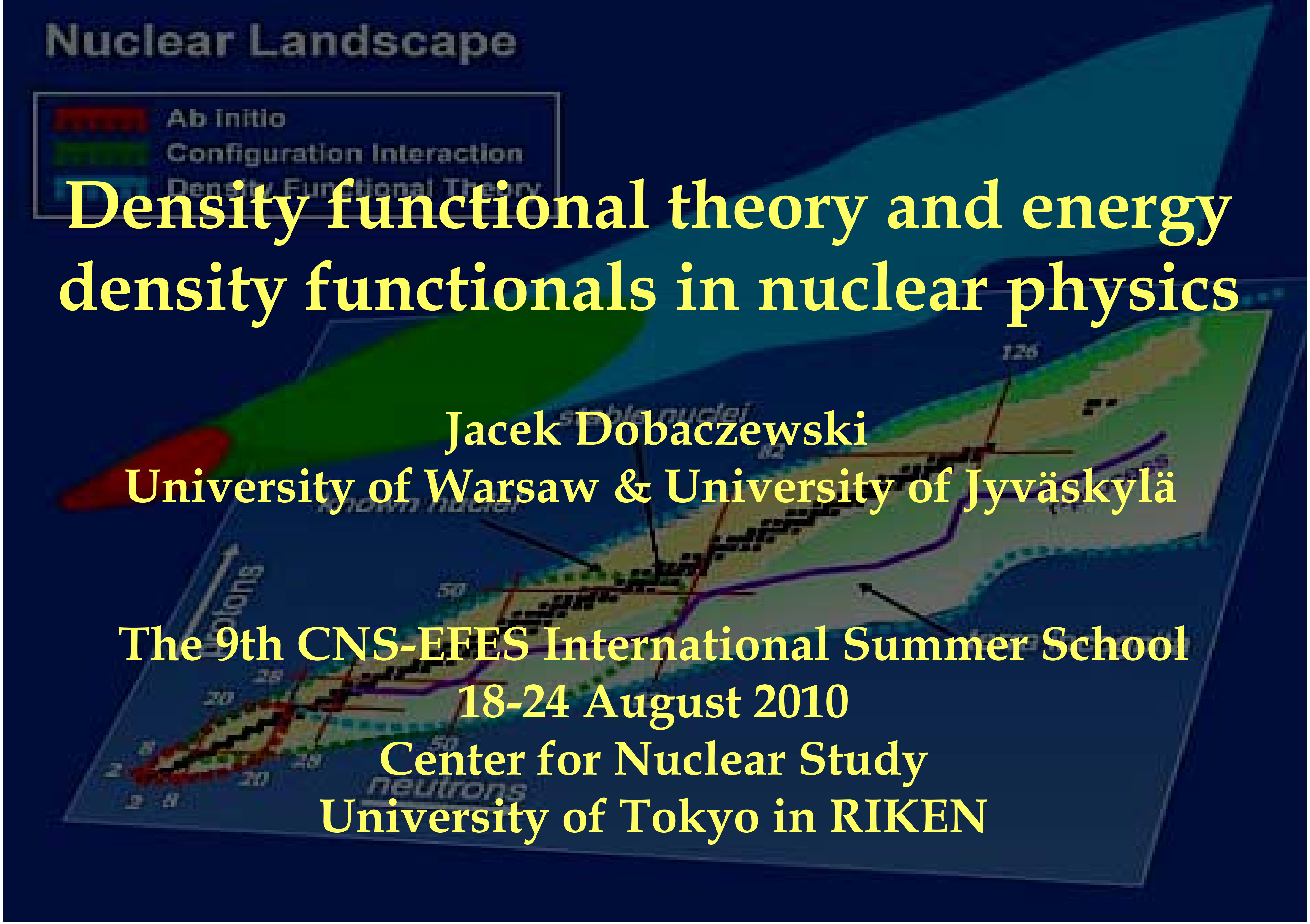

Density functional theory and energy density functionals in nuclear physics

Jacek Dobaczewski
University of Warsaw & University of Jyväskylä

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Center for Nuclear Study
University of Tokyo in RIKEN

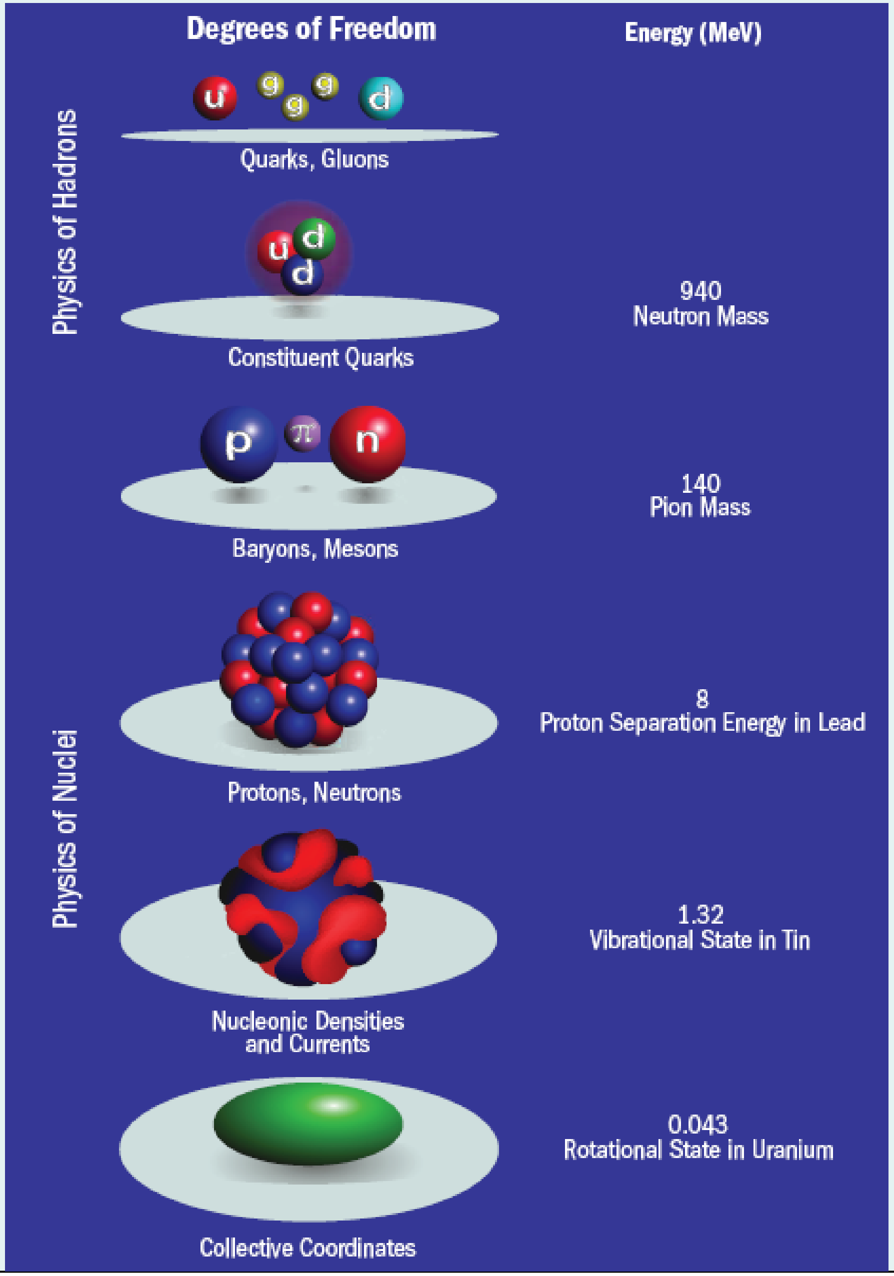
Reading material:

Jacek Dobaczewski:2004 RIA Summer School
http://www.fuw.edu.pl/~dobaczew/RIA.Summer.Lectures/slajd01.html
Jacek Dobaczewski:2005 Ecole Doctorale de Physique, Strasbourg
http://www.fuw.edu.pl/~dobaczew/Strasbourg/slajd01.html
Witek Nazarewicz:2007 Lectures at the University of Knoxville
http://www.phys.utk.edu/witek/NP622/NuclPhys622.html
Jacek Dobaczewski: 2008 the 18th Jyväskylä Summer School
http://www.fuw.edu.pl/~dobaczew/JSS18/JSS18.html
Jacek Dobaczewski: 2008 Euroschool on Exotic Beams
http://www.fuw.edu.pl/~dobaczew/Euroschool/Euroschool.html
Jacek Dobaczewski: 2008 Lectures at University of Jyväskylä
http://www.fuw.edu.pl/~dobaczew/FYSN305/FYSN305.html
Jacek Dobaczewski: 2009 Lectures at University of Stellenbosch
http://www.fuw.edu.pl/~dobaczew/Stellenbosch/dobaczewski_lecture.pdf

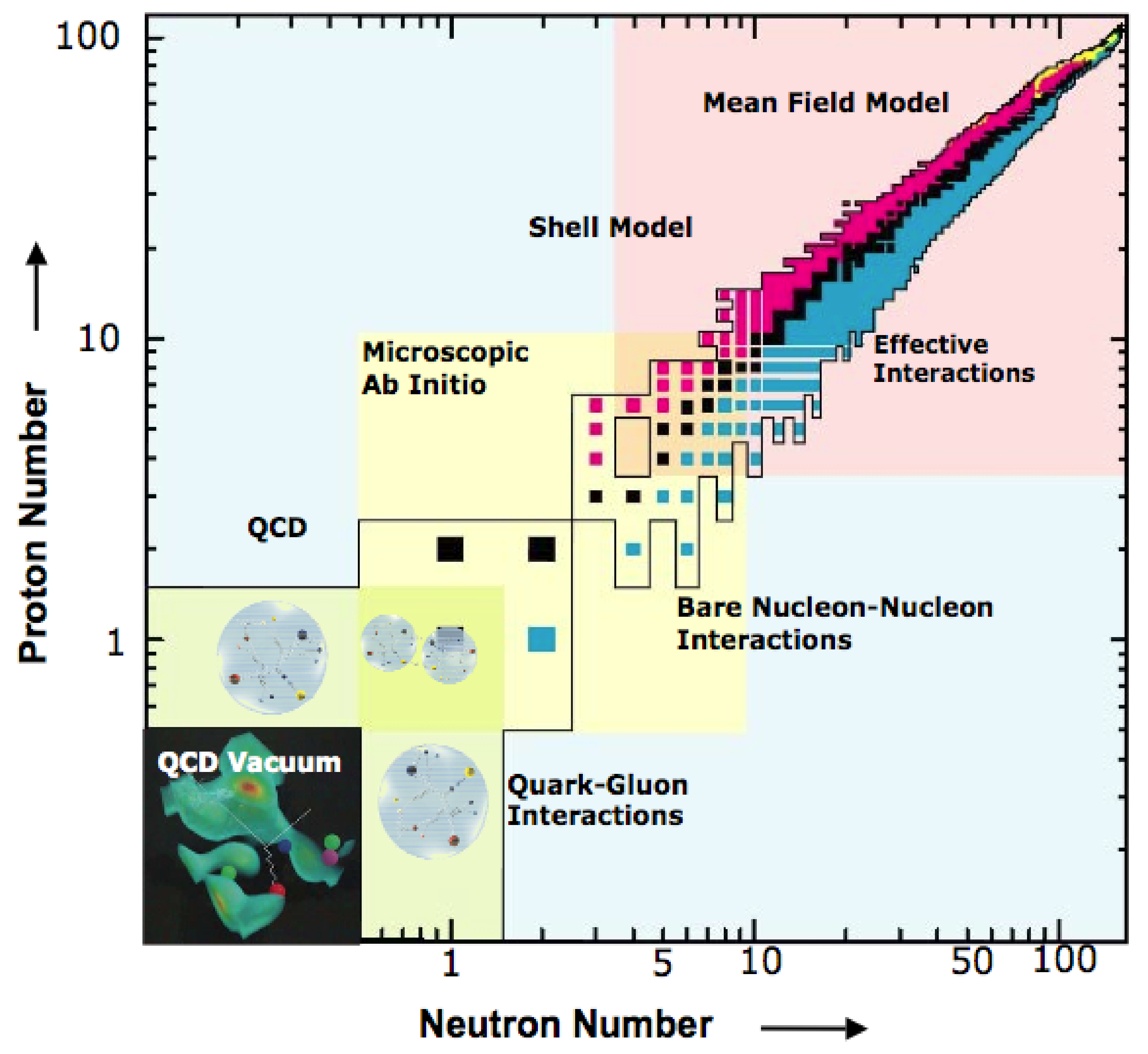
Home page: http://www.fuw.edu.pl/~dobaczew/

Energy scales in nuclear physics

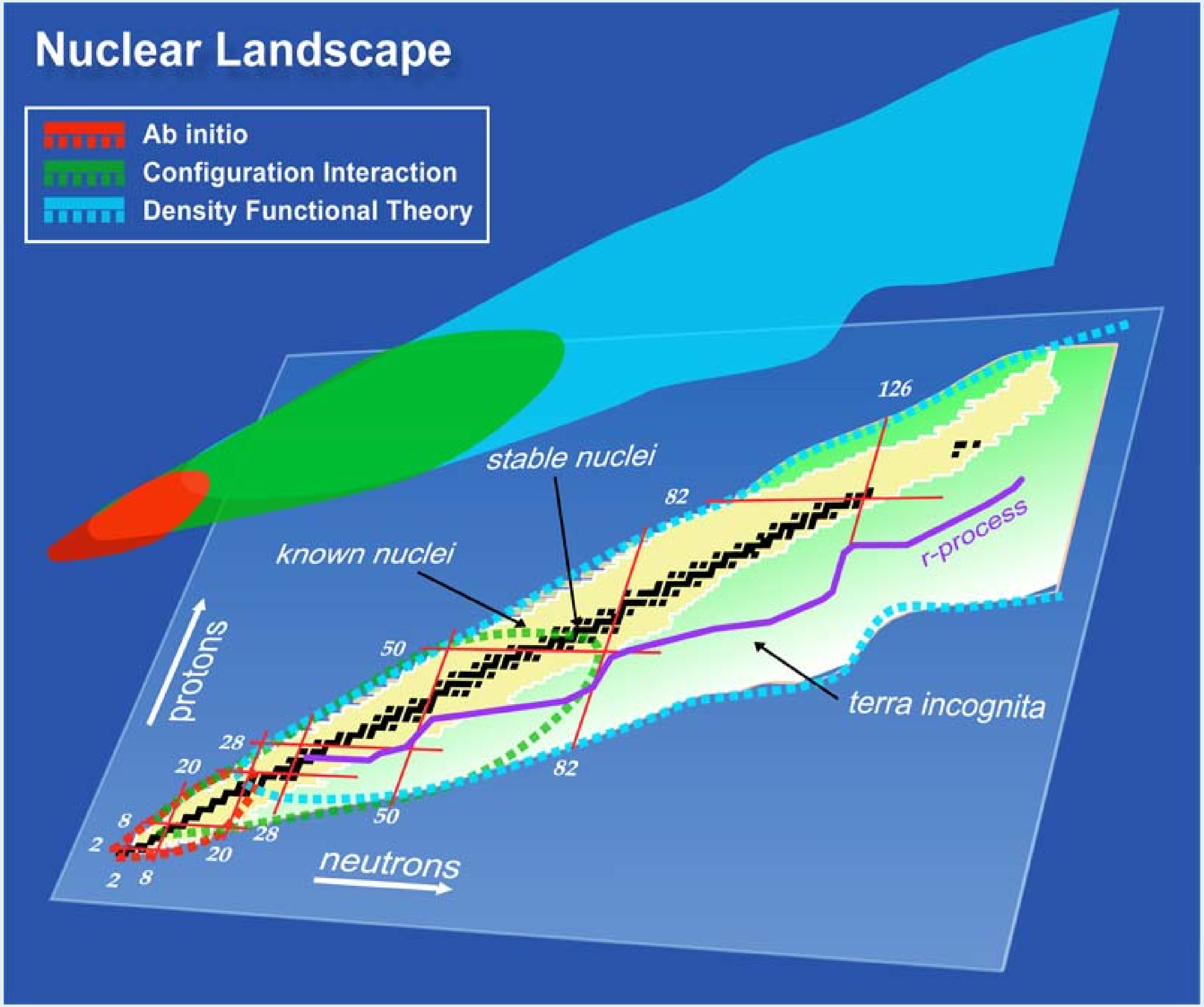
G. Bertsch *et al.*, SciDAC Review 6, 42 (2007)



Nuclear Structure

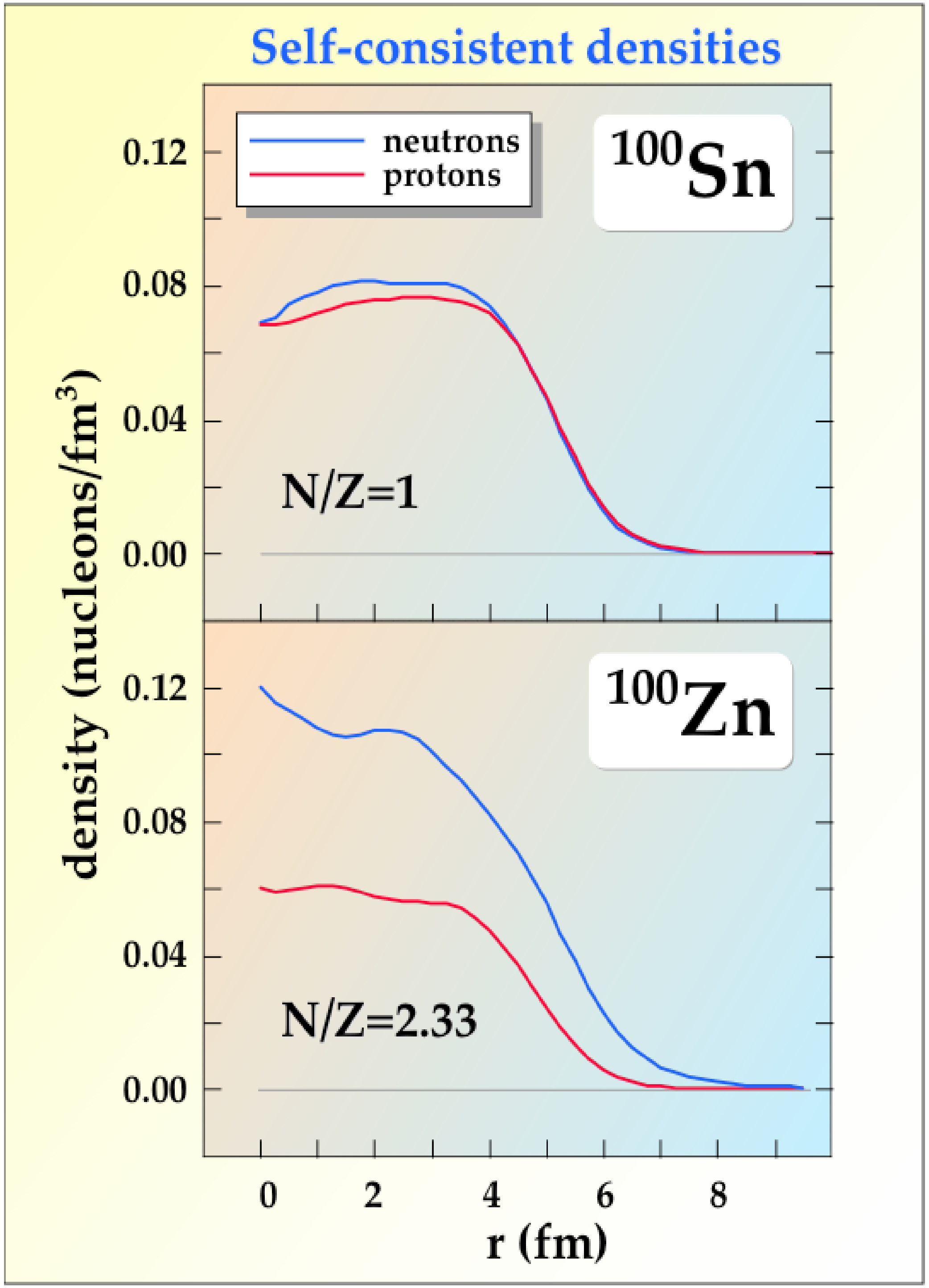

Mean Field Model
Shell Model
Effective Interactions
Microscopic Ab Initio
QCD
Bare Nucleon-Nucleon Interactions
QCD Vacuum
Quark-Gluon Interactions
Proton Number
Neutron Number
100
10
1
1
5
10
50
100

Universal Nuclear Energy Density Functional



UNEDF Collaboration, http://unedf.org/

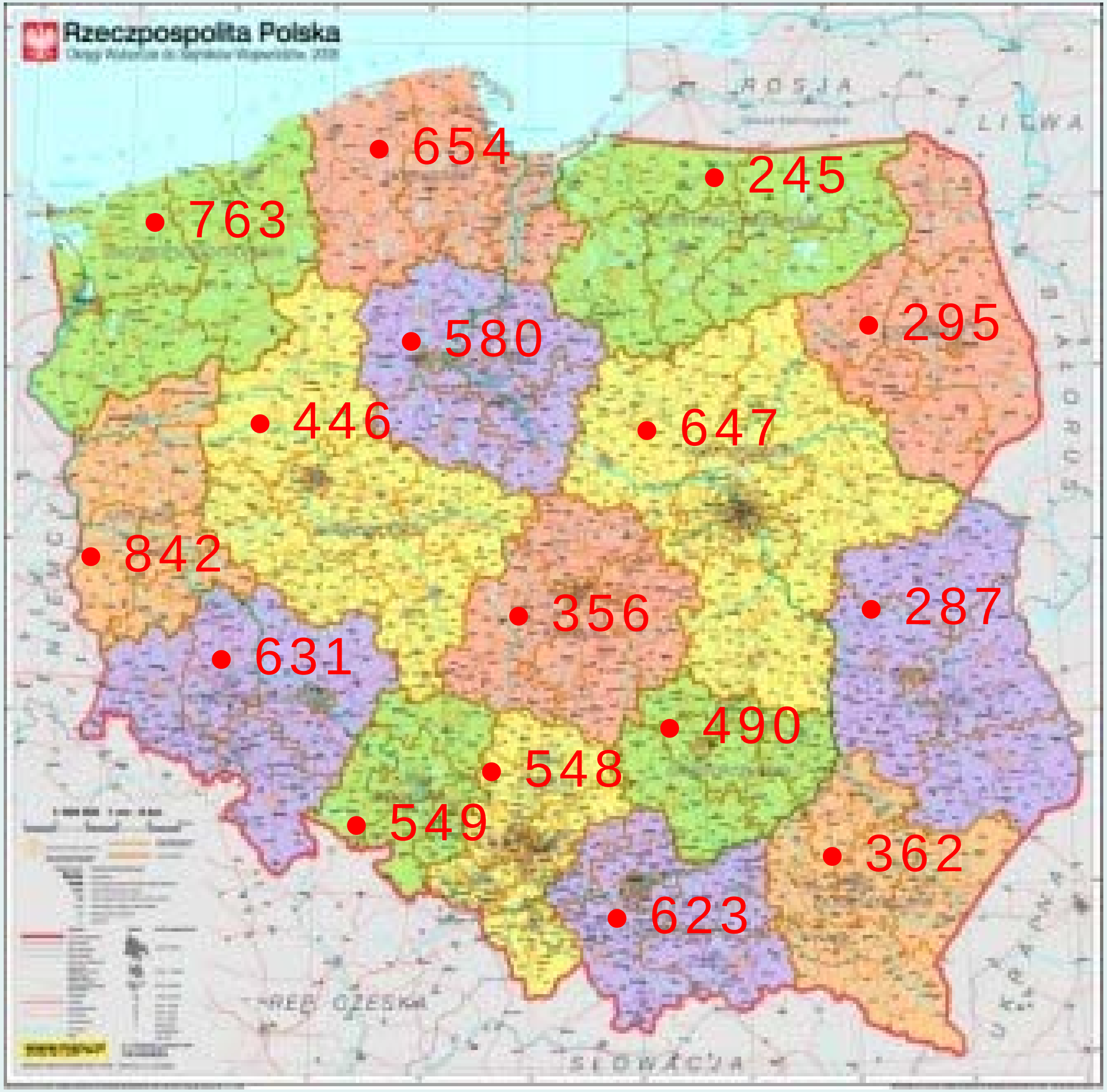
Mean-Field Theory ⇒ Density Functional Theory



Nuclear DFT

- two fermi liquids
- self-bound
- superfluid

- mean-field ⇒ one-body densities
- zero-range ⇒ local densities
- finite-range ⇒ gradient terms
- particle-hole and pairing channels
- Has been extremely successful. A broken-symmetry generalized product state does surprisingly good job for nuclei.



Price of land in Poland per voivodship

Price voivodship functional

Energy density functional

Price of land in Poland per district

↓

Price district functional

↓

Energy density functional

Price of land in Eurpe per country

Price country functional

Energy density functional

What is DFT?

Density Functional Theory:

A variational method that uses observables as variational parameters.

$$\delta\langle\hat{H} - \lambda\hat{Q}\rangle = 0$$

$$\Downarrow$$

$$E = E(Q)$$

for $E(\lambda) \equiv \langle\hat{H}\rangle$ and $Q(\lambda) \equiv \langle\hat{Q}\rangle$

Which DFT?

$$\delta\langle\hat{H} - \lambda\hat{Q}\rangle = 0 \Longrightarrow E = E(Q)$$

$$\delta\langle\hat{H} - \sum_k\lambda_k\hat{Q}_k\rangle = 0 \Longrightarrow E = E(Q_k)$$

$$\delta\langle\hat{H} - \int \mathrm{d}q\,\lambda(q)\hat{Q}(q)\rangle = 0 \Longrightarrow E = E[Q(q)]$$

$$\delta\langle\hat{H} - \int \mathrm{d}\vec{r}\,\lambda(\vec{r})\hat{\rho}(\vec{r})\rangle = 0 \Longrightarrow E = E[\rho(\vec{r})]$$

$$\text{for} \quad \hat{\rho}(\vec{r}) \quad = \quad \sum_{i=1}^{A}\delta(\vec{r} - \vec{r}_i)$$

$$\delta\langle\hat{H} - \int\!\!\int \mathrm{d}\vec{r}\mathrm{d}\vec{r}\,'\,\lambda(\vec{r},\vec{r}\,')\hat{\rho}(\vec{r},\vec{r}\,')\rangle = 0 \Longrightarrow E = E[\rho(\vec{r},\vec{r}\,')]$$

What is the DFT good for?

$$\delta\langle\hat{H} - \lambda\hat{Q}\rangle = 0$$

$$\Downarrow$$

$$E = E(Q)$$

Energy E is a function(al) of Q

1) **Exact:** Minimization of E(Q) gives the exact E and exact Q
2) **Impractical:** Derivation of E(Q) requires the full variation δ (bigger effort than to find the exact ground state)
3) **Inspirational:** Can we build useful models E′(Q) of the exact E(Q)?
4) **Experiment-driven:** E′(Q) works better or worse depending on the physical input used to build it.

Nuclear Energy Density Functionals

How the nuclear EDF is built?

$$E'[\rho(\vec{r})] = \int \mathrm{d}\vec{r}\,\mathcal{H}(\rho(\vec{r}))$$

LDA

Local energy density is a function of local density

$$E'[\rho(\vec{r},\vec{r}\,')] = \int\!\!\int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,'\,\mathcal{H}(\rho(\vec{r},\vec{r}\,'))$$

Gogny, M3Y,...

Non-local energy density is a function of non-local density

$$\mathcal{H}(\rho(\vec{r},\vec{r}\,')) = V(\vec{r}-\vec{r}\,')\Big[\rho(\vec{r})\rho(\vec{r}\,') - \rho(\vec{r},\vec{r}\,')\rho(\vec{r}\,',\vec{r})\Big]$$

How the nuclear EDF is built?

$$E' = \int d\vec{r}\, \mathcal{H}(\rho(\vec{r}), \tau(\vec{r}), \Delta\rho(\vec{r}), \ldots)$$

Skyrme, BCP, point-coupling,…

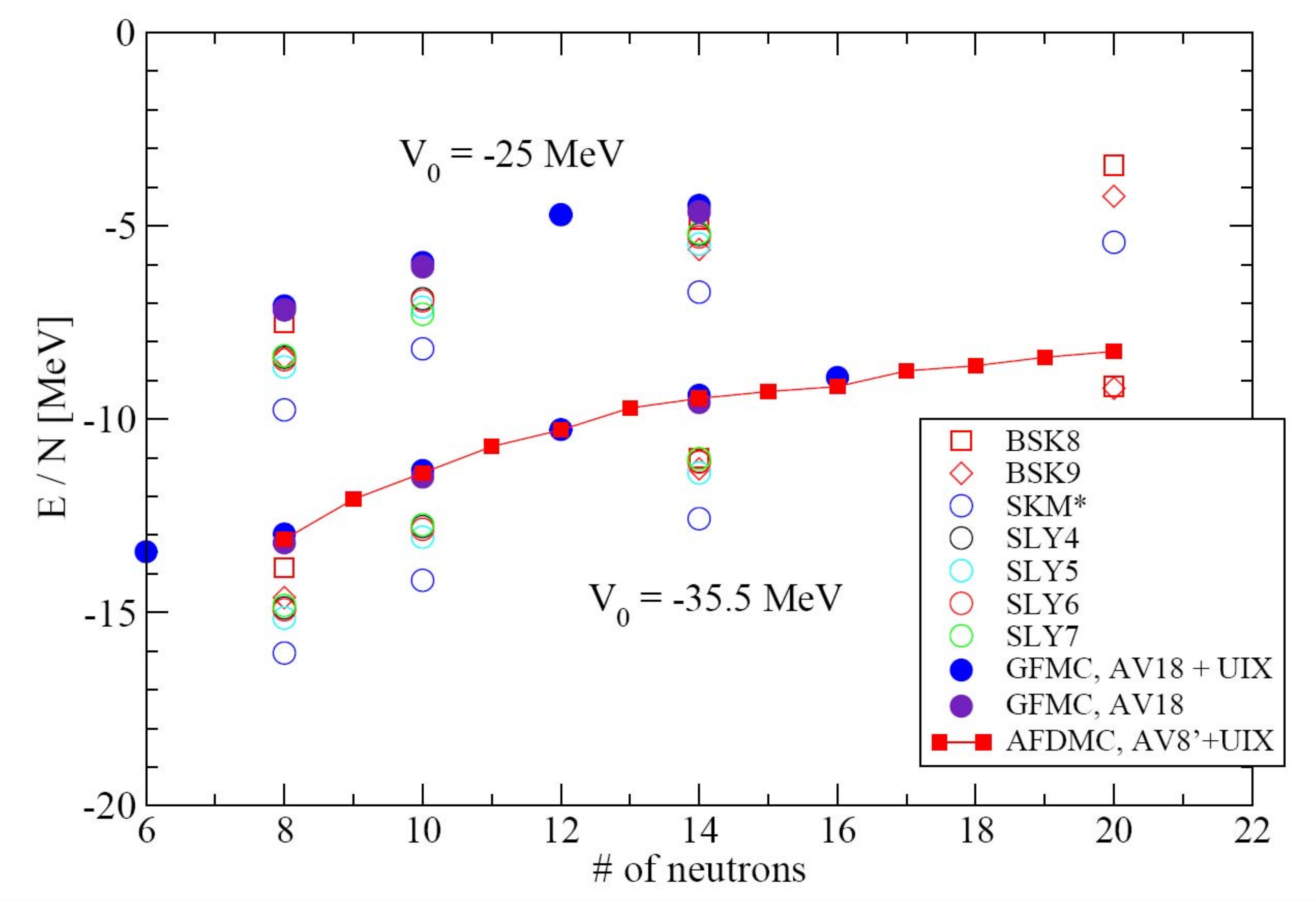
Quasi-local energy density is a function of local densities and gradients

$$E' = \int\int d\vec{r} d\vec{r}\,'\, \mathcal{H}(\rho(\vec{r}), \rho(\vec{r}\,'))$$

RMF (Hartree)

Non-local energy density is a function of local densities

Neutrons in external Woods-Saxon well



R.B. Wiringa & UNEDF Collaboration

Hohenberg-Kohn theorem

For any many-fermion state $|\Psi\rangle$ one can determine spatial distribution of particles $\rho(\vec{r})$ in the following way:

$$\rho(\vec{r}) = \langle\Psi|a^{+}(\vec{r})a(\vec{r})|\Psi\rangle = \int \mathrm{d}^3\vec{r}_1\ldots\mathrm{d}^3\vec{r}_A\Psi^*(\vec{r}_1\ldots\vec{r}_A)\left(\sum_{i=1}^{A}\delta(\vec{r}-\vec{r}_i)\right)\Psi(\vec{r}_1\ldots\vec{r}_A).$$

This creates a map

$$|\Psi\rangle \longrightarrow \rho(\vec{r})$$

and defines the class of states $\{|\Psi\rangle\}_{\rho(\vec{r})}$ that all have the same density distribution

$$\rho(\vec{r}) \longrightarrow \{|\Psi\rangle\}_{\rho(\vec{r})}\,.$$

Within the class of states $\{|\Psi\rangle\}_{\rho(\vec{r})}$ there is also a Slater determinant $|\Phi\rangle$, which has the same density distribution $\rho(\vec{r})$ as the other (correlated) states in the class. By minimizing the energy of the system within the class $\{|\Psi\rangle\}_{\rho(\vec{r})}$, we now define the energy-density-functional $\mathcal{E}[\rho(\vec{r})]$:

$$\mathcal{E}[\rho(\vec{r})] = \min_{\{|\Psi\rangle\}_{\rho(\vec{r})}} \langle\Psi|\hat{H}|\Psi\rangle.$$

It is then obvious that the exact ground-state energy E_0 is obtained by minimizing the functional $\mathcal{E}[\rho(\vec{r})]$ with respect to densities $\rho(\vec{r})$.

$$E_0 = \min_{\rho(\vec{r})} \mathcal{E}[\rho(\vec{r})].$$

Hohenberg-Kohn theorem (trivial version)

For any many-fermion state $|\Psi\rangle$ one can determine mean-square radius $\langle\vec{r}^2\rangle$ in the following way:

$$\langle\vec{r}^2\rangle = \int d^3\vec{r}_1\ldots d^3\vec{r}_A \Psi^*(\vec{r}_1\ldots\vec{r}_A)\left(\sum_{i=1}^{A}\vec{r}_i^2\right)\Psi(\vec{r}_1\ldots\vec{r}_A).$$

This creates a map

$$|\Psi\rangle \longrightarrow \langle\vec{r}^2\rangle$$

and defines the class of states $\{|\Psi\rangle\}_{\langle\vec{r}^2\rangle}$ that all have the same mean-square radius

$$\langle\vec{r}^2\rangle \longrightarrow \{|\Psi\rangle\}_{\langle\vec{r}^2\rangle}\,.$$

Within the class of states $\{|\Psi\rangle\}_{\langle\vec{r}^2\rangle}$ there are also Slater determinants $|\Phi\rangle$, which have the same mean-square radii $\langle\vec{r}^2\rangle$ as the other (correlated) states in the class. By minimizing the energy of the system within the class $\{|\Psi\rangle\}_{\langle\vec{r}^2\rangle}$, we now define the energy-density-functional $\mathcal{E}[\langle\vec{r}^2\rangle]$:

$$\mathcal{E}[\langle\vec{r}^2\rangle] = \min_{\{|\Psi\rangle\}_{\langle\vec{r}^2\rangle}} \langle\Psi|\hat{H}|\Psi\rangle.$$

It is then obvious that the exact ground-state energy E_0 is obtained by minimizing the functional $\mathcal{E}[\langle\vec{r}^2\rangle]$ with respect to mean-square radii $\langle\vec{r}^2\rangle$:

$$E_0 = \min_{\langle\vec{r}^2\rangle} \mathcal{E}[\langle\vec{r}^2\rangle].$$

Nuclear Energy Density Functional
(physical insight)

1° The energy-density functional that can be universal (valid for systems with any particle number) must depend at least on the local particle density:

$$\mathcal{E}'[\rho(\vec{r})] = \mathcal{E}[\rho(\vec{r})] - \lambda \int \mathrm{d}^3\vec{r}\rho(\vec{r}).$$

2° The energy-density functional that can describe shell effects must depend on the local kinetic density (Kohn-Sham approach):

$$\mathcal{E}[\rho(\vec{r}),\tau(\vec{r})] = \frac{\hbar^2}{2m}\int \mathrm{d}^3\vec{r}\tau(\vec{r}) + \mathcal{E}^{\mathrm{int}}[\rho(\vec{r})].$$

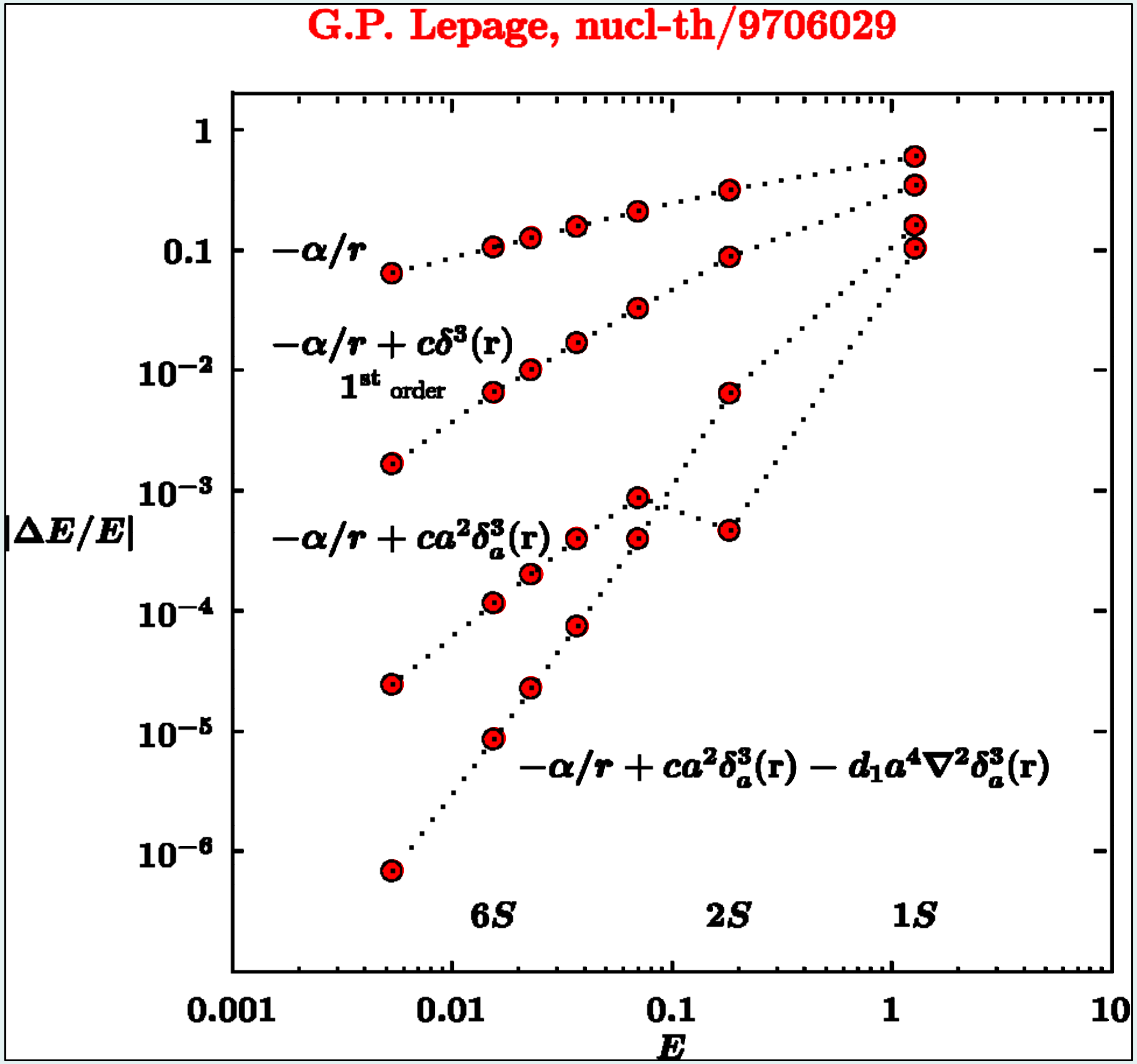
3° The energy-density functional that can describe effective-mass, surface, and spin-orbit effects must in addition depend on the gradient of density and spin-momentum density:

$$\mathcal{E}[\rho(\vec{r}),\tau(\vec{r}),\vec{\nabla}\rho(\vec{r}),J_{\mu\nu}(\vec{r})] = \frac{\hbar^2}{2m}\int \mathrm{d}^3\vec{r}\tau(\vec{r}) + \mathcal{E}^{\mathrm{int}}[\rho(\vec{r}),\vec{\nabla}\rho(\vec{r}),J_{\mu\nu}(\vec{r})].$$

4° The energy-density functional that can describe time-odd effects must in addition depend on time-odd densities.

Effective Theories

Hydrogen atom perturbed near the center


G.P. Lepage, nucl-th/9706029

Relative errors in the S-wave binding energies are plotted versus:

(i) the binding energy for the Coulomb theory

(ii) the Coulomb theory augmented with a delta function in first-order perturbation theory

(iii) the non-perturbative effective theory through a^2, and

(iv) the effective theory through a^4.

Dimensional analysis - regularization

Integrals

$$I_1 = \int_{-\infty}^{\infty} \mathrm{d}x \, \exp\left(-\frac{x^2}{a^2}\right), \qquad I_2 = \int_{-\infty}^{\infty} \mathrm{d}x \, \frac{1}{a^2 + x^2},$$

are equal to

$$I_1 = \kappa_1 \, a, \qquad I_2 = \kappa_2 \, a^{-1},$$

where κ's stand for dimensionless constants, because

$$\dim I_1 = \dim x = \dim a, \qquad \dim I_2 = \dim x^{-1} = \dim a^{-1}.$$

Explicitly, we have $\kappa_1 = \sqrt{\pi}$ and $\kappa_2 = \pi$.
Dimension of the δ distribution is $\dim \delta = \dim x^{-1}$, because

$$\int_{-\infty}^{\infty} \mathrm{d}x \, \delta(x) = 1.$$

Hence we have two possible *regularized* δ distributions:

$$\delta_a^{(1)}(x) = \frac{1}{\sqrt{\pi} a} \exp\left(-\frac{x^2}{a^2}\right), \qquad \delta_a^{(2)}(x) = \frac{a}{\pi} \frac{1}{a^2 + x^2},$$

or in three dimensions:

$$\delta_a^{(1)}(\vec{r}) = \frac{1}{\sqrt{\pi^3} a^3} \exp\left(-\frac{\vec{r}^2}{a^2}\right), \qquad \delta_a^{(2)}(\vec{r}) = \frac{a^3}{\pi^3} \frac{1}{(a^2 + x^2)(a^2 + y^2)(a^2 + z^2)}.$$

Dimensional analysis – the hydrogen-like atom

Hydrogen-like atom (one-electron) Hamiltonian reads

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta - \frac{\alpha}{r},$$

where $\alpha = Ze^2$.

Dimensions of terms are

$$\begin{aligned} \dim \hat{H} &= \dim E, \\ \dim \left[\frac{\hbar^2}{m}\right] &= \dim Er^2, \\ \dim \alpha &= \dim Er. \end{aligned}$$

Therefore

$$\begin{aligned} E &= \kappa_E \frac{\alpha^2 m}{2\hbar^2} = \kappa_E Z^2 \mathrm{Ry}, \\ \langle r^2 \rangle^{1/2} &= \kappa_r \frac{\hbar^2}{\alpha m} = \kappa_r \frac{a_0}{Z}, \end{aligned}$$

where Ry and a_0 are one Rydberg and Bohr's radius, respectively. For example, for the n-th radial state we have

$$E_n = -\frac{Z^2}{n^2}\mathrm{Ry}, \qquad r_n^{max} = \frac{n^2}{Z}a_0$$

Emission of long electromagnetic waves

(I) EXACT

For an arbitrary current $\vec{J}(\vec{x}', t')$:

$$\vec{A}(\vec{x}, t) = \frac{1}{c}\int \mathrm{d}^3\vec{x}' \int \mathrm{d}t' \, \frac{\delta(t' - (t - \frac{1}{c}|\vec{x}' - \vec{x}|))}{|\vec{x}' - \vec{x}|} \vec{J}(\vec{x}', t')$$

For harmonic currents (or a single Fourier component),

$$\vec{J}(\vec{x}, t) = \vec{J}(\vec{x}) e^{-i\omega t},$$

the fields are also harmonic,

$$\vec{A}(\vec{x}, t) = \vec{A}(\vec{x}) e^{-i\omega t},$$

and the amplitudes outside the sources read

$$\vec{A}(\vec{x}) = \frac{4\pi i}{c} \sum\nolimits_{lm} k^{l+1} h_l^{(1)}(kr) Y_{lm}(\theta, \phi) \vec{M}_{lm}(k)$$

for

$$\vec{M}_{lm}(k) = \frac{1}{k^l} \int \mathrm{d}^3\vec{x}' j_l(kr') Y^*_{lm}(\theta', \phi') \vec{J}(\vec{x}')$$

and $k = \omega / c$.

Emission of long electromagnetic waves

(II) APPROXIMATE

Details of the current distribution become totally invisible when a long wave, $kr' \ll 1$, is recorded at a large distance, $kr \gg 1$:

$$\vec{A}(\vec{x}) = \frac{4\pi}{c}\frac{e^{ikr}}{r}\sum_{lm}(-ik)^l Y_{lm}(\theta,\phi)\vec{M}_{lm}$$

for

$$\vec{M}_{lm} = \frac{1}{(2l+1)!!}\int \mathrm{d}^3\vec{x}' r'^l Y^*_{lm}(\theta',\phi')\vec{J}(\vec{x}')$$

Within the long wavelength approximation, only a few numbers (the multipole moments $\vec{M}_{lm}$) are needed to fully describe the emitted radiation. Details of current distribution inside the source become irrelevant.

Blue-sky problem - Compton scattering

(I) CLASSICAL EM: A charge q confined by a potential with eigen-frequency of ω_0, shaken by an external force F with frequency ω, radiates a wave with power P:

$$P = \frac{q^2F^2}{3c^3m^2}\frac{\omega^4}{(\omega^2-\omega_0^2)^2}$$

(II) QED: Sum of three 2nd order diagrams.
(III) EFT: The energy density $H^0_{\rm eff}$ of an atom in state Ψ reads:

$$H^0_{\rm eff} = \Psi^*\left(\frac{p^2}{2m}+e\phi\right)\Psi$$

When the atom is placed in an EM field it acquires additional energy density $H^1_{\rm eff}$ that must be a scalar, T-even, and P-even function of fields, i.e., for sufficiently weak fields:

$$H^1_{\rm eff} = -\frac{1}{2}\Psi^*\Psi\left(c_E\vec{E}^2+c_B\vec{B}^2\right)$$

Since the coupling constants c_E and c_B have dimensions of a volume, they must be related to the volume of the atom a_0^3 by: $c_E = \chi_E a_0^3$, $c_B = \chi_B a_0^3$ with dimensionless coupling constants χ_E and χ_B of the order of 1. Finaly, for the EM wave, $|\vec{E}|\sim\omega$ and $|\vec{B}|\sim\omega$ we obtain:

$$\frac{d\sigma}{d\Omega} = |\langle f|H^1_{\rm eff}|i\rangle|^2 \sim \omega^4a_0^6.$$

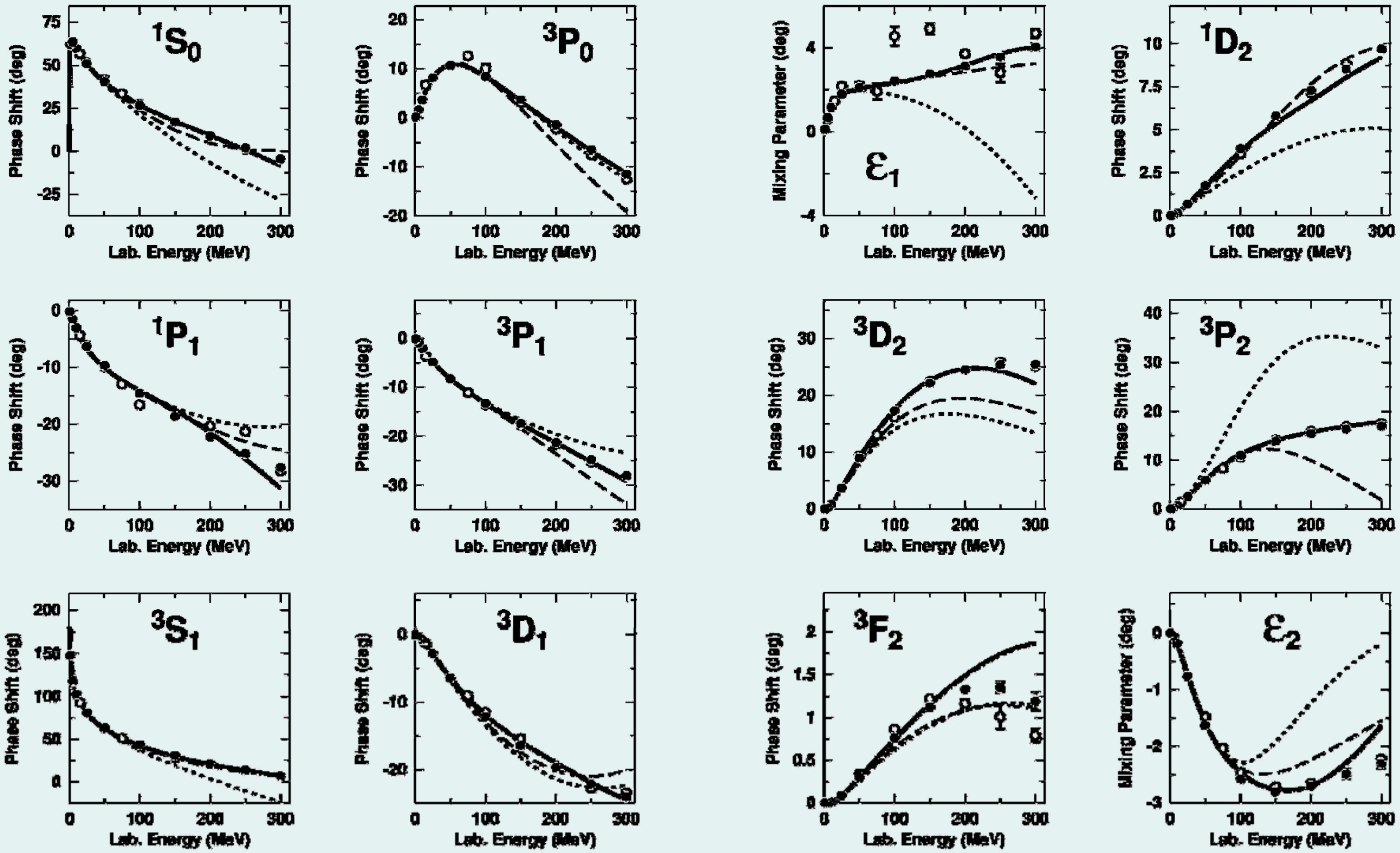
N^3LO in the chiral perturbation effective field theory

Table 1: Contact-gradient expansion for relative-coordinate two-particle matrix elements. Here $\vec{D}^2_M = (\vec{\nabla} \otimes \vec{\nabla})_{2M}$, $\vec{D}^0_0 = [(\boldsymbol{\sigma}(1) \otimes \boldsymbol{\sigma}(2))_2 \otimes D^2]_{00}$, $\vec{F}^3_M = (\vec{\nabla} \otimes \vec{D}^2)_{3M}$, $\vec{F}^1_M = [(\boldsymbol{\sigma}(1) \otimes \boldsymbol{\sigma}(2))_2 \otimes F^3]_{1M}$, $\vec{G}^4_M = (\vec{D}^2 \otimes \vec{D}^2)_{4M}$, $\vec{G}^2_M = [(\boldsymbol{\sigma}(1) \otimes \boldsymbol{\sigma}(2))_2 \otimes G^4]_{2M}$, and the scalar product of tensor operators is defined as $A^J \cdot B^J = \sum_{M=-J}^{M=J} (-1)^M A^J_M B^J_{-M}$.

Transitions	LO	NLO	NNLO	N^3LO
${}^3S_1 \leftrightarrow {}^3S_1$ or ${}^1S_0 \leftrightarrow {}^1S_0$	$\delta(\mathbf{r})$	$\overleftarrow{\nabla}^2\,\delta(\mathbf{r}) + \delta(\mathbf{r})\,\overrightarrow{\nabla}^2$	$\overleftarrow{\nabla}^2\,\delta(\mathbf{r})\,\overrightarrow{\nabla}^2$ $\overleftarrow{\nabla}^4\,\delta(\mathbf{r}) + \delta(\mathbf{r})\,\overrightarrow{\nabla}^4$	$\overleftarrow{\nabla}^4\,\delta(\mathbf{r})\,\overrightarrow{\nabla}^2 + \overleftarrow{\nabla}^2\,\delta(\mathbf{r})\,\overrightarrow{\nabla}^4$ $\overleftarrow{\nabla}^6\,\delta(\mathbf{r}) + \delta(\mathbf{r})\,\overrightarrow{\nabla}^6)$
${}^3S_1 \leftrightarrow {}^3D_1$		$\delta(\mathbf{r})\,\overrightarrow{D}^0 + \overleftarrow{D}^0\,\delta(\mathbf{r})$	$\overleftarrow{\nabla}^2\,\delta(\mathbf{r})\,\overrightarrow{D}^0 + \overleftarrow{D}^0\,\delta(\mathbf{r})\,\overrightarrow{\nabla}^2$ $\delta(\mathbf{r})\,\overrightarrow{\nabla}^2\overrightarrow{D}^0 + \overleftarrow{D}^0\overleftarrow{\nabla}^2\,\delta(\mathbf{r})$	$(\overleftarrow{\nabla}^4\,\delta(\mathbf{r})\,\overrightarrow{D}^0 + \overleftarrow{D}^0\,\delta(\mathbf{r})\,\overrightarrow{\nabla}^4$ $(\overleftarrow{\nabla}^2\,\delta(\mathbf{r})\,\overrightarrow{\nabla}^2\overrightarrow{D}^0 + \overleftarrow{D}^0\overleftarrow{\nabla}^2\,\delta(\mathbf{r})\,\overrightarrow{\nabla}^2$ $(\delta(\mathbf{r})\,\overrightarrow{\nabla}^4\overrightarrow{D}^0 + \overleftarrow{D}^0\overleftarrow{\nabla}^4\,\delta(\mathbf{r})$
${}^1D_2 \leftrightarrow {}^1D_2$ or ${}^3D_J \leftrightarrow {}^3D_J$			$\overleftarrow{D}^2 \cdot \delta(\mathbf{r})\,\overrightarrow{D}^2$	$\overleftarrow{D}^2\overleftarrow{\nabla}^2 \cdot \delta(\mathbf{r})\,\overrightarrow{D}^2 + \overleftarrow{D}^2 \cdot \delta(\mathbf{r})\,\overrightarrow{\nabla}^2\overrightarrow{D}^2$
${}^3D_3 \leftrightarrow {}^3G_3$				$(\overleftarrow{D}^2 \cdot \delta(\mathbf{r})\,\overrightarrow{G}^2 + \overleftarrow{G}^2 \cdot \delta(\mathbf{r})\,\overrightarrow{D}^2$
${}^1P_1 \leftrightarrow {}^1P_1$ or ${}^3P_J \leftrightarrow {}^3P_J$		$\overleftarrow{\nabla} \cdot \delta(\mathbf{r})\,\overrightarrow{\nabla}$	$\overleftarrow{\nabla}\overleftarrow{\nabla}^2 \cdot \delta(\mathbf{r})\,\overrightarrow{\nabla} + \overleftarrow{\nabla} \cdot \delta(\mathbf{r})\,\overrightarrow{\nabla}^2\overrightarrow{\nabla}$	$\overleftarrow{\nabla}\overleftarrow{\nabla}^2 \cdot \delta(\mathbf{r})\,\overrightarrow{\nabla}^2\overrightarrow{\nabla}$ $\overleftarrow{\nabla}\overleftarrow{\nabla}^4 \cdot \delta(\mathbf{r})\,\overrightarrow{\nabla} + \overleftarrow{\nabla} \cdot \delta(\mathbf{r})\,\overrightarrow{\nabla}^4\overrightarrow{\nabla}$
${}^3P_2 \leftrightarrow {}^3F_2$			$\overleftarrow{\nabla} \cdot \delta(\mathbf{r})\,\overrightarrow{F}^1 + \overleftarrow{F}^1 \cdot \delta(\mathbf{r})\,\overrightarrow{\nabla}$	$\overleftarrow{\nabla}\overleftarrow{\nabla}^2 \cdot \delta(\mathbf{r})\,\overrightarrow{F}^1 + \overleftarrow{F}^1 \cdot \delta(\mathbf{r})\,\overrightarrow{\nabla}^2\overrightarrow{\nabla})$ $\overleftarrow{\nabla} \cdot \delta(\mathbf{r})\,\overrightarrow{\nabla}^2\overrightarrow{F}^1 + \overleftarrow{F}^1\overleftarrow{\nabla}^2 \cdot \delta(\mathbf{r})\,\overrightarrow{\nabla}$
${}^1F_3 \leftrightarrow {}^1F_3$ or ${}^3F_J \leftrightarrow {}^3F_J$				$\overleftarrow{F}^3 \cdot \delta(\mathbf{r})\,\overrightarrow{F}^3$

W.C. Haxton, Phys. Rev. C77, 034005 (2008)

EFT phase-shift analysis



np phase parameters below 300 MeV lab. energy for partial waves with J=0,1,2. The solid line is the result at N^{3}LO. The dotted and dashed lines are the phase shifts at NLO and NNLO, respectively, as obtained by Epelbaum *et al*. The solid dots show the Nijmegen multi-energy np phase shift analysis and the open circles are the VPI single-energy np analysis SM99.

D.R. Entem and R. Machleidt Phys.Rev. C68 (2003) 041001

Many-fermion Hilbert space

Indistinguishability principle

We define the exchange operator $\hat{P}_{ij}$ as

$$\hat{P}_{ij}\Psi(x_1,\ldots,x_i,\ldots,x_j,\ldots,x_A)=\Psi(x_1,\ldots,x_j,\ldots,x_i,\ldots,x_A).$$

$\hat{P}_{ij}$ is hermitian and unitary:

$$\hat{P}_{ij}^{+}=\hat{P}_{ij}\quad,\qquad\hat{P}_{ij}^{2}=1,$$

and has eigenvalues equal only to $+1$ or -1.

> **Any measurement performed on states Ψ and $\hat{P}_{ij}\Psi$ must give the same result**

Hence:

$$\hat{P}_{ij}\Psi=p_{ij}\Psi\quad,\qquad p_{ij}=\pm1,$$

for all ij, and
$p_{ij}{=}{+}1$ for all ij, i.e., $\hat{P}_{ij}\Psi{=}\Psi$,
$p_{ij}{=}{-}1$ for all ij, i.e., $\hat{P}_{ij}\Psi{=}{-}\Psi$.

In nature, we have only two kinds of particles:
$\hat{P}_{ij}\Psi{=}\Psi \implies$ bosons
$\hat{P}_{ij}\Psi{=}{-}\Psi \implies$ fermions

Eigenstates of the many-body Hamiltonian $\hat{H}$ must simultaneously be eigenstates of $\hat{P}_{ij}$, i.e.,

$$\hat{P}_{ij}^{+}\hat{H}\hat{P}_{ij}=\hat{H}\quad\text{or}\quad[\hat{P}_{ij},\hat{H}]=0.$$

Fock space

Let us consider a (finite) space of single-particle states spanned by M wave-functions that form the one-body Hilbert space $\mathcal{H}_1$

$$\phi_1(x), \phi_2(x), \ldots, \phi_M(x),$$

which are orthogonal:

$$\int dx \phi^*_\mu(x)\phi_\nu(x) = \delta_{\mu\nu}.$$

Products of single-particle states $\phi_\mu(x_1)\phi_\nu(x_2)$ span the two-body space $\mathcal{H}_2 = \mathcal{H}_1 \otimes \mathcal{H}_1$; hence the two-body *fermion* space is spanned by antisymmetrized products:

$$\Phi_{\mu\nu}(x_1, x_2) = \frac{1}{\sqrt{2}} \left(\phi_\mu(x_1)\phi_\nu(x_2) - \phi_\mu(x_2)\phi_\nu(x_1)\right)$$

for $\mu < \nu$. Similarly, the A-body Hilbert space $\mathcal{H}_A$ is spanned by the wave-functions $\Phi_{\mu_1 \ldots \mu_A}(x_1, \ldots, x_A)$ (Slater determinants):

$$\Phi_{\mu_1 \ldots \mu_A}(x_1, \ldots, x_A) = (A!)^{-1/2} \sum_P (-1)^P \phi_{\mu_1}(x_{i_1}) \ldots \phi_{\mu_A}(x_{i_A}),$$

The set of Hilbert spaces $\mathcal{H}_1$,$\mathcal{H}_2$,...,$\mathcal{H}_M$ can now be completed with the zero-body Hilbert space $\mathcal{H}_0$ containing only one "wave-function" ϕ_{vac} called vacuum state, which gives the Fock space:

$$\boxed{\mathcal{H} := \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \ldots \oplus \mathcal{H}_M.}$$

Creation and annihilation operators

In the Fock space, the creation operators are defined as

$$a^+_\mu \Phi_{\mu_1\ldots\mu_A} := \begin{cases} 0 & \text{for} \quad \mu \in \{\mu_i\}, \\ \Phi_{\mu\mu_1\ldots\mu_A} & \text{for} \quad \mu \notin \{\mu_i\}. \end{cases}$$

Hence, their hermitian conjugates $a_\mu = (a^+_\mu)^+$ act on states $\Phi_{\mu\mu_1\ldots\mu_A}$ as the annihilation operators:

$$a_\mu \Phi_{\mu_1\ldots\mu_{A+1}} = \begin{cases} 0 & \text{for} \quad \mu \notin \{\mu_i\}, \\ (-1)^{k+1}\Phi_{\mu_1\ldots\overset{\text{no }\mu}{\smile}\ldots\mu_{A+1}} & \text{for} \quad \mu = \mu_k, \end{cases}$$

where symbol $\overset{\text{no }\mu}{\smile}$ denotes that index $\mu = \mu_k$ must be omitted.

Based on these definitions, one can derive the following anticommutation properties for $\{A, B\}{:=}AB{+}BA$:

$$\boxed{\begin{aligned} \{a^+_\mu, a^+_\nu\} &= 0, \\ \{a_\mu, a_\nu\} &= 0, \\ \{a_\mu, a^+_\nu\} &= \delta_{\mu\nu}, \end{aligned}}$$

which imply that in particular

$$(a^+_\mu)^2 = 0, \qquad (a_\mu)^2 = 0.$$ **The Pauli Principle!!**

Operators in the Fock space

We define the K-particle position-representation operator acting in the A-body Hilbert space as

$$\hat{F}_K = \sum_{j_1<\ldots<j_K}^{A} f(x_{j_1},\ldots,x_{j_K}),$$

where $f(x_{j_1},\ldots,x_{j_K})$ is a *symmetric* function to comply with the indistinguishability principle. By definition, in all Hilbert spaces with $A<K$, we have $\hat{F}_K=0$. Operator $\hat{F}_K=0$ is fully determined through its matrix elements in the A-body space for $A=K$. In particular,

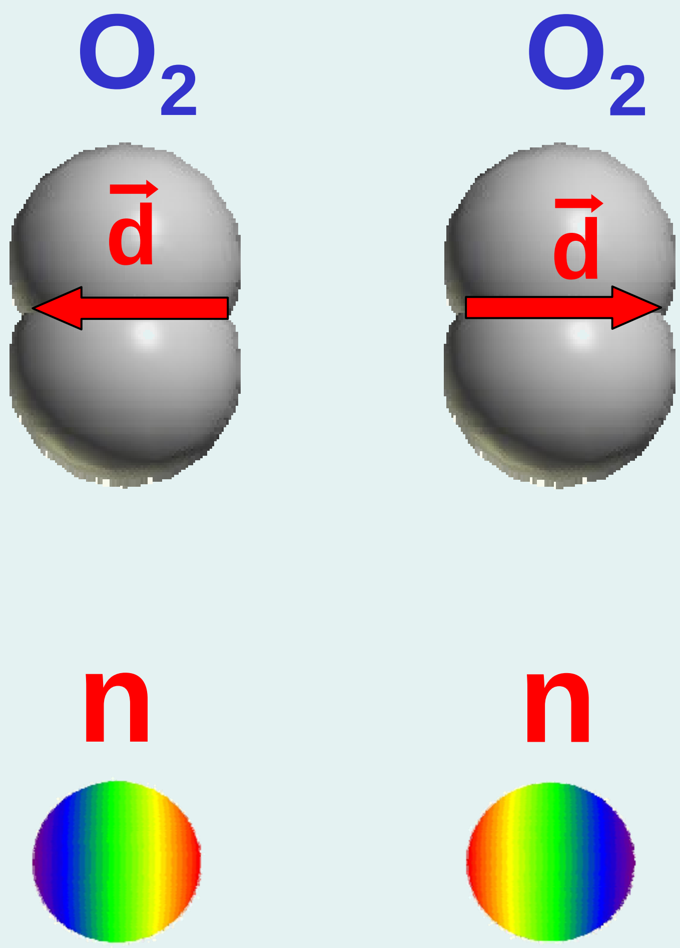
$$\begin{aligned}
F_{\mu\nu} &= \int \mathrm{d}x\,\phi^*_\mu(x) f(x)\phi_\nu(x), \\
F_{\mu\mu'\nu\nu'} &= \int \mathrm{d}x\mathrm{d}x'\,\phi^*_\mu(x)\phi^*_{\mu'}(x') f(x,x') \times \left(\phi_\nu(x)\phi_{\nu'}(x') - \phi_{\nu'}(x)\phi_\nu(x')\right),
\end{aligned}$$

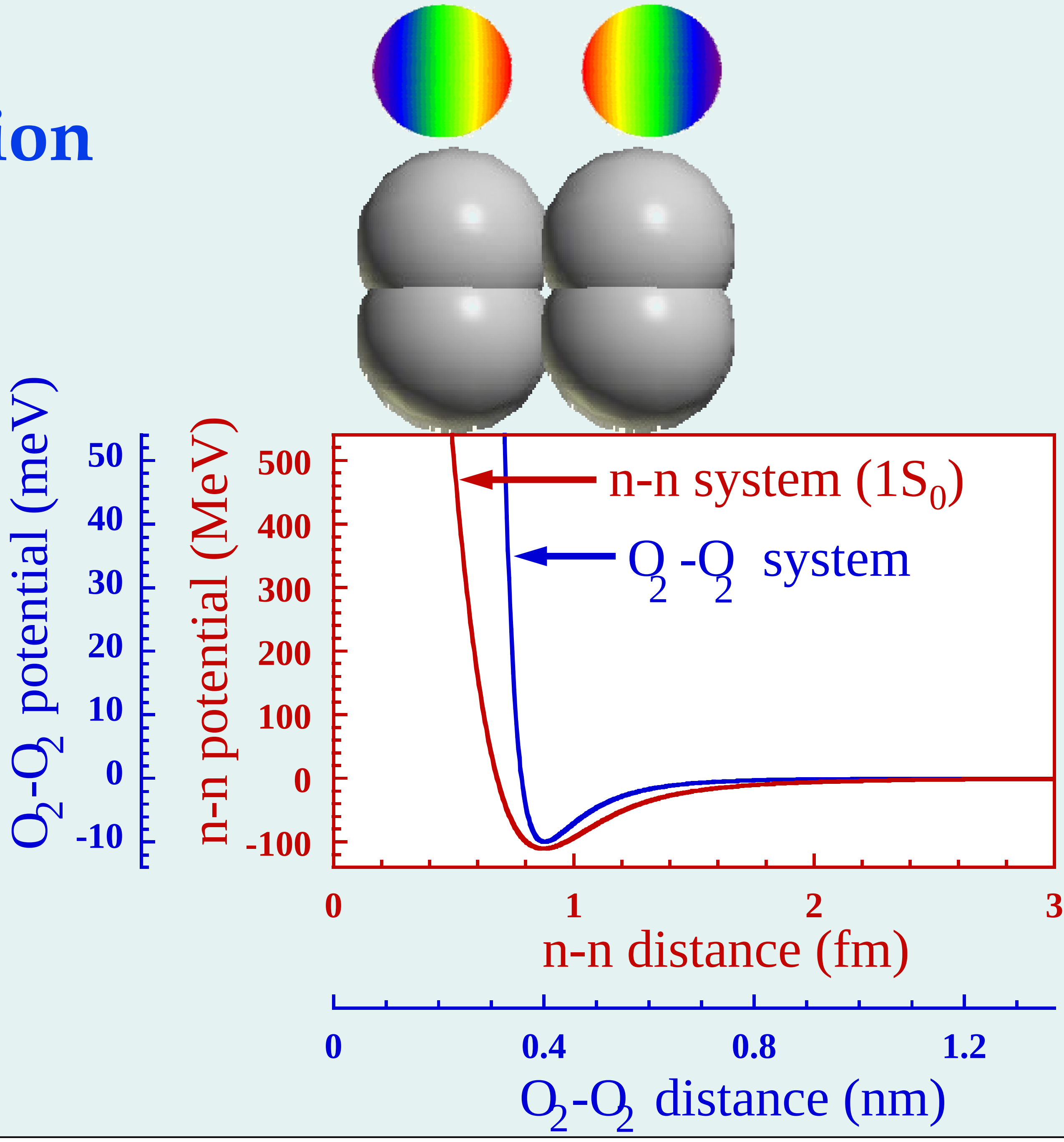
and

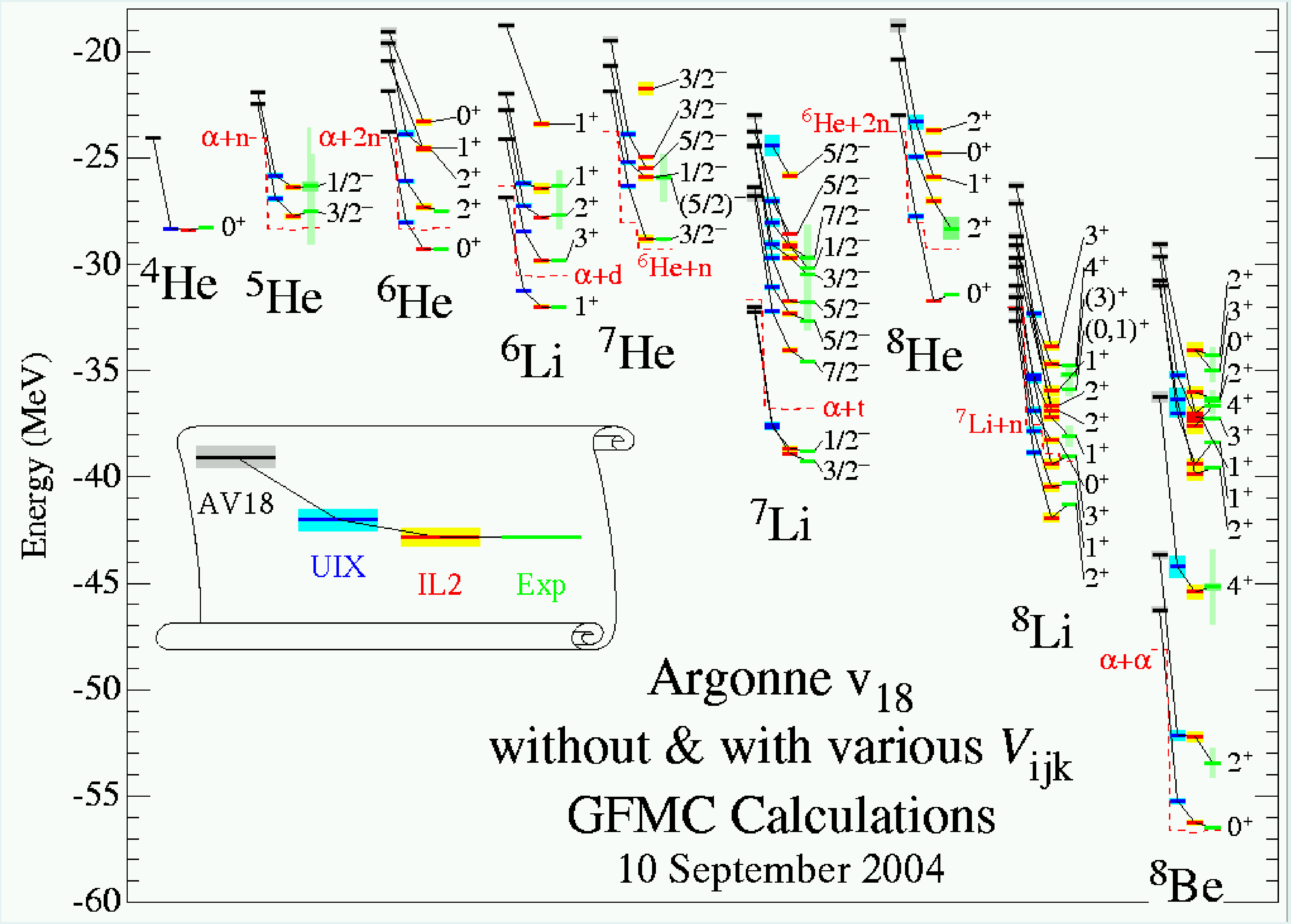
$$\begin{aligned}
\hat{F}_1 &= \sum_{\mu\nu} F_{\mu\nu} a^+_\mu a_\nu, \\
\hat{F}_2 &= \frac{1}{4}\sum_{\mu\mu'\nu\nu'} F_{\mu\mu'\nu\nu'} a^+_\mu a^+_{\mu'} a_{\nu'} a_\nu, \\
\hat{F}_3 &= \frac{1}{36}\sum_{\mu\mu'\mu''\nu\nu'\nu''} F_{\mu\mu'\mu''\nu\nu'\nu''} a^+_\mu a^+_{\mu'} a^+_{\mu''} a_{\nu''} a_{\nu'} a_\nu.
\end{aligned}$$

Note the inverted order of indices in $\hat{F}_2$ and $\hat{F}_3$!

n-n versus O_2-O_2 interaction







Argonne v_{18}

without & with various V_{ijk}

GFMC Calculations

10 September 2004

http://www.phy.anl.gov/theory/research/forces.html

Lessons learned

★ 1) Energy density functional exists due to the two-step variational method and gives exact ground state energy and its exact particle density.

★ 2) Whenever the energy scales (or range scales) between the interactions and observations are different, the observations can be described by a series of pseudopotentials with coupling constants adjusted to data (an effective theory).

Density-matrix expansion

Density matrices and Wick theorem

$$
\begin{aligned}
\langle\Phi|ABCD|\Phi\rangle = {} & \wick{\c1 A \c1 B \c2 C \c2 D} + \wick{\c1 A \c2 B \c1 C \c2 D} + \wick{\c1 A \c2 B \c2 C \c1 D} \\
& + \overbracket{A}\,\overbracket{B}\,\wick{\c1 C \c1 D} + \overbracket{A}\,\wick{\c1 B \overbracket{C} \c1 D} + \overbracket{A}\,\wick{\c1 B \c1 C}\,\overbracket{D} \\
& + \wick{\c1 A \c1 B}\,\overbracket{C}\,\overbracket{D} + \wick{\c1 A \overbracket{B} \c1 C \overbracket{D}} + \wick{\c1 A \overbracket{B}\,\overbracket{C} \c1 D} + \overbracket{A}\,\overbracket{B}\,\overbracket{C}\,\overbracket{D}\,.
\end{aligned}
$$

$$
\begin{aligned}
= {} & \langle\Phi|AB|\Phi\rangle\langle\Phi|CD|\Phi\rangle + c\langle\Phi|AC|\Phi\rangle\langle\Phi|BD|\Phi\rangle + \langle\Phi|AD|\Phi\rangle\langle\Phi|BC|\Phi\rangle \\
- {} & (1+c)\langle\Phi|A|\Phi\rangle\langle\Phi|B|\Phi\rangle\langle\Phi|C|\Phi\rangle\langle\Phi|D|\Phi\rangle.
\end{aligned}
$$

Density matrix and pairing tensor:

$$\rho_{\mu\nu} = \langle\Phi|a_\nu^+ a_\mu|\Phi\rangle = \wick{\c1 a_\nu^+ \c1 a_\mu}, \qquad \kappa_{\mu\nu} = \langle\Phi|a_\nu a_\mu|\Phi\rangle = \wick{\c1 a_\nu \c1 a_\mu},$$

Many-body Hamiltonian $\hat{H}$ and average energy E:

$$\hat{H} = \hat{T} + \hat{V} = \sum\nolimits_{\mu\nu} T_{\mu\nu} a_\mu^+ a_\nu + \tfrac{1}{4}\sum\nolimits_{\mu\lambda\nu\pi} V_{\mu\lambda\nu\pi} a_\mu^+ a_\lambda^+ a_\pi a_\nu,$$

$$
\begin{aligned}
E = \langle\Phi|\hat{H}|\Phi\rangle & = \sum\nolimits_{\mu\nu} T_{\mu\nu}\rho_{\nu\mu} + \tfrac{1}{2}\sum\nolimits_{\mu\lambda\nu\pi} V_{\mu\lambda\nu\pi}\left(\rho_{\nu\mu}\rho_{\pi\lambda} + \tfrac{1}{2}\kappa^*_{\mu\lambda}\kappa_{\nu\pi}\right) \\
& = \mathrm{Tr}\left(T\rho + \tfrac{1}{2}\Gamma\rho - \tfrac{1}{2}\Delta\kappa^*\right),
\end{aligned}
$$

Single-particle Hamiltonian h and self-consistent potential Γ:

$$\Gamma_{\mu\nu} = \sum\nolimits_{\lambda\pi} V_{\mu\lambda\nu\pi}\rho_{\pi\lambda} \quad , \quad h_{\mu\nu} = \frac{\partial E}{\partial\rho_{\nu\mu}} = T_{\mu\nu} + \Gamma_{\mu\nu}$$

Coulomb force – the direct self-consistent potential

$$V(\vec r_1\sigma_1,\vec r_2\sigma_2;\vec r\,'_1\sigma'_1,\vec r\,'_2\sigma'_2)=\delta(\vec r_1-\vec r\,'_1)\delta(\vec r_2-\vec r\,'_2)\frac{\delta_{\sigma_1,\sigma'_1}\delta_{\sigma_2,\sigma'_2}}{|\vec r_1-\vec r_2|}$$

We define the non-antisymmetrized matrix elements by

$$\begin{aligned}\tilde V_{\mu\lambda\nu\pi} &= \sum\!\!\!\!\!\!\!\int_{\vec r_1\sigma_1}\sum\!\!\!\!\!\!\!\int_{\vec r_2\sigma_2}\sum\!\!\!\!\!\!\!\int_{\vec r\,'_1\sigma'_1}\sum\!\!\!\!\!\!\!\int_{\vec r\,'_2\sigma'_2}\\ &\quad \phi^*_\mu(\vec r_1\sigma_1)\;\phi^*_\lambda(\vec r_2\sigma_2)\;V(\vec r_1\sigma_1,\vec r_2\sigma_2;\vec r\,'_1\sigma'_1,\vec r\,'_2\sigma'_2)\;\phi_\nu(\vec r\,'_1\sigma'_1)\;\phi_\pi(\vec r\,'_2\sigma'_2).\end{aligned}$$

Then, the *direct* selfconsistent potential reads:

$$\begin{aligned}\Gamma^{dir}_{\mu\nu} &= \sum_{\lambda\pi}\tilde V_{\mu\lambda\nu\pi}\rho_{\pi\lambda}\\ &= \sum_{\lambda\pi}\sum\!\!\!\!\!\!\!\int_{\vec r_1\sigma_1}\sum\!\!\!\!\!\!\!\int_{\vec r_2\sigma_2}\sum\!\!\!\!\!\!\!\int_{\vec r\,'_1\sigma'_1}\sum\!\!\!\!\!\!\!\int_{\vec r\,'_2\sigma'_2}\\ &\quad \phi^*_\mu(\vec r_1\sigma_1)\;\phi^*_\lambda(\vec r_2\sigma_2)\;V(\vec r_1\sigma_1,\vec r_2\sigma_2;\vec r\,'_1\sigma'_1,\vec r\,'_2\sigma'_2)\;\overset{\Big\downarrow}{\phi_\nu}(\vec r\,'_1\sigma'_1)\;\overset{\Big\downarrow}{\phi_\pi}(\vec r\,'_2\sigma'_2)\rho_{\pi\lambda}\\ &= \sum_{\lambda\pi}\sum\!\!\!\!\!\!\!\int_{\vec r_1\sigma_1}\sum\!\!\!\!\!\!\!\int_{\vec r_2\sigma_2}\sum\!\!\!\!\!\!\!\int_{\vec r\,'_1\sigma'_1}\\ &\quad \phi^*_\mu(\vec r_1\sigma_1)\;\phi^*_\lambda(\vec r_2\sigma_2)\delta(\vec r_1-\vec r\,'_1)\frac{\delta_{\sigma_1,\sigma'_1}}{|\vec r_1-\vec r_2|}\;\phi_\nu(\vec r\,'_1\sigma'_1)\;\phi_\pi(\vec r_2\sigma_2)\rho_{\pi\lambda}\\ &= \sum\!\!\!\!\!\!\!\int_{\vec r_1\sigma_1}\sum\!\!\!\!\!\!\!\int_{\vec r\,'_1\sigma'_1}\phi^*_\mu(\vec r_1\sigma_1)\left[\delta(\vec r_1-\vec r\,'_1)\delta_{\sigma_1,\sigma'_1}\sum\!\!\!\!\!\!\!\int_{\vec r_2\sigma_2}\frac{\rho(\vec r_2\sigma_2,\vec r_2\sigma_2)}{|\vec r_1-\vec r_2|}\right]\;\phi_\nu(\vec r\,'_1\sigma'_1).\end{aligned}$$

which gives $\Gamma^{dir}(\vec r_1)=\int_{\vec r_2}\frac{\rho(\vec r_2)}{|\vec r_1-\vec r_2|}$ **for** $\rho(\vec r_2)=\sum_{\sigma_2}\rho(\vec r_2\sigma_2,\vec r_2\sigma_2)$.

Coulomb force – the exchange self-consistent potential

$$V(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2;\vec{r}\,'_1\sigma'_1,\vec{r}\,'_2\sigma'_2) = \delta(\vec{r}_1-\vec{r}\,'_1)\delta(\vec{r}_2-\vec{r}\,'_2)\frac{\delta_{\sigma_1,\sigma'_1}\delta_{\sigma_2,\sigma'_2}}{|\vec{r}_1-\vec{r}_2|}$$

We define the non-antisymmetrized matrix elements by

$$\tilde{V}_{\mu\lambda\nu\pi} = \sum\!\!\!\!\!\!\!\int_{\vec{r}_1\sigma_1}\sum\!\!\!\!\!\!\!\int_{\vec{r}_2\sigma_2}\sum\!\!\!\!\!\!\!\int_{\vec{r}\,'_1\sigma'_1}\sum\!\!\!\!\!\!\!\int_{\vec{r}\,'_2\sigma'_2}$$

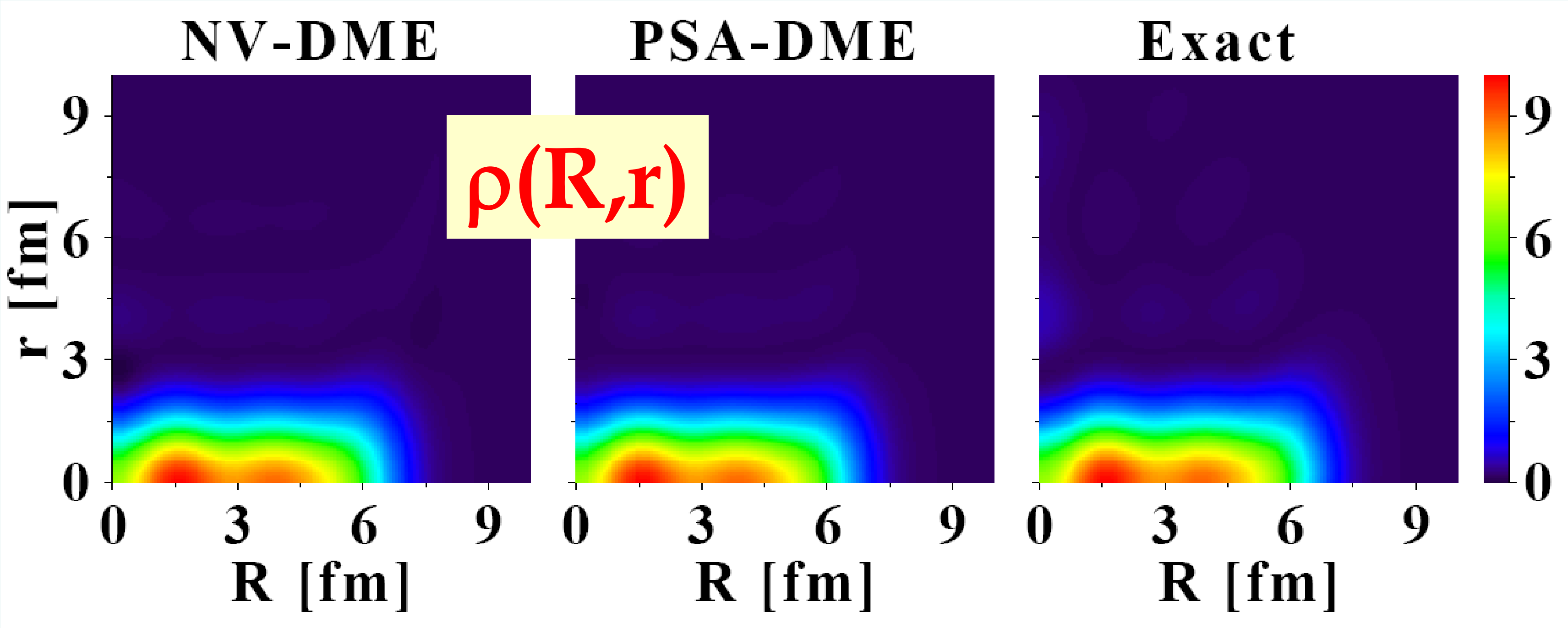
$$\phi^*_\mu(\vec{r}_1\sigma_1)\ \phi^*_\lambda(\vec{r}_2\sigma_2)\ V(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2;\vec{r}\,'_1\sigma'_1,\vec{r}\,'_2\sigma'_2)\ \phi_\nu(\vec{r}\,'_1\sigma'_1)\ \phi_\pi(\vec{r}\,'_2\sigma'_2).$$

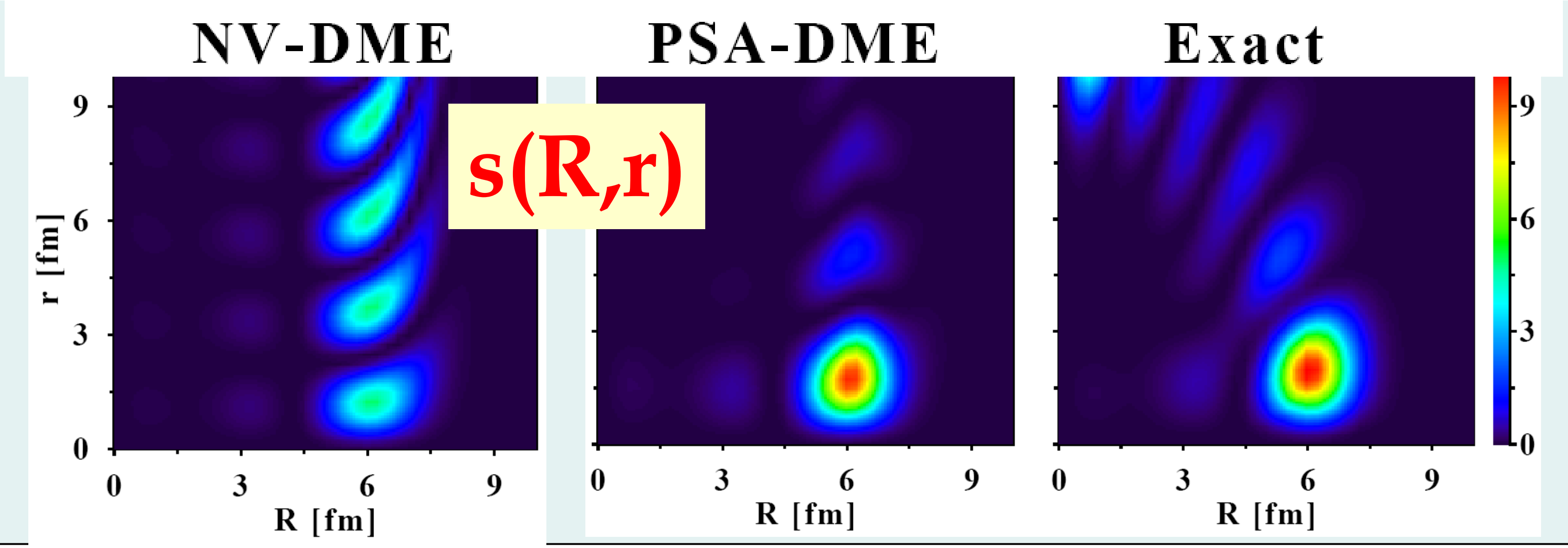
Then, the *exchange* selfconsistent potential reads:

$$\begin{aligned}
\Gamma^{exc}_{\mu\nu} &= \sum\nolimits_{\lambda\pi}\tilde{V}_{\mu\lambda\nu\pi}\rho_{\pi\lambda} \\
&= \sum\nolimits_{\lambda\pi}\sum\!\!\!\!\!\!\!\int_{\vec{r}_1\sigma_1}\sum\!\!\!\!\!\!\!\int_{\vec{r}_2\sigma_2}\sum\!\!\!\!\!\!\!\int_{\vec{r}\,'_1\sigma'_1}\sum\!\!\!\!\!\!\!\int_{\vec{r}\,'_2\sigma'_2} \\
&\qquad \phi^*_\mu(\vec{r}_1\sigma_1)\ \phi^*_\lambda(\vec{r}_2\sigma_2)\ V(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2;\vec{r}\,'_1\sigma'_1,\vec{r}\,'_2\sigma'_2)\ \phi_\pi(\vec{r}\,'_1\sigma'_1)\ \phi_\nu(\vec{r}\,'_2\sigma'_2)\rho_{\pi\lambda} \\
&= \sum\nolimits_{\lambda\pi}\sum\!\!\!\!\!\!\!\int_{\vec{r}_1\sigma_1}\sum\!\!\!\!\!\!\!\int_{\vec{r}_2\sigma_2} \\
&\qquad \phi^*_\mu(\vec{r}_1\sigma_1)\ \phi^*_\lambda(\vec{r}_2\sigma_2)\frac{1}{|\vec{r}_1-\vec{r}_2|}\ \phi_\pi(\vec{r}_1\sigma_1)\ \phi_\nu(\vec{r}_2\sigma_2)\rho_{\pi\lambda} \\
&= \sum\!\!\!\!\!\!\!\int_{\vec{r}_1\sigma_1}\sum\!\!\!\!\!\!\!\int_{\vec{r}_2\sigma_2}\phi^*_\mu(\vec{r}_1\sigma_1)\left[\frac{\rho(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2)}{|\vec{r}_1-\vec{r}_2|}\right]\ \phi_\nu(\vec{r}_2\sigma_2),
\end{aligned}$$

which gives $\Gamma^{exc}(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2) = \dfrac{\rho(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2)}{|\vec{r}_1-\vec{r}_2|}.$

Particle and spin densities in ^{208}Pb





B. Gebremariam *et al.*, Phys. Rev. C82, 014305 (2010)

Density-matrix expansion (Negele-Vautherin)
(or do we need the non-local density)

We begin by considering the simplest (and academic) case of fermions with no spin and no isospin. For an arbitrary non-local interaction $V(\vec{r}_1^{\,\prime},\vec{r}_2^{\,\prime};\vec{r}_1,\vec{r}_2)$ the Hartree-Fock interaction energy has the form

$$\mathcal{E}^{\rm int} = \tfrac{1}{2}\int \mathrm{d}^3\vec{r}_1^{\,\prime}\mathrm{d}^3\vec{r}_2^{\,\prime}\mathrm{d}^3\vec{r}_1\mathrm{d}^3\vec{r}_2 V(\vec{r}_1^{\,\prime},\vec{r}_2^{\,\prime};\vec{r}_1,\vec{r}_2)\times \left(\rho(\vec{r}_1,\vec{r}_1^{\,\prime})\rho(\vec{r}_2,\vec{r}_2^{\,\prime}) - \rho(\vec{r}_2,\vec{r}_1^{\,\prime})\rho(\vec{r}_1,\vec{r}_2^{\,\prime})\right),$$

while for a local interaction,

$$V(\vec{r}_1^{\,\prime},\vec{r}_2^{\,\prime};\vec{r}_1,\vec{r}_2) = \delta(\vec{r}_1^{\,\prime}-\vec{r}_1)\delta(\vec{r}_2^{\,\prime}-\vec{r}_2)V(\vec{r}_1,\vec{r}_2)$$

the interaction energy reduces to:

$$\mathcal{E}^{\rm int} = \tfrac{1}{2}\int \mathrm{d}^3\vec{r}_1\mathrm{d}^3\vec{r}_2 \overbrace{V(\vec{r}_1,\vec{r}_2)\left(\rho(\vec{r}_1)\rho(\vec{r}_2) - \rho(\vec{r}_2,\vec{r}_1)\rho(\vec{r}_1,\vec{r}_2)\right)}^{\text{Nonlocal energy density}},$$

where $\rho(\vec{r}_1) \equiv \rho(\vec{r}_1,\vec{r}_1)$ and $\rho(\vec{r}_2) \equiv \rho(\vec{r}_2,\vec{r}_2)$ are local densities.

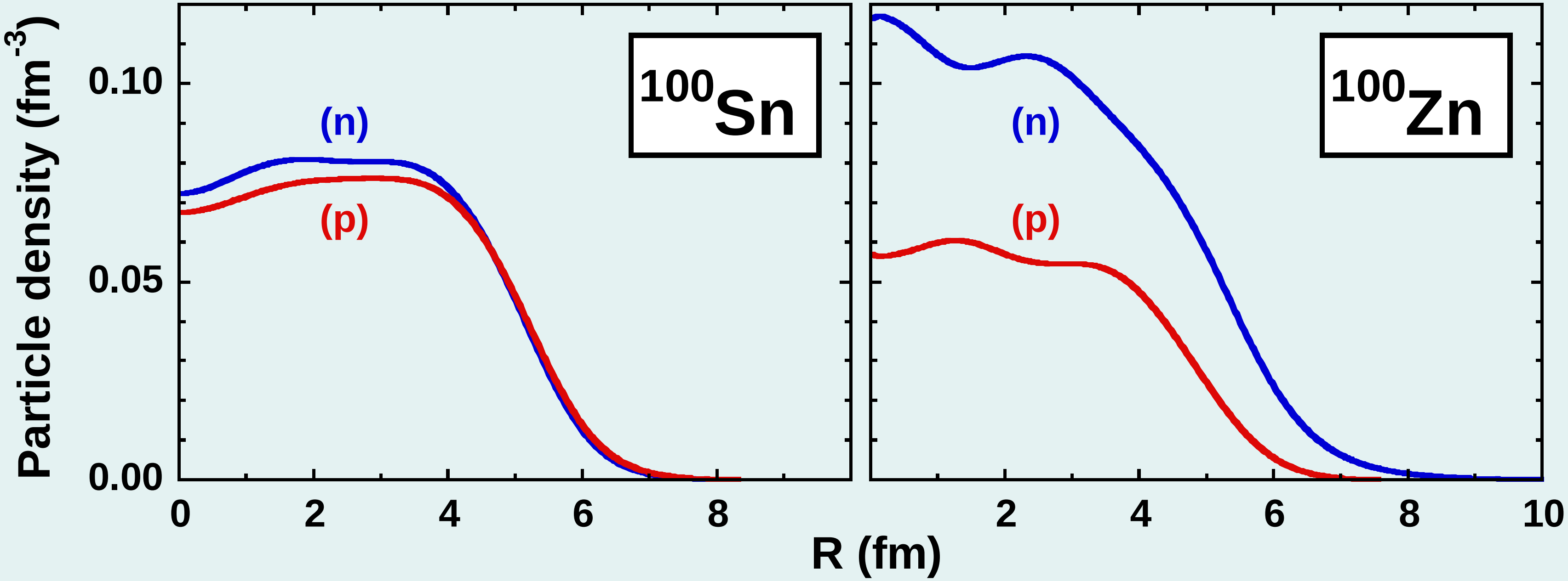
$$\mathcal{E}^{\rm int}_{\rm dir} = \tfrac{1}{2}\int \mathrm{d}^3\vec{r}_1\mathrm{d}^3\vec{r}_2 V(\vec{r}_1,\vec{r}_2)\rho(\vec{r}_1)\rho(\vec{r}_2),$$

$$\mathcal{E}^{\rm int}_{\rm exc} = \tfrac{1}{2}\int \mathrm{d}^3\vec{r}_1\mathrm{d}^3\vec{r}_2 V(\vec{r}_1,\vec{r}_2)\rho(\vec{r}_2,\vec{r}_1)\rho(\vec{r}_1,\vec{r}_2),$$

$$\mathcal{E}^{\rm int} = \mathcal{E}^{\rm int}_{\rm dir} - \mathcal{E}^{\rm int}_{\rm exc}.$$

J. D., B.G Carlsson, M. Kortelainen, J. Phys. G 37, 075106 (2010)

Nuclear densities as composite fields



Modern Mean-Field Theory ≡ Energy Density Functional

ρ, τ, $\overleftrightarrow{J}$, $\vec{j}$, $\vec{T}$, $\vec{s}$, $\vec{F}$,

- Hohenberg-Kohn
- Kohn-Sham
- Negele-Vautherin
- Landau-Migdal
- Nilsson-Strutinsky

mean field ⇒ one-body densities

zero range ⇒ local densities

finite range ⇒ non-local densities

Density-matrix expansion (2)

Denoting the standard total ($\vec{R}$) and relative ($\vec{r}$) coordinates and derivatives as

$$\begin{aligned} \vec{R} &= \tfrac{1}{2}(\vec{r}_1+\vec{r}_2), & \vec{\nabla} &= \frac{\partial}{\partial\vec{R}} = \frac{\partial}{\partial\vec{r}_1}+\frac{\partial}{\partial\vec{r}_2}, \\ \vec{r} &= \vec{r}_1-\vec{r}_2, & \vec{\partial} &= \frac{\partial}{\partial\vec{r}} = \frac{1}{2}\left(\frac{\partial}{\partial\vec{r}_1}-\frac{\partial}{\partial\vec{r}_2}\right), \end{aligned}$$

we have the expansion of local densities,

$$\begin{aligned} \rho(\vec{r}_1) = \rho(\vec{R}+\tfrac{1}{2}\vec{r}) &= \rho(\vec{R}) + \tfrac{1}{2}r^i\nabla_i\rho(\vec{R}) + \tfrac{1}{8}r^ir^j\nabla_i\nabla_j\rho(\vec{R}) + \ldots, \\ \rho(\vec{r}_2) = \rho(\vec{R}-\tfrac{1}{2}\vec{r}) &= \rho(\vec{R}) - \tfrac{1}{2}r^i\nabla_i\rho(\vec{R}) + \tfrac{1}{8}r^ir^j\nabla_i\nabla_j\rho(\vec{R}) + \ldots, \end{aligned}$$

and hence

$$\begin{aligned} \rho(\vec{r}_1)\rho(\vec{r}_2) = {} & \rho^2(\vec{R}) \\ & + \tfrac{1}{4}r^ir^j\left(\rho(\vec{R})\nabla_i\nabla_j\rho(\vec{R}) - [\nabla_i\rho(\vec{R})][\nabla_j\rho(\vec{R})]\right) \end{aligned}$$

where summation over repeated Cartesian indices i and j is assumed Assuming that the local potential $V(\vec{r}_1,\vec{r}_2)$ depends only on the di interacting particles, $V(\vec{r}_1,\vec{r}_2)=V(|\vec{r}_1-\vec{r}_2|)=V(r)$, the direct interac given by the integral of a local energy density,

Local energy density

$$\mathcal{E}^{\text{int}}_{\text{dir}} = \frac{1}{2}\int \mathrm{d}^3\vec{R}\,\overbrace{[V_0\rho^2 + \tfrac{1}{12}V_2(\rho\Delta\rho - (\vec{\nabla}\rho)^2)]} + \ldots,$$

where coupling constants, V_0 and V_2, are given by the lowest two moments of the interaction,

$$V_k = \int \mathrm{d}^3\vec{r}\, r^k V(r) = 4\pi\int \mathrm{d}r\, r^{k+2}V(r).$$

Density-matrix expansion (3)

In the exhange term, the range of the interaction is relevant only for the non-local dependence of the density matrix on space variables. As function of $\vec{r}$, the scale at which the density matrix varies is given by the Fermi momentum k_F. Hence, for short-range interactions one may expand $\rho(\vec{R},\vec{r})$ with respect to the variable $\vec{r}$, which gives

$$\rho(\vec{r}_1,\vec{r}_2) = \rho(\vec{R},\vec{r}) = \rho(\vec{R}) + r^i\partial_i\rho(\vec{R},\vec{r}) + \tfrac{1}{2}r^ir^j\partial_i\partial_j\rho(\vec{R},\vec{r}) + \ldots,$$

where derivatives ∂_i, are always calculated at r^i=0. This parabolic approximation does not ensure that $\rho(\vec{r}_1,\vec{r}_2)\longrightarrow 0$ for large $|\vec{r}|=|\vec{r}_1-\vec{r}_2|$. One can improve it by introducing three functions of $r=|\vec{r}|$, $\pi_0(r)$, $\pi_1(r)$, and $\pi_2(r)$ that vanish at large r, i.e., we define the LDA of the density matrix by:

$$\begin{aligned}\rho(\vec{r}_1,\vec{r}_2) = \rho(\vec{R},\vec{r}) = \pi_0(r)\rho(\vec{R}) &+ \pi_1(r)r^i\partial_i\rho(\vec{R},\vec{r}) \\ &+ \tfrac{1}{2}\pi_2(r)r^ir^j\partial_i\partial_j\rho(\vec{R},\vec{r}) + \ldots .\end{aligned}$$

Such a postulate has to be compatible with the Taylor expansion, which requires that

$$\pi_0(0) = \pi_1(0) = \pi_2(0) = 1 \quad \text{and} \quad \pi_0'(0) = \pi_1'(0) = \pi_0''(0) = 0.$$

Of course, for $\pi_0(r)$=$\pi_1(r)$=$\pi_2(r)$=1 one reverts to parabolic approximation.

Density-matrix expansion (4)

The product of nonlocal densities in the exchange integral now reads

$$\begin{aligned}\rho(\vec{r}_1,\vec{r}_2)\rho(\vec{r}_2,\vec{r}_1) &= \pi_0^2(r)\rho^2(\vec{R}) \\ &+ \pi_0(r)\pi_2(r)r^ir^j\{\rho(\vec{R})\partial_i\partial_j\rho(\vec{R},\vec{r}) - [\partial_i\rho(\vec{R},\vec{r})][\partial_j\rho(\vec{R},\vec{r})]\} + \ldots,\end{aligned}$$

where we have introduced a supplementary condition,

$$\pi_1^2(r) = \pi_0(r)\pi_2(r).$$

This condition ensures that the LDA of is compatible with the local gauge invariance; indeed only the difference of terms in curly brackets of is invariant with respect to the local gauge transformation,

$$\rho'(\vec{r}_1,\vec{r}_2) = e^{i\phi(\vec{r}_1)-i\phi(\vec{r}_2)}\rho(\vec{r}_1,\vec{r}_2).$$

Within the LDA one obtains the exchange interaction energy,

$$\mathcal{E}_{\text{exc}}^{\text{int}} = \tfrac{1}{2}\int \mathrm{d}^3\vec{R}\,\overbrace{[V_0^{00}\rho^2 + \tfrac{1}{12}V_2^{02}(\rho\Delta\rho - 4(\rho\tau - \vec{j}^{\,2}))]}^{\text{Local energy density}} + \ldots,$$

where τ and $\vec{j}$ are the standard kinetic energy and current densities, respectively, and the coupling constants V_0^{00} and V_2^{02} are given by the following moments of the interaction,

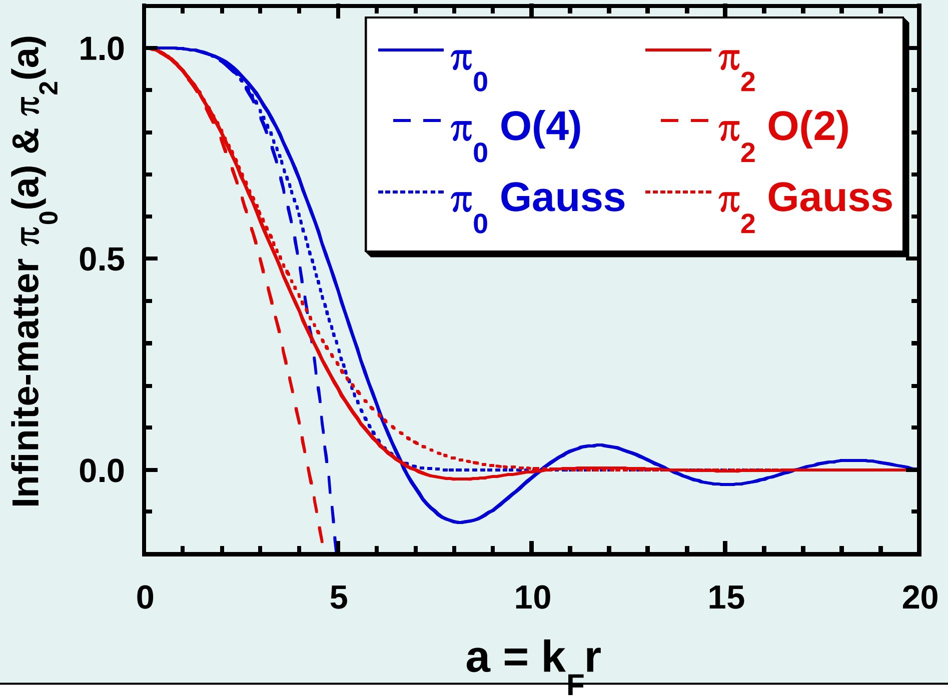
$$V_k^{ij} = \int \mathrm{d}^3\vec{r}\,r^k\pi_i(r)\pi_j(r)V(r) = 4\pi\int \mathrm{d}r\,r^{k+2}\pi_i(r)\pi_j(r)V(r).$$

Density-matrix expansion (6)

Auxiliary functions $\pi_0(r)$ and $\pi_2(r)$, which define the LDA, can be calculated *a posteriori*, to give the best possible approximation of a given density matrix $\rho(\vec{R},\vec{r})$. However, they can also be estimated *a priori* by making a momentum expansion around the Fermi momentum k_F of an infinite system (Negele and Vautherin):

$$\pi_0(r) = \frac{6j_1(k_Fr)+21j_3(k_Fr)}{2k_Fr} \quad , \quad \pi_2(r) = \frac{105j_3(k_Fr)}{(k_Fr)^3},$$

where $j_n(k_Fr)$ are the spherical Bessel functions. The standard Slater approximation corresponds to $\pi_0(r) = \frac{3j_1(k_Fr)}{k_Fr}$ and $\pi_2(r) = 0$.



J. D., B.G Carlsson, M. Kortelainen, J. Phys. G 37, 075106 (2010)

Exchange interaction energy in infinite matter

In the exchange term, the situation is entirely different. Here, the range of interaction matters in the non-local, relative direction $\vec{r}$. To get a feeling what are the properties of the one-body density matrix in this direction, we can calculate it for infinite matter,

$$\rho(\vec{x},\vec{y}) = \int_{|\vec{k}|<k_F} \mathrm{d}^3\vec{k}\, \frac{\exp(i\vec{k}\cdot\vec{x})}{\sqrt{8\pi^3}} \frac{\exp(-i\vec{k}\cdot\vec{y})}{\sqrt{8\pi^3}},$$

where the s.p. wave functions (plane waves) are integrated within the Fermi sphere of momenta $|\vec{k}| < k_F$. Obviously, $\rho(\vec{x},\vec{y})$ depends only on the relative coordinate, i.e.,

$$\rho(\vec{R},\vec{r}) = \frac{1}{2\pi^2 r}\int_0^{k_F} \mathrm{d}k\, k \sin(kr) = \frac{k_F^3}{6\pi^2}\left[3\frac{\sin(k_F r) - k_F r\cos(k_F r)}{(k_F r)^3}\right] = \frac{k_F^3}{6\pi^2}\left[3\frac{j_1(k_F r)}{k_F r}\right].$$

Function in square parentheses equals 1 at r=0, and has the first zero at $r \simeq 4.4934/k_F \simeq$ 3 fm, i.e., in the non-local direction the density varies on the same scale as it does in the local direction. Therefore, the quadratic expansion in the relative variable,

$$\rho(\vec{R},\pm\vec{r}) = \rho(\vec{R}) \pm r^i\partial_i\rho(\vec{R},\vec{r}) + \tfrac{1}{2}r^ir^j\partial_i\partial_j\rho(\vec{R},\vec{r}) + \ldots,$$

where derivatives ∂_i=$\partial/\partial r^i$ are always calculated at r^i=0, is, in principle, sufficient for the evaluation of the exchange interaction energy. However, we can improve it by introducing three universal functions of $r = |\vec{r}|$, $\pi_0(r)$, $\pi_1(r)$, and $\pi_2(r)$, which vanish at large r, i.e., we define the LDA by:

$$\rho(\vec{R},\pm\vec{r}) = \pi_0(r)\rho(\vec{R}) \pm \pi_1(r)r^i\partial_i\rho(\vec{R},\vec{r}) + \tfrac{1}{2}\pi_2(r)r^ir^j\partial_i\partial_j\rho(\vec{R},\vec{r}) + \ldots$$

Lessons learned

1) Energy density functional exists due to the two-step variational method and gives exact ground state energy and its exact particle density.

2) Whenever the energy scales (or range scales) between the interactions and observations are different, the observations can be described by a series of pseudopotentials with coupling constants adjusted to data (an effective theory).

3) In nuclei, the non-local energy density functionals can be replaced by the local ones. This is because the range of the interaction is shorter than the range of variations in the local and non-local density matrix.

Density-matrix expansion (5)

In summary:

$$\mathcal{E}^{\rm int}_{\rm dir} = \frac{1}{2}\int {\rm d}^3\vec{r}_1{\rm d}^3\vec{r}_2 V(\vec{r}_1,\vec{r}_2)\rho(\vec{r}_1)\rho(\vec{r}_2),$$

$$\mathcal{E}^{\rm int}_{\rm exc} = \frac{1}{2}\int {\rm d}^3\vec{r}_1{\rm d}^3\vec{r}_2 V(\vec{r}_1,\vec{r}_2)\rho(\vec{r}_2,\vec{r}_1)\rho(\vec{r}_1,\vec{r}_2),$$

$$\mathcal{E}^{\rm int} = \mathcal{E}^{\rm int}_{\rm dir} - \mathcal{E}^{\rm int}_{\rm exc}.$$

$$\mathcal{E}^{\rm int}_{\rm dir} = \frac{1}{2}\int {\rm d}^3\vec{R}[V_0\rho^2 + \frac{1}{12}V_2(\rho\Delta\rho - (\vec{\nabla}\rho)^2)] + \ldots,$$

$$V_k = \int {\rm d}^3\vec{r}\, r^k V(r) = 4\pi\int {\rm d}r\, r^{k+2}V(r).$$

$$\mathcal{E}^{\rm int}_{\rm exc} = \frac{1}{2}\int {\rm d}^3\vec{R}[V_0^{00}\rho^2 + \frac{1}{12}V_2^{02}(\rho\Delta\rho - 4(\rho\tau - \vec{j}^{\,2}))] + \ldots,$$

$$V_k^{ij} = \int {\rm d}^3\vec{r}\, r^k\pi_i(r)\pi_j(r)V(r) = 4\pi\int {\rm d}r\, r^{k+2}\pi_i(r)\pi_j(r)V(r).$$

Negele-Vautherin density-matrix expansion

We can apply the Negele-Vautherin DME to the general case of an arbitrary finite-range local nuclear interaction composed of the standard central, spin-orbit, and tensor terms:

$$\begin{aligned}\hat{V}(\vec{r}_1,\vec{r}_2) &= W(r)+B(r)P_\sigma-H(r)P_\tau-M(r)P_\sigma P_\tau \\ &+ \big[P(r)+Q(r)P_\tau\big]\vec{L}\cdot\vec{S}+\big[R(r)+S(r)P_\tau\big]S_{12},\end{aligned}$$

where $r=|\vec{r}|=|\vec{r}_1-\vec{r}_2|$, and

$$P_\sigma=\tfrac{1}{2}(1+\vec{\sigma}_1\cdot\vec{\sigma}_2), \qquad P_\tau=\tfrac{1}{2}(1+\vec{\tau}_1\circ\vec{\tau}_2),$$

$$\vec{L}=-i\hbar\vec{r}\times\vec{\partial}, \qquad \vec{S}=\tfrac{\hbar}{2}(\vec{\sigma}_1+\vec{\sigma}_2), \qquad S_{12}=\tfrac{3}{r^2}(\vec{\sigma}_1\cdot\vec{r})(\vec{\sigma}_2\cdot\vec{r})-\vec{\sigma}_1\cdot\vec{\sigma}_2.$$

After straightforward but lengthy calculations, one obtains the interaction energy in the form of a local integral, analogous to that for the Skyrme interaction,

$$\begin{aligned}\mathcal{E}^{\rm int} = \int \mathrm{d}^3\vec{R}\sum_{k=0}^{3}\Big[& C_t^\rho\rho_k^2+C_t^{\Delta\rho}\rho_k\Delta\rho_k+C_t^\tau\big(\rho_k\tau_k-\vec{j}_k^{\,2}\big) \\ & +C_t^s\vec{s}_k^{\,2}+C_t^{\Delta s}\vec{s}_k\cdot\Delta\vec{s}_k+C_t^T\big(\vec{s}_k\cdot\vec{T}_k-\mathsf{J}_{abk}\mathsf{J}_{abk}\big) \\ & +C_t^F\big(\vec{s}_k\cdot\vec{F}_k-\tfrac{1}{2}\mathsf{J}_{aak}\mathsf{J}_{bbk}-\tfrac{1}{2}\mathsf{J}_{abk}\mathsf{J}_{bak}\big)+C_t^{\nabla s}\big(\vec{\nabla}\cdot\vec{s}_k\big)^2 \\ & +C_t^{\nabla J}\big(\rho_k\vec{\nabla}\cdot\vec{J}_k+\vec{s}_k\cdot(\vec{\nabla}\times\vec{j}_k)\big)\Big],\end{aligned}$$

where $\rho_k\equiv\rho_{0k}$, $\tau_k\equiv\tau_{0bbk}$, $\vec{j}_{ak}\equiv j_{0ak}$, $\vec{s}_{ak}\equiv\rho_{ak}$, $\vec{T}_{ak}\equiv\tau_{abbk}$, $\vec{F}_{ak}\equiv\frac{1}{2}(\tau_{babk}+\tau_{bbak})$, $\mathsf{J}_{abk}\equiv j_{abk}$, and $\vec{J}_{ak}\equiv\epsilon_{abc}j_{cbk}$ are the standard local densities. The isoscalar ($t=0$) and isovector ($t=1$) coupling constants C_t correspond to $k=0$ and $k=1,2,3$, respectively.

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Negele-Vautherin density-matrix expansion

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The coupling constants of the local energy density are related to moments of the interaction:

$$8\begin{pmatrix} C_0^\rho \\ C_1^\rho \\ C_0^s \\ C_1^s \end{pmatrix} = \begin{pmatrix} 4 & 2 & -2 & -1 \\ 0 & 0 & -2 & -1 \\ 0 & 2 & 0 & -1 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} W_0 + M_{\nu 0}^{00} + \frac{1}{5} M_{\nu 2}^{02}\, k_F^2 \\ B_0 + H_{\nu 0}^{00} + \frac{1}{5} H_{\nu 2}^{02}\, k_F^2 \\ H_0 + B_{\nu 0}^{00} + \frac{1}{5} B_{\nu 2}^{02}\, k_F^2 \\ M_0 + W_{\nu 0}^{00} + \frac{1}{5} W_{\nu 2}^{02}\, k_F^2 \end{pmatrix},$$

$$96\begin{pmatrix} C_0^{\Delta\rho} \\ C_1^{\Delta\rho} \\ C_0^{\tau} \\ C_1^{\tau} \\ C_0^{\Delta s} \\ C_1^{\Delta s} \\ C_0^{T} \\ C_1^{T} \\ C_0^{F} \\ C_1^{F} \\ C_0^{\nabla s} \\ C_1^{\nabla s} \end{pmatrix} = \begin{pmatrix} 8 & -1 & 4 & -2 & -4 & 2 & -2 & 4 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & -2 & -4 & 0 & -2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 8 & 0 & -8 & 0 & -16 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & 2 & -2 & 0 & -4 & 1 & -2 & 2 \\ 0 & -1 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 1 & -2 & 0 \\ 0 & 4 & 0 & 0 & 0 & -8 & 0 & 0 & 0 & -4 & 0 & -8 \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12 & 0 & 24 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 12 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -12 & 3 & -6 & 6 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & -6 & 0 \end{pmatrix} \begin{pmatrix} W_2 \\ W_{\nu 2}^{02} \\ B_2 \\ B_{\nu 2}^{02} \\ H_2 \\ H_{\nu 2}^{02} \\ M_2 \\ M_{\nu 2}^{02} \\ \frac{4}{5}R_2 \\ \frac{4}{5}R_{\nu 2}^{02} \\ \frac{4}{5}S_2 \\ \frac{4}{5}S_{\nu 2}^{02} \end{pmatrix},$$

$$24\begin{pmatrix} C_0^{\nabla J} \\ C_1^{\nabla J} \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} P_2 + Q_{\nu 2}^{01} \\ Q_2 + P_{\nu 2}^{01} \end{pmatrix}.$$

All the coupling constants of the local energy density depend linearly on the following moments of potentials:

$$X_n = \int \mathrm{d}^3\vec{r}\, r^n X(r) \qquad X_{\nu n}^{ij} = \int \mathrm{d}^3\vec{r}\, r^n \nu_i(r)\nu_j(r) X(r),$$

where X stands for W, B, H, M, P, Q, R, or S.

Negele-Vautherin density-matrix expansion

In general, the number of moments is higher than the number of coupling constants, and all the coupling constants are independent. However, in the vacuum limit of $k_F = 0$, the direct and exchange moments equal to one another, namely, $X^{ij}_{\nu n} = X_n$, and the coupling constants collapse to:

$$8\begin{pmatrix} C_0^\rho \\ C_1^\rho \\ C_0^s \\ C_1^s \end{pmatrix} = \begin{pmatrix} 3 & 0 \\ -1 & -2 \\ -1 & 2 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} W_0 + M_0 \\ B_0 + H_0 \end{pmatrix},$$

$$96\begin{pmatrix} C_0^{\Delta\rho} \\ C_1^{\Delta\rho} \\ C_0^\tau \\ C_1^\tau \\ C_0^{\Delta s} \\ C_1^{\Delta s} \\ C_0^T \\ C_1^T \\ C_0^F \\ C_1^F \\ C_0^{\nabla s} \\ C_1^{\nabla s} \end{pmatrix} = \begin{pmatrix} 7 & 2 & -2 & 2 & 0 & 0 \\ -1 & -2 & -4 & -2 & 0 & 0 \\ 4 & 8 & -8 & -16 & 0 & 0 \\ 4 & 8 & 0 & 0 & 0 & 0 \\ -1 & 4 & 2 & -2 & -3 & 0 \\ -1 & 0 & 0 & -2 & 1 & -2 \\ 4 & 0 & -8 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & 0 \\ 0 & 0 & 0 & 0 & 12 & 24 \\ 0 & 0 & 0 & 0 & 12 & 0 \\ 0 & 0 & 0 & 0 & -9 & 0 \\ 0 & 0 & 0 & 0 & 3 & -6 \end{pmatrix} \begin{pmatrix} W_2 \\ B_2 \\ H_2 \\ M_2 \\ \frac{4}{5}R_2 \\ \frac{4}{5}S_2 \end{pmatrix},$$

$$24\begin{pmatrix} C_0^{\nabla J} \\ C_1^{\nabla J} \end{pmatrix} = \begin{pmatrix} 3 \\ 1 \end{pmatrix} \begin{pmatrix} P_2 + Q_2 \end{pmatrix}.$$

These coupling constants correspond exactly to those obtained for the Skyrme force, namely,

$$\begin{array}{lll} t_0 = W_0 + M_0, & t_1 = -\frac{1}{3}(W_2 + M_2), & t_2 = \frac{1}{3}(W_2 - M_2), \\ t_0x_0 = B_0 + H_0, & t_1x_1 = -\frac{1}{3}(B_2 + H_2), & t_2x_2 = \frac{1}{3}(B_2 - H_2), \\ t_e = \frac{1}{15}(S_2 - R_2), & t_o = \frac{1}{15}(S_2 + R_2), & W = -\frac{1}{6}(P_2 + Q_2) \end{array}$$

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Density-matrix expansion and the Skyrme force

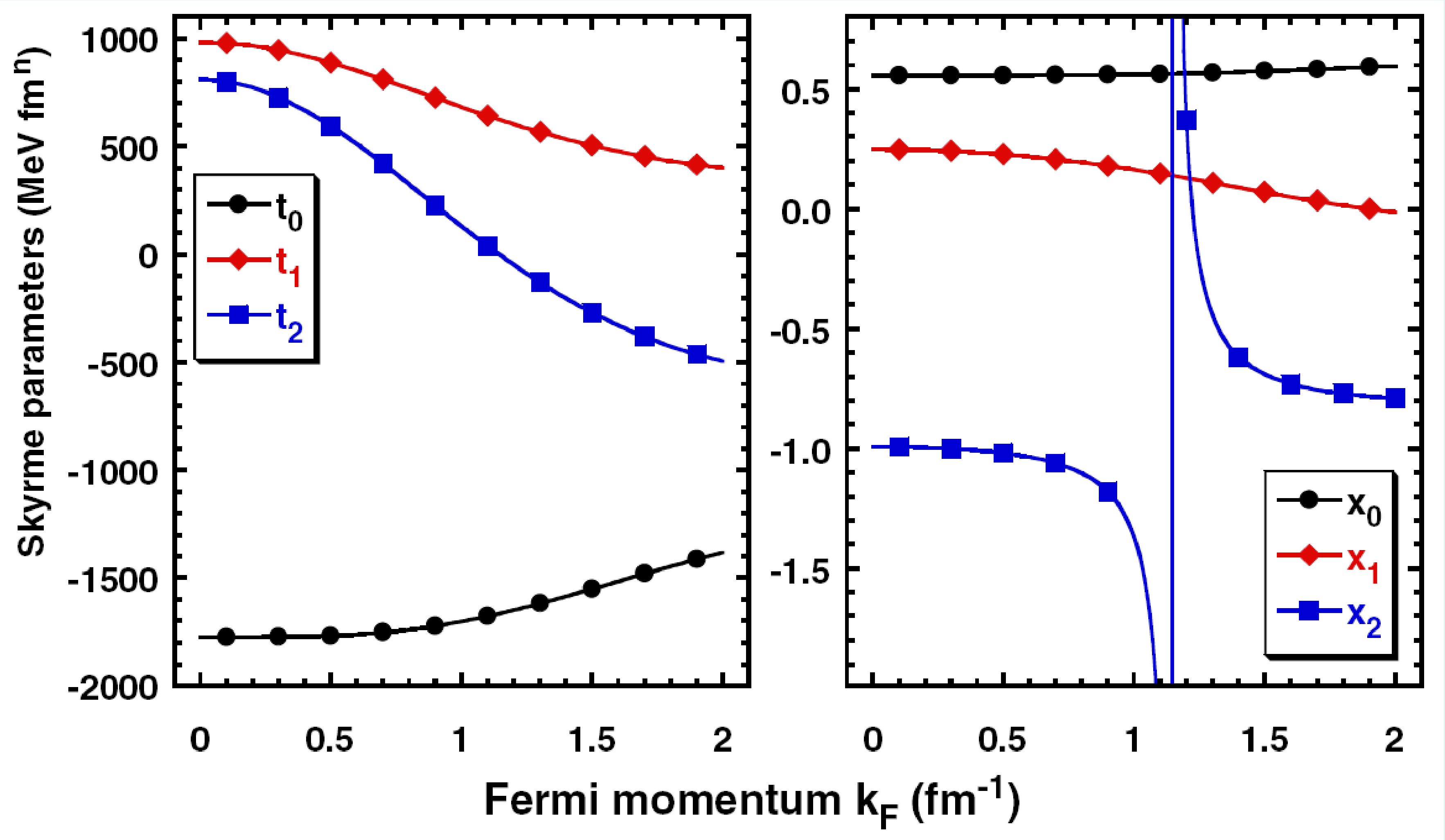
In general, the number of moments entering is higher than the number of final coupling constants, and all the coupling constants are independent from one another. On the other hand, for the quadratic Taylor expansion, which corresponds to $\pi_0(r)=\pi_2(r)=1$, the direct and exchange moments become equal to one onother, $X_k^{ij}=X_k$. Then, the coupling constants become dependent, and, in fact, half of them determines the other half. This is exactly the situation encountered when the energy density is calculated for the Skyrme interaction. Then one obtains:

$$
\begin{aligned}
3\begin{pmatrix} C_0^s \\ C_1^s \end{pmatrix} &= \begin{pmatrix} -2 & -3 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} C_0^\rho \\ C_1^\rho \end{pmatrix}, \\
24\begin{pmatrix} C_0^{\Delta s} \\ C_1^{\Delta s} \\ C_0^T \\ C_1^T \end{pmatrix} &= \begin{pmatrix} -12 & -12 & 3 & 9 \\ -4 & -4 & 3 & -3 \\ 16 & 48 & -4 & 12 \\ 16 & -16 & 4 & -12 \end{pmatrix}\begin{pmatrix} C_0^{\Delta\rho} \\ C_1^{\Delta\rho} \\ C_0^\tau \\ C_1^\tau \end{pmatrix}, \\
C_0^{\nabla J} &= 3C_1^{\nabla J}.
\end{aligned}
$$

It is obvious that the above relations among the coupling constants result from an oversimplified approximation to the exchange energy of a finite-range interaction. The Skyrme force parameters are given by the following relations:

$$
\begin{array}{rcl}
t_0 = W_0 + M_0 & , & t_0x_0 = B_0 + H_0, \\
3t_1 = -W_2 - M_2 & , & 3t_1x_1 = -B_2 - H_2, \\
3t_2 = W_2 - M_2 & , & 3t_2x_2 = B_2 - H_2, \\
6W = -P_2 - Q_2 & . &
\end{array}
$$

Negele-Vautherin density-matrix expansion



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Based on the Negele-Vautherin density-matrix expansion, we have derived the NLO Skyrme-functional parameters corresponding to the finite-range Gogny interaction. The method has been extended to derive the coupling constants of local N^{3}LO functionals

Negele-Vautherin density-matrix expansion

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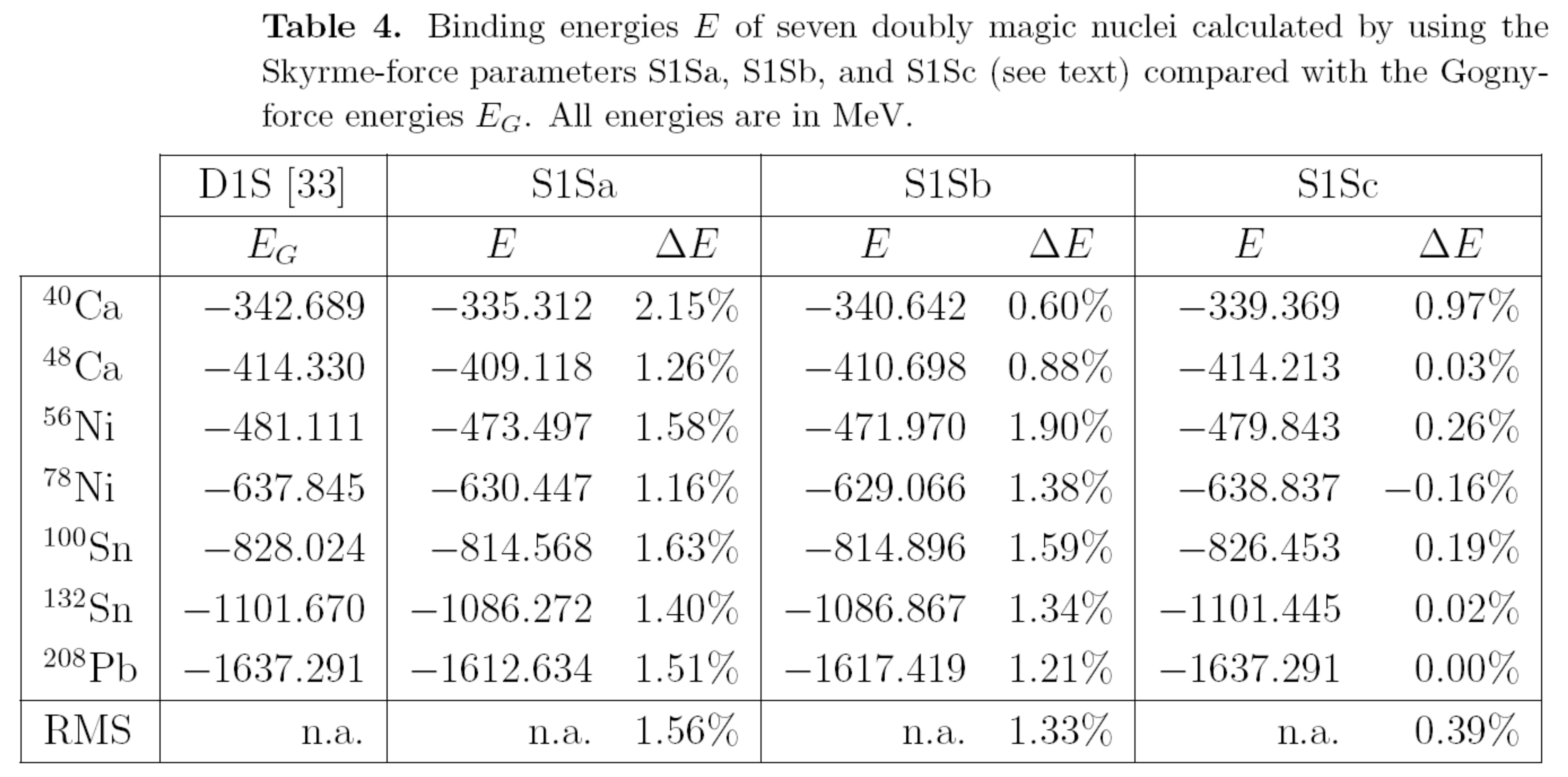
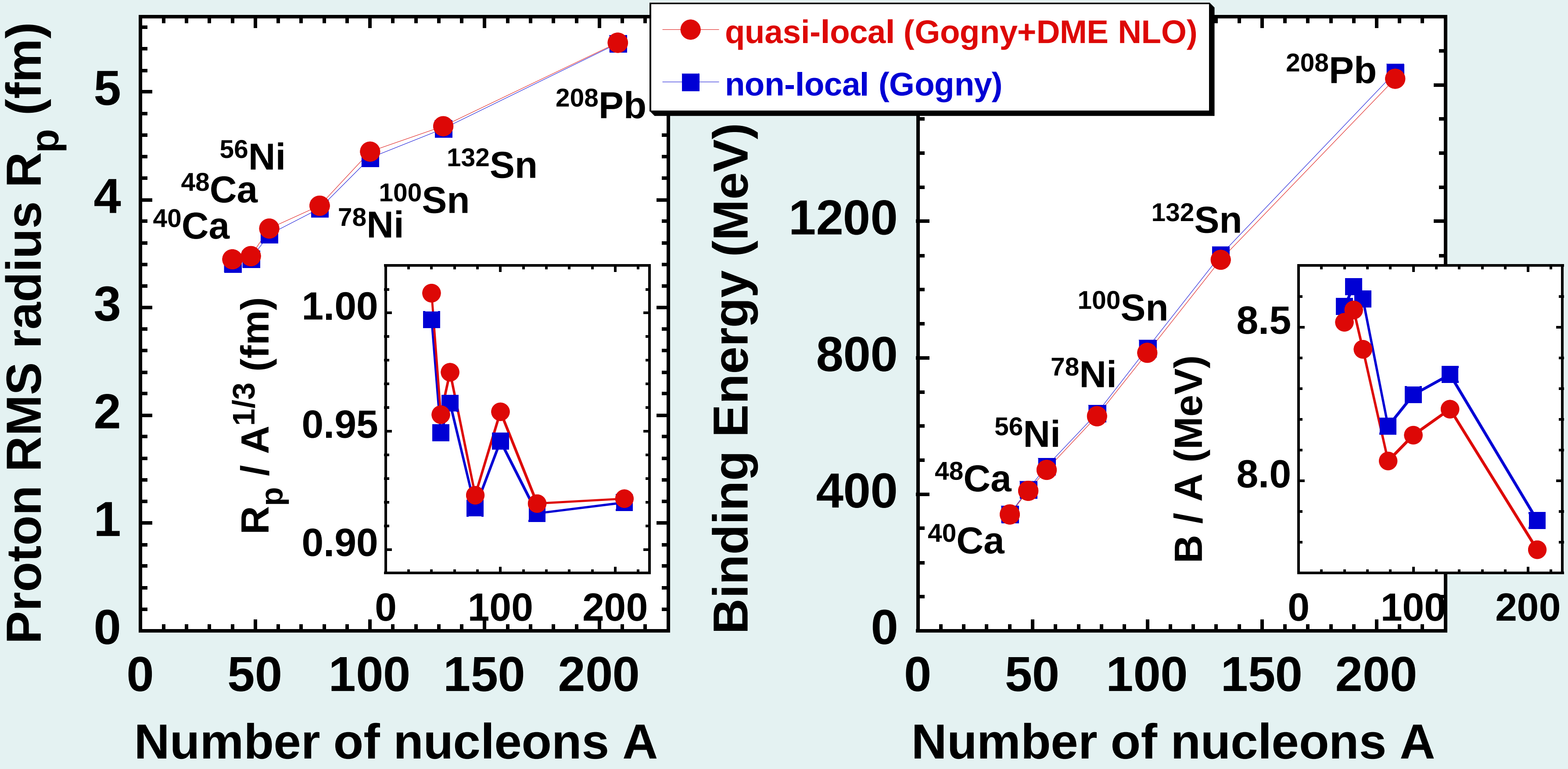


Table 4. Binding energies E of seven doubly magic nuclei calculated by using the Skyrme-force parameters S1Sa, S1Sb, and S1Sc (see text) compared with the Gogny-force energies E_G. All energies are in MeV.

	D1S [33]	S1Sa		S1Sb		S1Sc	
	E_G	E	ΔE	E	ΔE	E	ΔE
^{40}Ca	−342.689	−335.312	2.15%	−340.642	0.60%	−339.369	0.97%
^{48}Ca	−414.330	−409.118	1.26%	−410.698	0.88%	−414.213	0.03%
^{56}Ni	−481.111	−473.497	1.58%	−471.970	1.90%	−479.843	0.26%
^{78}Ni	−637.845	−630.447	1.16%	−629.066	1.38%	−638.837	−0.16%
^{100}Sn	−828.024	−814.568	1.63%	−814.896	1.59%	−826.453	0.19%
^{132}Sn	−1101.670	−1086.272	1.40%	−1086.867	1.34%	−1101.445	0.02%
^{208}Pb	−1637.291	−1612.634	1.51%	−1617.419	1.21%	−1637.291	0.00%
RMS	n.a.	n.a.	1.56%	n.a.	1.33%	n.a.	0.39%

Quasi-local vs. non-local functionals

The Negele-Vautherin density-matrix expansion (DME) up to NLO (2^{nd} order) applied to the Gogny non-local functional gives a Skyrme-like quasi-local functional. The results for self-consistent observables, obtained for both functionals are very similar.



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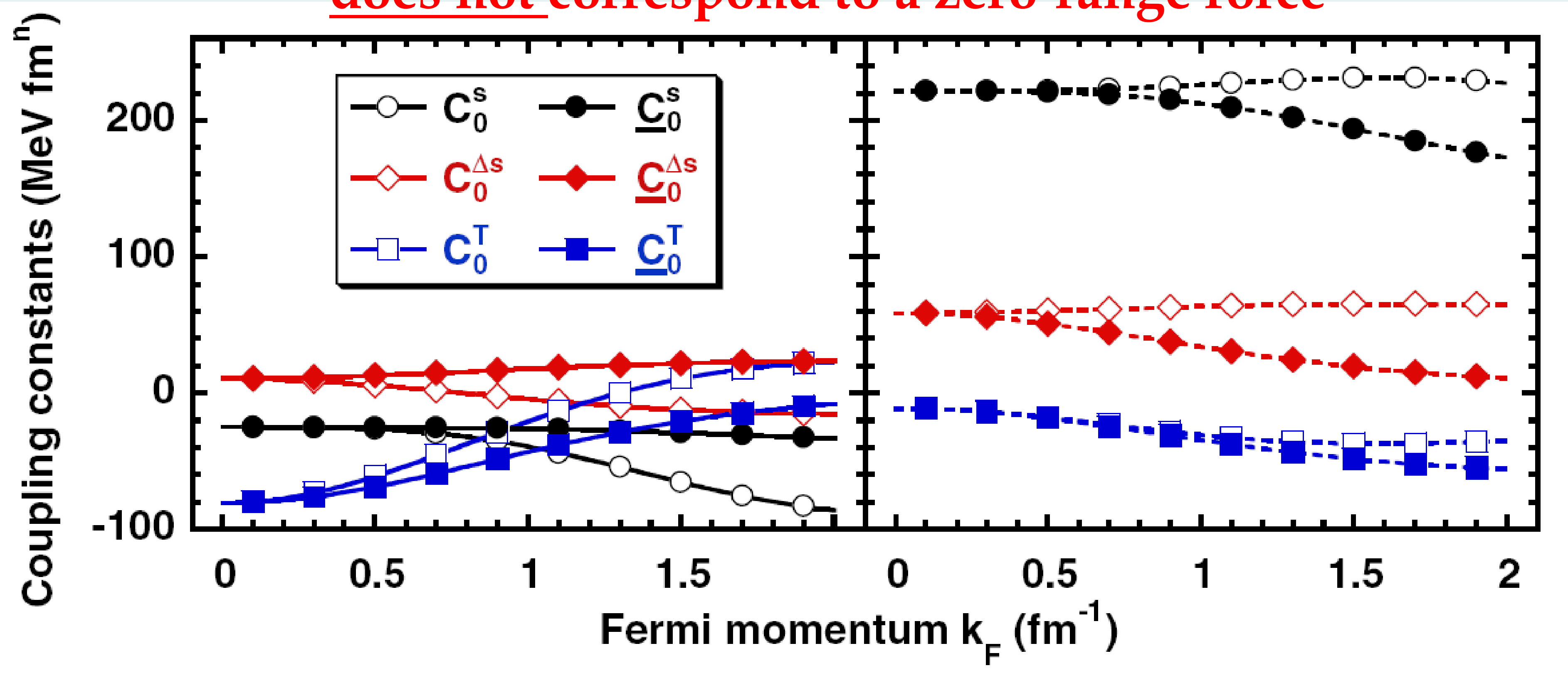
Negele-Vautherin density-matrix expansion

The quasi-local EDF derived from the finite-range force does not correspond to a zero-range force



Open symbols show the results obtained directly by using the Negele-Vautherin DME, whereas the full symbols show the results inferred from the time-even sector by using the Gogny-equivalent Skyrme force. Solid and dashed lines (left and right panels) show the values of the isoscalar and isovector coupling constants, respectively.

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Nuclear densities as composite fields

Density matrix:

$$\rho(\vec{r}\sigma,\vec{r}'\sigma') = \langle\Phi|a^{+}(\vec{r}'\sigma')a(\vec{r}\sigma)|\Phi\rangle$$

Scalar and vector part:

$$\begin{aligned} \rho(\vec{r},\vec{r}') &= \sum_{\sigma}\rho(\vec{r}\sigma,\vec{r}'\sigma) \\ \vec{s}(\vec{r},\vec{r}') &= \sum_{\sigma\sigma'}\rho(\vec{r}\sigma,\vec{r}'\sigma')\langle\sigma'|\vec{\sigma}|\sigma\rangle \end{aligned}$$

Symmetries:

$$\begin{aligned} \rho^{T}(\vec{r},\vec{r}') &= \rho^{*}(\vec{r},\vec{r}') &= \rho(\vec{r}',\vec{r}) \\ \vec{s}^{T}(\vec{r},\vec{r}') &= -\vec{s}^{*}(\vec{r},\vec{r}') &= -\vec{s}(\vec{r}',\vec{r}) \end{aligned}$$

Local densities:

Matter: $\rho(\vec{r}) = \rho(\vec{r},\vec{r})$

Momentum: $\vec{j}(\vec{r}) = (1/2i)[(\vec{\nabla}-\vec{\nabla}')\rho(\vec{r},\vec{r}')]_{r=r'}$

Kinetic: $\tau(\vec{r}) = [\vec{\nabla}\cdot\vec{\nabla}'\rho(\vec{r},\vec{r}')]_{r=r'}$

Spin: $\vec{s}(\vec{r}) = \vec{s}(\vec{r},\vec{r})$

Spin momentum: $J_{\mu\nu}(\vec{r}) = (1/2i)[(\nabla_{\mu}-\nabla'_{\mu})s_{\nu}(\vec{r},\vec{r}')]_{r=r'}$

Spin kinetic: $\vec{T}(\vec{r}) = [\vec{\nabla}\cdot\vec{\nabla}'\vec{s}(\vec{r},\vec{r}')]_{r=r'}$

Tensor kinetic: $\vec{F}(\vec{r}) = \frac{1}{2}[(\vec{\nabla}\otimes\vec{\nabla}'+\vec{\nabla}'\otimes\vec{\nabla})\cdot\vec{s}(\vec{r},\vec{r}')]_{r=r'}$

Local energy density: (no isospin, no pairing)

Density	Derivative	Symmetry			Energy density
		T	P	space	
$\rho(\vec{r})$		$+$	$+$	scalar	ρ^2
	$\vec{\nabla}\rho(\vec{r})$	$+$	$-$	vector	$\vec{\nabla}\rho\cdot\vec{J}$
	$\Delta\rho(\vec{r})$	$+$	$+$	scalar	$\rho\Delta\rho$
$\tau(\vec{r})$		$+$	$+$	scalar	$\rho\tau$
$J^{(0)}(\vec{r})$		$+$	$-$	scalar	$J^{(0)}J^{(0)}$
	$\vec{\nabla}J^{(0)}(\vec{r})$	$+$	$+$	vector	
$\vec{J}(\vec{r})$		$+$	$-$	vector	$\vec{J}^2$
	$\vec{\nabla}\cdot\vec{J}(\vec{r})$	$+$	$+$	scalar	$\rho\vec{\nabla}\cdot\vec{J}$
	$\vec{\nabla}\times\vec{J}(\vec{r})$	$+$	$+$	vector	
$J^{(2)}_{\mu\nu}(\vec{r})$		$+$	$-$	tensor	$\sum_{\mu\nu}J^{(2)}_{\mu\nu}J^{(2)}_{\mu\nu}$
$\vec{s}(\vec{r})$		$-$	$+$	vector	$\vec{s}^2$
	$\vec{\nabla}\cdot\vec{s}(\vec{r})$	$-$	$-$	scalar	$(\vec{\nabla}\cdot\vec{s})^2$
	$\vec{\nabla}\times\vec{s}(\vec{r})$	$-$	$-$	vector	$\vec{j}\cdot\vec{\nabla}\times\vec{s}$
	$\Delta\vec{s}(\vec{r})$	$-$	$+$	vector	$\vec{s}\cdot\Delta\vec{s}$
$\vec{j}(\vec{r})$		$-$	$-$	vector	$\vec{j}^2$
	$\vec{\nabla}\cdot\vec{j}(\vec{r})$	$-$	$+$	scalar	
	$\vec{\nabla}\times\vec{j}(\vec{r})$	$-$	$+$	vector	$\vec{s}\cdot\vec{\nabla}\times\vec{j}$
$\vec{T}(\vec{r})$		$-$	$+$	vector	$\vec{s}\cdot\vec{T}$
$\vec{F}(\vec{r})$		$-$	$+$	vector	$\vec{s}\cdot\vec{F}$

Nuclear Energy Density Functional

We consider the EDF in the form,

$$\mathcal{E} = \int d^3r \mathcal{H}(r),$$

where the energy density $\mathcal{H}(r)$ can be represented as a sum of the kinetic energy and of the potential-energy isoscalar ($t = 0$) and isovector ($t = 1$) terms,

$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(r) + \mathcal{H}_1(r),$$

which for the time-reversal and spherical symmetries imposed read:

$$\mathcal{H}_t(r) = C_t^\rho \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^{\Delta\rho} \rho_t \Delta \rho_t + \tfrac{1}{2} C_t^J J_t^2 + C_t^{\nabla J} \rho_t \nabla \cdot J_t.$$

Following the parametrization used for the Skyrme forces, we assume the dependence of the coupling parameters C_t^ρ on the isoscalar density ρ_0 as:

$$C_t^\rho = C_{t0}^\rho + C_{t\mathrm{D}}^\rho \rho_0^\alpha.$$

The standard EDF depends linearly on 12 coupling constants,

$$C_{t0}^\rho, \quad C_{t\mathrm{D}}^\rho, \quad C_t^\tau, \quad C_t^{\Delta\rho}, \quad C_t^{\mathrm{J}}, \quad \text{and} \quad C_t^{\nabla\mathrm{J}},$$

for $t = 0$ and 1.

Complete local energy density

The energy density can be written in the following form:

$$\mathcal{H}(\vec{r}) = \frac{\hbar^2}{2m}\tau_0(\vec{r}) + \sum\nolimits_{t=0,1}\left(\chi_t(\vec{r}) + \breve{\chi}_t(\vec{r})\right),$$

E. Perlińska, *et al.*,
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The p-h and p-p interaction energy densities, $\chi_t(\vec{r})$ and $\breve{\chi}_t$, for t=0 depend quadratically on the isoscalar densities, and for t=1 – on the isovector ones. Based on general rules of constructing the energy density, one obtains

Mean field

$$\begin{aligned}
\chi_0(\vec{r}) &= C_0^{\rho}\rho_0^2 + C_0^{\Delta\rho}\rho_0\Delta\rho_0 + C_0^{\tau}\rho_0\tau_0 \\
&+ C_0^{J0}J_0^2 + C_0^{J1}\vec{J}_0^2 + C_0^{J2}\underline{J}_0^2 + C_0^{\nabla J}\rho_0\vec{\nabla}\cdot\vec{J}_0 \\
&+ C_0^{s}\vec{s}_0^2 + C_0^{\Delta s}\vec{s}_0\cdot\Delta\vec{s}_0 + C_0^{T}\vec{s}_0\cdot\vec{T}_0 \\
&+ C_0^{j}\vec{j}_0^2 + C_0^{\nabla j}\vec{s}_0\cdot(\vec{\nabla}\times\vec{j}_0) \\
&+ C_0^{\nabla s}(\vec{\nabla}\cdot\vec{s}_0)^2 + C_0^{F}\vec{s}_0\cdot\vec{F}_0, \\
\chi_1(\vec{r}) &= C_1^{\rho}\vec{\rho}^{\,2} + C_1^{\Delta\rho}\vec{\rho}\circ\Delta\vec{\rho} + C_1^{\tau}\vec{\rho}\circ\vec{\tau} \\
&+ C_1^{J0}\vec{J}^2 + C_1^{J1}\vec{\vec{J}}^{\,2} + C_1^{J2}\underline{\vec{J}}^{\,2} + C_1^{\nabla J}\vec{\rho}\circ\vec{\nabla}\cdot\vec{\vec{J}} \\
&+ C_1^{s}\vec{\vec{s}}^{\,2} + C_1^{\Delta s}\vec{\vec{s}}\cdot\circ\Delta\vec{\vec{s}} + C_1^{T}\vec{\vec{s}}\cdot\circ\vec{\vec{T}} \\
&+ C_1^{j}\vec{\vec{j}}^{\,2} + C_1^{\nabla j}\vec{\vec{s}}\cdot\circ(\vec{\nabla}\times\vec{\vec{j}}) \\
&+ C_1^{\nabla s}(\vec{\nabla}\cdot\vec{\vec{s}})^2 + C_1^{F}\vec{\vec{s}}\cdot\circ\vec{\vec{F}},
\end{aligned}$$

where × stands for the vector product

Pairing

$$\begin{aligned}
\breve{\chi}_0(\vec{r}) &= \breve{C}_0^{s}|\breve{\vec{s}}_0|^2 + \breve{C}_0^{\Delta s}\Re(\breve{\vec{s}}_0^{\,*}\cdot\Delta\breve{\vec{s}}_0) \\
&+ \breve{C}_0^{T}\Re(\breve{\vec{s}}_0^{\,*}\cdot\breve{\vec{T}}_0) + \breve{C}_0^{j}|\breve{\vec{j}}_0|^2 \\
&+ \breve{C}_0^{\nabla j}\Re(\breve{\vec{s}}_0^{\,*}\cdot(\vec{\nabla}\times\breve{\vec{j}}_0)) \\
&+ \breve{C}_0^{\nabla s}|\vec{\nabla}\cdot\breve{\vec{s}}_0|^2 \\
&+ \breve{C}_0^{F}\Re(\breve{\vec{s}}_0^{\,*}\cdot\breve{\vec{F}}_0), \\
\breve{\chi}_1(\vec{r}) &= \breve{C}_1^{\rho}|\breve{\vec{\rho}}|^2 + \breve{C}_1^{\Delta\rho}\Re(\breve{\vec{\rho}}^{\,*}\circ\Delta\breve{\vec{\rho}}) \\
&+ \breve{C}_1^{\tau}\Re(\breve{\vec{\rho}}^{\,*}\circ\breve{\vec{\tau}}) \\
&+ \breve{C}_1^{J0}|\breve{\vec{J}}|^2 + \breve{C}_1^{J1}|\breve{\vec{\vec{J}}}|^2 \\
&+ \breve{C}_1^{J2}|\breve{\underline{\vec{J}}}|^2 \\
&+ \breve{C}_1^{\nabla J}\Re(\breve{\vec{\rho}}^{\,*}\circ\vec{\nabla}\cdot\breve{\vec{\vec{J}}}).
\end{aligned}$$

Mean-field equations

Mean-field potentials:

$$
\begin{aligned}
\Gamma_t^{\text{even}} &= -\vec{\nabla}\cdot M_t(\vec{r})\vec{\nabla} + U_t(\vec{r}) + \tfrac{1}{2i}\left(\overleftrightarrow{\nabla}\sigma\cdot\overleftrightarrow{B}_t(\vec{r}) + \overleftrightarrow{B}_t(\vec{r})\cdot\overleftrightarrow{\nabla}\sigma\right)\\
\Gamma_t^{\text{odd}} &= -\vec{\nabla}\cdot(\vec{\sigma}\cdot\vec{C}_t(\vec{r}))\vec{\nabla} + \vec{\sigma}\cdot\vec{\Sigma}_t(\vec{r}) + \tfrac{1}{2i}(\vec{\nabla}\cdot\vec{I}_t(\vec{r}) + \vec{I}_t(\vec{r})\cdot\vec{\nabla}) - \vec{\nabla}\cdot\vec{D}_t(\vec{r})\vec{\sigma}\cdot\vec{\nabla}
\end{aligned}
$$

where

$$
\begin{aligned}
U_t &= 2C_t^{\rho}\rho_t + 2C_t^{\Delta\rho}\Delta\rho_t + C_t^{\tau}\tau_t + C_t^{\nabla J}\vec{\nabla}\cdot\vec{J}_t,\\
\vec{\Sigma}_t &= 2C_t^{s}\vec{s}_t + 2C_t^{\Delta s}\Delta\vec{s}_t + C_t^{T}\vec{T}_t + C_t^{\nabla j}\vec{\nabla}\times\vec{j}_t, -2C_t^{\nabla s}\Delta\vec{s}_t + C_t^{F}\vec{F}_t - 2C_t^{\nabla s}\vec{\nabla}\times(\vec{\nabla}\times\vec{s}_t)\\
M_t &= C_t^{\tau}\rho_t,\\
\vec{C}_t &= C_t^{T}\vec{s}_t,\\
\overleftrightarrow{B}_t &= 2C_t^{J}\overleftrightarrow{J}_t - C_t^{\nabla J}\overleftrightarrow{\nabla}\rho_t,\\
\vec{I}_t &= 2C_t^{j}\vec{j}_t + C_t^{\nabla j}\vec{\nabla}\times\vec{s}_t,\\
\vec{D}_t &= C_t^{F}\vec{s}_t,
\end{aligned}
$$

Neutron and proton mean-field Hamiltonians:

$$
\begin{aligned}
h_n &= -\frac{\hbar^2}{2m}\Delta + \Gamma_0^{\text{even}} + \Gamma_0^{\text{odd}} + \Gamma_1^{\text{even}} + \Gamma_1^{\text{odd}},\\
h_p &= -\frac{\hbar^2}{2m}\Delta + \Gamma_0^{\text{even}} + \Gamma_0^{\text{odd}} - \Gamma_1^{\text{even}} - \Gamma_1^{\text{odd}}.
\end{aligned}
$$

HF equation for single-particle wave functions:

$$
h_\alpha\psi_{i,\alpha}(\vec{r}\sigma) = \epsilon_{i,\alpha}\psi_{i,\alpha}(\vec{r}\sigma) \quad\Longrightarrow\quad \rho_\alpha(\vec{r}\sigma,\vec{r}'\sigma') = \sum_{i=1}^{N}\psi_{i,\alpha}(\vec{r}\sigma)\psi_{i,\alpha}^{*}(\vec{r}'\sigma')
$$

where i numbers the neutron ($\alpha{=}n$) and proton ($\alpha{=}p$) eigenstates.

Lessons learned

1) Energy density functional exists due to the two-step variational method and gives exact ground state energy and its exact particle density.

2) Whenever the energy scales (or range scales) between the interactions and observations are different, the observations can be described by a series of pseudopotentials with coupling constants adjusted to data (an effective theory).

3) In nuclei, the non-local energy density functionals can be replaced by the local ones. This is because the range of the interaction is shorter than the range of variations in the local and non-local density matrix.

4) Systematic energy density functionals with derivative corrections can be constructed and the resulting self-consistent equations solved.

Applications

Phenomenological effective interactions

- Gogny force.*

$$\tilde{V}_{xyx'y'} = \delta(\vec{x}-\vec{x}')\delta(\vec{y}-\vec{y}')V(x,y),$$

where the tilde denotes a non-antisymmetrized matrix element ($V_{xyx'y'} = \tilde{V}_{xyx'y'} - \tilde{V}_{xyy'x'}$), and $V(x,y)$ is a sum of two Gaussians, plus a zero-range, density dependent part,

$$V(x,y) = \sum\nolimits_{i=1,2} e^{-(\vec{x}-\vec{y})^2/\mu_i^2} \times (W_i + B_iP_\sigma - H_iP_\tau - M_iP_\sigma P_\tau)$$

$$+t_3(1+P_\sigma)\delta(\vec{x}-\vec{y})\rho^{1/3}\left[\tfrac{1}{2}(\vec{x}+\vec{y})\right].$$

In this Equation, $P_\sigma = \frac{1}{2}(1+\vec{\sigma}_1\cdot\vec{\sigma}_2)$ and $P_\tau = \frac{1}{2}(1+\vec{\tau}_1\cdot\vec{\tau}_2)$ are, respectively, the spin and isospin exchange operators of particles 1 and 2, $\rho(\vec{r})$ is the total density of the system at point $\vec{r}$, and $\mu_i = 0.7$ and 1.2 fm, W_i, B_i, H_i, M_i, and t_3 are parameters.

- Skyrme force.*

$$\tilde{V}_{xyx'y'} = \Big\{t_0(1+x_0P^\sigma) + \tfrac{1}{6}t_3(1+x_3P^\sigma)\rho^\alpha\left(\tfrac{1}{2}(\vec{x}+\vec{y})\right)$$

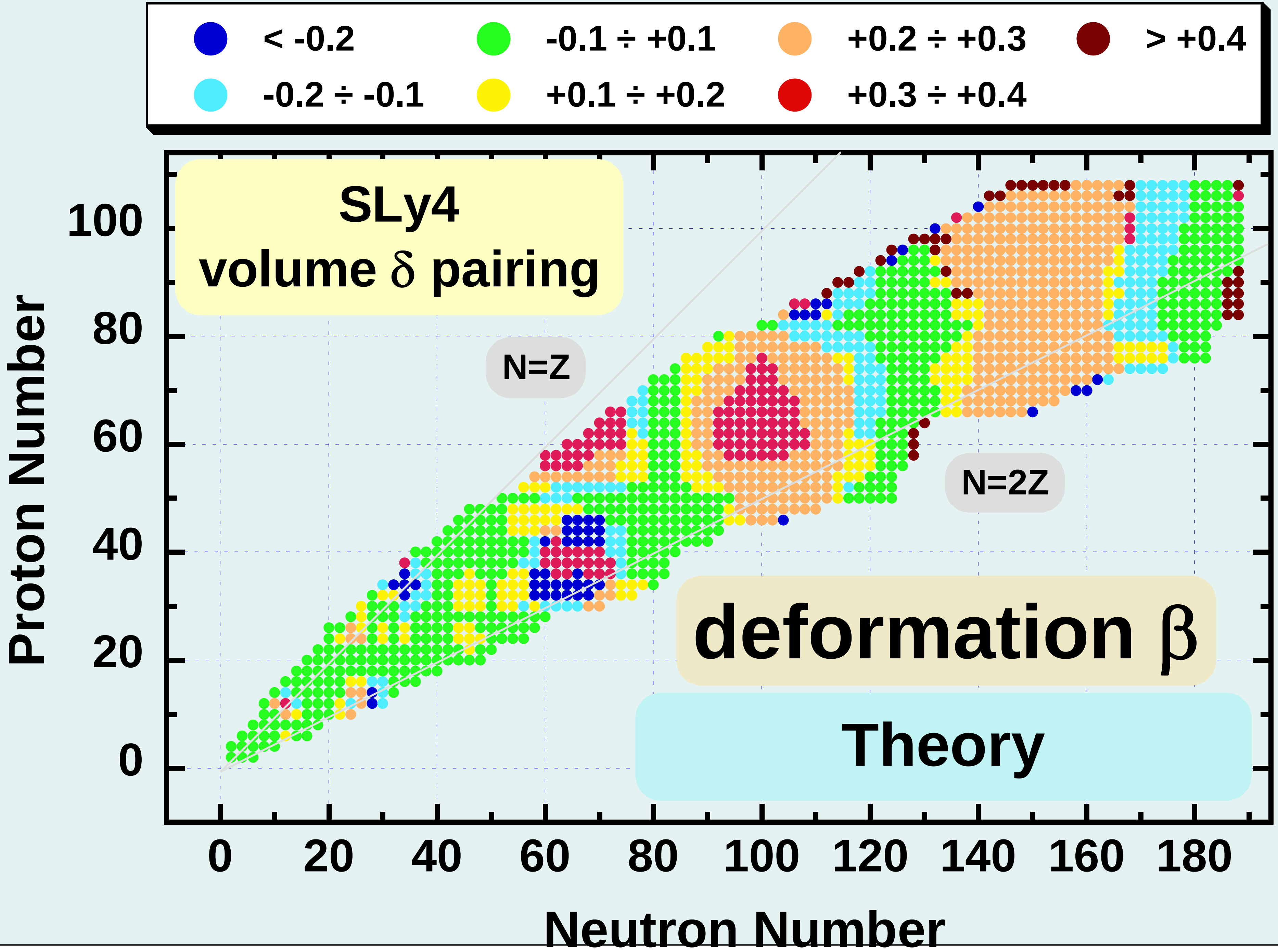
$$+\tfrac{1}{2}t_1(1+x_1P^\sigma)[\vec{k}^2+\vec{k}'^2] + t_2(1+x_2P^\sigma)\vec{k}^*\cdot\vec{k}'\Big\}\delta(\vec{x}-\vec{x}')\delta(\vec{y}-\vec{y}')\delta(\vec{x}-\vec{y}),$$

where the relative momentum operators read

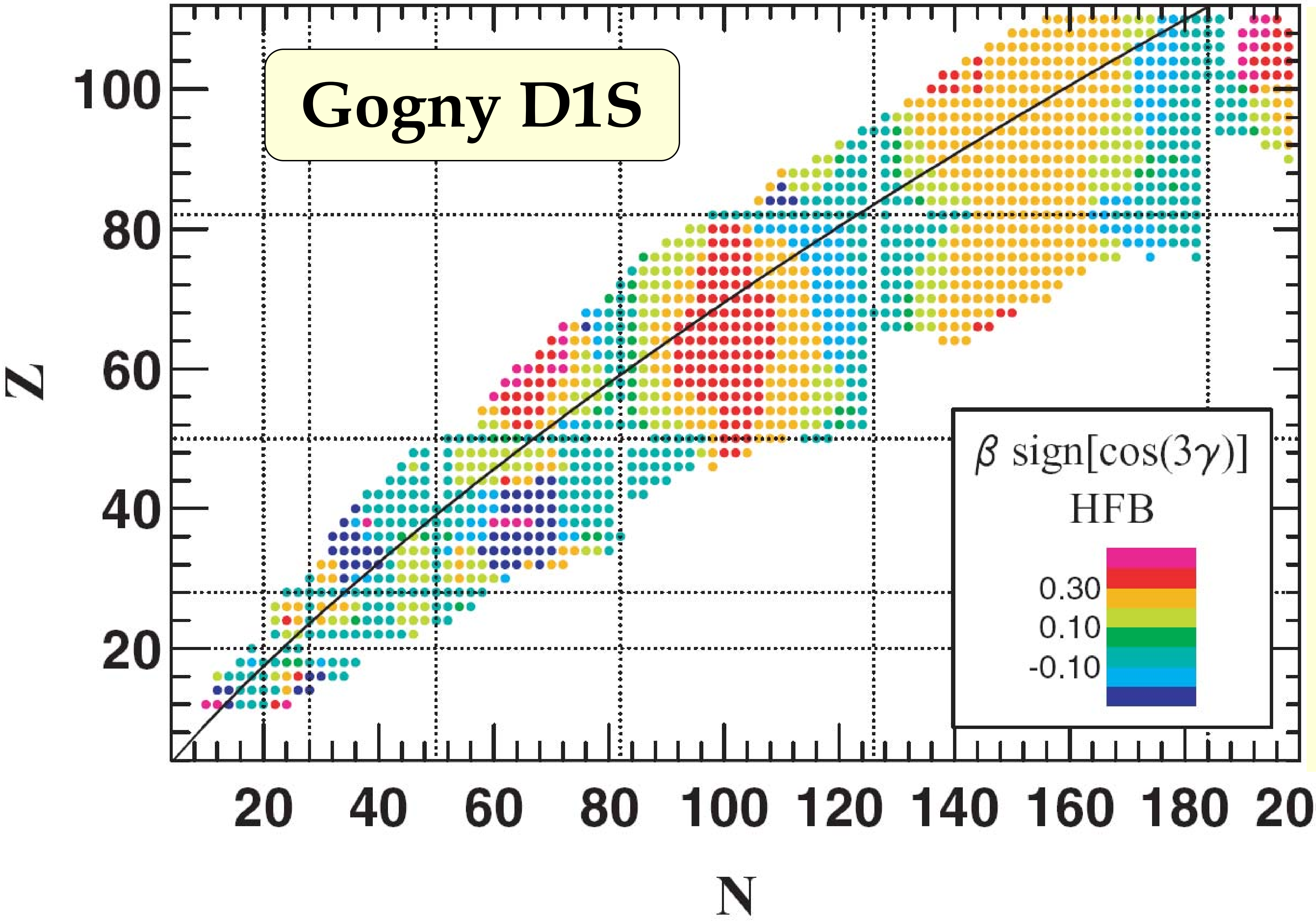
$$\hat{\vec{k}} = \frac{1}{2i}\left(\vec{\nabla}_x - \vec{\nabla}_y\right), \qquad \hat{\vec{k}}' = \frac{1}{2i}\left(\vec{\nabla}'_x - \vec{\nabla}'_y\right).$$

---

*We omit the spin-orbit and tensor terms for simplicity.

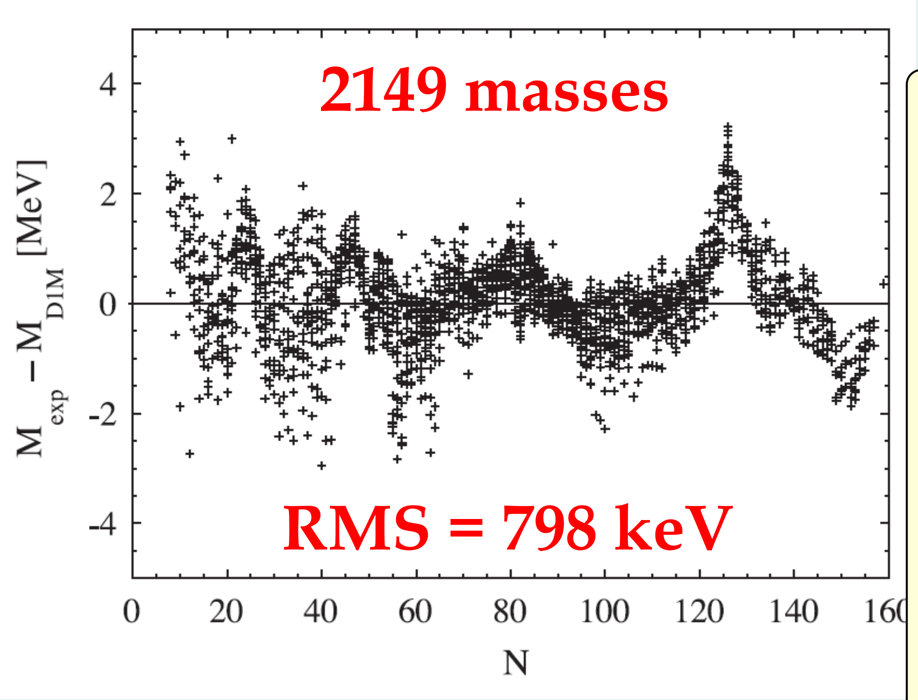


M.V. Stoitsov, *et al.*, Phys. Rev. C68, 054312 (2003)



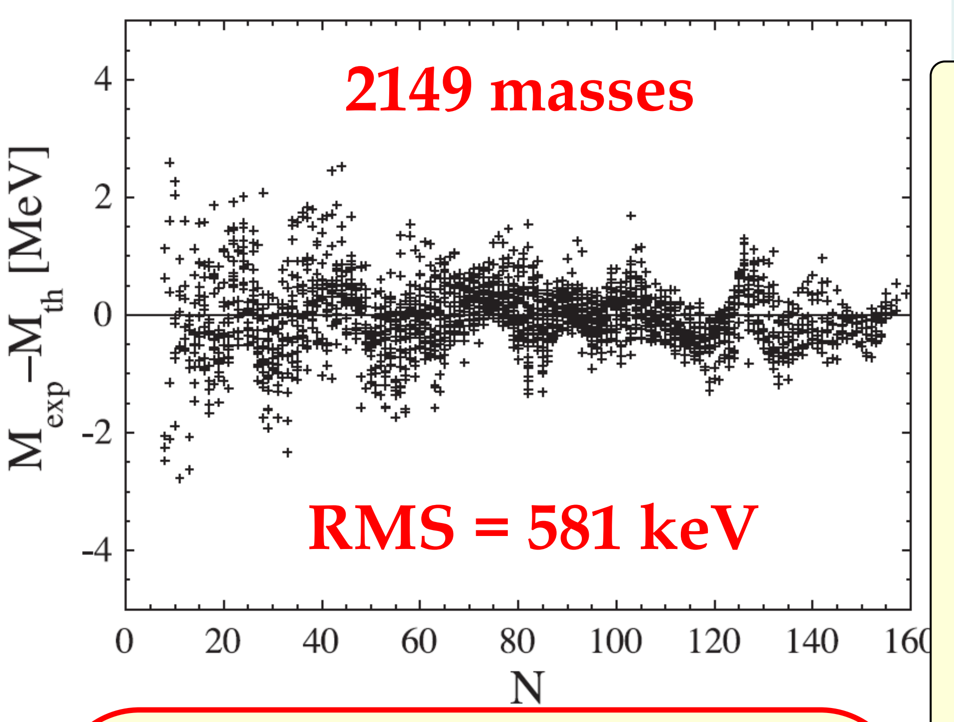
J.-P. Delaroche et al., Phys. Rev. C81, 014303 (2010)

Nuclear binding energies (masses)



The first Gogny HFB mass model. An explicit and self-consistent account of all the quadrupole correlation energies are included within the 5D collective Hamiltonian approach.

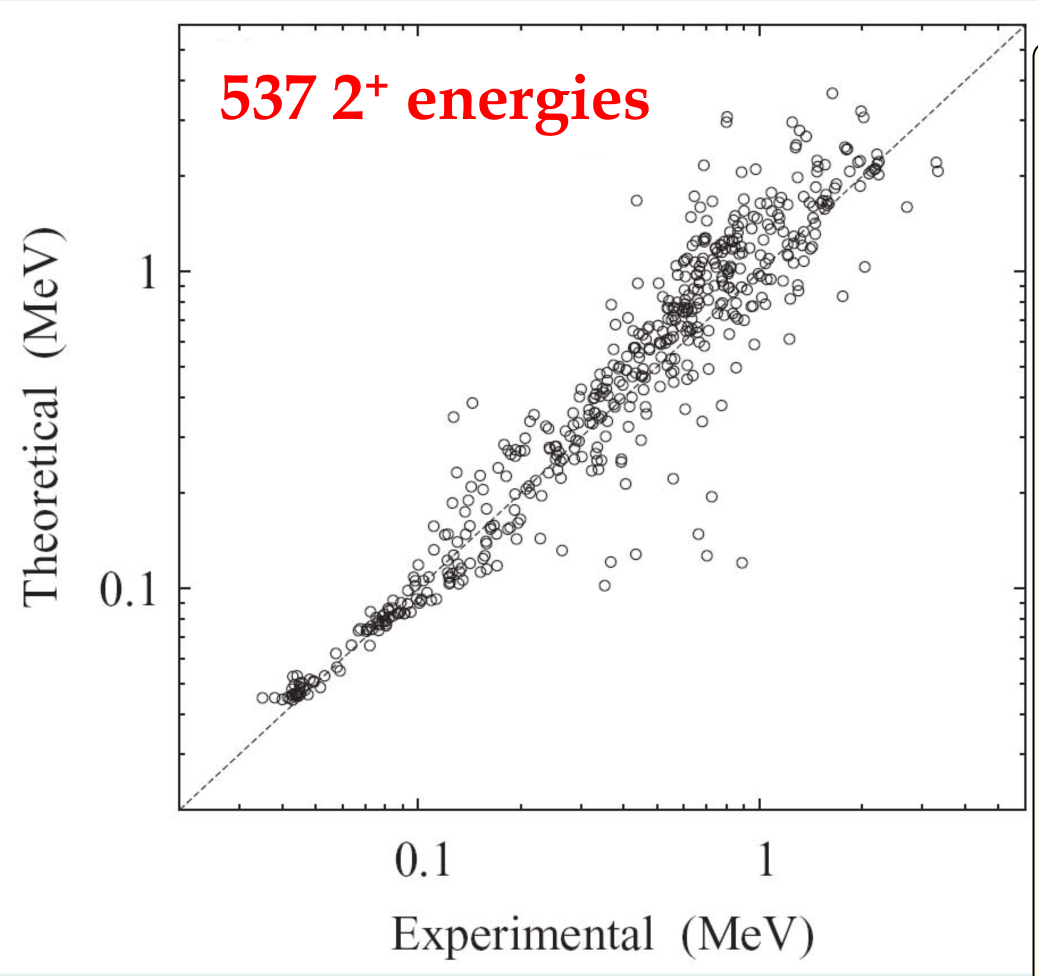
S. Goriely *et al.*, Phys. Rev. Lett. 102, 242501 (2009)



The new Skyrme HFB nuclear-mass model, in which the contact-pairing force is constructed from microscopic pairing gaps of symmetric nuclear matter and neutron matter.

S. Goriely *et al.*, Phys. Rev. Lett. 102, 152503 (2009)

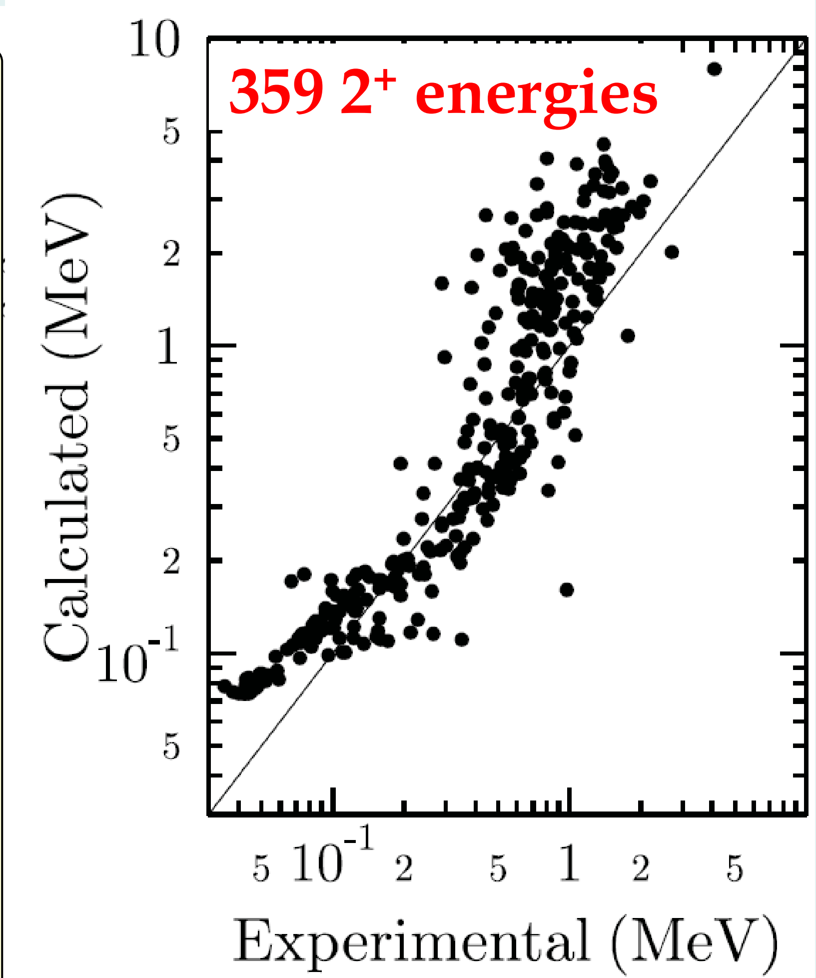
First 2^+ excitations of even-even nuclei



537 2^+ energies

J.-P. Delaroche *et al.*, Phys. Rev. C81, 014303 (2010)

Gogny HFB calculations plus the 5D collective Hamiltonian approach.

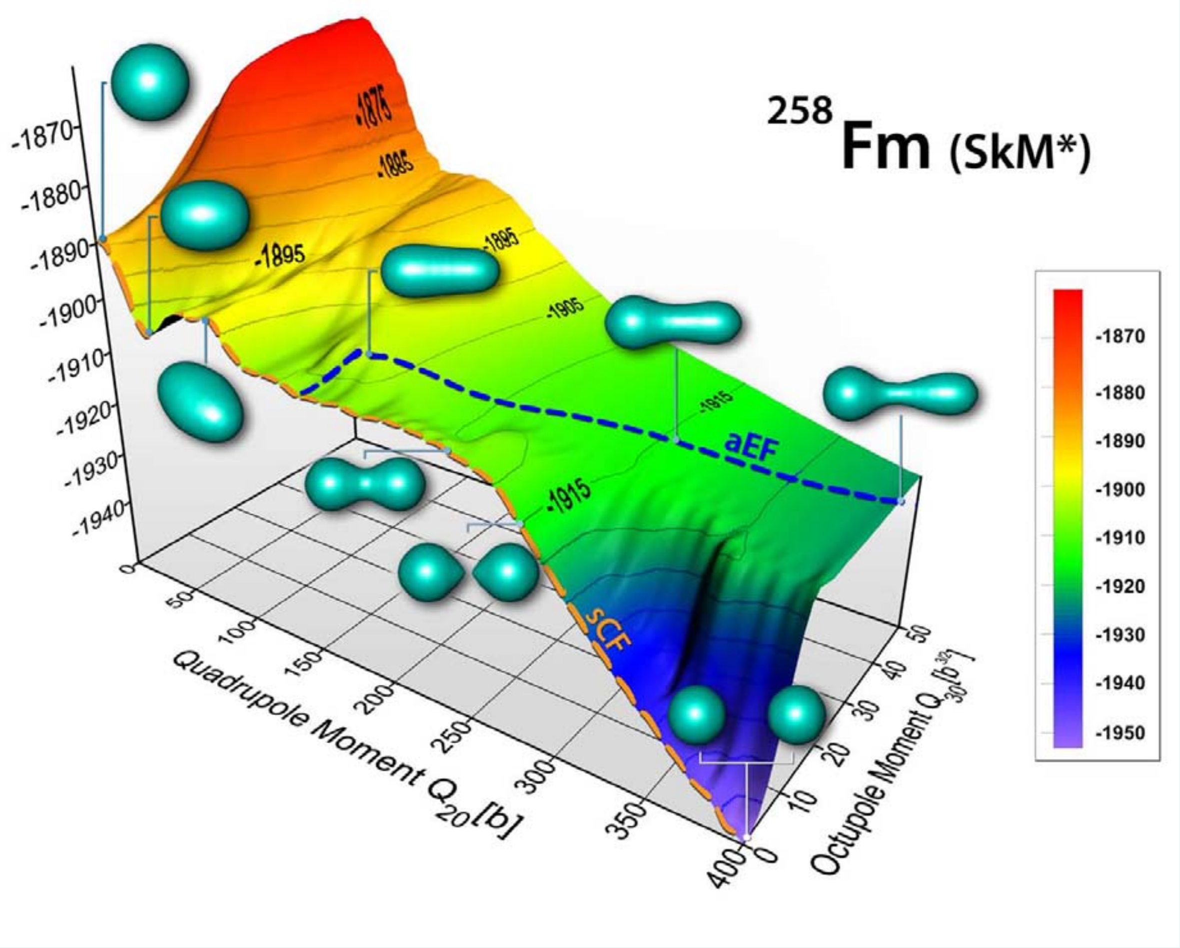


359 2^+ energies

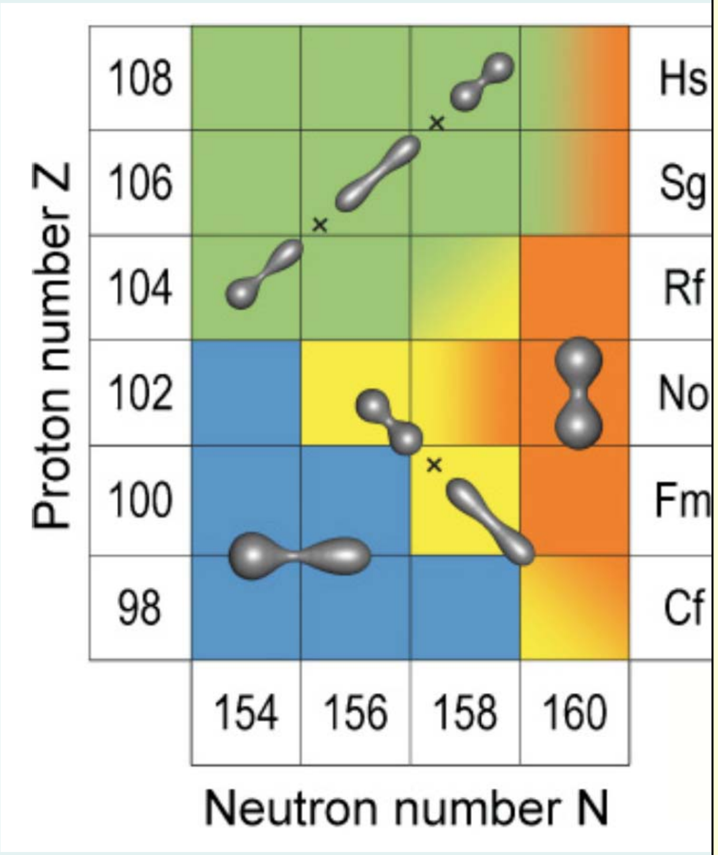
B. Sabbey *et al.*, Phys. Rev. C75, 044305 (2007)

Skyrme HF+BCS calculations plus the particle-number and angular-momentum projection and shape mixing.

Spontaneous fission



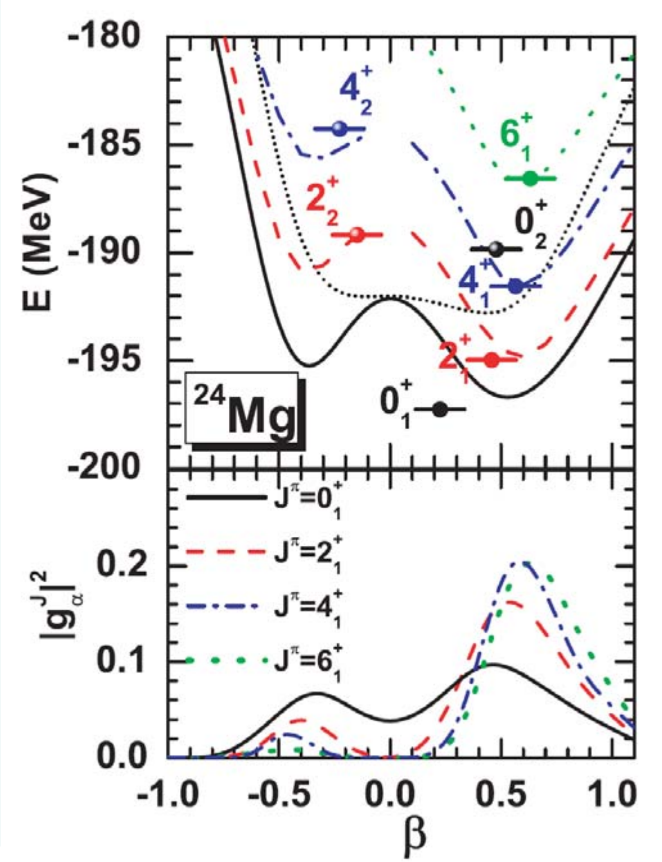
UNEDF collaboration: SciDAC Review 6, 42 (2007)



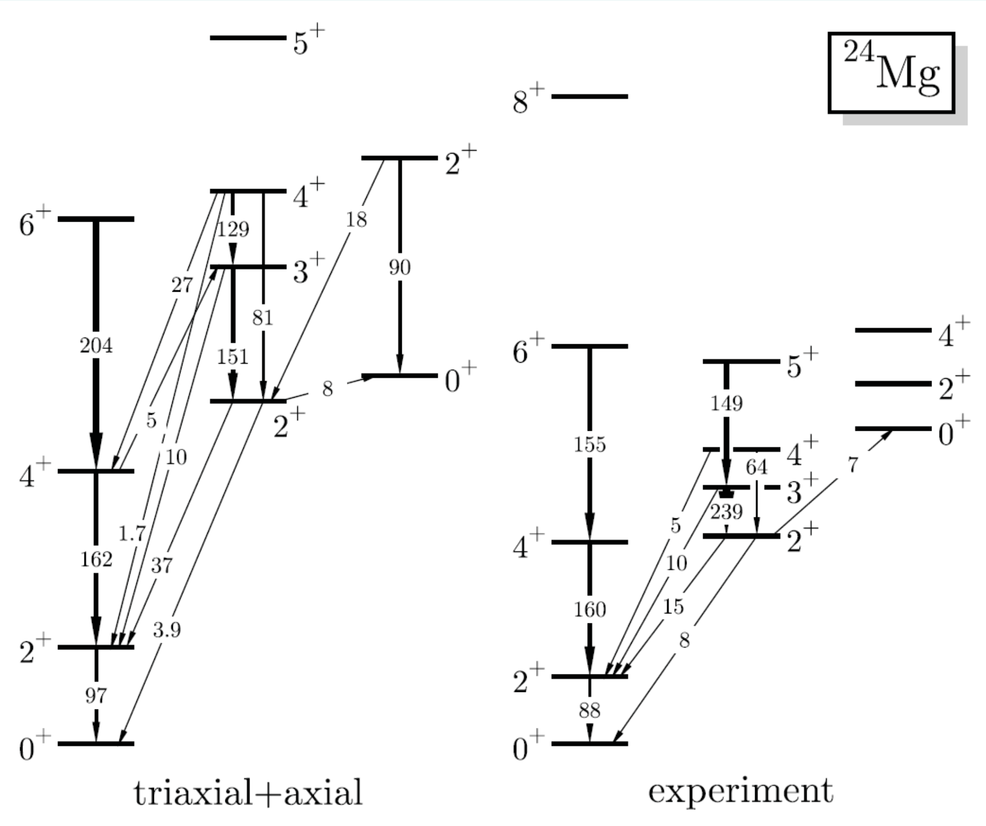
A. Staszczak *et al.*, Phys. Rev. C80, 014309 (2009)

Symmetry-unrestricted Skyrme HF+BCS calculations.

Collective states in even-even nuclei

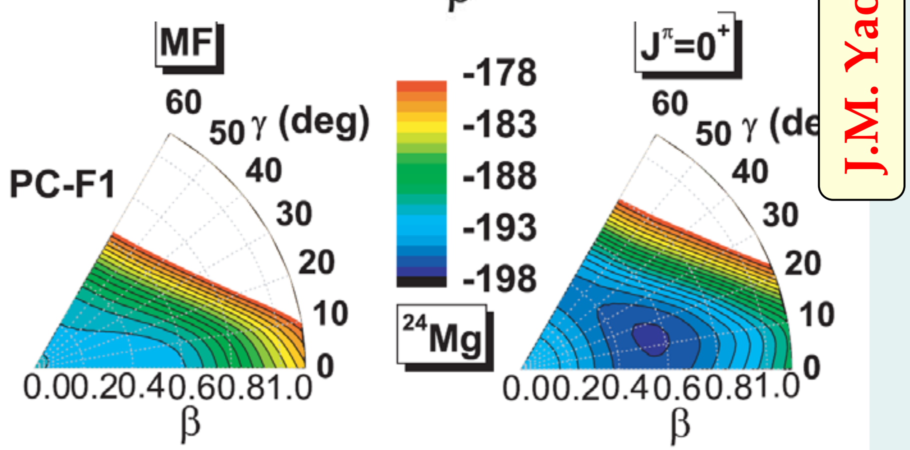


J.M. Yao *et al.*, **Phys. Rev. C81, 044311 (2010)**

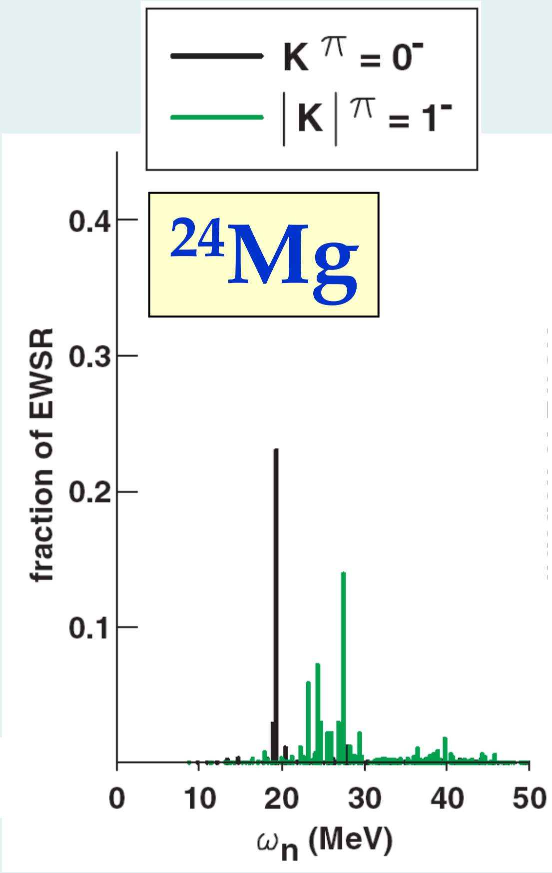


M. Bender *et al.*, **Phys. Rev. C78, 024309 (2008)**

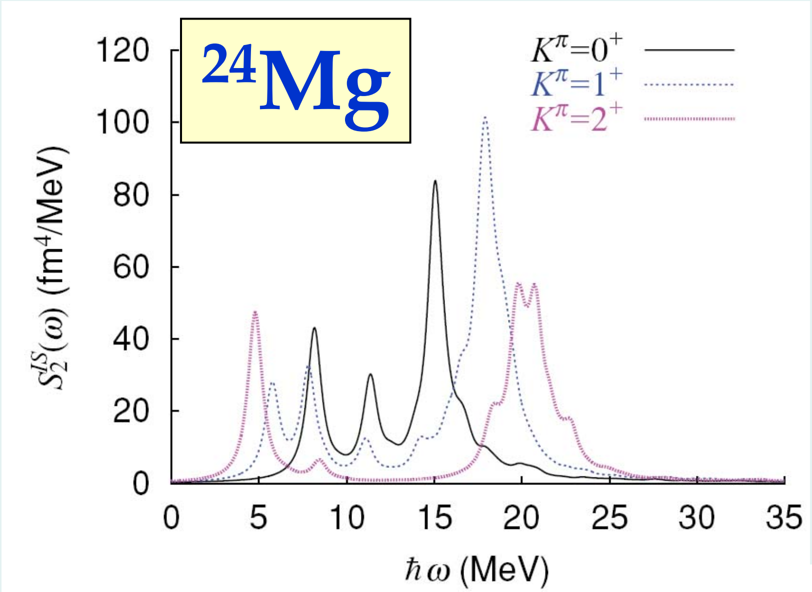
$$|\Psi_{NZ,JM}\rangle = \int d\beta d\gamma \sum_K f_K(\beta,\gamma) \times \hat{P}_N \hat{P}_Z \hat{P}_{JMK} |\Psi(\beta,\gamma)\rangle$$



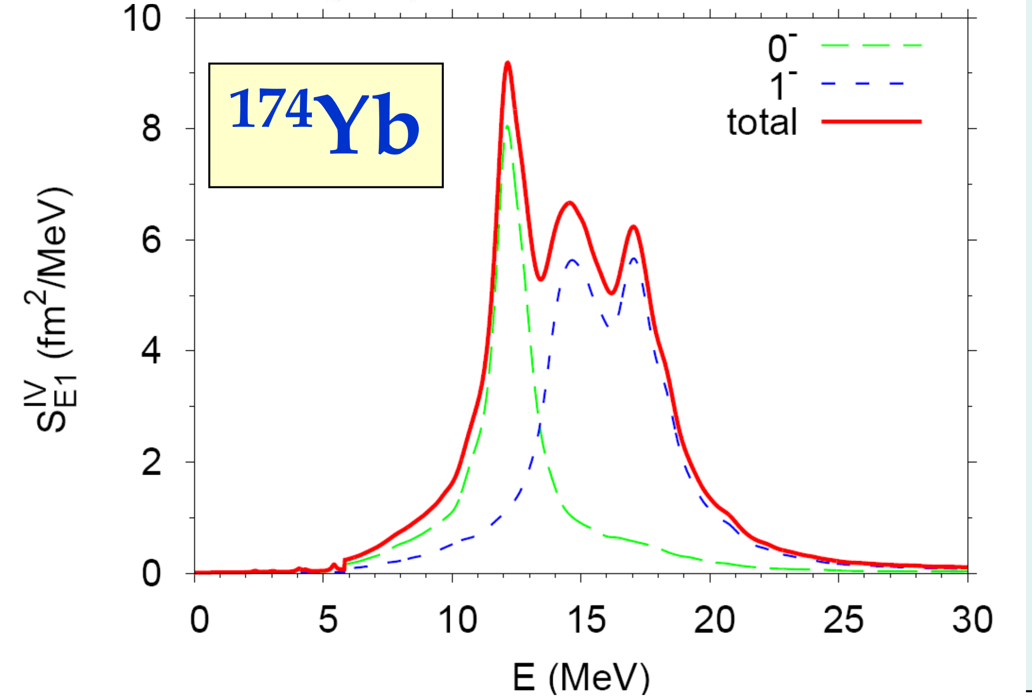
Giant resonances in deformed nuclei



S. Péru *et al.*, Phys. Rev. C77, 044313 (2008)



K. Yoshida *et al.*, Phys. Rev. C78, 064316 (2008)



J. Terasaki *et al.*, arXiv:1006.0010

Fast RPA and QRPA + Arnoldi method

Within RPA, let ρ denote the one-body projective density matrix, $\rho^2 = \rho$, and $h(\rho) = \partial E/\partial\rho$ denote the mean-field Hamiltonian calculated for ρ. The TDHF equation for $\rho(t)$ then reads:

$$i\hbar\frac{d}{dt}\rho = [h(\rho), \rho].$$

The RPA method approximates the TDHF solution by a single-mode vibrational state $\rho(t)$ in the vibrating mean field $h(t) = h(\rho(t))$:

$$\rho(t) = \rho_0 + \tilde{\rho}e^{-i\omega t} + \tilde{\rho}^+e^{i\omega t}, \qquad h(t) = h_0 + \tilde{h}e^{-i\omega t} + \tilde{h}^+e^{i\omega t}$$

where ρ_0 is the self-consistent solution, $[h_0, \rho_0] = 0$ for $h_0 = h(\rho_0)$, $\tilde{\rho}$ is the RPA amplitude, and $\tilde{h} = h(\tilde{\rho})$. This allows for transforming the TDHF into the RPA equation in the form

$$\hbar\omega\tilde{\rho} = \mathbb{H}_0\tilde{\rho} = [h_0, \tilde{\rho}] + [\tilde{h}, \rho_0],$$

by which the right-hand side becomes a linear operator $\mathbb{H}_0$ depending on ρ_0 and acting on $\tilde{\rho}$.

J. Toivanen *et al.*, Phys. Rev. C 81, 034312 (2010)

The RPA equation can be written explicitly in terms of the particle-hole and hole-particle matrix elements as:

$$\begin{aligned}\hbar\omega\,\tilde{\rho}_{\omega,mi} &= (\epsilon_m-\epsilon_i)\,\tilde{\rho}_{\omega,mi}+\tilde{h}_{\omega,mi}\,,\\ \hbar\omega\,\tilde{\rho}_{\omega,im} &= (\epsilon_i-\epsilon_m)\,\tilde{\rho}_{\omega,im}-\tilde{h}_{\omega,im}\,,\end{aligned}$$

We solve this problem by using an iterative method that during each iteration only needs to know the product of the RPA matrix and a density vector, that is, the right-hand sides of the preceding equations:

$$\begin{aligned}W^k_{mi} &= (\epsilon_m-\epsilon_i)\,X^k_{mi}+\tilde{h}_{mi}(\mathcal{X}^k,\mathcal{Y}^k)=\left(A\mathcal{X}^k+B\mathcal{Y}^k\right)_{mi}\,,\\ W'^k_{mi} &= (\epsilon_i-\epsilon_m)\,Y^k_{mi}-\tilde{h}_{im}(\mathcal{X}^k,\mathcal{Y}^k)=\left(-B'^*\mathcal{X}^k-A'^*\mathcal{Y}^k\right)_{mi}\,,\end{aligned}$$

where index k labels iterations and the mean fields $\tilde{h}(\mathcal{X}^k,\mathcal{Y}^k)$ depend linearly on the density vectors $\mathcal{X}^k$ and $\mathcal{Y}^k$. :

$$\begin{pmatrix}\mathcal{W}^k_+\\ \mathcal{W}'^{\,k}_+\end{pmatrix}=\begin{pmatrix}A & B\\ -B'^* & -A'^*\end{pmatrix}\begin{pmatrix}\mathcal{X}^k\\ \mathcal{Y}^k\end{pmatrix},\quad \begin{pmatrix}\mathcal{W}^k_-\\ \mathcal{W}'^{\,k}_-\end{pmatrix}=\begin{pmatrix}A & B\\ -B'^* & -A'^*\end{pmatrix}\begin{pmatrix}\mathcal{Y}^{k*}\\ \mathcal{X}^{k*}\end{pmatrix}$$

In exact arithmetic $A=A'$ and $B=B'$ and therefore either of these equations could be used in the iteration procedure with equivalent results. Nevertheless, below we use them both to stabilize the iteration process.

Fast and converging algorithm is obtained by using the following tricks:

1. Calculate the mean fields $\tilde{\rho}_{\omega,mi} \Longrightarrow \tilde{h}_{\omega,mi}$ in three steps that are exactly analogous to the HF method for ρ_0, namely:
   - $\psi_m(\vec{r}\sigma') = \sum_i \tilde{\rho}_{\omega,mi}\phi_i(\vec{r}\sigma)$, $\quad \tilde{\rho}(\vec{r}\sigma'\sigma) = \sum_m \phi_m(\vec{r}\sigma')\psi^*_m(\vec{r}\sigma)$
   - $\tilde{h}(\vec{r}\sigma'\sigma) = \delta E/\delta\tilde{\rho}^*(\vec{r}\sigma'\sigma)$
   - $\tilde{h}_{\omega,mi} = \int \mathrm{d}^3\vec{r}\sum_{\sigma'\sigma}\phi^*_m(\vec{r}\sigma')\tilde{h}(\vec{r}\sigma'\sigma)\phi_i(\vec{r}\sigma)$
2. Reduce the numerical errors in the matrix-vector products by symmetrization to get the final stabilized RPA matrix-vector product,

$$\begin{pmatrix} \mathcal{W}^k \\ \mathcal{W}'^k \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \mathcal{W}^k_+ - \mathcal{W}'^{k*}_- \\ \mathcal{W}'^k_+ - \mathcal{W}^{k*}_- \end{pmatrix}$$

3. Use the non-hermitian Arnoldi method instead of the non-hermitian Lanczos method, that is, orthogonalize each new basis vector against all previous basis vectors and their opposite norm partners:

$$\begin{pmatrix} \tilde{\mathcal{X}}^{k+1} \\ \tilde{\mathcal{Y}}^{k+1} \end{pmatrix} = \begin{pmatrix} \mathcal{W}^k \\ \mathcal{W}'^k \end{pmatrix} - \sum_{p=1}^{k}\begin{pmatrix} \mathcal{X}^p \\ \mathcal{Y}^p \end{pmatrix} a_{pk} + \sum_{p=1}^{k}\begin{pmatrix} \mathcal{Y}^{p*} \\ \mathcal{X}^{p*} \end{pmatrix} b_{pk}$$

   where a_{pk} and b_{pk} are the overlap matrices.

4. For the positive norm of the residual vector $\tilde{N}^{k+1} = \langle \tilde{X}^{k+1}, \tilde{Y}^{k+1} | \tilde{X}^{k+1}, \tilde{Y}^{k+1} \rangle > 0$, define the new normalized positive-norm basis vector as

$$X^{k+1}_{mi} = \frac{1}{\sqrt{\tilde{N}^{k+1}}} \tilde{X}^{k+1}_{mi}, \quad Y^{k+1}_{mi} = \frac{1}{\sqrt{\tilde{N}^{k+1}}} \tilde{Y}^{k+1}_{mi} .$$

If $\tilde{N}^{k+1} < 0$, the new normalized positive norm basis vector is defined as

$$X^{k+1}_{mi} = \frac{1}{\sqrt{-\tilde{N}^{k+1}}} \tilde{Y}^{k+1*}_{mi}, \quad Y^{k+1}_{mi} = \frac{1}{\sqrt{-\tilde{N}^{k+1}}} \tilde{X}^{k+1*}_{mi} .$$

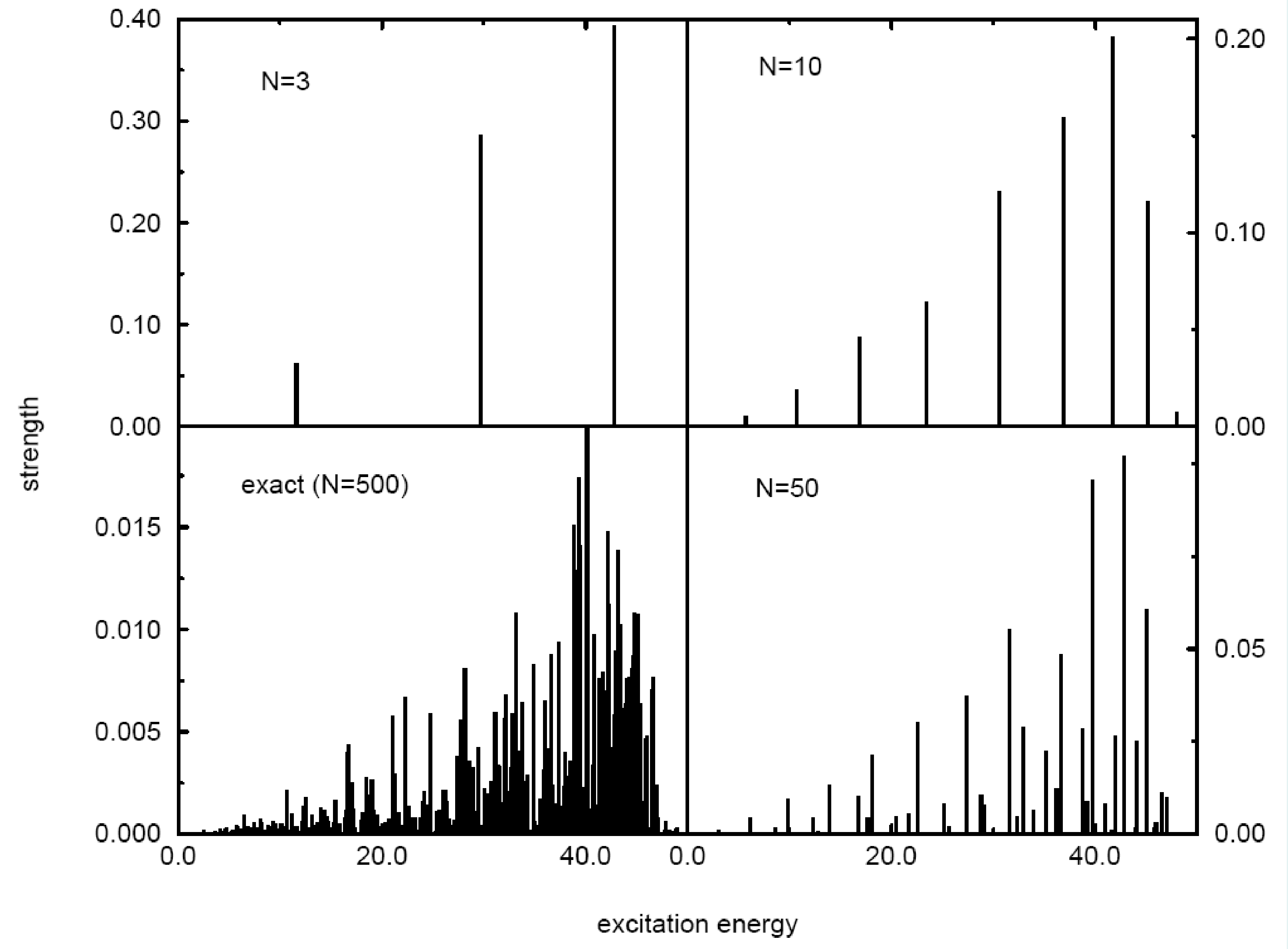
5. During the Arnoldi iteration orthogonalize the basis with respect to the position and momentum vectors:

$$\begin{pmatrix} \mathcal{X}_k \\ \mathcal{Y}_k \end{pmatrix}_{phys.} = \begin{pmatrix} \mathcal{X}_k \\ \mathcal{Y}_k \end{pmatrix} - \lambda \begin{pmatrix} \mathcal{P} \\ \mathcal{P}^* \end{pmatrix} - \mu \begin{pmatrix} \mathcal{R} \\ \mathcal{R}^* \end{pmatrix}$$

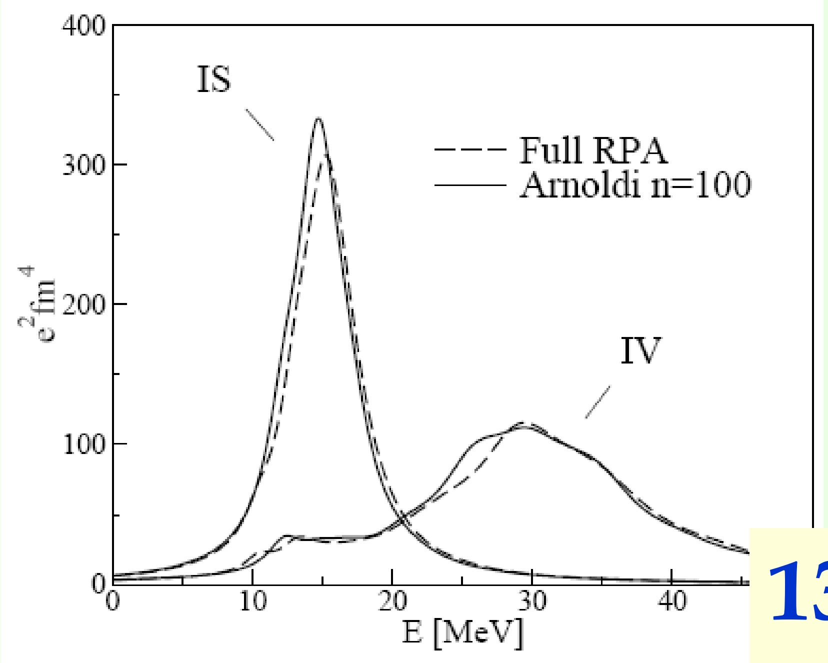
where the overlaps λ and μ are defined as

$$\lambda = \frac{\langle R, R^* | X^k, Y^k \rangle}{\langle R, R^* | P, P^* \rangle}, \quad \mu = -\frac{\langle P, P^* | X^k, Y^k \rangle}{\langle R, R^* | P, P^* \rangle} .$$

Figure taken from C. W. Johnson, G. F. Bertsch and W. D. Hazelton, Computer Physics Communications **120**, 155-161 (1999).



Fast RPA and QRPA + Arnoldi method



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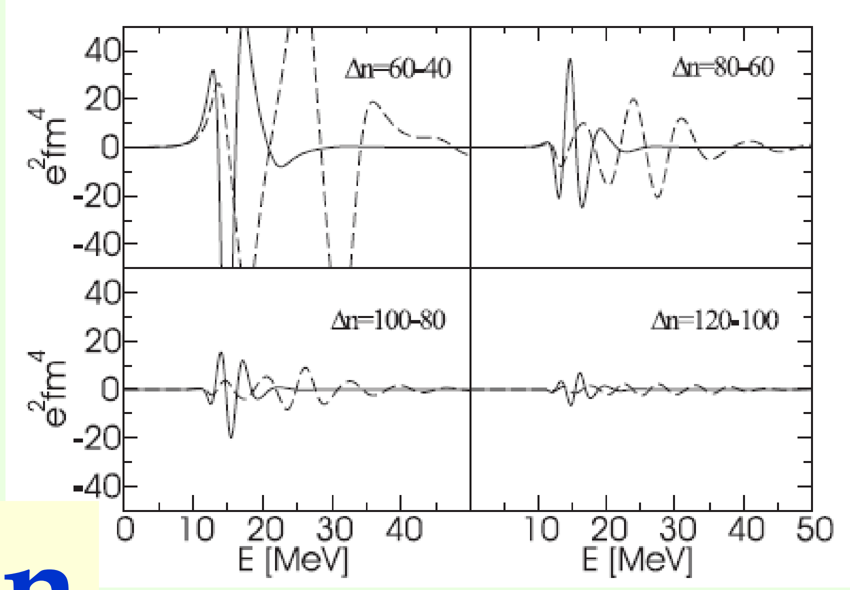
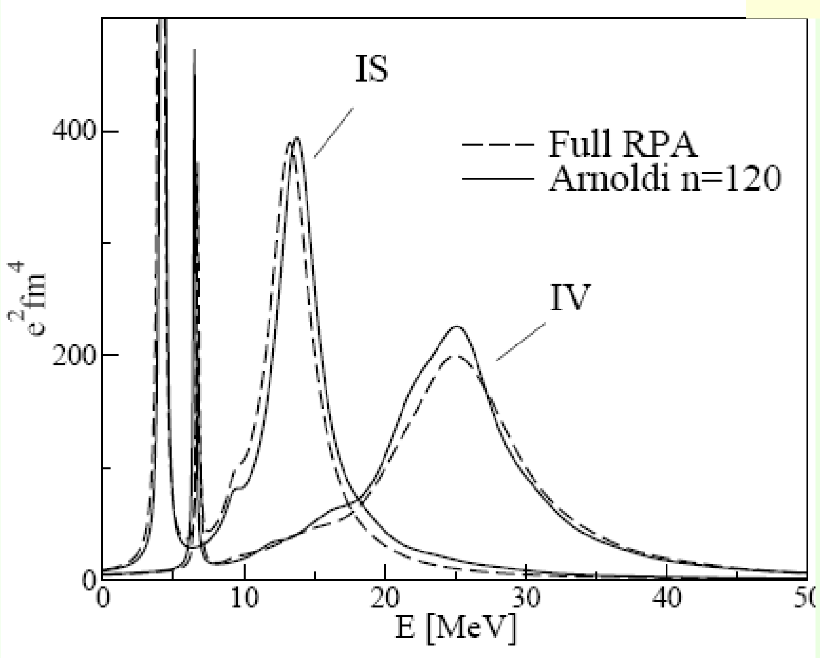


^{132}Sn



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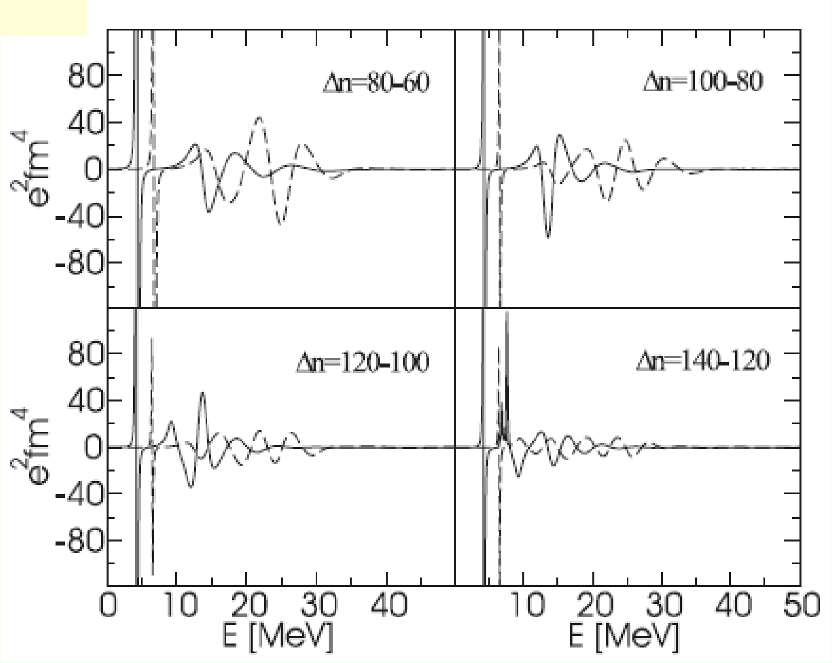
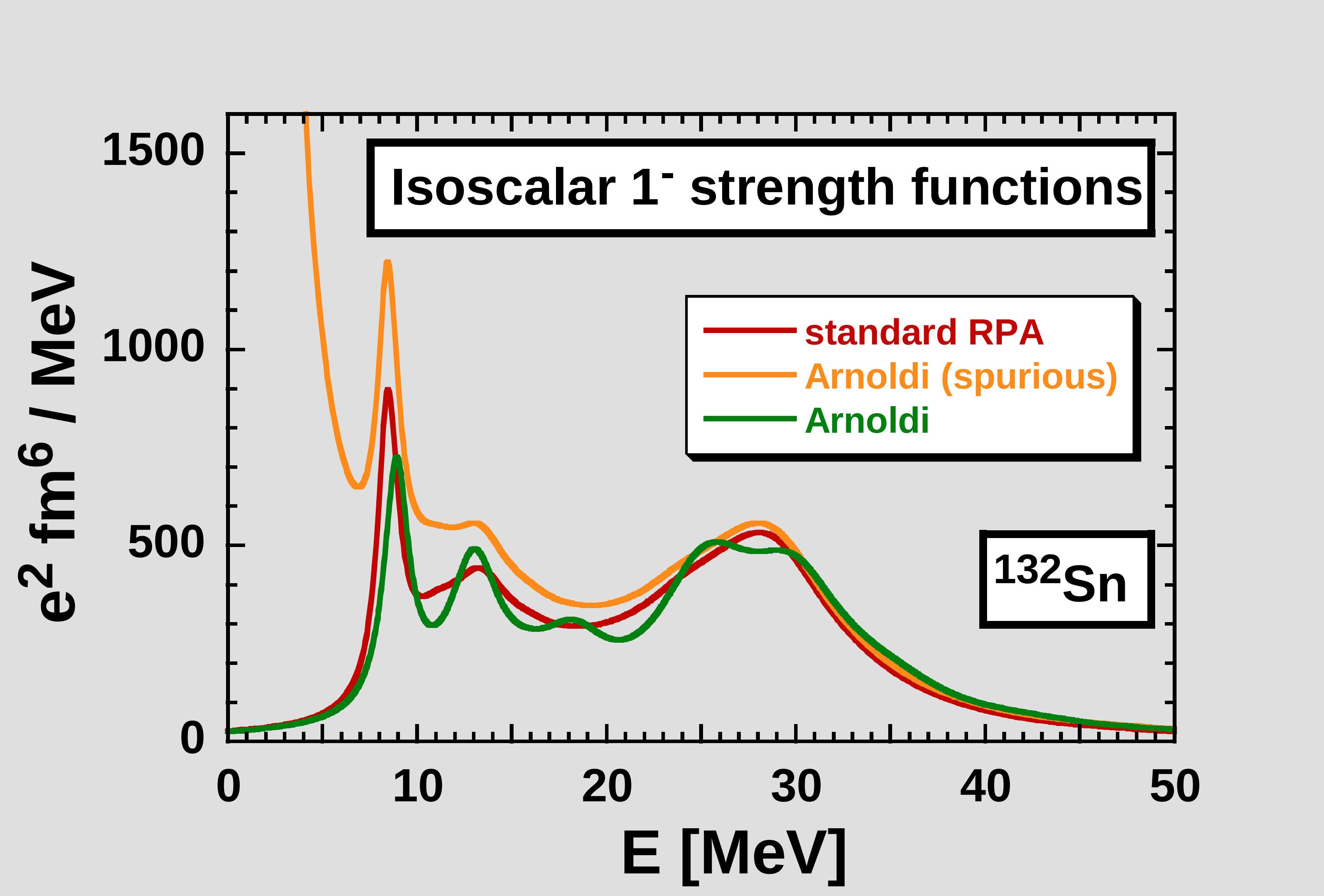


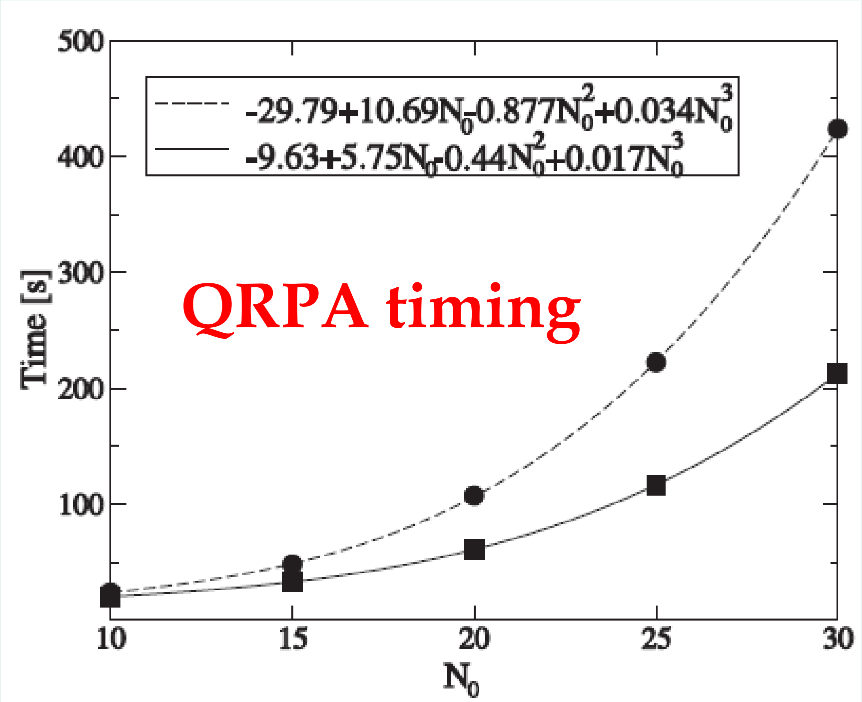
J. Toivanen *et al.*, Phys. Rev. C 81, 034312 (2010)

Removal of spurious modes



J. Toivanen *et al.*, Phys. Rev. C 81, 034312 (2010)

Scaling properties



☐ Spherical QRPA+Arnoldi scales linearly with the size of the single-particle space Ω.

☐ Deformed QRPA+Arnoldi expected to scale quadratically, that is, as Ω^2

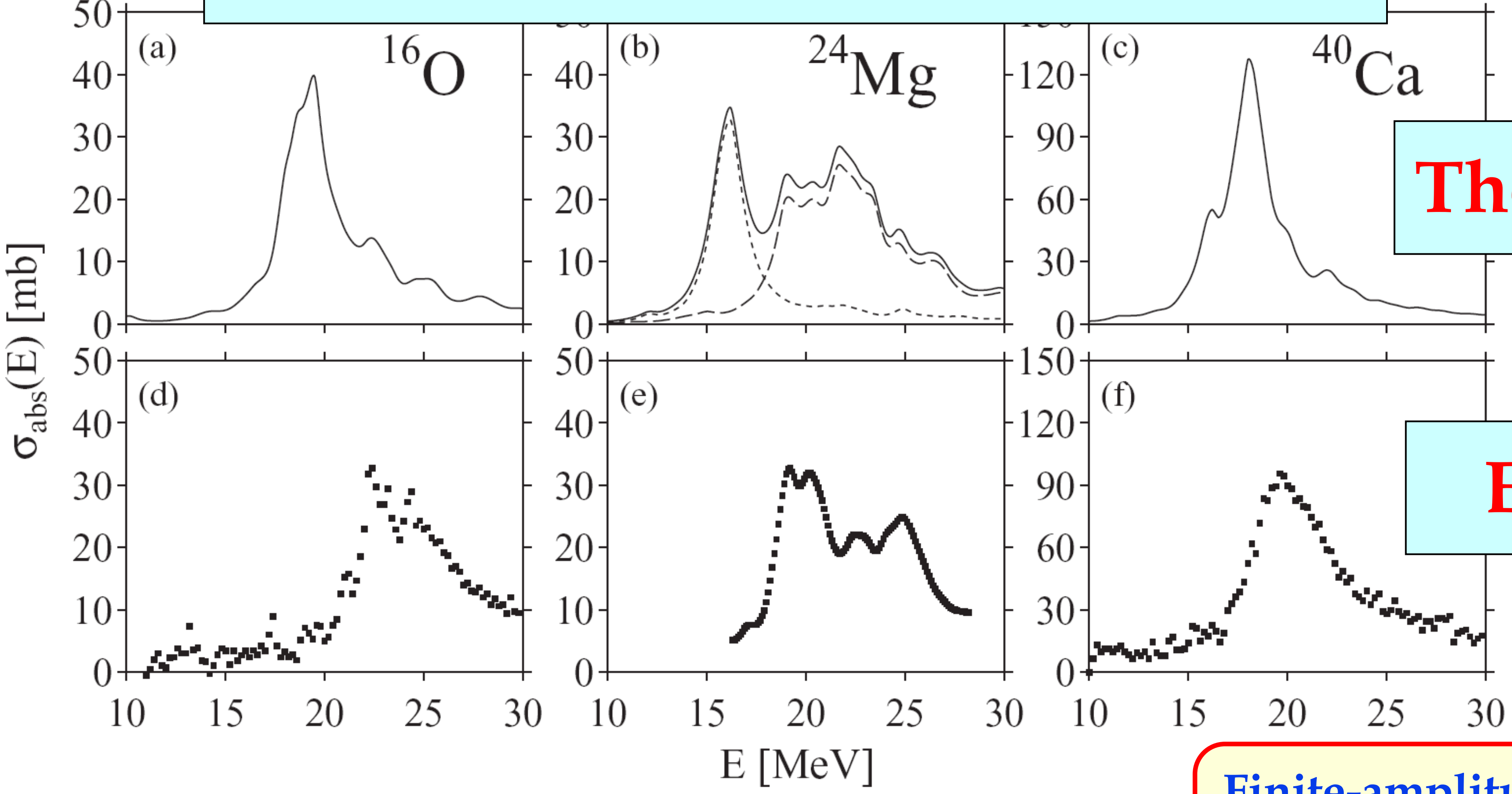
☐ Standard QRPA scales quartically, that is, as Ω^4 !

Future plans:

- Full implementation and testing of the spherical QRPA + Arnoldi method in the code HOSPHE with new-generation separable pairing interactions. Systematic calculations of multipole giant-resonance modes to be used in the EDF adjustments.
- Deformed QRPA + Arnoldi method implemented in the code HFODD. Systematic calculations of β-decay strengths functions and β-delayed neutron emission probabilities to be used in the EDF adjustments.

Iterative methods to solve (Q)RPA

Photoabsorption cross sections



Theory

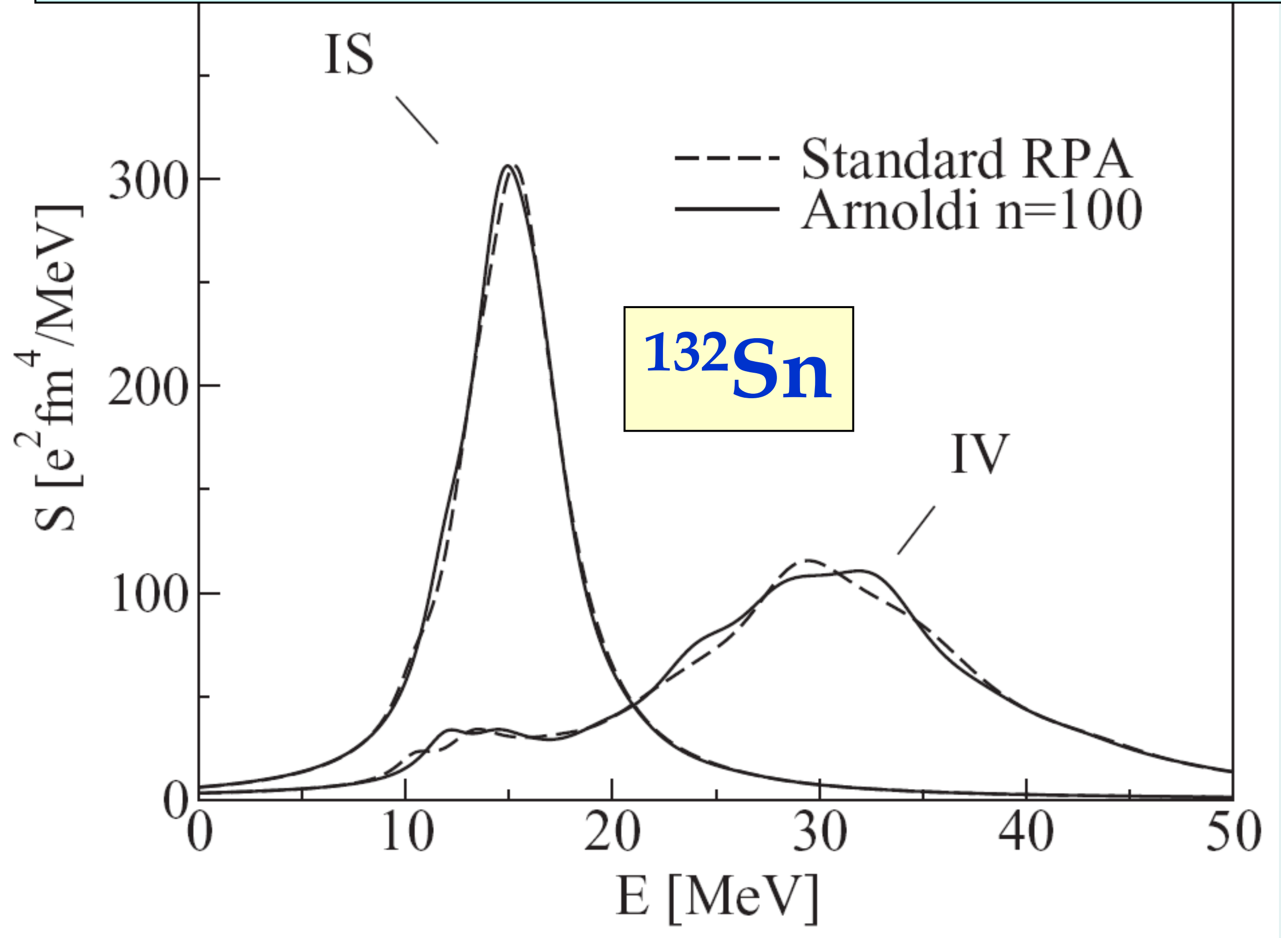
Exp

T. Inakura *et al.,* Phys. Rev. C80, 044301 (2009)

Finite-amplitude method to solve the QRPA equations.

Iterative methods to solve (Q)RPA

Monopole resonance

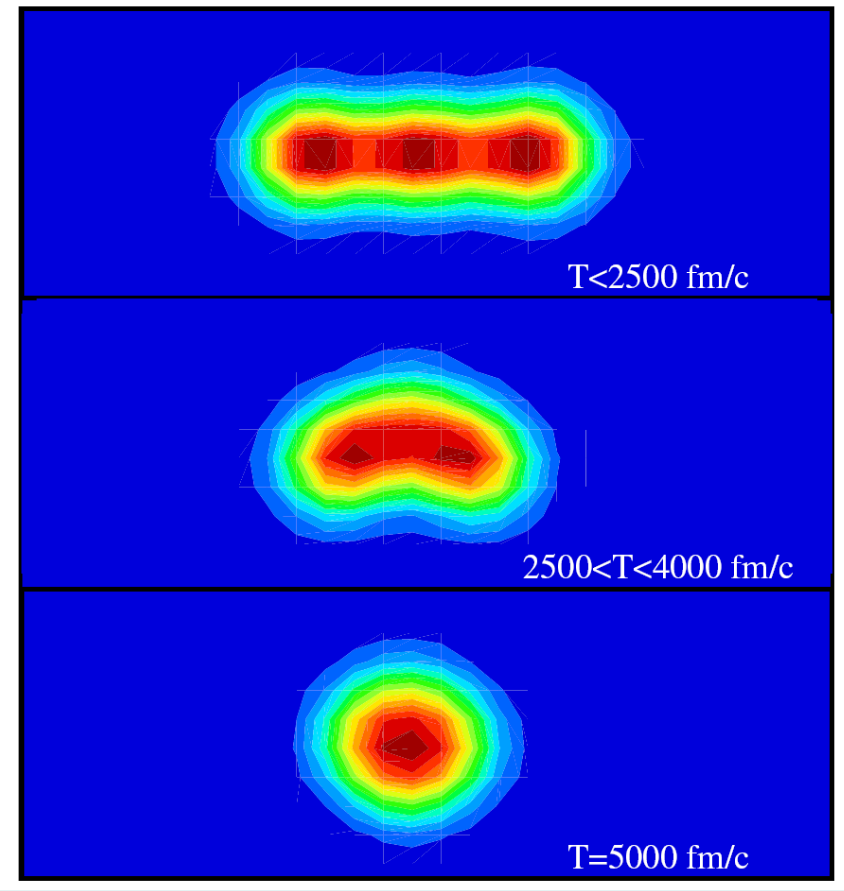


J. Toivanen *et al.*, Phys. Rev. C81, 034312 (2010)

Arnoldi method to solve the RPA equations.

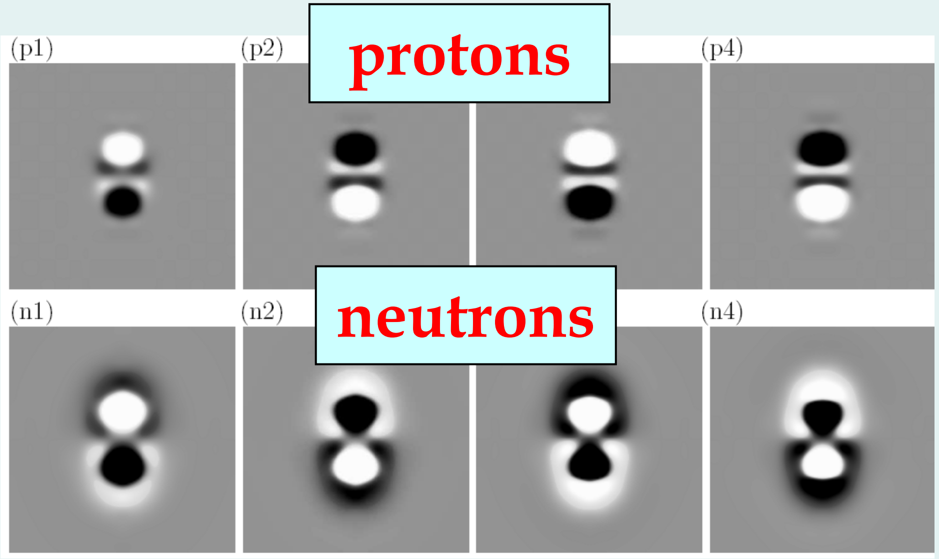
Time-dependent solutions

α– ^{8}Be collision (tip configuration)



A.S. Umar *et al.*, Phys. Rev. Lett. 104, 212503 (2010)

Dipole oscillations in ^{14}Be



T. Nakatsukasa *et al.*, Nucl. Phys. A788, 349 (2007)

UNEDF collaboration: Quantum Dynamics with TDSLDA, A. Bulgac, *et al.*, http://www.phys.washington.edu/groups/qmbnt/index.html

Nuclear Energy Density Functional

We consider the EDF in the form,

$$\mathcal{E} = \int d^3r \mathcal{H}(r),$$

where the energy density $\mathcal{H}(r)$ can be represented as a sum of the kinetic energy and of the potential-energy isoscalar ($t = 0$) and isovector ($t = 1$) terms,

$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(r) + \mathcal{H}_1(r),$$

which for the time-reversal and spherical symmetries imposed read:

$$\mathcal{H}_t(r) = C_t^\rho \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^{\Delta\rho} \rho_t \Delta \rho_t + \tfrac{1}{2} C_t^J J_t^2 + C_t^{\nabla J} \rho_t \nabla \cdot J_t.$$

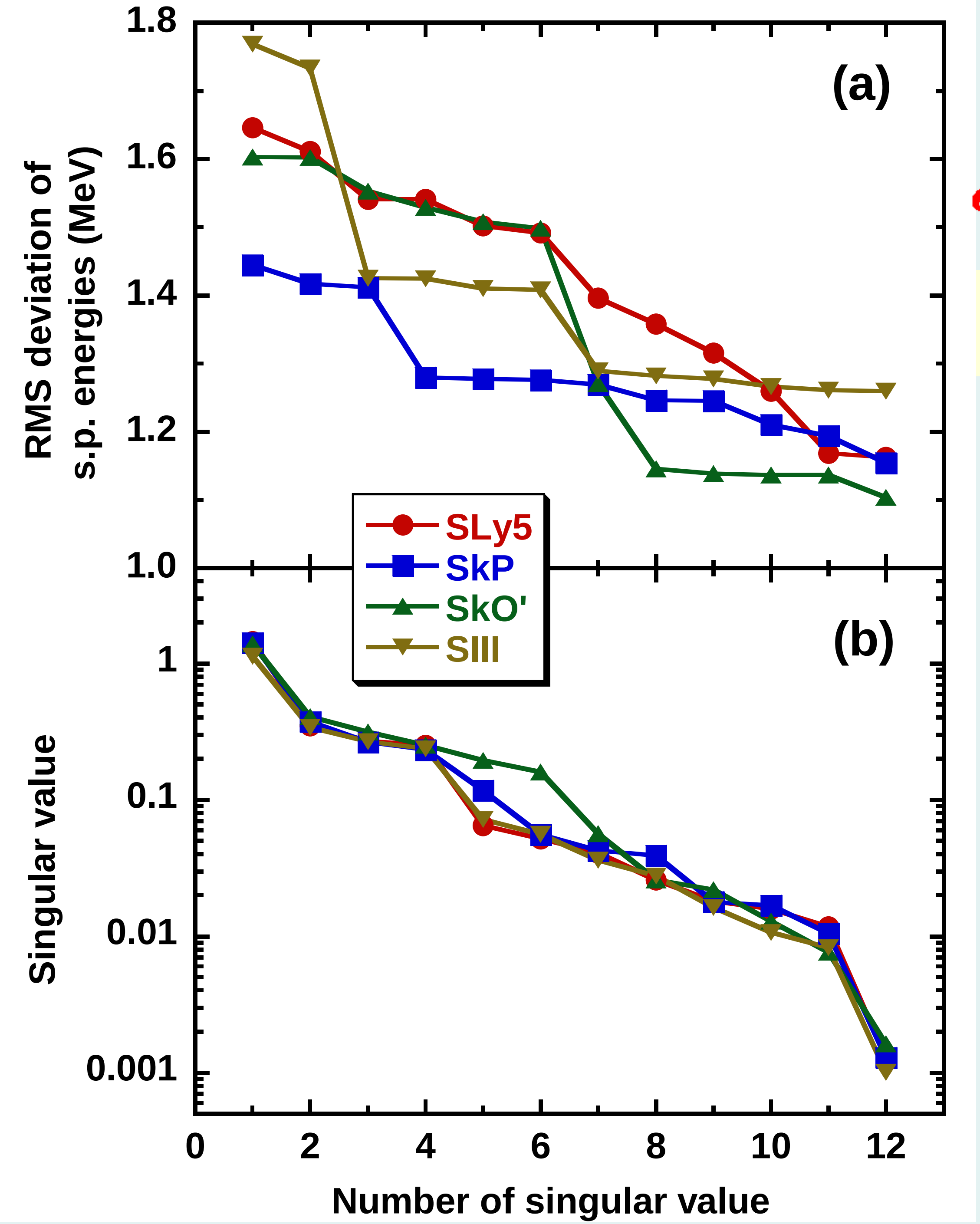
Following the parametrization used for the Skyrme forces, we assume the dependence of the coupling parameters C_t^ρ on the isoscalar density ρ_0 as:

$$C_t^\rho = C_{t0}^\rho + C_{t\mathrm{D}}^\rho \rho_0^\alpha.$$

The standard EDF depends linearly on 12 coupling constants,

$$C_{t0}^\rho, \quad C_{t\mathrm{D}}^\rho, \quad C_t^\tau, \quad C_t^{\Delta\rho}, \quad C_t^{\mathrm{J}}, \quad \text{and} \quad C_t^{\nabla \mathrm{J}},$$

for $t = 0$ and 1.



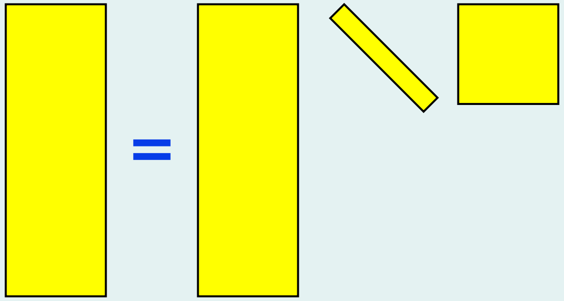
Fits of s.p. energies

$$\epsilon_i - \epsilon_i^{\mathrm{EXP}} = -\sum\nolimits_m \beta_{im}\Delta C_m,$$

EXP: M.N. Schwierz, I. Wiedenhover, and A. Volya, arXiv:0709.3525

Singular value decomposition

$$\beta_{im} = \sum\nolimits_\mu V_{i\mu} d_\mu U^T_{\mu m},$$

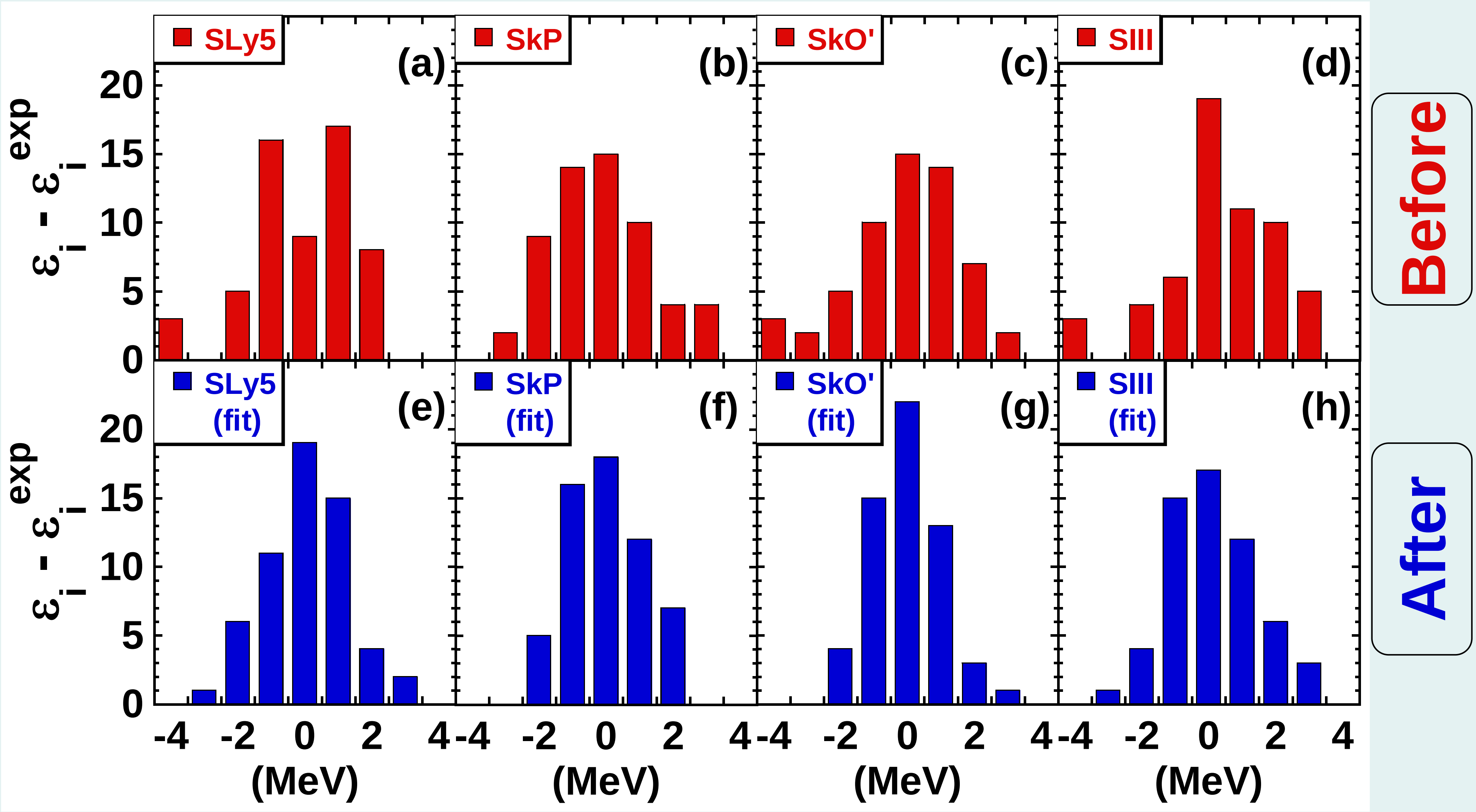


$$\sum\nolimits_i V_{i\mu} V_{i\nu} = \delta_{\mu\nu},$$

$$\sum\nolimits_m U_{m\mu} U_{m\nu} = \delta_{\mu\nu},$$

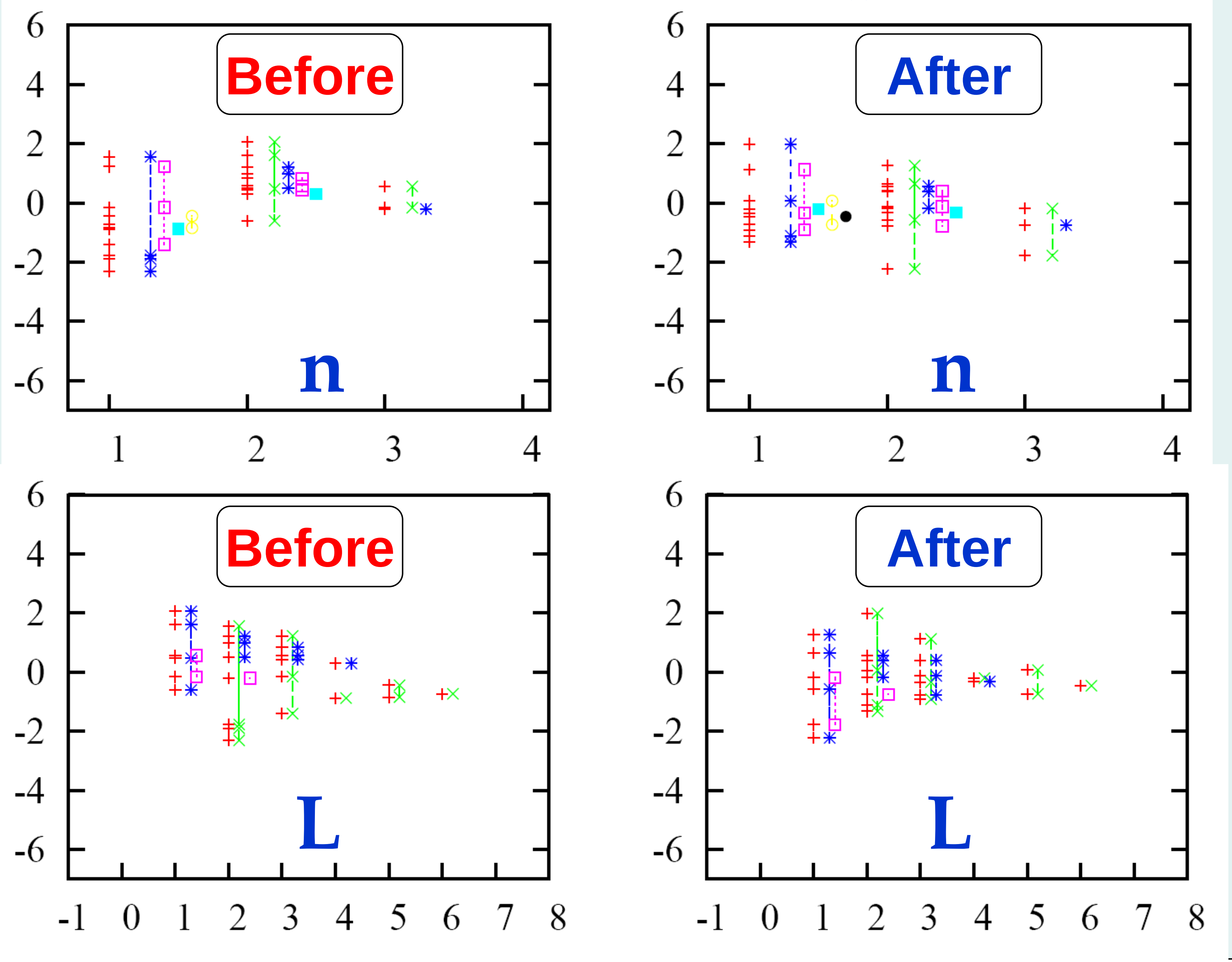
M. Kortelainen *et al.*, Phys. Rev. C77, 064307 (2008)

Fits of single-particle energies



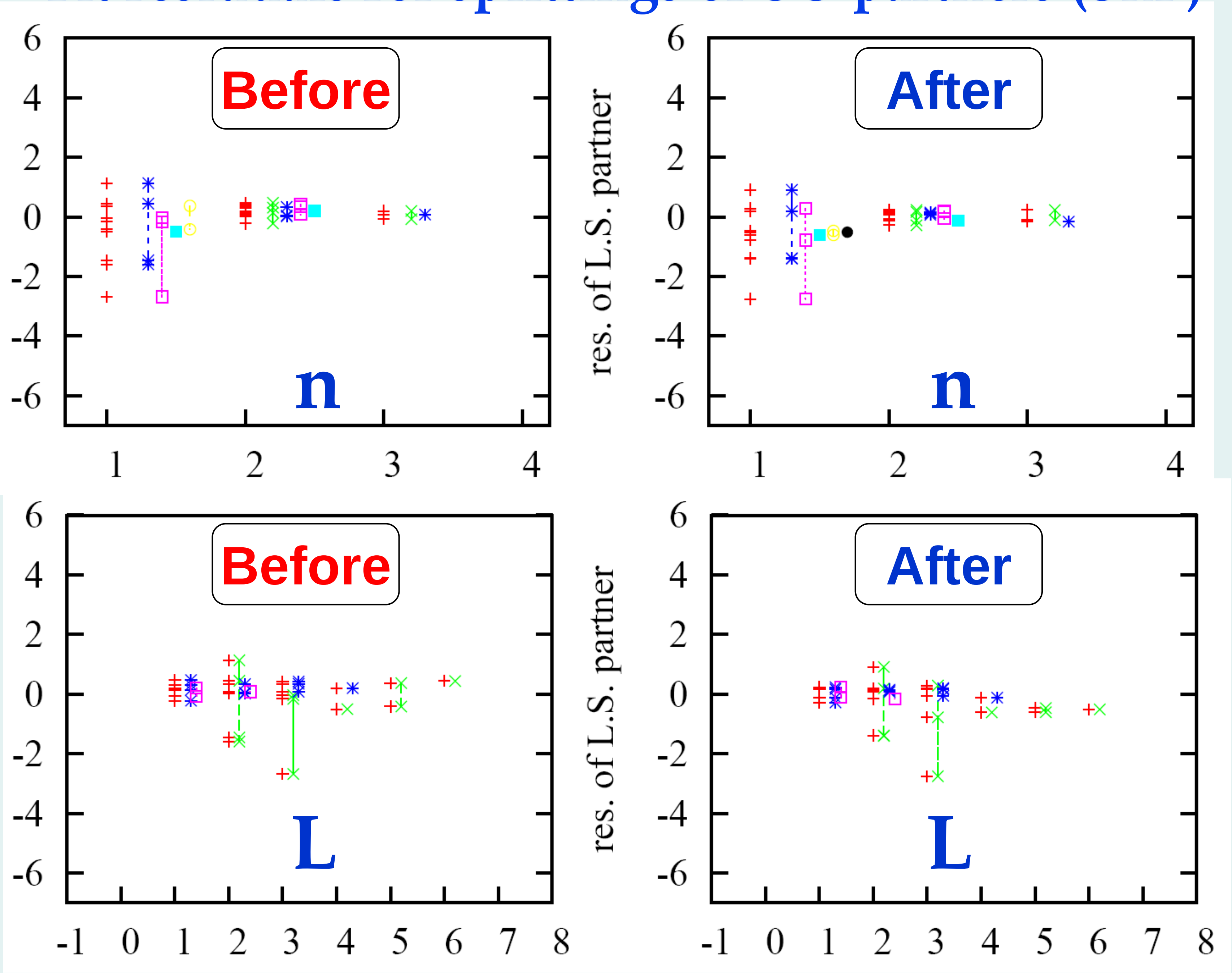
M. Kortelainen *et al.*, Phys. Rev. C77, 064307 (2008)

Fit residuals for centroids of SO partners (SkP)



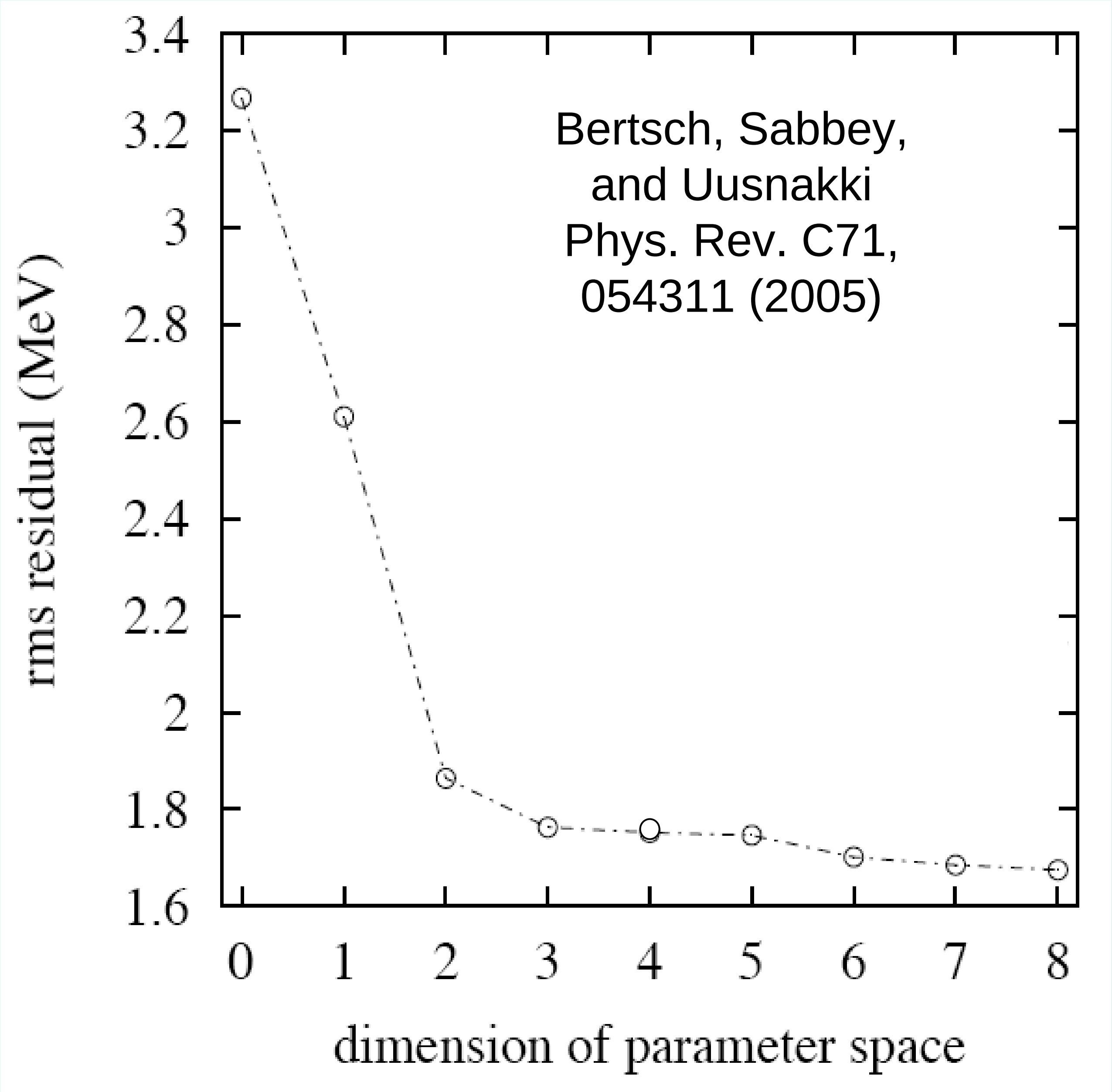
M. Kortelainen *et al.*, to be published

Fit residuals for splittings of SO partners (SkP)



M. Kortelainen *et al.*, to be published

How many parameters are really needed?



Global (masses)

SciDAC 2 UNEDF Project (USA)

http://www.unedf.org/

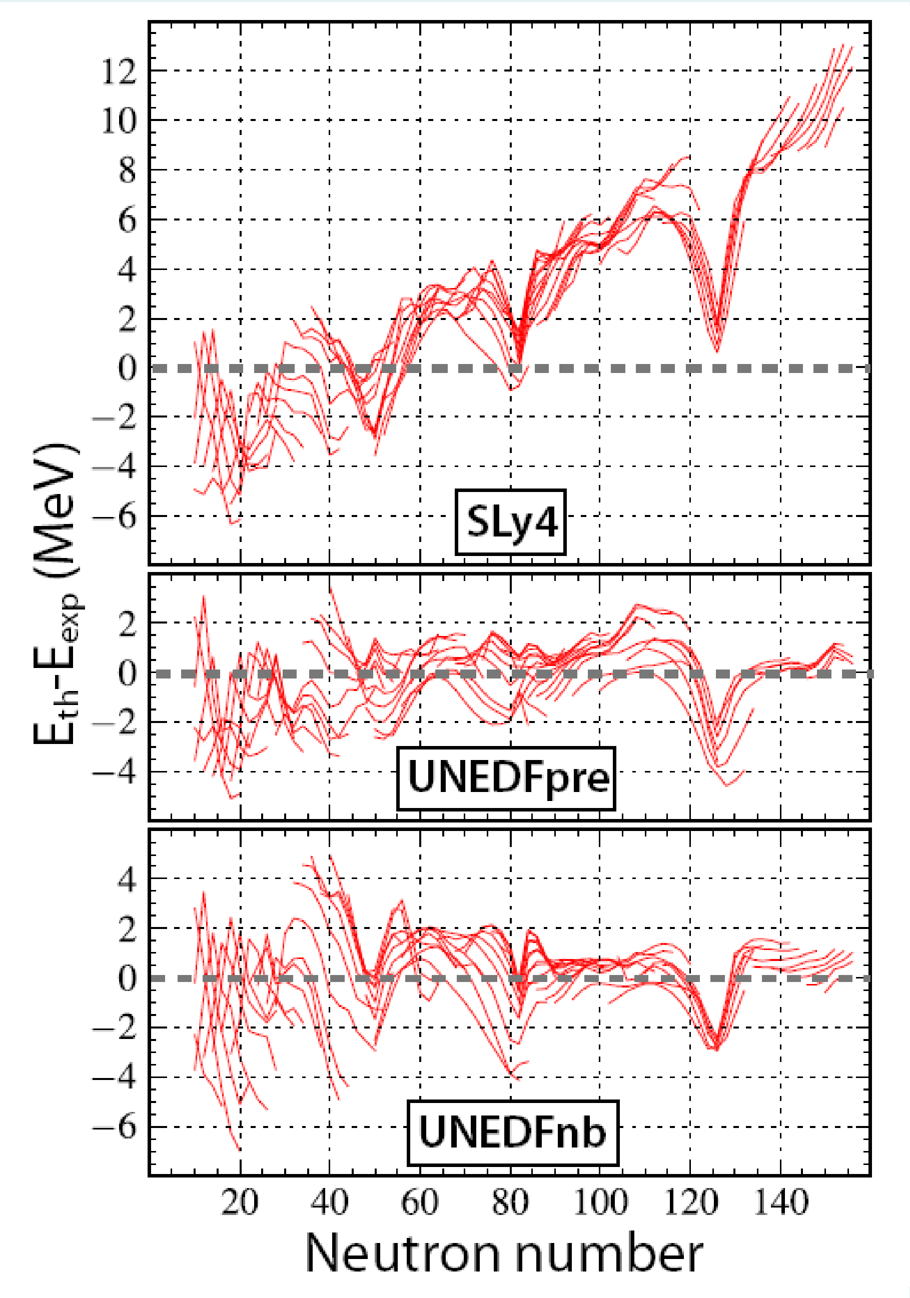
Building a Universal Nuclear Energy Density Functional

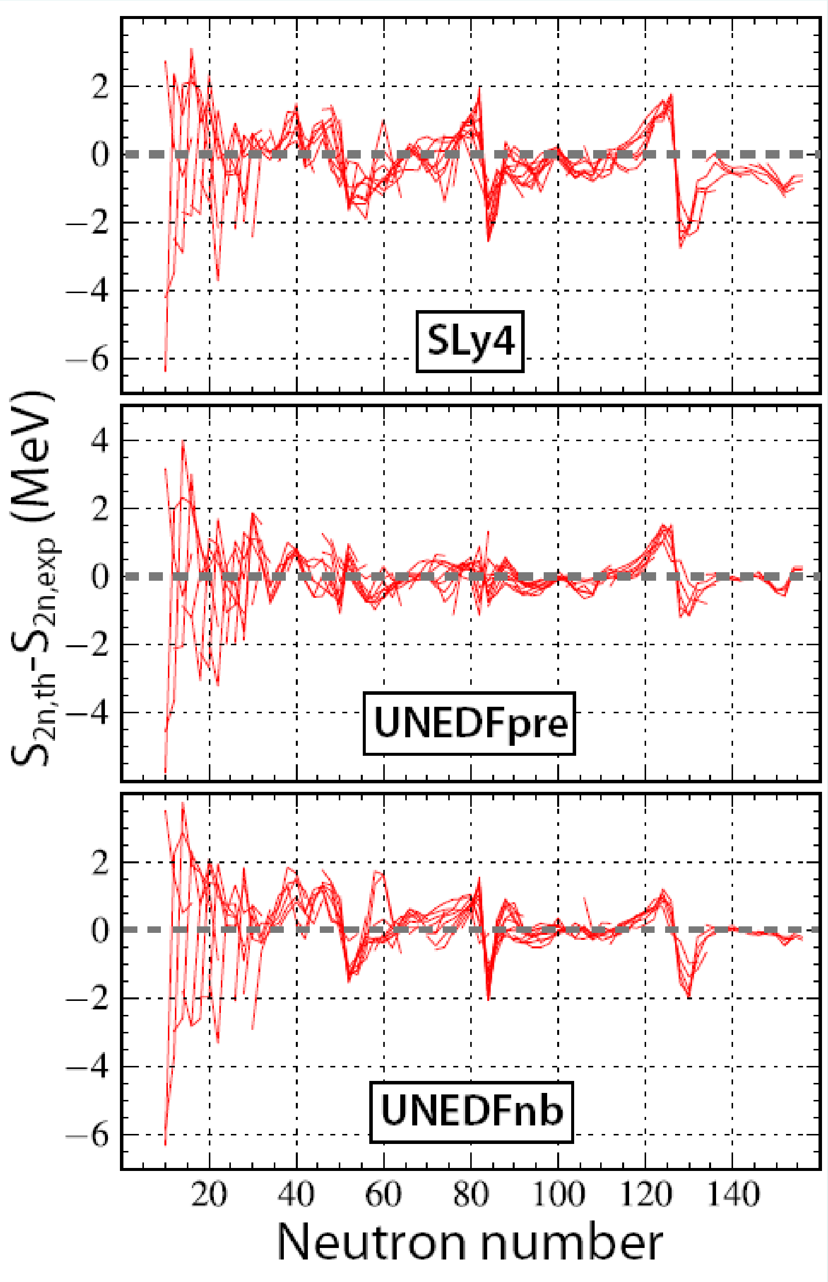
- Understand nuclear properties “for element formation, for properties of stars, and for present and future energy and defense applications”
- Scope is all nuclei, with particular interest in reliable calculations of unstable nuclei and in reactions
- Order of magnitude improvement over present capabilities
  - ➢ Precision calculations
- Connected to the best microscopic physics
- Maximum predictive power with well-quantified uncertainties

FIDIPRO Project (Finland)

http://www.jyu.fi/accelerator/fidipro/

UNEDF Skyrme Functionals





M. Kortelainen, *et al.*, arXiv:1005.5145

UNEDF Skyrme Functionals

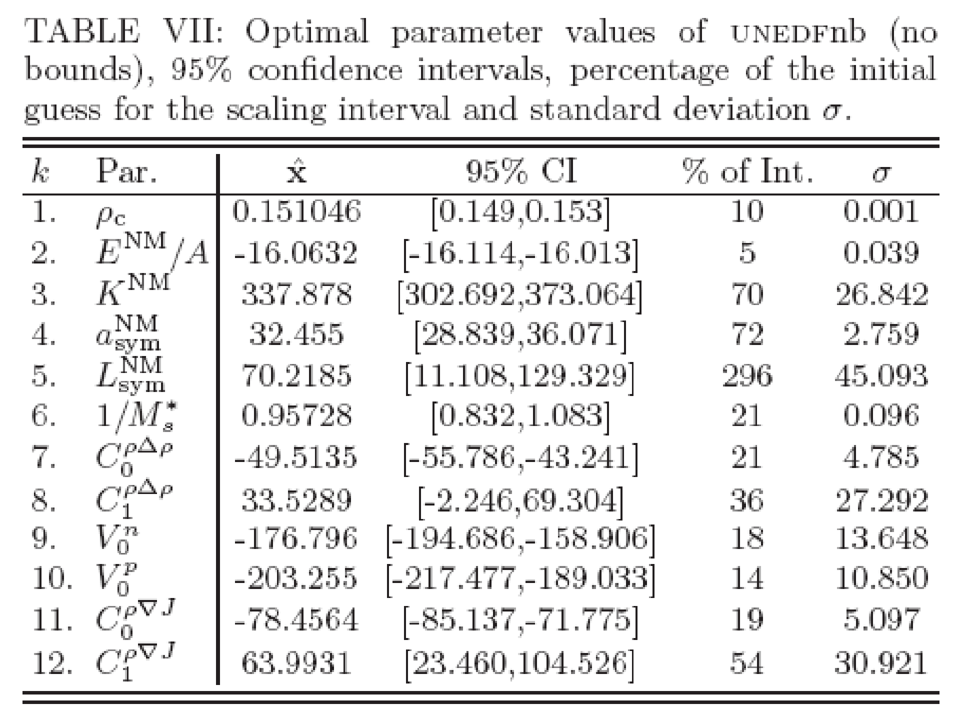
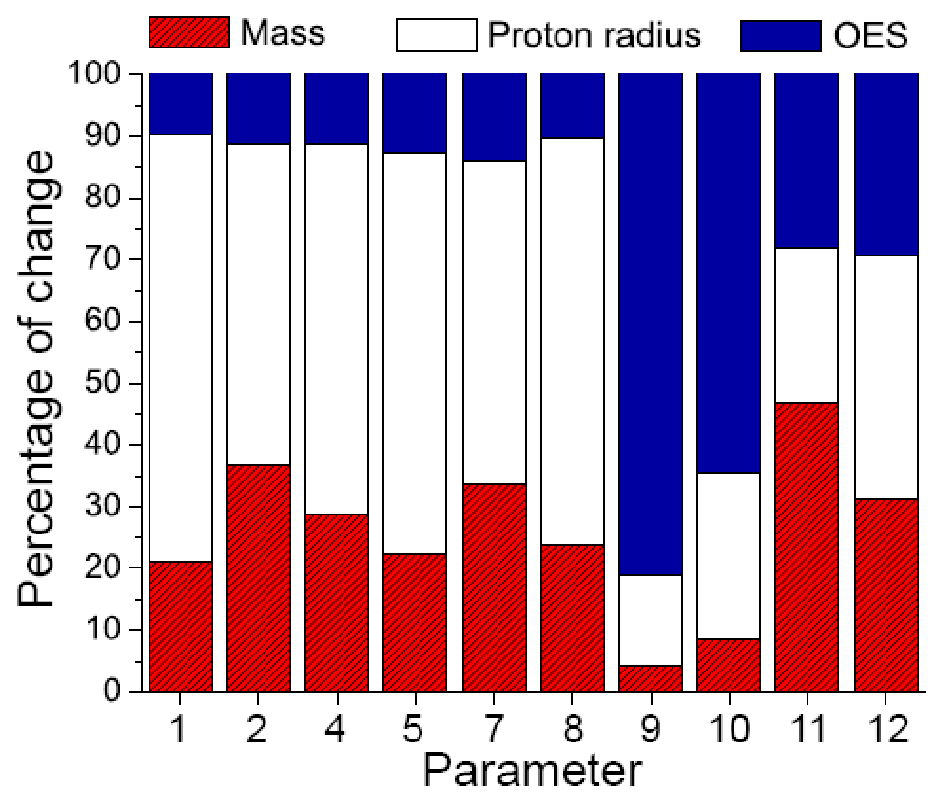


TABLE VII: Optimal parameter values of UNEDFnb (no bounds), 95% confidence intervals, percentage of the initial guess for the scaling interval and standard deviation σ.

k	Par.	$\hat{x}$	95% CI	% of Int.	σ
1.	ρ_c	0.151046	[0.149,0.153]	10	0.001
2.	E^{NM}/A	-16.0632	[-16.114,-16.013]	5	0.039
3.	K^{NM}	337.878	[302.692,373.064]	70	26.842
4.	a_{sym}^{NM}	32.455	[28.839,36.071]	72	2.759
5.	L_{sym}^{NM}	70.2185	[11.108,129.329]	296	45.093
6.	$1/M_s^*$	0.95728	[0.832,1.083]	21	0.096
7.	$C_0^{\rho\Delta\rho}$	-49.5135	[-55.786,-43.241]	21	4.785
8.	$C_1^{\rho\Delta\rho}$	33.5289	[-2.246,69.304]	36	27.292
9.	V_0^n	-176.796	[-194.686,-158.906]	18	13.648
10.	V_0^p	-203.255	[-217.477,-189.033]	14	10.850
11.	$C_0^{\rho\nabla J}$	-78.4564	[-85.137,-71.775]	19	5.097
12.	$C_1^{\rho\nabla J}$	63.9931	[23.460,104.526]	54	30.921



M. Kortelainen, *et al.*, arXiv:1005.5145

New functionals

Nuclear Energy Density Functional

We consider the EDF in the form,

$$\mathcal{E} = \int d^3r \mathcal{H}(r),$$

where the energy density $\mathcal{H}(r)$ can be represented as a sum of the kinetic energy and of the potential-energy isoscalar ($t = 0$) and isovector ($t = 1$) terms,

$$\mathcal{H}(r) = \frac{\hbar^2}{2m}\tau_0 + \mathcal{H}_0(r) + \mathcal{H}_1(r),$$

which for the time-reversal and spherical symmetries imposed read:

$$\mathcal{H}_t(r) = C_t^\rho \rho_t^2 + C_t^\tau \rho_t \tau_t + C_t^{\Delta\rho} \rho_t \Delta \rho_t + \tfrac{1}{2} C_t^J J_t^2 + C_t^{\nabla J} \rho_t \nabla \cdot J_t.$$

Following the parametrization used for the Skyrme forces, we assume the dependence of the coupling parameters C_t^ρ on the isoscalar density ρ_0 as:

$$C_t^\rho = C_{t0}^\rho + C_{t\mathrm{D}}^\rho \rho_0^\alpha.$$

The standard EDF depends linearly on 12 coupling constants,

$$C_{t0}^\rho,\quad C_{t\mathrm{D}}^\rho,\quad C_t^\tau,\quad C_t^{\Delta\rho},\quad C_t^{\mathrm{J}},\quad \text{and}\quad C_t^{\nabla\mathrm{J}},$$

for $t = 0$ and 1.

Derivatives of higher order: Negele & Vautherin density matrix expansion

Nr	Tensor	order n	rank L
1	1	0	0
2	∇	1	1
3	Δ	2	0
4	$[\nabla\nabla]_2$	2	2
5	$\Delta\nabla$	3	1
6	$[\nabla[\nabla\nabla]_2]_3$	3	3
7	Δ^2	4	0
8	$\Delta[\nabla\nabla]_2$	4	2
9	$[\nabla[\nabla[\nabla\nabla]_2]_3]_4$	4	4
10	$\Delta^2\nabla$	5	1
11	$\Delta[\nabla[\nabla\nabla]_2]_3$	5	3
12	$[\nabla[\nabla[\nabla[\nabla\nabla]_2]_3]_4]_5$	5	5
13	Δ^3	6	0
14	$\Delta^2[\nabla\nabla]_2$	6	2
15	$\Delta[\nabla[\nabla[\nabla\nabla]_2]_3]_4$	6	4
16	$[\nabla[\nabla[\nabla[\nabla[\nabla\nabla]_2]_3]_4]_5]_6$	6	6

Total derivatives $(\vec{\nabla}^m)_I$ up to N^{3}LO

Nr	Tensor	order n	rank L
1	1	0	0
2	k	1	1
3	k^2	2	0
4	$[kk]_2$	2	2
5	k^2k	3	1
6	$[k[kk]_2]_3$	3	3
7	$(k^2)^2$	4	0
8	$k^2[kk]_2$	4	2
9	$[k[k[kk]_2]_3]_4$	4	4
10	$(k^2)^2k$	5	1
11	$k^2[k[kk]_2]_3$	5	3
12	$[k[k[k[kk]_2]_3]_4]_5$	5	5
13	$(k^2)^3$	6	0
14	$(k^2)^2[kk]_2$	6	2
15	$k^2[k[k[kk]_2]_3]_4$	6	4
16	$[k[k[k[k[kk]_2]_3]_4]_5]_6$	6	6

Relative derivatives $(\vec{k}^n)_L$ up to N^{3}LO

$$\nabla = \nabla_1 + \nabla_2, \qquad k = \frac{1}{2i}\left(\nabla_1 - \nabla_2\right),$$

$$\rho_{v=0} = \rho(r_1, r_2), \qquad \rho_{v=1} = \vec{s}(r_1, r_2),$$

$$\rho_{nLvJ} = \left((\vec{k}^n)_L \rho_v\right)_J \text{ (primary)}, \; \rho_{mInLvJQ} = \left((\vec{\nabla}^m)_I \left((\vec{k}^n)_L \rho_v\right)_J\right)_Q \text{ (secondary)}$$

B.G. Carlsson *et al.*, Phys. Rev. C 78, 044326 (2008)

Energy density functional up to N^{3}LO

order	from ρ	from $\vec{s}$	T-even	T-odd	total
0	1	1	1	1	2
1	1	3	3	1	4
2	2	4	2	4	6
3	2	6	6	2	8
4	2	5	2	5	7
5	1	4	4	1	5
6	1	2	1	2	3
total	10	25	19	16	35

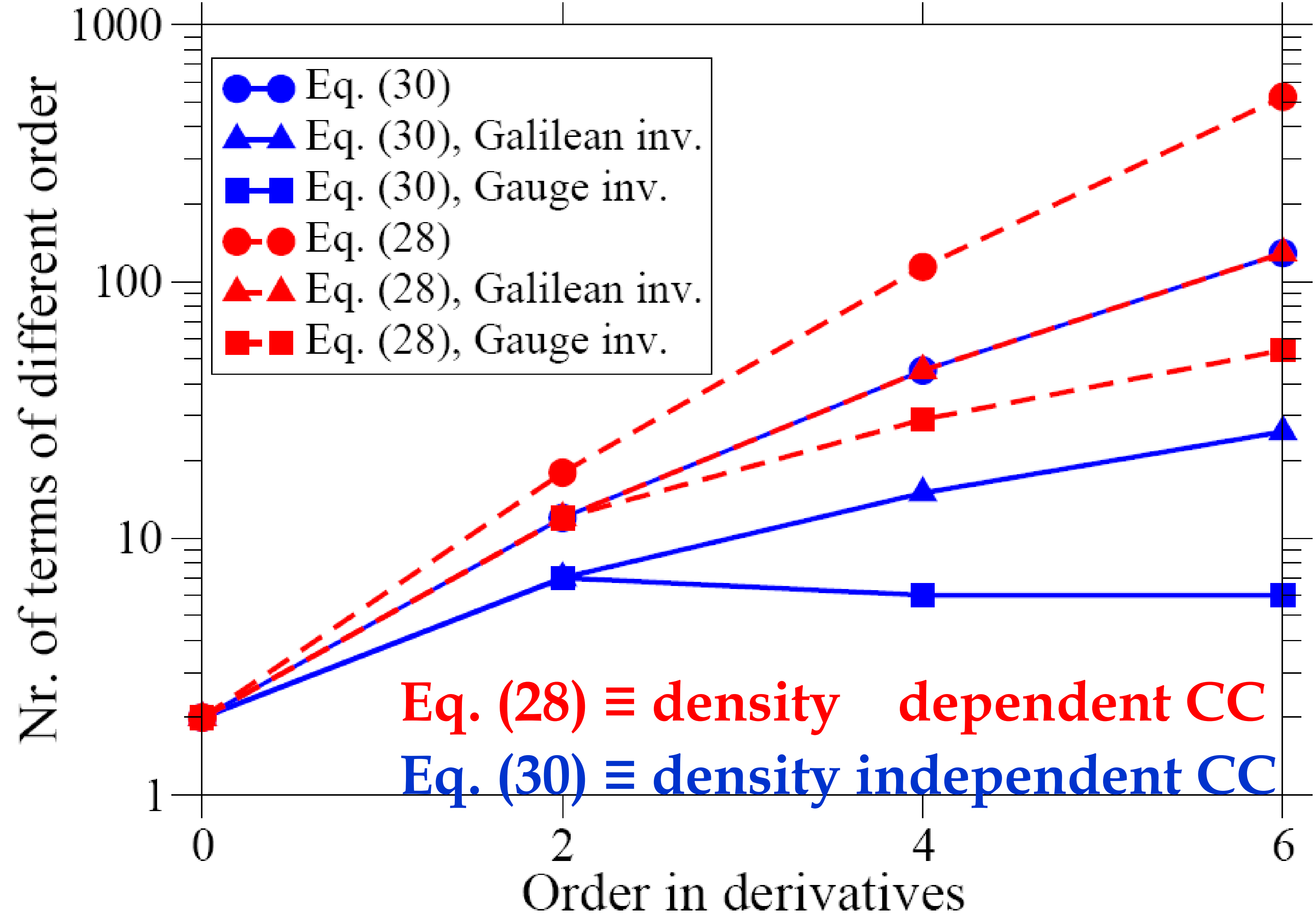
Numbers of primary ($m = 0$) local-densities up to N^{3}LO.

order	T-even	T-odd	total	Galilean invariant	Gauge invariant
0	1	1	2	2	2
2	6	6	12	7	7
4	22	23	45	15	6
6	64	65	129	26	6
N^{3}LO	93	95	188	50	21

Numbers of terms in the EDF up to N^{3}LO.

B.G. Carlsson *et al.*, Phys. Rev. C 78, 044326 (2008)

Numbers of terms in the density functional up to N^3LO



Eq. (28) ≡ density dependent CC

Eq. (30) ≡ density independent CC

B.G. Carlsson *et al.*, Phys. Rev. C 78, 044326 (2008)

Energy density functional for spherical nuclei (I)

B.G. Carlsson *et al.*, Phys. Rev. C 78, 044326 (2008)
Phys. Rev. C 81, 029904(E) (2010)

For conserved spherical, space-inversion, and time-reversal symmetries, all non-zero densities can be defined as:

$$\begin{aligned}
R_0 &= \rho, \\
R_2 &= \vec{k}^2\rho = \tau - \tfrac{1}{4}\Delta\rho, \\
\overleftrightarrow{R}_{2ab} &= \vec{k}_a\vec{k}_b\rho, \\
R_4 &= \vec{k}^4\rho, \\
\overleftrightarrow{R}_{4ab} &= \vec{k}^2\vec{k}_a\vec{k}_b\rho, \\
R_6 &= \vec{k}^6\rho,
\end{aligned}$$

and

$$\begin{aligned}
\vec{J}_{1a} &= (\vec{k}\times\vec{s})_a, \\
\vec{J}_{3a} &= \vec{k}^2(\vec{k}\times\vec{s})_a, \\
\overleftrightarrow{J}_{3abc} &= \vec{k}_a\vec{k}_b(\vec{k}\times\vec{s})_c + \vec{k}_b\vec{k}_c(\vec{k}\times\vec{s})_a \\
&+ \vec{k}_c\vec{k}_a(\vec{k}\times\vec{s})_b, \\
\vec{J}_{5a} &= \vec{k}^4(\vec{k}\times\vec{s})_a,
\end{aligned}$$

where $\vec{k}^2 = \sum_a \vec{k}_a\vec{k}_a$ and the Cartesian indices are defined as $a, b, c = x, y, z$. To lighten the notation, in these definitions we have omitted the arguments of local densities, $\vec{r}$, and limits of $\vec{r}\,' = \vec{r}$.

Numbers of terms of different orders in the EDF up to N^{3}LO, evaluated for the conserved spherical, space-inversion, and time-reversal symmetries. The last two columns give numbers of terms when the Galilean or gauge invariance is assumed, respectively.

order	Total	Galilean	Gauge
0	1	1	1
2	4	4	4
4	12	9	3
6	28	16	3
N^{3}LO	45	30	11

Energy density functional for spherical nuclei (II)

We can write the N^{3}LO spherical energy density as a sum of contributions from zero, second, fourth, and sixth orders:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_2 + \mathcal{H}_4 + \mathcal{H}_6,$$

where

$$\mathcal{H}_0 = C^0_{00} R_0 R_0,$$

$$\begin{aligned}\mathcal{H}_2 &= C^0_{20} R_0 \Delta R_0 + C^0_{02} R_0 R_2 \\ &+ C^0_{11} R_0 \vec{\nabla} \cdot \vec{J}_1, + C^1_{01} \vec{J}_1^2,\end{aligned}$$

Energy densities $\mathcal{H}_0$ and $\mathcal{H}_2$ correspond, of course, to the standard Skyrme functional with $C^0_{00} = C^\rho$, $C^0_{20} = C^{\Delta\rho} + \frac{1}{4} C^\tau$, $C^0_{02} = C^\tau$, $C^0_{11} = C^{\nabla J}$, and $C^1_{01} = C^{J1}$. At fourth order, the energy density reads

$$\begin{aligned}\mathcal{H}_4 &= C^0_{40} R_0 \Delta^2 R_0 + C^0_{22} R_0 \Delta R_2 \\ &+ C^0_{04} R_0 R_4 + C^2_{02} R_2 R_2 \\ &+ D^0_{22} R_0 \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + D^2_{02} \sum_{ab} \overleftrightarrow{R}_{2ab} \overleftrightarrow{R}_{2ab} \\ &+ C^1_{21} \vec{J}_1 \cdot \Delta \vec{J}_1 + C^1_{03} \vec{J}_1 \cdot \vec{J}_3 \\ &+ C^0_{31} R_0 \Delta \left(\vec{\nabla} \cdot \vec{J}_1 \right) + C^0_{13} R_0 \left(\vec{\nabla} \cdot \vec{J}_3 \right) \\ &+ C^2_{11} R_2 \left(\vec{\nabla} \cdot \vec{J}_1 \right) + D^2_{11} \sum_{ab} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{J}_{1b},\end{aligned}$$

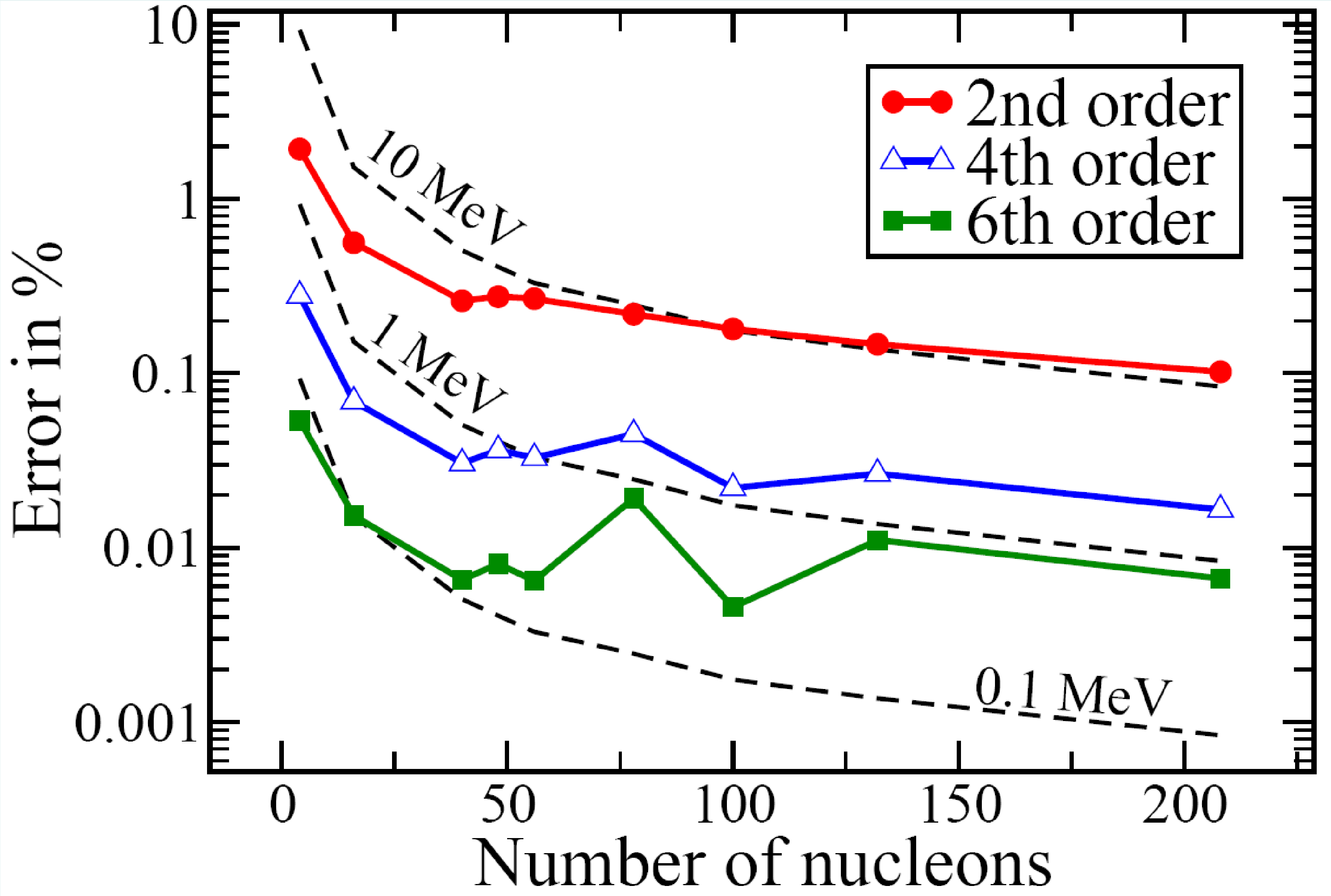
At sixth order, the energy density reads

$$\begin{aligned}\mathcal{H}_6 &= C^0_{60} R_0 \Delta^3 R_0 + C^0_{42} R_0 \Delta^2 R_2 \\ &+ C^0_{24} R_0 \Delta R_4 + C^0_{06} R_0 R_6 \\ &+ C^2_{22} R_2 \Delta R_2 + C^2_{04} R_2 R_4 \\ &+ D^0_{42} R_0 \Delta \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + D^0_{24} R_0 \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{4ab} \\ &+ D^2_{22} R_2 \sum_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + E^2_{22} \sum_{ab} \overleftrightarrow{R}_{2ab} \Delta \overleftrightarrow{R}_{2ab} \\ &+ E^2_{04} \sum_{ab} \overleftrightarrow{R}_{2ab} \overleftrightarrow{R}_{4ab} + C^1_{41} \vec{J}_1 \cdot \Delta^2 \vec{J}_1 + C^1_{23} \vec{J}_1 \cdot \Delta \vec{J}_3 \\ &+ C^1_{05} \vec{J}_1 \cdot \vec{J}_5 + C^3_{03} \vec{J}_3 \cdot \vec{J}_3 \\ &+ E^1_{23} \sum_{abc} \vec{J}_{1a} \vec{\nabla}_b \vec{\nabla}_c \overleftrightarrow{J}_{3abc} + D^3_{03} \sum_{abc} \overleftrightarrow{J}_{3abc} \overleftrightarrow{J}_{3abc} \\ &+ C^0_{51} R_0 \Delta^2 \left(\vec{\nabla} \cdot \vec{J}_1 \right) + C^0_{33} R_0 \Delta \left(\vec{\nabla} \cdot \vec{J}_3 \right) \\ &+ C^0_{15} R_0 \left(\vec{\nabla} \cdot \vec{J}_5 \right) + C^2_{31} R_2 \Delta \left(\vec{\nabla} \cdot \vec{J}_1 \right) \\ &+ C^2_{13} R_2 \left(\vec{\nabla} \cdot \vec{J}_3 \right) + C^4_{11} R_4 \left(\vec{\nabla} \cdot \vec{J}_1 \right) \\ &+ D^0_{33} R_0 \sum_{abc} \vec{\nabla}_a \vec{\nabla}_b \vec{\nabla}_c \overleftrightarrow{J}_{3abc} + D^2_{13} \sum_{abc} \overleftrightarrow{R}_{2ab} \vec{\nabla}_c \overleftrightarrow{J}_{3abc} \\ &+ D^2_{31} \sum_{ab} \overleftrightarrow{R}_{2ab} \Delta \vec{\nabla}_a \vec{J}_{1b} + E^2_{13} \sum_{ab} \overleftrightarrow{R}_{2ab} \vec{\nabla}_a \vec{J}_{3b} \\ &+ D^4_{11} \sum_{ab} \overleftrightarrow{R}_{4ab} \vec{\nabla}_a \vec{J}_{1b}.\end{aligned}$$

The energy densities above are given in terms of 45 $C^{n'}_{mn}$, $D^{n'}_{mn}$, and $E^{n'}_{mn}$.

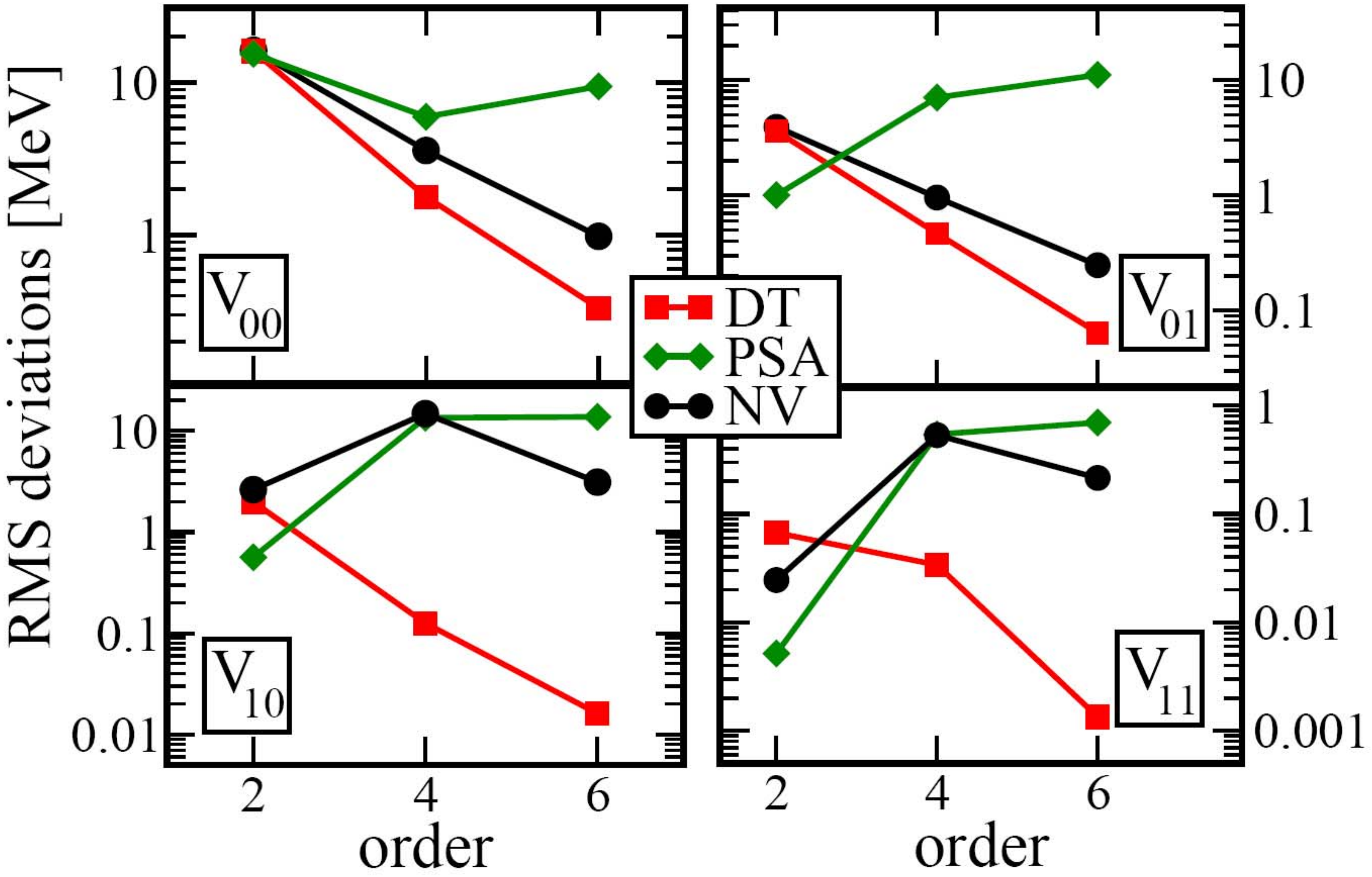
B.G. Carlsson *et al.*, Phys. Rev. C 78, 044326 (2008)
Phys. Rev. C 81, 029904(E) (2010)

Convergence of density-matrix expansions for nuclear interactions (the direct term)



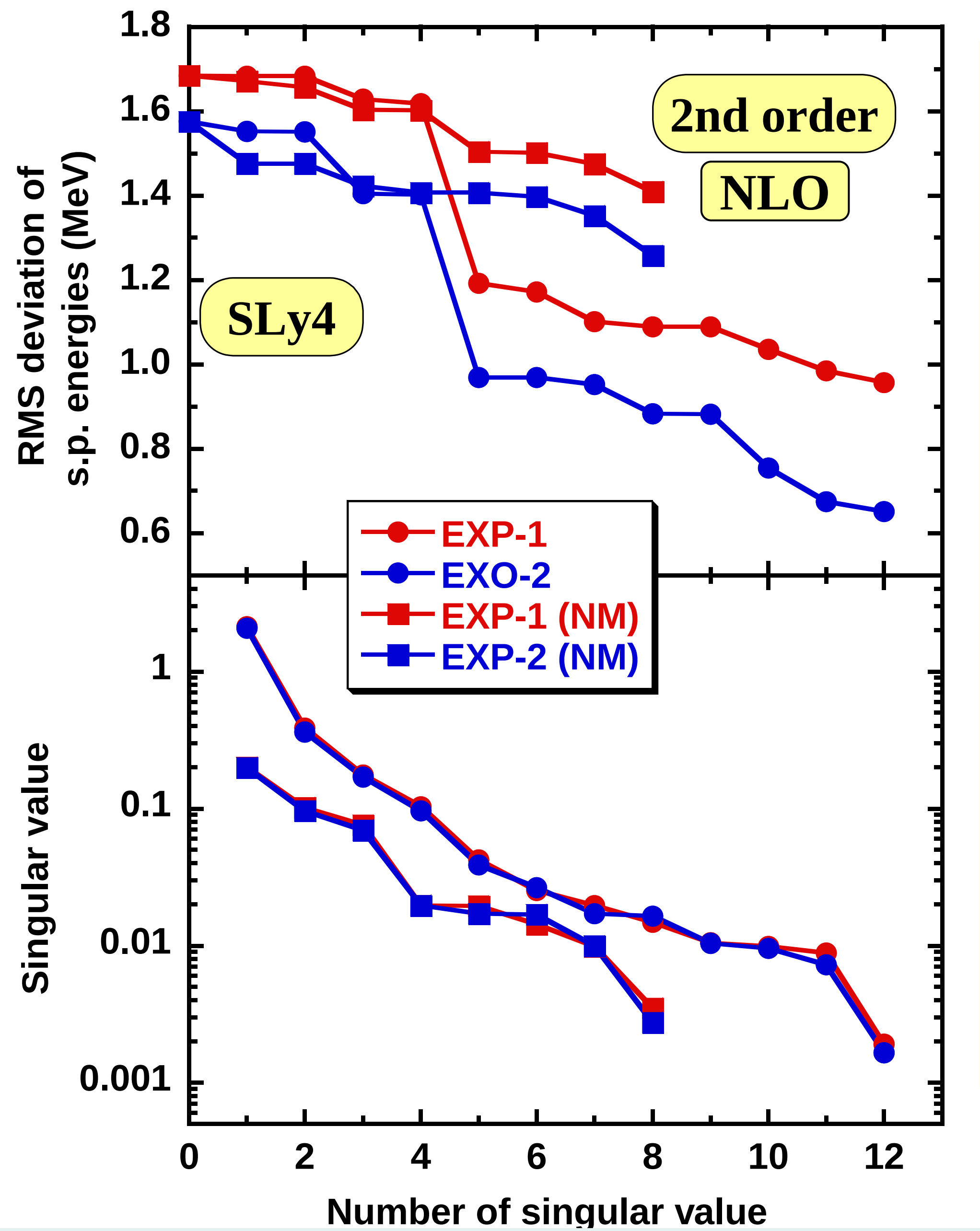
B.G. Calsson, J. Dobaczewski, arXiv:1003.2543

Convergence of density-matrix expansions for nuclear interactions (the exchange term)



B.G. Calsson, J. Dobaczewski, arXiv:1003.2543

Fits of s.p. energies – regression analysis



B.G. Carlsson *et al.*, to be published

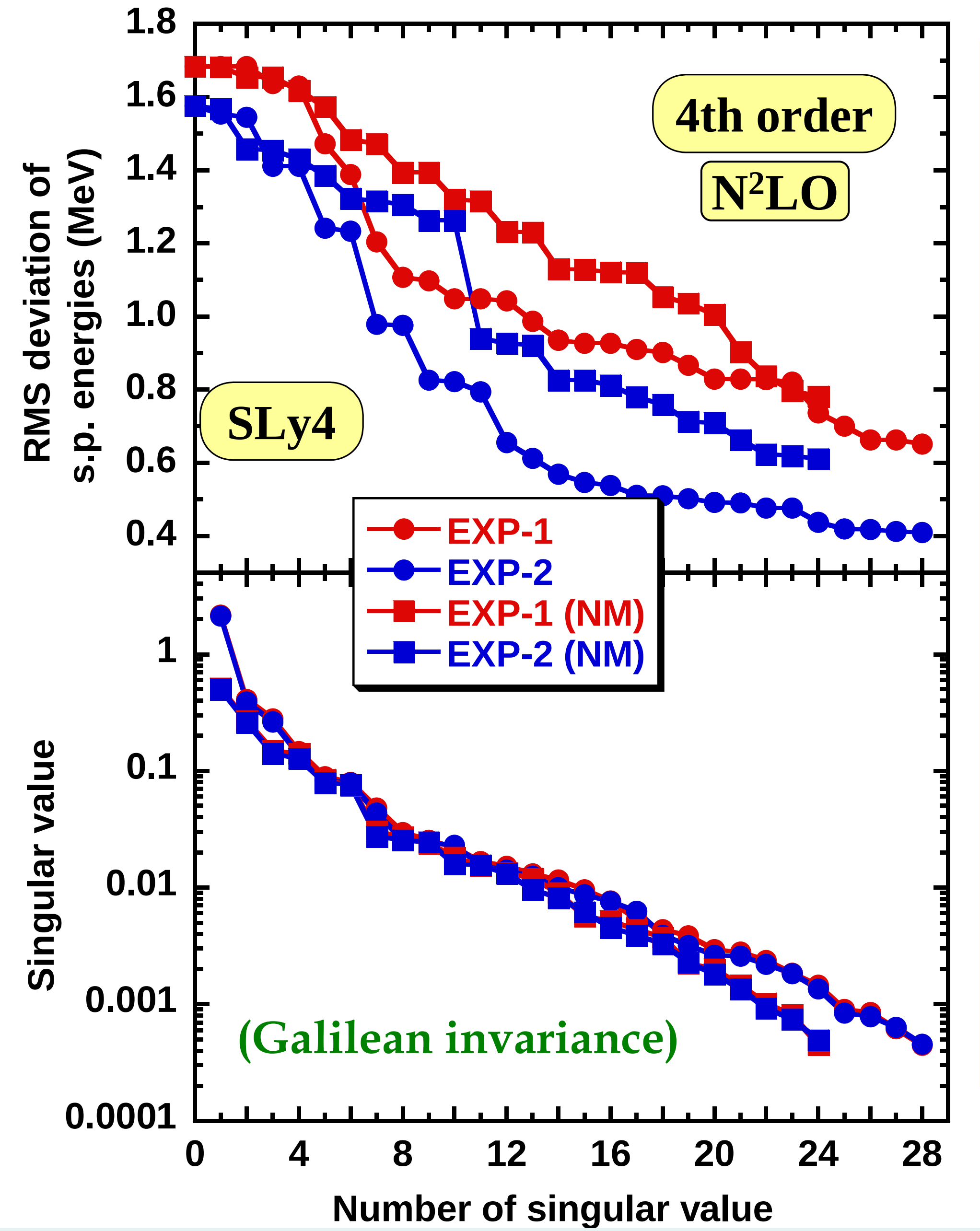
EXP-1:
M.N. Schwierz,
I. Wiedenhover, and
A. Volya, arXiv:0709.3525

EXP-2:
M.G. Porquet *et al.*,
to be published

NM:
Nuclear-matter
constraints on:

- saturation density
- energy per particle
- incompressibility
- effective mass

Fits of s.p. energies – regression analysis



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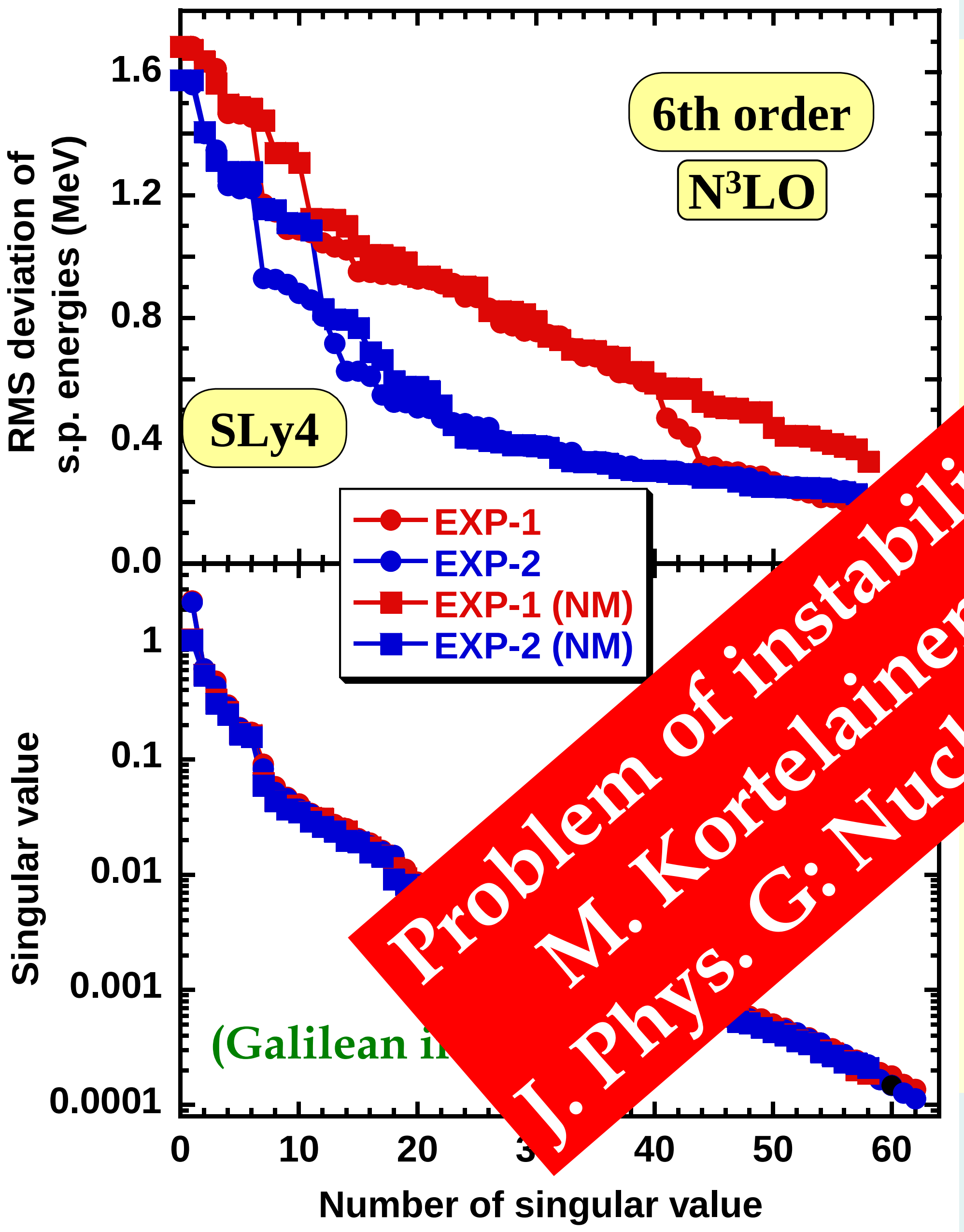

B.G. Carls
published

Problem of instabilities unsolved yet
M. Kortelainen and T. Lesinski
J. Phys. G: Nucl. Part. Phys. 37 064039

EXP-1:
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orquet *et al.*,
be published

NM:
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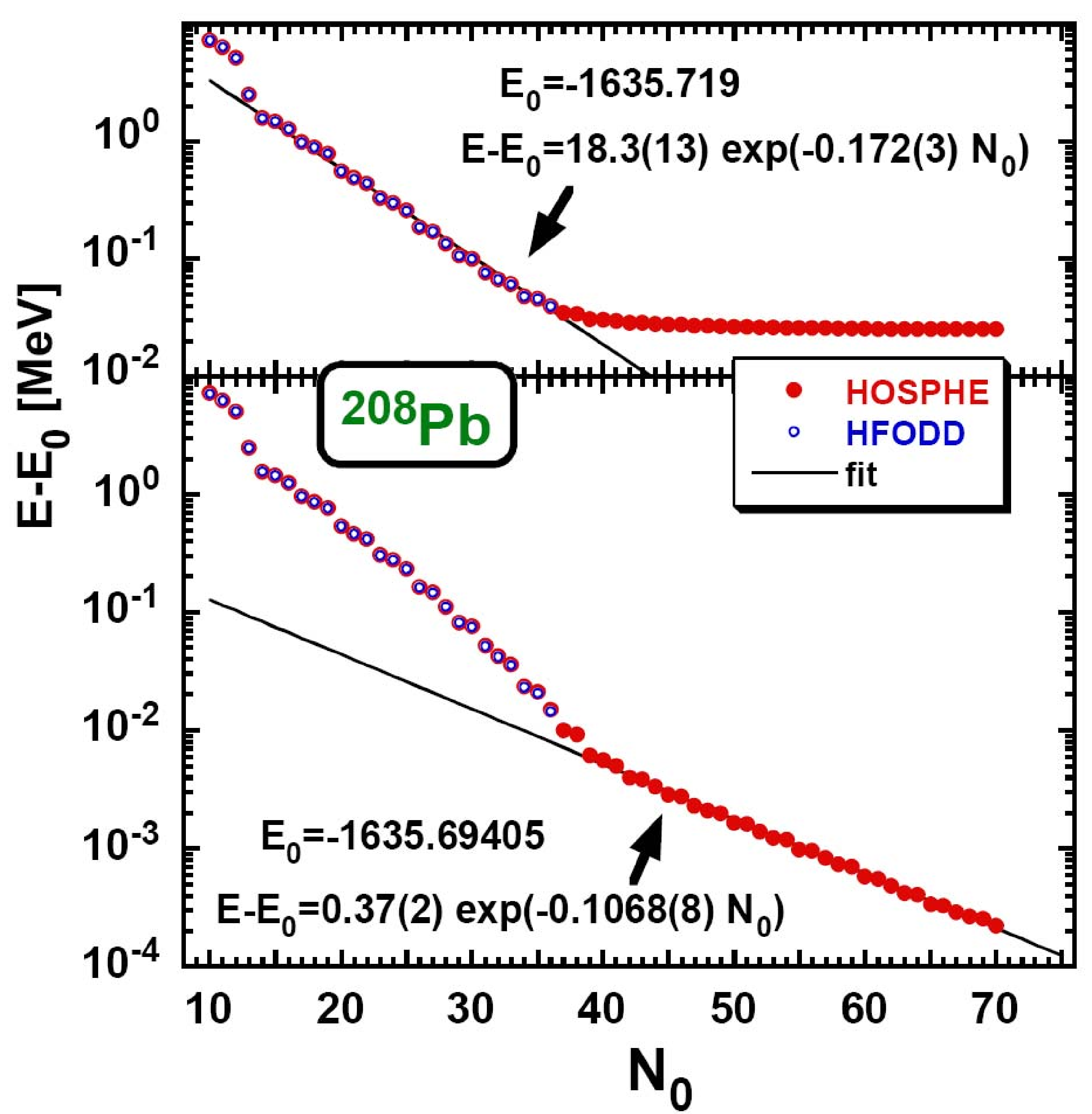
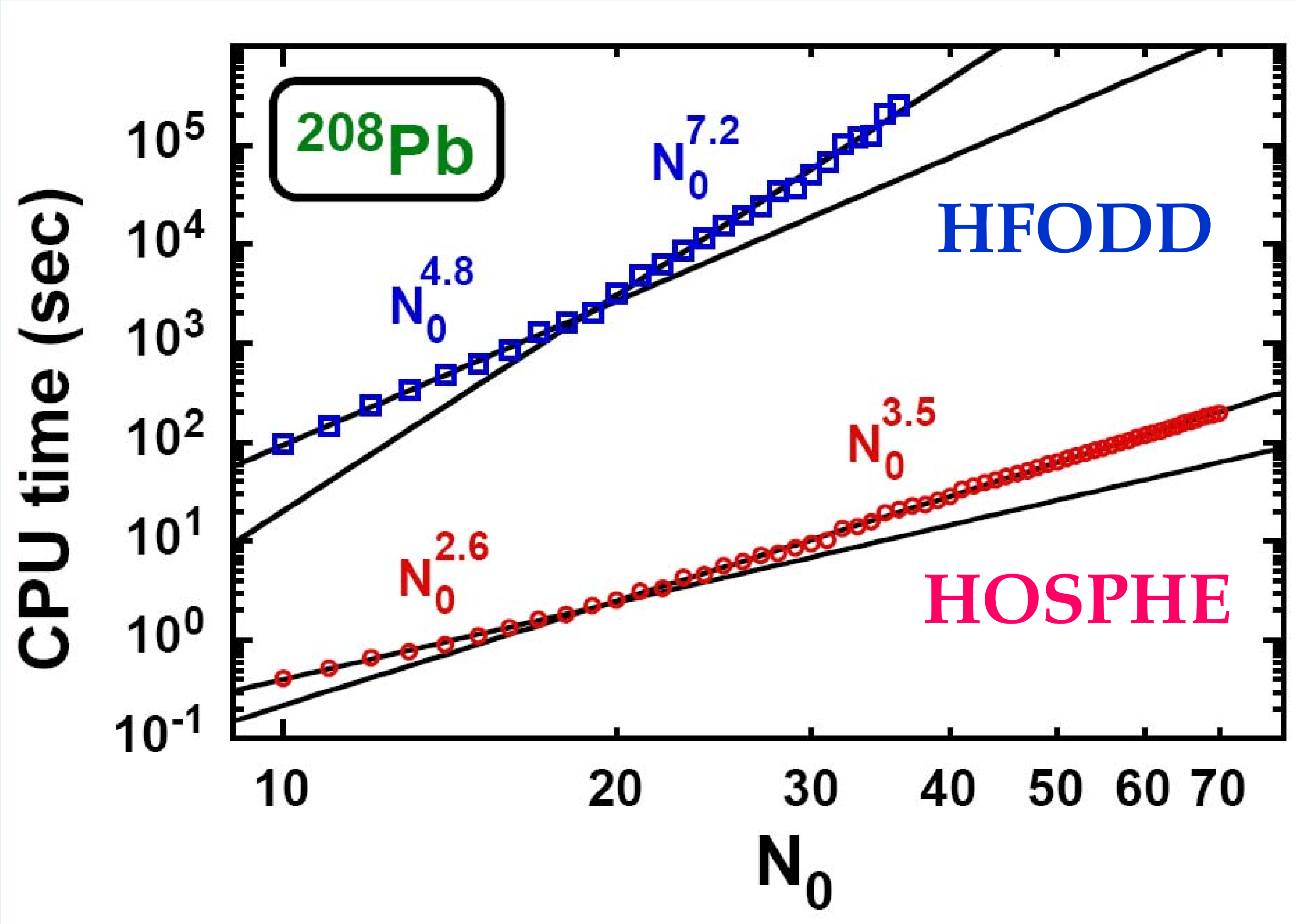


Program HOSPHE

Solution of self-consistent equations for the N^3LO nuclear energy density functional in spherical symmetry

B.G. Carlsson *et al.*, arXiv:0912.3230



Program HOSPHE

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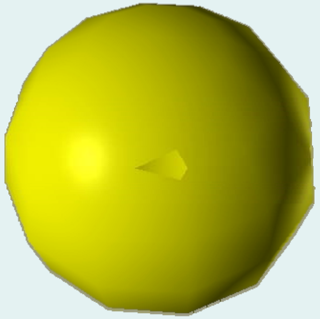
B.G. Carlsson *et al.*, arXiv:0912.3230

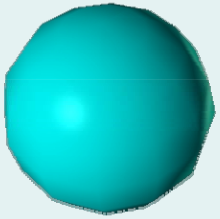
Spontaneous symmetry breaking

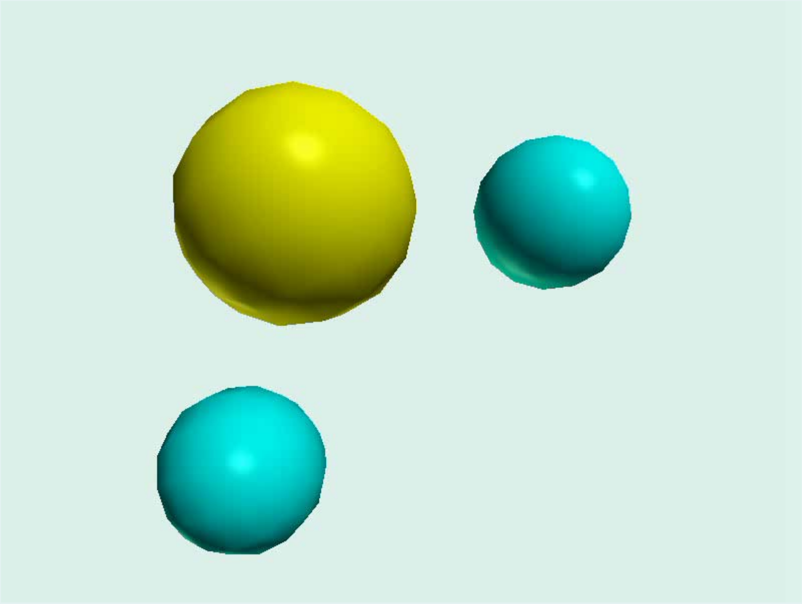
Ammonia molecule NH_3

Nitrogen atom

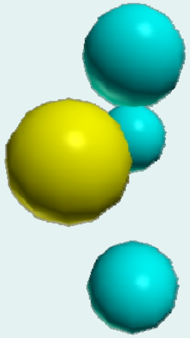


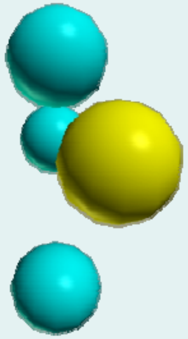
Hydrogen atom





$|L\rangle =$



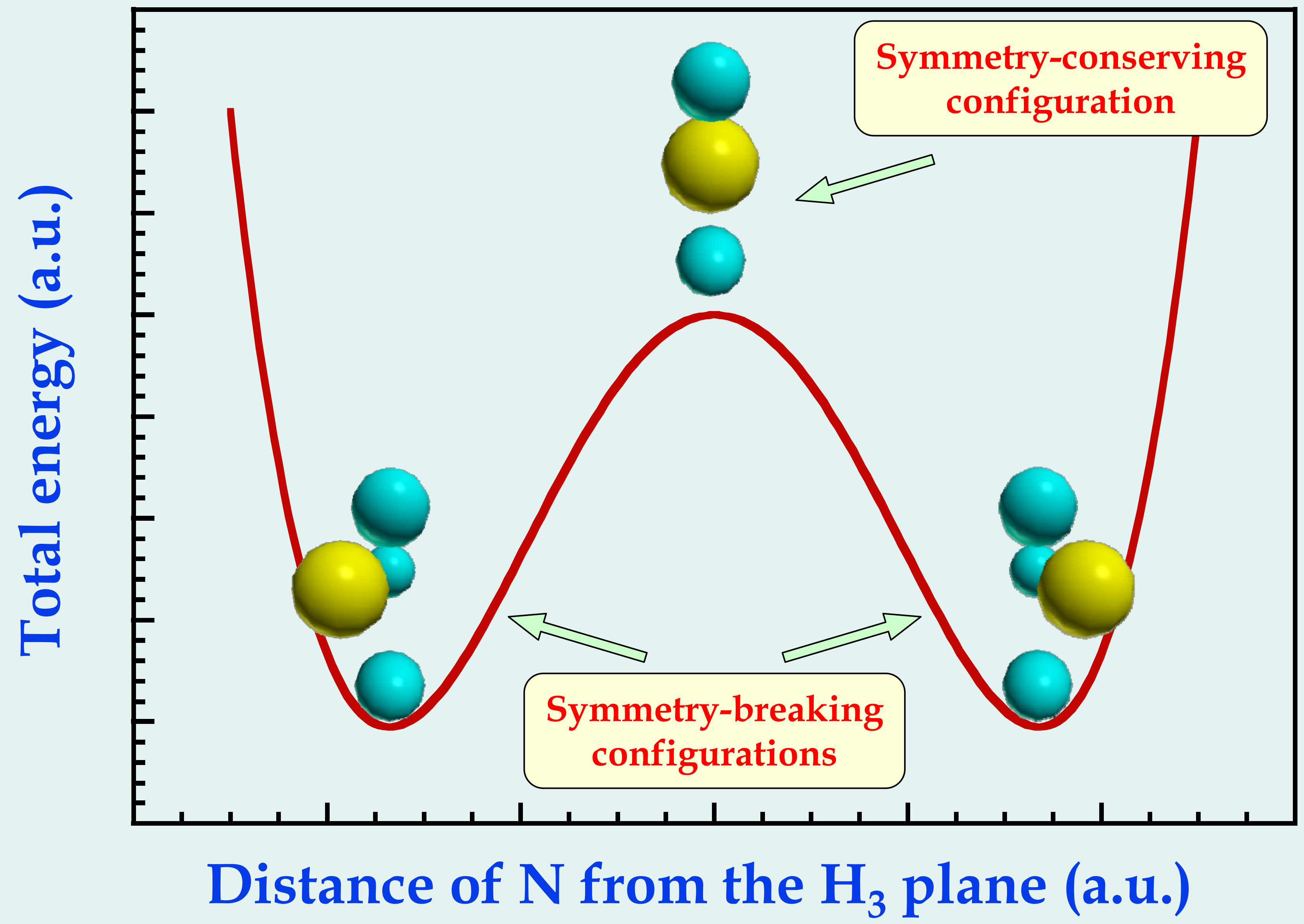


$= |R\rangle$

left state

right state

Ammonia molecule NH_3



Symmetry-conserving configuration

Symmetry-breaking configurations

Let P be the plane-reflection operator with respect to the H$_3$ plane, then

$$\begin{aligned} P|R\rangle &= |L\rangle \\ P|L\rangle &= |R\rangle \end{aligned}$$

Let us denote overlaps and matrix elements by

$$\begin{aligned} 1 &= \langle L|L\rangle = \langle R|R\rangle \\ \epsilon &= \langle L|R\rangle \\ E_0 &= \langle L|H|L\rangle = \langle R|H|R\rangle \\ \Delta &= \langle L|H|R\rangle \end{aligned}$$

In the non-orthogonal basis of $|L\rangle$, $|R\rangle$ the Hamiltonian matrix reads

$$H = \begin{pmatrix} E_0 & \Delta \\ \Delta & E_0 \end{pmatrix}$$

The eigenstates must correspond to the restored-symmetry states

$$|\pm\rangle = \frac{1}{\sqrt{2 \pm 2\epsilon}}(|L\rangle \pm R\rangle)$$

i.e.,

$$P|\pm\rangle = \pm|\pm\rangle$$

The eigenenergies read

$$E_\pm = \langle\pm|H|\pm\rangle = \frac{E_0 \pm \Delta}{1 \pm \epsilon}$$

States $|L\rangle$ and $R\rangle$ are wave packets, e.g.,

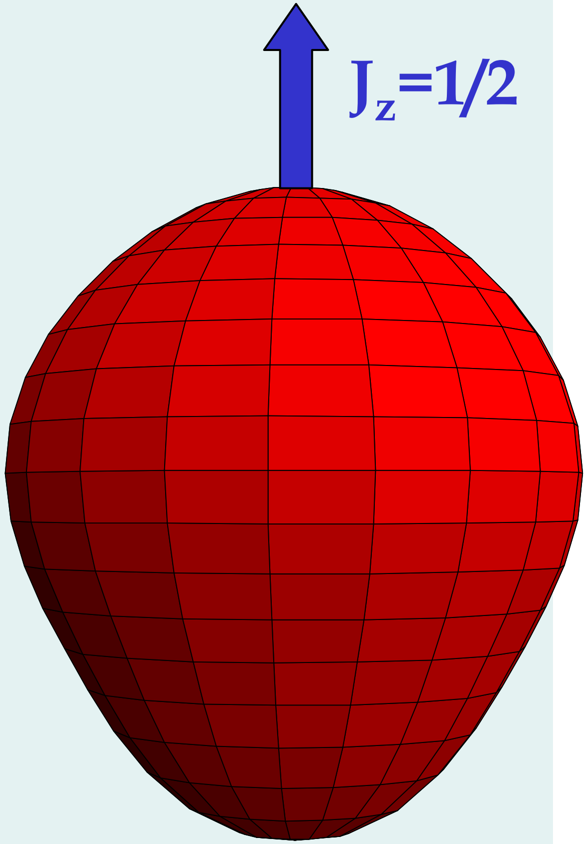
$$|L\rangle = \frac{1}{2}\left(\sqrt{2+2\epsilon}|+\rangle + \sqrt{2-2\epsilon}|-\rangle\right)$$

which evolve in time ($\epsilon = 0$ assumed) as:,

$$\boxed{|L,t\rangle = e^{iE_0 t/\hbar}\left(\cos(\Delta t/\hbar)|L,0\rangle + i\sin(\Delta t/\hbar)|R,0\rangle\right)}$$

Skyrme-Hartree-Fock
J. Dobaczewski, J. Engel,
Phys. Rev. Lett. 94, 232502 (2005)

Experiment
R.G. Helmer *et al.*, Nucl. Phys. A474 (1987) 77



β_{10} = 0.023
β_{20} = 0.161
β_{30} =–0.128
β_{40} = 0.091

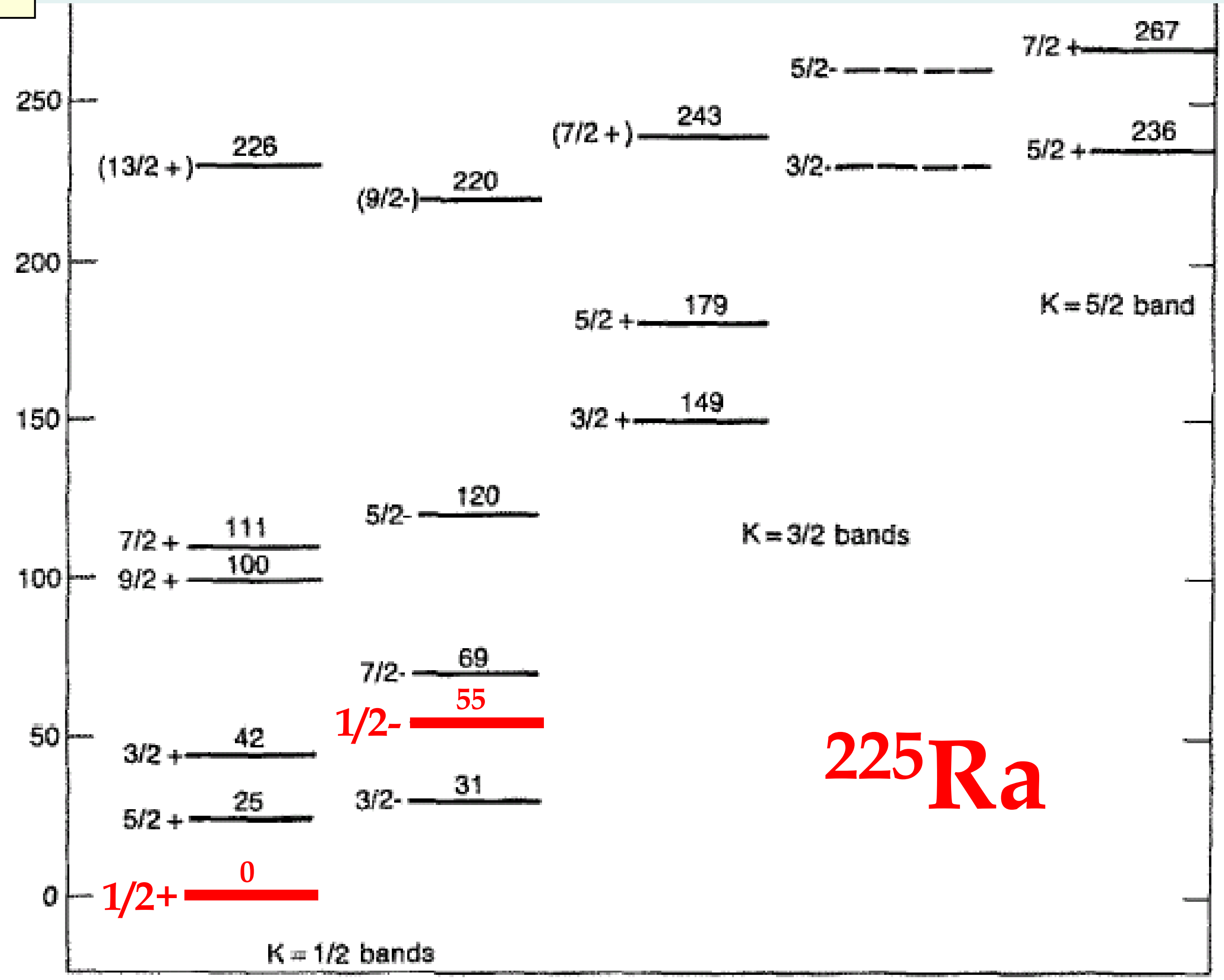


Fig. 5. Proposed grouping of the low-lying states of ^{225}Ra into rotational bands. The two members of the $K^\pi = \frac{3}{2}^-$ band have been reported in a study of the ^{225}Fr decay [20]; they are not observed in the present study.

	NH_3	^{225}Ra	ratio
-2Δ	0.1 meV	55 keV	1.8×10^{-9}
$T_{1/2}$ (Q.M.)	6.6 ps	0.012 as	5.5×10^{8}
$T_{1/2}$ (E.M.)	16 ks	~5 ns	3.2×10^{12}
D	0.76 e×nm	~0.1 e× fm	7.6×10^{-6}

Lessons learned

1) Energy density functional exists due to the two-step variational method and gives exact ground state energy and its exact particle density.

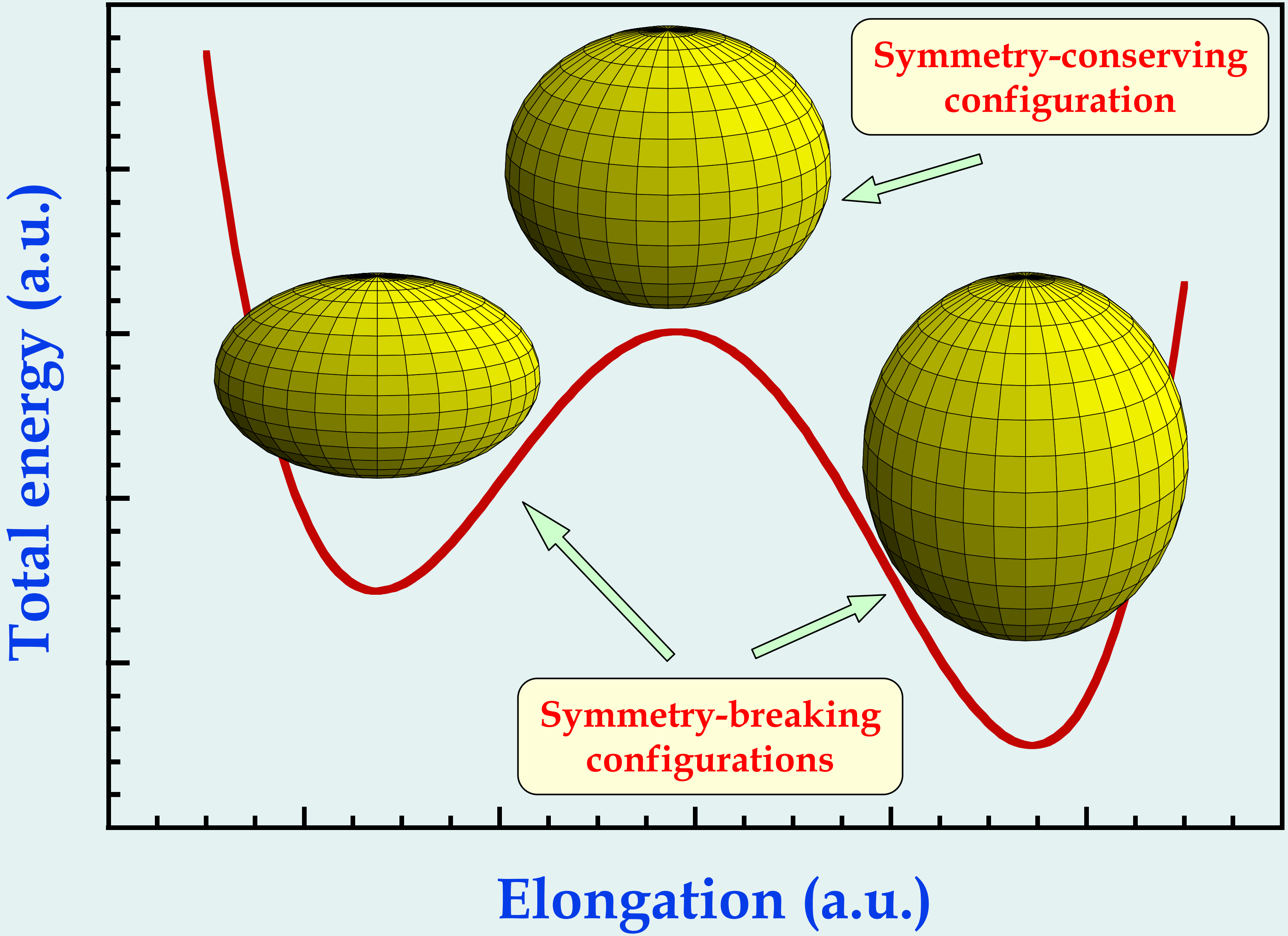
2) Whenever the energy scales (or range scales) between the interactions and observations are different, the observations can be described by a series of pseudopotentials with coupling constants adjusted to data (an effective theory).

3) In nuclei, the non-local energy density functionals can be replaced by the local ones. This is because the range of the interaction is shorter than the range of variations in the local and non-local density matrix.

4) Systematic energy density functionals with derivative corrections can be constructed and the resulting self-consistent equations solved.

5) In finite systems, the phenomenon of spontaneous symmetry breaking is best captured by the mean-field or energy-density-functional methods.

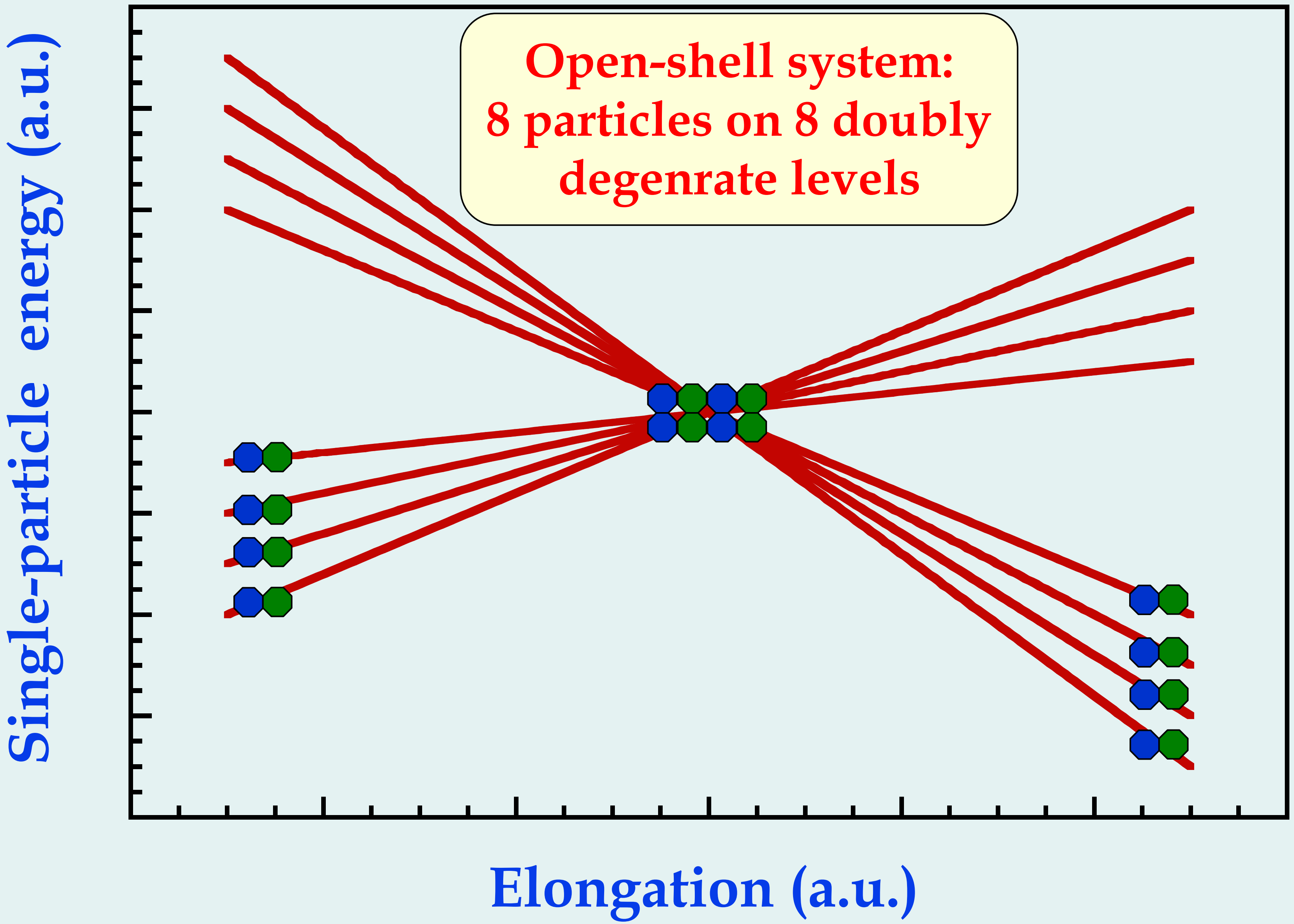
Nuclear deformation



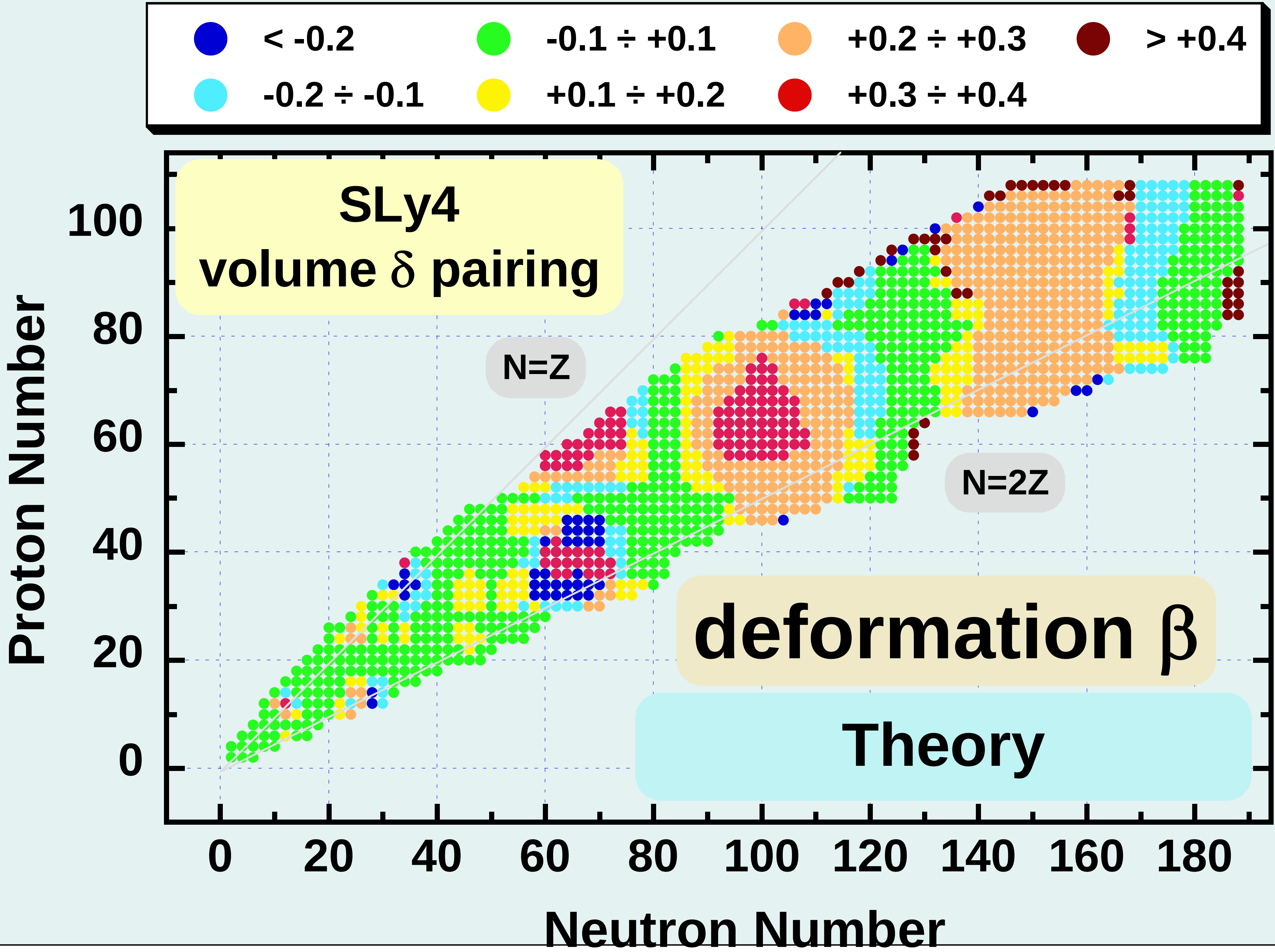
Symmetry-conserving configuration

Symmetry-breaking configurations

Origins of nuclear deformation



Open-shell system:
8 particles on 8 doubly
degenrate levels



SLy4
volume δ pairing

deformation β

Theory

M.V. Stoitsov, *et al.*, Phys. Rev. C68, 054312 (2003)

Jacek Dobaczewski

IFT UW

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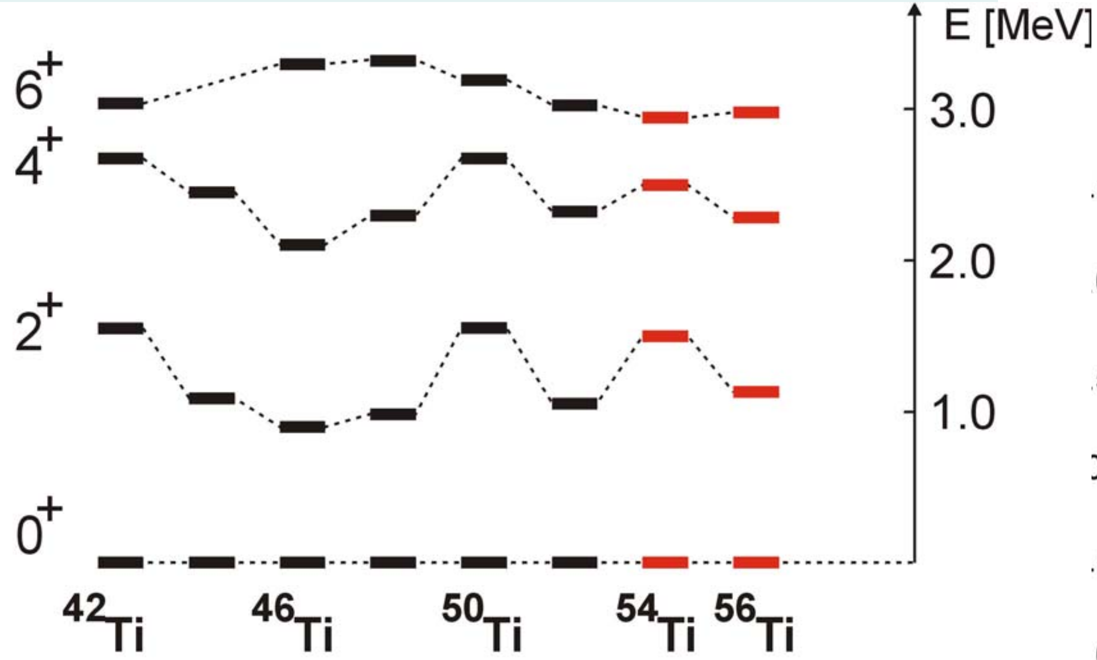
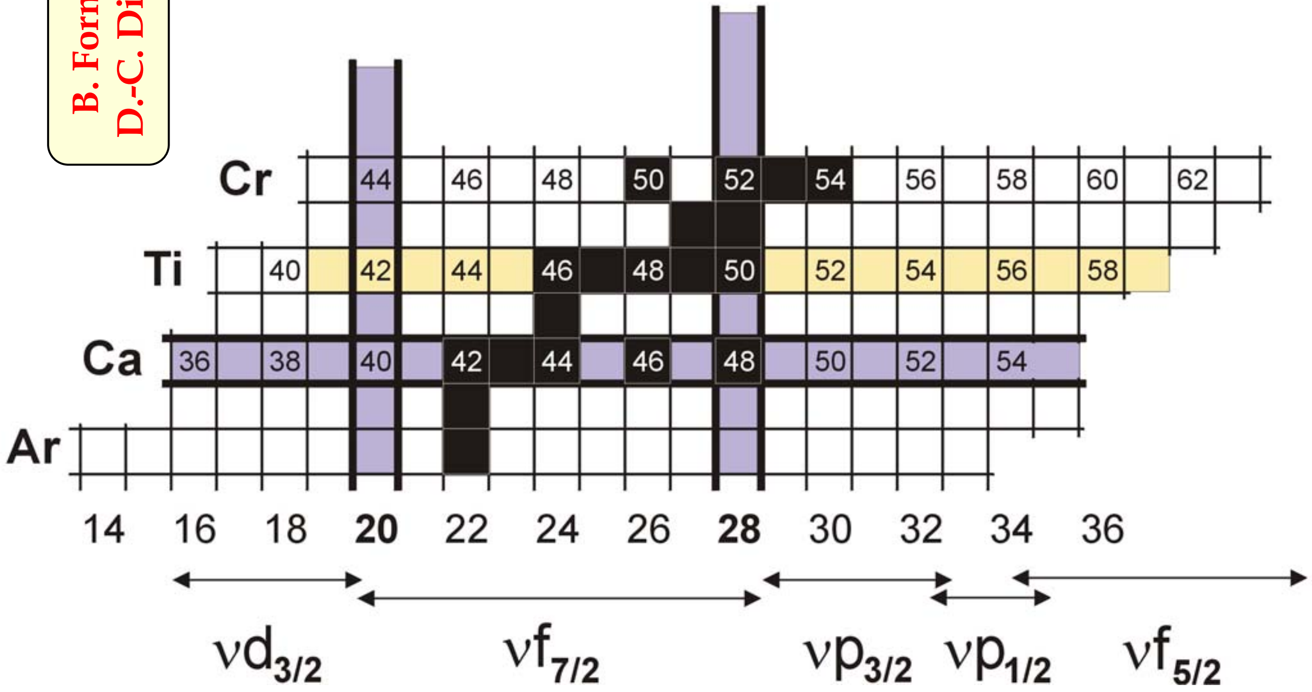
Tensor effects

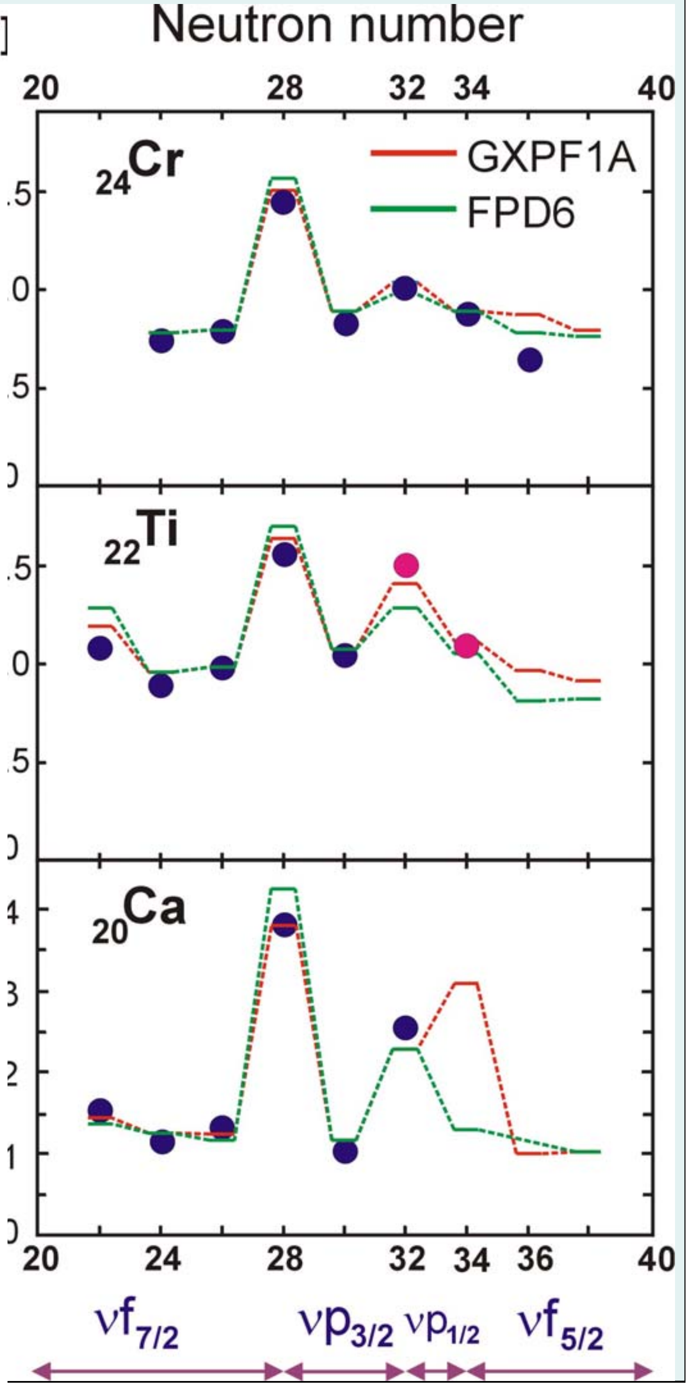
B. Fornal, XXIX Mazurian Lakes Conference on Physics (2005)

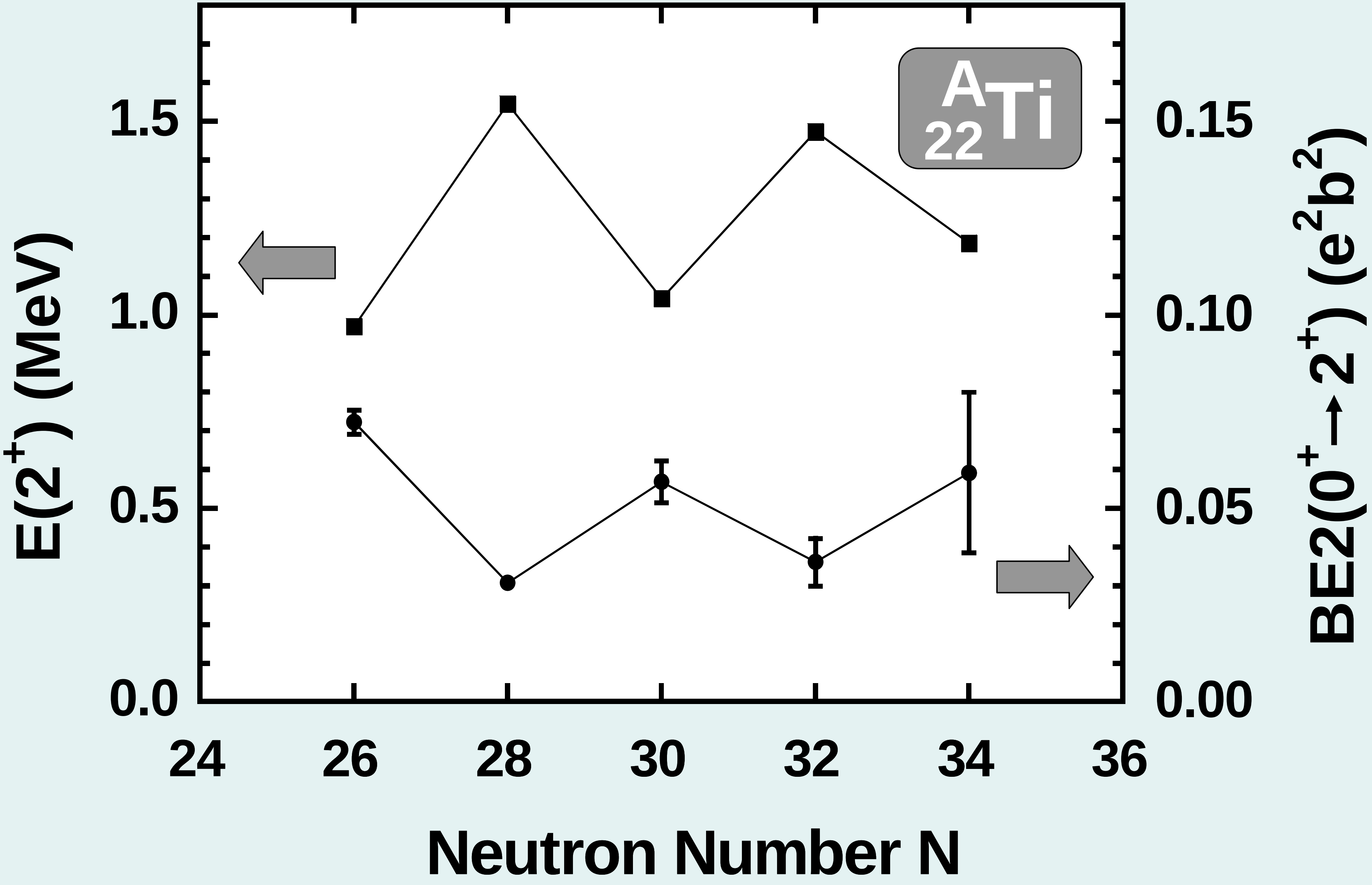
M.Honma et al., Eur. Phys. J. 25,s01 (2005) 499

B. Fornal *et al.*, Phys. Rev. C 70, 064304 (2004)
D.-C. Dinca *et al.*, Phys. Rev. C 71, 041302 (2005)

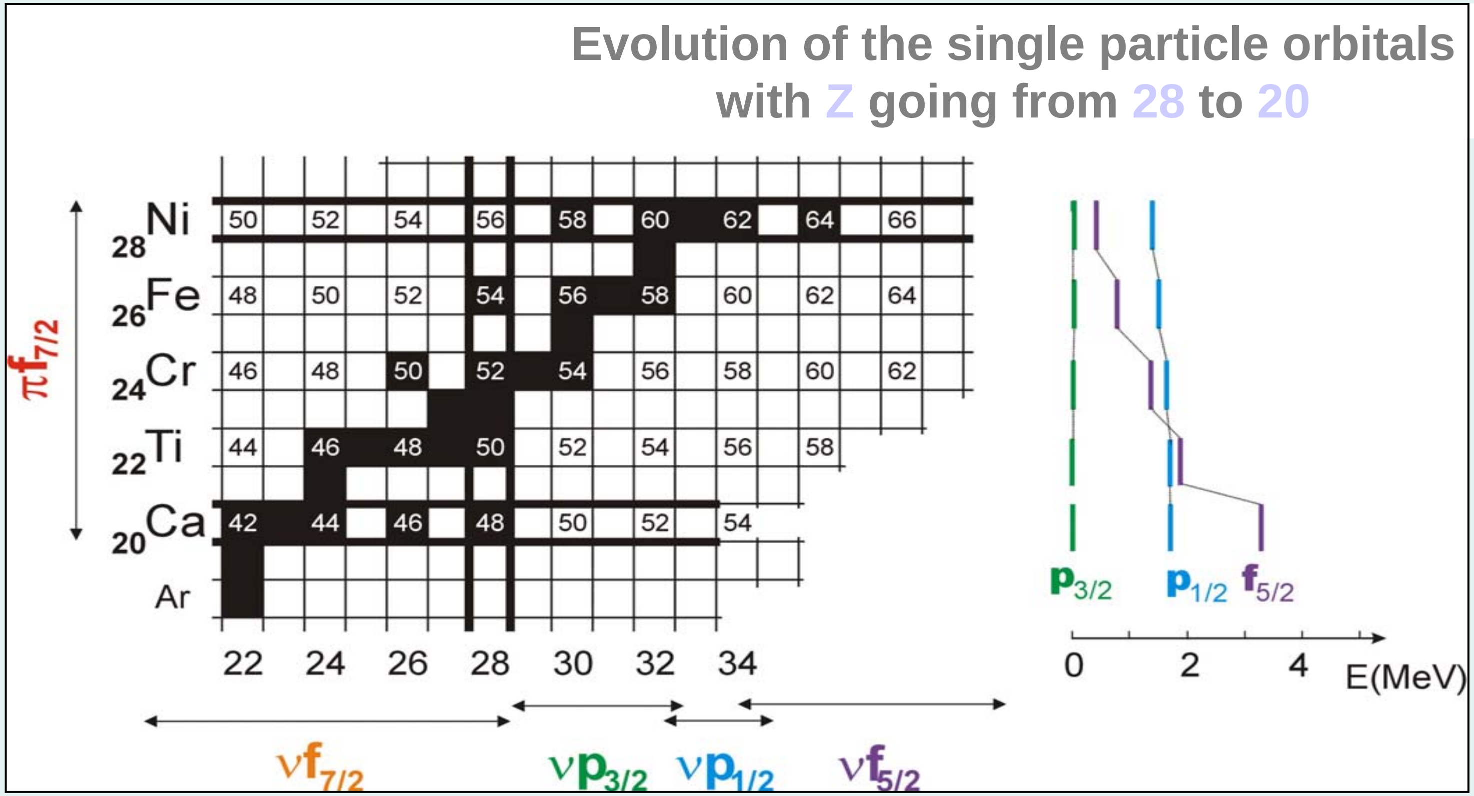








$^{A}_{22}$Ti
E(2^+) (MeV)
BE2($0^+ \rightarrow 2^+$) (e^2b^2)
Neutron Number N
0.0
0.5
1.0
1.5
0.00
0.05
0.10
0.15
24
26
28
30
32
34
36


Evolution of the single particle orbitals with Z going from 28 to 20

B. Fornal, XXIX Mazurian Lakes Conference on Physics (2005)

Tensor Interaction

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

V_T couples $j_>$ and $j_<$ orbitals and favors charge exchange processes

$$\pi f_{7/2} \leftrightarrow \nu f_{5/2}$$

T. Otsuka *et al.* Phys. Rev. Lett 87, 082502 (2001)

Tensor-even, tensor-odd, and spin-orbit interactions

$$\begin{aligned}
\hat{V}_{Te} &= \tfrac{1}{2}t_e\big[\hat{\vec{k}}' \cdot \hat{\mathbf{S}} \cdot \hat{\vec{k}}' + \hat{\vec{k}} \cdot \hat{\mathbf{S}} \cdot \hat{\vec{k}}\big] \\
\hat{V}_{To} &= t_o\hat{\vec{k}}' \cdot \hat{\mathbf{S}} \cdot \hat{\vec{k}} \\
\hat{V}_{SO} &= iW_0\hat{\vec{S}} \cdot \big[\hat{\vec{k}}' \times \hat{\vec{k}}\big]
\end{aligned}$$

where

$$\begin{aligned}
\hat{\mathbf{S}}^{ij} &= \tfrac{3}{2}\big[\vec{\sigma}_1^i\vec{\sigma}_2^j + \vec{\sigma}_1^j\vec{\sigma}_2^i\big] - \delta^{ij}\vec{\sigma}_1 \cdot \vec{\sigma}_2 \\
\hat{\vec{S}} &= \vec{\sigma}_1 + \vec{\sigma}_2
\end{aligned}$$

Tensor energy densities

For conserved spherical and time-reversal symmetries, averaged tensor and SO interactions give the following energy densities:

$$\begin{aligned} \mathcal{H}_T &= \tfrac{5}{8}[t_e \vec{J}_n \cdot \vec{J}_p + t_o(\vec{J}_0^2 - \vec{J}_n \cdot \vec{J}_p)] \\ \mathcal{H}_{SO} &= \tfrac{1}{4}[3W_0 \vec{J}_0 \cdot \vec{\nabla}\rho_0 + W_1 \vec{J}_1 \cdot \vec{\nabla}\rho_1] \end{aligned}$$

where the particle and SO densities read

$$\rho(r) = \frac{1}{4\pi r^3}\sum\nolimits_i v_i^2(2j_i+1)R_i^2(r)$$

$$J(r) = \frac{1}{4\pi r^3}\sum\nolimits_i v_i^2(2j_i+1)\left[j_i(j_i+1) - l_i(l_i+1) - \tfrac{3}{4}\right]R_i^2(r)$$

$$\vec{J} = \frac{\vec{r}}{r}J(r)$$

Single-particle spin-orbit potentials

$$C_0^J = \tfrac{5}{16}(3t_{\rm o} + t_{\rm e}), \qquad C_1^J = \tfrac{5}{16}(t_{\rm o} - t_{\rm e}),$$

$$C_0^{\nabla J} = -\tfrac{3}{4}W_0, \qquad C_1^{\nabla J} = -\tfrac{1}{4}W_1.$$

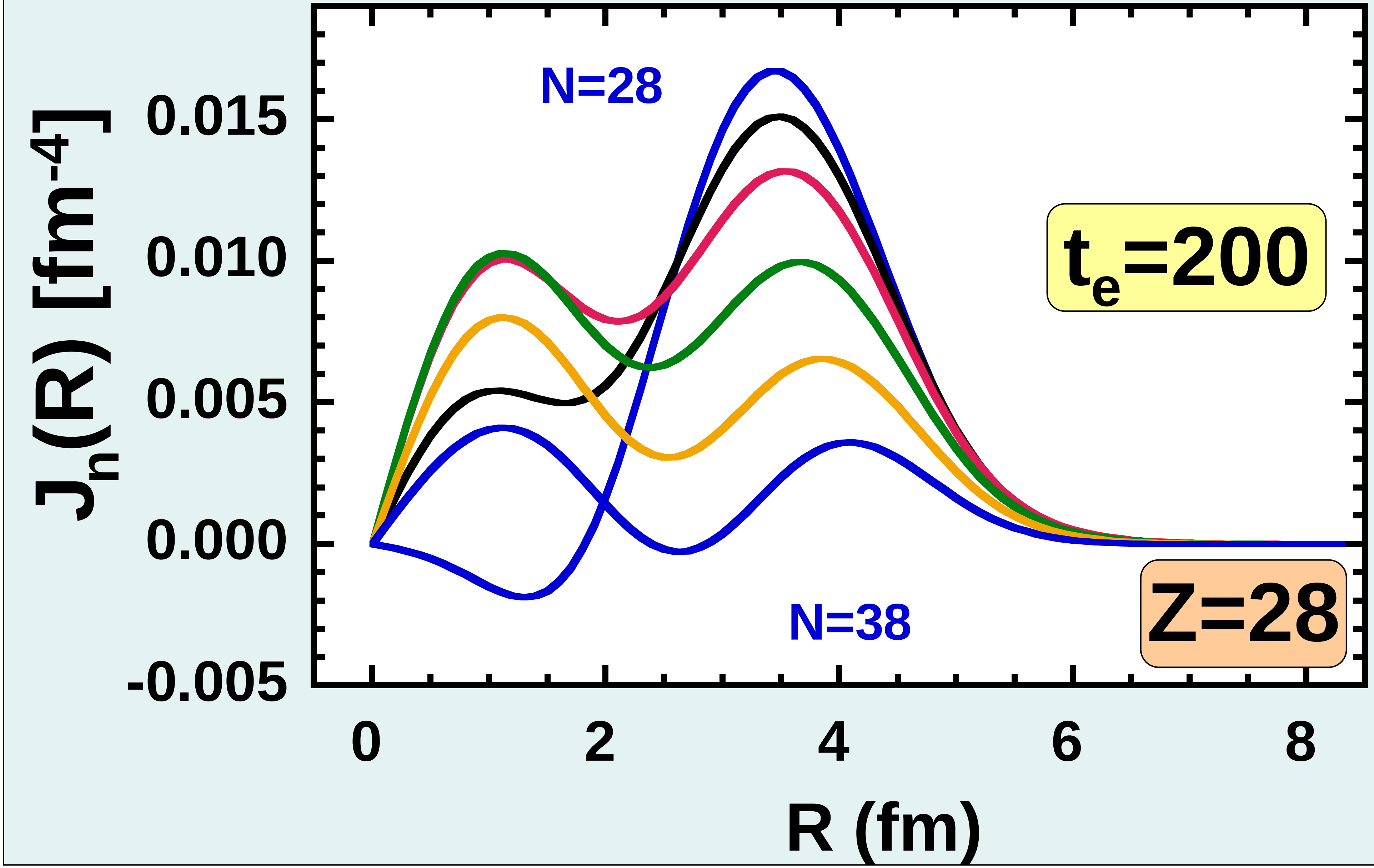
Variation of the energy densities with respect to
the single-particle wave functions gives
form factors of the single-particle spin-orbit potentials:

$$\vec{V}_p^{SO} = \frac{5t_e+5t_o}{8}\vec{J}_n + \frac{5t_o}{4}\vec{J}_p + \frac{3W_0-W_1}{4}\vec{\nabla}\rho_n + \frac{3W_0+W_1}{4}\vec{\nabla}\rho_p$$

$$\vec{V}_n^{SO} = \frac{5t_e+5t_o}{8}\vec{J}_p + \frac{5t_o}{4}\vec{J}_n + \frac{3W_0-W_1}{4}\vec{\nabla}\rho_p + \frac{3W_0+W_1}{4}\vec{\nabla}\rho_n$$

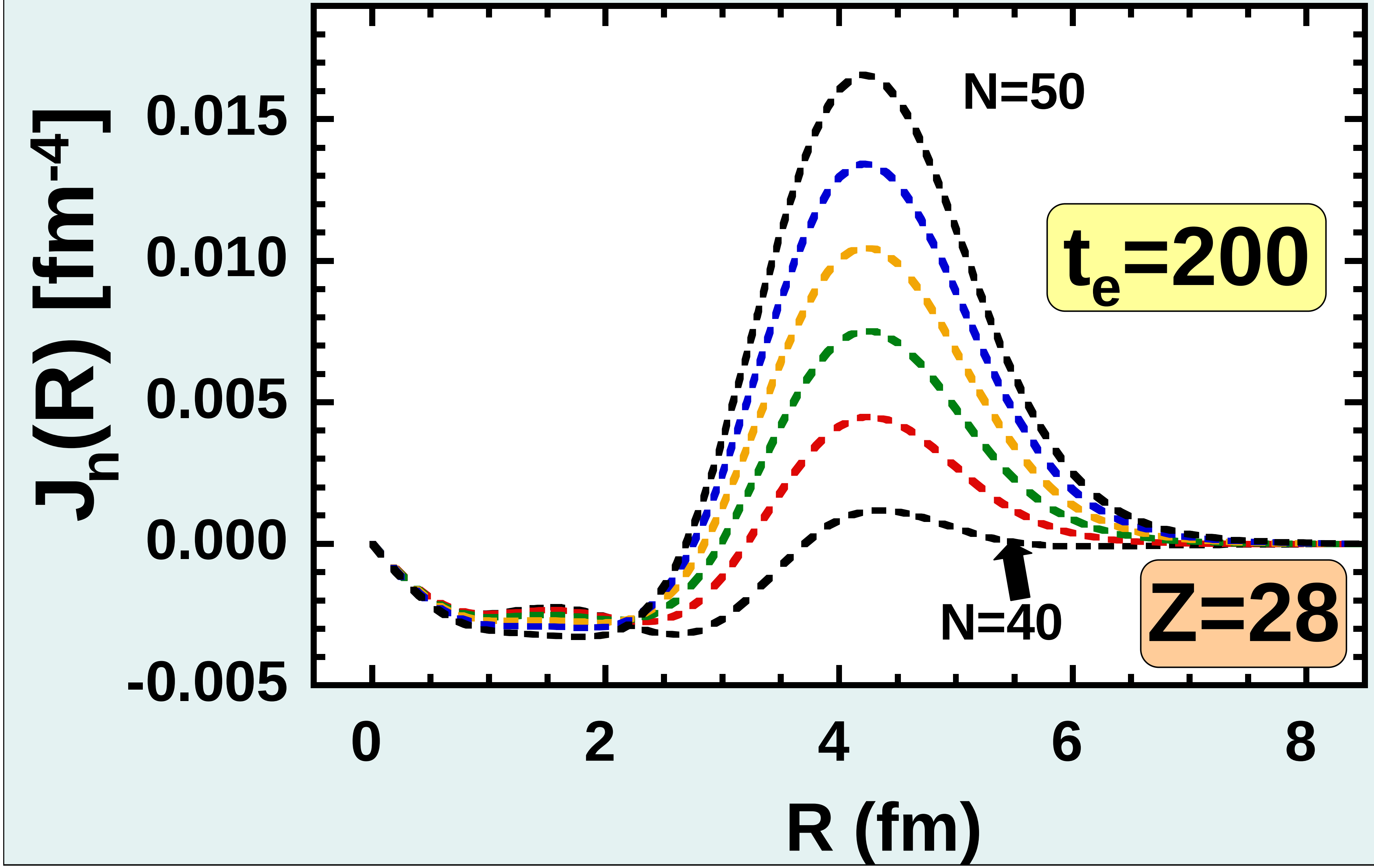
$$\hat{V}^{SO} = \frac{1}{r}V^{SO}(r)\hat{\vec{L}}\cdot\hat{\vec{S}} \quad \text{for} \quad \vec{V}^{SO} = \frac{\vec{r}}{r}V^{SO}(r)$$

Neutron S-O Density



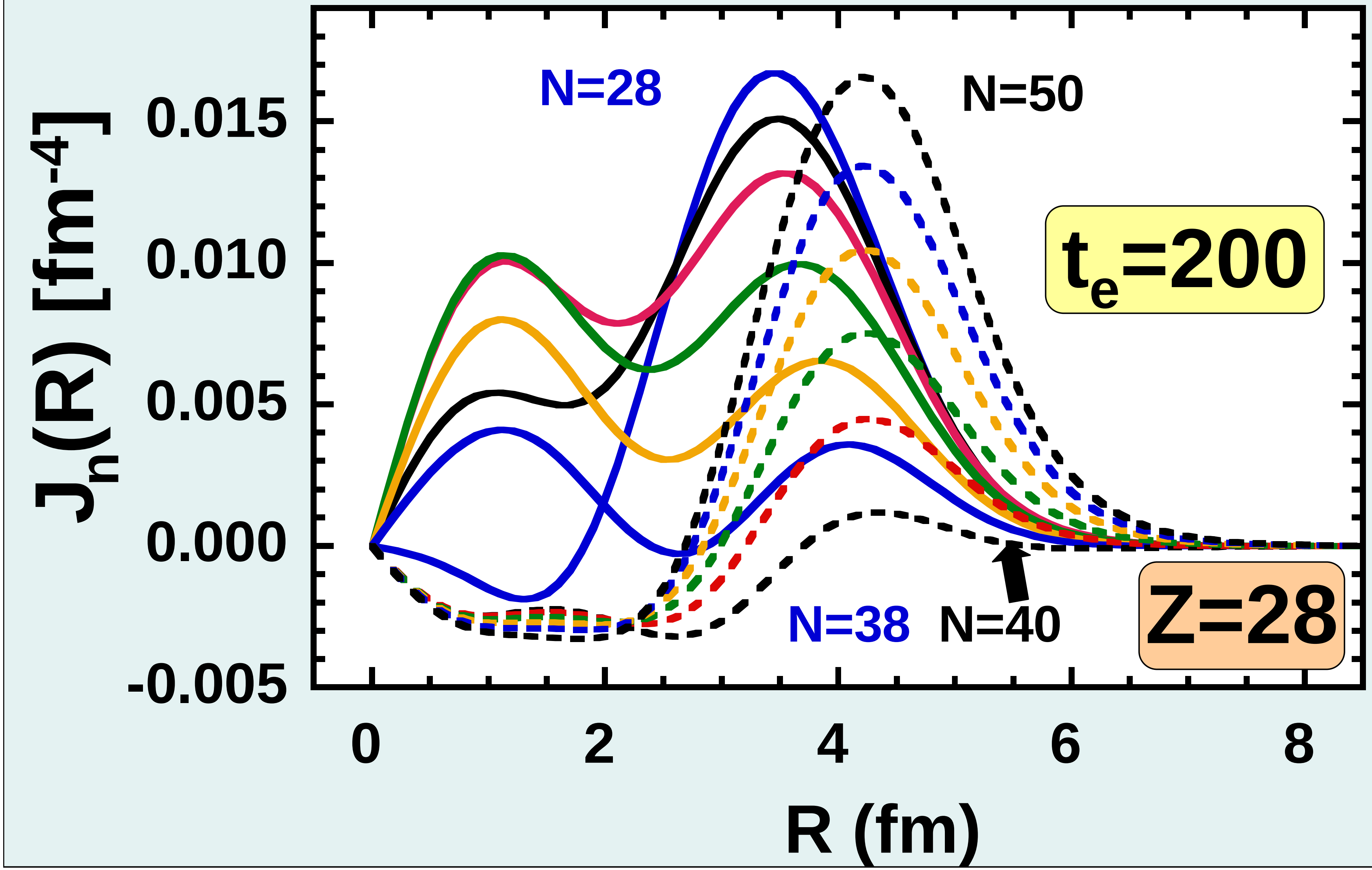
J. Dobaczewski, nucl-th/0604043

Neutron S-O Density

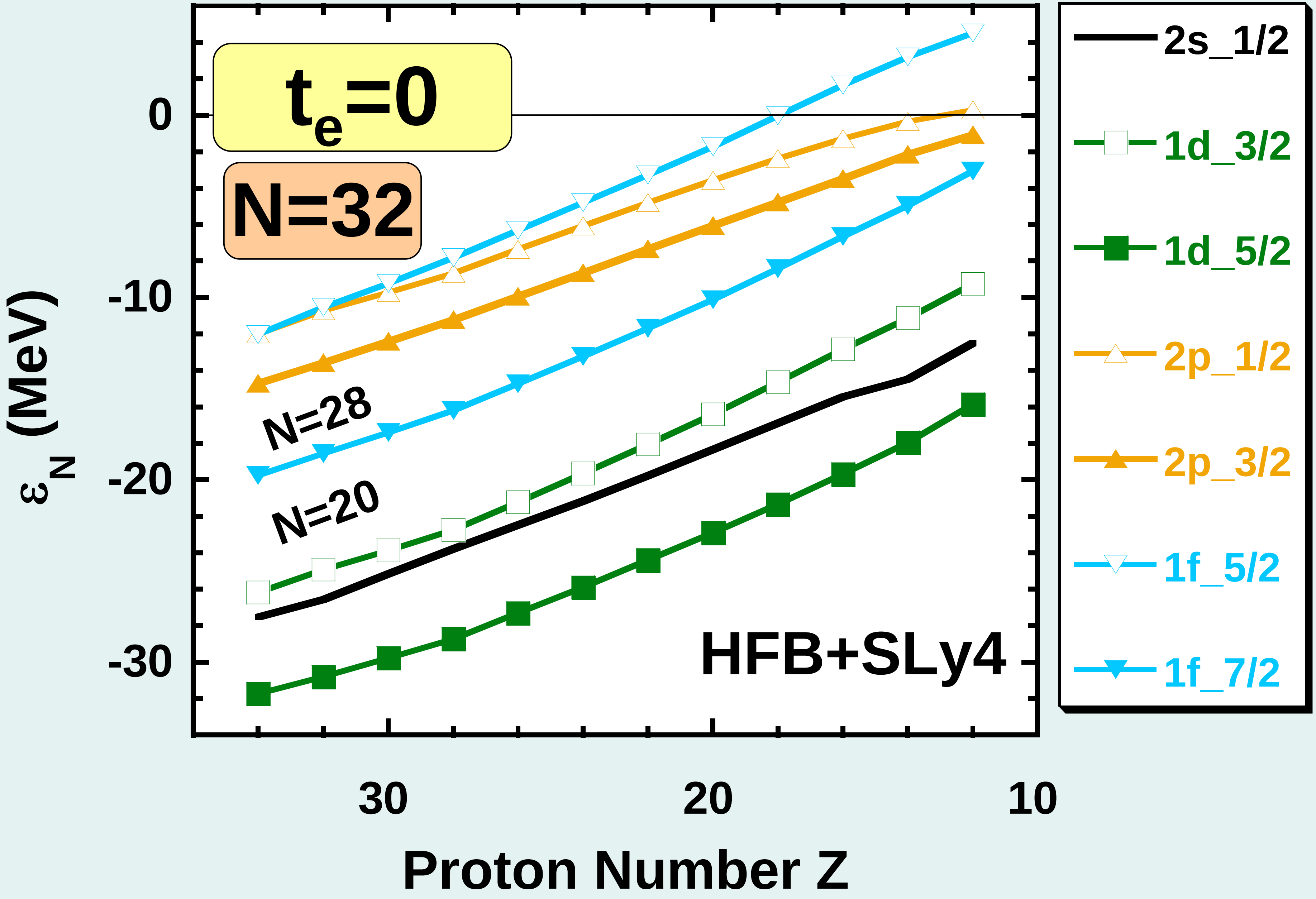


J. Dobaczewski, nucl-th/0604043

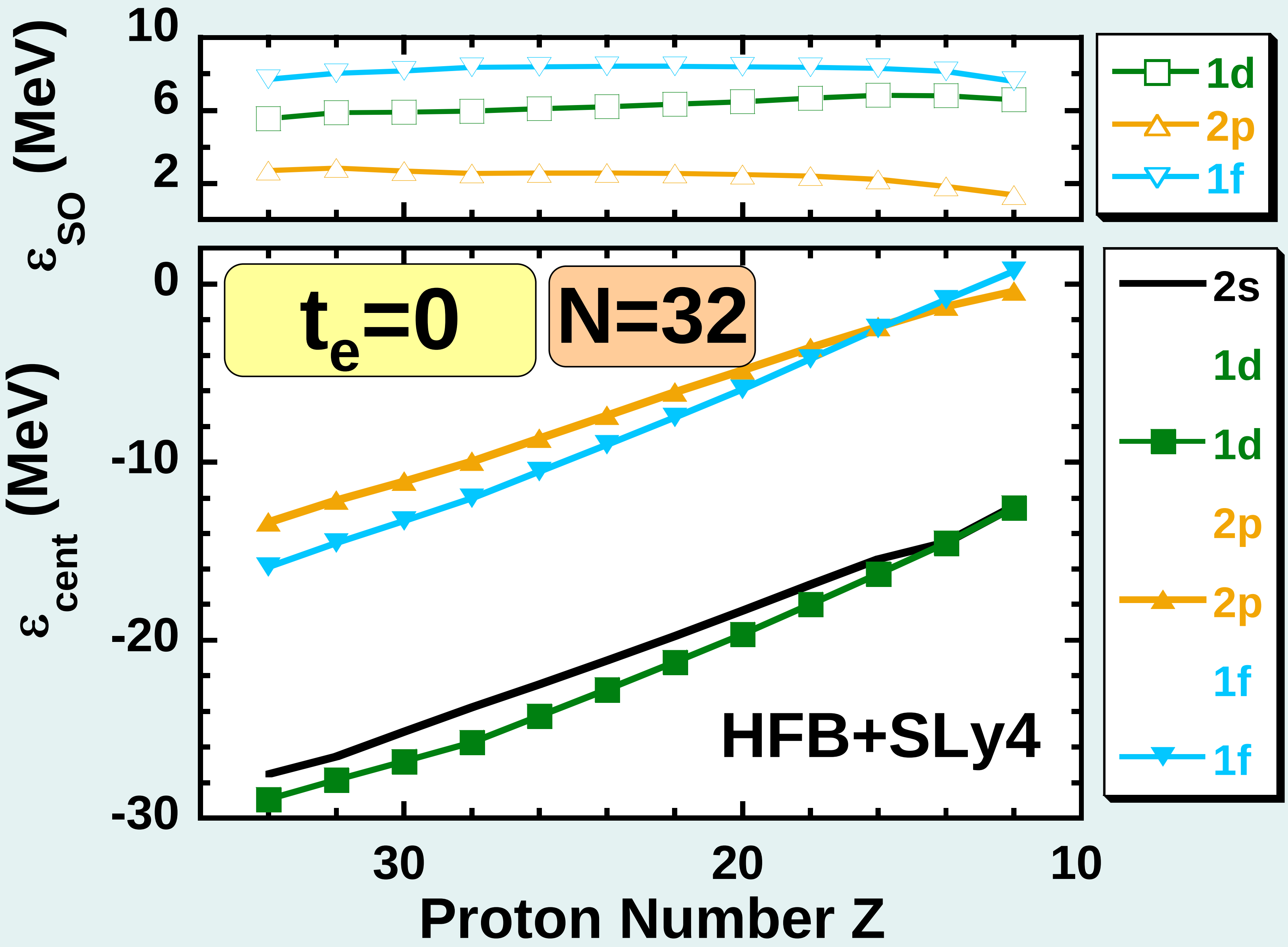
Neutron S-O Density



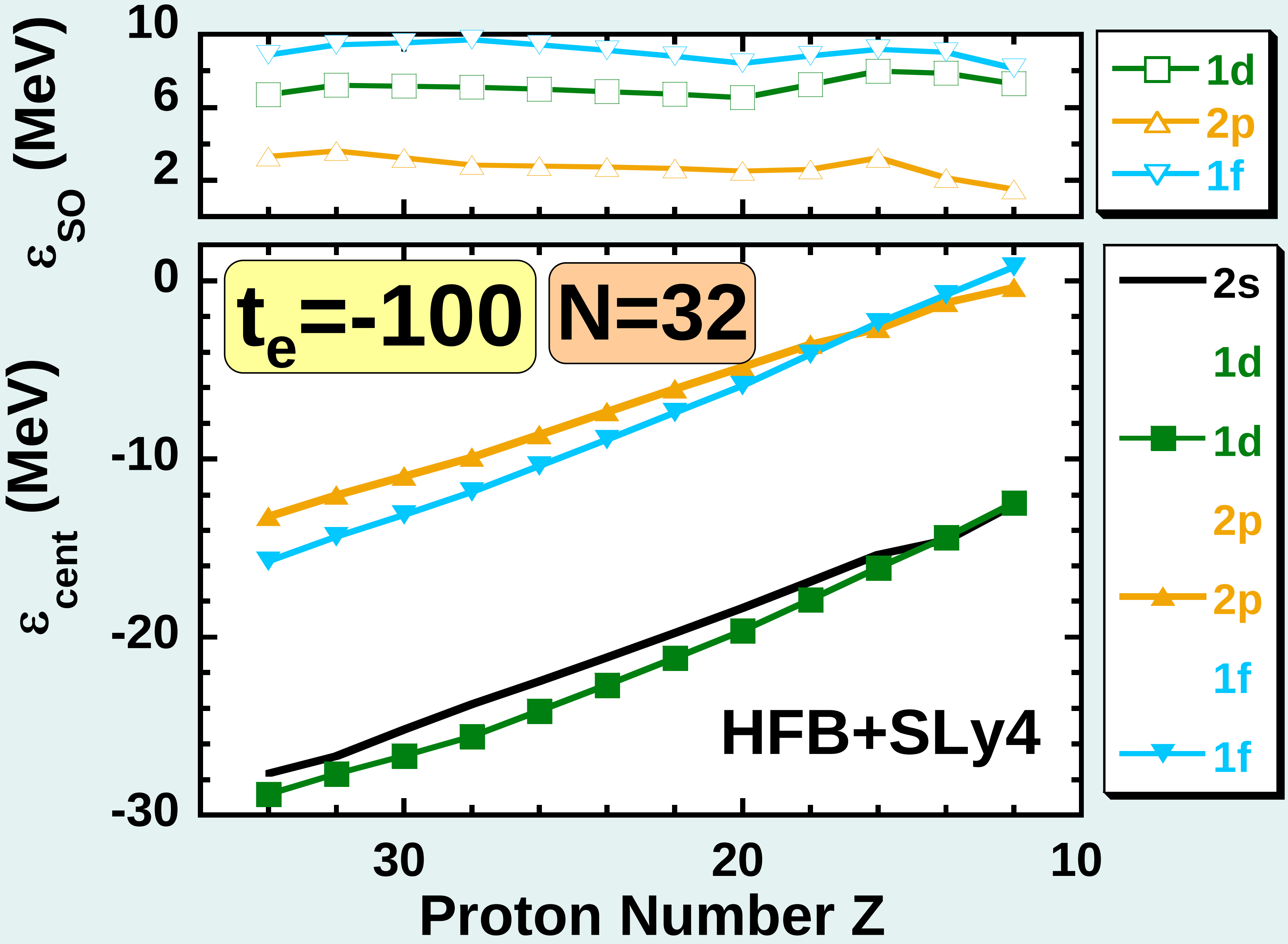
J. Dobaczewski, nucl-th/0604043



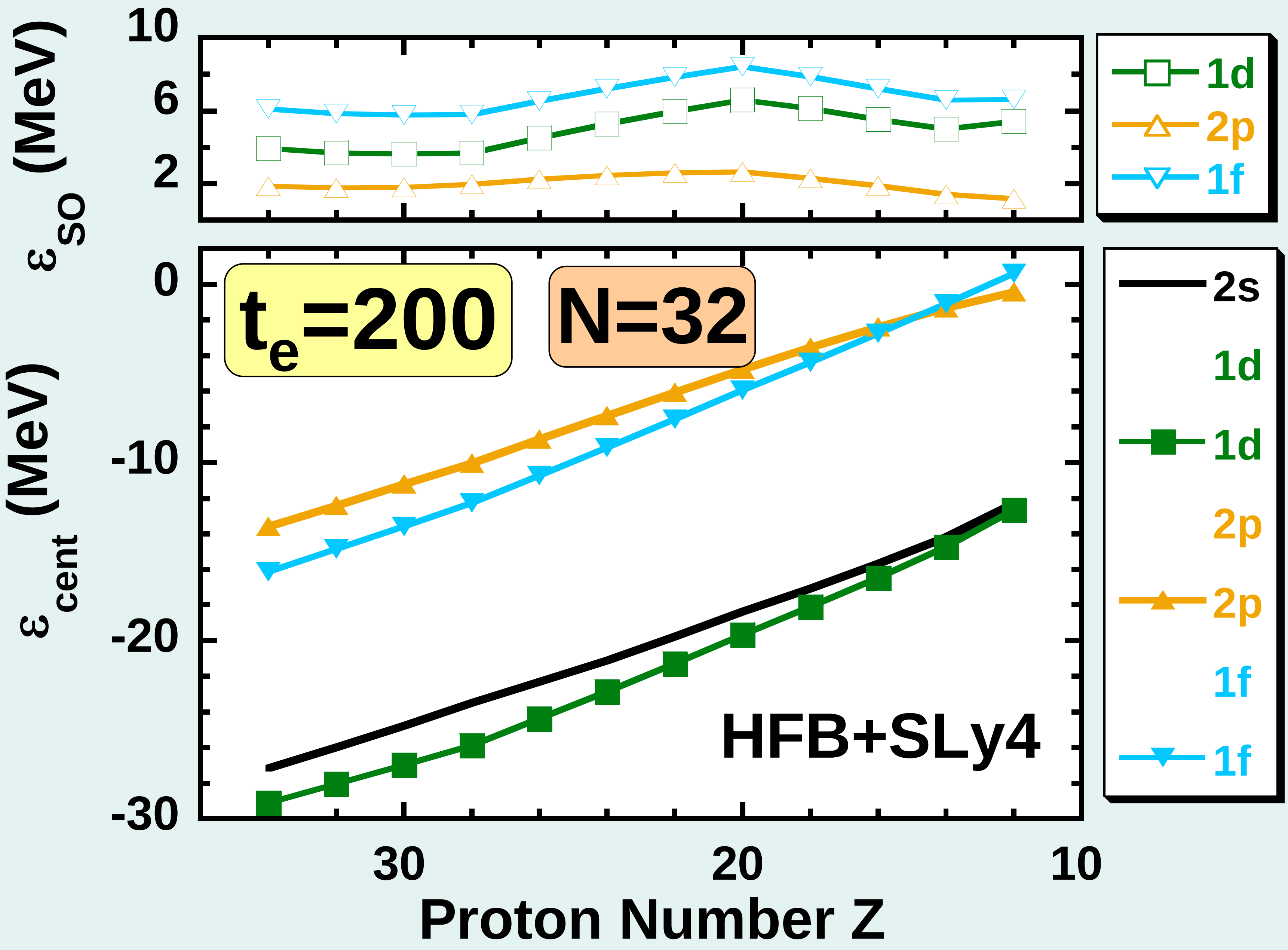
J. Dobaczewski, nucl-th/0604043



J. Dobaczewski, nucl-th/0604043



J. Dobaczewski, nucl-th/0604043



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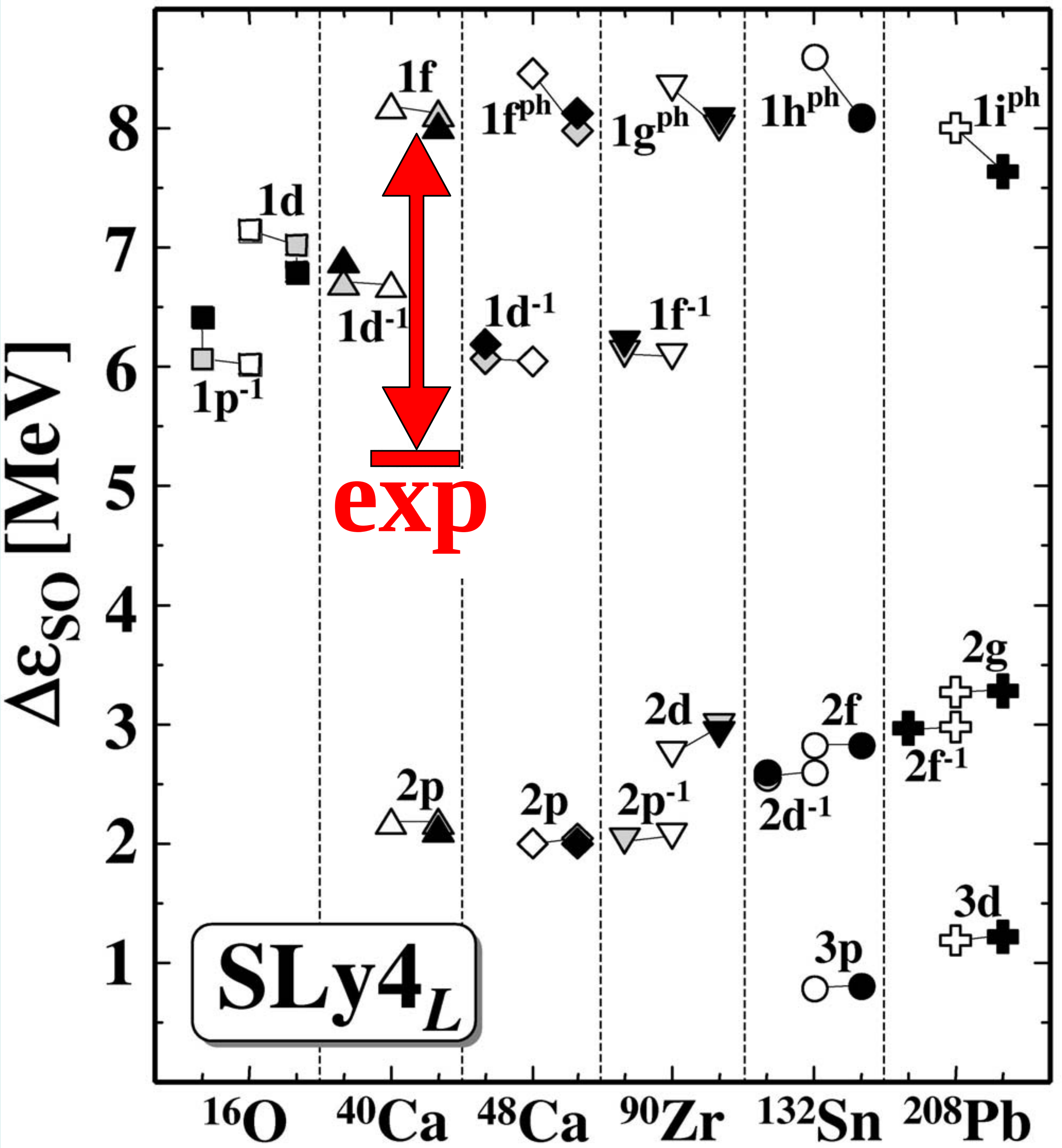
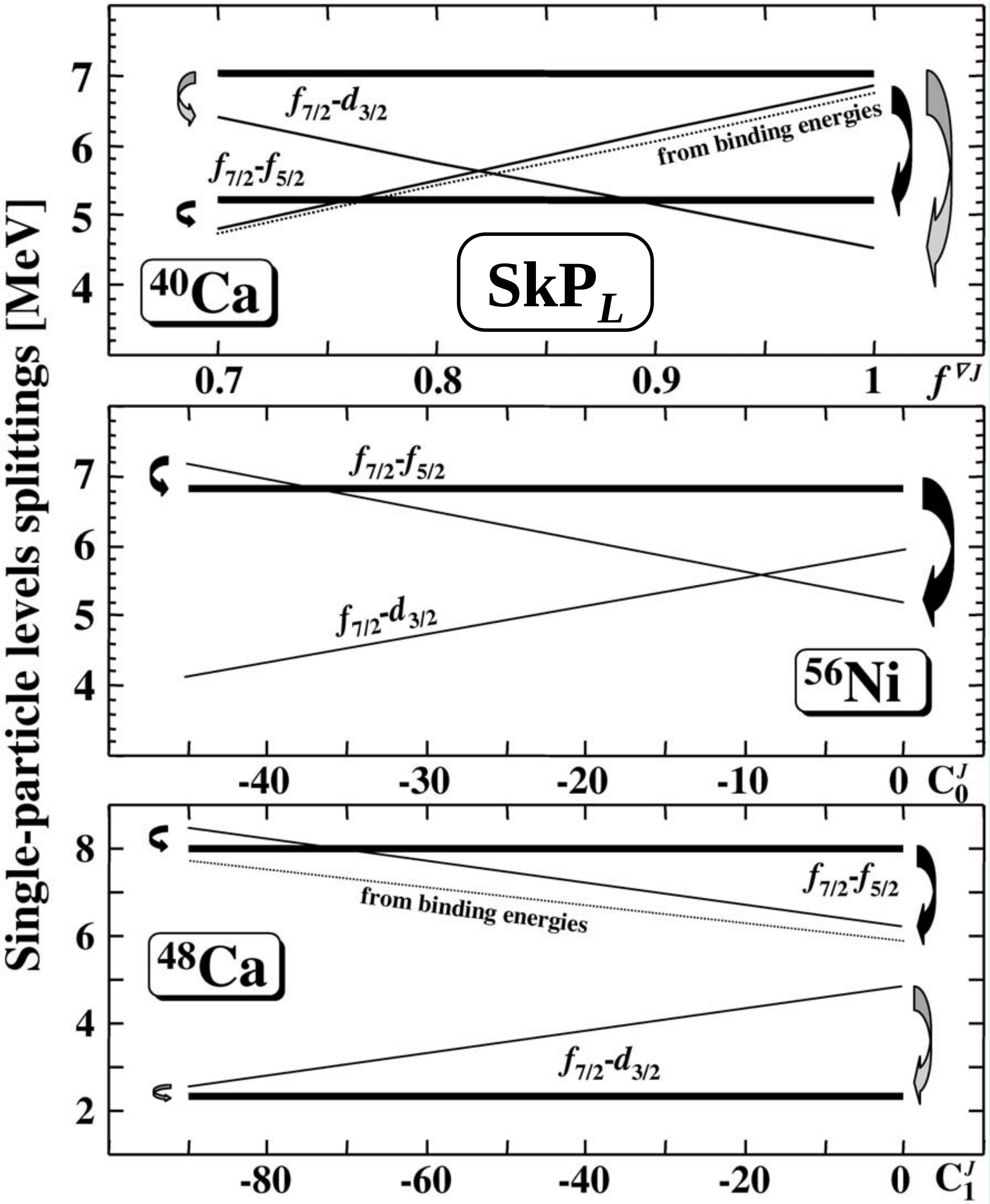


Polarization effects for neutron spin-orbit splitting

M. Zalewski *et al.*, Phys. Rev. C77, 024316 (2008)



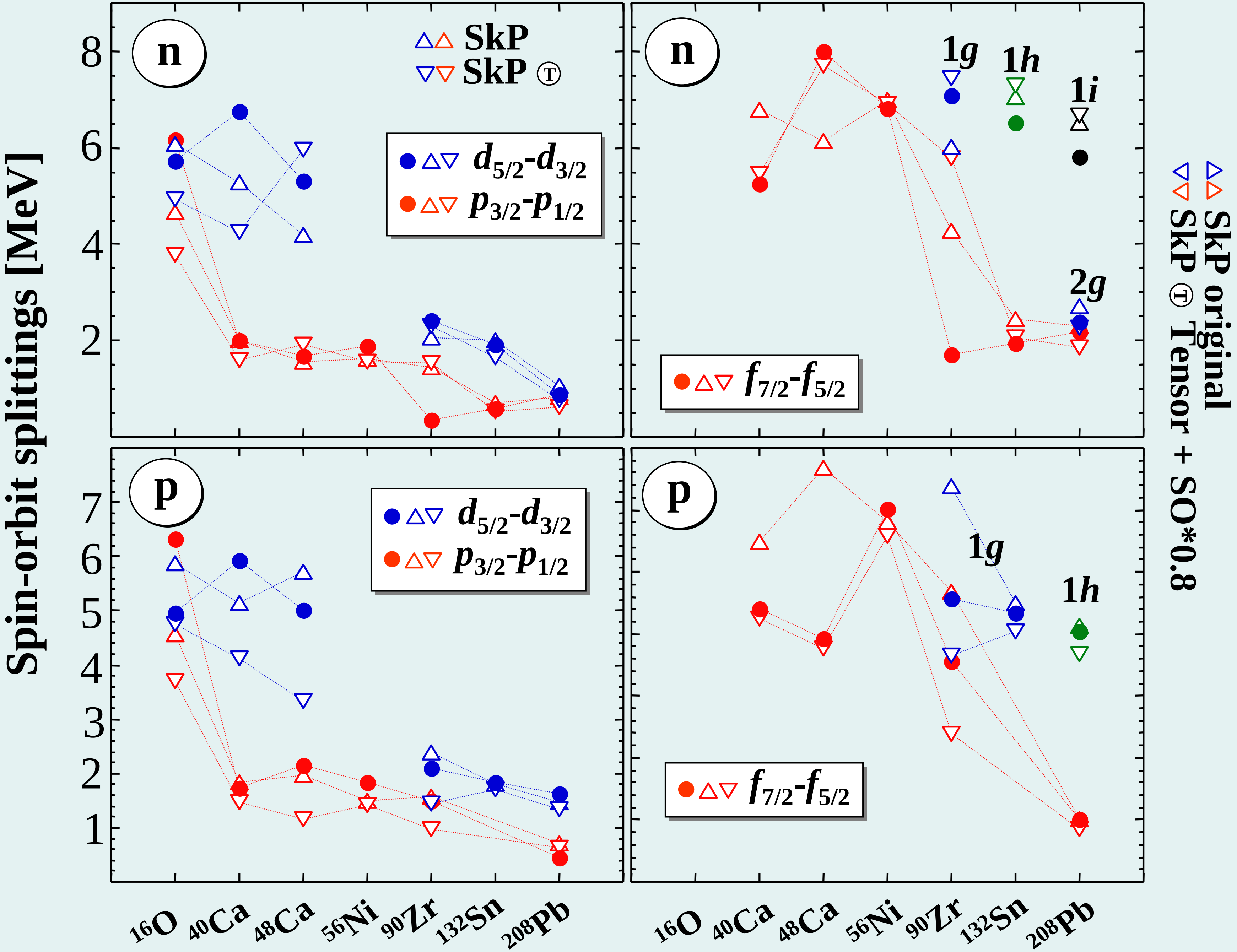
Fits of $C_0^{\nabla J}$, C_0^J, and C_1^J

M. Zalewski *et al.*, Phys. Rev. C77, 024316 (2008)

Fits of spin-orbit and tensor coupling constants

Skyrme force	$C_0^{\nabla J}$ [MeV fm^5]	$C_0^{\nabla J}/C_1^{\nabla J}$	C_0^J [MeV fm^5]	C_1^J [MeV fm^5]
SkP$_T$	-60.0	3	-38.6	-61.7
SLy4$_T$	-60.0	3	-45.0	-60.0
SkO$_T$	-61.8	-0.78	-33.1	-91.6

M. Zalewski *et al.*, Phys. Rev. C77, 024316 (2008)



M. Zalewski *et al.*, Phys. Rev. C77, 024316 (2008)

Jacek Dobaczewski

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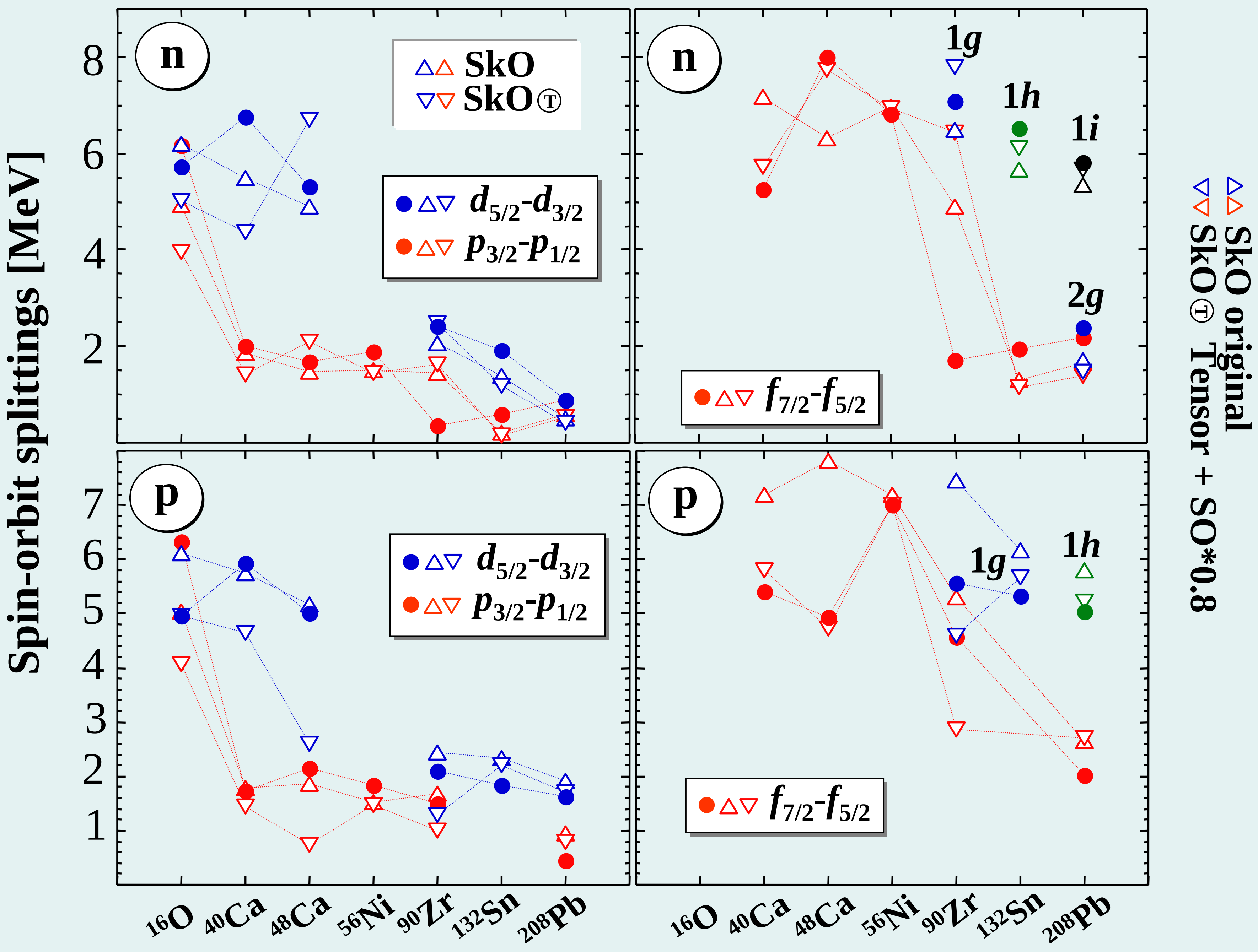

M. Zalewski *et al.*, Phys. Rev. C77, 024316 (2008)

Challenges

Collectivity

beyond mean field, ground-state correlations, shape coexistence, symmetry restoration, projection on good quantum numbers, configuration interaction, generator coordinate method, multi-reference DFT, etc....

$$E = \langle\Psi|\hat{H}|\Psi\rangle \simeq \int\!\!\int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,'\,\mathcal{H}(\rho(\vec{r},\vec{r}\,'))$$

True for mean field

$$\Downarrow$$

$$\text{for}\quad \rho(\vec{r},\vec{r}\,') = \frac{\langle\Psi|a^+(\vec{r}\,')a(\vec{r}\,')|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

$$\langle\Psi_1|\hat{H}|\Psi_2\rangle \simeq \int\!\!\int \mathrm{d}\vec{r}\,\mathrm{d}\vec{r}\,'\,\mathcal{H}(\rho_{12}(\vec{r},\vec{r}\,'))$$

$$\text{for}\quad \rho_{12}(\vec{r},\vec{r}\,') = \frac{\langle\Psi_1|a^+(\vec{r}\,')a(\vec{r}\,')|\Psi_2\rangle}{\langle\Psi_1|\Psi_2\rangle}$$

Extensions

★ **I. Range separation and exact long-range effects**

$$\mathcal{H}(\rho) = \mathcal{H}_{\text{long}}(\rho) + \mathcal{H}_{\text{short}}(\rho)$$

★ **II. Derivatives of higher order:**

$$\mathcal{H}(\rho) = \mathcal{H}(\rho, \tau, \tau_4, \tau_6, \Delta\rho, \Delta^2\rho, \Delta^3\rho, \ldots)$$

★ **III. Products of more than two densities:**

$$\mathcal{H}(\rho) = \mathcal{H}(\rho^2, \rho^3, \tau^2, \tau^3, \rho\tau, \rho^2\tau, \ldots)$$

Lessons learned

1) **Energy density functional exists due to the two-step variational method and gives exact ground state energy and its exact particle density.**

2) **Whenever the energy scales (or range scales) between the interactions and observations are different, the observations can be described by a series of pseudopotentials with coupling constants adjusted to data (an effective theory).**

3) **In nuclei, the non-local energy density functionals can be replaced by the local ones. This is because the range of the interaction is shorter than the range of variations in the local and non-local density matrix.**

4) **Systematic energy density functionals with derivative corrections can be constructed and the resulting self-consistent equations solved.**

5) **In finite systems, the phenomenon of spontaneous symmetry breaking is best captured by the mean-field or energy-density-functional methods.**

6) **Energy density functionals up to the second order in derivatives (Skyrme functionals) provide for a fair but not very precise description of global properties of nuclear ground states.**

Thank you