École Joliot-Curie

27 September - 3 October 2009

Lacanau - France

Strong interaction in the nuclear medium: new trends

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

Marcella Grasso

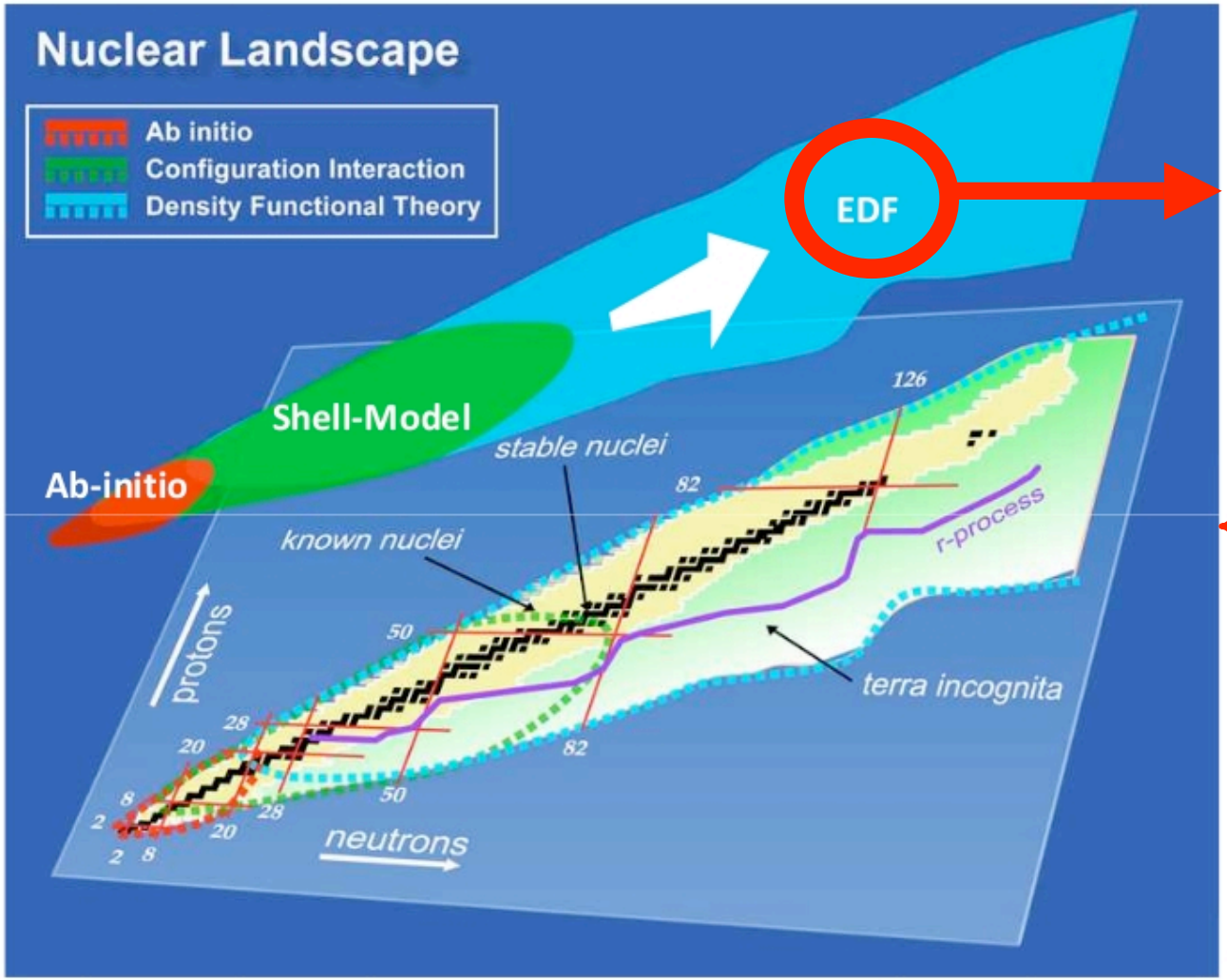
IPN Orsay

cnrs IN2P3
Institut national de physique nucléaire et de physique des particules

… see Introduction - Denis Lacroix

A unified theory for nuclear structure, reactions and stars

The Energy Density Functional (EDF) Concept



http://unedf.org/

- ***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,…***

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:

$$H = \sum_{\alpha\beta} a_\alpha^+ \langle \alpha | T | \beta \rangle a_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} a_\alpha^+ a_\beta^+ \langle \alpha\beta | V | \gamma\delta \rangle a_\delta a_\gamma + \dots ,$$

Approximations have to be done !!

α, β, γ, δ **sets of quantum numbers associated to the particles under study…**

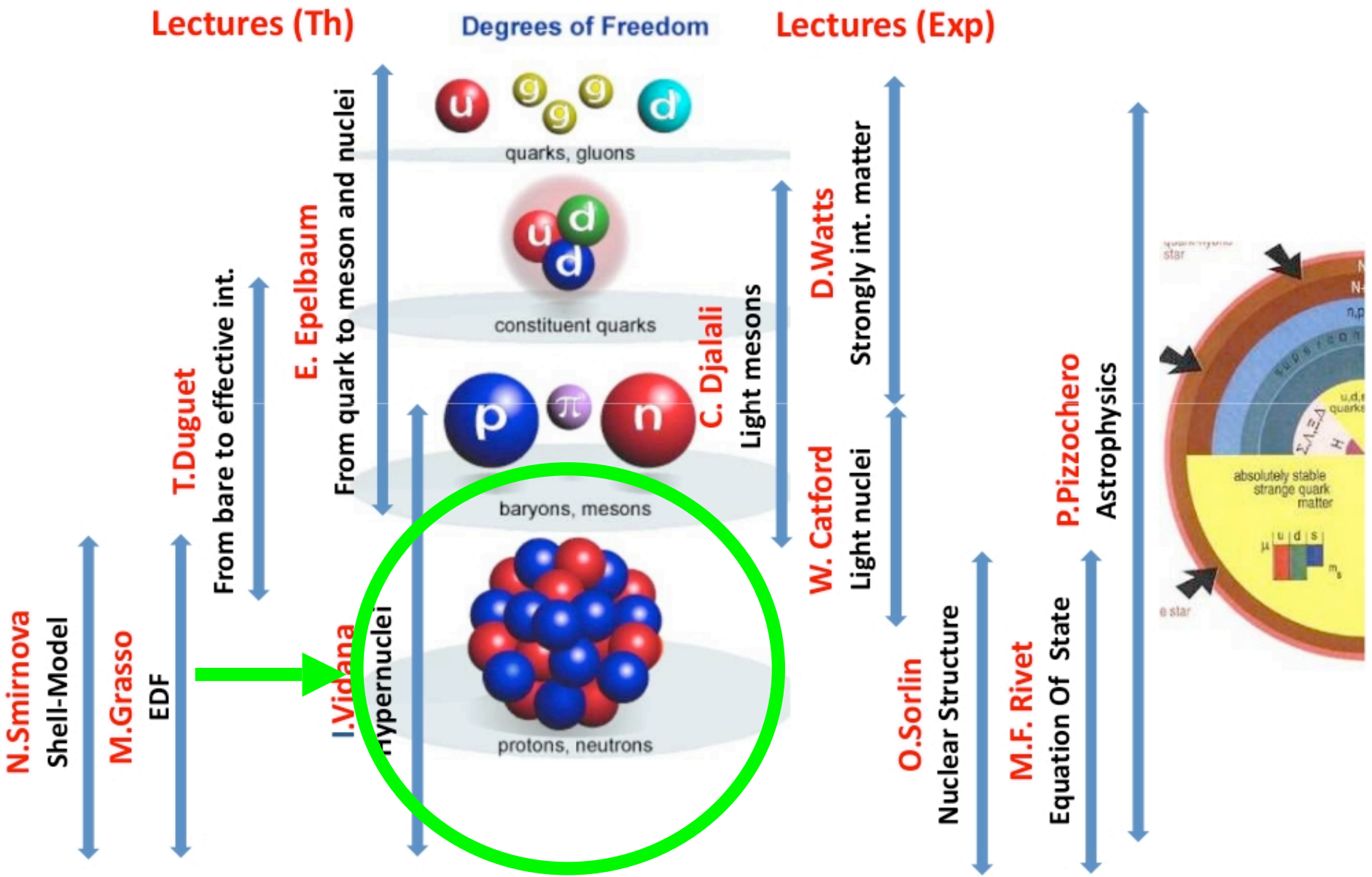
Which particles?

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

… see Introduction - Denis Lacroix

Summary

EJC2009 Lectures



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

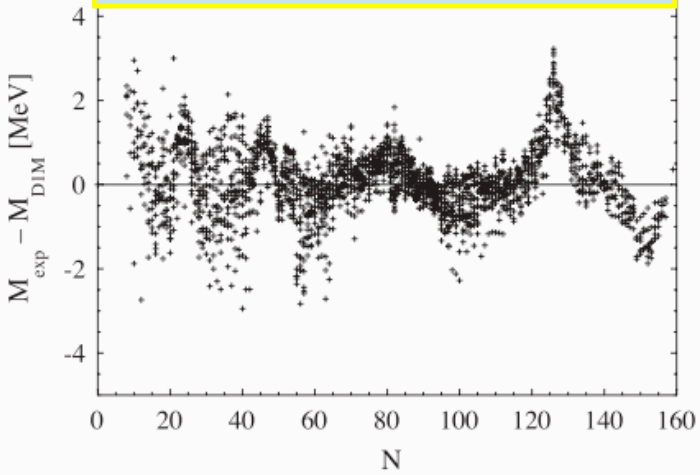


FIG. 1. Differences between measured [4] and D1M masses, as a function of the neutron number N.

Goriely, et al., PRL 102, 242501 (2009)

EDF using a zero-range interaction: Skyrme

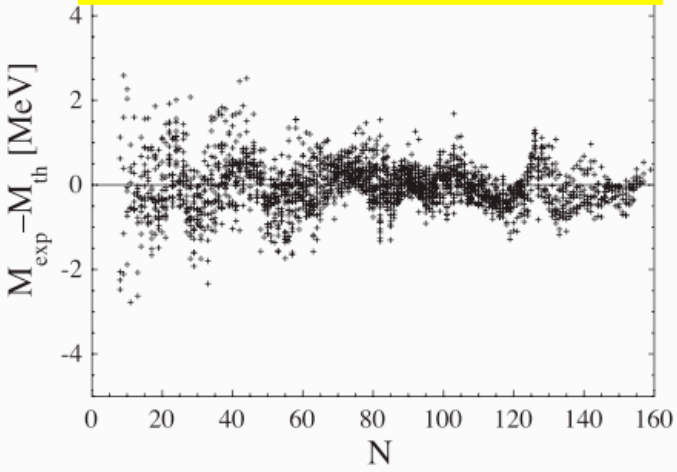


FIG. 2. Differences between measured [6] and HFB-17 masses, as function of N.

Goriely, et al., PRL 102, 152503 (2009)

Importance of nuclear masses in r-process nucleosynthesis : Arnould, et al., Phys. Rep. 450, 97 (2007)

[4] and [6] experimental values: Audi, Wapstra, and Thibault, Nucl. Phys. A729, 337 (2003)

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

$$S_{2n} = B(N,Z) - B(N-2,Z)$$

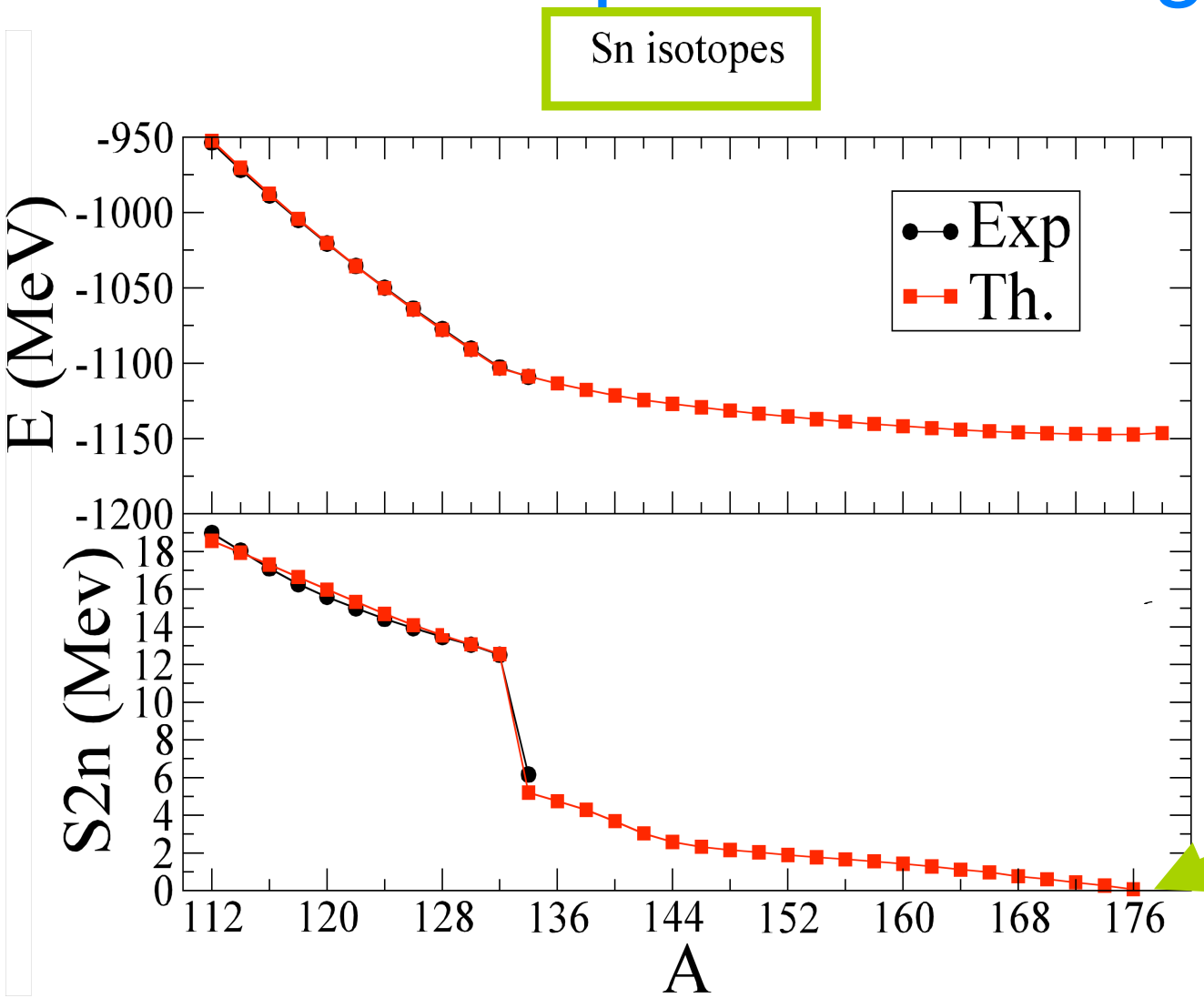
$$M(N,Z) = ZM_p + NM_n - B(N,Z)$$

$$S_n = B(N,Z) - B(N-1,Z)$$

- **Densities**

- **Single particle spectra** → **Energies and occupation probabilities?**

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



Mean field calculations (HFB) with a Skyrme force

DRIP LINE ?

Strongly model dependent!!!

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

$$S_{2n} = B(N,Z) - B(N-2,Z)$$

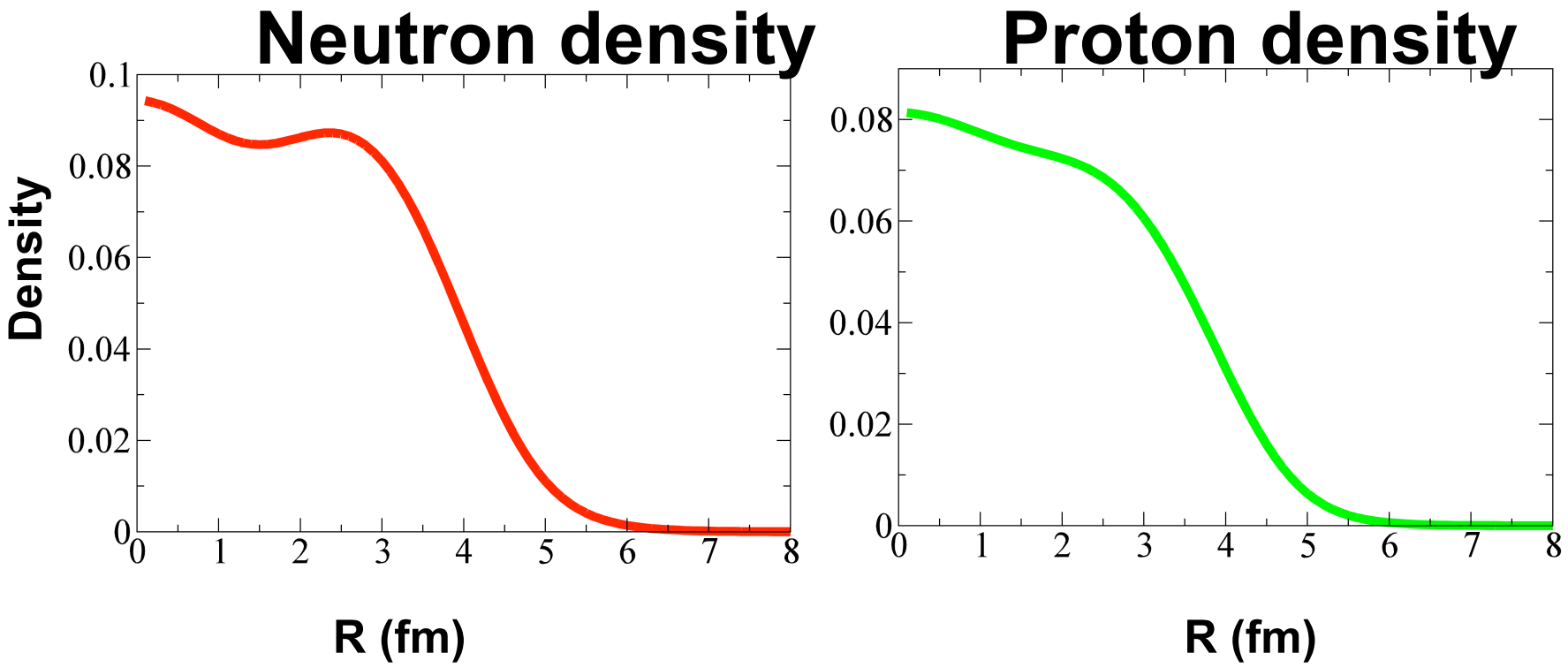
$$M(N,Z) = ZM_p + NM_n - B(N,Z)$$

$$S_n = B(N,Z) - B(N-1,Z)$$

- **Densities**

- **Single particle spectra** → **Energies and occupation probabilities?**

^{48}Ca density profiles. Spherical nucleus. Hartree-Fock with Skyrme



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

$$S_{2n} = B(N,Z) - B(N-2,Z)$$

$$M(N,Z) = ZM_p + NM_n - B(N,Z)$$

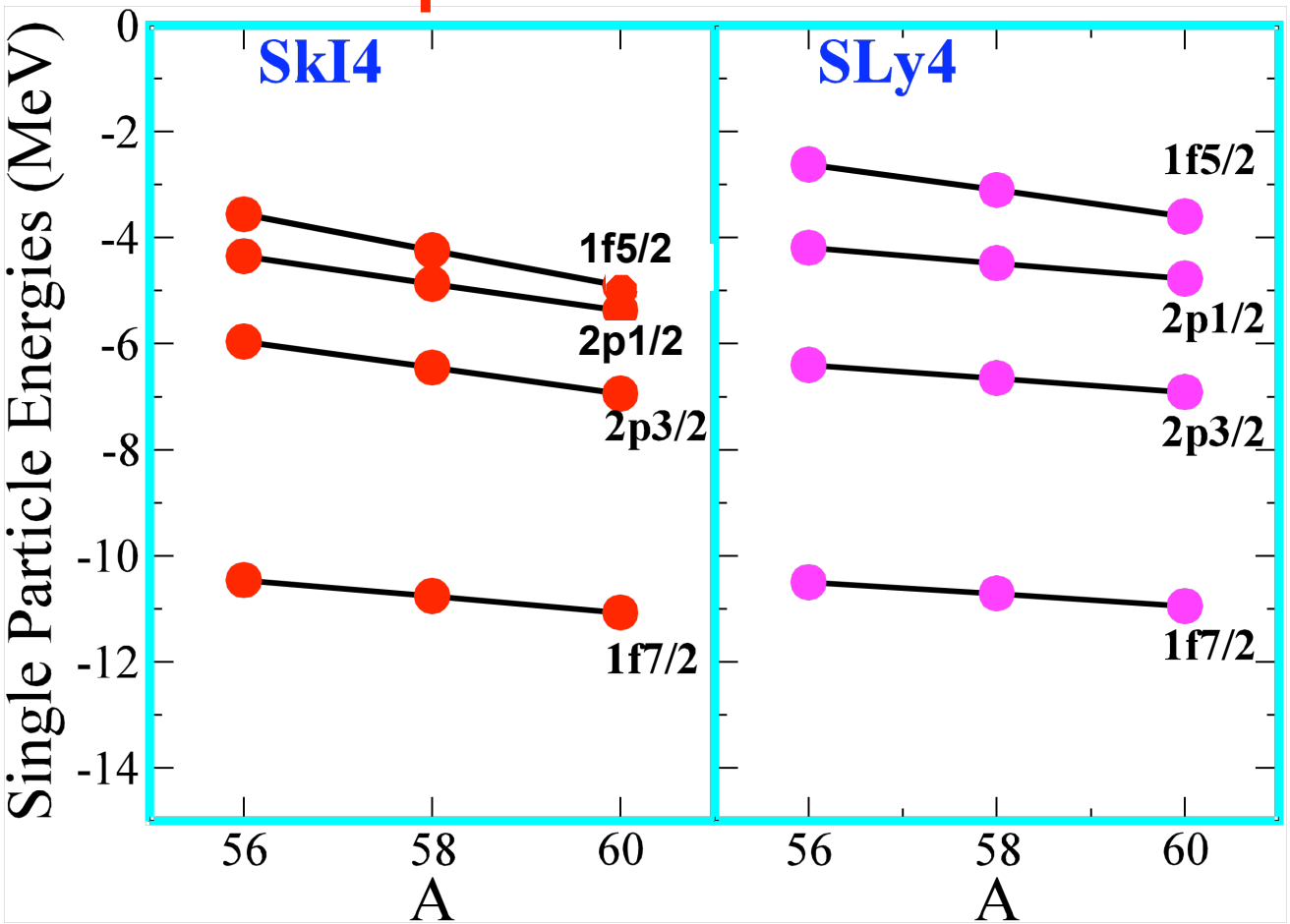
$$S_n = B(N,Z) - B(N-1,Z)$$

- **Densities**

- **Single particle spectra** → **Energies and occupation probabilities?**

Last neutron single-particle Hartree-Fock states

Ca isotopes



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

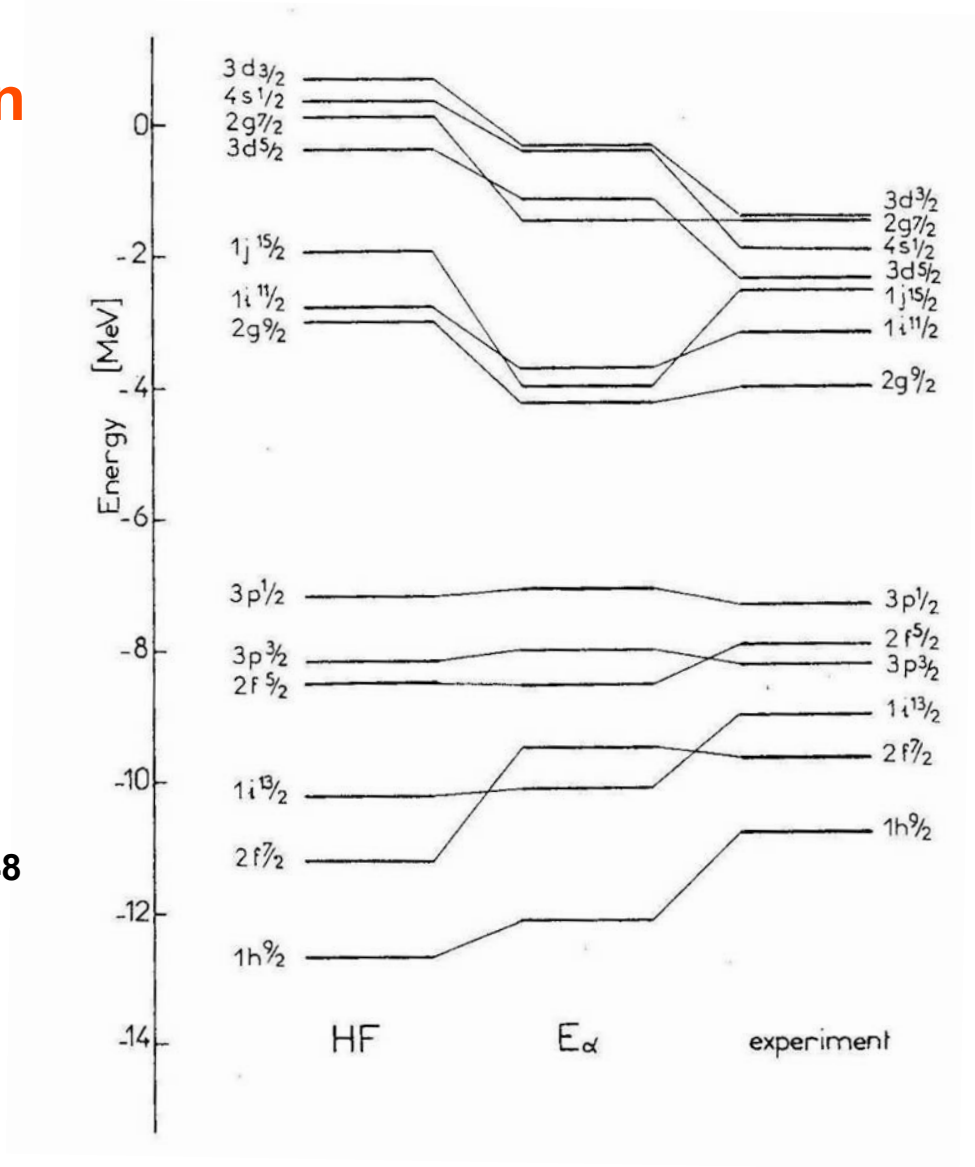
Why?

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



Bernard, Van Giai, Nucl. Phys. A 348 (1980), 75

These correlations also affect the excited states …

Particle-vibration coupling

E. Litvinova, et al.

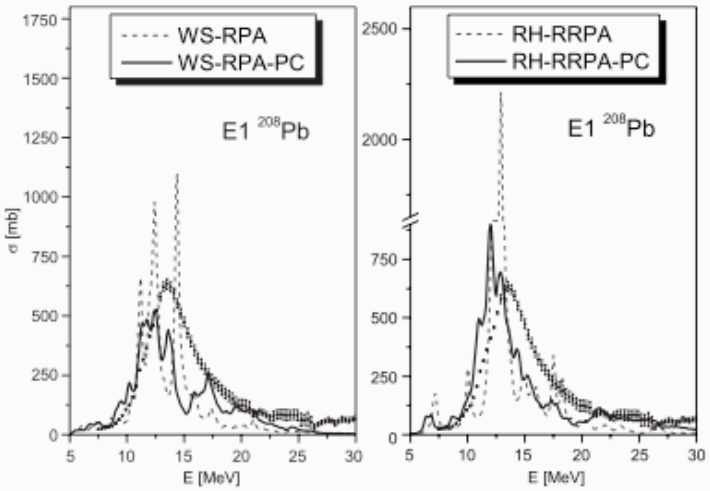


FIG. 4. Isovector $E1$ resonance in ^{208}Pb. Details are given in the text.

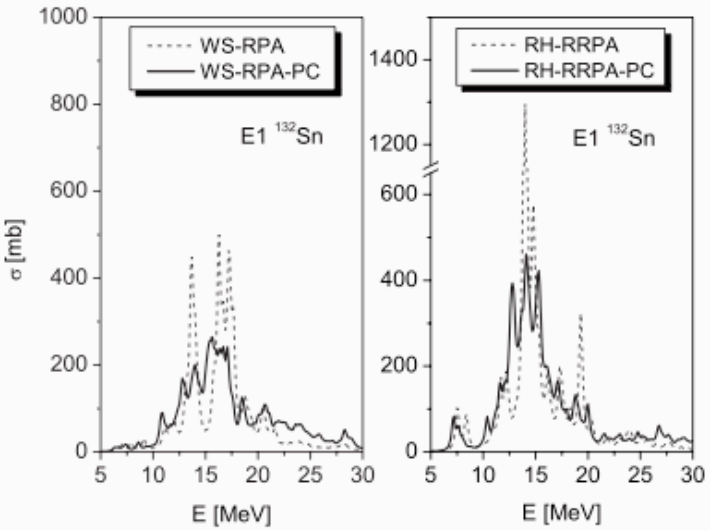


FIG. 5. Same as Fig. 4, but for ^{132}Sn.

^{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

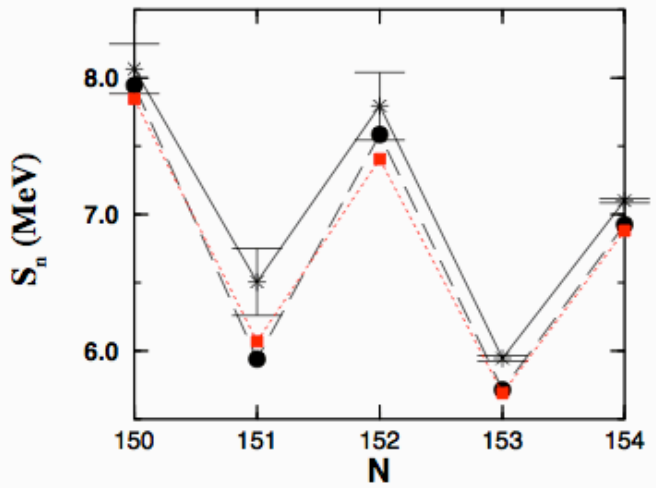


Figure 2: One neutron separation energy S_n for five ^{254}No isotopes. Stars with full line are for experiment with error bars, circles with long-dashed line for pairing 1 and squares with dotted line for pairing 2.

Sn = 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

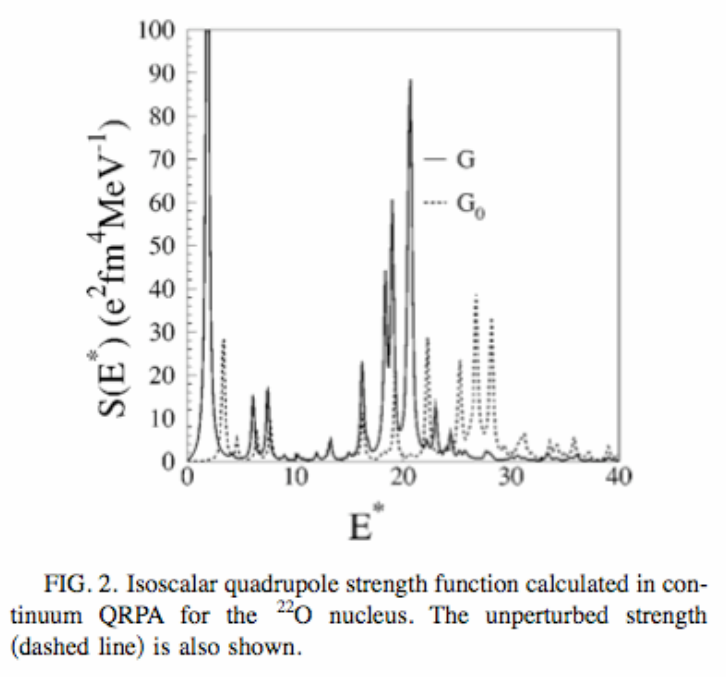
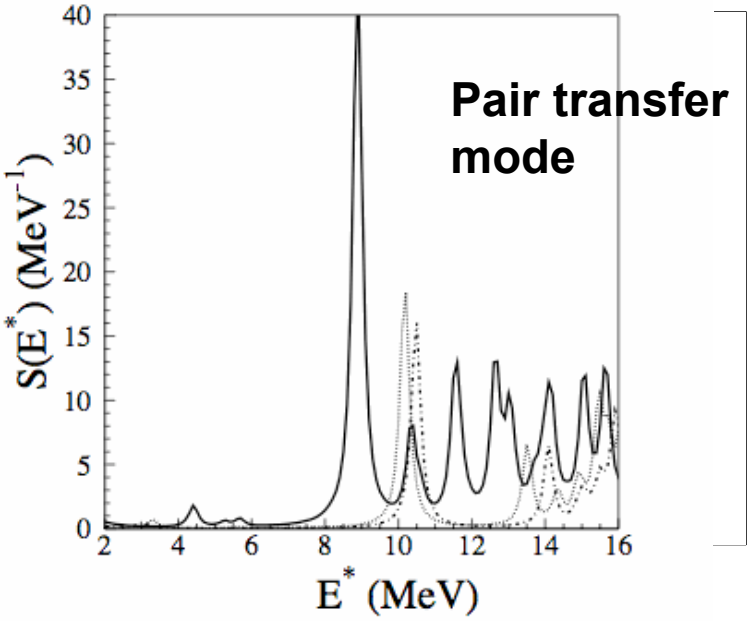


FIG. 2. Isoscalar quadrupole strength function calculated in continuum QRPA for the ^{22}O nucleus. The unperturbed strength (dashed line) is also shown.

Khan, Sandulescu, Grasso, and Van Giai, PRC 66, 024309 (2002)

Two-neutron 0^+ addition mode QRPA in particle-particle channel

Response function for ^{124}Sn



Khan, Grasso, Margueron, submitted PRC

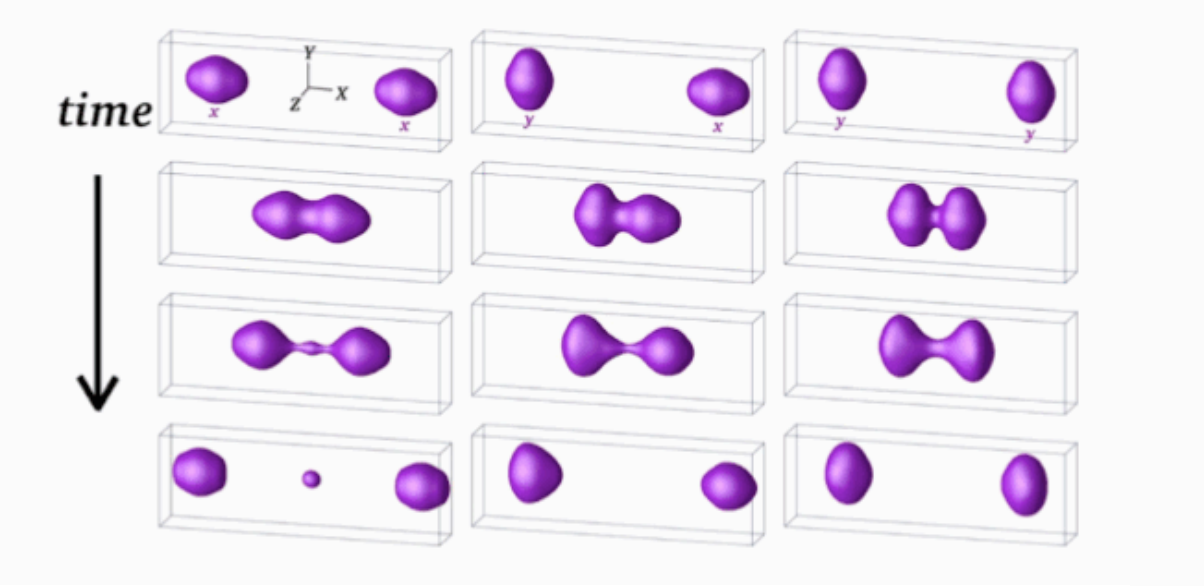
FIG. 5: QRPA response function for ^{124}Sn in the two neutrons 0^+ addition mode. The pure surface mode is in solid line, the η=0.65 mode is in dotted line, and the η=0.35 mode in dashed-dotted lines.

Dynamics. Beyond small amplitude oscillations. Time dependent approaches for the dynamics

Collision Dynamics of Two ^{238}U Atomic Nuclei

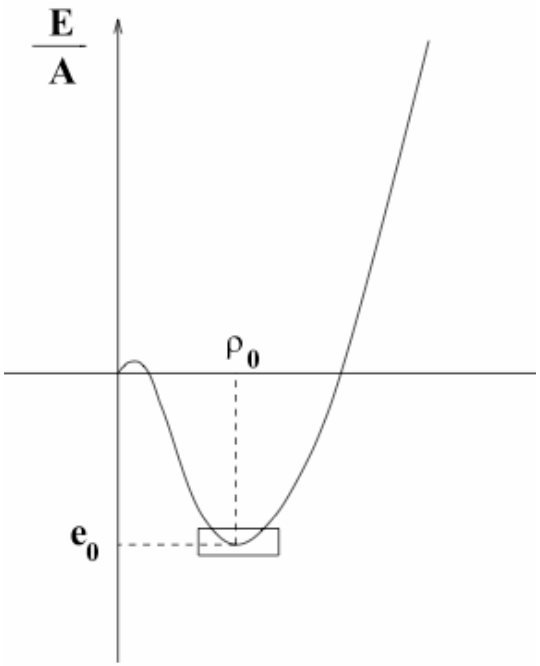
Time-dependent HF

Golabek and Simenel, PRL 103, 042701 (2009)

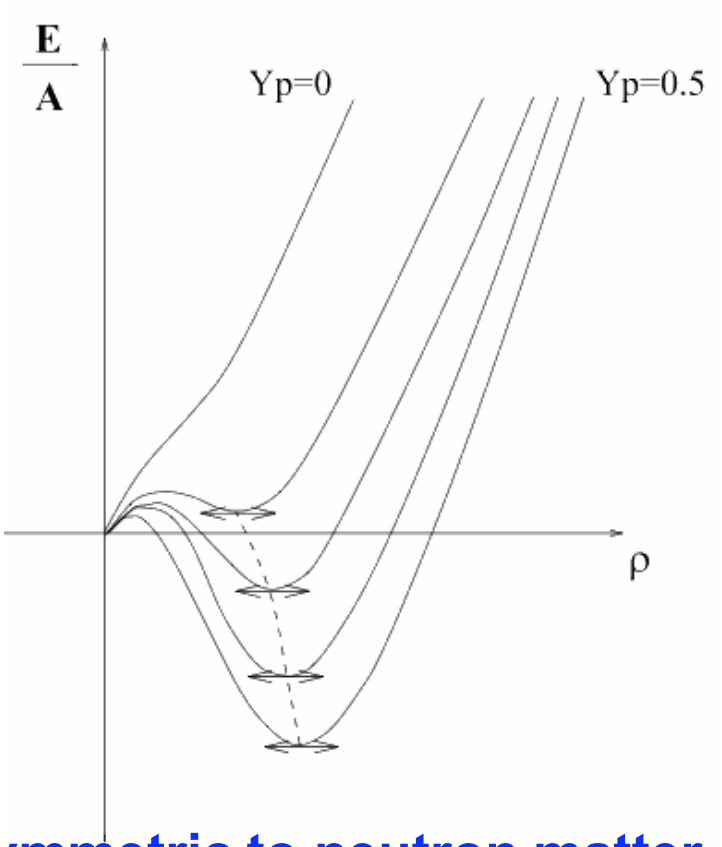


Properties of nuclear matter

With an EDF model (for instance from the Skyrme density functional) we can calculate the Equation of State (EoS) of nuclear matter



Symmetric

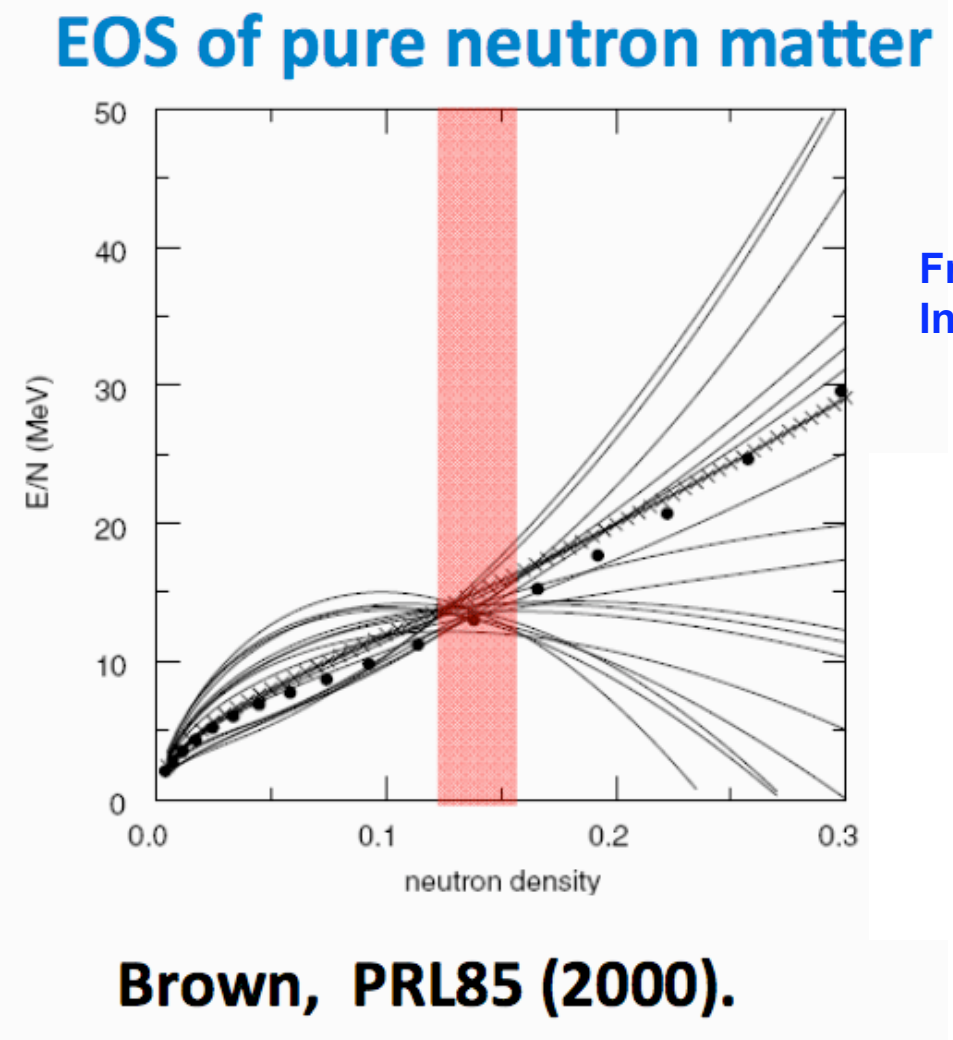


From symmetric to neutron matter. $Y_p=Z/A$

Isospin effects and density dependence

Differences 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)



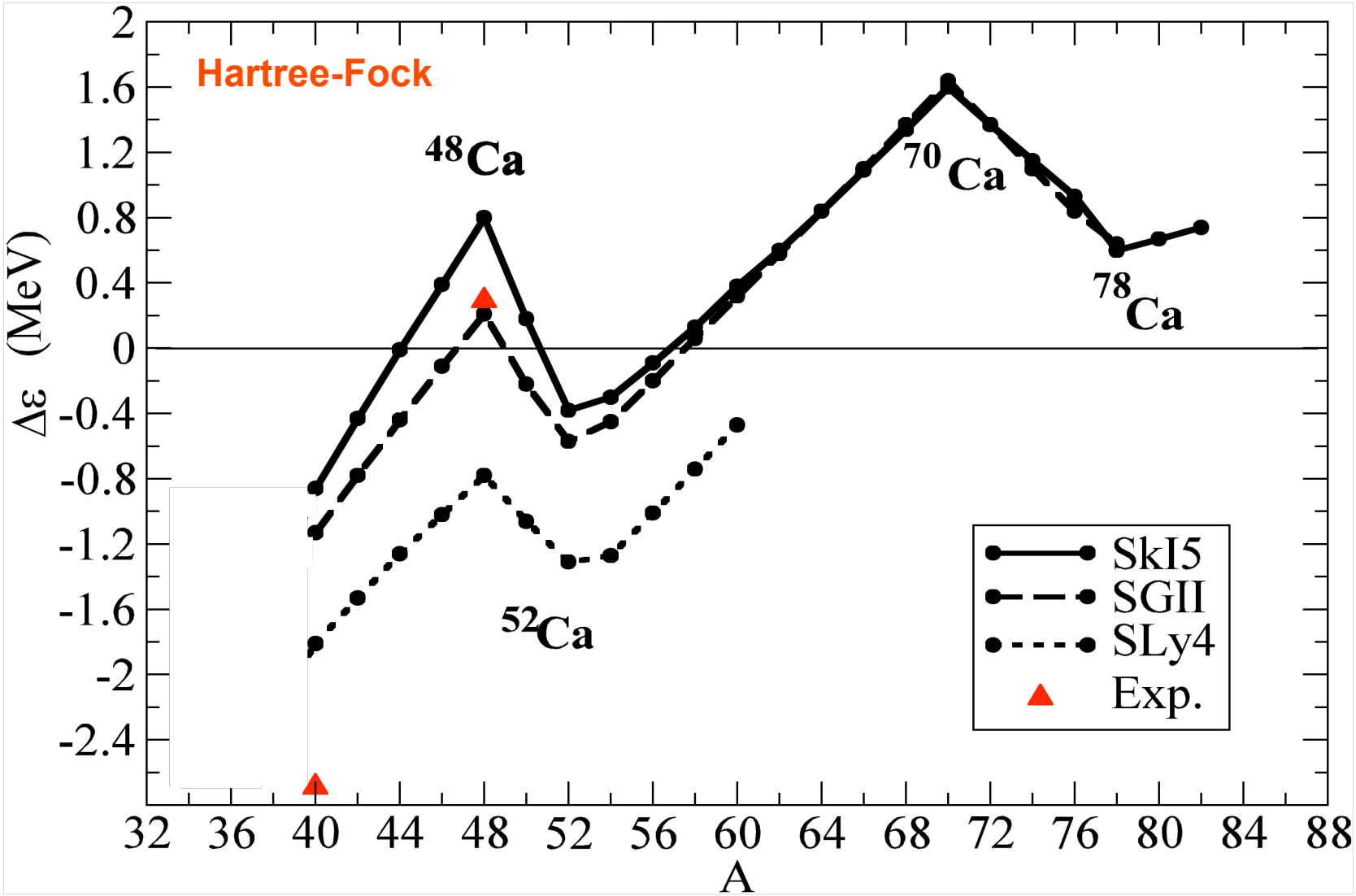
From Denis Lacroix. Introduction

Predicting power in EDF

1) strong model dependence in unknown regions

2) unluckily, model dependence in some cases also in known regions…one example…

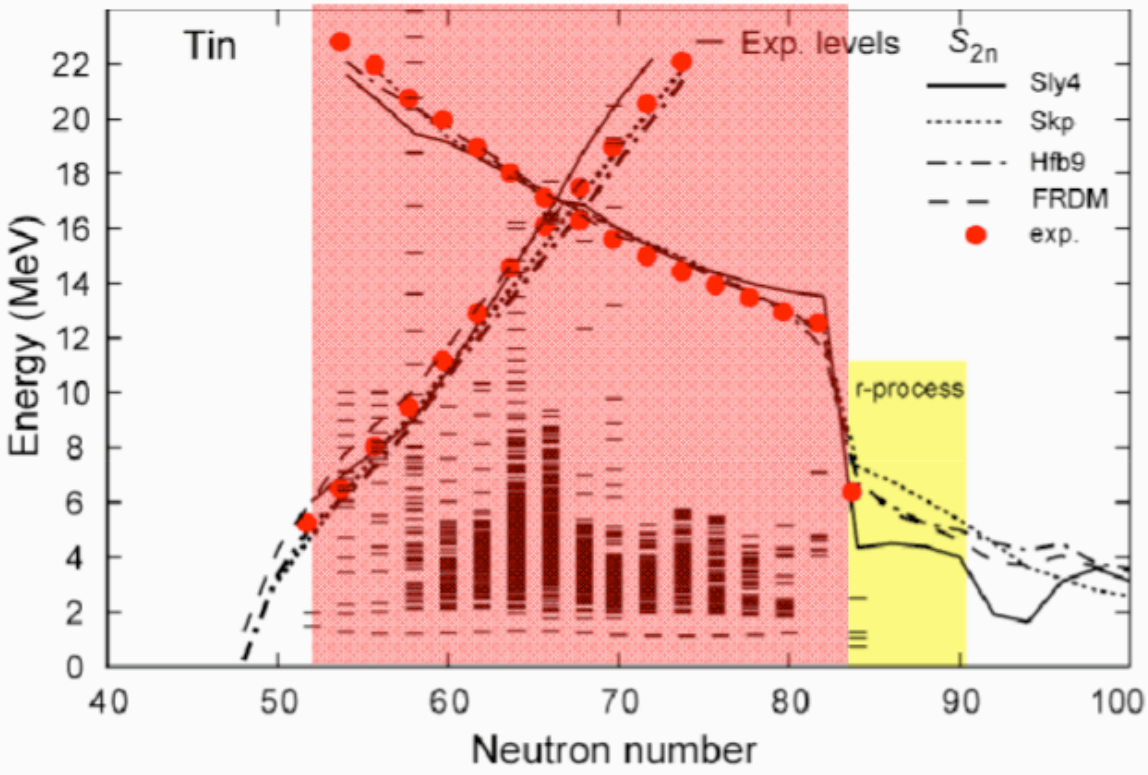
Energy difference between the proton states 2s1/2 and 1d3/2 in Ca isotopes



Grasso, Ma, Khan, Margueron, Van Giai, PRC 76, 044319 (2007)

From Introduction.
Denis Lacroix

S_{2n} and S_{2p} in Tin isotopic chain



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

Large uncertainty in unknown region

Nuclear structure / Astrophysics

Neutron stars. Very exotic nuclear systems (Pierre Pizzochero lecture of today)

Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Physics Reports 411 (2005) 325–375
PHYSICS REPORTS
www.elsevier.com/locate/physrep

Isospin asymmetry in nuclei and neutron stars☆

A.W. Steiner[a,b,*], M. Prakash[c], J.M. Lattimer[c], P.J. Ellis[a,✠]

and references therein

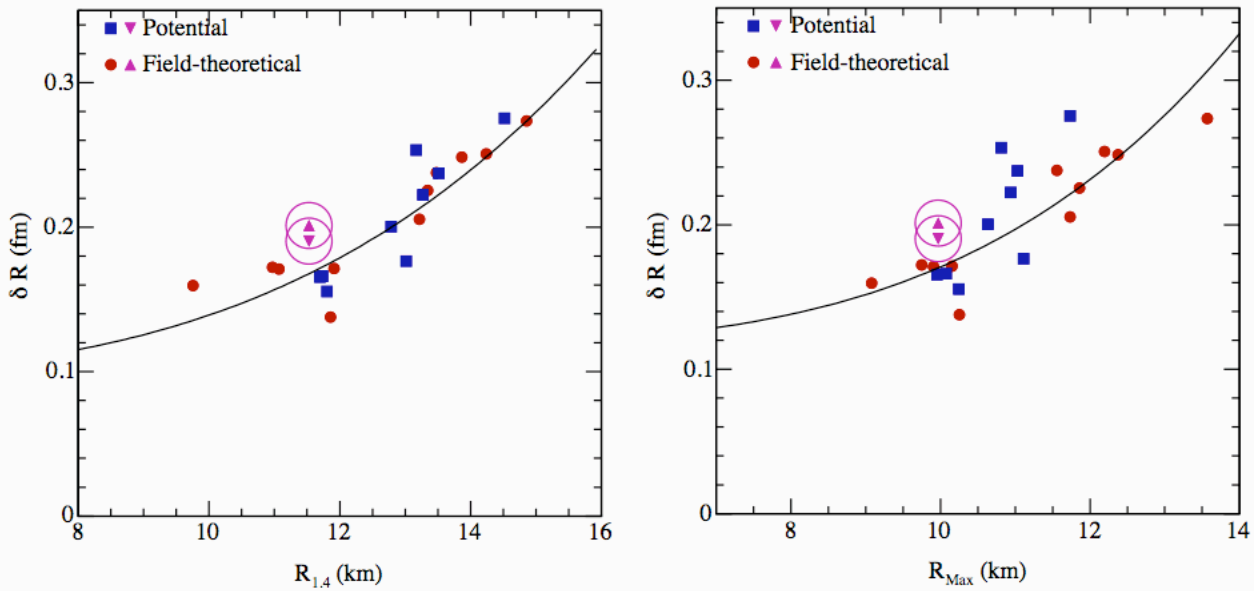


Fig. 16. Calculated neutron skin thickness δR of nuclei versus the radius of $1.4M_{\odot}$ stars (left panel) and of maximum mass stars (right panel). The solid lines are described in the text.

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

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

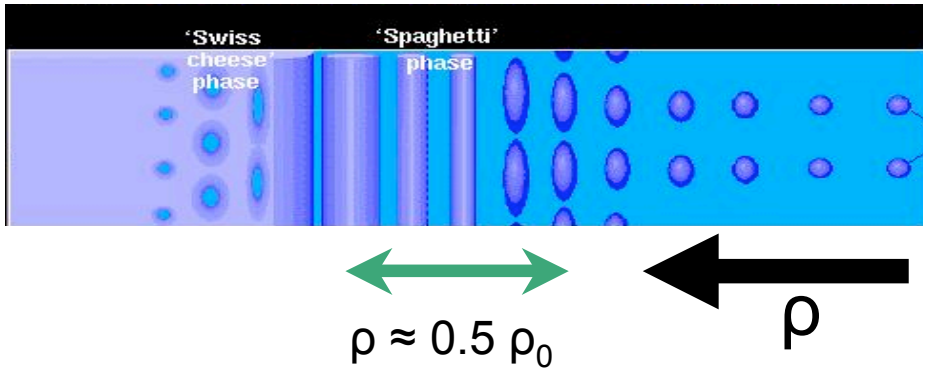
$\sim 2.5 \cdot 10^{14}\ g/cm^3$

Drip point for neutrons

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

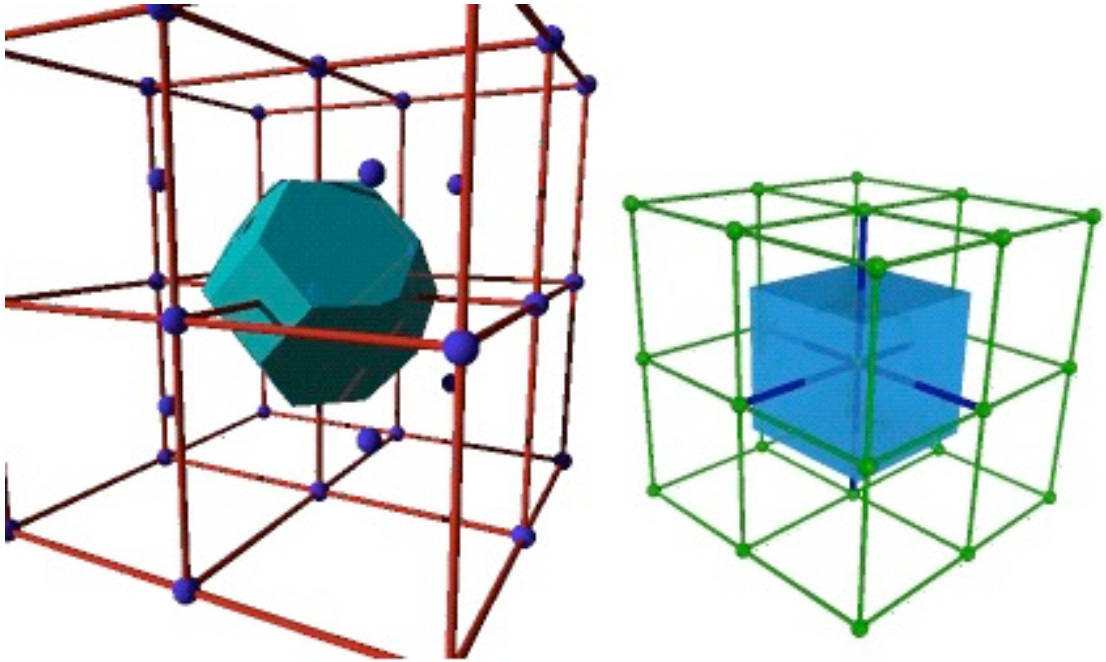
Inner crust: crystal of nuclear clusters in an electron sea and in a gas of superfluid neutrons

Outer crust: crystal of nuclei in an electron sea



β-stability condition -> $\mu_e = \mu_n - \mu_p$

Wigner-Seitz cell model



J.W. Negele and D. Vautherin, Nucl. Phys. A 207, 298 (1973)

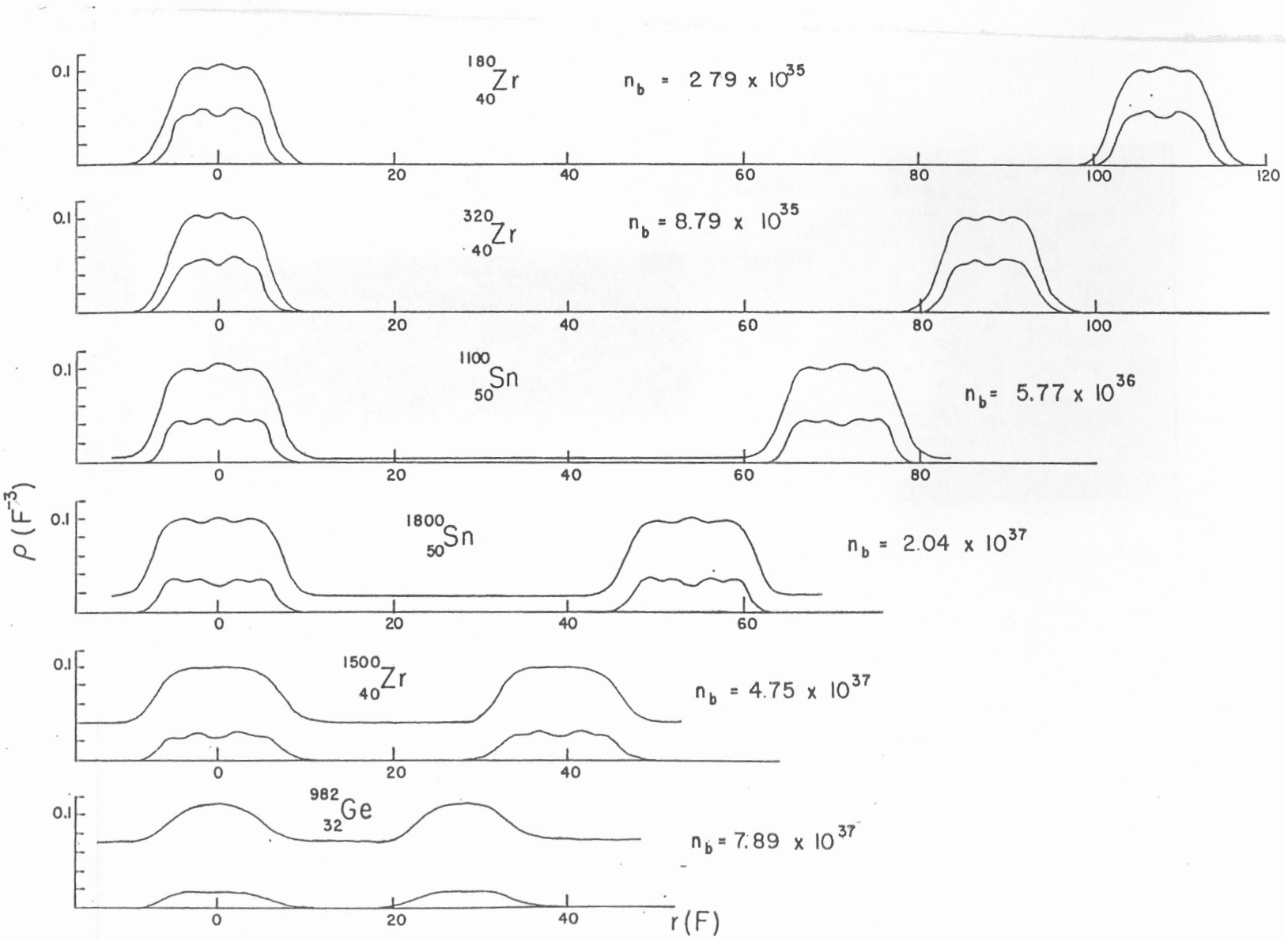
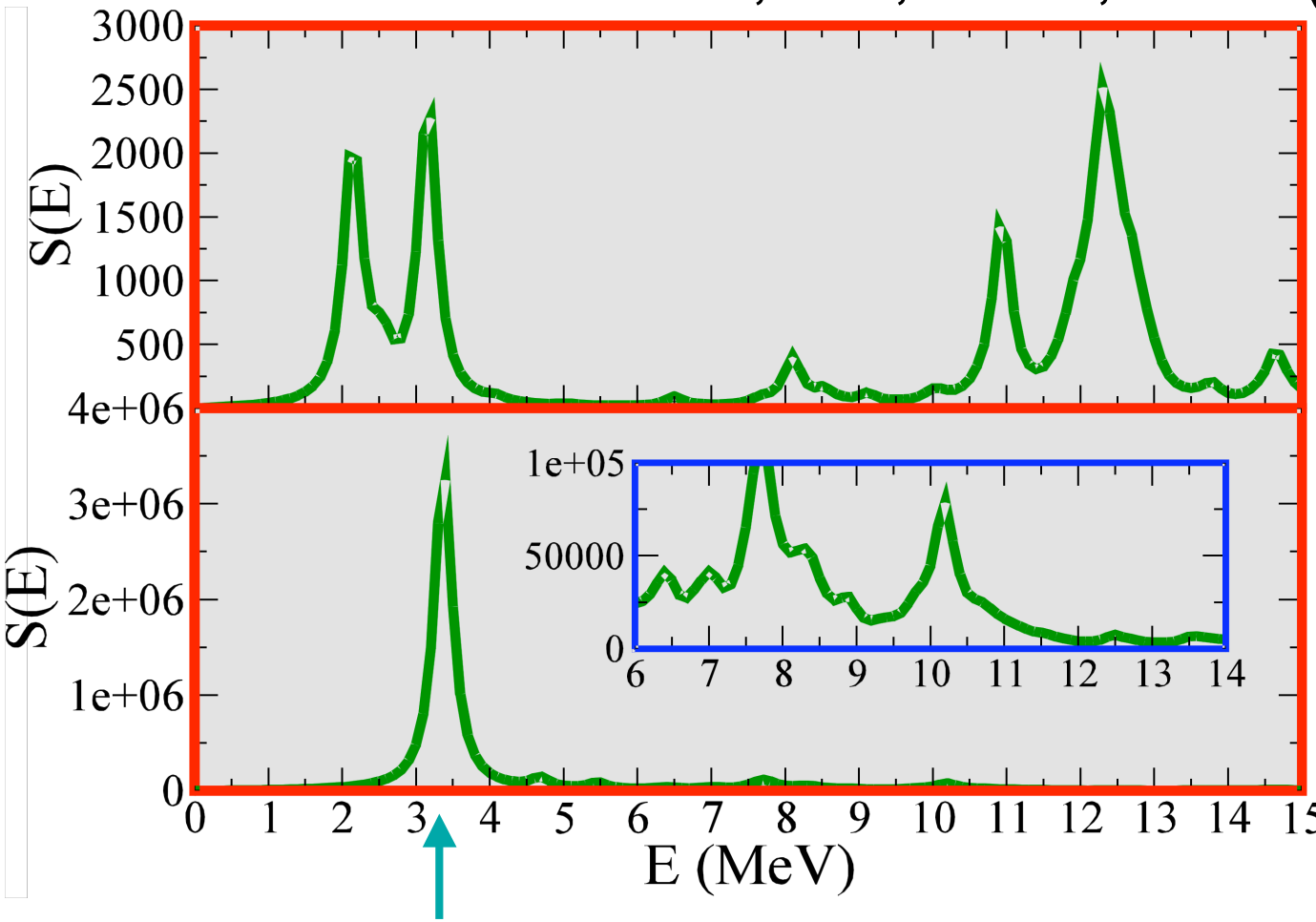


Fig. 3. Proton and neutron density distributions occurring along an axis joining the centers of two adjacent unit cells.

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



Collective mode

Nucleus ^{122}Zr

Wigner-Seitz cell (Z=40, N=1460,

R~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:

K. Capelle, A Bird's-Eye View of Density-Functional Theory, Brazilian Journal of Physics 36, 1318 (2006)

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 Schroedinger 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)

Hohenberg, Kohn, Phys. Rev. B 136, 864 (1964)

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

$$\left[\sum_i^N \left(-\frac{\hbar^2\nabla_i^2}{2m} + v(\mathbf{r}_i)\right) + \sum_{i<j} U(\mathbf{r}_i,\mathbf{r}_j)\right]\Psi(\mathbf{r}_1,\mathbf{r}_2\ldots,\mathbf{r}_N)$$

$$= E\Psi(\mathbf{r}_1,\mathbf{r}_2\ldots,\mathbf{r}_N),$$

- If the ground state density ρ_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 ρ_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 Schroedinger equation for non interacting particles: Kohn-Sham equations

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

Kinetic — Interaction — Functional related to the external potential

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

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

Exact

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

Minimization

$$v_S(\vec{r}) = v(\vec{r}) + v_{Hartree}(\vec{r}) + v_{xc}(\vec{r}).$$

We need E_{xc} to explicitely calculate $v_{xc}(\vec{r}) = \frac{\delta E_{xc}[\rho]}{\delta\rho(\vec{r})}$

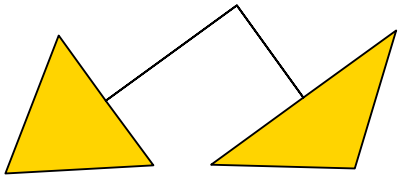
E_{xc} : Exchange-correlation part

$$\left[-\frac{\hbar^2\nabla^2}{2m} + v_S(\vec{r})\right]\varphi_i(\vec{r}) = \varepsilon_i\varphi_i(\vec{r}).$$

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 ?



Local density approximation is used (homogeneous system)

Gradient-corrections to implement LDA (derivatives of the density)

Old: perturbation theory

More recent: Quantum Monte Carlo calculations for the electron liquid

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:

$$V(\mathbf{r}_1,\mathbf{r}_2)=\sum_{i=1,2}\left[W_i+B_iP_\sigma-H_iP_\tau-M_iP_\sigma P_\tau\right]\mathrm{e}^{-r^2/\mu_i^2}$$ **Finite-range (gaussian form)**

$$+t_3\left(1+x_3P_\sigma\right)\left[\rho\left(\mathbf{R}\right)\right]^\alpha\delta(\mathbf{r})$$ **Density dependent (zero-range)**

$$+\mathrm{i}W_0\,\boldsymbol{\sigma}\cdot\left[\mathbf{P}'\times\delta(\mathbf{r})\,\mathbf{P}\right]$$ **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

$$V(\mathbf{r}_1,\mathbf{r}_2) =$$

$$t_0\,(1+x_0P_\sigma)\,\delta(\mathbf{r}) \qquad \text{central}$$

$$+\frac{1}{2}t_1\,(1+x_1P_\sigma)\left[\mathbf{P}'^2\delta(\mathbf{r})+\delta(\mathbf{r})\mathbf{P}^2\right]+t_2\,(1+x_2P_\sigma)\;\mathbf{P}'\cdot\delta(\mathbf{r})\mathbf{P} \qquad \text{non local}$$

$$+\frac{1}{6}t_3\,(1+x_3P_\sigma)\,[\rho\,(\mathbf{R})]^\alpha\,\delta(\mathbf{r}) \qquad \text{density dependent}$$

$$+\mathrm{i}W_0\,\sigma\cdot\left[\mathbf{P}'\times\delta(\mathbf{r})\,\mathbf{P}\right] \qquad \text{spin-orbit}$$

+ 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**

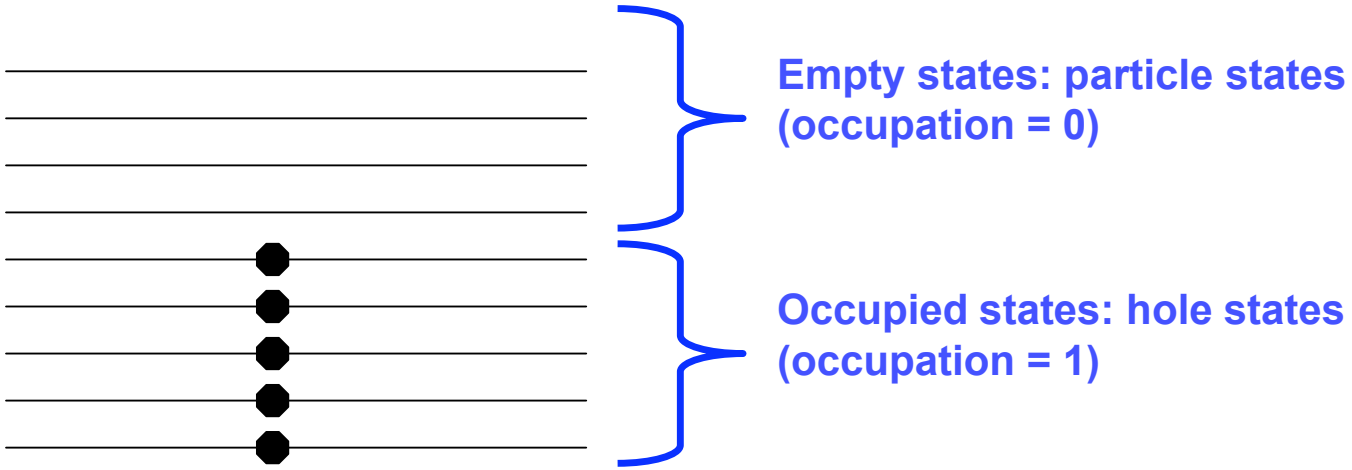
$$H = K + V \sim \sum_{i=1}^{A} \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} \sum_{i \neq j=1}^{A} V_{ij}^{\text{eff}}.$$

What is neglected in V is called residual interaction

- **Ground state wave function is chosen as a Slater determinant**

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

x -> space, spin and isospin coordinates



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:

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

For the Skyrme interaction:

$$\langle H \rangle = \int \mathcal{H}(\mathbf{r})\, \mathrm{d}\mathbf{r}$$

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

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

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

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

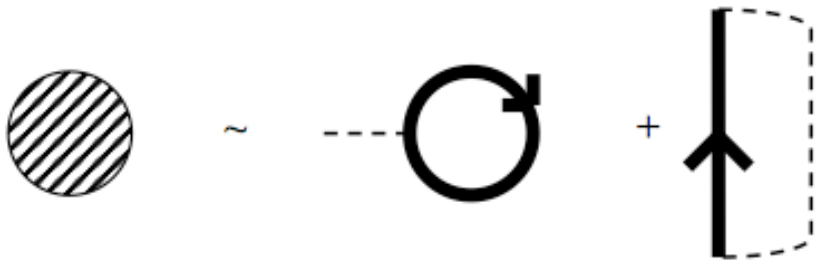
with:

$$\Gamma_H(\vec{r}) = \int d\vec{r}\,'\, v(\vec{r},\vec{r}\,')\rho(\vec{r}\,'), \qquad \text{Depending on local density}$$

$$\Gamma_{Ex}(\vec{r},\vec{r}\,') = -v(\vec{r},\vec{r}\,')\rho(\vec{r},\vec{r}\,'), \qquad \text{Depending on non-local density}$$

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

- DFT is formulated for a system in an external potential. Nuclei are self-bound. Generalizations of the theorems: Engel, PRC 75, 014306 (2007)
  Giraud et al., PRA 78, 032507 (2008)
  Giraud, PRC 77, 014311 (2008)

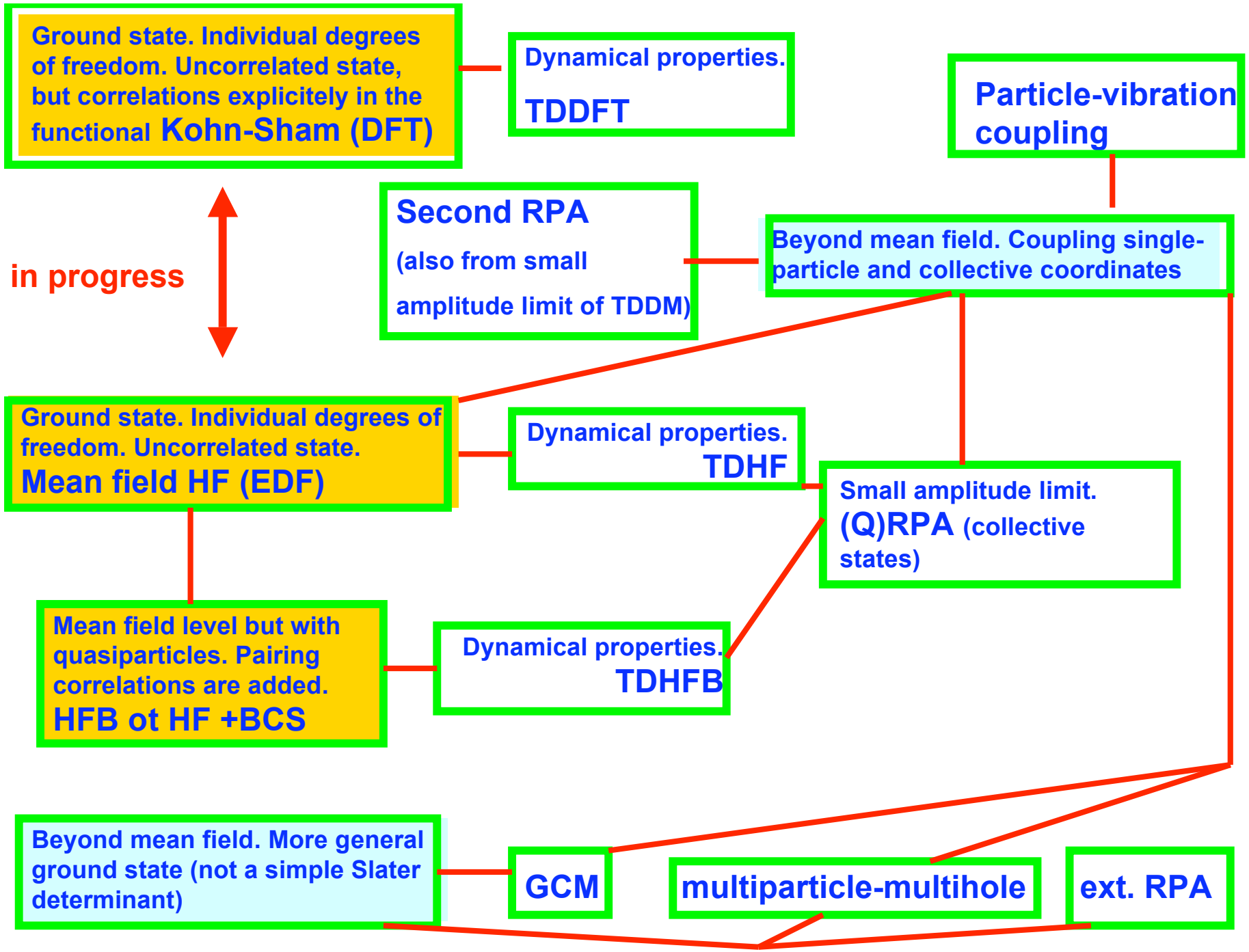
- In HF the exchange term is exactly calculated and the correlation part is totally missing (correlations included in an effective way by the fitting procedure of the interaction). In DFT correlations are always explicitly introduced.

- 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 explicitely in the functional Kohn-Sham (DFT)
Dynamical properties.
TDDFT
Particle-vibration coupling
in progress
Second RPA
(also from small amplitude limit of TDDM)
Beyond mean field. Coupling single-particle and collective coordinates
Ground state. Individual degrees of freedom. Uncorrelated state.
Mean field HF (EDF)
Dynamical properties.
TDHF
Small amplitude limit.
(Q)RPA (collective states)
Mean field level but with quasiparticles. Pairing correlations are added.
HFB ot HF +BCS
Dynamical properties.
TDHFB
Beyond mean field. More general ground state (not a simple Slater determinant)
GCM
multiparticle-multihole
ext. RPA