Strong interaction in the nuclear medium: new trends

Effective interactions and energy functionals: applications to nuclear systems – I

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A unified theory for nuclear structure, reactions and stars

The Energy Density Functional (EDF) Concept

- Mean field for ground state nuclear structure (HF, HFB,...)
- RPA and QRPA for small amplitude oscillations
- Beyond small amplitude oscillations: time-dependent mean field for dynamics (TDHF, TDHFB,...)
- Beyond-mean-field models (correlations): GCM, particle-vibration coupling, variational multiparticle-multihole configuration mixing, extensions of RPA, Second RPA,...

... see Introduction - Denis Lacroix
The atomic nucleus is a quantum many-body system
The Quantum Many-Body Problem

Schroedinger equation to solve (non relativistic case)

\[ H\Psi = E\Psi, \]

The Hamiltonian in second quantization is written as:

\[ H = \sum_{\alpha\beta} a_{\alpha}^+ \langle \alpha | T | \beta \rangle a_{\beta} + \frac{i}{2} \sum_{\alpha\beta\gamma\delta} a_{\alpha}^+ a_{\beta}^+ \langle \alpha\beta | V | \gamma\delta \rangle a_{\delta} a_{\gamma} + ... , \]

Approximations have to be done !!

\[ \alpha, \beta, \gamma, \delta \] sets of quantum numbers associated to the particles under study...
Which particles?

Which are the degrees of freedom taken into account in the nuclear many-body problem within EDF?
Overview of the first lecture

1. Applications of EDF to nuclear systems (effective interactions are used): some examples for nuclei and neutron stars

2. The many-body problem. A way to describe it: density functional theory (DFT)

3. The independent particle approximation

4. DFT. Kohn-Sham equations. From the many-body to a 1-body effective model - I

5. The basis of EDF. Phenomenological effective interactions in nuclear physics, Skyrme and Gogny

6. EDF. Hartree-Fock (HF) mean field with the Skyrme force. From the many-body to a 1-body effective model - II

7. DFT and EDF
1. Some applications
Ground state of nuclei. **Mean field: individual degrees of freedom**

- **Masses** → **Separation energies** → **Drip lines?**

\[ S_{2n} = B(N, Z) - B(N - 2, Z) \]
\[ M(N, Z) = ZM_p + NM_n - B(N, Z) \]
\[ S_n = B(N, Z) - B(N - 1, Z) \]

- **Densities**

- **Single particle spectra** → **Energies and occupation probabilities?**
MASSES. Hartree-Fock-Bogoliubov nuclear mass model. A microscopic mass model

- EDF using a finite-range interaction, Gogny
- EDF using a zero-range interaction: Skyrme

**FIG. 1.** Differences between measured [4] and D1M masses, as a function of the neutron number $N$.  
Goriely, et al., PRL 102, 242501 (2009)

**FIG. 2.** Differences between measured [6] and HFB-17 masses, as function of $N$.  
Goriely, et al., PRL 102, 152503 (2009)


**Masses** → **Separation energies** → **Drip lines?**

\[ S_{2n} = B(N, Z) - B(N - 2, Z) \]

\[ M(N, Z) = ZM_p + NM_n - B(N, Z) \]

\[ S_n = B(N, Z) - B(N - 1, Z) \]

**Densities**

**Single particle spectra** → **Energies and occupation probabilities?**
Mean field calculations (HFB) with a Skyrme force

Binding energy (top) and two-neutron separation energy (bottom)

Sn isotopes

DRIP LINE ?
Strongly model dependent!!!
Masses  ➔  Separation energies  ➔  Drip lines?

\[ S_{2n} = B(N, Z) - B(N - 2, Z) \]

\[ M(N, Z) = ZM_p + NM_n - B(N, Z) \]

\[ S_n = B(N, Z) - B(N - 1, Z) \]

Densities

Single particle spectra  ➔  Energies and occupation probabilities?

$^{48}\text{Ca}$ density profiles. Spherical nucleus. Hartree-Fock with Skyrme
Masses

Separation energies

Drip lines?

\[ S_{2n} = B(N, Z) - B(N - 2, Z) \]

\[ M(N, Z) = ZM_p + NM_n - B(N, Z) \]

\[ S_n = B(N, Z) - B(N - 1, Z) \]

Densities

Single particle spectra

Energies and occupation probabilities?
Can we predict single-particle energies and spectroscopic factors? We need to go beyond mean field (see next Lecture).

Why?

Grasso, Yoshida, Sandulescu, Van Giai, PRC 74, 064317 (2006)
Single-particle and collective degrees of freedom couple: beyond mean field
Effects of particle-vibration coupling on the single-particle spectrum

Neutron states in $^{208}$Pb


These correlations also affect the excited states ...
Particle-vibration coupling

E. Litvinova, et al.

**FIG. 4.** Isovector $E1$ resonance in $^{208}$Pb. Details are given in the text.

**FIG. 5.** Same as Fig. 4, but for $^{132}$Sn.

$^{208}$Pb  

$^{132}$Sn
At mean field level we can include pairing correlations to treat superfluid nuclei (BCS superfluidity -> Cooper pairs)

- Energy gap in excitation spectra
- Odd-even effect in binding energy
- Moments of inertia
Odd-even effect

No isotopes (Z=102)

Duguet et al. arXiv:nucl-th/0005040v1

Figure 2: One neutron separation energy $S_n$ for five $^{254}$No isotopes. Stars with full line are for experiment with error bars, circles with long-dashed line for pairing 1 and squares with dotted line for pairing 2.

$S_n = E(Z,N) - E(Z,N-1)$
Excitations. Collective degrees of freedom
Excitation modes (small amplitudes)

Quadrupole mode QRPA in particle-hole channel
Response function for $^{22}$O

Two-neutron $0^+$ addition mode QRPA in particle-particle channel
Response function for $^{124}$Sn

Khan, Sandulescu, Grasso, and Van Giai, PRC 66, 024309 (2002)
Dynamics. Beyond small amplitude oscillations. Time dependent approaches for the dynamics

Collision Dynamics of Two $^{238}\text{U}$ Atomic Nuclei

Time-dependent HF

Golabek and Simenel, PRL 103, 042701 (2009)
Properties of nuclear matter
With an EDF model (for instance from the Skyrme density functional) we can calculate the Equation of State (EoS) of nuclear matter. Isospin effects and density dependence differ between symmetric nuclear matter EoSs and neutron-rich matter EoSs (density dependence of symmetry energy).
EoSs can be very different at **low** and **high densities** (with respect to saturation density) (strong model dependence !!!) This is a problem, for instance, for treating nuclear systems at low density (crust of neutron stars)

**EOS of pure neutron matter**

![Graph showing EOS of pure neutron matter](image)

From Denis Lacroix. Introduction

Predicting power in EDF

1) strong model dependence in unknown regions

2) unluckily, model dependence in some cases also in known regions…one example…
Energy difference between the proton states 2s1/2 and 1d3/2 in Ca isotopes

Grasso, Ma, Khan, Margueron, Van Giai, PRC 76, 044319 (2007)
From Introduction.
Denis Lacroix

\[ S_{2n} \text{ and } S_{2p} \text{ in Tin isotopic chain} \]

http://www.nscl.msu.edu/future/isf

Large uncertainty in unknown region
Neutron stars. Very exotic nuclear systems (Pierre Pizzochero lecture of today)
Isospin asymmetry in nuclei and neutron stars

A.W. Steiner\textsuperscript{a, b, *}, M. Prakash\textsuperscript{c}, J.M. Lattimer\textsuperscript{c}, P.J. Ellis\textsuperscript{a, \#} and references therein

Fig. 16. Calculated neutron skin thickness $\delta R$ of nuclei versus the radius of $1.4M_\odot$ stars (left panel) and of maximum mass stars (right panel). The solid lines are described in the text.

Neutron skin thickness versus neutron star radius
Picture of the crust of a neutron star
Baym, Bethe, Pethick, NPA 175 (1971), 225

Inner crust: $0.001 \rho_0 \leq \rho \leq 0.5 \rho_0$

Saturation density

$\rho_0 = 0.16 \text{ fm}^{-3}$

$\sim 2.5 \cdot 10^{14} \text{ g/cm}^3$

Outer crust: crystal of nuclei in an electron sea

Drip point for neutrons

$\sim 4 \cdot 10^{11} \text{ g/cm}^3$

Inner crust: crystal of nuclear clusters in an electron sea and in a gas of superfluid neutrons

$\beta$-stability condition $\rightarrow \mu_e = \mu_n - \mu_p$

ρ = 0.5 ρ₀
Wigner-Seitz cell model
Fig. 3. Proton and neutron density distributions occurring along an axis joining the centers of two adjacent unit cells.
Collective mode

Low-lying quadrupole excitations. QRPA. Excitation spectrum and cooling time (see Monrozeau, et al., PRC 75, 065807 (2007))

Nucleus $^{122}$Zr

Wigner-Seitz cell ($Z=40$, $N=1460$, $R \approx 20$ fm)

Grasso, Khan, Margueron, Van Giai, NPA 807,1 (2008)
2. The quantum many-body problem. A way to describe it: density functional theory (DFT)

A nice text to start with:

Density functional theory (DFT). The Quantum Many-Body problem is solved by an energy minimization

- **Very currently used in physics and in chemistry** to calculate, for instance, band structure in solids and binding energies in molecules

- **1964** Hohenber-Kohn (HK) theorem(s)

- **1965** Kohn-Sham (KS) equations: one way to practically use DFT

- **1998** Nobel Prize in chemistry to W. Kohn (the father of the theory) and J. Pople (for numerical implementations in computational chemistry)
• The usual way to treat a problem is to solve the Schrödinger equation and construct all the mean values of the operators (for instance the density) with the calculated wave function.

• In DFT the procedure is inverted. The density (which is a mean value of an operator) plays a fundamental role in this theory.

• Functionals are used, that are functions of a function. If \( f(x) \) is a function, a functional \( F \) of the function \( f \), \( F[f] \), is any rule that associates a number to the function \( f \) for a given value of \( x \).
HK theorem(s)

Let us consider a system of interacting particles in an external potential $v$ (!!! in nuclear physics systems are self-bound !!!)

$$\left[ \sum_i^N \left( -\frac{\hbar^2 \nabla_i^2}{2m} + v(r_i) \right) + \sum_{i<j} U(r_i, r_j) \right] \Psi(r_1, r_2, \ldots, r_N)$$

$$= E \Psi(r_1, r_2, \ldots, r_N),$$

• If the ground state density $\rho_0$ is known, the ground state wave function and the external potential (up to an additive constant) can be determined

• For each potential $v$, a functional $E[\rho]$ exists which is minimized by $\rho_0$. Ground state energy $E_0$ is equal to $E[\rho_0]$

• If $\rho \neq \rho_0$, $E[\rho] \geq E_0$
3. The independent particle approximation
In nuclei: mean free path of nucleons in a nucleus is at least comparable with nuclear size (scattering experiments) (Pauli and uncertainty principle)

A nucleon does not ‘see’ directly all the other nucleons, but ‘feels’ an average potential that is constructed by all the other nucleons. Nucleons act as non interacting particles moving in an average single particle potential

Confirmation of the validity of the independent particle approximation: existence of shells and magic numbers (shell closure: binding energies, excitation spectra...)
4. DFT. From the many-body to a 1-body effective model – I Kohn-Sham equations

Kohn and Sham, Phys. Rev. A 140, 1133 (1965)
The energy minimization is transformed in the solution of a Schrödinger equation for non-interacting particles: **Kohn-Sham equations**

\[ E[\rho] = T[\rho] + U[\rho] + V[\rho]. \]

**Kinetic**  
**Interaction**  
**Functional related to the external potential**

\[ V[\rho] = \int d^3 \vec{r} \rho(\vec{r}) V(\vec{r}) \]

\[ E[\rho] = T_S[\{\phi_i[\rho]\}] + U_{\text{Hartree}}[\rho] + E_{xc}[\rho] + V[\rho]. \]

**Minimization**

\[ 0 = \frac{\delta E[\rho]}{\delta \rho(\vec{r})} = \frac{\delta T_S[\rho]}{\delta \rho(\vec{r})} + \frac{\delta V[\rho]}{\delta \rho(\vec{r})} + \frac{\delta U_{\text{Hartree}}[\rho]}{\delta \rho(\vec{r})} + \frac{\delta E_{xc}[\rho]}{\delta \rho(\vec{r})} = \frac{\delta T_S[\rho]}{\delta \rho(\vec{r})} + V(\vec{r}) + v_{\text{Hartree}}(\vec{r}) + v_{xc}(\vec{r}) \]

\[ v_S(\vec{r}) = v(\vec{r}) + v_{\text{Hartree}}(\vec{r}) + v_{xc}(\vec{r}). \]

**We need** \( E_{xc} \) **to explicitly calculate**

\[ E_{xc} : \text{Exchange-correlation part} \]

Equations to be solved. Non linear problem to be solved iteratively.
Choice of $E_{xc}[\rho]$

- The exchange part is sometimes introduced exactly
- The correlation part is always approximated
- How to choose the functional?

Old: perturbation theory
More recent: Quantum Monte Carlo calculations for the electron liquid

Local density approximation is used (homogeneous system)
Gradient-corrections to implement LDA (derivatives of the density)

See for instance: Perdew, Burke, Ernzerhof, PRL 77, 3865 (1996)
Fiolhais et al., A primer in DFT
5. The basis of EDF. Phenomenological effective interactions in nuclear physics, Skyrme and Gogny
The simple idea

• Construction of an effective phenomenological force that is chosen so as to reproduce global properties of some finite nuclei (binding energies and radii) and properties related to the EoS of nuclear matter (first of all saturation point)

• Form and parameters to choose

• For instance, to have in-medium effects (Pauli principle), we need the density-dependent term

• Correlations in the interaction contained in an effective way. Double counting when RPA is done?
Finite-range: Gogny interaction

It has been introduced from a realistic G matrix

**Standard form:**

\[
V(r_1, r_2) = \sum_{i=1,2} \left[ W_i + B_i P_{\sigma} - H_i \langle P_{\tau} \rangle - M_i \langle P_{\sigma} P_{\tau} \rangle \right] e^{-r^2/\mu_i^2} \\
+ t_3 \left[ 1 + x_3 P_{\sigma} \right] \left[ \rho(\mathbf{R}) \right]^{\alpha} \delta(r) \\
+ iW_0 \sigma \cdot \left[ \mathbf{P}' \times \delta(r) \mathbf{P} \right]
\]

**Finite-range (gaussian form)**

**Density dependent (zero-range)**

**Spin-orbit (zero-range)**

First parametrization: D1
Déchargé, Gogny, PRC 21, 1568 (1980)

Most used: D1S (fit also on fission barriers)
Berger, Girod, Gogny, NPA 502, 85c (1989)

A recent modification (towards finite-range in all terms): D1N
Chappert, Girod, Hilaire, Phis. Lett. B 668 (2008), 420
Zero-range: Skyrme interaction

Standard form

\[
V(r_1, r_2) = \begin{align*}
& t_0 (1 + x_0 P_\sigma) \delta(r) & \text{central} \\
& + \frac{1}{2} t_1 (1 + x_1 P_\sigma) \left[ P' \delta(r) + \delta(r) P^2 \right] & \text{non local} \\
& + t_2 (1 + x_2 P_\sigma) P' \cdot \delta(r) P & \\
& + \frac{1}{6} t_3 (1 + x_3 P_\sigma) [\rho(R)]^2 \delta(r) \\
& + i W_0 \sigma \cdot [P' \times \delta(r) P] & \text{spin-orbit}
\end{align*}
\]

+ several modifications

T.H.R. Skyrme, Phil. Mag. 1, 1043 (1956), Nucl. Phys. 9, 615 (1959)

First applications: Vautherin, Brink, PRC 5, 626 (1972)

Negele and Vautherin showed a connection between realistic forces and Skyrme phenomenological forces: Negele, Vautherin, PRC 5, 1472 (1972); ibid. C 11, 1031 (1975)
6. Hartree-Fock (HF) mean field with the Skyrme force. From the many-body to a 1-body effective model - II
Based on the independent particle approximation (effective 1-body problem). Non relativistic case here.

- A 1-body effective interaction has to be derived

\[ H = K + V \sim \sum_{i=1}^{A} \frac{p_i^2}{2m} + \frac{1}{2} \sum_{i \neq j}^{A} V_{ij}^{\text{eff}}. \]

What is neglected in \( V \) is called residual interaction.

- Ground state wave function is chosen as a Slater determinant

\[ \Psi_{HF}(x_1, \ldots, x_A) = \frac{1}{\sqrt{A!}} \det \left\{ \phi_{\alpha_1}(x_1)\phi_{\alpha_2}(x_2)\cdots\phi_{\alpha_A}(x_A) \right\}. \]

\( x \rightarrow \) space, spin and isospin coordinates

Empty states: particle states (occupation = 0)

Occupied states: hole states (occupation = 1)
The ground state wave function is obtained in a variational way by an energy minimization. Vautherin and Brink, PRC 5 (1972), 626. The HF energy is:

$$E_{\text{HF}} = \frac{\langle \Psi_{\text{HF}} | H | \Psi_{\text{HF}} \rangle}{\langle \Psi_{\text{HF}} | \Psi_{\text{HF}} \rangle}.$$ 

For the Skyrme interaction:

$$\langle H \rangle = \int \mathcal{H}(r) \, dr$$

Hamiltonian density: **ENERGY DENSITY FUNCTIONAL** (algebraic function of nucleon densities, kinetic energy densities and spin-orbit densities)

$$\mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{\text{eff}} + \mathcal{H}_{\text{fin}} + \mathcal{H}_{\text{so}} + \mathcal{H}_{\text{sg}} + \mathcal{H}_{\text{coul}}$$

Term 1: kinetic
Term 2: coming from the central part
Term 3: density dependent
Term 4: effective mass term
Term 5: coming from gradient terms (simulating finite range)
Term 6: spin-orbit coupling
Term 7: spin-gradient coupling (contains the tensor contribution)
Term 8: Coulomb
The variational principle leads to the HF equations

\[
\left\{-\frac{\hbar^2}{2m} \Delta + \Gamma_H(\vec{r})\right\} \phi_k(\vec{r}) + \int d\vec{r}' \Gamma_{Ex}(\vec{r}, \vec{r}') \phi_k(\vec{r}') = \varepsilon_k \phi_k(\vec{r}),
\]

with:

\[
\Gamma_H(\vec{r}) = \int d\vec{r}' v(\vec{r}, \vec{r}') \rho(\vec{r}'),
\]

Depending on local density

\[
\Gamma_{Ex}(\vec{r}, \vec{r}') = -v(\vec{r}, \vec{r}') \rho(\vec{r}, \vec{r}'),
\]

Depending on non-local density

Iterative procedure (non linear problem)

In terms of Feynman diagrams, the HF proper self-energy is described by the following graphs

First-order for the proper self-energy
7. DFT and EDF
In principle, in EDF the starting point is the Hamiltonian and the functional is derived from the interaction by applying the variational principle. In DFT the functional is chosen.


In HF the exchange term is exactly calculated and the correlation part is totally missing (correlations included in an effective way by the fitting procedure of the interaction). In DFT correlations are always explicitly introduced.

Symmetry breaking and restoration: a procedure currently used in EDF (not in DFT)

Single-particle energies have a physical meaning in HF, not in DFT-Kohn-Sham

Is there a time-dependent DFT? Yes, based on Runge-Gross theorem

Looking for a universal (?) functional (same concepts of DFT) in nuclear physics. What to take into account? Which correlations to put in?
Ground state. Individual degrees of freedom. Uncorrelated state, but correlations explicitly in the functional Kohn-Sham (DFT).

Mean field HF (EDF)

Dynamical properties.

TDDFT

Particle-vibration coupling

Second RPA
(also from small amplitude limit of TDDM)

Beyond mean field. Coupling single-particle and collective coordinates

Small amplitude limit. (Q)RPA (collective states)

Dynamical properties.

TDHF

Beyond mean field. More general ground state (not a simple Slater determinant)

Mean field level but with quasiparticles. Pairing correlations are added.

HFB or HF + BCS

Dynamical properties.

TDHFB

GCM

multiparticle-multihole

ext. RPA