

A hand is pointing at a colorful periodic table of elements. The table is divided into blocks of different colors: yellow, red, blue, and green. The text is overlaid on the image.

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

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- ▶ Some general comments on EDFs
- ▶ Motivation and present situation: example GTR
- ▶ Propose a new fitting protocol: Example with a Skyrme interaction

## Spin and Isospin excitations in Nuclei

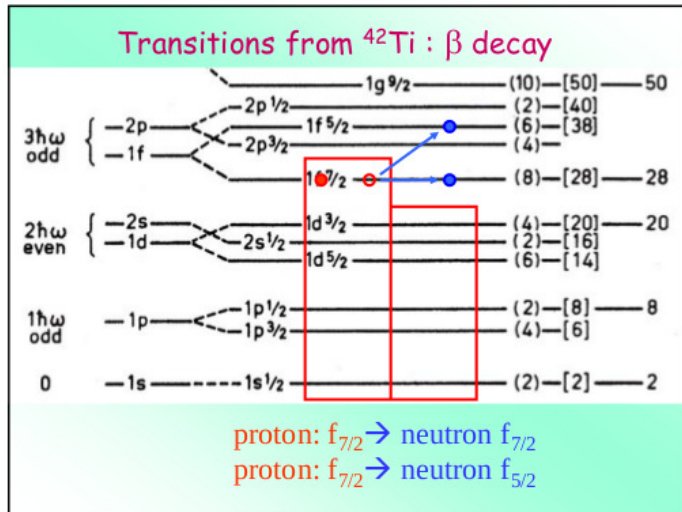
- ▶ **Nucleons** are fermions charac. by their spin and isospin
- ▶ **Nucleons** with spin (isospin) may **change their state** in **phase**: spin-scalar  $S=0$  modes (isospin-scalar  $T=0$  modes); or **out of phase**: spin-vector  $S=1$  modes (isospin-vector  $T=1$  modes)
- ▶ They can be **excited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

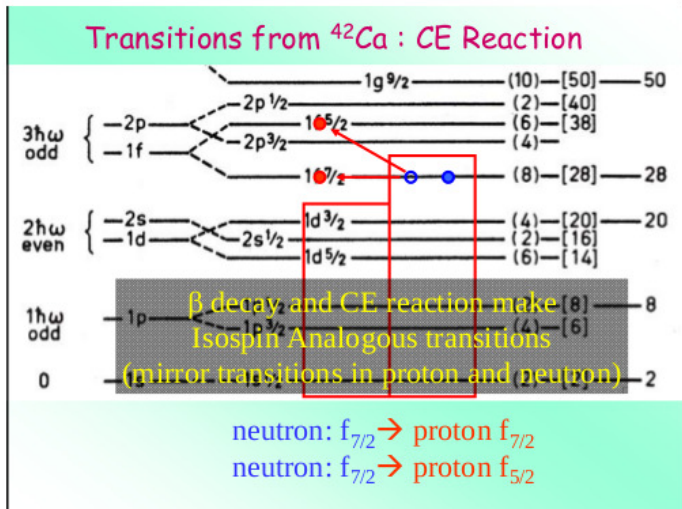
**Spin-isospin modes** of excitation (such as the **GTR**) give **direct information** on the spin-isospin channel of the **effective interaction** (or generator of our EDF)

## Example: $\beta$ -decay transition



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  $\beta$ -decay transitions give the same/similar information

## Therefore, (as we already know ... )

- ▶ allowed **GT** transitions mainly determine  **$\beta$ -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- $\beta$ -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 nuclear interactions in the medium** 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:

(remember 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.

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

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

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

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

# 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,

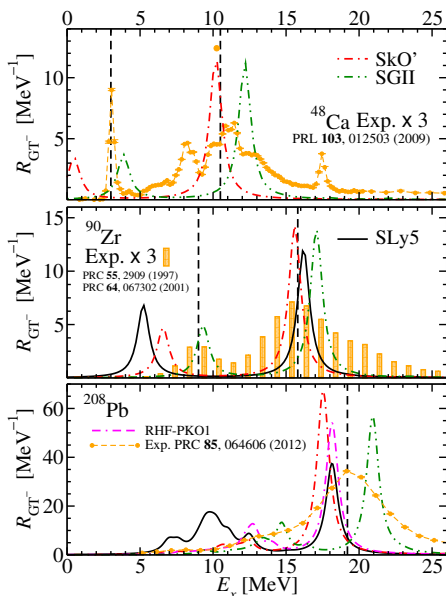
- ▶ there are still some **open problems** ... but we will concentrate here on how to

**improve the spin-isospin properties of our EDF**

# Motivation: Gamow Teller Resonance

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

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

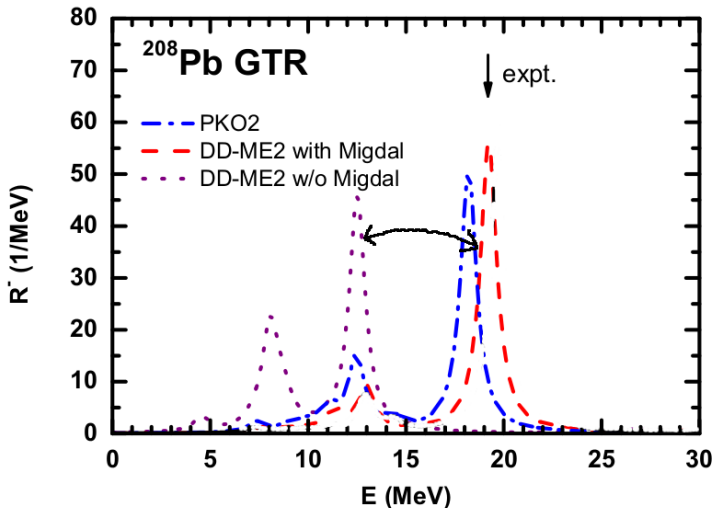


<sup>a</sup>PLB 106, 379 (1981), <sup>b</sup>PRC 60, 014316 (1999), <sup>c</sup>PRL 101, 122502 (2008), <sup>d</sup>PRC 69, 054303

# Motivation: Gamow Teller Resonance

Exchange (Fock) effects on GTR in relativistic models

Effect of Migdal term  $\rightarrow$  fitted to  $^{208}\text{Pb}$  in RH

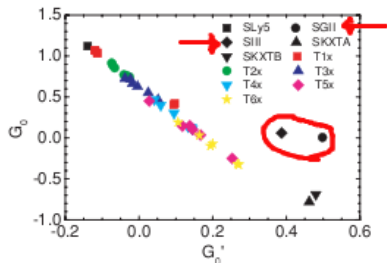


# Motivation: which gs properties are important for describing the $E_x^{GTR}$ ?

The study<sup>a</sup> 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

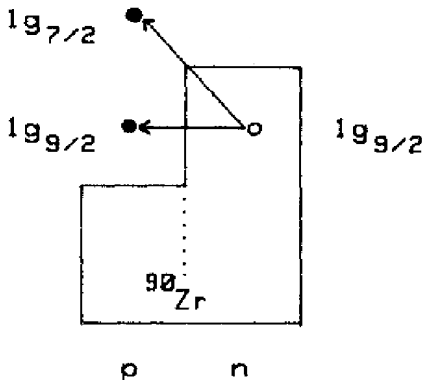
- ▶ Empirical indications<sup>b</sup> suggest that  $G'_0 > G_0 > 0$
- ▶ Not a very common feature within available Skyrme forces<sup>c</sup>



<sup>a</sup>M. Bender, J. Dobaczewski, J. Engel, and W. Nazarewicz, Phys. Rev. C **65**, 054322 (2002); <sup>b</sup>T. Wakasa, M. Ichimura, and H. Sakai, Phys. Rev. C **72**, 067303 (2005); T. Suzuki and H. Sakai, Phys. Lett. B **455**, 25 (1999), <sup>c</sup>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  $^{90}\text{Zr}$ .  
Transitions excited by  $\sigma\tau_-$  operator.



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

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

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)

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

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

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

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

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

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

$$H_{\text{SO}} = (1/2)W_0\mathbf{J} \cdot \nabla\rho + (1/2)W'_0(\mathbf{J} \cdot \mathbf{n} \nabla\rho_n + \mathbf{J}_p \cdot \nabla\rho_p)$$

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



# Fitting Protocol: Inspired on SLy5

$\chi^2$  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.

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

# Skyrme Aizu Milano interaction: SAMi

## Parameter set:

	value( $\sigma$ )	
$t_0$	-1877.75(75)	MeV fm <sup>3</sup>
$t_1$	475.6(1.4)	MeV fm <sup>5</sup>
$t_2$	-85.2(1.0)	MeV fm <sup>5</sup>
$t_3$	10219.6(7.6)	MeV fm <sup>3+3<math>\alpha</math></sup>
$x_0$	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)	
$\alpha$	0.25614(37)	

$\sigma$  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)

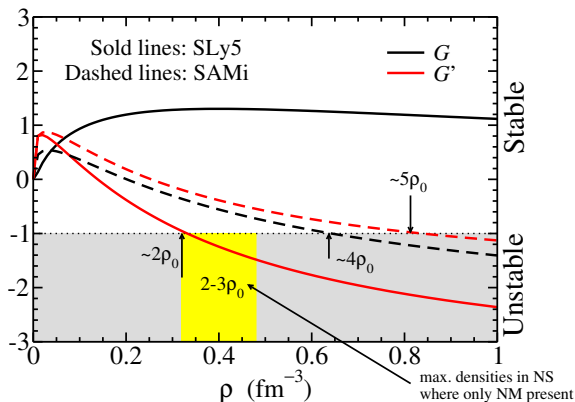
Prop.	value( $\sigma$ )	
$\rho_\infty$	0.159(1)	$\text{fm}^{-3}$
$e_\infty$	-15.93(9)	MeV
$m_{\text{IS}}^*$	0.6752(3)	
$m_{\text{IV}}^*$	0.664(13)	
J	28(1)	MeV
L	44(7)	MeV
$K_\infty$	245(1)	MeV
$G_0$	0.15	(fixed)
$G'_0$	0.35	(fixed)

# 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)]

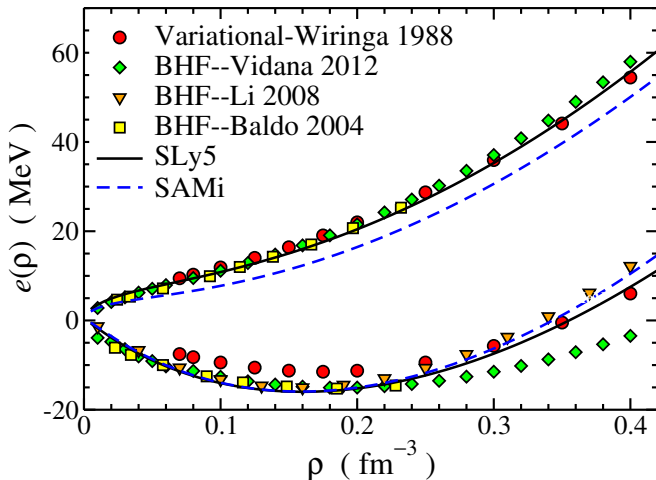
$$1 + G_0 > 0$$

$$1 + G'_0 > 0$$



# Results

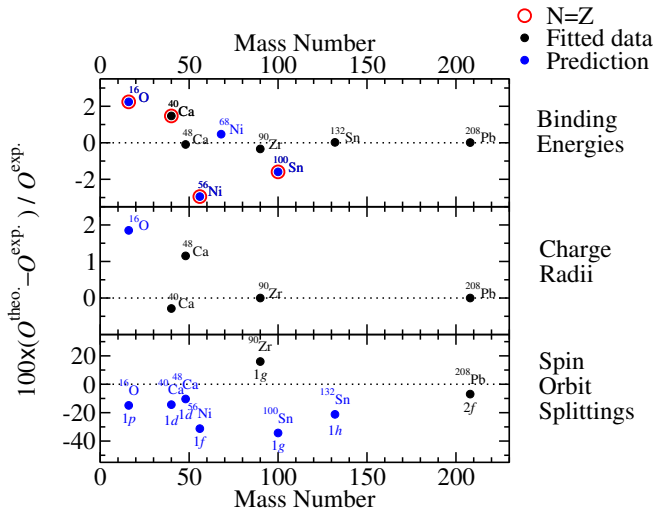
## Equation of State: SAMi vs *ab-initio* calculations



**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

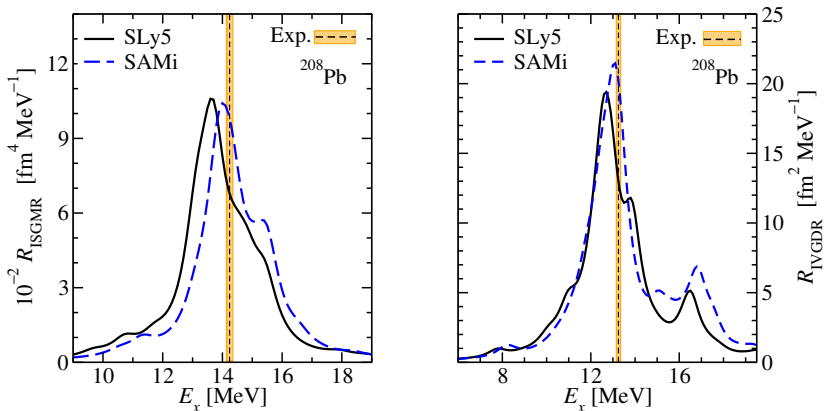
## Finite Nuclei: spherical double-magic nuclei



**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:  $E_c (\text{GMR}) = 14.24 \pm 0.11 \text{ MeV}$  [D. H. Youngblood, et al., Phys. Rev. Lett. **82**, 691 (1999)] and  $E_c (\text{GDR}) = 13.25 \pm 0.10 \text{ MeV}$  [N. Ryezayeva et al., Phys. Rev. Lett. **89**, 272502 (2002)].

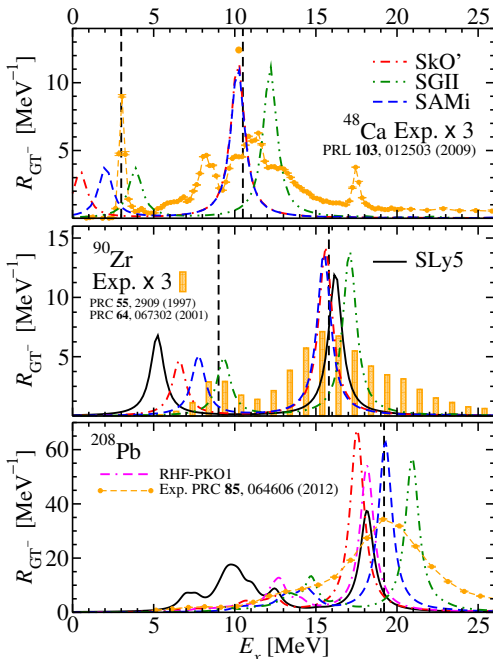
# Results

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

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

**Figure:** Gamow Teller strength

distributions in  $^{48}\text{Ca}$  (upper panel),  $^{90}\text{Zr}$  (middle panel) and  $^{208}\text{Pb}$  (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

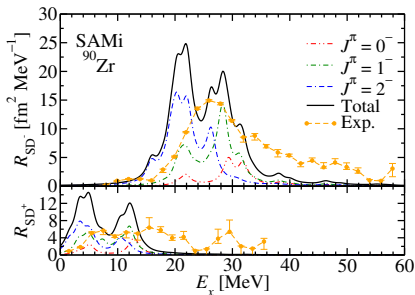
## Spin Dipole Resonances in $^{90}\text{Zr}$ and $^{208}\text{Pb}$

Operator:

$$\sum_{i=1}^A \sum_M \tau_{\pm}(i) r_i^L [Y_L(\hat{r}_i) \otimes \sigma(i)]_M$$

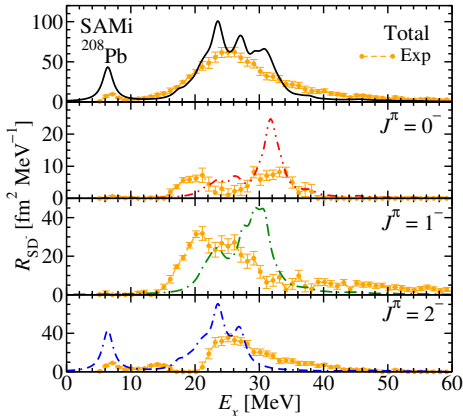
Sum Rule:

$$\int [R_{SD-}(E) - R_{SD+}(E)] dE = \frac{9}{4\pi} (N \langle r_N^2 \rangle - Z \langle r_P^2 \rangle)$$



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 **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)

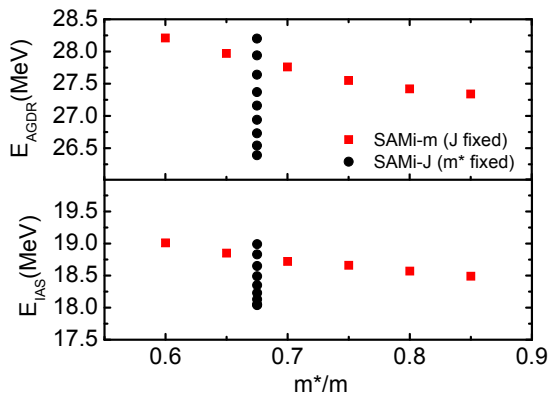
- ▶ In analogy with **differential geommetry** it is **convenient** to consider the **properties of a function** ( $\chi^2(\mathbf{p})$ ) as being **properties of the space** in the variables  $\mathbf{p}$ .
- ▶ The fundamental **invariant** in **non-Euclidean** space is  $\Delta s^2 = \Delta \mathbf{p}^T \mathbf{A} \Delta \mathbf{p}$  ( $\mathbf{A}$  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
- ▶  $\Delta s^2$ : square of the generalized distance produced by  $\Delta \mathbf{p}$
- ▶  $\Delta s$ : the number of standard deviations  $\Delta \mathbf{p}$  away from  $\mathbf{p}_0$  (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,  $\Delta d^2 = \mathbf{g}^T \mathcal{M}^{-1} \mathbf{g}$ )
- ▶  $\Delta d^2$ : 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  $\mathbf{p}_{i+1} = \mathbf{p}_i - \mathcal{M}_i^{-1} \mathbf{g}_i$  where  $\mathbf{g}_i$  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 $G'_0$

- ▶ **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  $\Delta$ -h excitations**  $\Rightarrow$  it may **contribute to the GTR**.
- ▶ The **experimental analysis of  $^{90}\text{Zr}$**   $\Rightarrow$  **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  $\Rightarrow$  **hard to excite the  $\Delta$**  in the nuclear medium.