On the ab-initio derivation of covariant density functionals

Thessaloniki, Apr. 12, 2019

Peter Ring

Technical University Munich
Excellence Cluster "Origin of the Universe"
Beijing University

- Covariant Density Functional Theory (CDFT) is a universal tool for the description of nuclear structure
- One uses phenomenological input (masses, radii)
- One finds large uncertainties far from stability.
- One also needs ‚ab-initio' results

  for infinite nuclear matter

  for finite nuclear systems
- We use Relativistic Brueckner-Hartree-Fock theory

  as an ab-initio starting point.
- neutron-drops can be used as meta-data, providing information for the determination of the tensor force

Content:

1) Systematic investigations on present functionals

2) Semi-microscopic density functionals

3) Single particle energies and tensor forces

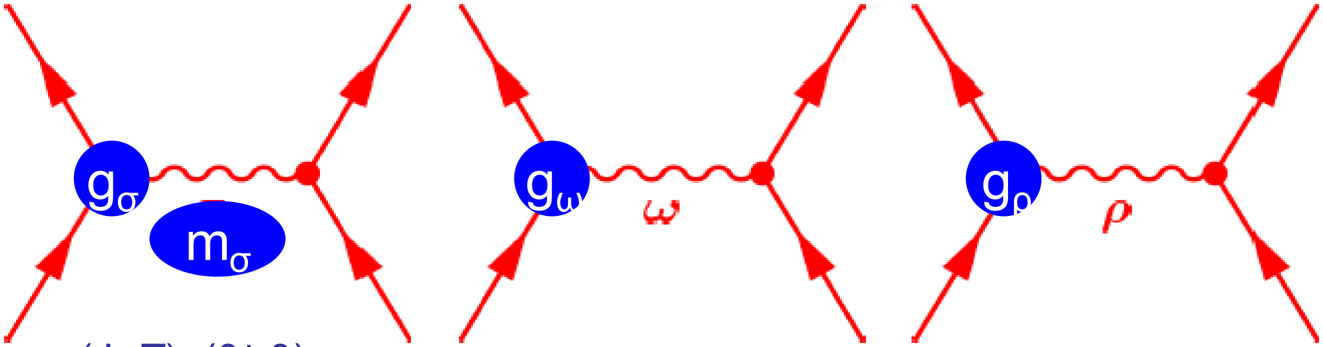
4) Relativistic Brueckner-Hartree-Fock in finite nuclei

5) Neutron drops and tensor forces

Covariant DFT is based on the Walecka model:

$E[\rho]$

This model has only four parameters:



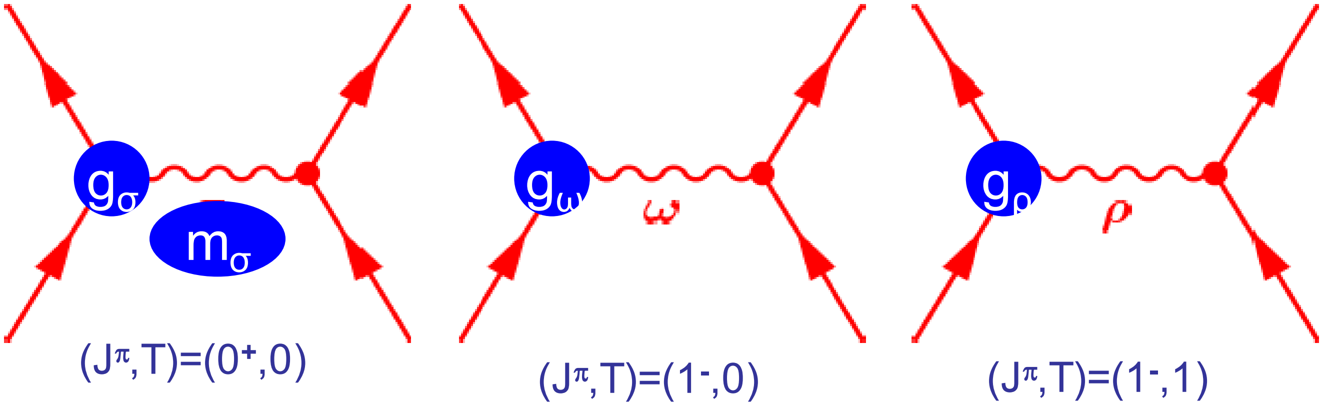
$(J^\pi,T)=(0^+,0)$ $(J^\pi,T)=(1^-,0)$ $(J^\pi,T)=(1^-,1)$

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

Covariant DFT is based on the Walecka model:

$E[\rho]$

This model has only four parameters:

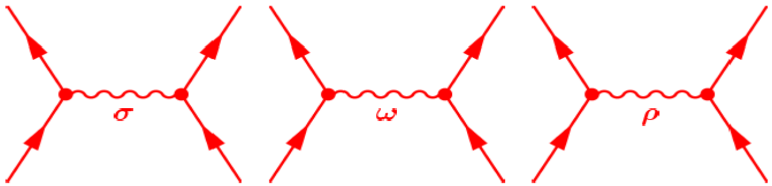


$$S(r) = g_\sigma \sigma(r) \qquad V(r) = g_\omega \omega(r) + g_\rho \rho(r) + eA(r)$$

Density dependent parameters: $g_i \rightarrow g_i(\boldsymbol{\rho})$

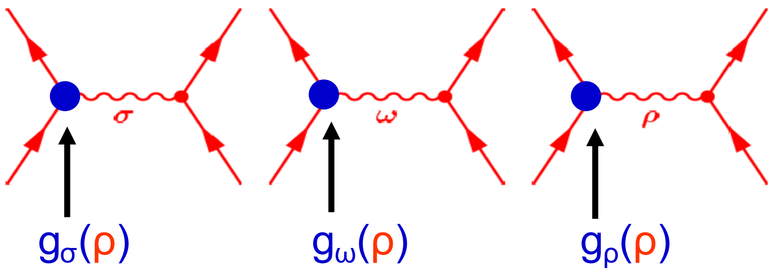
3 types of covariant density functionals:

a)



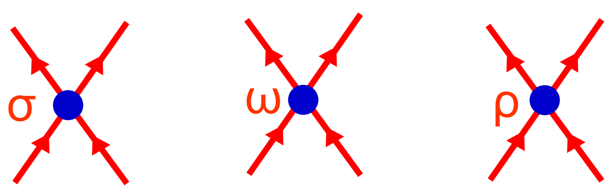
+ non-linear meson couplings
NL3, PK1, FSU….

b)



density dependent couplings
TW, DD-ME2, DD-MEδ….

c)



point-coupling models
PC-F1, DD-PC1, PC-PK1…

+ derivative terms

Concept of a microscopic derivation:

The basic idea is the local density approximation:

Starting from the microscopic energy functional for the homogeneous system (nuclear matter) gradient terms, terms depending on currents are added:

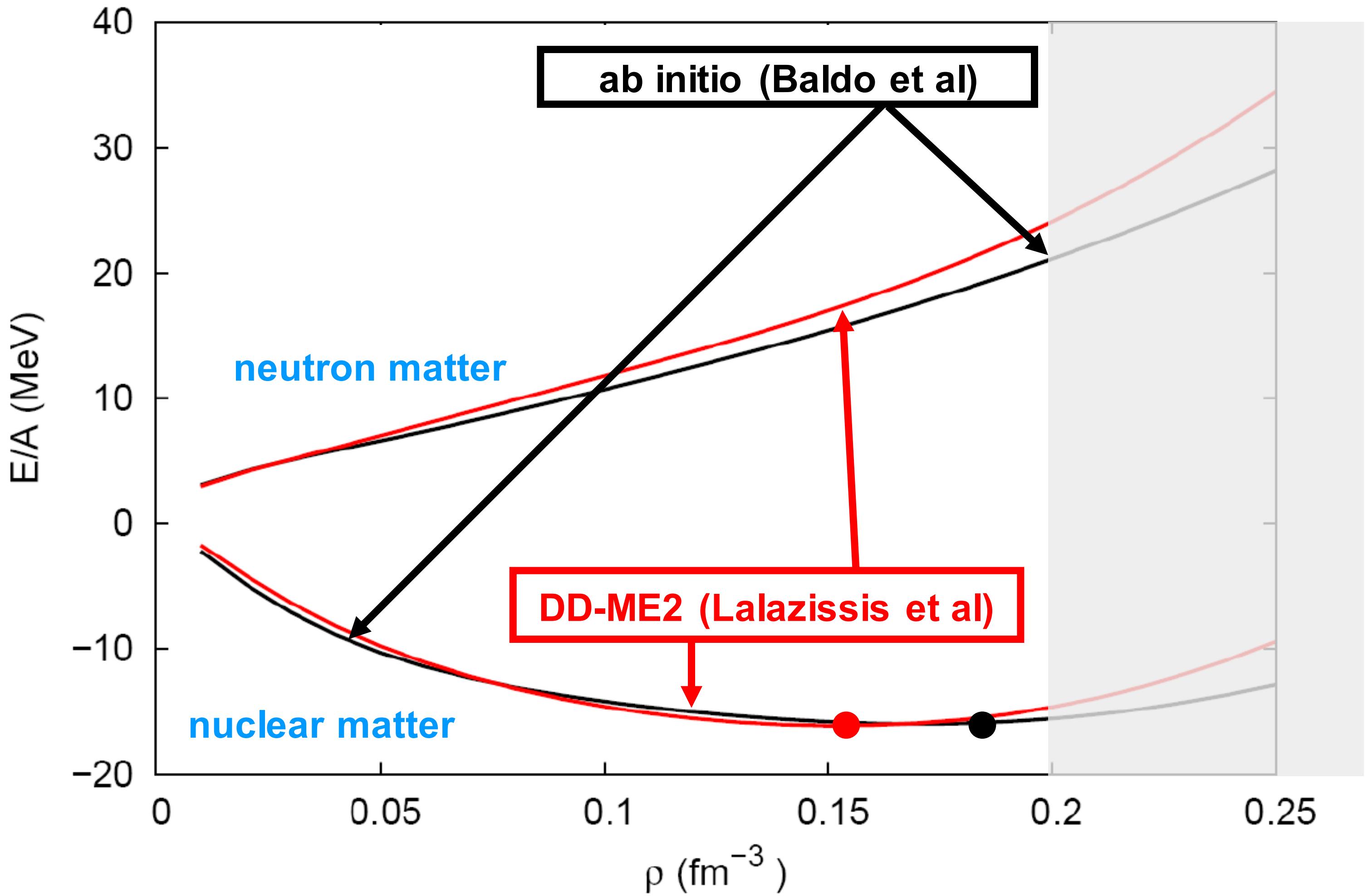
$$E[\rho] = E_\infty[\rho] + \text{gradient terms}$$

ab initio

few parameters fitted

Fayans (1998), Baldo et al (2008) (BCPM), Roca-Maza et al (2011) (DD-MEδ)

Comparison with ab initio calculations:

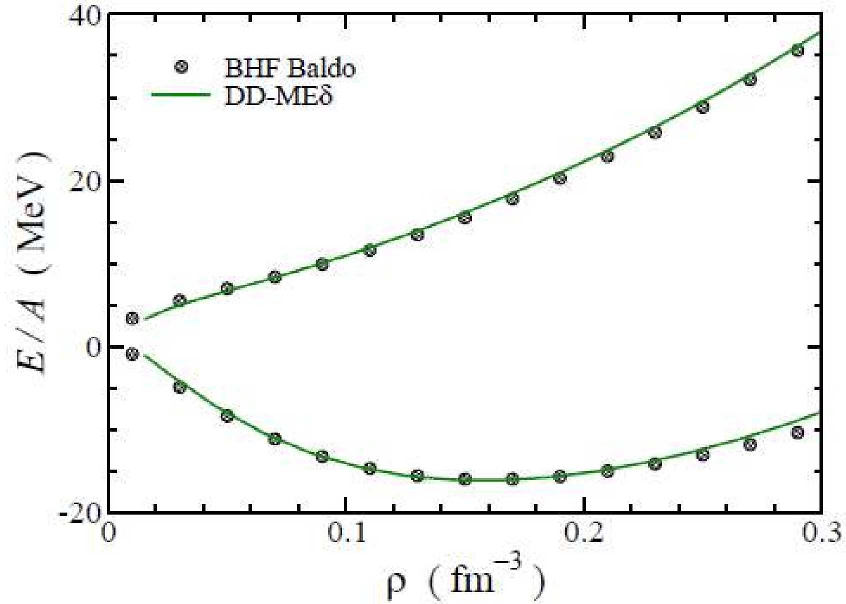


we find excellent agreement with ab initio calculations of Baldo et al.

Semi-microscopic functional with a δ-meson:

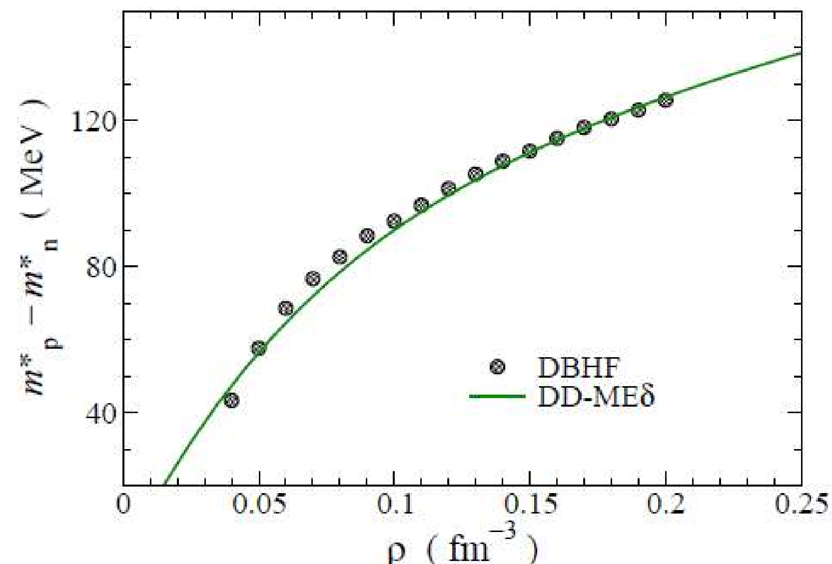
(a) The density dependence of the 4 vertices $g_i(\rho)$ ($i=\sigma,\omega,\delta,\rho$) is determined ab-initio by Brueckner $E_{SM}(\rho)$, $E_{NM}(\rho)$, $m^*_p(\rho) - m^*_n(\rho)$

(b) The 4 parameters $g_i(\rho_s)$ ($i = \sigma, \omega, \rho$) and m_σ are fitted to a set of finite nuclei



Parameter set: **DD-MEδ**

Result: the parameters of the δ-meson can be compensated completly by the parameters of the ρ-meson. They have no influence on present structure data



Roca-Maza et al (2011)

^{208}Pb

4 digits: ^{208}Pb: E=1626.690 MeV
7 digits: ^{208}Pb: E=1633.471 MeV

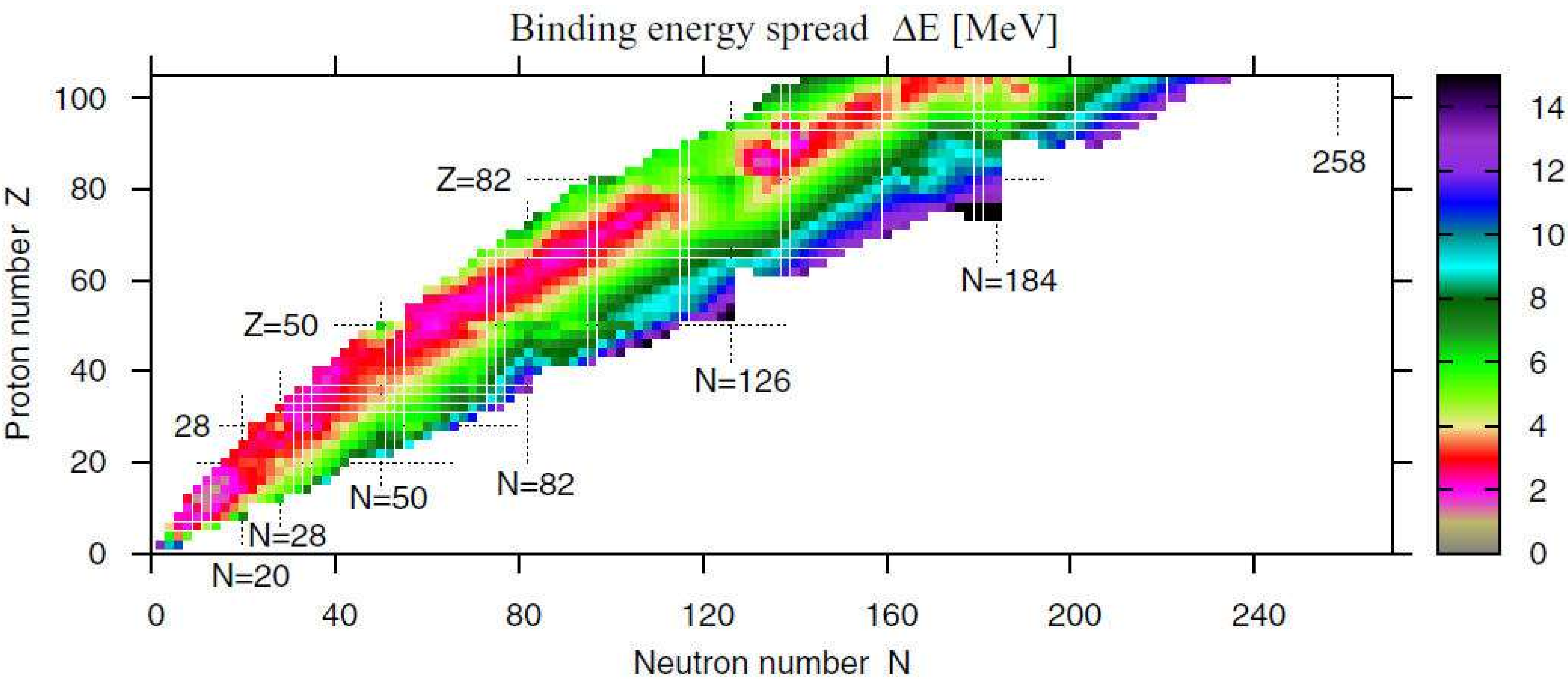
Difference **6.781 MeV**

DD-MEδ

				T=1	
E_S	=	-30.014 GeV	-100.0 %	– 0.173 GeV	(δ)
E_V	=	+24.642 GeV	+ 82.1 %	+ 0.275 GeV	(ρ)
E_C	=	+0.828 GeV	+ 0.3 %		
E_{kin}	=	+2.916 GeV	+ 9.7 %		
E_{CM}	=	-0.006 GeV	-0.02 %		
E_{tot}	**=**	**-1.633 GeV**	**- 5.4 %**		

required accuracy: 100 keV ≡ $3.3 \cdot 10^{-6}$

Binding energy spread over 4 classes of functionals: NL3*, DD-ME2, DD-MEδ, DD-PC1



Agbemava, Afanasjev, Ray, P. R., Phys. Rev. C89, 54320 (2014)

Problem

single particle energies ⟺ tensor forces

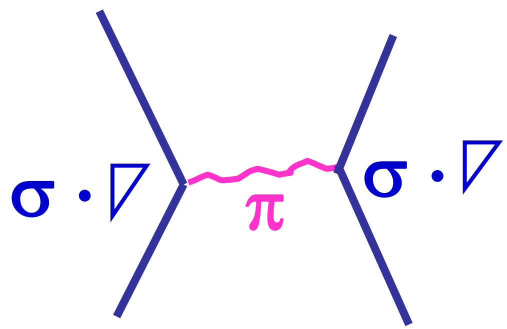
Tensor interaction by pion exchange:

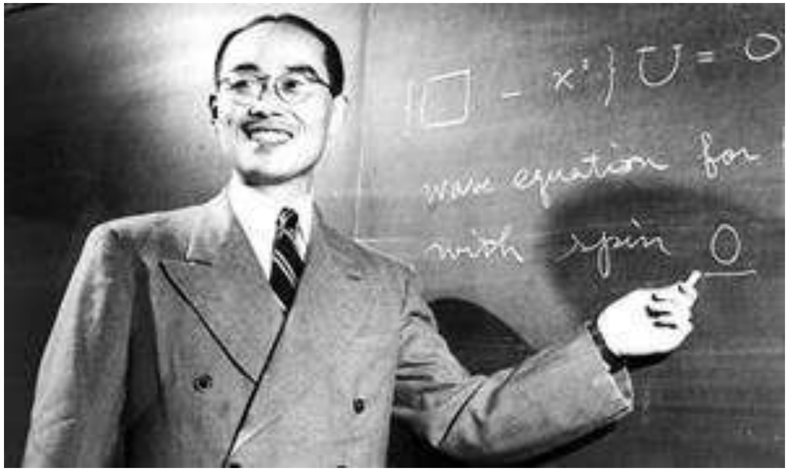
$$V_T = (\tau_1 \tau_2)\,(\,[\sigma_1 \sigma_2]^{(2)}\,Y^{(2)}(\Omega)\,)\,Z(r)$$

contributes only to **S=1** states

relative motion

π meson : primary source

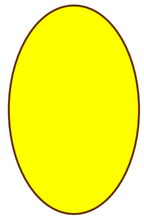




Yukawa

thanks to Takaharu Otsuka

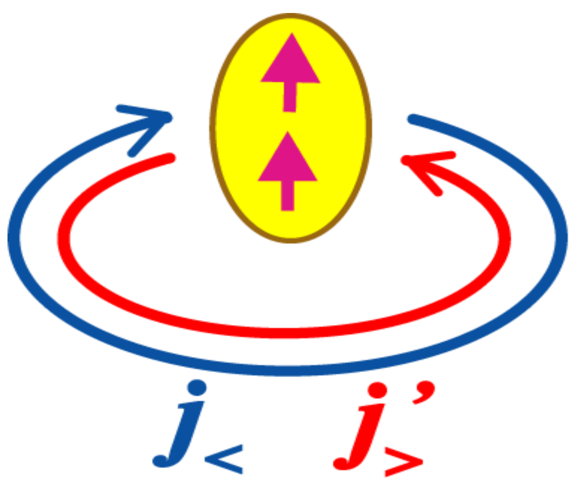
Monopole effects due to the tensor force:



wave function of relative motion

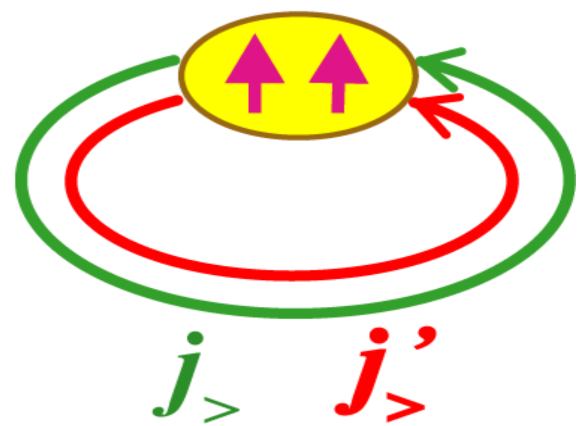
↑↑ spin of the nucleon

large relative momentum



attractive

small relative momentum



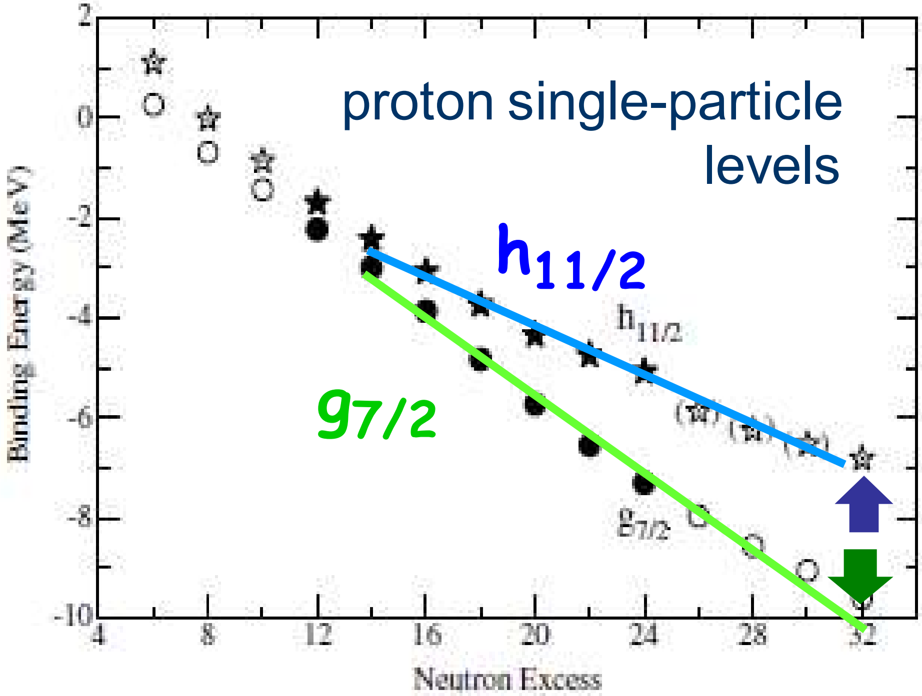
repulsive

$$j_> = \ell + \frac{1}{2}, \quad j_< = \ell - \frac{1}{2}$$

Otsuka et al, PRL 95, 232502 (2005)

An example are the Sb isotopes (Z=51):

Experiment: J. P. Schiffer et al., Phys. Rev. Lett, 92 162501, (2004)



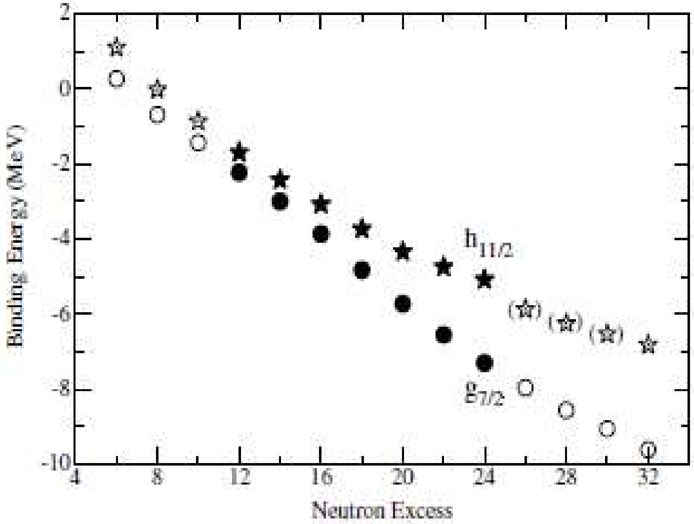
change is driven by neutrons in $1h_{11/2}$

$h_{11/2}$ - $h_{11/2}$ repulsive

$h_{11/2}$ - $g_{7/2}$ attractive

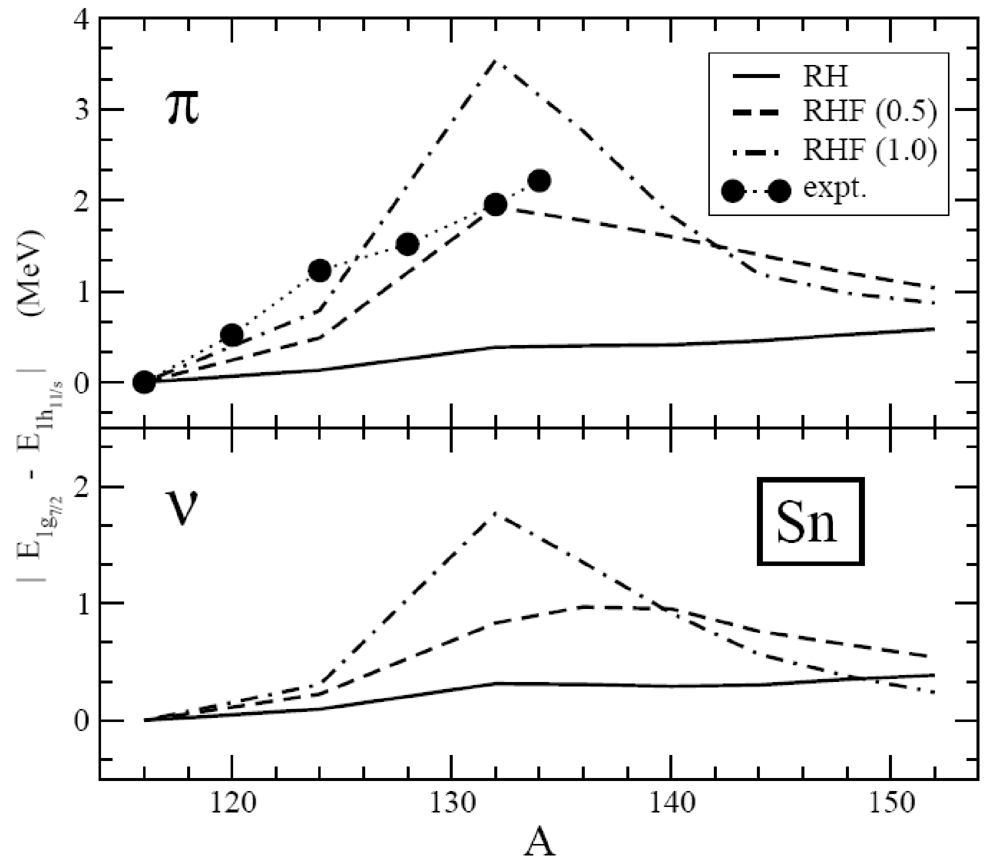
tensor force increases splitting by ~ 2 MeV

Without tensor, no EDF (Skyrme, Gogny, RMF) explains these facts.



Experiment:
J. P. Schiffer et al., Phys. Rev. Lett, 92 162501, (2004)

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

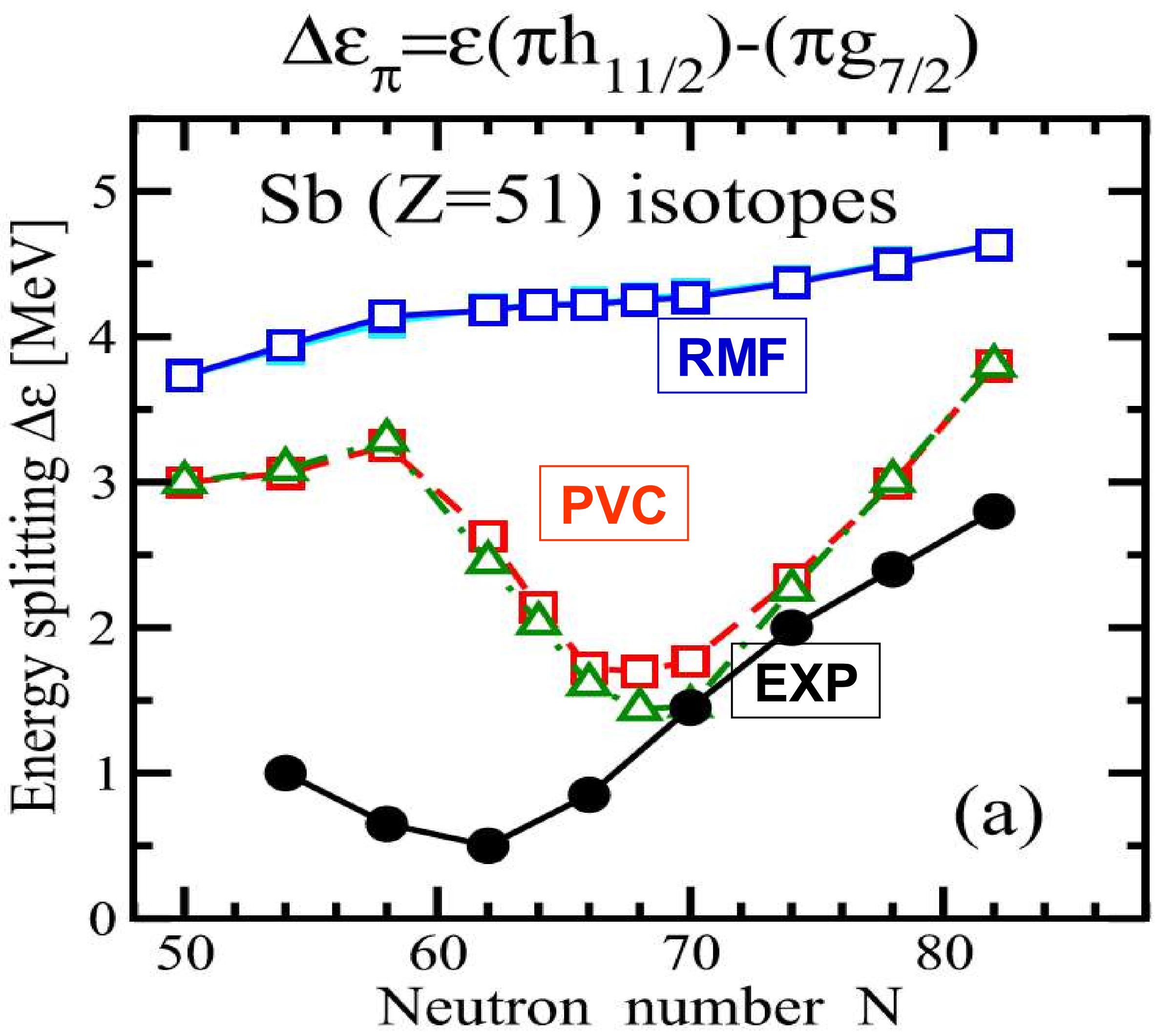


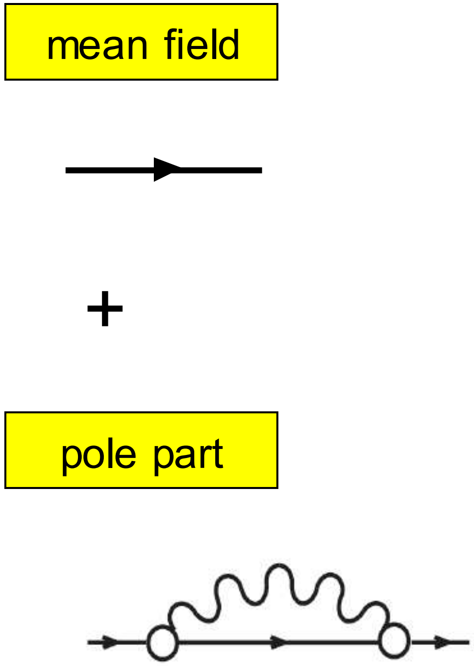
Effect of a tensor force in Relativistic Hartree-Fock

RH → RHF

Theory: Lalazissis, Karatzikos, Serra, Otsuka, P.R., Phys. Rev. C89, 041301 (2009)

Influence of Particle-Vibrational Coupling





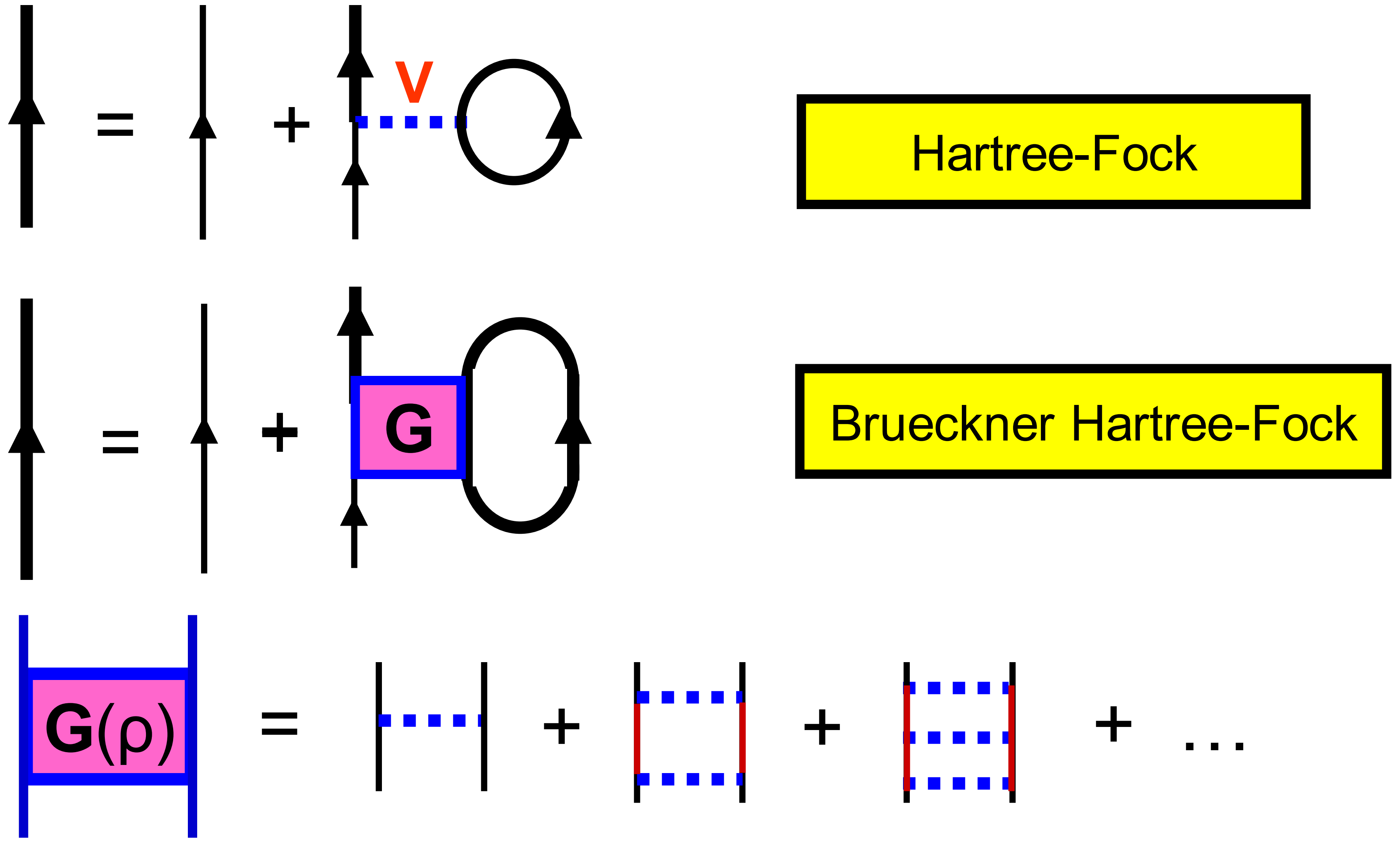
Experiment: J. P. Schiffer et al., Phys. Rev. Lett, 92 162501, (2004)
Theory: A.V. Afanasjev, E. Litvinova, Phys. Rev. C92, 044307 (2015)

- It is very difficult to determine the tensor force from experimental data.

- Can we use a microscopic input ?

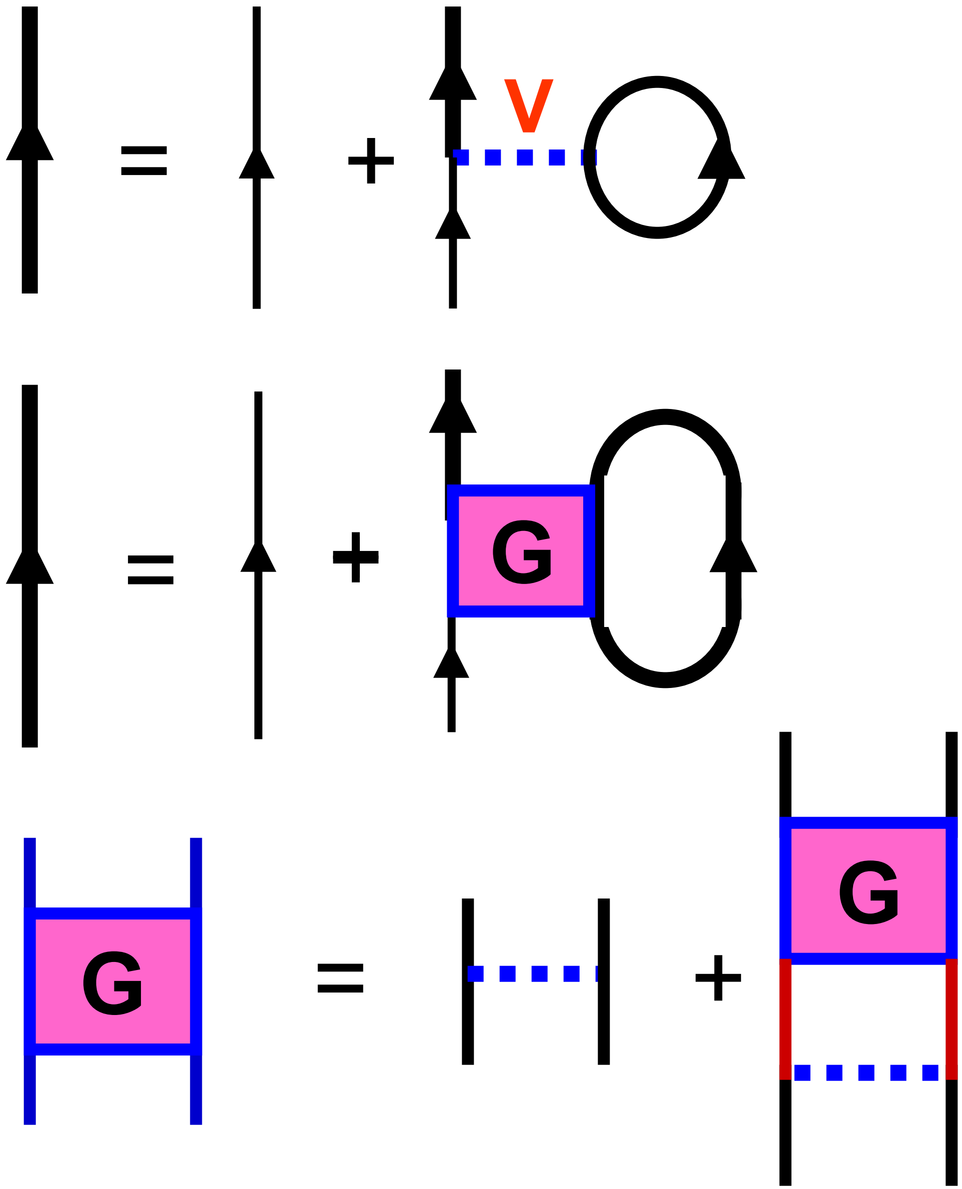
  i. e. an ab-initio derivation

Ab-initio: Relativistic Brueckner Hartree-Fock:



Summing up all ladder diagramms

Ab-initio: Relativistic Brueckner Hartree-Fock:



Hartree-Fock

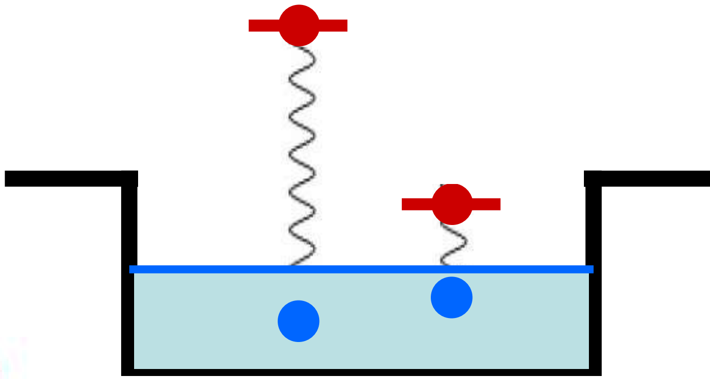
Brueckner Hartree-Fock

Bethe-Goldstone

Bethe-Goldstone equation:

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

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



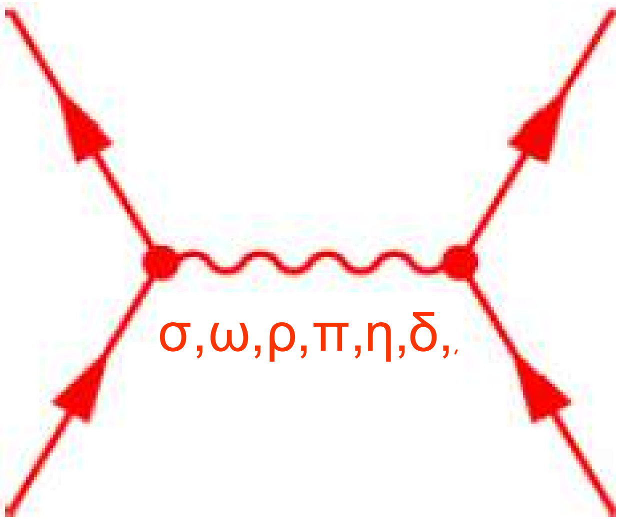
$$G(\omega) = V + V P_F(\omega) G(\omega)$$

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

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

Is solved in each step of the iteration

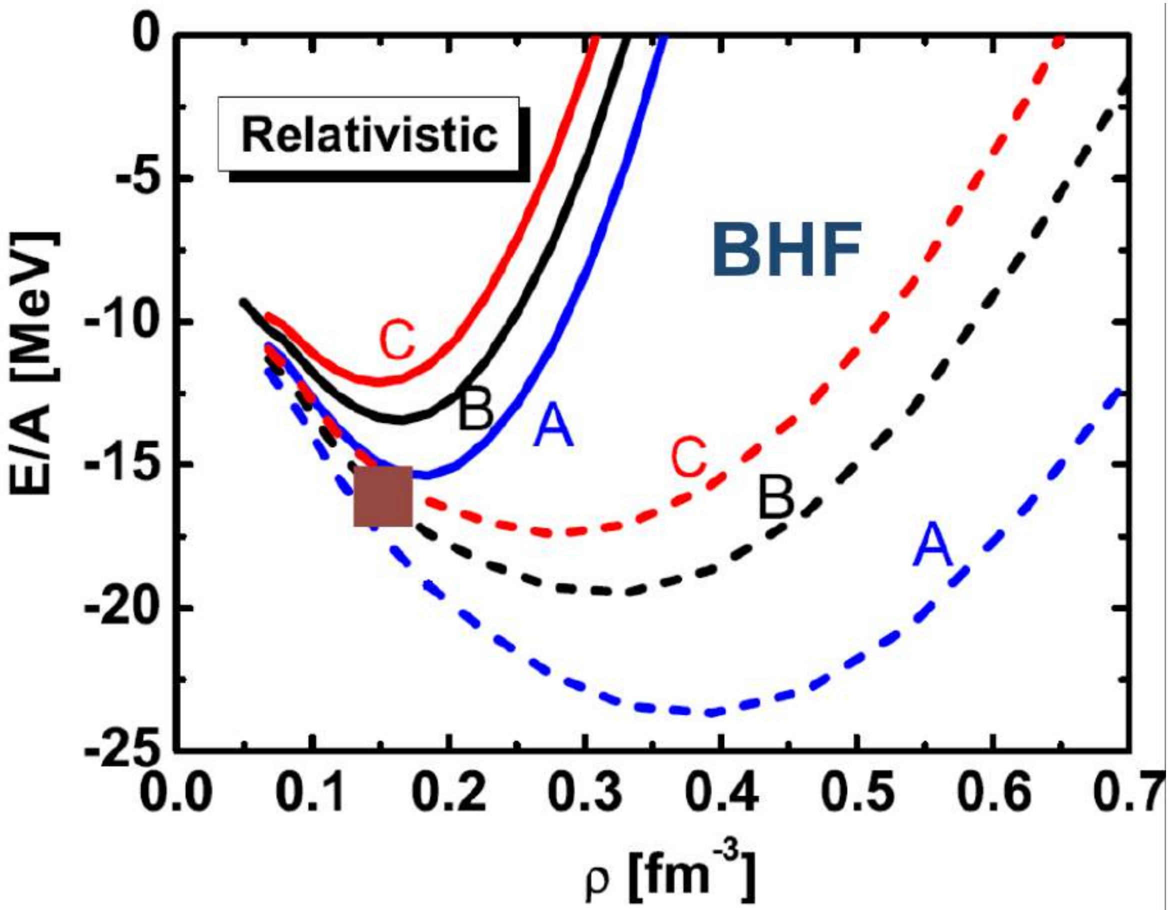
Bare nucleon-nucleon force:



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



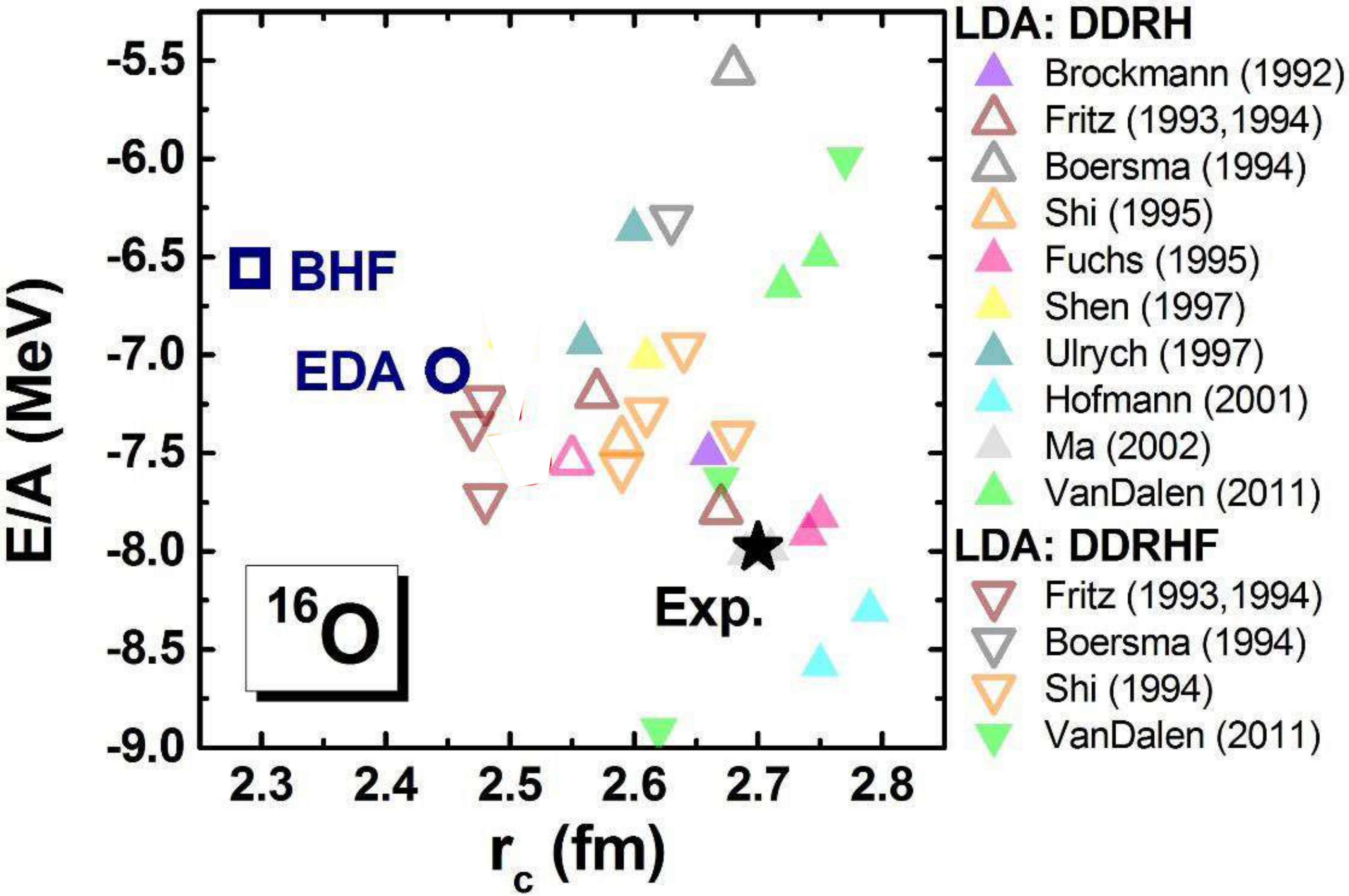
Brockmann and Machleidt, PRC **42**, 1965 (1990).

Local density approximation (LDA):

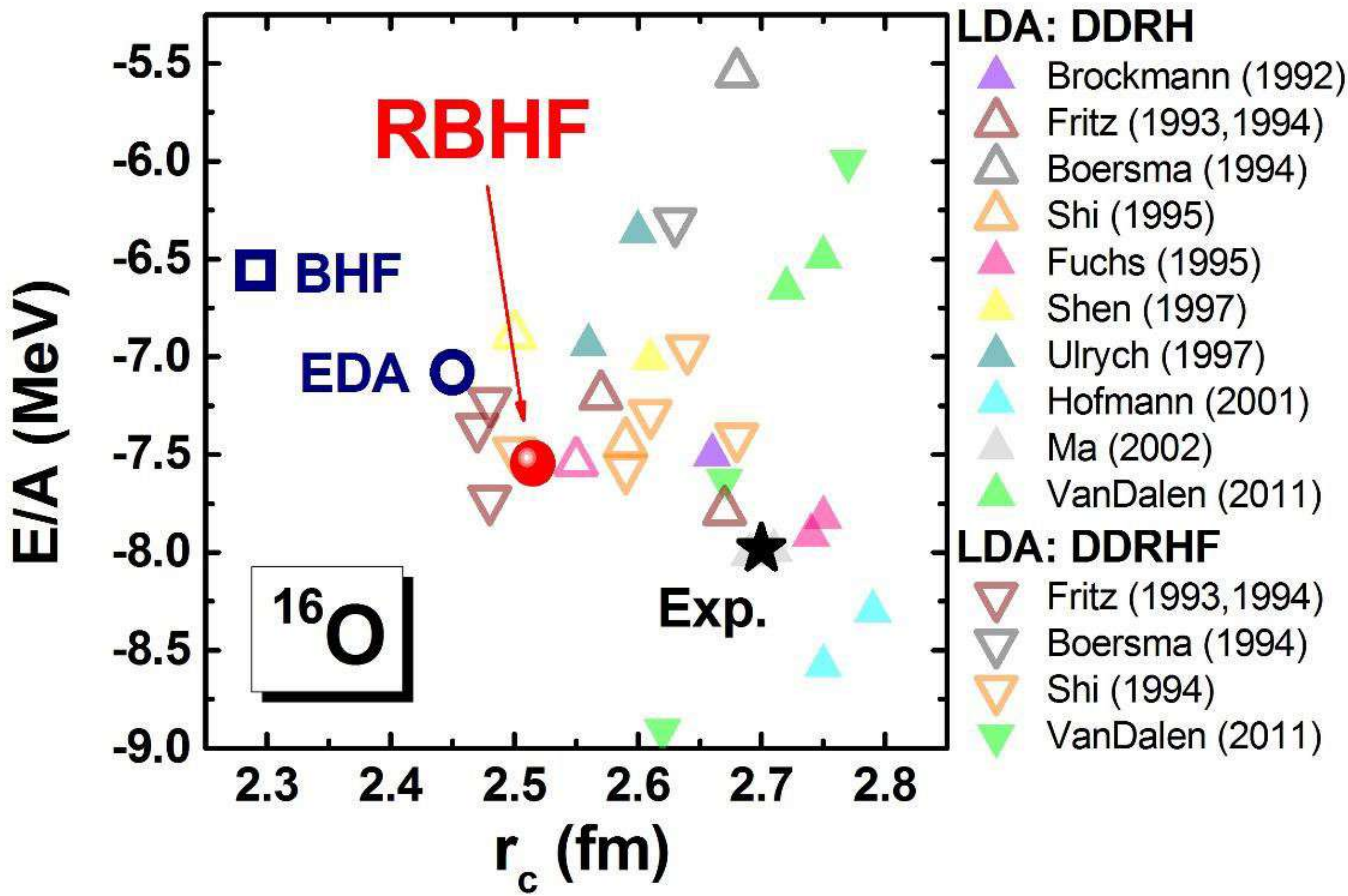
1. solve the Brueckner-Hartree-Fock equations in nuclear matter at various densities ρ
2. map the density dependent results on a Walecka model with density dependent couplings
3. this yields → $g_\sigma(\rho), g_\omega(\rho), \ldots$
4. but: this mapping is not unique !

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

Relativistic BHf for finite nuclei:



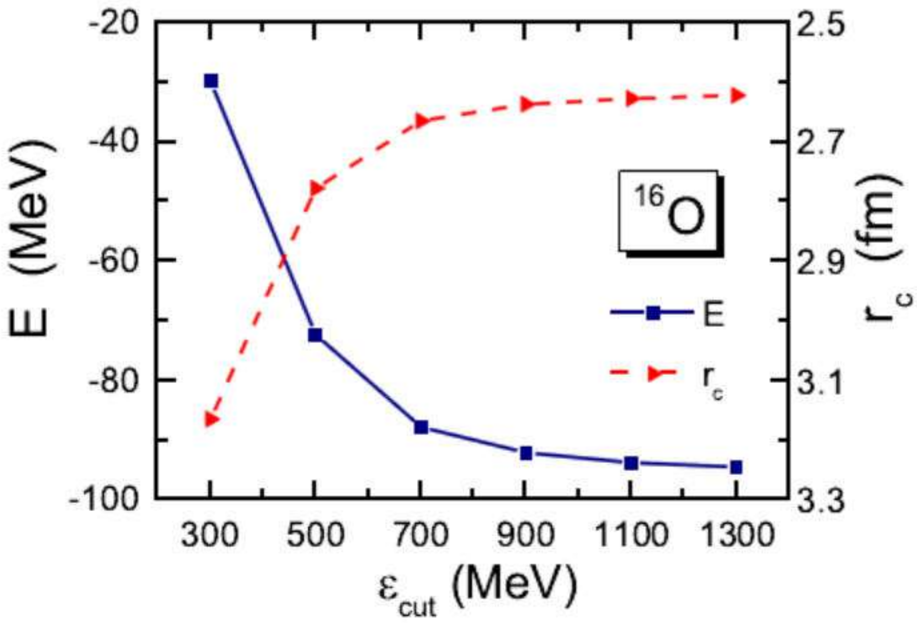
Relativistic BHf for finite nuclei:

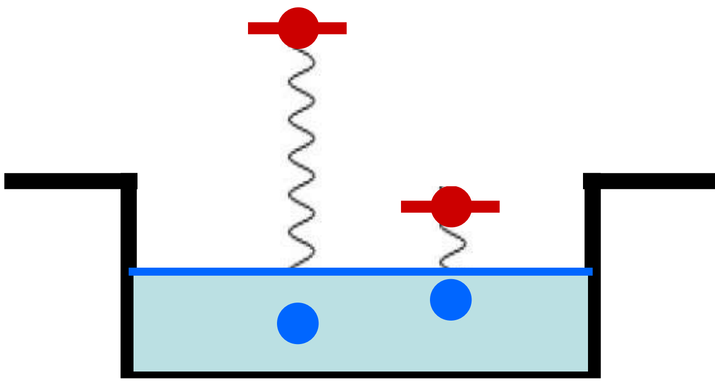


Results for ^{16}O

S.H. Shen et al, PRC 96, 014316 (2017)

Convergenge with the cuf-off in single particle energy:

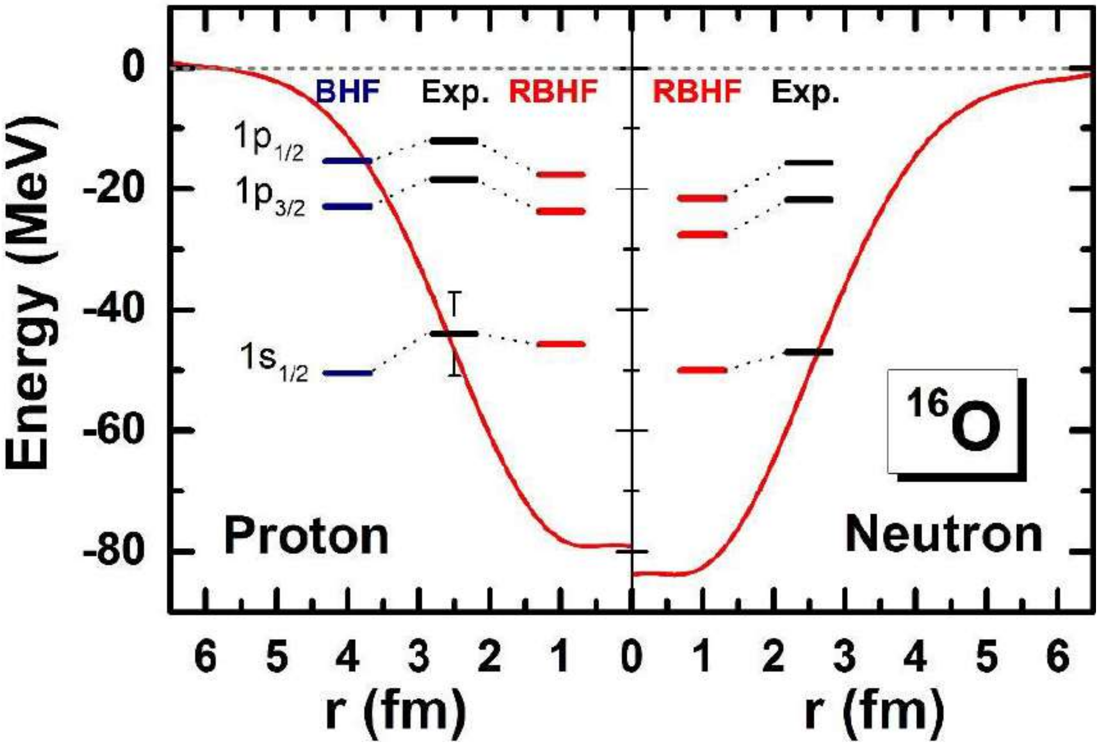




Results for ^{16}O:

	E (MeV)	r_c (fm)	r_m (fm)	$\Delta E^{ls}_{\pi 1p}$ (MeV)	
Exp.	−127.6	2.70	2.54	6.3	
DDRHF, PKO1	−128.3	2.68	2.54	6.4	Long et al, (2006)
DDRHF, PKA1	−127.0	2.80	2.67	6.0	Long et al, (2007)
RBHF, Bonn A	**−120.2**	**2.53**	**2.39**	**5.3**	
RBHF (DWS)	−120.7	2.52	2.38	6.0	
BHF, AV18	−134.2	–	1.95	13.0	Hu et al, (2017)
CC, N^3LO	−120.9	–	2.30	–	Hagen et al, (2009)
IM-SRG, N^3LO	−122.9	–	–	–	Hergert et al, (2013)
NCSM, N^3LO	−119.7	–	–	–	Roth et al, (2011)
SCGF, N^3LO	−122.0	–	–	–	Cipollone et al, (2013)
NLEFT, N^2LO	−121.4	–	–	–	Laehde et al, (2014)
QMC, N^2LO	−87.0	2.76	–	–	Lonardoni et el, (2018)

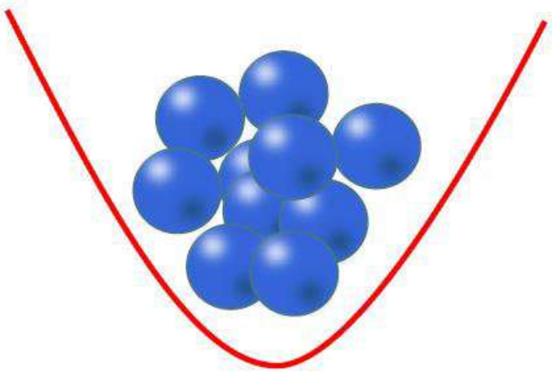
Single particle spectrum:



Shen, Hu, HZL, Meng, Ring, Zhang, *Chin. Phys. Lett.* **33**, 102103 (2016)

- a first *ab initio* calculations for finite nuclei in the **relativistic** scheme
- **Spin-orbit** splitting is reproduced well from the bare interaction
- **benchmark** for various LDA calculations

Neutron drops:



A neutron drop is a multi-neutron system confined in an external field.

Why neutron drops?

- simple, can be accessed by many ab initio methods
- an ideal environment for studying neutron rich system

Pudliner et al., *PRL* **76**, 2416 (1996)
Gandolfi, Carlson, Pieper, *PRL* **106**, 012501 (2011)
Maris et al., *PRC* **87**, 054318 (2013)
Potter et al., *PLB* **739**, 445 (2014)
Zhao & Gandolfi, *PRC* **94**, 041302(R) (2016)
……

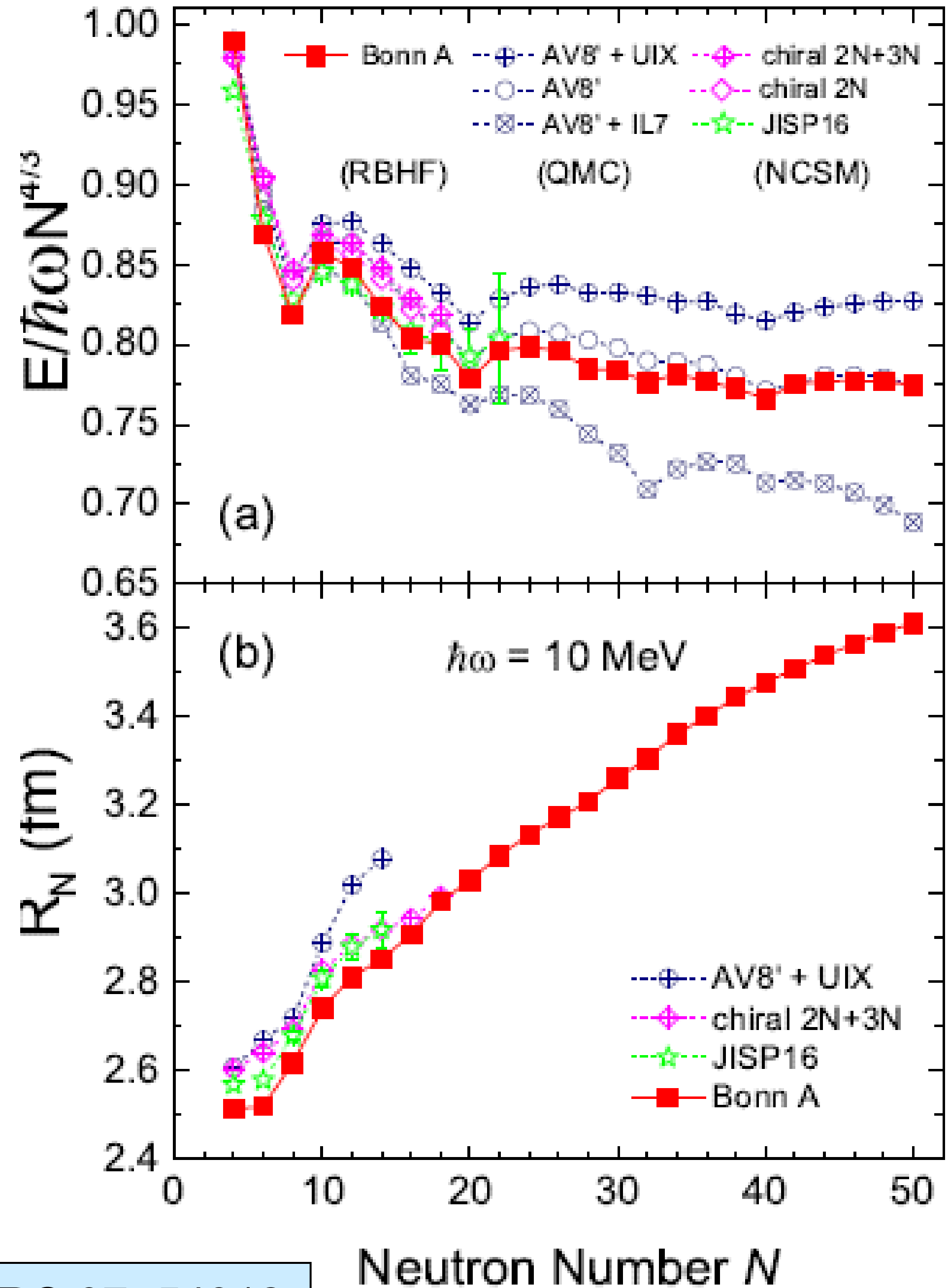
- Relativistic Hartree-Fock (RHF) equation with **external field**

$$(T + U + U_{\rm ex})|a\rangle = e_a|a\rangle, \qquad U_{ij} = \sum_{c=1}^{A} \langle ic|\bar{G}(W)|jc\rangle$$

Neutron drops:

Binding energy:

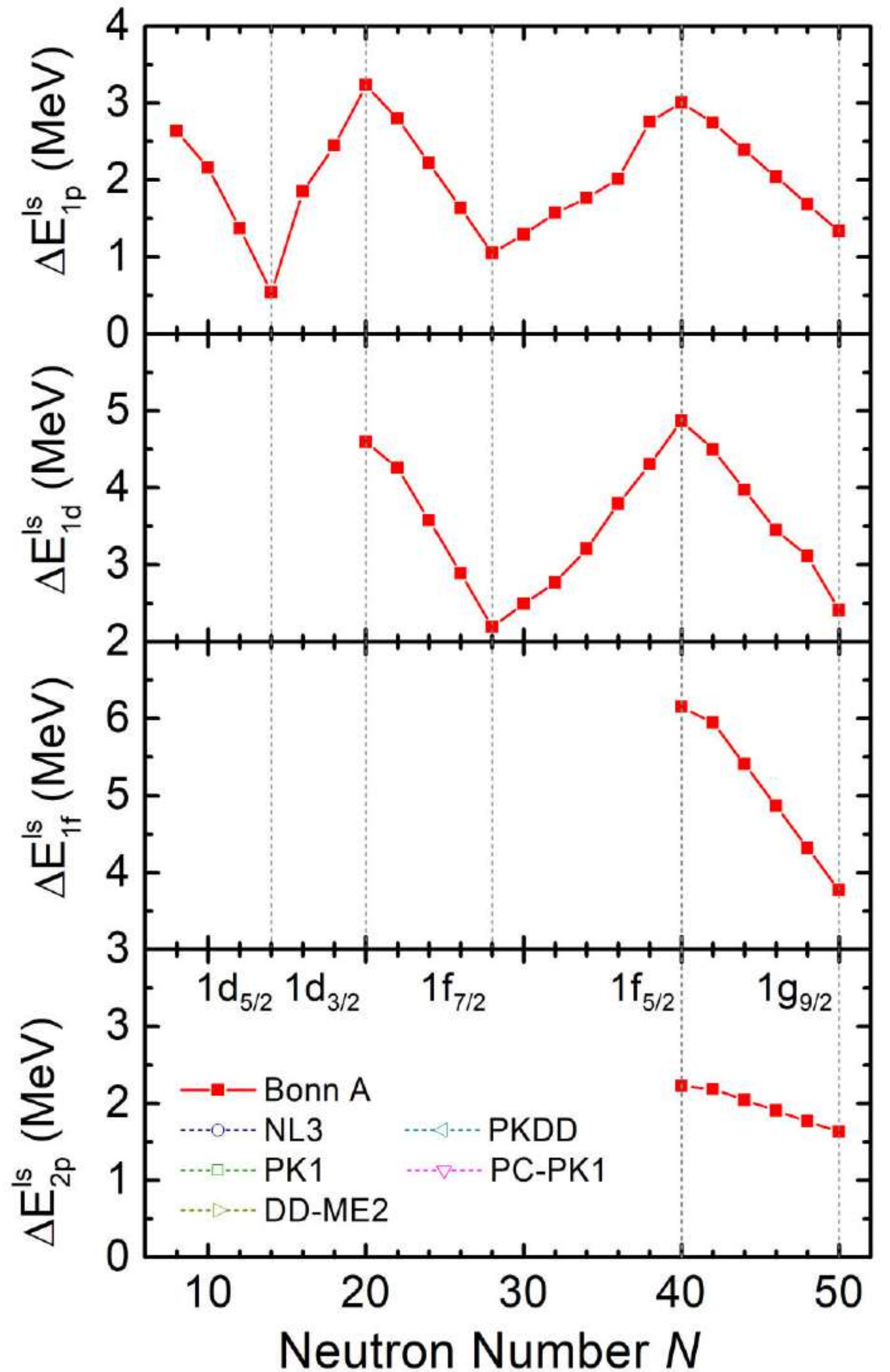
Radius:



Shen, Liang, Meng, PR, Zhang, PRC 97, 54312

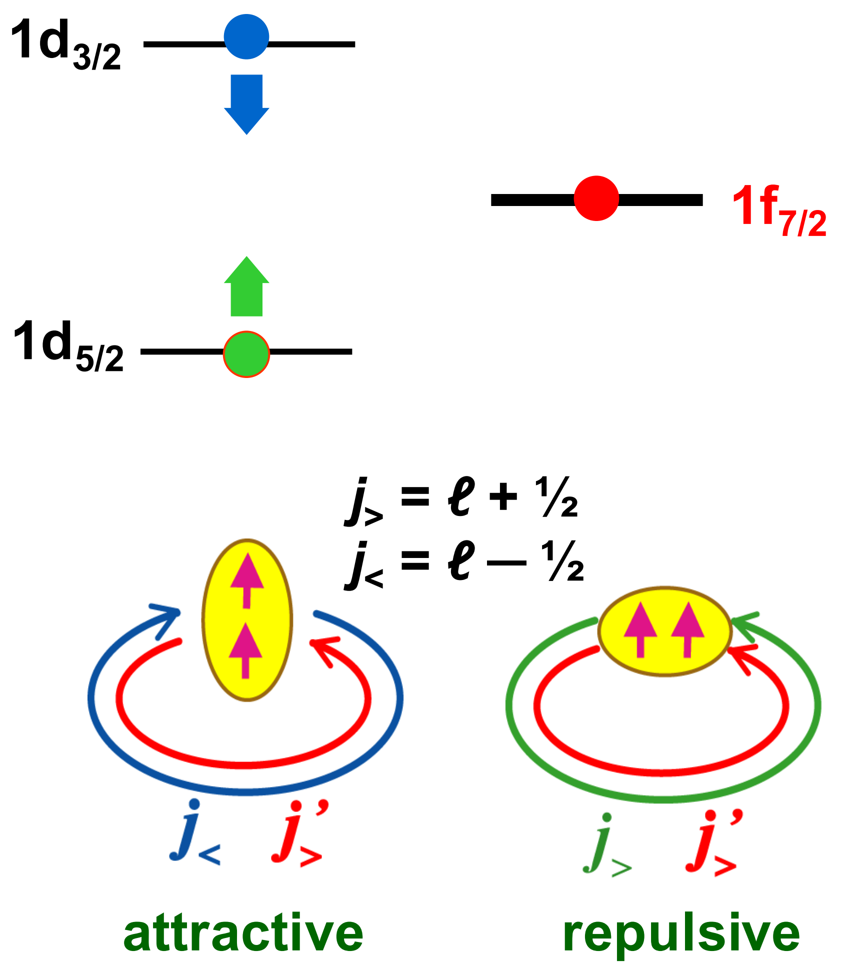
Spin-orbit splitting in neutron drops:

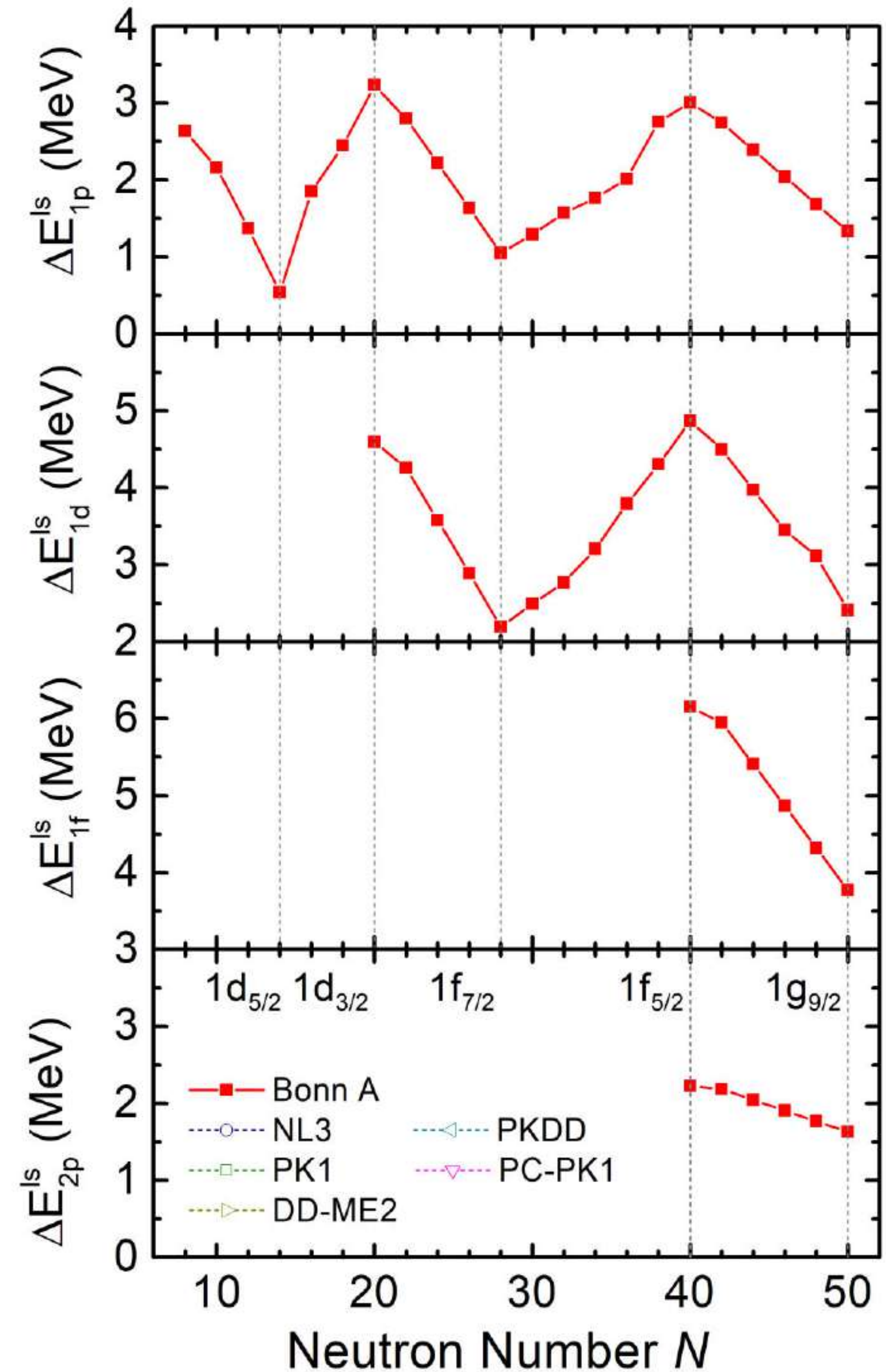
full relativistic BHF



Shen et al, PLB 778, 344 (2018)

Spin-orbit splitting in neutron drops:

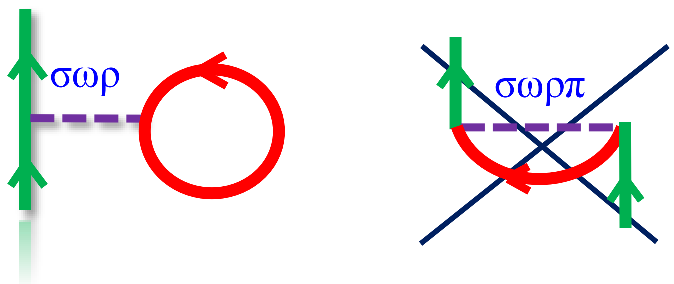


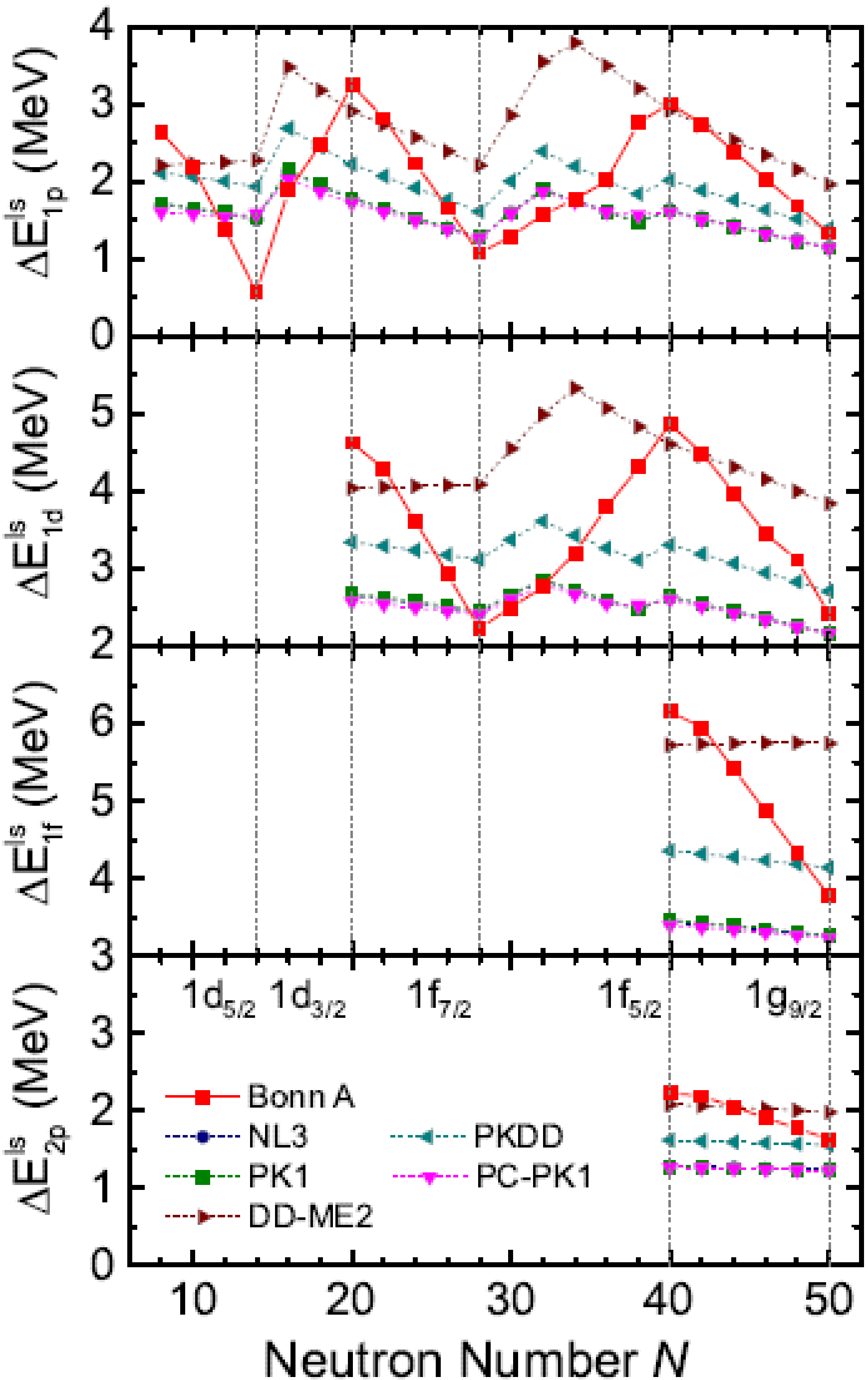


Otsuka *et al.*, PRL 95, 232502 (2005)

Spin-orbit splitting in neutron drops:

- Comparison with **phenomenological** relativistic mean-field (**RMF**) density functionals.



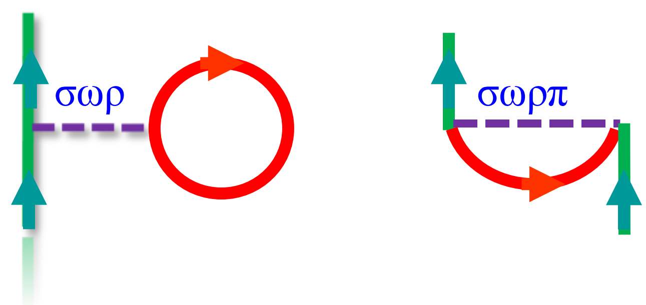


☐ **None of them can reproduce this tensor behavior!**

Shen et al, PLB 778, 344 (2018)

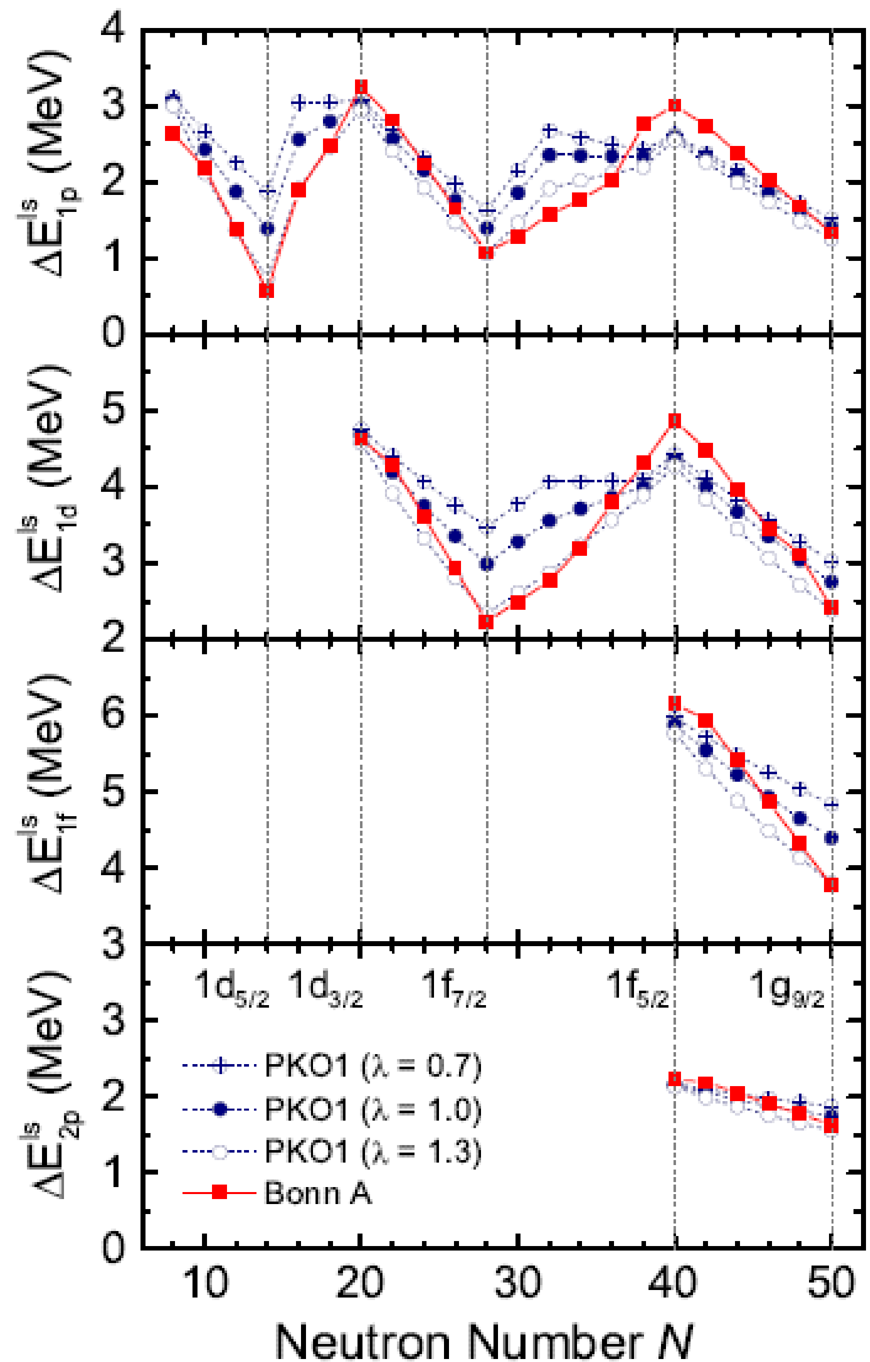
Effect of tensor force in covariant DFT

- Comparison with **phenomenological** relativistic Hartree-Fock (**RHF**) density functionals.



- **RHF** (PKO1)shows the same pattern, due to the ***π*NN tensor interaction**.
- Neither RBHF nor CDFT includes **beyond-mean-field effects**

➔ **it is a fair comparison!**



Conclusions

- Covariant DFT is very successful (8-10 parameters)
- Semi-microscopic with only 4 parameters uses microscopic input from nuclear matter
- 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) RBHF in local density approximation not unique
  b) RBHF fully self-consistent,
  c) neutron drops shows the influence of tensor force

How to improve the results?

- Other relativistic NN-forces ?
- Relativistic NNN-forces ?
- Extended Brueckner theory (3 hole lines …)?
- …

Outlook for the future:

- simplify the calculations:

  Brueckner theory with renormalized forces ($V_{low\ k}$) …

  Local density approximation under control
- heavy nuclei and the tensor force
- open shell nuclei: pairing, deformation
- optical potential
- short range correlations

Thanks to my collaborators:

Shihang Shen (Beijing)
Jie Meng (Beijing)
S.Q. Zhang (Beijing)
Haozhao Liang (RIKEN)

X.L. Ren (Beijing)
K.W. Li (Beijing)
B.W. Long (Beijing)
L.S. Geng (Beijing)

M. Serra†
S. Karatzikos (Thessaloniki)
G. A. Lalazissis (Thessaloniki)
T. Otsuka (Tokyo)

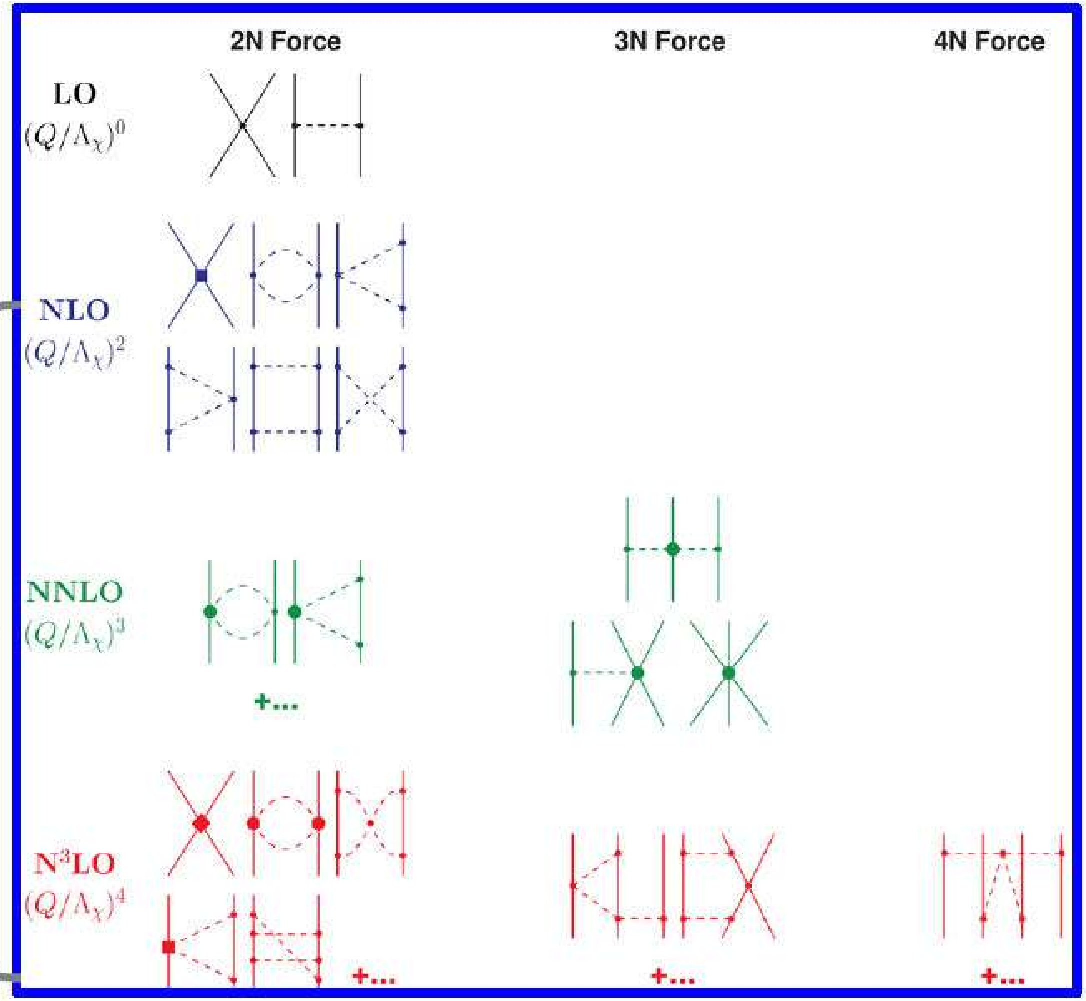
A. Afanasjev (Mississippi)
X. Roca Maza (Milano)
X. Vinas (Barcelona)
P. Schuck (Orsay)

Hierarchy of chiral nuclear force

$$V = V_{2N}^{\mathrm{LO}}$$

High order contributions

Not included at present



R.Machleidt, Phys.Rept.503(2011)1

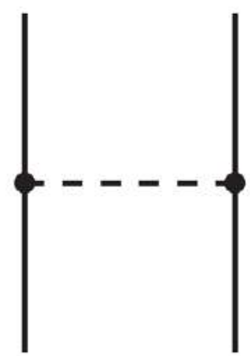
Xiulei Ren, Kaiwen Li, Bingwei Long, Lisheng Geng, P.R., Jie. Meng

A relativistic version of chiral perturbation theory:

$$V = V_{2N}^{\mathrm{LO}}$$

$$= V_{\mathrm{CTP}} + V_{\mathrm{OPEP}}$$

Contact Potential (CTP)



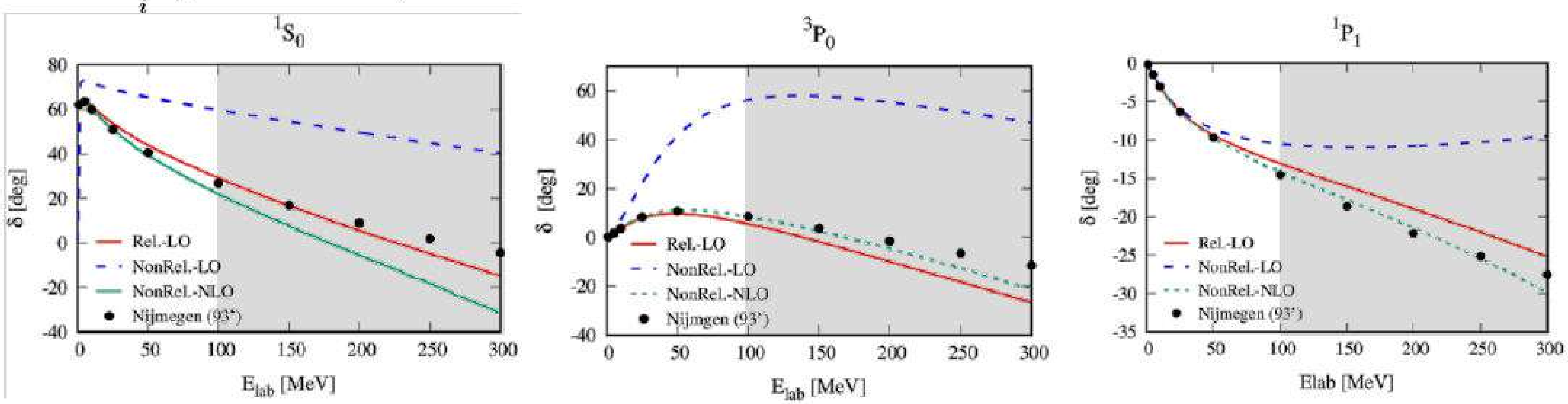
One-Pion Exchange Potential (OPEP)

A relativistic version of chiral perturbation theory:

	Relativistic Chiral NF	**Non-relativistic Chiral NF**	
Chiral order	LO	LO	NLO*
No. of LECs	5	2	9
$\tilde{\chi}^2$/d.o.f.	**2.9**	**147.9**	**2.5**

$$\tilde{\chi}^2 = \sum_i \left(\delta_i^{\text{Theory}} - \delta_i^{\text{Nij93}}\right)^2 .$$

*E. Epelbaum, et. al., NPA(2000)



- Relativistic chiral NF at LO **can be comparable with** the nonrelativistic case up to NLO
- Relativistic chiral NF provides a **more efficient description** of the phase shifts.

Xiulei Ren, Kaiwen Li, Bingwei Long, Lisheng Geng, P.R., Jie Meng, arXiv:1611.04875