

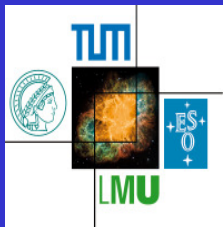
On the way to an *ab-initio* derivation of Covariant Density Functional Theory and Relativistic Brueckner-Hartree-Fock Theory in Finite Nuclei

RIKEN, June 11, 2014

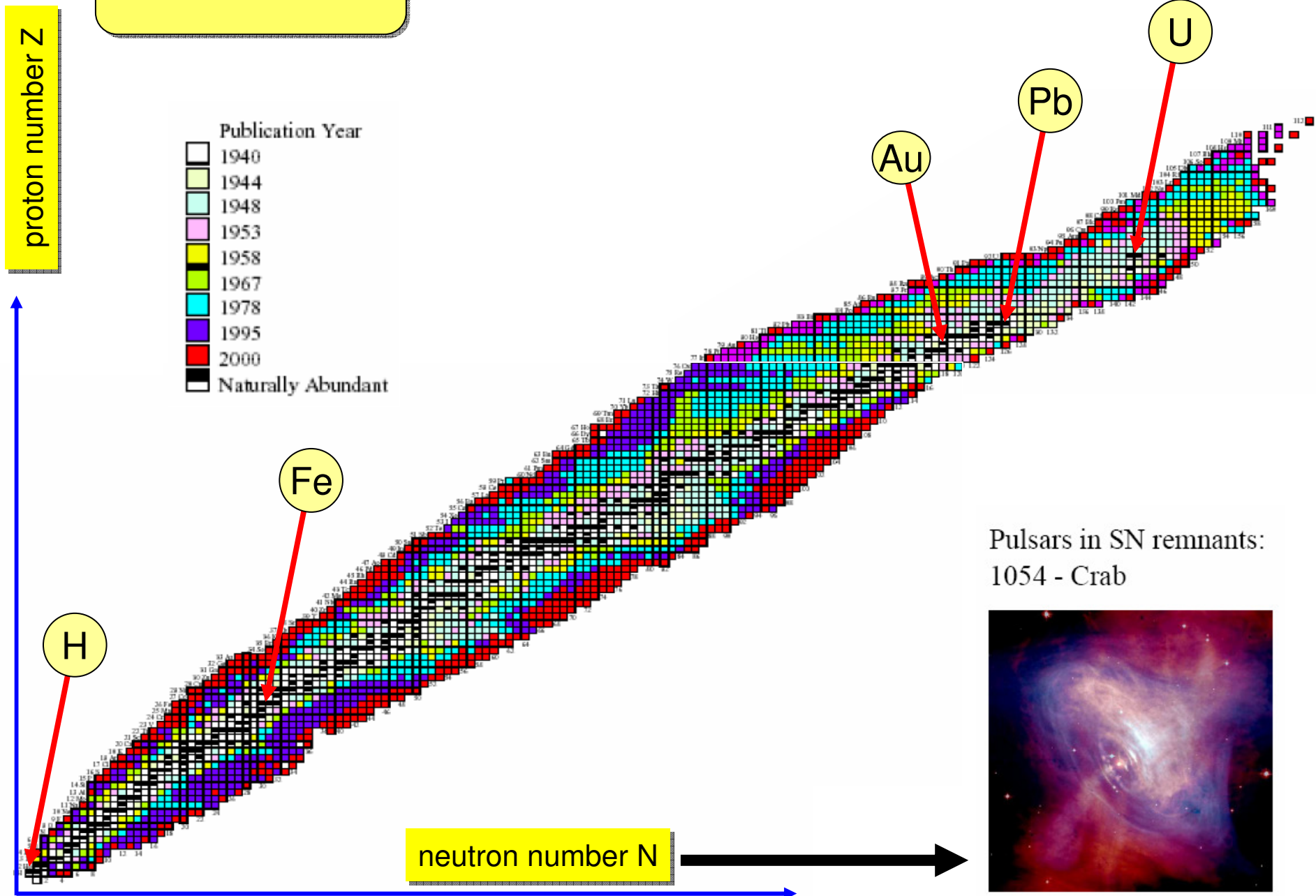
Peter Ring

Technical University Munich
Excellence Cluster “Origin of the Universe”
Peking University

Collaborators: Jinniu Hu, Jie Meng



Motivation:



Density functional theory (DFT) for manybody quantum systems

The manybody problem is mapped onto a one-body problem:

Density functional theory starts from the

Hohenberg-Kohn theorem:

„The exact ground state energy $E[\rho]$ is a universal functional for the local density $\rho(\mathbf{r})$ “

Kohn-Sham theory starts

with a density dependent self-energy:

and the single particle equation:

with the exact density:

$$\begin{aligned} h(\mathbf{r}) &= \frac{\delta E[\rho]}{\delta \rho(\mathbf{r})} \\ h(\mathbf{r})|\varphi_i\rangle &= \varepsilon_i|\varphi_i\rangle \\ \rho(\mathbf{r}) &= \sum_i^A |\varphi_i(\mathbf{r})|^2 \end{aligned}$$

In Coulombic systems the functional is derived *ab initio*

Content:

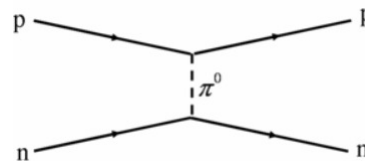
- **Motivation**
- **Early ideas to the ab-initio problem (1956/57)**
- **Brueckner-Hartree-Fock as the mother of nuclear DFT**
- **Covariant DFT and new semi-microscopic versions**
- **Ab-initio theory of pairing ?**
- **The problem of the tensor force**
- **Dirac-Brueckner-HF in finite nuclei,
first applications in light nuclei**
- **Open questions and list of wishes**

Early ideas to ab initio theories in nuclei.

What was known in 1954 ?

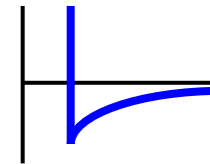
- The nucleus consists of **protons and neutrons** interacting by the **strong force**:

meson exchange:



Yukawa 1935

hard core at short distances

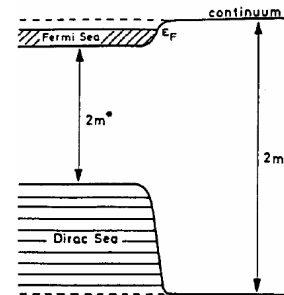


- Saturation** properties (Bethe-Weizsaecker)
- Shell structure** (Goeppert-Mayer, Jensen 1948) with very large **spin-orbit**
- Hartree-Fock does not work !
- Odd-even** staggering,
- Moments of inertia** in rotational bands too small (Inglis)

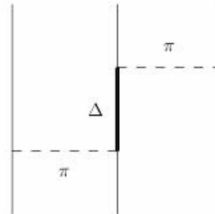
New ideas around 1956/1957:

- Bethe-Goldstone-Brueckner (1957):
the **effective interaction G** within the nucleus is very weak

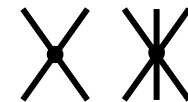
- Dürr-Teller (1956):
relativistic single particle model:



- Fujita Miyazawa (1957):
three-body force:

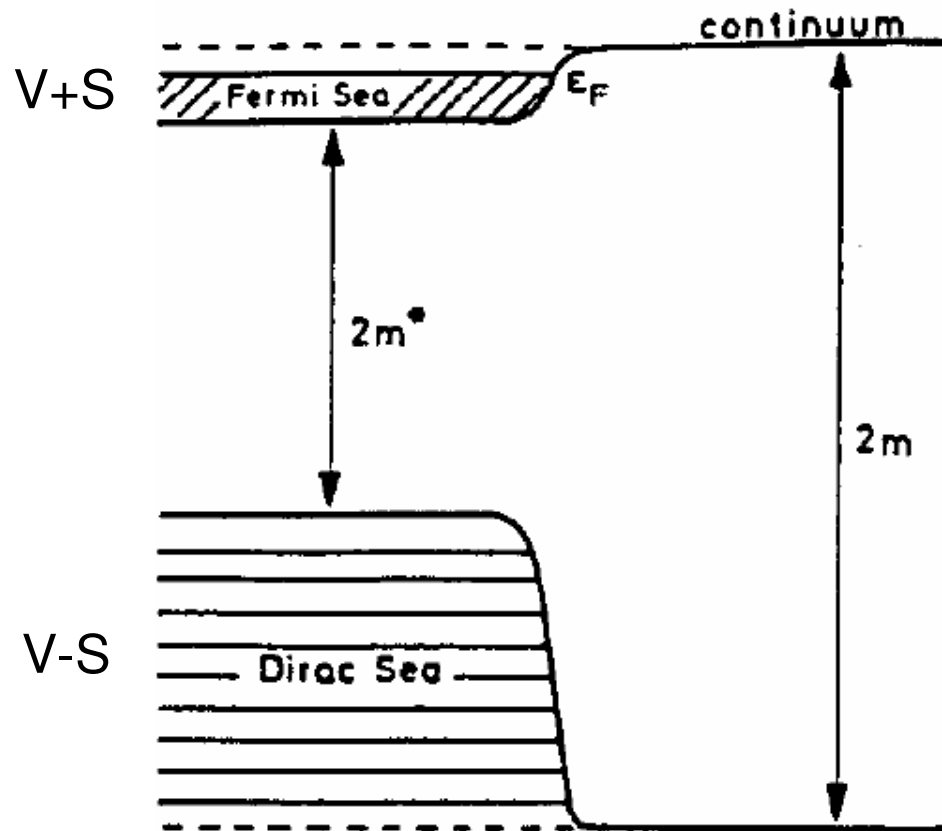


- Skyrme (1957):
model with **zero range**: twobody, threebody, tensor



- Arima & Horie (1954): first configuration mixing calculations
- BCS (1957).

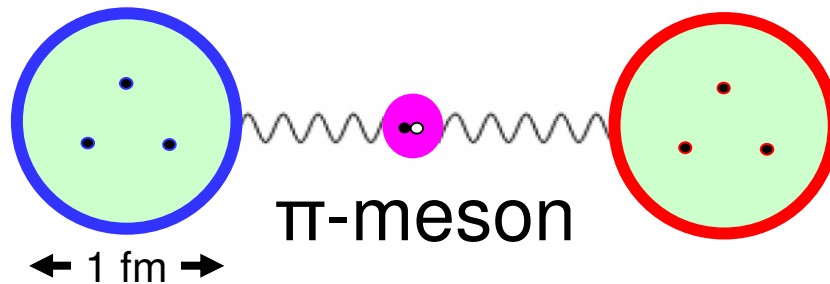
Relativistic model of Duerr and Teller (1956):



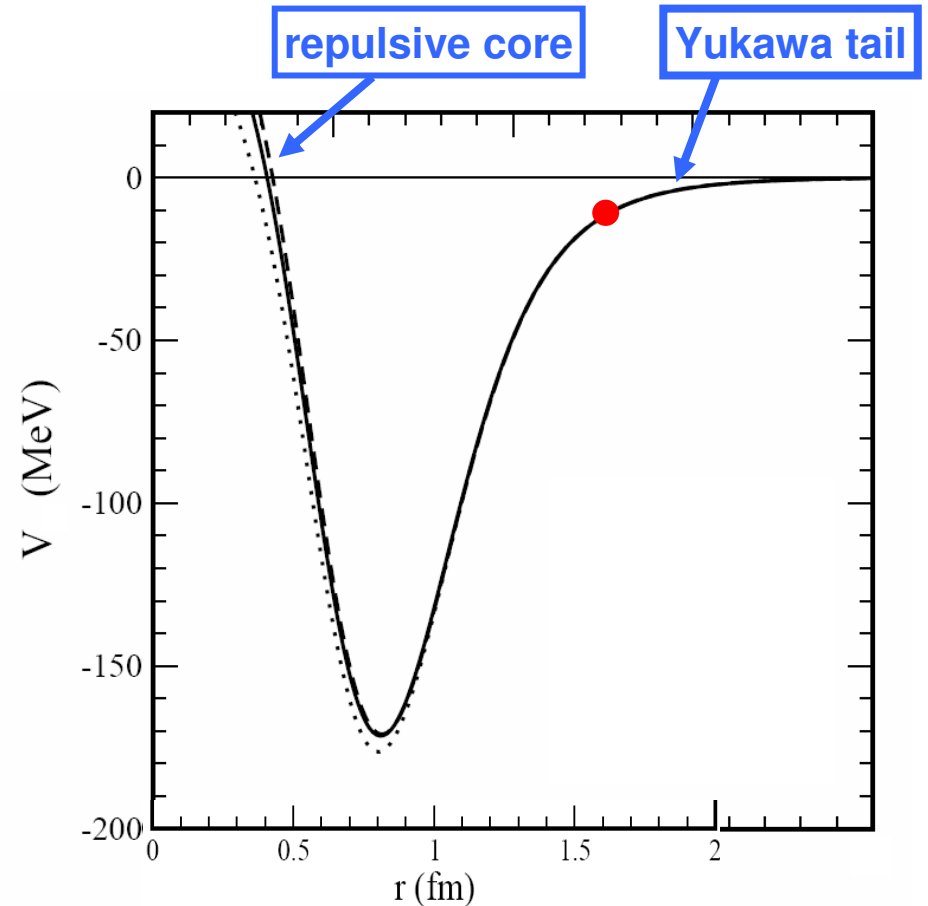
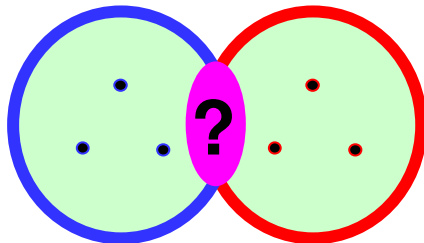
Large **scalar** field (attractive)
Large **vector** field (repulsive)
Rel. **saturation** mechanism
Shallow potential
Non-relativistic kinematics
Large **Spin-orbit** term

The bare nucleon-nucleon interaction:

distance > 1 fm: attractive



distance < 0.8 fm: repulsive

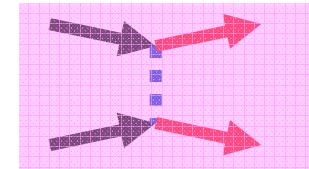
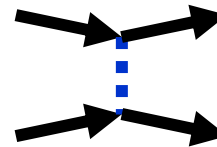


Three-body forces

Brueckner theory (1958):

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

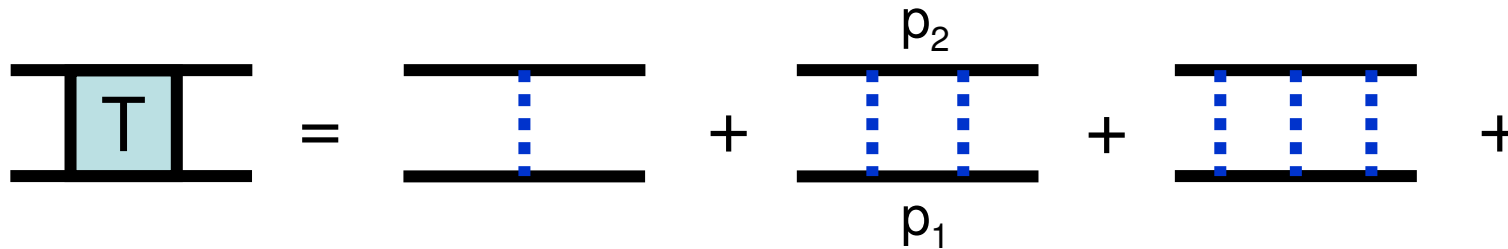
- The nucleons in the interior of the nuclear medium do not feel the same **bare force V** , as the nucleons feel in free space.
- They feel an **effective force G** .
- The **Pauli principle** prohibits the scattering into states, which are already occupied in the medium.
- Therefore this force **$G(\rho)$** 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:

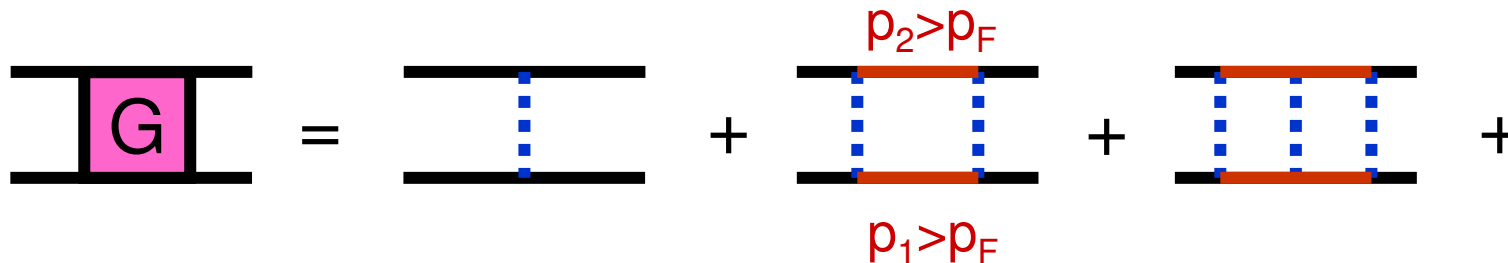
Lippmann-Schwinger-Eq.

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



Scattering in the nuclear medium:

Bethe-Goldstone-Eq.



Ab initio in nuclear matter:

- Variational method:
- Greens function:
- Chiral perturbation theory:
- Quantum Monte Carlo
- Brueckner theory:

Akmal PRC 1998

Dickhoff PPNP 2004

Kaiser NPA 2002

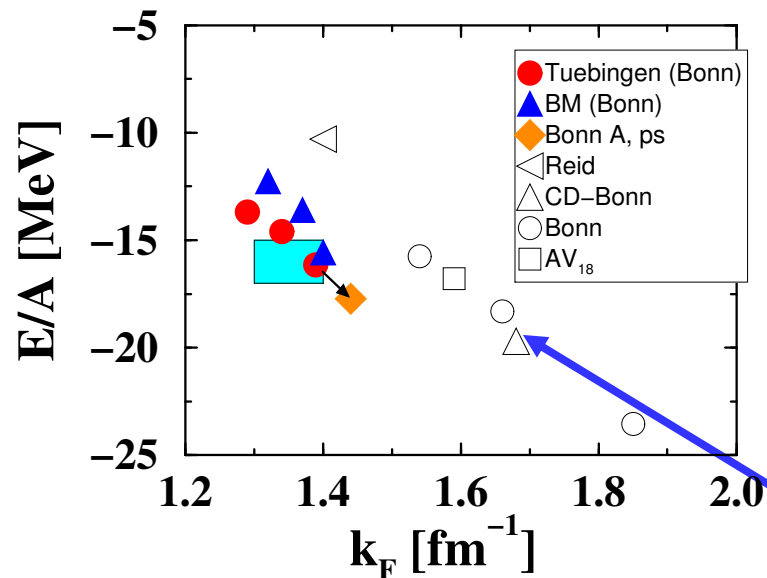
Gandolfi arXiv 2014

Baldo RPP 2012

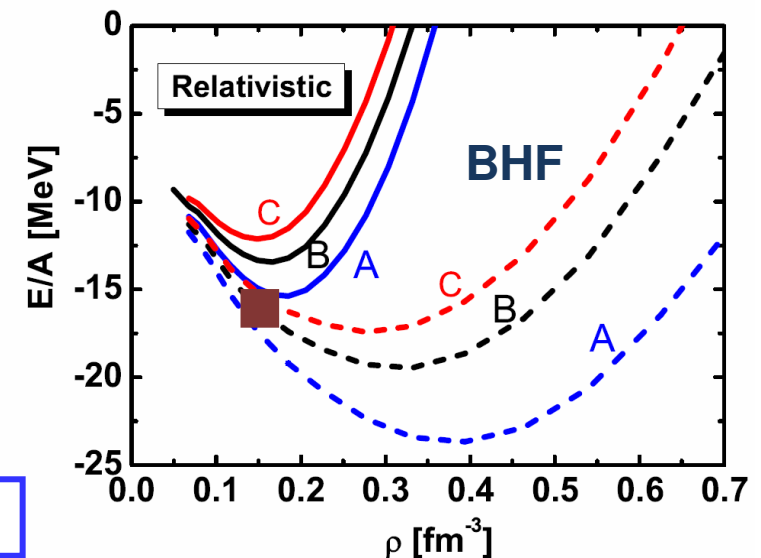
+ NNN-forces

- Relativistic Brueckner theory:

Brockmann PRC 1990



Coester-line



Density functional theory in nuclei:

In nuclei DFT has been introduced by **effective Hamiltonians**:
by [Vautherin and Brink \(1972\)](#) using the Skyrme model as a vehicle

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

Based on the philosophy of Bethe, Goldstone, and Brueckner
one has in the nuclear interior a density dependent interaction $G(\rho)$

At present, the ansatz for $E(\rho)$ 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
- Connection to QCD: (large scalar and vector fields: $\sim \pm 400$ MeV)
- Lorentz covariance restricts the number of phenomen. parameters...

Covariant DFT is based on the Walecka model

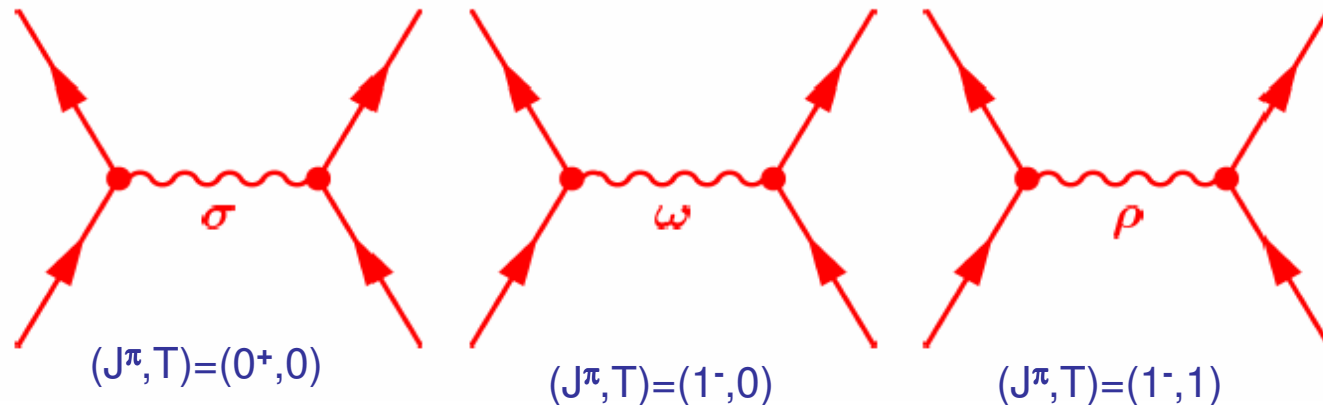
Dürr and Teller, Phys.Rev. 101 (1956)

Walecka, Phys.Rev. C83 (1974)

Boguta and Bodmer, Nucl.Phys. A292 (1977)

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

$$E[\rho]:$$



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

sigma-meson:
attractive scalar field

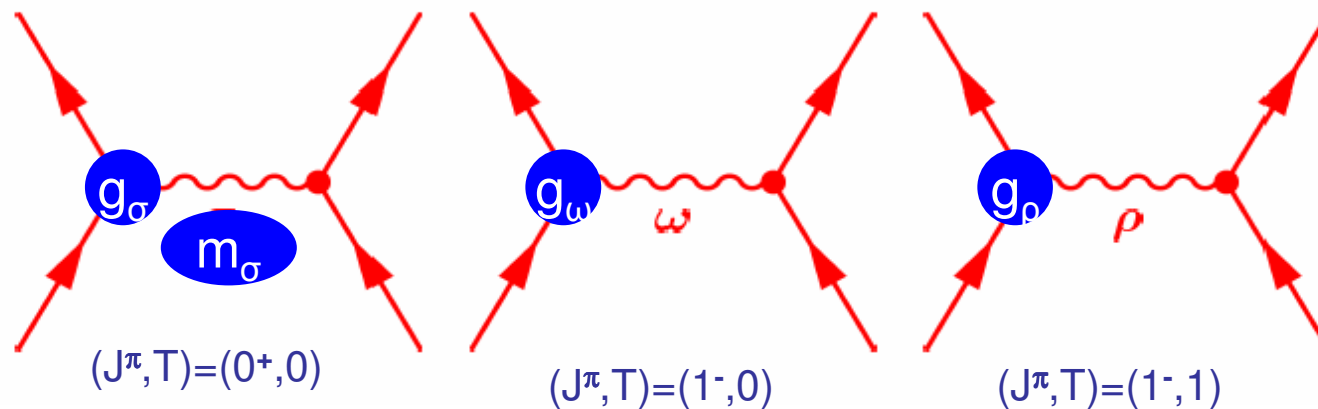
$$V(\mathbf{r}) = g_\omega \omega(\mathbf{r}) + g_\rho \vec{\tau} \vec{\rho}(\mathbf{r}) + eA(\mathbf{r})$$

omega-meson:
short-range repulsive

rho-meson:
isovector field

Covariant DFT is based on the Walecka model

This model has **only four parameters**:

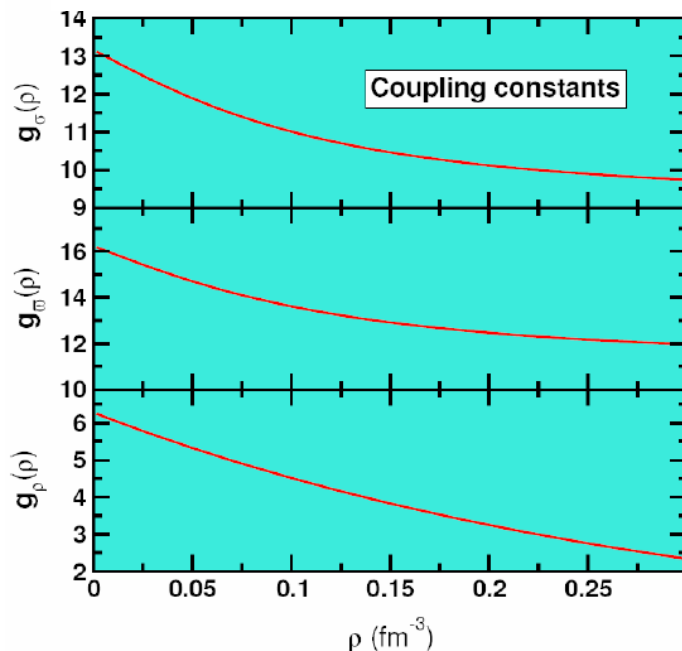


$$S(r) = g_\sigma \sigma(r) \quad V(r) = g_\omega \omega(r) + g_\rho \rho(r) + eA(r)$$

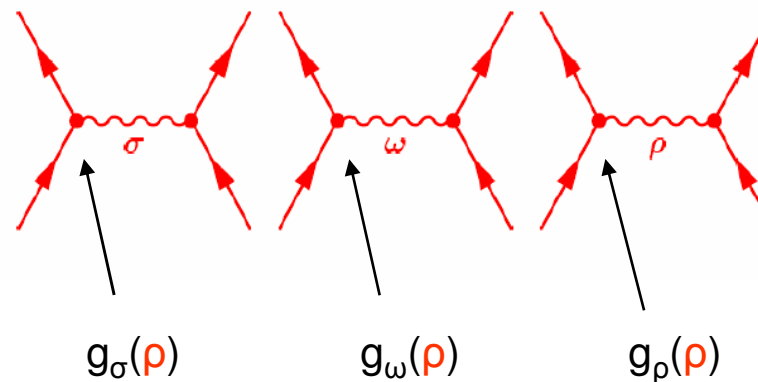
Effective density dependence:

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:



adjusted to ground state properties of finite nuclei

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

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

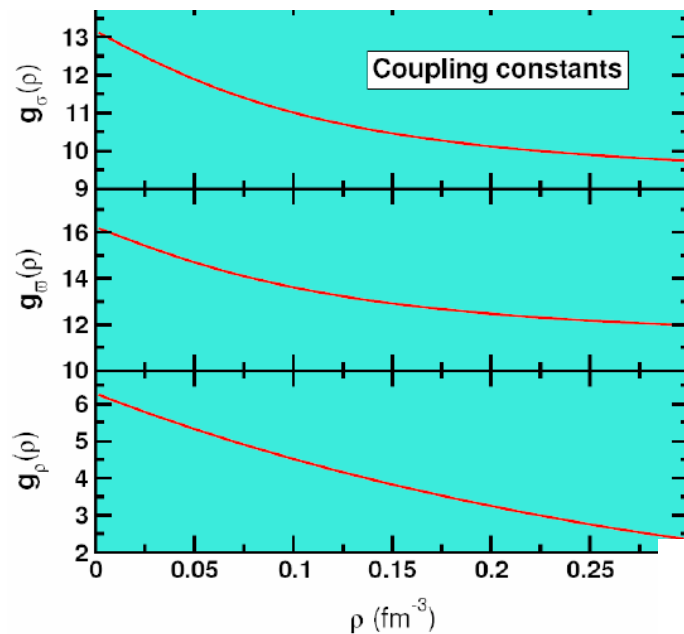
Lalazissis, Niksic, Vretenar, P.R., PRC **78**, 034318 (2008):

DD-ME1

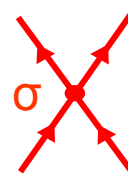
DD-ME2

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):

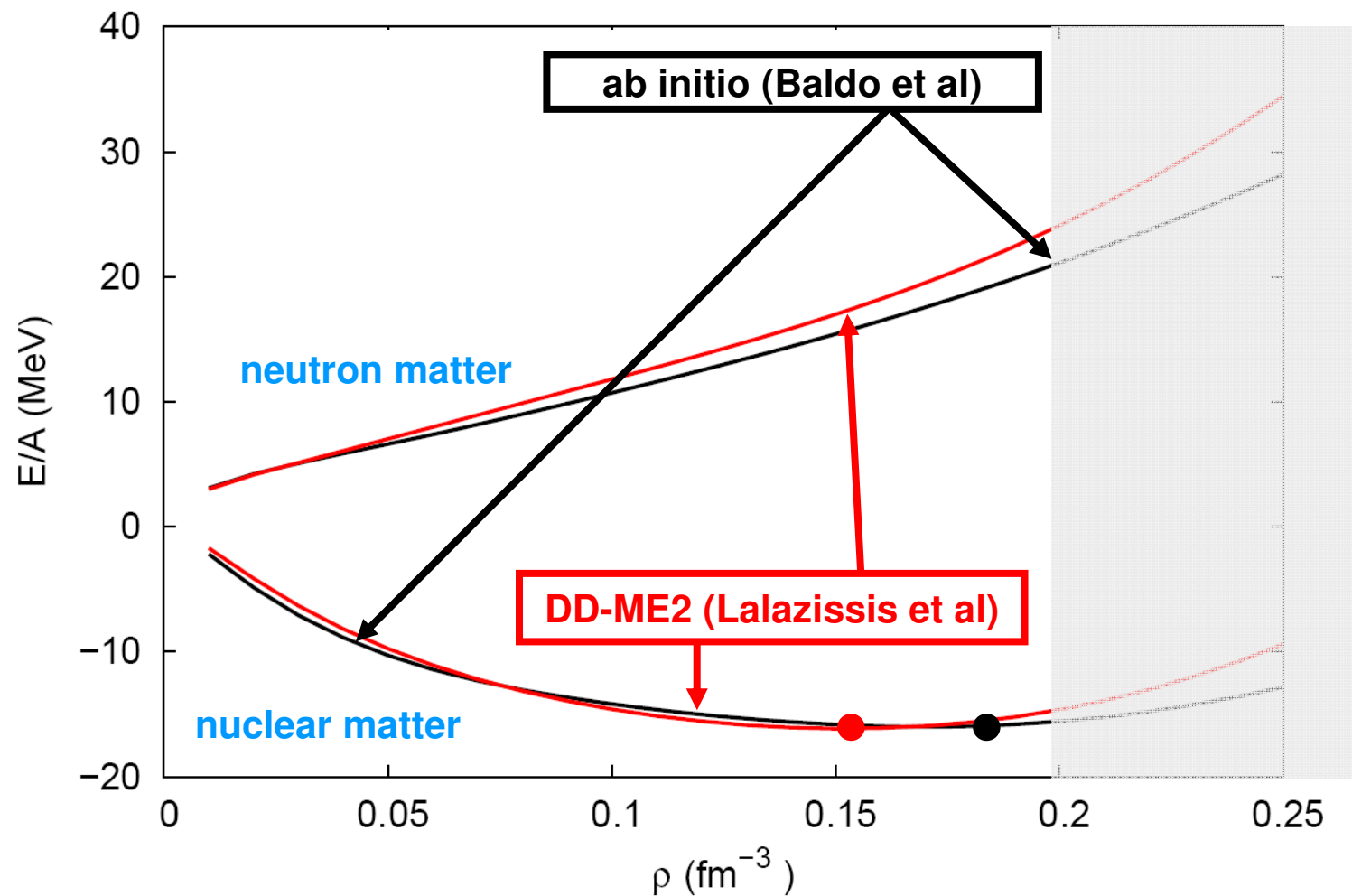
Zhao, Li, Yao, Meng, J. Meng, archiv 1002.1789

PC-F1

DD-PC1

PC-PK1

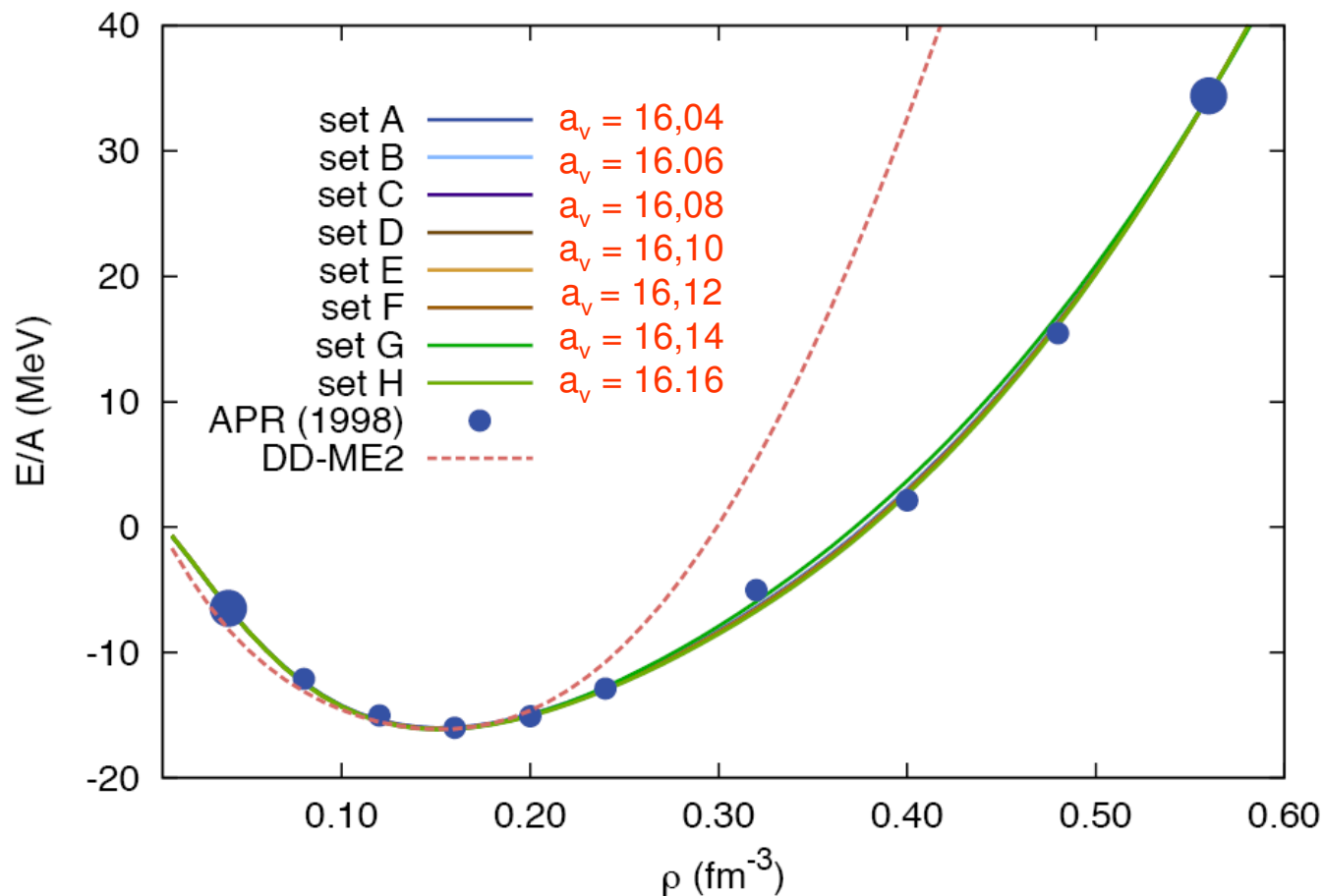
Comparison with ab initio calculations:



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

Semi-microscopic covariant density functionals:

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



$\rho_{\text{sat}} = 0.152 \text{ fm}^{-3}$
 $m^* = 0.58m$
 $K_{\text{nm}} = 230 \text{ MeV}$
 $a_4 = 33 \text{ MeV}$

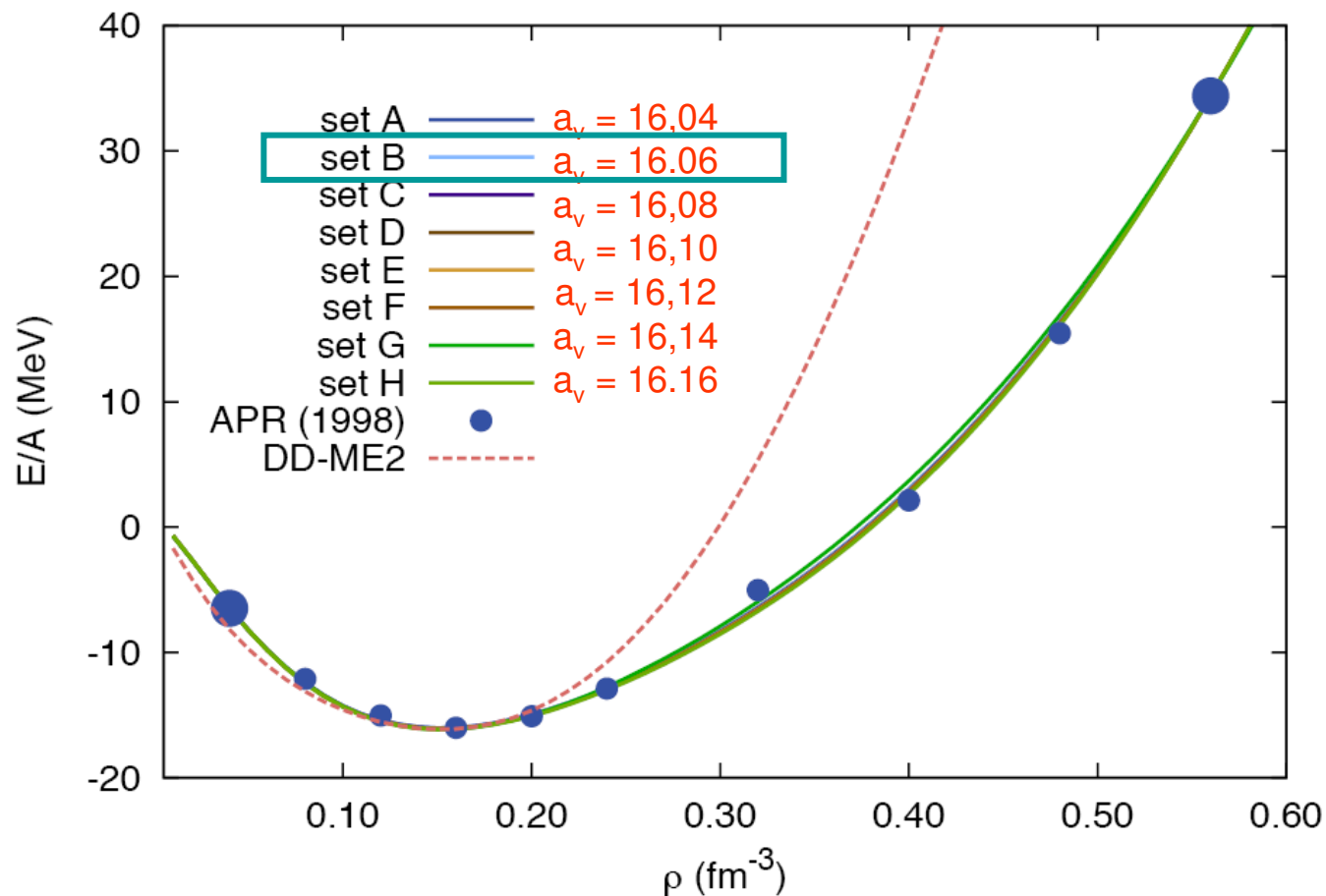
Niksic et al, (2008)

DD-PC1

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

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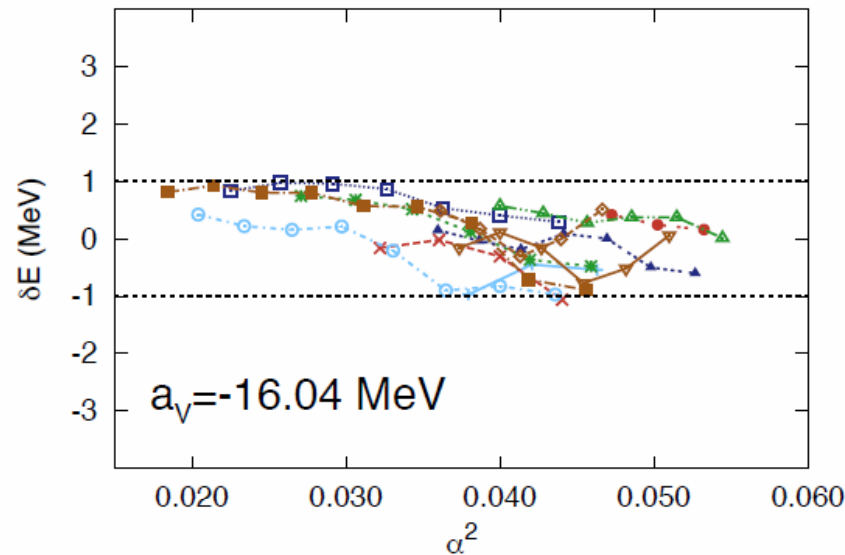
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Adjusting the model parameters

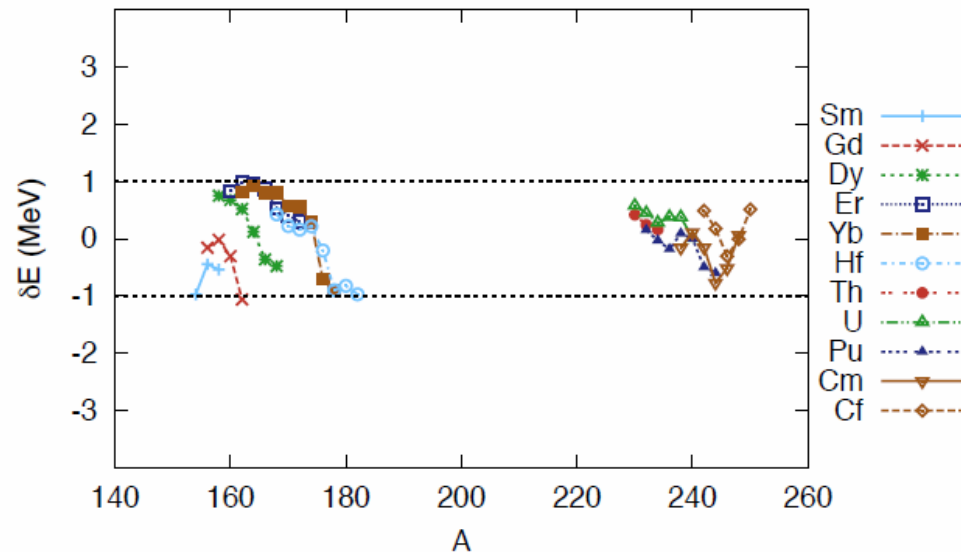


Rare-earth region

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)

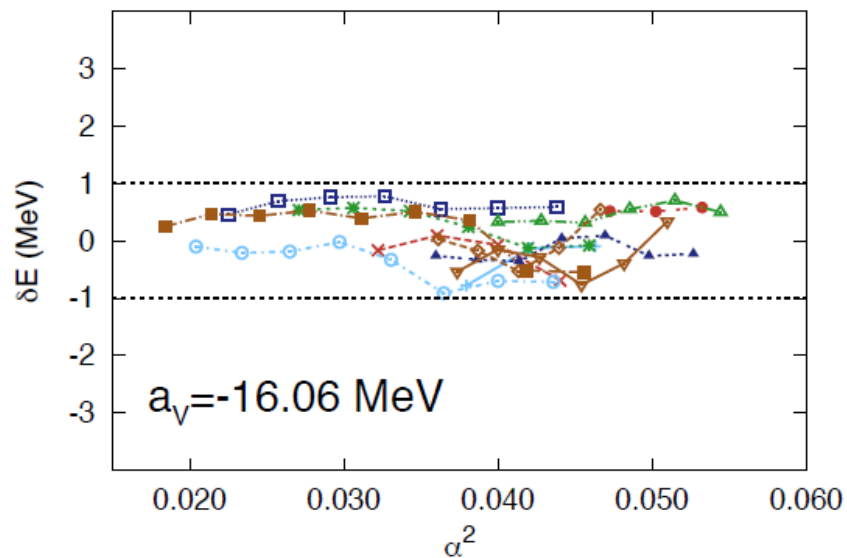


Total

64 isotopes

T. Niksic et al, (2008)

Adjusting the model parameters

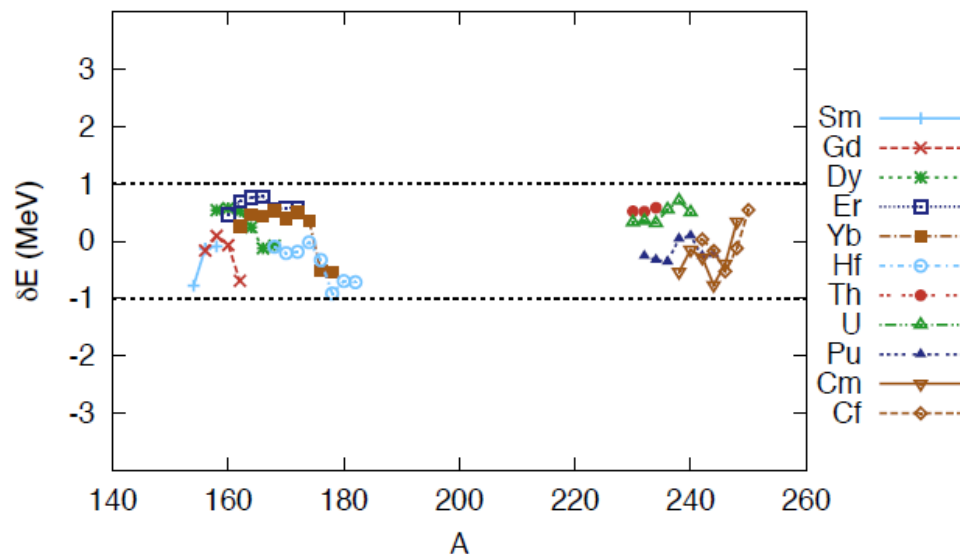


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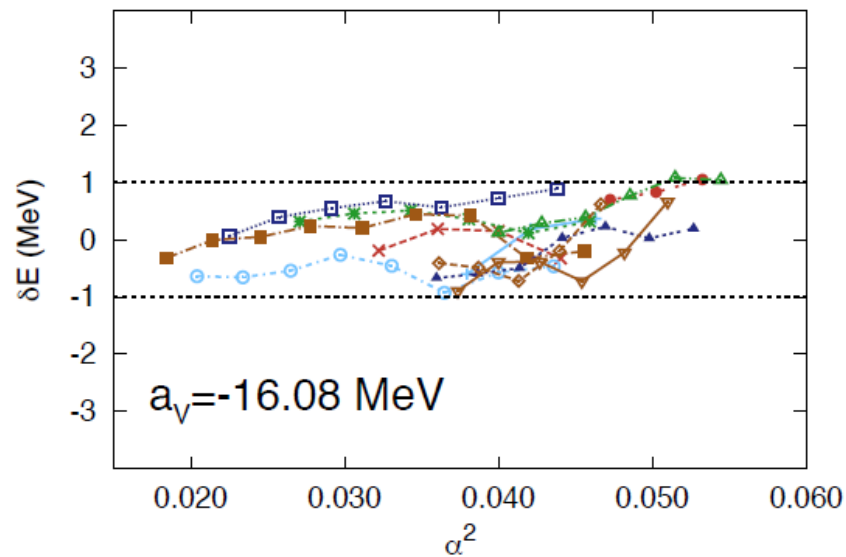


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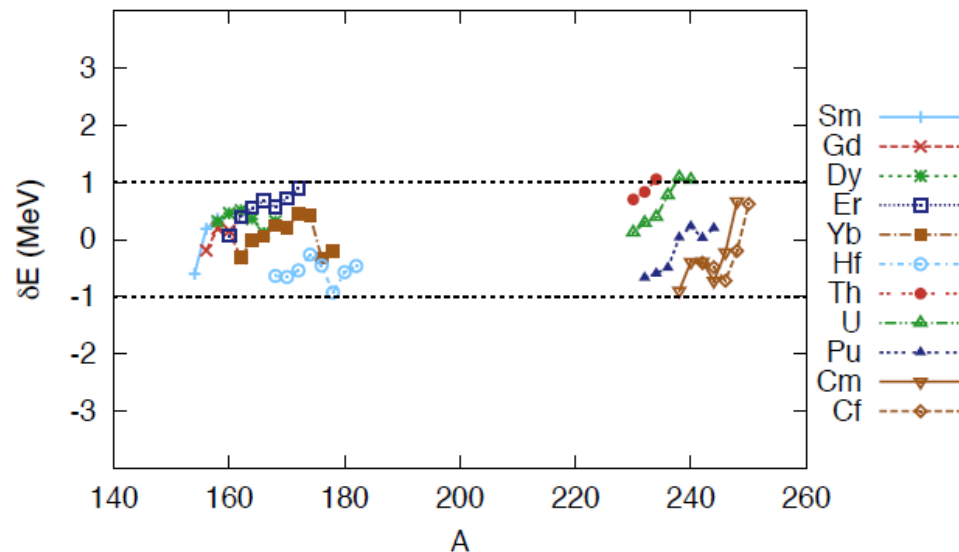


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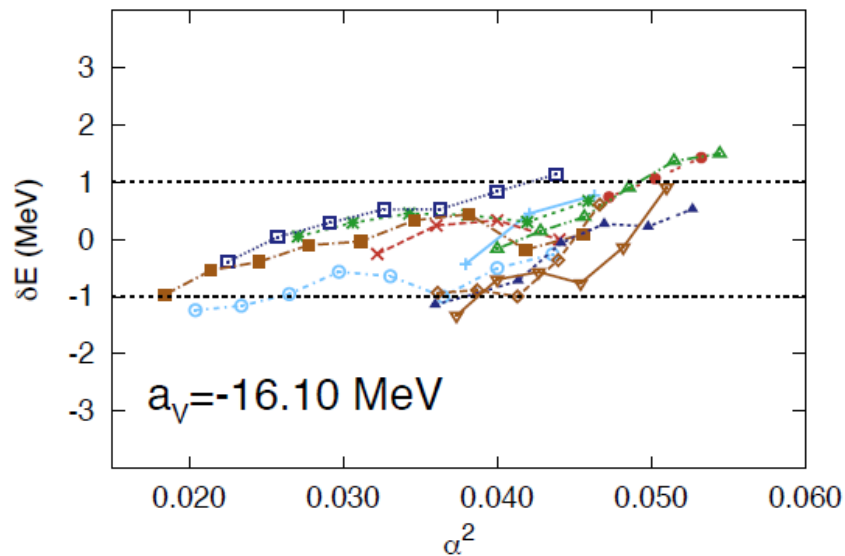


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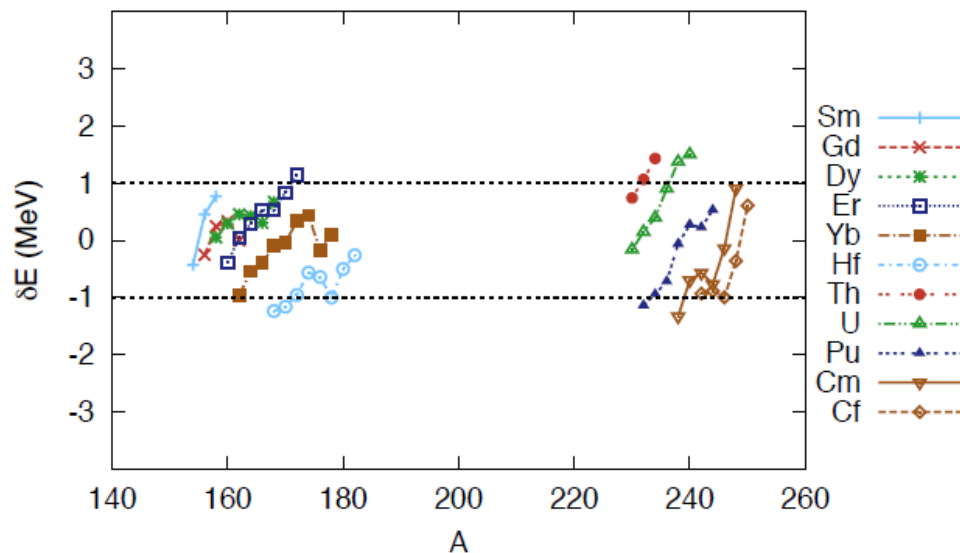


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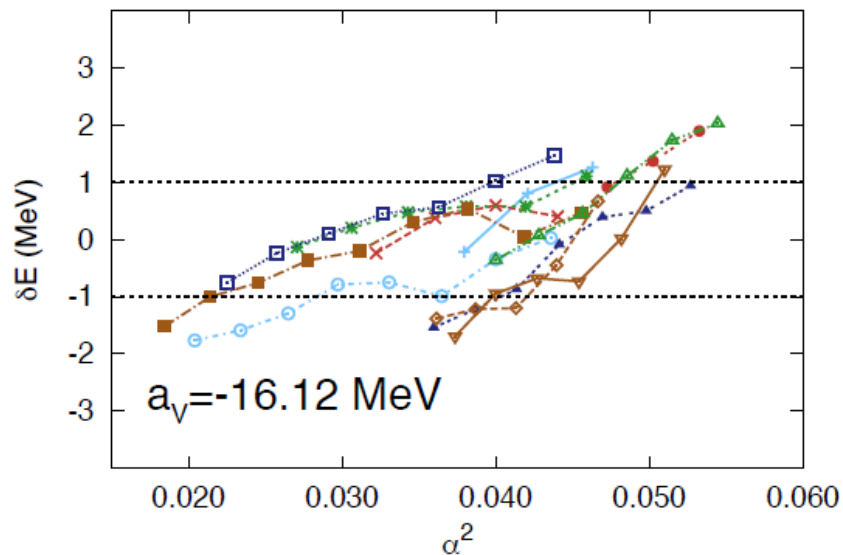


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T. Niksic et al, (2008)

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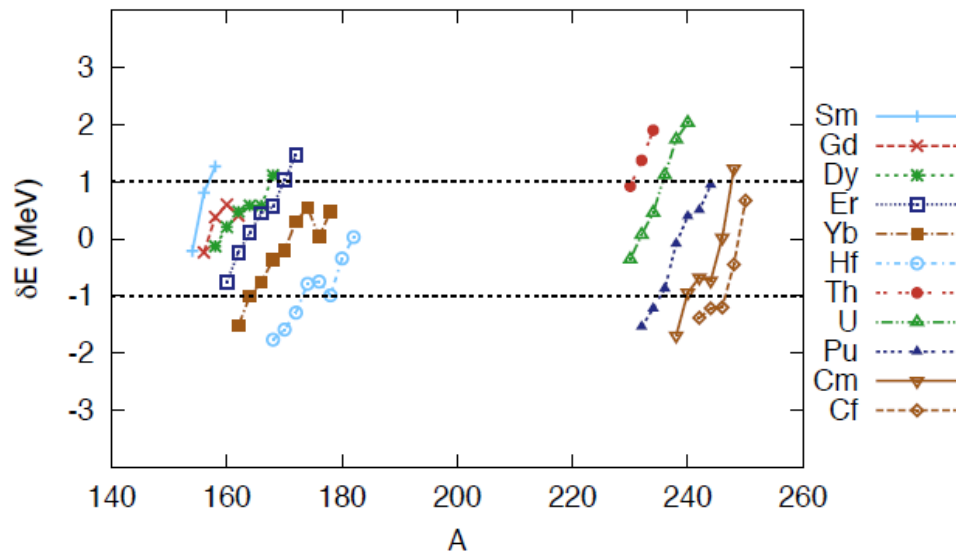


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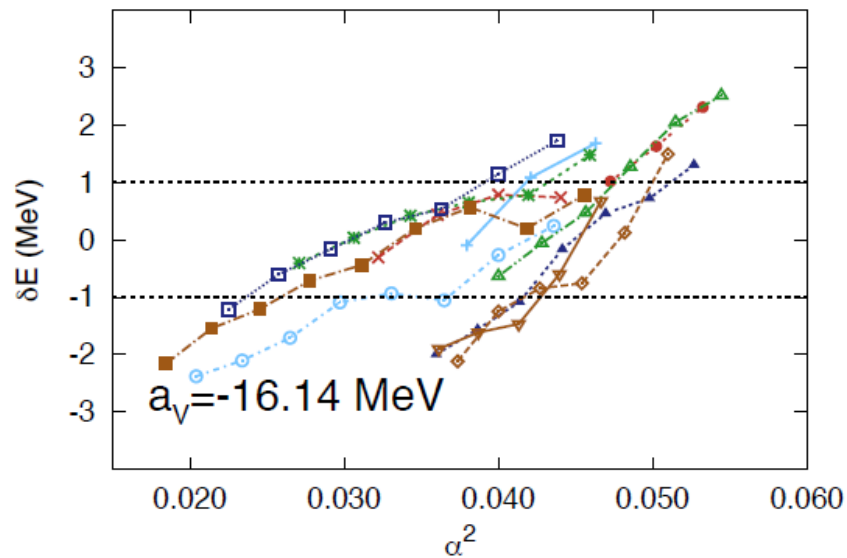


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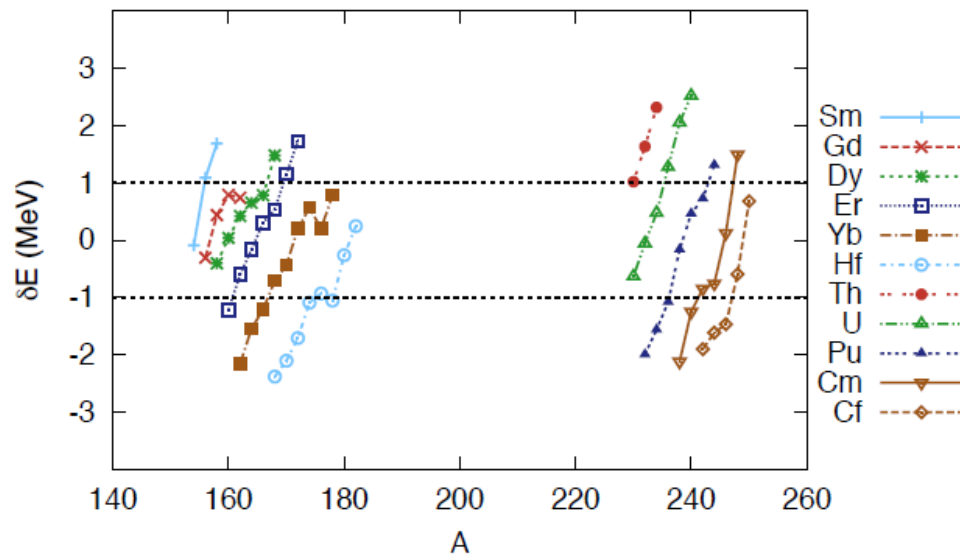


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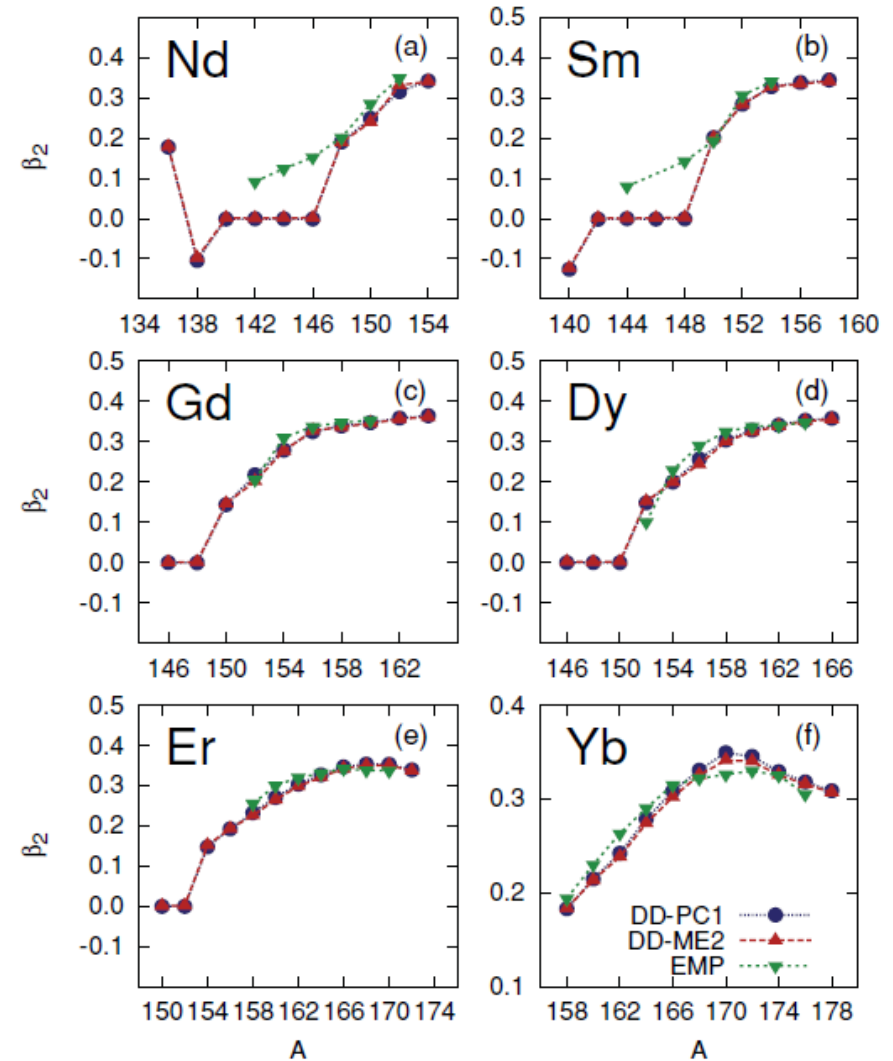
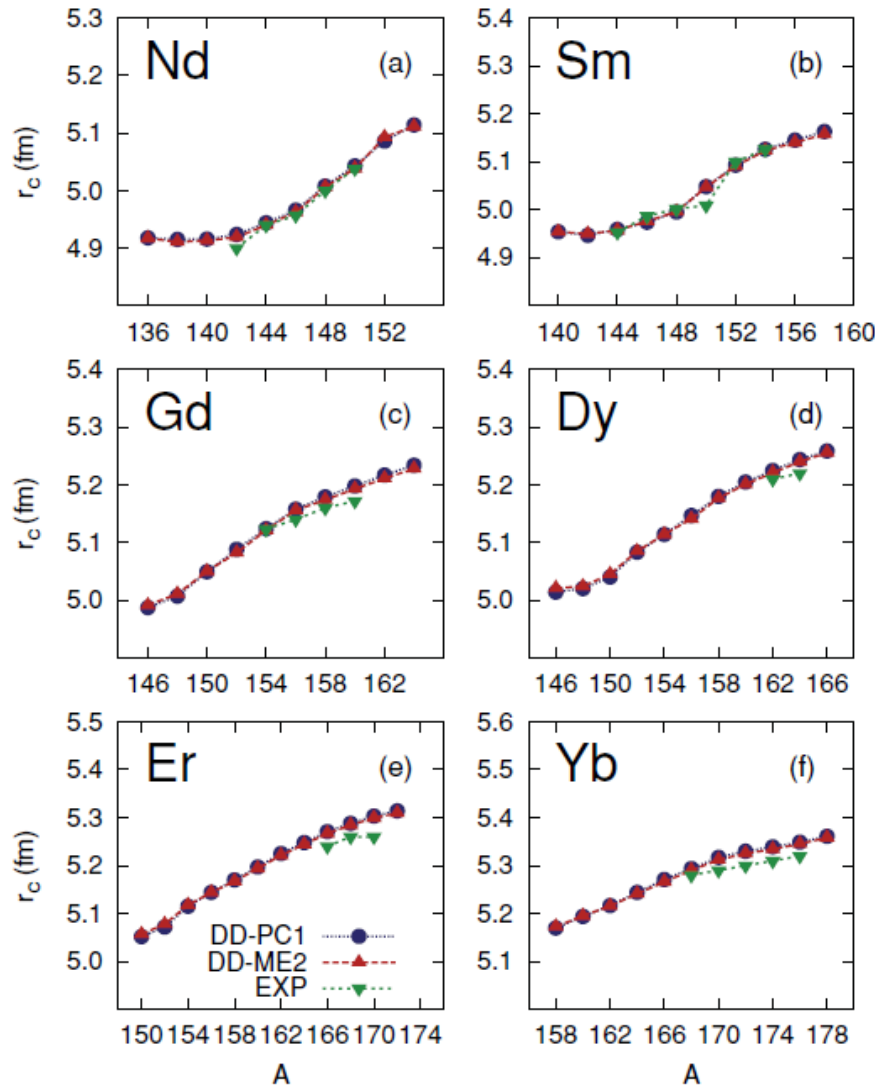
Total

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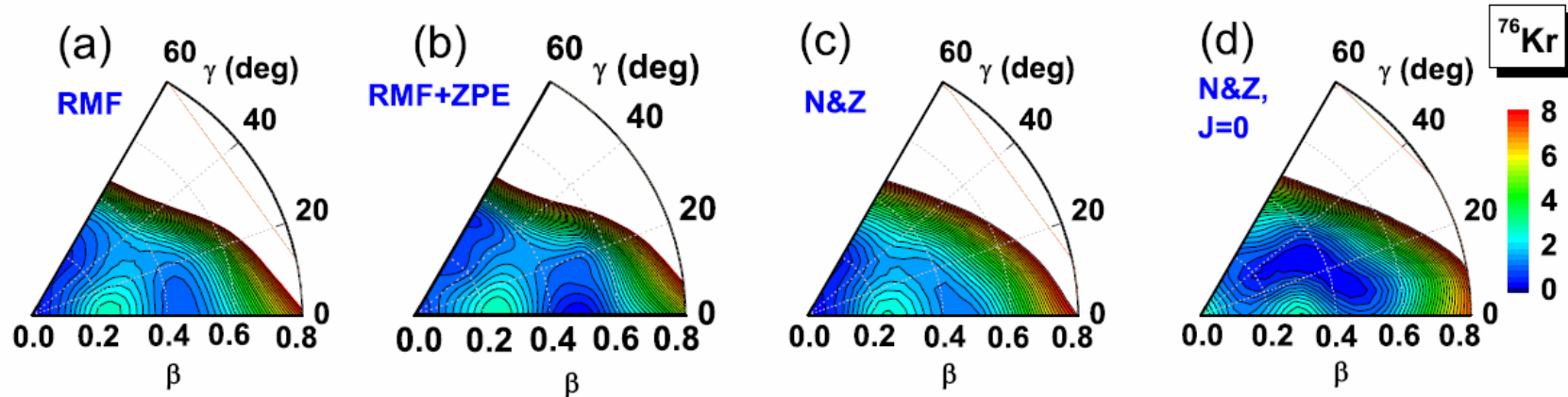
T. Niksic et al, (2008)

DD-PC1: isotope shifts and deformation parameters:

T. Niksic et al, PRC (2008)



Transitional nuclei: DFT beyond mean field:



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

Projection on J and N:

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

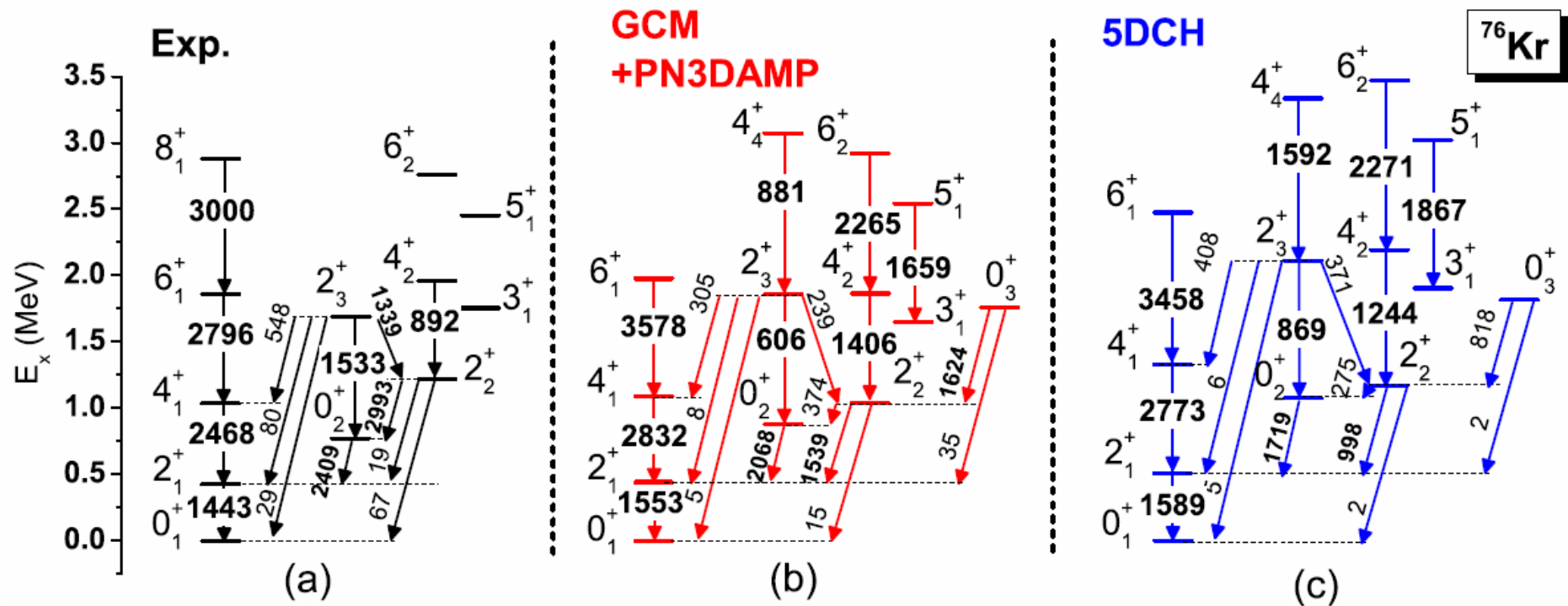
Bohr Hamiltonian: $H = -\frac{\partial}{\partial q} \frac{1}{2B(q)} \frac{\partial}{\partial q} + V(q) + V_{corr}(q)$

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

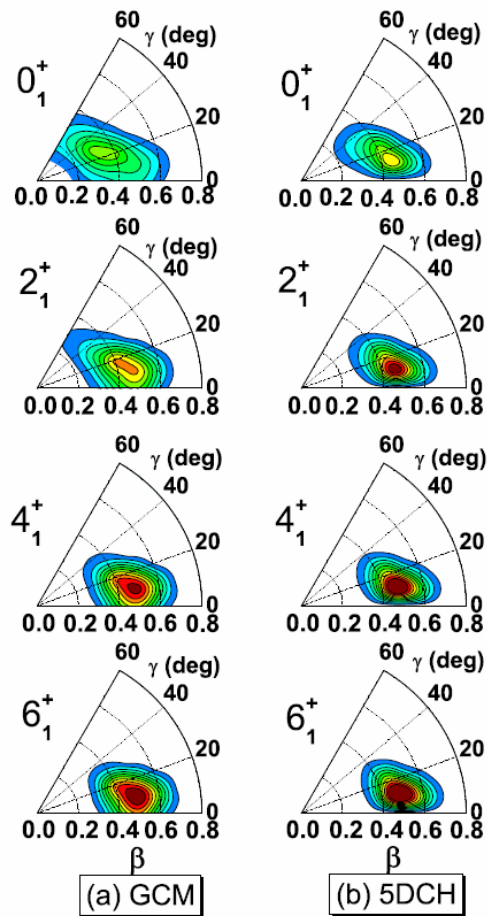
Spectra: GCM (7D)

Bohr Hamiltonian (5DCH)

PC-PK1

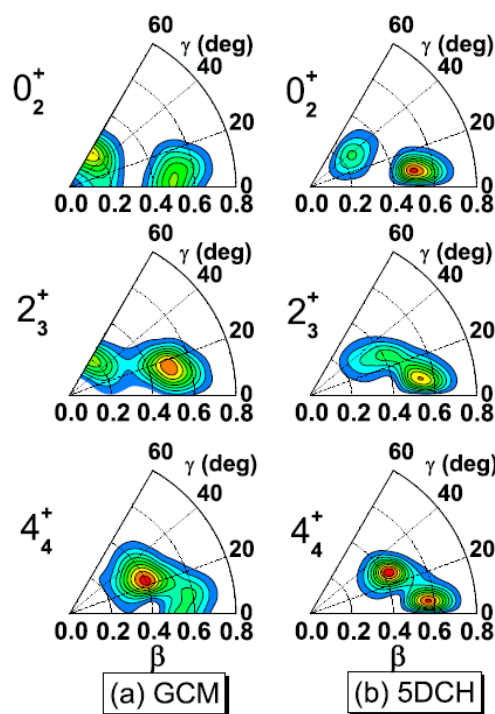


J.M. Yao et al, PRC (2014)



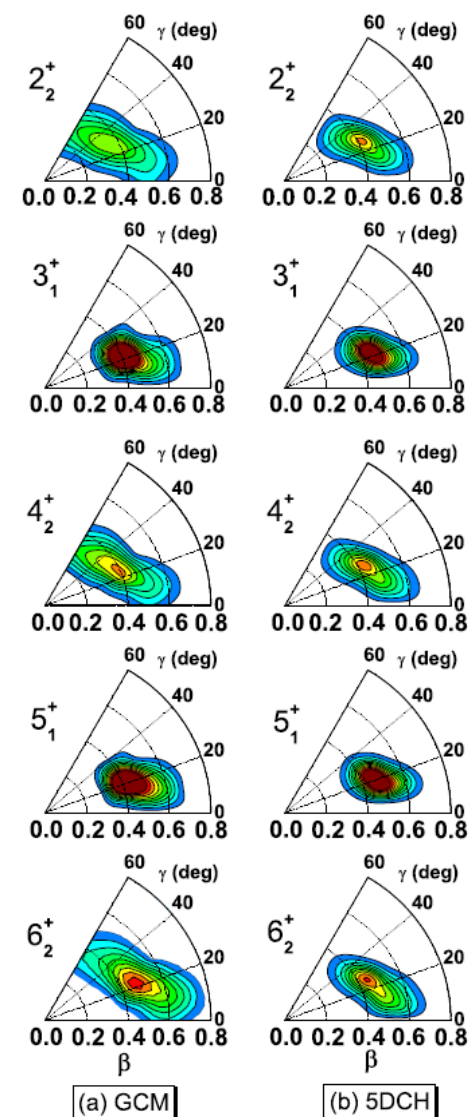
ground state band

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

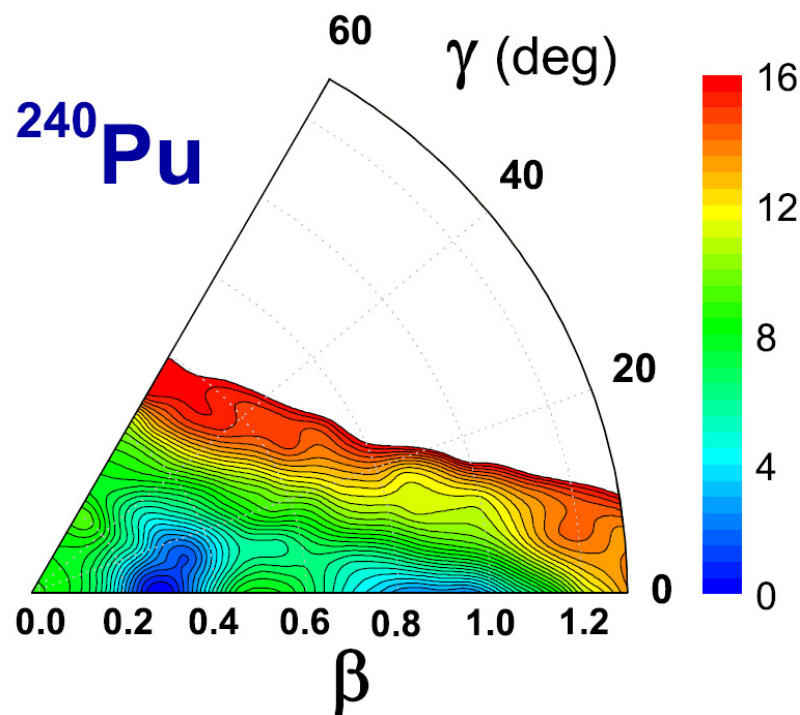


quasi- β band

wave functions



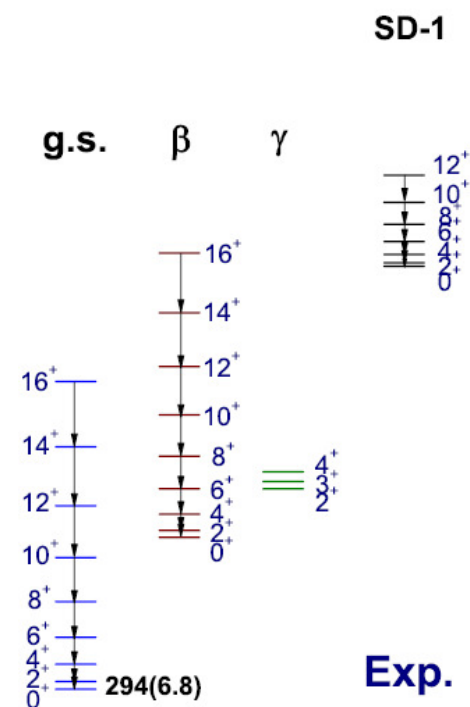
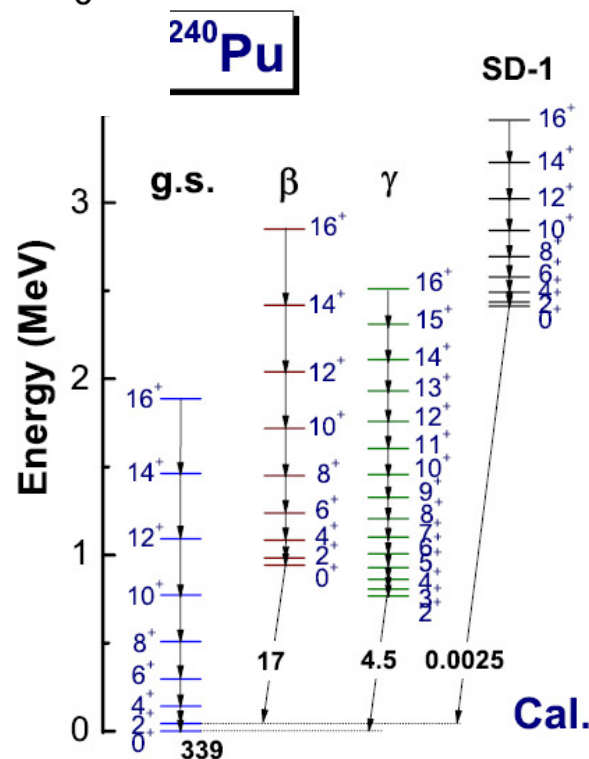
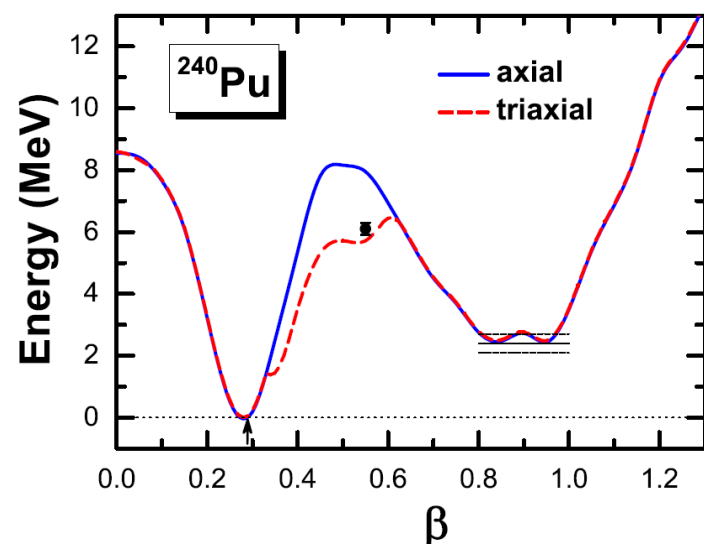
quasi- γ band



Fission barrier and super-deformed bands in ^{240}Pu

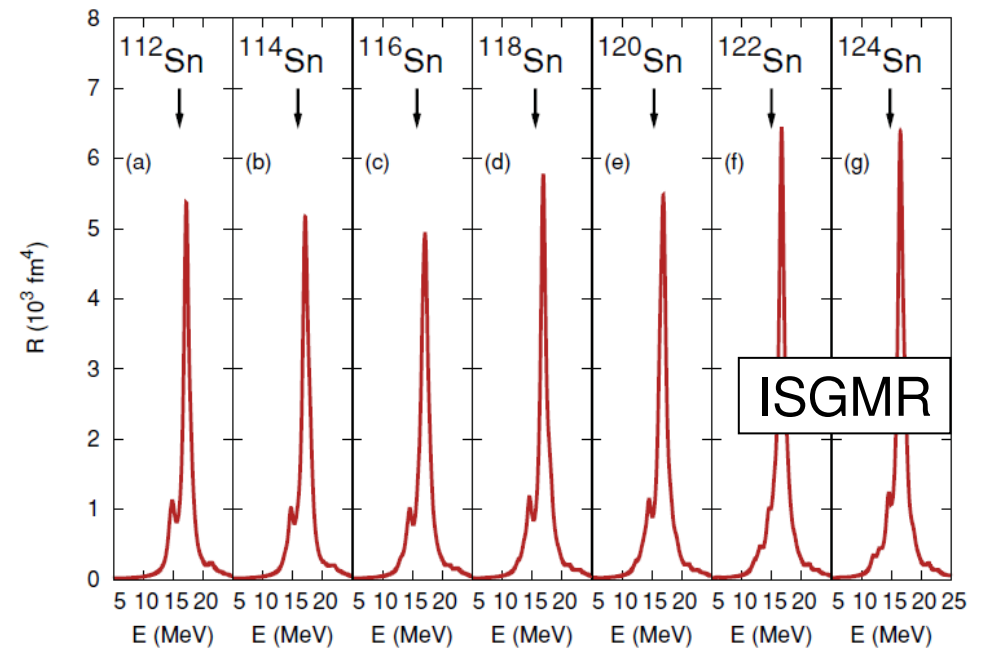
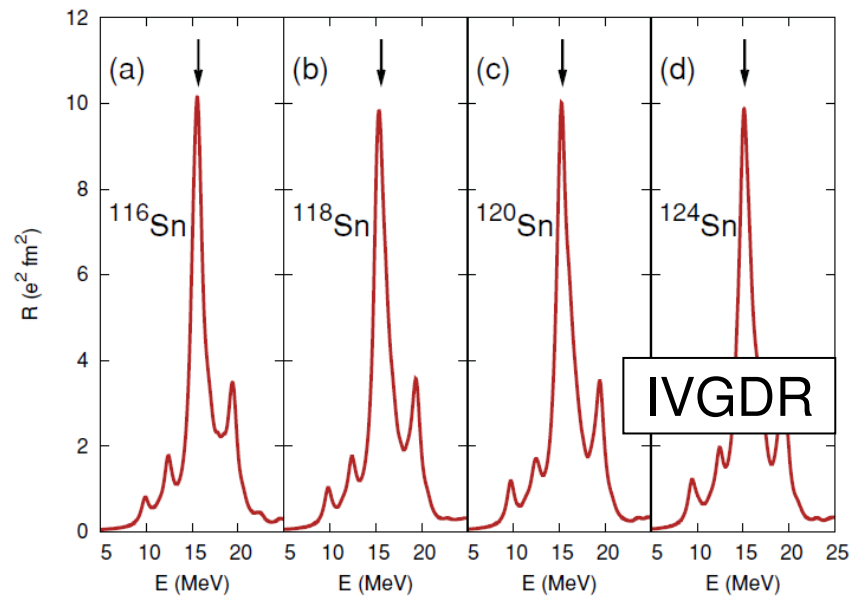
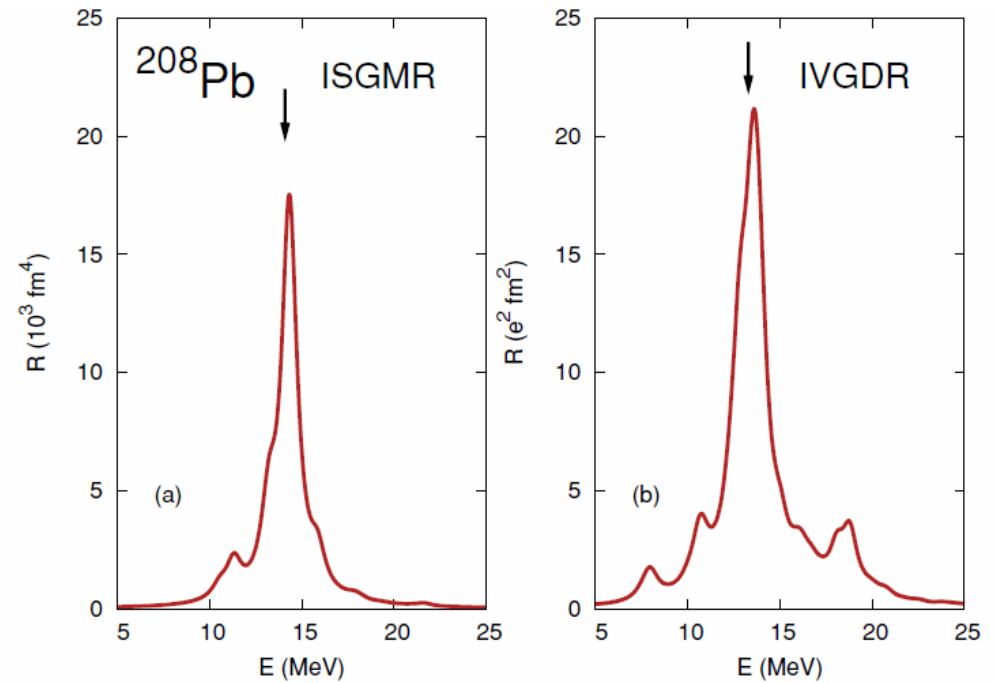
Zhipan Li et al, PRC (2010)

DD-PC1



DD-PC1: Giant resonances:

T. Niksic et al, PRC (2008)



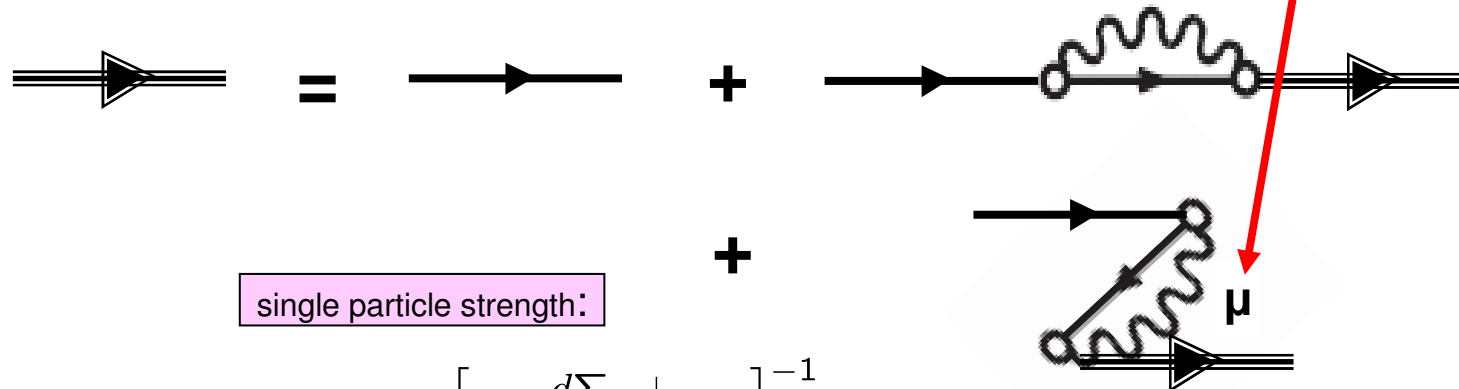
Particle-vibrational coupling: energy dependent self-energy

$$\Sigma = S + V + \Sigma(\omega)$$

mean field

pole part

RPA-modes

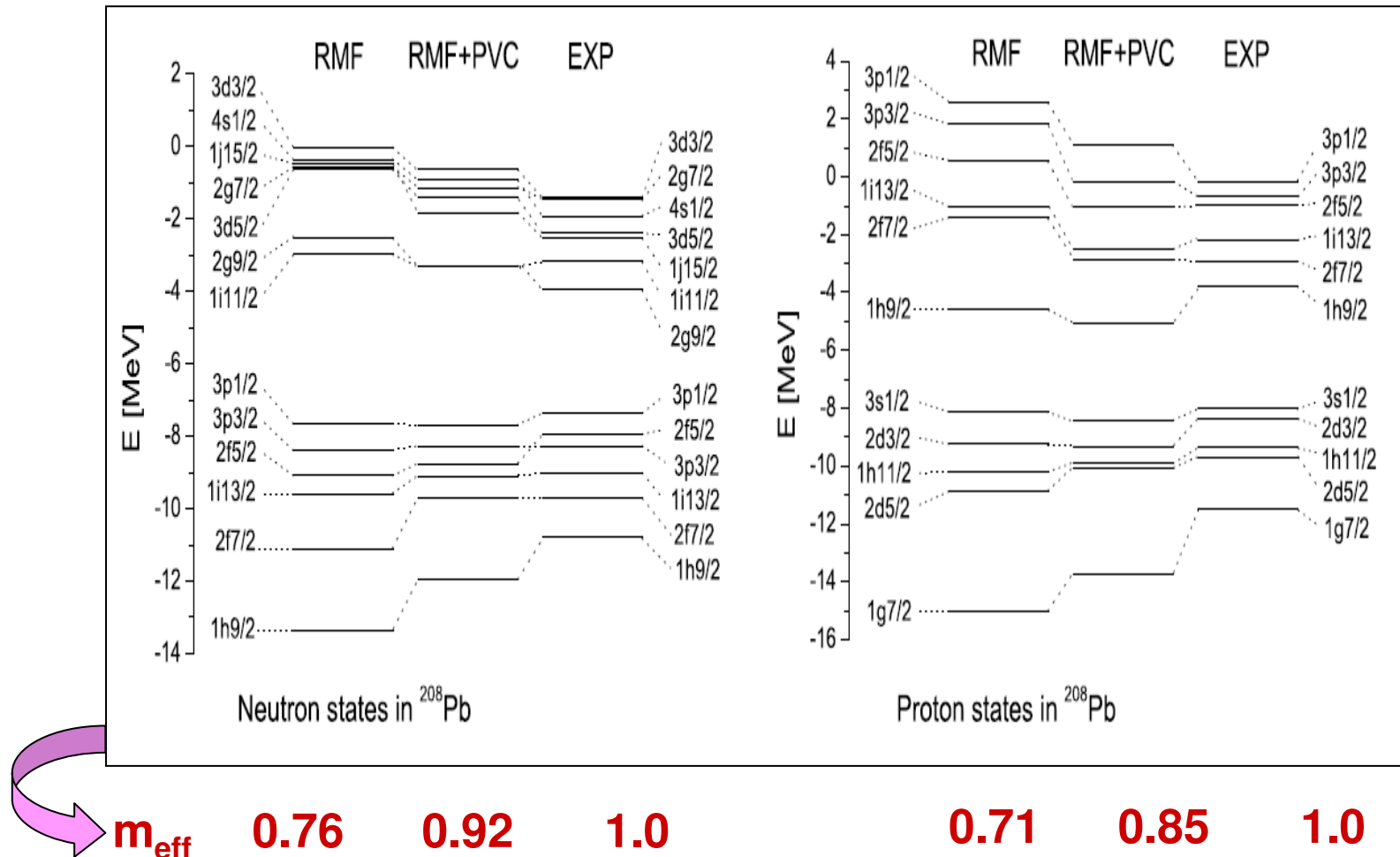


single particle strength:

$$z_\nu = \left[1 - \frac{d\Sigma_{\nu\nu}}{d\omega} \Big|_{\omega=\epsilon_\nu} \right]^{-1}$$

Density functional theory - Landau-Migdal theory

Single particle spectrum in the Pb region

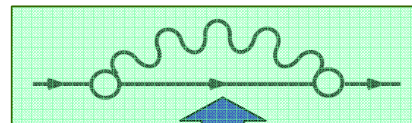


E. Litvinova, P.R., PRC 73, 44328 (2006)

Width of Giant Resonances:

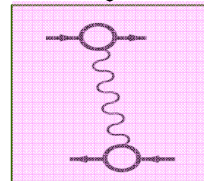
The full response contains energy dependent parts coming from vibrational couplings.

$$V(\omega) = \frac{\delta\Sigma(\omega)}{\delta\rho}$$

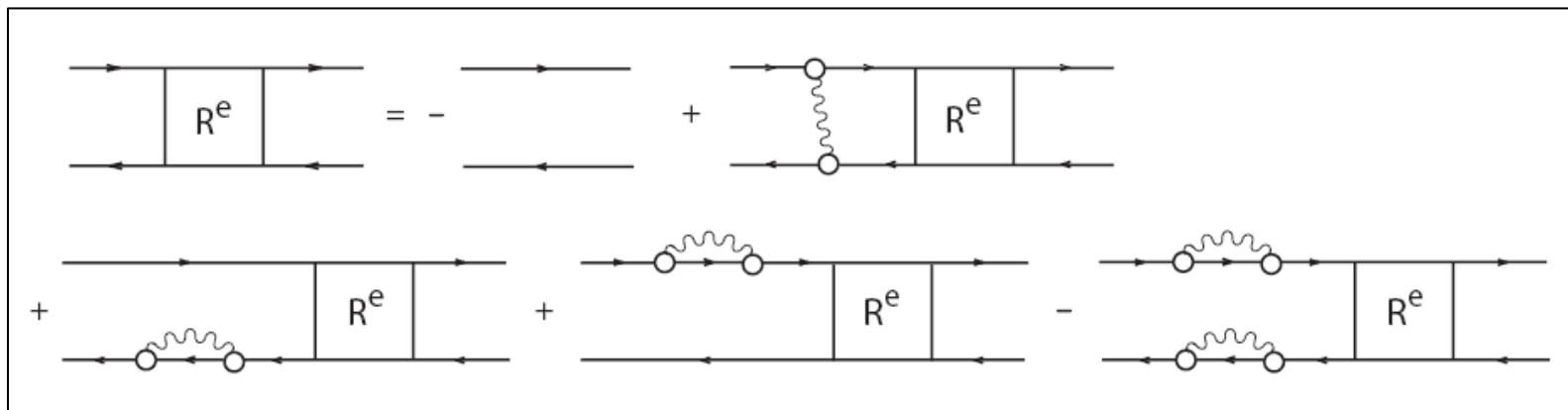


Self energy

ph-phonon amplitudes(QRPA)



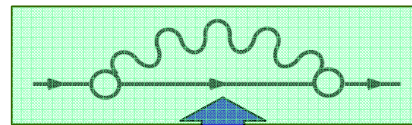
induced interaction



Width of Giant Resonances:

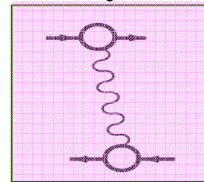
The full response contains energy dependent parts coming from vibrational couplings.

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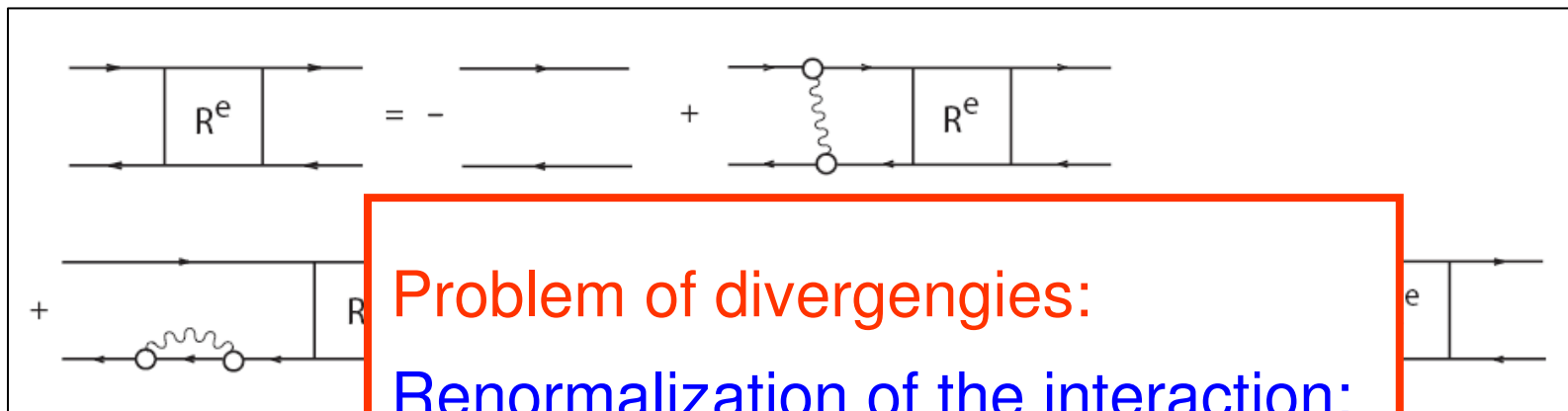


Self energy

ph-phonon amplitudes(QRPA)



induced interaction

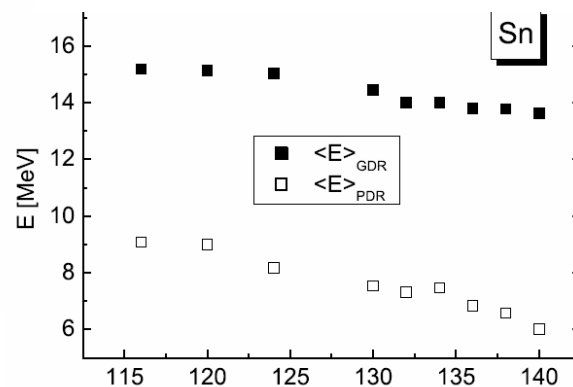
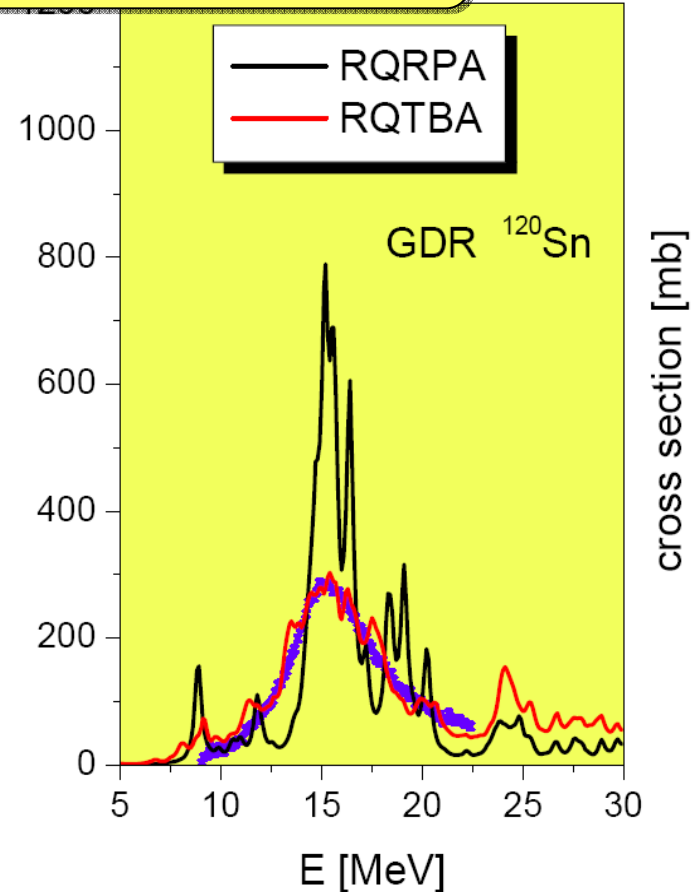
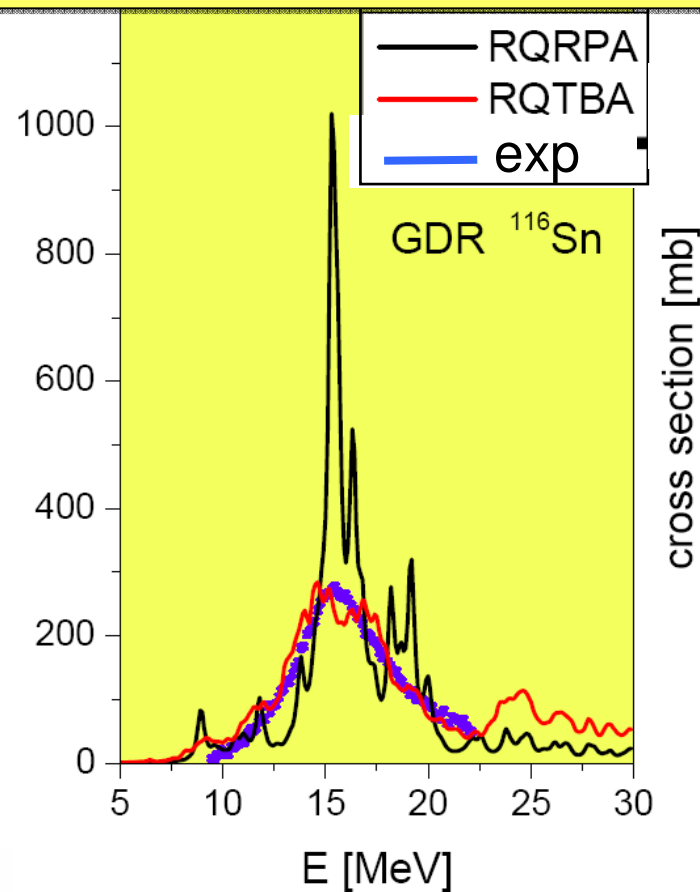


Problem of divergencies:

Renormalization of the interaction:

$$V(\omega) \rightarrow V_{\text{RPA}} + V(\omega) - V(0)$$

Coupling to complex configurations in the GDR:



centroid energies for
GDR and PDR

Litvinova, P.R. Tselyaev, PRC 78, 14312 (2008)

Litvinova, P.R. Tselyaev, Langanke, PRC 79, 054312 (2009)

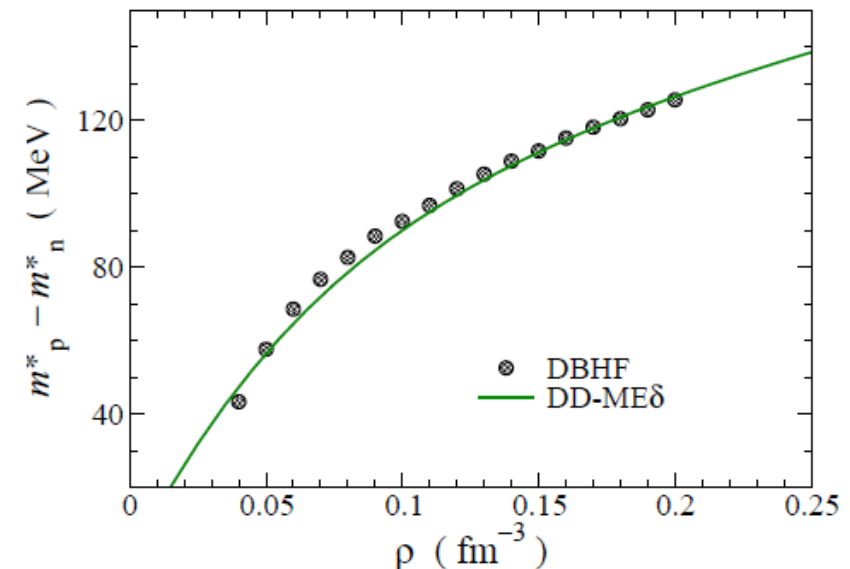
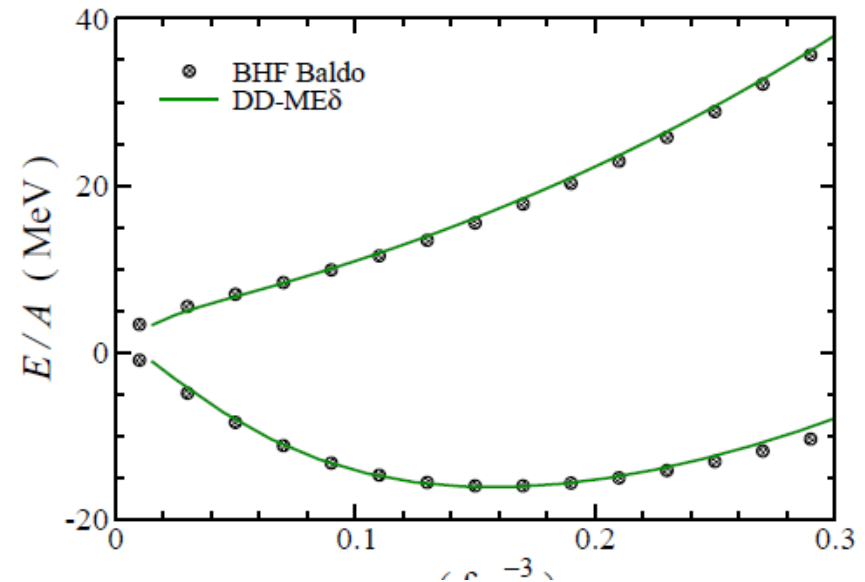
Ab-initio parameter set with δ -meson ($J=0, T=1$):

- (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 $g_\sigma(\rho_0)$, $g_\omega(\rho_0)$, $g_\rho(\rho_0)$, and m_σ are fitted to a set of finite nuclei

Parameter set: **DD-ME δ**

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

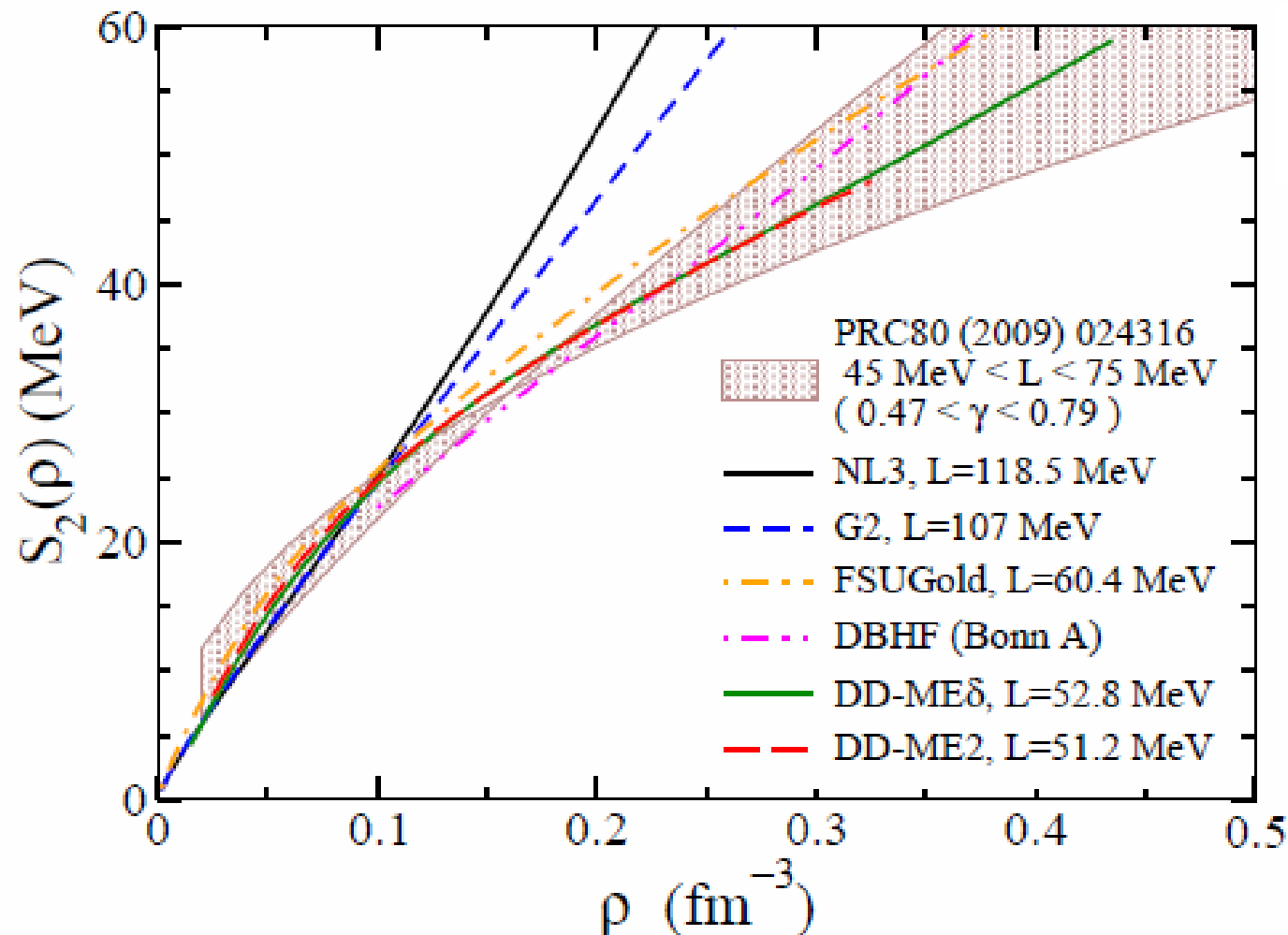
Roca-Maza et al, PRC 84, 54309 (2011)



symmetry energy $S_2(\rho)$:

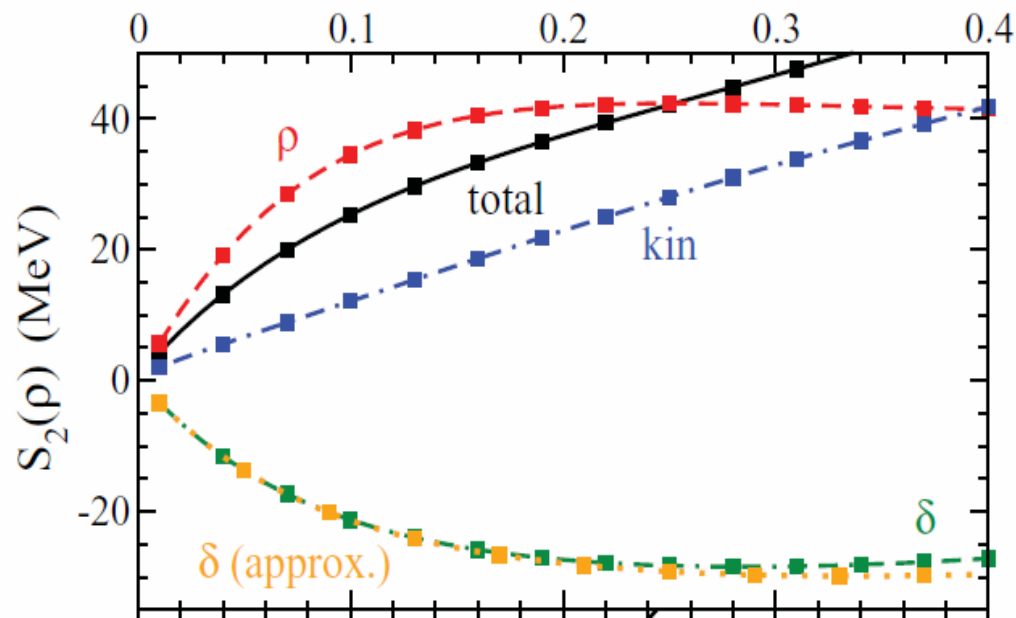
$$\rho = \rho_n + \rho_p \quad \alpha = \frac{\rho_n - \rho_p}{\rho_n + \rho_p}$$

$$E(\rho_n, \rho_p) = E(\rho, \alpha) = E(\rho, 0) + \alpha^2 S_2(\rho) + \dots$$



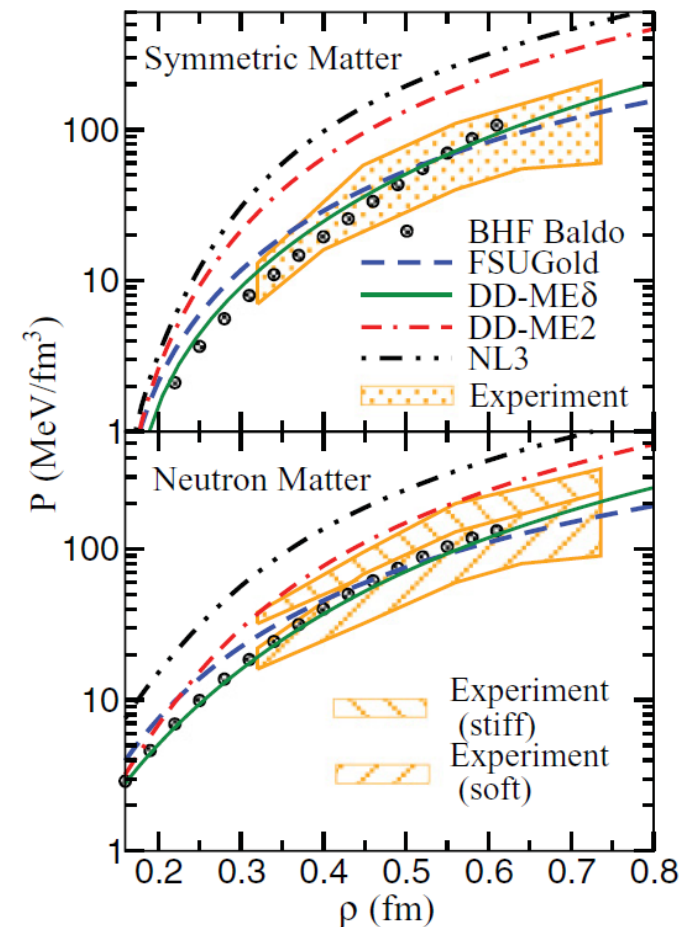
$$L(\rho) \equiv 3\rho \frac{dS_2(\rho)}{d\rho}$$

δ -meson and the symmetry energy $S_2(\rho)$:



$$S_2(\rho) \equiv S_2^{\text{kin}}(\rho) + S_2^{\rho}(\rho) + S_2^{\delta}(\rho),$$

δ -meson and EoS at high densities



effective pairing forces:

seniority force, constant G
zero range; δ -force

pairing part of Gogny D1S

Gonzales-Llarena et al, PLB 379, 13 (1996)

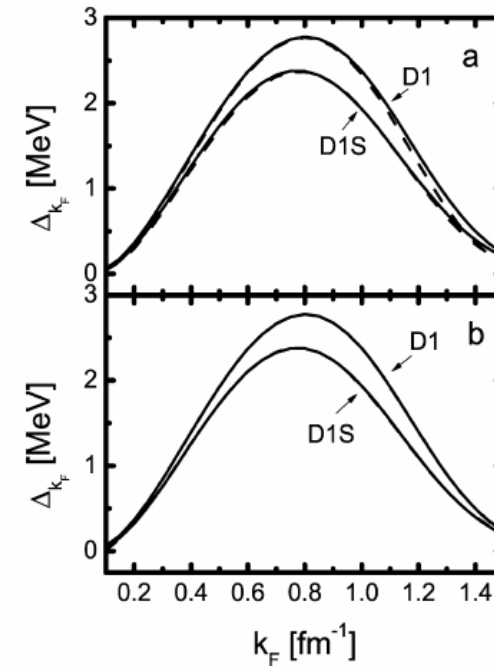
Gogny equivalent separable force:

Tian, Ma, P.R. PLB 676, 44 (2009)

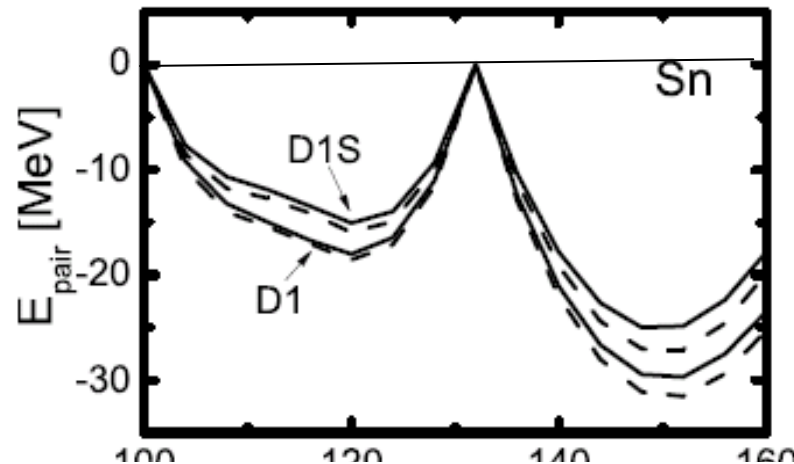
$$V_{pp}(\mathbf{r}_1\mathbf{r}_2, \mathbf{r}'_1, \mathbf{r}'_2) = -G \delta(\mathbf{R} - \mathbf{R}') e^{-(\alpha r)^2} e^{-(\alpha r')^2}$$

where $\mathbf{R} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2), \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$

nucl. matter:



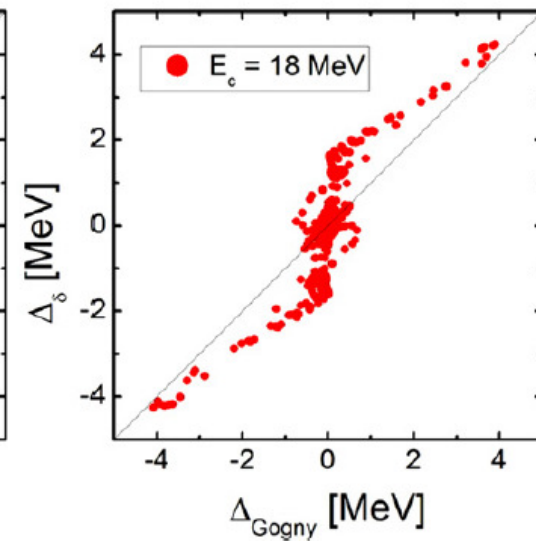
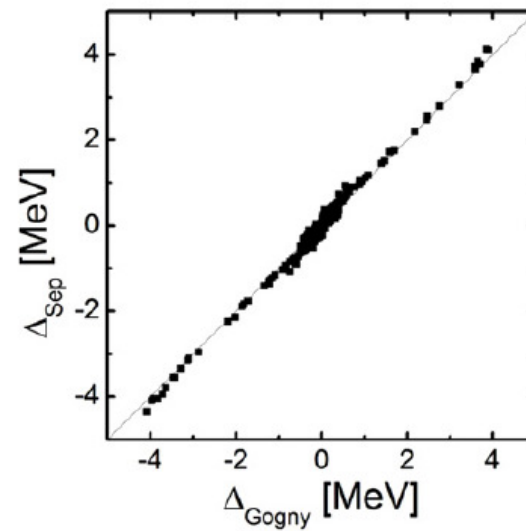
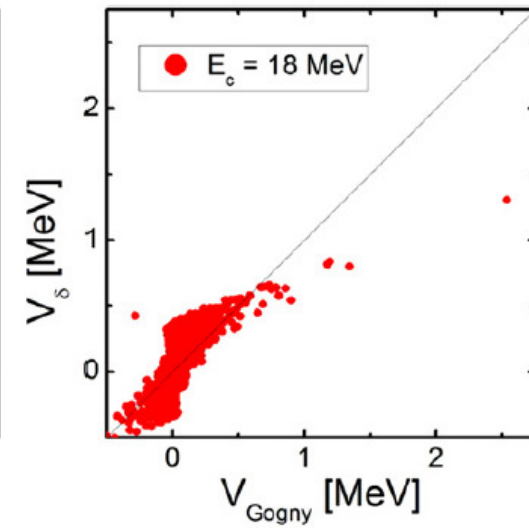
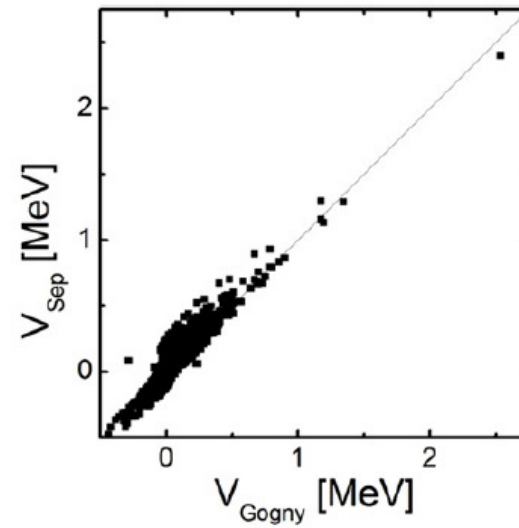
finite nuclei:



$$V_{121'2'}^0 = -G \sum_N V_{12}^N V_{1'2'}^N$$

effective pairing forces:

$$V_{121'2'}^0 = -G \sum_N V_{12}^N V_{1'2'}^N$$

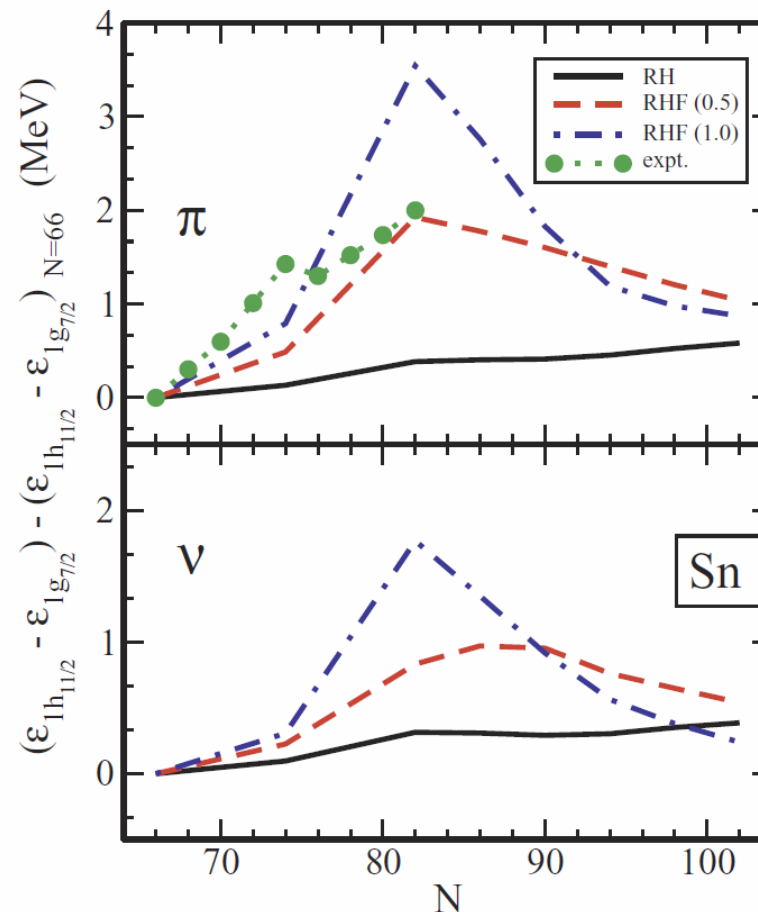


Single-particle energy splittings in Sn-isotopes:

$$\epsilon_{1h_{11/2}} - \epsilon_{1g_{7/2}}$$

Effect of a tensor force in
Relativistic Hartree-Fock

RH $\rightarrow$ RHF



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

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

Relativistic Hartree-Fock equation in a basis:

Relativistic Hartree-Fock (RHF) equation:

Lalazissis, Serra et al, Phys. Rev. C89, 041301 (2009)

$$\sum_{n'} \left(\alpha \cdot p + \beta M + \beta \Gamma_{nn'}^{HF} \right) \psi_{n'} = \epsilon_n \psi_n$$

where $\Gamma_{nn'}^{HF}$ is related with the density matrix $\rho_{nn'}$

$$\Gamma_{nn'}^{HF} = V_{nmm'n'} \rho_{mm'} - V_{nmm'n'} \rho_{mm'}$$

RHF equation in HO basis

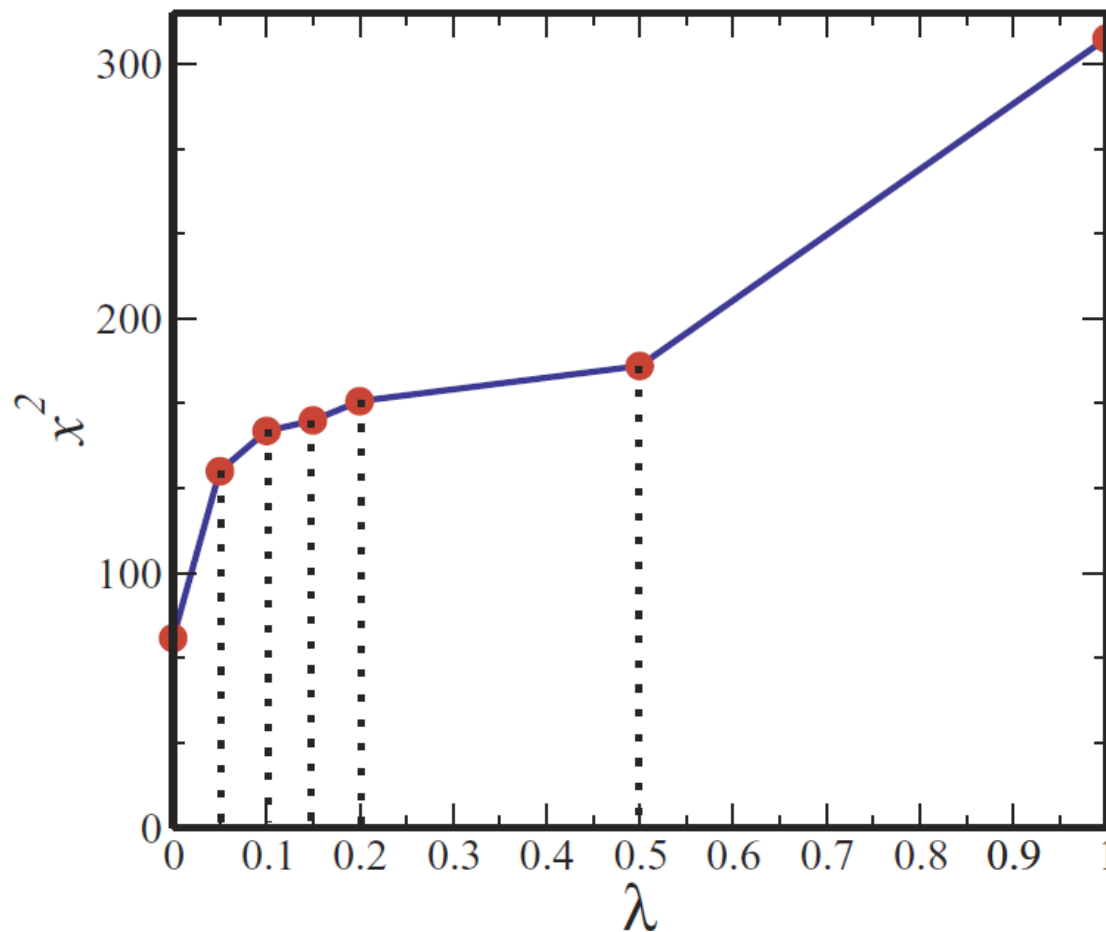
$$\begin{pmatrix} A_{nn'}^{RHF} & B_{n\bar{n}'}^{RHF} \\ B_{\bar{n}n}^{RHF} & C_{\bar{n}\bar{n}'}^{RHF} \end{pmatrix} \begin{pmatrix} f_{n'}^{(a)} \\ g_{\bar{n}'}^{(a)} \end{pmatrix} = \epsilon_a \begin{pmatrix} f_n^{(a)} \\ g_{\bar{n}}^{(a)} \end{pmatrix}$$

where

$$\psi_a = \begin{pmatrix} \sum_{n=1}^{n_{\max}} f_n^{(a)} R_{nl_a}(r) \\ \sum_{\bar{n}=1}^{\bar{n}_{\max}} g_{\bar{n}}^{(a)} R_{\bar{n}\bar{l}_a}(r) \end{pmatrix}$$

$$\begin{aligned} A_{nn'}^{RHF} &= (\alpha \cdot p + \beta M)_{nn'} + \sum_b \sum_{m,m'} f_m^{(b)} f_{m'}^{(b)} (v_{nmm'm'} - v_{nmm'n'}) \\ B_{n\bar{n}'}^{RHF} &= (\alpha \cdot p + \beta M)_{n\bar{n}'} + \sum_b \sum_{m,\bar{m}'} f_m^{(b)} g_{\bar{m}'}^{(b)} (v_{nm\bar{n}'\bar{m}'} - v_{nm\bar{m}'\bar{n}'}) \\ C_{\bar{n}\bar{n}'}^{RHF} &= (\alpha \cdot p + \beta M)_{\bar{n}\bar{n}'} + \sum_b \sum_{\bar{m},\bar{m}'} g_{\bar{m}}^{(b)} g_{\bar{m}'}^{(b)} (v_{\bar{n}\bar{m}\bar{n}'\bar{m}'} - v_{\bar{n}\bar{m}\bar{m}'\bar{n}'}) \end{aligned}$$

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



no pion

full pion

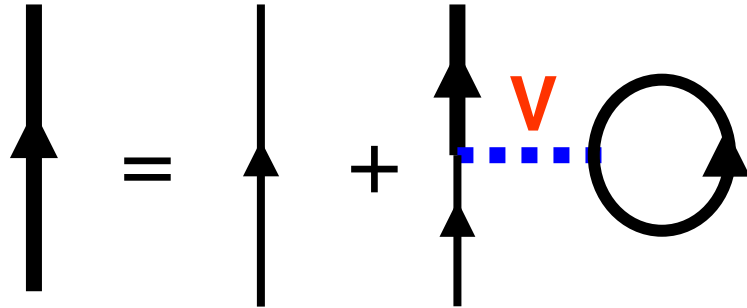
Lalazissis, Karatzikos, Serra, Otsuka, P.R., PRC 80 , 041301(R) (2009)

Further observations :

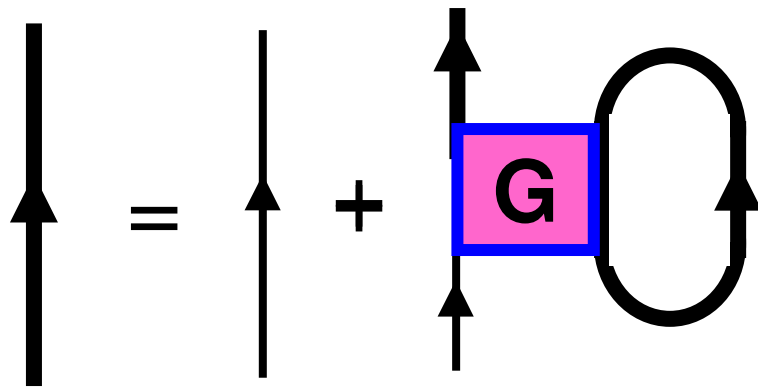
- **effective single particle energies in shell-model calculations show specific trends due to the tensor force, which agrees with many data (Otsuka, Schiffer, Greavy)**
- **the same trend can be found qualitatively if one adds a the pion with an effective coupling constant in fully selfconsistent RHF calculations (Lalazissis, Long)**
- **particle-vibrational coupling is also important**

How can we determine the tensor ?

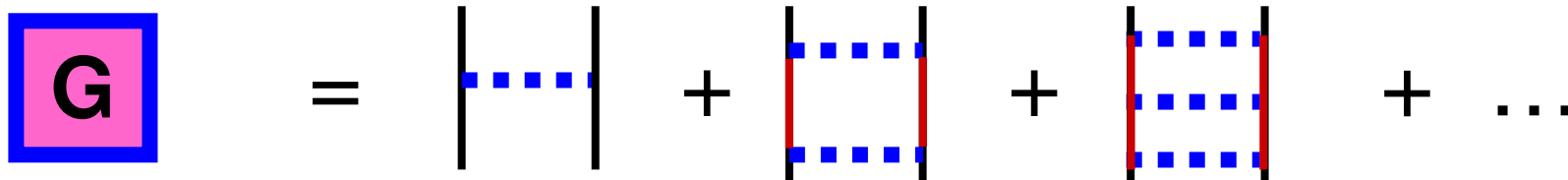
Ab-initio: Relativistic Brueckner Hartree-Fock:



Hartree-Fock



Brueckner Hartree-Fock



Summing up all ladder diagramms

Bethe-Goldstone equation:

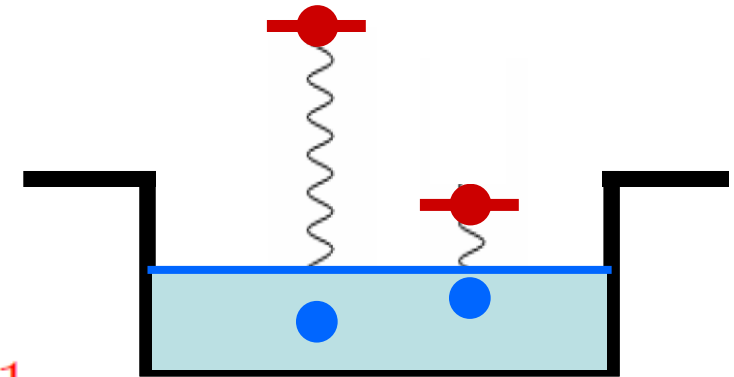
- ω is the starting energy
- V is realistic interaction
- Q_F is the Pauli operator

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

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

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

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



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

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

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:

Relativistic Brueckner Hartree-Fock (RBHF) equation

$$\sum_{n'} \left(\alpha \cdot p + \beta M + \beta \Gamma_{nn'}^{BHF} \right) \psi_{n'} = \epsilon_n \psi_n$$

where $\Gamma_{nn'}^{BHF}$ is related with the density matrix $\rho_{nn'}$

$$\Gamma_{nn'}^{BHF} = G_{nmm'n'} \rho_{mm'} - G_{nmm'n'} \rho_{mm'}$$

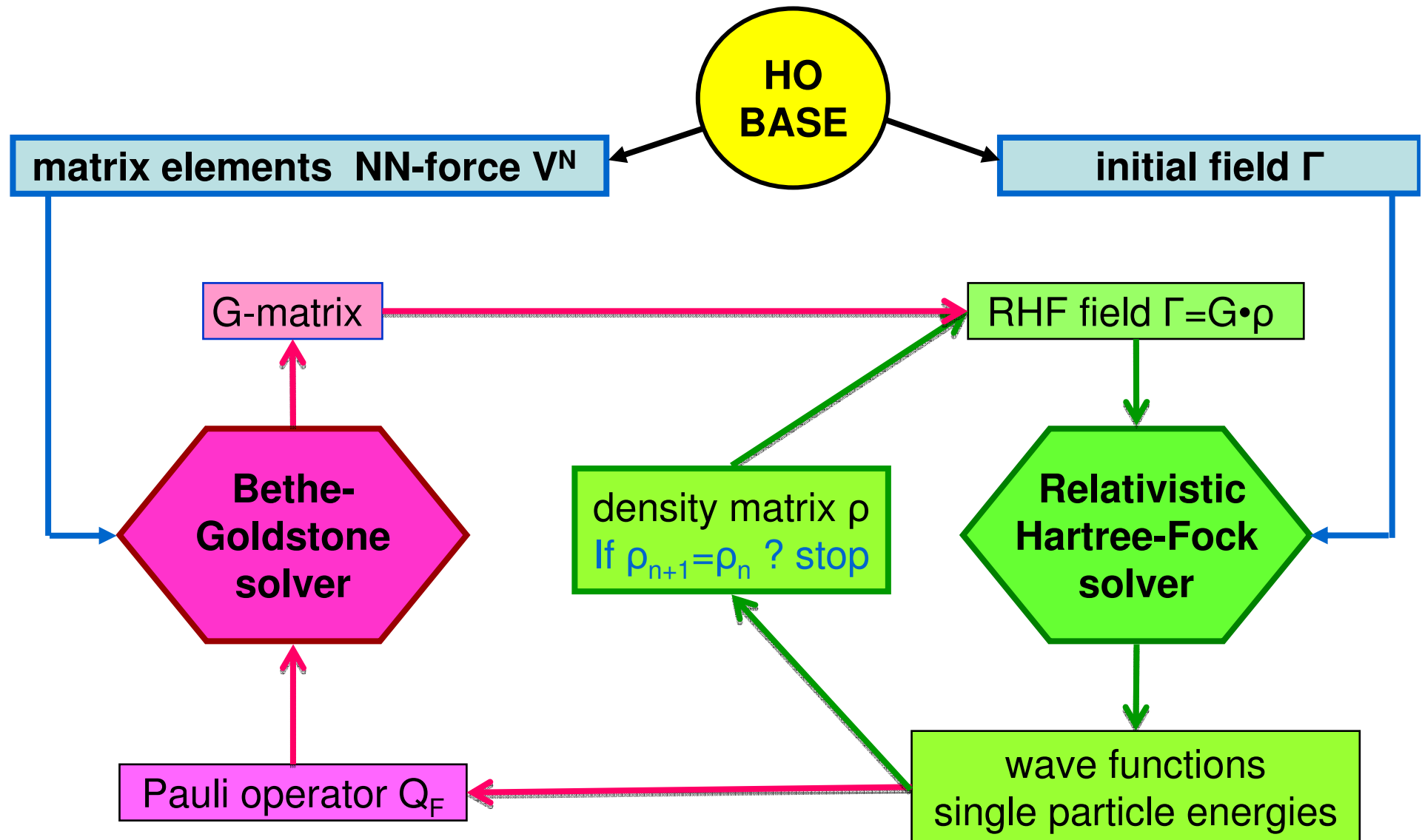
RHF equation in HO basis

$$\begin{pmatrix} A_{nn'}^{BHF} & B_{n\bar{n}'}^{BHF} \\ B_{\bar{n}n}^{BHF} & C_{\bar{n}\bar{n}'}^{BHF} \end{pmatrix} \begin{pmatrix} f_{n'}^{(a)} \\ g_{\bar{n}'}^{(a)} \end{pmatrix} = \epsilon_a \begin{pmatrix} f_n^{(a)} \\ g_{\bar{n}}^{(a)} \end{pmatrix}$$

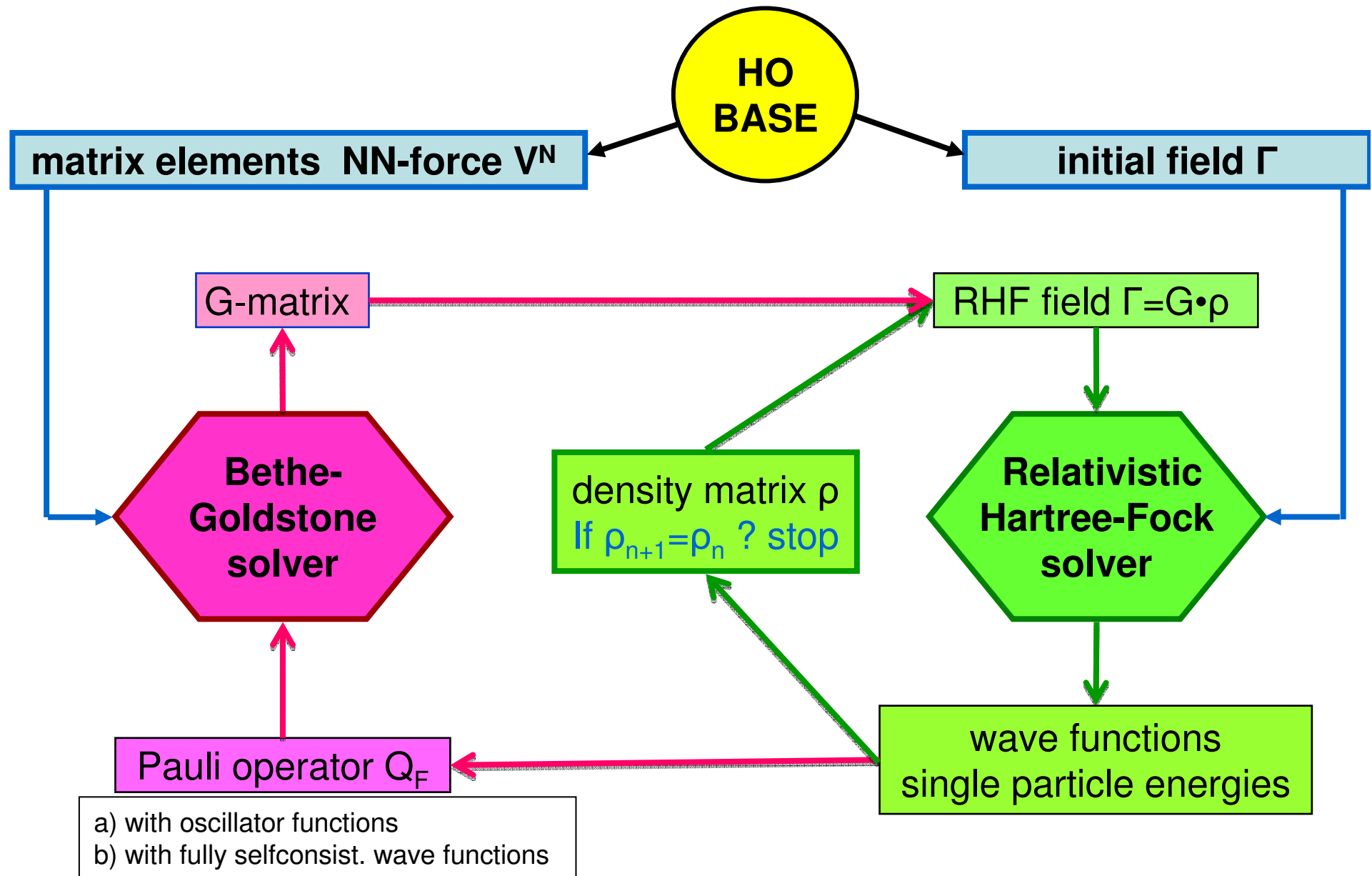
where

$$\begin{aligned} A_{nn'}^{BHF} &= (\alpha \cdot p + \beta M)_{nn'} + \sum_b \sum_{m,m'} f_m^{(b)} f_{m'}^{(b)} G_{nmm'n'} \\ B_{n\bar{n}'}^{BHF} &= (\alpha \cdot p + \beta M)_{n\bar{n}'} + \sum_b \sum_{m,\bar{m}'} f_m^{(b)} g_{\bar{m}'}^{(b)} G_{nm\bar{n}'\bar{m}'} \\ C_{\bar{n}\bar{n}'}^{BHF} &= (\alpha \cdot p + \beta M)_{\bar{n}\bar{n}'} + \sum_b \sum_{\bar{m},\bar{m}'} g_{\bar{m}}^{(b)} g_{\bar{m}'}^{(b)} G_{\bar{n}\bar{m}\bar{n}'\bar{m}'} \end{aligned}$$

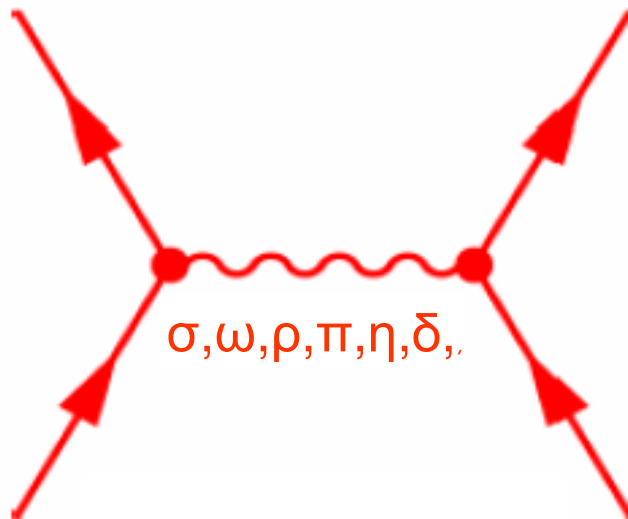
Flow chart for RBHF theory in finite nuclei:



Flow chart for RBHF theory in finite nuclei:



Bare nucleon-nucleon force:



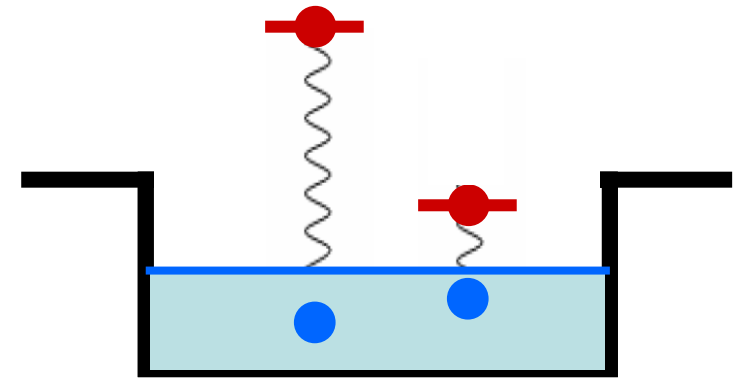
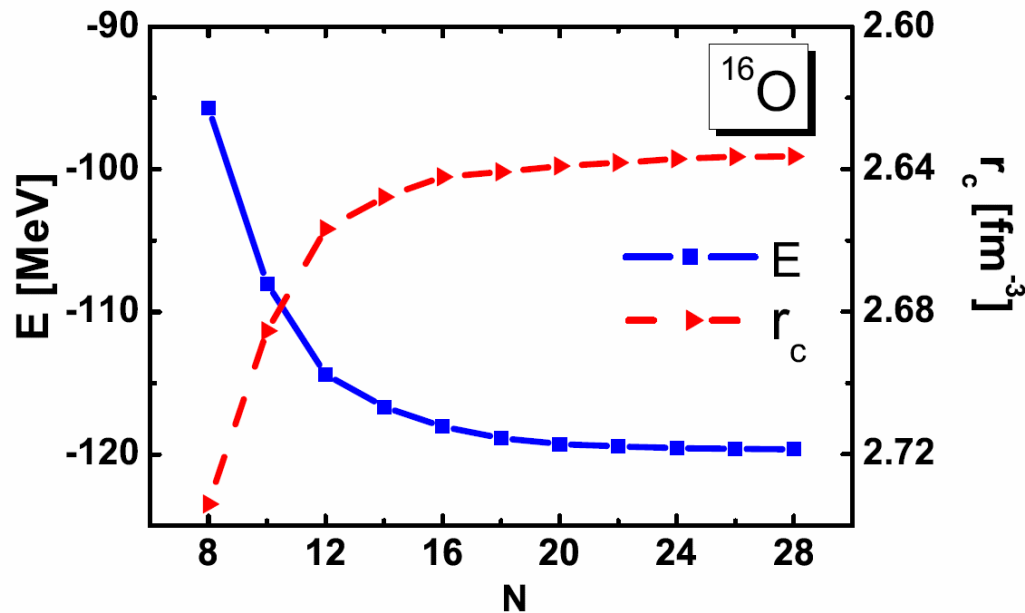
Brockmann and Machleidt, PRC **42**, 1965 (1990).

Meson Parameters	m_α (MeV)	Potential A		Potential B		Potential C	
		$g_\alpha^2/4\pi$	Λ_α (GeV)	$g_\alpha^2/4\pi$	Λ_α (GeV)	$g_\alpha^2/4\pi$	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

Results for ^{16}O

J. Hu, J. Meng, P. Ring to be published.

Convergence with the number of oscill. shells N :



Rel. HF code: Milena Serra, PRC 80, 41301 (2009)
Slater integrals: Horie and Sasaki, PTP 25, 475 (1961)

Local density approximation:

Bonn A

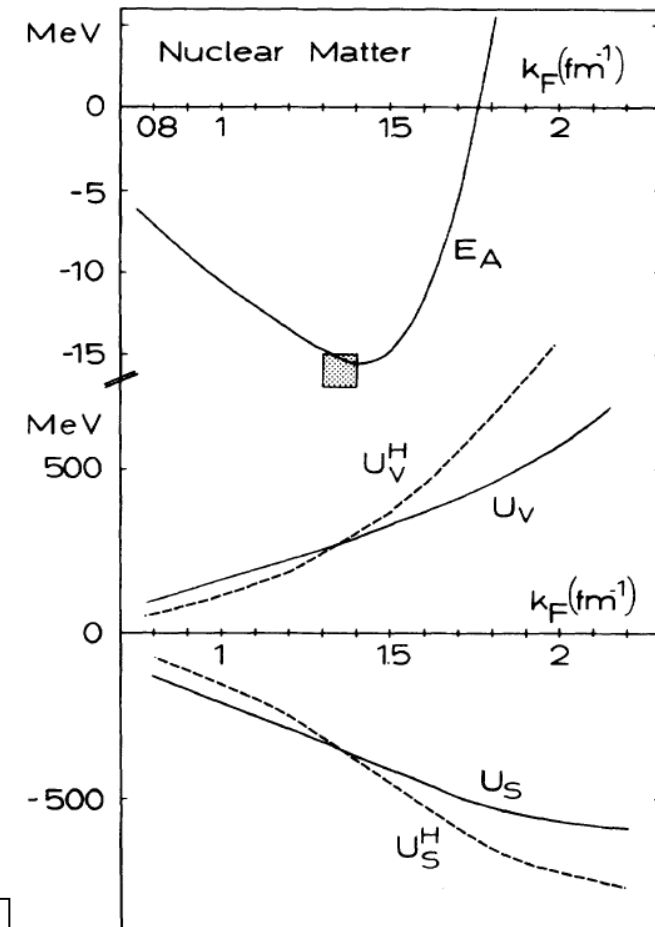
E/A Binding energy per particle
in Rel. Brückner-Hartree-Fock

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

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

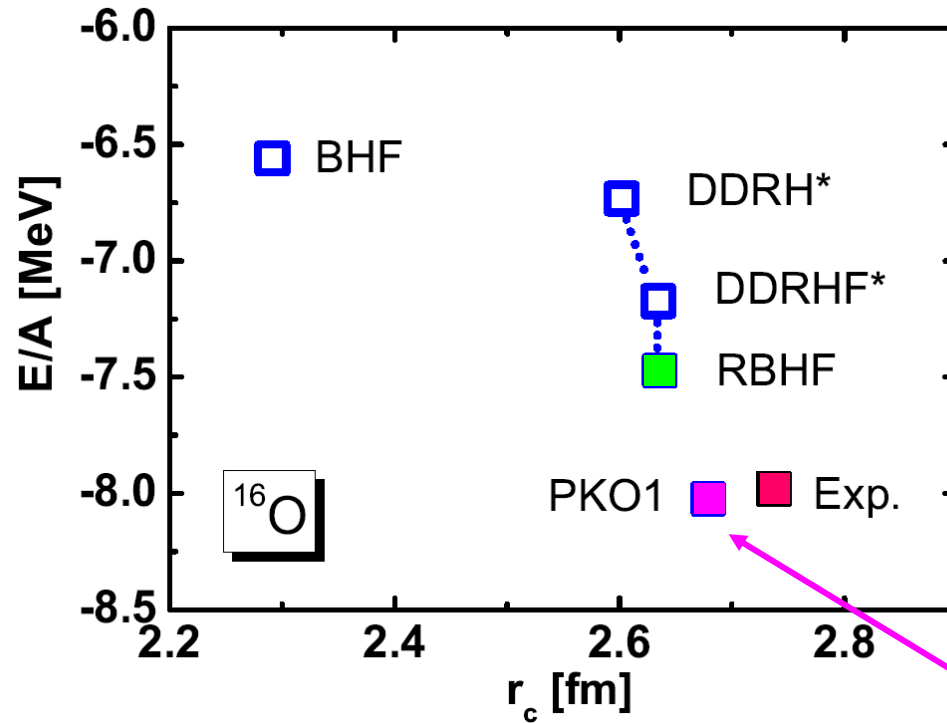
U_S^H, U_V^H : scalar and vector potential
in Relativistic Hartree

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



Results for ^{16}O

J. Hu, J. Meng, P. Ring to be published.



DDRH*: $g(\rho)$ in RH for finite nuclei is adjusted to the self-energy $\Sigma(\rho)$ Rel. BHF in nuclear matter with the density ρ

DDRHF*: $g(\rho)$ in RHF for finite nuclei is adjusted to the self-energy $\Sigma(\rho)$ Rel. BHF in nuclear matter with the density ρ

Results for ^{16}O

J. Hu, J. Meng, P. Ring to be published.

Fitted: PKO1:

	EXP.	RBHF	BHF	PKO1
E (MeV)	-127.62	-119.552	-104.96	-128.33
r_c (fm)	2.737	2.6357	2.291	2.693
$\varepsilon_{1p_{1/2}} - \varepsilon_{1p_{3/2}}$ (MeV)	6.3	4.1	7.5	6.4

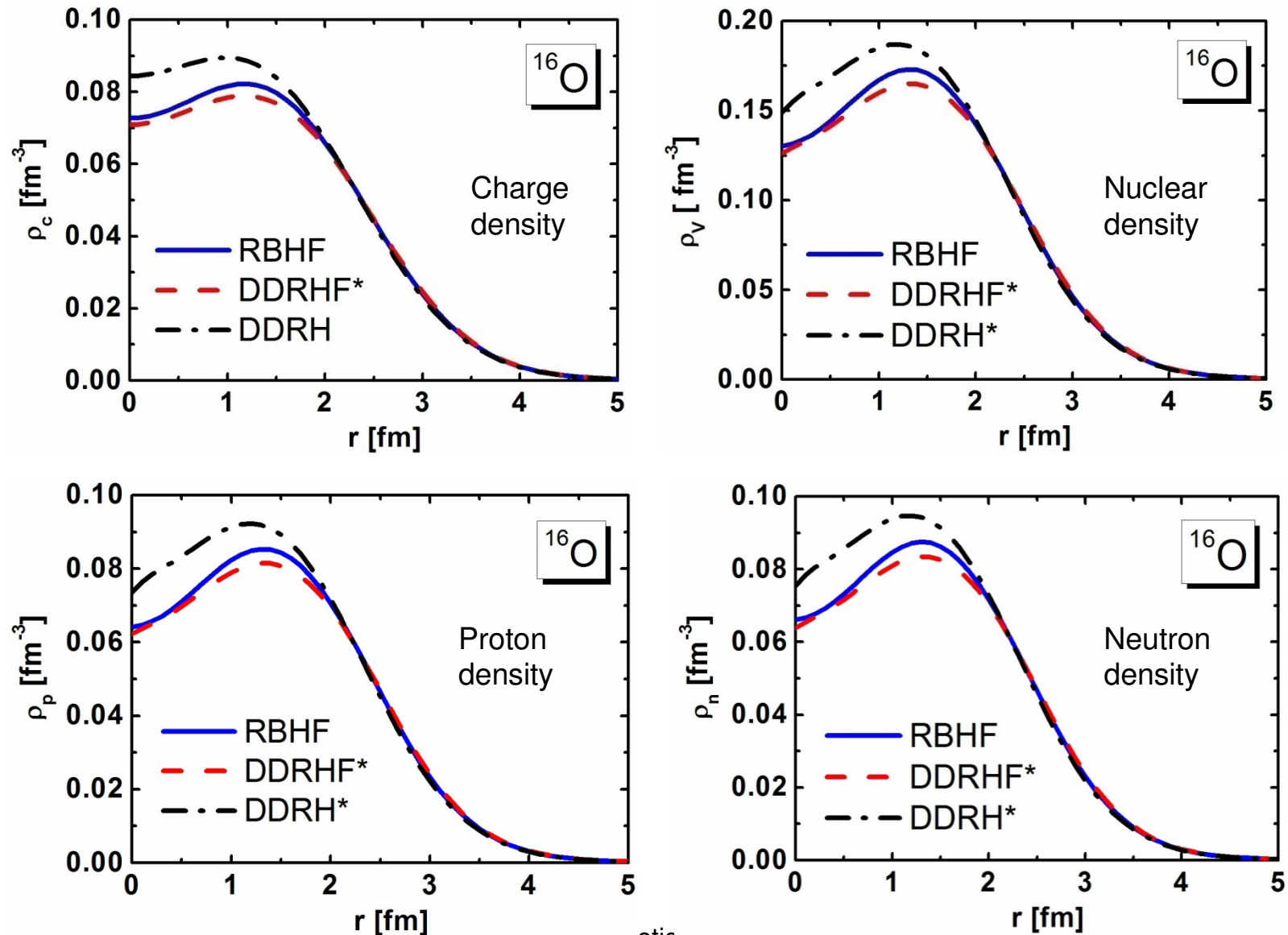
Ab-initio: Bonn A

	EXP.	DDRH*	DDRHF*	RBHF	CC N3LO
E (MeV)	-127.62	-107.72	-114.76	-119.55	-120.8
r_c (fm)	2.737	2.602	2.634	2.636	
$\varepsilon_{1p_{1/2}} - \varepsilon_{1p_{3/2}}$ (MeV)	6.3	5.2	4.8	4.1	

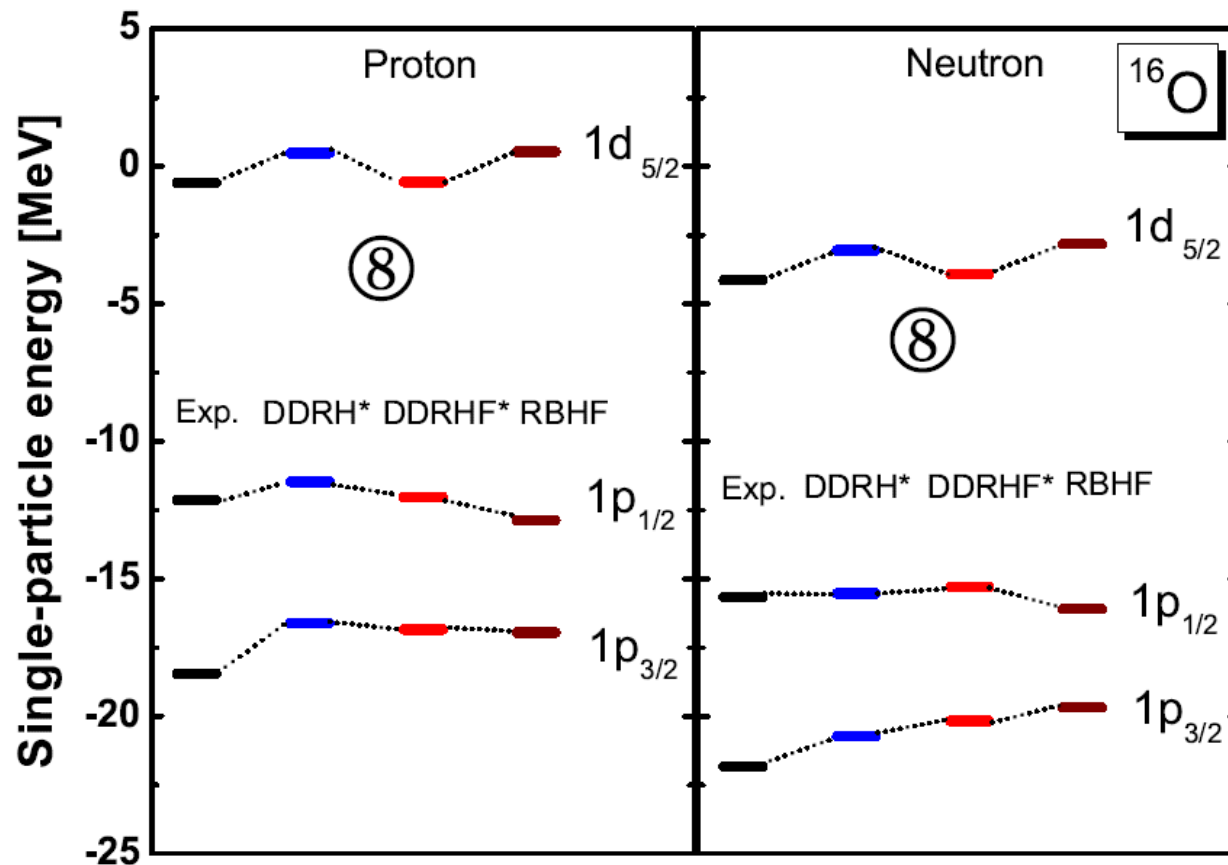
Hagen et al, PRC 80 (2009).

Nuclear densities in Brueckner theories:

The densities of ^{16}O in different theories

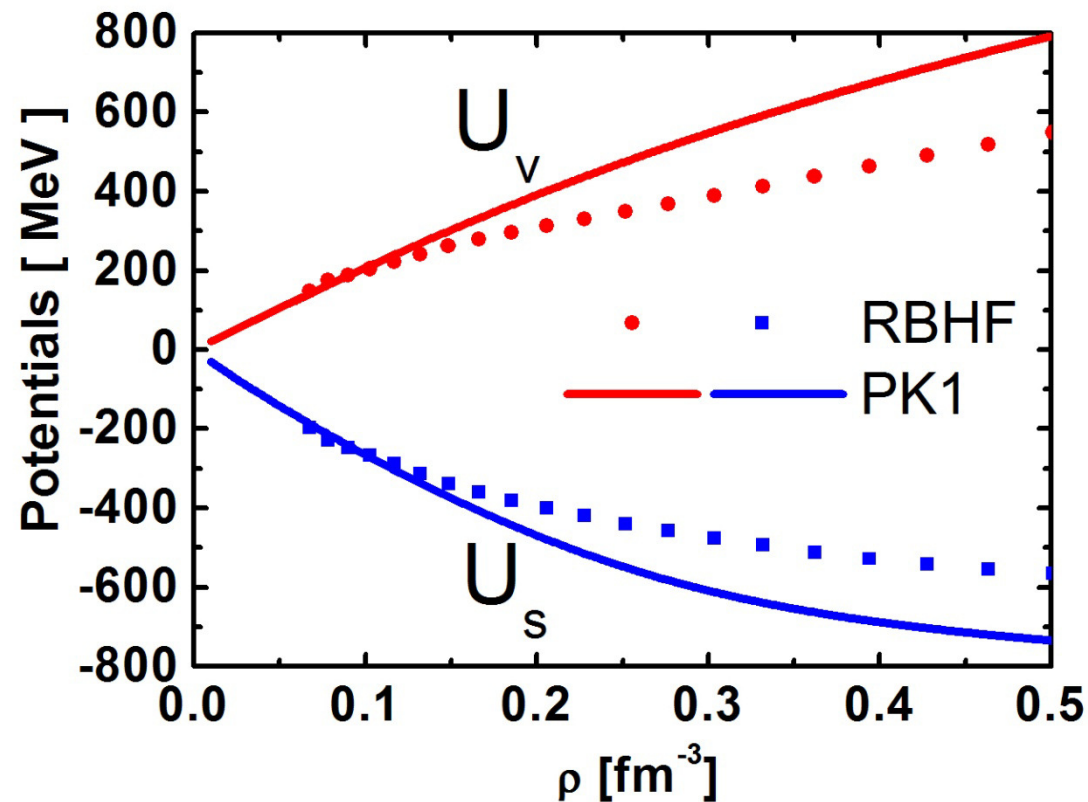


Single particle spectra for ^{16}O :



Spin-Orbit-splitting in RBHF theory:

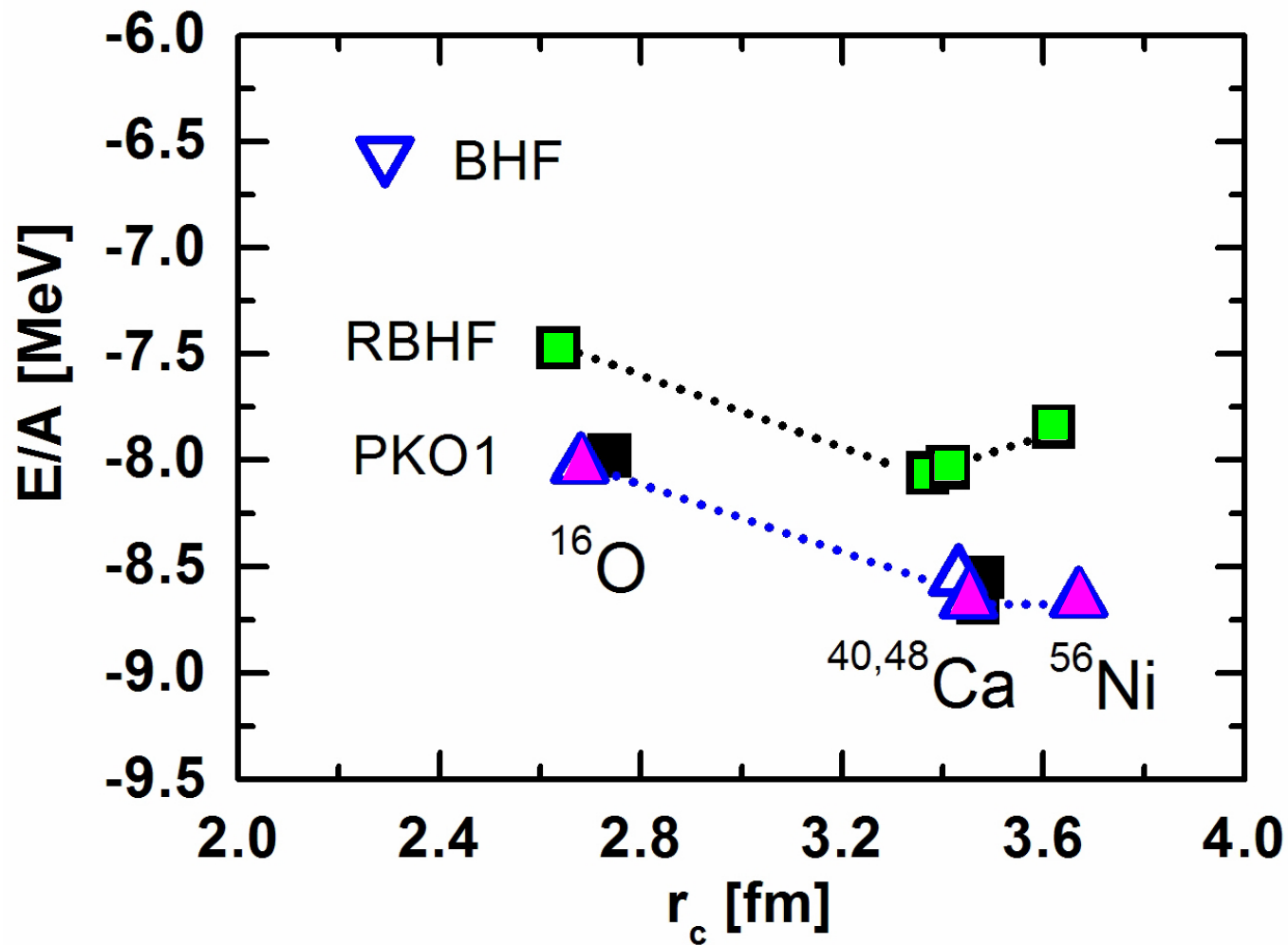
The scalar and vector potentials in RMF and RBHF theories:



Spin-orbit force in RMF theory:

$$U_{s.o.} \propto (U_v - U_s) \vec{L} \cdot \vec{S}$$

Properties for heavier nuclei in RBHF theory:



Properties for heavier nuclei in RBHF theory:

The ground state properties of other nuclei in RBHF theory

	E (MeV)			r_c (fm)			$\varepsilon_{1p_{1/2}} - \varepsilon_{1p_{3/2}}$ (MeV)		
	Exp.	RBHF	PKO1	Exp.	RBHF	PKO1	Exp.	RBHF	PKO1
^{14}C	−105.73	−98.49	−106.66	2.50	2.42	2.45	—	4.6	6.6
^{14}O	−98.73	−91.51	−100.48	—	2.67	2.68	—	—	—
^{40}Ca	−342.05	−322.41	−341.93	3.48	3.37	3.43	7.2	5.7	6.5
^{48}Ca	−416.16	−385.62	−415.62	3.47	3.41	3.45	4.3	3.1	6.2
^{56}Ni	−483.95	−439.26	−484.61	—	3.62	3.67	—	1.2	1.8

The deviations of binding energy between experiment and RBHF

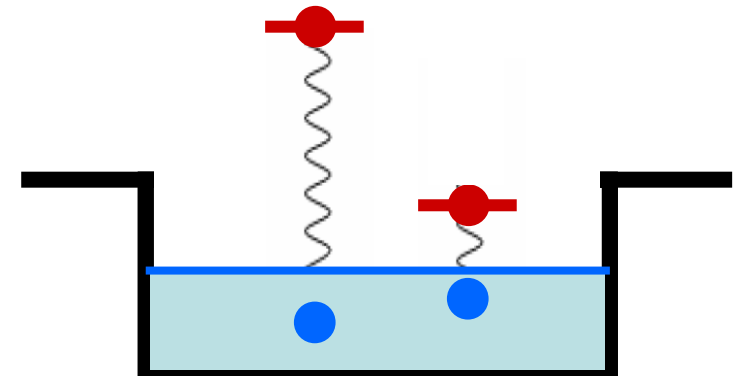
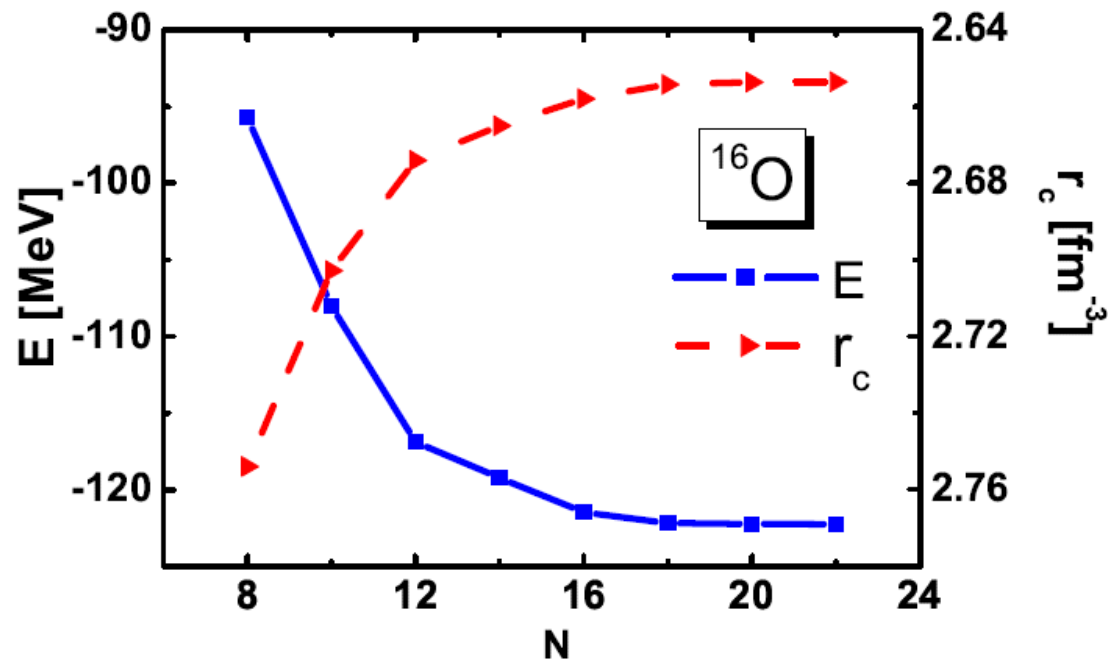
	^{14}C	^{14}O	^{16}O	^{40}Ca	^{48}Ca	^{56}Ni
$(E_{\text{exp.}} - E_{\text{RBHF}})/E_{\text{exp.}}(\%)$	6.85	7.31	6.32	5.74	7.34	9.23

- There is less than 10% underbinding in RBHF as compared with data
- The spin-orbit splitting is relatively small

Results for ^{16}O

J. Hu, J. Meng, P. Ring to be published.

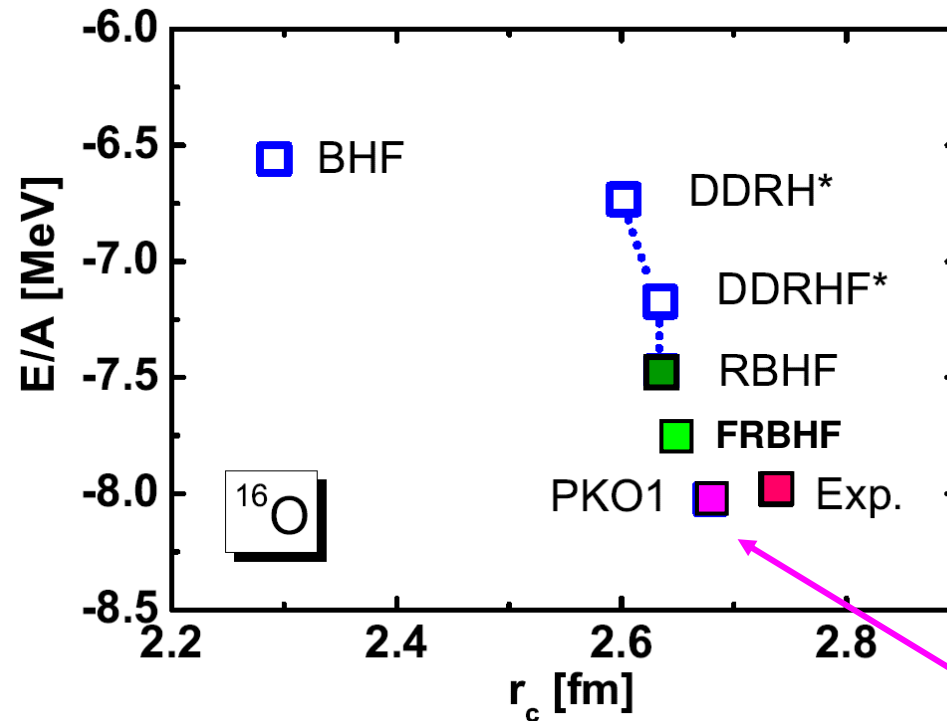
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Rel. HF code: Milena Serra, PRC 80, 41301 (2009)
Slater integrals: Horie and Sasaki, PTP 25, 475 (1961)

Results for ^{16}O

J. Hu, J. Meng, P. Ring to be published.



fitted

DDRH*: $g(\rho)$ in RH for finite nuclei is adjusted to the self-energy $\Sigma(\rho)$ Rel. BHF in nuclear matter with the density ρ

DDRHF*: $g(\rho)$ in RHF for finite nuclei is adjusted to the self-energy $\Sigma(\rho)$ Rel. BHF in nuclear matter with the density ρ

Results for ^{16}O

J. Hu, J. Meng, P. Ring to be published.

Fitted: PKO1:

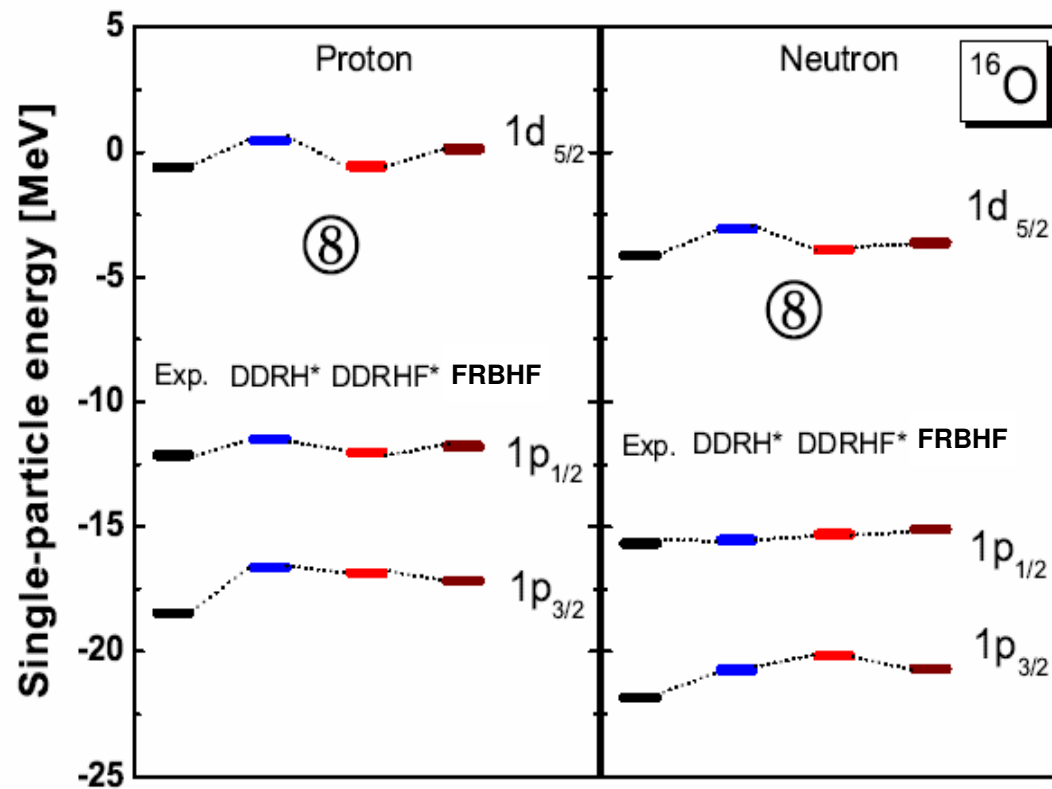
	EXP.	RBHF	BHF	PKO1
E (MeV)	-127.62	-119.552	-104.96	-128.33
r_c (fm)	2.737	2.6357	2.291	2.693
$\varepsilon_{1p_{1/2}} - \varepsilon_{1p_{3/2}}$ (MeV)	6.3	4.1	7.5	6.4

Ab-initio: Bonn A

	EXP.	DDRH*	DDRHF*	RBHF	FRBHF	CC N3LO
E (MeV)	-127.62	-107.72	-114.76	-119.55	-122.27	-120.8
r_c (fm)	2.737	2.602	2.634	2.636	2.653	
ΔE_{1p}^{ls} (MeV)	6.3	5.2	4.8	4.1	5.4	

Hagen et al, PRC 80 (2009).

Single particle spectra for ^{16}O :



Conclusions

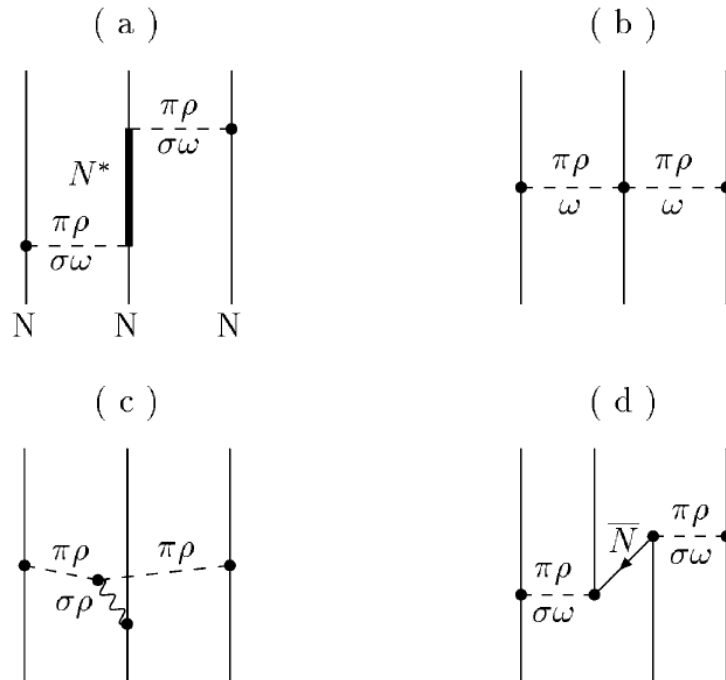
- Covariant density functional theory is very successful
- So far it is **phenomenological** (8-10 parameters)
- Semi-microscopic with only 4 parameters uses **microscopic input** (density dependence from BHF...)
- For the required accuracy (10^{-4}) we need fine-tuning
- Problem of additional terms in the Lagrangian (e.g. **tensor**)
- **Full ab initio** calculations in finite nuclei possible:
 - a) Hartree-Fock potential in **local density appr.**
 - b) Pauli operator expressed in **oscillator wave func.**
 - c) Full selfconsistent Rel. Brückner Hartree Fock.

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

Outlook

- Heavy nuclei without spin-saturation
- Importance of the tensor force
- Other microscopic forces (covariant chiral forces ?)
- Pairing and open shell nuclei
- Saxon-Woods basis
- Deformed nuclei
- Optical potential
-
- Importance of higher order in the hole-line expansion?
- Importance of three-body forces in relativistic systems?

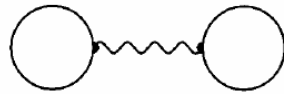
Microscopic origin of three body forces ?



W. Zuo, Lejeune, Lombardo, Mathiot, NPA 2002

- The major part comes from the anti-nucleon (relativistic),
- but the rest is not completely negligible, particular at high densities

Higher order terms in the hole-line expansion: (Bethe-Brueckner-Goldstone expansion)

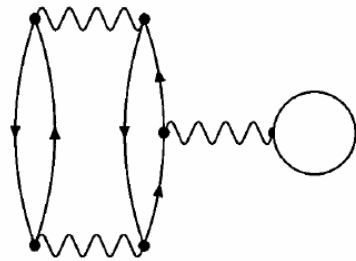


(c)

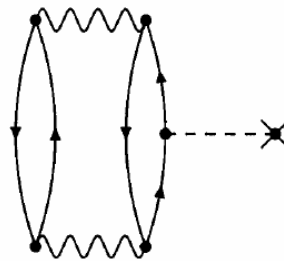


(d)

BHF

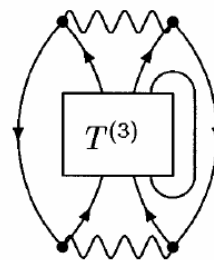
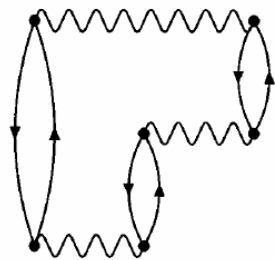


(e)



(f)

BBP-theorem



Bethe-Fadeev-eq.

Song et al PRL 8, (1998)

My Wishlist to “ab-initio” specialists:

- Microscopic pairing in nuclear matter:
 $\Delta_F(\rho)$, the **gap at the Fermi surface** for
symmetric nuclear matter in the 1S_0 channel
- Fully **relativistic chiral NN-forces**:
This would connect much better to QCD than
chiral symmetry.

Thanks to my collaborators:

Jinniu Hu (Beijing)
Jie Meng (Beijing)

M. Serra[†]

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

E. Litvinova (WMU, Kalamzoo, USA)
V. Tselyaev (St. Petersburg)

D. Vretenar (Zagreb)
T. Niksic (Zagreb)

Y. Tian (CIAE, Beijing)
Z.Y. Ma (CIAE, Beijing)

J. M. Yao (Chongqing)
Z. P. Li (Chongqing)
K. Hagino (Sendai)

X. Roca-Maza (Milano)
X. Vinas. (Barcelona)
P. Schuck (Orsay)