Nuclear equation of state from ground and excited state properties of nuclei

2.-Theoretical models, associated errors and correlations

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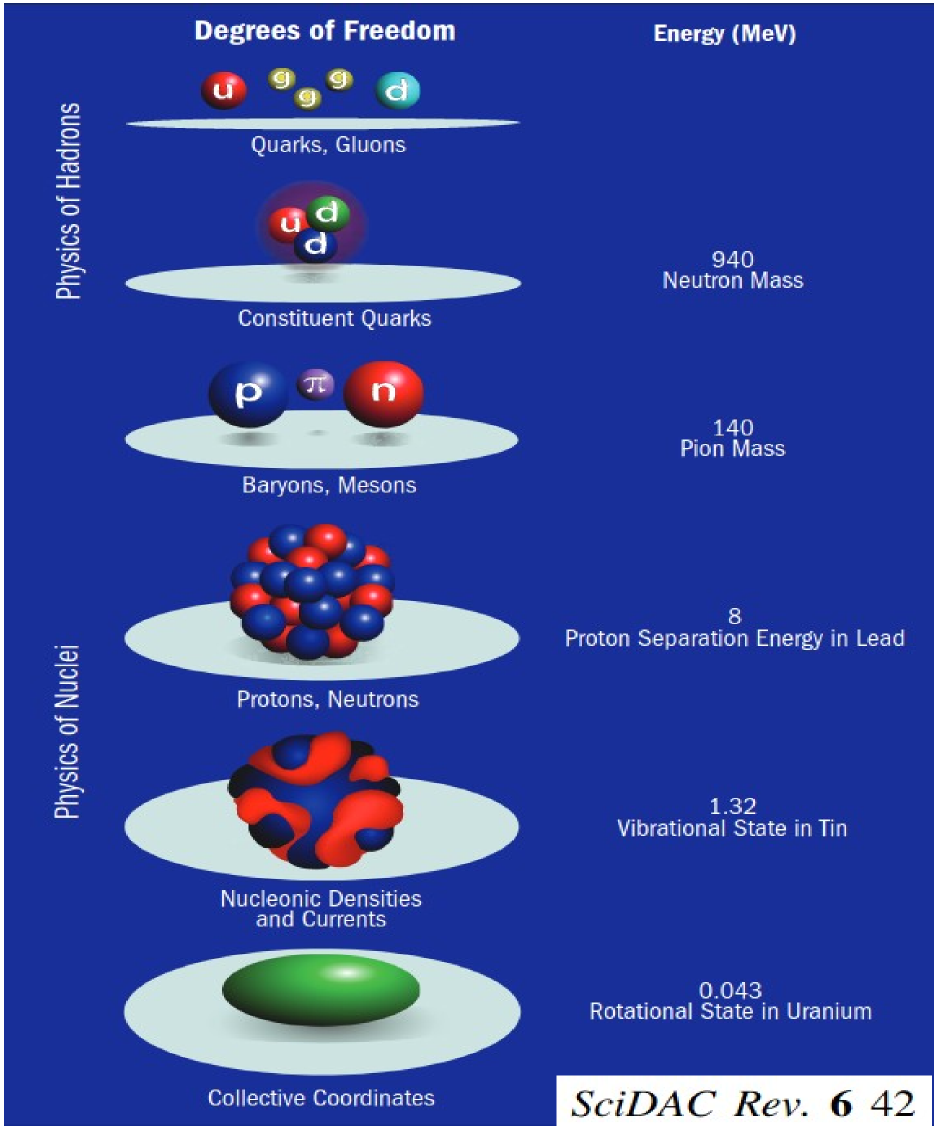
France September 4th-9th

How are we dealing with the nuclear many-body problem?

→ Ab inito methods

→ Density Functional Theory

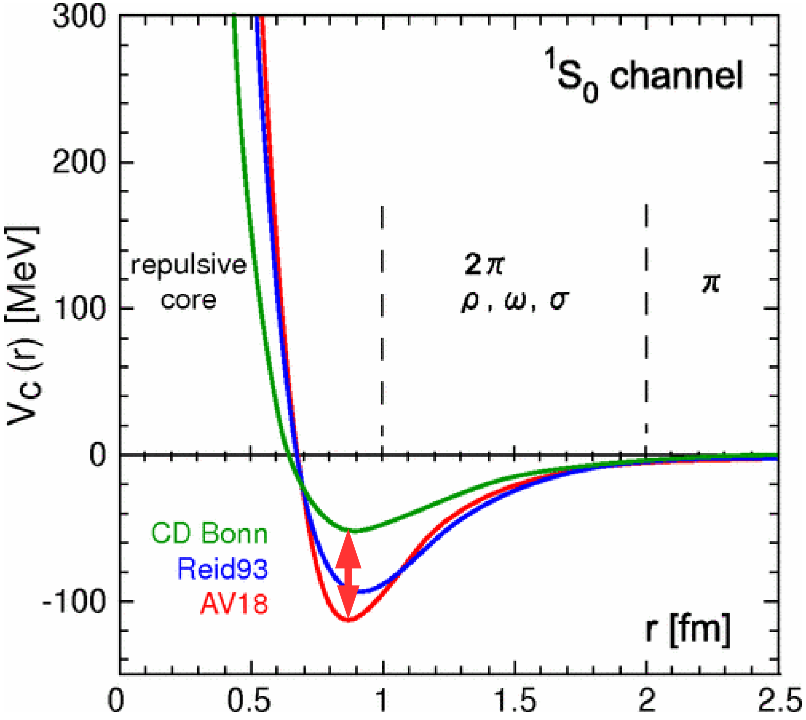
→ …



Nuclear Many-Body Problem:
Nuclear interaction

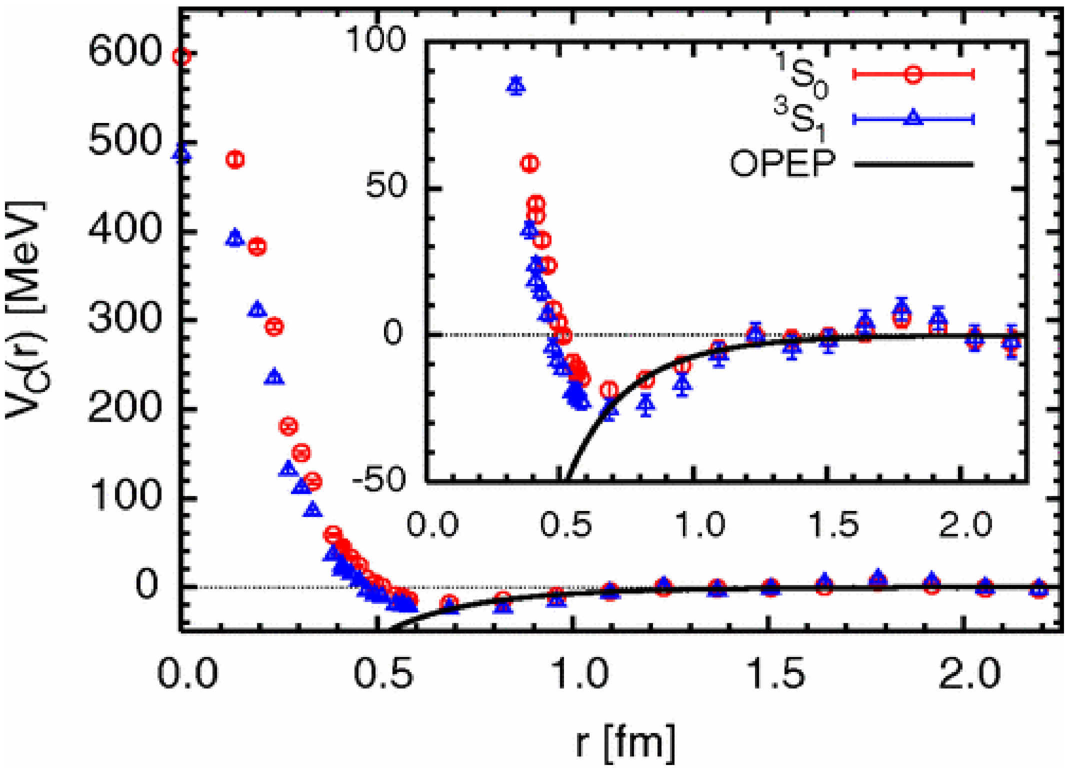
Underlying interaction: the “so called” **residual strong interaction** = **nuclear force** has **not** been **derived yet** (with the precision needed) from first principles as **QCD** is **non-perturbative** at the **low-energies** (~ below $m_\pi \approx 140$ MeV) relevant for the description of nuclei.

Phenomenological



Nuclear Force from Lattice QCD - N. Ishii, S. Aoki, and T. Hatsuda Phys. Rev. Lett. 99, 022001 (2007)

Lattice QCD (m_π/m_ρ~0.6)



$\Delta V(r_{min}) \approx 60$ MeV !! → **different saturation energy**

Similar to CD-Bonn $V(r_{min}) \approx -40$ MeV but postion of the **minimum diff. → diff. saturation density** (m_π/m_ρ~0.6 scaled to physical value 140/775≈0.18)

Chiral effective field theory:

Building the interaction from QCD

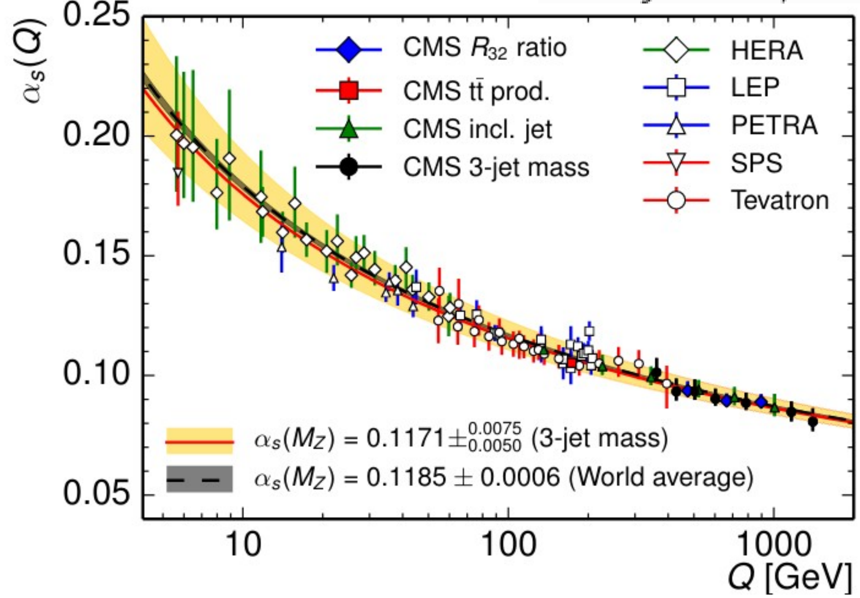
QCD non-perturbative at low energies (below ~ m_π) $\alpha_s \rightarrow 1$ or larger (breaking scale $\Lambda_{QCD} \sim m_\pi$).

$$\alpha_s(Q) = \frac{6\pi}{33 - 2N_f} \log^{-1}\left[\frac{Q}{\Lambda_{QCD}}\right]$$

S. Bethke, Prog. Part. Nucl. Phys. **58**, 351 (2007).

$$\mathscr{L}_{QCD} = \sum_{f=u,d,s} \left(\bar{q}_f i \not{D} q_f - m_f \bar{q}_f q_f\right) - \frac{1}{2} \mathrm{Tr}\, G_{\mu\nu} G^{\mu\nu},$$

Eur. Phys. J. C **75**, 186



Chiral symmetry: rotating left-handed and the right-handed quark fields independently makes no difference to the theory:

$$\psi_L \rightarrow \psi_L \quad \text{and} \quad \psi_R \rightarrow e^{i\theta_R}\psi_R.$$

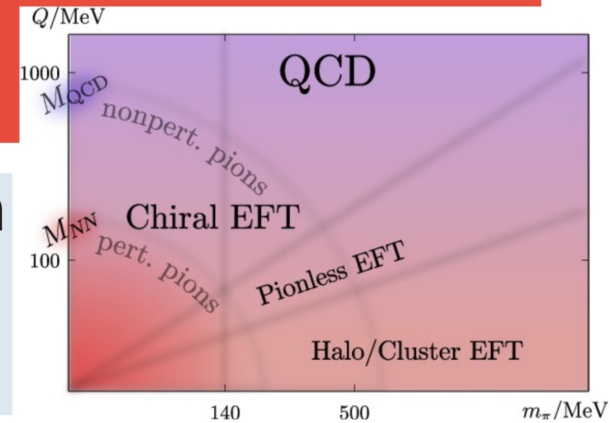
$$\psi_L \rightarrow e^{i\theta_L}\psi_L \quad \text{and} \quad \psi_R \rightarrow \psi_R$$

Chiral symmetry in QCD is **explicitly broken** due to the non zero-quark masses and, even in the Chiral limit ($m_{quarks} \rightarrow 0$), it is **spontaneously broken.** Exp. evidence due to the absence of parity doublets [e.g. ρ (1^-) and δ (1^+) mesons has very different masses]

→ **Pseudo-Goldston bosons** with finite mass: pions, kaons, …

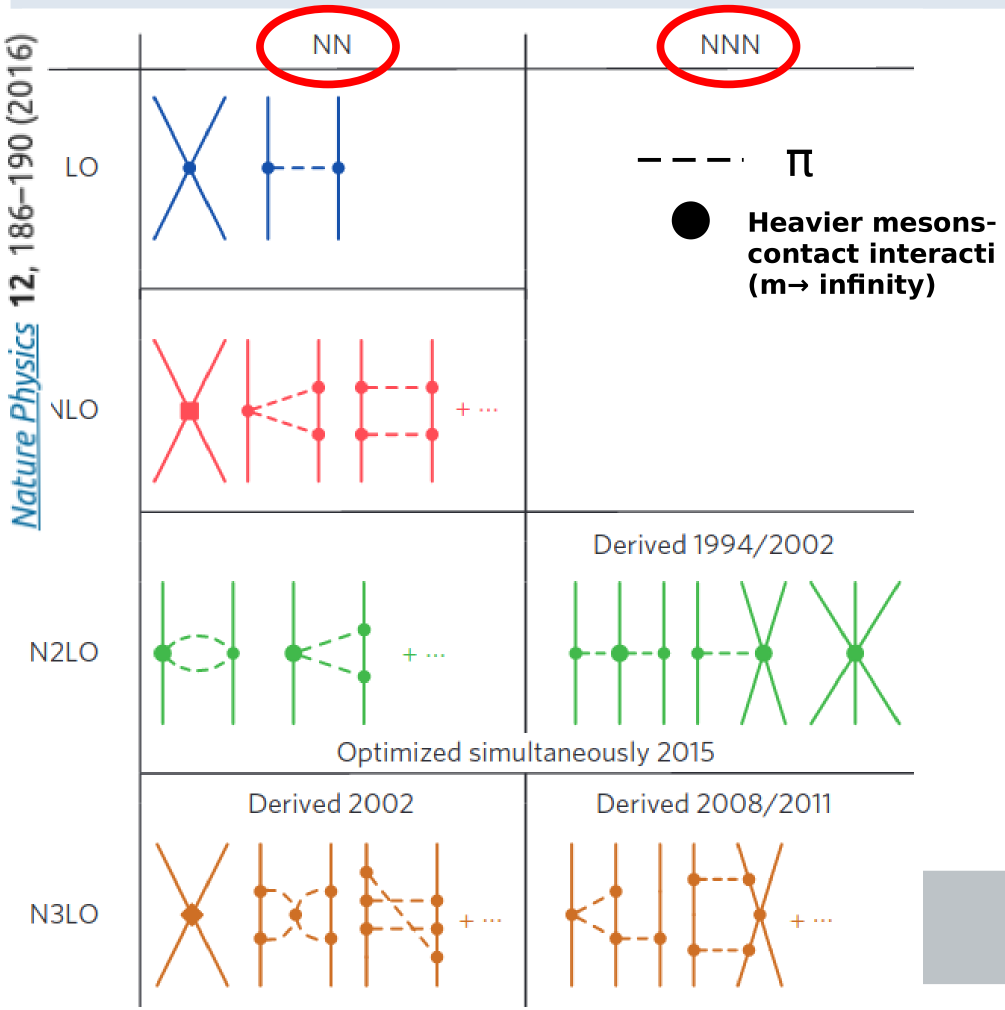
Chiral effective field theory
Building the interaction from QCD

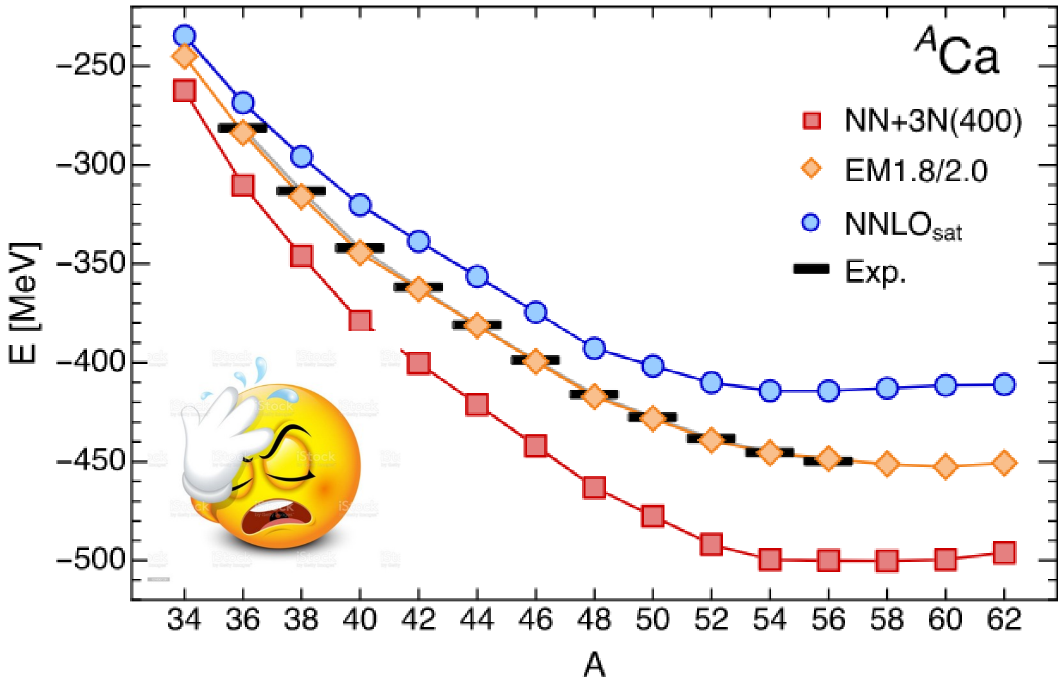
H.-W. Hammer, Sebastian König, and U. van Kolck
Rev. Mod. Phys. **92**, 025004 – Published 23 June 2020



Chiral EFT for nuclei: pions + nucleons with breaking scale Λ~500 MeV

[there exist also other possibilities such as pionless Chiral EFT or pions+Delta+nucleons]





Determination of the **EFT** parameters is **not unique** → different Hamiltonians that agree with experimental data on NN scattering and 3N data **do not agree** on the prediction of many body data (e.g. Ca isotopes Z=20)

Many-body methods:

Nuclei are made from few to hundreds of nucleons!

Once the **Hamiltonian** has been built, a **many-body method** is needed to **calculate nuclei**

Main many-body approaches seem to agree well if the same Hamiltonian is assumed:

→ No core shell model (**NCSM**)

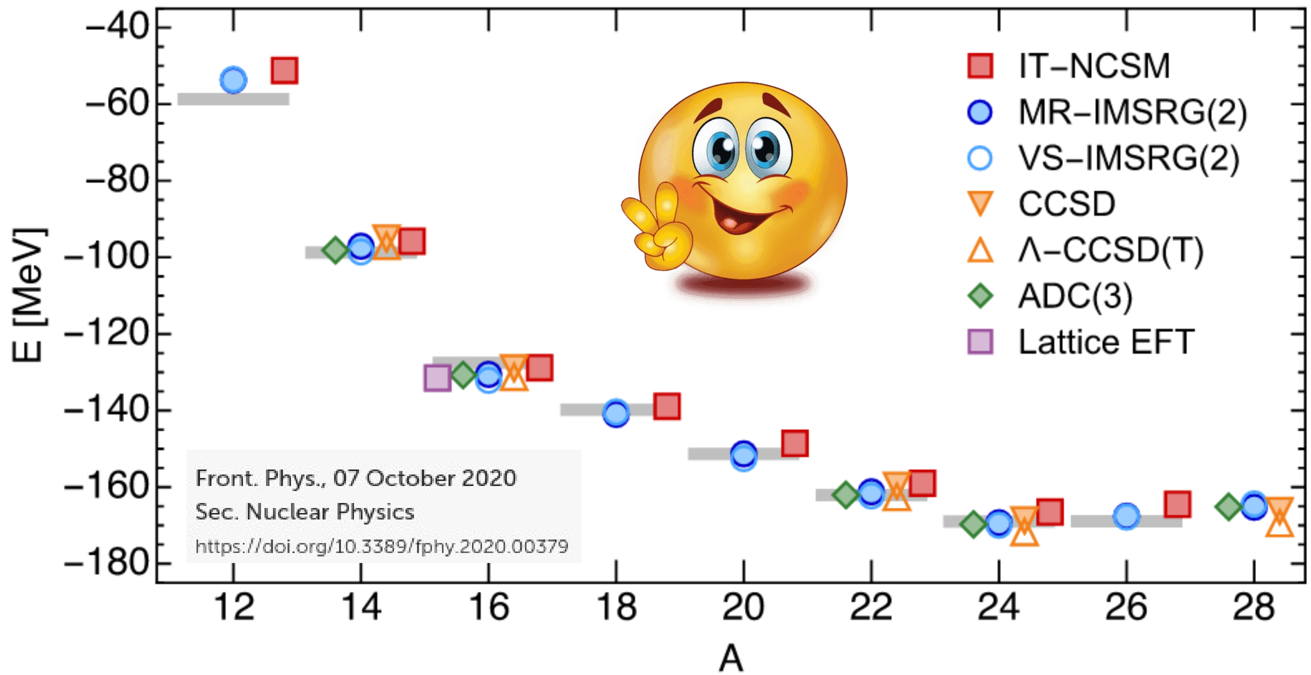
→ In medium similarity renormalization group (**IMSRG**)

→ Coupled cluster (**CC**)

→ Algebraic Diagrammatic Construction (**ADC** for <u>Self-Consistent Green's Functions</u>)

→ Quantum Monte Carlo (**QMC**)

→ Many-body perturbation theory (**MBPT**)



Ground-state energies of the **oxygen (Z=8)** isotopes for **various many-body approaches**, using the **same chiral NN+3N(400) Hamiltonian**. Gray bars indicate experimental data.

DENSITY FUNCTIONAL THEORY
Hohenberg-Kohn theorems
P.Hohenberg, W. Kohn, Phys. Rev. 136, B864 (1964)

→ Assuming a system of **interacting fermions** in a confining **external potential**, there exist a **universal** functional **F[ρ]** of the fermion density **ρ**:

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

→ and it can be shown that

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

so **E[ρ]** has a **minimum** for the **exact ground-state density** where it assumes the **exact energy** as a value.

Kohn-Sham realization

$F[\rho] \rightarrow T_{\text{non-int.}}[\rho] + V_{KS}[\rho]$

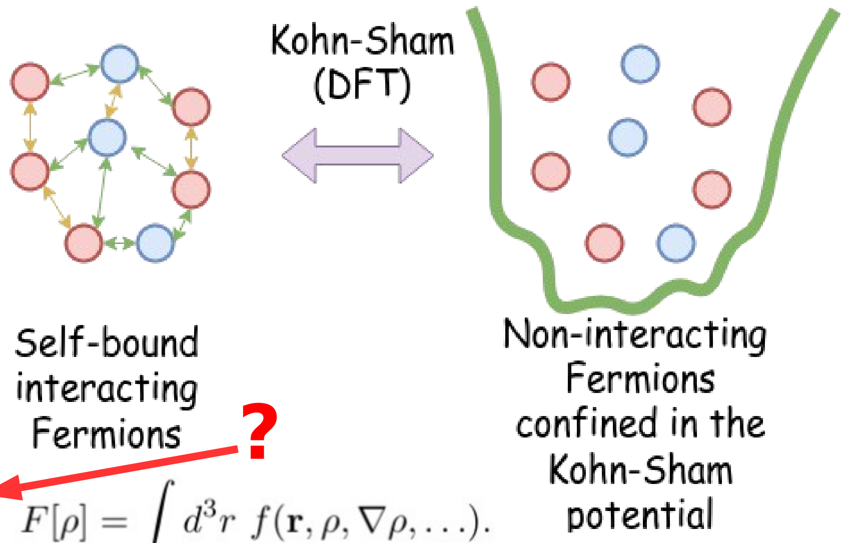
In nuclei no need of external confining potential

For **any interacting system**, there exists a <u>**local**</u> **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**:

$$\rho_{\text{exact}}(\vec{r}) = \rho_{\text{KS}}(\vec{r}) = \sum_{i=1}^{A} |\phi(\vec{r})|^2$$

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

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



$$F[\rho] = \int d^3r \; f(\mathbf{r}, \rho, \nabla\rho, \ldots).$$

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

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

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

Time dependent DFT for the study of GR

Linear Response Theory (Ring&Schuck)

Perturbing the initial static Hamiltonian H_0 with a small **time dependent operator F(t)**:

$$\mathcal{H} = \mathcal{H}_0 + F(t) \qquad F(t) = f\exp(-i\omega t) + f^\dagger \exp(i\omega t)$$

Will produce variations on the **static density ρ_0 linear with the external operator F(t)** in first approximation:

$$\delta\rho(t) = \delta\rho\exp(-i\omega t) + \delta\rho^\dagger \exp(i\omega t)$$

Writting the **Schroedinger equation using commutators**

$$\mathcal{H} = \sum_i h(i)$$

$$h\Psi(t) = i\hbar\dot{\Psi}(t) \rightarrow [h,\rho] = i\hbar\dot{\rho}$$

$$h_0\Psi = \varepsilon\Psi \rightarrow [h_0,\rho_0] = 0$$

$$[h_0 + F(t), \rho_0 + \delta\rho(t)] = i\hbar\delta\dot{\rho}$$

Time dependent DFT for the study of GR

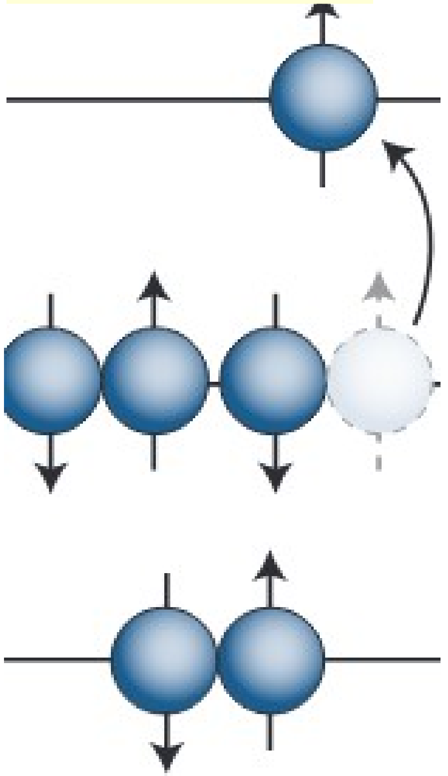
Linear Response Theory (Ring&Schuck)

Keeping the **linear terms** in the **perturbation** (F) and imposing that a Slater determinant satisfies **$\rho^2=\rho$** (only for **particle-hole** or **hole-particle** excitations [**GR→ Many coherent ph excitations!**]) one could find:

$$(\omega - \epsilon_m + \epsilon_i)\delta\rho_{mi} = f_{mi} + \sum_{m'i'} V_{mi'im'}\delta\rho_{m'i'} + V_{mm'ii'}\delta\rho_{im'}$$

$$(\omega - \epsilon_i + \epsilon_m)\delta\rho_{im} = f_{im} + \sum_{m'i'} V_{imi'mm'}\delta\rho_{m'i'} + V_{im'mi'}\delta\rho_{im'}$$

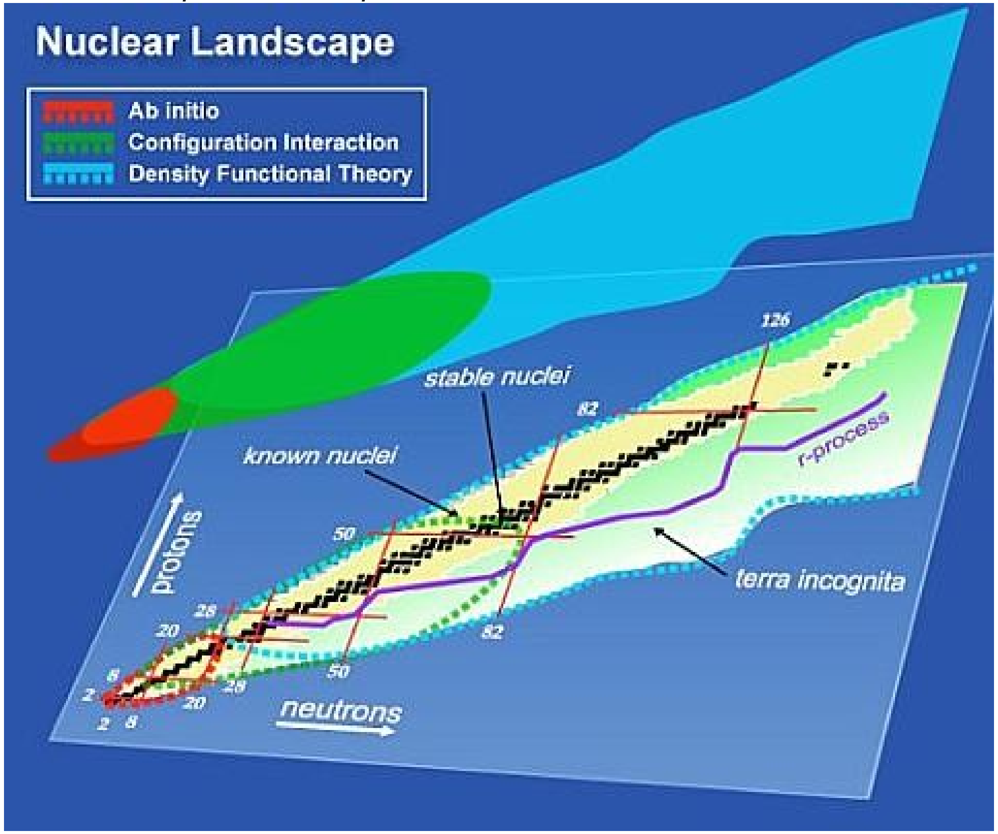
$$V_{kl'lk'} = \sum_{kk'} \left.\frac{\partial h_{kl}}{\partial \rho_{k'l'}}\right|_{\rho^{(0)}} = \left.\frac{\partial^2 E}{\partial \rho_{lk}\partial \rho_{k'l'}}\right|_{\rho^{(0)}}$$



For **F→ 0** and solving the Eqs. for **δρ** one finds the **Random Phase Approximation** where the knowledge of **E[ρ] is suffiient**, no need to impose H.

Advantadges and disadvantages of DFT

UNEDF http://unedf.mps.ohio-state.edu/



→ **ADVANTAGES OF DFT:**

• **exact theory** that can be applied to the **whole nuclear chart**

• **many-body** problem mapped onto a **one-body** problem without the need of explicitly involving inter-nucleon interactions!!! (computational cost and interpretation of observables 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)

→ **DISADVANTAGES OF DFT:**

• 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 attempts already exist)

• **no systematic** way of **improvement** (evaluate syst. Errors) so far.

Nuclear DFT: example

Write an **energy density functional (EDF)** in terms of the **relevant denisties for the nuclear problem**: baryon density (ρ), spin density (s) and density currents (j); **keeping the basic symmetries** (time reversal invariance, invariance under space reflections and rotational invariance, as well as Galilean or Lorentz invariance).

$$\mathcal{E}[\rho(\vec{r}),\tau(\vec{r}),\vec{\nabla}\rho(\vec{r}),\vec{J}(\vec{r}),\ldots] = \frac{\hbar^2}{2m}\int d\vec{r}\,\tau^2(\vec{r}) + \mathcal{E}^{\text{pot}}[\rho(\vec{r}),\tau(\vec{r}),\vec{\nabla}\rho(\vec{r}),\vec{J}(\vec{r}),\ldots] + \mathcal{E}^{\text{Coul}}[\rho(\vec{r})]$$

A bit of history:

→ In **nuclear physics EDFs** have been derived from **two body interactions** evaluated at the **Hartree-Fock** level (expectation value of the Hamiltonian assuming a Slater determinant for the wave function)

→ However, one may well **invent directly an EDF** without the need of deriving it from a Hamiltonian.

Nuclear DFT: example

How do I calculate the EoS?

→ **uniform matter:** derivative terms of the density will be zero!! Among them spin-orbit currents (J).

→ **Kinetic energy:** uniform Fermi gas

→ **Spin-saturated**: spin denisties zero.

→ **No Coulomb**

EoS with a simplfied Skyrme EDF:

δ=0 symmetric nuclear matter ($\rho_n=\rho_p$)
δ=1 neutron matter ($\rho=\rho_n$; $\rho_p=0$)

$$e(\rho,\delta) = \frac{E}{A} = \frac{\mathcal{E}}{\rho} = \frac{3}{5}\frac{\hbar^2}{2m}\left(\frac{3\pi^2}{2}\right)^{2/3}\rho^{2/3} f_{5/3}$$

← **Free Fermi gas** with degeneracy 4 (2 from spin and 2 from isospin)

$$+ \frac{1}{8} t_0 \rho \left[2(x_0+2) - (2x_0+1) f_2\right]$$

← $t_0(1+x_0P_\sigma)\delta(\vec{r}_1-\vec{r}_2)$

$$+ \frac{1}{48} t_0 \rho^{\alpha+1}\left[2(x_3+2) - (2x_3+1) f_2\right]$$

← $\frac{1}{6}t_3(1+x_3P_\sigma)\rho^\alpha\delta(\vec{r}_1-\vec{r}_2)$

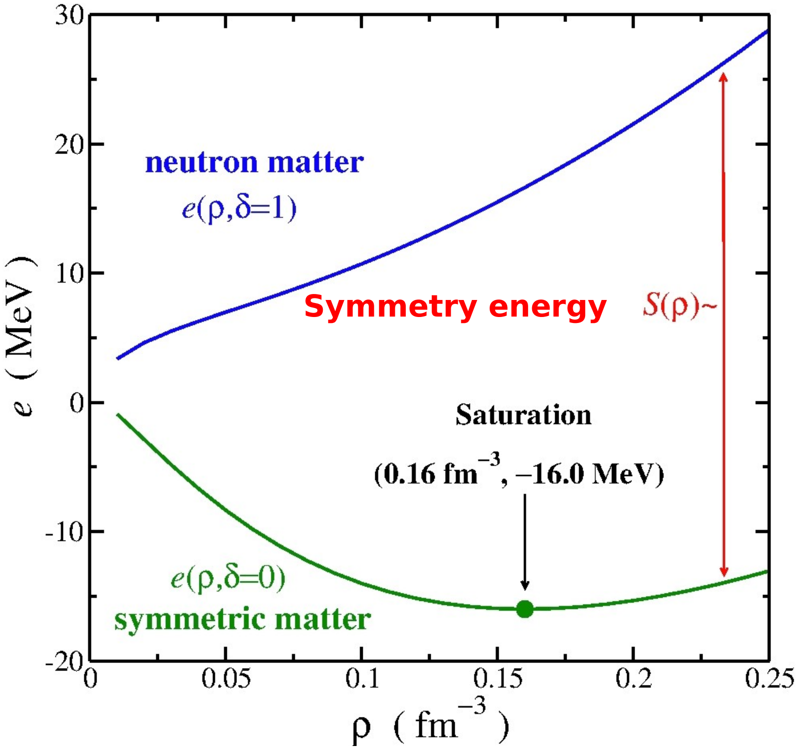
Parameters of the model: t_0, x_0, t_3, x_3, and α typically fitted to experimental data on binding energies and charge radii

$$f_a \equiv \frac{1}{2}\left[(1+\delta)^a + (1-\delta)^a\right]$$

Reminder: Nuclear EoS

Unpolarized **nuclear matter** at zero temperature (10^{10}K→1MeV) is defined as the **energy** per **nucleon** (*e*) as a function of the **neutron** (ρ_n) and **proton** (ρ_p) **densities** as (*isospin conserving* $V_{nn} = V_{pp} = V_{np}$):

$$e(\rho,\delta) = e(\rho,0) + S(\rho)\delta^2 + \mathcal{O}[\delta^4] \quad \text{where } \rho = \rho_n + \rho_p \text{ and } \delta = \frac{\rho_n - \rho_p}{\rho}$$



It is customary to **expand *e(ρ,δ)*** around nuclear **saturation density** ρ_0 ~ 0.16 fm^{-3}

$$e(\rho,0) = e(\rho_0,0) + \frac{1}{2}K_0 x^2 + \mathcal{O}[\rho^3] \text{ where } x = \frac{\rho-\rho_0}{3\rho_0}$$

$$S(\rho) = J + Lx + \frac{1}{2}K_{\text{sym}}x^2 + \mathcal{O}[\rho^3,\delta^4]$$

K_0 → how **compressible** is symmetric matter at ρ_0

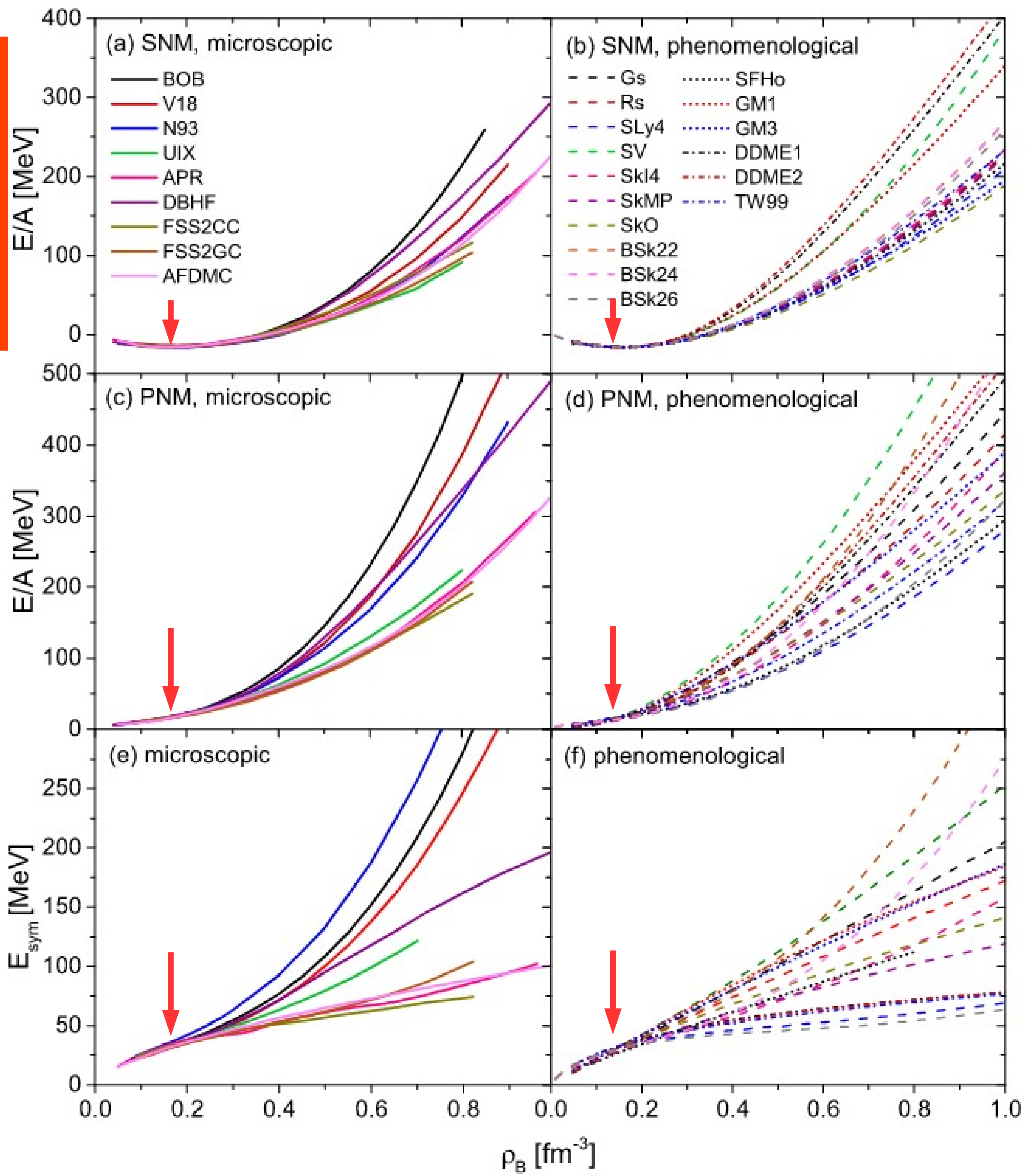
J → **penalty energy** for converting all **protons into neutrons** in symmetric matter at ρ_0

L → **neutron pressure** in neutron matter at ρ_0

Nuclear EoS as predicted by modern nuclear models

Discrepancies among models, not only for large densities

$$e(\rho,1) \approx e(\rho,0) + S(\rho)$$
$$S(\rho) \approx e(\rho,1) - e(\rho,0)$$



Determination of the parameters; theoretical errors and correlations

→ **Chiral EFT** expansion **allows** for the **estimation** of the **errors** associated to a given truncation in the determination of the Hamiltonian.

→ Most **many-body techniques** (except EDF) **allow** to **estimate** the **error** associated to the method by evaluating the following (and more complex) terms. Analogous to the expansion in the interaction, think about (many-body) perturbation theory.

→ **All nuclear models are effective** and, thus, **parameters must be determined (fitted to experiment).**

→ **Two statistic approaches to this problem in the literature:**

Frequentists concentrate on having methods guaranteed to work most of the time, given minimal assumptions. Based on the ratio of times we expect an event to occur (#successes / #experiment)

Bayesians try to make inferences that take into account all available information and answer the question of interest given the particular data set. Based on individual's degree of belief of the occurrence of an event

Frequentist inference:

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 $\mathcal{A}$

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

- 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: two typical EDF fitting protocols

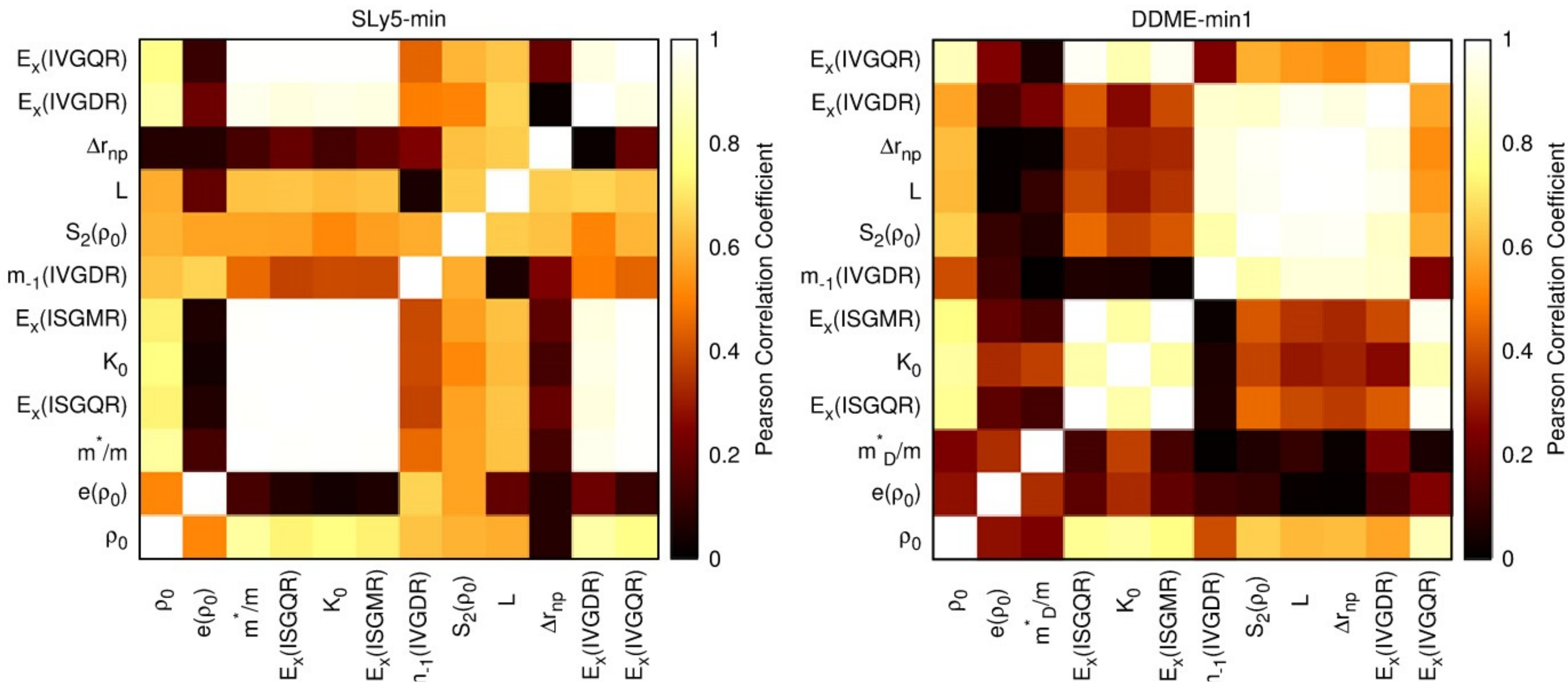
SLy5-min: use constant error for a given observable

- **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.

Associated covariance matrix



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 $\rightarrow$ 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 $\rightarrow$ 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 $\rightarrow$ corr. may weaken

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

Some numerical results

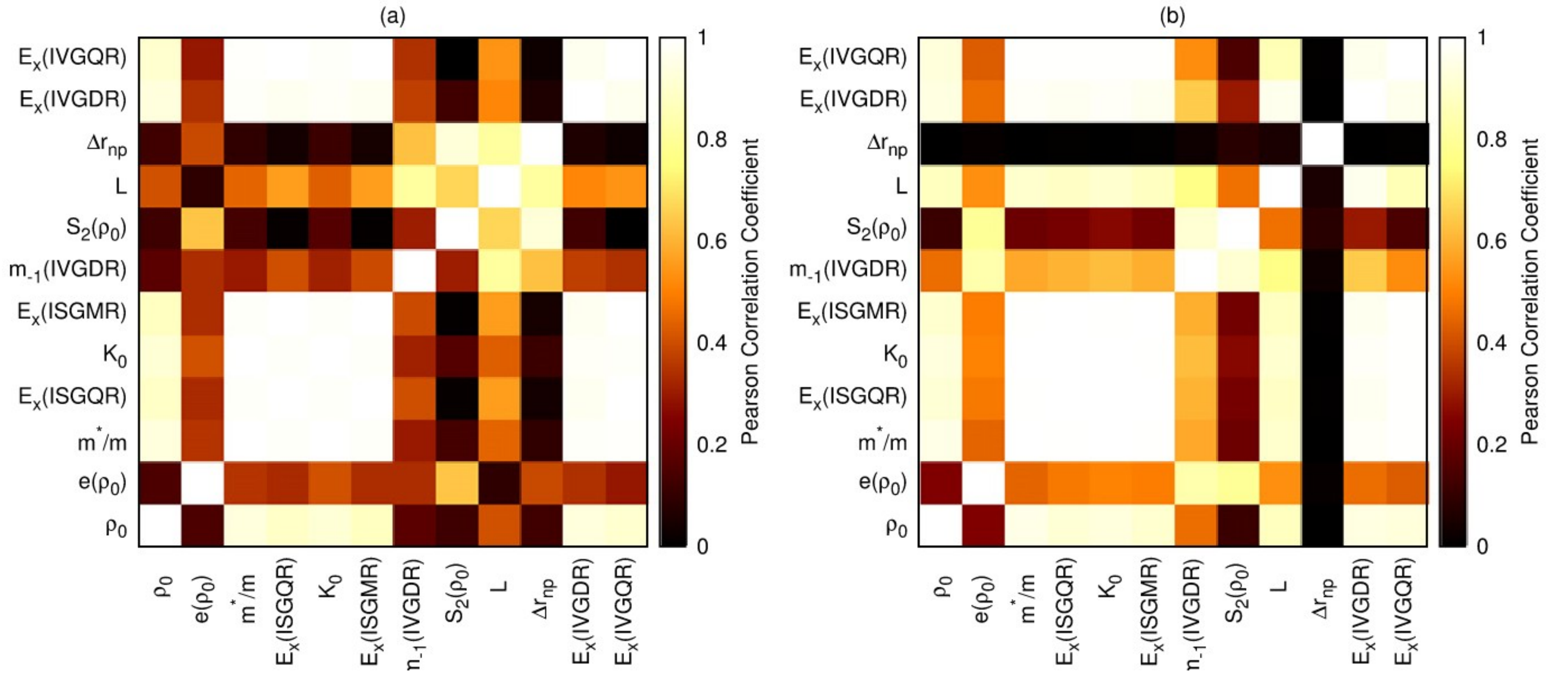
A	SLy5-min A_0		SLy5-min $\sigma(A_0)$	DDME-min1 A_0		DDME-min1 $\sigma(A_0)$	units
SNM							
ρ_0	0.162	$\pm$	0.002	0.150	$\pm$	0.001	fm^{-3}
$e(\rho_0)$	−16.02	$\pm$	0.06	−16.18	$\pm$	0.03	MeV
m^*/m	0.698	$\pm$	0.070	0.573	$\pm$	0.008	
J	32.60	$\pm$	0.71	33.0	$\pm$	1.7	MeV
K_0	230.5	$\pm$	9.0	261	$\pm$	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...**

Modifing the χ² artificially:

→ **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



- 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:

Beyond statistical errors there exist other types of errors!

Differences among equally “good” models

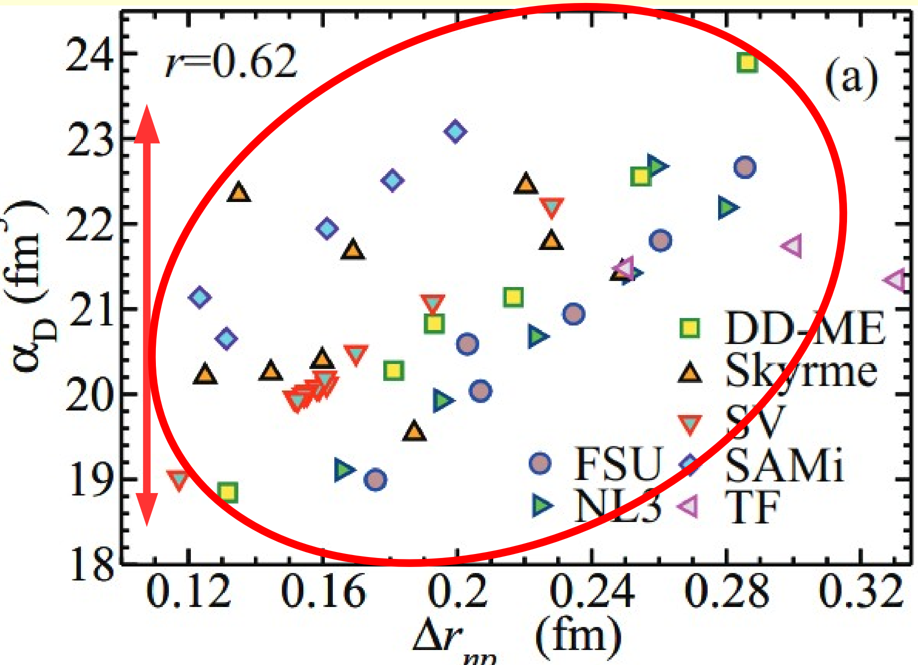
*** Up to now statistical errors from the fit. Is that the whole story?**

$$\sigma^2 = \sigma^2_{\text{stat}} + \sigma^2_{\text{syst}}$$

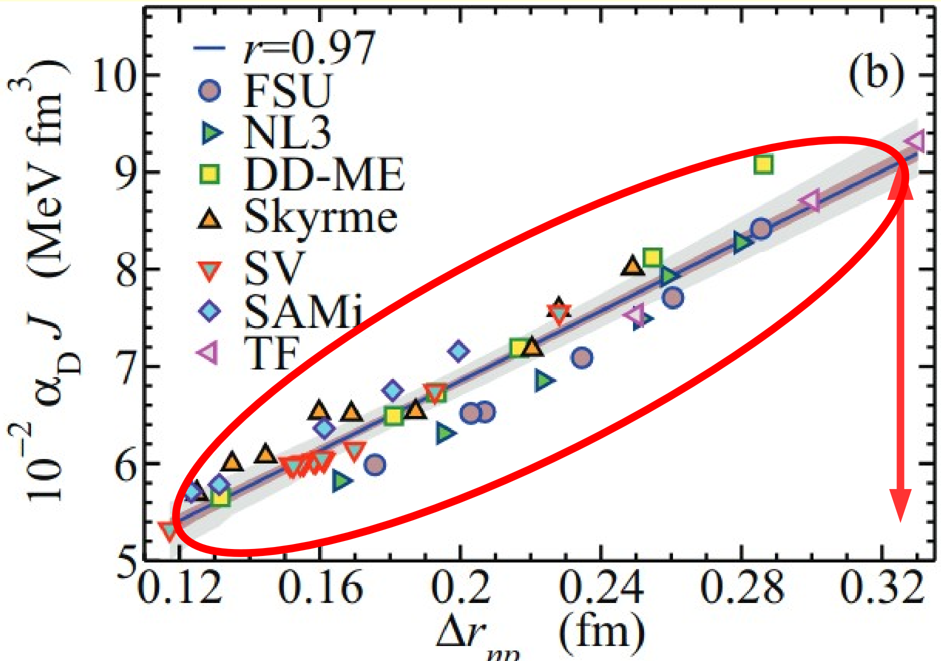
*** Differences between theory and experiment:** model error or systematic theoretical error → not allways possible.

*** Differences among (reasonable) models → proxy to model error**

Model errors large



Correlation between models low



Correlation between models high

Model errors large

Reminder from yesterday:
Dipole polarizability (Giant Dipole Resonance)

→ Calculate the polarizzability (α), **proportional to m_{-1}** from the **dielectric theorem** and **Droplet Model** ($J=a_A$)

$$\alpha_D = \frac{8\pi e^2}{9} m_{-1}(E1)$$

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

J. Meyer, P. Quentin, and B. Jennings, Nucl. Phys. A **385**, 269

$$a_{\rm sym}(A) = \frac{J}{1+x_A}, \quad \text{with} \quad x_A = \frac{9J}{4Q}A^{-1/3} \qquad \Delta r_{np}^{\rm DM} = \frac{2r_0}{3J}[J - a_{\rm sym}(A)]A^{1/3}(I - I_C)$$

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

Polarizability must increase with the mass (for the dipole $A^{5/3}$, for the quadrupole $A^{7/3}$ and so on) and **surface symmetry energy** and **decrease** with the **bulk symmetry energy**