ECT* 30 June 2005

NUCLEAR ENERGY DENSITY FUNCTIONAL
constrained by
LOW-ENERGY QCD

Wolfram Weise
TUMünchen

Paolo Finelli   Stefan Fritsch   Norbert Kaiser   Dario Vretenar

- PRELUDE:
  an example of CHIRAL PERTURBATION THEORY at work

\- **SCALAR FIELD** and scalar form factor of the **NUCLEON** -

- NUCLEAR (CHIRAL) DYNAMICS

\- **In-medium CHIRAL PERTURBATION THEORY** and beyound -

\- **DENSITY FUNCTIONAL** strategies -

\- In-medium **QCD CONDENSATES** and **SPIN-ORBIT INTERACTION** -

\- Applications to **NUCLEAR MATTER** and **FINITE NUCLEI** -

LOW - ENERGY QCD

- **NUCLEI:** aggregates of quarks and gluons in the HADRONIC (low T) phase of QCD

- CONFINEMENT at $\mathbf{T} < \mathbf{T_{crit}} \simeq \mathbf{170}$ MeV

  ➡ Eigenstates of $\mathbf{H_{QCD}}$ are (colour-singlet) HADRONS

- Spontaneously broken CHIRAL SU(2) x SU(2) SYMMETRY:

  ➡ non-trivial VACUUM $|0\rangle$: CHIRAL (QUARK) CONDENSATE

  $$|\langle\bar{\mathbf{q}}\mathbf{q}\rangle| \simeq 1.5\, fm^{-3}$$

  ➡ low-mass collective excitations : GOLDSTONE BOSONS (PIONS)
  ... interact weakly at low energy / momentum

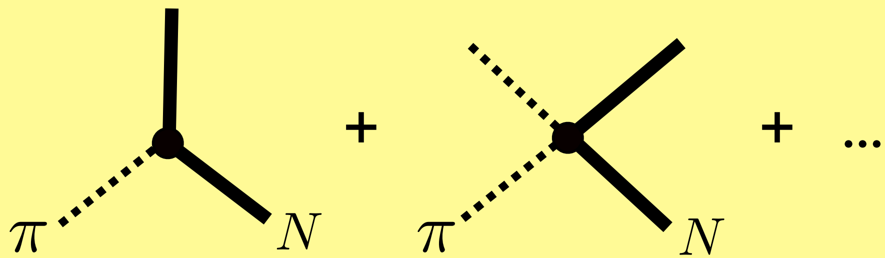
  ➡ order parameter: PION DECAY CONSTANT $\mathbf{f}_\pi = 92.4\, MeV$

  ➡ characteristic MASS GAP in the hadron spectrum: $4\pi\, \mathbf{f}_\pi \sim 1\, GeV$

PION-NUCLEON EFFECTIVE LAGRANGIAN

$$\mathcal{L}_N = \bar{\Psi}_N \left[i\gamma_\mu(\partial^\mu - i\mathcal{V}^\mu) - M_0 + g_A \gamma_\mu \gamma_5 \mathcal{A}^\mu \right] \Psi_N + \ldots$$

$$- \bar{\Psi}_N \, \mathcal{S} \, \Psi_N + \ldots$$ higher orders



effects of $\mathbf{\Delta(1230)}$;
short distance physics

$$\mathcal{A}^\mu = \frac{1}{2f_\pi} \vec{\tau} \cdot \partial^\mu \vec{\pi} + \ldots \; ; \quad \mathcal{V}^\mu = \frac{1}{4f_\pi^2} \vec{\tau} \cdot (\vec{\pi} \times \partial^\mu \vec{\pi}) + \ldots \; ; \quad \mathcal{S} = \sigma_N \left(1 - \frac{\vec{\pi}^2}{2f_\pi^2} + \ldots \right)$$

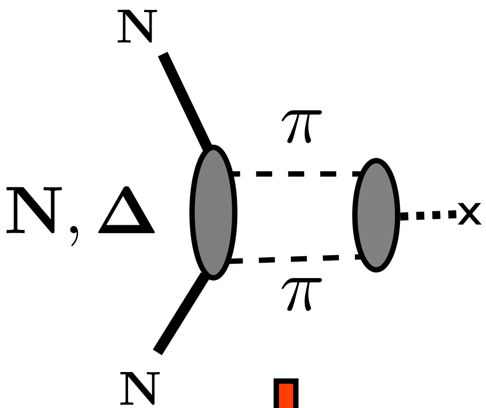
AXIAL VECTOR　　VECTOR　　SCALAR

$$\mathbf{f}_\pi = \mathbf{92.4\,MeV} \qquad \mathbf{g_A} = \mathbf{1.267}$$

$$\sigma_N = \langle N | \mathbf{m_u \, \bar{u}u + m_d \, \bar{d}d} | N \rangle \simeq \mathbf{50\,MeV}$$

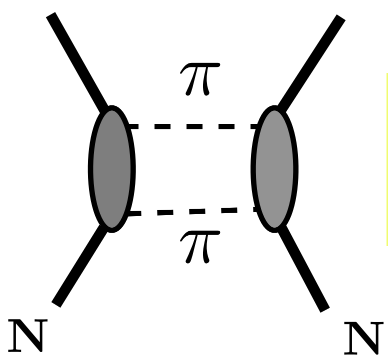
SCALAR FORMFACTOR of the NUCLEON

$$\sigma_N(Q^2) = \sigma_N - Q^2 \int_{4m_\pi^2}^{\infty} dt \, \frac{\eta(t)}{t(Q^2+t)}$$



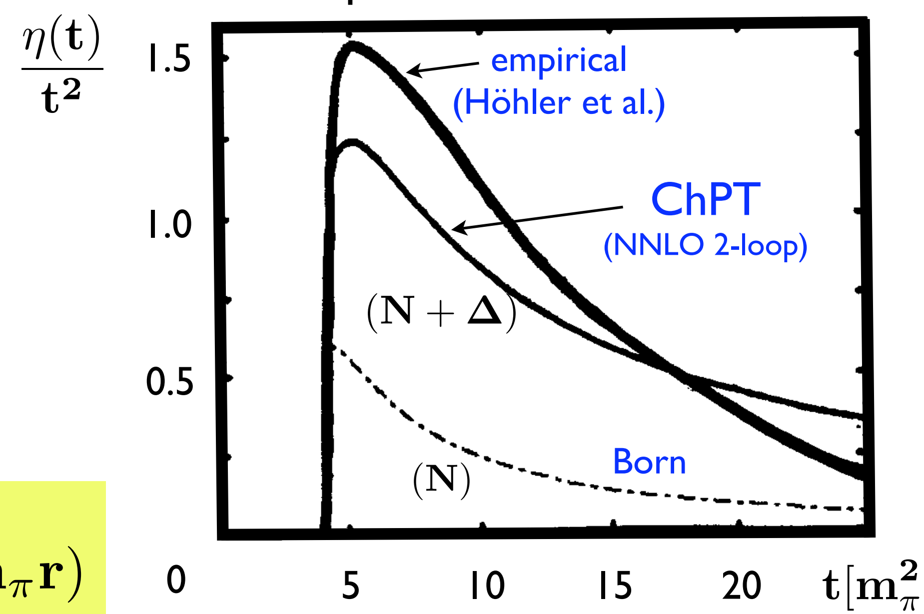
strong SCALAR field

van der Waals - type NN interaction



$$V(r) \sim \frac{e^{-2m_\pi r}}{r^6} P(m_\pi r)$$

spectral distribution



N. Kaiser
Phys. Rev. C68 (2003) 025202

Earlier phenomenology:

"2nd order tensor force"
G.E. Brown & T.T.S. Kuo ('65)

"Spin-isospin polarizability of the nucleon"
M. Ericson & A. Figureau ('81)

SCALAR RADIUS of the NUCLEON:

$$\sqrt{\langle r_s^2 \rangle} \simeq 1.3\ \mathrm{fm}$$

(Gasser, Leutwyler, Sainio (1991))

CHIRAL DYNAMICS and the NUCLEAR MANY-BODY PROBLEM

N. Kaiser, S. Fritsch, W.W. (2002 - 2003)

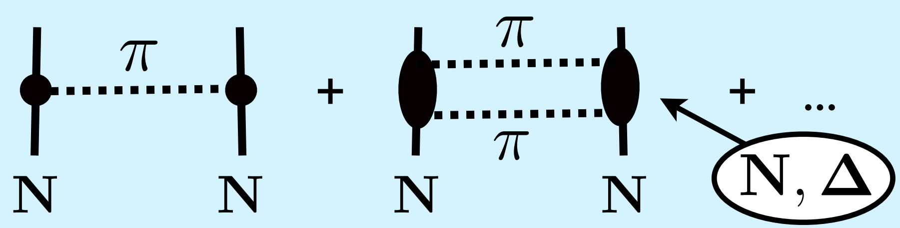
- additional relevant scale: Fermi momentum

  “small” scales: $\mathbf{k_F \sim 2m_\pi \sim M_\Delta - M_N << 4\pi\, f_\pi^2}$

- treat PIONS and DELTA isobars as EXPLICIT degrees of freedom

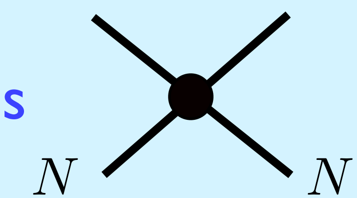
- IN-MEDIUM CHIRAL PERTURBATION THEORY

  ➡ pion exchange processes in the presence of a filled Fermi sea



“ in medium”

  ➡ short-distance dynamics: contact interactions



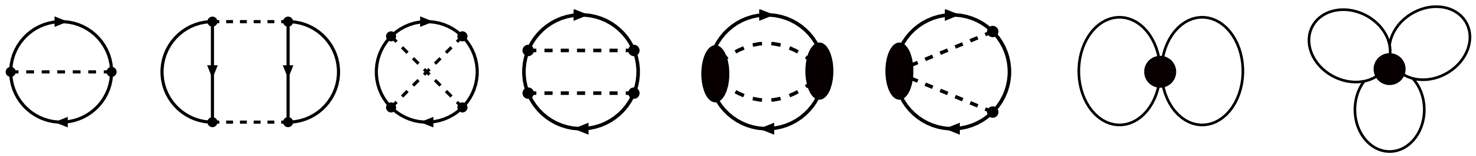
- IN-MEDIUM nucleon propagator:

$$(\gamma \cdot p + M)\left[\frac{i}{p^2 - M^2 + i\epsilon} - 2\pi\delta(p^2 - M^2)\theta(p_0)\theta(k_F - |\mathbf{p}|)\right]$$

- Expansion of ENERGY DENSITY in powers of Fermi momentum k_F

NUCLEAR MATTER

- Expansion of ENERGY DENSITY in powers of Fermi momentum k_F



$$\frac{\mathbf{E(k_F)}}{\mathbf{A}} = \sum_{\mathbf{n}} \mathcal{F}_{\mathbf{n}}(\mathbf{k_F}/\mathbf{m}_\pi, \mathbf{k_F}/\mathbf{\Delta})\ \mathbf{k_F^n}$$

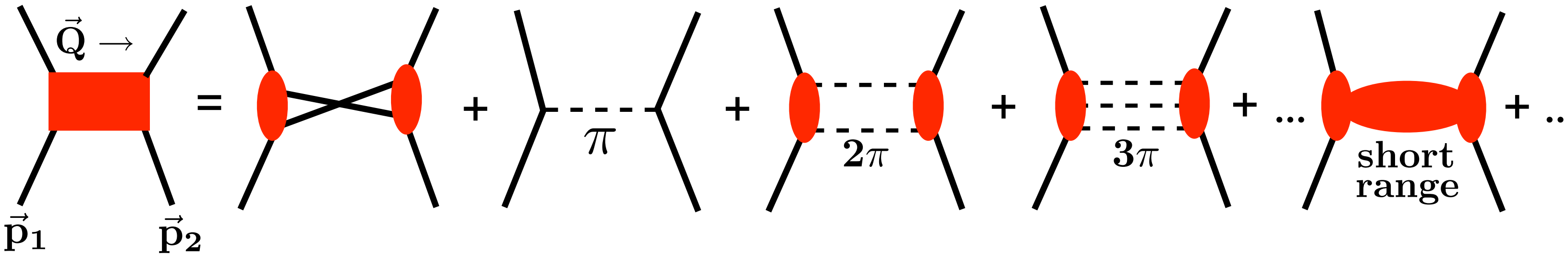
$$= \frac{\mathbf{3}}{\mathbf{10}} \frac{\mathbf{k_F^2}}{\mathbf{M_N}} + \mathcal{C}_3 \frac{\mathbf{k_F^3}}{\mathbf{M_N^2}} + \mathcal{C}_4 \frac{\mathbf{k_F^4}}{\mathbf{M_N^3}} + \mathcal{C}_5 \frac{\mathbf{k_F^5}}{\mathbf{M_N^4}} + \mathcal{C}_6 \frac{\mathbf{k_F^6}}{\mathbf{M_N^5}} + \mathcal{O}(\mathbf{k_F^7})$$

- 2 low-energy (subtraction) constants / contact terms included in $\mathcal{C}_3$ and $\mathcal{C}_5$
- $\mathcal{C}_4$: model-independent
- $\mathcal{C}_6$: 3 - body contact terms at $\mathcal{O}(\mathbf{k_F^6})$
- at low densities: agreement with universal "V(low-k)" from realistic NN potentials

S.K. Bogner, T.T.S. Kuo, A. Schwenk; Phys. Reports 386 (2003) 1

EFFECTIVE INTERACTION: SCALES at WORK

- Nucleon-nucleon amplitude "in-medium"

$\mathbf{T(Q^2; k_F)}$ 

particle-hole excitations — one- and two-pion exchange — short-distance dynamics

- Spectral representation:

$$\mathbf{T(Q^2; k_F) = T^{(0)} + \frac{Q^2}{\pi} \sum_n \int_{\mu_n^2}^{\infty} dt \, \frac{\eta_n(t; k_F)}{t(t + Q^2)}}$$

- $|\vec{\mathbf{p}}_{1,2}| \leq \mathbf{k_F}$, $\mathbf{Q \sim k_F}$:

➡ treat terms with $\mu_n \leq \mathbf{k_F}$ EXPLICITLY (long and intermediate range)

➡ approximate integrals with $\mu_n > \mathbf{Q \sim k_F}$ as $\mathbf{\frac{Q^2}{\pi} \sum_n \int_{\mu_n^2}^{\infty} dt \, \frac{\eta_n(t; k_F)}{t^2}}$

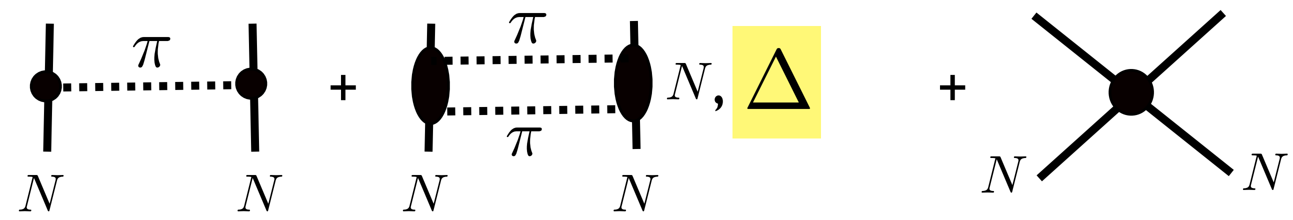
CONTACT term $\mathbf{T^{(0)}}$ plus finite range corrections $\sim \mathbf{Q^2 \langle r_n^2 \rangle}$

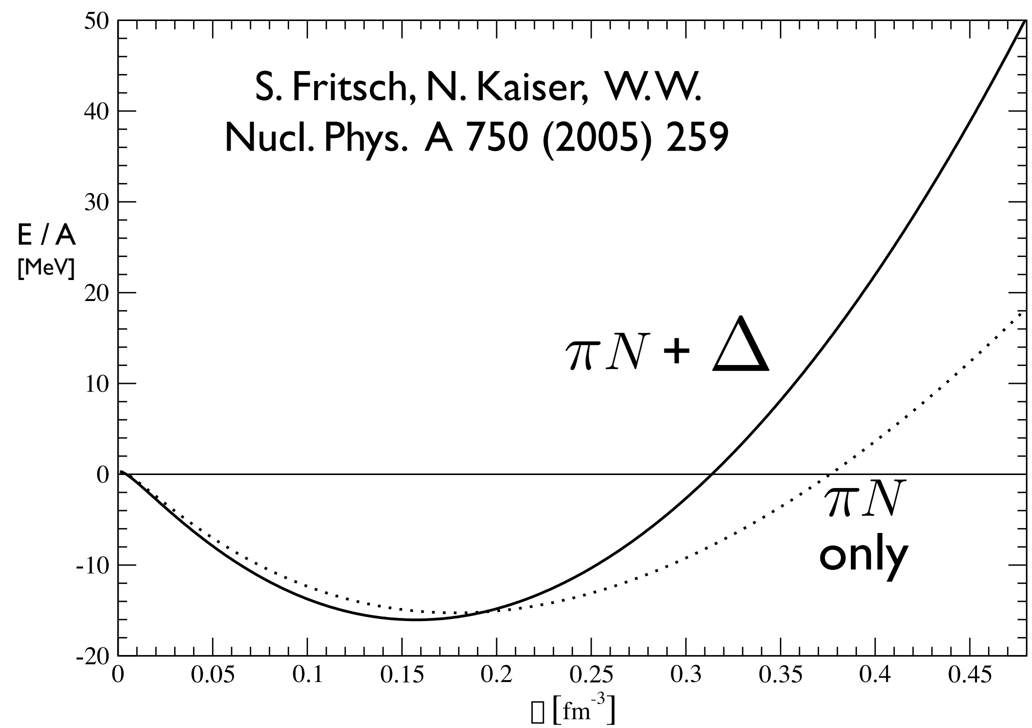
ROLE of Δ(1232)

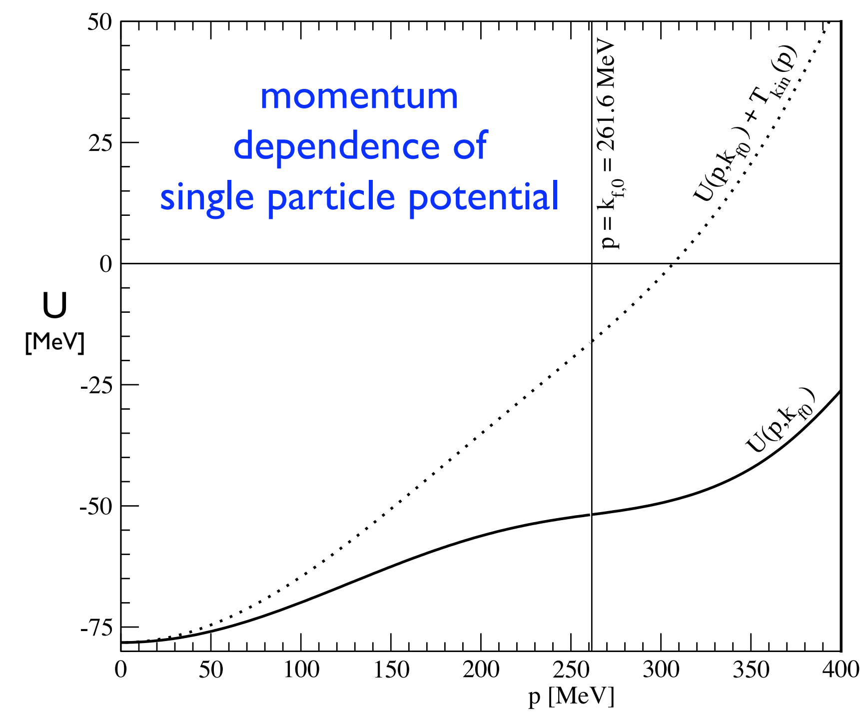
- **Mass difference** $\mathbf{M_\Delta - M_N \sim k_f \sim 2m_\pi << 4\pi\, f_\pi}$

"small scale"; large SPIN-ISOSPIN POLARIZABILITY of the nucleon:

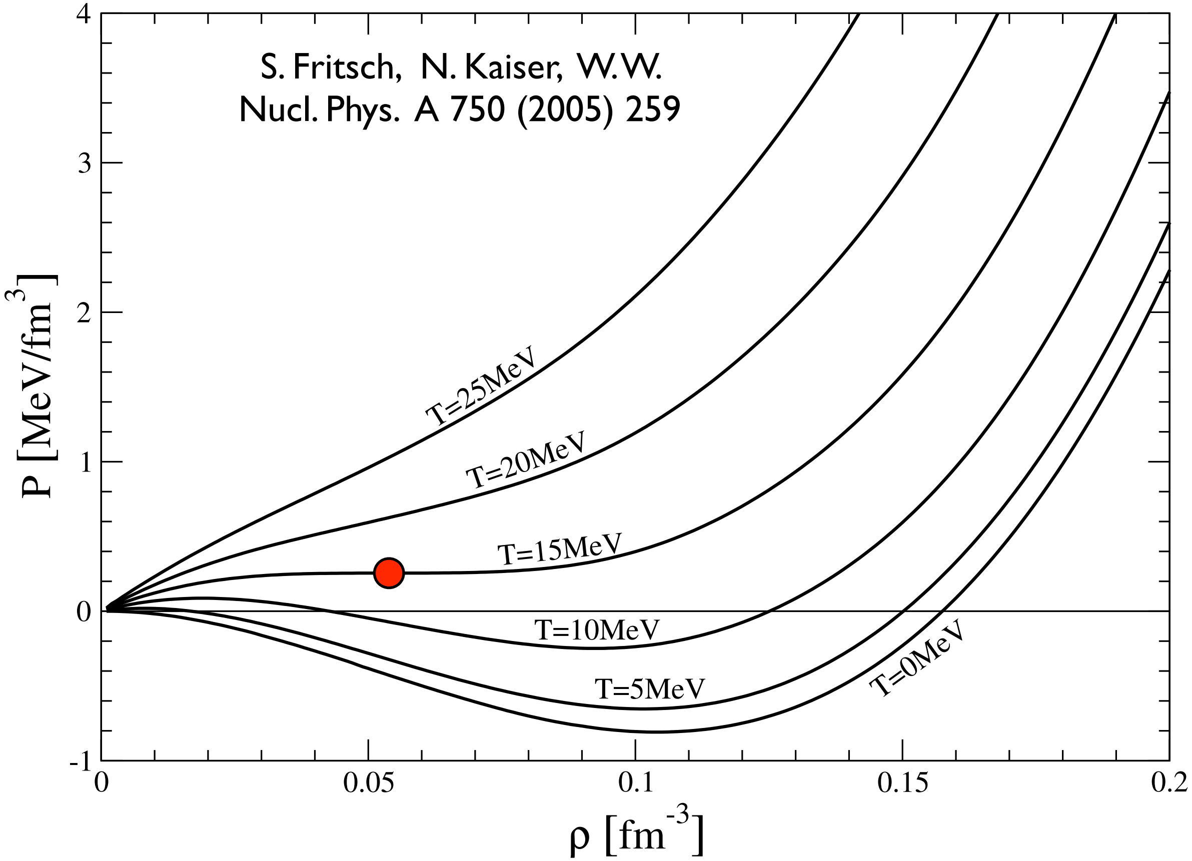
$$\chi_\Delta = \frac{\mathbf{g_A^2}}{\mathbf{f_\pi^2 (M_\Delta - M_N)}} \simeq \mathbf{5\,fm^3}$$



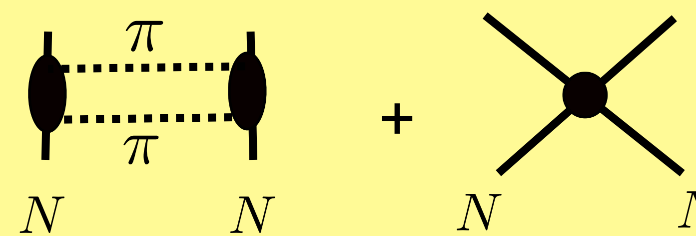




NUCLEAR THERMODYNAMICS



CHIRAL PION DYNAMICS
("Pionic van der Waals + Pauli")

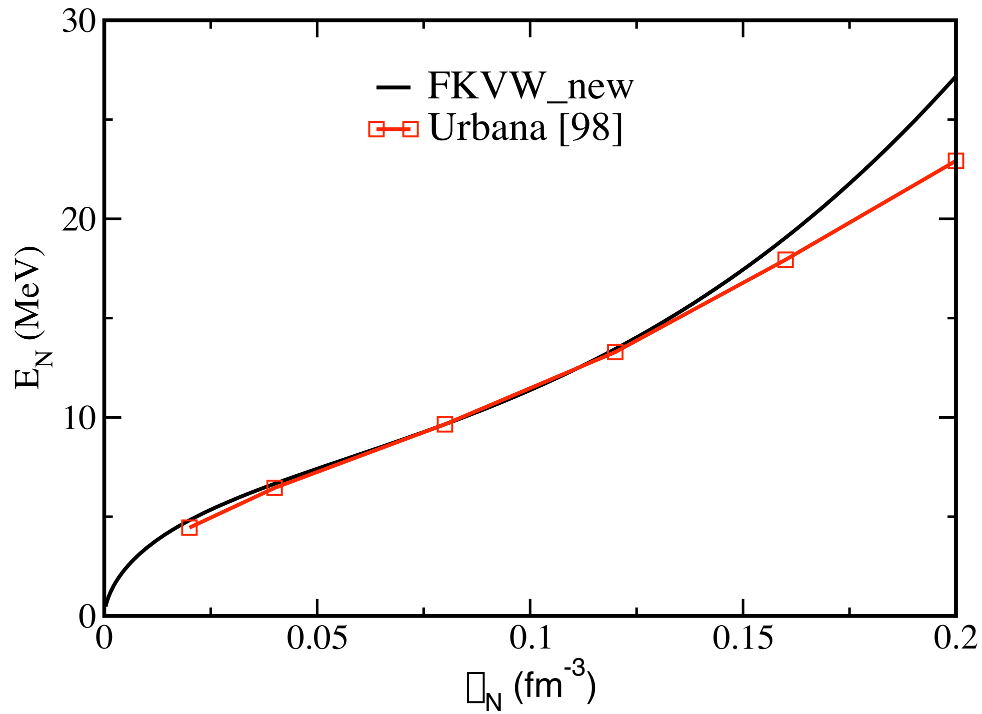


... plus contact terms

Liquid - Gas Transition at
Critical Temperature T_c = 15 MeV
(empirical: T_c = 16 - 18 MeV)

NEUTRON MATTER

- Isospin - dependent forces primarily from two-pion exchange
- 2 low-energy (subtraction) constants / contact terms



P. Finelli, N. Kaiser, D.Vretenar, W.W.
Nucl. Phys. A 735 (2004) 449
and preprint (2005)

- Asymmetry energy for isospin - asymmetric nuclear matter:

$\mathcal{A} = \mathbf{34.0\,MeV}$ (empirical: $\mathcal{A} = \mathbf{33 - 36\,MeV}$)

INHOMOGENOUS SYSTEMS: connection with (non-relativistic) density functional

S. Fritsch, N. Kaiser, W.W.: Nucl. Phys. A 724 (2003) 47, Nucl. Phys. A 750 (2005) 259

local density

$$\rho(\vec{\mathbf{r}}) = \frac{2\mathbf{k_F^3}(\vec{\mathbf{r}})}{3\pi^2} = \sum_{\alpha\in\mathbf{F}} \psi_\alpha^\dagger(\vec{\mathbf{r}})\psi_\alpha(\vec{\mathbf{r}})$$

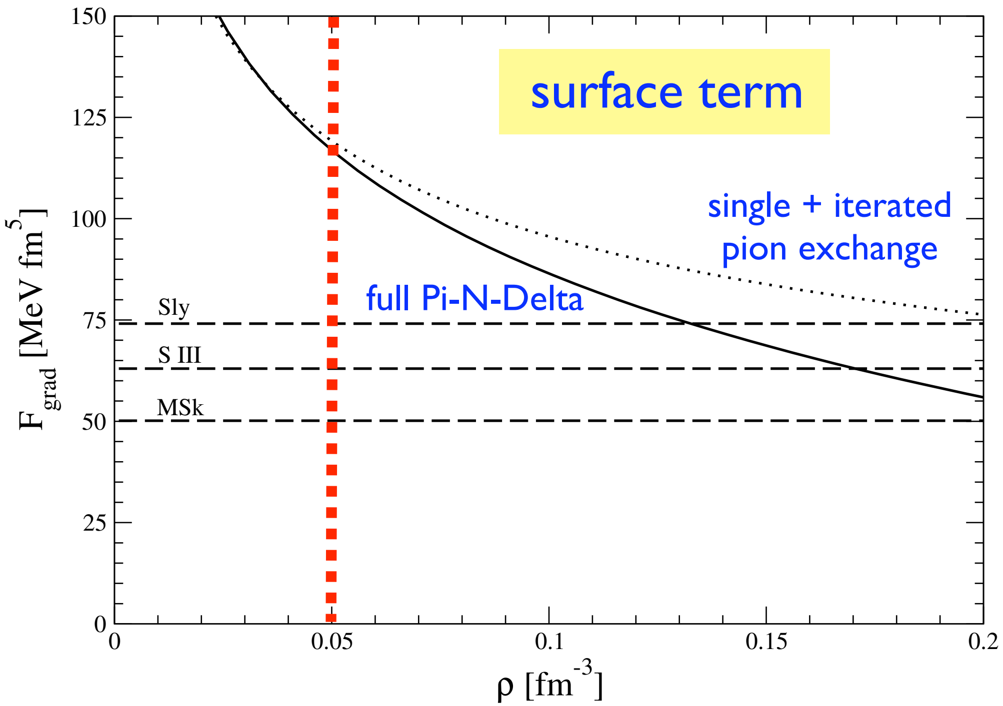
kinetic energy density

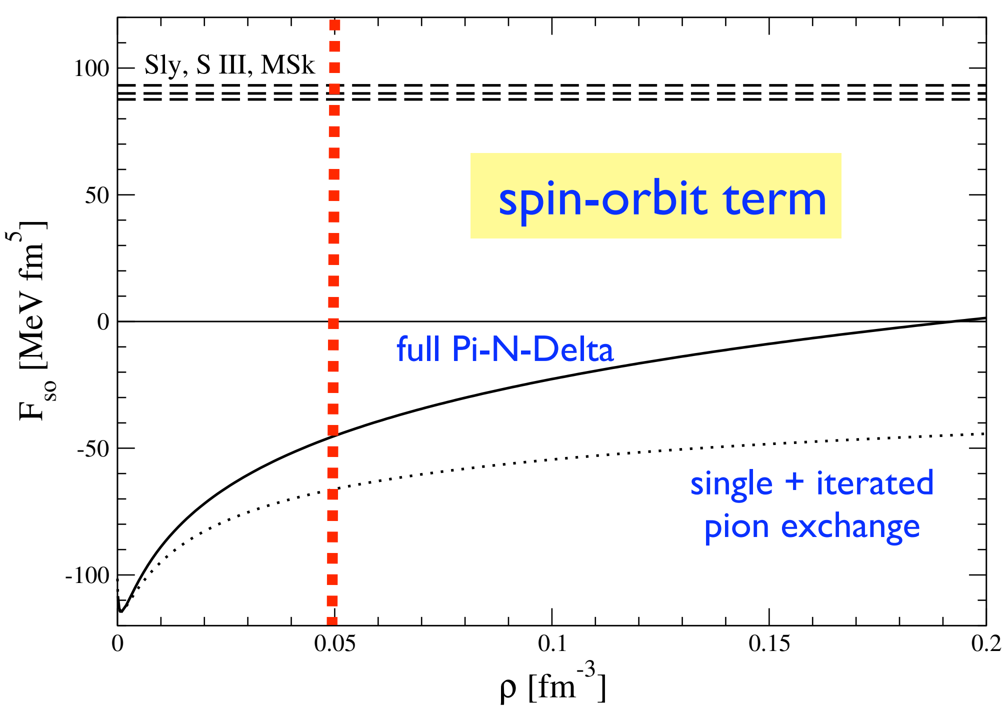
$$\tau(\vec{\mathbf{r}}) = \sum_{\alpha\in\mathbf{F}} \nabla\psi_\alpha^\dagger(\vec{\mathbf{r}})\cdot\nabla\psi_\alpha(\vec{\mathbf{r}})$$

spin-orbit density

$$\mathbf{J}(\vec{\mathbf{r}}) = \sum_{\alpha\in\mathbf{F}} \psi_\alpha^\dagger(\vec{\mathbf{r}})i\vec{\sigma}\times\nabla\psi_\alpha(\vec{\mathbf{r}})$$

$$\mathcal{E}[\rho,\tau,\mathbf{J}] = \frac{\mathbf{E}(\mathbf{k_F})}{\mathbf{A}}\rho + \left(\tau - \frac{3}{5}\rho\,\mathbf{k_F^2}\right)\left[\frac{1}{2\mathbf{M_N}} - \mathbf{F}_\tau(\mathbf{k_F})\right] + (\nabla\rho)^2\,\mathbf{F_{grad}}(\mathbf{k_F}) + \nabla\rho\cdot\mathbf{J}\,\mathbf{F_{so}}(\mathbf{k_F}) + \ldots$$





FINITE NUCLEI: DENSITY FUNCTIONAL STRATEGIES

- ... towards a relativistic DENSITY FUNCTIONAL ...

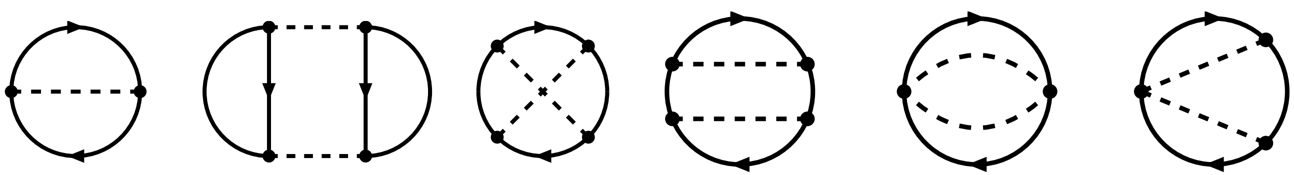
(see e.g.: R. Furnstahl et al., B. Serot, in: Lecture Notes in Phys. 641 (2004))

... constrained by
(in-medium) CHIRAL PERTURBATION THEORY and QCD SUM RULES

(P. Finelli, N. Kaiser, D. Vretenar, W. W., Eur. Phys. J. A 17 (2003) 573, Nucl. Phys. A 735 (2004) 449)

$$\mathbf{E}[\rho] = \mathbf{E_{kin}} + \int \mathbf{d^3x}\,[\mathcal{E}^{(\mathbf{0})}(\rho) + \mathcal{E}_{\mathbf{exc}}(\rho)] + \mathbf{E_{coul}} \quad ; \qquad \rho = \sum_{i=1}^{A} |\psi_i\rangle\langle\psi_i|$$

- $\mathcal{E}_{\mathbf{exc}}(\rho)$: from in-medium ChPT ("Pionic fluctuations")



- $\mathcal{E}^{(\mathbf{0})}(\rho)$: strong SCALAR and VECTOR mean fields generated by IN-MEDIUM changes of QCD CONDENSATES

(Drukarev, Levin (1990); Cohen, Furnstahl, Griegel (1991))

$$\mathbf{\Sigma_S^{(0)}} = \mathbf{M}^*(\rho) - \mathbf{M} = -\mathbf{M}\frac{\sigma_\mathbf{N}}{\mathbf{2m_q}}\frac{\rho_\mathbf{S}}{|\langle\bar{\mathbf{q}}\mathbf{q}\rangle_{\mathbf{vacuum}}|} \sim -\frac{\mathbf{M}}{\mathbf{3}}\frac{\rho}{\rho_\mathbf{0}}\,; \qquad \mathbf{\Sigma_V^{(0)}} \simeq -\mathbf{\Sigma_S^{(0)}}$$

FINITE NUCLEI
- contd. -

- construct equivalent Effective Lagrangian with DENSITY DEPENDENT four-point couplings:

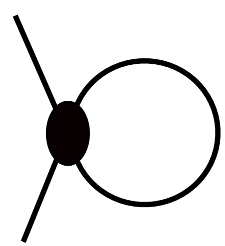
$$\mathcal{L}_{eff} = \bar{\Psi}(i\gamma\cdot\partial - M)\Psi - \frac{1}{2}\sum_{i=S,V,\dots} G_i(\hat{\rho})(\bar{\Psi}\Gamma_i\Psi)^2$$

$$-\frac{1}{2}\sum_{i=S,V,\dots} D_i(\hat{\rho})(\partial\bar{\Psi}\Gamma_i\Psi)^2 + \mathcal{L}_{e.m.}$$

$$\Gamma_S = \mathbf{1}\ , \quad \Gamma_V = \gamma^\mu\ , \quad \dots$$

- matching at the level of nucleon self-energies:

$$\Sigma_i(\rho) = G_i(\rho)\cdot\rho$$



+ re-arrangement terms

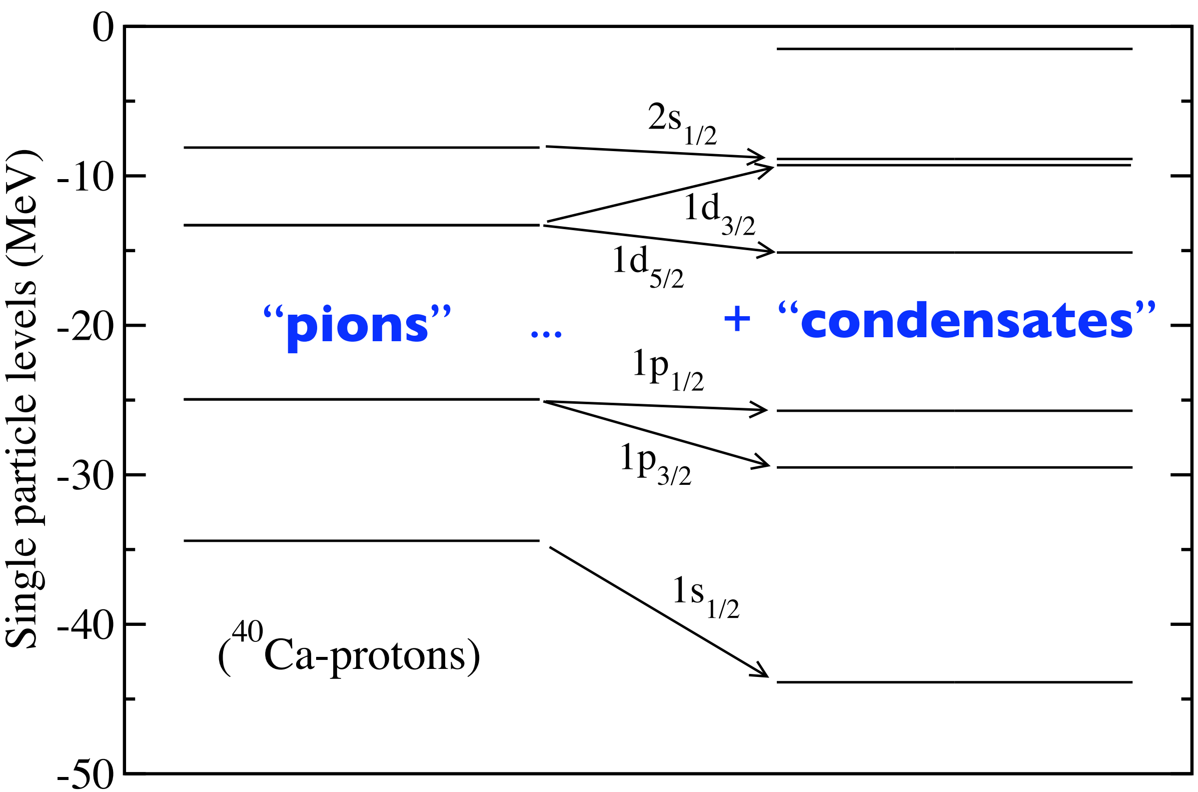
- solve self-consistent Dirac equations for single-particle orbits

(relativistic analog of Kohn-Sham equations)

- apply corrections: CM energy , pairing (rel. Hartree-Bogoliubov)

Example: SINGLE PARTICLE SPECTRUM of ^{40}Ca

P. Finelli, N. Kaiser, D.Vretenar, W.W.: Nucl. Phys. A 735 (2004) 449



SPIN-ORBIT splitting from strong "CONDENSATE" SCALAR & VECTOR mean fields:

$$\Sigma_S^{(0)}(\rho) \simeq -0.35\,\text{GeV}\left(\frac{\rho_s}{\rho_0}\right)$$

$$\Sigma_V^{(0)}(\rho) \simeq +0.34\,\text{GeV}\left(\frac{\rho}{\rho_0}\right)$$

(SPIN-ORBIT interaction proportional to SCALAR minus VECTOR)

BINDING from CHIRAL DYNAMICS

(mainly regularized two-pion exchange "van der Waals + Pauli")

$$\Sigma_{S,V}^{(\pi)}(\rho) \simeq -75\,\text{MeV}\left(\frac{\rho}{\rho_0}\right)\left[1 - 0.38\left(\frac{\rho}{\rho_0}\right)^{1/3} - 0.27\left(\frac{\rho}{\rho_0}\right)^{2/3} + 0.09\left(\frac{\rho}{\rho_0}\right)\right]$$

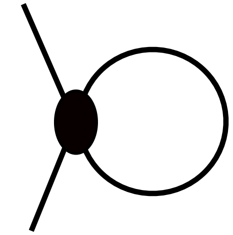
+ surface (derivative) term

PARAMETERS and their interpretation

- single particle potential:

$$\mathbf{U = S + V = G_S^{(0)}\rho_S + G_V^{(0)}\rho + \Delta U}$$

$$\mathbf{\Delta U = g_3 \frac{k_F^3}{\Lambda^2} + g_4 \frac{k_F^4}{\Lambda^3} + g_5 \frac{k_F^5}{\Lambda^4} + g_6 \frac{k_F^6}{\Lambda^5}}$$

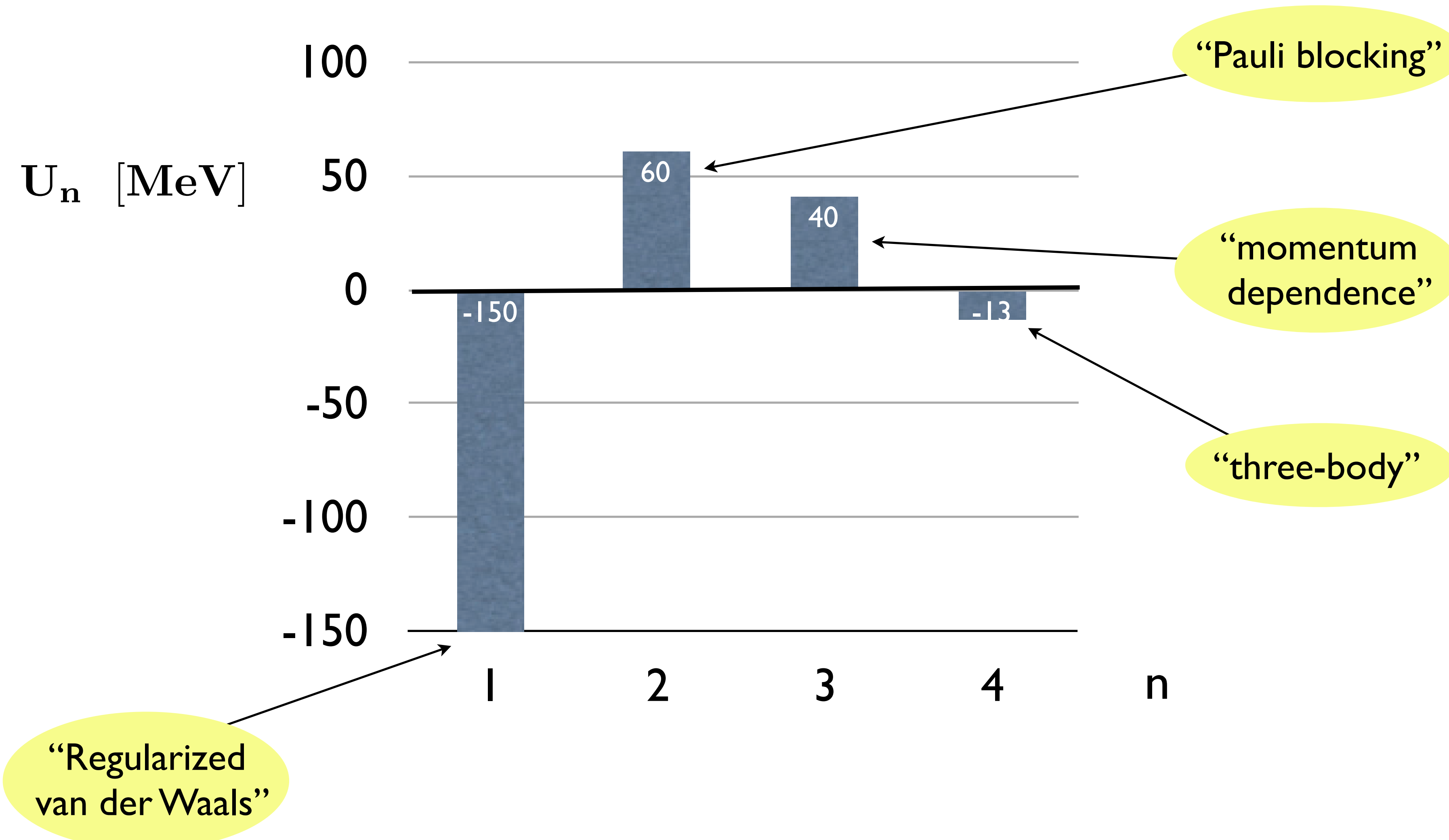


$(\mathbf{\Lambda = 0.6\,GeV})$

	coupling	fine-tuned	expected / predicted	
condensate fields	$\mathbf{G_S^{(0)}}$	$-\,\mathbf{11.5\,fm^2}$	$-\,\mathbf{(11.0 \pm 1.5)\,fm^2}$	**QCD sum rules**
	$\mathbf{G_V^{(0)}}$	$\mathbf{11.0\,fm^2}$	$\mathbf{(10.5 \pm 1.5)\,fm^2}$	
nuclear chiral (pion) dynamics:	$\mathbf{g_3}$	$-\,\mathbf{3.04}$	$-\,\mathbf{3.31}$	**in-medium ChPT**
van der Waals + Pauli + short range (contact) terms	$\mathbf{g_4}$	$\mathbf{2.95}$	$\mathbf{2.95}$	model-independent
	$\mathbf{g_5}$	$\mathbf{2.48}$	$\mathbf{2.48}$	
	$\mathbf{g_6}$	$-\,\mathbf{4.00}$	–	
	$\mathbf{D_S}$	$-\,\mathbf{0.76}$	$-\,\mathbf{0.7}$	surface (derivative) term

Central (isoscalar) SINGLE PARTICLE POTENTIAL of a typical HEAVY NUCLEUS

$$\mathbf{U}(\mathbf{r}) = \mathbf{U_1}\frac{\rho(\mathbf{r})}{\rho_\mathbf{0}} + \mathbf{U_2}\left(\frac{\rho(\mathbf{r})}{\rho_\mathbf{0}}\right)^{\mathbf{4/3}} + \mathbf{U_3}\left(\frac{\rho(\mathbf{r})}{\rho_\mathbf{0}}\right)^{\mathbf{5/3}} + \mathbf{U_4}\left(\frac{\rho(\mathbf{r})}{\rho_\mathbf{0}}\right)^{\mathbf{2}}$$

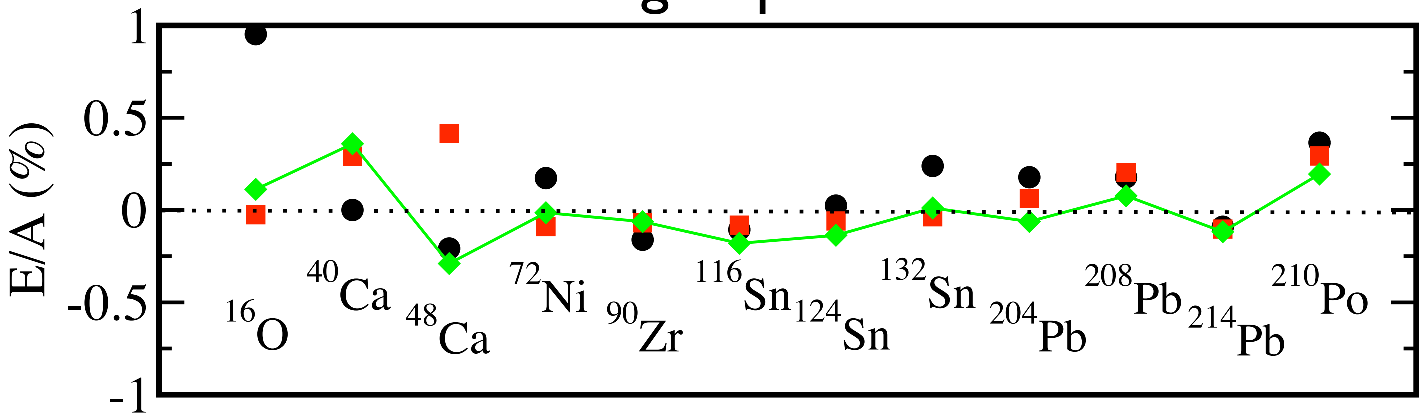


RESULTS (part I)

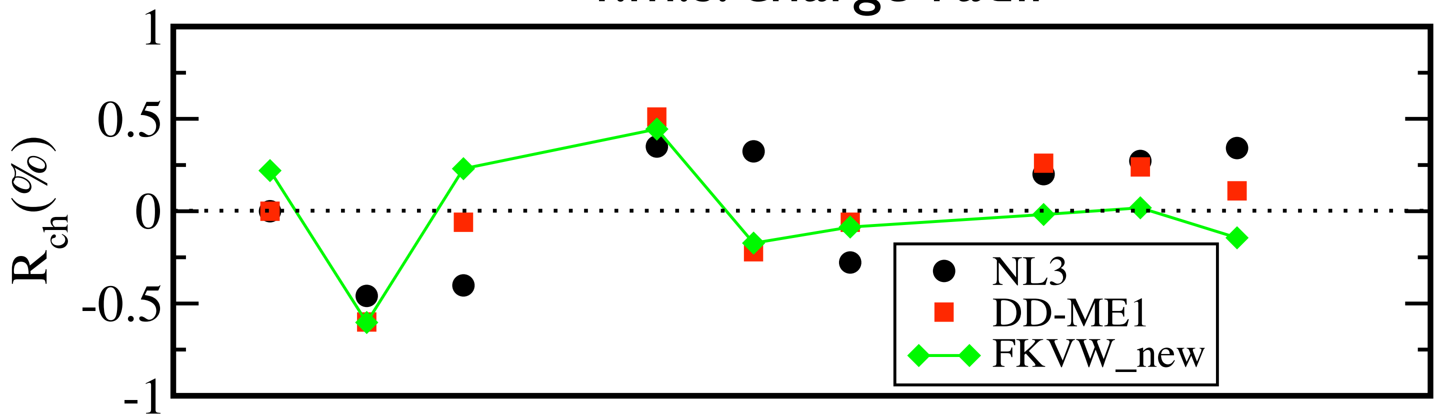
P. Finelli, N. Kaiser, D.Vretenar, W.W.: Nucl. Phys. A 735 (2004) 449
and preprint (2005)

deviations (in %) between calculated and measured

energies per nucleon



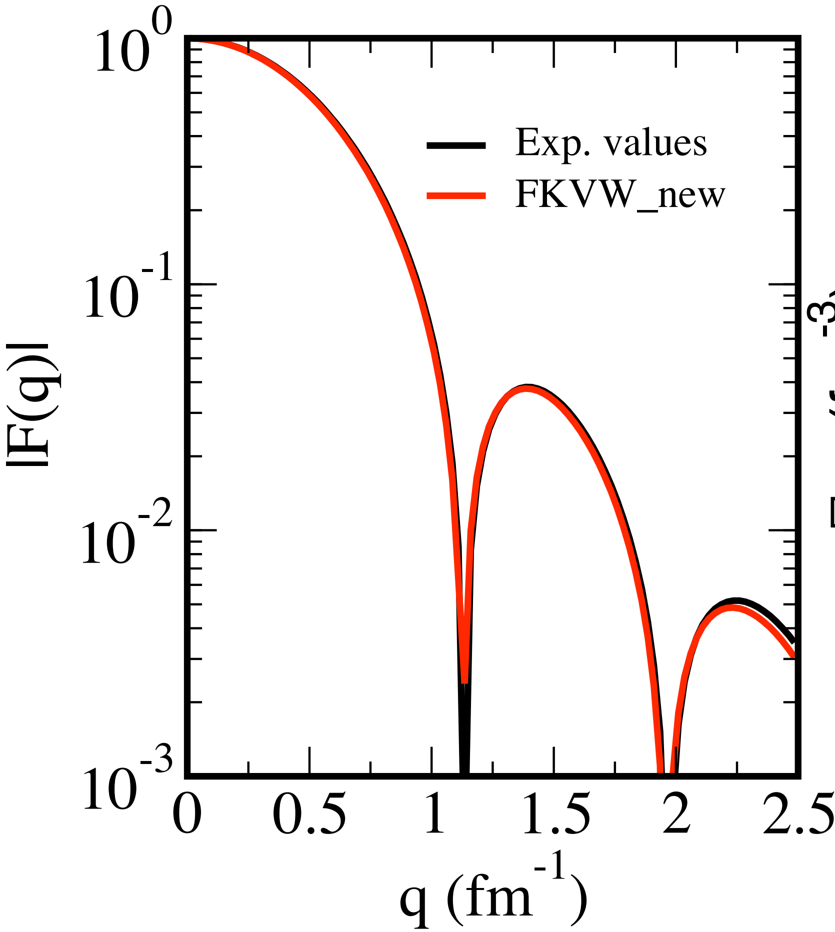
r.m.s. charge radii

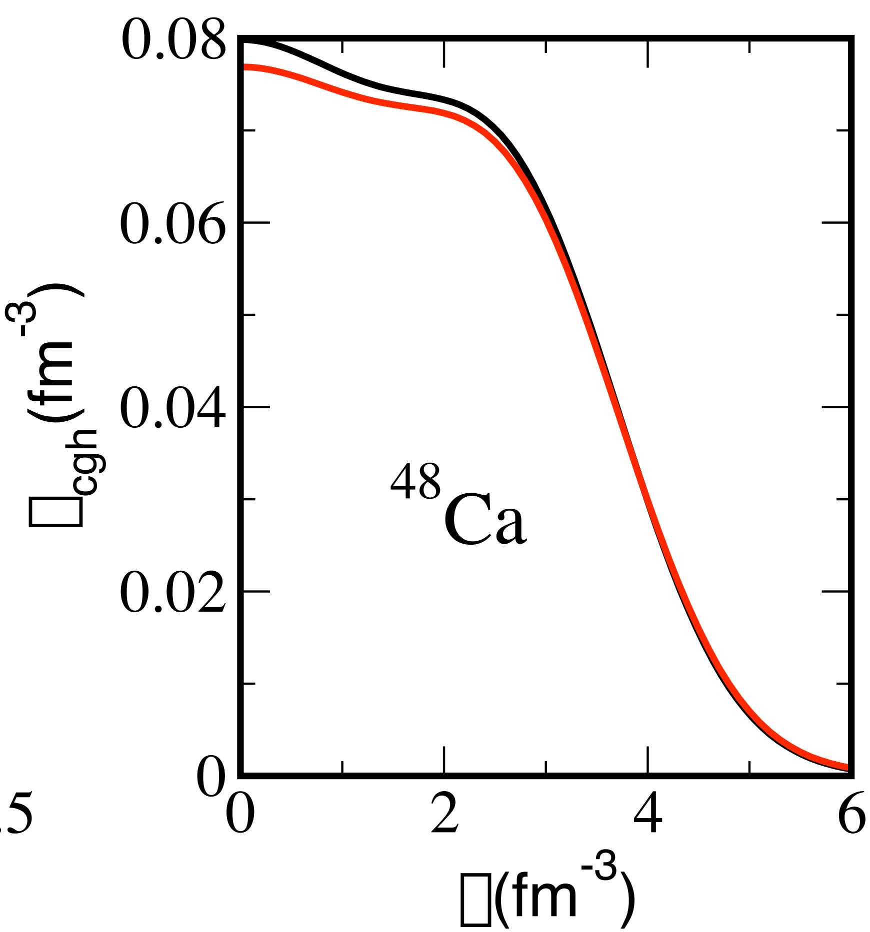


RESULTS (part II)

P. Finelli, N. Kaiser, D.Vretenar, W.W. : preprint (2005)

charge density of ^{48}Ca

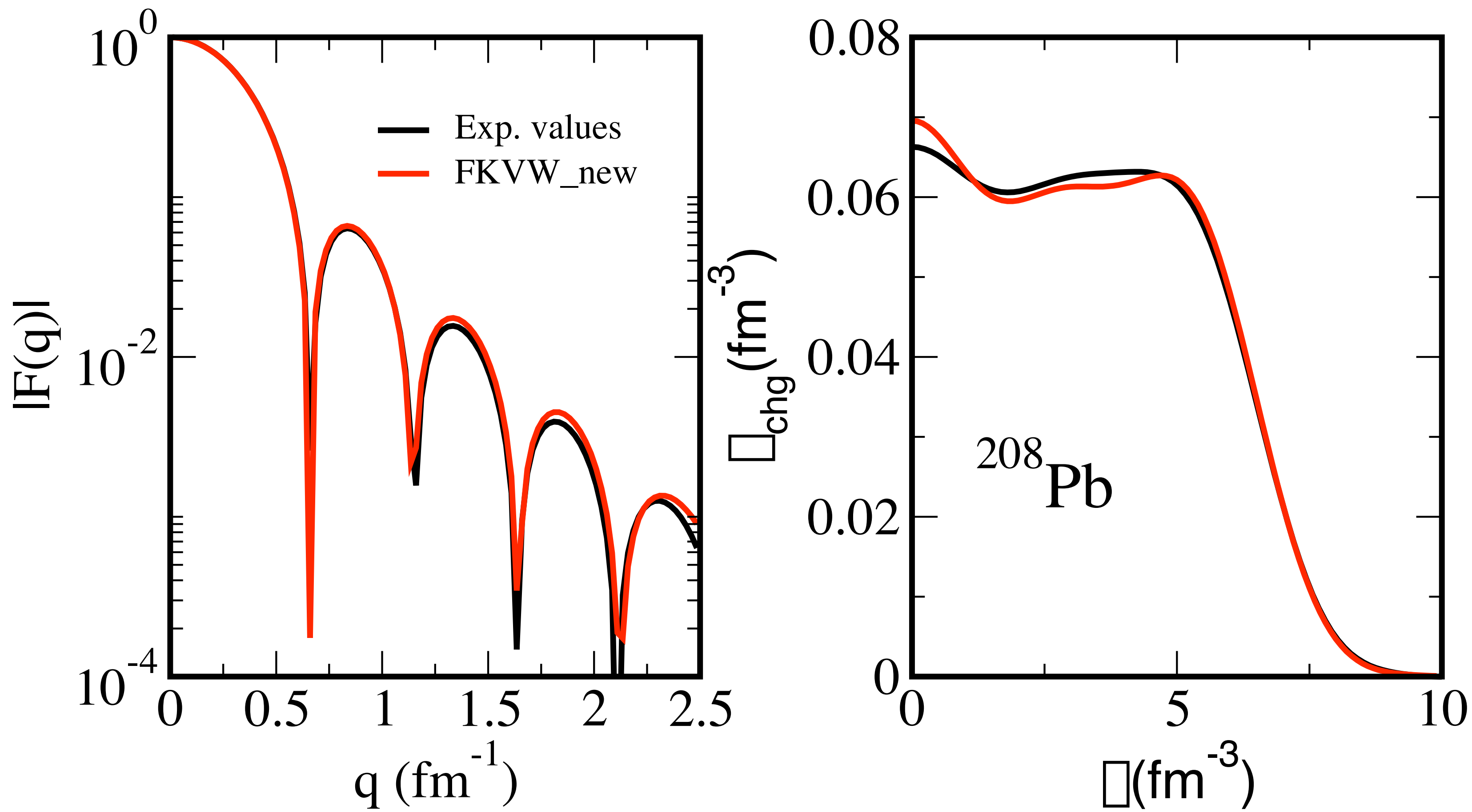




RESULTS (part III)

P. Finelli, N. Kaiser, D.Vretenar, W.W. : preprint (2005)

charge density of ^{208}Pb

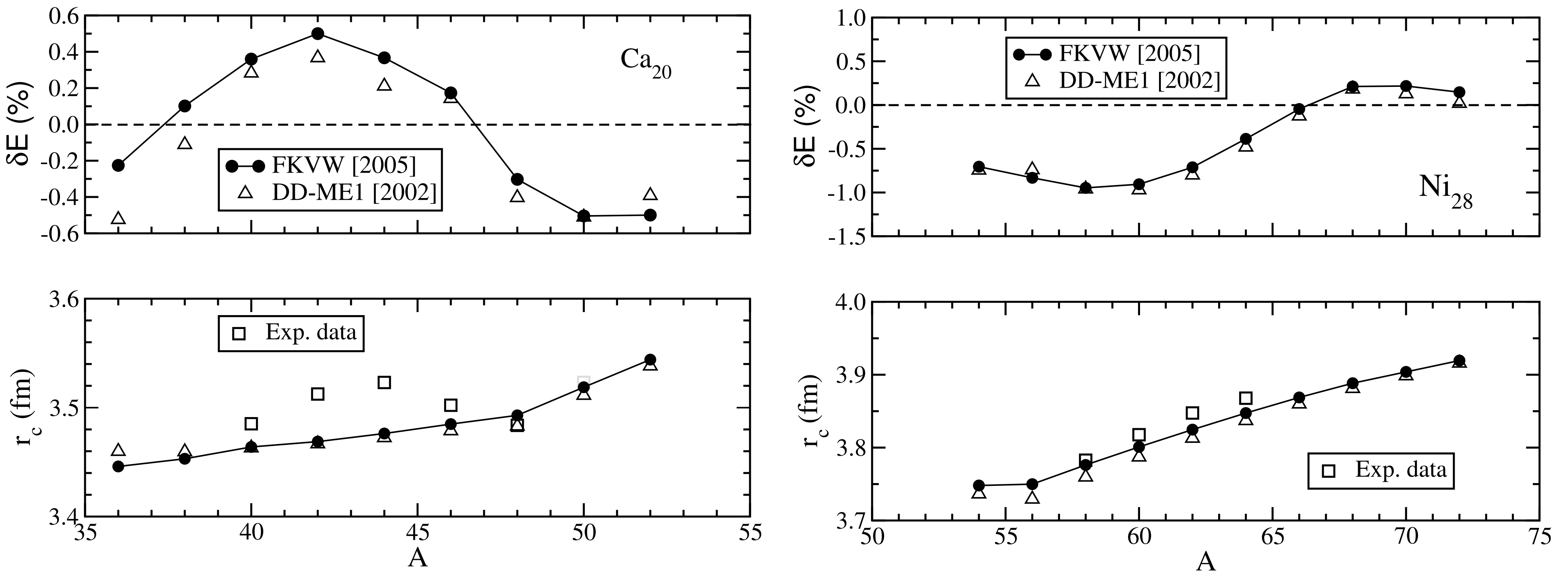


RESULTS (part IV)

P. Finelli, N. Kaiser, D.Vretenar, W.W. : preprint (2005)

ISOSPIN dependence:

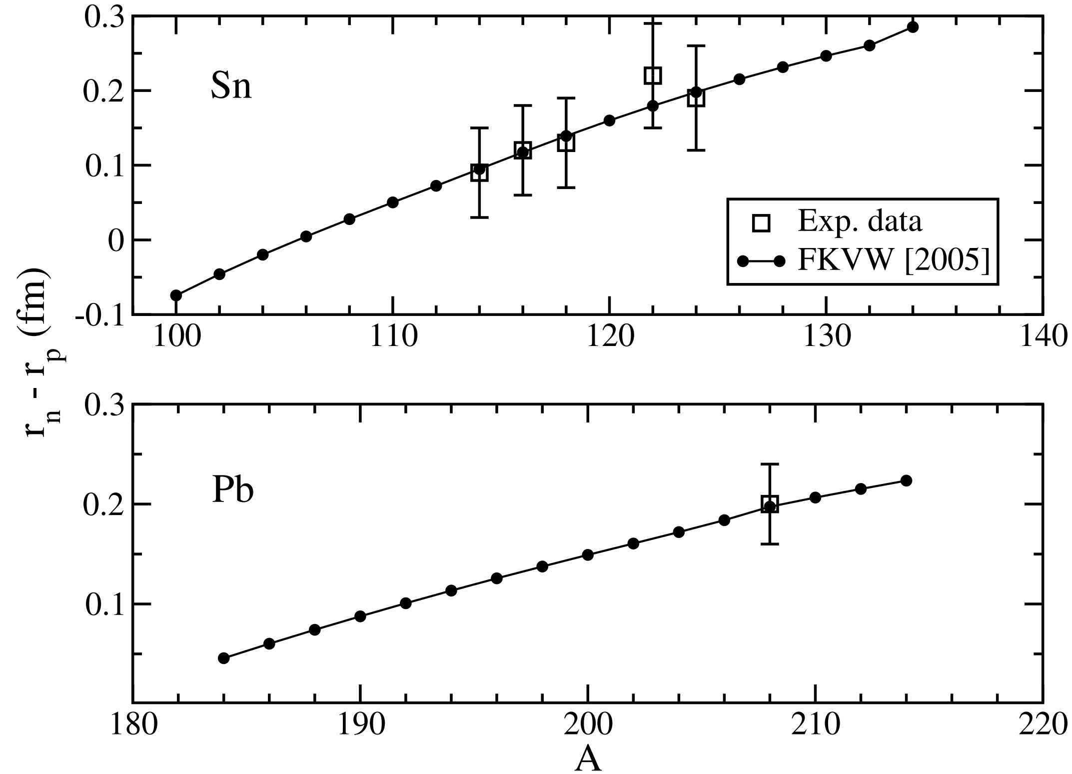
Ca and Ni isotopes

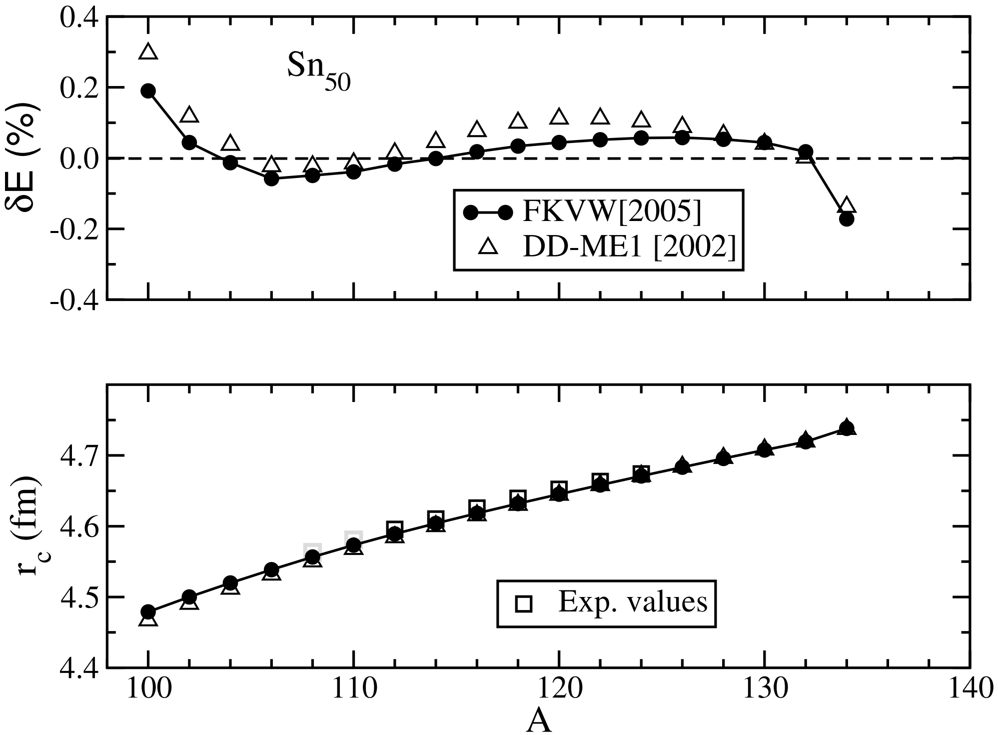


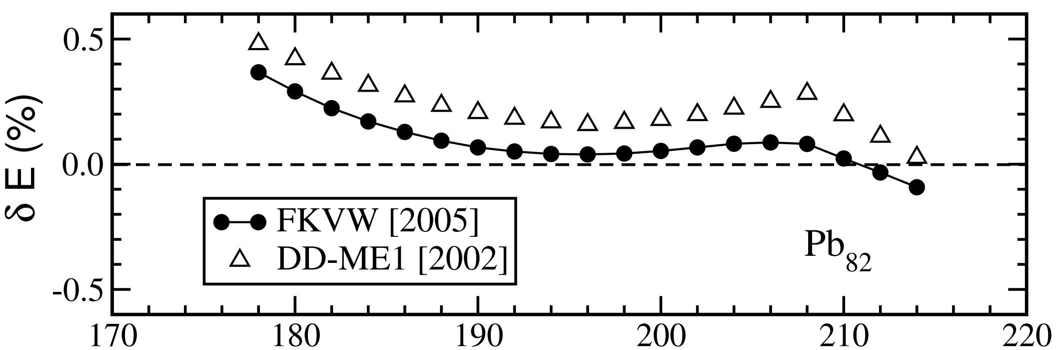
RESULTS (part V)

ISOSPIN dependence:

Sn and Pb isotopes





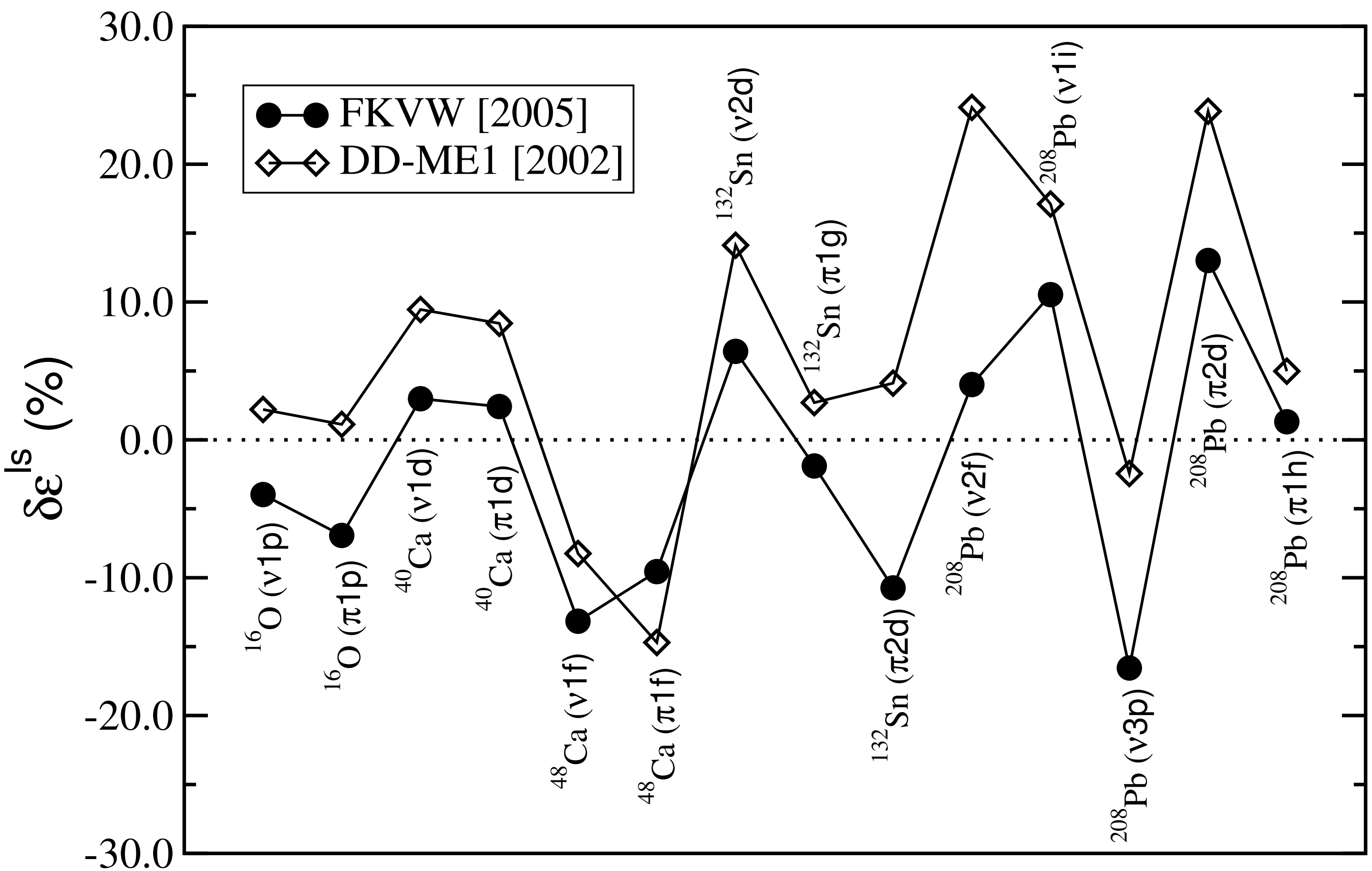


RESULTS (part VI)

P. Finelli, N. Kaiser, D.Vretenar, W.W. : Nucl. Phys. A 735 (2004) 449
and preprint (2005)

SPIN - ORBIT splittings

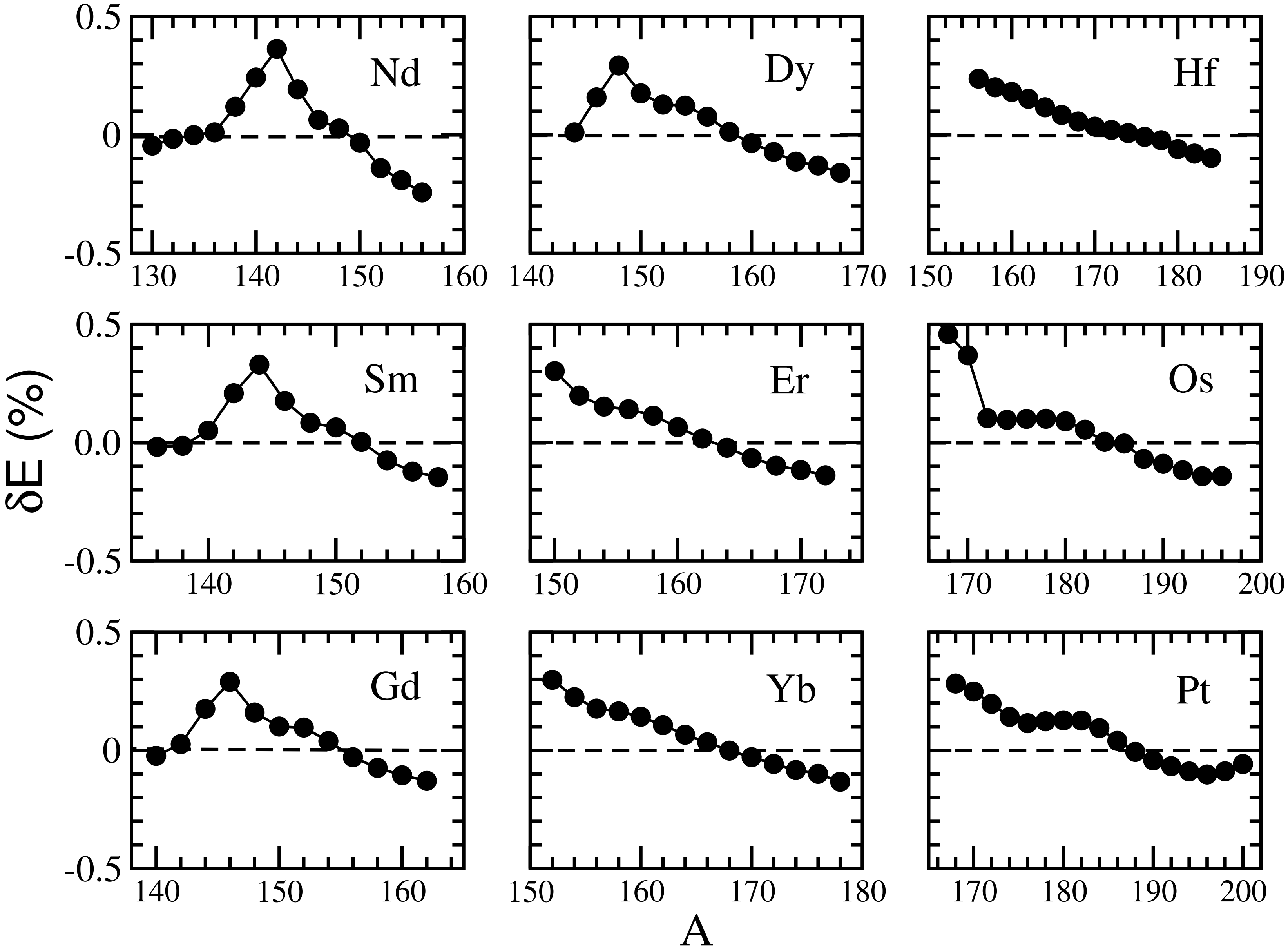
deviations (in %) between calculated and measured



RESULTS (part VII)

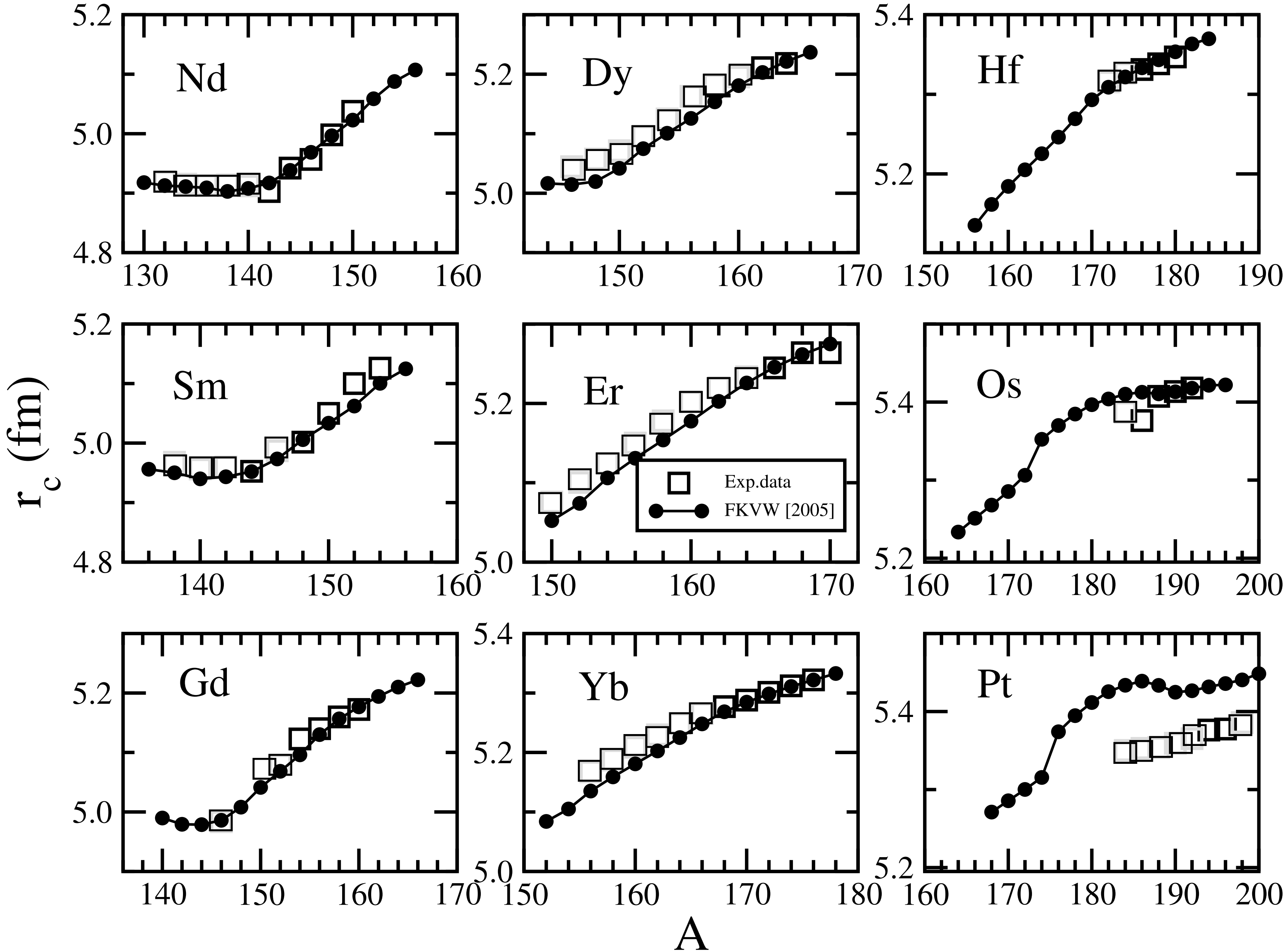
P. Finelli, N. Kaiser, D.Vretenar, W.W. : preprint (2005)

DEFORMED NUCLEI: binding energies



RESULTS (part VIII)

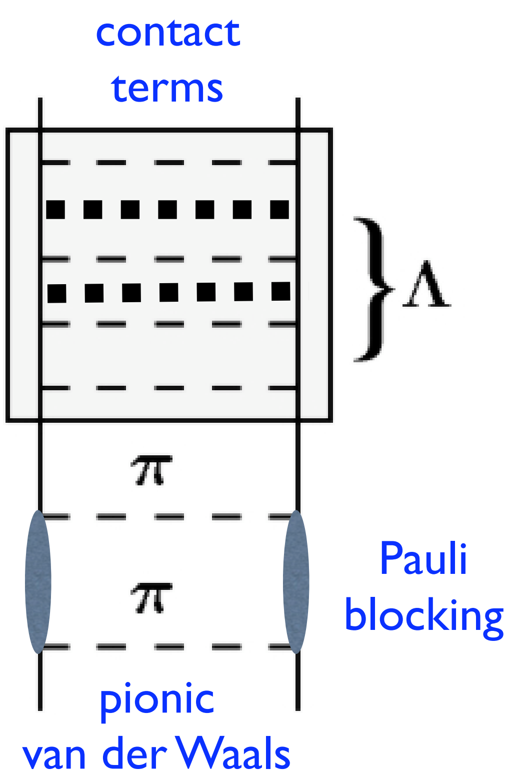
DEFORMED NUCLEI: charge radii

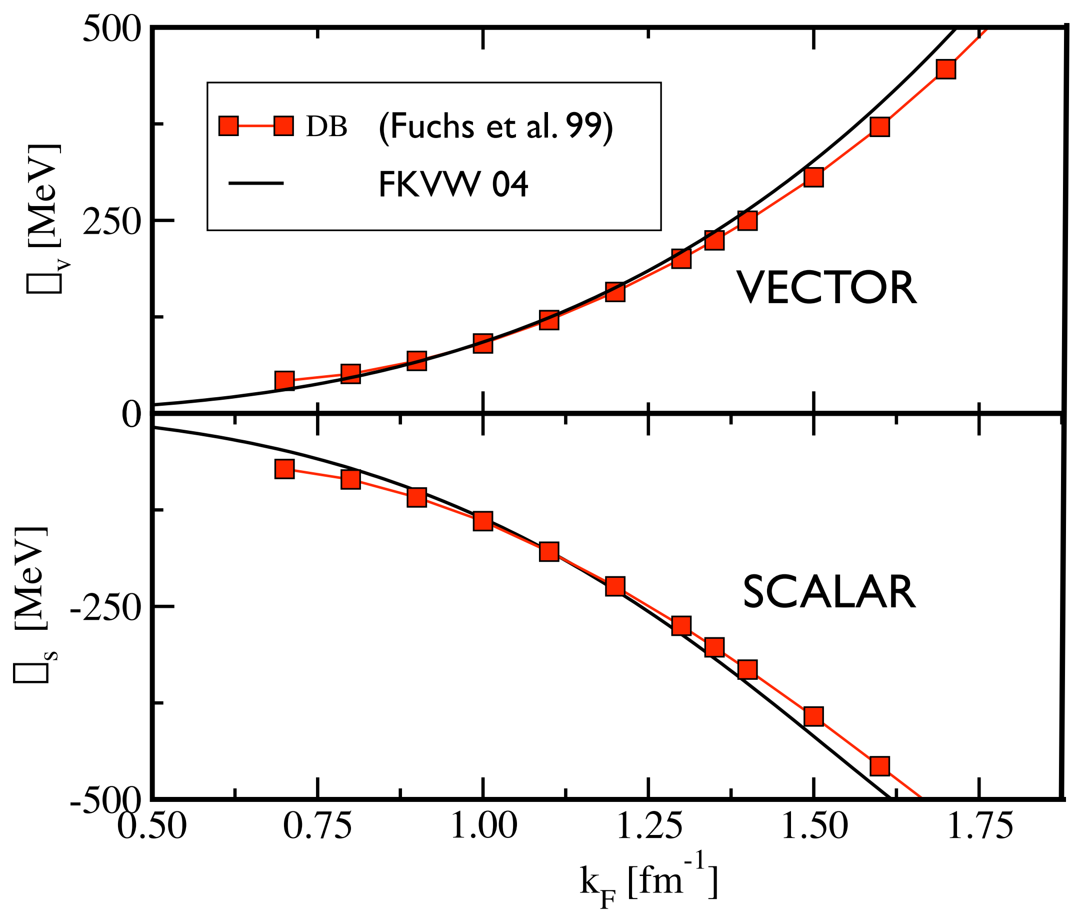


SUMMARY & CONCLUSIONS

- ... on the way to a density functional approach for nuclear many-body systems, constrained by LOW-ENERGY QCD
- BINDING and SATURATION primarily from PION DYNAMICS ("Pionic van der Waals + Pauli")
- SPIN-ORBIT interaction: strong SCALAR and VECTOR mean fields consistent with in-medium QCD CONDENSATES
- HEAVY NUCLEI and chains of isotopes: correct ISOSPIN dependence, primarily from 2-pion-dynamics
- PERTURBATIVE (chiral) approach plus contact terms seems to work
- agreement with results from Dirac-Brueckner theory (where comparable)

Comparison with DIRAC-BRUECKNER calculations

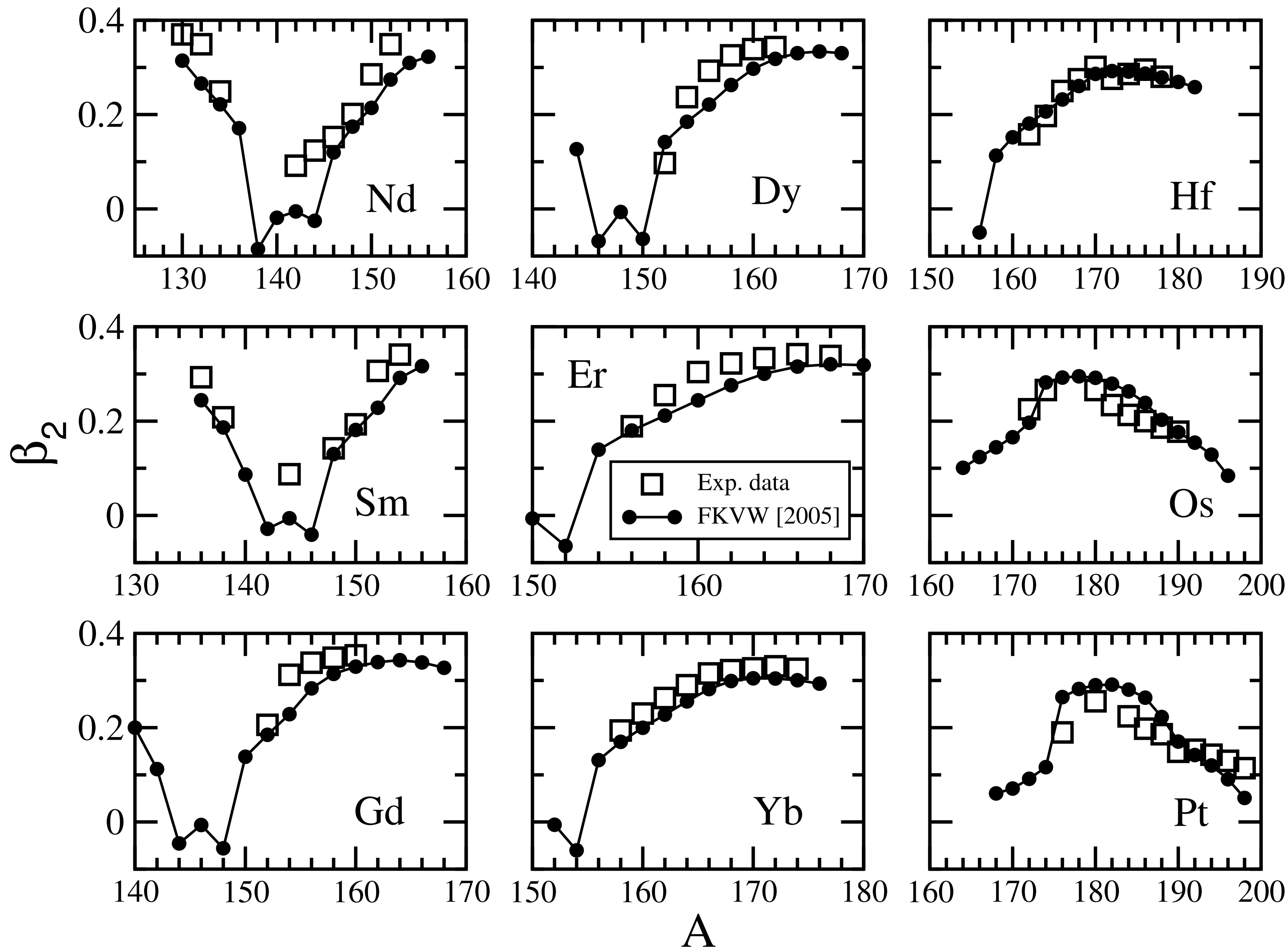




- "trivial" density dependence from short-distance / in-medium condensate dynamics (⇒ contact terms)
- "non-trivial" density dependence from intermediate and long-range pion dynamics ("van der Waals") plus Pauli blocking

RESULTS (part IX)

DEFORMED NUCLEI: ground state deformations



QCD SUM RULES at FINITE DENSITY

(Drukarev, Levin (1990); Cohen, Furnstahl, Griegel (1991))

- In-medium QCD SUM RULES, leading order:

$$\Sigma_S^{(0)} = -\frac{8\pi^2}{\Lambda_B^2}\left[\langle\bar{q}q\rangle_\rho - \langle\bar{q}q\rangle_0\right] = \frac{8\pi^2}{\Lambda_B^2}\,\frac{-\sigma_N}{m_u + m_d}\rho_s\ , \qquad \Sigma_V^{(0)} = +\frac{64\pi^2}{3\Lambda_B^2}\langle q^\dagger q\rangle_\rho = \frac{32\pi^2}{\Lambda_B^2}\rho$$

- ... use Ioffe's formula $M_N = -\frac{8\pi^2}{\Lambda_B^2}\langle\bar{q}q\rangle_0$

  and Gell-Mann, Oakes, Renner relation $(m_u + m_d)\langle\bar{q}q\rangle_0 = -m_\pi^2 f_\pi^2$

$$\rightarrow \quad \Sigma_S^{(0)} = M_N^*(\rho) - M_N(\rho) = -\frac{\sigma_N M_N}{m_\pi^2 f_\pi^2}\rho_s \equiv G_S^{(0)}\rho_s$$

$$\rightarrow \quad \Sigma_V^{(0)} = \frac{4(m_u + m_d)M_N}{m_\pi^2 f_\pi^2}\rho \equiv G_V^{(0)}\rho$$

$$\rightarrow \quad \frac{\Sigma_S^{(0)}}{\Sigma_V^{(0)}} = -\frac{\sigma_N}{4(m_u + m_d)}\left(\frac{\rho_s}{\rho}\right) \simeq -1$$