Relativistic nuclear energy density functional constrained by low-energy QCD

[Nucl. Phys. A**735** (2004) 449; nucl-th/0509040]

Paolo Finelli[†], N. Kaiser[†], D. Vretenar[*], W. Weise[†]

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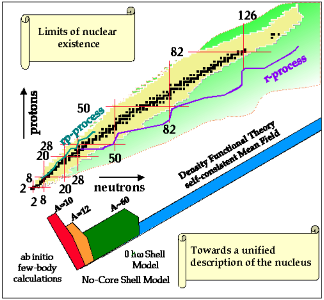
Seattle, 27 september 2005

Looking for a *universal* energy functional



- Lect. Not. in Phys. **641**
- Rev. Mod. Phys. **75** (2003) 121
- Rev. Mod. Phys. **75** (2003) 1021
- Phys. Rep. **409** (2005) 101
- RIA theory Blue book (2005) [http://www.orau.org/ria/RIATG]

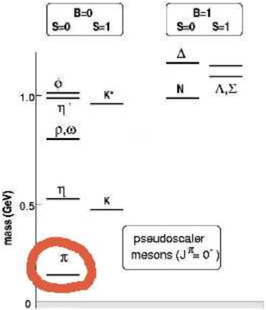
Advantages of an energy functional:

- Clear physical picture
- Same interaction for all atomic nuclei
- Easy implementation
- Common framework for stable and unstable nuclei

Signatures of QCD at low energy

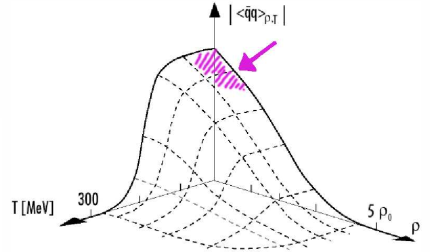
Paolo Finelli†, N. Kaiser†, D. Vretenar*, W. Weise†

Goldstone modes



Pions as low-energy d.o.f.
Long-range physics should be explicitly treated

Quark condensate



At $T \simeq 0$, $\langle\bar{q}q\rangle_\rho$ is large ($\simeq 1.8\ \mathrm{fm}^{-3}$) and modifies nucleon properties

Inspiration from Kohn-Sham theory

In atomic physics

- Relativistic Kohn-Sham functional
  [Dreizler, Lect. Not. in Phys. **620**]

$$\mathcal{E}_0[j^\mu] = T_{kin}[j^\mu] + \mathcal{E}_{ext} + \mathcal{E}_{Hartree}[j^\mu] + \mathcal{E}_{exc}[j^\mu]$$

Strategy: isolate the (in principle) tractable dominant contributions from the **exc**-energy that contains crucial many-body effects $\Longmapsto$ the success relies on $\mathcal{E}_{\mathbf{exc}}$ determination.

- Local Density Approximation (LDA)

$$\mathcal{E}_{exc}^{LDA} = \int d^3x \; \epsilon_{hom}^{xc}(\rho_0)\Big|_{\rho_0 \to \rho(\mathbf{x})}$$

Our proposal

Working scheme:

- Relativistic nuclear Kohn-Sham functional

$$\mathcal{E}_0[j^\mu] = T_{free}[j^\mu] + \mathcal{E}^{(0)}[j^\mu] + \mathcal{E}_{exc}[j^\mu] + \mathcal{E}_{coul}[j^\mu]$$

- $\mathcal{E}^{(0)}$: Large scalar and vector fields, arising from the in-medium changes of the chiral condensate $\langle \bar{q}q \rangle$ and the quark density $\langle q^\dagger q \rangle$, act as background fields (0).

- $\mathcal{E}_{exc} \rightarrow \mathcal{E}^{\pi}_{exc}$: The exchange correlation term is described in terms of pion-nucleon interaction (within the framework of in-medium ChPT).

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Nuclear interaction

Background fields

[Prog. Part. Nucl. Phys. **35** (1995) 221; **27** (1991) 77]

$$\Sigma_S^{(0)} \simeq -\frac{\sigma_N M_N}{m_\pi^2 f_\pi^2}\rho + \dots$$

$$\Sigma_V^{(0)} \simeq \frac{4(m_u + m_d)M_N}{m_\pi^2 f_\pi^2}\rho + \dots$$

Of approximately equal magnitude (300 MeV) but of opposite sign $\Longmapsto$ **origin of the spin-orbit interaction**

Background fields: in-medium QCD sum rules

In-medium nucleon self-energies

$$\Sigma_S^{(0)} = -\frac{8\pi^2}{\Lambda_B^2}[\langle\bar{q}q\rangle_\rho - \langle\bar{q}q\rangle_0] = -\frac{8\pi^2}{\Lambda_B^2}\,\frac{\sigma_N}{m_u+m_d}\rho_s$$

$$\Sigma_V^{(0)} = \frac{64\pi^2}{3\Lambda_B^2}\langle q^\dagger q\rangle_\rho = \frac{32\pi^2}{\Lambda_B^2}\rho$$

Strong scalar and vector mean fields generated by in-medium changes of QCD condensates

- Scalar self-energy

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

- Vector self-energy

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

- Estimates

$$\frac{\Sigma_S^{(0)}}{\Sigma_V^{(0)}} = \frac{G_S^{(0)}\rho_s}{G_V^{(0)}\rho} = -\frac{\sigma_N}{4(m_u+m_d)}\frac{\rho_s}{\rho} \simeq -1$$

Ioffe's sum rule

$$M_N = -\frac{8\pi^2}{\Lambda_B^2}\langle\bar{q}q\rangle_0$$

GMOR relation

$$(m_u+m_d)\langle\bar{q}q\rangle_0 = -m_\pi^2 f_\pi^2$$

Spin-orbit from in-medium QCD sum rules

Equation of motion

$$\begin{pmatrix} [\Sigma_S^{(0)} + \Sigma_V^{(0)}] & -i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla} \\ -i\boldsymbol{\sigma}\cdot\boldsymbol{\nabla} & [-\Sigma_S^{(0)} + \Sigma_V^{(0)}] \end{pmatrix} \begin{pmatrix} \phi_k \\ \chi_k \end{pmatrix} = \begin{pmatrix} \bar{\epsilon}_k & 0 \\ 0 & 2M_N + \bar{\epsilon}_k \end{pmatrix} \begin{pmatrix} \phi_k \\ \chi_k \end{pmatrix}$$

Non-relativistic reduction

$$\Bigg(\underbrace{-\boldsymbol{\nabla}\frac{1}{2M_N^{eff}(r)}\boldsymbol{\nabla}}_{Kinetic} + \underbrace{\Sigma_V^{(0)} + \Sigma_S^{(0)}}_{Central} + \underbrace{\frac{1}{r}\frac{d}{dr}\left(\frac{1}{2M_N^{eff}(r)}\right)\mathbf{l}\cdot\boldsymbol{\sigma}}_{Spin-orbit} \Bigg)\phi_k = \bar{\epsilon}_k\phi_k$$

$$\text{If } \Sigma_S^{(0)}/\Sigma_V^{(0)} \simeq -1 \quad \begin{cases} Central & \Sigma_V^{(0)} + \Sigma_S^{(0)} \simeq 0 \\ Spin-orbit & M_N^{eff}(r) \simeq M_N - \frac{1}{2}\underbrace{(\Sigma_V^{(0)} - \Sigma_S^{(0)})}_{\simeq 600/700 \text{ MeV}} \end{cases}$$

Nuclear interaction

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[Prog. Part. Nucl. Phys. **35** (1995) 221; **27** (1991) 77]

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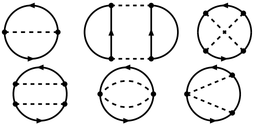
Exchange correlation term

[Nucl. Phys. A**750** (2005) 259]

The nuclear matter energy density is calculated at three loop order, including medium and Δ-insertions.



Exchange correlation term: in-medium ChPT

Key ingredient: In-medium propagator

$$= (\not{p} + M_N) \quad \left[\frac{i}{p^2 - M_N^2 + i\epsilon} \quad -2\pi\delta(p^2 - M_N^2)\theta(k_f - |\vec{p}^2|)\theta(p_0)\right]$$

full vacuum medium

- Expansion of $\bar{E}(k_f) = \mathcal{E}(k_f)/A$ in powers of $\frac{q}{Q}$ with

$q = k_f, m_\pi, M_\Delta - M_N$	small momentum	≤ 300 MeV
$Q = M_N, 4\pi, f_\pi$	large momentum	$\simeq 1$ GeV

- $\bar{E}(k_f)$ can be written as:

$$\bar{E}(k_f) = \frac{3k_f^2}{10M_N} - \alpha\left(\frac{k_f}{m_\pi}\right)\frac{k_f^3}{M_N^2} + \beta\left(\frac{k_f}{m_\pi}\right)\frac{k_f^4}{M_N^3} + \ldots$$

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Exchange correlation term: in-medium ChPT

First step: no delta intermediate states

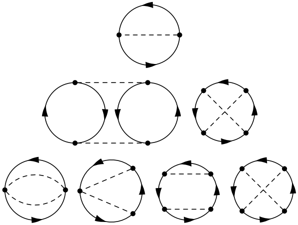
[Nucl. Phys. A**697** (2002) 255; Nucl. Phys. A**700** (2002) 343; Nucl. Phys. A**724** (2003) 47]

Kinetic energy $\mathcal{O}(q^2)$

$1\pi -$ exchange $\mathcal{O}(q^3)$

Iterated $1\pi -$ exchange $\mathcal{O}(q^4)$

Irreducible $2\pi -$ exchange $\mathcal{O}(q^5)$

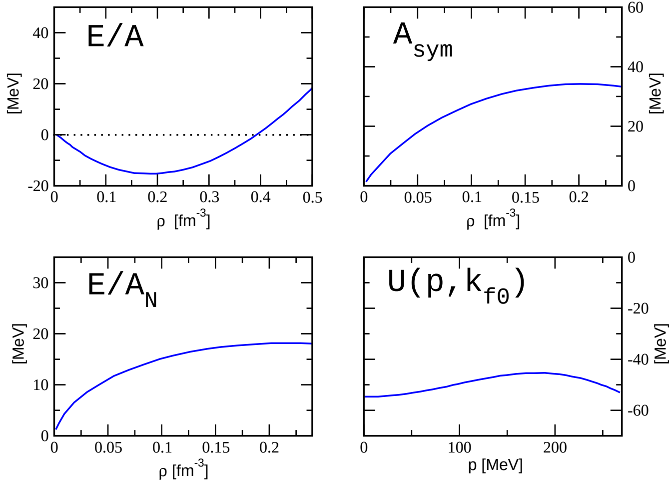


Regularization

A single contact term  (or an equivalent cut-off $\Lambda \simeq 2\pi f_\pi$) at order k_f^3 adjusted to empirical saturation point.

Encodes unresolved short-distance information.

Exchange correlation term: in-medium ChPT



$\rho_{sat} = 0.178\ \text{fm}^{-3}$, $\bar{E} = -15.3$ MeV, $K = 255$ MeV,

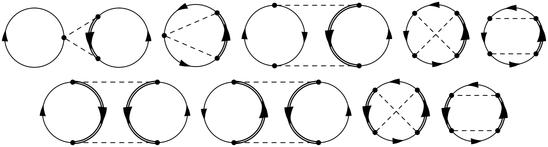
$A_{sym} = 33.8$ MeV, $U(0, k_{f0}) = -53.2$ MeV

Exchange correlation term: in-medium ChPT

Inclusion of Delta-intermediate states

[Nucl. Phys. A**750** (2005) 259]

Irreducible 2π-exchange:



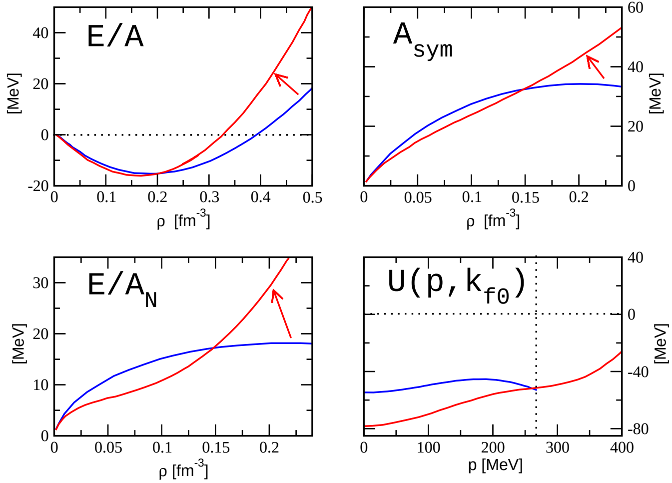
Divergent momentum space loop integrals are regularized by (few) subtraction constants

$$\Delta \bar{E}(k_f)^{(ct)} = b_3 \frac{k_f^3}{\Lambda^2} + b_5 \frac{k_f^5}{\Lambda^4} + b_6 \frac{k_f^6}{\Lambda^5}$$

$$\Delta \bar{S}_2(k_f)^{(ct)} = a_3 \frac{k_f^3}{\Lambda^2} + a_5 \frac{k_f^5}{\Lambda^4} + a_6 \frac{k_f^6}{\Lambda^5}$$

with $\Lambda = 2\pi f_\pi \simeq 0.58$ MeV

Exchange correlation term: in-medium ChPT



$\rho_{sat} = 0.157\ \mathrm{fm}^{-3}$, $\bar{E} = -16.0$ MeV, $K = 304$ MeV,

$A_{sym} = 34.0$ MeV, $U(0, k_{f0}) = -78.2$ MeV

Formalism

Functional : $\mathcal{E}_0[\hat{\rho}] = \mathcal{E}_{free}[\hat{\rho}] + \mathcal{E}^{(0)}[\hat{\rho}] + \mathcal{E}^{\pi}_{exc}[\hat{\rho}] + \mathcal{E}_{coul}[\hat{\rho}]$

$$\mathcal{E}_{free}[\hat{\rho}] = \int d^3x\, \langle\phi_0|\bar{\psi}[-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + M_N]\psi|\phi_0\rangle$$ **Free**

$$\mathcal{E}^{(0)}[\hat{\rho}] = \frac{1}{2}\int d^3x\, [\langle\phi_0|G_S^{(0)}(\bar{\psi}\psi)^2|\phi_0\rangle + \langle\phi_0|G_V^{(0)}(\bar{\psi}\gamma_\mu\psi)^2|\phi_0\rangle]$$ **BG**

$$\begin{aligned}\mathcal{E}^{\pi}_{exc}[\hat{\rho}] = \frac{1}{2}\Big\{&\int d^3x\, [\langle\phi_0|G_S^{\pi}(\hat{\rho})(\bar{\psi}\psi)^2|\phi_0\rangle + \langle\phi_0|G_V^{\pi}(\hat{\rho})(\bar{\psi}\gamma_\mu\psi)^2|\phi_0\rangle] \\ &+ \int d^3x\, [\langle\phi_0|G_{TS}^{\pi}(\hat{\rho})(\bar{\psi}\vec{\tau}\psi)^2|\phi_0\rangle + \langle\phi_0|G_{TV}^{\pi}(\hat{\rho})(\bar{\psi}\gamma_\mu\vec{\tau}\psi)^2|\phi_0\rangle] \\ &- \int d^3x\, [\langle\phi_0|D_S^{\pi}(\boldsymbol{\nabla}\bar{\psi}\psi)^2|\phi_0\rangle + \langle\phi_0|D_V^{\pi}(\boldsymbol{\nabla}\bar{\psi}\gamma_\mu\psi)^2|\phi_0\rangle]\Big\}\end{aligned}$$ **Pions**

$$\mathcal{E}_{coul}[\hat{\rho}] = \frac{1}{2}\int d^3x\, \langle\phi_0|A^\mu e\frac{1+\tau_3}{2}(\bar{\psi}\gamma_\mu\psi)|\phi_0\rangle$$ **Coulomb**

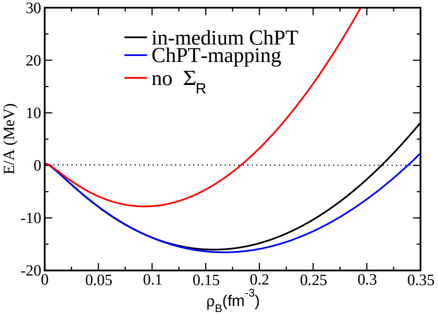
Equation of motion

$$[-i\beta\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + M_N + \gamma_0\Sigma_V^0 + \gamma_0\tau_3\Sigma_{TV}^0 + \gamma_0\Sigma_R^0 + \Sigma_S + \tau_3\Sigma_{TS}]\psi_k = \epsilon_k\psi_k$$

How to include in-medium ChPT calculations

Application of the Hugenholtz-Van Hove theorem:

... for a system with zero pressure (i.e. a Fermi liquid at absolute zero) the Fermi energy is equal to the average energy per particle E/N of the system.



Rearrangement terms (Σ_R^0) can not be neglected

[Phys. Rev. C**52** (1995) 3043]

Density-dependent couplings

$$G(\rho) = \overbrace{\underbrace{\mathbf{g_3}(b_3, a_3, G_S^{(0)}, G_V^{(0)})}_{ChPT}}^{QCD\ Sum\ Rules} + \underbrace{\mathbf{g}_4\rho^{1/3}}_{ChPT} + \underbrace{\mathbf{g}_5(b_5, a_5)\rho^{2/3}}_{ChPT} + \overbrace{\underbrace{\mathbf{g}_6(b_6, a_6)\rho}_{ChPT}}^{high\ order}$$

Background terms		
	Fit FKVW	QCD SR
$G_S^{(0)}$ [fm^2]	- 11.5	-11.0
$G_V^{(0)}$ [fm^2]	11.0	11.0
Counter terms / Pionic fluctuations		
	Fit FKVW	ChPT
b_3	-2.93	-3.05
a_3	2.20	2.16
b_5	0	0
a_5	0	-3.5
b_6	-5.68	-2.83
a_6	-0.13	2.83
$D_S^{(\pi)}$ [fm^4]	-0.76	-0.7

- nice agreement for the QCD SR estimates
- truncation at order k_f^6 is not adequate for finite nuclei

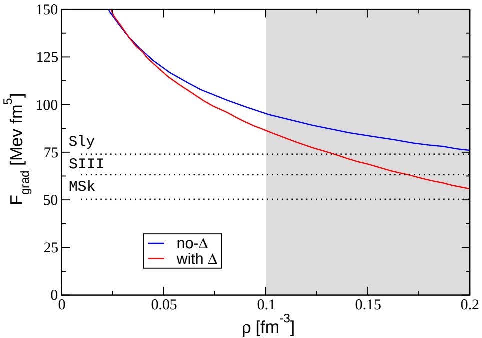
Gradient terms

Inhomogeneous systems: a density-matrix expansion could be used to derive

$$\mathcal{E}(\rho, \boldsymbol{\nabla}\rho) = \rho\,\bar{E}(k_f) + (\boldsymbol{\nabla}\rho)^2\, F_\nabla(k_f) + \ldots$$

To estimate our derivative term $D_S^{(\pi)}$, we approximate F_∇ by a costant

$$D_S^{(\pi)} = -2F_\nabla = -0.7\ \text{fm}^4 \simeq -140\ \text{MeVfm}^5$$



- Anoumalous behaviour close to zero density due to *chiral singularities*

  $$\lim_{\rho\to 0} F_\nabla = 340\ \text{Mevfm}^5$$

- The shaded area represents a region where calculations are *under control*

This estimate -0.7 fm^4 is in good agreement with the fitted value -0.76 fm^4

In practice...

Functional : $\mathcal{E}_0[\hat{\rho}] = \mathcal{E}_{free}[\hat{\rho}] + \mathcal{E}^{(0)}[\hat{\rho}] + \mathcal{E}^{\pi}_{exc}[\hat{\rho}] + \mathcal{E}_{coul}[\hat{\rho}]$

$\Downarrow$

Antisymmetrized single particle (qp) basis Ψ_n

$\Downarrow$

Dirac equation of motion (RHB)

$$\begin{pmatrix} \hat{h}_D - M_N - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}_D + M_N + \lambda \end{pmatrix} \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix} = E_k \begin{pmatrix} U_k(\mathbf{r}) \\ V_k(\mathbf{r}) \end{pmatrix}$$

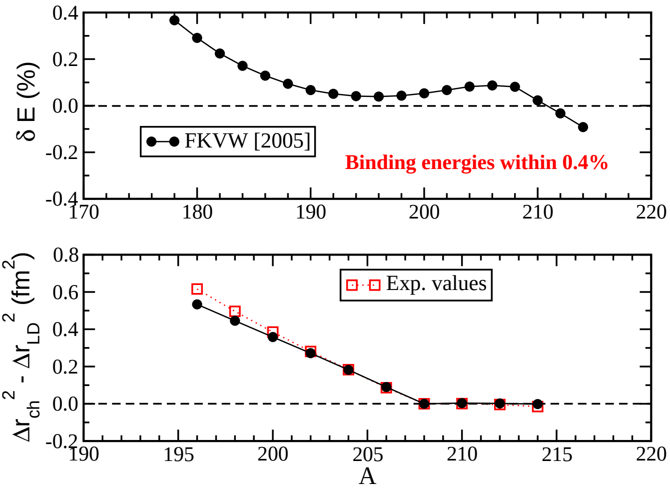
$\Downarrow$

Self-consistent calculations

$\Downarrow$

Observables, check with experimental data

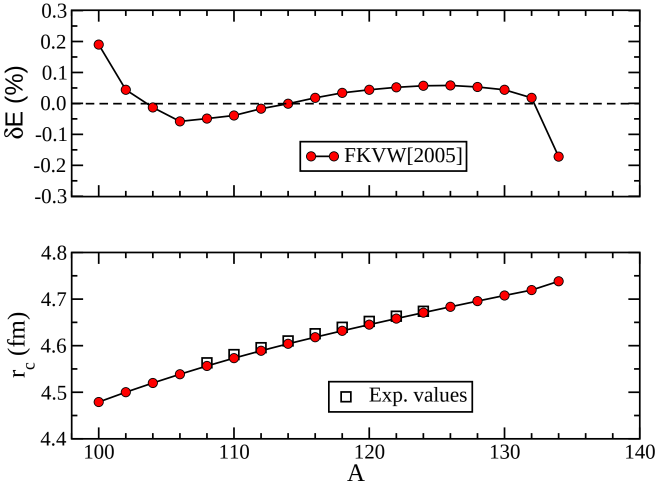
Lead isotopes



Exp. data:

Audi, Wapstra and Thibault (2003), Nadiakov, Marinova and Gangrsky (1994)

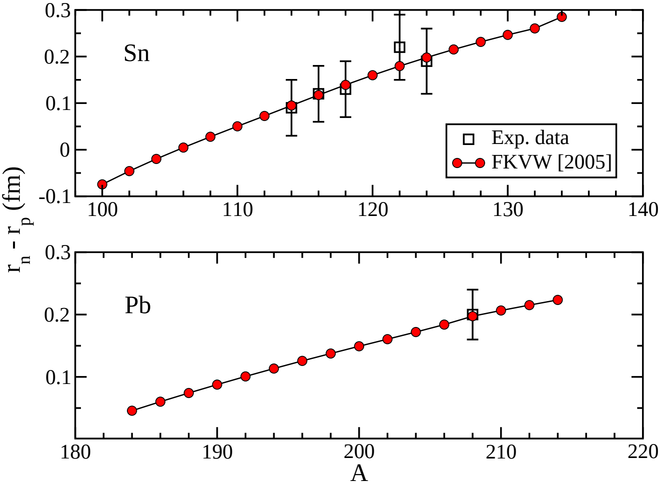
Tin isotopes



Exp. data:

Audi, Wapstra and Thibault (2003), Nadiakov, Marinova and Gangrsky (1994)

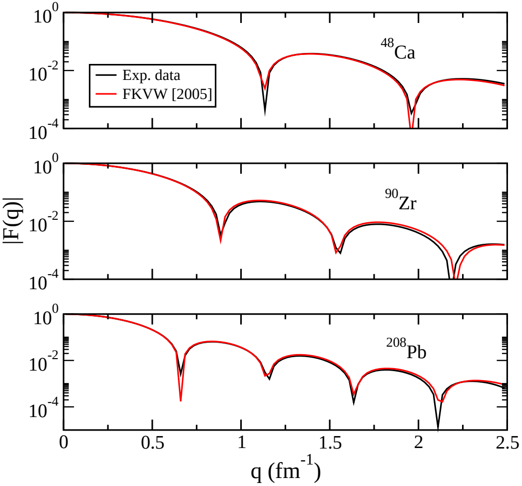
Neutron and proton radii (Tin and Lead isotopes)



Exp. data:

Krasznahorkay et al. (1999), Krasznahorkay et al. (1994)

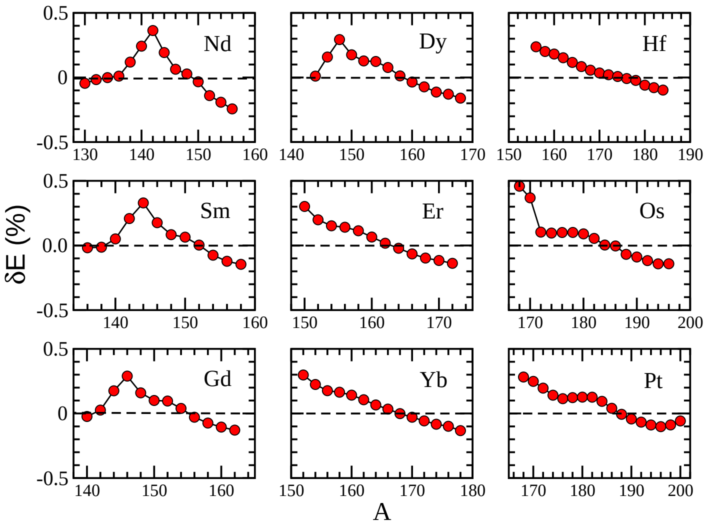
Form factors



Exp. data:

De Vries, De Jager and De Vries (1987)

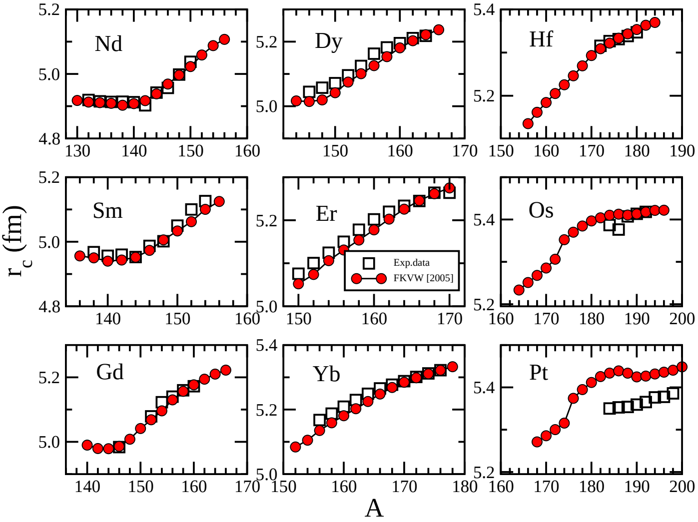
Binding energies



Exp. data:

Audi, Wapstra and Thibault (2003)

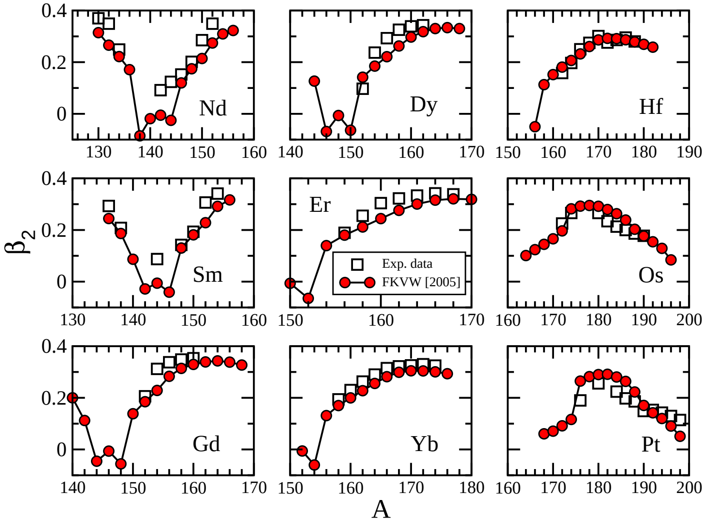
Charge radii



Exp. data:

Nadiakov, Marinova and Gangrsky (1994)

Deformations



Exp. data:

Raman, Nestor and Tikkanen (2001)

Perspectives

Present:

- Successful description of ground-state properties in finite nuclei
- Linking to the low-energy phenomenology of QCD

Future:

- Hypernucley
- Collective motions (QRPA)
- Clear identification of the three-body term

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Self-energies

From the variation of the vertex functionals

$$\frac{\delta \mathcal{L}_{int}}{\delta \bar{\psi}} = \frac{\partial \mathcal{L}_{int}}{\partial \bar{\psi}} + \frac{\partial \mathcal{L}_{int}}{\partial \hat{\rho}} \frac{\delta \hat{\rho}}{\delta \bar{\psi}} \quad \text{with} \quad \frac{\delta \hat{\rho}}{\delta \bar{\psi}} = \frac{\partial \hat{\rho}}{\partial \bar{\psi}} = \gamma_\mu \hat{u}^\mu \psi \quad \text{and} \quad \hat{\rho}\hat{u}^\mu = j^\mu$$

the self-energies are defined as

$$\begin{aligned}
\Sigma_V &= [G_V^{(0)} + G_V^{(\pi)}(\rho)]\rho + eA^0 \frac{1+\tau_3}{2} \\
\Sigma_{TV} &= G_{TV}^{(\pi)}(\rho)\, \rho_3 \\
\Sigma_S &= [G_S^{(0)} + G_S^{(\pi)}(\rho)]\rho_S + D_S^{(\pi)} \boldsymbol{\nabla}^2 \rho_S \\
\Sigma_{TS} &= G_{TS}^{(\pi)}(\rho)\, \rho_{S3}\ , \\
\Sigma_R &= \frac{1}{2} \left\{ \frac{\partial G_V^{(\pi)}(\rho)}{\partial \rho} \rho^2 + \frac{\partial G_S^{(\pi)}(\rho)}{\partial \rho} \rho_S^2 + \right. \\
&\qquad \left. \frac{\partial G_{TV}^{(\pi)}(\rho)}{\partial \rho} \rho_3^2 + \frac{\partial G_{TS}^{(\pi)}(\rho)}{\partial \rho} \rho_{S3}^2 \right\}
\end{aligned}$$

Self-energies

$$U(p,k_f) - U_I(p,k_f)\tau_3\delta + \mathcal{O}(\delta^2) \quad \text{with} \quad \delta = \frac{\rho^n - \rho^p}{\rho^n + \rho^p}$$

where

$$U(k_f; b_3, b_5, b_6) \quad = \quad [c_3 + 2b_3]\,\frac{k_f^3}{\Lambda^2} + c_4\,\frac{k_f^4}{\Lambda^3} + \left[c_5 + \frac{8}{3}b_5\right]\frac{k_f^5}{\Lambda^4} + [c_6 + 3b_6]\,\frac{k_f^6}{\Lambda^5}$$

and

$$U_I(k_f, a_3, a_5, a_6, b_5) \quad = \quad [d_3 + 2a_3]\,\frac{k_f^3}{\Lambda^2} + d_4\,\frac{k_f^4}{\Lambda^3} + \left[d_5 + 2a_5 - \frac{10}{9}b_5\right]\frac{k_f^5}{\Lambda^4} + [d_6 + 2a_6]\,\frac{k_f^6}{\Lambda^5}$$

Comparison

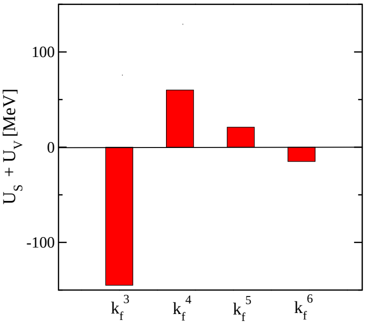
$$\left\{ \begin{array}{c} \Sigma_S^{\rm ChPT}(k_f,\rho) = \frac{1}{2}U(k_f,k_f) \\ \Sigma_V^{\rm ChPT}(k_f,\rho) = \frac{1}{2}U(k_f,k_f) \\ \Sigma_{TS}^{\rm ChPT}(k_f,\rho) = -\frac{1}{2}U_I(k_f,k_f)\delta \\ \Sigma_{TV}^{\rm ChPT}(k_f,\rho) = -\frac{1}{2}U_I(k_f,k_f)\delta \end{array} \right.$$

$$\begin{aligned} \Sigma_S^{\rm PC}(k_f,\rho) &= G_S^{(\pi)}(\rho)\,\rho_S \\ \Sigma_V^{\rm PC}(k_f,\rho) &= G_V^{(\pi)}(\rho)\,\rho \\ &\quad + \frac{1}{2}\left\{\frac{\partial G_V^{(\pi)}(\rho)}{\partial\rho}\rho^2 + \frac{\partial G_S^{(\pi)}(\rho)}{\partial\rho}\rho_S^2\right\} \\ \Sigma_{TS}^{\rm PC}(k_f,\rho) &= G_{TS}^{(\pi)}(\rho)\,\rho_{S3} \\ \Sigma_{TV}^{\rm PC}(k_f,\rho) &= G_{TV}^{(\pi)}(\rho)\,\rho_3 \end{aligned}$$

Influence of the three-body term

Central potential

$$U(\mathbf{r}) = U_3 \frac{\rho(\mathbf{r})}{\rho(0)} + U_4 \left(\frac{\rho(\mathbf{r})}{\rho(0)}\right)^{4/3} + U_5 \left(\frac{\rho(\mathbf{r})}{\rho(0)}\right)^{5/3} + U_6 \left(\frac{\rho(\mathbf{r})}{\rho(0)}\right)^{2}$$

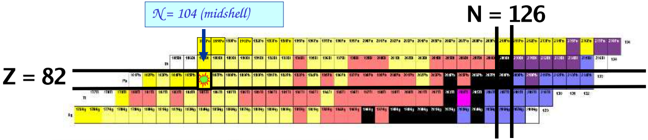


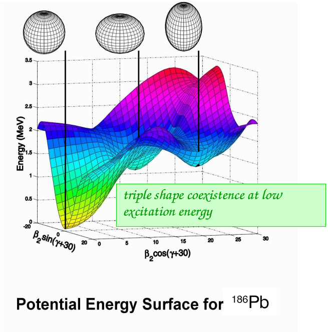
- Almost no contribution from background fields

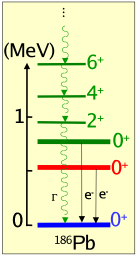
$$U^{(0)} = G_S^{(0)} \rho_S + G_V^{(0)} \rho \simeq 0$$

- Convergence still to be achieved
- Terms of order $\rho^{4/3}$ and $\rho^{5/3}$ are free-parameters

Shape coexistence: experimental status

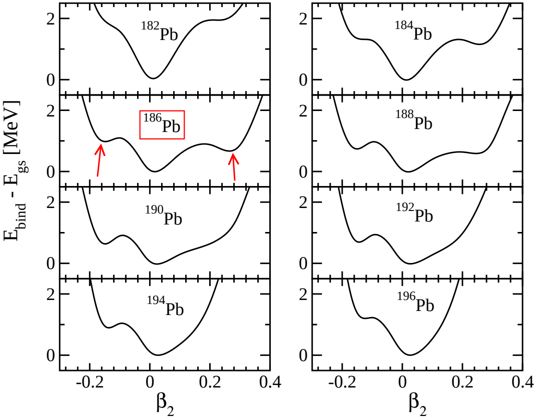






A. Andreyev et al., Nature 405 (2000) 430

Shape coexistence: theoretical overview



$$E = \langle \hat{H} \rangle - \sum_{q=p,n} \lambda_q \langle \hat{N}_q \rangle + \frac{1}{2} \sum_a C_a (\langle \hat{Q}_a \rangle - \mu_a)^2$$