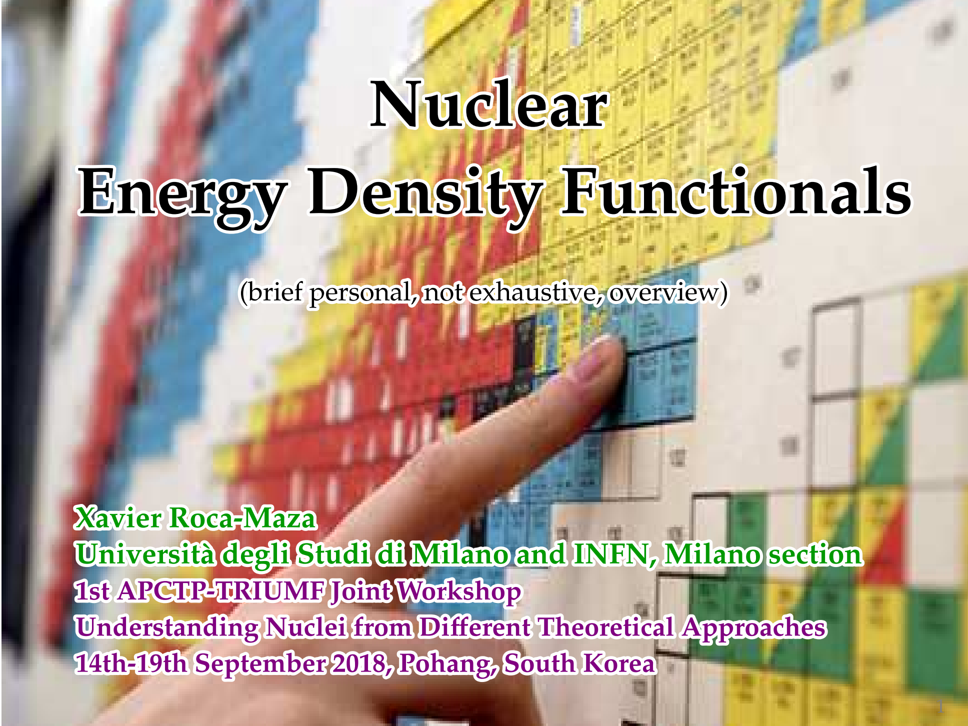

Nuclear Energy Density Functionals

(brief personal, not exhaustive, overview)

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1st APCTP-TRIUMF Joint Workshop
Understanding Nuclei from Different Theoretical Approaches
14th-19th September 2018, Pohang, South Korea

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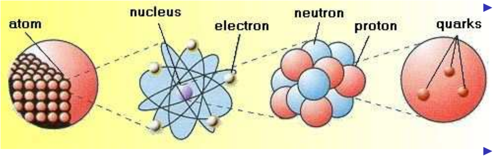
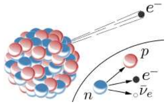
The Nuclear Many-Body Problem

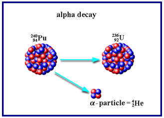
- **Nucleus:** from few to more than 200 strongly interacting and **self-bound fermions** (**neutrons and protons**).
- **Complex systems**: **spin, isospin, pairing, deformation,** ...
- **3 of the 4 fundamental forces in nature** are contributing to the nuclear phenomena (**as a whole driven by the strong interaction**).



- Nuclei: self-bound system by the strong interaction [In the binding energy $B_{coul} \sim -B_{strong}/(3 \text{ to } 10)$]
- β−decay: weak process

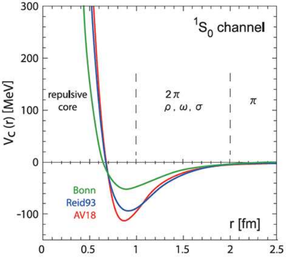


- α−decay: interplay between the strong and electromagnetic interaction



The Nuclear Many-Body Problem

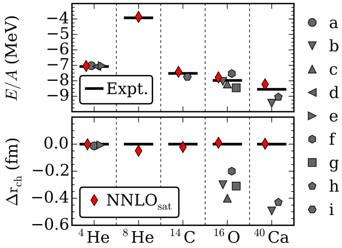
- **Underlying interaction:** the “so called” **residual strong interaction = nuclear force**, **the one acting effectively between nucleons**, has **not been derived yet** from first principles as **QCD is non-perturbative** at the low-energies relevant for the description of nuclei.

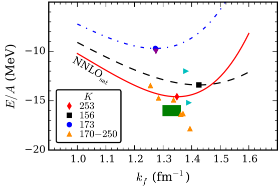


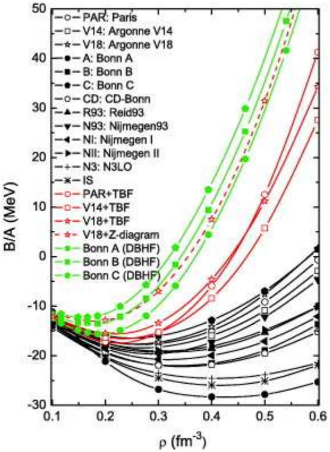
The nuclear force in practice: effective potential fitted to **few-body physics**. **3 Body force are needed.** **4 Body?**

Motivation: The Nuclear Many-Body Problem

- **State-of-the-art many-body** calc. based on **these type of potentials** are **not conclusive** yet although **great advances have been achieved**:





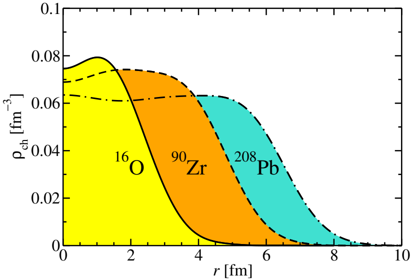


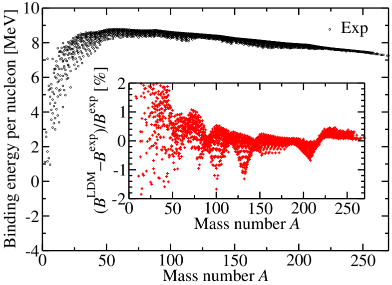
[A. Ekström, *et al.* PRC 91, 051301(R)]

[Z.H. Li, *et al.*, PRC 74 (2006) 047304]

- **Which param. of the residual strong interaction should we use?**
- **Which many-body technique is the most suitable?**

Motivation: The Nuclear Many-Body Problem





[X. Roca-Maza and N.Paar, PPNP 101 (2018) 96-176]

- **Saturation originates from the short-range** $\Rightarrow R \approx A^{1/3}$. A simple fit: $\langle r^2_{ch}\rangle^{1/2} = \sqrt{\frac{3}{5}}1.21(1)A^{-1/3}$ with a **r.m.s.** $\approx$ 0.07 **fm**
- Uniform sphere with average nucleon interdistance of $2 \times r_0 = 2 \times 1.21$ fm and density $\rho_0 \approx 0.14(2)$ fm^{-3}

- $B(A,Z) = (a_V - a_S A^{-1/3})A - a_C \frac{Z(Z-1)}{A^{1/3}} - (a_A - a_{AS} A^{-1/3})\frac{(A-2Z)^2}{A} + \ldots$

A simple fit: $a_V = 15.6(4)$ MeV, $a_S = 18(1)$ MeV, $a_C = 0.70(2)$ MeV $a_A = 28(3)$ MeV and $a_{AS} = 26(12)$ MeV with a **r.m.s. < 3 MeV**

Very simple model gets the right saturation point

Hohenberg-Kohn theorem

The original theorem and its proof can be found in **P. Hohenberg, W. Kohn, Phys. Rev. 136, B864 (1964)**.

• Assuming a **system of interacting fermions** in some external potential, there exist a **universal functional** $F[\rho]$ of the fermion density ρ:

$$E[\rho] = \langle\Psi|T + V + V_{ext}|\Psi\rangle = F[\rho] + \int V_{ext}(r)\rho(r)d\vec{r}$$

• and it can be shown that:

$$\min_{\Psi}\langle\Psi|T + V + V_{ext}|\Psi\rangle = \min_{\rho} E[\rho]$$

so $E[\rho]$ has a minimum at the exact ground-state density where it assumes the exact energy as a value.

Kohn-Sham realization ($F[\rho] \to T[\rho]$)

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

$$\rho_{exact}(\vec{r}) = \rho_{KS}(\vec{r}) = \sum_{i}^{occ} |\phi_i(\vec{r})|^2$$

where ϕ are single-particle orbitals and the total wave-function correspond to a Slater determinant. The $E[\rho]$ **is unique**

$$E_{KS}[\rho] = T[\rho] + \int V_{KS}(r)\rho(r)d\vec{r}$$

where $T[\rho]$ **is the kinetic energy of the non-interacting system** and for which the variational equation

$$\frac{\delta E[\rho]}{\delta \rho} = 0 = \frac{\delta T[\rho]}{\delta \rho} + V_{KS}$$

yields to the **exact ground state density and energy**

Kohn-Sham realization

- The Kohn-Sham potential V_{KS} is customary splitted in the literature in three pieces:

$$V_{KS} = V_{ext} + V_{Hartree} + V_{xc}$$

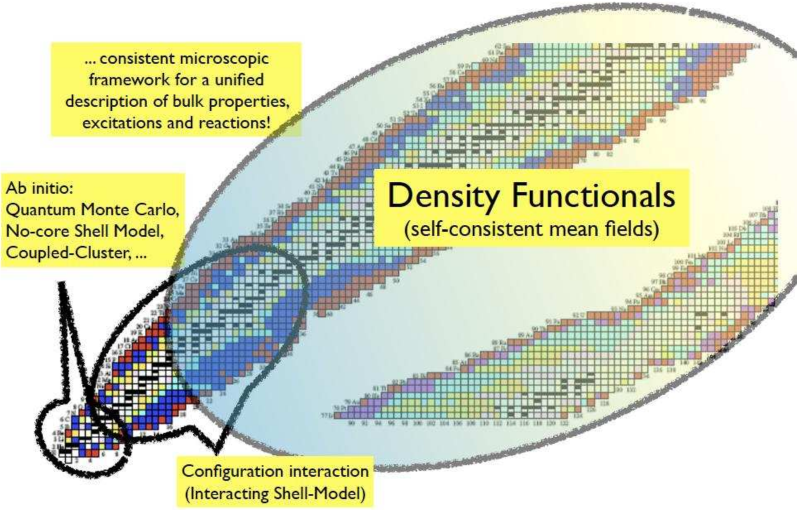
in **nuclei** $V_{ext} = 0$, the **Hartree** contribution to $E[\rho]$ is **easy** to calculate once an interaction $v(r)$ has been asumed

$$E_{Hartree} = \frac{1}{2}\int d\vec{r}\int d\vec{r}'\rho(r)v(r-r')\rho(r')$$

and the **exchage-correlation** is the less known.

- **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 EDFs neglect explicit correlation effects** $V_{cx} = V_F$. **Included implicitely in the fitting parameters of the model.**

Applicability of nuclear E[ρ] as compared to other methods



Advantadges and disadvantages of DFT

- exact theory that can be applied to the whole nuclear chart
- many-body problem mapped onto a one body problem without explicitly involving inter-nucleon interactions!!! (computational cost and interpretation of observbles in terms of single-particle properties)
- HK generalised in (almost all) possible ways: time dependence, degenerate ground-state, magnetic systems, finite T, relativistic case ...
- any one body observable is within the DFT framework (this includes also some sum rules related to nuclear excitations)

- various proofs of HK theorems do not give any clue on how to build the functional.
- no direct connection with realistic NN or NNN interaction if current approaches to EDF are not improved (some atempts already exist)
- no systematic way of improvement (evaluate syst. errors).

(traditional) Nuclear Energy Density Functionals

- Traditional realization of a NEDF: **Effective interactions** solved at the **Hartree-Fock or Mean-Field fitted to experimental data in many-body system** ⇒ **successful** in the description of properties such as **masses, nuclear radii, deformations,** E_x **/ sum rules in Giant Resonances ...**

$$\min_\rho E[\rho] = \min_\Psi \langle \Psi | \mathcal{H} | \Psi \rangle \approx \min_\Phi \langle \Phi | \mathcal{H}_{HF} | \Phi \rangle = \min_\rho E_{HF}[\rho]$$

- **Connection with KS is via** $V_{KS} \equiv V_H + V_F$
- remember: Ψ exact wave-function; Φ Slater determinant; ρ one-body density matrix ↔ one-body observables

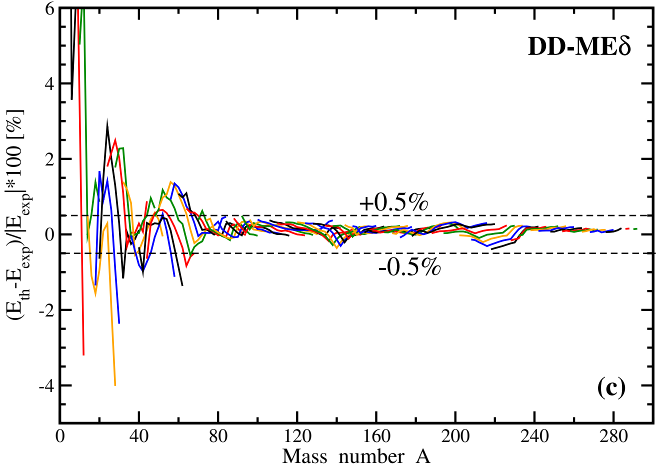
Main types of models:

- **Relativistic** based on Lagrangians where effective mesons carry the interaction (π, σ, ω...).
- **Non-relativistic** based on effective Hamiltonians (Yukawa, Gaussian or zero-range forces)

⇒ **Both give similar results and in both cases density dependence of the interaction (=3N, 4N, ...) improves results**

Examples: Binding energies

Relativistic model by Milano and Barcelona groups

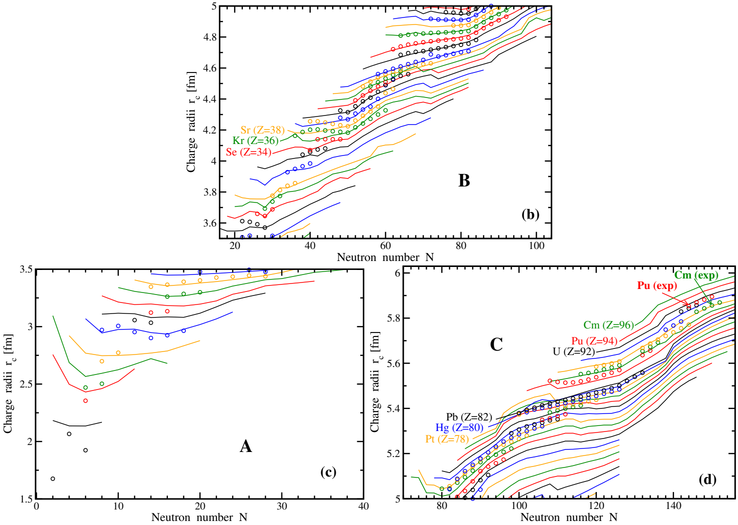


[PHYSICAL REVIEW C 89, 054320 (2014)]

Remarkable accuracy on thousands of measured binding energies

Examples: Charge radii

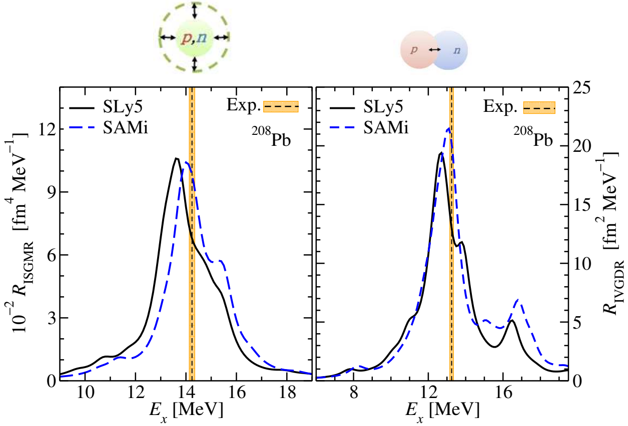
Theory-lines / Experiment - circles



[PHYSICAL REVIEW C 89, 054320 (2014)]

Examples: Giant Monopole and Dipole Resonances

Non-relativistic model by Milano and Aizu (Japan) groups

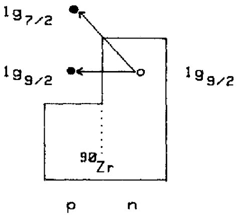


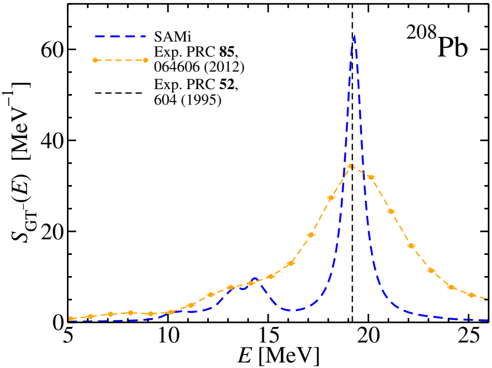
R = nuclear response function (in dipole resonance is related with the probability of a photon absorption by the nucleus or σ_γ)

Good description excitation energy and integrated R but not the width of the resonance.

Examples: Gamow Teller Resonance

Gamow-Teller Resonance driven by nuclear force (**analogous transitions to β−decay**).





[Phys.Rev. C86 (2012) 031306]

Summary: [X. Roca-Maza and N.Paar, PPNP 101 (2018) 96-176]

Model	Type	N^o par.	ρ_0 [fm^{-3}]	e_0 [MeV]	K_0 [MeV]	J [MeV]	L [MeV]	σ_M [MeV]
FRDM12	Mac-Mic	38 [a]	–	−16.195	240	32.5(5)	53(15)	0.559 [b]
WS4 [c]	Mac-Mic	18	–	−15.58(1)	235(11)	29.7(3)	59(10)	0.298 [d]
HFB24	EDF	30 [e]	0.1578	−16.048	245.5	30.0	46.4	0.549 [f]
UNEDF1	EDF	12	0.1587(4)	−15.800	220.0	29.0(6)	40(13)	1.88 [g]
DD-PC1	EDF	9	0.154	−16.12	238	35.6	113	2.01 [h]
Rel. var.			3%	4%	9%	20%	80%	

[a] 21 fixed from other considerations than fit to masses;
[b] With respect to AME2003;
[c] Estimated properties;
[d] With respect to AME2012;
[e] Some of them fixed *a propri*;
[f] Only even-even nuclei with $N, Z > 8$ have been considered and compared with AME2003;
[g] Only even-even nuclei with $N, Z > 8$ have been considered;
[h] Only even-even nuclei with $Z \leqslant 104$ have been considered and compared to AME2012.

- **Mac-Mic** models: most accurate models in masses
- Traditional **EDFs**: ~10 parameters and based on HF
- **HFB24** is based on a traditional EDF strategy plus several phenomenological parameters, some fixed before the fit to some *intelligent guess*

Summary: [X. Roca-Maza and N.Paar, PPNP 101 (2018) 96-176]

EoS par.	Observable	Range	Comments
ρ_0	$\langle r_{ch}^2\rangle^{1/2}$	0.154-0.159	Most accurate EDFs on $M(N,Z)$ and $\langle r_{ch}^2\rangle^{1/2}$
e_0	$M(N,Z)$	-16.2 - -15.6	Most accurate EDFs on $M(N,Z)$ and $\langle r_{ch}^2\rangle^{1/2}$
K_0	$M(N,Z)$	220-245	Most accurate EDFs on $M(N,Z)$ and $\langle r_{ch}^2\rangle^{1/2}$
	ISGMR	220-260	From EDFs in closed shell nuclei (Colò)
	ISGMR	250-315	Blaizot's formula (Stone)
	ISGMR	~ 200	EDF describing also open shell nuclei (Avogadro)
J	$M(N,Z)$	29-35.6	Most accurate EDFs on $M(N,Z)$ and $\langle r_{ch}^2\rangle^{1/2}$
	IVGDR	$\sim 24.1(8) + L/8$	From EDF analysis [$S(\rho = 0.1\ \mathrm{fm}^{-3})$ = 24.1(8) MeV] (Trippa)
	PDS	30.2-33.8	From EDF analysis (Klimkiewicz)
	PDS	31.0-33.6	From EDF analysis (Carbone)
	α_D	$24.5(8) + 0.168(7)L$	From EDF analysis ^{208}Pb
	α_D	30-35	From EDF analysis
	IAS and Δr_{np}	30.2-33.7	From EDF analysis (Danielewicz)
	AGDR	31.2-35.4	From EDF analysis
	PDS, α_D, IVGQR, AGDR	32-33	From EDF analysis (Paar)
	compilation	29.0-32.7	Astrophys. J. 771 (1) (2013) 51
	compilation	30.7-32.5	PLB 727 (1) (2013) 276âĂŞ281
	compilation	28.5-34.9	RMP 89 (2017) 015007

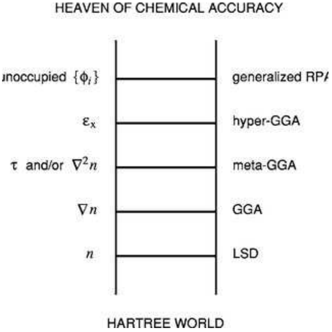
Summary: [X. Roca-Maza and N.Paar, PPNP 101 (2018) 96-176]

EoS par.	Observable	Range	Comments
L	$M(N,Z)$	27-113	Most accurate EDFs on $M(N,Z)$ $\langle r_{ch}^2 \rangle^{1/2}$
	ρ_n	40-110	proton-^{208}Pb scattering (Zenihiro)
	ρ_n	0-60	π photoproduction (^{208}Pb) (Tarbert)
	ρ_n	30-80	antiprotonic at. (EDF analysis) (Centelles,Warda)
	ρ_{weak}	> 20	Parity violating scattering (PREx)
	PDS	32-54	From EDF analysis (Klimkiewicz)
	PDS	49.1-80.5	From EDF analysis (Carbone)
	α_D	20-66	From EDF analysis
	IVGQR and ISGQR	19-55	From EDF analysis
	IAS and Δr_{np}	35-75	From EDF analysis (Danielewicz)
	AGDR	75.2-122.4	From EDF analysis
	PDS, α_D, IVGQR, AGDR	45.2-54.6	From EDF analysis (Paar)
	compilation	40.5-61.9	Astrophys. J. 771 (1) (2013) 51
	compilation	42.4-75.4	PLB 727 (1) (2013) 276âĂŞ281
	compilation	30.6-86.8	RMP 89 (2017) 015007
K_τ	ρ_n	-620 - -400	antiprotonic at. (EDF analysis) (Centelles)
	ISGMR	-650 - -450	α-scattering Sn isotopes (Li)
	ISGMR	-630 - -480	α-scattering Cd isotopes (Patel)
	ISGMR	-840 - -350	Blaizot's formula (Stone)

$K_\tau = K_{sym} + L\left(\frac{K'}{K_0} - 6\right)$ or as it has been customary in different analyses $K_\tau = K_{sym} - 6L$, neglecting K'

EDFs from ab initio?

- (kind of) analogy with Coulomb DFT (see for review: PPNP 64 (2010) 120)



1. Present-day, e.g., Skyrme EDFs (including ρ and $\nabla\rho$). [DONE!]
2. Generalized Skyrme (additional gradient and density dependences, with new constraints from microscopic theory (e.g., neutron drops).
3. Functionals that merge the long-range parts (from χEFT) with a Skyrme functional.
4. point 3 from a low-momentum potential that is evolved from χEFT NN and NNN interactions.

5. Full orbital-based DFT based on low-momentum interactions.

- Determine V_{KS} from $\rho_{ab\ initio}$ via inverse KS problem (see below)

EDFs from ab initio?

Example 1: DD-MEδ functional $\mathcal{L} = \mathcal{L}_N + \mathcal{L}_M + \mathcal{L}_{int}$

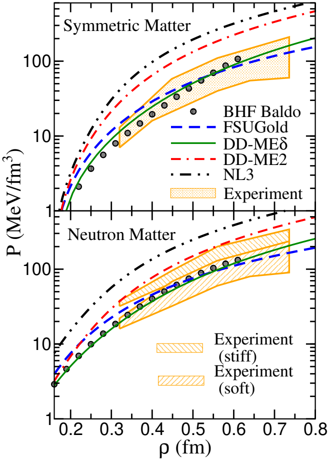
$$\mathcal{L}_N = \bar{\psi}\left(i\gamma_\mu \partial^\mu - m\right)$$

$$\mathcal{L}_M = \frac{1}{2}\left(\partial_\mu \sigma \partial^\mu \sigma - m_\sigma^2 \sigma^2\right) + \frac{1}{2}\left(\partial_\mu \vec{\delta} \partial^\mu \vec{\delta} - m_\sigma^2 \vec{\delta}^2\right) - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} - \frac{1}{2} m_\omega^2 \omega_\mu \omega^\mu - \frac{1}{4}\vec{R}_{\mu\nu}\vec{R}^{\mu\nu} - \frac{1}{2} m_\rho^2 \vec{\rho}_\mu \vec{\rho}^\mu - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}$$

$$\mathcal{L}_{int} = g_\sigma \bar{\psi}\sigma\psi + g_\delta \bar{\psi}\vec{\tau}\vec{\delta}\psi - g_\omega \bar{\psi}\gamma_\mu \omega^\mu \psi - g_\rho \bar{\psi}\gamma_\mu \vec{\tau}\vec{\rho}^\mu \psi - e\bar{\psi}\gamma_\mu A^\mu \psi$$

field strength tensors for the vector fields are

$\Omega^{\mu\nu} = \partial^\mu \omega^\nu - \partial^\nu \omega^\mu$ and correspondingly $\vec{R}^{\mu\nu}$ and $F^{\mu\nu}$.



- EoS from BHF fixes the density dep. coupling constants g's
- 4 parameters left to fix B (r.m.s. 2 MeV) and R_{ch} (r.m.s. 0.02 fm)
- Expected to be better in extrapolations, not the case...

EDFs from ab initio?

Example 2: BCP functional $E[\rho] = T_0 + E_\infty + E_{S.O.} + E_C + E_{FR}$

$$T_0 = \frac{\hbar^2}{2m}\sum |\vec{\nabla}\Psi|^2$$

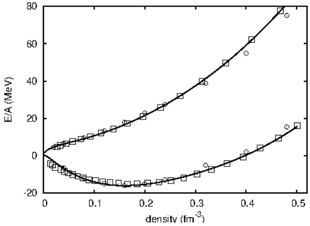
$$E_C = \frac{1}{2}\int d^3r d^3r' \frac{\rho_p(r)\rho_p(r')}{|r-r'|} - \frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3}\int d^3r \rho_p(r)^{4/3}$$

$$E_\infty[\rho] = \int d^3r[P_s(\rho)(1-\beta^2) + P_n(\rho)\beta^2]\rho$$

(P's fifth order polynomials)

$$E_{FR}[\rho] = \frac{1}{2}\int d^3r d^3r' \rho(r)\nu(r-r')\rho(r') - \frac{1}{2}\int d^3r d^3r' \rho(r)\rho(r')$$

(interaction gaussian type depending on three parameters)



PLB 663 (2008) 390-394

- EoS from BHF fix coefficinets of polynomial
- 4 parameters left to fix B (r.m.s. 2 MeV), R_{ch} (r.m.s. 0.03 fm) and spin-orbit splittings
- Expected to be better in extrapolations, not the case...

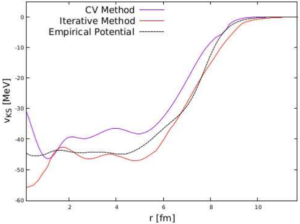
Inverse Kohn-Sham problem

Determine V_{KS} from ρ_{exp}

Non-linear problem, not well-defined (Hadamard criteria), numerically difficult

Methods: essentially two.

- **Iterative:** algebraic inversion of KS equation.
  - Simple to implement. Direct KS equation solved at each step.
  - Too sensitive to initial guess.



G. Accorto Master Thesis

- **Variational:** constrained minimization of the non-interacting kinetic energy.

  [Remember from KS: $\frac{\delta T[\rho]}{\delta \rho} = -V_{KS}$]
  - Difficult to implement. KS equation not need to be solved.
  - No sensitivity to initial guess.

Conclusions

- **Effective interactions** solved at **Hartree-Fock or Mean-Field** level have been shown to be **successful** in the description of all nuclei (**masses, nuclear sizes, deformations, Giant Resonances...**
- These **effective models** can be understood as an **approximate realization of a nuclear energy density functional** $E[\rho] \Rightarrow$ **exact functional exist**.
- **EDFs from ab initio starts to be explored.**

Thank you!