Mapping the minefield: problems and challenges within the EDF framework

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Workshop on
"Nuclear energy density functional method: going beyond the minefield"

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Outline

1. Which type EDF of approach?
   1. self-consistent mean field / single-reference EDF approach
   2. horizontal expansion (multi reference EDF approach)
   3. vertical expansion: QRPA and beyond
2. Functional form
   1. relativistic or non-relativistic EDFs?
   2. EDF of local or non-local densities?
   3. Which kind of terms has to be considered for better phenomenology?
   4. Not every form can be safely/meaningfully used in each type of EDF approach!
   5. Do we need dedicated parameter sets for each type of approach?
   6. What do density dependences actually represent?
   7. What about the Pauli principle?
3. Instabilities
   1. Landau-type instabilities
   2. Finite-size instabilities
   3. Others: Shell-structure / BCS-BEC / . . . instability
   4. Divergence of QRPA & beyond correlation energy when increasing the model space
   5. Divergence of pairing correlations when increasing the model space
   6. Cutoff procedures are in general representation-dependent
   7. Not all instabilities are resolved by all numerical representations - feature or bug?
4. Numerical challenges of large-scale applications
5. How far can EDF approaches been pushed . . .
   1. . . . concerning phenomena to be described
   2. . . . concerning observables to be described

Disclaimer

- The following presentation assumes that the audience has working knowledge of the nuclear EDF approach. There will be only very few equations. A formal introduction into the many flavours of the nuclear EDF method touched upon and the analysis precise mathematical nature of the problems mentioned in what follows would require a one-week course.
- The following is my personal and biased view of the many open conceptual and practical problems with using the nuclear EDF method that prevents practitioners from major advances.
- Most, if not all, of these problems are connected. Attempts to avoid one problem usually leads to at least one new problem at a different place.
- Still, some of the problems that will be addressed below are easier to ignore than others.

What is the nuclear EDF method?

In spite of popular belief, the nuclear EDF method is not a variant of Density Functional Theory as used for electronic systems.
As a reminder, the Hohenberg-Kohn theorems in their most basic form (for non-degenerate ground states in the absence of a magnetic fields)

1. *The ground state expectation value of any physical observable of a many-electron system is a unique functional of the electron density* $\rho(\mathbf{r})$
2. *The total energy functional has a minimum, the ground state energy* E_0*, in correspondence to the ground state density* $\rho_0(\mathbf{r})$*.*

Hohenberg, Kohn, PR 136 (1964) B864

Made practical when calculating the density and kinetic density from an auxiliary product state that provides yields $\rho_0(\mathbf{r})$.

Kohn, Sham, Phys. Rev. A 140 (1965) 1133;

1998 Nobel Prize in Chemistry

The theorems do not cover what is done by all practitioners

- symmetry-breaking calculations (in the sense of working with densities that do not adopt the symmetries (J, N, Z, parity, translational invariance, . . . of the nuclear wave function
- There is no room for a "beyond-mean-field DFT" for the ground state

In the end, the contradiction boils down to (isolated) nuclei being self-bound systems, while electronic systems are bound by an external potential (usually generated by atomic nuclei). The various extensions of DFT to spin-polarised systems, paired systems, systems with currents coupling to external potentials, ensemble averages, do not change this issue.

Engel, PRC 75 (2007) 014306; Barnea, PRC76 (2007) 067302;

Messud, Bender, Suraud, PRC 80 (2009) 054314;

Messud, PRC 87 (2013) 024302;

Kievsky, Orlandini, Gattibigio, PRA (2021) L030801;

What is the nuclear EDF method?

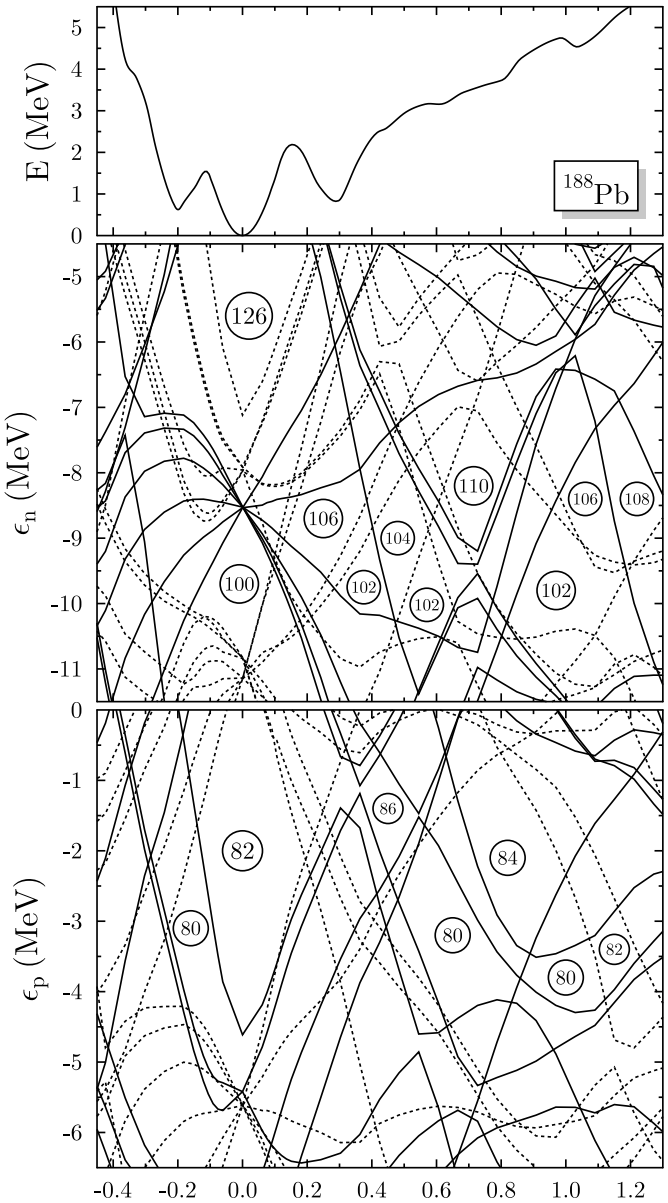
What is the concept underlying the nuclear EDF method?

- Phenomenological functional of one body densities generated by some auxiliary state?
- Wave-function based method based on the expectation value of an effective interaction evaluated for an an auxiliary state?

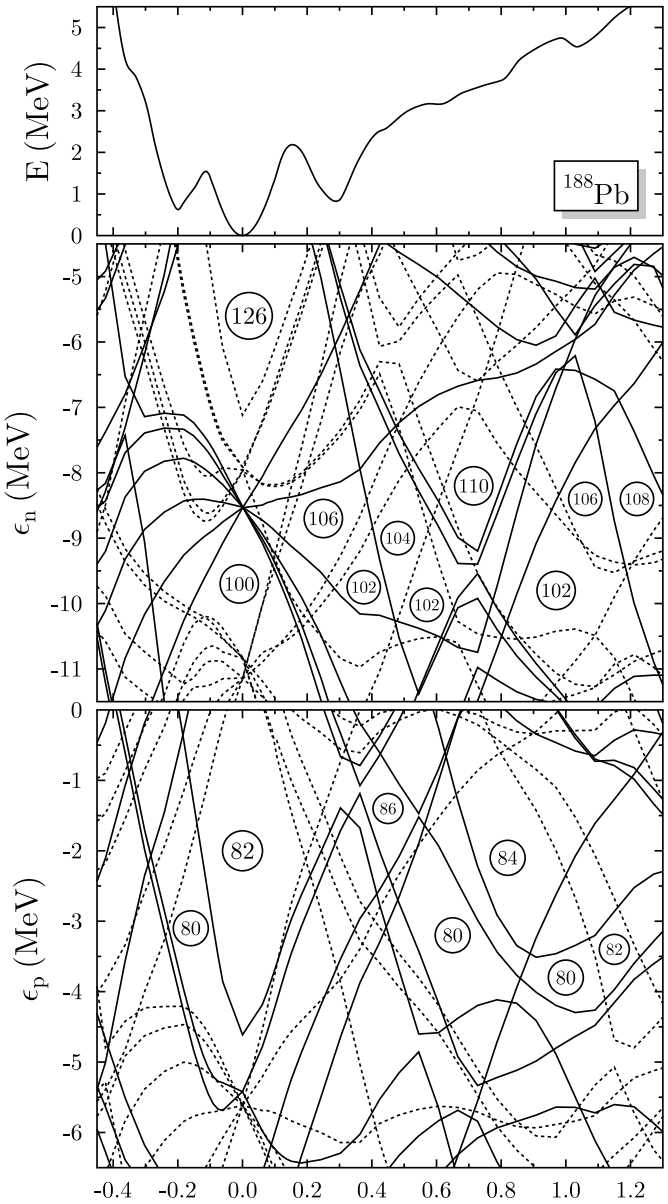
What kind of auxiliary state?

- Single-reference (self-consistent mean field)?
- Multi-reference?
- Summation of diagrams?
- Something entirely different?

Horizontal vs. vertical expansion of correlations



Horizontal vs. vertical expansion of correlations



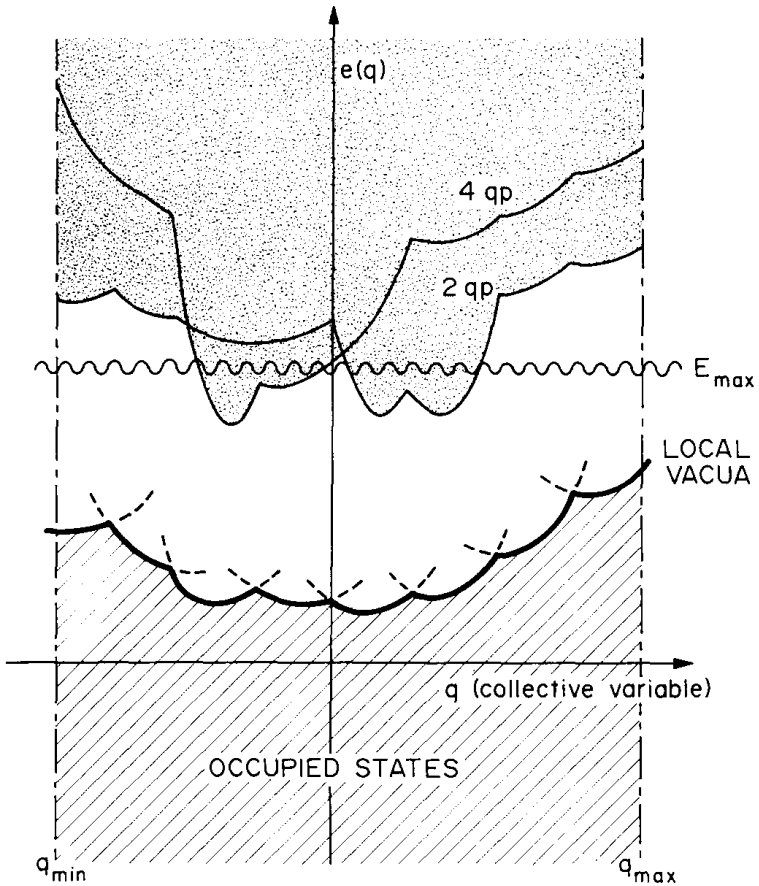


Fig. 1. Schematic plot of the energy versus the collective variable. The dark envelopes show the positions of the local vacua. The domain of the collective variable is defined by q_{min}, q_{max} and the energy cut E_{max}.

Dönau *et al*, NPA496 (1989) 333.

Some questions on horizontal expansions

By "horizontal expansion", I mean symmetry restoration and mixing of low-lying quasiparticle vacua differing in some set of collective coordinates

- This establishes a configuration mixing
- What are the relevant degrees of freedom?
  - N-projection, Z-projection, J projection, parity projection, projection on the centre-of-mass, isospsin-projection (and subsequent mixing of different multiplets connected by isospin-breaking pieces of the Hamiltonian, ...
  - Mixing shapes with different (axial and non-axial) quadrupole / octupole / hexadecapole / ... moments, mean-square radii, pairing gaps, low-lying quasi-particle excitations ...
- Phrased differently, where to stop for which phenomenon / nucleus / ... ?
- PAV or VAP?

- Can this be done with the same EDF?
- Can MR effects be absorbed into the EDF for SR calculations?

Some questions on horizontal expansions

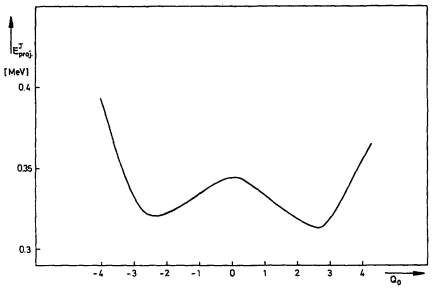
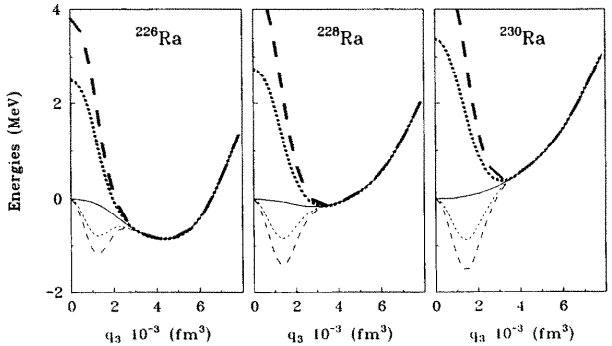
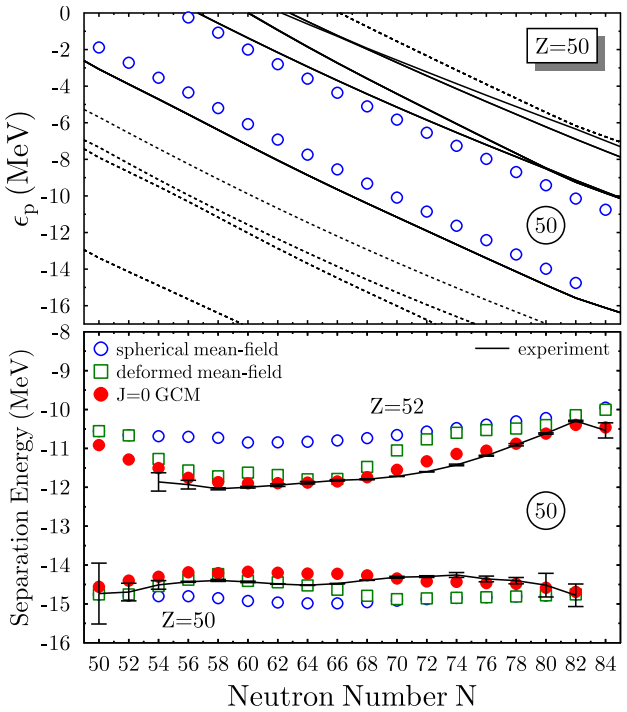


Fig. 1. Angular momentum projected ($J = 0$) energy as a function of the quadrupole moment Q_0 (eq. (19)) for the nucleus ^{150}Sn.

Dalafi, NPA 252 (1975) 42



Egido, Robledo, NPA 524 (1991) 65

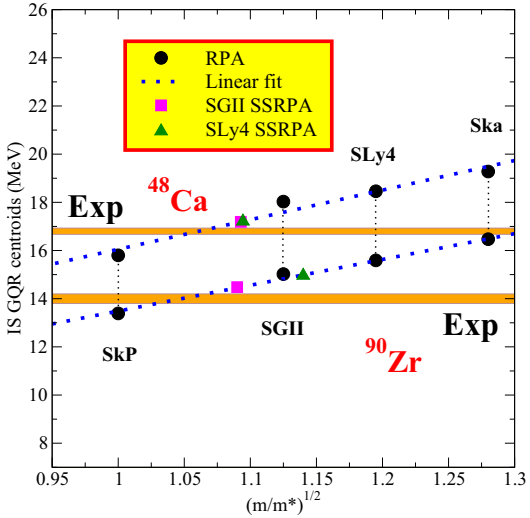


Bender, Bertsch, Heenen, PRC 78 (2008) 054312

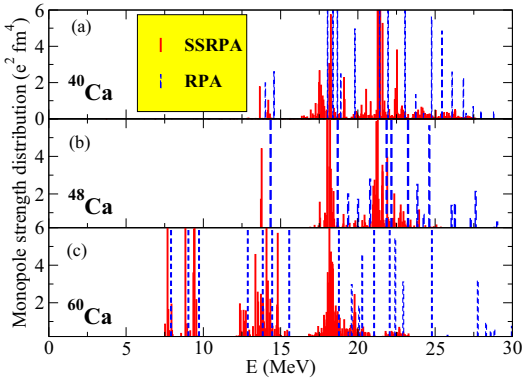
Some questions on vertical expansions

Which vertical expansion?

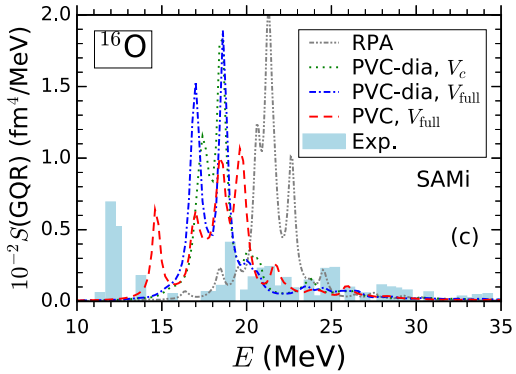
- QRPA?
- Some flavour of Second QRPA?
- Particle-vibration coupling of some sort?
- Multi-Configuration Hartree-Fock / variational multiparticle-multihole configuration mixing method



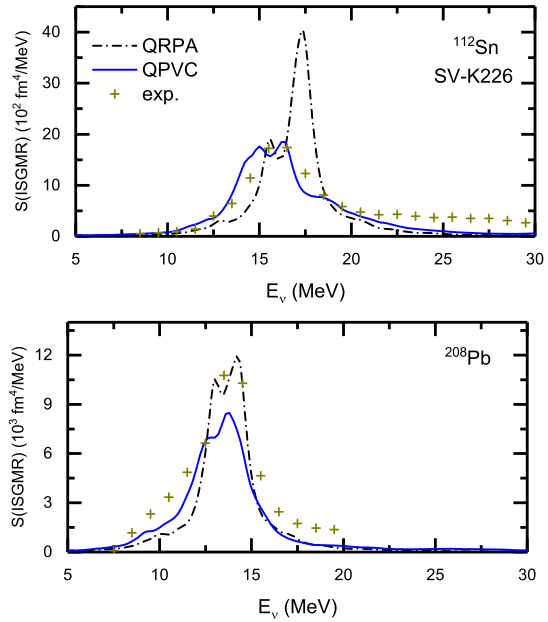
Grasso, Gambacurta, Vasseur, PRC98 (2018) 051303(R)



Gambacurta, Grasso, Sorlin, PRC100 (20120) 014317



Shen, Colò, Roca-Maza, PRC 101 (2020) 044316



Li, Niu, Colò, PRL131 (2023) 082501

What does this imply for the adjustment of EDFs on data?

- Going beyond the mean field in a horizontal expansion adds correlation energy (and modifies other observables) for each added collective degree of freedom.
- (not shown) Particle-vibration coupling changes the relative positions of low-lying states often interpreted as "single-particle states"
- Whatever the method, the impact of going beyond (Q)RPA significantly changes observables used to phenomenologically deduce nuclear matter properties from giant resonances (incompressibility, effective mass, . . .)

Which degrees of freedom in EDF?

- relativistic or non-relativistic?
- contact forces with gradients or finite range or a combination of both?
- If finite range, which form factor (Gaussian, Yukawa, ...)?
- exact exchange?
- different particle-hole and particle-particle interactions?
- density dependences?
- many-body forces?
- isospin-breaking nuclear terms?
- How to treat the electromagnetic interaction (Coulomb exchange, correlation energy, relativistic corrections, magnetic effects, intrinsic form factors, ...)

- Is there a constructive scheme that establishes a hierarchy of terms (with respect to gradients, 2-body vs. 3-body vs. 4-body terms) beyond the naive expectation that importance decreases with the complexity of the terms?
- Can we expect that coupling constants take a "natural size"?

An example of "naive dimensional analysis" based on chiral EFT adapted to nuclear EDFs:

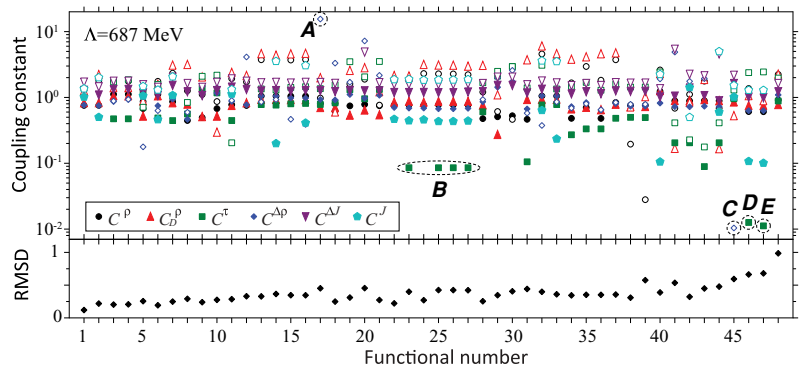


FIG. 2. (Color online) Scaled coupling constants $|C_t^\sigma|$ at $\Lambda = 687$ MeV (top) and contributions of individual functionals to the total RMS value (bottom). The filled symbols refer to the isoscalar coupling constants and empty symbols to the isovector ones. The ordering of functionals by index is the same as in Table I.

index 40 = SkP

Kortelainen, Furnstahl, Nazarewicz, Stoitsov, PRC 82 (2010) 011304(R)

True contact pseudo-potential $t_0\,(1+x_0\hat{P}_\sigma)\,\delta(\mathbf{r}-\mathbf{r}')$

$$\begin{aligned}\mathcal{E} &= \int d^3r\,\Big\{\tfrac{3}{8}\,t_0\,\rho_0^2(\mathbf{r}) - \tfrac{1}{8}\,t_0\,(1+2x_0)\,\rho_1^2(\mathbf{r}) - \tfrac{1}{8}\,t_0\,(1-2x_0)\,\mathbf{s}_0^2(\mathbf{r}) \\ &\quad -\tfrac{1}{8}\,t_0\,\mathbf{s}_1^2(\mathbf{r}) + \tfrac{1}{8}\,t_0\,(1+x_0)\,\check{\mathbf{s}}_0(\mathbf{r})\cdot\check{\mathbf{s}}_0^*(\mathbf{r}) + \tfrac{1}{8}\,t_0\,(1-x_0)\,\check{\rho}_1(\mathbf{r})\,\check{\rho}_1^*(\mathbf{r})\Big\}\end{aligned}$$

(see Perlinska *et al.* PRC 69 (2004) 014316 for definition of $\check{\mathbf{s}}_0(\mathbf{r})$ and $\check{\rho}_1(\mathbf{r})$)

Functional with contact vertices:

$$\begin{aligned}\mathcal{E} &= \int d^3r\,\Big\{C_0^\rho[\rho_0,\ldots]\,\rho_0^2(\mathbf{r}) + C_1^\rho[\rho_0,\ldots]\,\rho_1^2(\mathbf{r}) + C_0^s[\rho_0,\ldots]\,\mathbf{s}_0^2(\mathbf{r}) \\ &\quad + C_1^s[\rho_0,\ldots]\,\mathbf{s}_1^2(\mathbf{r}) + C_0^{\check{s}}[\rho_0,\ldots]\,\check{\mathbf{s}}_0(\mathbf{r})\cdot\check{\mathbf{s}}_0^*(\mathbf{r}) + C_1^{\check{\rho}}[\rho_0,\ldots]\,\check{\rho}_1(\mathbf{r})\,\check{\rho}_1^*(\mathbf{r})\Big\}\end{aligned}$$

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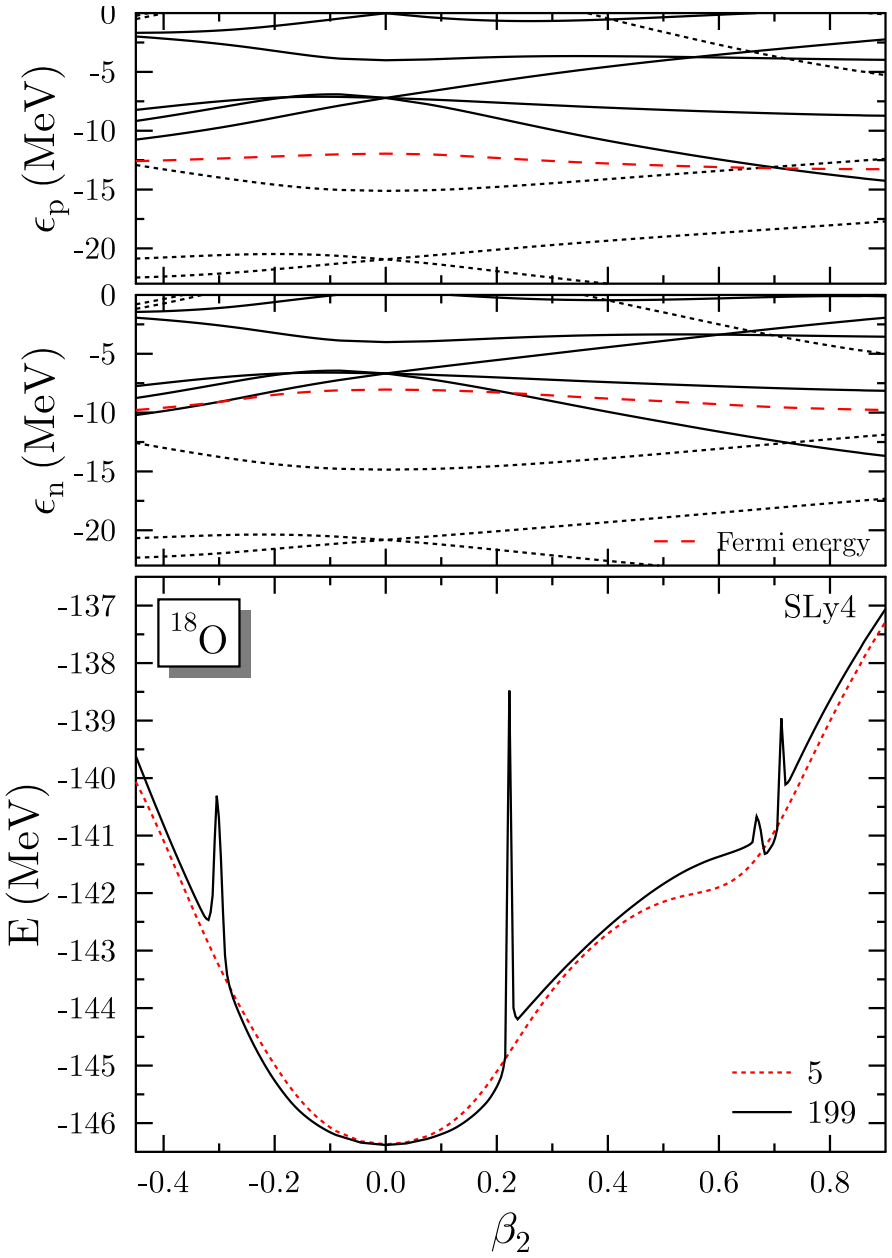
Coulomb interaction $\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}$

$$\mathcal{E} = \frac{1}{2}\iint d^3r\,d^3r'\,\frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\Big[\rho_p(\mathbf{r})\rho_p(\mathbf{r}') - \rho_p(\mathbf{r},\mathbf{r}')\rho_p(\mathbf{r}',\mathbf{r}) + \kappa_p^*(\mathbf{r},\mathbf{r}')\kappa_p(\mathbf{r},\mathbf{r}')\Big]$$

Approximate Coulomb functionals

$$\mathcal{E} = \frac{e^2}{2}\iint d^3r\,d^3r'\,\frac{\rho_p(\mathbf{r})\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} - \frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}\int d^3r\,\rho_p^{4/3}(\mathbf{r})$$

Breaking the Pauli principle causes problems



- pure particle-number projection
- first hints from Hamiltonian-based approaches

  Dönau, PRC 58 (1998) 872; Almehed, Frauendorf, Dönau, PRC 63 (2001) 044311; Anguiano, Egido, Robledo NPA696 (2001) 467
- Subsequent analysis in a strict energy density functional (EDF) framework and of EDF-specific consequences

  Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC 76 (2007) 054315; Lacroix, Duguet, Bender, PRC 79 (2009) 044318; Bender, Duguet, Lacroix, PRC 79 (2009) 044319; Duguet, Bender, Bennaceur, Lacroix, Lesinski, PRC 79 (2009) 044320
- Same problem in different disguise found already earlier for EDF kernels between HFB vacua and two-quasiparticle states

  Tajima, Flocard, Bonche, Dobaczewski, Heenen, NPA542 (1992) 355
- Also found in angular-momentum projection

The origin of the problem in a nutshell

- All standard energy density functionals (EDF) used for mean-field models and beyond do not correspond to the expectation value of a Hamiltonian for at least one of the following reasons:
  - density dependences
  - the use of different effective interactions in the particle-hole and pairing parts of the energy functional
  - the omission, approximation or modification of specific exchange terms

  that are all introduced for phenomenological reasons and/or the sake of numerical efficiency.
- consequence: breaking of the exchange symmetry ("Pauli principle") under particle exchange when calculating the energy, leading to non-physical interactions of a given nucleon or pair of nucleons with itself, or of three nucleons among themselves etc.
- the resulting self-interactions and self-pairing-interactions remain (usually) hidden in the mean field
- in the extension to symmetry-restored GCM, these terms cause
  - discontinuities and divergences in symmetry-restored energy surfaces
  - breaking of sum rules in symmetry restoration
  - potentially multi-valued EDF in case of standard density-dependences

Many-body forces or density dependences? I

- Based on a back-of-the-envelope estimate, Weisskopf [NP3 (1957) 423] pointed out that any pure two-body interaction – irrespective of its form – fitted to reproduce – at the mean-field level – the empirical values for the saturation density ρ_{sat} and binding energy per particle E/A of the model system of homogeneous symmetric and spin-symmetric infinite nuclear matter necessarily leads to an isocalar effective mass $m_0^*/m \approx 0.4$ that is much smaller than what is expected from empirical data.

$\Rightarrow$ Need for higher-order terms.

- There are many indications that there are *genuine* three-body forces acting in nuclear many-body systems.
- From a modern point of view, any attempt to renormalise the "bare" NN and NNN interaction to an effective interaction acting only below a given cutoff scale necessarily leads to *induced* three-body (and higher many-body) forces. Although it cannot be expected that the nuclear EDF can be directly connected to the "bare" interaction in this way, it nevertheless represents by construction such a renormalised effective interaction; hence, implying the presence of induced three-body (and higher) forces.
- Any approach that is "beyond the mean field" in the diagrammatic sense leads in one way or the other to a k_F dependence of the total binding energy (and in principle also an energy dependence, but that is irrelevant for the present discussion).

Many-body forces or density dependences? II

- The Brueckner-HF formalism when applied to infinite nuclear matter yields a k_F-dependent G matrix, which in local density approximation (LDA) can be translated into a density-dependent effective in-medium interaction via the relation $k_F = (\frac{3}{2}\pi^2\rho)^{1/3}$ for the Fermi energy in homogeneous symmetric and spin-symmetric infinite nuclear matter [H. S. Köhler, NPA258 (1976) 301].
- Also, the density-matrix expansion (DME) of exchange terms leads to complicated density dependences of the resulting effective interaction for Hartree calculations.

- Skyrme proposed a combination of two-, three- and four-body contact interactions (with density- independent coupling constants).
- Skyrme's simple gradientless contact three-body force

$$v^{3b} = u_0 \left(\hat{\delta}_{r_1 r_3} \, \hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2} \, \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_2 r_1} \, \hat{\delta}_{r_3 r_1} \right) . \tag{1}$$

  In the absence of proton-neutron mixing, the EDF reads

$$\mathcal{E}^{3b} = \frac{3}{4} u_0 \int d^3 r \left[\rho_n \left(\rho_p^2 - \mathbf{s}_p^2 + \tilde{\rho}_p^* \tilde{\rho}_p \right) + \rho_p \left(\rho_n^2 - \mathbf{s}_n^2 + \tilde{\rho}_n^* \tilde{\rho}_n \right) \right] \tag{2}$$

  The absence of contributions that are trilinear in the same isospin is a consequence of the Pauli principle: a gradientless contact force only acts between nucleons in relative s waves, such that the contributions to the energy have to come from two nucleons of same isospin but opposite spin and a third nucleon of opposite isospin and arbitrary spin [Waroquier et al, PRC 13 (1976) 1664].
- Gradientful contact three-body forces were considered later [Liu, PLBB60, 9 (1975); Onishi and Negele NPA301, 336 (1978); Waroquier et al, PRC 19 (1979) 1983, NPA404 (1983) 269, NPA404 (1983) 298; Arima et al, NPA459 (1986) 286; Zheng et al, AP201 (1990) 342; Liu et al, NPA534 (1991) 1, NPA534 (1991) 58; Sadoudi et al, PR88 (2013) 064326].

Skyrme's contact 3-body force vs. a density-dependent two-body force I

- A simple gradientless contact three-body force fails to provide realistic K_∞, leads to repulsive pairing matrix elements [Zamick, Proc. Int. Conf. on Nuclear Structure and Spectroscopy, Amsterdam (1974), p. 24; Arima, NPA354 (1981) 19c] and leads to an infinite-wavelength spin-instability signalled by the Landau parameter $g_0 < -1$ [Chang PLB56 (1975) 205]. The third of these problems disappears when re-interpreting the 3-body force as a density-dependent 2-body force.

- A density dependent two-body force is obtained multiplying Skyrme's t_0 term by $\frac{1}{3}\left[\rho_n(\mathbf{R}) + \rho_p(\mathbf{R})\right]$, where $\hat{P}_\sigma$ is the spin exchange operator and $\mathbf{R} \equiv \frac{1}{2}(\mathbf{r} + \mathbf{r}')$ the mean position of the two nucleons

$$v^{2b,dd:I} = \tfrac{1}{3}\, t_3 \left(1 + x_3 \hat{P}_\sigma\right) \left[\rho_n(\mathbf{R}) + \rho_p(\mathbf{R})\right] \hat{\delta}_{r_1 r_2} \tag{3}$$

The corresponding EDF reads

$$\begin{aligned}
\mathcal{E}_{t_3} \;=\; \int d^3r \Big\{ & \tfrac{1}{12} t_3 (1 - x_3) \left[\left(\rho_n^2 - \mathbf{s}_n^2 + \tilde{\rho}_n^* \tilde{\rho}_n\right) \rho_n + \left(\rho_p^2 - \mathbf{s}_p^2 + \tilde{\rho}_p^* \tilde{\rho}_p\right) \rho_p \right] \\
& + \tfrac{1}{12} t_3 (1 - x_3) \left[\left(\rho_n^2 - \mathbf{s}_n^2 + \tilde{\rho}_n^* \tilde{\rho}_n\right) \rho_p + \left(\rho_p^2 - \mathbf{s}_p^2 + \tilde{\rho}_p^* \tilde{\rho}_p\right) \rho_n \right] \\
& + \tfrac{1}{6} t_3 \left(1 + \tfrac{x_3}{2}\right) \left(\rho_n^2\, \rho_p + \rho_n\, \rho_p^2\right) + \tfrac{1}{12} t_3 \left(\rho_n \mathbf{s}_n \cdot \mathbf{s}_p + \mathbf{s}_n \cdot \mathbf{s}_p \rho_p\right) \Big\} .
\end{aligned} \tag{4}$$

- The expression in red is what is obtained from genuine three-body force (2).
- The expressions in blue and purple have an isospin structure that is not obtained from a genuine three-body force (2). Choosing $x_3 = +1$ in order to suppress the term in blue also sets the desired term in red to zero. The term in purple can only be set to zero by setting $t_3 = 0$, a choice which sets all terms to zero.
- The expression in brown has the correct isospin structure for the time-even terms, but has no spin or pairing terms it can correctly combine with.
- Altogether, a gradientless three-body contact force cannot be exactly mapped onto a density-dependent gradientless contact two-body force, which is not unexpected.

- To obtain the same HF energy in a time-reversal invariant system (where $\mathbf{s}_q = \tilde{\rho}_q = 0$), one has to set $x_3 = +1$. This suppresses the pairing term altogether. The EDF then reads

$$\mathcal{E}_{t_3,x_3=1} = \int d^3r \left\{ \tfrac{3}{12} t_3 \left(\rho_n^2 \rho_p + \rho_n \rho_p^2\right) + \tfrac{1}{12} t_3 \left(\rho_n \mathbf{s}_n \cdot \mathbf{s}_p + \mathbf{s}_n \cdot \mathbf{s}_p \rho_p\right) \right\}. \quad (5)$$

  which evidently differs from the expression from a true three-body force (2)

$$\mathcal{E}^{3b} = \tfrac{3}{4} u_0 \int d^3r \left[\rho_n \left(\rho_p^2 - \mathbf{s}_p^2 + \tilde{\rho}_p^* \tilde{\rho}_p\right) + \rho_p \left(\rho_n^2 - \mathbf{s}_n^2 + \tilde{\rho}_n^* \tilde{\rho}_n\right) \right]$$

- From a phenomenological point of view this has been excellent news. Following the suggestion of Vautherin and Brink [PRC5 (1972) 626] to re-interpret the three-body force of early parameterisations like SIII as a density-dependent two-body force that gives the same result for time-reversal-conserving HF states, the difference in spin structure between (2) and (5) suppresses the (Landau type) spin-instability of these parameterisations.
- However, as results for homogeneous isotropic spin-saturated infinite matter are not affected, the incompressibility K_∞ remains non-physically high.

- The incompressibility can be lowered to its empirical value by taking a fractional power $\alpha < 1/n$ of the density entering the density dependence $\left[\rho_n(\mathbf{R}) + \rho_p(\mathbf{R})\right]^\alpha$ of the coupling constant, as can be motivated by the structure of the expression for the Brueckner G matrix [Köhler, NPA258 (1976) 301]

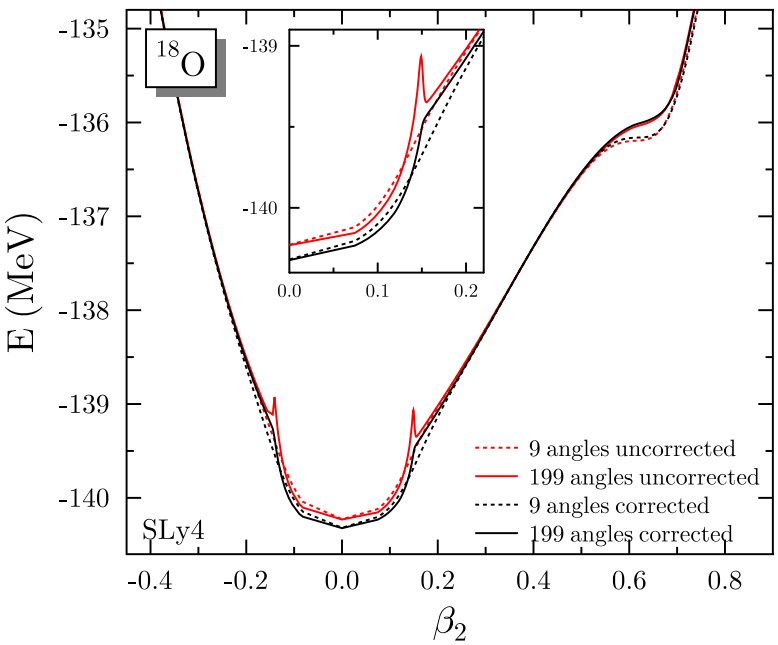
$$v^{2b,dd} = \tfrac{1}{3}\, t_3 \left(1 + x_3 \hat{P}_\sigma\right) \left[\rho_n(\mathbf{R}) + \rho_p(\mathbf{R})\right]^\alpha \hat{\delta}_{r_1 r_2} \tag{6}$$

  which leads to the EDF

$$\begin{aligned}\mathcal{E}_{t_3} \quad = \quad & \int d^3 r \left\{ \tfrac{1}{12} t_3 (1 - x_3) \left[\left(\rho_n^2 - \mathbf{s}_n^2 + \tilde{\rho}_n^* \tilde{\rho}_n\right) + \left(\rho_p^2 - \mathbf{s}_p^2 + \tilde{\rho}_p^* \tilde{\rho}_p\right) \right] (\rho_n + \rho_p)^\alpha \right. \\ & \left. + \tfrac{1}{6} t_3 \left(1 + \tfrac{x_3}{2}\right) \rho_n \rho_p \left(\rho_n + \rho_p\right)^\alpha + \tfrac{1}{12} t_3 \mathbf{s}_n \cdot \mathbf{s}_p \left(\rho_n + \rho_p\right)^\alpha \right]. \end{aligned} \tag{7}$$

- Köhler's Ska and Skb with $\alpha = 1/3$, SkM with$\alpha = 1/6$ [Krivine et al, NPA336 (1980) 155].
- Such density dependence with $\alpha = 1/3$ has also always been used with the Gogny force making the additional choice $x_3 = +1$ in order to suppress local $T = 1$ pairing terms that would diverge when solving the HFB equations for like-particle pairing.
- For all widely-used standard Skyrme parameterisations, only the coupling constant of the gradientless two-body term is chosen to be density dependent. Extensions tried concern density-dependences of gradient terms [Krewald et al, NPA281 (1977) 166; Farine et al, NPA696 (2001) 396; Chamel et al, PRC80 (2009) 065804] using two density dependences [Farine et al, NPA696 (2001) 396; Cochet et al, NPA731(2004) 34; Lesinski et al, PRC74 (2006) 044315] density-dependence with different isospin structure [Dutta et al, NPA458 (1986) 77] and different forms [Erler et al, PR82 (2010) 044307].

Non-viability of non-analytical density dependences

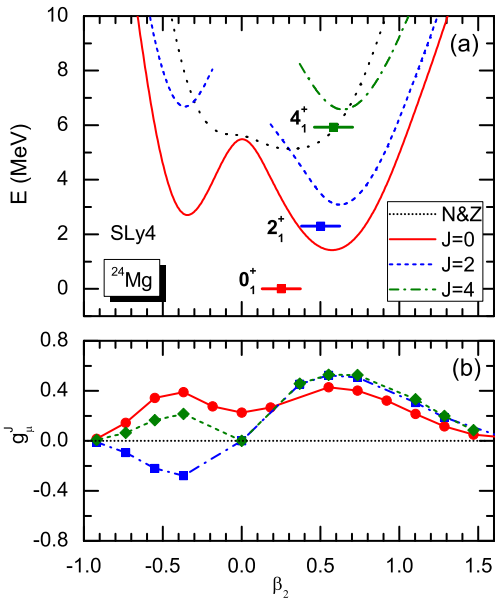


Duguet, Lacroix, Bender, Bennaceur, Lesinski, PRC 79 (2009) 044320

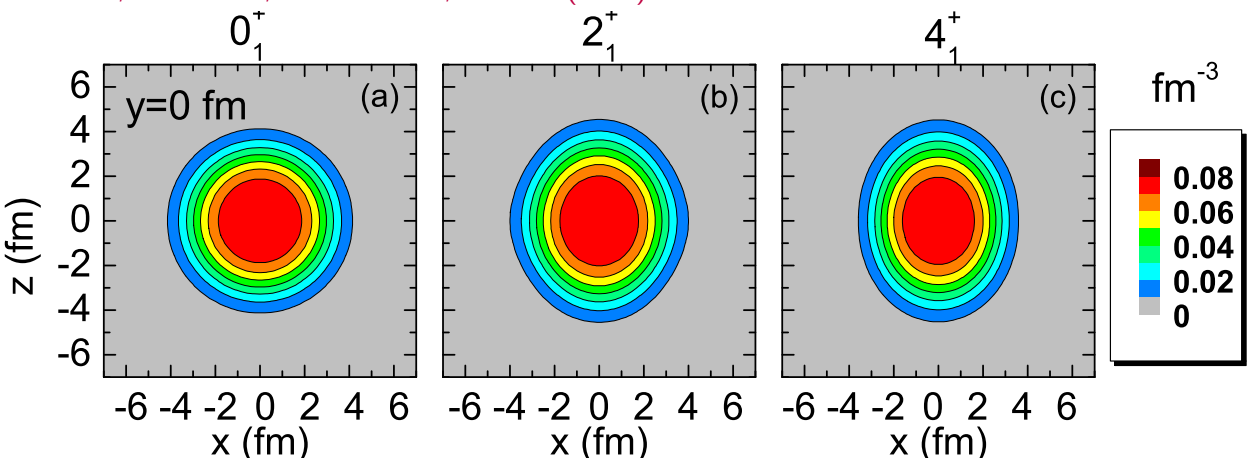
- in symmetry restored GCM, the local densities $\rho^{qq'}(\mathbf{r})$ are in general complex
- $\left[\rho^{qq'}(\mathbf{r})\right]^{\alpha}$ is a multi-valued non-analytical function
- spurious contribution from branch cuts (see Dobaczewski *et al.* PRC76 (2007) 054315, and Duguet *et al.* PRC79 (2009) 044320 for complex plane analysis)
- (partial) workaround when conserving specific symmetries: use particle-number projected densities for density dependence instead

Density dependences cannot be on laboratory densities

Using a prescription that combines transition/mixed densities and laboratory densities for restoration of spatial symmetries leads to problems with nuclear saturation as these objects have different spatial distribution.

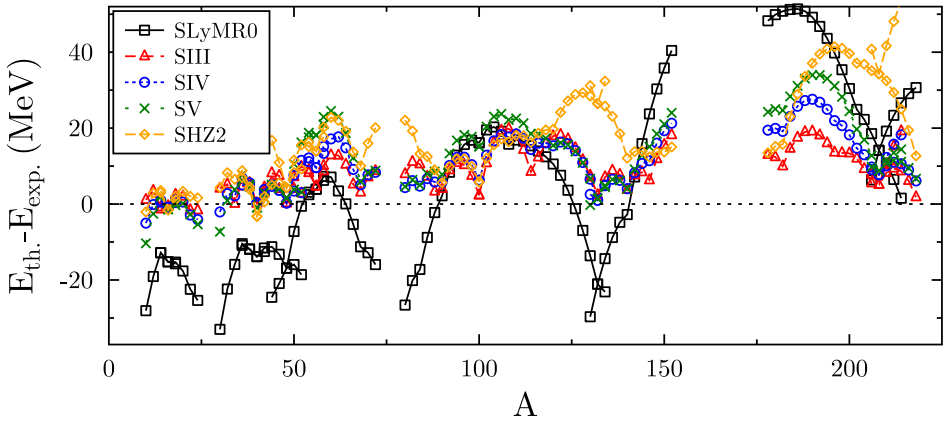


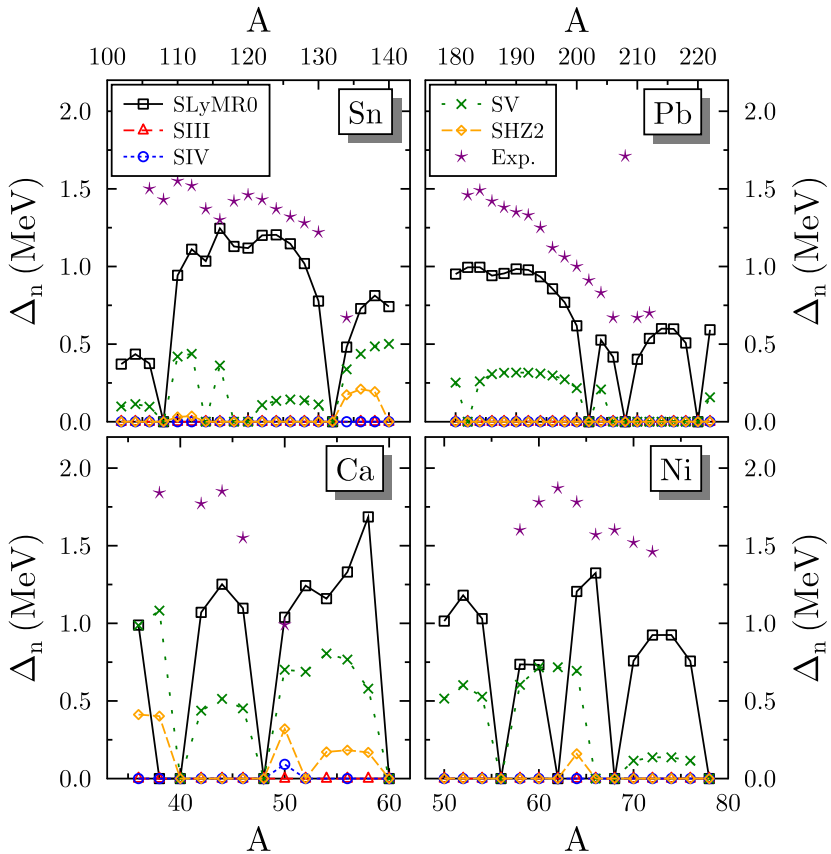
J. M. Yao, M. Bender, P.-H. Heenen, PRC 91 (2015) 024301



Contour plots of the 3D proton densities (in fm^{-3}) in the $y = 0$ plane for the 0^+_1 (a), 2^+_1 (b), 4^+_1 (c) states (with $M = 0$) in ^{24}Mg.

Simple 3+4-body have problems with phenomenology: SLyMR0



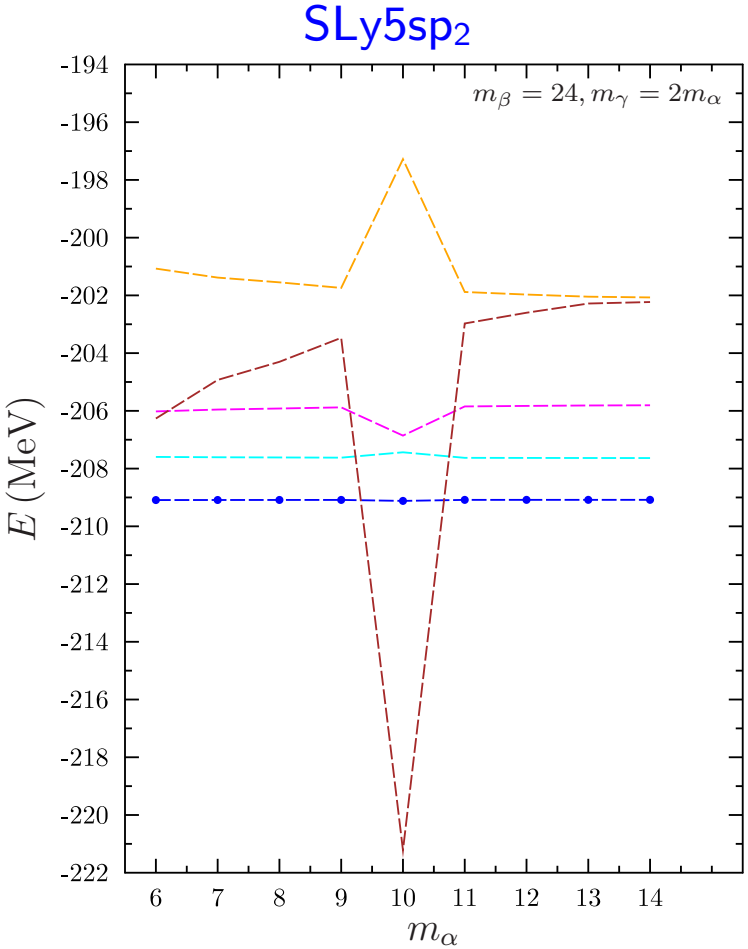


- it is impossible to fulfill the usual nuclear matter constraints , to have stable interactions and attractive pairing
- no "best fit" possible
- very bad performance compared to standard general functionals

Sadoudi, Bender, Bennaceur, Davesne, Jodon, and Duguet, Physica Scripta T154 (2013) 014013

Density dependence with particle-number projected density

Dependence on the number of discretization points chosen for Euler angles when projecting the same blocked triaxial state of ^{25}Mg which is practically pure $K = 5/2$, with SLy5sp$_2$ and SLyMR0.

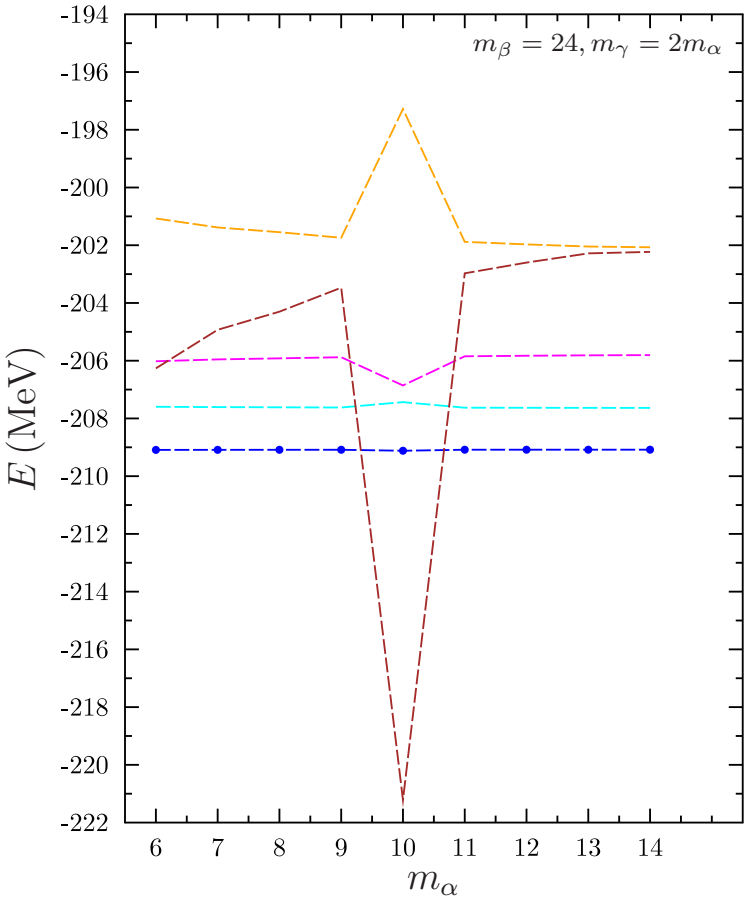


- effective interaction: standard density-dependent Skyrme (SLy5sp2) taking all exchange and pairing terms into account, courtesy of K. Bennaceur (unpublished, 2012).
- exact Coulomb exchange and Coulomb pairing
- particle-number projected (mixed) density entering the linear density dependence $\rho^\alpha = \rho$
- No obvious problems when projecting and mixing time-reversal invariance conserving HFB states.
- On a very small level, projected energies depend on the number of discretization points and sumrules might not be fulfilled.
- unrealistic decomposition into J, K components when projecting *time-reversal-invariance breaking* HFB states (where the particle-number projected mixed densities are *complex*)

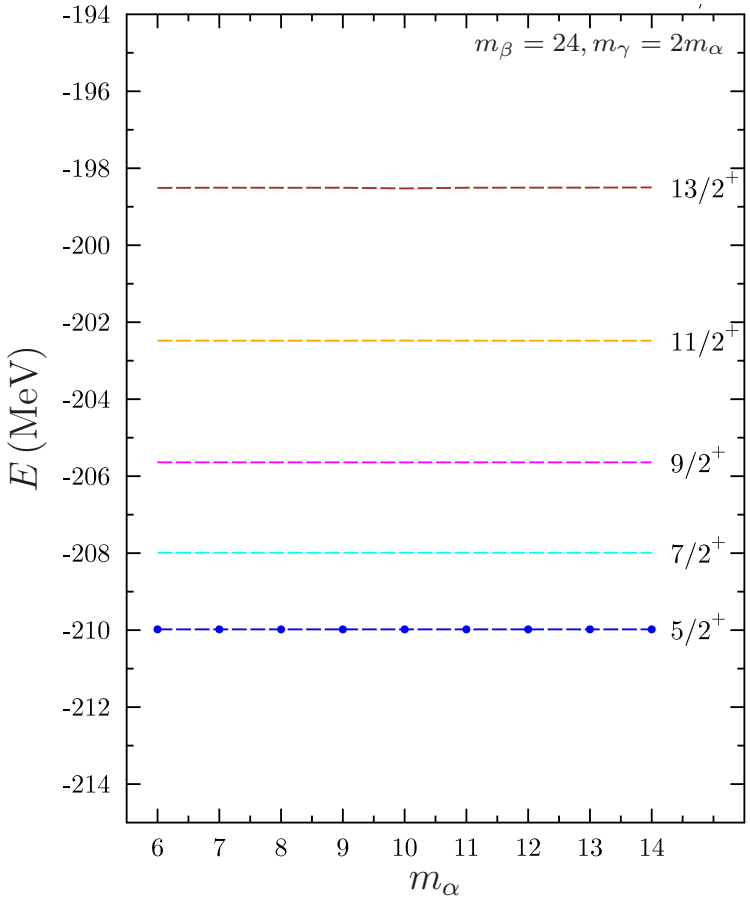
Discretization dependence

Dependence on the number of discretization points chosen for Euler angles when projecting the same blocked triaxial state of ^{25}Mg which is practically pure $K = 5/2$, with SLy5sp$_2$ and SLyMR0.

SLy5sp$_2$

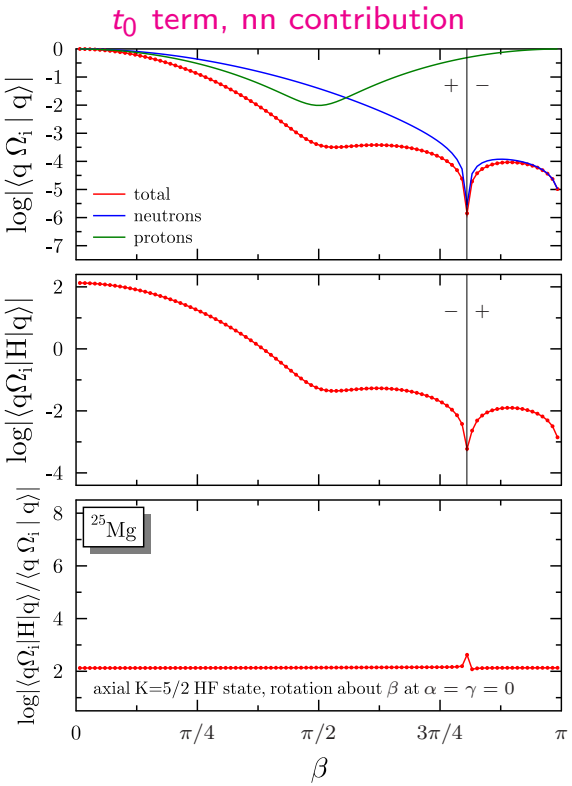


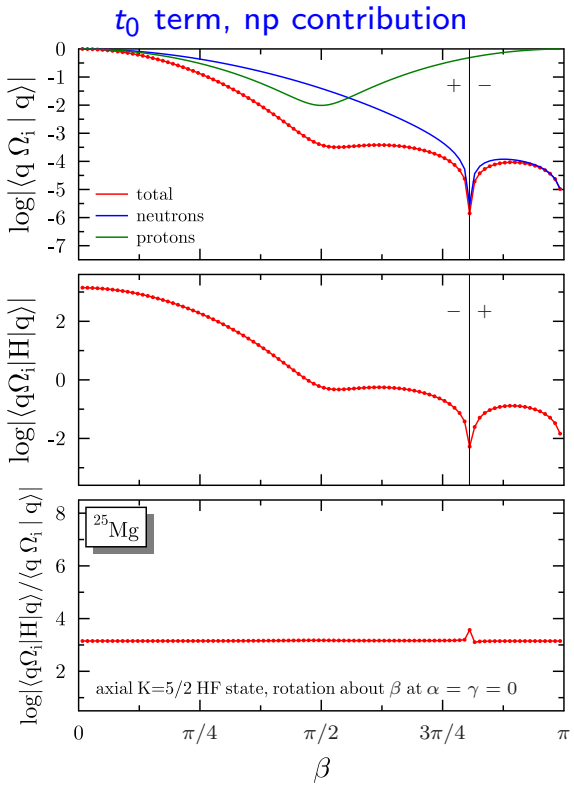
SLyMR0

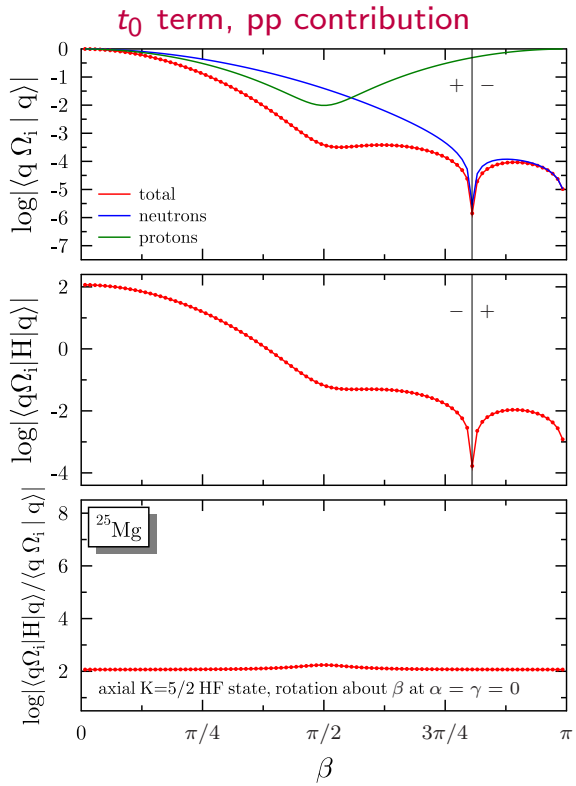


M. Bender, unpublished.

^{25}Mg, HF, $K = 5/2$: projection of the t_0 term of the Skyrme Hamiltonian



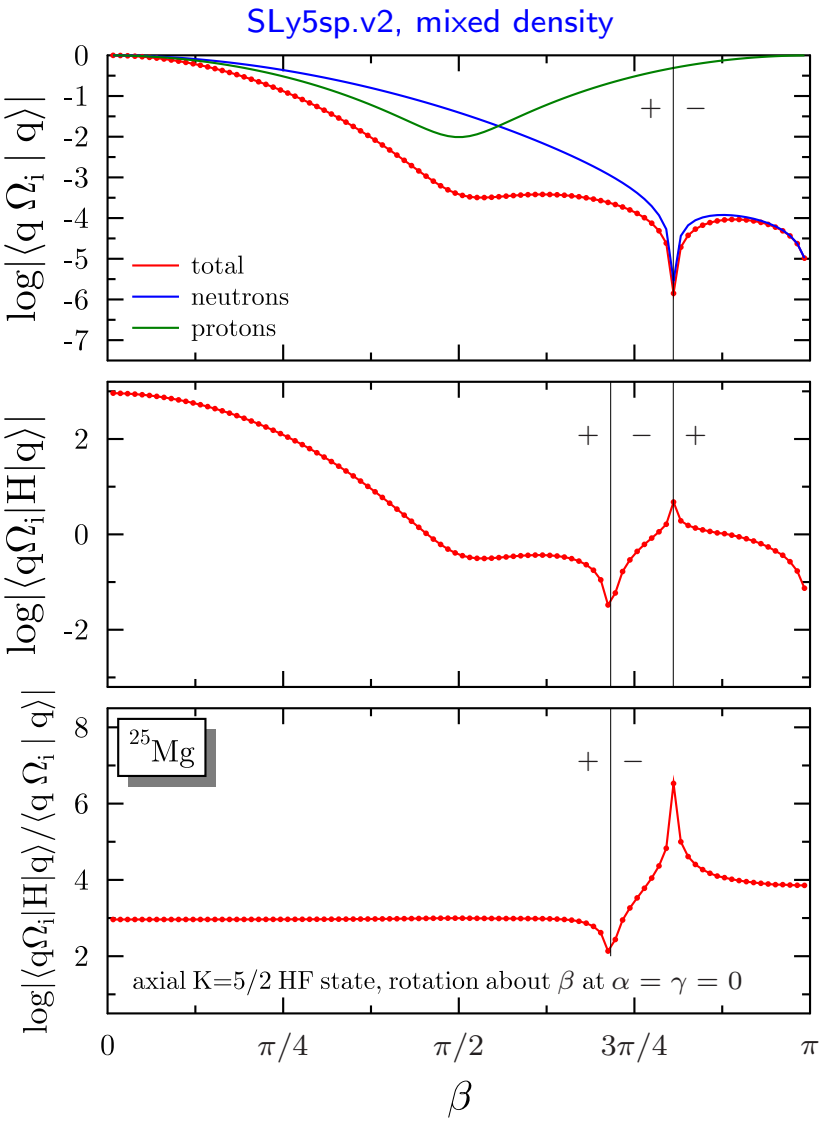




$$
\begin{aligned}
E_{t_0}^{LR} &= \langle \mathrm{L}|t_0\,(1+x_0\hat{P}_\sigma)\,\hat{\delta}^{\mathbf{r}}|\mathrm{R}\rangle \\
&= \tfrac{1}{4}t_0(1-x_0)\int d^3r\left[\rho_n^{LR}(\mathbf{r})\,\rho_n^{LR}(\mathbf{r}) - \mathbf{s}_n^{LR}(\mathbf{r})\cdot\mathbf{s}^{LR}(\mathbf{r}) + \tilde{\rho}_n^{RL*}(\mathbf{r})\,\tilde{\rho}_n^{LR}(\mathbf{r})\right]\langle \mathrm{L}_n|\mathrm{R}_n\rangle\,\langle \mathrm{L}_p|\mathrm{R}_p\rangle \\
&\quad + \int d^3r\left[\tfrac{1}{2}t_0\left(1+\tfrac{x_0}{2}\right)\rho_n^{LR}(\mathbf{r})\,\rho_p^{LR}(\mathbf{r}) + \tfrac{1}{4}t_0\mathbf{s}_n^{LR}(\mathbf{r})\cdot\mathbf{s}_p^{LR}(\mathbf{r})\right]\langle \mathrm{L}_n|\mathrm{R}_n\rangle\,\langle \mathrm{L}_p|\mathrm{R}_p\rangle \\
&\quad + \tfrac{1}{4}t_0(1-x_0)\int d^3r\left[\rho_p^{LR}(\mathbf{r})\,\rho_p^{LR}(\mathbf{r}) - \mathbf{s}_p^{LR}(\mathbf{r})\cdot\mathbf{s}_p^{LR}(\mathbf{r}) + \tilde{\rho}_p^{RL*}(\mathbf{r})\,\tilde{\rho}_p^{LR}(\mathbf{r})\right]\langle \mathrm{L}_n|\mathrm{R}_n\rangle\,\langle \mathrm{L}_p|\mathrm{R}_p\rangle
\end{aligned}
$$

where $|\mathrm{L}\rangle = \hat{R}(\alpha,\beta,\gamma)|\mathrm{R}\rangle$ with $|\mathrm{R}\rangle = |\mathrm{R}_n\rangle \otimes |\mathrm{R}_p\rangle$ and analogous for $|\mathrm{L}\rangle$.

^{25}Mg, HF, $K = 5/2$: projection of the t_3 term of a density-dependent Skyrme Hamiltonian

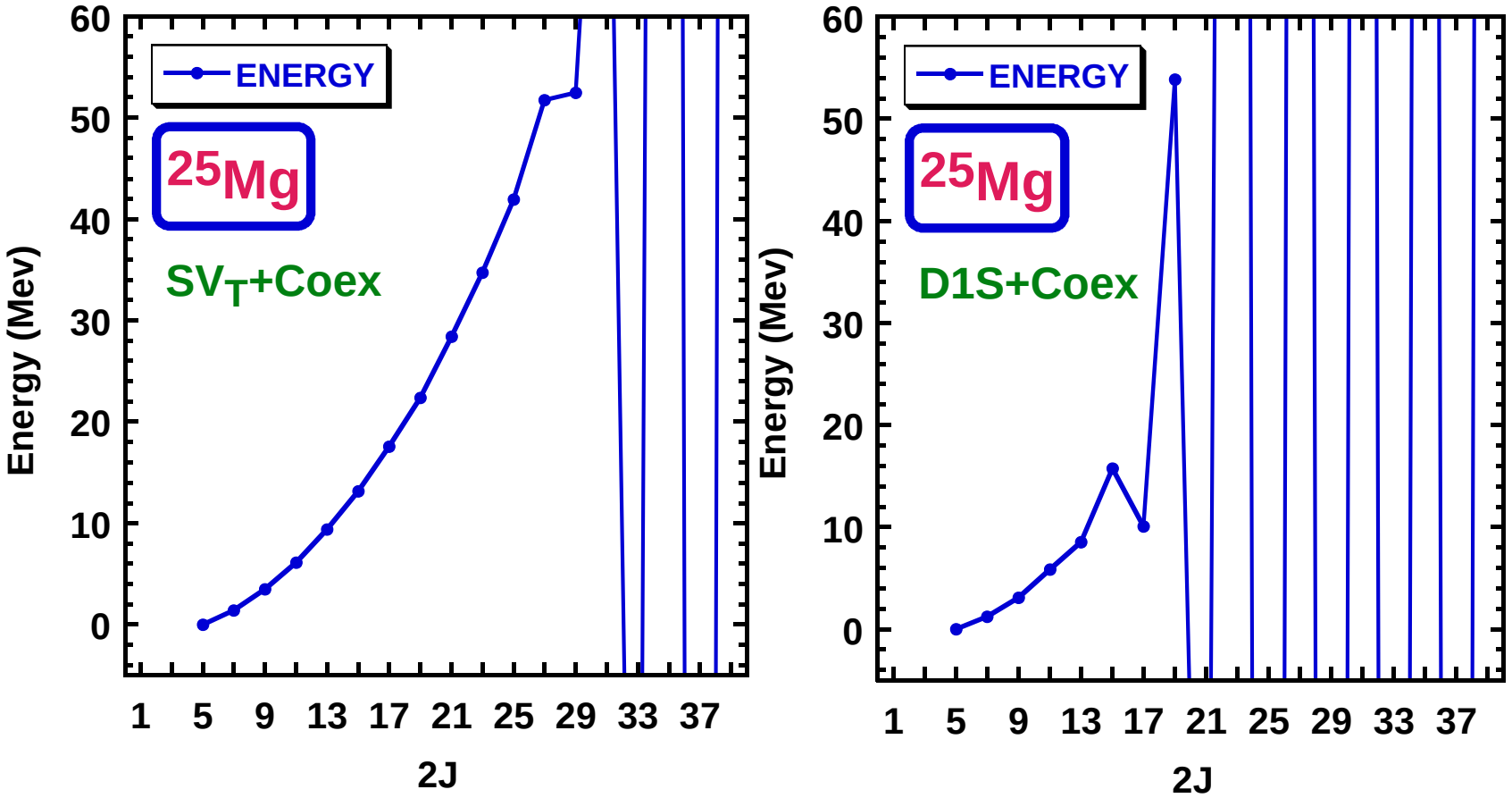


For a parameterization with $x_3 = 1$ and in the limit of Slater determinants, the energy kernel of the density-dependent part of the Skyrme interaction reads

$$
\begin{aligned}
E^{LR}_{t_3} \quad = \quad & \int d^3r \left[\tfrac{1}{2} t_3 \left(1 + \tfrac{x_3}{2}\right) \rho^{LR}_n(\mathbf{r})\, \rho^{LR}_p(\mathbf{r}) \right. \\
& \left. + \tfrac{1}{4} t_3\, \mathbf{s}^{LR}_n(\mathbf{r}) \cdot \mathbf{s}^{LR}_p(\mathbf{r}) \right] \\
& \times \left[\rho^{LR}_n(\mathbf{r}) + \rho^{LR}_p(\mathbf{r}) \right]^{\alpha} \\
& \times \langle \mathsf{L}_n | \mathsf{R}_n \rangle \, \langle \mathsf{L}_p | \mathsf{R}_p \rangle
\end{aligned}
$$

Same in HFODD

J. Dobaczewski, private communication, 18/03/2017



Self-interaction in a nut-shell:

- A many-body system shall not gain binding through the interaction of a given article with itself.

  early papers by Hartree and Fock

  S. Stringari and D. M. Brink, NPA 304, 307 (1978)

  P. Perdew and A. Zunger, PRB 23, 5048 (1981)

  D. Lacroix, T. Duguet, and M. Bender, PRC 79, 044318 (2009); M. Bender, T. Duguet, and D. Lacroix, PRC 79, 044319 (2009)

- The interaction part of the EDF has to vanish in the one-body limit

$$\lim_{A\to 1} \mathcal{E} \to \mathcal{E}_{\text{kin}} \qquad \Leftrightarrow \qquad \lim_{A\to 1} \mathcal{E}_{\text{Skyrme}} \to 0$$

- Similarly, the 3-body contribution to the EDF has to vanish in the 2-body limit
- Automatically fulfilled for HF-expectation values of true operators
- Similar concept ("self-pairing") for paired systems: "A correlated pair shall not gain energy by pair-interaction with itself", automatically fulfilled for HFB-expectation values of true operators

  M. Bender, T. Duguet, and D. Lacroix, PRC 79, 044319 (2009)

Self-interactions in SR calculations

This can be summarized in the form of polarization corrections to energies of odd states δE,

$$E^{A\pm1} = E^{A} \pm e_\lambda + \delta E, \tag{20}$$

or polarization corrections to s.p. energies δe_λ,

$$E^{A\pm1} = E^{A} \pm (e_\lambda + \delta e_\lambda), \tag{21}$$

is nonzero, and explicitly appears in Eq. (43). This leads to corrections to s.p. energies now having the form,

$$\delta e_\lambda = \pm\delta E = \pm\left(\delta E^{\lambda}_{\rm SIF} + E^{\lambda}_{\rm SI}\right), \tag{46}$$

where, based on the analogy with Eq. (37), the first term can be called self-interaction-free (SIF) polarization correction,

SI $\equiv$ self-interaction
SIF $\equiv$ self-interaction-free

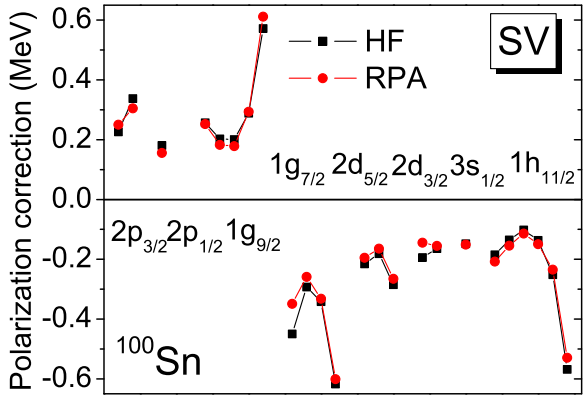


FIG. 1. (Color online) Comparison of polarization corrections of selected orbitals in ^{100}Sn, determined using the HF and RPA methods and Skyrme EDF SV [48]; see text. Lines connect the values obtained for different projections of the angular momentum $|m_\lambda| = \frac{1}{2}, \ldots, j_\lambda$ (from left to right).

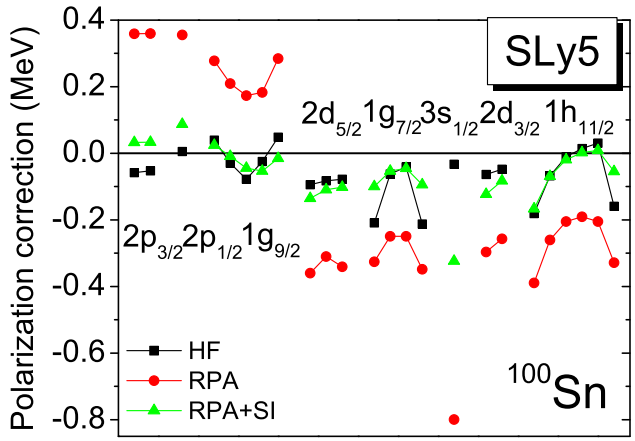


FIG. 5. (Color online) Same as in Fig. 1, but for the Skyrme EDF SLy5 [49]. The RPA results correspond to the SIF terms in Eq. (46), whereas RPA + SI denotes both SIF and SI contributions combined.

D. Tarpanov, J. Toivanen, J. Dobaczewski, and B. G. Carlsson, PRC89 (2014) 014307

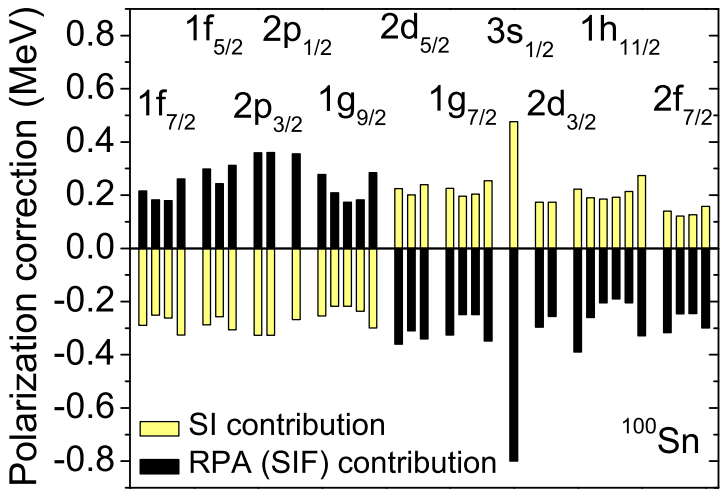


FIG. 6. (Color online) The SIF and SI contributions to the polarization corrections of Eq. (46), calculated in ^{100}Sn for the Skyrme EDF SLy5.

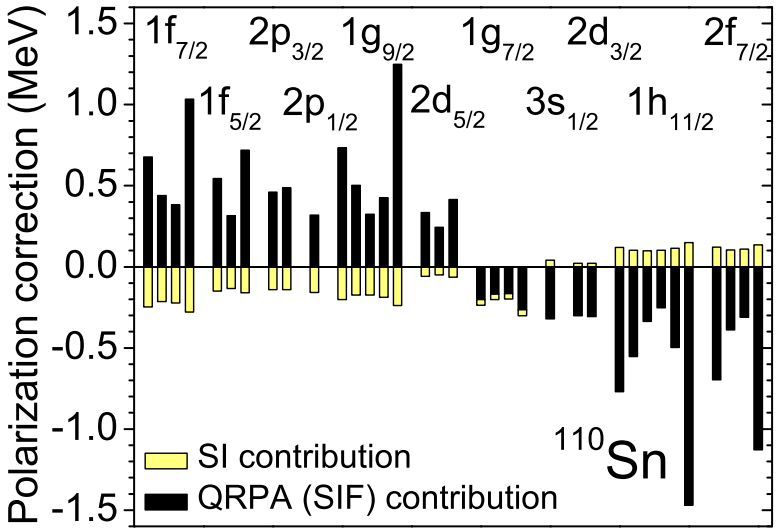


FIG. 10. (Color online) Same as in Fig. 6, but for ^{110}Sn.

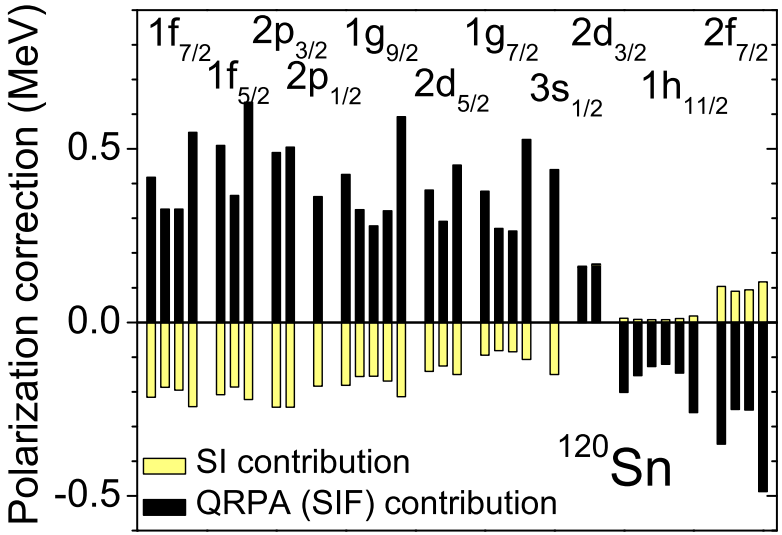


FIG. 11. (Color online) Same as in Fig. 6, but for ^{120}Sn.

D. Tarpanov, J. Toivanen, J. Dobaczewski, and B. G. Carlsson, PRC89 (2014) 014307

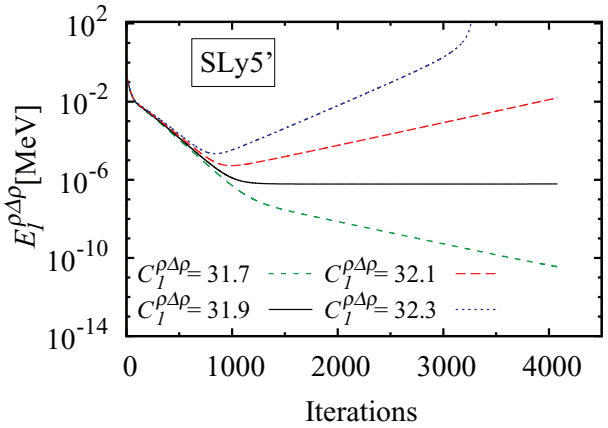


FIG. 3. (Color online) Contribution of $E_1^{\rho\Delta\rho}$ to the binding energy of ^{40}Ca as a function of the number of iterations. Four modified SLy5′ [34] parametrizations with values of $C_1^{\rho\Delta\rho}$ around its critical value $C_{1,\mathrm{crit}}^{\rho\Delta\rho}$ are represented. Calculations are performed with the EV8 code for a value $dx = 0.4$ fm of the Cartesian mesh. During the iterations, the Coulomb term in the EDF is switched off, such that the exact value of $E_1^{\rho\Delta\rho}$ should be zero for ^{40}Ca.

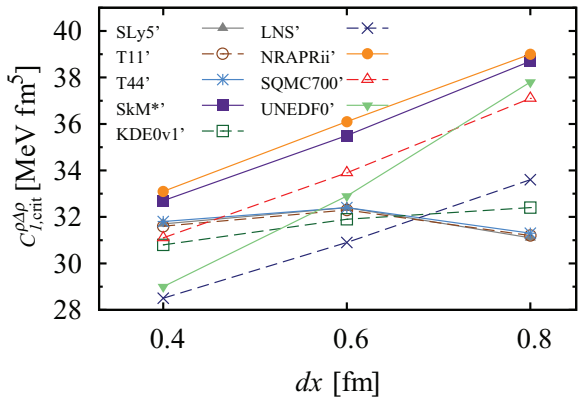
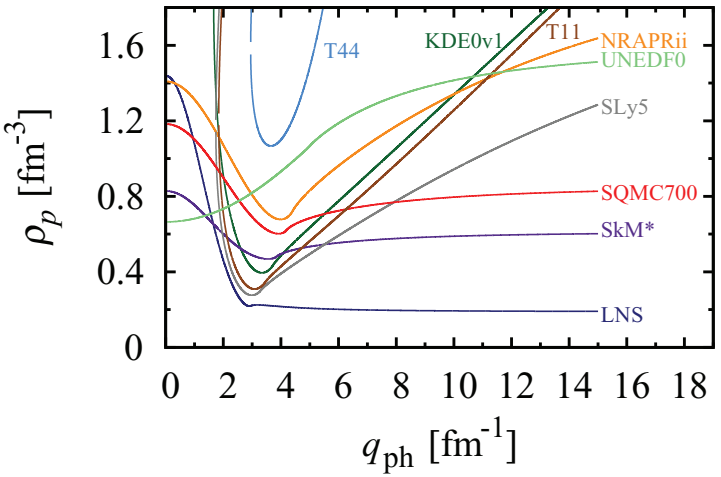
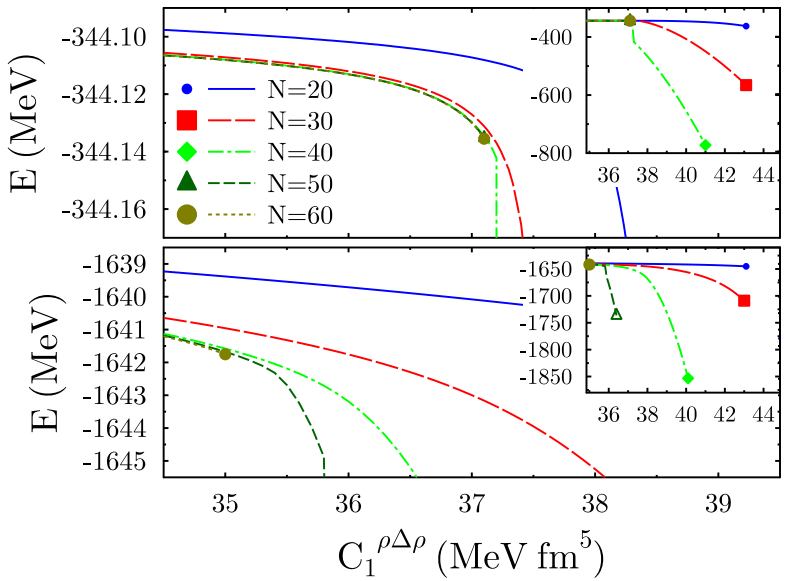


FIG. 4. (Color online) $C_{1,\mathrm{crit}}^{\rho\Delta\rho}$ obtained for ^{40}Ca with the EV8 code for the various (modified) parametrizations as a function of the step size dx.

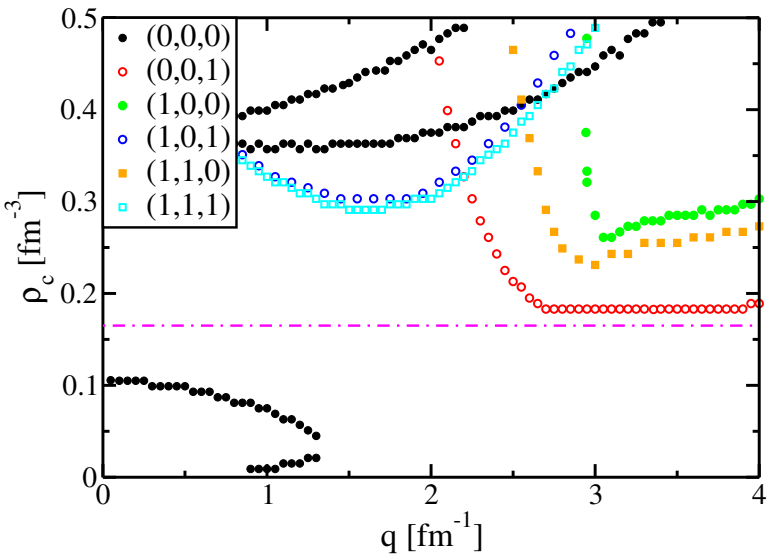


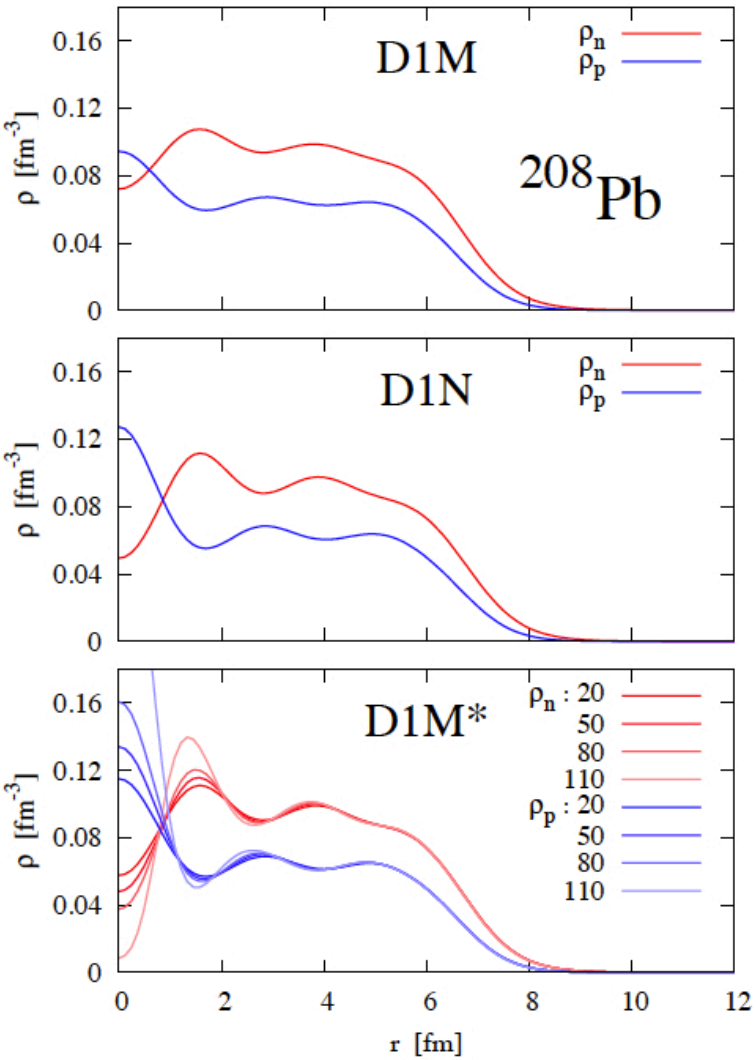


Hellemans, Pastore, Duguet, Bennaceur, Davesne, Meyer, Bender, Heenen, PRC 88 (2013) 064323

Finite-size isospin instabilities

- In the context of standard Skyrme EDFs, finite-size instabilities in the isospin channel are triggered by the $\rho_1(\mathbf{r})\Delta\rho_1(\mathbf{r}) = [\nabla\rho_1(\mathbf{r})]^2$ terms.
- Finite-size instabilities can be detected calculating linear response of infinite nuclear matter
- Finite-size instabilities can also be found for finite-range interactions





Martini, De Pace, Bennaceur, EPJA 55 (2019) 150

Finite-size spin instabilities

Convergence problems:

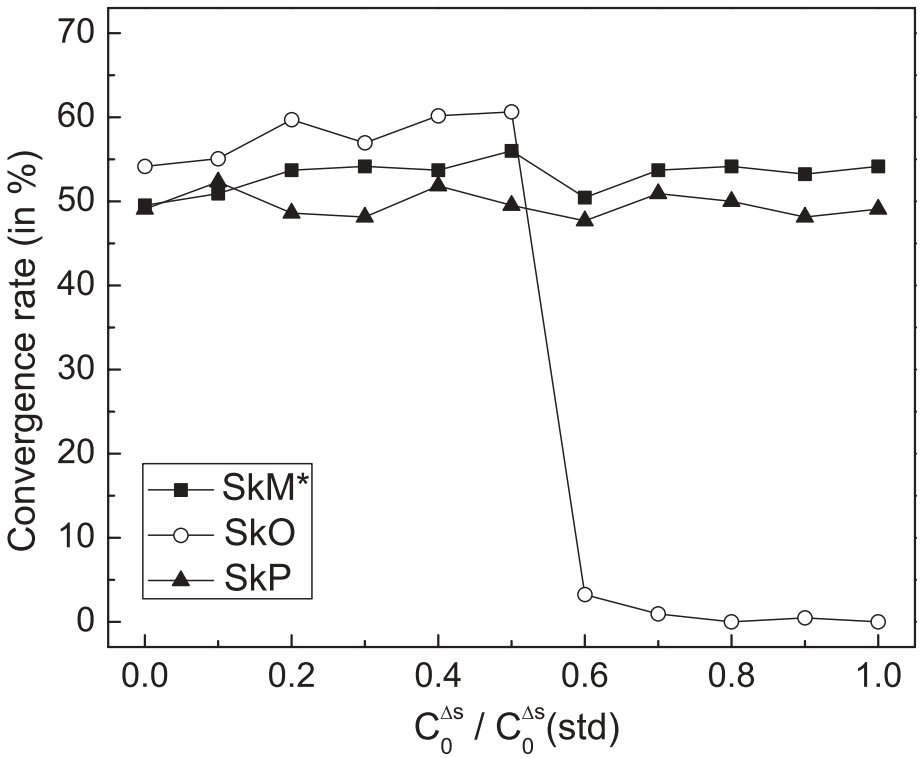
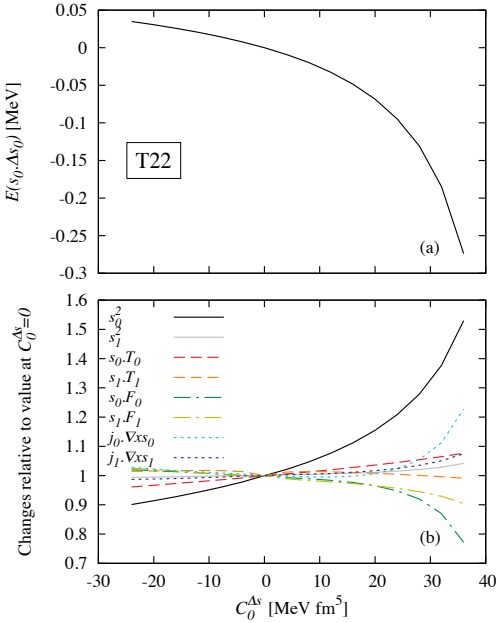


FIG. 9. Convergence rate of HFB equations with SkP, SkO, and SkM* functionals for one-quasiproton states in odd-A Ho isotopes with $88 \leqslant N \leqslant 104$ as a function of the scalar-isoscalar coupling constant $C_0^{\Delta s}$. See text for details.

Schunck, Dobaczewski, McDonnell, Moré, Nazarewicz, Sarich, and Stoitsov PRC 81 (2010) 024316

See also Pototzky, Erler, Reinhard, Nesterenko, EPJ A 46 (2010) 299

And divergences:



(a) Dependence of the $C_0^{\Delta s}\mathbf{s}_0 \cdot \Delta\mathbf{s}_0$ term of a variant of the T22 parameterisation on the value of $C_0^{\Delta s}$ for the $\langle \hat{J}_z \rangle = 54\hbar$ state in the yrast superdeformed rotational band of ^{194}Hg.

(b) Dependence of all other time-odd terms containing the spin density $\mathbf{s}_t$ relative to their value at $C_0^{\Delta s} = 0$ in the same calculations.

Hellemans, Heenen and Bender, PRC 85 (2012) 014326

Finite-size spin instabilities

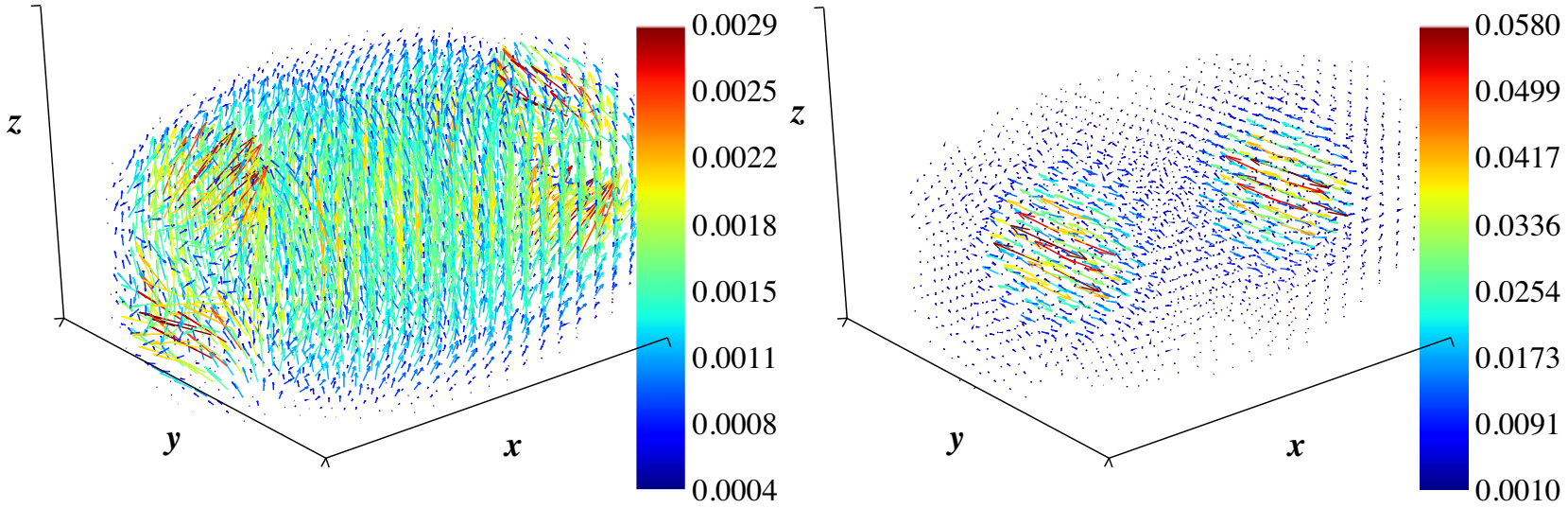


FIGURE 2. (color online) Left: The isoscalar spin density s_0 obtained with a modified T22 parameterization (see text) with $C_0^{\Delta s} = 0$ for the $J_z = 54\hbar$ state in the ground superdeformed band of ^{194}Hg at convergence. Right: Same as the panel on the left, but for $C_0^{\Delta s} = 40$ MeV fm^5 at a few iterations before the code crashes.

Hellemans, Heenen and Bender, AIP Conf. Proc. 1491 (2012) 242

Finite-size spin instabilities – linear response

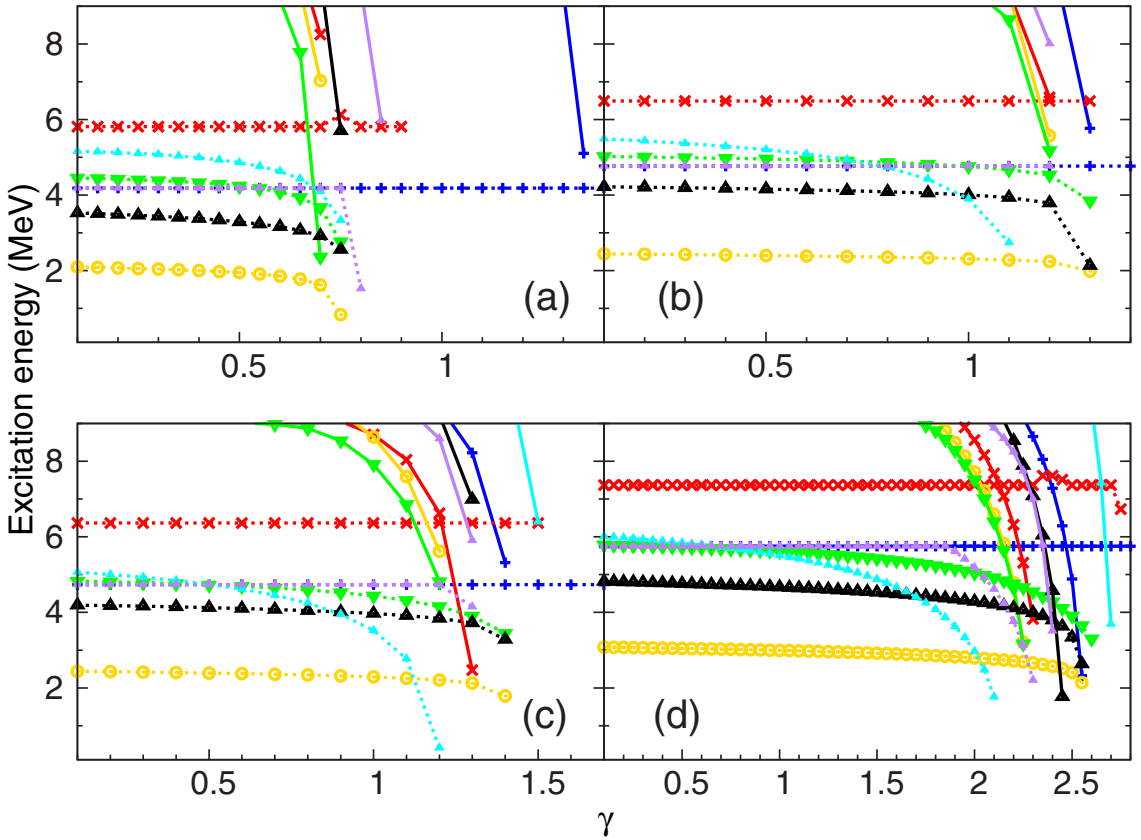


FIG. 3. (Color online) Evolution phonons in ^{56}Ni as a function of the multiplicative factor γ for T44 (a), SLy5 (b), BSk27 (c), and SIII (d). The caption is the same as that for Fig. 2.

- RPA calculation of lowest state of multipolarity $J^{\pm}$ in ^{56}Ni
- Skyrme parameterisation T44, SLy5, BSk27, SIII
- nominal coupling constant of the $\gamma\, C_t^{s\Delta s} \int d^3r\, \mathbf{s}_t \Delta \mathbf{s}_t$ term is rescaled by factor γ

Pastore, Tarpanov, Davesne, and Navarro, PRC 92 (2015) 024305

Can be correlated to linear response in infinite matter

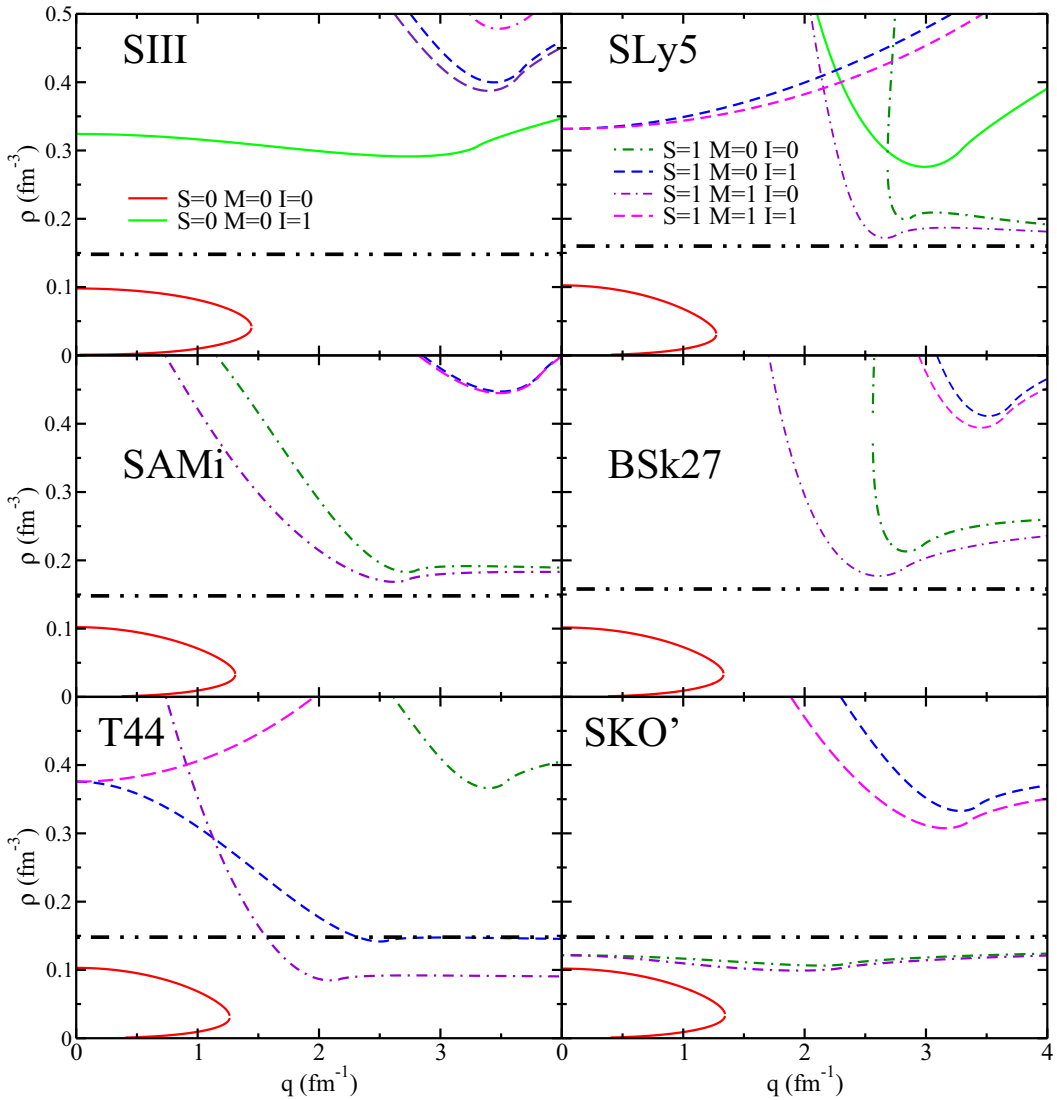


FIG. 7. (Color online) Instabilities in SNM for the functionals considered in the present article. The dashed-dotted horizontal line stands for the saturation density of the functional. See text for details.

Pastore, Tarpanov, Davesne, and Navarro, PRC 92 (2015) 024305

Unexpected instabilities: "spin-orbit coexistence"

$\mathbf{J}_q$ is not a bulk property, but a shell effect. It varies rapidly between near-zero and substantial values. Multiplying a large $\mathbf{J}_q$ with a large coupling constant leads to a large contribution to the spin-orbit potential

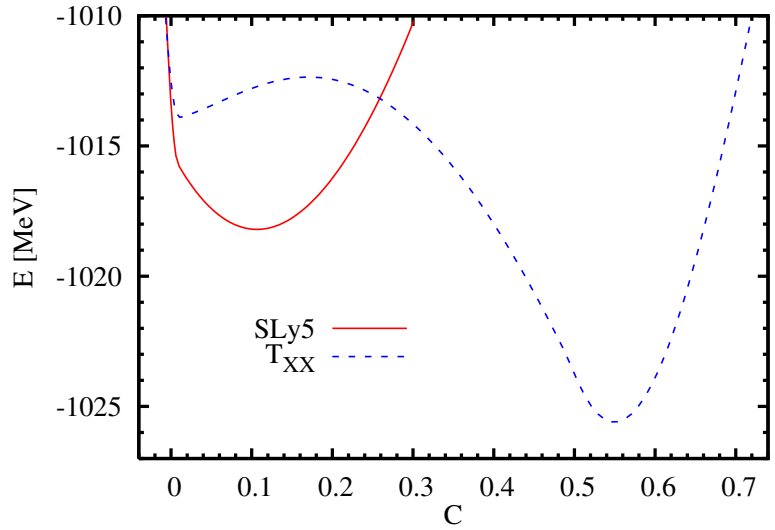
$$W_n(r) = -\frac{W_0}{2}\left(2\nabla\rho_n + \nabla\rho_p\right) + \alpha\, J_n + \beta\, J_p$$

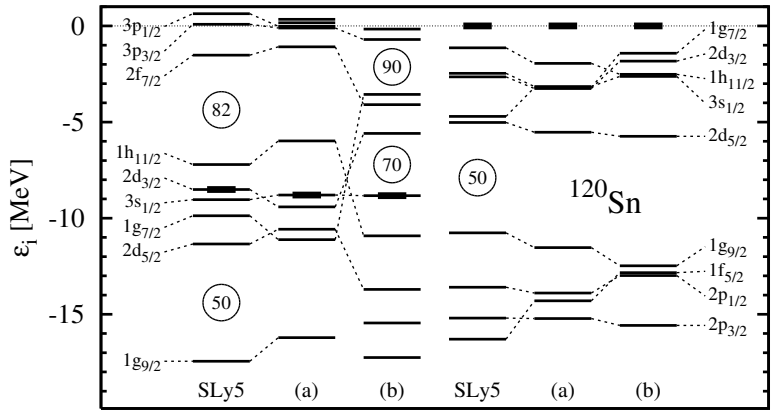
which (3) might switch levels originating from different j shells, which further increases $\mathbf{J}$. Feed this back to (1) and you have an instability towards unrealistic spectra

- fits in many regions of the parameter space not covered by our parameter sets have this instability
- there is even "spin-orbit current coexistence"
- constraint on

$$C = \int d^3r\; \mathbf{J}_n \cdot \nabla\rho_n$$

- TXX: parameter set with $C_0^J = -157.57\,\mathrm{MeV\,fm^5}$ and $C_1^J = -114.88\,\mathrm{MeV\,fm^5}$.
- $\alpha = C_0^J + C_1^J$, $\beta = C_0^J - C_1^J$.





Lesinski, Bender, Bennaceur, Duguet, Meyer PRC 76 (2007) 014312

In the strong-coupling limit, there are two different ways of coupling two single-article states $\Psi_k(\mathbf{r})$ with good j_z out of a Kramers-degenerate doublet

$$\hat{J}_z\Psi_1(\mathbf{r}) = K_1\Psi_1(\mathbf{r}) \qquad \text{with } K_1 = \langle\Psi_1|\hat{L}_z|\Psi_1\rangle + \langle\Psi_1|\hat{S}_z|\Psi_1\rangle$$
$$\hat{J}_z\Psi_2(\mathbf{r}) = K_2\Psi_2(\mathbf{r}) \qquad \text{with } K_2 = \langle\Psi_2|\hat{L}_z|\Psi_2\rangle + \langle\Psi_2|\hat{S}_z|\Psi_2\rangle$$

to a two-particle state with good j_z

$$\hat{J}_z\Psi_1(\mathbf{r})\Psi_2(\mathbf{r}') = (K_1+K_2)\Psi_1(\mathbf{r})\Psi_2(\mathbf{r}')$$
$$\hat{J}_z\Psi_1(\mathbf{r})\Psi_{\bar{2}}(\mathbf{r}') = (K_1-K_2)\Psi_1(\mathbf{r})\Psi_{\bar{2}}(\mathbf{r}')$$

(plus two others related to these by time-reversal).

- [C. J. Gallagher, PR 126 (1962) 1525]: For the lower 2qp state in well-deformed even-even nuclei $\left|\langle\Psi_1|\hat{S}_z|\Psi_1\rangle + \langle\Psi_2|\hat{S}_z|\Psi_2\rangle\right|$ is minimal (anti-parallel spins)
- [C. J. Gallagher and S. A. Moszkowski, PR 111 (1958) 1282]: For the lower 2qp state in odd-odd nuclei $\left|\langle\Psi_1|\hat{S}_z|\Psi_1\rangle + \langle\Psi_2|\hat{S}_z|\Psi_2\rangle\right|$ is maximal (parallel spins)
  see also [J. Boisson, R. Piepenbring, and W. Ogle, Phys. Rep. 26 (1976) 99]

The impact of time-odd terms on energies of 2qp states

Robledo, Bernard, Bertsch, PRC 89 (2014) 021303(R)

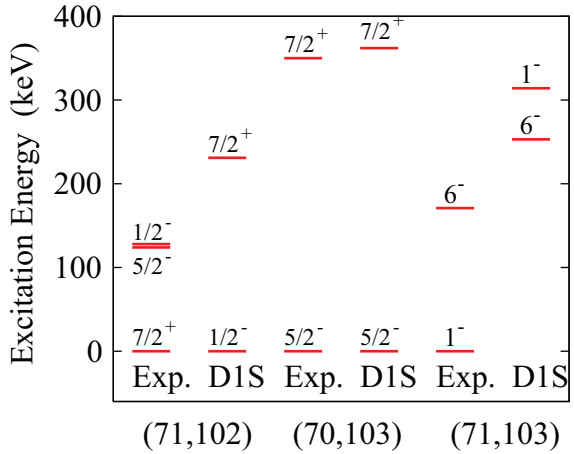


FIG. 1. (Color online) Low-lying band heads in the spectra of the nucleus ^{174}Lu and odd-A neighbors: ^{173}Lu (left), ^{173}Yb (center), and ^{174}Lu (right). Due to the inversion of the lowest proton quasiparticle energies, the ground-state doublet in ^{174}Lu is not the lowest two-quasiparticle configuration in the calculated spectrum. Lower energy calculated configurations are not shown.

- [404] $\downarrow_p$ [512] $\uparrow_n$ coupled to 1^- or 6^-
- Gogny force
- density-dependent term (called "3-body" for whatever reason) is identified as likely origin of the wrong sign of the matrix element of the spin-spin interaction
- Skyrme SLy4 gives same for this nucleus (MB, unpublished)

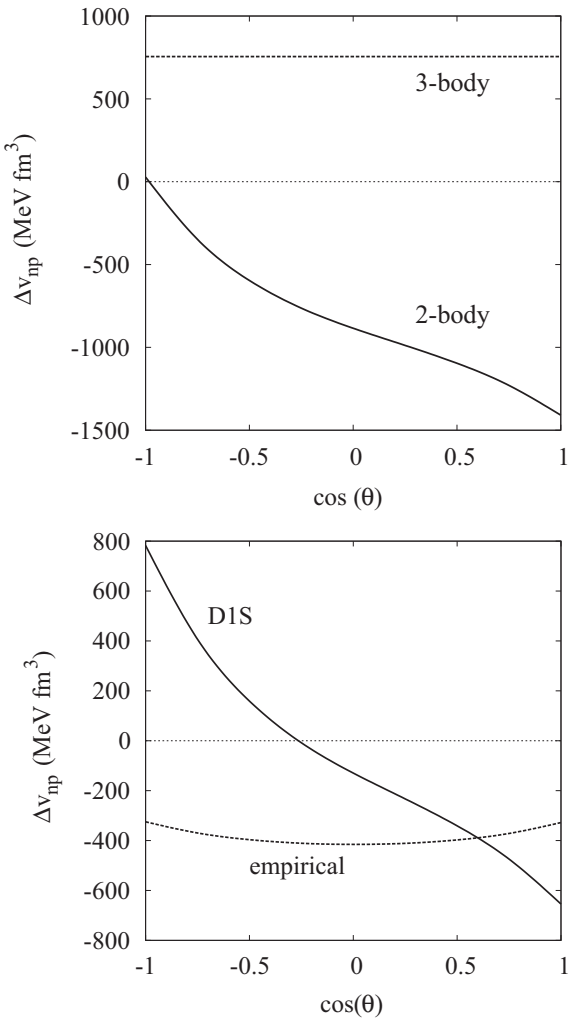


FIG. 2. Matrix elements of the effective neutron-proton interaction from the D1S Gogny energy functional at nuclear matter density, $\rho = 0.16$ fm^{-3}. In the upper panel, the individual contributions of the two- and three-body terms from Eqs. (3) and (4) are shown. In the lower panel, the total for the D1S is shown in comparison to the empirical Δv_{np} discussed in Refs. [10,18].

And there is still more

When preparing the transparencies, I expected that I ran out of time by now, so here is a short list of further issues:

- How to calculate observables in the context of an effective EDF? Do we need effective operators for other observables as well?
- Which is the range of densities, momenta, ... at which an EDF that describes finite nuclei can be meaningfully applied? How to consistently define cutoffs?
- Is large-amplitude motion described by the same EDF formalism as stationary states?
- How to make efficient use of modern high-performance computation? (see talk by WR)
- Add your own problems and worries.

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The work presented here would have been impossible without my collaborators with whom I struggled with these problems over the past 19 years

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formal aspects of the big picture

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design and implementation of code extensions

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development and benchmarking of new functionals

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