Covariant density functions in nuclear physics and their microscopic origin

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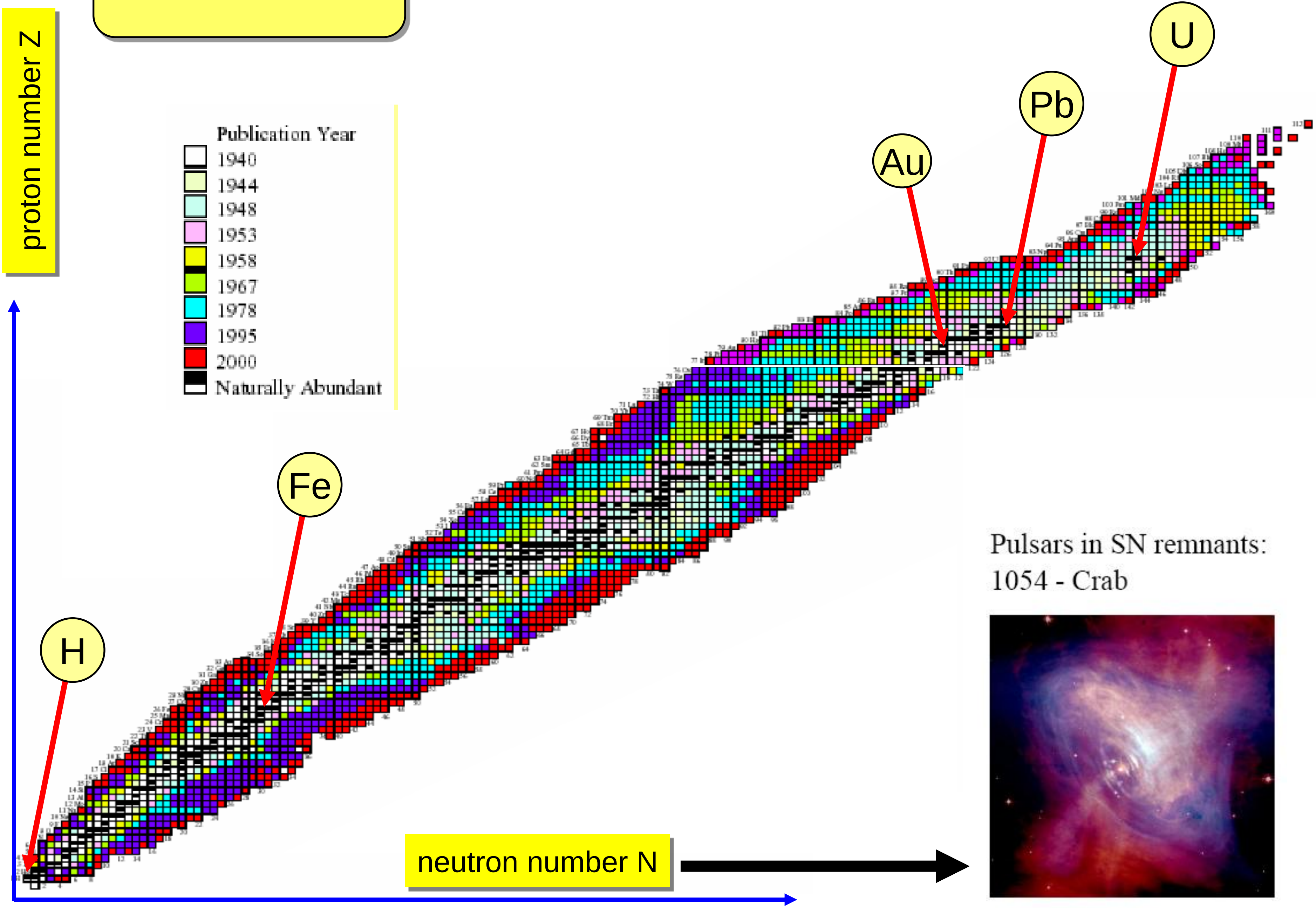
Content:

- **Motivation**
- **Phenomenological covariant density functionals**
- **Semi-microscopic density functionals**
- **Why do we need a fully microsopic theory ?**
- **Relativistic Brueckner-Hartree-Fock**

  In infinite nuclear matter
  In finite nuclei: local density approximation
  RBHF-theory in a Dirac-Woods-Saxon Basis
  Full self-consistent RBHF-theory
- **Applications for ^{4}He, ^{16}O, ^{40}Ca**
- **Outlook**

Motivation:



Pulsars in SN remnants:
1054 - Crab

Density functional theory for manybody quantum systems

Density functional theory starts from the

Hohenberg-Kohn theorem:

„The exact ground state energy E[ρ] is a
universal functional for the local density ρ(r)“

Kohn-Sham theory starts

with a density dependent self-energy:

and the single particle equation:

with the exact density:

$$h(\mathbf{r}) = \frac{\delta E[\rho]}{\delta \rho(\mathbf{r})}$$

$$h(\mathbf{r})|\varphi_i\rangle = \varepsilon_i |\varphi_i\rangle$$

$$\rho(\mathbf{r}) = \sum_i^A |\varphi_i(\mathbf{r})|^2$$

In Coulombic systems the functional is derived *ab initio*

Density functional theory is very successful in nuclei:

In nuclei DFT has been introduced by **effective Hamiltonians**:
by Vautherin and Brink (1972)

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

Based on the philosophy of Bethe, Goldstone, and Brueckner
one has a in the nuclear interior a density dependen interaction G(ρ)

At present the ansatz for E(ρ) is phenomenological:

- Skyrme: non-relativistic, zero range
- Gogny: non-relativistic, finite range (Gaussian)
- CDFT: Covariant density functional theory:

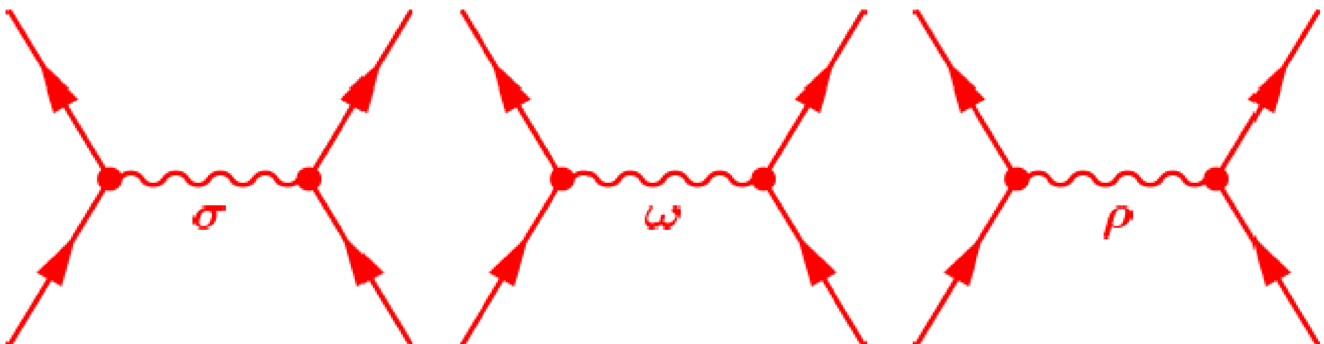
- Spin-orbit automatically included
- New saturation mechanism (scalar different from vector density)
- Proper treatment of time-odd components (nuclear magnetism)
- Pseudospin symmetry

….

Covariant density functional theory

$E[\rho]$

The nuclear fields are obtained by coupling the nucleons through the exchange of effective mesons through an effective Lagrangian.



$(J^\pi,T)=(0^+,0)$ $(J^\pi,T)=(1^-,0)$ $(J^\pi,T)=(1^-,1)$

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

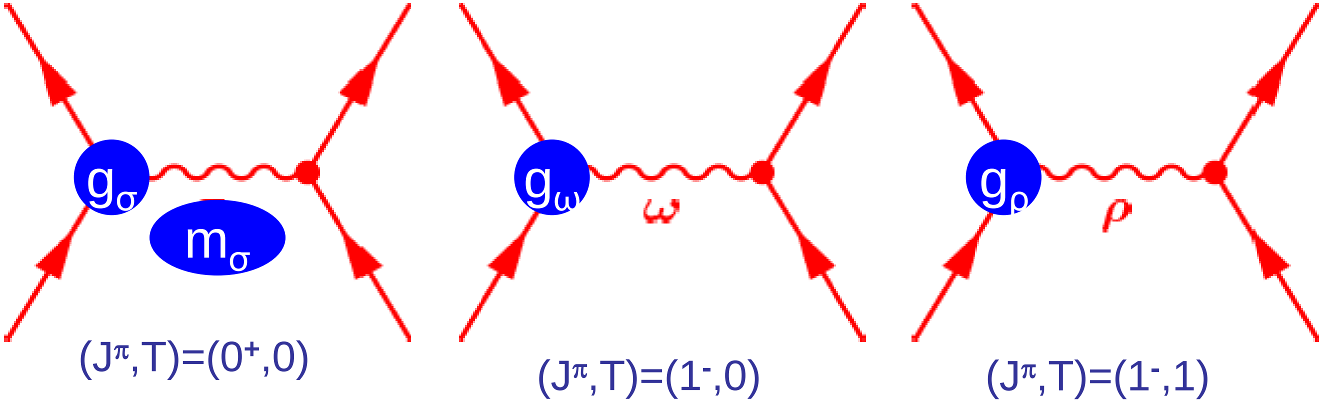
sigma-meson: attractive scalar field

omega-meson: short-range repulsive

rho-meson: isovector field

Covariant DFT is based on the Walecka model

This model has only four parameters:

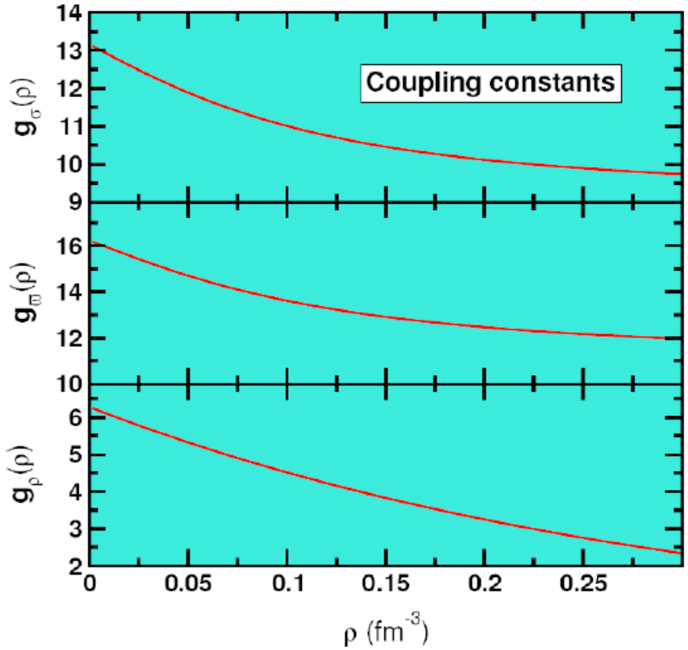


$$S(r) = g_\sigma \sigma(r) \qquad V(r) = g_\omega \omega(r) + g_\rho \rho(r) + eA(r)$$

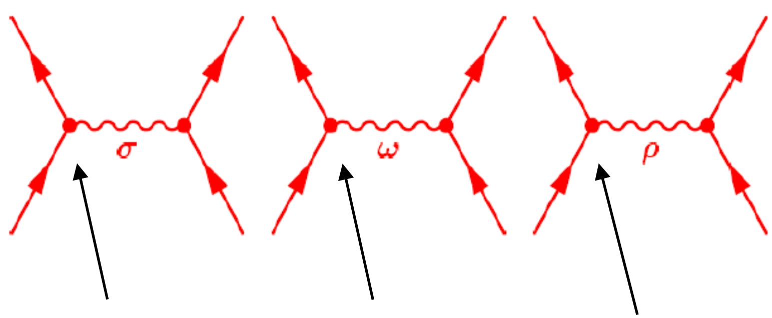
Effective density dependence:

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

non-linear meson coupling: **NL3, PK1 ….**



Effective interactions with medium-dependent couplings:



$g_\sigma(\rho)$ $g_\omega(\rho)$ $g_\rho(\rho)$

adjusted to ground state properties of finite nuclei

Typel, Wolter, NPA **656**, 331 (1999)
Niksic, Vretenar, Finelli, P.R., PRC **66**, 024306 (2002): **DD-ME1**
Lalazissis, Niksic, Vretenar, P.R., PRC 78, 034318 (2008): **DD-ME2**

Effective density dependence:

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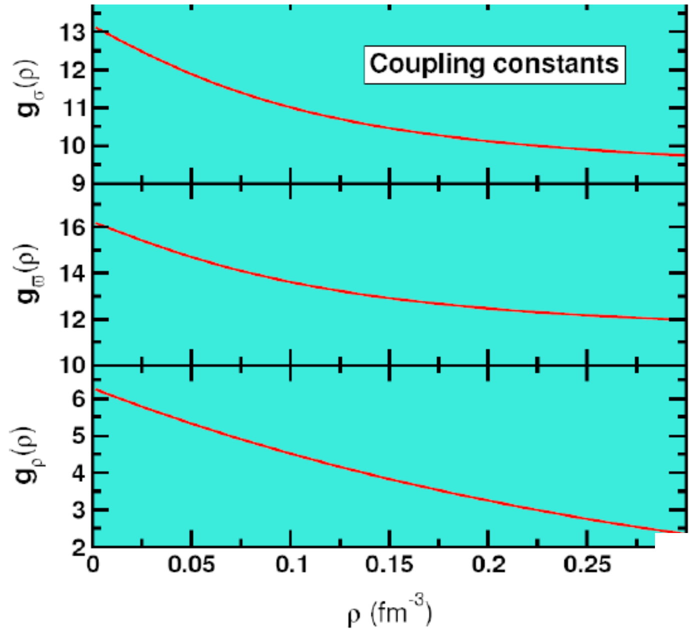


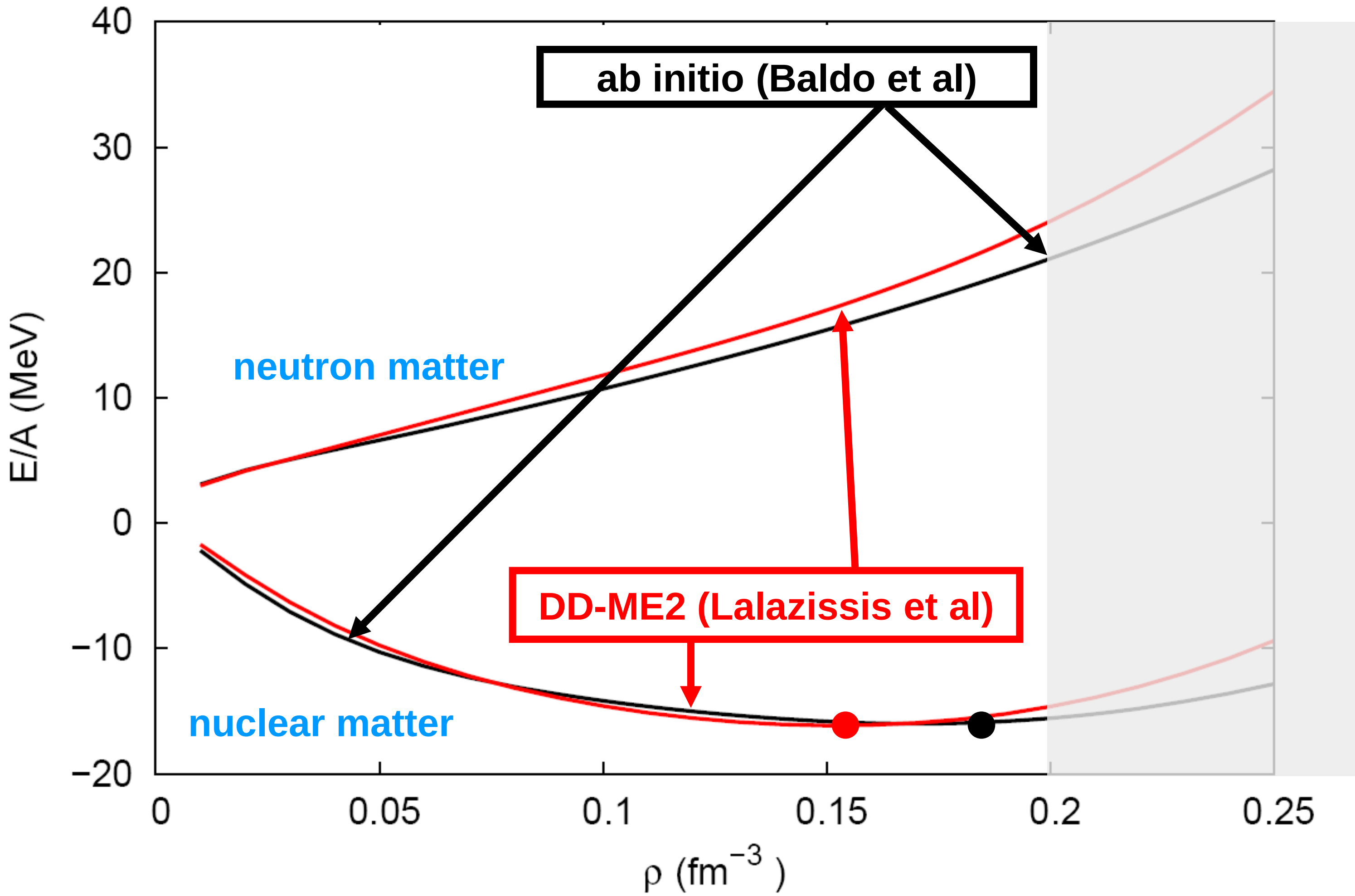
Point-coupling models
with derivative term: $D \; (\bar\psi\psi)\Delta(\bar\psi\psi)$

$G_\sigma(\rho)$ $G_\omega(\rho)$ $G_\rho(\rho)$

adjusted to ground state properties of finite nuclei

Manakos and Mannel, Z.Phys. **330**, 223 (1988)
Bürvenich, Madland, Maruhn, Reinhard, PRC **65**, 044308 (2002): **PC-F1**
Niksic, Vretenar, P.R., PRC 78, 034318 (2008): **DD-PC1**
Zhao, Li, Yao, Meng, J. Meng, PRC 82, 054319 (2010) **PC-PK1**

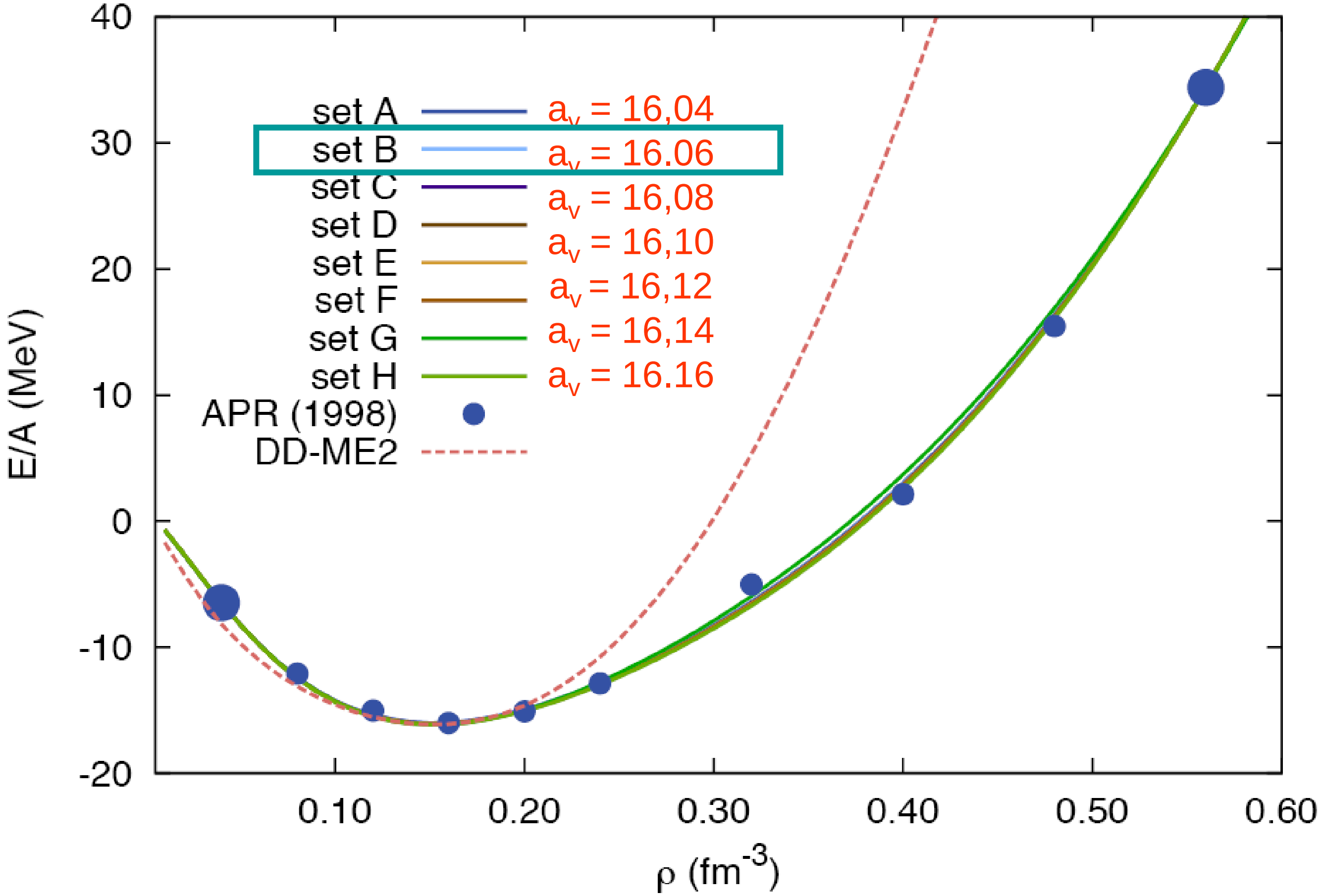
Comparison with ab initio calculations:



we find excellent agreement with ab initio calculations of Baldo et al.

Semi-microscopic relativistic functionals

point coupling model is fitted to microscopic nuclear matter
and to masses of 64 deformed nuclei:



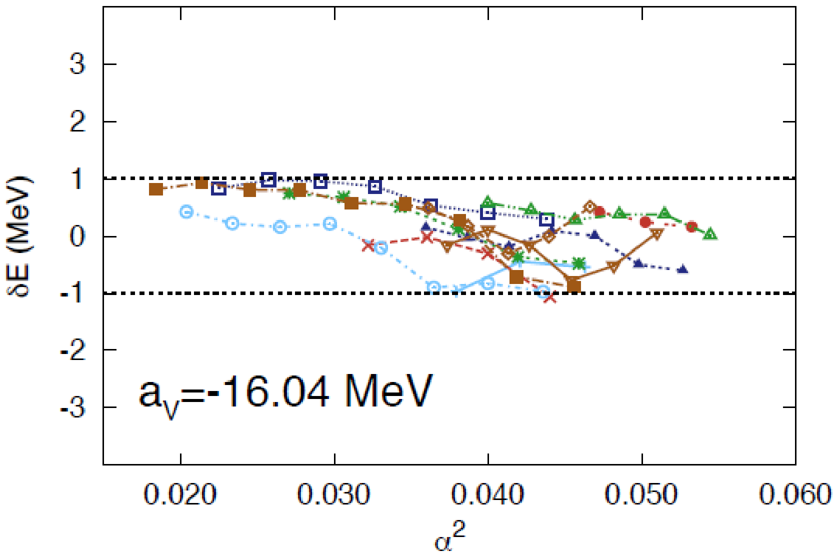
ρ_{sat} = 0.152 fm^{-3}
m^* = 0.58m
K_{nm} = 230 MeV
a_4 = 33 MeV

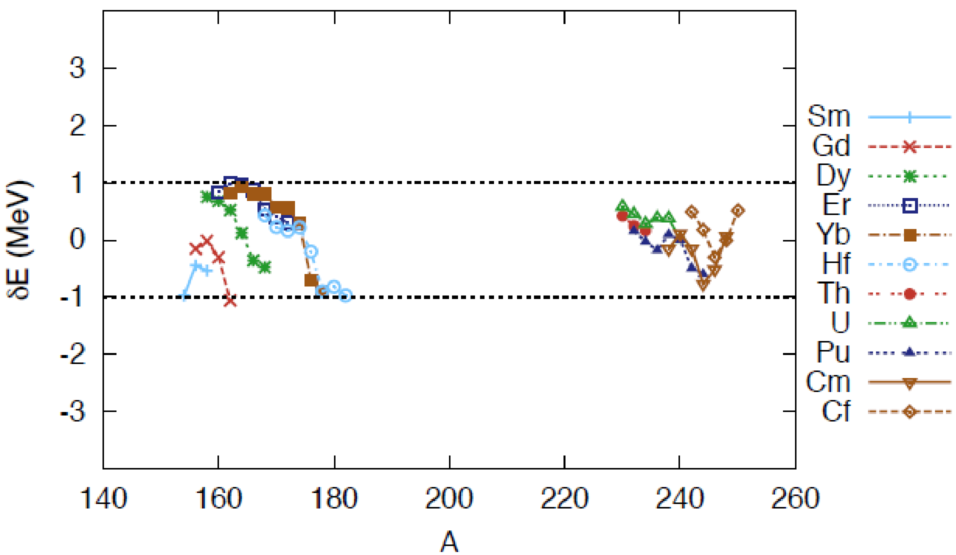
Niksic et al, (2008)

DD-PC1

A. Akmal, V.R. Pandharipande, and D.G. Ravenhall, PRC. 58, 1804 (1998).

Adjusting the model parameters





Rare-earth region

Sm (Z=62), Gd (Z=64), Dy (Z=66), Er (Z=68), Yb (Z=70), Hf (Z=72)

Actinides

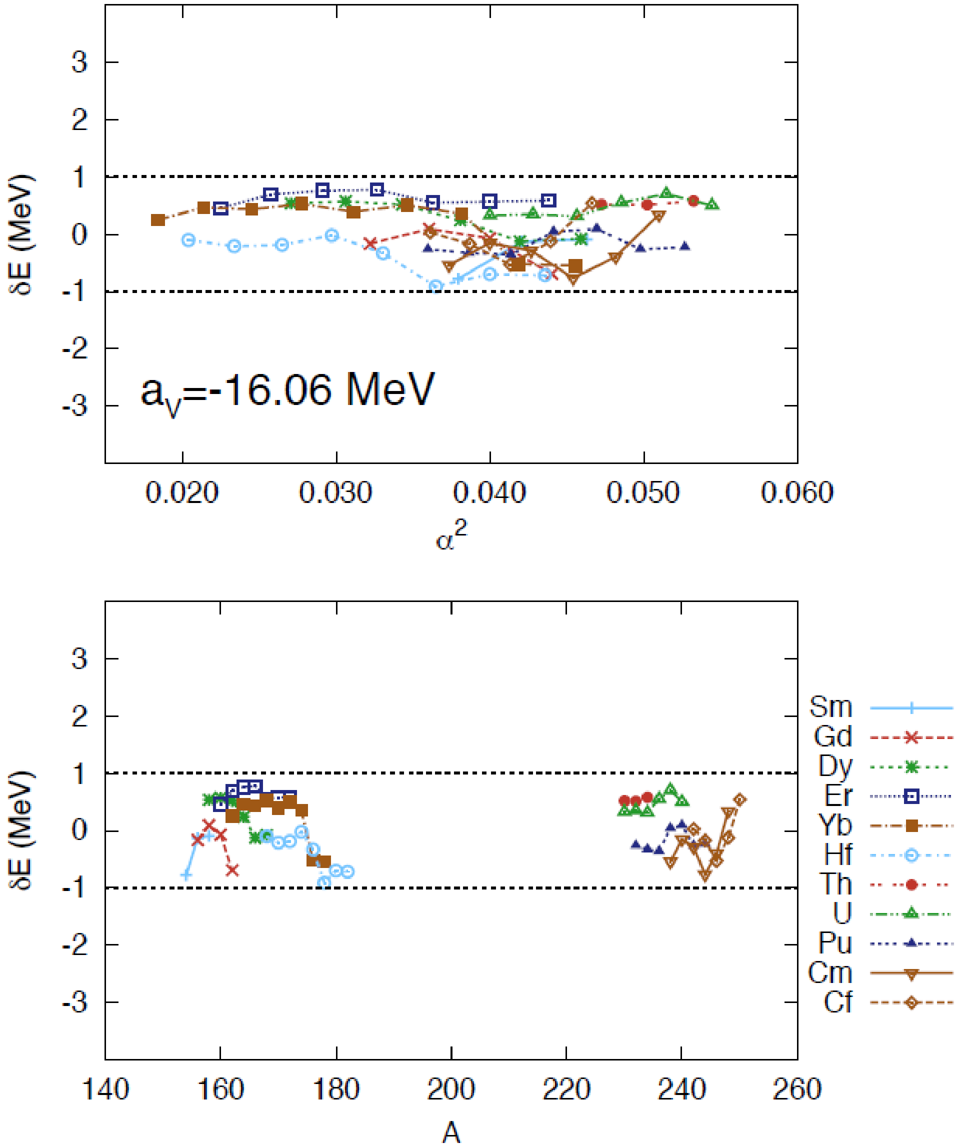
Th (Z=90), U (Z=92), Pu (Z=94), Cm (Z=96), Cf (Z=98)

Total

64 isotopes

T. Niksic

Adjusting the model parameters



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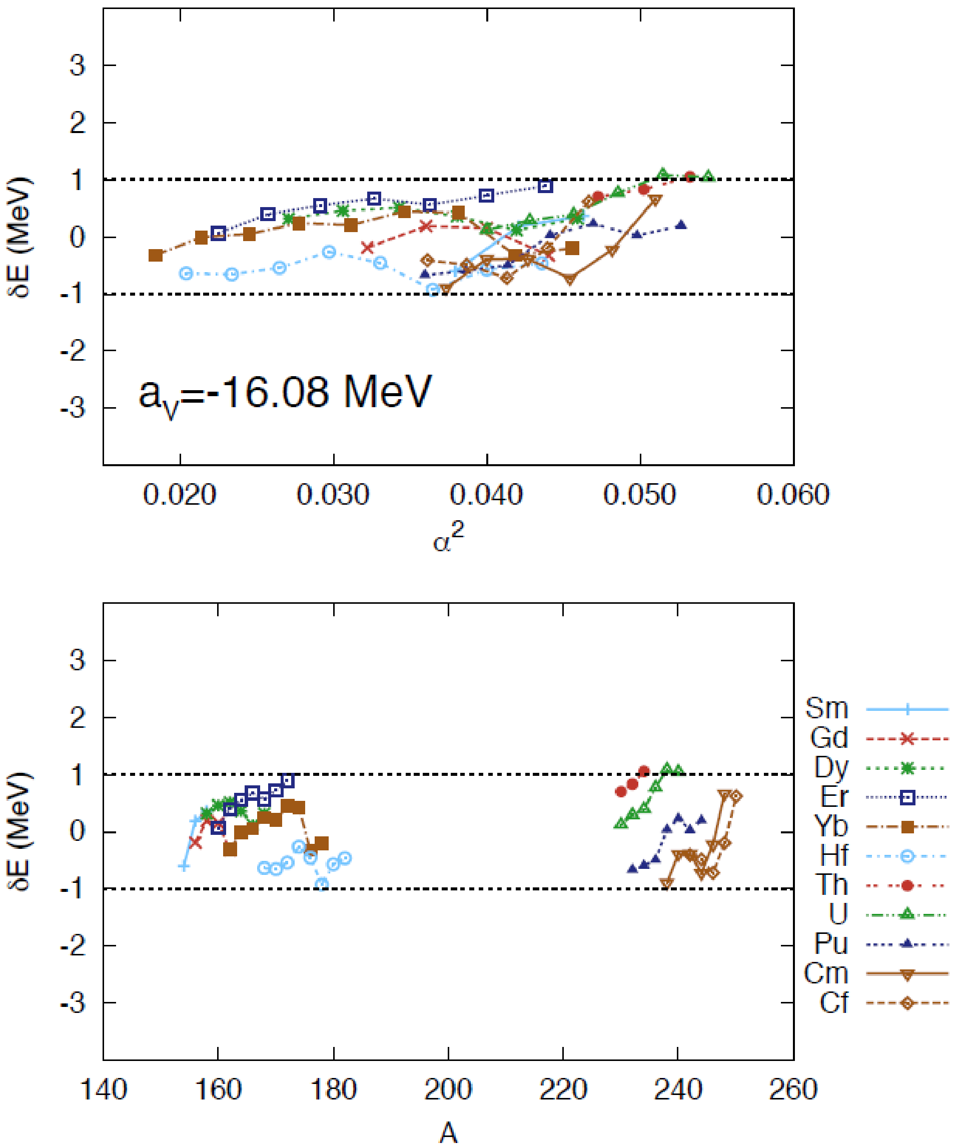

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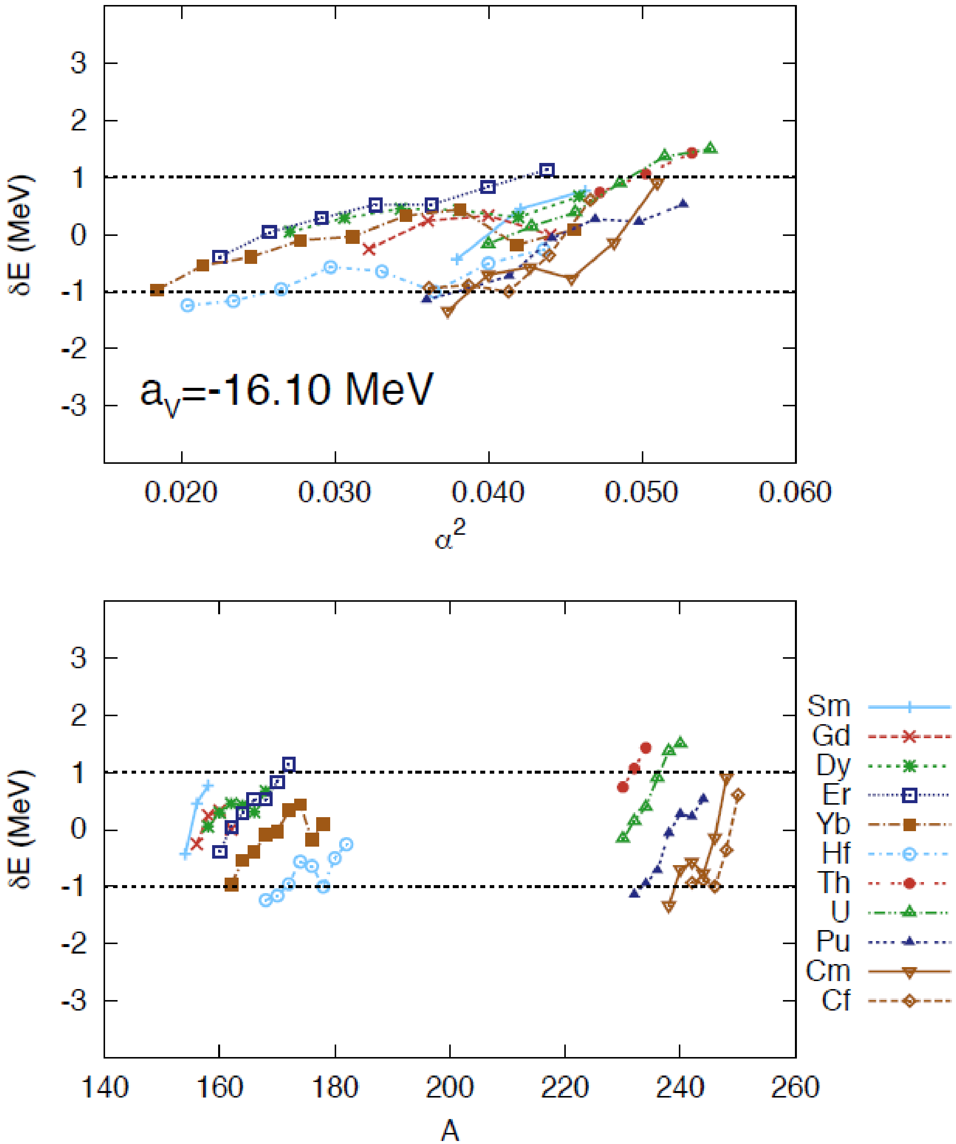

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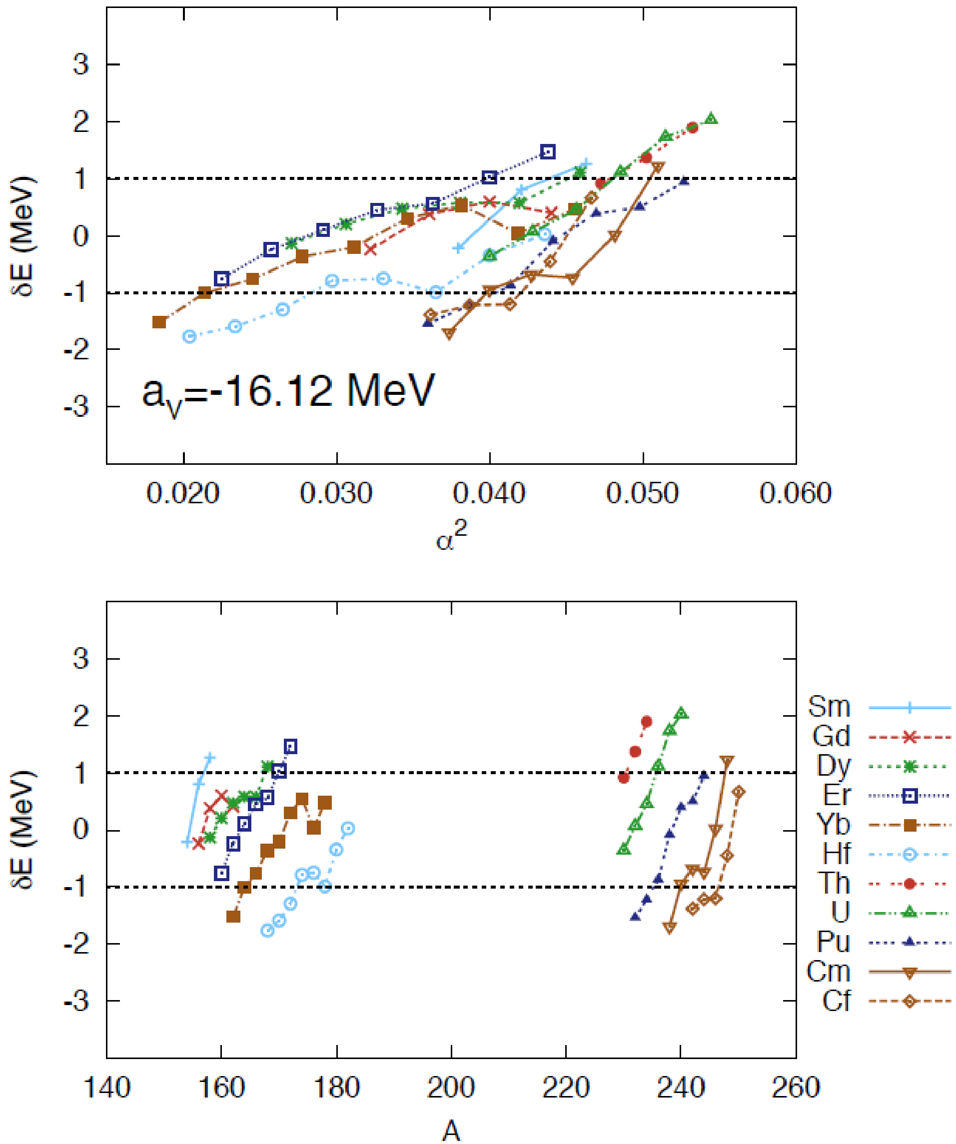

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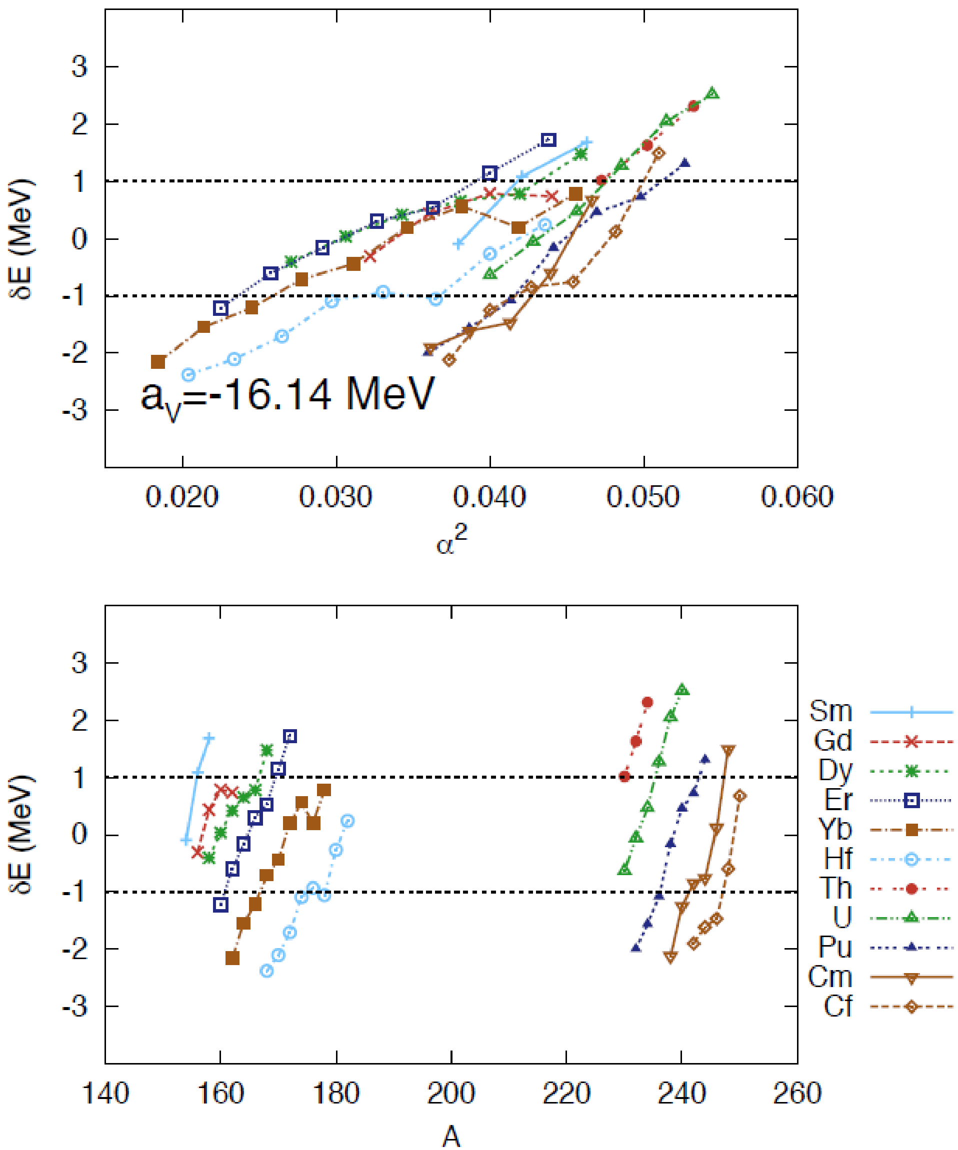

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Total

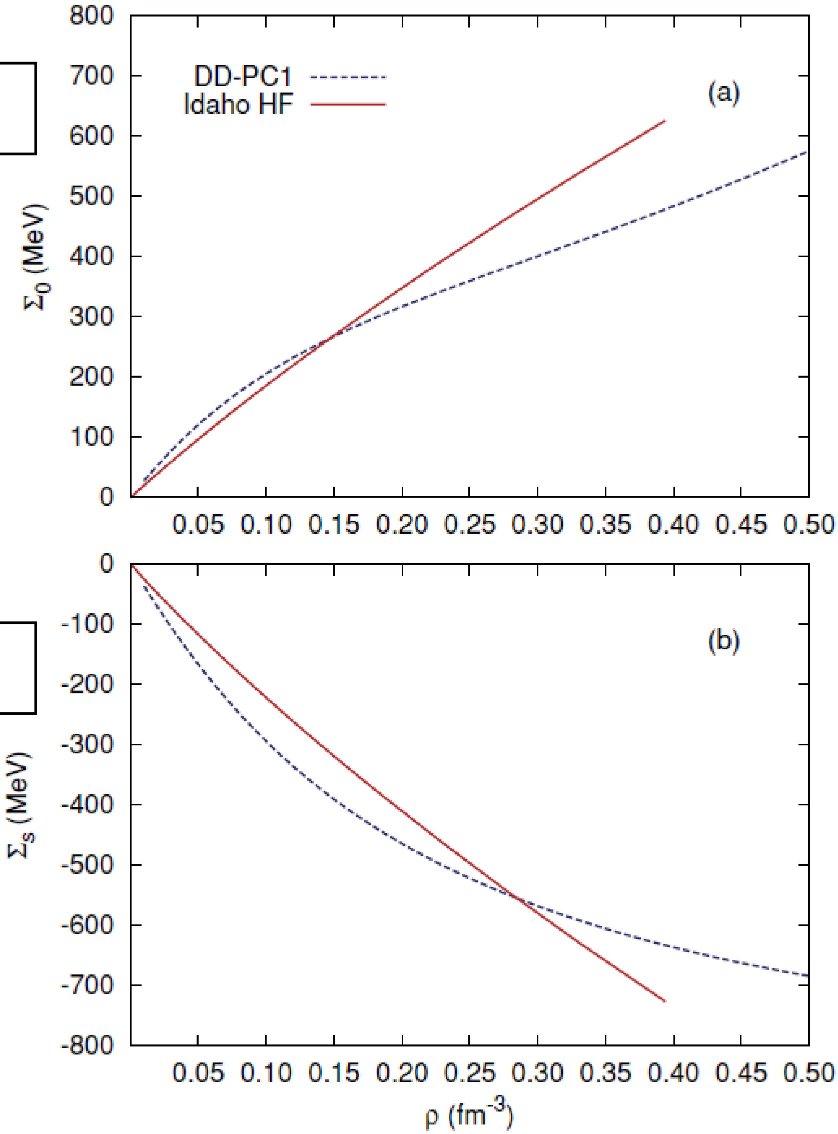
64 isotopes

T. Niksic

DD-PC1 and microscopic self energies:

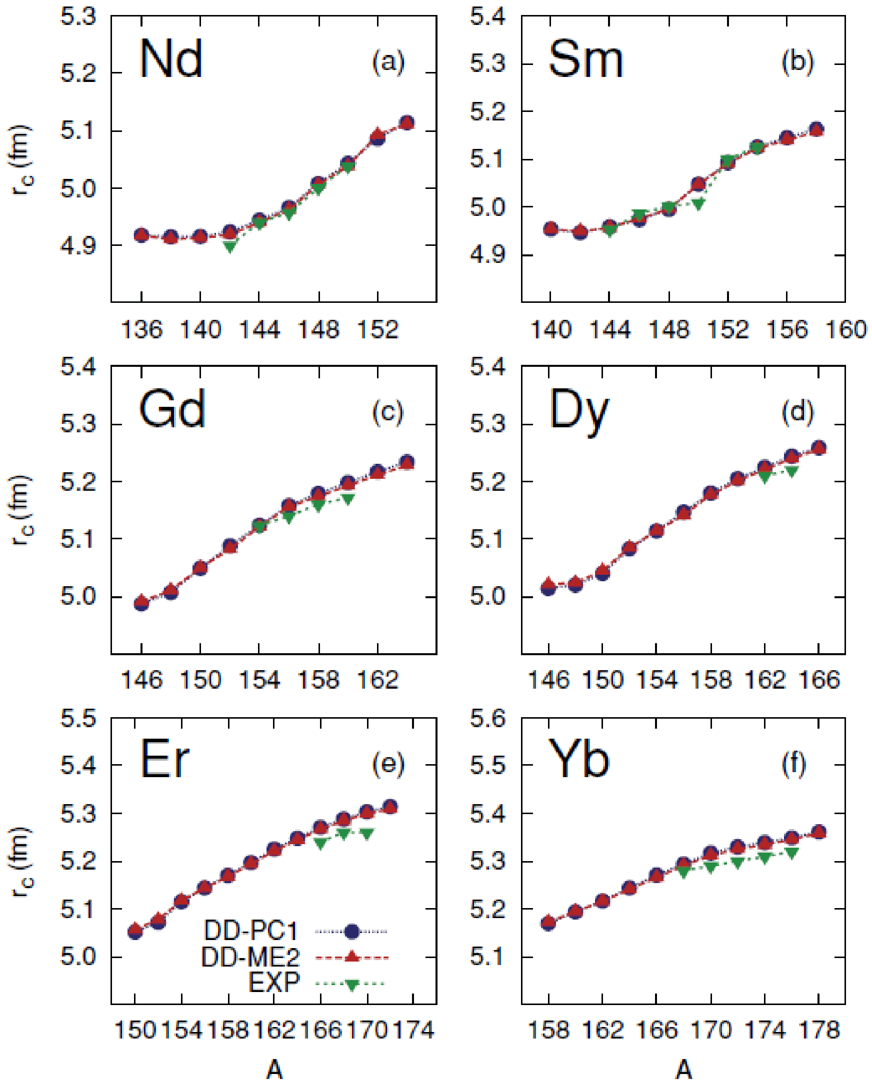
Vector self energy $V(\rho)$:

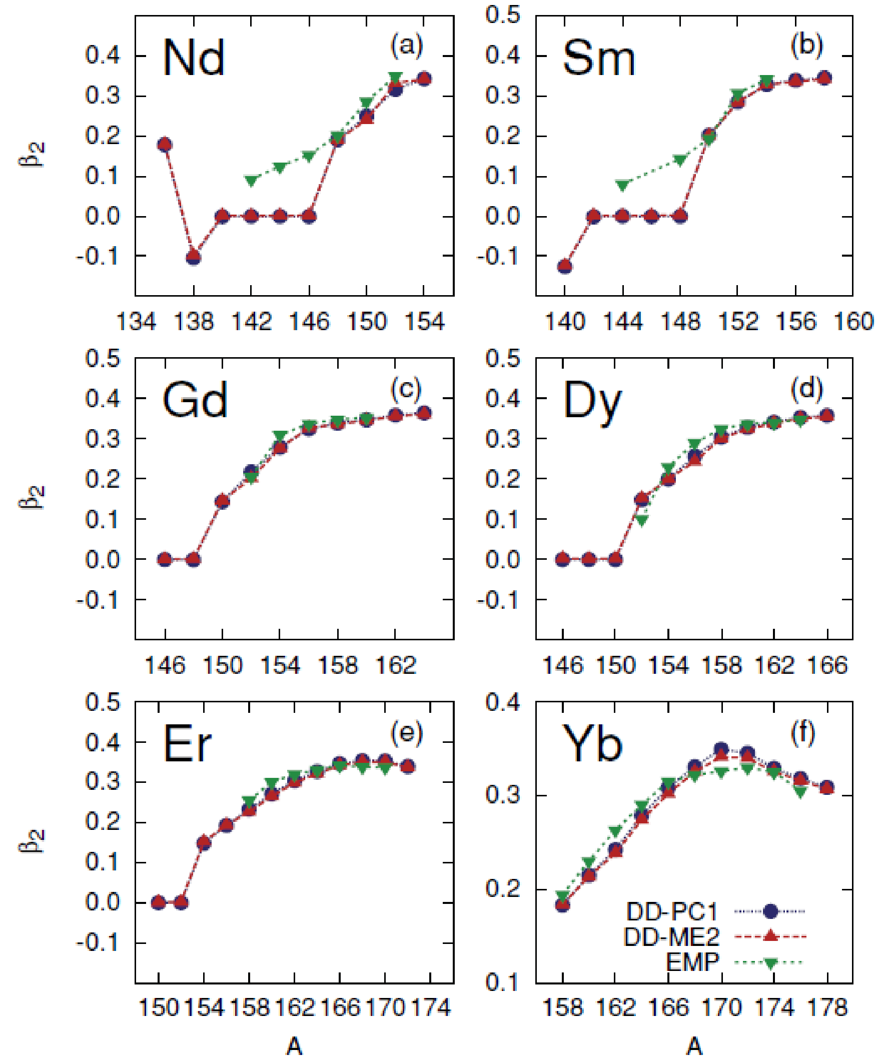
Scalar self energy $S(\rho)$:



T. Niksic

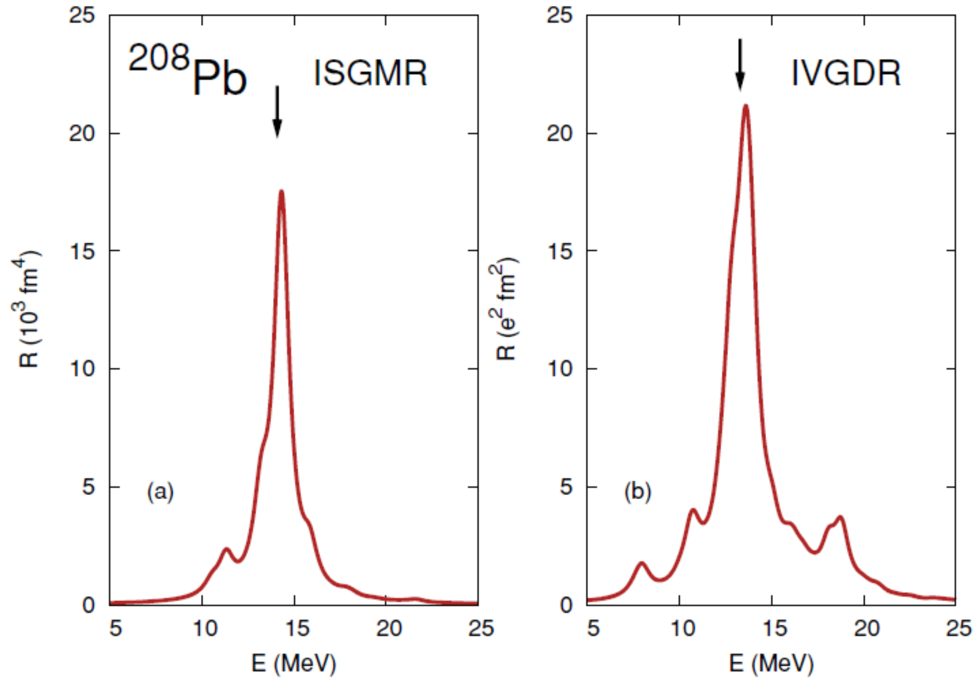
DD-PC1: isotope shifts and deformation parameters

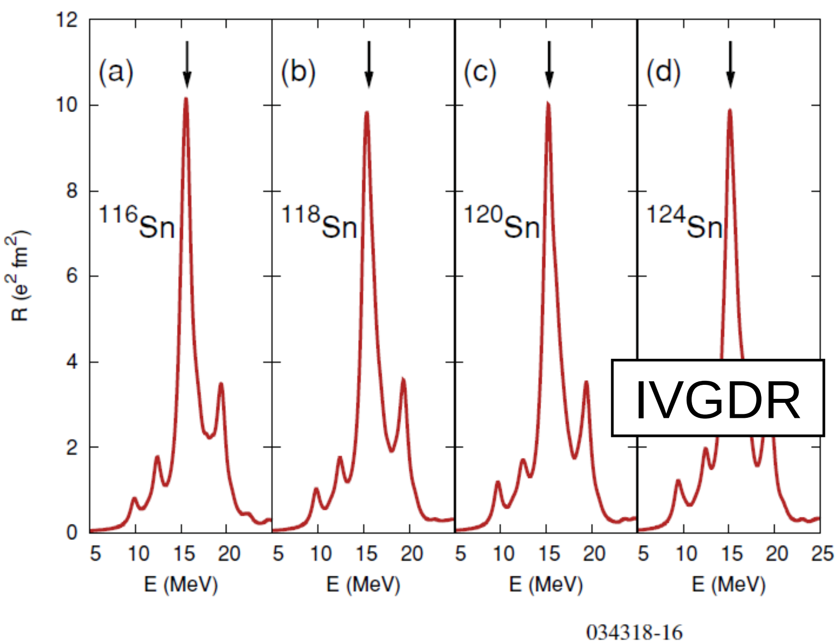


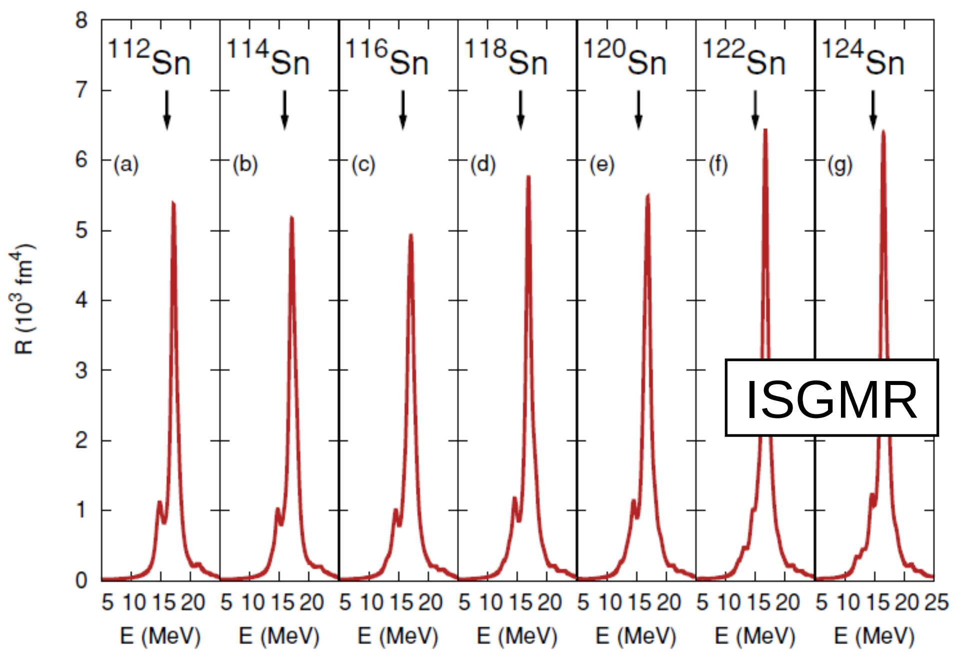


DD-PC1
Giant resonances:

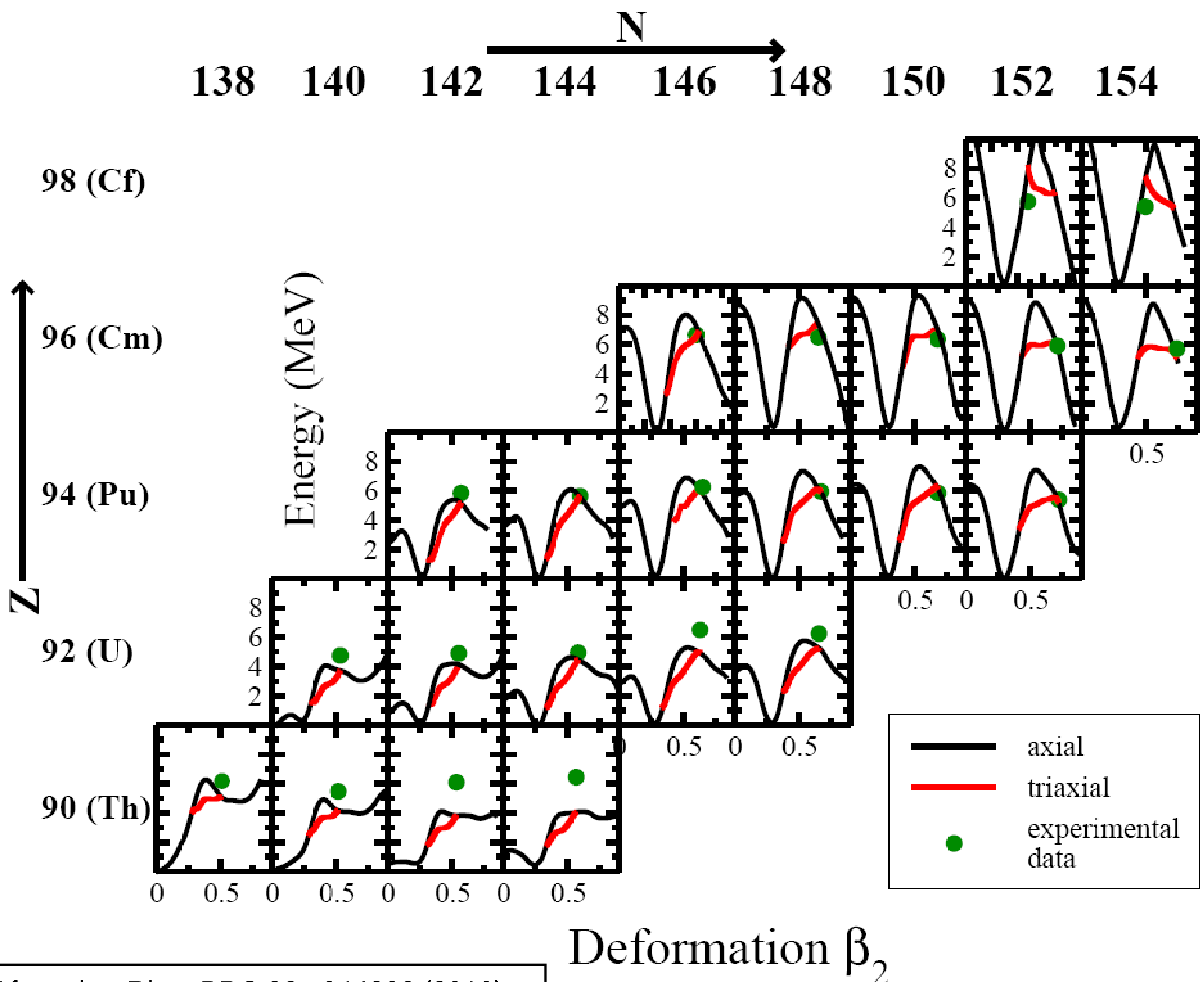
T. Niksic et al, (2008)







Fission barriers for triaxially deformed shapes:



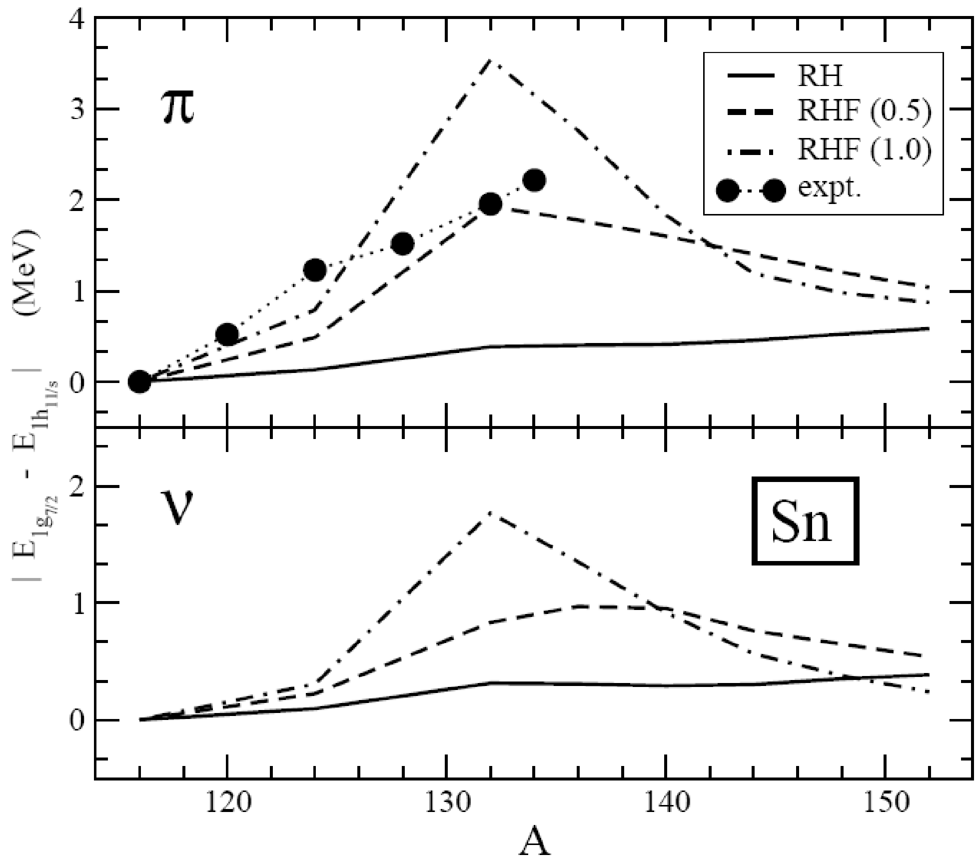
Abusara, Afanasjev, Ring, PRC 82, 044303 (2010).

Single-particle energy splittings in Sn-isotopes:

$E_{1h_{11/2}} - E_{1g_{7/2}}$

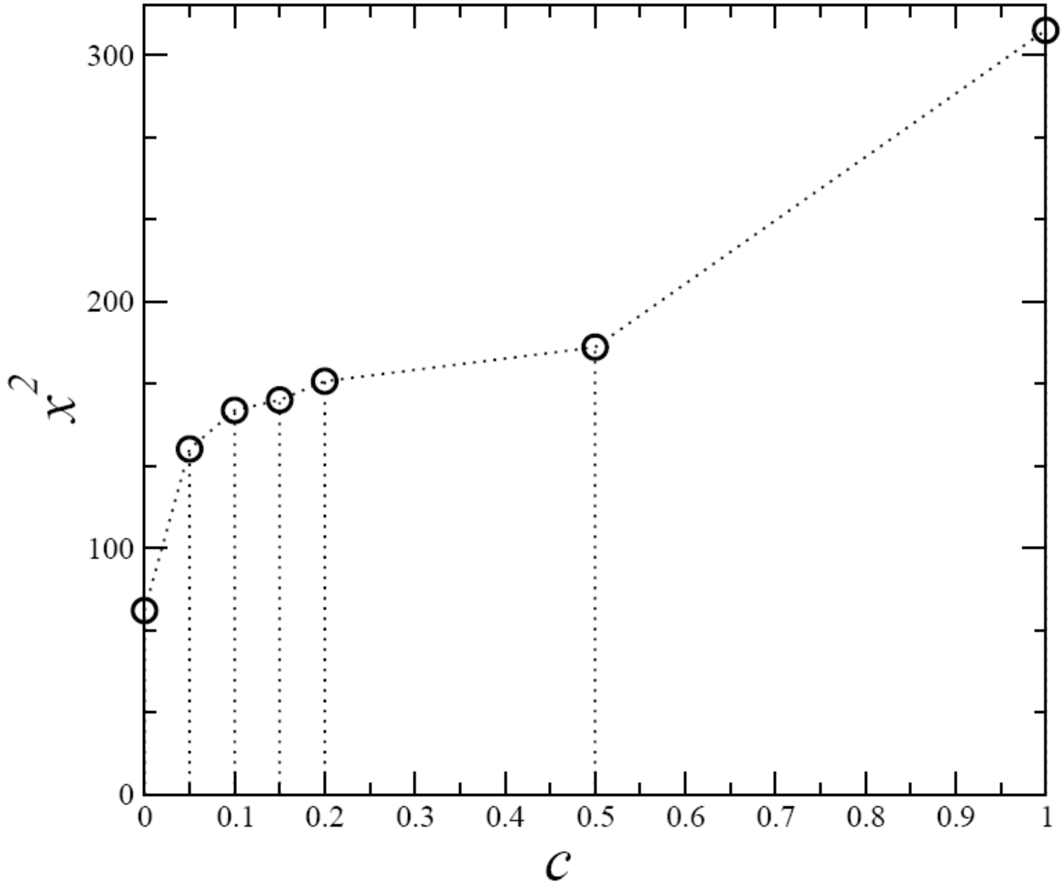
Effect of a tensor force in Relativistic Hartree-Fock

RH → RHF



Experiment: J. P. Schiffer et al., Phys. Rev. Lett, 92 162501, (2004)
Theory: G. A. Lalazissis, T.Otsuka et al, Phys. Rev. C89, 041301 (2009)

Fit to masses and radii (as DD-ME2) + c $L_{\pi N}$

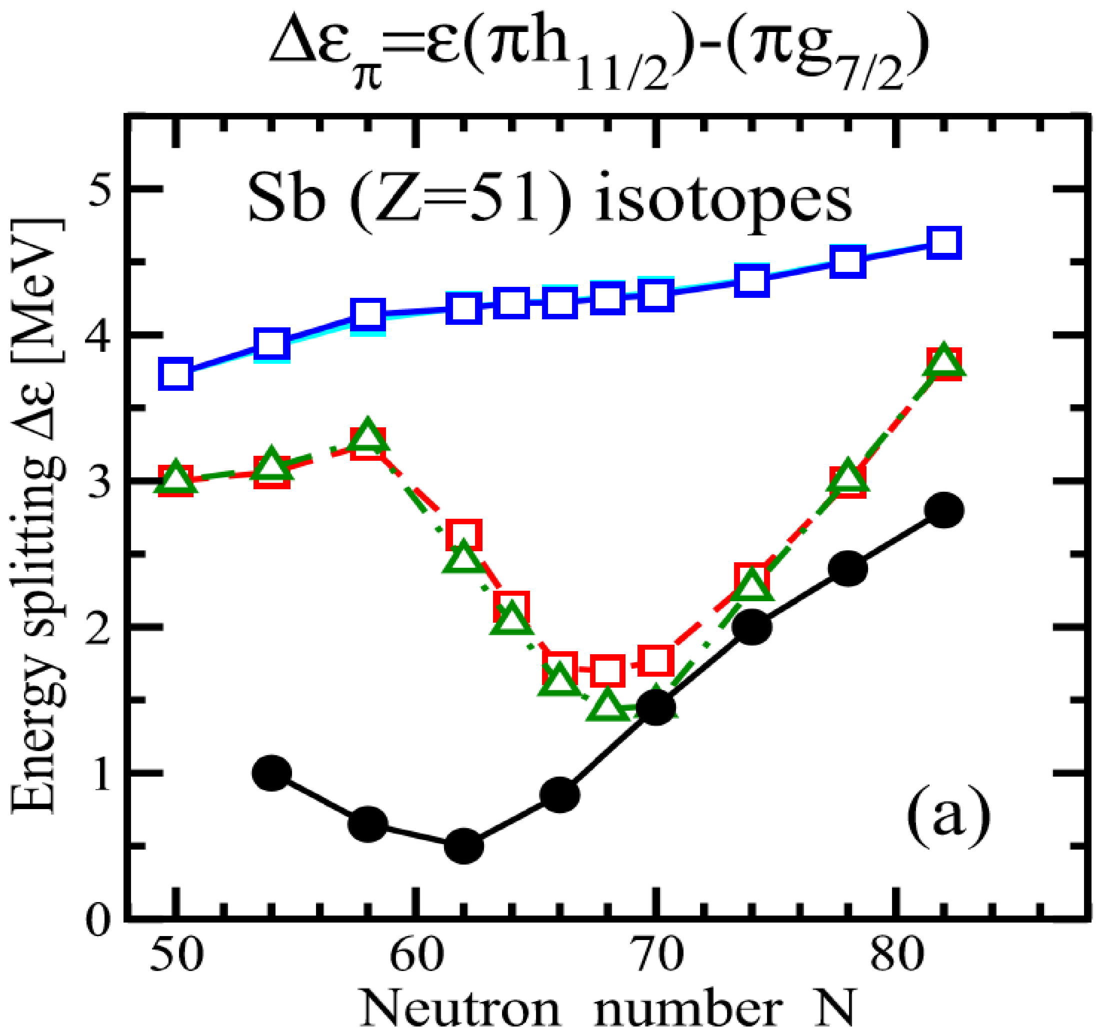


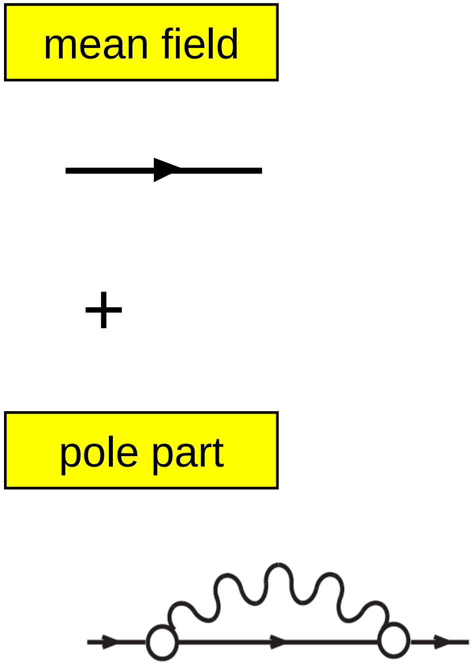
no pion

full pion

Lalazissis, Karatzikos, Serra, Otsuka, P.R., PRC 80 , 041301(R) (2009)

Influence of Particle-Vibrational Coupling





Experiment: J. P. Schiffer et al., Phys. Rev. Lett, 92 162501, (2004)
Theory: A.V. Afanasjev, E. Litvinova, Phys. Rev. C92, 044307 (2015)

Further observations :

- effective single particle energies in shell-model calculations show specific trends due to the tensor force, which agrees with many data (Otsuka, Schiffer, Greavy)

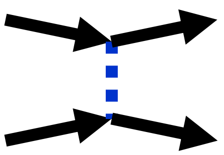
- the same trend can be found qualitatively if one adds a the pion with an effective coupling constant in fully selfconsistent RHF calculations (Lalazissis, Long)

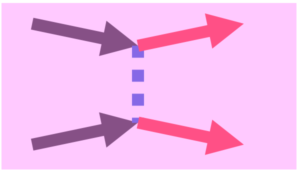
- particle-vibrational coupling is also important

How important are effective tensor forces?

Brueckner theory (1958):

Brueckner,Gammel, Phys. Rev. 109, 1023 (1958)



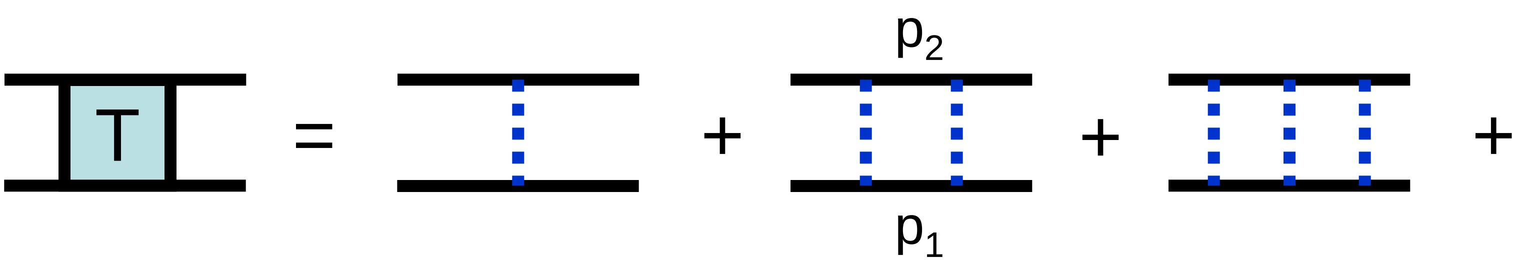


- The nucleons in the interior of the nuclear medium do not feel the same bare force V, as the nucleons feel in free space.
- They feel an effective force G.
- The Pauli principle prohibits the scattering into states, which are already occupied in the medium.
- Therefore this force G(ρ) depends on the density
- This force G is much weaker than bare force V.
- Nucleons move nearly free in the nuclear medium and feel only a strong attraction at the surface (shell model)

Free nucleon-nucleon scattering:

Lippmann-Schwinger-Eq.

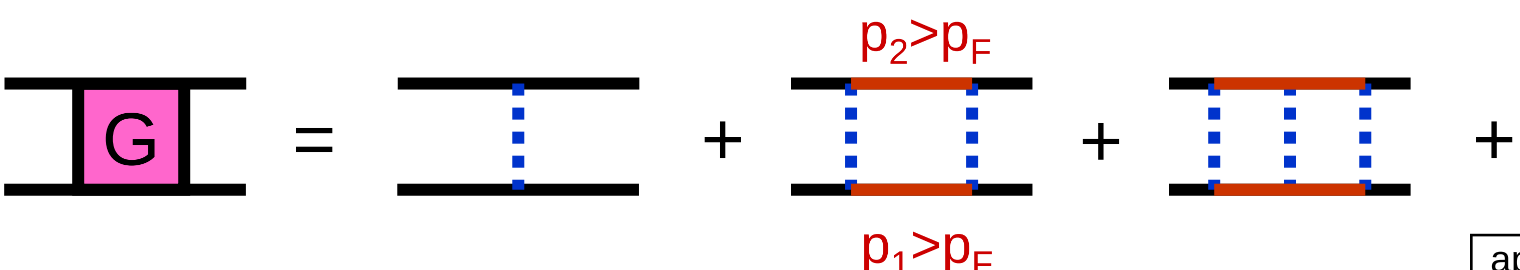
$$\langle \mathbf{k}_1\mathbf{k}_2|T|\mathbf{k}_1'\mathbf{k}_2'\rangle = \langle \mathbf{k}_1\mathbf{k}_2|V|\mathbf{k}_1'\mathbf{k}_2'\rangle + \sum_{\mathbf{p}_1\mathbf{p}_2}\langle \mathbf{k}_1\mathbf{k}_2|V|\mathbf{p}_1\mathbf{p}_2\rangle \frac{1}{E-\frac{\mathbf{p}_1^2}{2m}-\frac{\mathbf{p}_2^2}{2m}+i\eta}\langle \mathbf{p}_1\mathbf{p}_2|T|\mathbf{k}_1'\mathbf{k}_2'\rangle$$



exact

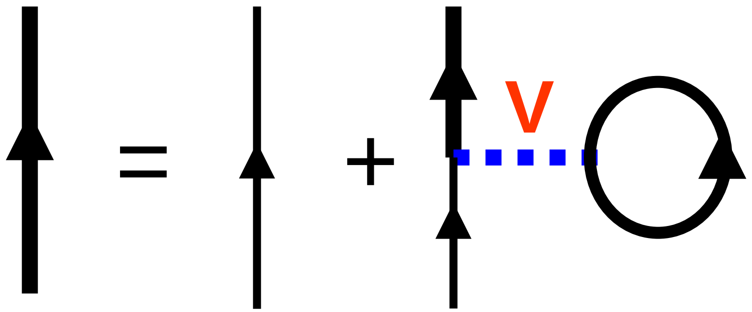
Scattering in the nuclear medium:

Bethe-Goldstone-Eq.

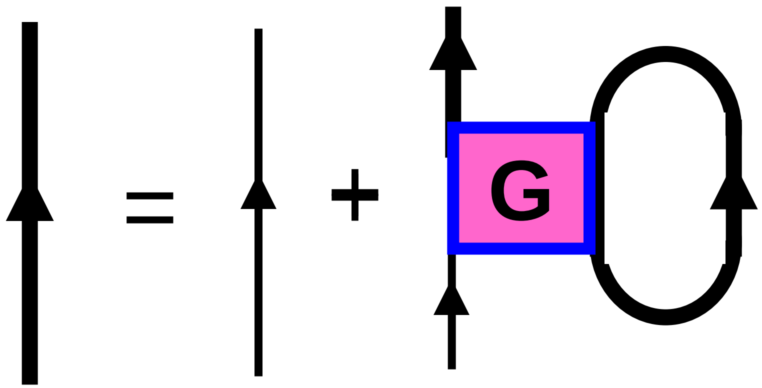


approximation

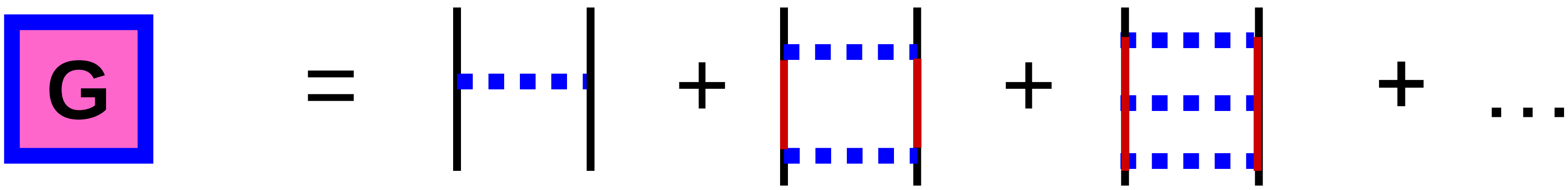
Ab-initio: Relativistic Brueckner Hartree-Fock:



Hartree-Fock



Brueckner Hartree-Fock



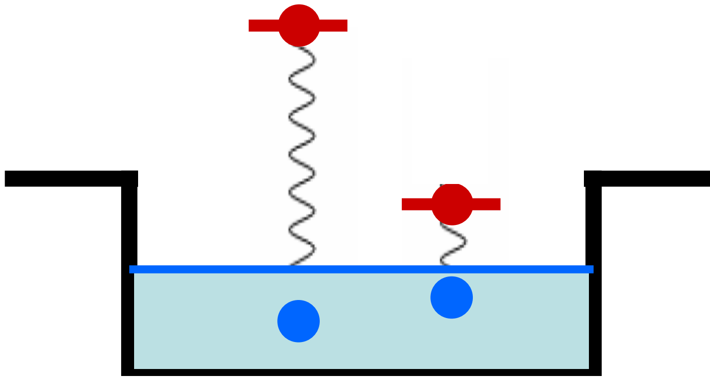
Summing up all ladder diagramms

Bethe-Goldstone equation:

- ω is the starting energy
- V is realistic interaction
- Q_F is the Pauli operator

$$G(\omega) = V + VQ_F \frac{1}{\omega - H_{HF}} Q_F G(\omega)$$

$$G(\omega) = V + V P_F(\omega) G(\omega)$$



$$P_F(\omega) = \sum_{m_1 m_2 > \varepsilon_F} |m_1 m_2\rangle \frac{1}{\omega - \varepsilon_{m_1} - \varepsilon_{m_2}} \langle m_1 m_2|$$

$$G(\omega) = \frac{1}{1 - V P_F(\omega)} V$$

Is solved in each step of the iteration

Solution of the Bethe-Goldstone equation:

Bethe-Goldstone equation in basis space

$$\langle ab|G(\omega)|a'b'\rangle = \langle ab|\bar{V}^N|a'b'\rangle + \sum_{\varepsilon_m \varepsilon_n > \varepsilon_F} \frac{\langle ab|\bar{V}^N|mn\rangle\langle mn|G(\omega)|a'b'\rangle}{\omega - \varepsilon_m - \varepsilon_n},$$

where ε_F is the Fermi energy, $\omega = \varepsilon_a + \varepsilon_b$ is the starting energy and $|mn\rangle$ are intermediate states.

Bethe-Goldstone equation in plane wave basis

$$G^{\alpha}_{ll'}(kk'K\omega) = V^{\alpha}_{ll'}(kk') + \sum_{ll'} \int \frac{d^3q}{(2\pi)^3} V^{\alpha}_{ll'}(kq) \frac{Q(q,K)}{\omega - H_0} G^{\alpha}_{ll'}(qk'K\omega)$$

where α is a shorthand notation for J, S, L and T.

Matrix inversion method

$$G = \left(1 - \frac{V}{\omega - H_0}\right)^{-1} V$$

RBHF theory in finite nuclei:

$$(\boldsymbol{\alpha p} + \beta M + U)|a\rangle = \varepsilon_a |a\rangle$$

Normal Hartree-Fock:

$$U_{ab}^{\mathrm{HF}} = \sum_{c=1}^{A} \langle ac|\bar{V}|bc\rangle$$

Brueckner-Hartree-Fock:

$$U_{ab}^{\mathrm{BHF}} = \sum_{c=1}^{A} \langle ac|\bar{G}(\omega)|bc\rangle$$

RBHF theory in finite nuclei:

$$(\boldsymbol{\alpha p} + \beta M + U)|a\rangle = \varepsilon_a|a\rangle$$

Bethe-Brandow-Petschek Theorem:

$$U_{ab}^{\mathrm{BHF}} = \frac{1}{2}\sum_{c=1}^{A}\langle ac|\bar{G}(\varepsilon_a + \varepsilon_c) + \bar{G}(\varepsilon_b + \varepsilon_c)|bc\rangle$$

$$\text{for}\quad \varepsilon_a < \varepsilon_F,\ \varepsilon_b < \varepsilon_F$$

$$U_{ab}^{\mathrm{BHF}} = \sum_{c=1}^{A}\langle ac|\bar{G}(\varepsilon_a + \varepsilon_c)|bc\rangle$$

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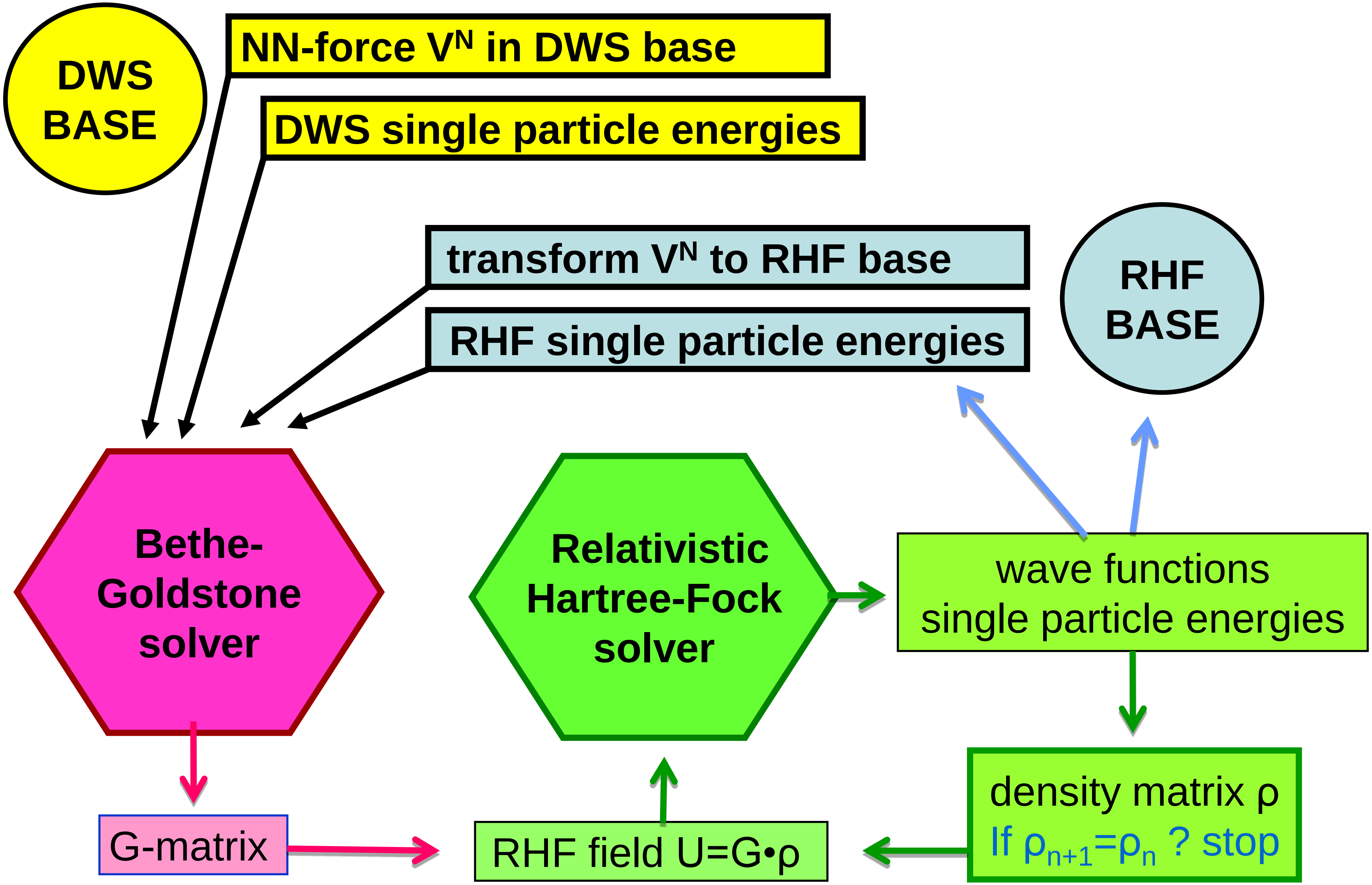
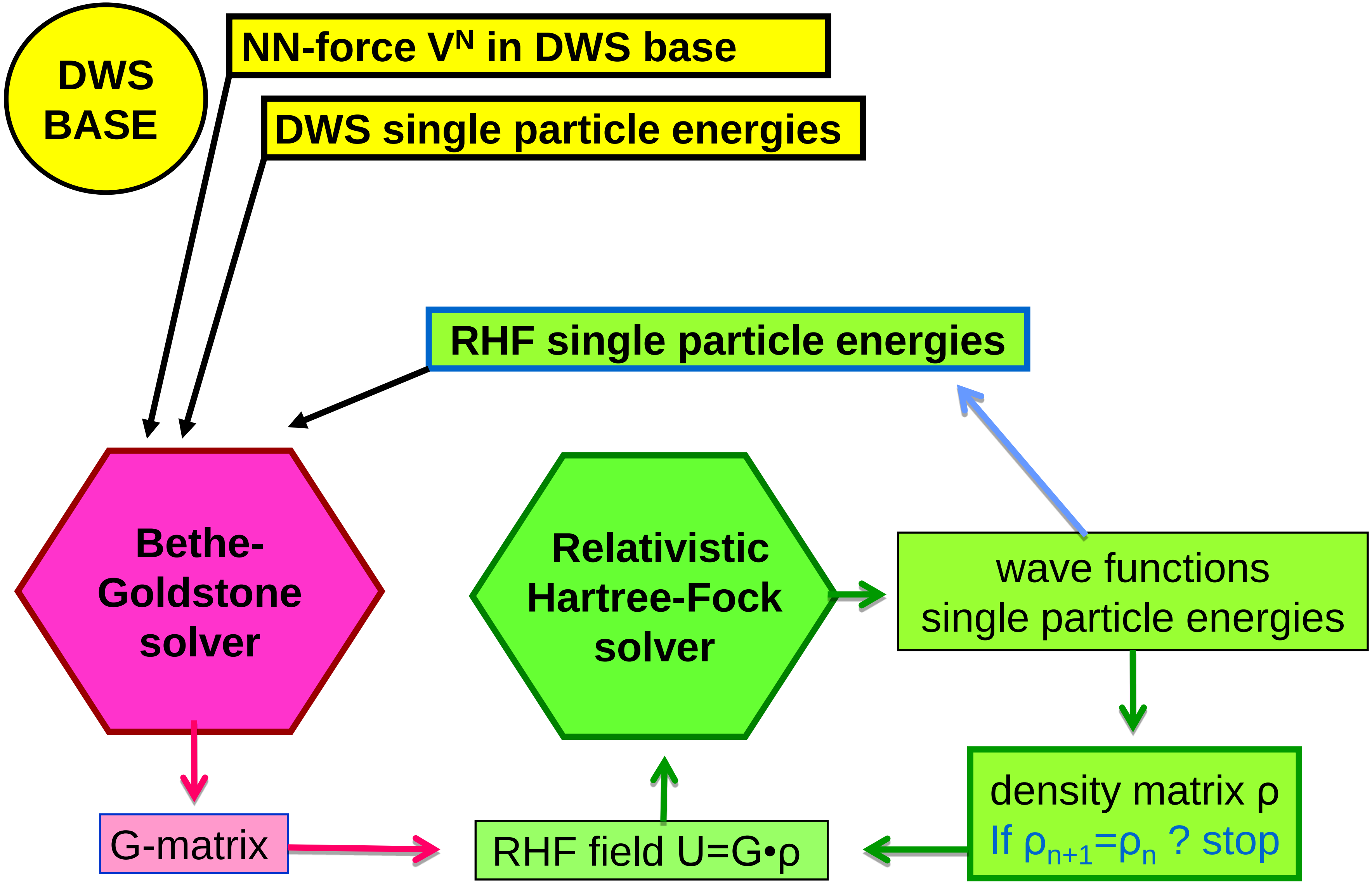
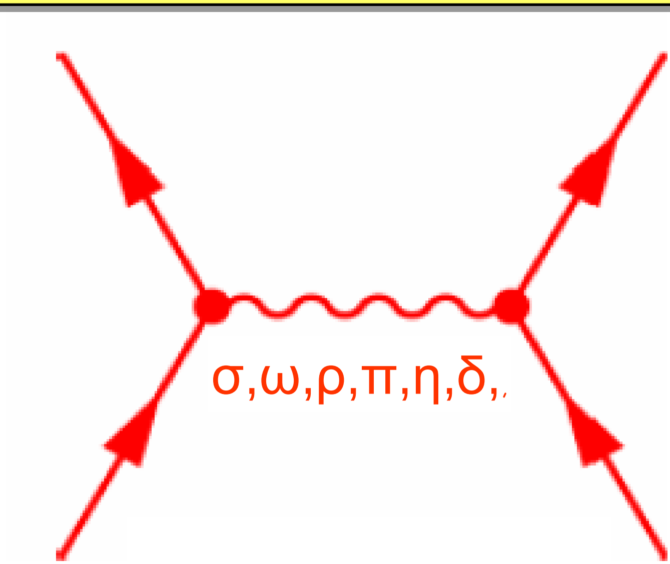
Flow chart for RBHF theory in finite nuclei:



Simpification with fixed DWS-basis:



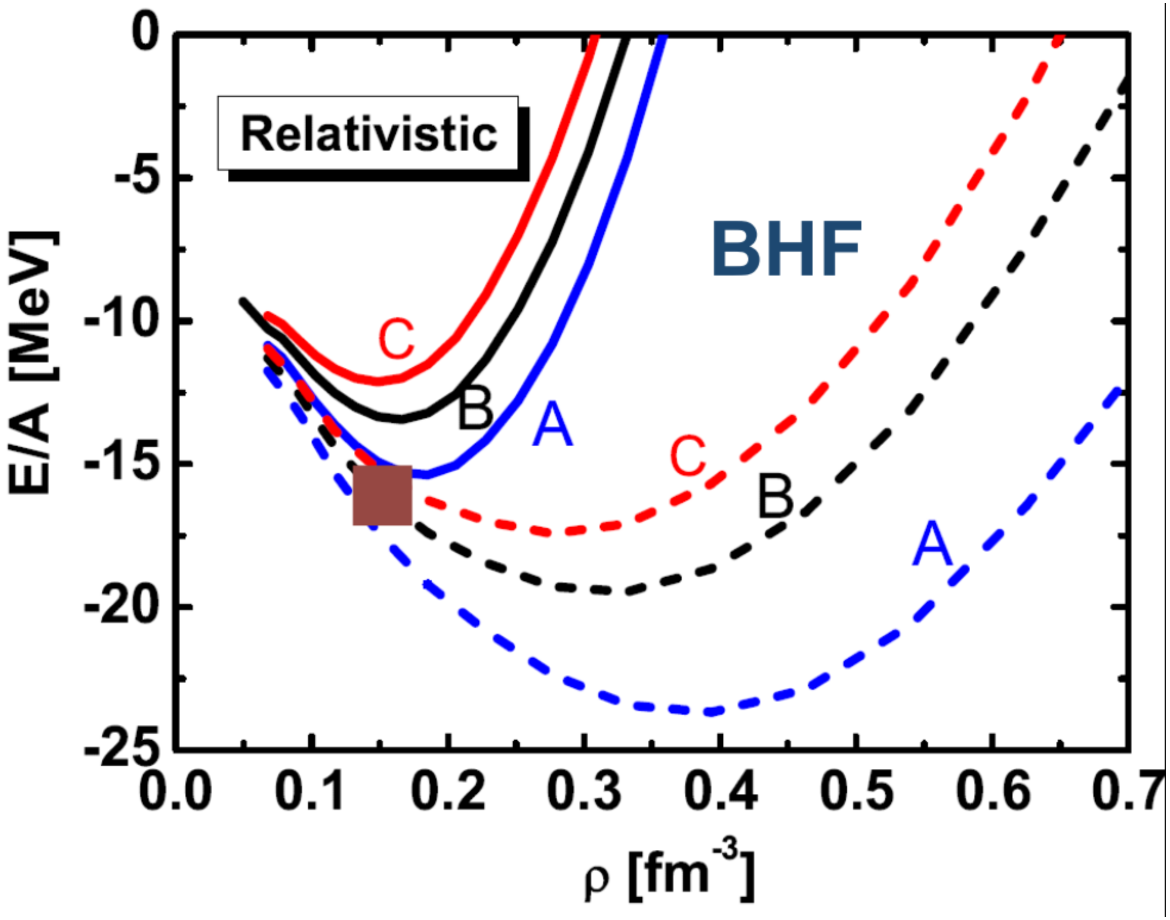
Bare nucleon-nucleon force:



Brockmann and Machleidt, PRC **42**, 1965 (1990).

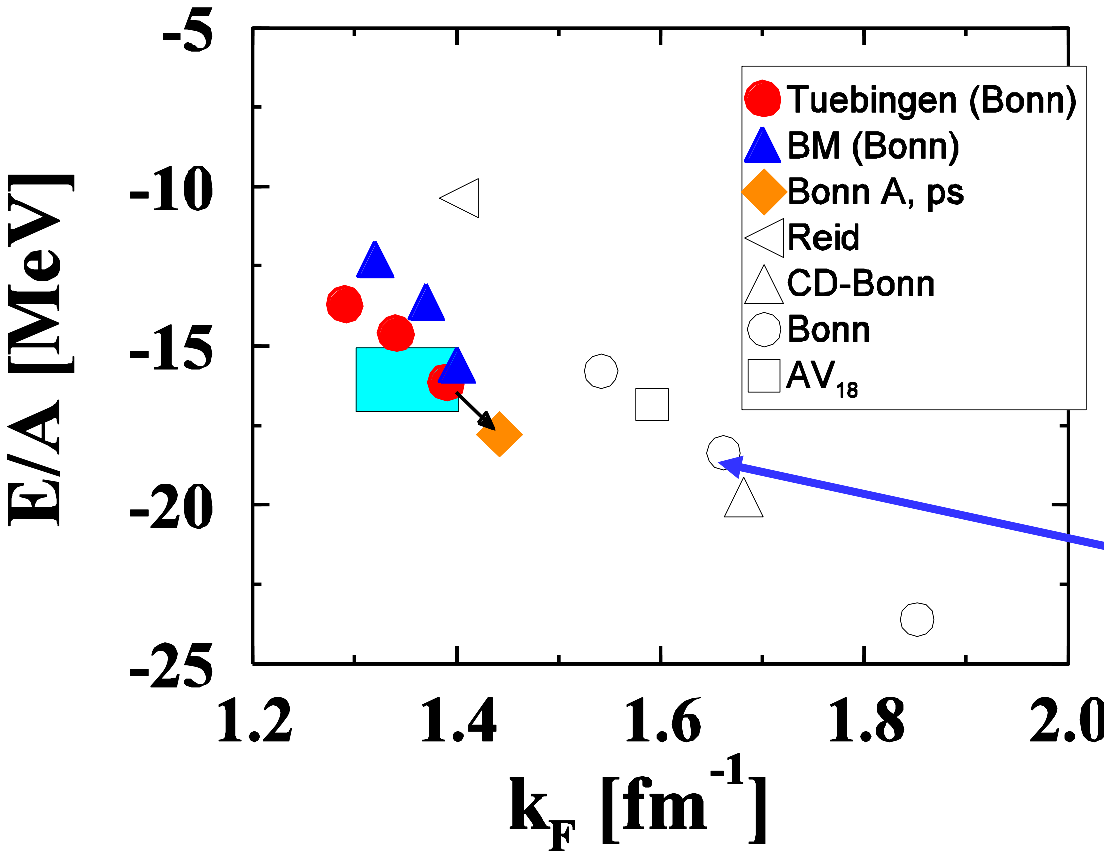
Meson Parameters	m_α (MeV)	Potential A $g_\alpha^2/4\pi$	Potential A Λ_α (GeV)	Potential B $g_\alpha^2/4\pi$	Potential B Λ_α (GeV)	Potential C $g_\alpha^2/4\pi$	Potential C Λ_α (GeV)
π	138.03	14.9	1.05	14.6	1.2	14.6	1.3
η	548.8	7	1.5	5	1.5	3	1.5
ρ	769	0.99	1.3	0.95	1.3	0.95	1.3
ω	782.6	20	1.5	20	1.5	20	1.5
δ	983	0.7709	2.0	3.1155	1.5	5.0742	1.5
σ	550	8.3141	2.0	8.0769	2.0	8.0279	1.8

Dirac-Brueckner-Hartree-Fock in nuclear matter



Brockmann and Machleidt, PRC **42**, 1965 (1990).

Dirac-Brueckner-Hartree-Fock in nuclear matter



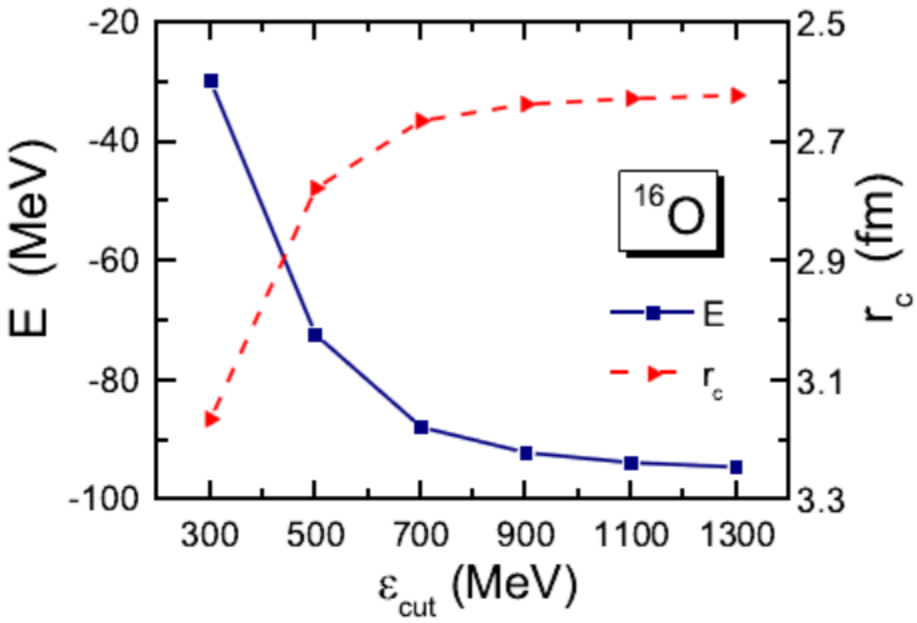
C. Fuchs, LNP (2004)

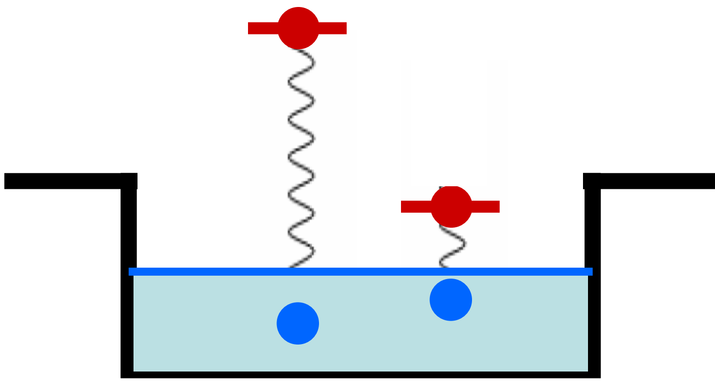
Coester-line

Results for ^{16}O

S.H. Shen et al, to be published.

Convergenge with the cuf-off in single particle energy:





Local density approximation:

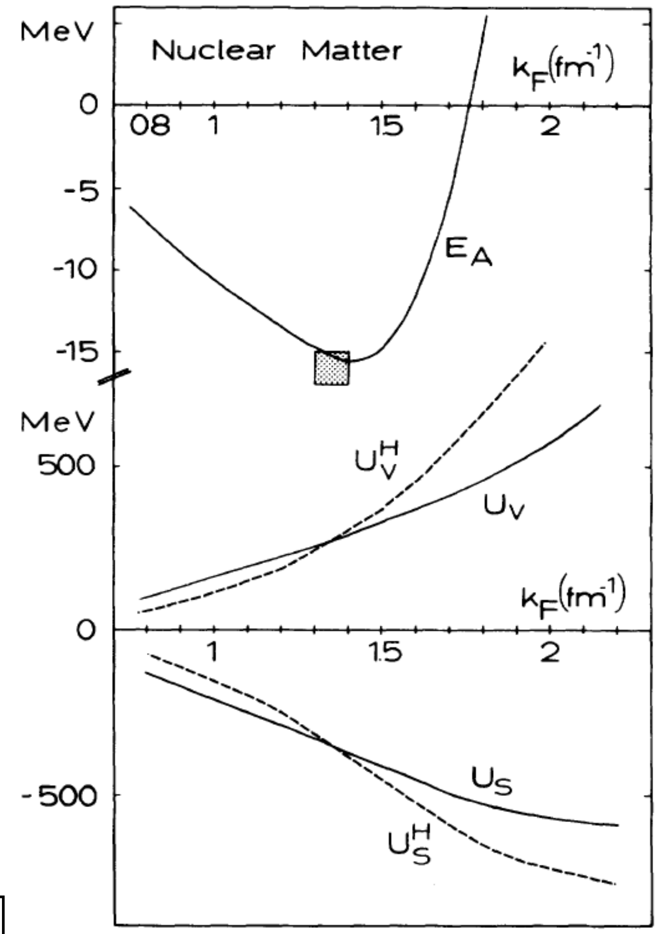
Bonn A

E/A Binding energy per particle
in Rel. Brückner-Hartree-Fock

U_S, U_V: scalar and vector potential $\Sigma(\rho)$
in Rel. Brueckner-Hartree-Fock
for nuclear matter with density ρ

$\rightarrow$ $g_\sigma(\rho)$ and $g_\omega(\rho)$

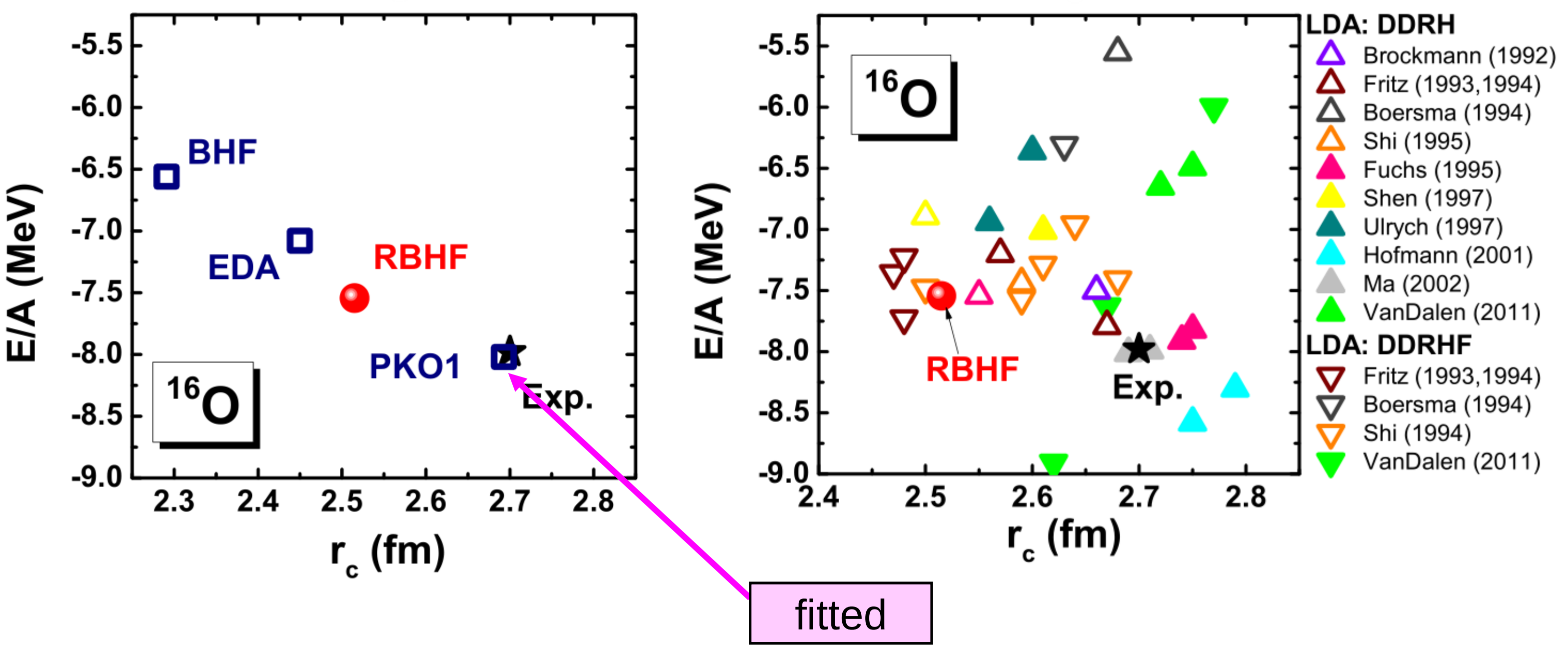
U^H_S, U^H_V: scalar and vector potential
in Relativistic. Hartree



Brockmann and Toki, PRL **68**, 3408 (1992).

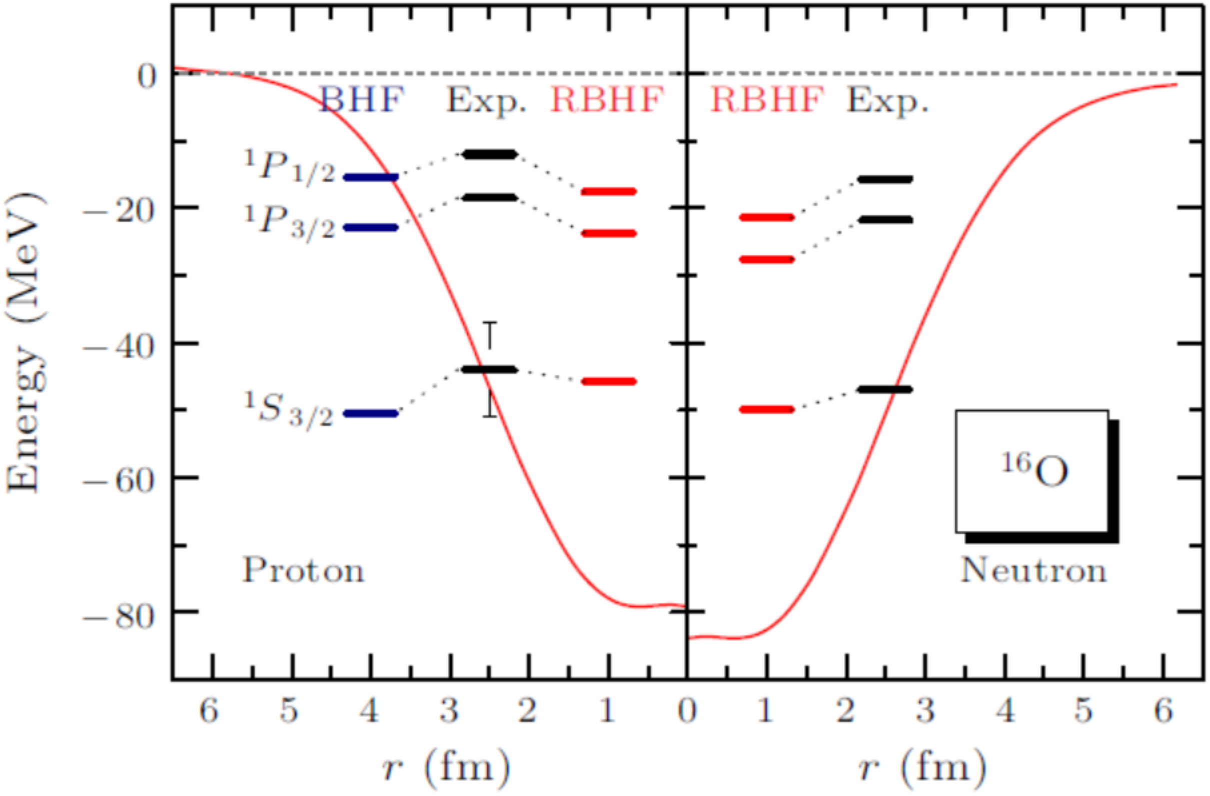
Bulk properties of ^{16}O:

- Energy per particle and charge radius of ^{16}O calculated by RBHF, non-relativistic BHF Müther1990PRC , BHF with EDA Müther1990PRC, RHF with PKO1 Long2010PLB (left); and RBHF with LDA (right) :



- Relativistic effect is very important to improve the description.
- There is a big uncertainty between different LDA calculations.

DWS-basis


BHF
Exp.
RBHF
RBHF
Exp.
$^1P_{1/2}$
$^1P_{3/2}$
$^1S_{3/2}$
0
−20
−40
−60
−80
Energy (MeV)
Proton
Neutron
^{16}O
6 5 4 3 2 1 0 1 2 3 4 5 6
r (fm)
r (fm)

^{16}O

	E (MeV)	r_c (fm)	r_m (fm)	$\Delta E^{ls}_{\pi 1p}$ (MeV)
Exp. [84–87]	−127.6	2.70	2.54(2)	6.3
RBHF, Bonn A	−113.5	2.56	2.42	5.4
RBHF (DWS) [63]	−120.7	2.52	2.38	6.0
DDRHF, PKO1 [70]	−128.3	2.68	2.54	6.4
DDRHF, PKA1 [88]	−127.0	2.80	2.67	6.0
BHF [89], AV18	−134.2		1.95	13.0
CC [91], N^3LO	−120.9		2.30	
NCSM [90], N^3LO	−119.7(6)			
NLEFT [93], N^2LO	−121.4(5)			

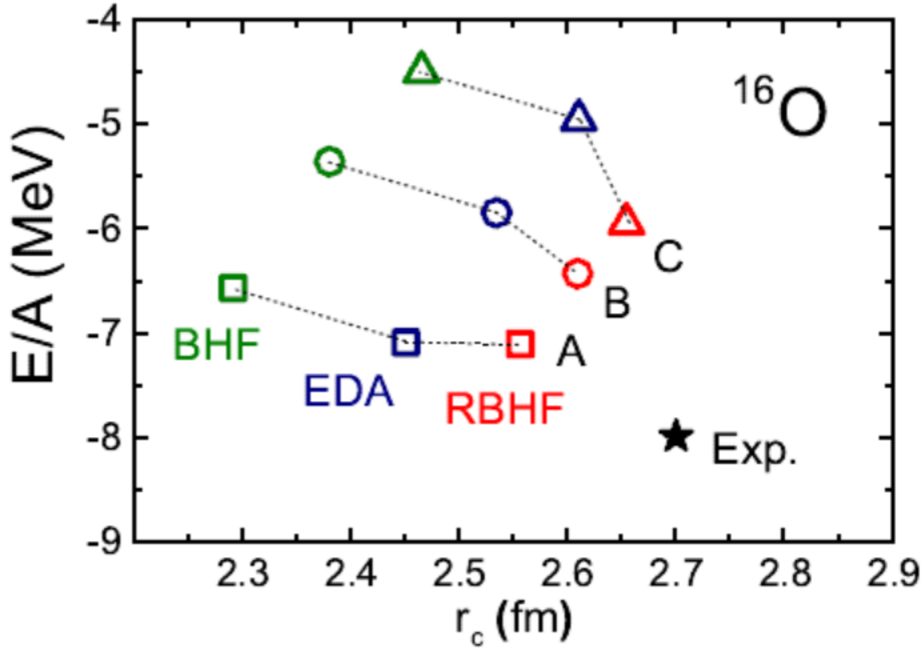
^{4}He

	E (MeV)	r_c (fm)	r_p (fm)
Exp. [84, 85, 99]	−28.30	1.68	1.46
RBHF (PBV), Bonn A	−35.05	1.83	1.64
RBHF (PAV), Bonn A	−26.31	1.90	1.73
DDRHF, PKO1 [70]	−28.45	1.90	1.72
DDRHF, PKA1 [88]	−28.28	2.06	1.90
FY [100], CD-Bonn	−26.26		
FY [101], N^4LO	−24.27(6)		1.547(2)
NCSM [102], N^3LO	−25.39(1)		1.515(2)
NLEFT [93], N^2LO	−25.60(6)		
BHF [89], AV18	−25.90		

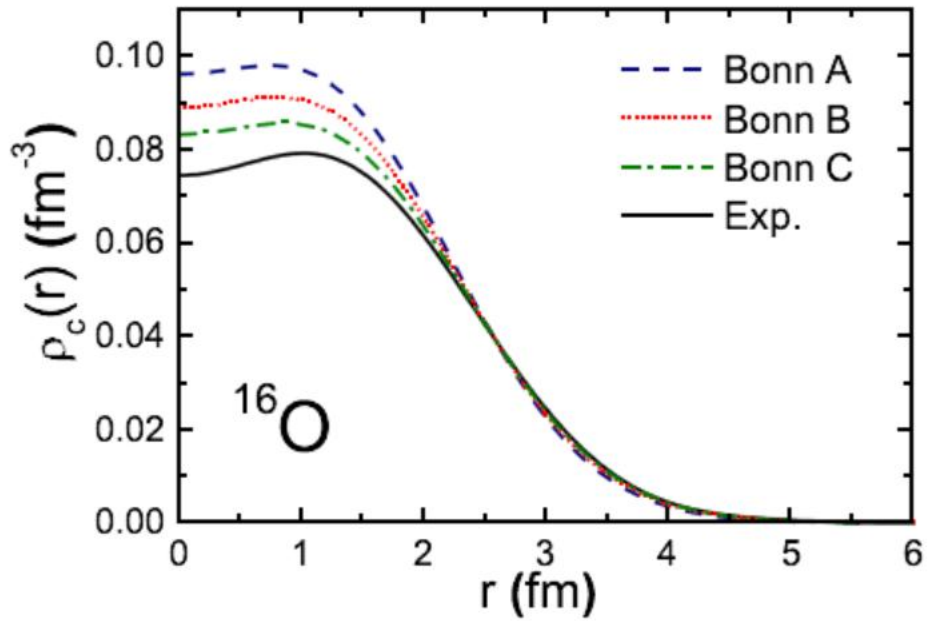
^{40}Ca

	E (MeV)	r_c (fm)	r_m (fm)	$\Delta E^{ls}_{\pi 1d}$ (MeV)
Exp. [84, 85, 87]	-342.1	3.48		6.6 ± 2.5
RBHF , Bonn A	-290.8	3.23	3.11	5.8
DDRHF, PKO1 [70]	-343.3	3.44	3.33	6.6
DDRHF, PKA1 [88]	-341.7	3.53	3.41	7.2
BHF [89], AV18	-552.1		2.20	24.9
NCSM [105], AV18	-461.8		2.27	
CC [106], AV18	-502.9			
CC [107], N^{3}LO	-345.2			

Self-consistent basis



Self-consistent basis



Conclusions

- Covariant density functional theory is very successful
- So far it is phenomenological (8-10 parameters)
- Semi-microscopic with only 4 parameters uses microscopic input (density dependence from BHF…)
- For the required accuracy (10^{-4}) we need fine-tuning
- In order to understand the phenomenological models and to decide about additional terms in the Lagrangian (e.g. tensor) we need ab-initio derivations
- Rel. Brueckner-Hartree-Fock calculations in finite nuclei:

  a) Rel. Brueckner-Hartree-Fock in local density approximation

  b) Rel. Brueckner-Hartree-Fock in a Dirac-Woods-Saxon basis

  c) Rel. Brueckner-Hartree-Fock fully selfconsistent

  we solve the Bethe-Goldstone equation
  in each step of the iteration selfconsistently.

Outlook

- Heavy nuclei and the tensor force
- Other microscopic forces
- Pairing and open shell nuclei
- Deformed nuclei
- Optical potential
-
- Three-body forces ?
- Beyond Brueckner ?

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