Covariance analysis for Nuclear Energy Density Functionals

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Table of contents:

- **Brief Introduction**
  - **Some comments on EDFs**
  - **The nuclear EoS**
  - **EoS parameters and nuclear observables:**
    some physical insights
- **Statistic uncertainties in EDFs:**
  - **Comments on the theory**
  - **Example: Relativistic versus non-Relativistic**
  - **Example: Modifying the χ^2**
- **Systematic uncertainties in EDFs:**
  - **Example: dipole polarizability**
- **Conclusions**

INTRODUCTION

Nuclear Energy Density Functionals:

Main types of successful EDFs are derived from Hartree-Fock (mean-field) calculations based on an effective interaciton

Relativistic mean-field models, based on Lagrangians where effective mesons carry the interaction:

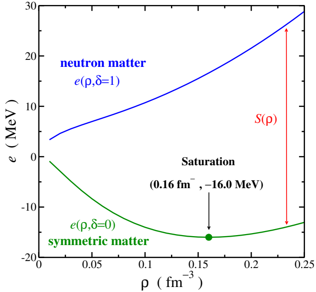
$$\begin{aligned}\mathcal{L}_{int} \quad &= \bar{\Psi}\Gamma_\sigma(\bar{\Psi},\Psi)\Psi\Phi_\sigma \quad +\bar{\Psi}\Gamma_\delta(\bar{\Psi},\Psi)\boldsymbol{\tau}\Psi\Phi_\delta \\ &-\bar{\Psi}\Gamma_\omega(\bar{\Psi},\Psi)\gamma_\mu\Psi A^{(\omega)\mu} \quad -\bar{\Psi}\Gamma_\rho(\bar{\Psi},\Psi)\gamma_\mu\tau\Psi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

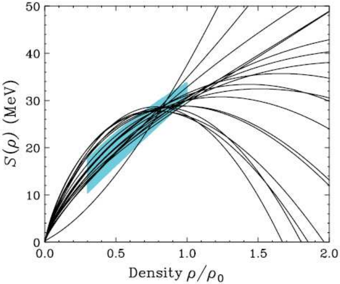
Non-relativistic mean-field models, based on Hamiltonians where effective interactions are proposed and tested:

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

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

The Nuclear Equation of State: Infinite System





* The nuclear EoS can be written in good approximation as:

$$e(\rho, \beta) \approx e(\rho, \beta = 0) + S(\rho)\beta^2 \text{ where } \beta \equiv \frac{\rho_n - \rho_p}{\rho_n + \rho_p}$$

* SNM can be expanded around ρ_0 and define some useful parameters:

$$e(\rho, 0) \approx e(\rho_0, 0) + K\varepsilon^2 \text{ where } \varepsilon \equiv \frac{\rho_0 - \rho}{3\rho_0}$$

* Symmetry energy can be also expanded around ρ_0 and define some useful parameters:

$$S(\rho) \approx J - L\varepsilon + K_{sym}\varepsilon^2$$

EoS parameters from nuclear observables

We expect that EDFs provide a good description of nuclear masses, densities and collective oscillation frequencies around the g.s. (GR excitation energies)

For guidance, some physical insights may be obtained from simple models while studyting microscopically a given observable:

- Within LDM $B(A, Z)$ determine very precisely $e(\rho_0, 0) \equiv e_0$

$$\frac{\delta e_0}{e_0} \sim 1\% \Rightarrow \delta B(^{208}\text{Pb}) \sim 30 \text{ MeV}$$

  A small change on $e(\rho_0, 0)$ *will predict unrealistic* B *in a heavy nucleus*

- The **interior density** (ρ_0) in most of existing nuclei is 0.16 fm^{-3}

$$\frac{\delta \rho_0}{\rho_0} \sim 5\% \Rightarrow \delta r(^{208}\text{Pb}) \sim \delta r_0 A^{1/3} \sim 0.1 \text{ fm}$$

  A small change will predict not very good r *and this will/may also affect* B

EoS parameters from nuclear observables

- Within the DM,
  * $\Delta r_{np} \propto r_0 I A^{1/3} L/J \Rightarrow$ information on J and L

Some properties are directly related to the restoring force in nuclear excitations:

- The nuclear matter incompressibility K strongly depends on:
  * $E(\text{ISGMR}) \propto \sqrt{K_A}$
  * K_A should depend on K (leptodermus expansion extensively used in literature $K_A \approx K + K_{surf} A^{-1/3} + K_\tau I^2 + K_C Z^2 A^{-4/3} + ...$)
- Within a simple HO model for the ISGQR **(B&M)**
  * $E(\text{ISGQR}) \propto \sqrt{m/m^*}\hbar\omega_0$
- Within a simple HO model for the IVGDR **(B&M)**
  * $E(\text{IVGDR}) \propto \sqrt{S(\langle\rho\rangle)}$ at some subsaturation density $\Rightarrow$ information on both J and L
- Within a simple HO model for the IVGQR **(B&M)**
  * $E(\text{IVGQR})$ shoude depend on $\sqrt{m/m^*}\hbar\omega_0$ and $\sqrt{S(\langle\rho\rangle)}$ at some subsaturation denisty $\Rightarrow$ information on both J and L

EoS parameters from nuclear observables

Dipole polarizability: a macroscopic approach

electric polarizability measures tendency of the nuclear charge distribution to be distorted $\left(\alpha \sim \frac{\text{electric dipole moment}}{\text{external electric field}}\right)$

- The dielectric theorem establishes that the m_{-1} moment can be comput ed from the expectation value of the Hamiltonian in the constrained ground stat e $\mathcal{H}' = \mathcal{H} + \lambda\mathcal{D}$.

Adopting the Droplet Model:

$$m_{-1} \approx \frac{A\langle r^2\rangle^{1/2}}{48J}\left(1 + \frac{15}{4}\frac{J}{Q}A^{-1/3}\right)$$

within the same model, connection with the neutron skin thickness:

$$\alpha_D \approx \frac{A\langle r^2\rangle}{12J}\left[1 + \frac{5}{2}\frac{\Delta r_{np} + \sqrt{\frac{3}{5}}\frac{e^2 Z}{70J} - \Delta r_{np}^{\text{surface}}}{\langle r^2\rangle^{1/2}(I - I_C)}\right]$$

So now we know which correlations we expect to see in the plots!

Isovector properties in nuclei

- **In the past** (and present), **neutron properties** in stable medium and heavy nuclei have been mainly measured by using **strongly interacting probes** and $(N - Z)/A$ **explored is small**.

$$\Downarrow$$

Limited knowledge of isovector properties
(we expect large extrapolation errors as compared to IS)

- **At present**,
  - the use of **RIBs** has opened the possibility of measuring properties of **exotic nuclei** $\Rightarrow$ **more info on large** $N - Z$
  - **parity violating elastic electron scattering** (PVES), a **model independent technique**, has allowed to estimate the **weak form factor at low** q of a stable heavy nucleus like ^{208}Pb

$$\Downarrow$$

Promising perspectives for the near future
(So we need to reliably assess the quality of our extrapolations!)

STATISTIC UNCERTAINTIES IN EDFs

Covariance analysis: χ^2 test

- Observables $\mathcal{O}$ used to calibrate the parameters $\mathbf{p}$

$$\chi^2(\mathbf{p}) = \sum_{i=1}^{m} \left(\frac{\mathcal{O}_i^{\text{theo.}} - \mathcal{O}_i^{\text{ref.}}}{\Delta \mathcal{O}_i^{\text{ref.}}} \right)^2$$

- Assuming that the χ^2 can be approximated by an hyper-parabola around the minimum $\mathbf{p}_0$,

$$\chi^2(\mathbf{p}) - \chi^2(\mathbf{p}_0) \approx \frac{1}{2} \sum_{i,j}^{n} (p_i - p_{0i}) \partial_{p_i} \partial_{p_j} \chi^2 (p_j - p_{0j})$$

where $\mathcal{M} \equiv \frac{1}{2} \partial_{p_i} \partial_{p_j} \chi^2$ (curvature m.) and $\mathcal{E} \equiv \mathcal{M}^{-1}$ (error m.).

- errors between predicted observables $\mathcal{A}$

$$\Delta \mathcal{A} = \sqrt{\sum_{i}^{n} \partial_{p_i} A \mathcal{E}_{ii} \partial_{p_i} A}$$

- correlations between predicted observables,

$$c_{AB} \equiv \frac{C_{AB}}{\sqrt{C_{AA} C_{BB}}}$$

where, $C_{AB} = \overline{(A(\mathbf{p}) - \overline{A})(B(\mathbf{p}) - \overline{B})} \approx \sum_{ij}^{n} \partial_{p_i} A \mathcal{E}_{ij} \partial_{p_j} B$

Example on two different fitting protocols and models:

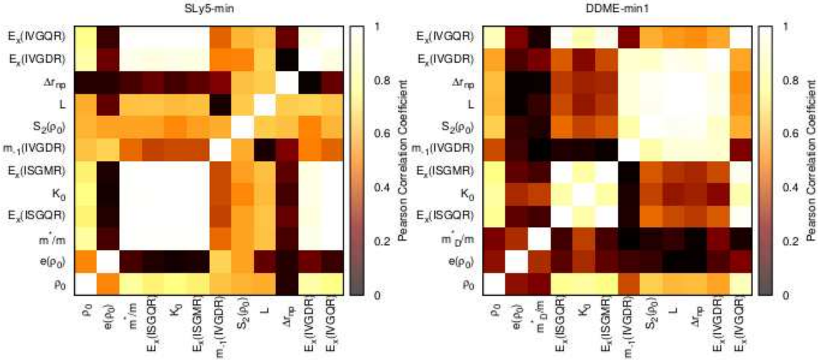
SLy5-min: use constant error for a given observable

- **Binding energies** of ^{40,48}Ca, ^{56}Ni, ^{130,132}Sn and ^{208}Pb with a fixed adopted error of **2 MeV**
- the **charge radius** of ^{40,48}Ca, ^{56}Ni and ^{208}Pb with a fixed adopted error of **0.02 fm**
- the **neutron matter** Equation of State calculated by Wiringa *et al.* (1988) for densities between 0.07 and 0.40 fm^{-3} with an adopted error of **10%**
- the **saturation energy** ($e(\rho_0) = -16.0 \pm 0.2$ MeV) and **density** ($\rho_0 = 0.160 \pm 0.005$ fm^{-3}) of symmetric nuclear matter.

DD-ME-min1: use relative error for all observables

- **binding energies, charge radii, diffraction radii and surface thicknesses** of 17 even-even spherical nuclei, ^{16}O, ^{40,48}Ca, ^{56,58}Ni, ^{88}Sr, ^{90}Zr, ^{100,112,120,124,132}Sn, ^{136}Xe, ^{144}Sm and ^{202,208,214}Pb. The assumed errors of these observables are **0.2%, 0.5%, 0.5%, and 1.5%**, respectively.

Covariance analysis: SLy5-min and DD-ME-min1



Some examples on correlations between:

* e_0 and $S(\rho_0) = J$: $e_n(\rho_0) \approx e_0 + J$. SLy5 fits e_n, DD-ME does not → Corr./Non Corr.

* Δr_{np} and E_x**(IVGDR)**: E_x(IVGDR) depends on $S(\langle\rho\rangle) \sim J - L\langle\varepsilon\rangle$ and κ in a non-linear way → corr. may weaken

* Δr_{np} and E_x**(IVGQR)**: E_x(IVGQR) depends on $S(\langle\rho\rangle) \sim J - L\langle\varepsilon\rangle$ and m^*/m a non-linear way → corr. may weaken

* $\Delta r_{np} \propto L/J$ is **strongly correlated** with **J** and **L** but **NOT** with $\alpha_D \sim a/J + bL/J$ → corr. may weaken

Covariance analysis: SLy5-min and DD-ME-min1

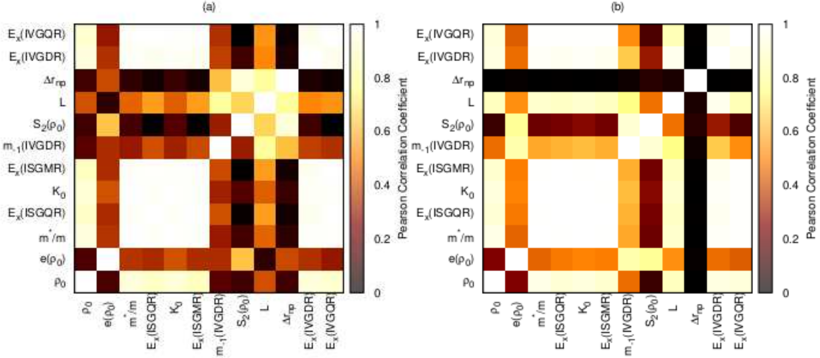
	SLy5-min			DDME-min1			
A	A_0		$\sigma(A_0)$	A_0		$\sigma(A_0)$	units
SNM							
ρ_0	0.162	$\pm$	0.002	0.150	$\pm$	0.001	fm^{-3}
$e(\rho_0)$	-16.02	$\pm$	0.06	-16.18	$\pm$	0.03	MeV
m^*/m	0.698	$\pm$	0.070	0.573	$\pm$	0.008	
J	32.60	$\pm$	0.71	33.0	$\pm$	1.7	MeV
K_0	230.5	$\pm$	9.0	261	$\pm$	23	MeV
L	47.5	$\pm$	4.5	55	$\pm$	16	MeV
^{208}Pb							
E_x^{ISGMR}	14.00	$\pm$	0.36	13.87	$\pm$	0.49	MeV
E_x^{ISGQR}	12.58	$\pm$	0.62	12.01	$\pm$	1.76	MeV
Δr_{np}	0.1655	$\pm$	0.0069	0.20	$\pm$	0.03	fm
E_x^{IVGDR}	13.9	$\pm$	1.8	14.64	$\pm$	0.38	MeV
m_{-1}^{IVGDR}	4.85	$\pm$	0.11	5.18	$\pm$	0.28	MeV^{-1} fm^2
E_x^{IVGQR}	21.6	$\pm$	2.6	25.19	$\pm$	2.05	MeV

Statistical uncertainties depend on the fitting protocol, that is on the **data (or pseudo-data) and associated errors used for the fits: Let us see an example...**

Covariance analysis: modifying the χ^2

→ **SLy5-a:** χ^2 as in SLy5-min except for the neutron EoS (relaxed the required accuracy = increasing associated error).

→ **SLy5-b:** χ^2 as in SLy5-min except the neutron EoS (not employed) and used instead a tight constraint on the Δr_{np} in ^{208}Pb

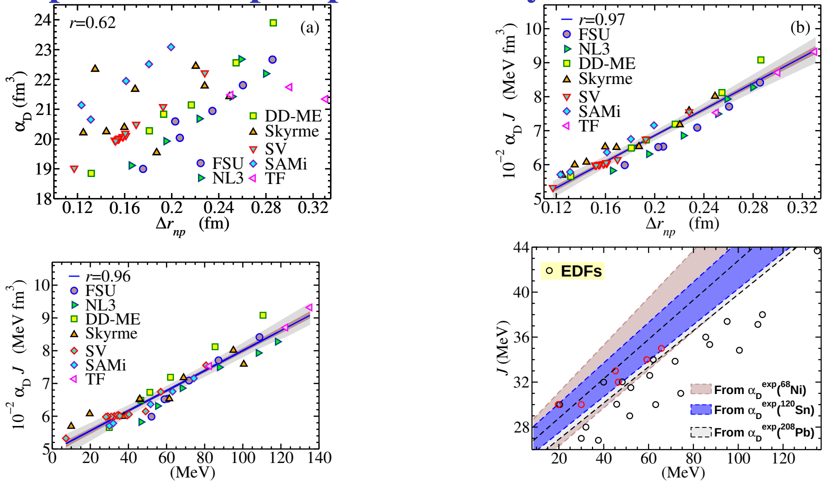


J. Phys. G: Nucl. Part. Phys. 42 034033 (2015).

- When a **constraint** on a property is **relaxed**, **correlations** of other observables with such a property should become **larger** → **SLy5-a: α_D is now better correlated with Δr_{np}**
- When a **constraint** on a property is **enhanced** —artificially or by an accurate experimental measurement— **correlations** of other observables with such a property should become **small** → **SLy5-b: Δr_{np} is not correlated with any other observable**

SYSTEMATIC UNCERTAINTIES IN EDFs

Example on the dipole polarizability:



* **Combine statistic and systematic** studies for a reasonable estimate of theoretical errors

* Add to that **physical understanding** of the problem to get reliable information

CONCLUSIONS

Conclusions:

Everything is χ^2 dependent

Which observables to fit?

- might masses be enough for the determination of an accurate EDF? (this will avoid us worry on adopted errors)
- most of EDFs are derived from a Mean-Field calculation based on an effective interaction $\rightarrow$ better to fit spherical/deformed nuclei; nuclei with small $E_{correlation}$; avoid very light systems?

What about adopted errors?

- they are crucial: results of the covariance analysis may strongly depend on them
- many groups *traditionally* adopt errors depending on their particular experience

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