Nuclear Energy Density Functionals

From Stable to Weakly-Bound Nuclei

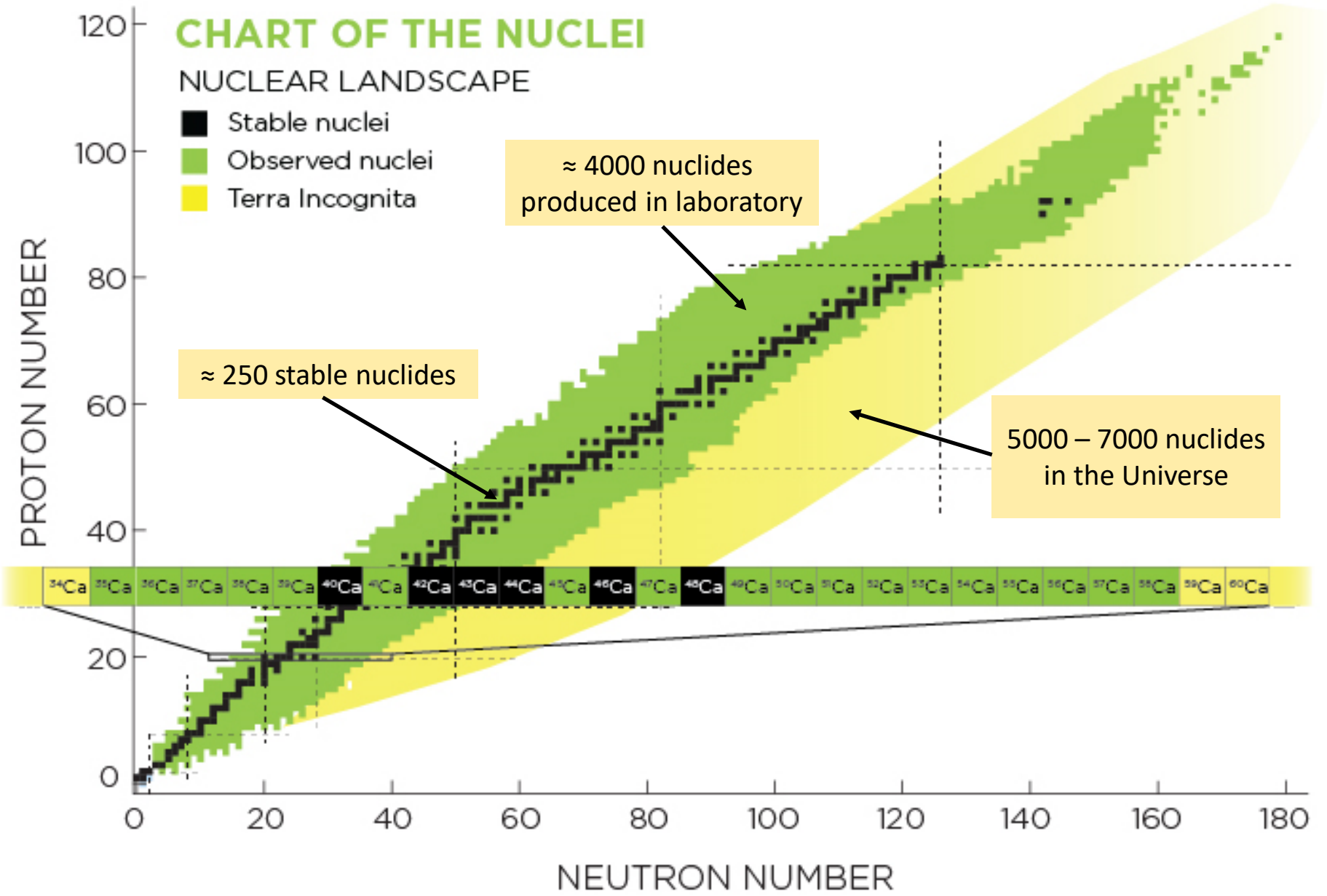


CHART OF THE NUCLEI
NUCLEAR LANDSCAPE
Stable nuclei
Observed nuclei
Terra Incognita
≈ 4000 nuclides produced in laboratory
≈ 250 stable nuclides
5000 – 7000 nuclides in the Universe
PROTON NUMBER
NEUTRON NUMBER
0
20
40
60
80
100
120
140
160
180

Elements of Density Functional Theory

DFT is the most popular method for electronic structure calculations of many-electron systems. No other method achieves comparable accuracy at the same computational cost.

A. The Hohenberg-Kohn Theorem

In ground-state DFT one is interested in systems of N interacting electrons described by the Hamiltonian:

$$
\begin{aligned}
H &= T + V + V_{ee} \\
&= -\sum_{i=1}^{N} \frac{\nabla_i^2}{2} + \sum_{i=1}^{N} v(\mathbf{r}_i) + \frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}
\end{aligned}
$$

The Hohenberg-Kohn theorem:

1. The ground-state (GS) wave function is a unique functional of the GS density:

$$\Psi_0(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \Psi[n_0(\vec{r})]$$

2. The GS energy:

$$E_0 \equiv E[n_0] = \langle \Psi[n_0] | \hat{H} | \Psi[n_0] \rangle$$

and the GS density n_0 of a system characterized by the external potential v_0 can be obtained from a variational principle which involves only the density:

$$E_0 = E_{v_0}[n_0] < E_{v_0}[n]$$

3. There exists a functional F[n] such that the energy functional can be written as:

$$E_{v_0}[n] = F[n] + \int d^3r \; v_0(\vec{r}) n(\vec{r})$$

The functional F[n] is universal → for a given particle-particle interaction it is independent of the potential $v_0(r)$ of the particular system ⇒ it has the same functional form for all systems.

The explicit density dependence of F[n] is not known!

B. Kohn-Sham DFT

Consider an auxiliary system of N *non-interacting* particles described by the Hamiltonian:

$$H_s = T + V_s$$

HK theorem ⇒ there exists a unique energy functional:

$$E_s[n] = T_s[n] + \int d^3r \; v_s(\mathbf{r}) n(\mathbf{r})$$

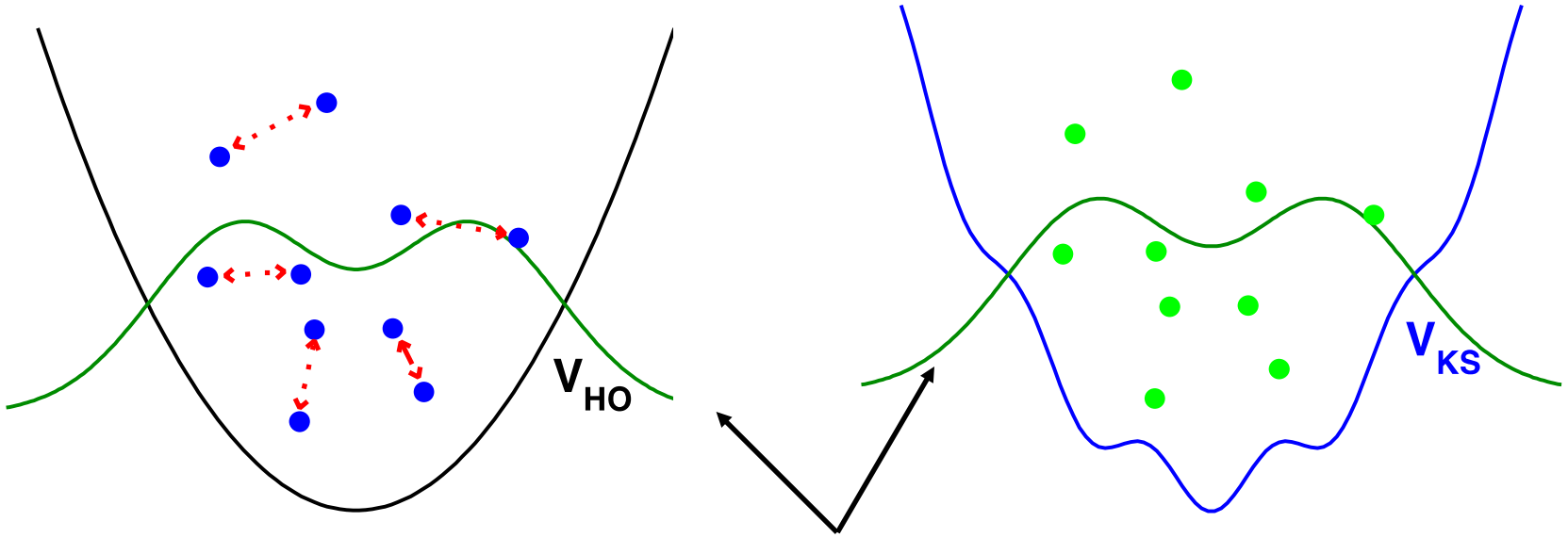
for which the variational equation yields the exact ground-state density $n_s(r)$ that corresponds to H_s.
$T_s[n]$ - universal kinetic energy functional of non-interacting particles.

For any interacting system, there exists a local single-particle (Kohn-Sham) potential $v_s(r)$, such that the exact ground-state density of the interacting system equals the ground-state density of the auxiliary problem:

$$n(\mathbf{r}) = n_s(\mathbf{r}) \equiv \sum_{i}^{occ} |\phi_i(\mathbf{r})|^2$$

Interacting system

Non-interacting system



Same density profiles

The single-particle orbitals are solutions of the Kohn-Sham equations:

$$\left[-\nabla^2/2 + v_s(\mathbf{r})\right]\phi_i(\mathbf{r}) = \varepsilon_i\phi_i(\mathbf{r})$$

The Hohenberg-Kohn functional is partitioned:

$$F[n] = T_s[n] + U[n] + E_{xc}[n]$$

Kinetic energy of the non-interacting system

Hartree term

Exchange-correlation energy which, by definition, includes everything else!

$$U[n] = \frac{1}{2}\int d^3r \int d^3r' \, \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

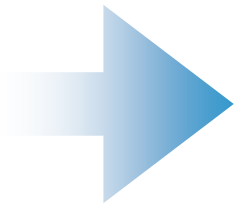
→ classical electrostatic energy of the charge distribution n(r).

The Kohn-Sham potential:

$$v_s[n(\mathbf{r})] = v(\mathbf{r}) + \int d^3r' \, \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + v_{xc}[n(\mathbf{r})]$$

where the *exchange-correlation potential* is defined by:

$$v_{xc}[n(\mathbf{r})] = \frac{\delta E_{xc}[n]}{\delta n(\mathbf{r})}$$



self-consistent Kohn-Sham DFT: includes correlations and therefore goes beyond the HF. It has the advantage of being a *local scheme*.

The practical usefulness of the Kohn-Sham scheme depends entirely on whether accurate approximations for E_{xc} can be found!

C. Approximations for E_{xc}

The true E_{xc} is a universal functional of the density, i.e. it has the same functional form for all systems.

(i) local density approximation (LDA):

$$E_{xc}^{LDA}[n] = \int d^3r \; n(\mathbf{r}) e_{xc}^{unif}(n(\mathbf{r}))$$

where $e^{unif}_{xc}(n)$ is the exchange-correlation energy per particle of the homogeneous electron gas with spatially uniform density n.

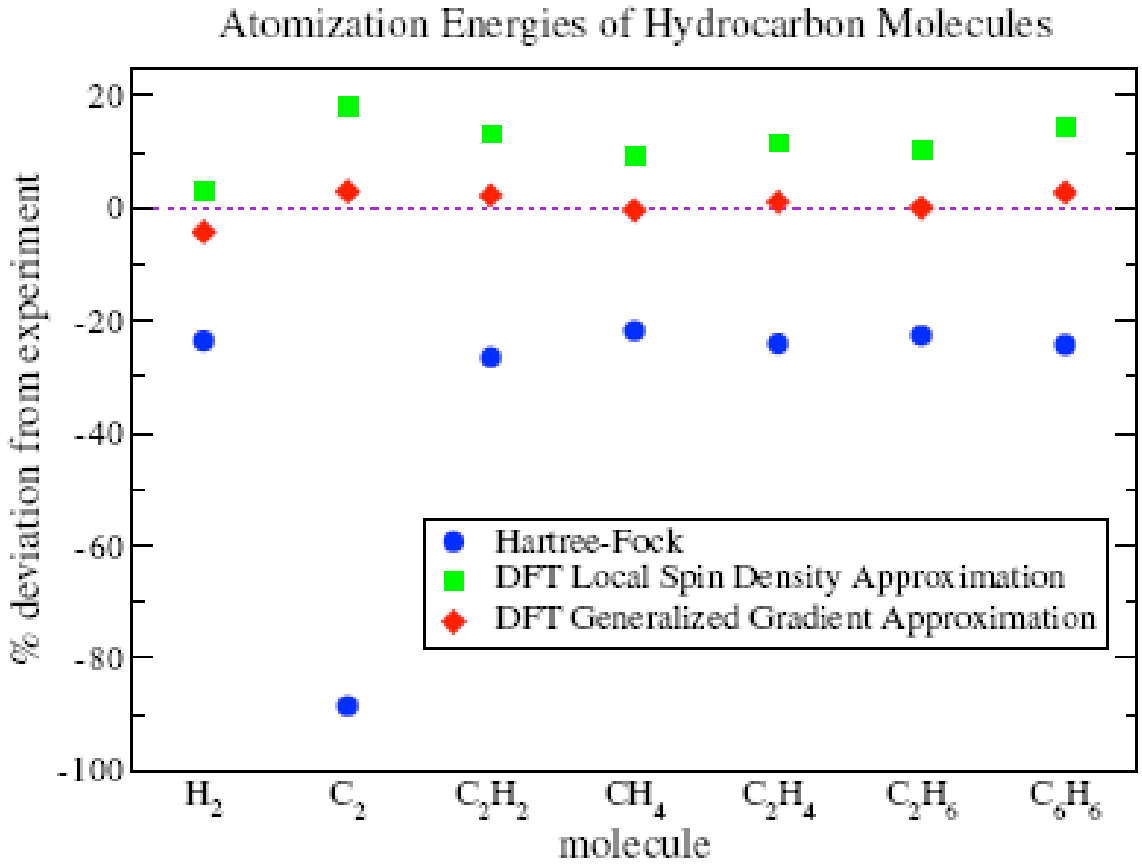
(ii) generalized gradient approximations (GGAs):

$$E_{xc}^{GGA}[n] = \int d^3r f(n(\mathbf{r}), \nabla n(\mathbf{r}))$$

→ the function f in GGA is not unique and many different forms have been considered.

Exchange-correlation functional:

Heaven of chemical accuracy



unoccupied $\{\Psi_i\}$

ε_x

τ and/or $\nabla^2\rho$

$\nabla\rho$

ρ

generalized RPA

hyper-GGA

meta-GGA

GGA

LDA

Hartree world

Ladder of DFT approximations for E_{xc}

Nuclear Energy Density Functionals

Nuclear Energy Density Functionals: the many-body problem is mapped onto a one body problem without explicitly involving inter-nucleon interactions!

The *self-consistent mean-field* approach to nuclear many-body problem is analogous to *Kohn-Sham DFT*, and provides a unified microscopic description of the structure of stable nuclei and systems far from stability.

The exact universal energy density functional is approximated with *powers and gradients of ground-state nucleon densities and currents.*

Local densities and currents

The full density matrix can be decomposed into four separate spin-isospin terms:

$$\begin{aligned}
&\rho(\mathbf{r}\sigma\tau, \mathbf{r}'\sigma'\tau') \\
&\quad = \frac{1}{4}\Bigg\{ \Big[\rho_{00}(\mathbf{r},\mathbf{r}')\,\delta_{\sigma\sigma'} + \mathbf{s}_{00}(\mathbf{r},\mathbf{r}')\cdot\boldsymbol{\sigma}_{\sigma'\sigma}\Big]\,\delta_{\tau\tau'} \\
&\qquad + \sum_{\alpha=-1}^{+1}\Big[\rho_{1\alpha}(\mathbf{r},\mathbf{r}')\,\delta_{\sigma\sigma'} + \mathbf{s}_{1\alpha}(\mathbf{r},\mathbf{r}')\cdot\boldsymbol{\sigma}_{\sigma'\sigma}\Big](\tau_{\tau'\tau})_\alpha\Bigg\}
\end{aligned}$$

where: $\boldsymbol{\sigma}_{\sigma'\sigma} = (\sigma'|\hat{\boldsymbol{\sigma}}|\sigma) \quad , \quad \boldsymbol{\tau}_{\tau'\tau} = (\tau'|\hat{\boldsymbol{\tau}}|\tau)$

For pure proton and neutron states only the α = 0 components of the isovector densities contribute.

There are six local densities and currents that can be derived from the full density matrix. We omit the second index in the densities, and with T=0 or 1:

Local densities and currents:

T=0 density:

$$\rho_0(\mathbf{r}) = \rho_0(\mathbf{r},\mathbf{r}) = \sum_{\sigma\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma\tau)$$

T=1 density:

$$\rho_1(\mathbf{r}) = \rho_1(\mathbf{r},\mathbf{r}) = \sum_{\sigma\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma\tau)\,\tau$$

T=0 spin density:

$$\mathbf{s}_0(\mathbf{r}) = \mathbf{s}_0(\mathbf{r},\mathbf{r}) = \sum_{\sigma\sigma'\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma'\tau)\,\boldsymbol{\sigma}_{\sigma'\sigma}$$

T=1 spin density:

$$\mathbf{s}_1(\mathbf{r}) = \mathbf{s}_1(\mathbf{r},\mathbf{r}) = \sum_{\sigma\sigma'\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma'\tau)\,\boldsymbol{\sigma}_{\sigma'\sigma}\,\tau$$

Current:

$$\mathbf{j}_T(\mathbf{r}) = \tfrac{i}{2}(\nabla' - \nabla)\,\rho_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

Spin-current tensor:

$$\mathcal{J}_T(\mathbf{r}) = \tfrac{i}{2}(\nabla' - \nabla) \otimes \mathbf{s}_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

Kinetic density:

$$\tau_T(\mathbf{r}) = \nabla\cdot\nabla'\,\rho_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

Kinetic spin-density:

$$\mathbf{T}_T(\mathbf{r}) = \nabla\cdot\nabla'\,\mathbf{s}_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

The Skyrme energy density functional

In the Skyrme KS approach, the total binding energy is given by the sum of the kinetic energy, the Skyrme energy functional that models the effective interaction between nucleons, the Coulomb energy, the pair energy, and corrections for spurious motions:

$$E = E_{\rm kin} + \int d^3r\, \mathcal{E}_{\rm Sk} + E_{\rm Coul} + E_{\rm pair} - E_{\rm corr}$$

The Skyrme energy functional:

$$\mathcal{E}_{\rm Sk} = \sum_{T=0,1} \left(\mathcal{E}_T^{\rm even} + \mathcal{E}_T^{\rm odd} \right)$$

Contains only time-even dens.

Dependence on time-odd currents

Density-dependent coefficients

$$\mathcal{E}_T^{\rm even} = C_T^{\rho} \rho_T^2 + C_T^{\Delta\rho}\, \rho_T \Delta\rho_T + C_T^{\tau}\, \rho_T \tau_T + C_T^{J} \mathcal{J}_T^2 + C_T^{\nabla J}\, \rho_T\, \nabla\cdot\mathbf{J}_T$$

$$\mathcal{E}_T^{\rm odd} = C_T^{s}\, \mathbf{s}_T^2 + C_T^{\Delta s}\, \mathbf{s}_T\cdot\Delta\mathbf{s}_T + C_T^{sT}\, \mathbf{s}_T\cdot\mathbf{T}_T + C_T^{\nabla s}\, (\nabla\cdot\mathbf{s}_T)^2 + C_T^{j}\, \mathbf{j}_T^2 + C_T^{\nabla j}\, \mathbf{s}_T\cdot\nabla\times\mathbf{j}_T$$

does not contribute for even-even nuclei!

PAIRING CORRELATIONS

The pairing-energy functional:

$$E_{\rm pair} = \sum_{q=p,n} \frac{V_q}{4} \int d^3r \left[1 - \left(\frac{\rho(\mathbf{r})}{\rho_c}\right)^{\beta}\right] \tilde{\rho}_q^2(\mathbf{r})$$

corresponds to the density-dependent two-body zero-range local pairing force:

$$v_{\rm pair} = \frac{V_0}{2}(1 - \hat{P}_\sigma) \left[1 - \left(\frac{\rho(\mathbf{r}_1)}{\rho_c}\right)^{\beta}\right] \delta(\mathbf{r}_1 - \mathbf{r}_2)$$

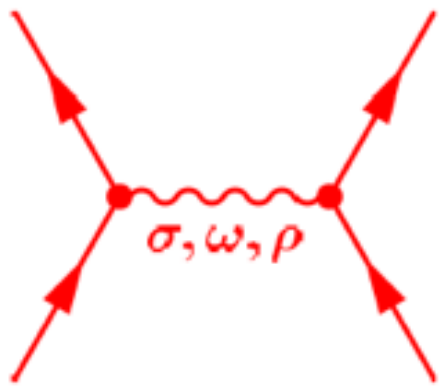
Volume pairing
$\rho_c \to \infty$

Surface pairing
$\rho_c \approx \rho_{nm}$

The pairing strengths $V_{p,n}$ are adjusted phenomenologically to reproduce the odd-even staggering of energies in selected chains of nuclei.

Relativistic Energy Density Functionals

FINITE RANGE



CONTACT INTERACTION

The explicit meson-exchange picture is merely a convenient representation of low-energy NN interactions, and the finite-range meson degrees of freedom can be replaced by contact nucleon-nucleon interactions in the corresponding channels.

Kinematical relativistic effects are small in nuclei, but the different behavior of the large Lorentz scalar and vector potentials leads to large dynamical relativistic interaction effects in the nuclear matter energy density (natural saturation mechanism!)

Relativistic energy density functionals:

The elementary building blocks are two-fermion terms of the general type:

$$(\bar{\psi}\mathcal{O}_\tau\Gamma\psi) \qquad \mathcal{O}_\tau \in \{1, \tau_i\} \qquad \Gamma \in \{1, \gamma_\mu, \gamma_5, \gamma_5\gamma_\mu, \sigma_{\mu\nu}\}$$

... isoscalar and isovector four-currents and scalar densities:

$$\begin{aligned}
j_\mu &= \langle\phi_0|\overline{\psi}\gamma_\mu\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\gamma_\mu\psi_k \ , \\
\vec{j}_\mu &= \langle\phi_0|\overline{\psi}\gamma_\mu\vec{\tau}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\gamma_\mu\vec{\tau}\psi_k \ , \\
\rho_S &= \langle\phi_0|\overline{\psi}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\psi_k \ , \\
\vec{\rho}_S &= \langle\phi_0|\overline{\psi}\vec{\tau}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\vec{\tau}\psi_k
\end{aligned}$$

where $|\phi_0\rangle$ is the nuclear ground state.

Four-fermion (contact) interaction terms in the various isospace-space channels

isoscalar-scalar: $(\bar{\psi}\psi)^2$

isoscalar-vector: $(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi)$

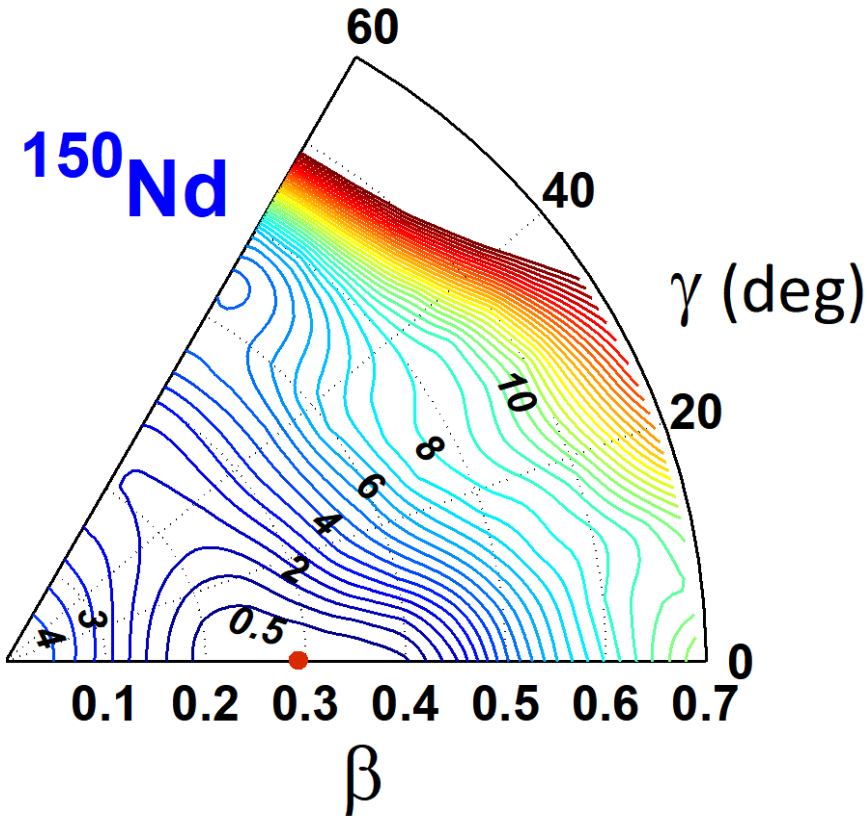
isovector-scalar: $(\bar{\psi}\vec{\tau}\psi)\cdot(\bar{\psi}\vec{\tau}\psi)$

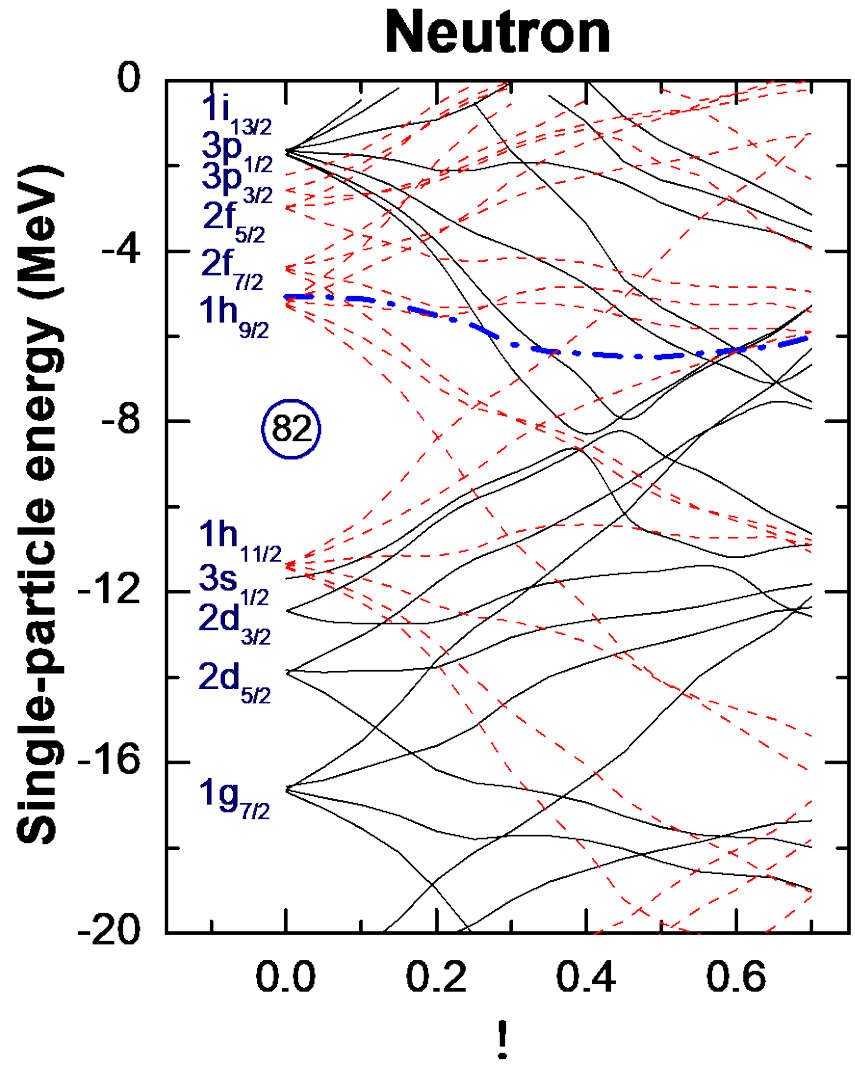
isovector-vector: $(\bar{\psi}\vec{\tau}\gamma_\mu\psi)\cdot(\bar{\psi}\vec{\tau}\gamma^\mu\psi)$

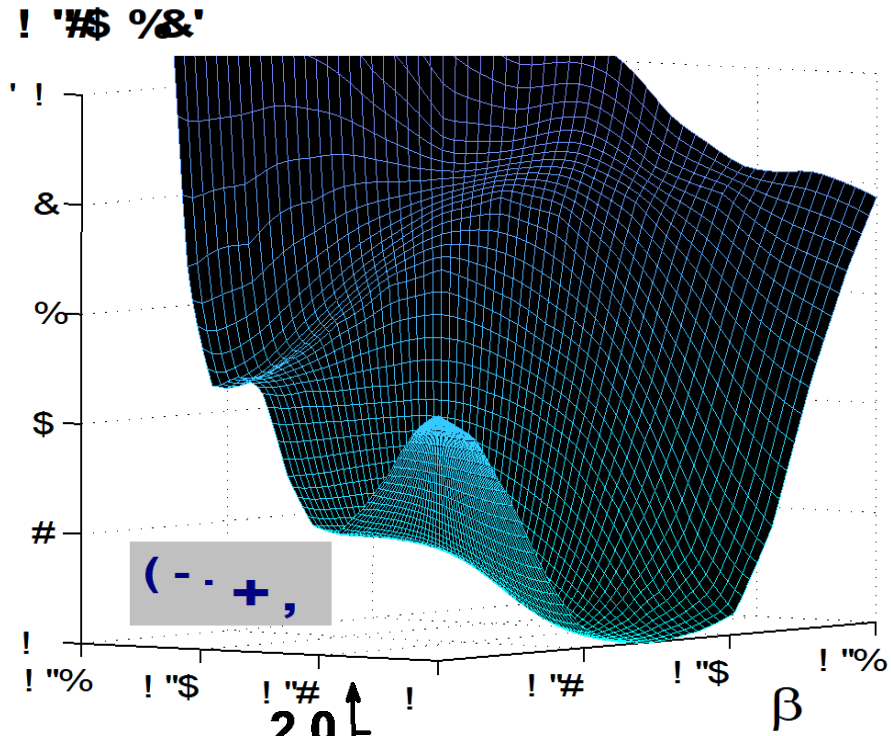
Empirical ground-state properties of finite nuclei can only determine a small set of parameters in the expansion of an effective Lagrangian in powers of fields and their derivatives.

Already at lowest order one finds more parameters than can be uniquely determined from data.

✔ an intuitive interpretation of mean-field results in terms of *intrinsic shapes* and *single-particle states*

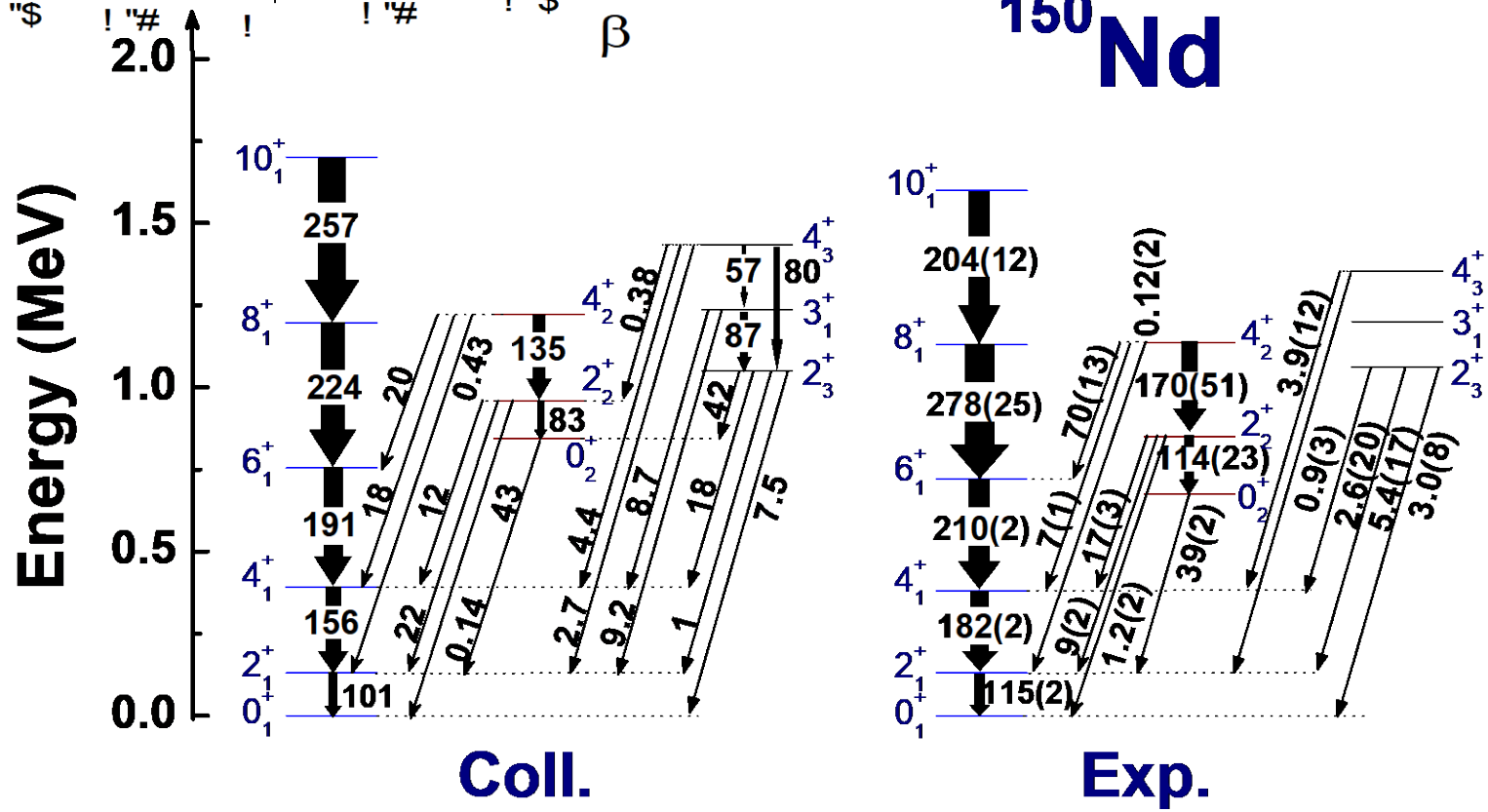






✔ the *full model space* of occupied states can be used; no distinction between core and valence nucleons, *no need for effective charges!*

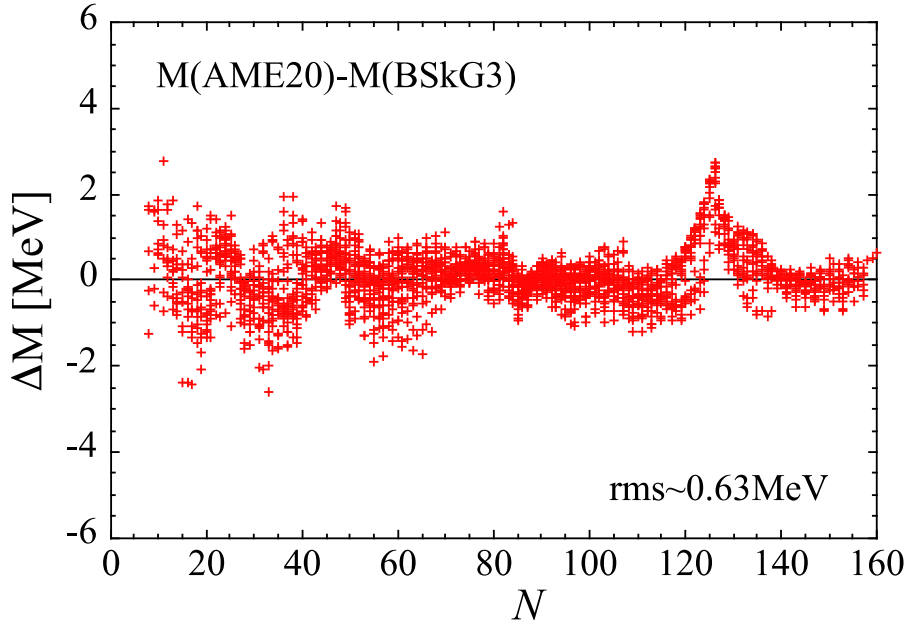
^{150}Nd

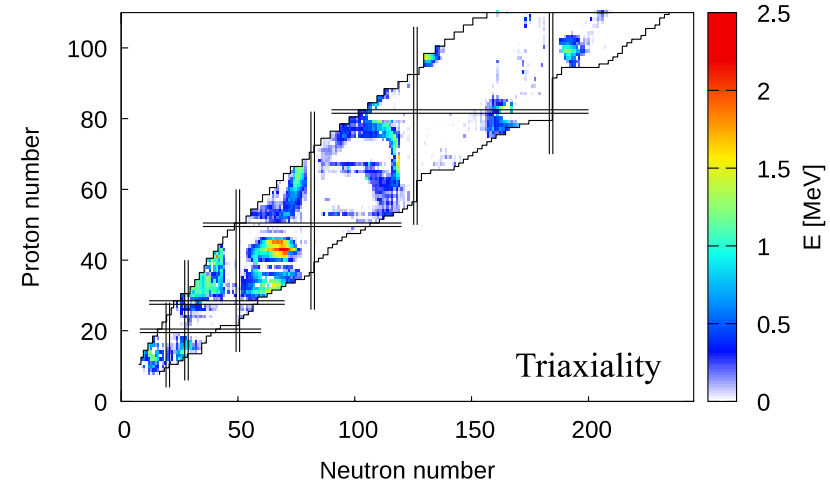


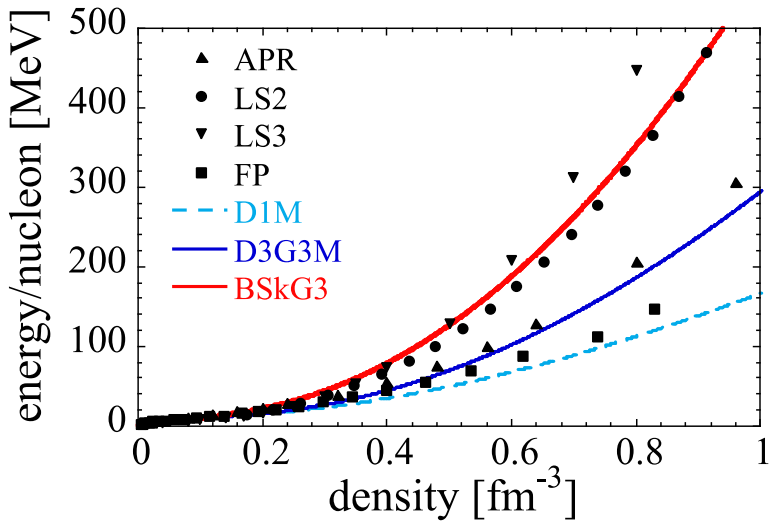
✔ *universal density functionals* can be applied to all nuclei over the entire nuclide chart!

New Skyrme-HFB mass model: BSkG3

- Triaxiality, time-reversal symmetry breaking & octupole GS deformation
- Microscopic pairing from "realistic" calculations
- Stiff EoS (NS M_{max}~2.26M_o)
- Accurate masses: σ(2457*M*)=0.63MeV







Grams, Ryssens et al. (EPJA 59, 270, 2023)

Self-consistent mean-field models

Mean-field approximation: the dynamics of the nuclear many-body system is represented by independent nucleons moving in a self-consistent potential.

Self-consistent potential: corresponds to the actual density distribution for a given nucleus.

Advantages of the SCMF approach:

- ✧ use of global effective nuclear interactions (used for all nuclei!)
- ✧ can be applied to arbitrarily heavy systems, including superheavy nuclei
- ✧ intuitive picture of intrinsic shapes

Finite Nuclei

The ground-state of a nucleus is described by the stationary self-consistent solution of the single-nucleon Dirac equation, the relativistic analogue of the Kohn-Sham equation, obtained from the variation of the Lagrangian:

$$\left[\gamma_\mu(i\partial^\mu - \Sigma^\mu - \Sigma^\mu_R) - (m + \Sigma_S)\right]\psi = 0$$

with the nucleon self-energies defined by the relations:

$$\Sigma^\mu = \alpha_V(\rho_v)j^\mu + e\frac{(1-\tau_3)}{2}A^\mu$$

$$\Sigma^\mu_R = \frac{1}{2}\frac{j^\mu}{\rho_v}\left\{\frac{\partial\alpha_S}{\partial\rho}\rho_s^2 + \frac{\partial\alpha_V}{\partial\rho}j_\mu j^\mu + \frac{\partial\alpha_{TV}}{\partial\rho}\vec{j}_\mu\vec{j}^\mu\right\}$$

$$\Sigma_S = \alpha_S(\rho_v)\rho_s - \delta_S\Box\rho_s$$

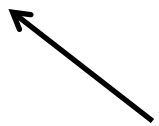
$$\Sigma^\mu_{TV} = \alpha_{TV}(\rho_v)\vec{j}^\mu$$

⇒ the isoscalar and isovector 4-currents and scalar density:

$$j_\mu = \langle \phi_0 | \bar{\psi} \gamma_\mu \psi | \phi_0 \rangle = \sum_{k=1}^{N} v_k^2 \; \bar{\psi}_k \gamma_\mu \psi_k$$

$$\vec{j}_\mu = \langle \phi_0 | \bar{\psi} \gamma_\mu \vec{\tau} \psi | \phi_0 \rangle = \sum_{k=1}^{N} v_k^2 \; \bar{\psi}_k \gamma_\mu \vec{\tau} \psi_k$$

$$\rho_S = \langle \phi_0 | \bar{\psi} \psi | \phi_0 \rangle = \sum_{k=1}^{N} v_k^2 \; \bar{\psi}_k \psi_k$$



occupation factor

For an even-even system, time reversal invariance forbids currents in the nucleus
⇒ the spatial components of the vector fields vanish.

Pairing correlations and Hartree-(Fock)-Bogoliubov theory

Ground-state properties of open-shell nuclei → pairing correlations must be taken into account, either in the BCS approximation, or in the full HFB theory.

…the relativistic Hartree-Bogoliubov (RHB) equations:

Pairing field

Quasiparticle energy

$$\begin{pmatrix} \hat{h}_D - m - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}_D^* + m + \lambda \end{pmatrix} \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix} = E_k \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix}$$

Dirac hamiltonian

nucleon mass

chemical potential

The RHB equations are solved self-consistently, with potentials determined in the mean-field approximation.