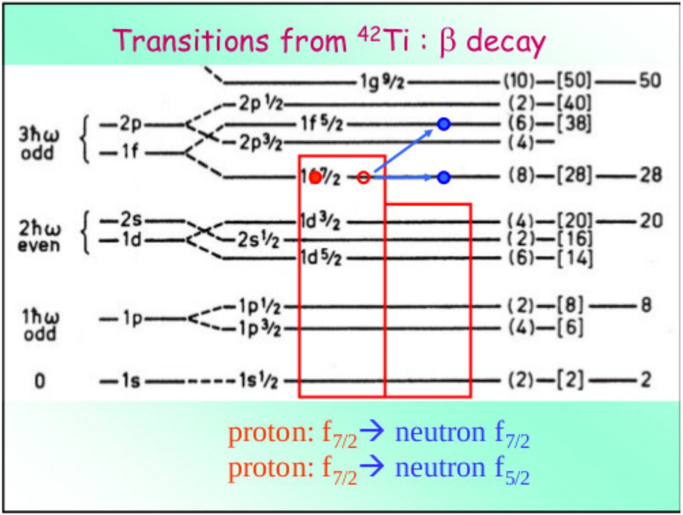
- **Nucleons** are fermions charac. by their spin and isospin
- **Nucleons** with spin (isospin) may **change their state** in **phase**: spin-scalar S=0 modes (isospin-scalar T=0 modes); or **out of phase**: spin-vector S=1 modes (isospin-vector T=1 modes)
- They can be **excited by strong probes** (charge-exhange 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 $\hat{O} \sim \sigma\tau$)

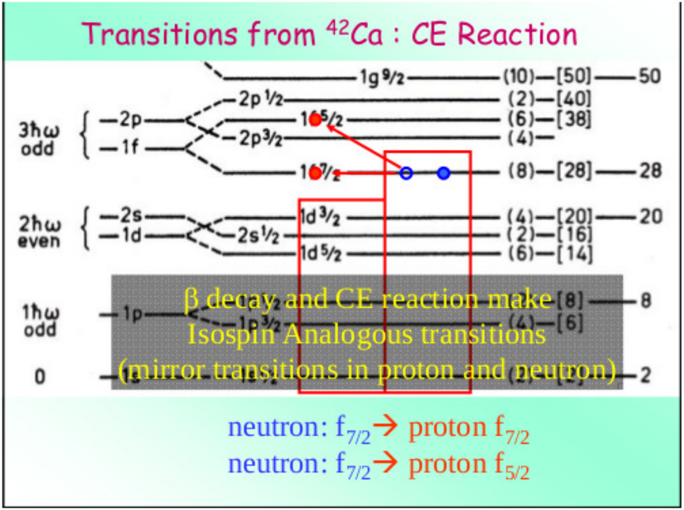
Spin-isospin modes of excitation (such as the **GTR**) give **direct information** on the spin-isospin channel of the **effective interaction** (or generator of our EDF)

Example: β−decay transition



Courtesy of Y. Fujita; taken from his lectures http://www.mi.infn.it/~colo/lectures/lectures.html

Example: Gamow Teller transition



Courtesy of Y. Fujita; taken from his lectures 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 detemine **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 ρ_0
- Calculate potential V_{eff} from ρ_0
- Solve single particle (Schrödinger) equation and find single particle wave functions ϕ_i
- Use ϕ_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.

$$\begin{aligned}\mathcal{L}_{int} \quad &= \bar{\Psi}\Gamma_\sigma(\bar{\Psi},\Psi)\Psi\Phi_\sigma \quad &+\bar{\Psi}\Gamma_\delta(\bar{\Psi},\Psi)\boldsymbol{\tau}\Psi\Phi_\delta \\ &-\bar{\Psi}\Gamma_\omega(\bar{\Psi},\Psi)\gamma_\mu\Psi A^{(\omega)\mu} \quad &-\bar{\Psi}\Gamma_\rho(\bar{\Psi},\Psi)\gamma_\mu\tau\Psi A^{(\rho)\mu} \\ &-e\bar{\Psi}\hat{Q}\gamma_\mu\Psi A^{(\gamma)\mu}\end{aligned}$$

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

$$V^{\text{eff}}_{\text{Nucl}} = V^{\text{long}-\text{range}}_{\text{attractive}} + V^{\text{short}-\text{range}}_{\text{repulsive}} + V_{\text{SO}}$$

- Fitted **parameters contain** (important) **correlations beyond the mean-field**
- Nuclear energy functionals are **phenomenological** $\rightarrow$ **not directly connected to any NN** (or NNN) **interaction**

Drawbacks on current EDFs ???

On the one side,

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

On the other side,

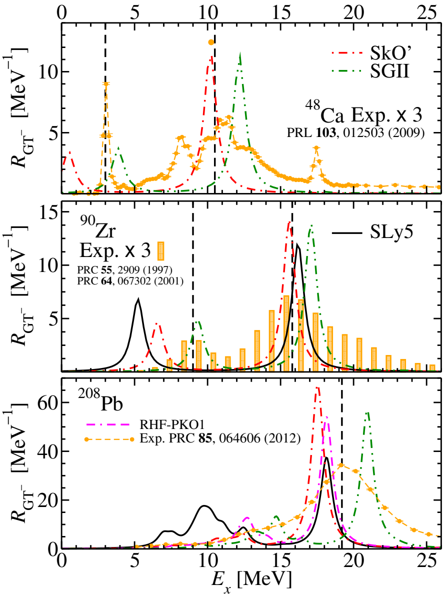
- there are still some **open problems** ... but we will concentrate here on how to

  improve the spin-isospin properties of our EDF

Motivation: Gamow Teller Resonance

The E_x is not properly described in H(F)+RPA

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

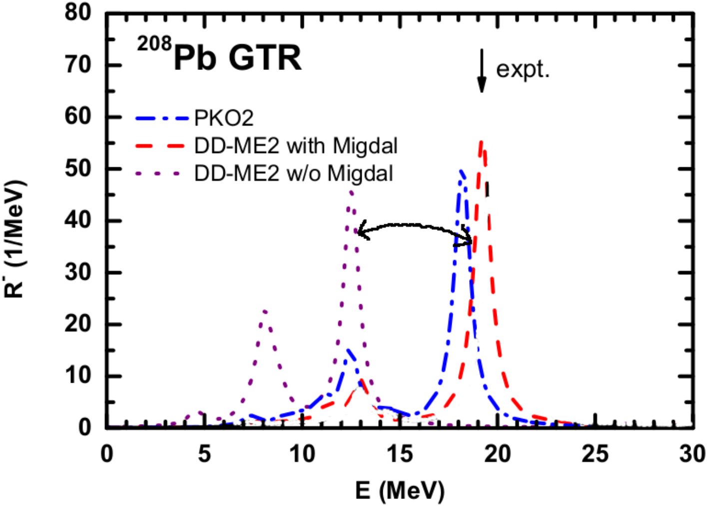


[a] PLB **106**, 379 (1981), [b] PRC **60**, 014316 (1999), [c] PRL **101**, 122502 (2008), [d] PRC 69, 054303

Motivation: Gamow Teller Resonance

Exchange (Fock) effects on GTR in relativistic models

Effect of Migdal term → fitted to ^{208}Pb in RH

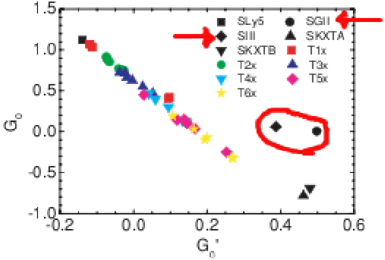


Motivation: which gs properties are important for describing the E_x^{GTR}?

The study[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

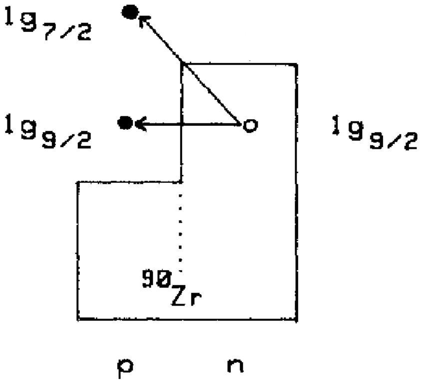
- Empirical indications[b] suggest that $G'_0 > G_0 > 0$
- **Not a very common feature** within available Skyrme forces[c]



[a] M. Bender, J. Dobaczewski, J. Engel, and W. Nazarewicz, Phys. Rev. C **65**, 054322 (2002); [b] T. Wakasa, M. Ichimura, and H. Sakai, Phys. Rev. C **72**, 067303 (2005); T. Suzuki and H. Sakai, Phys. Lett. B **455**, 25 (1999), [c] Li-Gang Cao, G. Colo, and H. Sagawa, Phys. Rev. C **81**, 044302 (2010)

Why spin-orbit splittings are important in E_x^{GTR}?

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



$$E_x^1 \approx \epsilon_{\pi 1 g_{7/2}} - \epsilon_{\nu 1 g_{9/2}} + \epsilon_{ph}^1 \qquad E_x^2 \approx \epsilon_{\pi 1 g_{9/2}} - \epsilon_{\nu 1 g_{9/2}} + \epsilon_{ph}^2$$

$$\Delta E_x \approx \Delta\epsilon_{\pi 1 g} + \Delta\epsilon_{ph}$$

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)

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

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

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

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

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

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

$$H_{SO} = (1/2)W_0\mathbf{J}\cdot\nabla\rho + (1/2)W_0'(\mathbf{J}\cdot_{\mathbf{n}}\nabla\rho_n + \mathbf{J_p}\cdot\nabla\rho_p)$$

$$H_{sg} = -(1/16)(t_1x_1 + t_2x_2)\mathbf{J}^2 + (1/16)(t_1 - t_2)(\mathbf{J_n}^2 + \mathbf{J_p}^2)$$

Fitting Protocol: Inspired on SLy5

χ^2 definition: $\chi^2 = \frac{1}{N_{data}} \sum_i^{N_{data}} \frac{(\mathcal{O}_i^{theo.} - \mathcal{O}_i^{data})^2}{(\Delta\mathcal{O}_i^{data})^2}$

Landau-Migdal parameters in infinite nuclear matter G_0 and G_0' fixed to **0.15** and **0.35**, respectively, at ρ_0.

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

$\mathcal{O}_i$	$\Delta\mathcal{O}_i$	
B	1.00 MeV	^{40,48}Ca, ^{90}Zr, ^{132}Sn and ^{208}Pb
r_c	0.01 fm	^{40,48}Ca, ^{90}Zr and ^{208}Pb
ΔE_{SO}	$0.04\times\mathcal{O}_i$	$\pi 1g$ in ^{90}Zr and $\pi 2f$ in ^{208}Pb
$e_n(\rho)$	$0.20\times\mathcal{O}_i$	R. B. Wiringa *et al.*, PRC **38**, 1010 (1988)

Skyrme Aizu Milano interaction: SAMi

Parameter set:

	value(σ)	
t_0	−1877.75(75)	MeV fm^3
t_1	475.6(1.4)	MeV fm^5
t_2	−85.2(1.0)	MeV fm^5
t_3	10219.6(7.6)	MeV $fm^{3+3\alpha}$
x_0	0.320(16)	
x_1	−0.532(70)	
x_2	−0.014(15)	
x_3	0.688(30)	
W_0	137(11)	
W_0'	42(22)	
α	0.25614(37)	

σ is the one standard deviation $\Delta\mathbf{p}$ defined as
$\chi^2(\mathbf{p}_0 + \Delta\mathbf{p}) - \chi^2(\mathbf{p}_0) = 1$

Skyrme Aizu Milano interaction: SAMi

But those, where not the actual fitted parameters

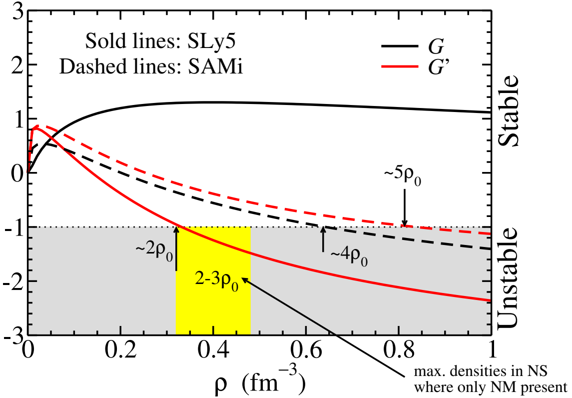
- we found **convenient** to use as parameters **nuclear matter** saturation properties instead.
- provides a more **transparent control on the parameter space** you would like to explore
- the **conversion** from nuclear matter parameters to the Skyrme interaction parameters is **one to one** (**Note:** we convert all parameters of the interaction contributing to NM)

Prop.	value(σ)	
ρ_∞	0.159(1)	fm^{-3}
e_∞	−15.93(9)	MeV
m^*_{IS}	0.6752(3)	
m^*_{IV}	0.664(13)	
J	28(1)	MeV
L	44(7)	MeV
K_∞	245(1)	MeV
G_0	0.15	(fixed)
G'_0	0.35	(fixed)

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)]

$$1 + G_0 > 0 \qquad 1 + G'_0 > 0$$



Results

Equation of State: SAMi vs *ab*–initio calculations

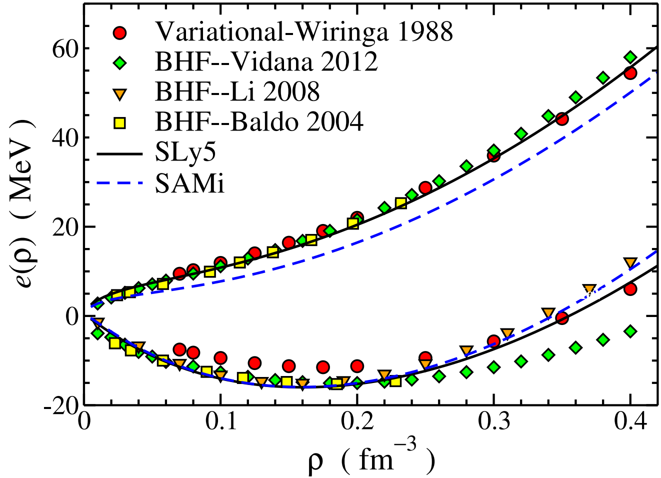


Figure: Neutron and symmetric matter EoS as predicted by the HF SAMi (dashed line) and SLy5 (solid line) interactions and by the benchmark microscopic calculations of R. B. Wiringa *et al.*, PRC **38**, 1010 (1988) (circles). State-of-the-art BHF calculations are shown by diamonds I. Vidaña, private communication, triangles Z. H. Li *et al.*, Phys. Rev. C **77**, 034316 (2008) and squares M. Baldo *et al.*, Nucl. Phys. A **736**, 241 (2004).

Results

Finite Nulcei: spherical double-magic nuclei

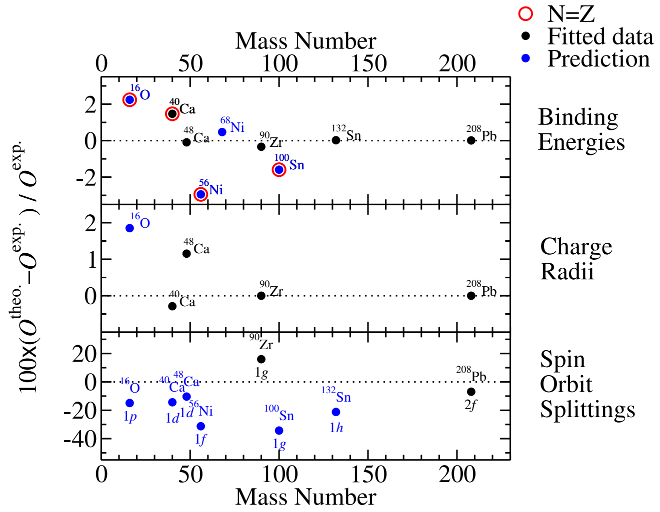


Figure: Finite nuclei properties as predicted by the HF SAMi (black circles) and some predictions (blue circles) for spherical double-magic nuclei. Experimental data taken from Refs. G. Audi *et al.*, NPA **729**, 337 (2003), I. Angeli, ADNDT **87**, 185 (2004), M. Zalewski *et al.*, PRC **77**, 024316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

Results

Giant Monopole and Dipole Resonances in ^{208}Pb

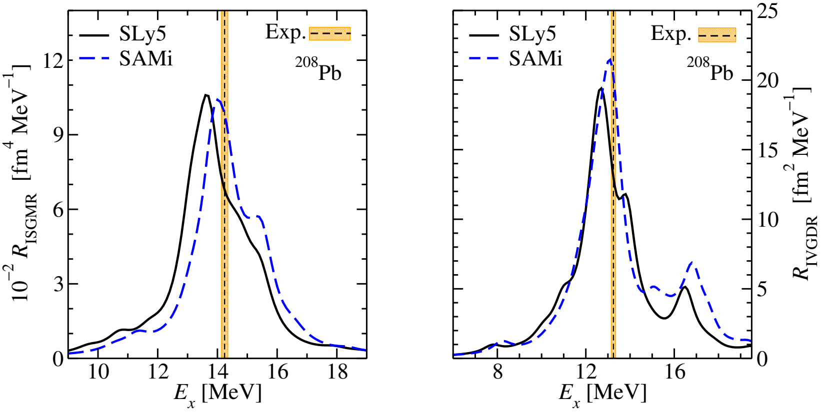


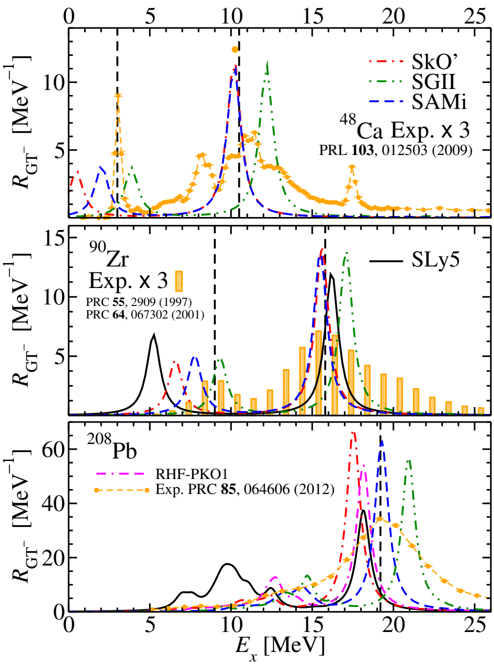
Figure: Strength function at the relevant excitation energies in ^{208}Pb as predicted by SLy5 and the SAMi interaction for GMR and GDR. A Lorentzian smearing parameter equal to 1 MeV is used. Experimental data for the centroid energies are also shown: $E_c(GMR) = 14.24 \pm 0.11$ MeV [D. H. Youngblood,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

Results

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

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

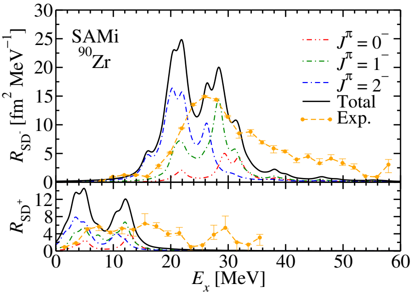
Figure: Gamow Teller strength distributions in ^{48}Ca (upper panel), ^{90}Zr (middle panel) and ^{208}Pb (lower panel) as measured in the experiment [T. Wakasa *et al.*, Phys. Rev. C **55**, 2909 (1997), K. Yako *et al.*, Phys. Rev. Lett. **103**, 012503 (2009), A. Krasznaborkay *et al.*, Phys. Rev. C **64**, 067302 (2001), H. Akimune *et al.*, Phys. Rev. C **52**, 604 (1995) and T. Wakasa et al., Phys. Rev. C **85**, 064606 (2012)] and predicted by SLy5, SkO', SGII and SAMi forces.



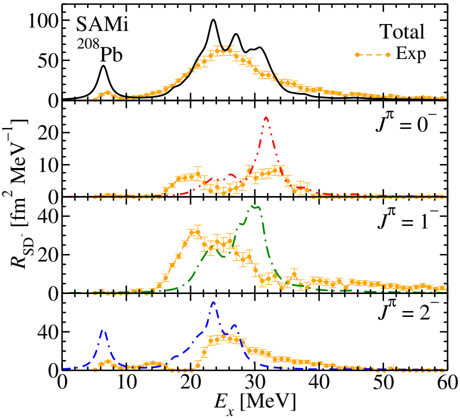
Results

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

Operator:
$\sum_{i=1}^{A} \sum_{M} \tau_{\pm}(i) r_i^L [Y_L(\hat{r}_i) \otimes \sigma(i)]_{JM}$
Sum Rule:
$\int [R_{SD-}(E) - R_{SD+}(E)] dE = \frac{9}{4\pi} (N \langle r_n^2 \rangle - Z \langle r_p^2 \rangle)$



Experiment: K. Yako *et al.*, Phys. Rev. C **74**, 051303(R) (2006). A Lorentzian smearing parameter 2 MeV is used.



Experiment: T. Wakasa *et al.*, Phys. Rev. C **85**, 064606 (2012). A Lorentzian smearing parameter 2 MeV is used.

Conclusions:

- We have **remainded** 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 descrive 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 $\rightarrow$ 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

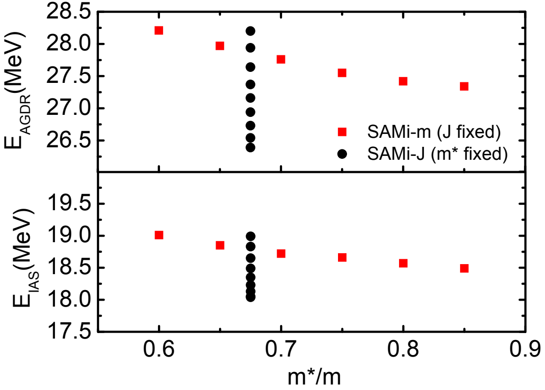
Algorithm: variable metric method (MINUIT)

- In analogy with **differential geommetry** it is **convenient** to consider the **properties of a function** ($\chi^2(\mathbf{p})$) as being **properties of the space** in the variables $\mathbf{p}$.
- The fundamental **invariant** in **non-Euclidean** space is $\Delta s^2 = \Delta\mathbf{p}^{\mathrm{T}} A \Delta\mathbf{p}$ (A covariant metric tensor $\Rightarrow$ **determines properties of the space**).
- The **Hessian** matrix ($\mathcal{M}$) behave as a covariant tensor under coordiante transformations $\Rightarrow$ will be our metric
- Δs^2: square of the generalized distance produced by $\Delta\mathbf{p}$
- Δs: the number of standard deviations $\Delta\mathbf{p}$ away from $\mathbf{p_0}$ (optimal set of parameters)

Algorithm: variable metric method (MINUIT)

- **Vertical distance** Δd^2: the other invariant quantity build with the contravariant tensor $\mathcal{M}^{-1}$ (named covariant matrix, $\Delta d^2 = \mathbf{g}^T \mathcal{M}^{-1} \mathbf{g}$)
- Δd^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 critrion**
- If $\chi^2(\mathbf{p})$ **is not quadratic in p**, but more complex, $\mathcal{M}$ is non-constant with variations of **p**: **Variable Metric Method**
- One does a kind of Newton-Raphson $\mathbf{p}_{i+1} = \mathbf{p}_i - \mathcal{M}_i^{-1} \mathbf{g}_i$ where g_i is the gradient vector evaluated at $\mathbf{p}_i$ and $\mathcal{M}_{i+1}^{-1}$ is usualy 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'

- **Gamow-Teller Resonance** using RPA based on the Woods-Saxon potential have been studied and the **Landau-Migdal parameters estimated by comparing experiment** with theoretical calculations in Refs. [T. Wakasa, M. Ichimura, and H. Sakai, Phys. Rev. C **72**, 067303 (2005) and T. Suzuki and H. Sakai, Phys. Lett. B **455**, 25 (1999)].
- 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**: $\int [R_{GT^-}(E) - R_{GT^+}(E)] dE = 3(N - Z)$
- 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 Δ−h excitations** ⇒ it may **contribute to the GTR**.
- The **experimental analysis of ^{90}Zr** ⇒ **quenching** (2/3) has to be **mainly attributed to 2p-2h** coupling and not to Δ−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 Δ−h states are hundreds of MeV above the GT ⇒ **hard to excite the Δ** in the nuclear medium.