

Phenomenological descriptions in Nuclear Physics.

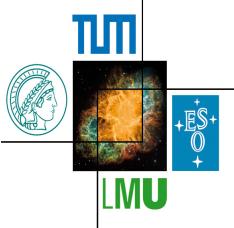
**Zhuhai,
Nov 22, 2023**

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Excellence Cluster “Origins”
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TECHNIS



- Motivation
- Macroscopic description of nuclei
- Microscopic description
- Nuclear density functional theory
- Applications for nuclear ground states
- Density functional theory for excited states
- Conclusions

proton number Z

Publication Year

- 1940
- 1944
- 1948
- 1953
- 1958
- 1967
- 1978
- 1995
- 2000
- Naturally Abundant

Fe

H

neutron number N

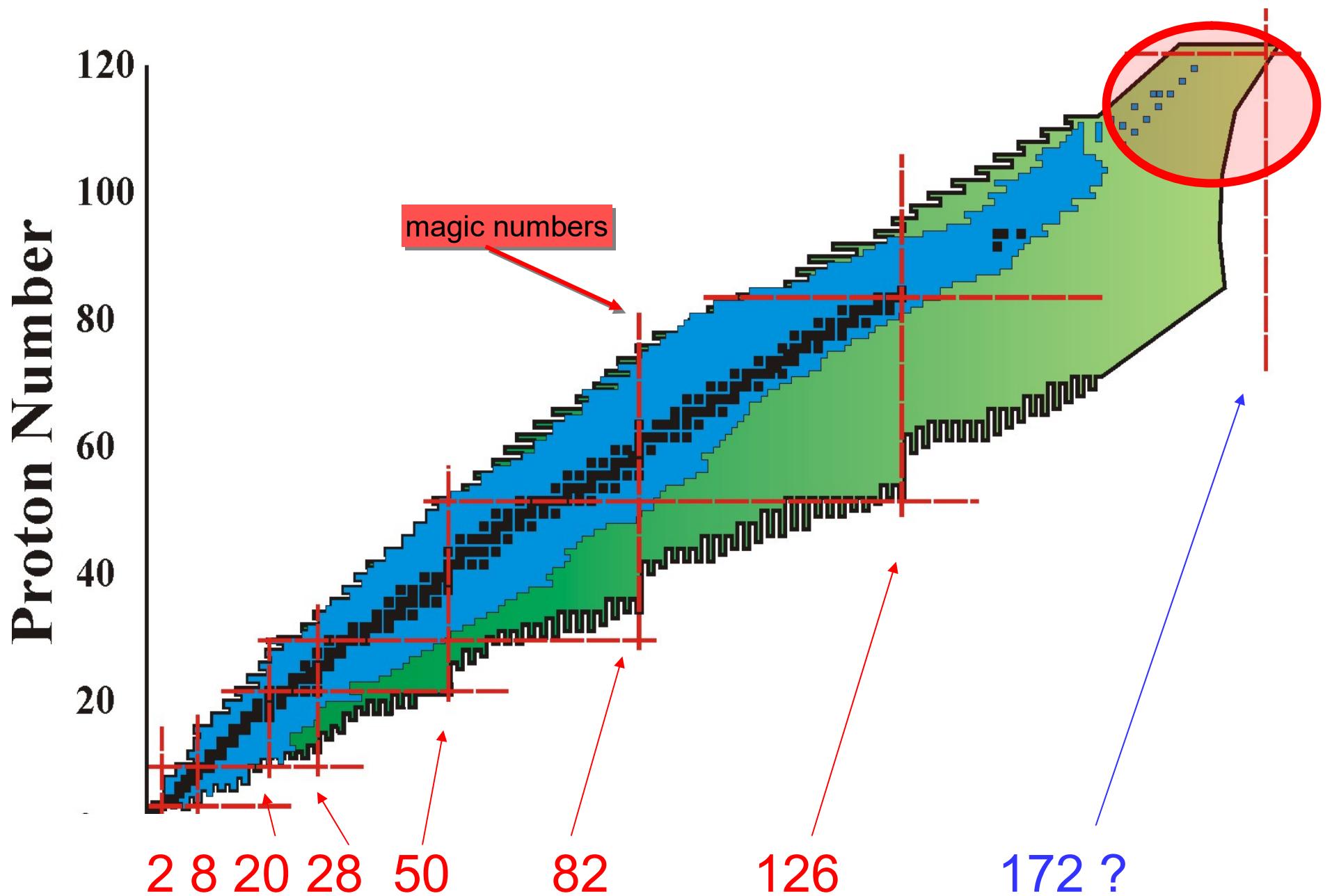
Au

Pb

U

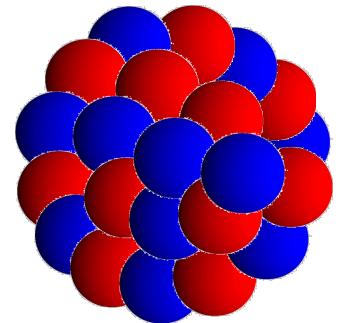
Pulsars in SN remnants:
1054 - Crab





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- Concluding remarks

Which forces act in the nucleus?

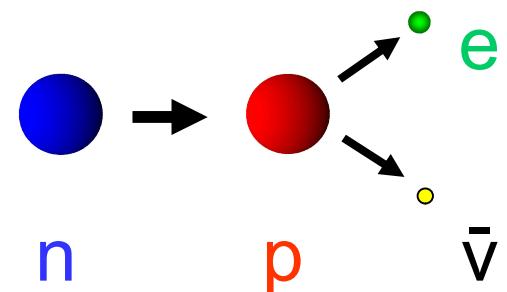


the **Coulomb force** repels the protons

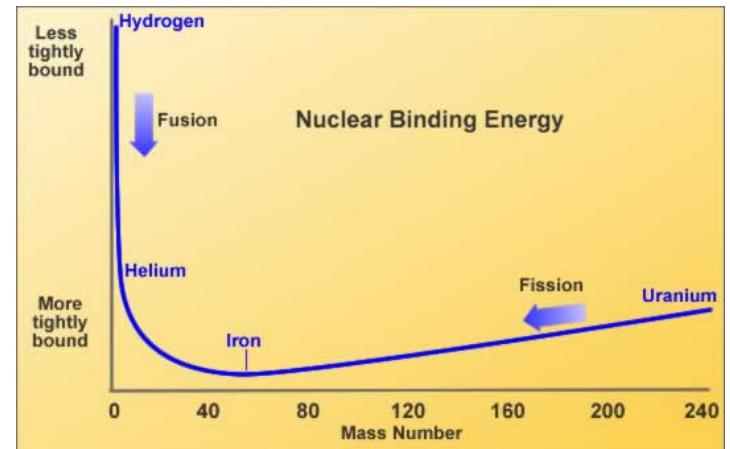
the **strong interaction** ("nuclear force") causes binding
it is stronger for pn-systems than for nn-systems

neutrons alone form no bound states
exception: neutron stars (**gravitation!**)

the **weak interaction** causes β -decay:



Phaenomenological description of the binding energy in nuclei: (Bethe-Weizsäcker-formula)



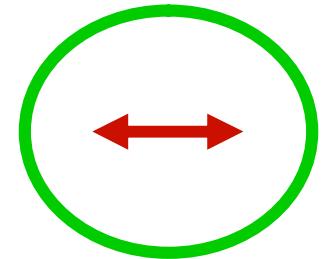
$$B(N,Z) = - a_V \cdot V - a_S \cdot S + a_C \cdot Z^2/R + a_I \cdot (N-Z)^2/A + \dots$$

surface tension

- bindes
- prefers sphere $\sim A^{2/3}$

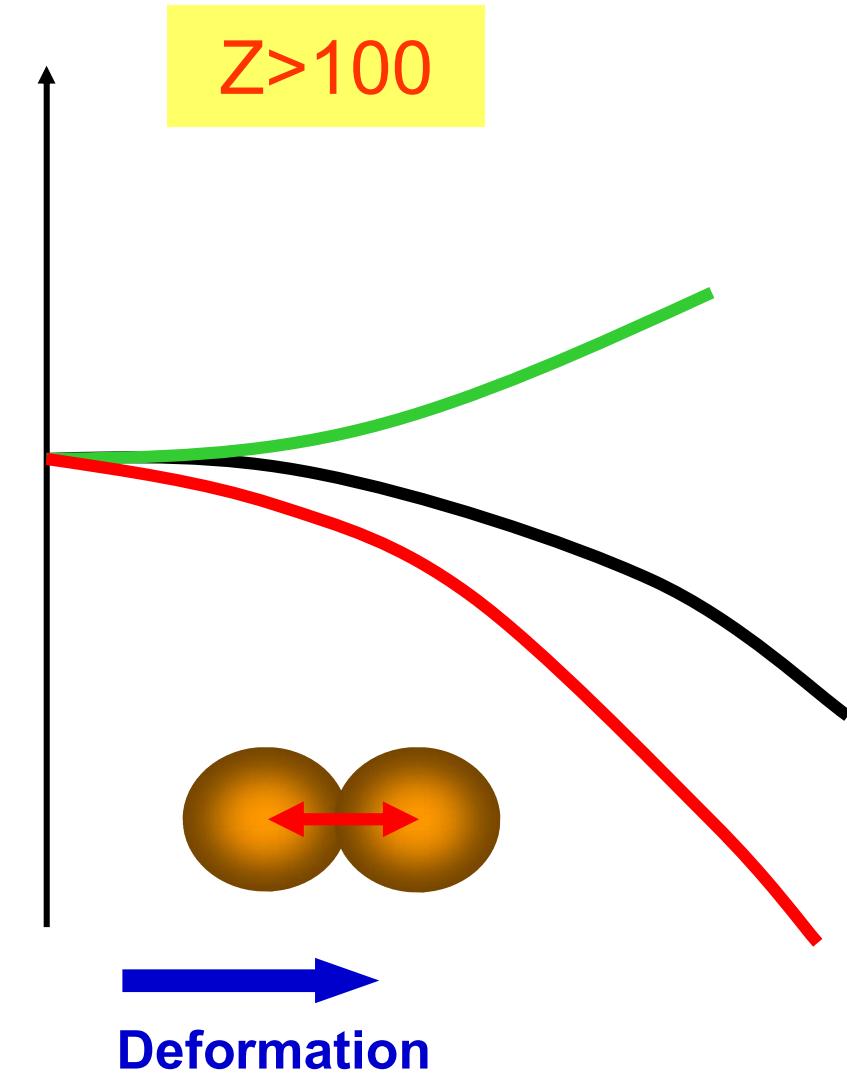
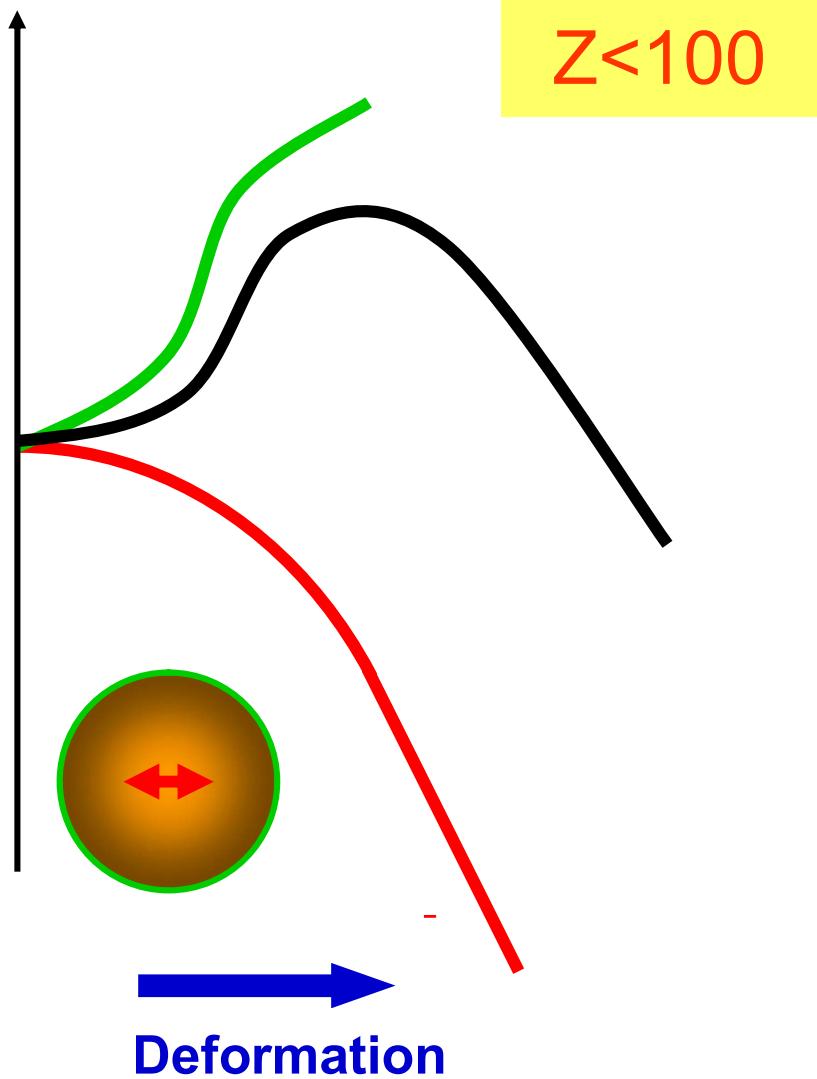
Coulomb repulsion

drives the nucleus
towards fission $\sim Z^2/A^{1/3}$



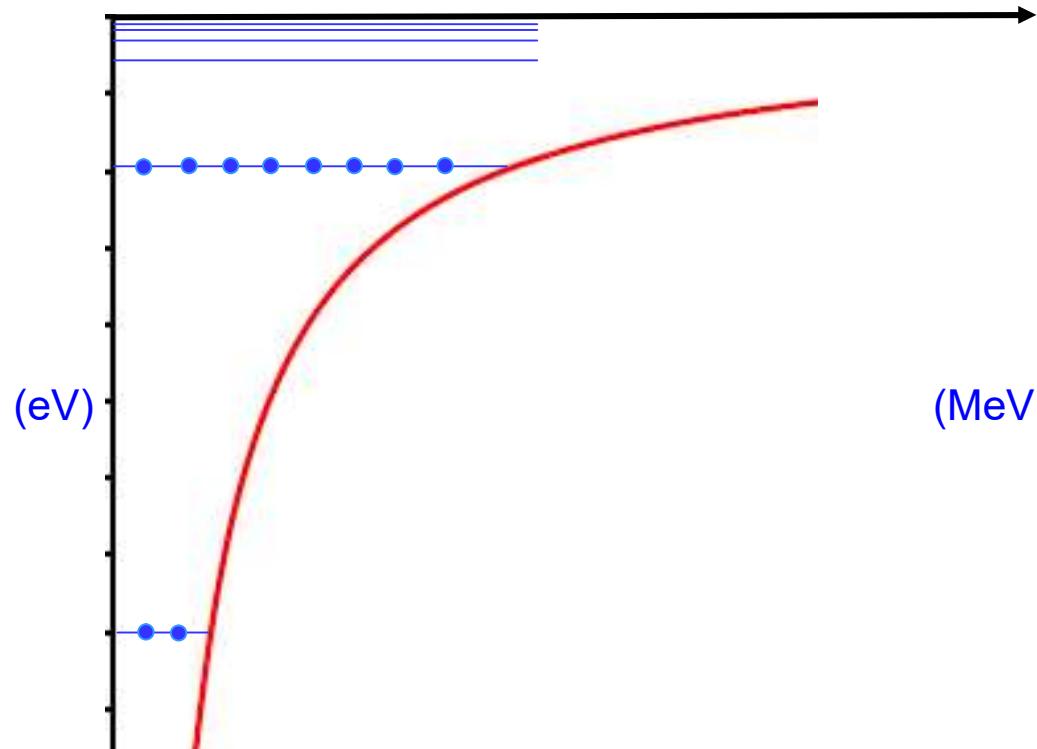
The stability of nuclei is defined
by the interplay between surface tension
and Coulomb repulsion

classical nuclear droplet



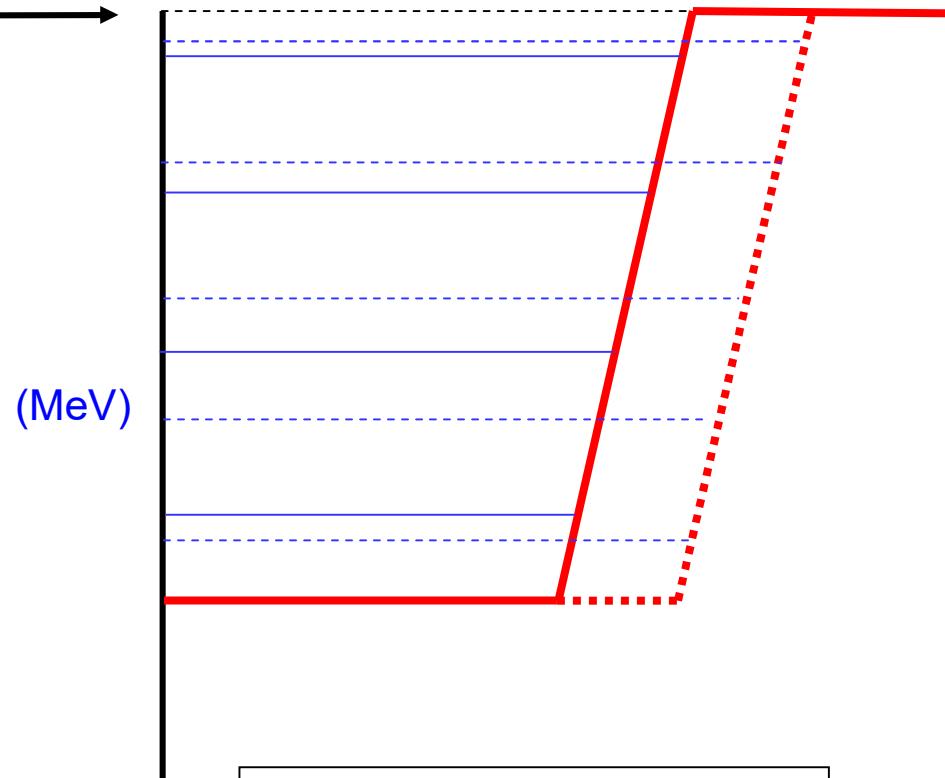
shell effects:

atoms

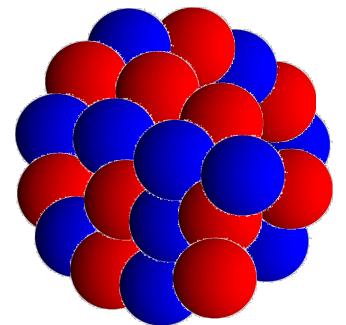


central potential
small spin-orbit

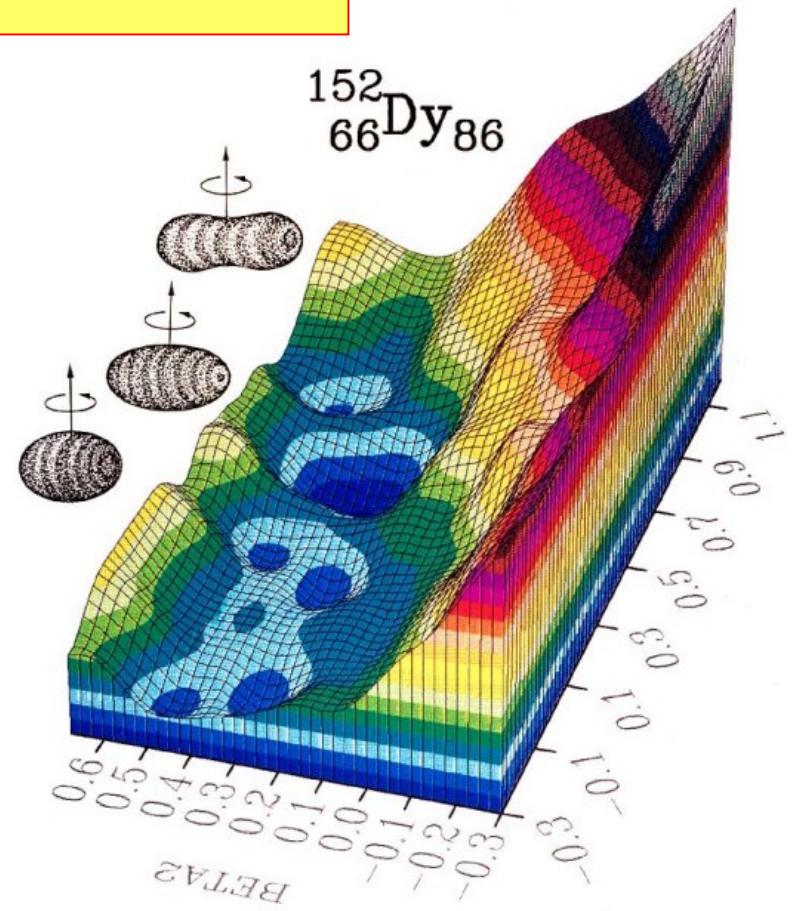
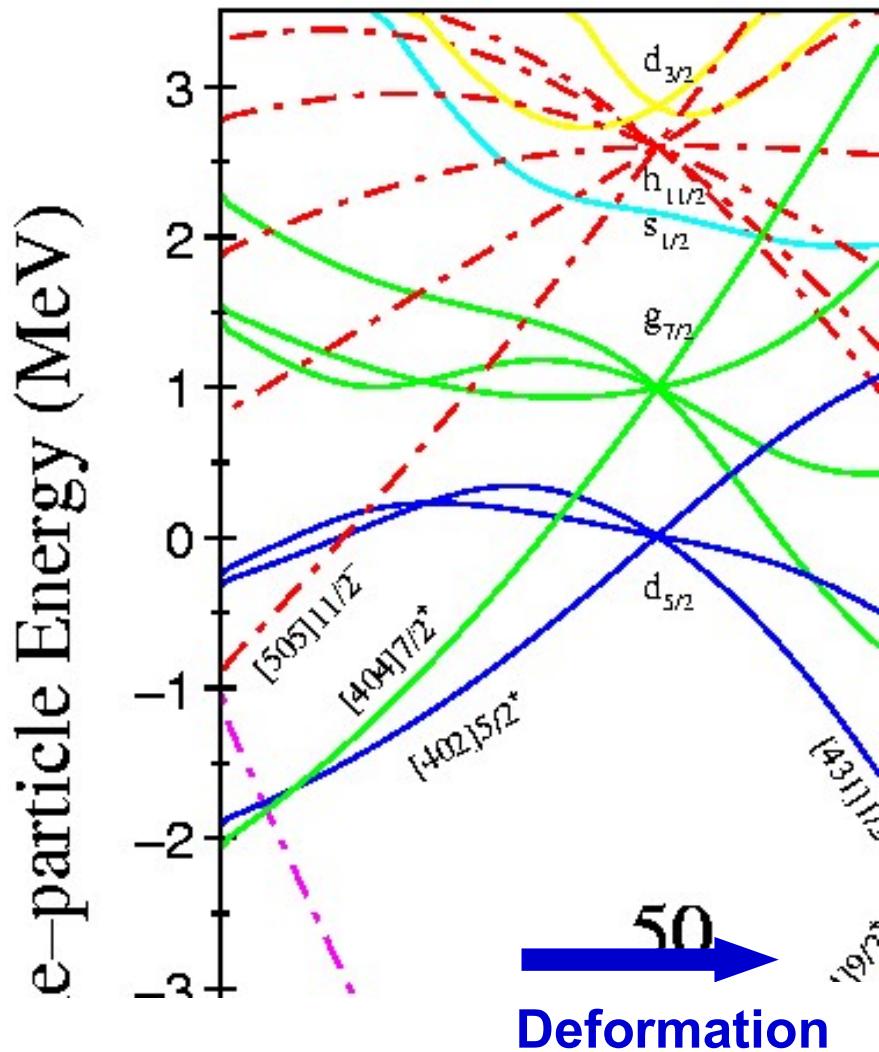
nuclei



self-bound system
large spin-orbit



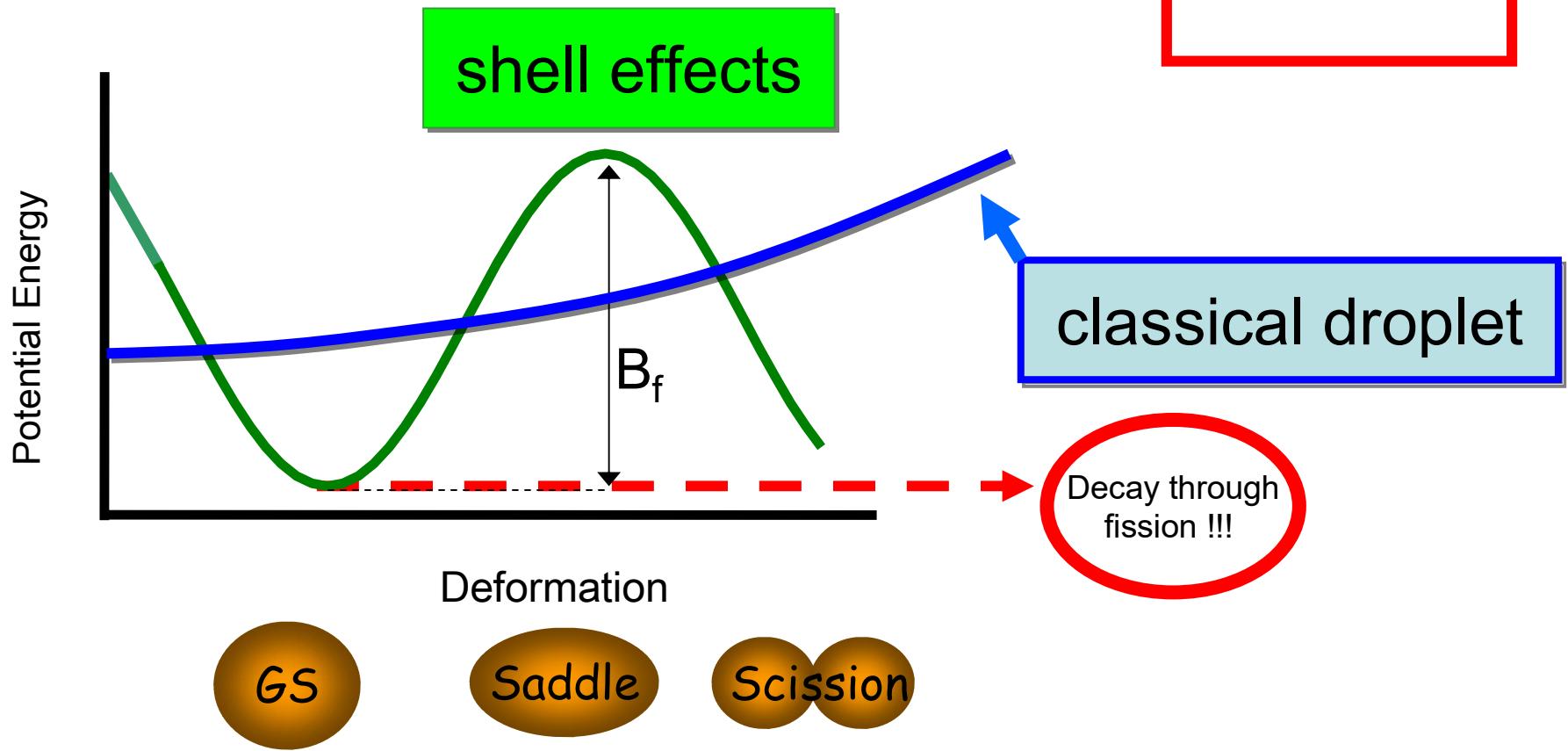
Quantummechanical Shell Effects



Shell effects lead to a new stability at specific protonen- or neutron numbers (**magic numbers**)

Microscopic-macroscopic models

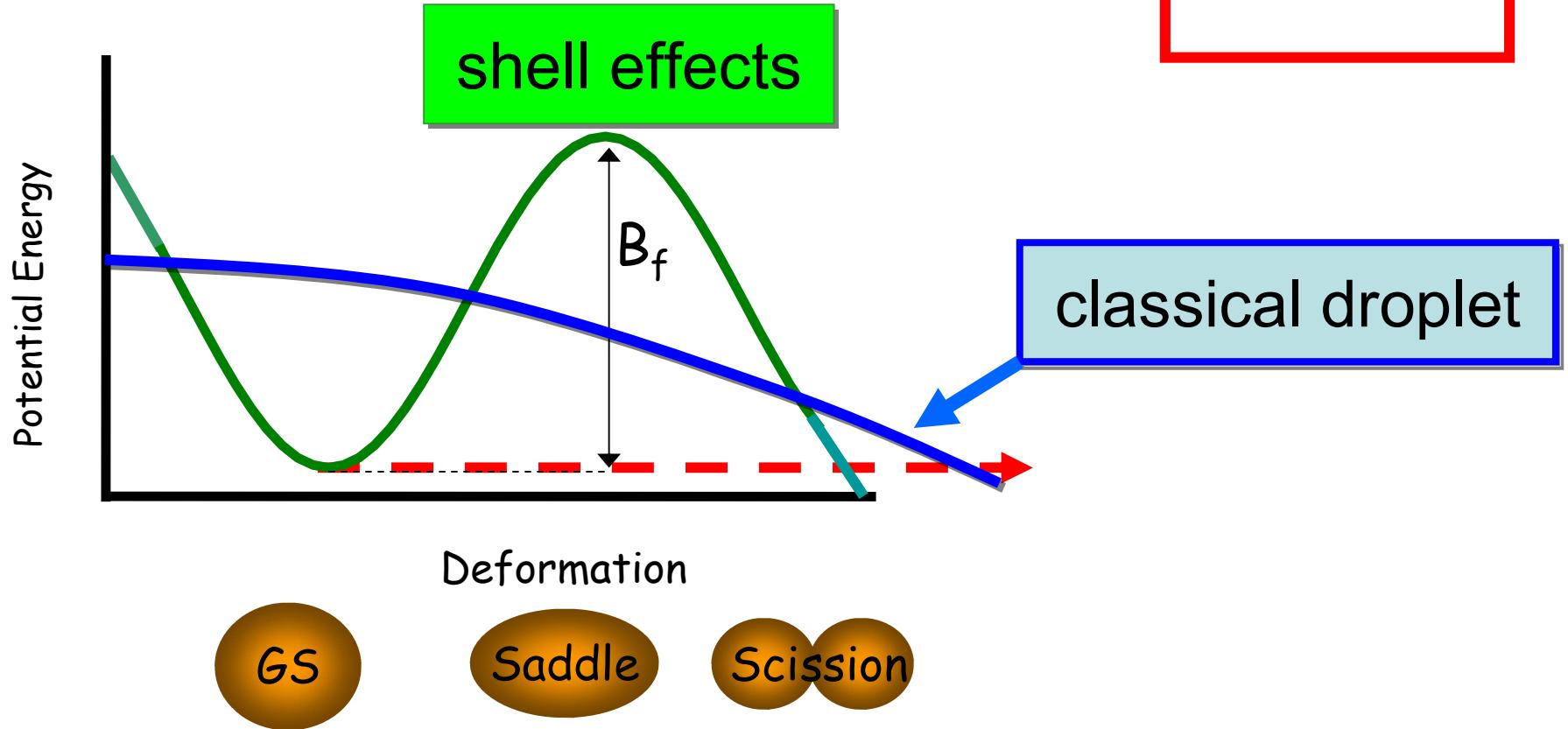
$Z < 100$



Elements with $Z < 100$ are stabilized by surface energy and shell effects

Quantum mechanical shell effects

$Z > 100$



Elements with $Z > 100$ are stabilized only by shell effects

Microscopic-macroscopic models (Mic-Mac):

$$E(\beta) = E_{LDM}(\beta) + E_{osc}(\beta)$$

$E_{LDM}(\beta)$ = liquid-drop energy at deformation β

$E_{osc}(\beta)$ = Strutinsky shell correction at def. β

Review: Peter Møller, EPJA 2023

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ab-initio: 3 scales

> 1 GeV

- **QCD:** non-linear gauge theory, **quarks, gluons**
- confinement, running coupling constant
- at low energies **non-perturbative**
- effective degrees of freedom: nucleon, pion

~ 200 MeV

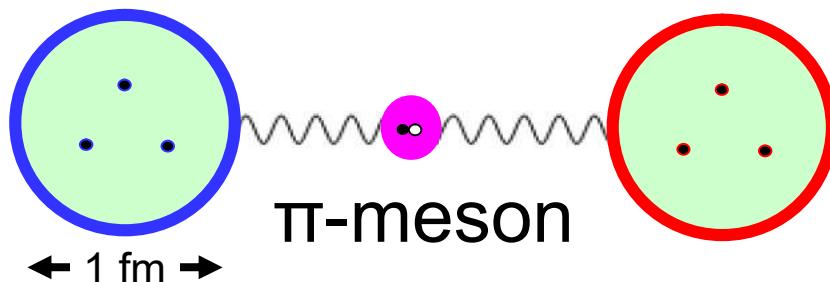
- effective Lagrangian in **nucleons and pions**
- parameters (LEC) so far phenomenological
- non renormalizable
- at low momenta: **chiral perturbation theory: xPT**
- → bare nucleon-nucleon interaction: e.g. **N³LO**

- renormalized forces (soft forces)
- effective forces within the nucleus
- depend on configuration, dependent on density
- **configuration mixing, density functional theory**

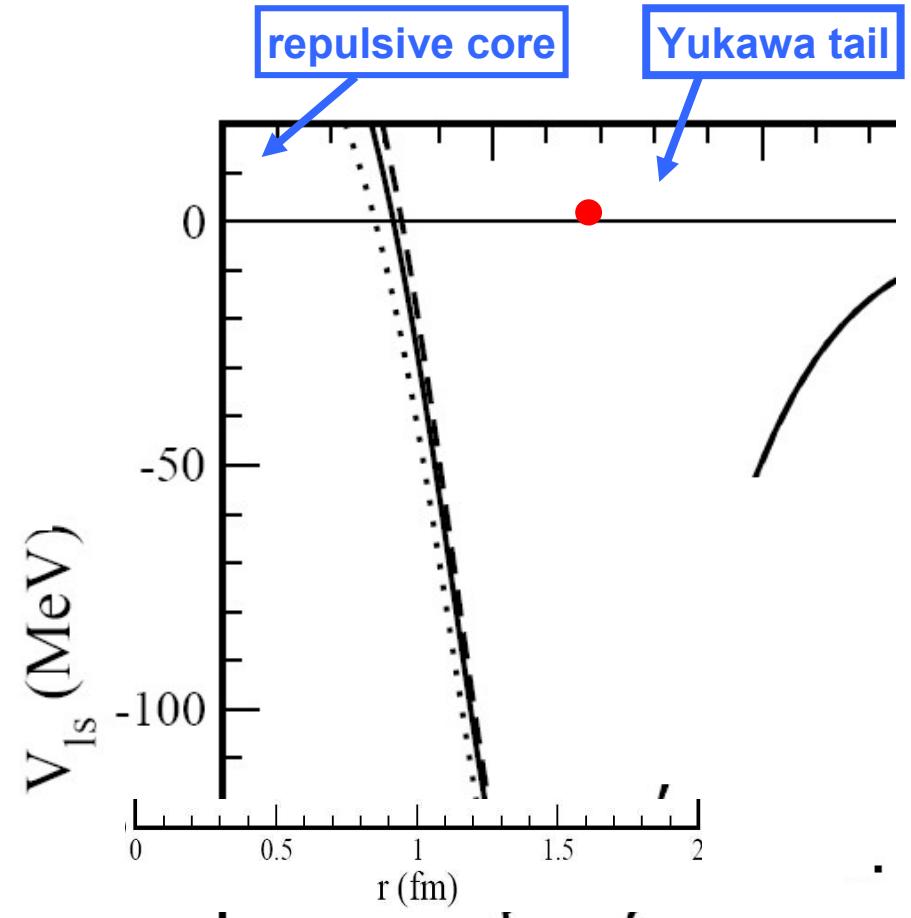
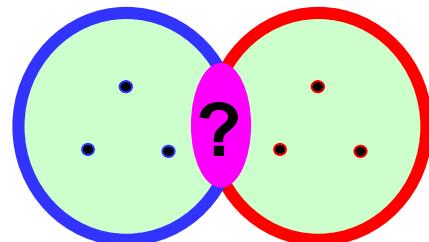
~ 0.1 - 1 MeV

The bare nucleon-nucleon interaction:

distance > 1 fm: attractive



distance < 0.8 fm: repulsive



three-body forces

What is special in nuclei?

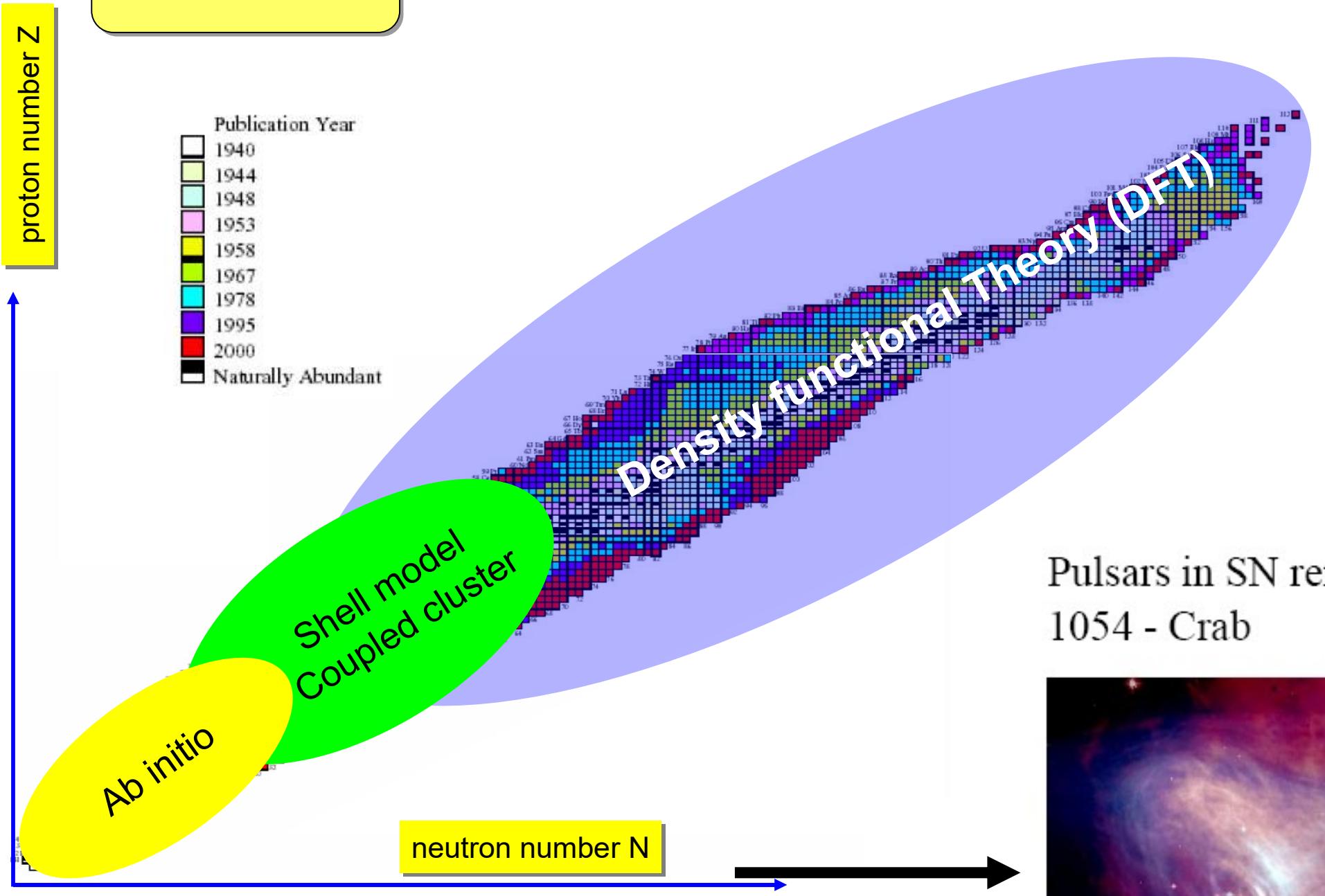
- size: nuclei are very small objects:

$$\Delta x^2 \Delta p^2 \geq \frac{\hbar^2}{4} \quad E_{kin} \geq 10 \frac{fm^2}{r^2} \text{ MeV} = 10^{-5} \frac{nm^2}{r^2} \text{ eV}$$

- spin and isospin degrees: 4^A possibilities
- complicated interaction:
strongly repulsive, tensor-forces, 3-body-forces
- many particles: Pauli principle:
effective interaction inside the nucleus is quenched (Brueckner)
- required accuracy (for masses):

$$100 \text{ keV} / 1000 \text{ MeV} \approx 10^{-4}$$

Motivation:



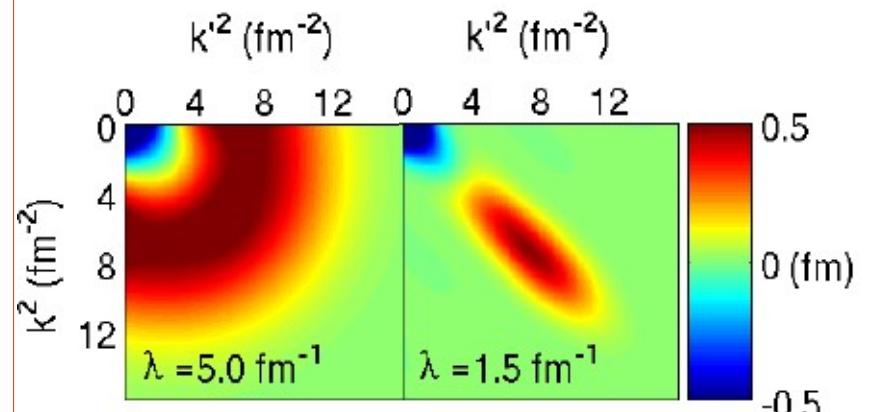
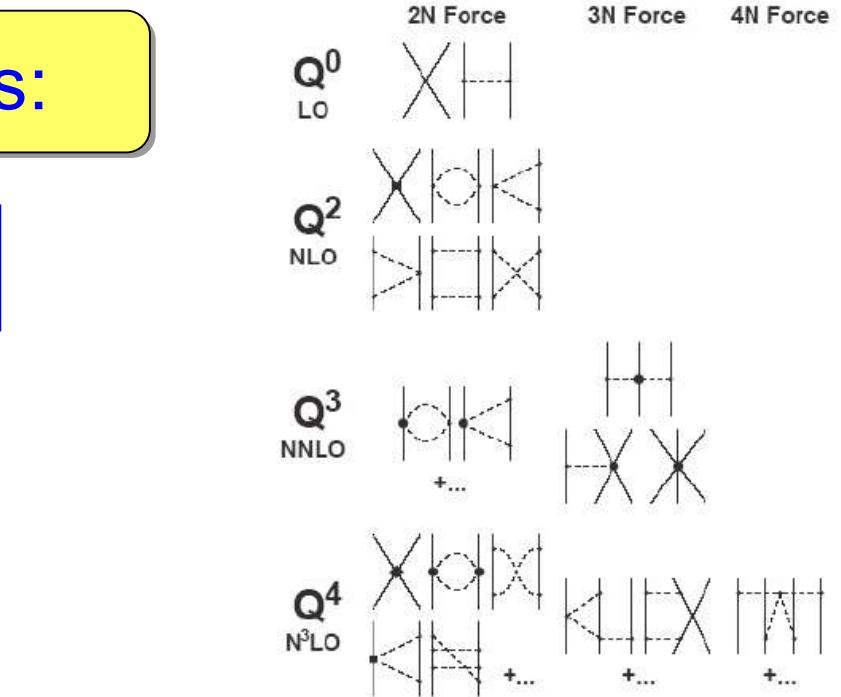
Forces for ab-initio calculations:

Ab initio forces NN+NNN (e.g. N3LO)

Entem,Machleit (Idaho-potential)
Epelbaum et al

Renormalization

- Brueckner G-Matrix
- Li - Suzuki
- SRG (similarity renormalization group method)
- UCOM (unitary correlator operator method)



Furnstahl et al

Manybody methods:

NN+NNN (e.g. N3LO)

- Greens-Function Monte Carlo (GFMC)

- No-Core Shell Model (NCSM)

- Coupled cluster methods (CC)

- Variational methods

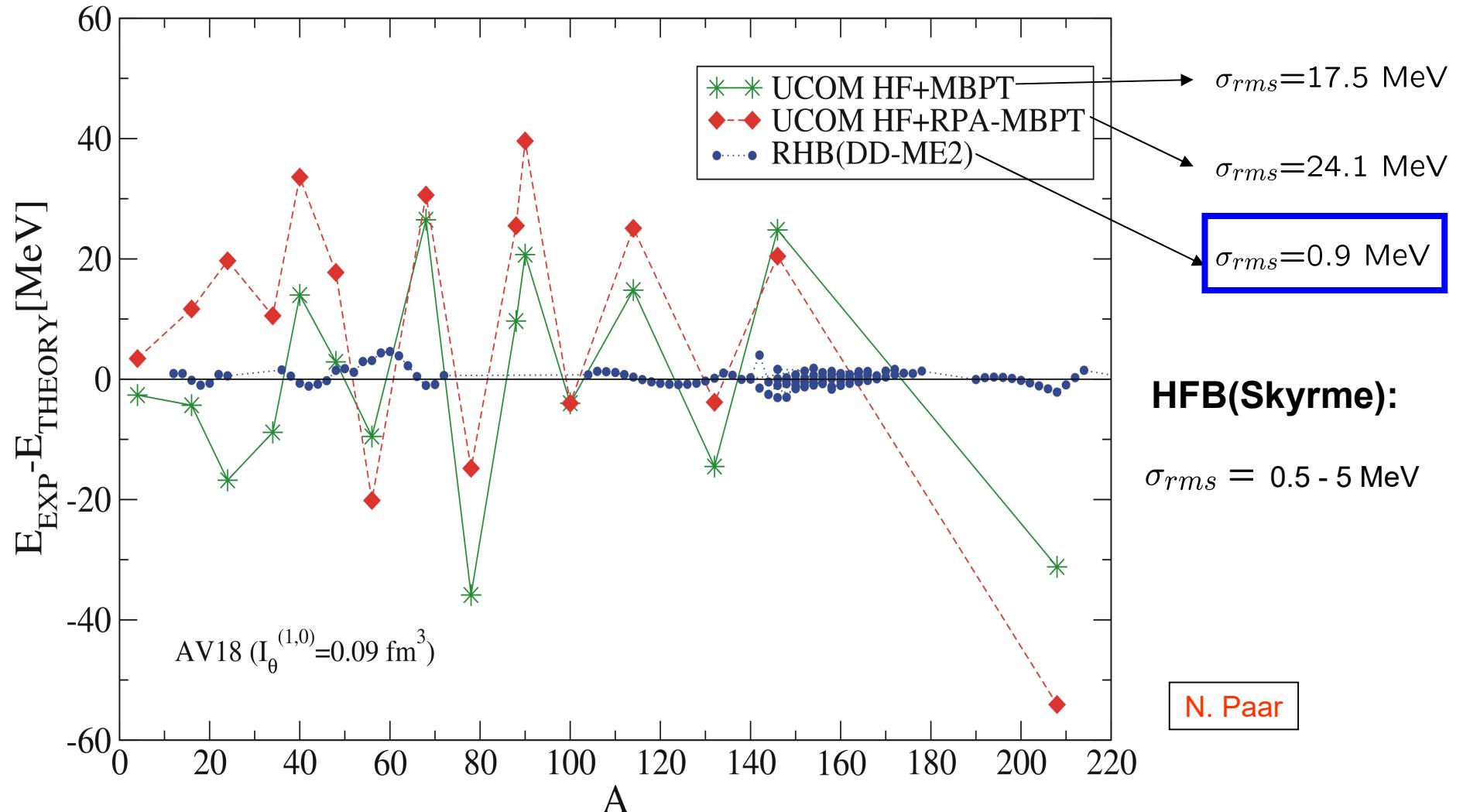
- Hartree-Fock + perturbation theory

Renormalized forces

Two types of NNN forces:
- from bare NNN-forces
- from the renormalization

Example:

UCOM-masses / DFT-masses



Ab-initio masses can and should not be compared with phenomenological masses !!!

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Concepts of density functional theory

$$E = \langle \Psi | \hat{H} | \Psi \rangle = \langle \Phi | \hat{H}_{eff} | \Phi \rangle = E[\hat{\rho}]$$

$|\Phi\rangle$ Slater determinant \Leftrightarrow $\hat{\rho}$ density matrix

$$|\Phi\rangle = \mathcal{A}(\varphi_1(\mathbf{r}_1) \cdots \varphi_A(\mathbf{r}_A)) \quad \hat{\rho}(\mathbf{r}, \mathbf{r}') = \sum_{i=1}^A |\varphi_i(\mathbf{r})\rangle\langle\varphi_i(\mathbf{r}')|$$

Mean field:

$$\hat{h} = \frac{\delta E}{\delta \hat{\rho}}$$

Eigenfunctions:

$$\hat{h}|\varphi_i\rangle = \varepsilon_i |\varphi_i\rangle$$

Interaction:

$$\hat{V} = \frac{\delta^2 E}{\delta \hat{\rho} \delta \hat{\rho}}$$

General aspects of density functional theory

- * $\hat{H}_{eff} = \hat{H}$ (**Hartree-Fock**) fails in nuclear physics
- * \hat{H}_{eff} contains **correlations** (e.g. Brueckner correlations)
- * \hat{H}_{eff} is **density dependent**
- * \hat{H}_{eff} can contain **symmetry restauration**: $\Rightarrow P^I \hat{H}_{eff} P^I$
- * \hat{H}_{eff} can contain **coupling to vibrations**: $\Rightarrow \hat{H}_{eff}(E)$
- * $E[\hat{\rho}]$ is **more general** than \hat{H}_{eff}
- * **Time-dependent DFT:**
$$\delta \int dt \left\langle \Phi(t) \left| i\partial_t \right| \Phi(t) \right\rangle - E[\hat{\rho}(t)] \right\rangle = 0$$

Hohenberg-Kohn theorem (1963):

The exact energy of a quantum mechanical many body system is a functional of the local density $\rho(\mathbf{r})$

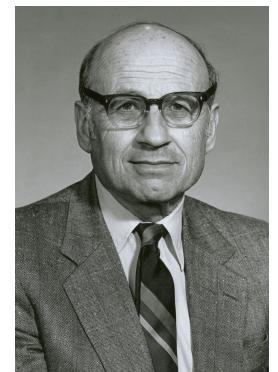
$$E[\rho] = \langle \Psi | H | \Psi \rangle$$



Hohenberg

This functional is universal. It does not depend on the system, only on the interaction.

One obtains the exact density $\rho(\mathbf{r})$ by a variation of the functional with respect to the density



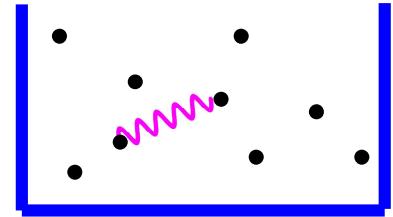
Kohn

note:

$\rho(\mathbf{r})$ is a function of 3 variables.

$\Psi(\mathbf{r}_1 \dots \mathbf{r}_N)$ is a function of $3N$ variables.

Many-body system in an external field $U(r)$:



We consider a realistic many-body system in an external field $U(r)$ and a two- (or three-) body interaction $V(r_i, r_k)$. The total energy E_{tot} of the system depends on $U(r)$: It is a **functional** of $U(r)$:

$$E_{\text{tot}} = \langle \hat{T} + \hat{V} + \hat{U} \rangle = \langle \hat{T} + \hat{V} \rangle + \int \rho(\mathbf{r}) U(\mathbf{r}) d^3r = E_{\text{tot}}[U(\mathbf{r})]$$

in the same way we obtain the density: $\rho = \rho[U]$

Inverting this relation we can introduce a **Legendre transformation** replacing the independent function $U(r)$ by the density $\rho(r)$: $U = U[\rho]$

$$E_{\text{tot}}[U] \Rightarrow E_{\text{HK}}[\rho]$$

$$F(V) \rightarrow G(P) = F + PV$$

$$\begin{aligned} E_{\text{HK}}[\rho] &= E_{\text{tot}}[U] - \int \rho(\mathbf{r}) U(\mathbf{r}) d^3r \\ &= \langle \hat{T} + \hat{V} + \hat{U} \rangle - \langle \hat{U} \rangle = E \end{aligned}$$

Legendre transformations in thermodynamics:

Free energy: $F(T, V)$ depends on the volume

Pressure: $P(V) = -\frac{\partial F}{\partial V}$

Inversion: $V = V(P)$

Gibbs energy: $G(T, P) = F(T, V(P)) + PV(P)$

$$F(T, V) \Rightarrow G(T, P)$$

In many-body systems:

$$V \Rightarrow -U(\mathbf{r})$$

$$P \Rightarrow \rho(\mathbf{r})$$

Decomposition of the HK-functional:

In practical applications the functional $E_{HK}[\rho]$ is decomposed into three parts:

$$E_{HK}[\rho] = E_{ni}[\rho] + E_H[\rho] + E_{xc}[\rho]$$

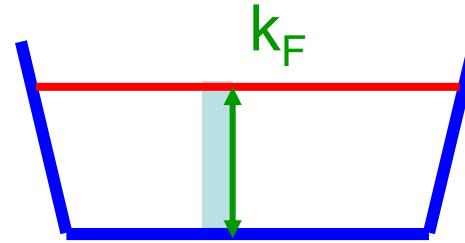
The Hartree term is simple: $E_H[\rho] = \frac{1}{2} \int \rho(\mathbf{r}) V(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') d^3r d^3r'$

The non interacting part: $E_{ni}[\rho] = E_{HK}[\rho]_{V=0}$

The exchange-correlation part is the rest: $E_{xc}[\rho] = E_{HK}[\rho] - E_{ni}[\rho] - E_H[\rho]$

E_{xc} is less important and often approximated, but for modern calculations it plays an essential rule.

Thomas Fermi approximation:



Thomas and Fermi used the **local density approximation** (LDA) to get an analytical expression for the non-interacting term. They calculated the kinetic energy density of a homogeneous system with constant density ρ

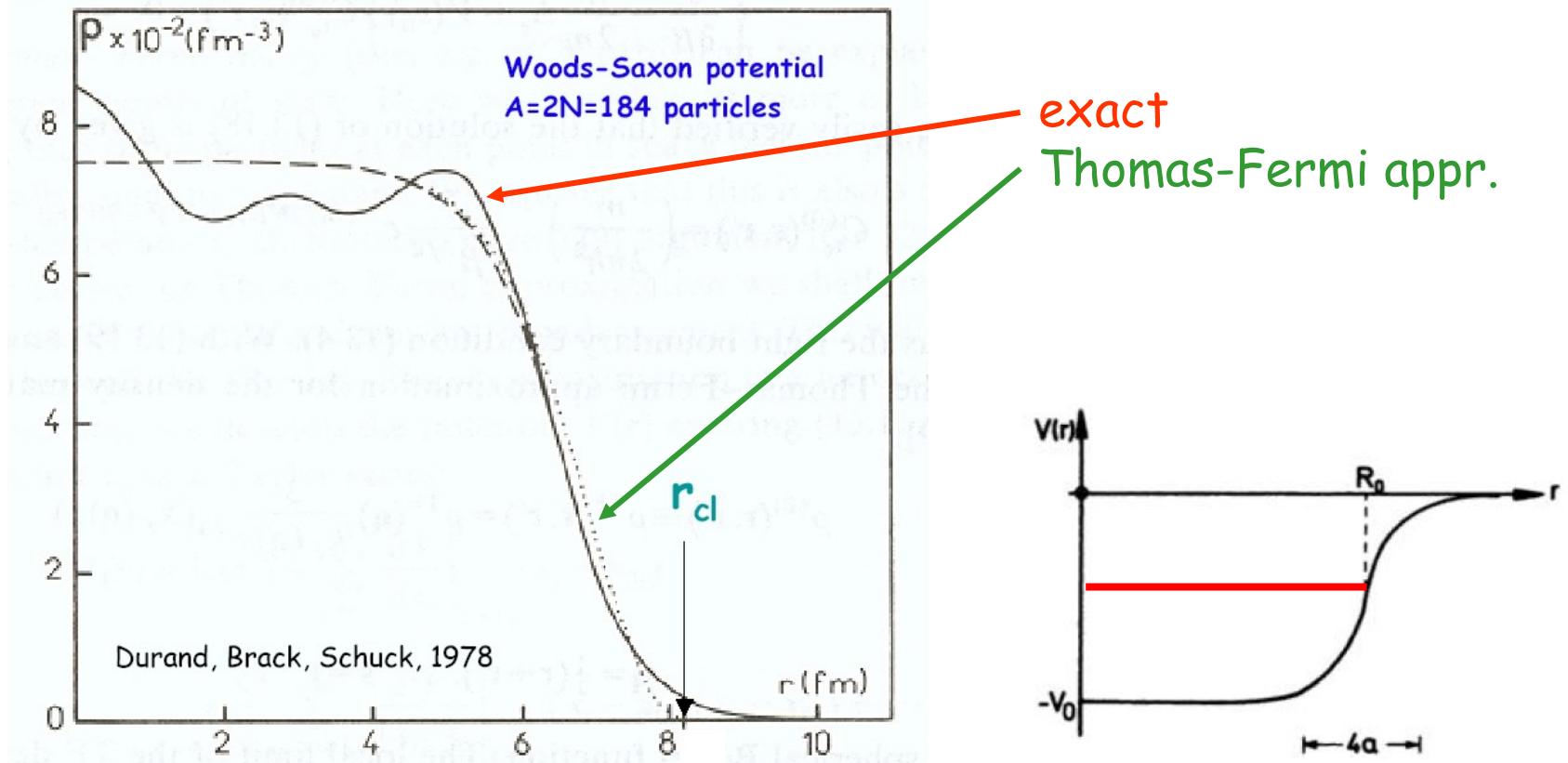
$$\frac{E}{V} = \gamma \int_{k < k_F} \frac{(\hbar k)^2}{2m} d^3k = \frac{\hbar^2}{2m} \frac{3}{5} \left(\frac{6\pi^2}{\gamma} \right)^{\frac{2}{3}} \rho^{\frac{5}{3}}$$

where γ is the spin/isospin degeneracy. One finds:

$$E_{ni}^{(TF)}[\rho] = \frac{\hbar^2}{2m} \frac{3}{5} \left(\frac{6\pi^2}{\gamma} \right)^{\frac{2}{3}} \int \rho^{\frac{5}{3}}(r) d^3r$$

This is not very good (molecules are never bound) and therefore one added later on gradient terms containing $\nabla\rho$ and $\Delta\rho$. This method is called **Extended Thomas Fermi (ETF)** theory. However, these are all asymptotic expansions and one always ends up with semi-classical approximations. **Shell effects** are never included.

Example for Thomas Fermi approximation:



Kohn-Sham theory:

In order to reproduce shell structure Kohn and Sham introduced a auxiliary single particle potential $V_{\text{eff}}(\mathbf{r})$, which is defined by the condition, that after the solution of the single particle eigenvalue problem

$$\left\{ -\frac{\hbar^2}{2m}\Delta + V_{\text{eff}}(\mathbf{r}) \right\} \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r})$$

the density obtained as $\sum_{i=1}^A |\varphi_i(\mathbf{r})|^2 = \rho(\mathbf{r})$ is the exact density

Obviously to each density $\rho(\mathbf{r})$ there exist such a potential $V_{\text{eff}}(\mathbf{r})$.

The non interacting part of the energy functional is given by:

$$E_{\text{ni}}[\rho] = \int \frac{\hbar^2}{2m} \tau(\mathbf{r}) d^3r = \int \frac{\hbar^2}{2m} \sum_{i=1}^A |\nabla \varphi_i(\mathbf{r})|^2 d^3r = \sum_{i=1}^A \varepsilon_i - \int V_{\text{eff}}(\mathbf{r}) \rho(\mathbf{r}) d^3r$$

and obviously we have:

$$V_{\text{eff}}(\mathbf{r}) = -\frac{\delta}{\delta \rho} E_{\text{ni}}[\rho] = -\frac{\delta}{\delta \rho} (E_{\text{HK}} - E_{\text{H}} - E_{\text{xc}})$$

Determinant of $V_{\text{eff}}(\mathbf{r})$:

In principle we can find $V_{\text{eff}}(\mathbf{r})$ by calculating the functional derivatives:

$$V_{\text{eff}}(\mathbf{r}) = -\frac{\delta}{\delta\rho}E_{\text{HK}} + \frac{\delta}{\delta\rho}E_{\text{H}} + \frac{\delta}{\delta\rho}E_{\text{xc}}$$

$$V_{\text{eff}}(\mathbf{r}) = U(\mathbf{r}) + V_H(\mathbf{r}) + V_{\text{xc}}(\mathbf{r})$$

with the Hartree potential:

$$V_H(\mathbf{r}) = \int V(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}')d^3r$$

and the exchange-correlation potential:

$$V_{\text{xc}}(\mathbf{r}) = \frac{\delta}{\delta\rho}E_{\text{xc}}$$

of course it all depends on the knowledge or on the approximation of the functional for the **exchange-correlation energy**

Kohn-Sham functional:

$$E_{\text{KS}}(\rho, \tau) = \int \frac{\hbar^2}{2m}\tau(\mathbf{r})d^3r + E_{\text{H}}(\rho) + E_{\text{xc}}(\rho)$$

Practical applications:

The Kohn-Sham scheme involves the following steps

- a) determine a good approximation for the functional $E_{XC}[\rho]$
- b) start with some initial guess for ρ_0
- c) calculate from this ρ_0 the potentials $V_H(r)$ and $V_{xc}(r)$ and $V_{eff}(r)$
- d) solve the single particle Schrödinger equation for $V_{eff}(r)$ and obtain the wave functions $\phi_i(r)$
- e) use these single particle wave functions to calculate the density $\rho_1(r)$ in the next step of the iteration
- f) repeat this cycle until convergence is achieved:

$$E[\rho] \Rightarrow \boxed{\hat{h} = \frac{\delta E}{\delta \rho}} \Rightarrow \boxed{\hat{h}\varphi_i = \varepsilon_i \varphi_i} \Rightarrow \boxed{\rho = \sum_{i=1}^A |\varphi_i|^2}$$


Remarks to the Kohn-Sham method:

We have the following remarks to the Kohn-Sham method

- 1) The method is exact under the condition that $V_{xc}[\rho]$ is known.
- 2) The single particle wave functions $\phi_i(r)$ and the single particle energies ϵ_i are only auxiliary quantities. They have nothing to do with experiment. We only obtain the exact total energy and the exact density, i.e. quantities accessible by the density $\rho(r)$.
- 3) The method works rather well even for shell structures

Methods to get a good approximation for the functional $E_{xc}[\rho]$

- 1) phenomenological formulas
- 2) in the local density approximation (LDA) the E_{xc} is calculated exactly by Monte-Carlo techniques for a homogeneous electron gas with density ρ . In the inhomogeneous system the LDA is used. An example: The binding energy of the Ar-atom is reproduced by the Thomas Fermi method with an accuracy of 20 %, by Kohn-Sham method with LDA approximation of 0.5 %.
- 3) there exist many more sophisticated techniques nowadays

Density functional theory in nuclei:

- In nuclei DFT has been introduced by **effective Hamiltonians**:

$$E = \langle \Psi | H | \Psi \rangle \approx \langle \Phi | \hat{H}_{eff}(\hat{\rho}) | \Phi \rangle = E[\hat{\rho}]$$

Skyrme
Gogny
Rel. DFT

- More degrees of freedom: **spin, isospin, relativistic, pairing**

- Nuclei are **self-bound systems**.

The exact density is a constant. $\rho(r) = \text{const}$

Hohenberg-Kohn theorem is true, but useless

$\rho(r)$ has to be replaced by the **intrinsic density**:

$$\rho_I(\vec{r}) = \rho(\vec{r} + \vec{R}_{CM}) \quad \text{with} \quad \vec{R}_{CM} = \frac{1}{A} \sum_i \vec{r}_i$$

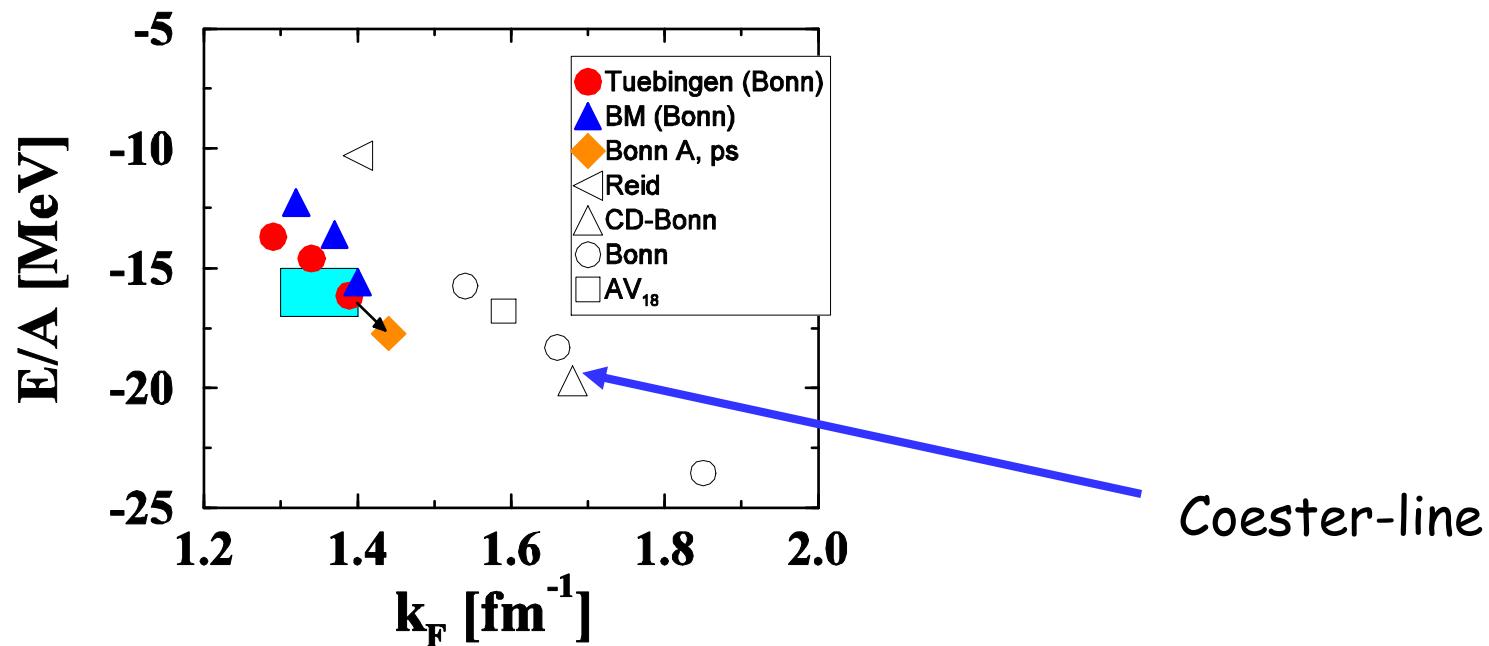
- Density functional theory in nuclei is probably **not exact**, but a very good approximation.

General properties of nuclear self-consistent mean field theories

- At present the nuclear energy functionals are **phenomenological** and not connected to any NN- or NNN-interaction.
- There is a large **spin-orbit** term
- The functionals are expressed in terms of powers and gradients of the ground state density using the principles of **symmetry** and **simplicity**
- **Relativistic functionals** (Covariant DFT) include the spin automatically therefore they have considerably less parameters

Why covariant?

- 1) Large spin-orbit splitting in nuclei
- 2) Large fields $V \approx 350$ MeV, $S \approx -400$ MeV
- 3) Success of Relativistic Brueckner
- 4) Success of intermediate energy proton scatt.
- 5) relativistic saturation mechanism
- 6) consistent treatment of time-odd fields
- 7) Pseudo-spin Symmetry
- 8) Connection to underlying theories ?
- 9) As many symmetries as possible



Relativistic densities:

In the **relativistic treatment**, one has to deal with four-component Dirac spinor wave functions. Consequently, there are 16 independent bilinear covariants:

$$\bar{\psi}(\mathbf{r})\Gamma\psi(\mathbf{r})$$

This gives the following local densities:

$$\Gamma^s = 1$$

scalar density

$$\Gamma_\mu^v = \gamma_\mu$$

vector density

$$\Gamma_{\mu\nu}^t = (i/2)(\gamma_\mu\gamma_\nu - \gamma_\nu\gamma_\mu)$$

tensor density

$$\Gamma^\rho = \gamma_5$$

pseudoscalar density

$$\Gamma_\mu^a = \gamma_\mu\gamma_5$$

axial density

(which have isoscalar and isovector components.) In most applications, only three densities are required:

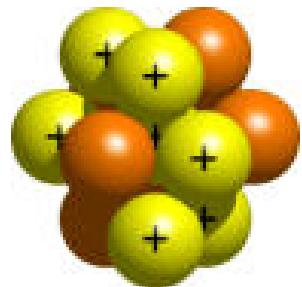
$$\bar{\psi}\psi (\sigma)$$

$$\bar{\psi}\gamma^\mu\psi (\omega)$$

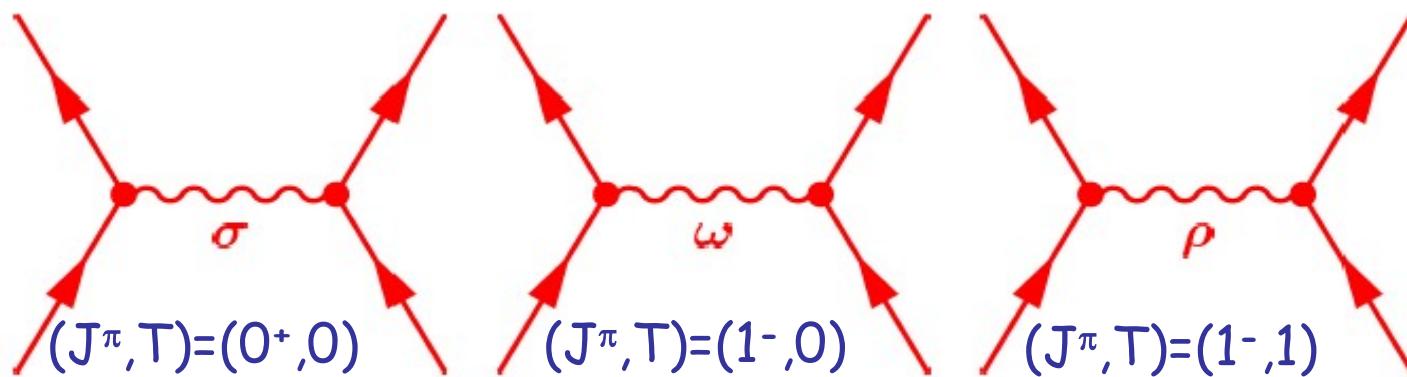
$$\bar{\psi}\gamma^\mu\vec{\tau}\psi (\rho)$$

Walecka model

$$E[\rho]$$



Nucleons are coupled by exchange of mesons through an **effective Lagrangian** (EFT)



$$S(\mathbf{r}) = g_\sigma \sigma(\mathbf{r})$$

↑
Sigma-meson:
attractive scalar field

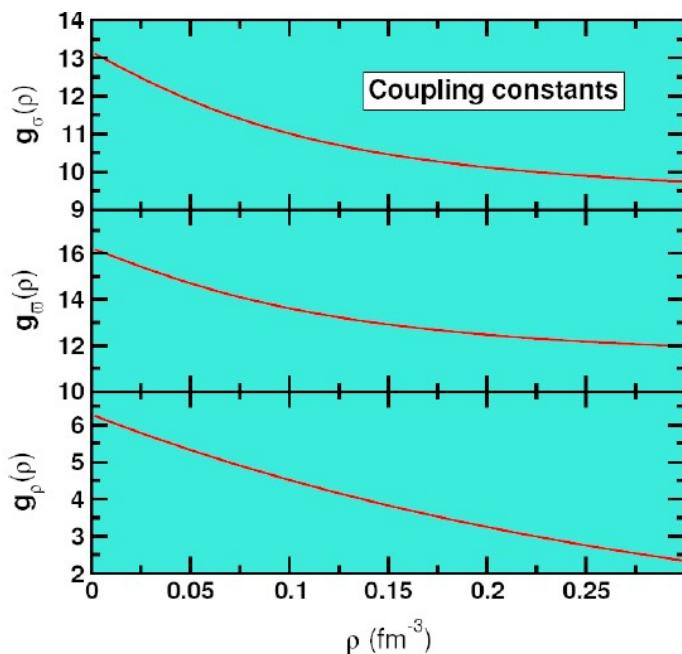
$$V(\mathbf{r}) = g_\omega \omega(\mathbf{r}) + g_\rho \vec{\tau} \vec{\rho}(\mathbf{r}) + eA(\mathbf{r})$$

↑
Omega-meson:
short-range repulsive

↑
Rho-meson:
isovector field

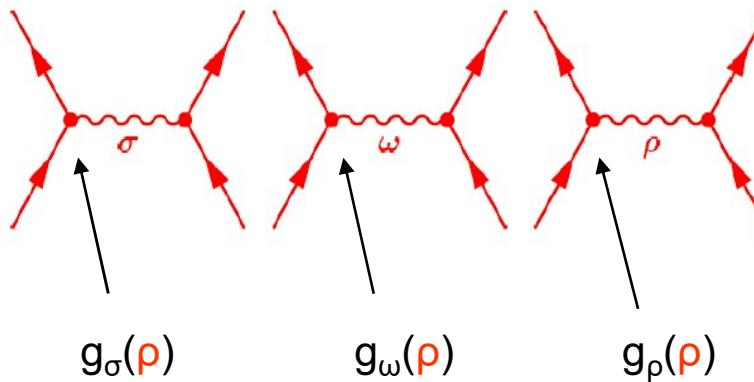
Effective density dependence:

The basic idea comes from **ab initio** calculations
density dependent coupling constants include Brueckner correlations
and threebody forces



non-linear meson coupling: **NL3**

Effective interactions with medium-dependent couplings:



adjusted to ground state properties of finite nuclei

TypeI, Wolter, NPA **656**, 331 (1999)

Niksic, Vretenar, Finelli, P.R., PRC **66**, 024306 (2002):

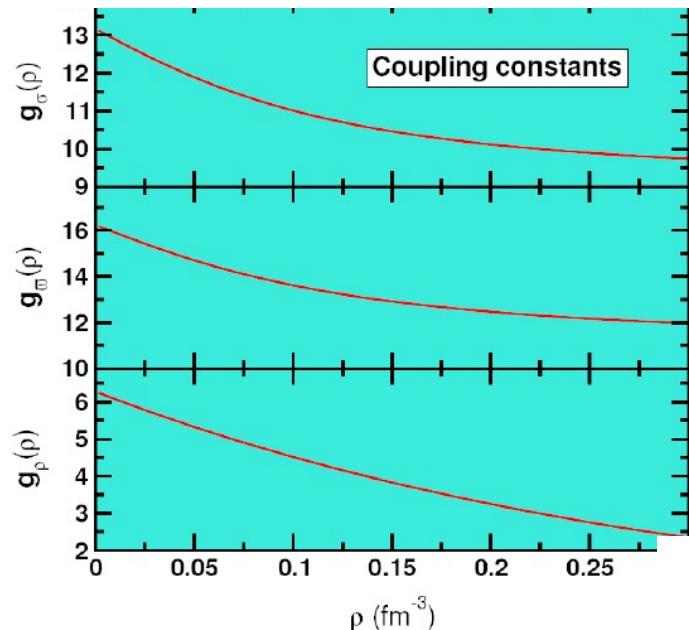
Lalazissis, Niksic, Vretenar, P.R., PRC **78**, 034318 (2008):

DD-ME1

DD-ME2

Effective density dependence:

The basic idea comes from **ab initio** calculations
density dependent coupling constants include Brueckner correlations
and threebody forces



Point-coupling models
with derivative term: D $(\bar{\psi}\psi)\Delta(\bar{\psi}\psi)$



$$G_\sigma(\rho)$$



$$G_\omega(\rho)$$



$$G_\rho(\rho)$$

adjusted to ground state properties of finite nuclei

Manakos and Mannel, Z.Phys. **330**, 223 (1988)

Bürvenich, Madland, Maruhn, Reinhard, PRC **65**, 044308 (2002):

Niksic, Vretenar, P.R., PRC 78, 034318 (2008):

Zhao, Li, Yao, Meng, J. Meng, archiv 1002.1789

PC-F1

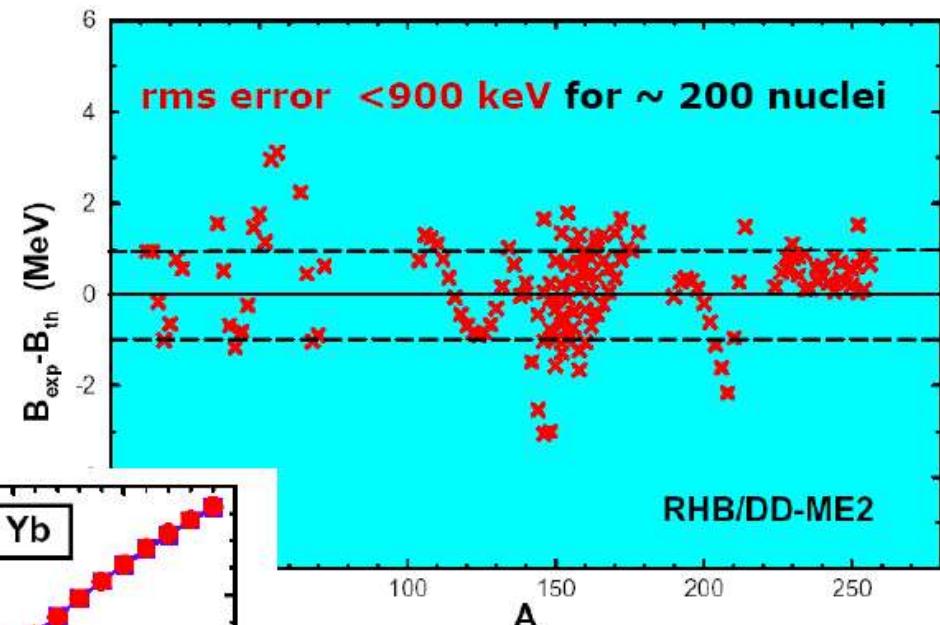
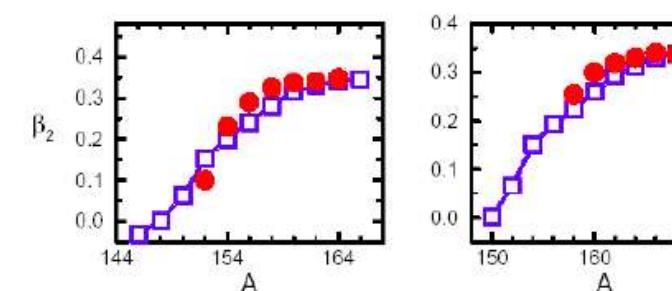
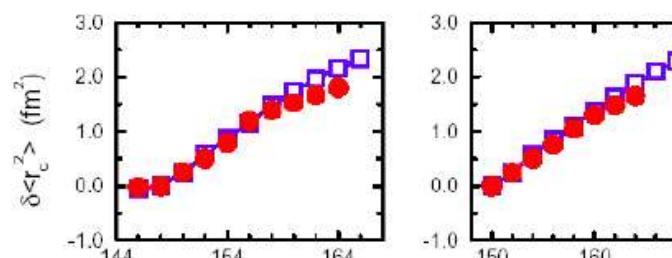
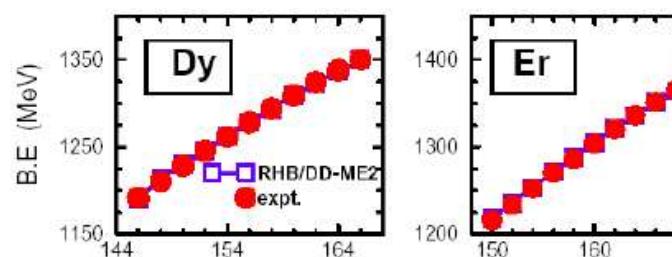
DD-PC1

PC-PK1

- Motivation
- Mic-mac models of nuclei
- Microscopic description
- Nuclear density functional theory
- Applications for nuclear ground states
- Density functional theory for excited states
- Concluding remarks

Relativistic Hartree-Bogoliubov calculations: DD-ME2 + Gogny DIS pairing

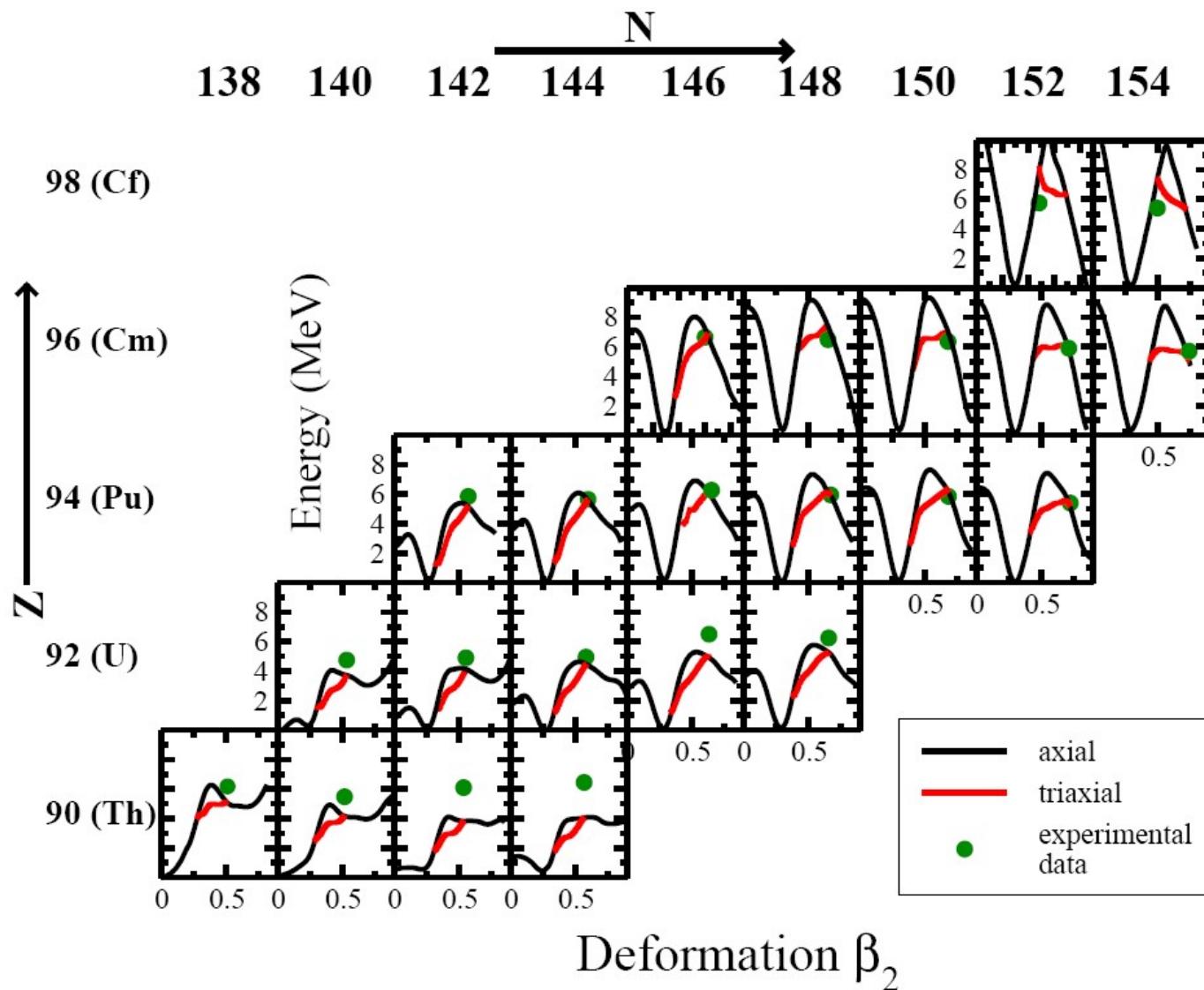
Absolute deviations of the calculated binding energies from experimental values:



Binding energies, charge isotope shifts and quadrupole deformations of isotopic chains in the rare-earth region.

Phys. Rev. C **71**, 024312 (2005)

Fission barriers for triaxially deformed shapes:



Comparision between DFT and Mic-Mac:

- Mic-mac is **more successfull**
e.g. superdeformation, super-heavy elements
- Mic-mac contains has **more parameters** but only **one** parameter set
- DFT has **many** parameter sets
- Skyrme (>200), Gogny (1-2), CDFT (>10 growing)
- but perhaps an **ab-initio** derivation
- Ab-initio values **will never precise** enough

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Time dependent density functional theory:

Runge-Gross Theorem (1984):

$$\int dt \{ \langle \Phi(t) | i\partial_t | \Phi(t) \rangle - E[\rho(t), t] \} = 0$$

quasi-static approx: $E[\rho(t), t] = E_{HK}[\rho(t)]$



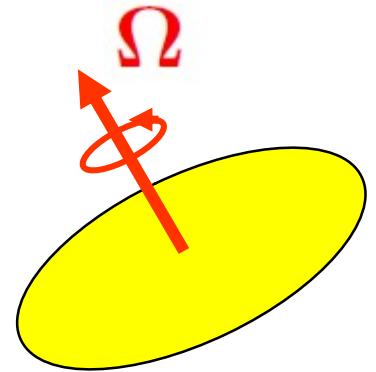
$$i\partial_t \hat{\rho} = [\hat{h}(\hat{\rho}) + \hat{f}, \hat{\rho}]$$

time-dependent mean field equations

Rotational excitations:

We assume that the time-dependence is given by a rotation with constant velocity Ω

$$\rho(\mathbf{r}, t) = e^{-i\Omega j t} \rho(\mathbf{r}) e^{i\Omega j t}$$



This leads to quasi-static Kohn-Sham equations in the rotations frame

Cranking model: Inglis (1956):

$$[-\nabla^2/2m + v[\rho](\mathbf{r}) - \Omega \mathbf{j}] \varphi_i(\mathbf{r}) = \varepsilon_i(\Omega) \varphi_i(\mathbf{r})$$

with the exact intrinsic density $\rho(\mathbf{r}) = \sum_{i=1}^A |\varphi_i(\mathbf{r})|^2$

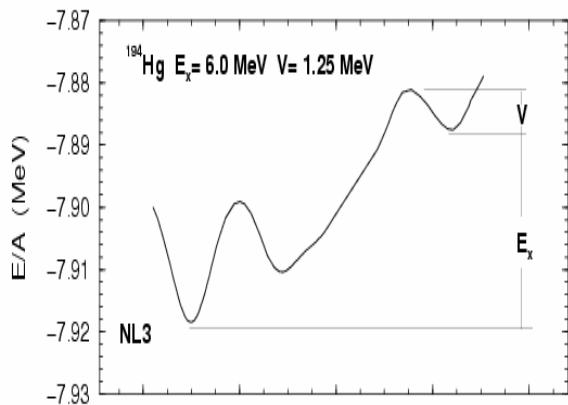
Here we assume, that $v[\rho](\mathbf{r})$ is the static Kohn-Sham potential ("adiabatic approximation")

Rotational Excitations in superdef. nuclei

$$I(\Omega) = \langle \Phi((\Omega)|\hat{j}|\Phi((\Omega)) \rangle$$

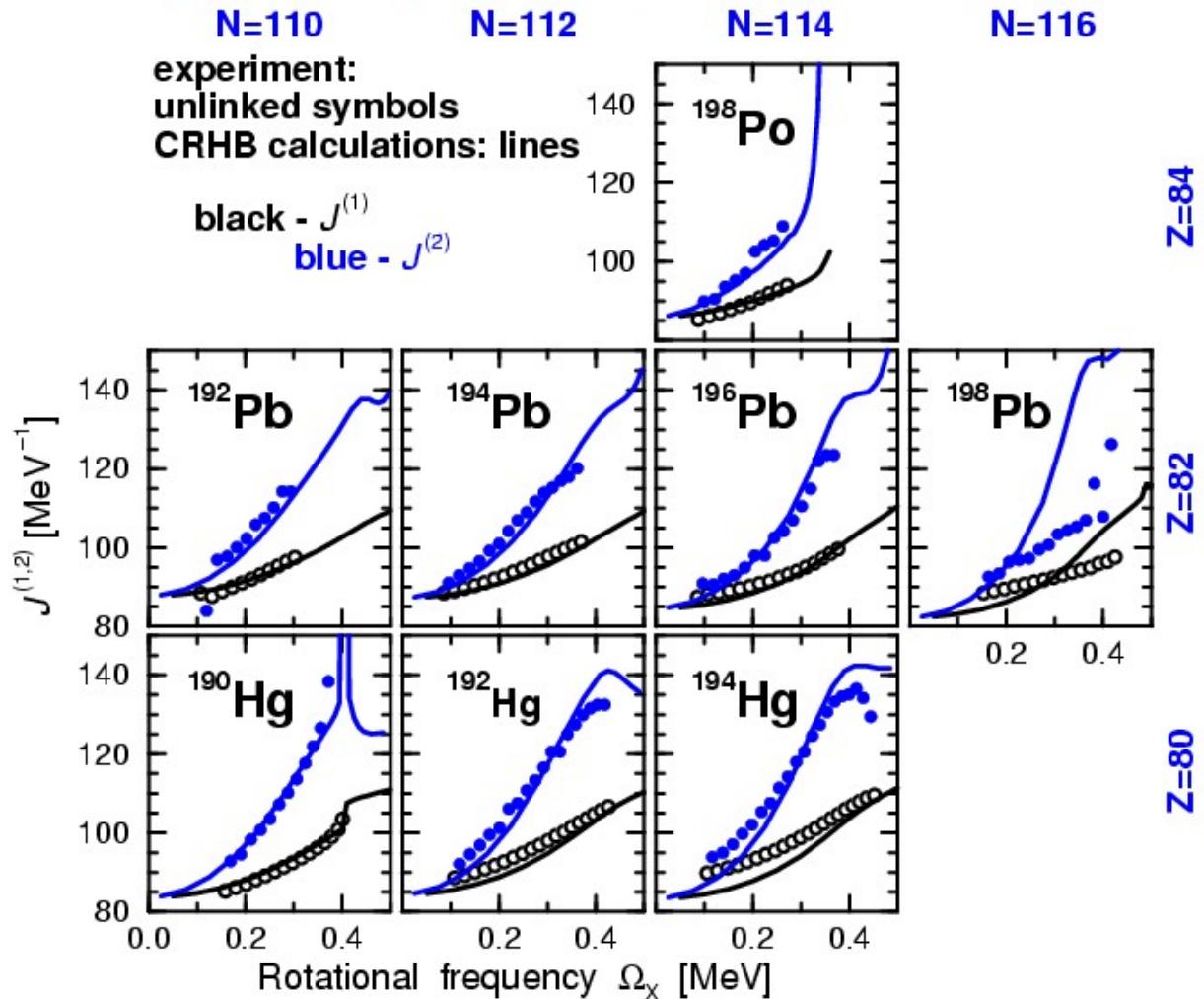
moment of inertia:

$$\mathcal{J}^1(\Omega) = \frac{I(\Omega)}{\Omega}; \quad \mathcal{J}^2(\Omega) = \frac{dI(\Omega)}{d\Omega}$$



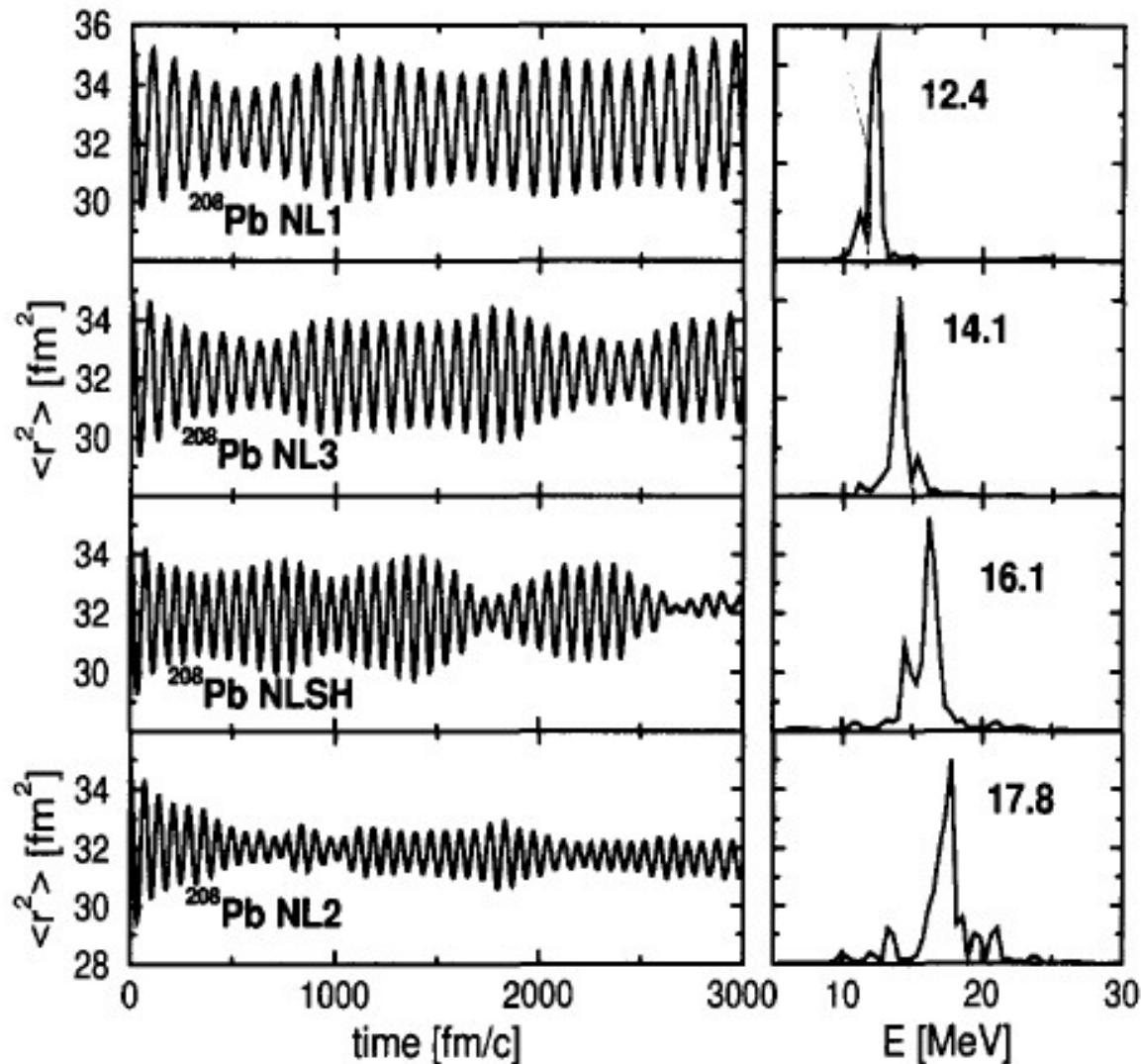
= 6.02
 Exp: E_x = 6.0
 NL3: = 6.9
 Gogny: = 5.0
 Skyrme: = 4.6
 WS:

A.V.Afanasjev, P. Ring, J. Konig
 Phys. Rev. C60 (1999) 051303; Nucl. Phys. A 676 (2000) 196



$$\langle \Phi(t) | r^2 | \Phi(t) \rangle$$

Breathing mode: ^{208}Pb



$$K_\infty = 211$$

$$K_\infty = 271$$

$$K_\infty = 355$$

Small amplitude limit gives RPA:

Small amplitude limit:

$$\hat{\rho}(t) = \hat{\rho}^{(0)} + \delta\hat{\rho}(t)$$

ground-state density

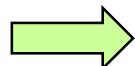
$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \hbar\omega \begin{pmatrix} X \\ Y \end{pmatrix}$$

$\delta\rho_{ph}, \delta\rho_{ah}$

$\delta\rho_{hp}, \delta\rho_{ha}$

RPA matrices:

$$A_{minj} = (\epsilon_n - \epsilon_i)\delta_{mn}\delta_{ij} + \frac{\partial h_{mi}}{\partial \rho_{nj}}, \quad B_{minj} = \frac{\partial h_{mi}}{\partial \rho_{jn}}$$



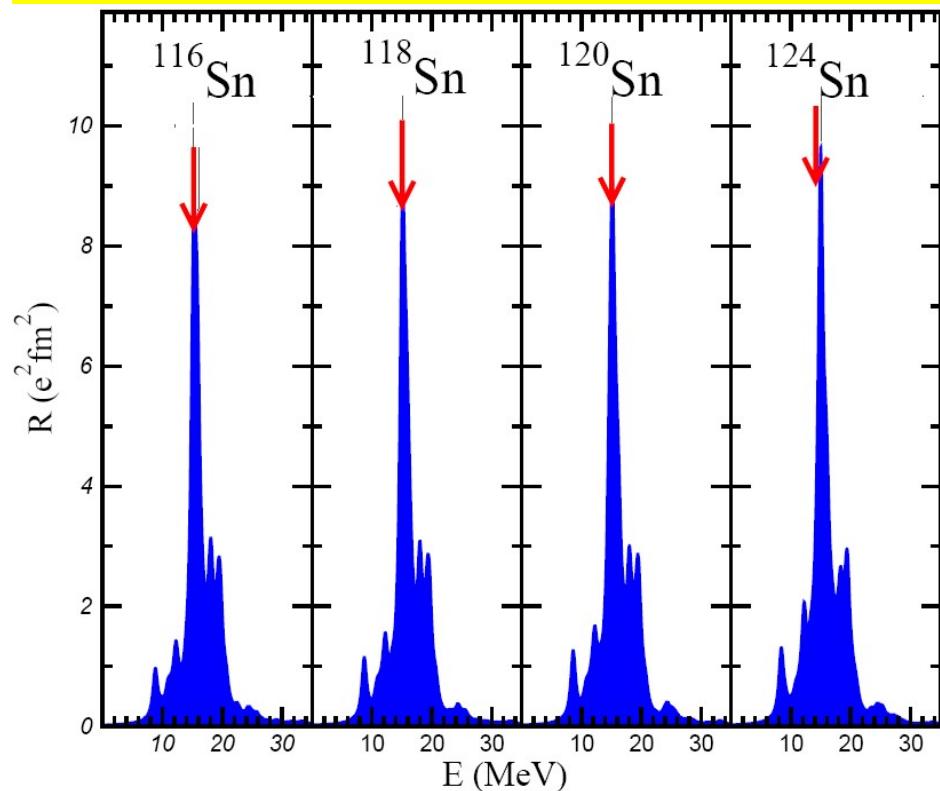
the same effective interaction determines
the Dirac-Hartree single-particle spectrum and
the residual interaction

Interaction:

$$\hat{V} = \frac{\delta^2 E}{\delta \hat{\rho} \delta \hat{\rho}}$$

In superfluid systems: quasiparticle RPA

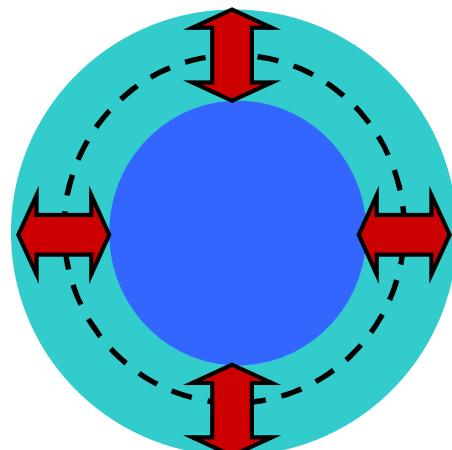
Relativistic (Q)RPA calculations of giant resonances



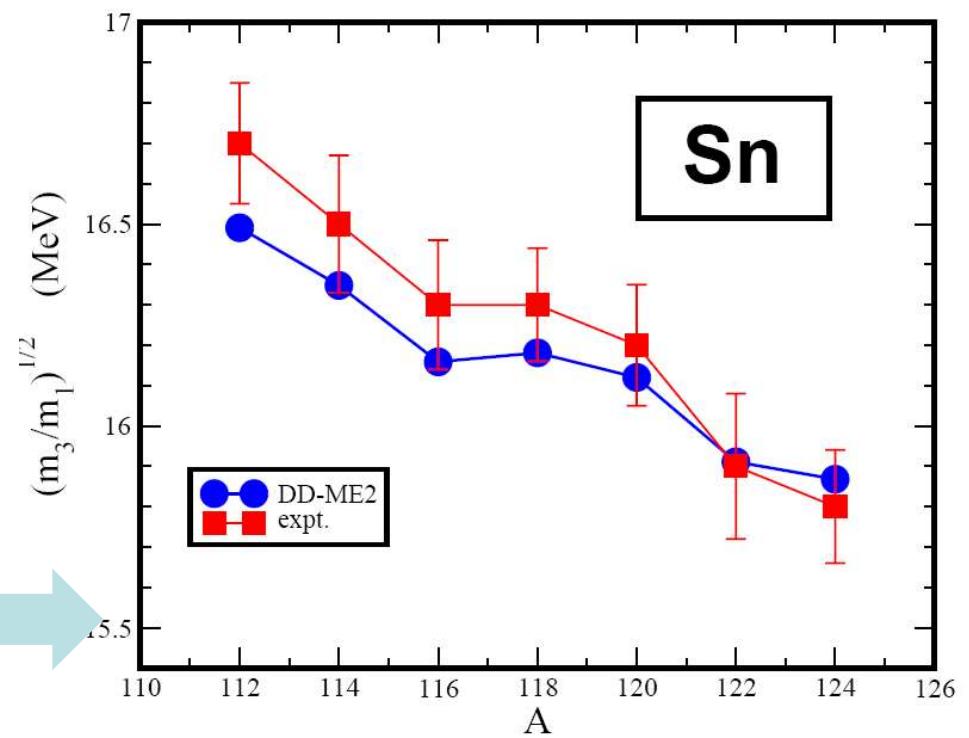
Sn isotopes: DD-ME2 effective interaction + Gogny pairing

Isovector dipole response

protons neutrons



Isoscalar
monopole
response

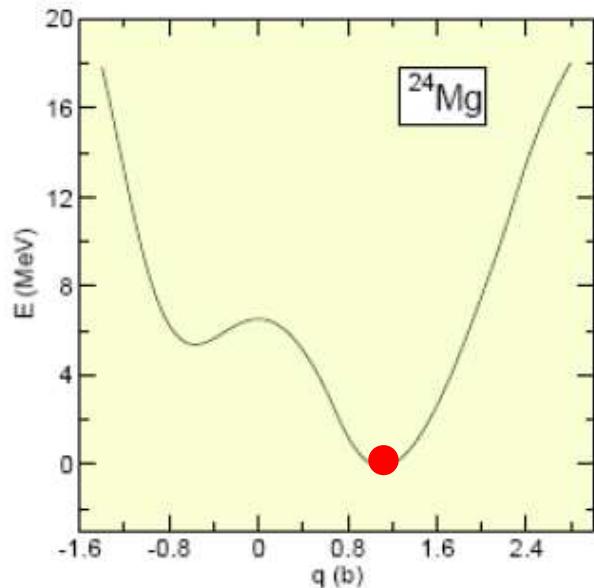


Large-amplitude collect. Motion (LACM)

GCM-method

$$\langle \delta\Phi | \hat{H} - q\hat{Q} | \Phi \rangle = 0$$

→ $|q\rangle = |\Phi(q)\rangle$



Constraint Hartree Fock produces deformed w.f.
depending on the generator coordinate q

GCM wave function is a superposition
of Slater determinants

$$|\Psi\rangle = \int dq f(q) |q\rangle$$

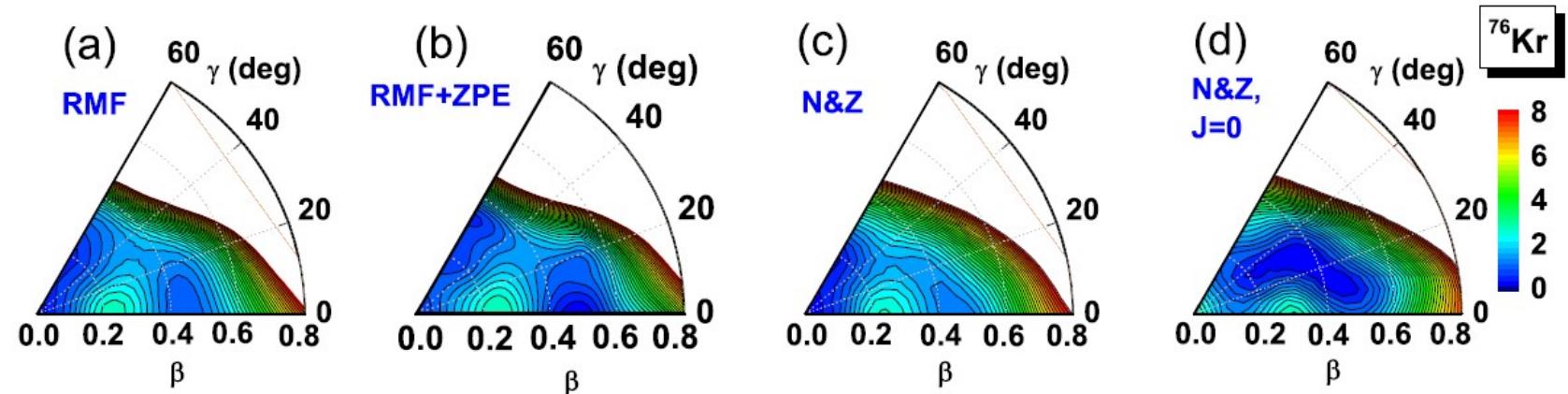
Hill-Wheeler equation:

$$\int dq' [\langle q | H | q' \rangle - E \langle q | q' \rangle] f(q') = 0$$

with projection:

$$|\Psi\rangle = \int dq f(q) \hat{P}^N \hat{P}^I |q\rangle$$

Transitional nuclei: DFT beyond mean field:



Generator-Coordinates: $q = (\beta, \gamma)$

Projection on J and N :

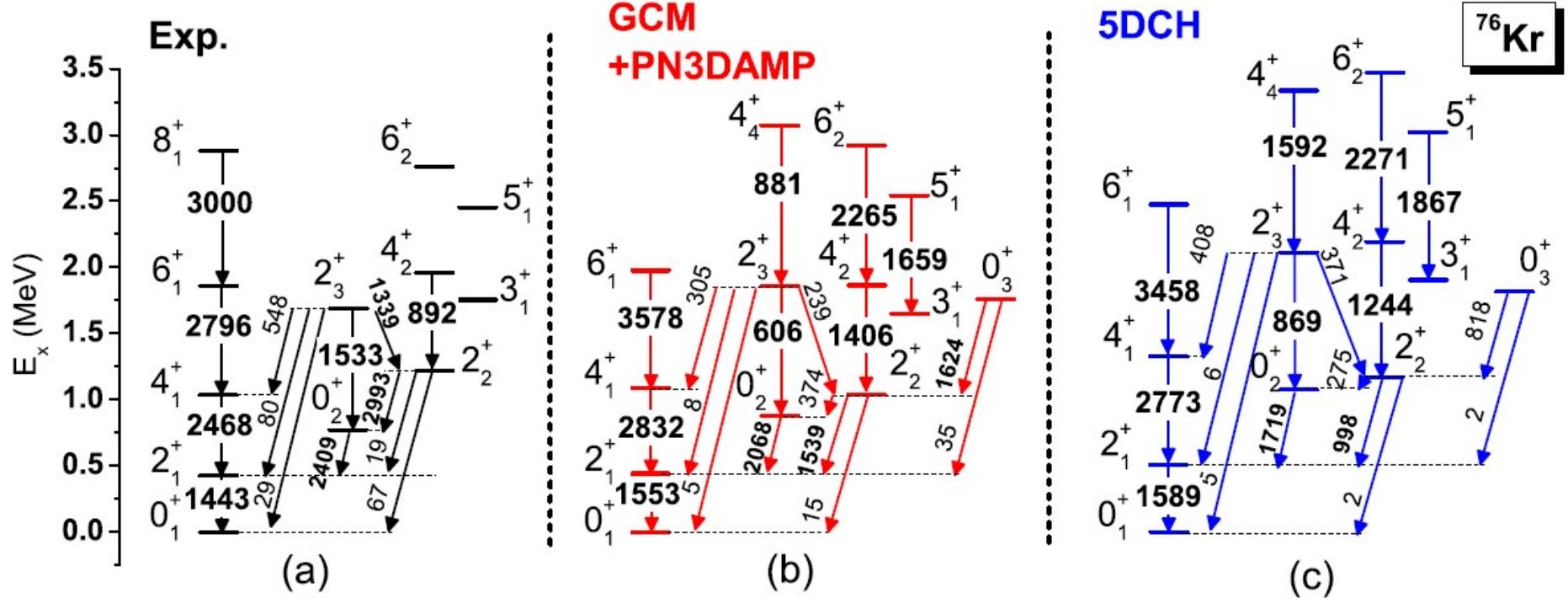
$$|JNZ; \alpha\rangle = \sum_{q,K} f_\alpha^{JK}(q) \hat{P}_{MK}^J \hat{P}^N \hat{P}^Z |q\rangle,$$

Bohr Hamiltonian: $H = -\frac{\partial}{dq} \frac{1}{2B(q)} \frac{\partial}{dq} + V(q) + V_{corr}(q)$

J.M. Yao et al, PRC (2014)

Spectra: GCM (7D)
Bohr Hamiltonian (5DCH)

PC-PK1



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- Nuclei: strongly interacting many-body systems
- Mic-mac models very successful
- Microscopic description with effective forces
- Nuclear density functional theory
- Applications for ground states
- Applications for excited states
- Future:
 - more detailed ab-initio calculations
 - ab-initio derivations for density functionals

Thank you