Nuclear Structure Theory (lecture II)

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Glossary part 1 : DFT for Coulomb systems

According to Lévy and Lieb, for a system of fermions, it is possible to define an exact functional that relates energy and particle density:

$$E_{\text{exact}} = E[\rho]$$

In the case of electron systems, the **Coulomb interaction is known**. Density Functional Theory (DFT) was created initially (only) for electronic systems.

The lowest-order approximation for the energy (i.e. Hartree-Fock) is known but is not the DFT energy! There are also a few exact results for electrons.

Electronic DFT is called *ab initio*. Nonetheless, existing functionals usually include empirical parameters.

The electronic many-body problem

We are concerned with a quantum system governed by a Hamiltonian:

$$H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}\sum_{i\neq j=1}^{N} V(i,j) + V_{\text{ext}}(i)$$

In the case of nuclei and electrons, clearly:

$$H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m_e}\nabla_i^2 + \frac{1}{2}\sum_{i\neq j=1}^{N} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} + \sum_{i=1}^{N}\sum_{\alpha=1}^{M} \frac{Z_\alpha e^2}{|\vec{r}_i - \vec{R}_\alpha|}$$

Yet, the *N*-electron problem cannot be solved exactly even though the Coulomb force is known.

The Hohenberg-Kohn theorem

The original theorem and its proof can be found in P. Hohenberg, W. Kohn, Phys. Rev. 136, B864 (1964). They have in mind a system of interacting fermions ($H = T + V$) in some external potential V_{ext}.

a) There exist a functional of the fermion density

$$E_{V_{\rm ext}}[\rho] = \langle \Psi | T + V + V_{\rm ext} | \Psi \rangle = F[\rho] + \int d^3r \; V_{\rm ext}(r)\rho(r)$$

and the part denoted by F is universal (for nuclei, it would be the only part).

b) It holds:

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

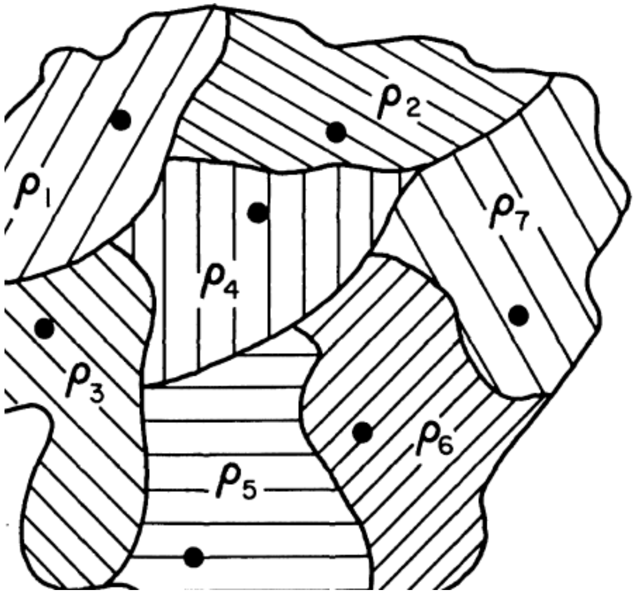
The variational principle is written for the density. The w.f. may be even too large to write !! (Try as an exercise to estimate its dimension...)

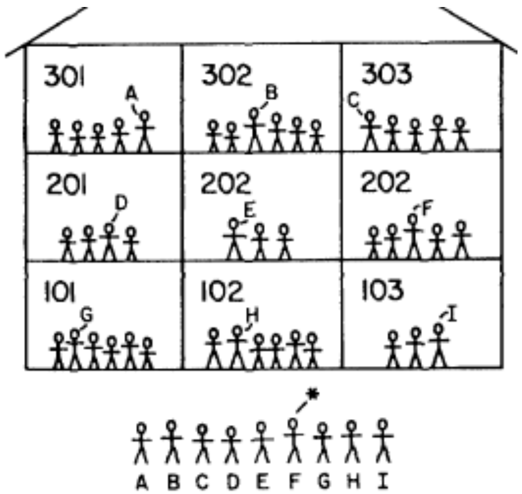
The constrained search approach by Lévy-Lieb

$$E_0 = \min_\Psi \langle \Psi | H | \Psi \rangle,$$

$$E_0 = \min_\rho \left(\min_{\Psi \to \rho} \langle \Psi | H | \Psi \rangle \right) = \min_\rho E[\rho],$$

$$E[\rho] = \min_{\Psi \to \rho} \langle \Psi | H | \Psi \rangle.$$





We consider all w.f.'s that correspond to a specific density with the symbol

$$\Psi \to \rho$$

"instead of finding the tallest child in the school by lining all of them in the yard, we just line in the yard the tallest pupils of each class..."

The simplest functional (EDF)

Non-interacting uniform gas
(either electrons
or protons+neutrons = symmetric nuclear matter)

$$\phi_k = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{r}} \quad k_F = \left(\frac{3\pi^2\rho}{2}\right)^{1/3}$$

$$E = T = \sum_k t_{kk} = 4\frac{\Omega}{(2\pi)^3} \int d^3k \int d^3r \ \phi^*_{\vec{k}}(\vec{r}) \left(-\frac{\hbar^2}{2m}\nabla^2\right) \phi_{\vec{k}}(\vec{r})$$

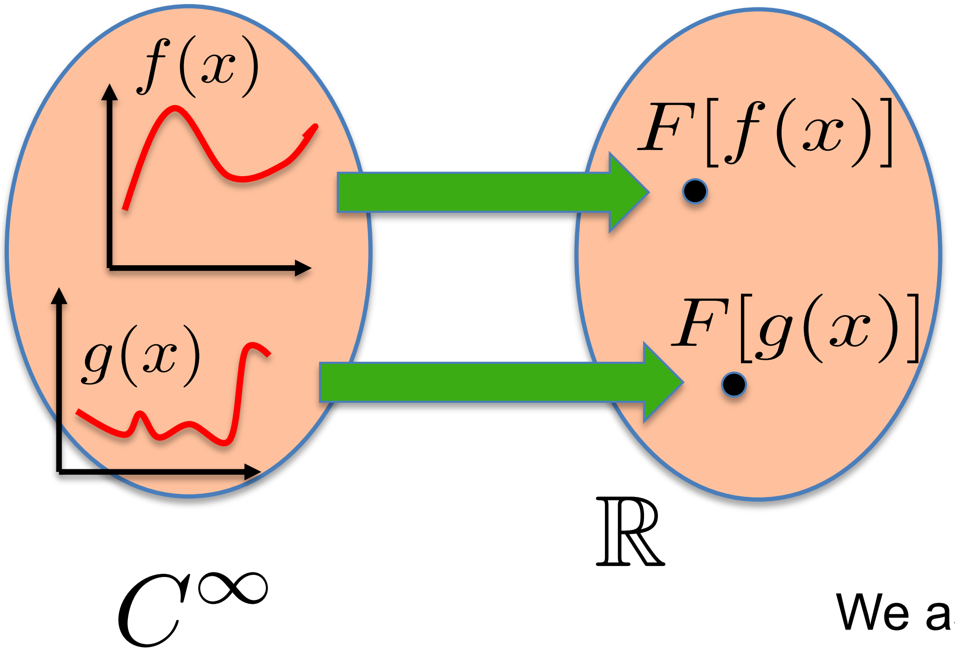
$$E = \frac{\Omega}{2\pi^3} \int_0^{k_F} 4\pi k^2 dk \ \frac{1}{\Omega} \left(\frac{\hbar^2 k^2}{2m}\right) \int d^3r \ 1 = \frac{2}{\pi^2}\frac{\hbar^2}{2m}\frac{k_F^5}{5}\Omega.$$

$$E = \int d^3r \ C\rho^{5/3}$$

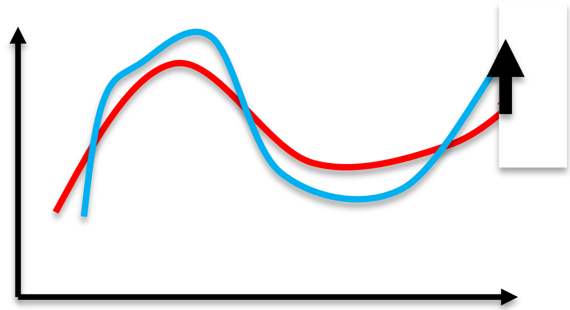
$$E = \int \mathcal{E}[\rho] \ d^3r$$

Energy density = $\mathcal{E}$

Functionals and functional derivative



$$f(x) + \epsilon\eta(x)$$



We assume that for any $\eta(x)$ we can write

$$F\left[f(x) + \epsilon\eta(x)\right] = F[f] + \frac{dF}{d\epsilon}[f+\epsilon\eta]\bigg|_{\epsilon=0} \epsilon + \ldots$$

$$\frac{dF}{d\epsilon}[f+\epsilon\eta]\bigg|_{\epsilon=0} = \int dx \, \frac{\delta F}{\delta f(x)} \eta(x)$$

Functional derivative

Analogy with the partial derivative:

$$\delta F = \frac{dF}{d\epsilon}[f+\epsilon\eta]\Big|_{\epsilon=0}\epsilon = \int dx\ \frac{\delta F}{\delta f(x)}\epsilon\eta(x) \quad \Longleftrightarrow \quad \delta F = \sum_i \frac{\delta F}{\delta f_i}\delta f_i$$

Equivalent formula:

$$\frac{\delta F}{\delta f(y)} = \lim_{\epsilon\to 0}\frac{F[f(x)+\epsilon\delta(x-y)] - F[f(x)]}{\epsilon} \qquad \frac{\delta F}{\delta f_j} = \lim_{\epsilon\to 0}\frac{F[f_j+\epsilon\delta_{ij}] - F[f_j]}{\epsilon}$$

Practical rules:

$$F = \int dx\ g(x)f(x) \quad \Rightarrow \quad \frac{\delta F}{\delta f(x)} = g(x)$$

$$F = \int dx\ h[f(x)] \quad \Rightarrow \quad \frac{\delta F}{\delta f(x)} = \frac{\partial h}{\partial f}(x)$$

Exercise for students:

a) Prove the formulas in these two slides (#7 and #8);

b) Prove: $F = \int dx\ g[f(x), f'(x)] \quad \Rightarrow \quad \frac{\delta F}{\delta f(x)} = \frac{\partial g}{\partial f} - \frac{d}{dx}\frac{\partial g}{\partial f'}$

(you know it from Euler-Lagrange equation!)

The Kohn-Sham (KS) scheme

We assume that the density can be expressed in terms of **single-particle orbitals**, and that the kinetic energy has the simple form:

$$\rho(\vec{r}) = \sum_i \phi_i^*(\vec{r})\phi_i(\vec{r}) \qquad T = \sum_i \int d^3r\ \phi_i^*(\vec{r}) \left(-\frac{\hbar^2\nabla_i^2}{2m} \right) \phi_i(\vec{r})$$

We have said that the energy must be minimized, but we add a constraint associated with the fact that we want **orbitals that form an orthonormal set** (Lagrange multiplier):

$$E - \sum_i \varepsilon_i \int d^3r\ \phi_i^*(\vec{r})\phi_i(\vec{r}) = T + F[\rho] + \int d^3r\ V_{\rm ext}(\vec{r})\rho(\vec{r}) - \sum_i \varepsilon_i \int d^3r\ \phi_i^*(\vec{r})\phi_i(\vec{r})$$

The variation of this quantity, $(\delta/\delta\phi^*)... = 0$ produces a Schrödinger-like equation:

$$\left(-\frac{\hbar^2\nabla_i^2}{2m} + \frac{\delta F}{\delta\rho} + V_{\rm ext} \right) \phi_i(\vec{r}) = \varepsilon_i\phi_i(\vec{r})$$

$$h\phi_i = \varepsilon_i\phi_i$$

"DFT is an exactification of Hartree-Fock" (W. Kohn).

Glossary part 2: DFT for nuclei

In the case of nuclei, we do not have (yet) a "fundamental Hamiltonian" to start from. All EDFs are based on an *ansatz* for the form of *E*, and a parameter fit.

All started with the invention of HF with effective forces. At a given point, these forces have been seen only as a way to "generate" a total energy from $\langle \Phi | T + V | \Phi \rangle$. Thus, there is no considerable difference between HF and KS-DFT.

Skyrme...

Gogny...

...and covariant

EDFs

Skyrme force or "pseudo-potential"

attraction **short-range repulsion**

$$v_{\rm Skyrme} = t_0\,(1 + x_0 P_\sigma)\,\delta(\vec{r}_1 - \vec{r}_2) + \frac{1}{2}t_1\,(1 + x_1 P_\sigma)\left(\vec{k}^{\dagger 2}\delta(\vec{r}_1 - \vec{r}_2) + \delta(\vec{r}_1 - \vec{r}_2)\vec{k}^2\right)$$

$$+\; t_2\,(1 + x_2 P_\sigma)\,\vec{k}^\dagger \cdot \delta(\vec{r}_1 - \vec{r}_2)\vec{k} + \frac{1}{6}t_3\,(1 + x_3 P_\sigma)\,\delta(\vec{r}_1 - \vec{r}_2)\rho^\alpha\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right)$$

$$+\; iW_0\,(\sigma_1 + \sigma_2)\cdot \vec{k}^\dagger \times \delta(\vec{r}_1 - \vec{r}_2)\vec{k}$$

$$\vec{k} = -\frac{i}{2}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right)$$

- There are velocity-dependent terms which mimic the finite-range.
- The last term is a zero-range spin-orbit.
- In total: 10 free parameters to be fitted (typically).

Skyrme force as a generator of an EDF

Let us see how it works with a **simplified force in the case of even-even nuclei.**

$$V_{\mathrm{Skyrme}} = \left[t_0 + \frac{t_3}{6}\rho^{\alpha}\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)\right]\delta(\vec{r}_1-\vec{r}_2)$$

$$E_{\mathrm{Skyrme}} = \frac{1}{2}\sum_{ij}\langle ij|V(1-P_{12})|ij\rangle = \frac{1}{2}\sum_{ij}\int d^3r_1 d^3r_2\ \phi_i^*(\vec{r}_1)\phi_j^*(\vec{r}_2)[\ldots]\delta(\vec{r}_1-\vec{r}_2)(1-P_M P_\sigma P_\tau)\phi_i(\vec{r}_1)\phi_j(\vec{r}_2)$$

$$P_M = 1 \qquad P_\sigma = \frac{1+\vec{\sigma}_1\cdot\vec{\sigma}_2}{2} \qquad P_\tau = \delta(q_i, q_j)$$

$$E_{\mathrm{Skyrme}} = \frac{1}{2}\sum_{ij}\int d^3r\ \phi_i^*(\vec{r})\phi_j^*(\vec{r})[t_0 + \frac{t_3}{6}\rho^{\alpha}](1-\frac{1}{2}\delta(q_i,q_j))\phi_i(\vec{r})\phi_j(\vec{r})$$

$$E = \frac{1}{2}\int d^3r\ (t_0 + \frac{t_3}{6}\rho^{\alpha}(r))(\rho^2(r) - \frac{1}{2}\rho_p^2(r) - \frac{1}{2}\rho_n^2(r))$$

Exercise: add T and derive the KS equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + U_q\right)\phi_{q,i} = \varepsilon_i\phi_{q,i} \qquad U = \frac{\delta E}{\delta\rho_q}$$

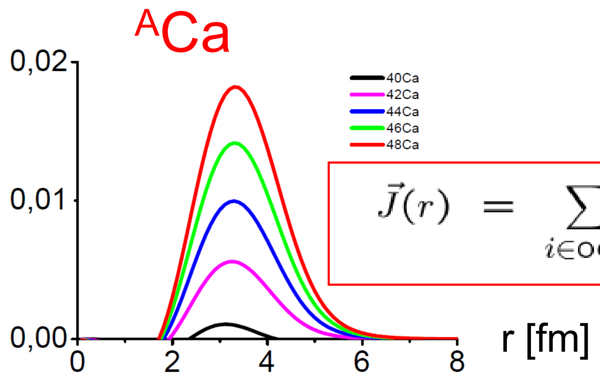
EDF from the full V_{skyrme} (even-even case)

$$\vec{k} = -\frac{i}{2}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right)$$ produces: $$\phi \vec{\nabla} \phi \quad \Rightarrow \quad \vec{\nabla}\rho$$

Other quadratic terms: $$\nabla^2 \rho = 2 \sum_i \phi_i^* \nabla^2 \phi_i + 2\tau \qquad \tau = \sum_i |\vec{\nabla}\phi_i|^2$$

The **spin** operators lead to:

$$\vec{J} = \sum_{i,\sigma,\sigma'} \phi_i^\dagger \vec{\nabla}\phi_i \times \langle \sigma' | \vec{\sigma} | \sigma \rangle$$



$$\vec{J}(r) = \sum_{i \in \mathrm{occ}} 2(2j_i + 1) \langle \vec{\ell} \cdot \vec{s} \rangle \frac{\vec{r}}{r^4} u_i^2(r)$$

$$\mathcal{E}^{\mathrm{Skyrme}} = C^{\rho\rho}[\rho]\rho^2 + C^{\rho\tau}\rho\tau + C^{J^2}\vec{J}^{\,2} + C^{(\nabla\rho)^2}\left(\vec{\nabla}\rho\right)^2 + C^{\rho\vec{\nabla}\cdot\vec{J}}\rho\vec{\nabla}\cdot\vec{J}$$

$$E = \int d^3r \ \left[\mathcal{E}^{\text{kin}} + \mathcal{E}^{\text{Skyrme}} + \mathcal{E}^{\text{pairing}} + \mathcal{E}^{\text{Coulomb}}\right]$$

The complete Skyrme EDF including the odd case is complicated.

$$\begin{aligned}
\mathcal{E} = \int d^3r \mathcal{H}(\boldsymbol{r}) = \int d^3r \sum_{t=0,1} \Bigg\{ & C_t^{\rho}[\rho_0]\rho_t^2 + C_t^{s}[\rho_0]\boldsymbol{s}_t^2 + C_t^{\Delta\rho}\rho_t \boldsymbol{\nabla}^2\rho_t \\
& + C_t^{\nabla s}(\boldsymbol{\nabla}\cdot\boldsymbol{s})^2 + C_t^{\Delta s}\boldsymbol{s}_t\cdot\boldsymbol{\nabla}^2\boldsymbol{s}_t + C_t^{\tau}(\rho_t\tau_t - \boldsymbol{j}_t^2) \\
& + C_t^{T}\left(\boldsymbol{s}_t\cdot\boldsymbol{T}_t - \sum_{\mu,\nu=x}^{z} J_{t,\mu\nu}J_{t,\mu\nu}\right) \\
& + C_t^{F}\left[\boldsymbol{s}_t\cdot\boldsymbol{F}_t - \frac{1}{2}\left(\sum_{\mu=x}^{z} J_{t,\mu\mu}\right)^2 - \frac{1}{2}\sum_{\mu,\nu=x}^{z} J_{t,\mu\nu}J_{t,\nu\mu}\right] \\
& + C_t^{\nabla\cdot J}\left(\rho_t\boldsymbol{\nabla}\cdot\boldsymbol{J}_t + \boldsymbol{s}_t\cdot\boldsymbol{\nabla}\times\boldsymbol{j}_t\right) \Bigg\}
\end{aligned}$$

P.D. Stevenson, M.C. Barton, PPNP 104, 142 (2019)

Pairing: not discussed here.

Coulomb: known. Exchange is often approximated (e.g.: Slater approximation).

Gogny forces

$$v_{\text{Gogny}} = \sum_{j=1}^{2} e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_j^2}} \left(W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau\right)$$

$$+t_0\,(1+x_0 P_\sigma)\,\delta(\vec{r}_1-\vec{r}_2)\rho^\alpha\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right) + iW_{ls}\,(\sigma_1+\sigma_2)\cdot\vec{k}^\dagger\times\delta(\vec{r}_1-\vec{r}_2)\vec{k}$$

- There are two Gaussians with different ranges that are supposed to create nuclear saturation.
- The introduction of a density-dependent term seems unavoidable. This suggests that v_{Gogny} is also a pseudo-potential (EDF generator).
- The great advantage of the Gogny force is that it seems adequate not only for the HF/KS equations but to describe *nuclear superfluidity* as well.

Exercise: derive the HF or KS equation with v equal to the sum of the two Gaussians

$$E_{\text{Gogny}} = \langle\Phi|T+V|\Phi\rangle = \int \mathcal{E}^{\text{Gogny}}$$

Fitting the EDF parameters

- Empirical saturation point
- Masses of nuclei
- Charge radii of nuclei

$$\chi^2(\vec{p}\,) = \sum_{k=1}^{N_{\rm data}} \frac{\left(O_k^{\rm th.}(\vec{p}\,) - O_k^{\rm exp.}\right)^2}{(\Delta O)^2}$$

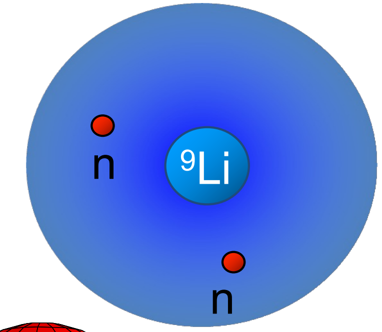
- More pseudo-observables like the equation of state of neutron matter
- More observables: excited states
- *A bit outside DFT philosophy: single-particle states and spin-orbit splittings*

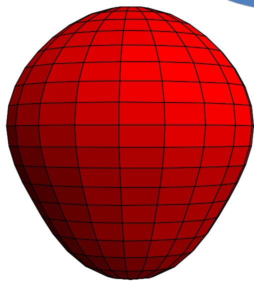
χ-square fitting is one widely used option to obtain the EDF parameters

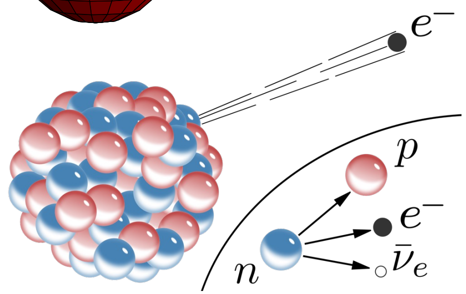
Increasing number of studies that employ Bayesian techniques (parameter distributions)

Status of DFT (short summary)

- Error on **masses** of the order of 1 MeV.
- (Controlled) predictions of **drip lines** and **super heavy** nuclei.
- Trends of **charge radii and deformations** fairly well reproduced.
- **Extrapolation to neutron matter and neutron stars.**
- Steady progress in the study of theoretical errors and of correlations among EDF parameters.
- Techniques based on **symmetry restoration** are available.
- **Giant resonances, charge-exchange transitions** are studied**.**
- Interest in **reactions, large amplitude phenomena like fission**.
- Merging with *ab initio.*

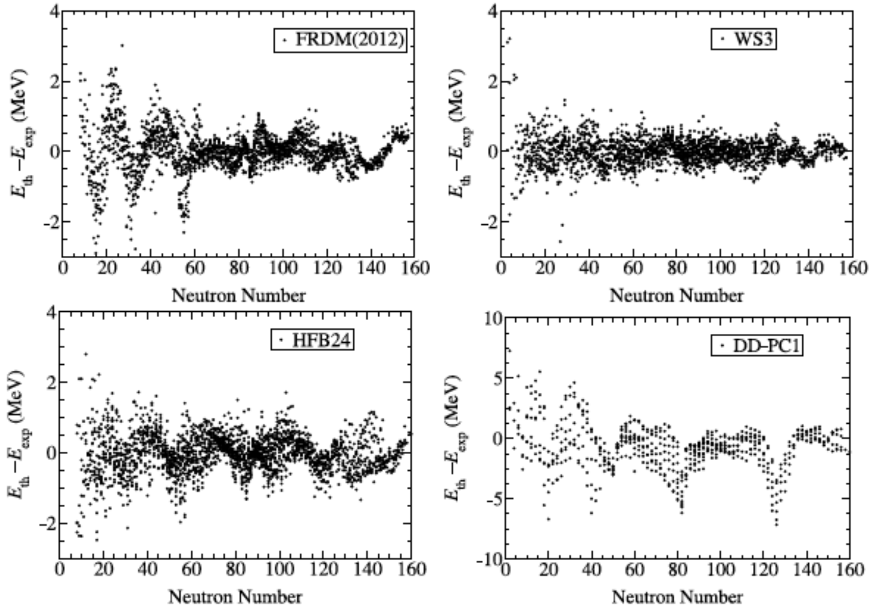






Much about this in the lectures by Iain, Magda.

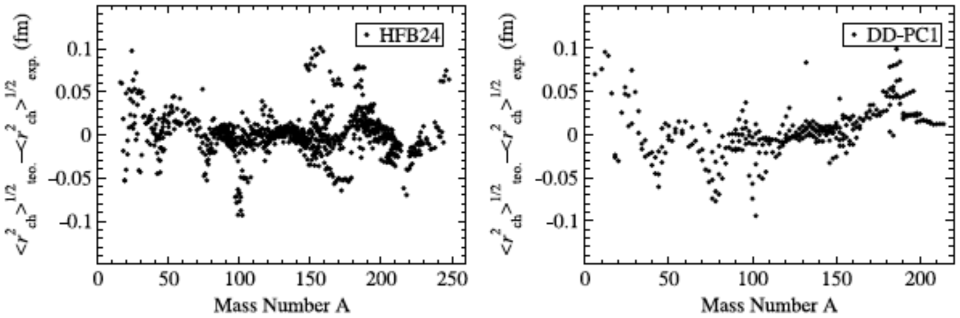
Masses and charge radii of atomic nuclei

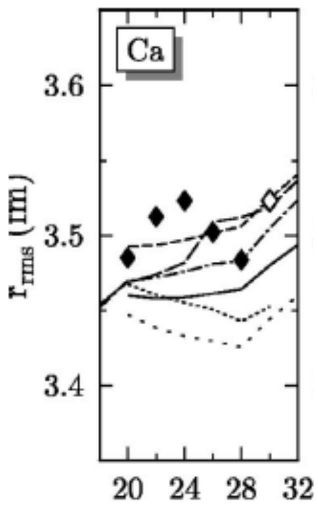


Model	Type	Nº par.	σ_M [MeV]
FRDM(2012)	Mac-Mic	38[a]	0,559[b]
WS4[c]	Mac-Mic	18	0,298[d]
HFB24	EDF	30[e]	0,549[f]
UNEDF1	EDF	12	1,88[g]
DD-PC1	EDF	9	2,01[h]

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

Masses: typical errors ≈ MeV. "Arches" show up.



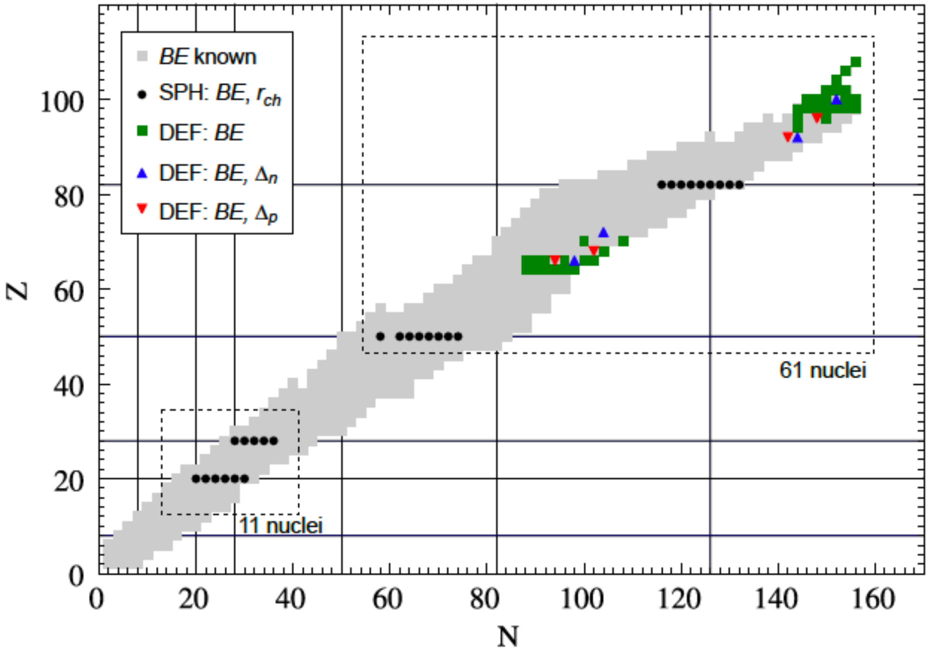


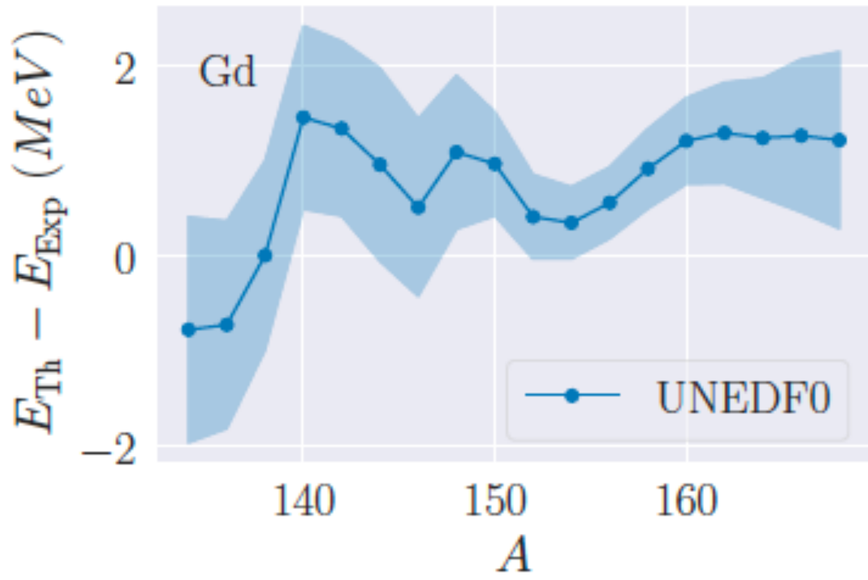
From M. Bender

For radii the pictures is somehow more blurred. More fingerprints of the basic limitations of the current EDFs.

See slides by Iain

Error propagation





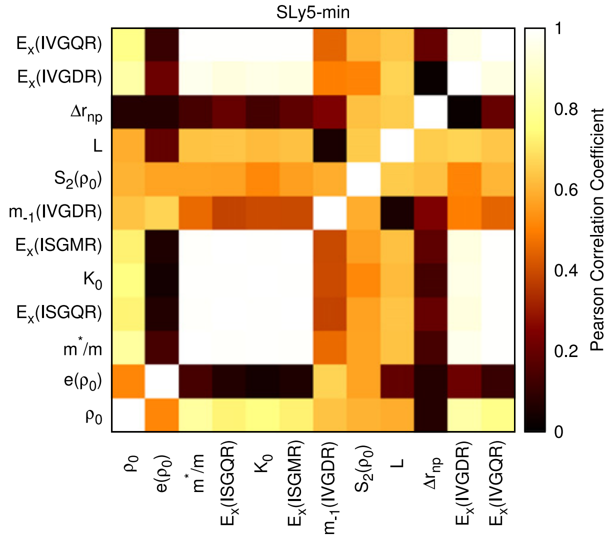
UNEDF0
Phys. Rev. C 82, 024313 (2010)

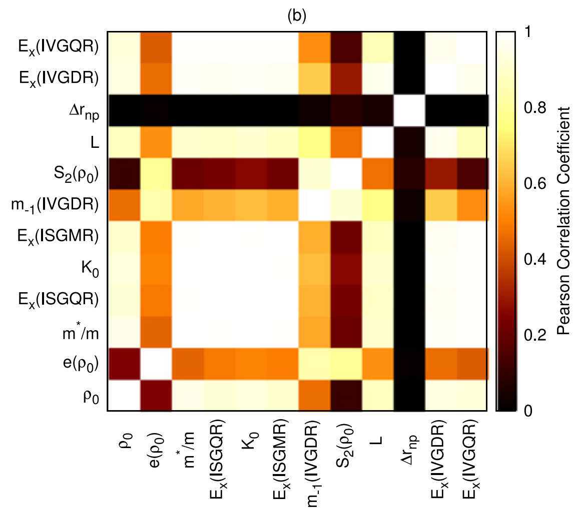
J. Phys. G 44, 044008 (2017)

Correlations

Covariance analysis for energy density functionals and instabilities

X Roca-Maza[1], N Paar[2] and G Colò[1]

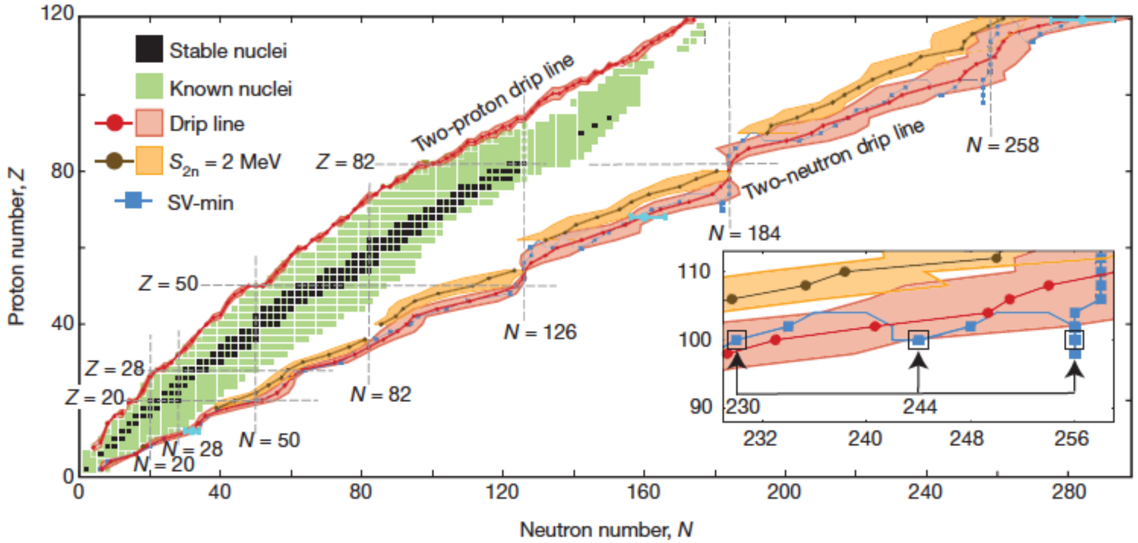




When a strong constraint is imposed on A, the correlations with other properties become very small.

The drip lines

J. Erler *et al.*, Nature 486, 509 (2012) - SEDF



A.V. Afanasjev *et al.*, Phys. Lett. B726, 680 (2013) - CEDF

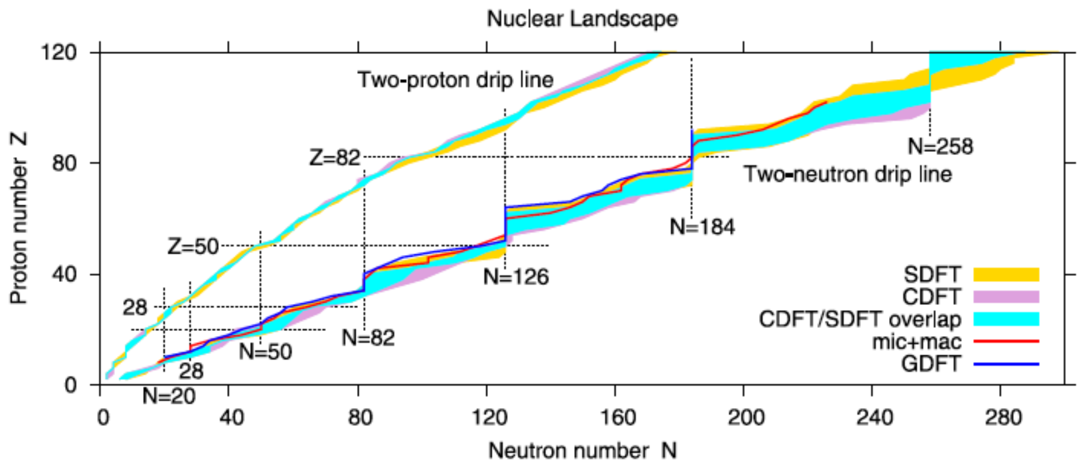


Fig. 4. The comparison of the uncertainties in the definition of two-proton and two-neutron drip lines obtained in CDFT and SDFT. The shaded areas are defined by the extremes of the predictions of the corresponding drip lines obtained with different parametrizations. The blue shaded area shows the area where the CDFT and SDFT results overlap. Non-overlapping regions are shown by dark yellow and plum colors for SDFT and CDFT, respectively. The results of the SDFT calculations are taken from the supplement to Ref. [2]. The two-neutron drip lines obtained by microscopic + macroscopic (FRDM [3]) and Gogny D1S DFT [5] calculations are shown by red and blue lines, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this Letter.)

How to not get lost

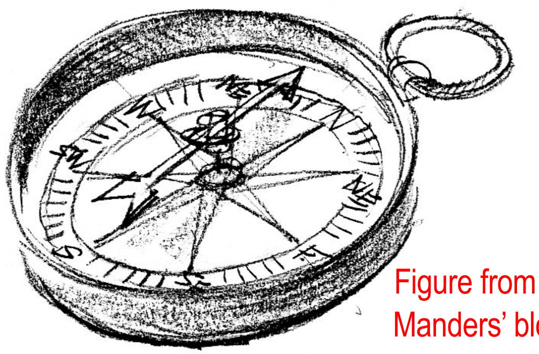


Figure from J. Manders' blog

In the case of axial quadrupole deformations:

$$\frac{\delta R}{R} \sim \beta$$

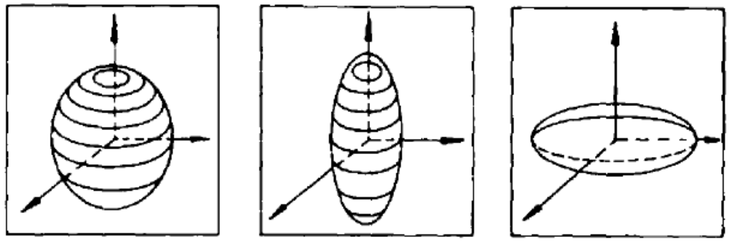
Intrinsic quadrupole moment $\langle Q \rangle \sim \beta$

There are non-axial deformations:

$$\delta R_x = R\left(\frac{\pi}{2}, 0\right) - R_0 = R_0\sqrt{\frac{5}{4\pi}}\beta cos\left(\gamma - \frac{2\pi}{3}\right)$$

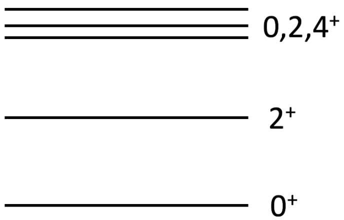
$$\delta R_y = R\left(\frac{\pi}{2}, \frac{\pi}{2}\right) - R_0 = R_0\sqrt{\frac{5}{4\pi}}\beta cos\left(\gamma + \frac{2\pi}{3}\right)$$

$$\delta R_z = R\left(0, 0\right) - R_0 = R_0\sqrt{\frac{5}{4\pi}}\beta cos\ \gamma$$

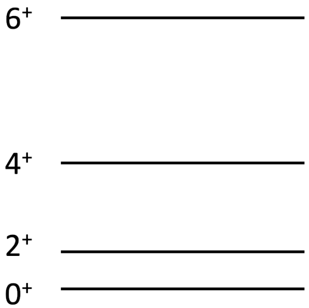


Some nuclei display "paradigmatic" spectra: (i) **spherical nuclei which vibrate** or (ii) **deformed nuclei which rotate**

$$E \sim \frac{\hbar}{2\mathcal{I}} J(J+1)$$



Vibrational spectra



Rotational spectra

Nuclear Physics

Interest in OTHER deformations

How to not get lost

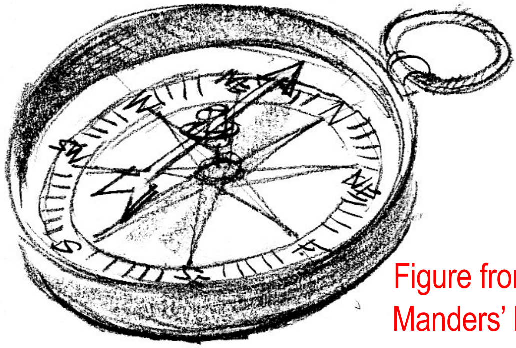
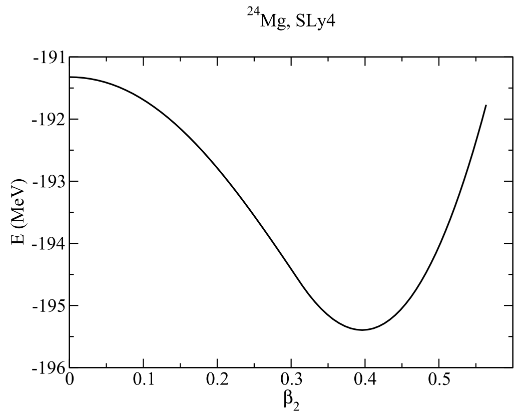
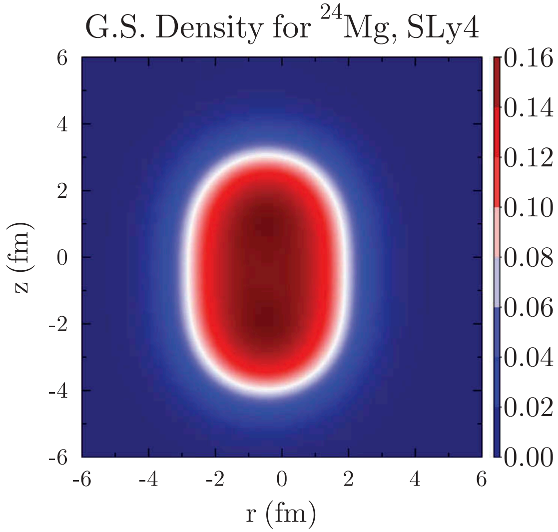


Figure from J. Manders' blog

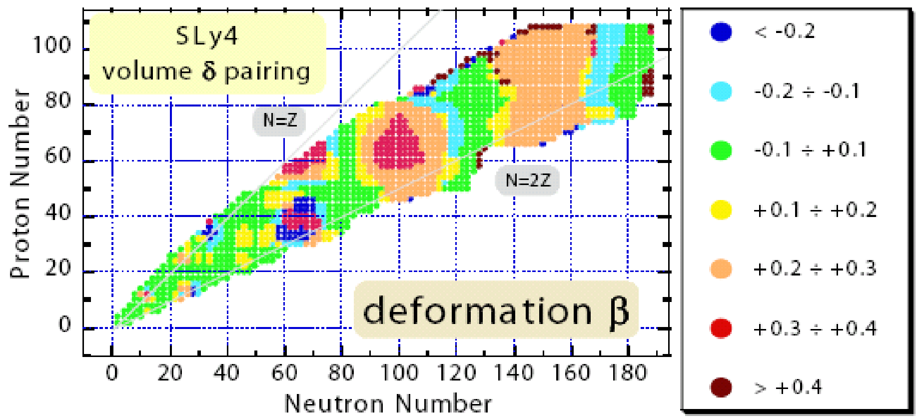


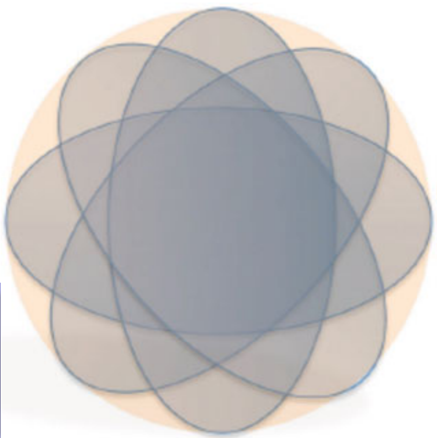


CONSTRAINED calculations:

$$H' = H - \lambda Q$$

They provide the whole energy surface.





Symmetry restoration in the lab frame

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This paper compiles the model parameters and zero-temperature properties of an extensive collection of published theoretical nuclear interactions, including 255 non-relativistic (Skyrme-like) forces, 270 relativistic mean field (RMF) and point-coupling (RMF-PC) forces, and 13 Gogny-like forces. This forms the most exhaustive tabulation of model parameters to date. The properties

In spite of the "proliferation" of EDFs, one should keep in mind that many of them have been built with limited purpose(s), or are outdated, or have been improved by the same authors who first introduced them.