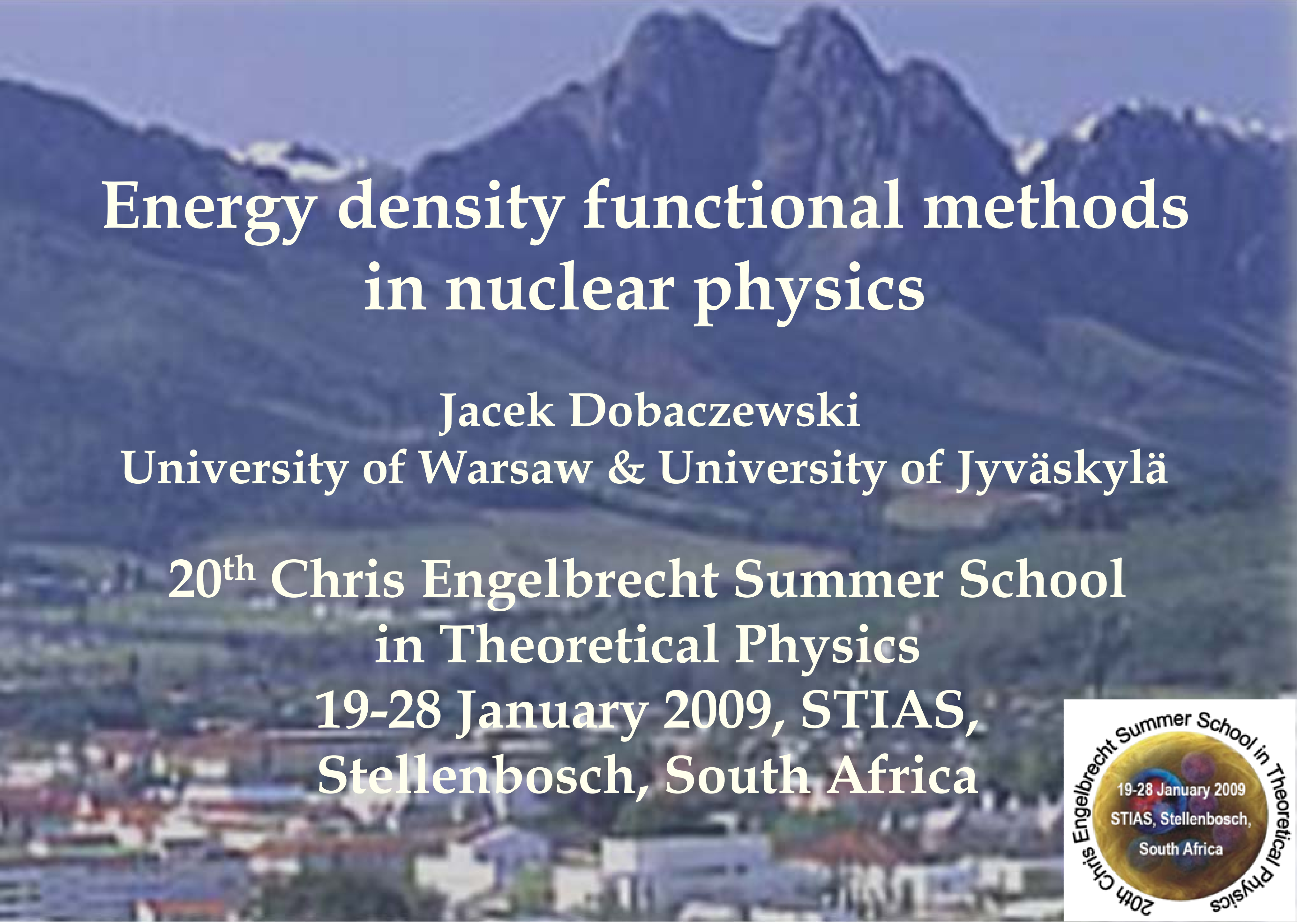

Energy density functional methods in nuclear physics

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20th Chris Engelbrecht Summer School
in Theoretical Physics
19-28 January 2009, STIAS,
Stellenbosch, South Africa

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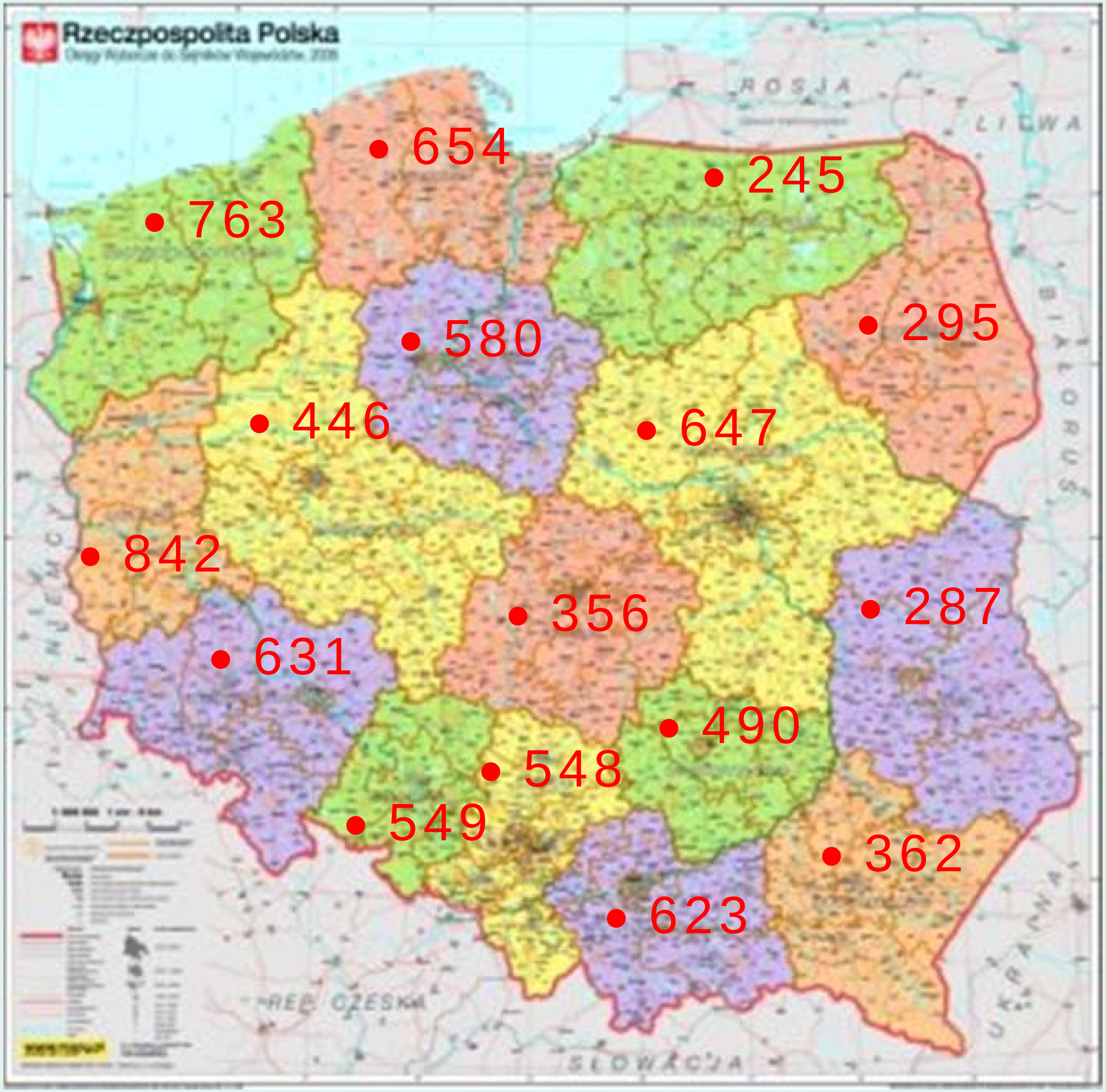
Reading materials:

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:1986-2005 draft of a book (in Polish)
http://www.fuw.edu.pl/~dobaczew/Czesc057d.pdf

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

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

Hohenberg-Kohn theorem

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

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

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:

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

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):

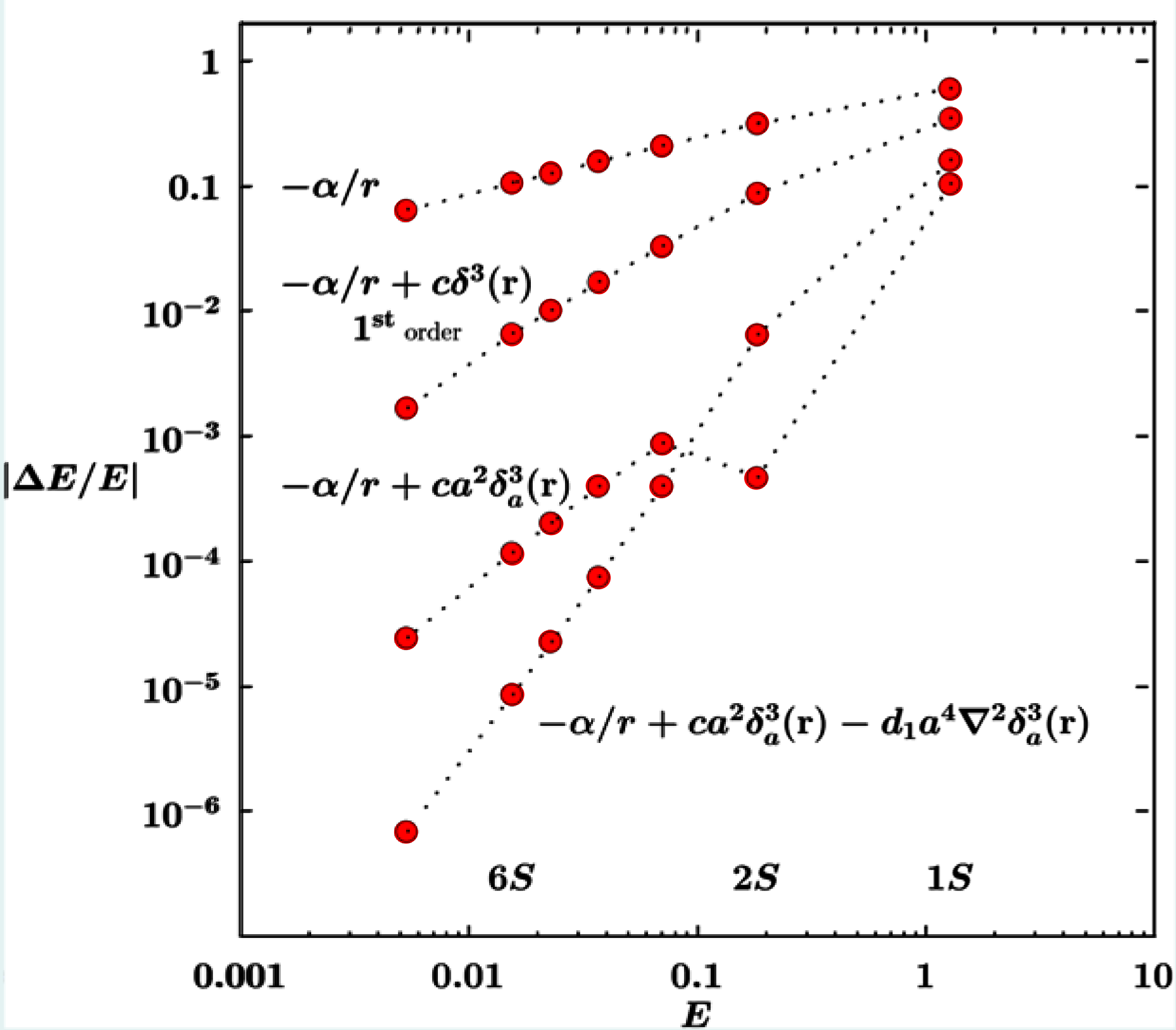
$$\mathcal{E}[\rho(\vec{r}),\tau(\vec{r})] = \frac{\hbar^2}{2m}\int \mathrm{d}^3\vec{r}\tau(\vec{r}) + \mathcal{E}^{\mathrm{int}}[\rho(\vec{r})].$$

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.

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, $kr \gg 1$:

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

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:

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

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

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

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

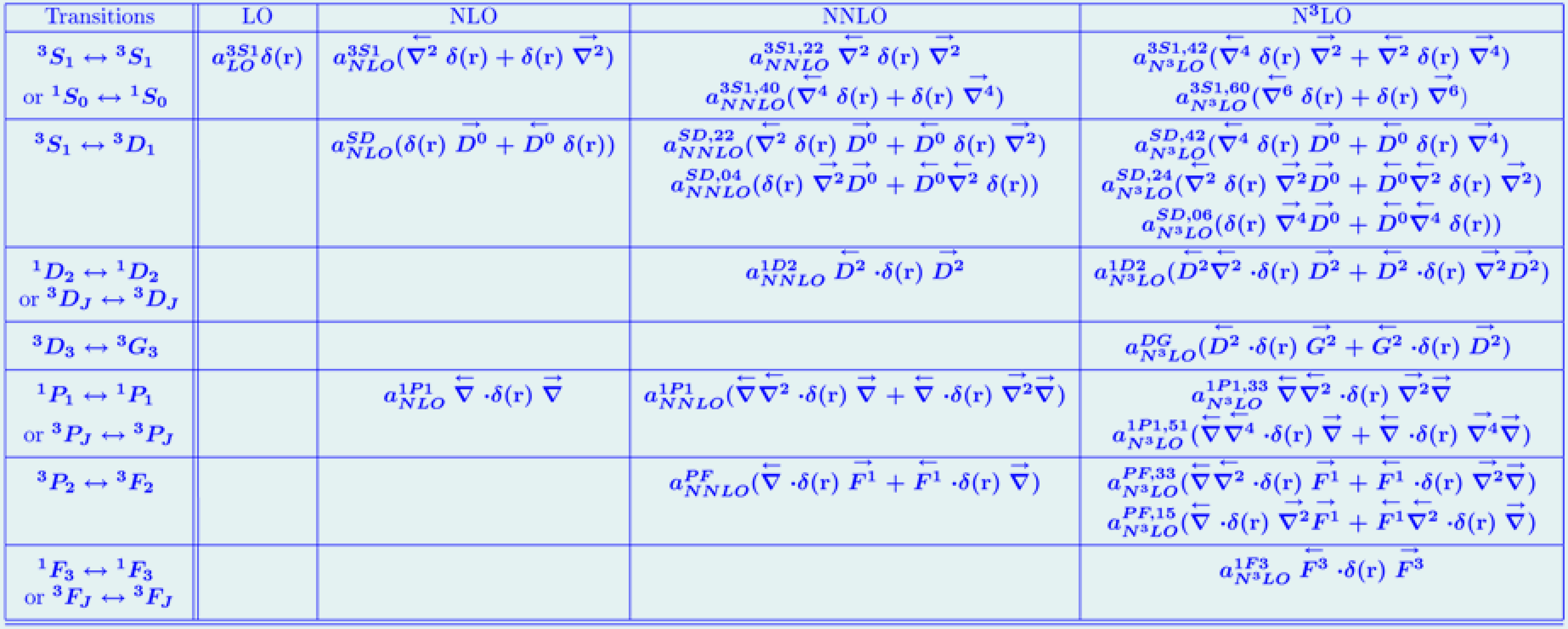
$$H^1_{\text{eff}} = -\frac{1}{2} \Psi^* \Psi \left(c_E \vec{E}^2 + c_B \vec{B}^2 \right)$$

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: $c_E = \chi_E a_0^3 \quad , \quad c_B = \chi_B a_0^3$ 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:

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

N^3LO in the chiral perturbation effective field theory

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



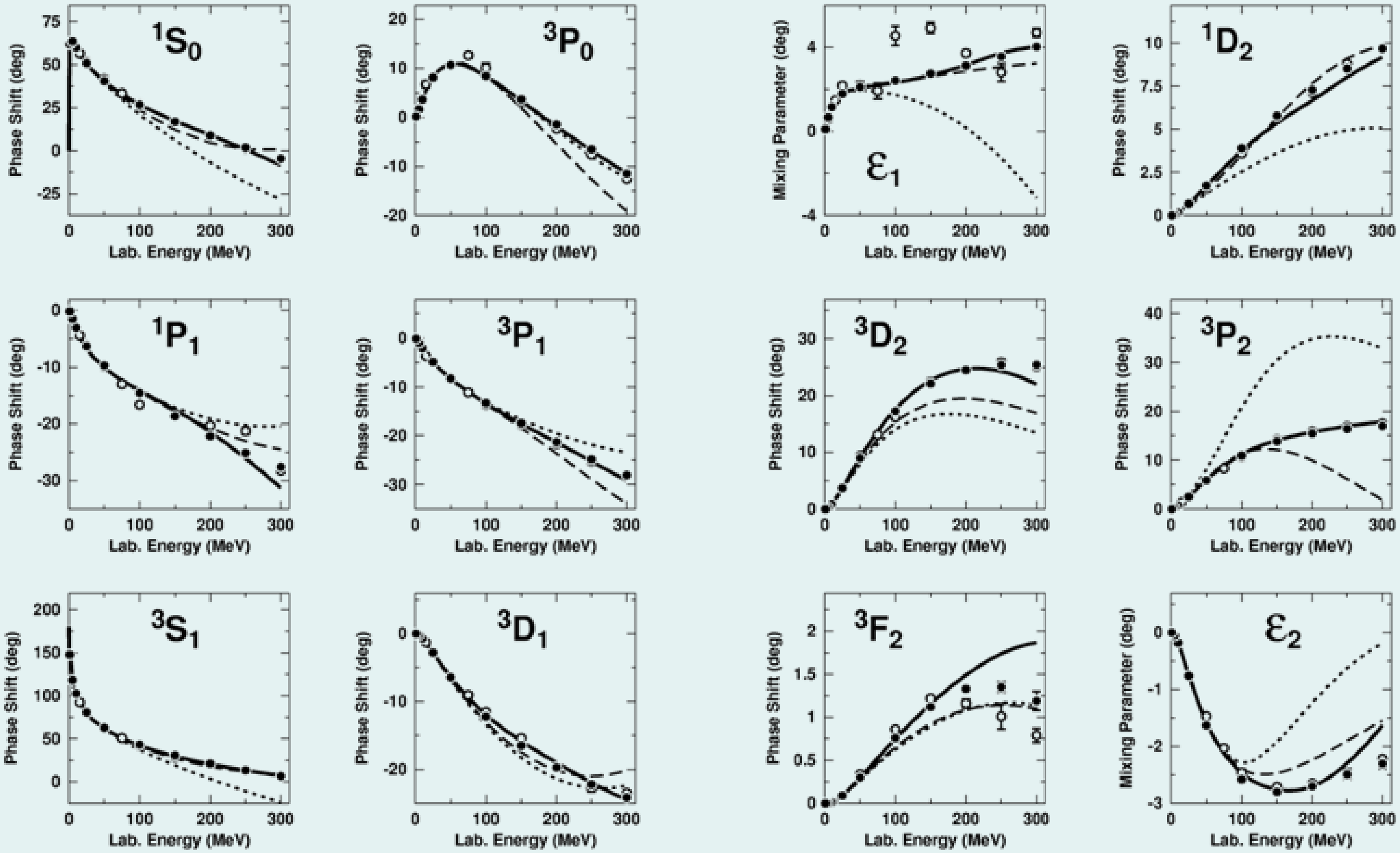
Transitions	LO	NLO	NNLO	N^3LO
${}^3S_1 \leftrightarrow {}^3S_1$ or ${}^1S_0 \leftrightarrow {}^1S_0$	$a^{3S1}_{LO}\delta(\mathrm{r})$	$a^{3S1}_{NLO}(\overleftarrow{\nabla}^2\ \delta(\mathrm{r}) + \delta(\mathrm{r})\ \overrightarrow{\nabla}^2)$	$a^{3S1,22}_{NNLO}\ \overleftarrow{\nabla}^2\ \delta(\mathrm{r})\ \overrightarrow{\nabla}^2$ $a^{3S1,40}_{NNLO}(\overleftarrow{\nabla}^4\ \delta(\mathrm{r}) + \delta(\mathrm{r})\ \overrightarrow{\nabla}^4)$	$a^{3S1,42}_{N^3LO}(\overleftarrow{\nabla}^4\ \delta(\mathrm{r})\ \overrightarrow{\nabla}^2 + \overleftarrow{\nabla}^2\ \delta(\mathrm{r})\ \overrightarrow{\nabla}^4)$ $a^{3S1,60}_{N^3LO}(\overleftarrow{\nabla}^6\ \delta(\mathrm{r}) + \delta(\mathrm{r})\ \overrightarrow{\nabla}^6)$
${}^3S_1 \leftrightarrow {}^3D_1$		$a^{SD}_{NLO}(\delta(\mathrm{r})\ \overrightarrow{D}^0 + \overleftarrow{D}^0\ \delta(\mathrm{r}))$	$a^{SD,22}_{NNLO}(\overleftarrow{\nabla}^2\ \delta(\mathrm{r})\ \overrightarrow{D}^0 + \overleftarrow{D}^0\ \delta(\mathrm{r})\ \overrightarrow{\nabla}^2)$ $a^{SD,04}_{NNLO}(\delta(\mathrm{r})\ \overrightarrow{\nabla}^2\overrightarrow{D}^0 + \overleftarrow{D}^0\overleftarrow{\nabla}^2\ \delta(\mathrm{r}))$	$a^{SD,42}_{N^3LO}(\overleftarrow{\nabla}^4\ \delta(\mathrm{r})\ \overrightarrow{D}^0 + \overleftarrow{D}^0\ \delta(\mathrm{r})\ \overrightarrow{\nabla}^4)$ $a^{SD,24}_{N^3LO}(\overleftarrow{\nabla}^2\ \delta(\mathrm{r})\ \overrightarrow{\nabla}^2\overrightarrow{D}^0 + \overleftarrow{D}^0\overleftarrow{\nabla}^2\ \delta(\mathrm{r})\ \overrightarrow{\nabla}^2)$ $a^{SD,06}_{N^3LO}(\delta(\mathrm{r})\ \overrightarrow{\nabla}^4\overrightarrow{D}^0 + \overleftarrow{D}^0\overleftarrow{\nabla}^4\ \delta(\mathrm{r}))$
${}^1D_2 \leftrightarrow {}^1D_2$ or ${}^3D_J \leftrightarrow {}^3D_J$			$a^{1D2}_{NNLO}\ \overleftarrow{D}^2 \cdot\delta(\mathrm{r})\ \overrightarrow{D}^2$	$a^{1D2}_{N^3LO}(\overleftarrow{D}^2\overleftarrow{\nabla}^2 \cdot\delta(\mathrm{r})\ \overrightarrow{D}^2 + \overleftarrow{D}^2 \cdot\delta(\mathrm{r})\ \overrightarrow{\nabla}^2\overrightarrow{D}^2)$
${}^3D_3 \leftrightarrow {}^3G_3$				$a^{DG}_{N^3LO}(\overleftarrow{D}^2 \cdot\delta(\mathrm{r})\ \overrightarrow{G}^2 + \overleftarrow{G}^2 \cdot\delta(\mathrm{r})\ \overrightarrow{D}^2)$
${}^1P_1 \leftrightarrow {}^1P_1$ or ${}^3P_J \leftrightarrow {}^3P_J$		$a^{1P1}_{NLO}\ \overleftarrow{\nabla} \cdot\delta(\mathrm{r})\ \overrightarrow{\nabla}$	$a^{1P1}_{NNLO}(\overleftarrow{\nabla}\overleftarrow{\nabla}^2 \cdot\delta(\mathrm{r})\ \overrightarrow{\nabla} + \overleftarrow{\nabla} \cdot\delta(\mathrm{r})\ \overrightarrow{\nabla}^2\overrightarrow{\nabla})$	$a^{1P1,33}_{N^3LO}\ \overleftarrow{\nabla}\overleftarrow{\nabla}^2 \cdot\delta(\mathrm{r})\ \overrightarrow{\nabla}^2\overrightarrow{\nabla}$ $a^{1P1,51}_{N^3LO}(\overleftarrow{\nabla}\overleftarrow{\nabla}^4 \cdot\delta(\mathrm{r})\ \overrightarrow{\nabla} + \overleftarrow{\nabla} \cdot\delta(\mathrm{r})\ \overrightarrow{\nabla}^4\overrightarrow{\nabla})$
${}^3P_2 \leftrightarrow {}^3F_2$			$a^{PF}_{NNLO}(\overleftarrow{\nabla} \cdot\delta(\mathrm{r})\ \overrightarrow{F}^1 + \overleftarrow{F}^1 \cdot\delta(\mathrm{r})\ \overrightarrow{\nabla})$	$a^{PF,33}_{N^3LO}(\overleftarrow{\nabla}\overleftarrow{\nabla}^2 \cdot\delta(\mathrm{r})\ \overrightarrow{F}^1 + \overleftarrow{F}^1 \cdot\delta(\mathrm{r})\ \overrightarrow{\nabla}^2\overrightarrow{\nabla})$ $a^{PF,15}_{N^3LO}(\overleftarrow{\nabla} \cdot\delta(\mathrm{r})\ \overrightarrow{\nabla}^2\overrightarrow{F}^1 + \overleftarrow{F}^1\overleftarrow{\nabla}^2 \cdot\delta(\mathrm{r})\ \overrightarrow{\nabla})$
${}^1F_3 \leftrightarrow {}^1F_3$ or ${}^3F_J \leftrightarrow {}^3F_J$				$a^{1F3}_{N^3LO}\ \overleftarrow{F}^3 \cdot\delta(\mathrm{r})\ \overrightarrow{F}^3$

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

Jacek Dobaczewski

JYVÄSKYLÄN YLIOPISTO

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

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:

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

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 $\begin{array}{ll} p_{ij}{=}{+}1 & \text{for all } ij\text{, i.e., } \hat{P}_{ij}\Psi{=}\Psi, \\ p_{ij}{=}{-}1 & \text{for all } ij\text{, i.e., } \hat{P}_{ij}\Psi{=}{-}\Psi. \end{array}$

In nature, we have only two kinds of particles: $\begin{array}{lll} \hat{P}_{ij}\Psi{=}\Psi & \Longrightarrow & \text{bosons} \\ \hat{P}_{ij}\Psi{=}{-}\Psi & \Longrightarrow & \text{fermions} \end{array}$

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:

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

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:

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

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

$$a^+_\mu \Phi_{\mu_1 \ldots \mu_A} := \begin{cases} 0 & \text{for} \quad \mu \in \{\mu_i\}, \\ \Phi_{\mu\mu_1 \ldots \mu_A} & \text{for} \quad \mu \not\in \{\mu_i\}. \end{cases}$$

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

$$a_\mu \Phi_{\mu_1 \ldots \mu_{A+1}} = \begin{cases} 0 & \text{for} \quad \mu \not\in \{\mu_i\}, \\ (-1)^{k+1} \Phi_{\mu_1 \ldots \overset{\text{no } \mu}{\smile} \ldots \mu_{A+1}} & \text{for} \quad \mu = \mu_k, \end{cases}$$

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 $\{A, B\} := AB + BA$:

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

which imply that in particular

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

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,

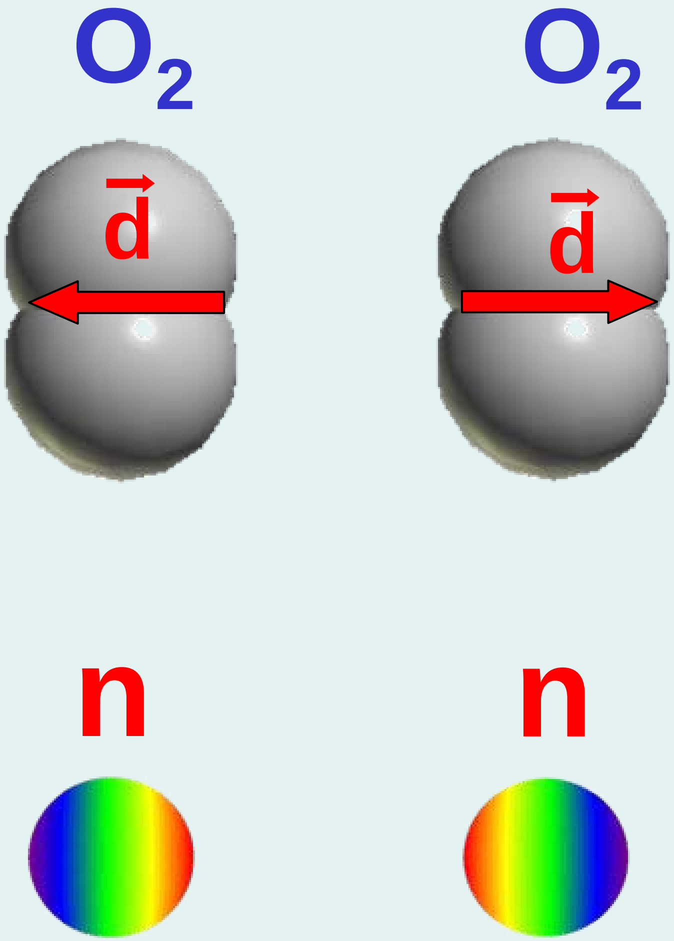
$$\begin{aligned} F_{\mu\nu} &= \int \mathrm{d}x\,\phi^*_\mu(x) f(x)\phi_\nu(x), \\ F_{\mu\mu'\nu\nu'} &= \int \mathrm{d}x\mathrm{d}x'\,\phi^*_\mu(x)\phi^*_{\mu'}(x') f(x,x') \times \left(\phi_\nu(x)\phi_{\nu'}(x') - \phi_{\nu'}(x)\phi_\nu(x')\right), \end{aligned}$$

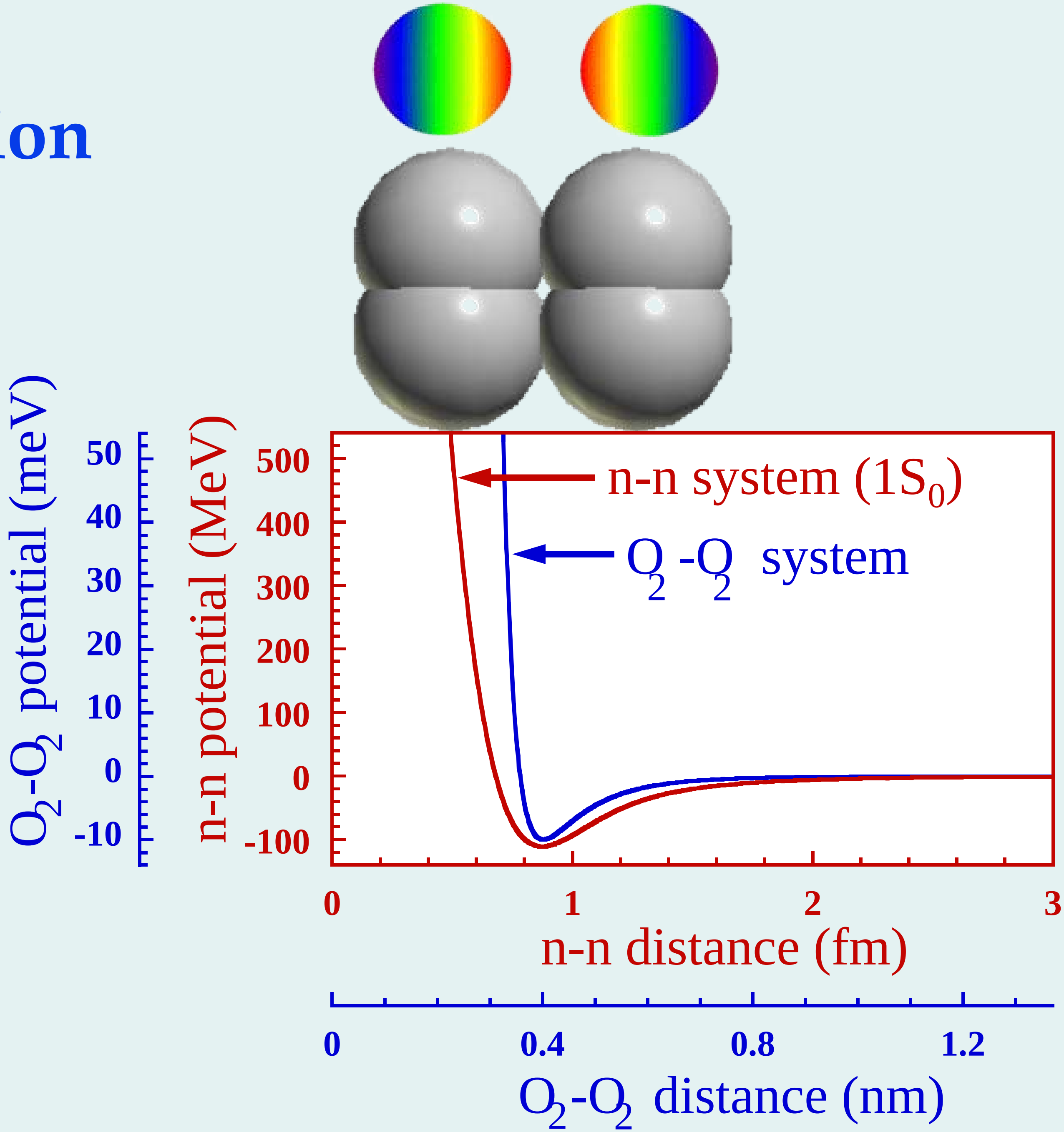
and

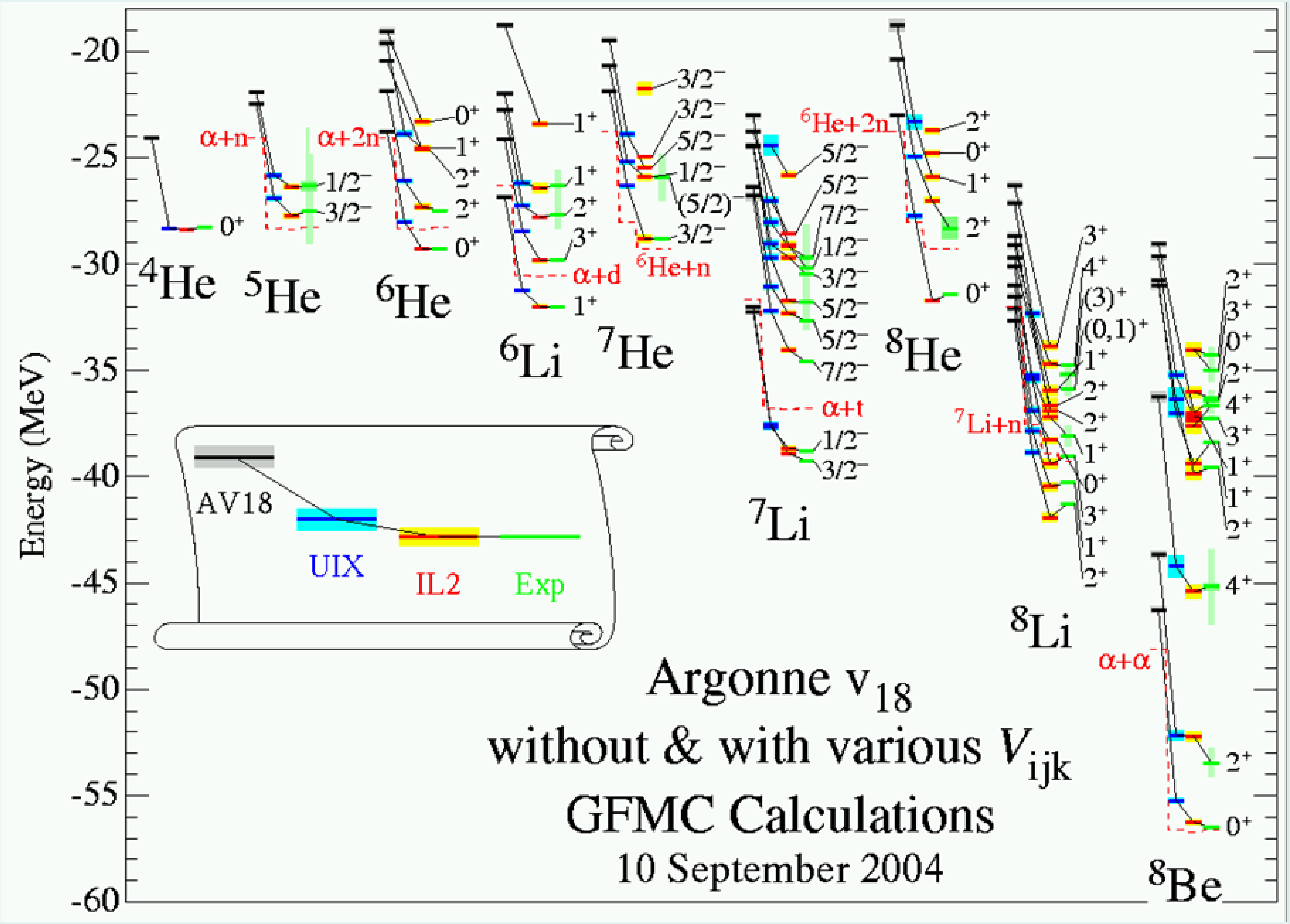
$$\begin{aligned} \hat{F}_1 &= \sum_{\mu\nu} F_{\mu\nu} a^+_\mu a_\nu, \\ \hat{F}_2 &= \frac{1}{4}\sum_{\mu\mu'\nu\nu'} F_{\mu\mu'\nu\nu'} a^+_\mu a^+_{\mu'} a_{\nu'} a_\nu, \\ \hat{F}_3 &= \frac{1}{36}\sum_{\mu\mu'\mu''\nu\nu'\nu''} F_{\mu\mu'\mu''\nu\nu'\nu''} a^+_\mu a^+_{\mu'} a^+_{\mu''} a_{\nu''}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

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

Thouless theorem for even states

Any even product state that is non-orthogonal to the vacuum $|0\rangle$ can be uniquely represented as:

$$|\Phi\rangle_{\text{even}} = \mathcal{N} \exp\left(-\tfrac{1}{2}\sum_{\mu\nu} Z^+_{\mu\nu} a^+_\mu a^+_\nu\right)|0\rangle, \qquad \text{where} \qquad Z^T = -Z.$$

The Thouless theorem is an immediate consequence of the Gauss factorization:

Any proper Bogoliubov transformation $\hat{\mathcal{A}}$ for det $A{\neq}0$ can be uniquely represented as:

$$\hat{\mathcal{A}} = \exp\left(-\hat{\mathcal{Z}}^+\right)\exp\left(\hat{\mathcal{D}}\right)\exp\left(\hat{\mathcal{Z}}'\right),$$

for

$$\begin{aligned}
\hat{\mathcal{Z}}^+ &= \tfrac{1}{2}\sum_{kl}\mathcal{Z}^+_{kl}c^+_k c_l = \tfrac{1}{2}\sum_{\mu\nu}Z^+_{\mu\nu}a^+_\mu a^+_\nu, \\
\hat{\mathcal{D}} &= \tfrac{1}{2}\sum_{kl}\mathcal{D}_{kl}c^+_k c_l = \sum_{\mu\nu}D_{\mu\nu}a^+_\mu a_\nu - \tfrac{1}{2}\mathrm{Tr}D, \\
\hat{\mathcal{Z}}' &= \tfrac{1}{2}\sum_{kl}\mathcal{Z}'_{kl}c^+_k c_l = \tfrac{1}{2}\sum_{\mu\nu}Z'_{\mu\nu}a_\mu a_\nu,
\end{aligned}$$

i.e.,

$$\mathcal{Z}^+ = \begin{pmatrix} 0 & Z^+ \\ 0 & 0 \end{pmatrix}, \quad \mathcal{D} = \begin{pmatrix} D & 0 \\ 0 & -D^T \end{pmatrix}, \quad \mathcal{Z}' = \begin{pmatrix} 0 & 0 \\ Z' & 0 \end{pmatrix},$$

where matrices Z and Z' are antisymmetric.

Gauss factorization

The Gauss factorization can easily be proved for the matrix Bogoliubov transformation:

$$\mathcal{A} = \exp\left(-\mathcal{Z}^{+}\right)\exp\left(\mathcal{D}\right)\exp\left(\mathcal{Z}'\right).$$

First we note that squares of matrices $\mathcal{Z}$ i $\mathcal{Z}'$ are equal to zero; hence by Taylor expanding the exponents we have:

$$\mathcal{A} = \begin{pmatrix} A & B^* \\ B & A^* \end{pmatrix} = \begin{pmatrix} 1 & -Z^+ \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \exp(D) & 0 \\ 0 & \exp(-D^T) \end{pmatrix}\begin{pmatrix} 1 & 0 \\ Z' & 1 \end{pmatrix},$$

and therefore

$$\begin{aligned} A &= \exp(D) - Z^+\exp(-D^T)Z', \\ B^* &= -Z^+\exp(-D^T), \\ B &= \exp(-D^T)Z', \\ A &= \exp(-D^T). \end{aligned}$$

which gives

$$\begin{aligned} \exp(D) &= (A^+)^{-1}, \\ Z &= BA^{-1}, \\ Z' &= (A^*)^{-1}B, \end{aligned}$$

while the remaining relation is automatically fulfilled:

$$\begin{aligned} \exp(D) - Z^+\exp(-D^T)Z' &= (A^+)^{-1} - (A^+)^{-1}B^+A^*(A^*)^{-1}B \\ &= (A^+)^{-1}(1 - B^+B) = A, \end{aligned}$$

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 matrices and Wick theorem

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

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

Density matrix and pairing tensor:

$$
\rho_{\mu\nu} = \langle\Phi|a^+_\nu a_\mu|\Phi\rangle = \overbracket{a^+_\nu a_\mu}, \qquad \kappa_{\mu\nu} = \langle\Phi|a_\nu a_\mu|\Phi\rangle = \overbracket{a_\nu a_\mu},
$$

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

$$
\hat{H} = \hat{T} + \hat{V} = \sum_{\mu\nu} T_{\mu\nu} a^+_\mu a_\nu + \frac{1}{4}\sum_{\mu\lambda\nu\pi} V_{\mu\lambda\nu\pi} a^+_\mu a^+_\lambda a_\pi a_\nu ,
$$

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

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

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

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

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

Then, the *direct* selfconsistent potential reads:

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

which gives $\Gamma^{dir}(\vec r_1)=\displaystyle\int_{\vec r_2}\frac{\rho(\vec r_2)}{|\vec r_1-\vec r_2|}$ 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:

$$\begin{aligned}\Gamma^{exc}_{\mu\nu}&=\sum\nolimits_{\lambda\pi}\tilde V_{\mu\lambda\nu\pi}\rho_{\pi\lambda}\\&=\sum\nolimits_{\lambda\pi}\sum\!\!\!\!\!\!\int_{\vec r_1\sigma_1}\sum\!\!\!\!\!\!\int_{\vec r_2\sigma_2}\sum\!\!\!\!\!\!\int_{\vec r\,'_1\sigma'_1}\sum\!\!\!\!\!\!\int_{\vec r\,'_2\sigma'_2}\\&\quad\phi^*_\mu(\vec r_1\sigma_1)\;\phi^*_\lambda(\vec r_2\sigma_2)\;V(\vec r_1\sigma_1,\vec r_2\sigma_2;\vec r\,'_1\sigma'_1,\vec r\,'_2\sigma'_2)\;\overset{\Downarrow}{\phi_\pi}(\vec r\,'_1\sigma'_1)\;\overset{\Downarrow}{\phi_\nu}(\vec r\,'_2\sigma'_2)\rho_{\pi\lambda}\\&=\sum\nolimits_{\lambda\pi}\sum\!\!\!\!\!\!\int_{\vec r_1\sigma_1}\sum\!\!\!\!\!\!\int_{\vec r_2\sigma_2}\\&\quad\phi^*_\mu(\vec r_1\sigma_1)\;\phi^*_\lambda(\vec r_2\sigma_2)\frac{1}{|\vec r_1-\vec r_2|}\;\phi_\pi(\vec r_1\sigma_1)\;\phi_\nu(\vec r_2\sigma_2)\rho_{\pi\lambda}\\&=\sum\!\!\!\!\!\!\int_{\vec r_1\sigma_1}\sum\!\!\!\!\!\!\int_{\vec r_2\sigma_2}\phi^*_\mu(\vec r_1\sigma_1)\left[\frac{\rho(\vec r_1\sigma_1,\vec r_2\sigma_2)}{|\vec r_1-\vec r_2|}\right]\;\phi_\nu(\vec r_2\sigma_2),\end{aligned}$$

which gives $\Gamma^{exc}(\vec r_1\sigma_1,\vec r_2\sigma_2)=\dfrac{\rho(\vec r_1\sigma_1,\vec r_2\sigma_2)}{|\vec r_1-\vec r_2|}.$

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 $V(\vec{r}_1',\vec{r}_2';\vec{r}_1,\vec{r}_2)$ the Hartree-Fock interaction energy has the form

$$\begin{aligned}\mathcal{E}^{\text{int}} &= \tfrac{1}{2}\int \mathrm{d}^3\vec{r}_1'\mathrm{d}^3\vec{r}_2'\mathrm{d}^3\vec{r}_1\mathrm{d}^3\vec{r}_2 V(\vec{r}_1',\vec{r}_2';\vec{r}_1,\vec{r}_2)\times \\ &\qquad (\rho(\vec{r}_1,\vec{r}_1')\rho(\vec{r}_2,\vec{r}_2') - \rho(\vec{r}_2,\vec{r}_1')\rho(\vec{r}_1,\vec{r}_2'))\end{aligned}$$

while for a local interaction,

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

the interaction energy reduces to:

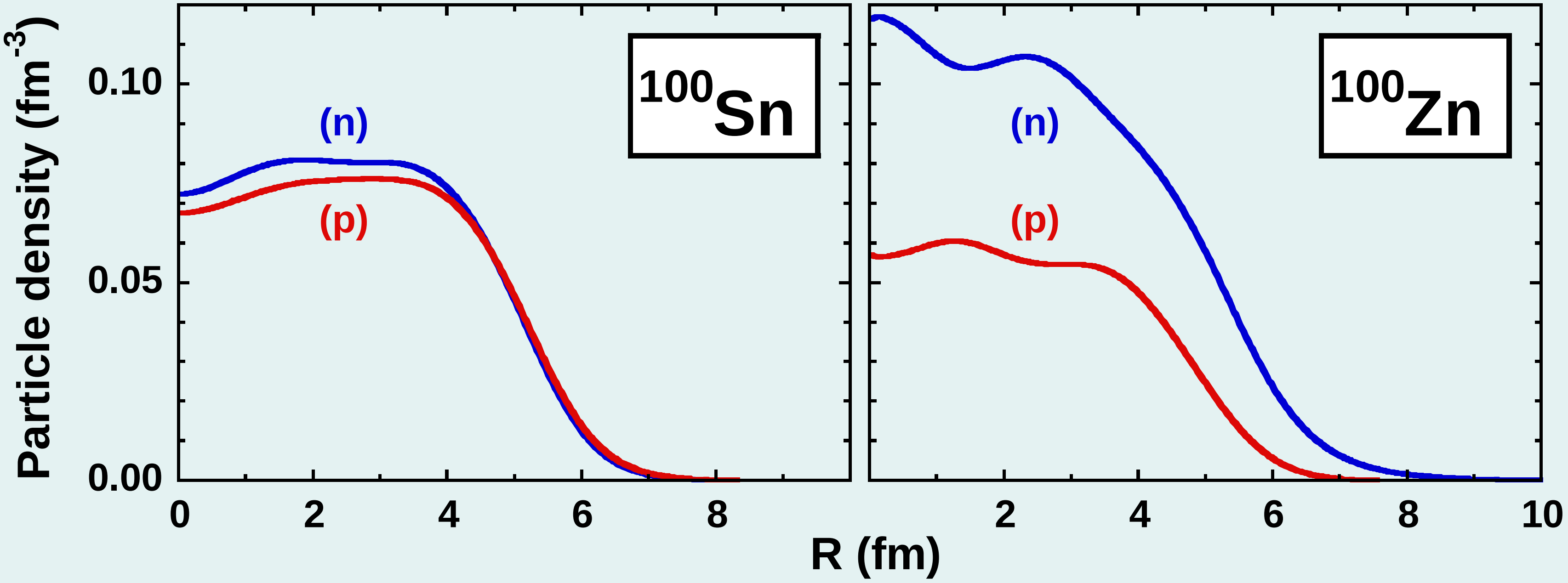
$$\mathcal{E}^{\text{int}} = \tfrac{1}{2}\int \mathrm{d}^3\vec{r}_1\mathrm{d}^3\vec{r}_2 \overbrace{V(\vec{r}_1,\vec{r}_2)(\rho(\vec{r}_1)\rho(\vec{r}_2) - \rho(\vec{r}_2,\vec{r}_1)\rho(\vec{r}_1,\vec{r}_2))}^{\text{Nonlocal energy density}},$$

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.

$$\begin{aligned}\mathcal{E}^{\text{int}}_{\text{dir}} &= \tfrac{1}{2}\int \mathrm{d}^3\vec{r}_1\mathrm{d}^3\vec{r}_2 V(\vec{r}_1,\vec{r}_2)\rho(\vec{r}_1)\rho(\vec{r}_2), \\ \mathcal{E}^{\text{int}}_{\text{exc}} &= \tfrac{1}{2}\int \mathrm{d}^3\vec{r}_1\mathrm{d}^3\vec{r}_2 V(\vec{r}_1,\vec{r}_2)\rho(\vec{r}_2,\vec{r}_1)\rho(\vec{r}_1,\vec{r}_2),\end{aligned}$$

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

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

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

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

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

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

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

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,

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

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,

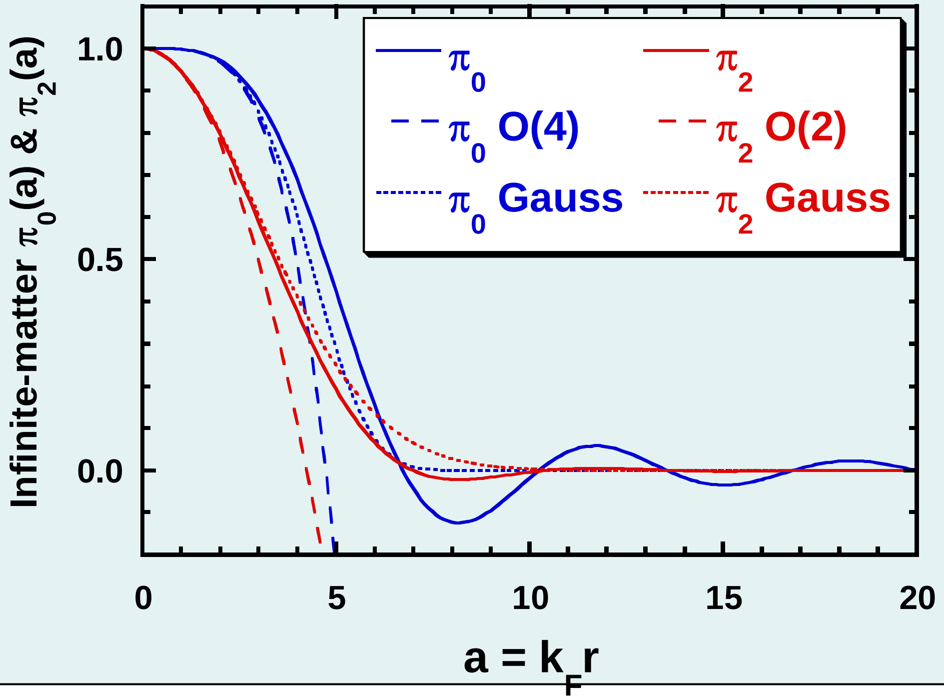
$$V_k^{ij} = \int \mathrm{d}^3\vec{r}\, r^k \pi_i(r)\pi_j(r)V(r) = 4\pi\int \mathrm{d}r\, r^{k+2}\pi_i(r)\pi_j(r)V(r).$$

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 $\pi_2(r) = 0$.



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 $r \simeq 4.4934/k_F \simeq 3\,\mathrm{fm}$, 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 $\partial_i{=}\partial/\partial r^i$ 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:

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

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

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

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

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

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

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

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:

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

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

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,

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

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

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 μ_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.

Density-matrix expansion (7)

We can now repeat derivations performed in the previous section for an arbitrary finite-range local nuclear interaction composed of the standard central, spin-orbit, and tensor terms,

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

where $r{=}|\vec{r}|{=}|\vec{r}_1{-}\vec{r}_2|$, $P_\sigma{=}\frac{1}{2}(1{+}\vec{\sigma}_1{\cdot}\vec{\sigma}_2)$, $P_\tau{=}\frac{1}{2}(1{+}\vec{\tau}_1{\cdot}\vec{\tau}_2)$, $\vec{L}{=}{-}i\hbar\vec{r}{\times}\vec{\partial}$, $\vec{S}{=}\frac{\hbar}{2}(\vec{\sigma}_1{+}\vec{\sigma}_2)$, and $S_{12}{=}3(\vec{\sigma}_1\cdot\vec{r})(\vec{\sigma}_2\cdot\vec{r})/r^2{-}\vec{\sigma}_1\cdot\vec{\sigma}_2$. After straightforward calculations, one obtains the interaction energy in the form of a local integral,

$$\begin{aligned}\mathcal{E}^{\text{int}} = \int\text{d}^3\vec{r}\sum\nolimits_{t=0,1}[&C_t^\rho\rho_t^2+C_t^{\Delta\rho}\rho_t\Delta\rho_t+C_t^\tau(\rho_t\tau_t-\vec{j}_t^{\,2}) \\ &+C_t^s\vec{s}_t^{\,2}+C_t^{\Delta s}\vec{s}_t\cdot\Delta\vec{s}_t+C_t^T(\vec{s}_t\cdot\vec{T}_t-\overset{\leftrightarrow}{J}_t^{\,2}) \\ &+C_t^{\nabla J}(\rho_t\vec{\nabla}\cdot\vec{J}_t+\vec{s}_t\cdot(\vec{\nabla}\times\vec{j}_t))]\end{aligned}$$

Density-matrix expansion (8)

$$8\begin{pmatrix} C_0^\rho \\ C_1^\rho \\ C_0^s \\ C_1^s \end{pmatrix} = \begin{pmatrix} 4 & 2 & -2 & -1 \\ 0 & 0 & -2 & -1 \\ 0 & 2 & 0 & -1 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} W_0 + M_0^{00} \\ B_0 + H_0^{00} \\ H_0 + B_0^{00} \\ M_0 + W_0^{00} \end{pmatrix},$$

$$96\begin{pmatrix} C_0^{\Delta\rho} \\ C_1^{\Delta\rho} \\ C_0^{\tau} \\ C_1^{\tau} \\ C_0^{\Delta s} \\ C_1^{\Delta s} \\ C_0^{T} \\ C_1^{T} \end{pmatrix} = \begin{pmatrix} 8 & -1 & 4 & -2 & -4 & 2 & -2 & 4 \\ 0 & -1 & 0 & -2 & -4 & 0 & -2 & 0 \\ 0 & 4 & 0 & 8 & 0 & -8 & 0 & -16 \\ 0 & 4 & 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & 2 & -2 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & -2 & 0 \\ 0 & 4 & 0 & 0 & 0 & -8 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} W_2 \\ W_2^{02} \\ B_2 \\ B_2^{02} \\ H_2 \\ H_2^{02} \\ M_2 \\ M_2^{02} \end{pmatrix},$$

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

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

$$X_k = \int \mathrm{d}^3\vec{r}\, r^k X(r),$$

$$X_k^{ij} = \int \mathrm{d}^3\vec{r}\, r^k \pi_i(r)\pi_j(r) X(r),$$

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

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:

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

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	$\vec{s}\cdot\vec{F}$

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.*,
Phys. Rev. C69 (2004) 014316

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

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

where × stands for the vector product

Pairing

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

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:

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

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.

II. Derivatives of higher order up to N^{3}LO

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

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

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

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

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

Energy density functional up to N^3LO

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

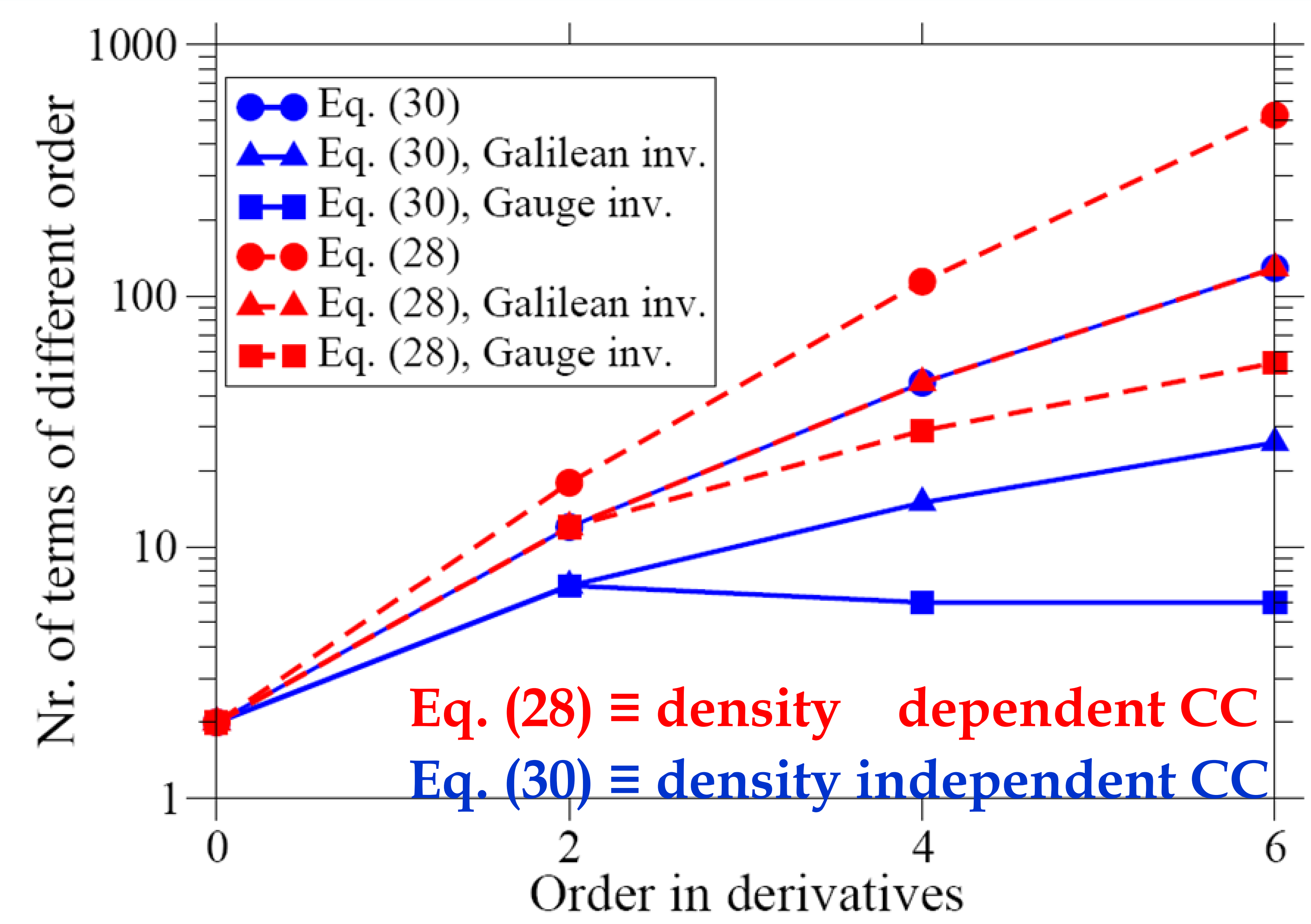
Numbers of primary ($m = 0$) local-densities up to N^3LO.

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^3LO	93	95	188	50	21

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

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

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

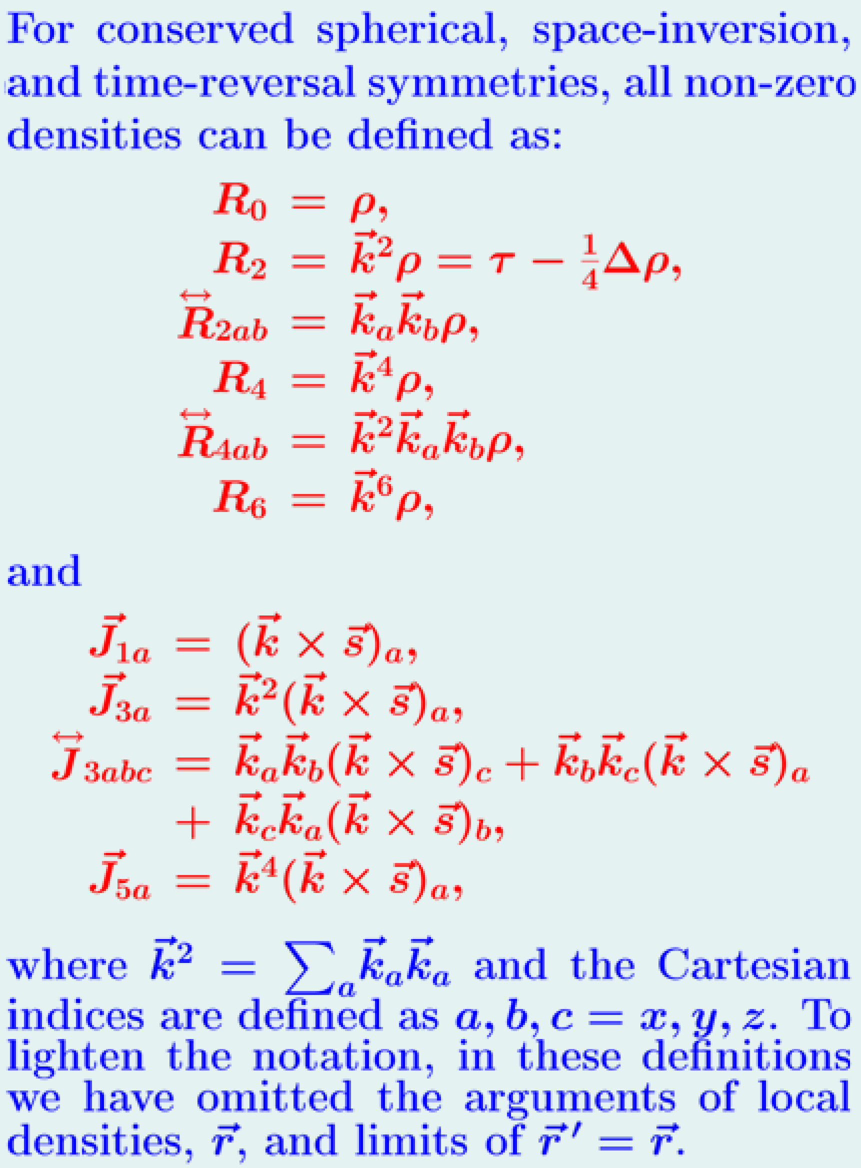


Eq. (28) ≡ density dependent CC

Eq. (30) ≡ density independent CC

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

Energy density functional for spherical nuclei (I)



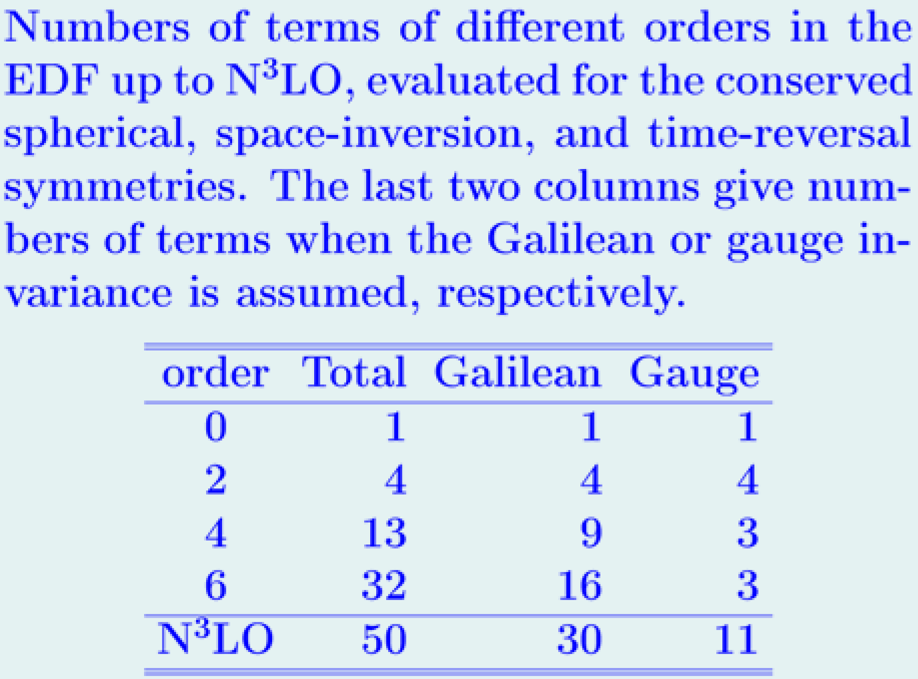
For conserved spherical, space-inversion, and time-reversal symmetries, all non-zero densities can be defined as:

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

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	13	9	3
6	32	16	3
N^{3}LO	50	30	11

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

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

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

$$\begin{aligned} \mathcal{H}_2 &= C^0_{20} R_0 \Delta R_0 + C^0_{02} R_0 R_2 \\ \text{[0.5ex]} &+ C^0_{11} R_0 \vec{\nabla} \cdot \vec{J}_1, + C^1_{01} \vec{J}_1^2, \end{aligned}$$

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

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

At sixth order, the energy density reads

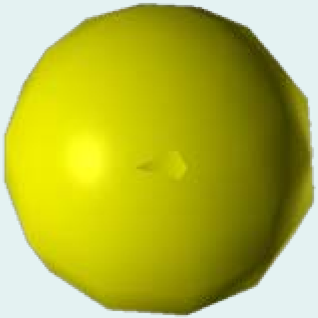
$$\begin{aligned} \mathcal{H}_6 &= C^0_{60} R_0 \Delta^3 R_0 + C^0_{42} R_0 \Delta^2 R_2 \\ &+ C^0_{24} R_0 \Delta R_4 + C^0_{06} R_0 R_6 \\ &+ C^2_{22} R_2 \Delta R_2 + C^2_{04} R_2 R_4 \\ &+ D^0_{42} R_0 \Delta \sum\nolimits_{ab} \vec{\nabla}_a \vec{\nabla}_b \overleftrightarrow{R}_{2ab} + D^0_{24}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

The energy densities above are given in terms of 50 coupling constants $C^{n'}_{mn}$, $D^{n'}_{mn}$, $E^{n'}_{mn}$, and $F^{n'}_{mn}$.

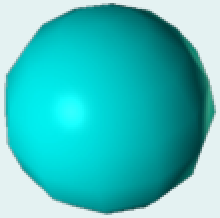
B.G. Carlsson *et al.*, C 78, 044326 (2008)

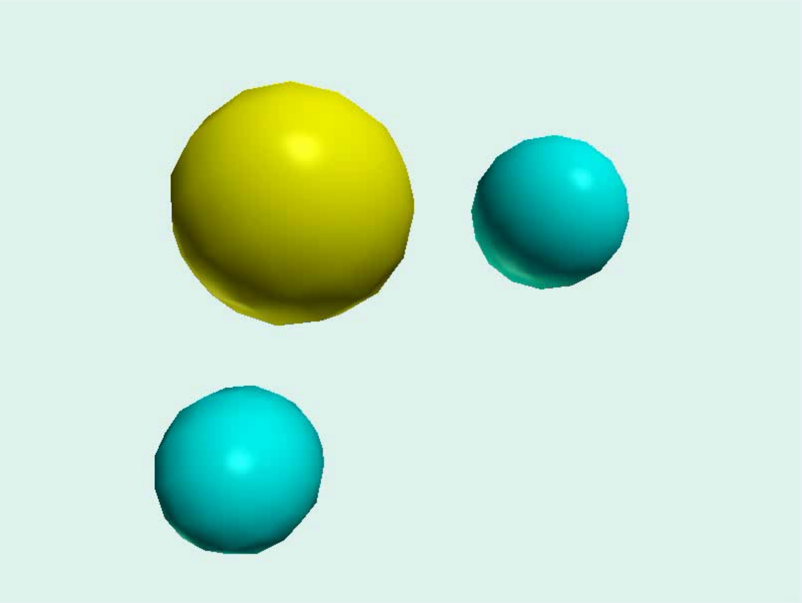
Ammonia molecule NH_3

Nitrogen atom

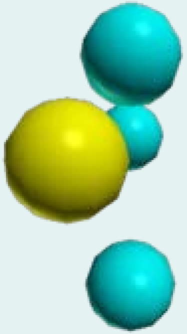


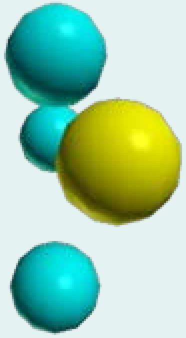
Hydrogen atom





$|L\rangle =$



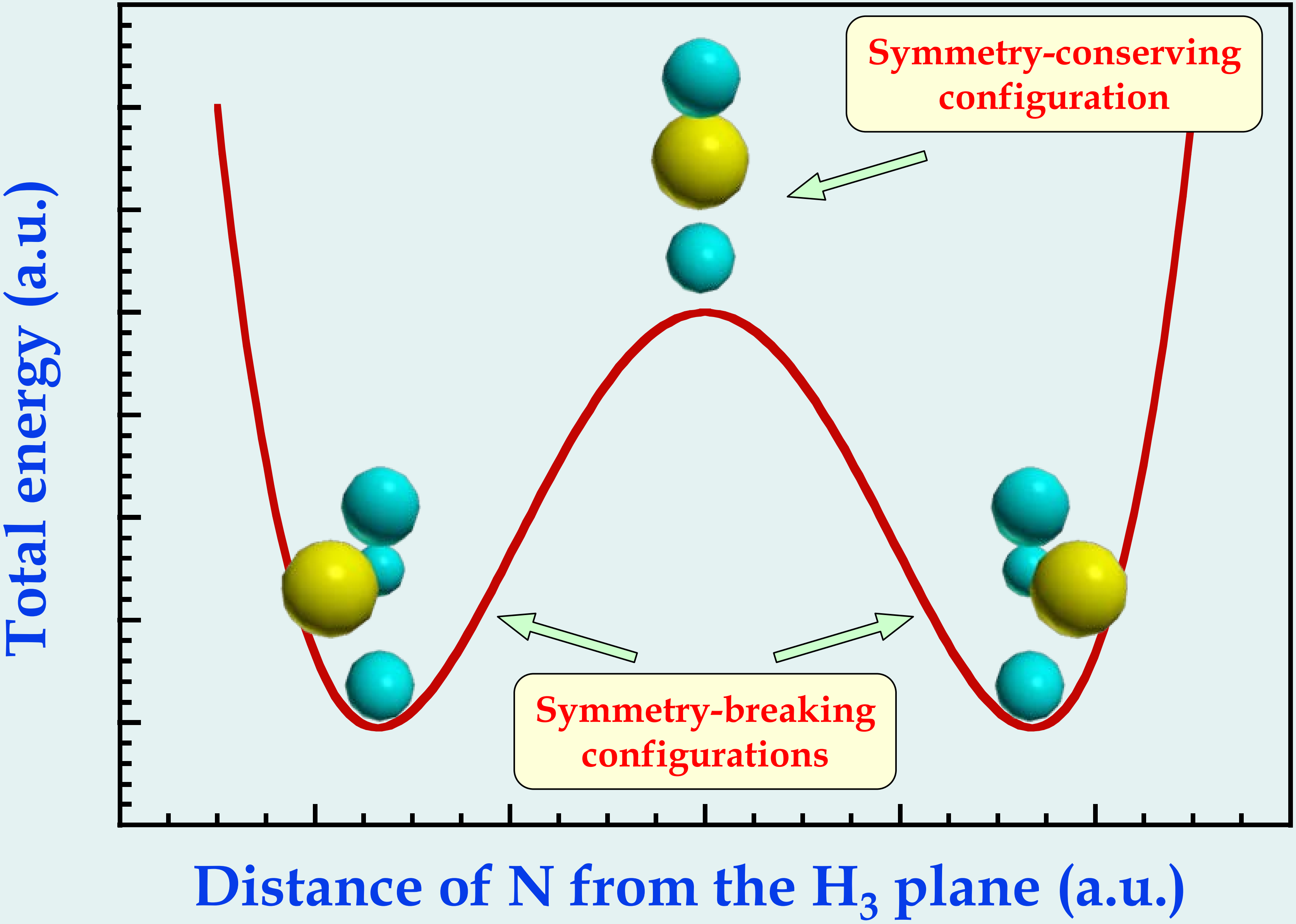


$= |R\rangle$

left state

right state

Ammonia molecule NH_3



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.,

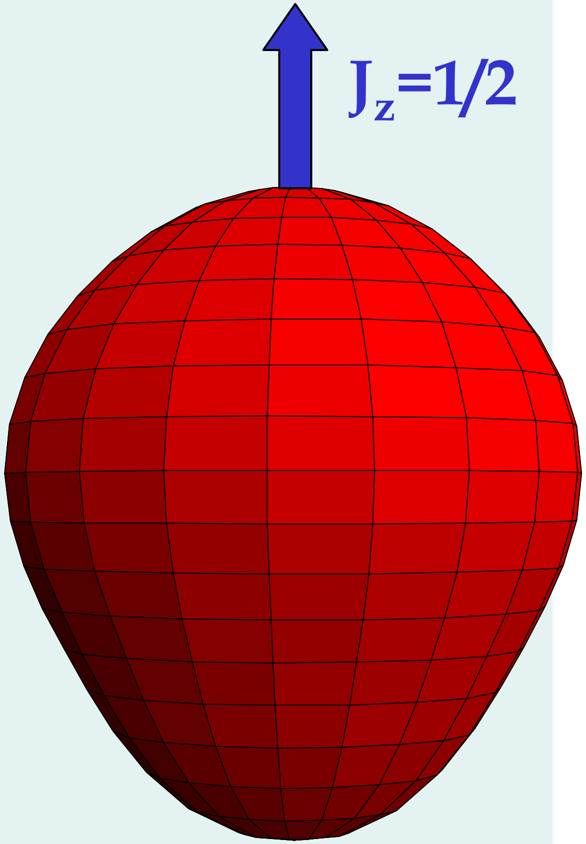
$$|L\rangle = \frac{1}{2}\left(\sqrt{2+2\epsilon}|+\rangle + \sqrt{2-2\epsilon}|-\rangle\right)$$

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

$$\boxed{|L,t\rangle = e^{iE_0t/\hbar}\left(\cos(\Delta t/\hbar)|L,0\rangle + i\sin(\Delta t/\hbar)|R,0\rangle\right)}$$

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

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



$$\beta_{10} = 0.023$$
$$\beta_{20} = 0.161$$
$$\beta_{30} = -0.128$$
$$\beta_{40} = 0.091$$

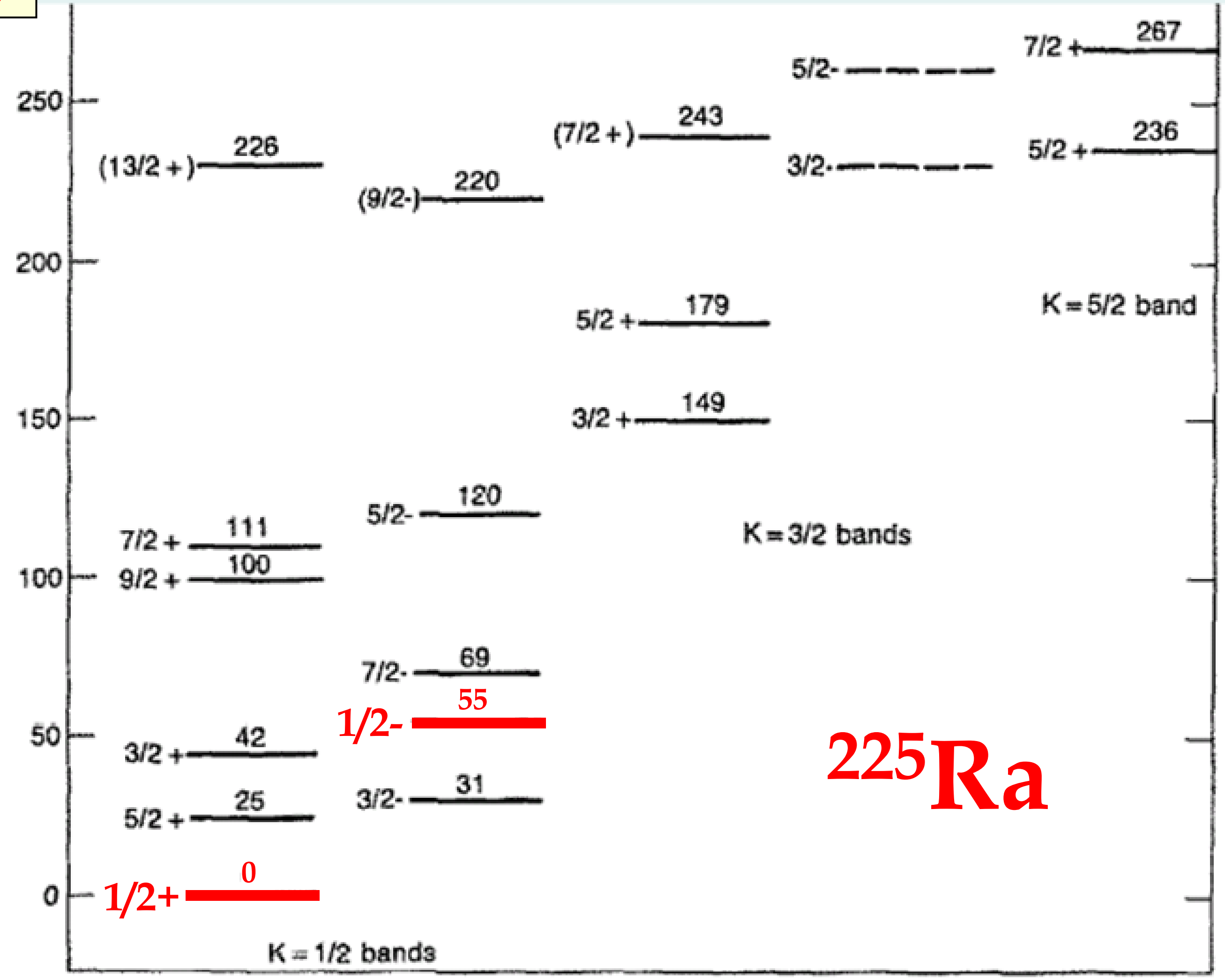


Fig. 5. Proposed grouping of the low-lying states of ^{225}Ra into rotational bands. The two members of the $K^\pi = \frac{3}{2}^-$ band have been reported in a study of the ^{225}Fr decay [20]; they are not observed in the present study.

	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.

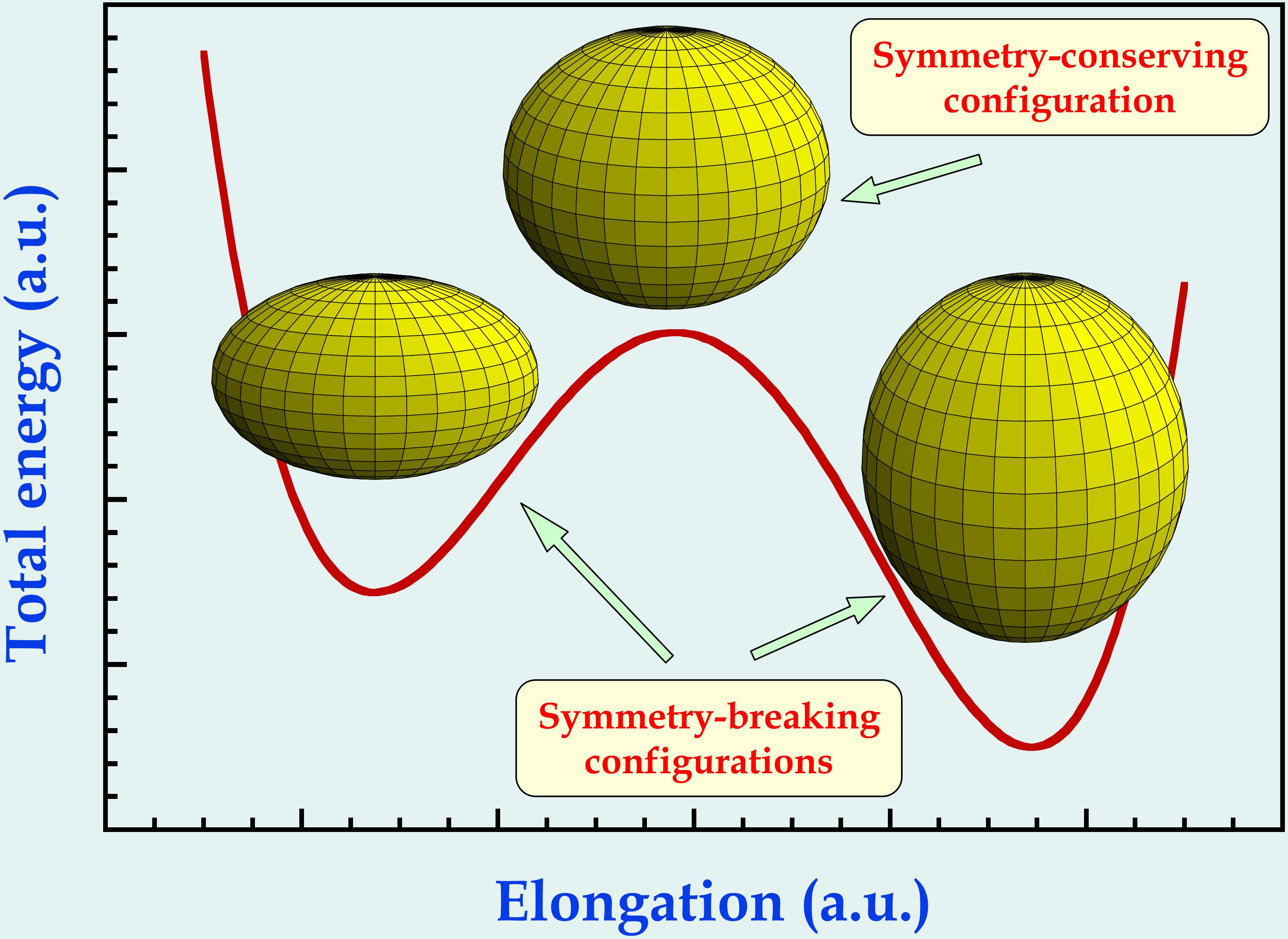
2) Whenever the energy scales (or range scales) between the interactions and observations are different, the observations can be described by a series of pseudopotentials with coupling constants adjusted to data (an effective theory).

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.

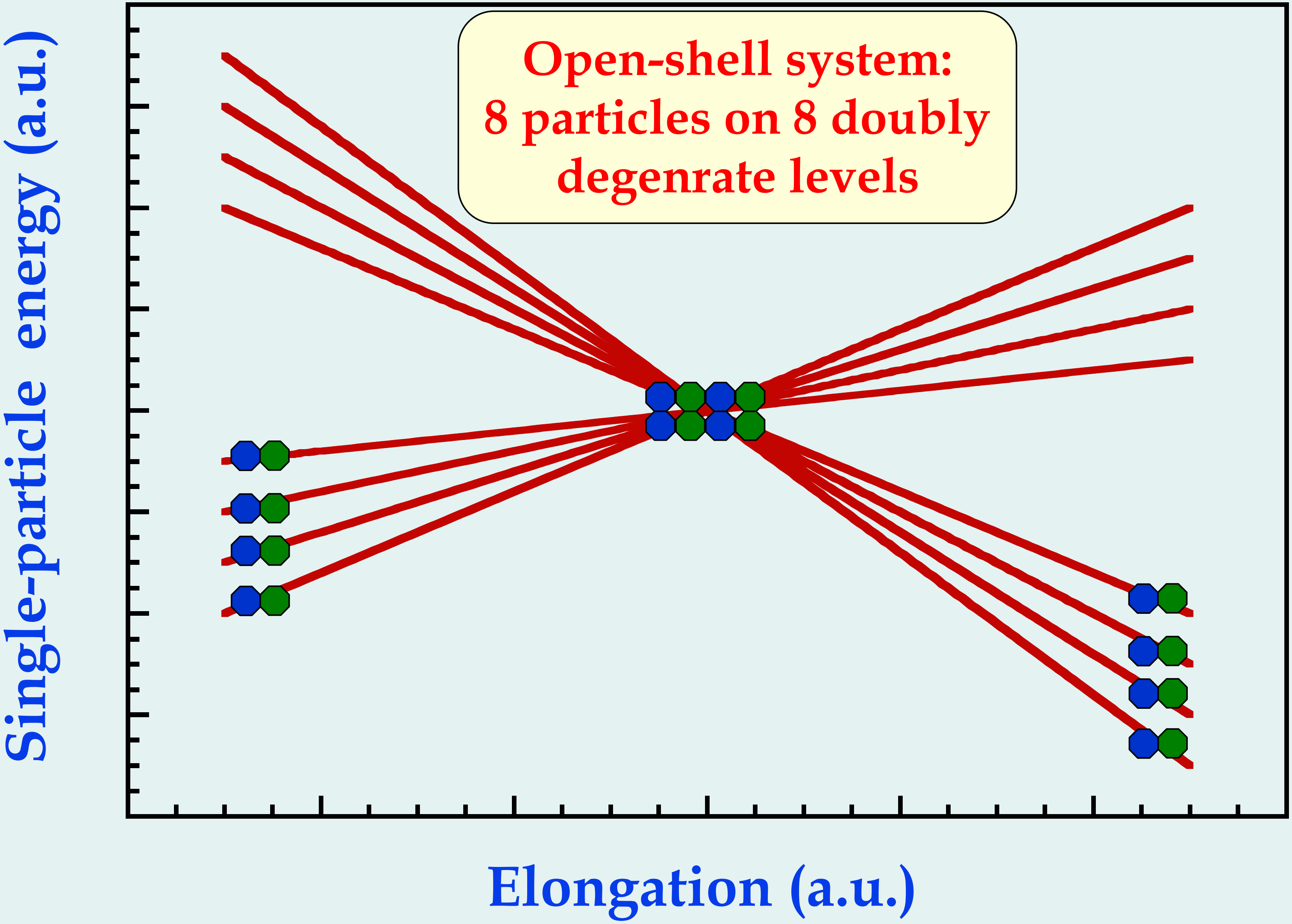
Nuclear deformation

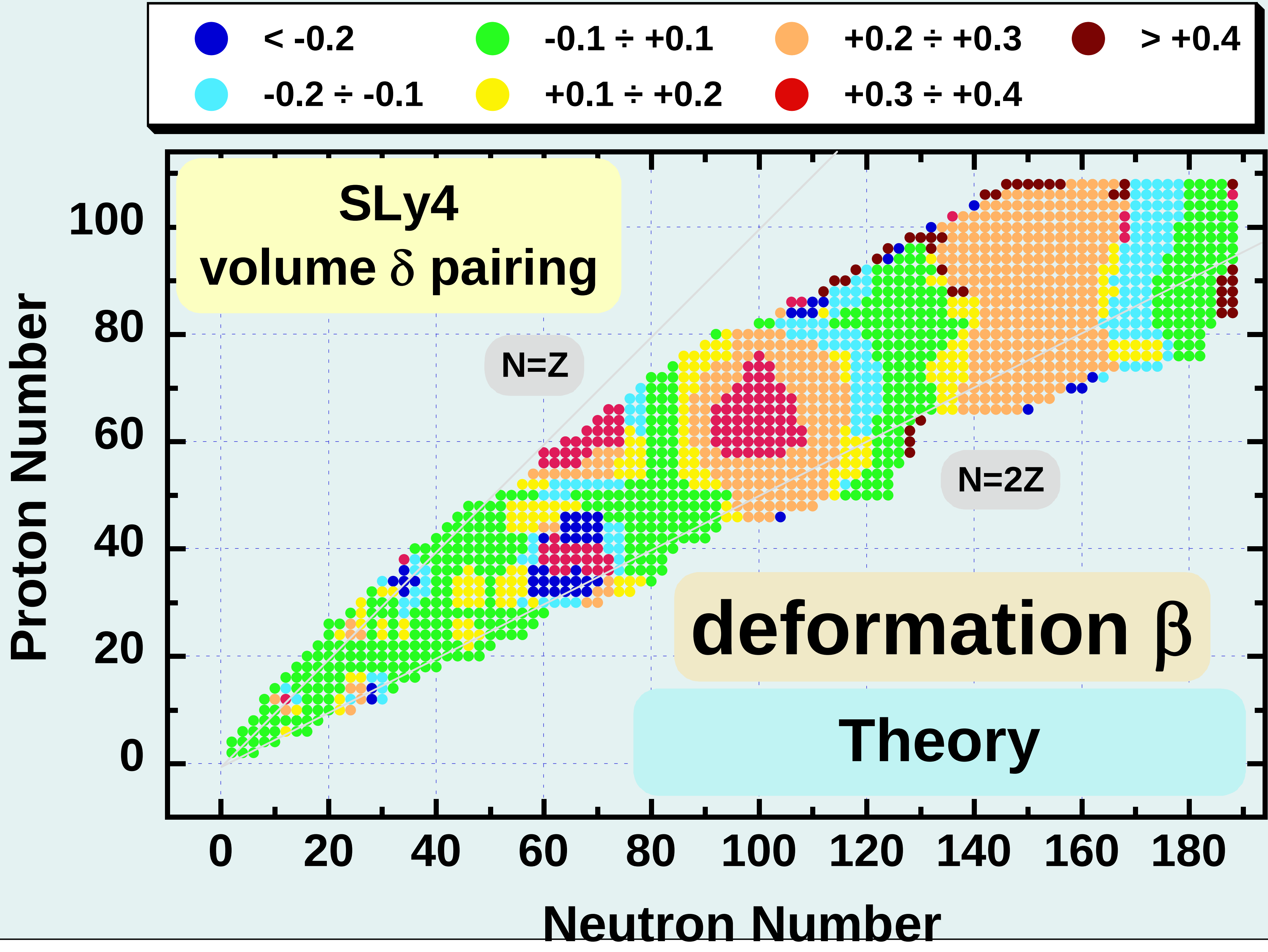


Symmetry-conserving configuration

Symmetry-breaking configurations

Origins of nuclear deformation


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

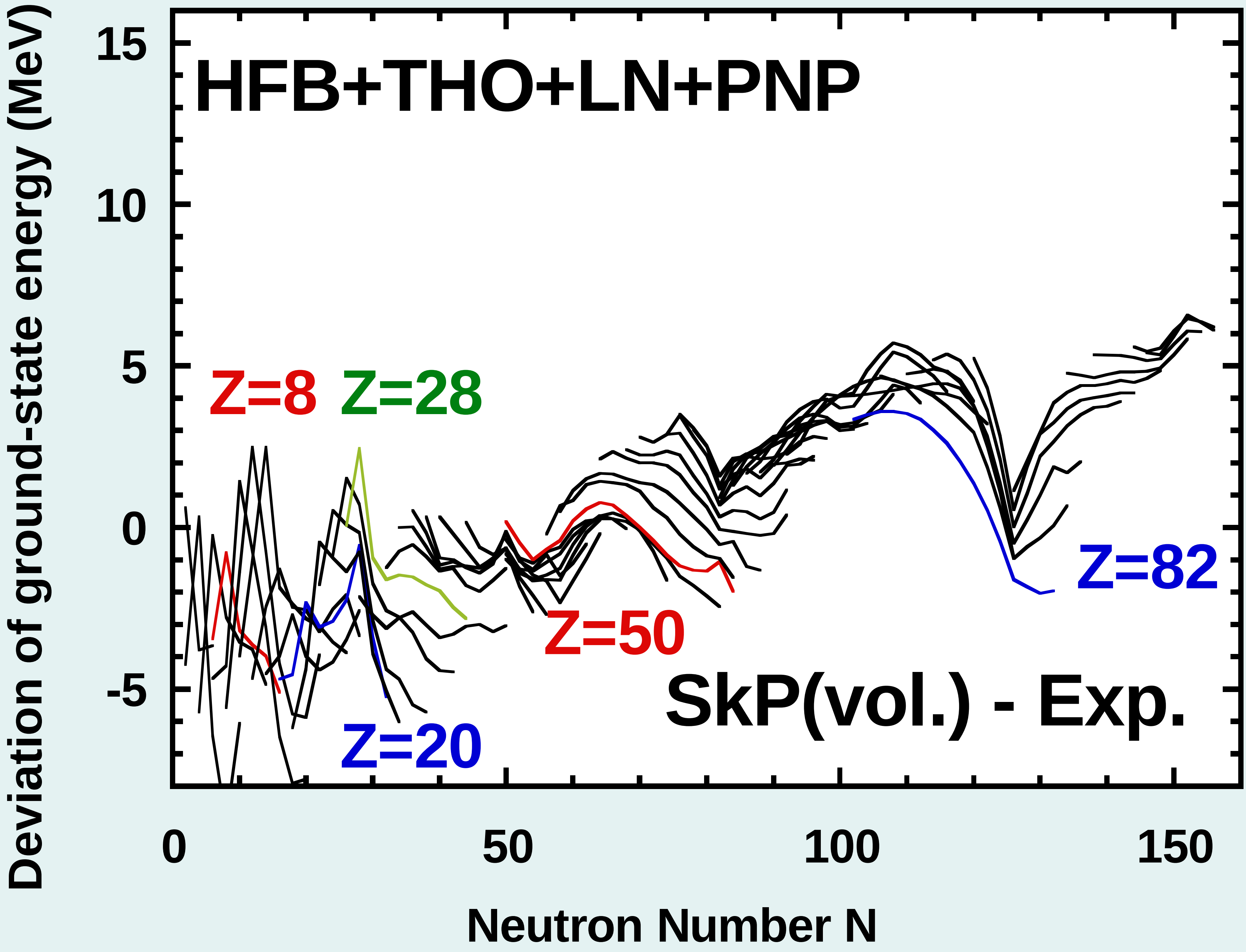


SLy4
volume δ pairing

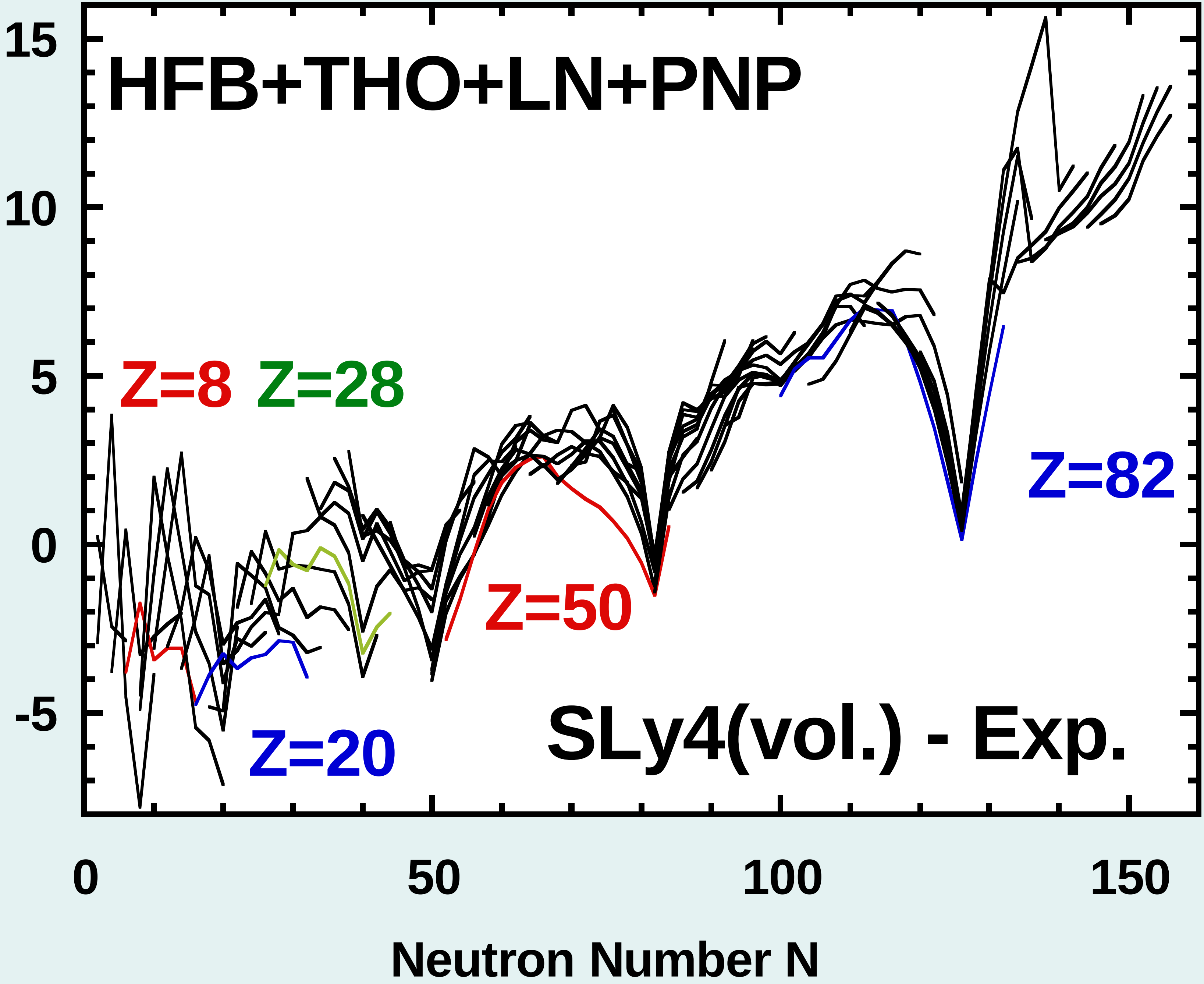
deformation β

Theory

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

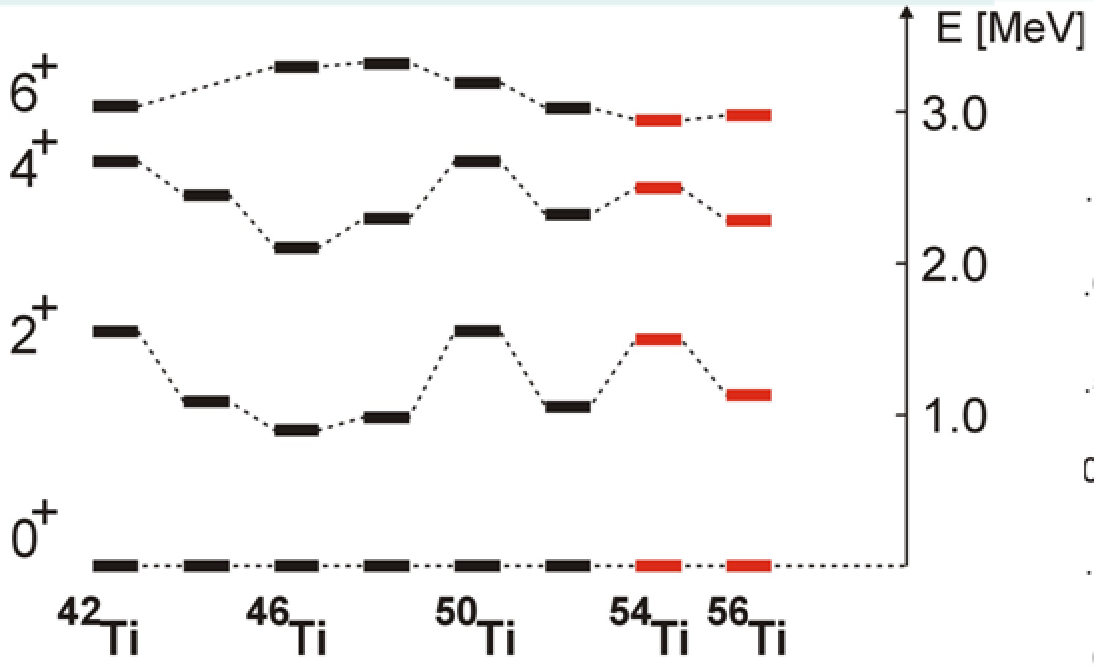


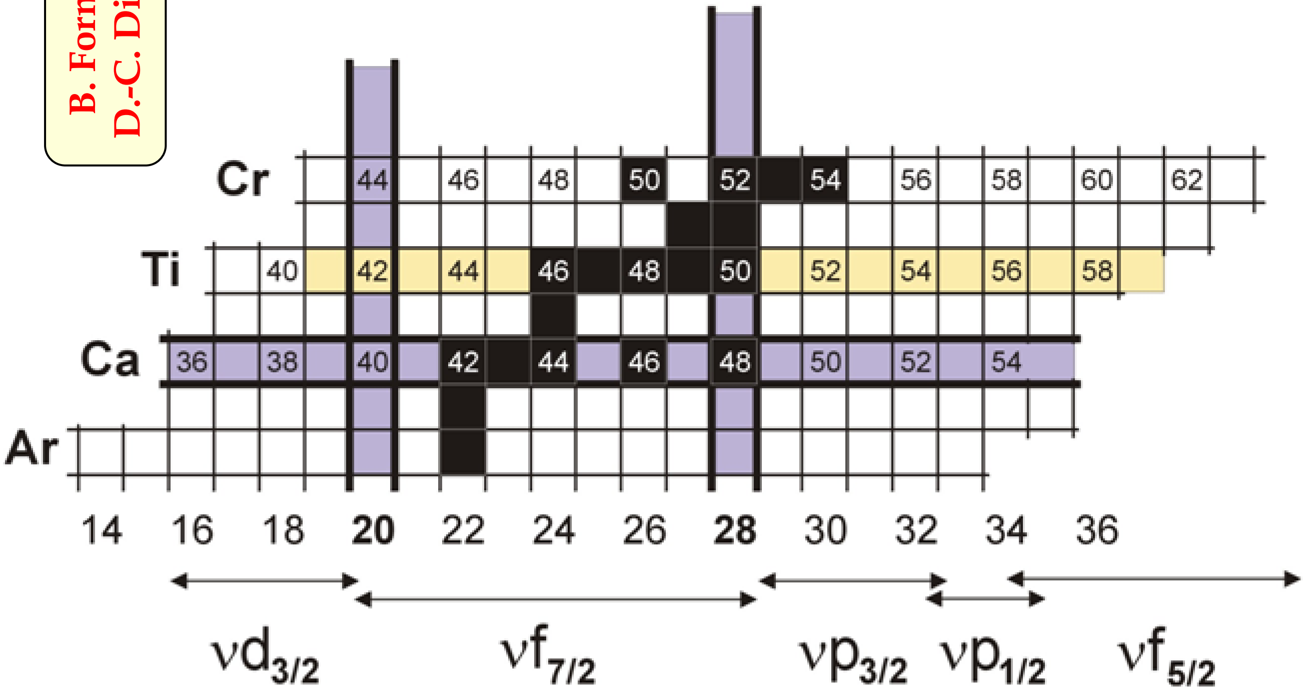
J. Dobaczewski, M.V. Stoitsov, W. Nazarewicz,
AIP Conf. Proc. 726, p. 51, nucl-th/0404077

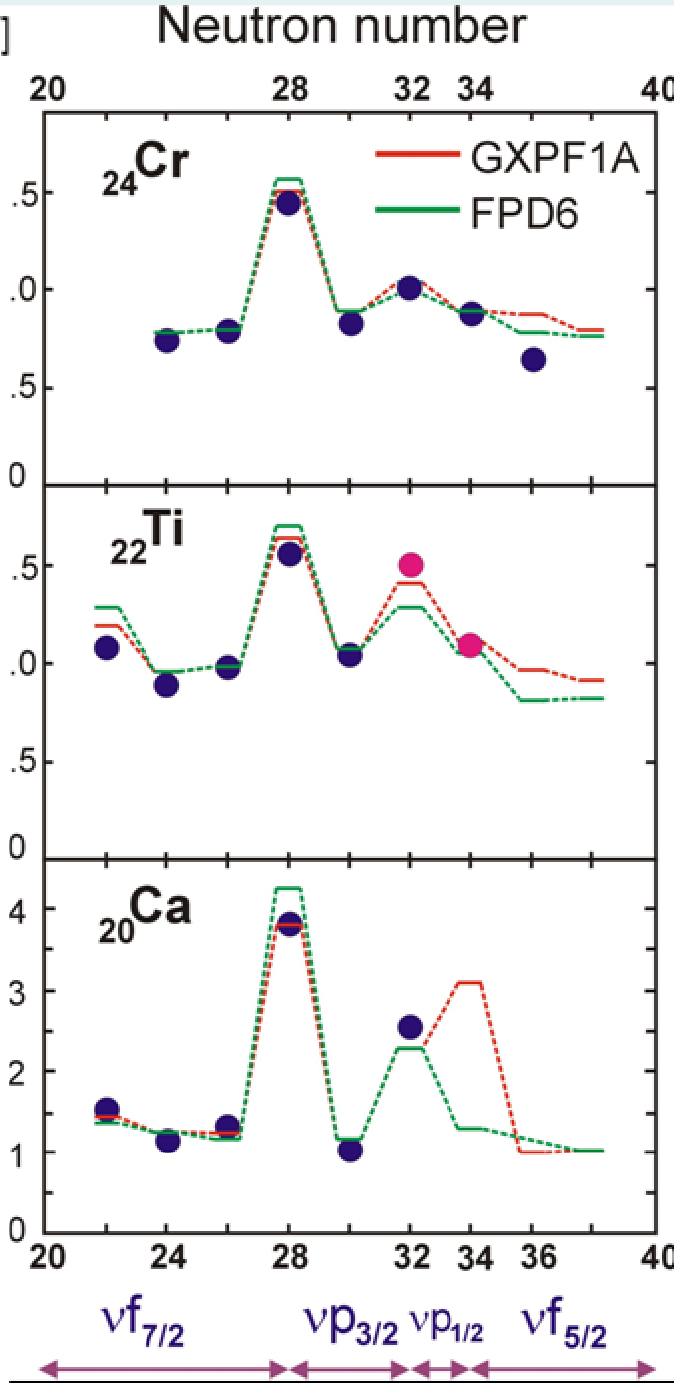


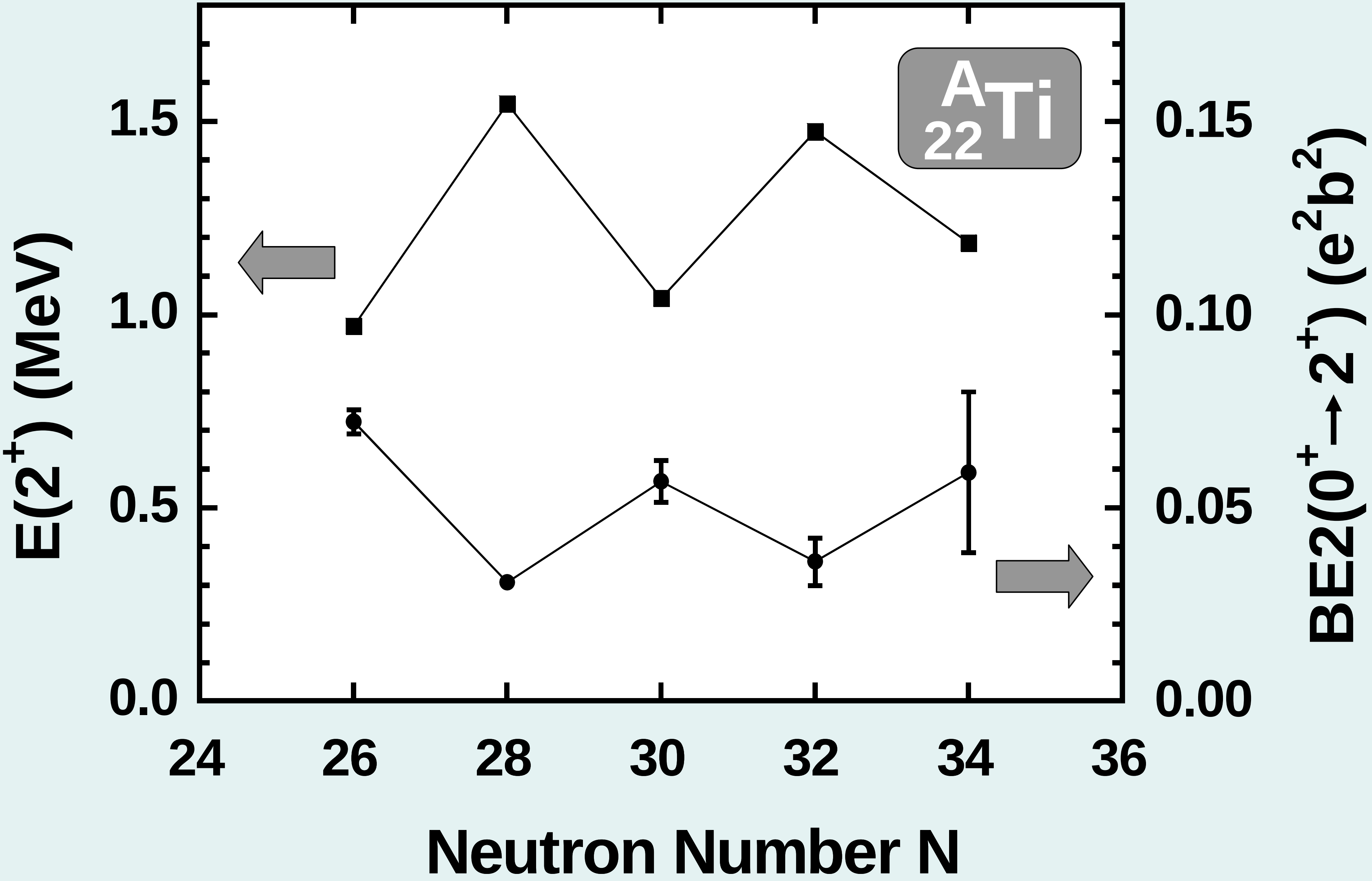
J. Dobaczewski, M.V. Stoitsov, W. Nazarewicz, AIP Conf. Proc. 726, p. 51, nucl-th/0404077

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

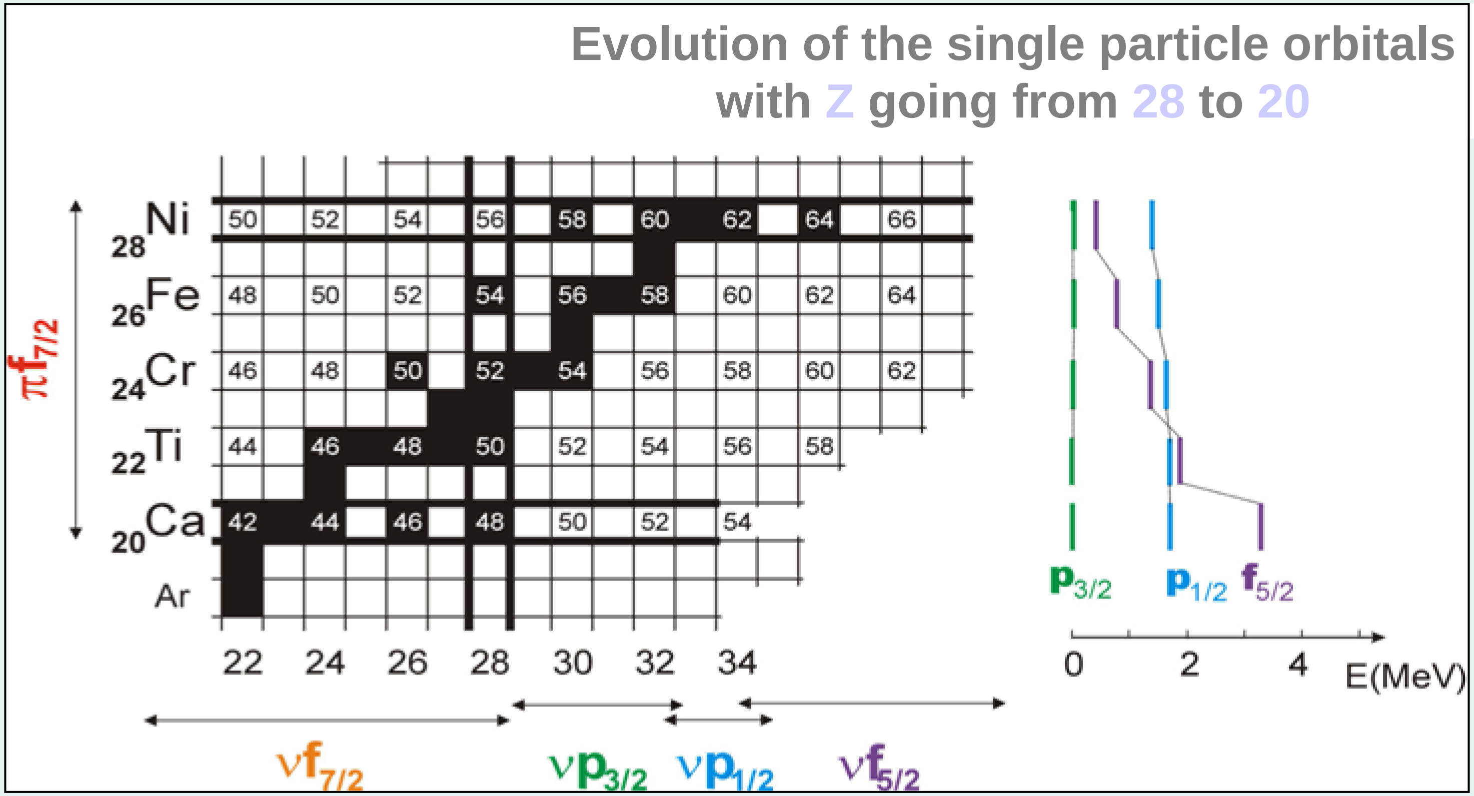








$^{A}_{22}Ti$
E(2$^+$) (MeV)
BE2(0$^+$→2$^+$) (e^{2}b^2)
0.0
0.5
1.0
1.5
0.00
0.05
0.10
0.15
24
26
28
30
32
34
36
Neutron Number N



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

$$
\begin{aligned}
\hat{V}_{Te} &= \tfrac{1}{2}t_{\mathrm{e}}[\hat{\vec{k}}' \cdot \hat{\mathsf{S}} \cdot \hat{\vec{k}}' + \hat{\vec{k}} \cdot \hat{\mathsf{S}} \cdot \hat{\vec{k}}] \\
\hat{V}_{To} &= t_{\mathrm{o}}\hat{\vec{k}}' \cdot \hat{\mathsf{S}} \cdot \hat{\vec{k}} \\
\hat{V}_{SO} &= iW_0\hat{\vec{S}} \cdot [\hat{\vec{k}}' \times \hat{\vec{k}}]
\end{aligned}
$$

where

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

Tensor energy densities

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

$$\mathcal{H}_T = \frac{5}{8}\left[t_e \vec{J}_n \cdot \vec{J}_p + t_o\left(\vec{J}_0^2 - \vec{J}_n \cdot \vec{J}_p\right)\right]$$

$$\mathcal{H}_{SO} = \frac{1}{4}\left[3W_0 \vec{J}_0 \cdot \vec{\nabla}\rho_0 + W_1 \vec{J}_1 \cdot \vec{\nabla}\rho_1\right]$$

where the particle and SO densities read

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

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

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

Single-particle spin-orbit potentials

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

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

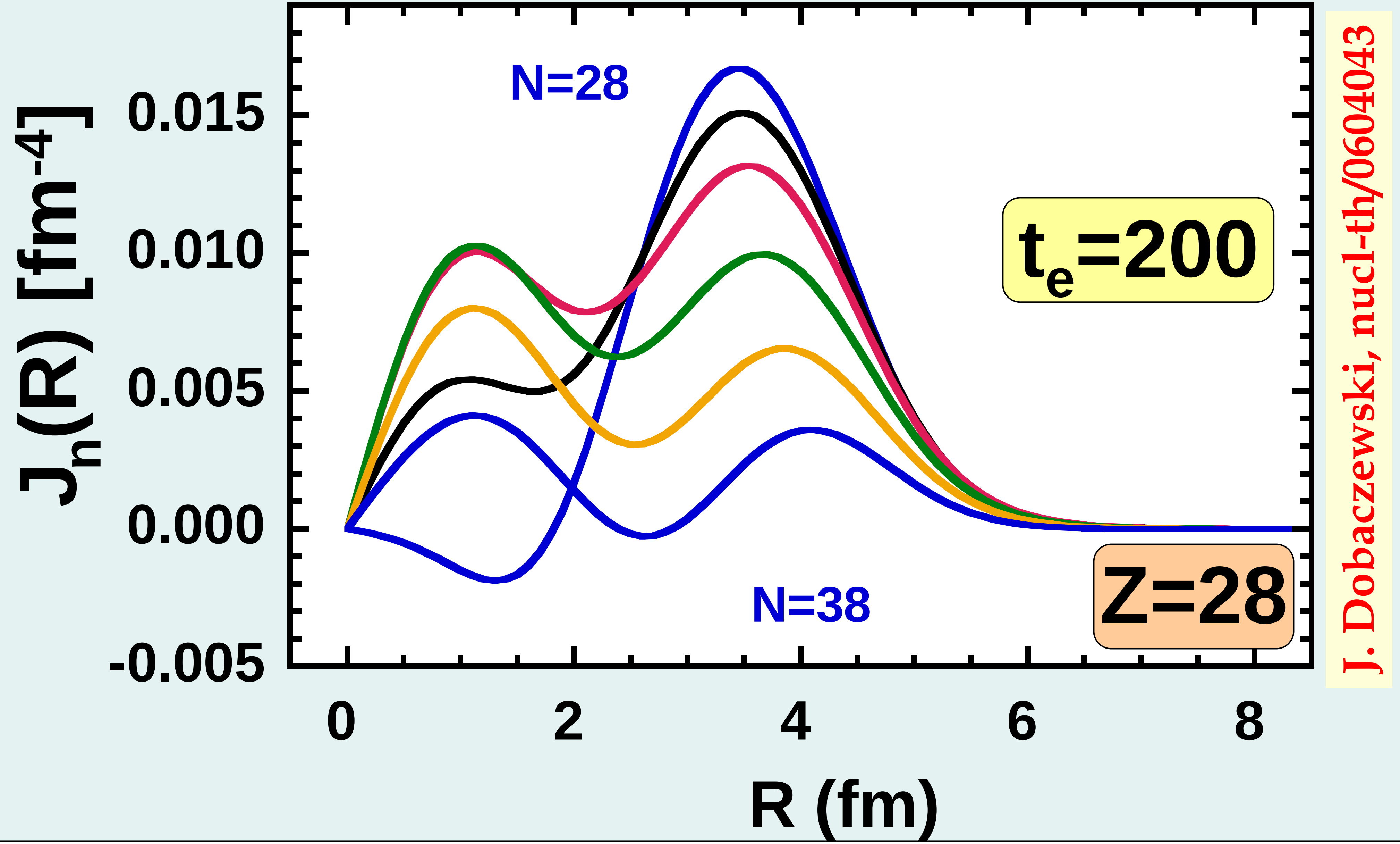
Variation of the energy densities with respect to the single-particle wave functions gives form factors of the single-particle spin-orbit potentials:

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

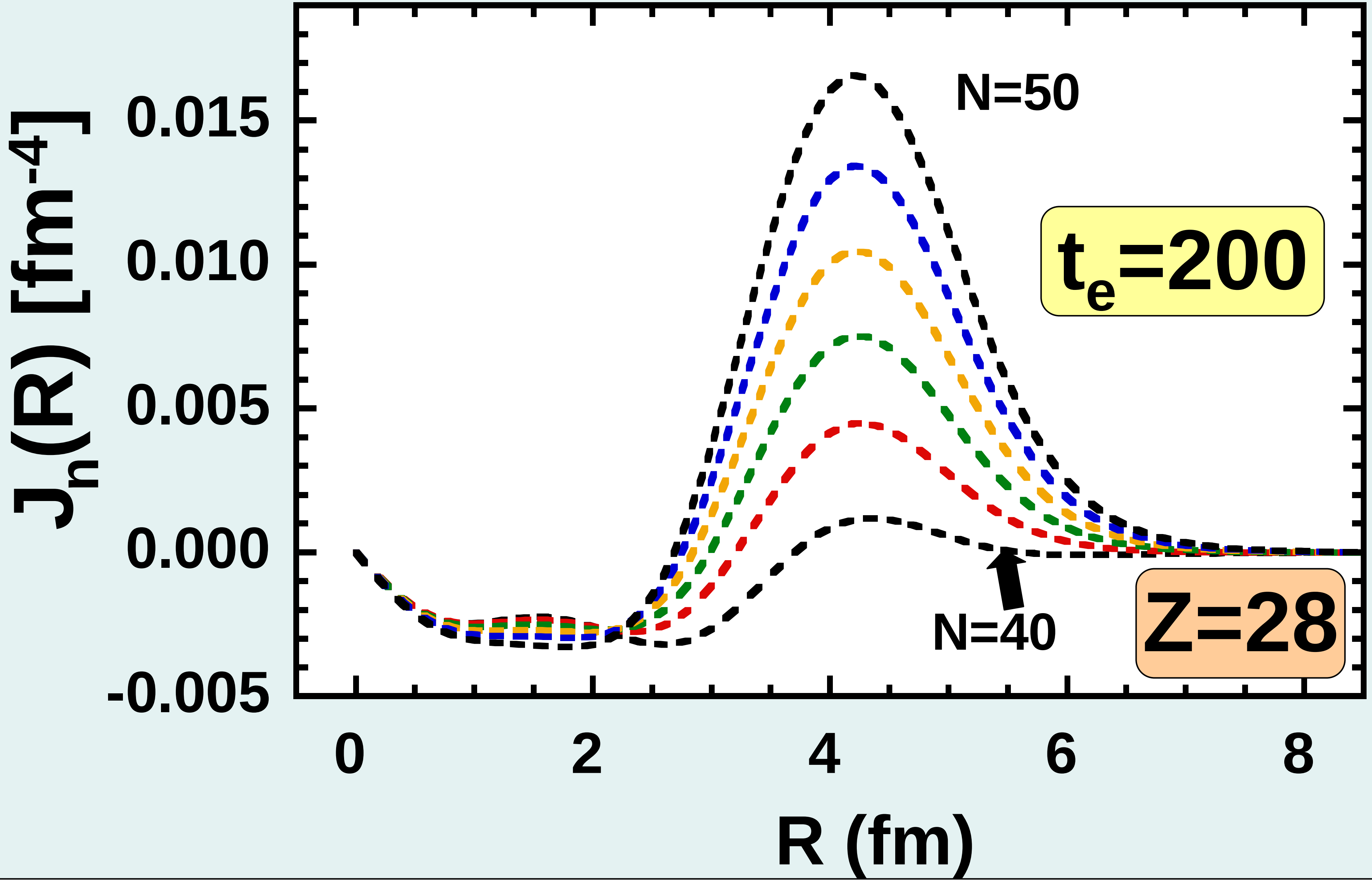
$$\vec{V}_n^{SO} = \frac{5t_e+5t_o}{8}\vec{J}_p + \frac{5t_o}{4}\vec{J}_n + \frac{3W_0-W_1}{4}\vec{\nabla}\rho_p + \frac{3W_0+W_1}{4}\vec{\nabla}\rho_n$$

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

Neutron S-O Density

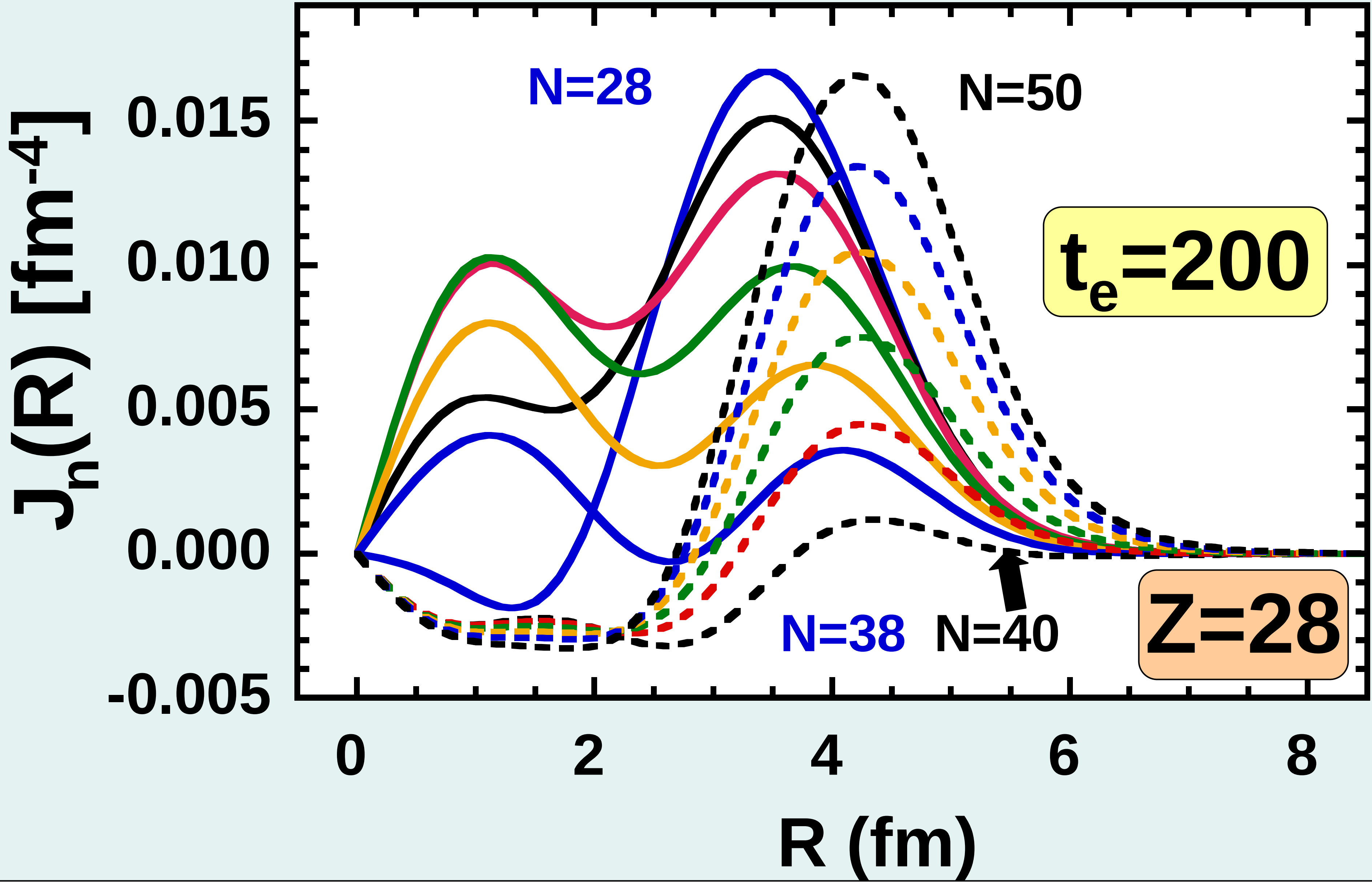


Neutron S-O Density

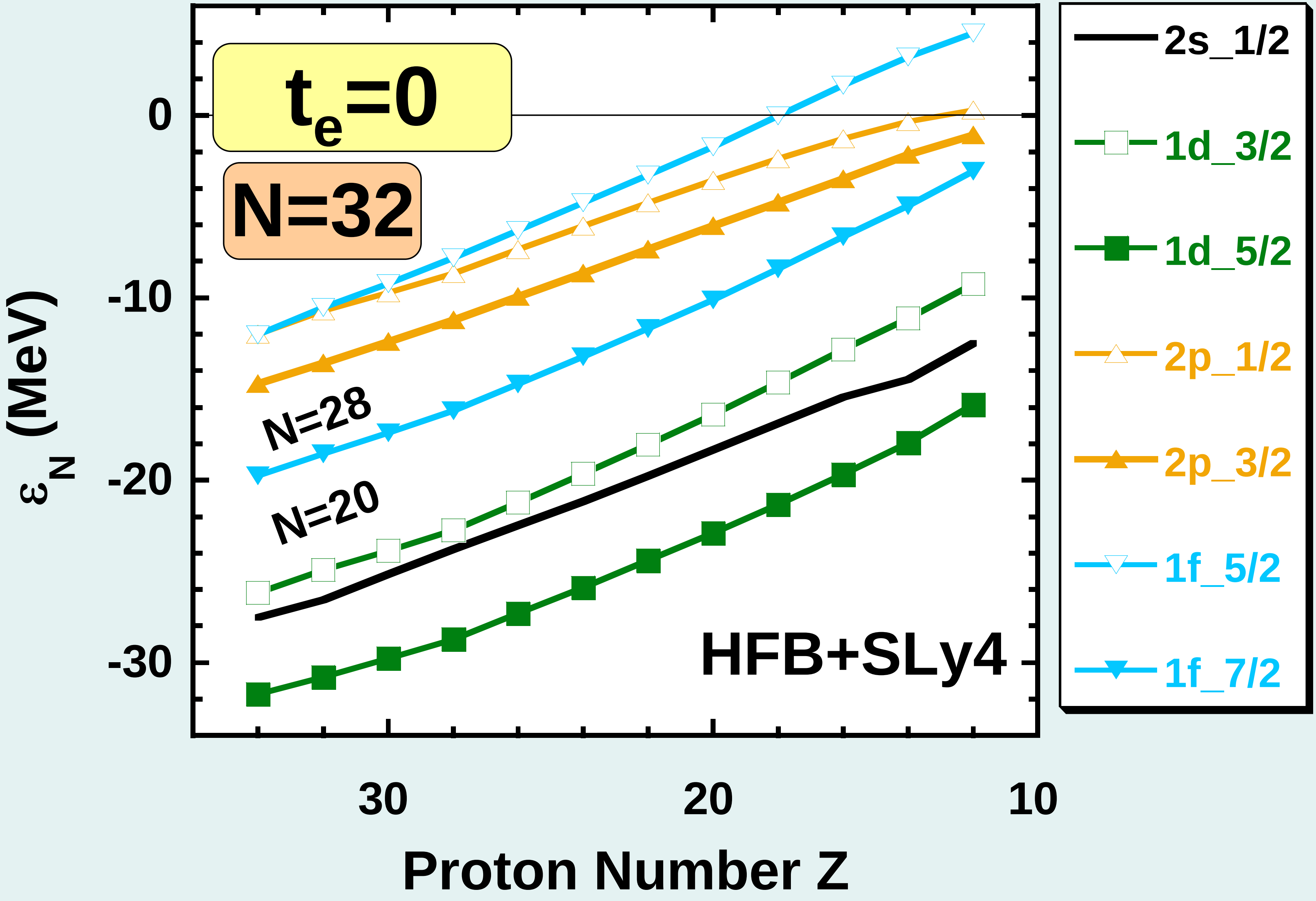


J. Dobaczewski, nucl-th/0604043

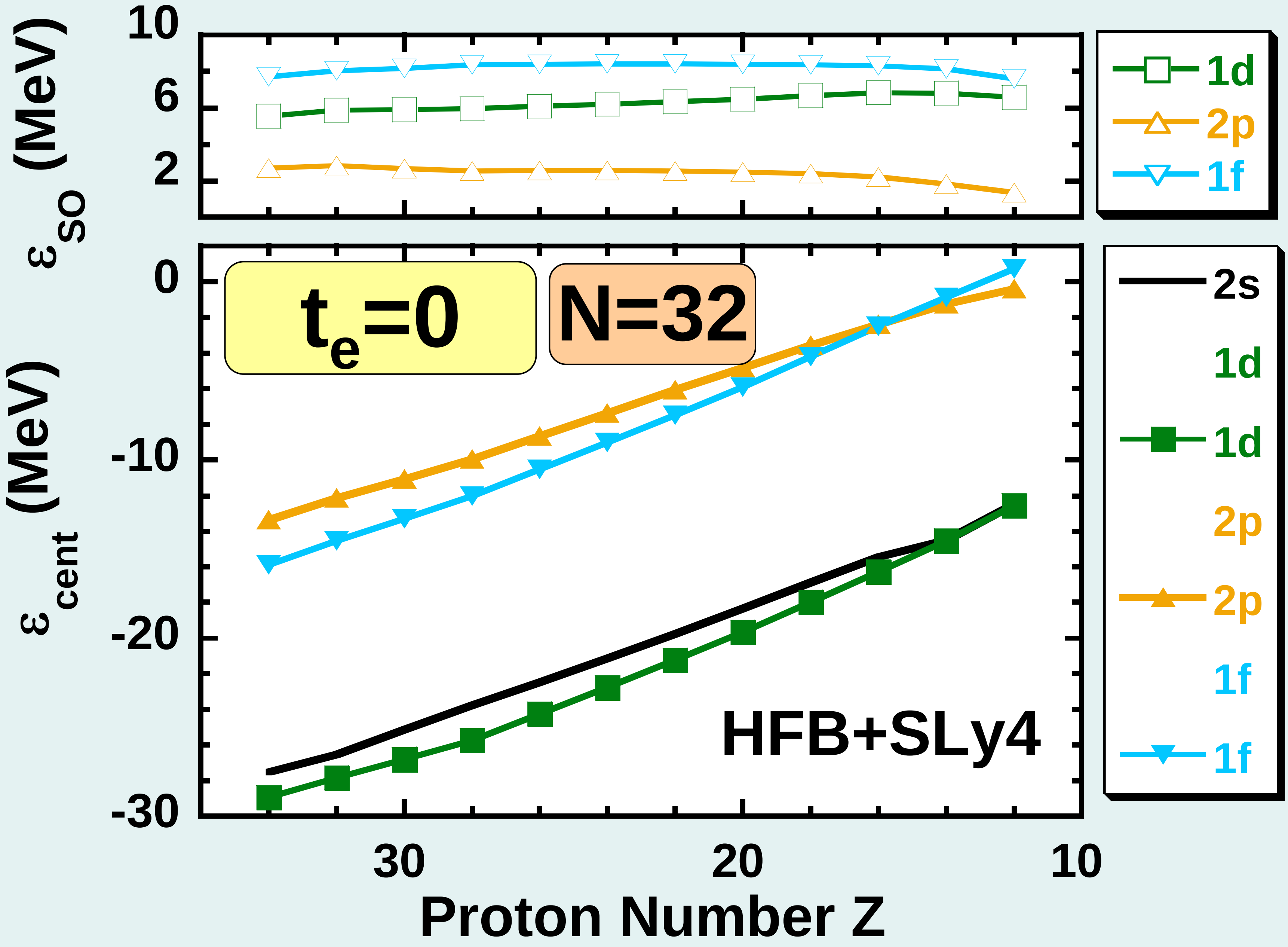
Neutron S-O Density



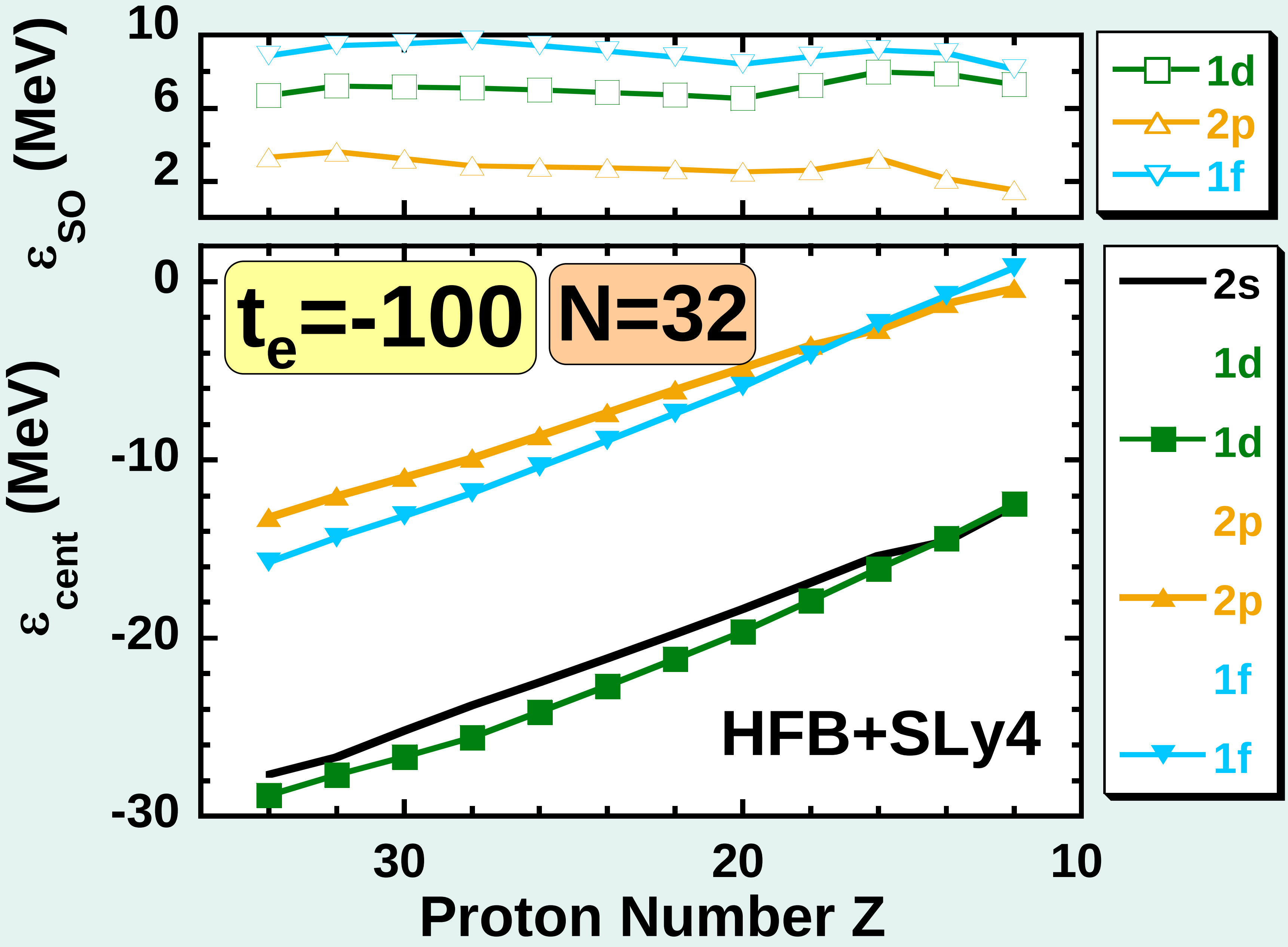
J. Dobaczewski, nucl-th/0604043



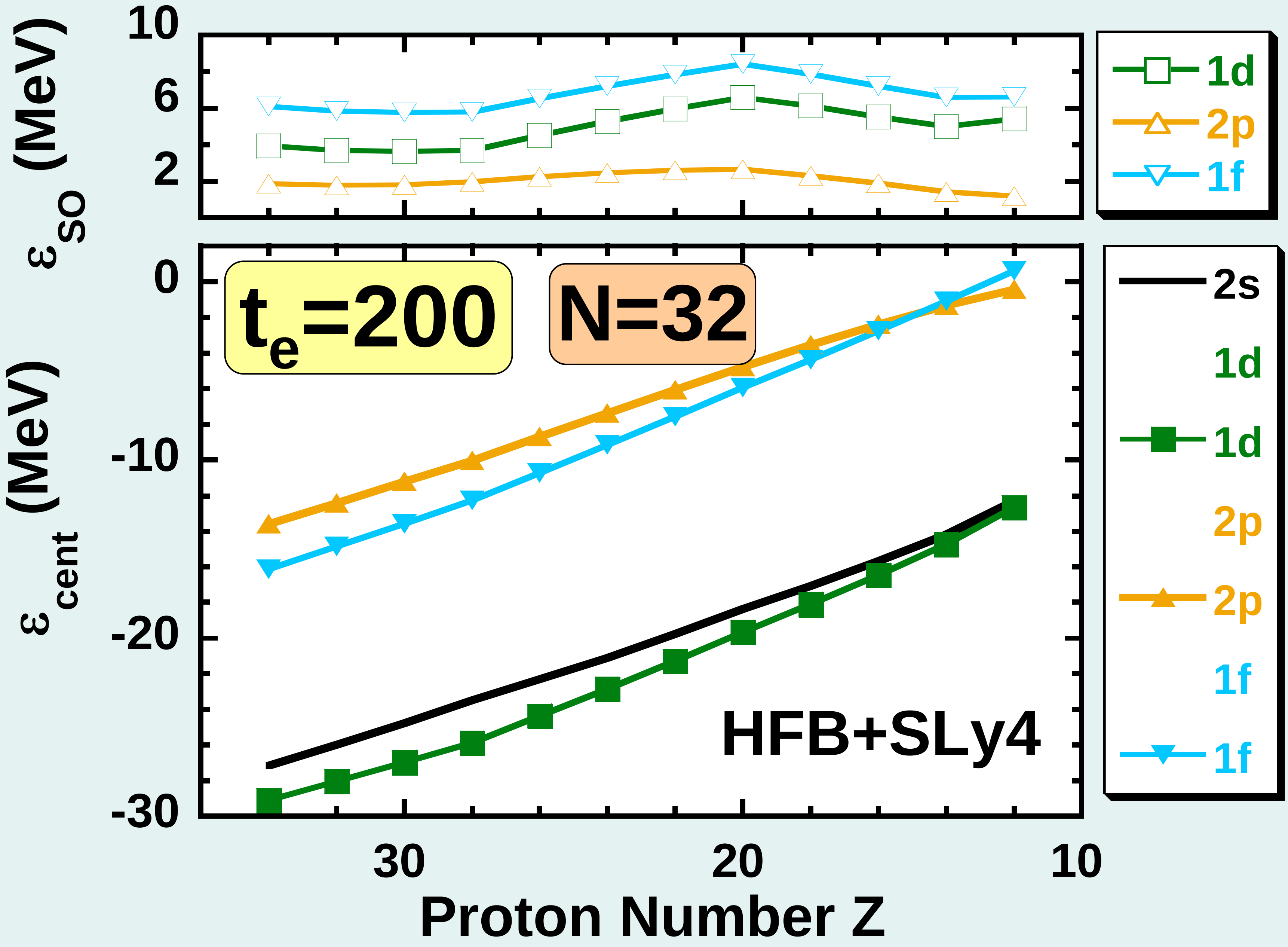
J. Dobaczewski, nucl-th/0604043



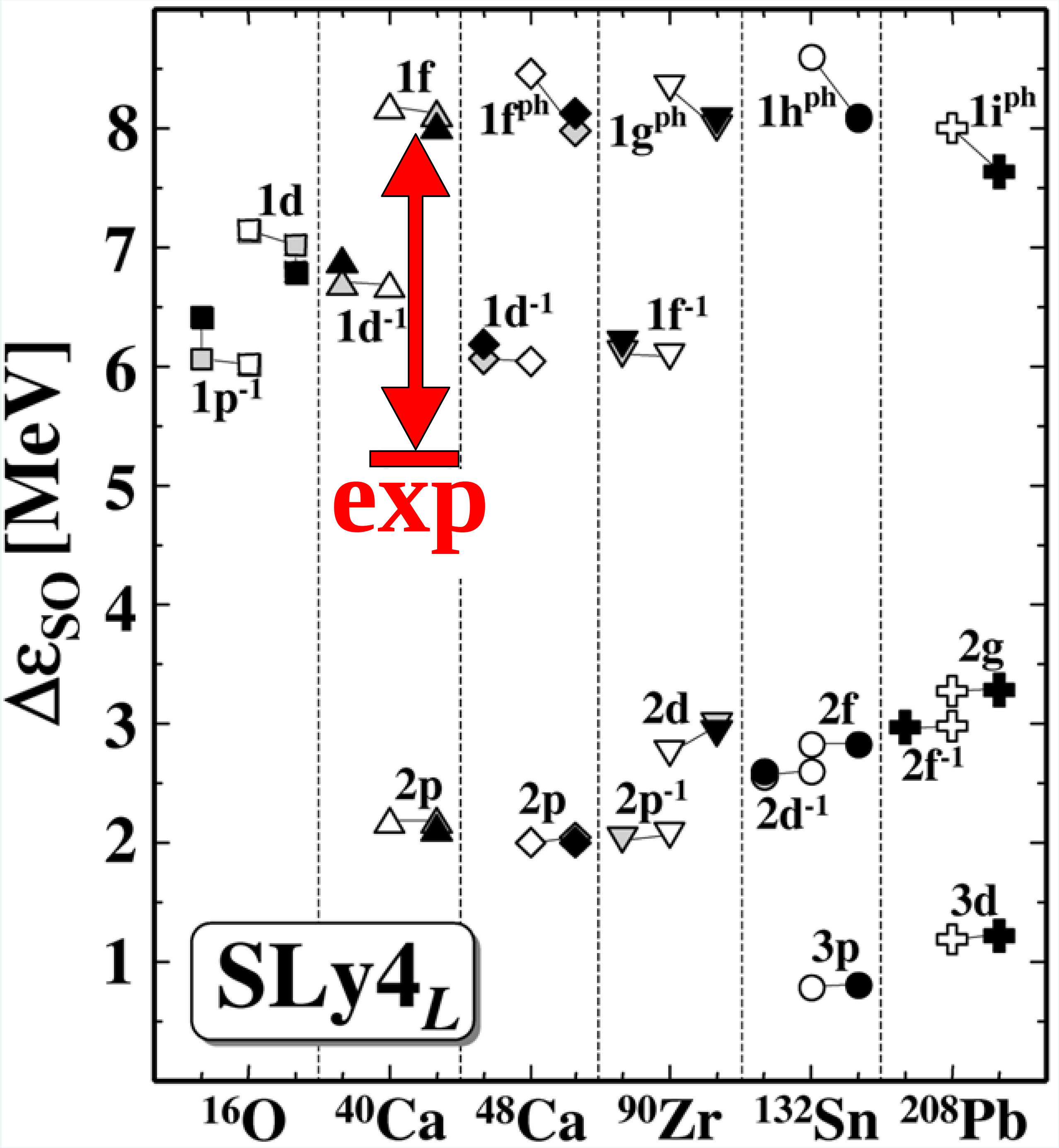
J. Dobaczewski, nucl-th/0604043



J. Dobaczewski, nucl-th/0604043



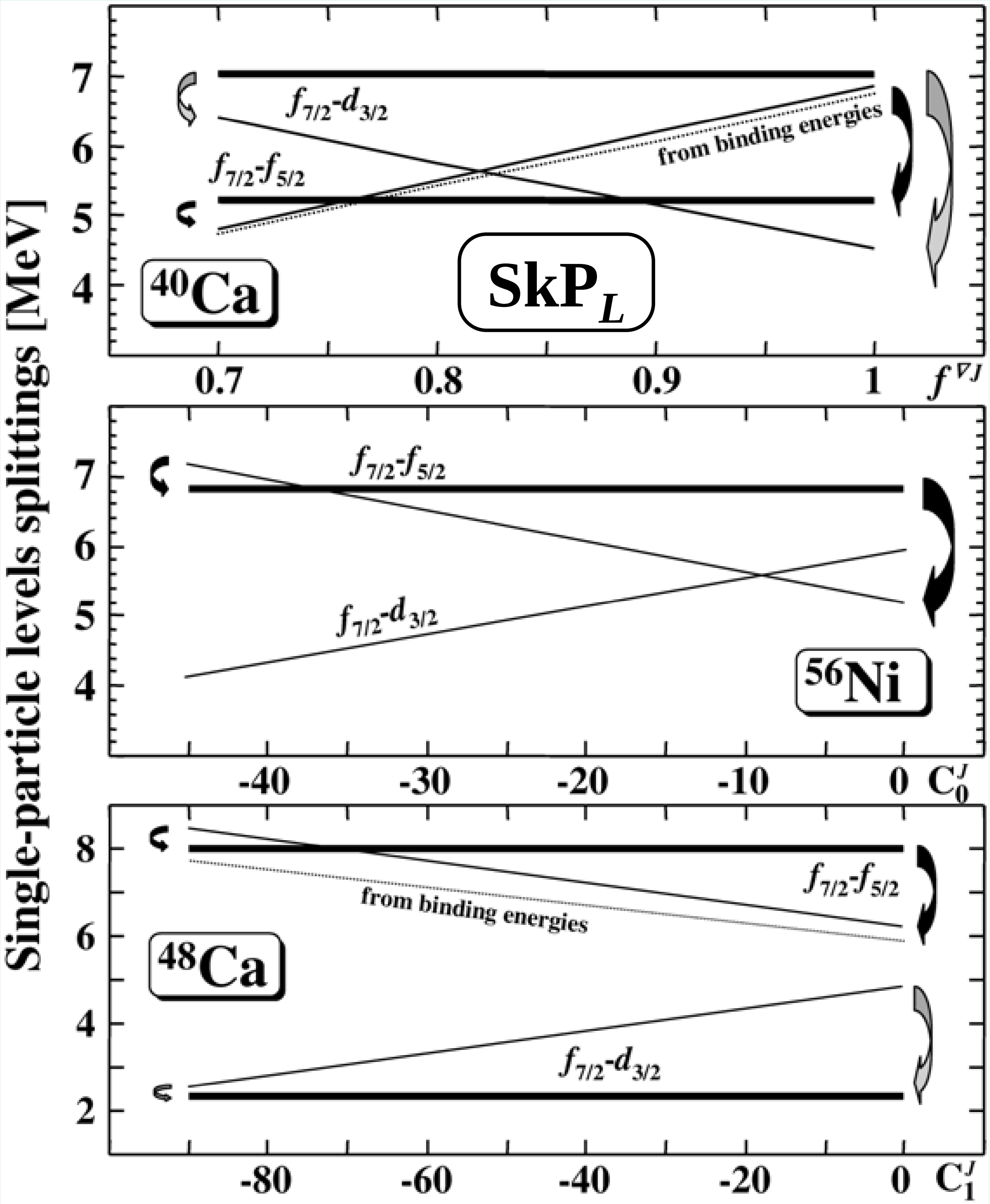
J. Dobaczewski, nucl-th/0604043



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

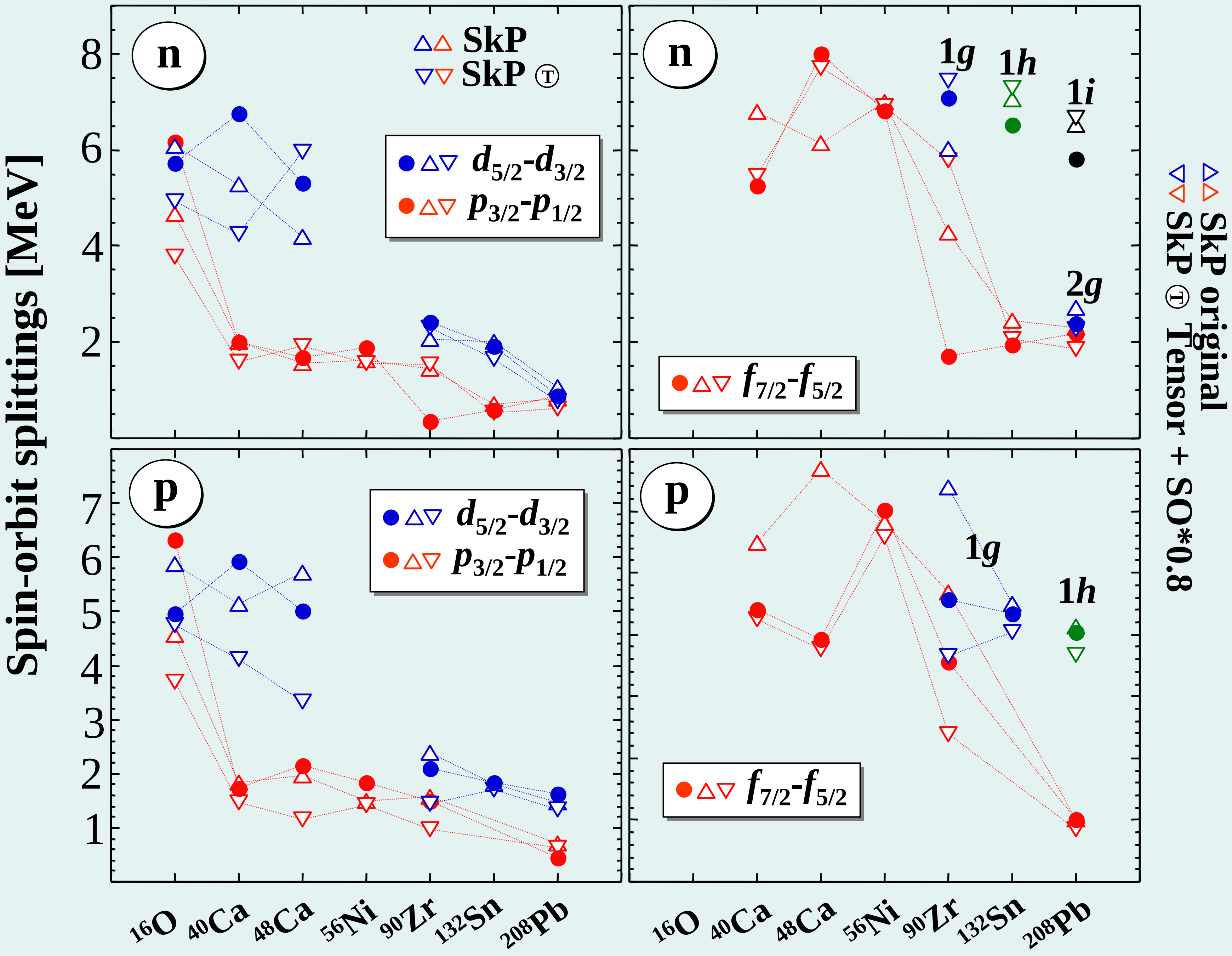


M. Zalewski *et al.*, Phys. Rev. C77, 024316 (2008)

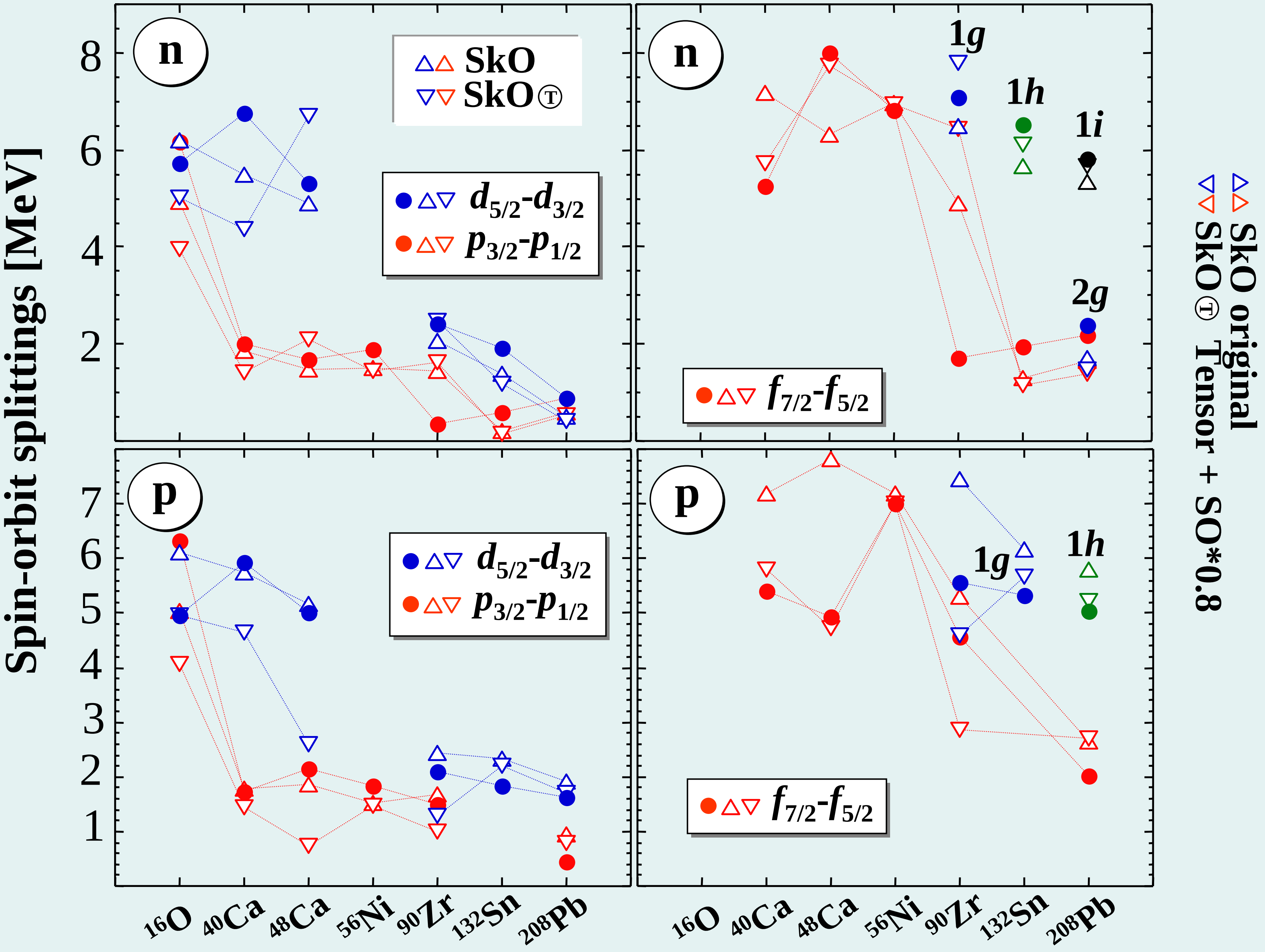
Fits of spin-orbit and tensor coupling constants

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.*, arXiv:0801.0924

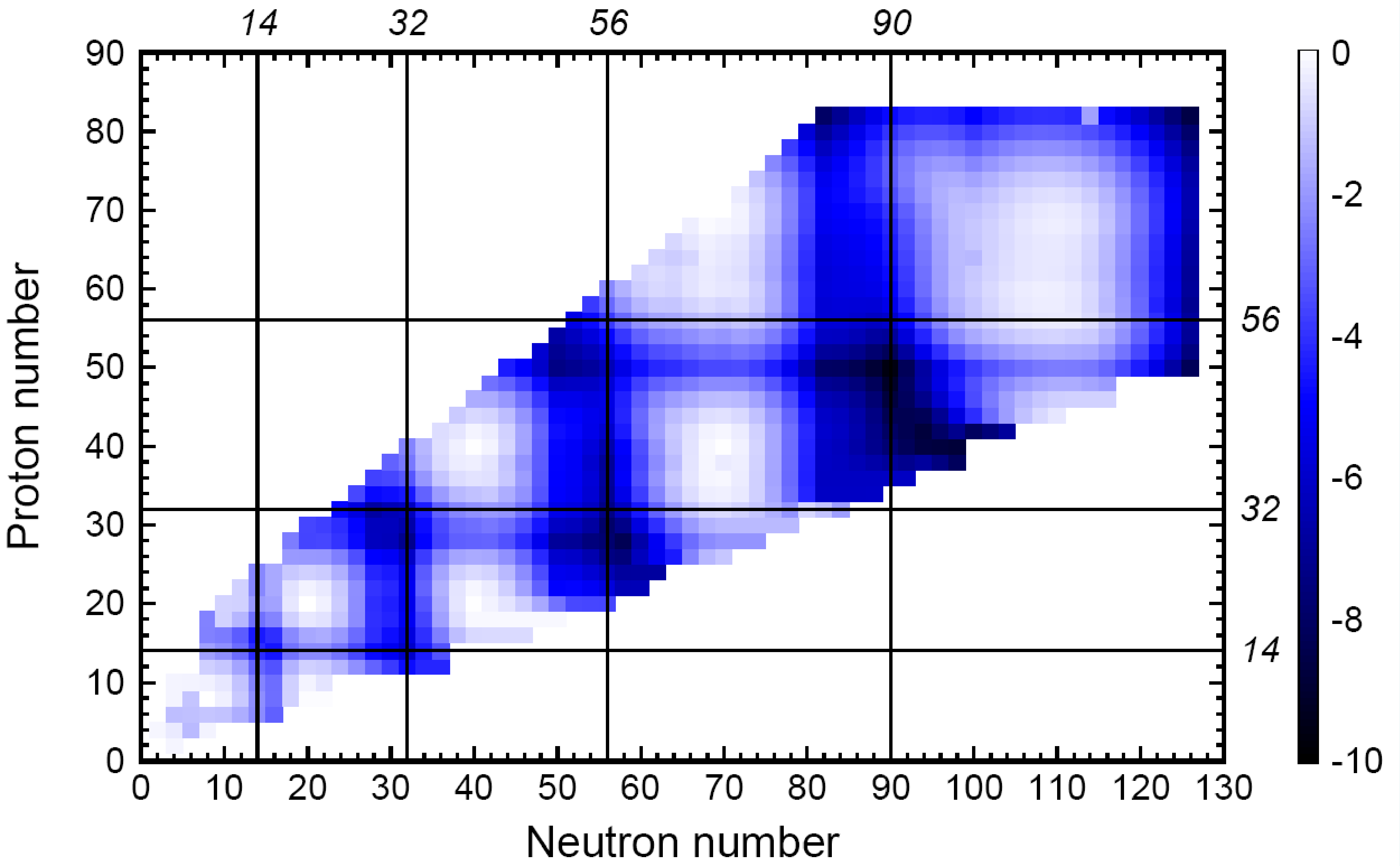


M. Zalewski *et al.*, arXiv:0801.0924

Jacek Dobaczewski

JYVÄSKYLÄN YLIOPISTO

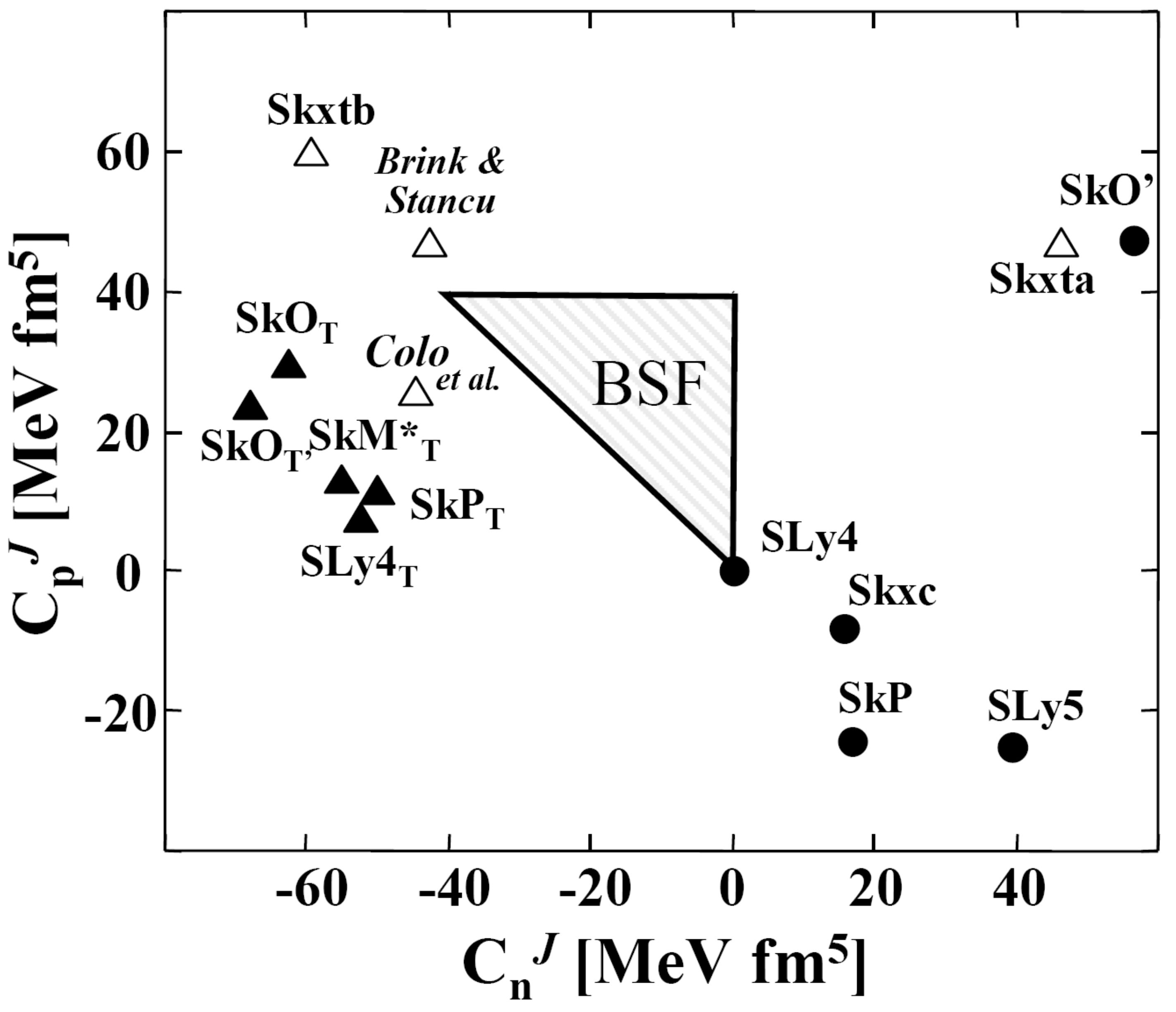
Tensorial magic numbers



W. Satuła, *et al.*, to be published

Tensor contribution to the total binding energy calculated using spherical Hartree-Fock-Bogolybov model with the $\mathrm{SLy4_T}$ functional

Tensor coupling constants



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

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

Hartree-Fock interaction energy

Neglecting for simplicity the spin-isospin degrees of freedom, we can write the HF interaction energy in the form

$$E_{\text{int}} = \frac{1}{2}\int \mathrm{d}^3\vec{x}\,\mathrm{d}^3\vec{y}\,\mathrm{d}^3\vec{x}'\mathrm{d}^3\vec{y}'\;\tilde{V}(\vec{x},\vec{y};\vec{x}',\vec{y}')\left(\rho(\vec{x}',\vec{x})\rho(\vec{y}',\vec{y}) - \rho(\vec{x}',\vec{y})\rho(\vec{y}',\vec{x})\right).$$

For local effective interaction, the non-antisymmetrized matrix element $\tilde{V}(\vec{x},\vec{y};\vec{x}',\vec{y}')$ is given by the potential $V(\vec{x},\vec{y})$, i.e., $\tilde{V}(\vec{x},\vec{y};\vec{x}',\vec{y}') = \delta(\vec{x}-\vec{x}')\delta(\vec{y}-\vec{y}')V(\vec{x},\vec{y})$, and the interaction energy reads

$$E^{\text{int}} = \frac{1}{2}\int \mathrm{d}^3\vec{x}\,\mathrm{d}^3\vec{y}\,V(\vec{x},\vec{y})\left(\rho(\vec{x},\vec{x})\rho(\vec{y},\vec{y}) - \rho(\vec{x},\vec{y})\rho(\vec{y},\vec{x})\right).$$

The first term (direct) depends only on the local density matrix (equal arguments), while the second term (exchange) involves the full one-body density matrix.
It is therefore convenient to represent the one-body density matrix as

$$\rho(\vec{x},\vec{y}) = \rho(\vec{R},\vec{r}), \qquad \text{where} \qquad \vec{R} = \tfrac{1}{2}(\vec{x}+\vec{y}) \quad \text{and} \quad \vec{r} = \vec{x}-\vec{y}.$$

Denoting the local density by single argument, $\rho(\vec{R}) = \rho(\vec{x},\vec{x}) = \rho(\vec{R},\vec{0})$, and noting that by translational invariance the potential $V(\vec{x},\vec{y}) = V(\vec{x}-\vec{y})$ depends only on the relative coordinate, we have

$$E^{\text{int}} = E^{\text{int}}_{\text{dir}} + E^{\text{int}}_{\text{exch}} = \frac{1}{2}\int \mathrm{d}^3\vec{R}\,\mathrm{d}^3\vec{r}\,V(\vec{r})[\rho(\vec{R}+\tfrac{1}{2}\vec{r})\rho(\vec{R}-\tfrac{1}{2}\vec{r}) - \rho(\vec{R},\vec{r})\rho(\vec{R},-\vec{r})].$$

Direct interaction energy

In the direct term,

$$E^{\text{int}}_{\text{dir}} = \tfrac{1}{2}\int \mathrm{d}^3\vec{R}\,\mathrm{d}^3\vec{r}\,\overbrace{V(\vec{r})[\rho(\vec{R}+\tfrac{1}{2}\vec{r})\rho(\vec{R}-\tfrac{1}{2}\vec{r})]}^{\text{Nonlocal energy density}},$$

we can use the fact that the range of the effective force is smaller than the typical distance at which the density changes. Hence, for the purpose of evaluating the direct interaction energy, the density can be approximated by the quadratic expansion,

$$\rho(\vec{R}\pm\tfrac{1}{2}\vec{r}) = \rho(\vec{R}) \pm \tfrac{1}{2}r^i\nabla_i\rho(\vec{R}) + \tfrac{1}{8}r^ir^j\nabla_i\nabla_j\rho(\vec{R}) + \ldots$$

and

$$\rho(\vec{R}+\tfrac{1}{2}\vec{r})\rho(\vec{R}-\tfrac{1}{2}\vec{r}) = \rho^2(\vec{R}) + \tfrac{1}{4}r^ir^j(\rho(\vec{R})\nabla_i\nabla_j\rho(\vec{R}) - [\nabla_i\rho(\vec{R})][\nabla_j\rho(\vec{R})]) + \ldots,$$

where $\nabla_i{=}\partial/\partial R^i$. This expansion gives [for scalar interactions $V(\vec{r}) = V(|\vec{r}|) = V(r)$] the direct interaction energy:

$$E^{\text{int}}_{\text{dir}} = \tfrac{1}{2}\int \mathrm{d}^3\vec{R}\,\overbrace{[V_0\rho^2 + \tfrac{1}{4}V_2(\rho\Delta\rho - (\vec{\nabla}\rho)^2)]}^{\text{Local energy density}} + \ldots,$$

where coupling constants V_0 and V_2 are given by the moments of the interaction:

$$V_0 = 4\pi\int \mathrm{d}r r^2 V(r) \quad \text{and} \quad V_2 = \tfrac{4}{3}\pi\int \mathrm{d}r r^4 V(r).$$

Exchange interaction energy (I)

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.,

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

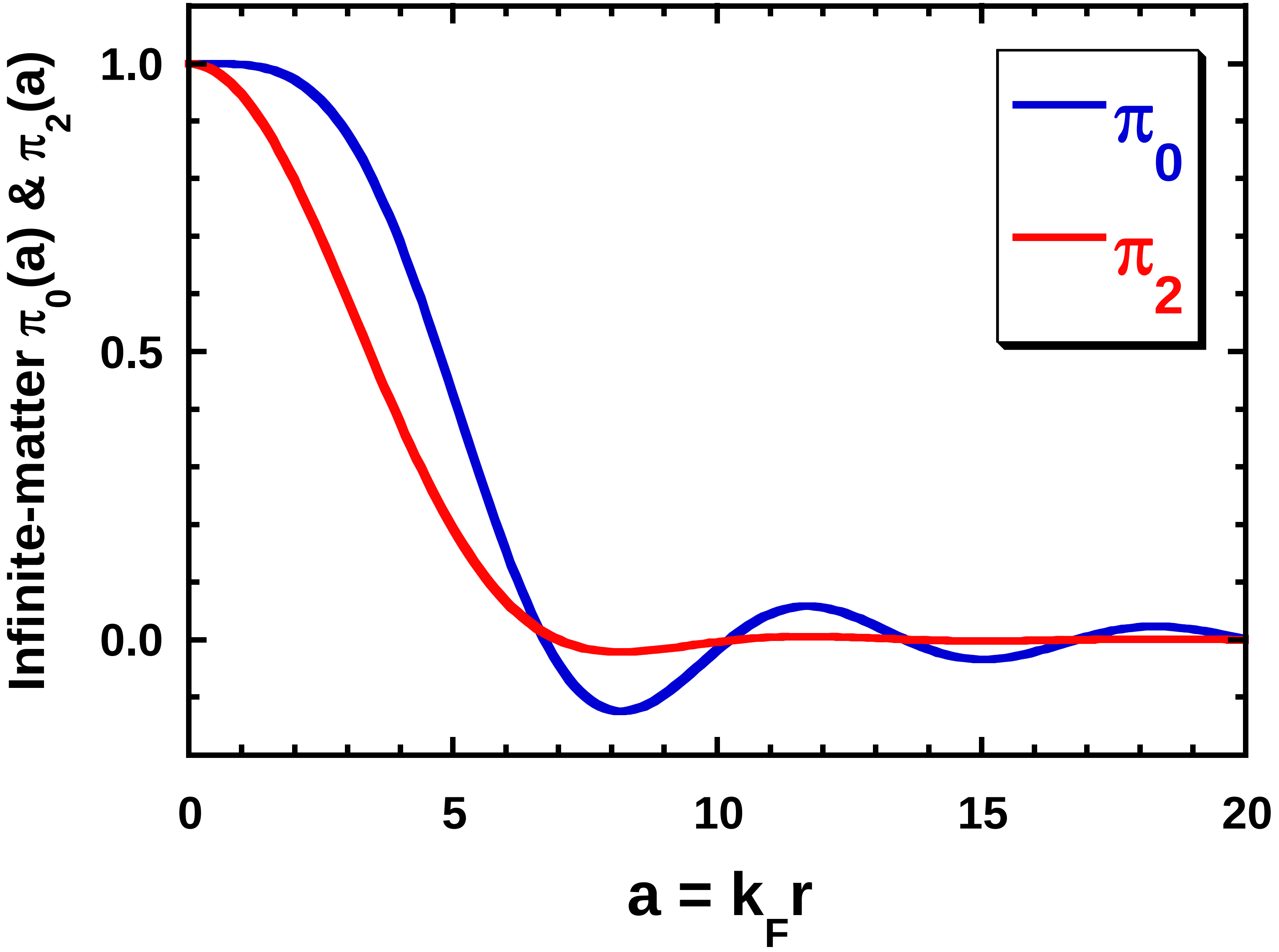
Function in square parentheses equals 1 at $r{=}0$, and has the first zero at $r \simeq 4.4934/k_F \simeq 3\,\mathrm{fm}$, i.e., in the non-local direction the density varies on the same scale as it does in the local direction. Therefore, the quadratic expansion in the relative variable,

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

where derivatives $\partial_i{=}\partial/\partial r^i$ 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:

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

Density matrix in the non-local direction



Exchange interaction energy (II)

Since for small r, this equation must be compatible with the Taylor expansion, the auxiliary functions must fulfill conditions at r=0,

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

In order to conserve the local-gauge-invariance properties, we also require that

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

The auxiliary functions $\pi_0(r)$ and $\pi_2(r)$ 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 momentum expansion around the Fermi momentum k_F. This gives the density-matrix expansion (DME) of Negele and Vatherin, in which

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

where $j_n(k_Fr)$ are the spherical Bessel functions. The term depending on the non-local density in the exchange integral gives the exchange interaction energy:

$$E_{\text{exch}}^{\text{int}}=-\tfrac{1}{2}\int \overbrace{\mathrm{d}^3\vec{R}[V_0'\rho^2+\tfrac{1}{4}V_2'(\rho\Delta\rho-4(\rho\tau-\vec{j}^2))]}+\ldots,$$

Local energy density

where coupling constants V_0' and V_2' read

$$V_0'=4\pi\int drr^2\pi_0^2(r)V(r)\quad\text{and}\quad V_2'=\tfrac{4}{3}\pi\int drr^4\pi_0(r)\pi_2(r)V(r).$$

Energy density functional in the 2$^{\rm nd}$ order (Skyrme)

Nr	$\rho_{n'L'v'J'}$	$(\vec{\nabla}^m)_I$	ρ_{nLvJ}	Skyrme
1	$[\rho]_0$	Δ	$[\rho]_0$	$\rho\Delta\rho$
2	$[\rho]_0$	1	$\left[k^2\rho\right]_0$	$\rho\tau$
1	$[ks]_0$	1	$[ks]_0$	$\left(J^{(0)}\right)^2$
2	$[ks]_1$	1	$[ks]_1$	$\left(J^{(1)}\right)^2$
3	$[ks]_2$	1	$[ks]_2$	$\left(J^{(2)}\right)^2$
1	$[\rho]_0$	∇	$[ks]_1$	$\rho\vec{\nabla}\cdot\vec{J}$

Time-even 2nd order terms.

Nr	$\rho_{n'L'v'J'}$	$(\vec{\nabla}^m)_I$	ρ_{nLvJ}	Skyrme
1	$[k\rho]_1$	1	$[k\rho]_1$	$\vec{j}^2$
1	$[s]_1$	Δ	$[s]_1$	$\vec{s}\Delta\vec{s}$
2	$[s]_1$	$[\nabla\nabla]_2$	$[s]_1$	$\left(\vec{\nabla}\cdot\vec{s}\right)^2$
3	$[s]_1$	1	$\left[k^2s\right]_1$	$\vec{s}\cdot\vec{T}$
4	$[s]_1$	1	$\left[[kk]_2\,s\right]_1$	$\vec{s}\cdot\vec{F}$
1	$[k\rho]_1$	∇	$[s]_1$	$\vec{s}\cdot\vec{\nabla}\times\vec{j}$

Time-odd 2nd order terms.

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Energy density functional in the 4th order

Nr	$\rho_{n'L'v'J'}$	$(\vec{\nabla}^m)_I$	ρ_{nLvJ}
1	$[\rho]_0$	Δ^2	$[\rho]_0$
2	$[\rho]_0$	Δ	$[k^2\rho]_0$
3	$[\rho]_0$	$[\nabla\nabla]_2$	$[[kk]_2\,\rho]_2$
4	$[\rho]_0$	1	$[k^4\rho]_0$
5	$[k^2\rho]_0$	1	$[k^2\rho]_0$
6	$[[kk]_2\,\rho]_2$	1	$[[kk]_2\,\rho]_2$
1	$[ks]_0$	Δ	$[ks]_0$
2	$[ks]_0$	$[\nabla\nabla]_2$	$[ks]_2$
3	$[ks]_0$	1	$[k^2ks]_0$
4	$[ks]_1$	Δ	$[ks]_1$
5	$[ks]_1$	$[\nabla\nabla]_2$	$[ks]_1$
6	$[ks]_1$	$[\nabla\nabla]_2$	$[ks]_2$
7	$[ks]_1$	1	$[k^2ks]_1$
8	$[ks]_2$	Δ	$[ks]_2$
9	$[ks]_2$	$[\nabla\nabla]_2$	$[ks]_2$
10	$[ks]_2$	1	$[k^2ks]_2$
11	$[ks]_2$	1	$[k\,[kk]_2]_3\,s]_2$
1	$[\rho]_0$	$\Delta\nabla$	$[ks]_1$
2	$[\rho]_0$	∇	$[k^2ks]_1$
3	$[k^2\rho]_0$	∇	$[ks]_1$
4	$[[kk]_2\,\rho]_2$	∇	$[ks]_1$
5	$[[kk]_2\,\rho]_2$	∇	$[ks]_2$

Nr	$\rho_{n'L'v'J'}$	$(\vec{\nabla}^m)_I$	ρ_{nLvJ}
1	$[k\rho]_1$	Δ	$[k\rho]_1$
2	$[k\rho]_1$	$[\nabla\nabla]_2$	$[k\rho]_1$
3	$[k\rho]_1$	1	$[k^2k\rho]_1$
1	$[s]_1$	Δ^2	$[s]_1$
2	$[s]_1$	$(\Delta)\,[\nabla\nabla]_2$	$[s]_1$
3	$[s]_1$	Δ	$[k^2s]_1$
4	$[s]_1$	$[\nabla\nabla]_2$	$[k^2s]_1$
5	$[s]_1$	Δ	$[[kk]_2\,s]_1$
6	$[s]_1$	$[\nabla\nabla]_2$	$[[kk]_2\,s]_1$
7	$[s]_1$	$[\nabla\nabla]_2$	$[[kk]_2\,s]_2$
8	$[s]_1$	$[\nabla\nabla]_2$	$[[kk]_2\,s]_3$
9	$[s]_1$	1	$[k^4s]_1$
10	$[s]_1$	1	$[(k^2)\,[kk]_2\,s]_1$
11	$[k^2s]_1$	1	$[k^2s]_1$
12	$[k^2s]_1$	1	$[[kk]_2\,s]_1$
13	$[[kk]_2\,s]_1$	1	$[[kk]_2\,s]_1$
14	$[[kk]_2\,s]_2$	1	$[[kk]_2\,s]_2$
15	$[[kk]_2\,s]_3$	1	$[[kk]_2\,s]_3$
1	$[k\rho]_1$	$\Delta\nabla$	$[s]_1$
2	$[k\rho]_1$	∇	$[k^2s]_1$
3	$[k\rho]_1$	∇	$[[kk]_2\,s]_1$
4	$[k\rho]_1$	∇	$[[kk]_2\,s]_2$
5	$[k^2k\rho]_1$	∇	$[s]_1$

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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.