Nuclear Energy Density Functionals

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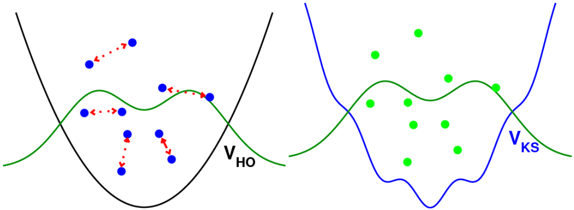
Density Functional Theory: Kohn-Sham realization

For **any interacting system**, there **exists** a **local single-particle potential** $V_{KS}(r) = V_{ext} + V_H + V_{xc}$, such that the **exact ground-state density** of the **interacting** system **equals** the ground-state density of the auxiliary **non-interacting** system.



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- **Kohn-Sham scheme depends entirely on whether accurate approximations for V_{xc} can be found.**
- Due to V_{xc}, the KS goes **beyond a simple HF** ($V_{HF} = V_H + V_F$) and it has the **advantage of being local**.

Nuclear Energy Density Functionals:

Main types of successful EDFs derived from the Hartree-Fock (mean-field) approximation

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

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

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

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

- 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,

- **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**) ⇒ have been shown to be **accurate in the description of binding energies, charge radii and the excitation energies of different Giant resonances**

On the other side,

- there are still some **open problems**.

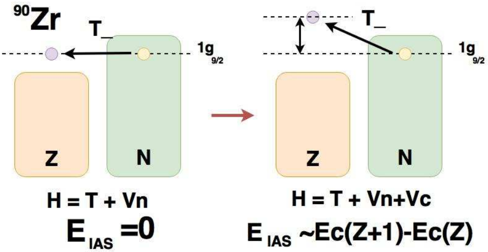
> **We briefly overview here recent improvements on the Skyrme functional in the spin and isospin channels**

Spin and Isospin excitations in Nuclei

We aim at improving the current description of the...

- **Isobaric Analog state**: **isospin mode** conected with **isospin symmetry breaking** in nuclei and with the **neutron skin** thickness of heavy nuclei ⇒ **properties of the nuclear EoS**.
- **Gamow Teller Resonance**: **spin-isospin mode**. **Analogous transitions to $\beta-$decay**. Sensitive to the **isospin channel of the functional** and on the **spin-orbit splittings**
- **Spin Dipole Giant Resonance**: **spin-dipole mode** connected with the isospin properties of the **EoS** and sensitive to the **tensor interaciton**.

The isobaric analog state energy: E_{IAS}



- **Analog state** can be defined: $|A\rangle = \frac{T_-|0\rangle}{\langle 0|T_+T_-|0\rangle}$
- **Displacement energy or** E_{IAS}

$$E_{IAS} = E_A - E_0 = \langle A|\mathcal{H}|A\rangle - \langle 0|\mathcal{H}|0\rangle = \frac{\langle 0|T_+[\mathcal{H},T_-]|0\rangle}{\langle 0|T_+T_-|0\rangle}$$

$E_{IAS} \neq 0$ **only due to Isospin Symmtry Breaking terms** $\mathcal{H}$

E_{IAS}^{exp} **usually accuratelly measured !**

Coulomb direct contribution: very simple model

- Assuming indepentent particle model and good isospin for $|0\rangle$ ($\langle 0|T_+T_-|0\rangle = 2T_0 = N - Z$)

$$E_{IAS} \approx E_{IAS}^{C,\mathrm{direct}} = \frac{1}{N-Z}\int [\rho_n(\vec{r}) - \rho_p(\vec{r})]\, U_C^{\mathrm{direct}}(\vec{r})d\vec{r}$$

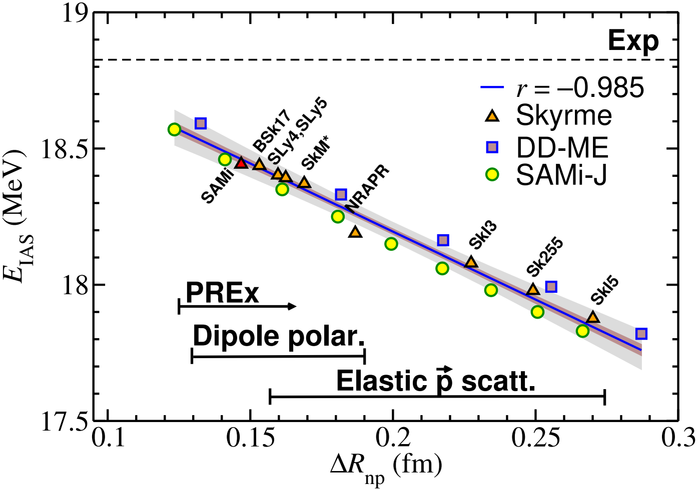
where $U_C^{\mathrm{direct}}(\vec{r}) = \int \frac{e^2}{|\vec{r}_1 - \vec{r}|}\rho_{ch}(\vec{r}_1)d\vec{r}_1$

- Assuming also a uniform neutron and proton distributions of radius R_n and R_p respectively, and $\rho_{ch} \approx \rho_p$ one can find

$$E_{IAS} \approx E_{IAS}^{C,\mathrm{direct}} \approx \frac{6}{5}\frac{Ze^2}{R_p}\left(1 - \sqrt{\frac{5}{12}}\frac{N}{N-Z}\frac{\Delta r_{np}}{R_p}\right)$$

One may expect: **the larger the Δr_{np} (stiff EoS around saturation) the smallest E_{IAS}**

E_{IAS} in Energy Density Functionals (No Corr.)



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Nuclear models (EDFs) where the nuclear part is isospin symmetric and U_{ch} is calculated from the ρ_p

Corrections: within self-consistent HF+RPA

Within the **HF+RPA** one can **estimate** the E_{IAS} accounting (in an effective way) for **short-range correlations and effects of the continuum** (if a large sp base is adopted).

• **Coulomb exchange** exact (usually Slater approx.):

$$U_C^{x,\text{exact}} \varphi_i(\vec{r}) = -\frac{e^2}{2} \int d^3 r' \, \frac{\varphi_j^*(\vec{r}\,')\varphi_j(\vec{r})}{|\vec{r} - \vec{r}\,'|} \varphi_i(\vec{r}\,')$$

• The **electromagnetic spin-orbit** correction to the nucleon single-particle energy (non-relativistic),

$$\varepsilon_i^{\text{emso}} = \frac{\hbar^2 c^2}{2 m_i^2 c^4} \langle \vec{l}_i \cdot \vec{s}_i \rangle x_i \int \frac{1}{r} \frac{dU_C}{dr} |R_i(r)|^2$$

where x_i: $g_p - 1$ for Z and g_n for N; $g_n = -3.82608545(90)$ and $g_p = 5.585694702(17)$, $R_i \to R_{nl}$ radial wf.

Corrections:

- **Finite size** effects (assuming spherical symmetry):

$$\rho_{ch}(q) = \left(1 - \frac{q^2}{8m^2}\right)\left[G_{E,p}(q^2)\rho_p(q) + G_{E,n}(q^2)\rho_n(q)\right]$$
$$- \frac{\pi q^2}{2m^2}\sum_{l,t}\left[2G_{M,t}(q^2) - G_{E,t}(q^2)\right]\langle\vec{l}\cdot\vec{s}\rangle\int_0^\infty dx\frac{j_1(qx)}{qx}|R_{nl}(x)x^2|^2$$

- **Vacuum polarization:** lowest order correction in the fine-structure constant to the Coulomb potential $\frac{eZ}{r}$:

$$V_{vp}(\vec{r}) = -\frac{2}{3}\frac{\alpha e^2}{\pi}\int d\vec{r}'\frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}\mathcal{K}_1\left(\frac{2}{\lambdabar_e}|\vec{r}-\vec{r}'|\right)$$

where e is the fundamental electric charge, α the fine-structure constrant, $\lambdabar_e$ the reduced Compton electron wavelength and

$$\mathcal{K}_1(x) \equiv \int_1^\infty dt e^{-xt}\left(\frac{1}{t^2} + \frac{1}{2t^4}\right)\sqrt{t^2-1}$$

Corrections:

- **Isospin symmetry breaking** (Skyrme-like): **two parts**
  (contact interaction)

charge symmetry breaking $+$

$V_{\rm CSB} = V_{nn} - V_{pp}$

$V_{\rm CSB}(\vec{r}_1, \vec{r}_2) \equiv \frac{1}{4}\,[\tau_z(1) + \tau_z(2)]\, s_0 (1 + y_0 P_\sigma)$

τ_z Pauli in isospin space; P_σ are the usual projector operators in spin space.

charge independence breaking*

$V_{\rm CIB} = \frac{1}{2}\left(V_{nn} + V_{pp}\right) - V_{pn}$

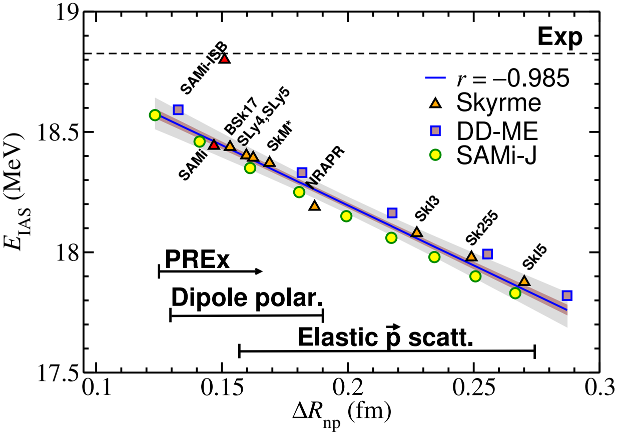
$V_{\rm CIB}(\vec{r}_1, \vec{r}_2) \equiv \frac{1}{2}\tau_z(1)\tau_z(2) u_0 (1 + z_0 P_\sigma)$

* general operator form $\tau_z(1)\tau_z(2) - \frac{1}{3}\vec{\tau}(1)\cdot\vec{\tau}(2)$.

Our prescription $\tau_z(1)\tau_z(2)$ not change structure of HF+RPA.

- Opposite to the other corrections, **ISB contributions depends on new parameters that need to be determined!**

SAMi-ISB: E_{IAS}



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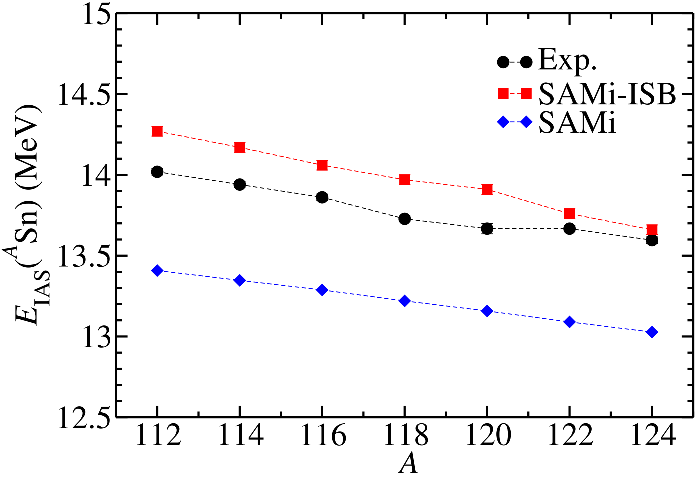
Measurement of Δr_{np} → determine ISB in the nuclear medium (or the other way around).

SAMi-ISB: E_{IAS} in the Sn isotopic chain



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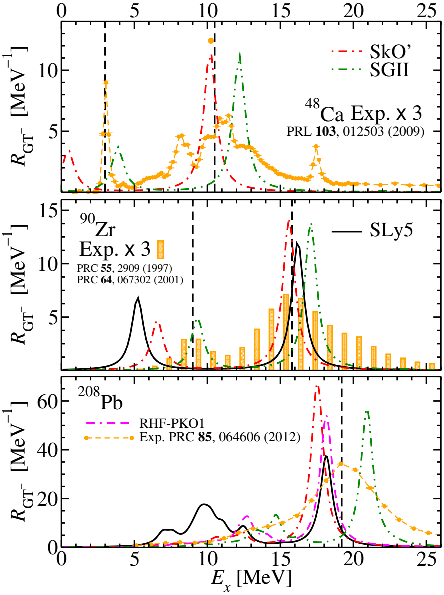
These corrections have been implemented on top of a Skyrme functional: SAMi. Let us discuss about SAMi in some detail.

Motivation for SAMi: 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*



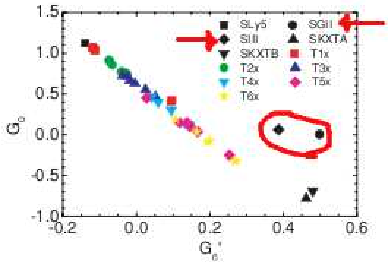
[a] PLB **106**, 379 (1981), [b] PRC **60**, 014316 (1999), [c] PRL **101**, 122502 (2008), [d] PRC 69, 054303

Motivation SAMi: 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)

Skyrme Aizu Milano interaction: SAMi

Parameter set and nuclear matter properties:

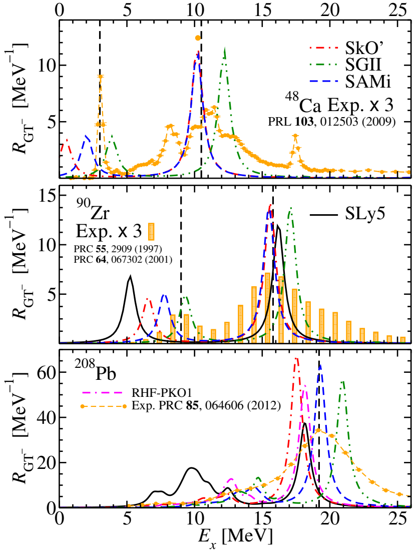
Table: SAMi parameter set and saturation properties with the estimated standard deviations inside parenthesis

	value(σ)			value(σ)	
t_0	$-1877.75(75)$	MeV fm^3	ρ_∞	0.159(1)	fm^{-3}
t_1	475.6(1.4)	MeV fm^5	e_∞	$-15.93(9)$	MeV
t_2	$-85.2(1.0)$	MeV fm^5	m^*_{IS}	0.6752(3)	
t_3	10219.6(7.6)	MeV $fm^{3+3\alpha}$	m^*_{IV}	0.664(13)	
x_0	0.320(16)		J	28(1)	MeV
x_1	$-0.532(70)$		L	44(7)	MeV
x_2	$-0.014(15)$		K_∞	245(1)	MeV
x_3	0.688(30)		G_0	0.15	(fixed)
W_0	137(11)		G'_0	0.35	(fixed)
W'_0	42(22)				
α	0.25614(37)				

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

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

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.



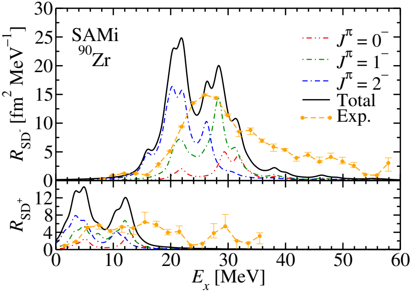
SAMi: Spin Dipole Resonances in ^{90}Zr and ^{208}Pb

Operator:

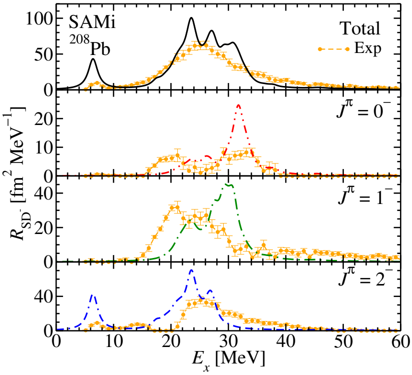
$\sum_{i=1}^{A} \sum_{M} \tau_{\pm}(i) r_i^L \left[Y_L(\hat{r}_i) \otimes \boldsymbol{\sigma}(i)\right]_{JM}$

Sum Rule:

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



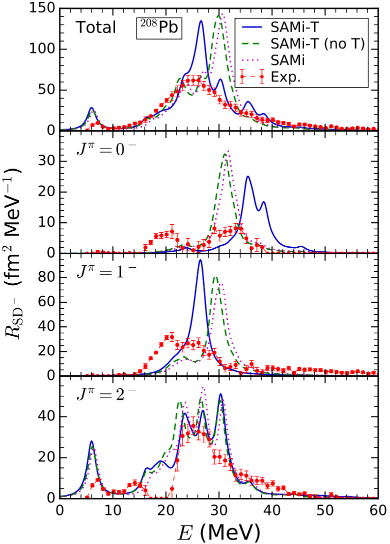
K. Yako *et al.*, Phys. Rev. C **74**, 051303(R) (2006)

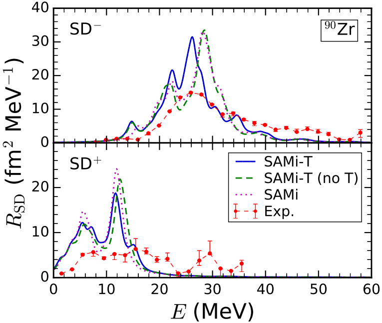


T. Wakasa *et al.*, Phys. Rev. C **85**, 064606 (2012)

Tensor is missing: different channels not well described

SAMi-T: Spin Dipole Resonances in ^{90}Zr and ^{208}Pb with tensor force Shihang Shen et al., work in progress

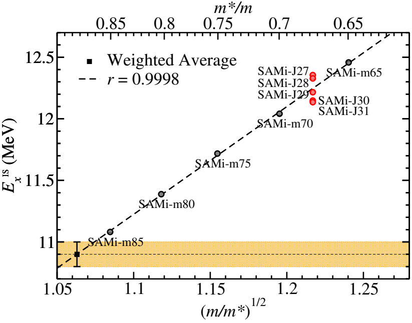


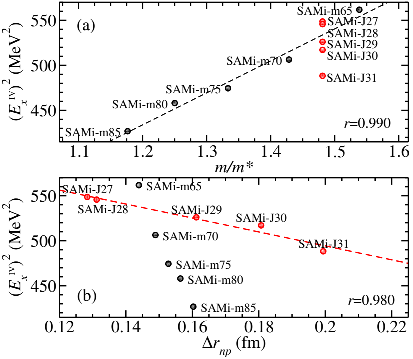


- Tensor force included and guided by ab initio calculations on neutron and neutro-proton drops.
- 1^- is the channel clearly improved by including the tensor force

SAMi families: insights on correlations

- **Isoscalar and isovector Giant Quadrupole resonances**





Phys. Rev. C 87, 034301 (2013)

- See also studies on the isovector Giant Dipole Resonance (Phys.Rev. C85 (2012) 041302, Phys. Rev. C 88, 024316 (2013), Phys. Rev. C 92, 064304 (2015)), the Antianalog Giant Dipole resonance (Phys. Rev. C 92, 034308 (2015), Phys. Rev. C 94, 044313 (2016)) or the Pygmy Dipole (arXiv:1807.10118).

Conclusions:

- **SAMi functionals account** for the most relevant quantities in order to improve the description of **charge-exchange nuclear resonances**
- **SAMi** and **SAMi-T**: **GTR** in ^{48}Ca and the **GTR**, and **SDR** in ^{90}**Zr** and ^{208}**Pb** are predicted with **good accuracy** by **SAMi** and **further improved** by **SAMi-T**
- **SAMi-ISB** functional reproduces the **experimental IAS** excitation energy in ^{208}**Pb** (and Sn isotopes) as well as a **neutron skin** in agreement with other experiments.
- **SAMi-J and SAMi-m** systematically varied interactions are useful in **studying correlations**.
- **SAMi based functionals** do **not deteriorate** the description of other **nuclear observables**
- **applicability in nuclear physics and astrophysics**

Thank you for your attention!