Parametrizing the nuclear EDF: the troubles with and without density dependences

Michael Bender

Institut de Physique Nucléaire de Lyon
CNRS/IN2P3 & Université de Lyon & Université Lyon 1
69622 Villeurbanne, France

First meeting of the WG3 of the GDR RESANET

CEA/Saclay/DPhN, Orme des merisiers, build. 703, room 135

13 November 2018

The Skyrme energy density functional at NLO

In Skyrme-EDF jargon, NLO means "next-to-leading order in gradients", i.e. the terms in the EDF contain zero (LO) or two (NLO) gradients. There are efforts to construct extended EDFs with four (N2LO) and six (N3LO) gradients. There is no reason to expect that this refers to a strict hierarchy in physical relevance, but it nevertheless refers a hierarchy in computational complexity.

$$\mathcal{E} = \mathcal{E}_{\rm kin} + \mathcal{E}_{\rm Skyrme} + \mathcal{E}_{\rm Coul} + \mathcal{E}_{\rm pair} + \mathcal{E}_{\rm corr}$$

$$\begin{aligned}
\mathcal{E}_{\rm Skyrme} = \int {\rm d}^3 r \sum_{t=0,1} \sum_{t_3=-t}^{+t} \Big\{ & C_t^{\rho\rho}[\rho_0]\rho_{tt_3}\,\rho_{t\,-t_3} + C_t^{\rho\tau}(\rho_{tt_3}\,\tau_{t\,-t_3} - \mathbf{j}_{tt_3}\cdot\mathbf{j}_{t\,-t_3}) \\
& + C_t^{\rho\Delta\rho}\rho_{tt_3}\Delta\rho_{t\,-t_3} + C_t^{ss}[\rho_0]\mathbf{s}_{tt_3}\cdot\mathbf{s}_{t\,-t_3} + C_t^{s\Delta s}\mathbf{s}_{tt_3}\cdot\Delta\mathbf{s}_{t\,-t_3} \\
& + C_t^{sT}\Big(\mathbf{s}_{tt_3}\cdot\mathbf{T}_{t\,-t_3} - \sum_{\mu,\nu=x,y,z}\mathbf{J}_{\mu\nu;tt_3}\mathbf{J}_{\mu\nu;t\,-t_3}\Big) \\
& + C_t^{\rho\nabla J}\big(\rho_{tt_3}\nabla\cdot\mathbf{J}_{t\,-t_3} + \mathbf{s}_{tt_3}\cdot\nabla\times\mathbf{j}_{t\,-t_3}\big) \\
& + C_t^{sF}\Big(\mathbf{s}_{tt_3}\cdot\mathbf{F}_{t\,-t_3} - \frac{1}{2}\sum_{\mu,\nu=x,y,z}\mathbf{J}_{\mu\nu;tt_3}\mathbf{J}_{\nu\mu;t\,-t_3} - \frac{1}{2}\sum_{\mu,\nu=x,y,z}\mathbf{J}_{\mu\mu;tt_3}\mathbf{J}_{\nu\nu;t\,-t_3}\Big) \\
& + C_t^{\nabla s\nabla s}\big(\nabla\cdot\mathbf{s}_{tt_3}\big)\big(\nabla\cdot\mathbf{s}_{t-t_3}\big)\Big\}
\end{aligned}$$

Local densities

$$
\begin{aligned}
\rho_q(\mathbf{r}) &= \rho_q(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}\,, \\
\tau_q(\mathbf{r}) &= \nabla\cdot\nabla'\,\rho_q(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}\,, \\
J_{q,\mu\nu}(\mathbf{r}) &= -\tfrac{i}{2}\left(\nabla_\mu-\nabla'_\mu\right)s_{q,\nu}(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}\,, \\
\mathbf{s}_q(\mathbf{r}) &= \mathbf{s}_q(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}\,, \\
\mathbf{T}_q(\mathbf{r}) &= \boldsymbol{\nabla}\cdot\boldsymbol{\nabla}'\,\mathbf{s}_q(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}\,, \\
F_{q,\mu}(\mathbf{r}) &= \tfrac{1}{2}\sum_\nu(\nabla_\mu\cdot\nabla'_\nu+\nabla_\nu\cdot\nabla'_\mu)\,s_{q,\nu}(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}\,, \\
\mathbf{j}_q(\mathbf{r}) &= -\tfrac{i}{2}\left(\nabla_\mu-\nabla'_\mu\right)\rho_q(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}\,.
\end{aligned}
$$

$$\mathcal{E}_{\text{Skyrme}} = \langle \text{HF} | \hat{t} + \hat{v}^{\text{central}} + \hat{v}^{\text{LS}} + \hat{v}^{\text{tensor}} | \text{HF} \rangle$$

- central

$$\begin{aligned}
\hat{v}^{\text{central}} \quad = \quad & t_0 \,(1 + x_0 \hat{P}_\sigma)\, \delta + \tfrac{1}{6}\, t_3 \,(1 + x_3 \hat{P}_\sigma)\, \rho^\alpha \, \delta \\
& + \tfrac{1}{2}\, t_1 \,(1 + x_1 \hat{P}_\sigma)\big(\hat{\mathbf{k}}'^2 \, \delta + \delta \, \hat{\mathbf{k}}^2\big) \\
& + t_2 \,(1 + x_2 \hat{P}_\sigma)\, \hat{\mathbf{k}}' \cdot \delta \, \hat{\mathbf{k}} \\
& + \tfrac{1}{6}\, t_3 \,(1 + x_3 \hat{P}_\sigma)\, \rho_0^\alpha \, \delta
\end{aligned}$$

- spin-orbit

$$\hat{v}^{\text{LS}} \quad = \quad i W_0 \,(\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2) \cdot \hat{\mathbf{k}}' \times \delta \, \hat{\mathbf{k}}$$

- tensor

$$\begin{aligned}
\hat{v}^{\text{tensor}} \quad = \quad & \tfrac{1}{2} t_e \Big\{ \big[3(\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\mathbf{k}}')(\hat{\boldsymbol{\sigma}}_2 \cdot \hat{\mathbf{k}}') - (\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2)\,(\hat{\mathbf{k}}')^2\big]\, \delta \\
& \qquad + \delta \,\big[3(\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\mathbf{k}})(\hat{\boldsymbol{\sigma}}_2 \cdot \hat{\mathbf{k}}) - (\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2)\,(\hat{\mathbf{k}})^2\big] \Big\} \\
& + \tfrac{1}{2} t_o \Big\{ \big[3(\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\mathbf{k}}')\, \delta\, (\hat{\boldsymbol{\sigma}}_2 \cdot \hat{\mathbf{k}}) + 3(\hat{\boldsymbol{\sigma}}_2 \cdot \hat{\mathbf{k}}')\, \delta\, (\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\mathbf{k}}) - 2(\hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2)\, \hat{\mathbf{k}}' \cdot \hat{\mathbf{k}}\big] \Big\}
\end{aligned}$$

The force

$$v = \sum_{i=1}^{2} \left[W_i + B_i \hat{P}_\sigma - H_i \hat{P}_\tau - M_i \hat{P}_\sigma \hat{P}_\tau \right] e^{-\mathbf{r}^2/\mu_i^2}$$
$$+ t_0 \left(1 + x_0 \hat{P}_\sigma\right) \rho^\alpha(\mathbf{R})\, \delta(\mathbf{r})$$
$$+ \mathrm{i} W_{LS} \left(\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2\right) \cdot \hat{\mathbf{k}}' \times \delta(\mathbf{r}) \hat{\mathbf{k}}$$

The functional

$$\mathcal{E} = \int d^3\mathbf{r} \int d^3\mathbf{r}' \sum_{t=0,1} \sum_{i=1}^{2} e^{-(\mathbf{r}-\mathbf{r}')^2/\mu_i^2} \Big[A_{it}^{\rho\rho}\, \rho_t(\mathbf{r})\, \rho_t(\mathbf{r}') + A_{it}^{ss}\, \mathbf{s}_t(\mathbf{r}) \cdot \mathbf{s}_t(\mathbf{r}')$$
$$+ B_{it}^{\rho\rho}\, \rho_t(\mathbf{r}, \mathbf{r}')\, \rho_t(\mathbf{r}', \mathbf{r}) + B_{it}^{ss}\, \mathbf{s}_t(\mathbf{r}, \mathbf{r}') \cdot \mathbf{s}_t(\mathbf{r}', \mathbf{r}) \Big]$$
$$+ \int d^3\mathbf{r} \sum_{t=0,1} \left[C_t^{\rho\rho}[\rho_0]\, \rho_t \rho_t + C_t^{ss}[\rho_0]\, \mathbf{s}_t \cdot \mathbf{s}_t + C_t^{\rho\nabla J} \left(\rho_t \boldsymbol{\nabla} \cdot \mathbf{J}_t + \mathbf{j}_t \cdot \boldsymbol{\nabla} \times \mathbf{s}_t \right) \right]$$

A bilinear EDF is not enough I

- 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 ρ_{sat} and E/A of homogeneous symmetric and spin-symmetric infinite nuclear matter necessarily leads to $m_0^*/m \approx 0.4$, which is incompatible with empirical data. For a modern analysis see [Davesne, Navarro, Meyer, Bennaceur, Pastore, PRC 97 (2018) 044304].

$\Rightarrow$ need for higher-order terms in the density matrix when aiming at a description of nuclear properties (at the mean-field level with effective interactions built for that purpose). But what kind of terms is missing that describes which physics phenomenon?

A bilinear EDF is not enough I

- There are many indications that there are genuine three-body (and four-body, . . .) forces acting in nuclear many-body systems.
- From a modern point of view, any attempt to renormalize 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. Nuclear EDFs are not (yet) constructed this way, but the in can be expected that many-body forces find their way into it.
- Any approach that is "beyond the mean field" in a 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).
- In particular, 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 [Köhler, NPA258 (1976) 301].
- The density-matrix expansion (DME) of exchange terms of finite-range interactions leads either to complicated density dependences of the resulting effective interaction for Hartree calculations [Negele & Vautherin, PRC5 (1972) 1472; PRC11 (1975) 1031; Gebremariam, Duguet, Bogner, PRC 82(2010) 014305; NPA851 (2011) 17; Stoitsov et al, PRC82 (2010) 054307] or higher-order momentum dependences [Carlsson & Dobaczewski, PRL105 (2010) 122501].

Density dependence vs. three-body force I

- 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

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

  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, meaning here 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, Duguet, Meyer, Bender, PRC88 (2013) 064326].

- A 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 a spin-instability signalled by the Landau parameter $g_0 < -1$ [Chang PLB56 (1975) 205; Bäckman, Jackson, Speth, PLB 56 (1975) 209; Passler, NPA 257 (1976) 253; Stringari, Leoardi, Brink, NPA 269 (1976) 87]. The last problem disappears when re-interpreting the 3-body force as a density-dependent 2-body force.

Density dependence vs. three-body force II

- 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

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

- Terms in red have the structure of those from a genuine three-body force (2).
- Terms 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 get rid of the pairing terms and to obtain the same energy in a time-reversal invariant system ($\mathbf{s}_q = 0$) requires $x_3 = +1$

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

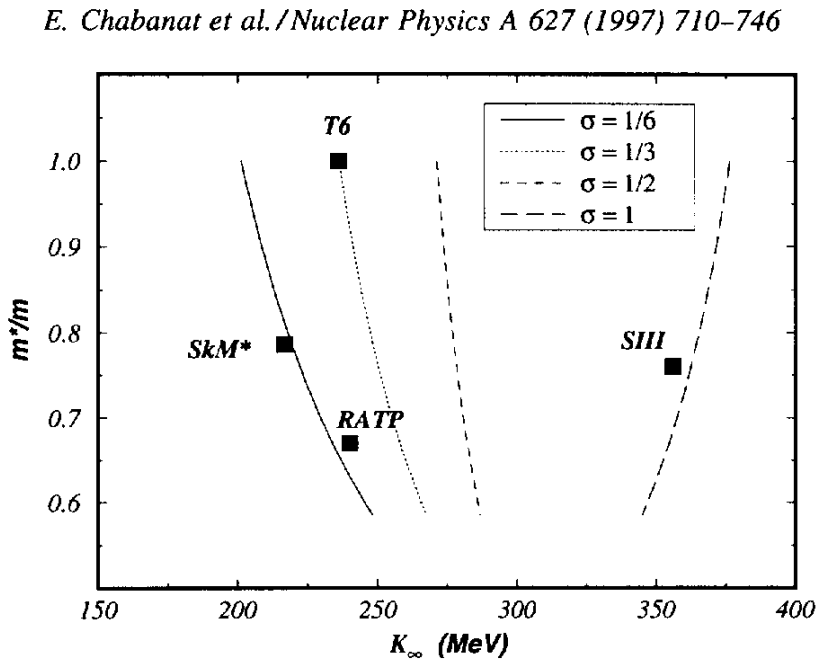
  which evidently differs from the expression from a true three-body force (2)

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

- 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.

Density dependence vs. three-body force IV

- However, as results for homogeneous isotropic spin-saturated infinite matter are not affected, the incompressibility K_∞ remains non-physically high.



Density dependence vs. three-body force V

- 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

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

- Köhler's Ska and Skb with $\alpha = 1/3$, SkM has $\alpha = 1/6$ [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 the divergence of the contact pairing terms when solving HFB equations.
- 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].

Density dependence vs. three-body force I

Unfortunately, practitioners of nuclear EDF methods did not live happily ever after.

Self-interactions from density-dependent terms

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
  Stringari and Brink, NPA 304, 307 (1978)
  Perdew and Zunger, PRB 23, 5048 (1981)

  Lacroix, Duguet, and Bender, PRC 79, 044318 (2009); Bender, Duguet, and 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

  Bender, Duguet, Lacroix, PRC 79, 044319 (2009)

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:

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

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:

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

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

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

Self-interactions from density-dependent terms

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

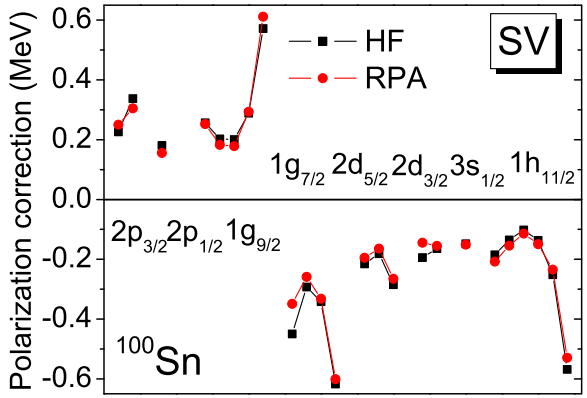


FIG. 1. (Color online) Comparison of polarization corrections of selected orbitals in ^{100}Sn, determined using the HF and RPA methods and Skyrme EDF SV [48]; see text. Lines connect the values obtained for different projections of the angular momentum $|m_\lambda| = \frac{1}{2}, \ldots, j_\lambda$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

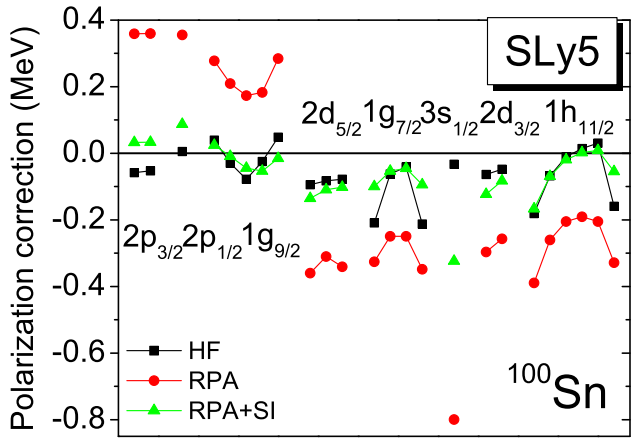


FIG. 5. (Color online) Same as in Fig. 1, but for the Skyrme EDF SLy5 [49]. The RPA results correspond to the SIF terms in Eq. (46), whereas RPA + SI denotes both SIF and SI contributions combined.

Tarpanov, Toivanen, Dobaczewski, Carlsson, PRC89 (2014) 014307

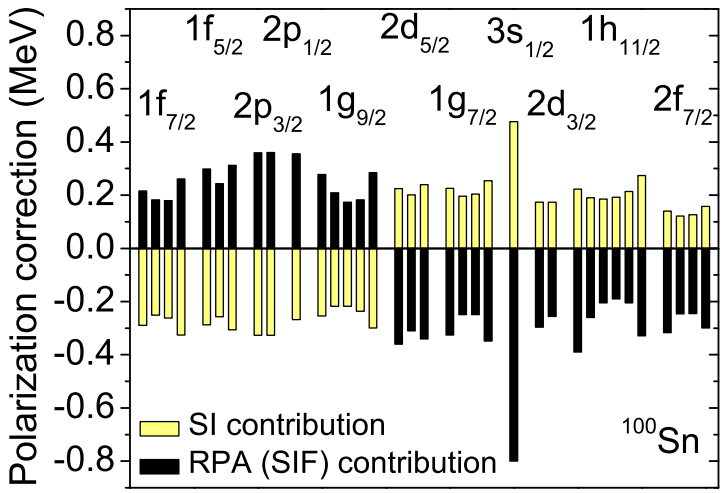


FIG. 6. (Color online) The SIF and SI contributions to the polarization corrections of Eq. (46), calculated in ^{100}Sn for the Skyrme EDF SLy5.

Tarpanov, Toivanen, Dobaczewski, Carlsson, PRC89 (2014) 014307

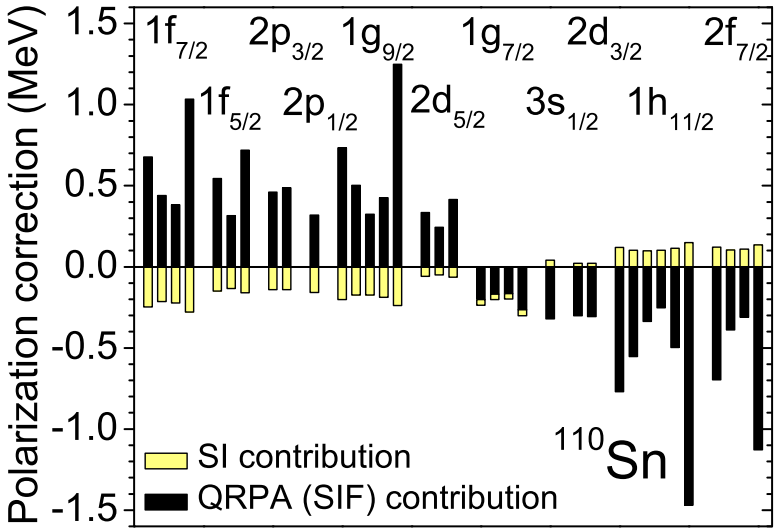


FIG. 10. (Color online) Same as in Fig. 6, but for ^{110}Sn.

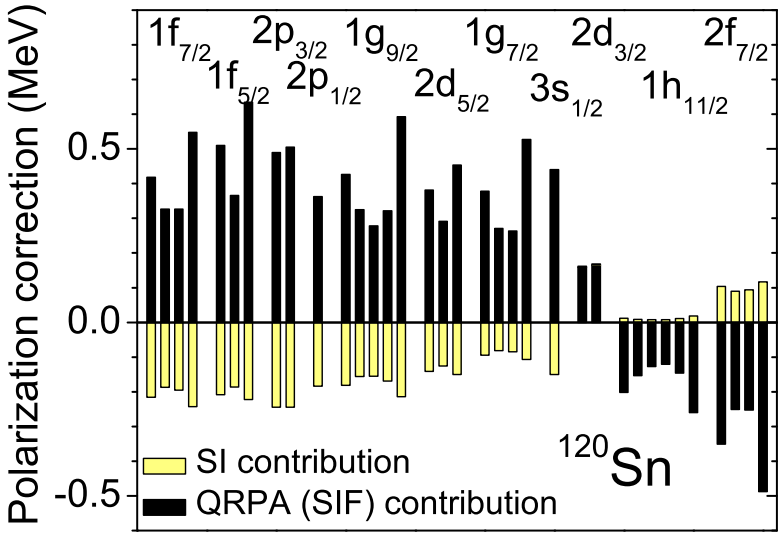
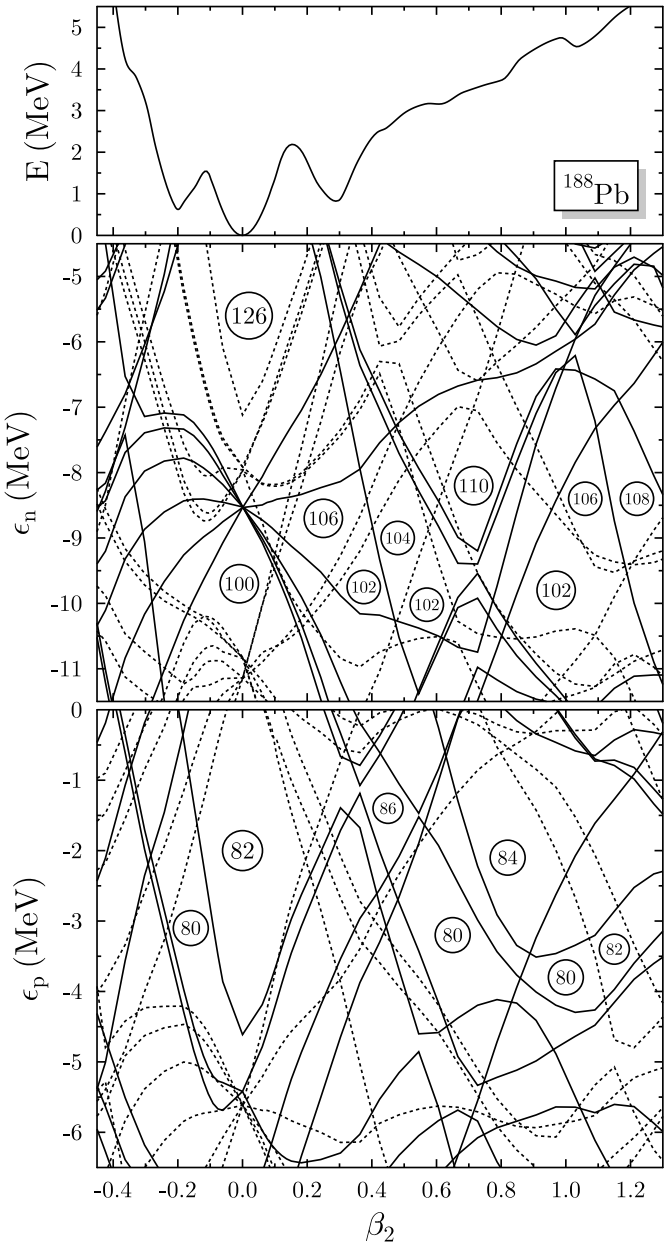
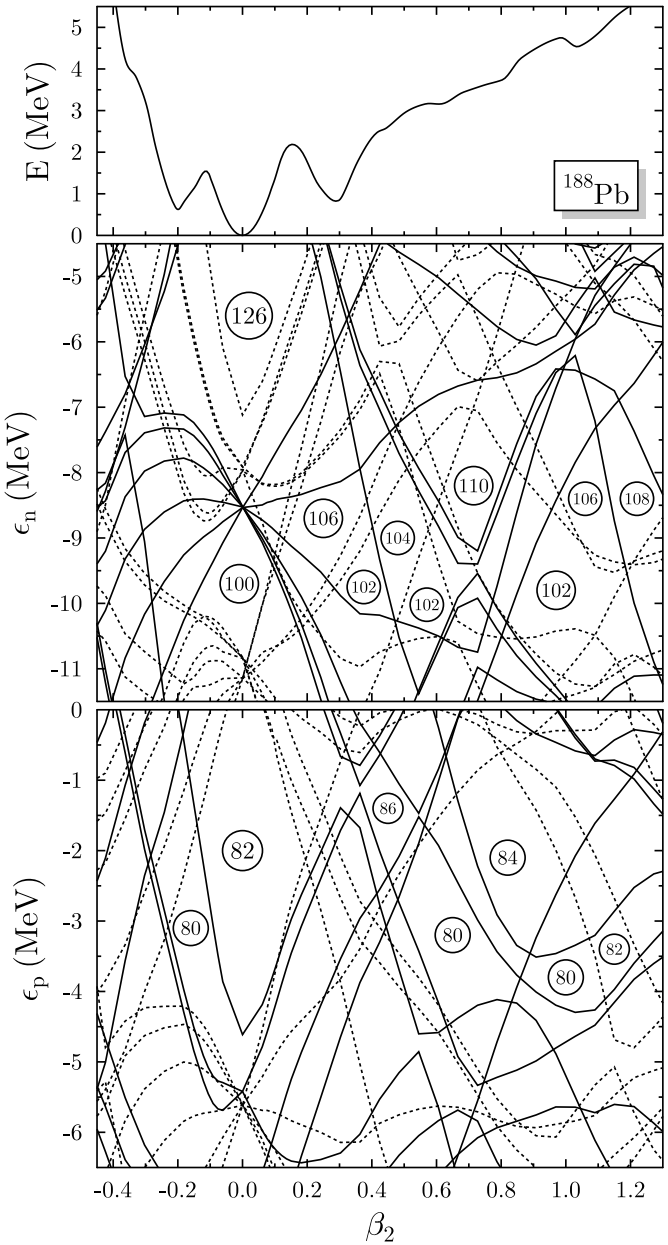


FIG. 11. (Color online) Same as in Fig. 6, but for ^{120}Sn.

MR EDF: Horizontal vs. vertical expansion of correlations



MR EDF: Horizontal vs. vertical expansion of correlations



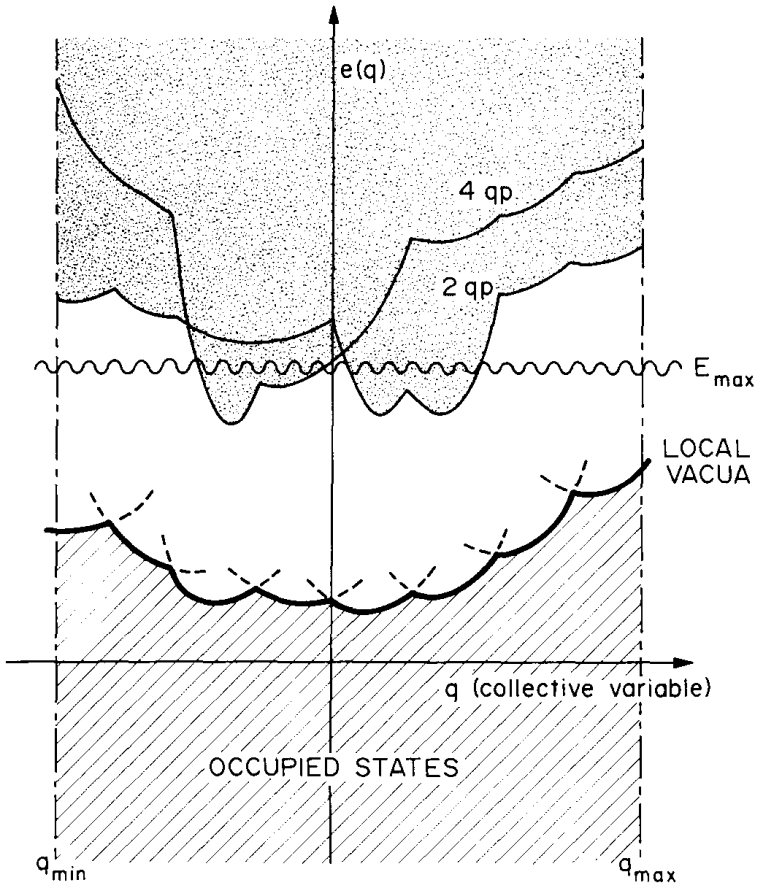


Fig. 1. Schematic plot of the energy versus the collective variable. The dark envelopes show the positions of the local vacua. The domain of the collective variable is defined by q_{min}, q_{max} and the energy cut E_{max}.

F. Dönau *et al*, NPA496 (1989) 333.

particle-number projector

$$\hat{P}_{N_0} = \frac{1}{2\pi}\int_0^{2\pi} d\phi_N \underbrace{e^{-i\phi_N N_0}}_{\text{weight}} \overbrace{e^{i\phi_N \hat{N}}}^{\text{rotation in gauge space}}$$

angular-momentum restoration operator

$$\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2}\int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \, \sin(\beta) \int_0^{2\pi} d\gamma \underbrace{\mathcal{D}^{*J}_{MK}(\alpha,\beta,\gamma)}_{\text{Wigner function}} \overbrace{\hat{R}(\alpha,\beta,\gamma)}^{\text{rotation in real space}}$$

K is the z component of angular momentum in the body-fixed frame.
Projected states are given by

$$|JMq\rangle = \sum_{K=-J}^{+J} f_J(K)\, \hat{P}^J_{MK}\, \hat{P}^Z\, \hat{P}^N\, |\mathrm{MF}(q)\rangle = \sum_{K=-J}^{+J} f_J(K)\, |JM(qK)\rangle$$

$f_J(K)$ is the weight of the component K and determined variationally

Axial symmetry (with the z axis as symmetry axis) allows to perform the α and γ integrations analytically, while the sum over K collapses, $f_J(K) \sim \delta_{K0}$

Superposition of projected self-consistent mean-field states $|\mathrm{MF}(\mathbf{q})\rangle$ differing in a set of collective and single-particle coordinates $\mathbf{q}$

$$|NZJM\nu\rangle = \sum_{\mathbf{q}} \sum_{K=-J}^{+J} f^{NZ}_{J,\kappa}(\mathbf{q},K)\, \hat{P}^{J}_{MK}\, \hat{P}^{Z}\, \hat{P}^{N}\, |\mathrm{MF}(\mathbf{q})\rangle = \sum_{\mathbf{q}} \sum_{K=-J}^{+J} f^{NZ}_{J\nu}(\mathbf{q},K)\, |NZ\, JM(\mathbf{q}K)\rangle$$

with weights $f^{NZ}_{J\nu}(\mathbf{q},K)$.

$$\frac{\delta}{\delta f^{*}_{J\nu}(\mathbf{q},K)} \frac{\langle NZ\, JM\nu|\hat{H}|NZ\, JM\nu\rangle}{\langle NZ\, JM\nu|NZ\, JM\nu\rangle} = 0 \quad \Rightarrow \quad \text{Hill-Wheeler-Griffin equation}$$

$$\sum_{\mathbf{q}'} \sum_{K'=-J}^{+J} \left[\mathcal{H}^{NZ}_{J}(\mathbf{q}K,\mathbf{q}'K') - E^{NZ}_{J,\nu}\, \mathcal{I}^{NZ}_{J}(\mathbf{q}K,\mathbf{q}'K')\right] f^{NZ}_{J,\nu}(\mathbf{q}'K') = 0$$

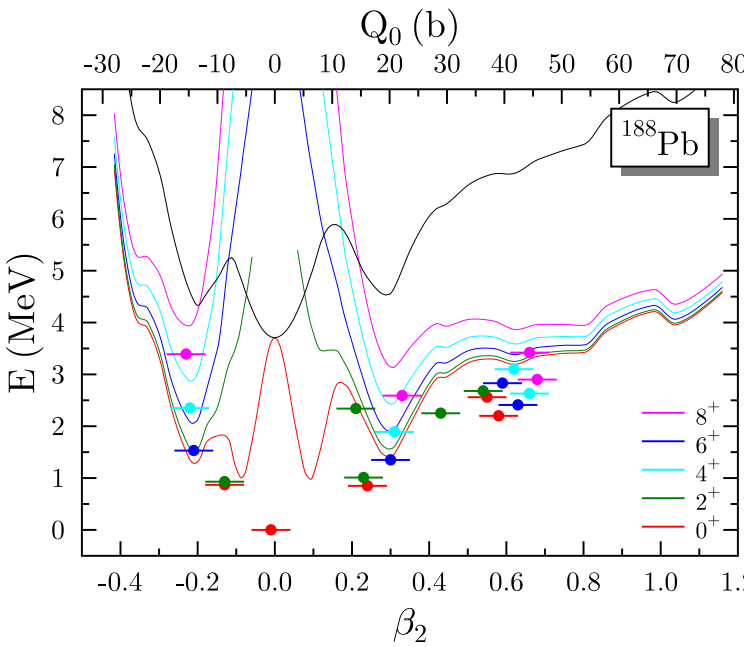
with

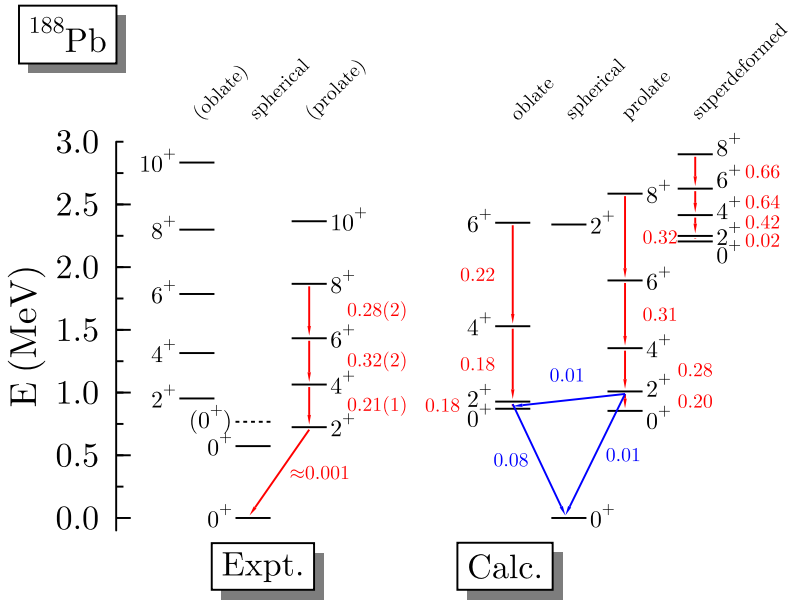
$$\mathcal{H}_{J}(\mathbf{q}K,\mathbf{q}'K') = \langle NZ\, JM\, \mathbf{q}K|\hat{H}|NZ\, JM\, \mathbf{q}'K'\rangle \quad \text{energy kernel}$$
$$\mathcal{I}_{J}(\mathbf{q}K,\mathbf{q}'K') = \langle NZ\, JM\, \mathbf{q}K|NZ\, JM\, \mathbf{q}'K'\rangle \quad \text{norm kernel}$$

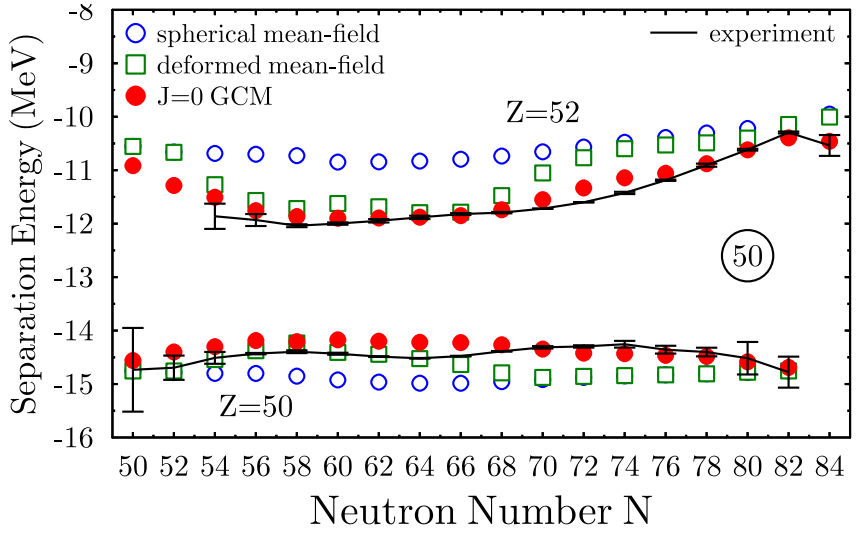
Angular-momentum projected GCM gives the

- correlated ground state for each value of J
- spectrum of excited states for each J

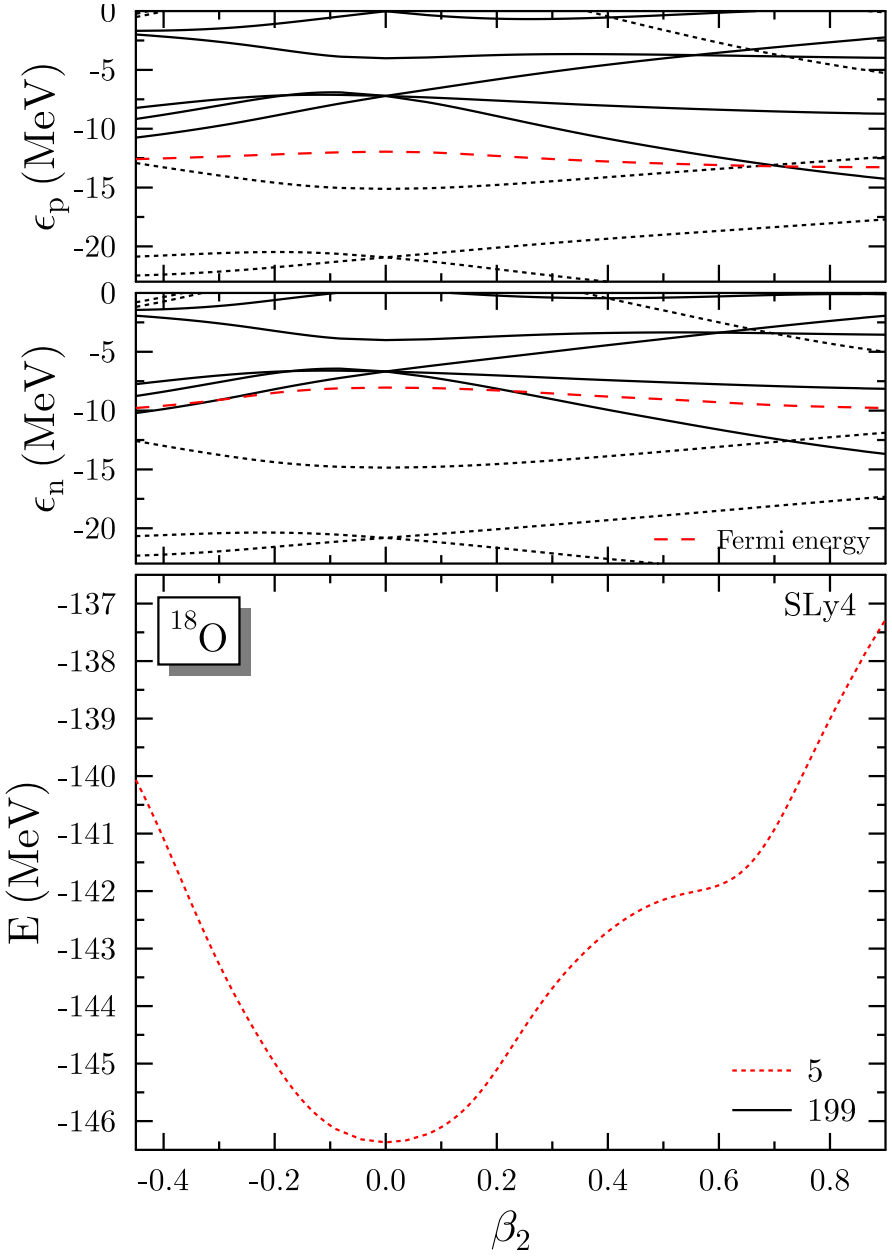
MR EDF: typical applications





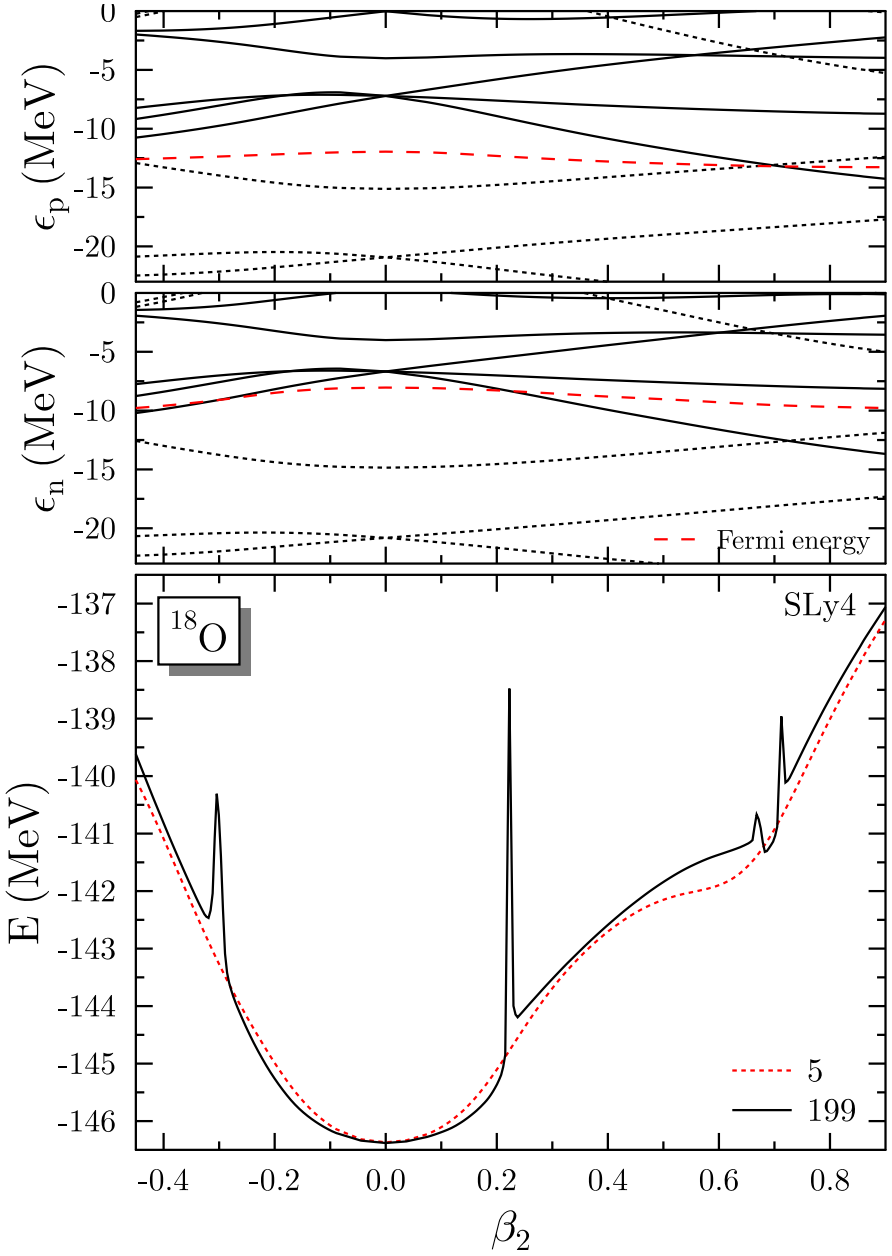


Problems with density dependences



- pure particle-number projection

Problems with density dependences



- 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
- First analysis in a strict energy density functional (EDF) framework and of EDF-specific consequences by Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC 76 (2007) 054315
- Further analysis of the EDF case by Lacroix, Duguet, Bender, PRC 79 (2009) 044318; Bender, Duguet, Lacroix, PRC 79 (2009) 044319; Duguet, Bender, Bennaceur, Lacroix, Lesinski, PRC 79 (2009) 044320; Bender, Avez, Duguet, Heenen, Lacroix, *in preparation*

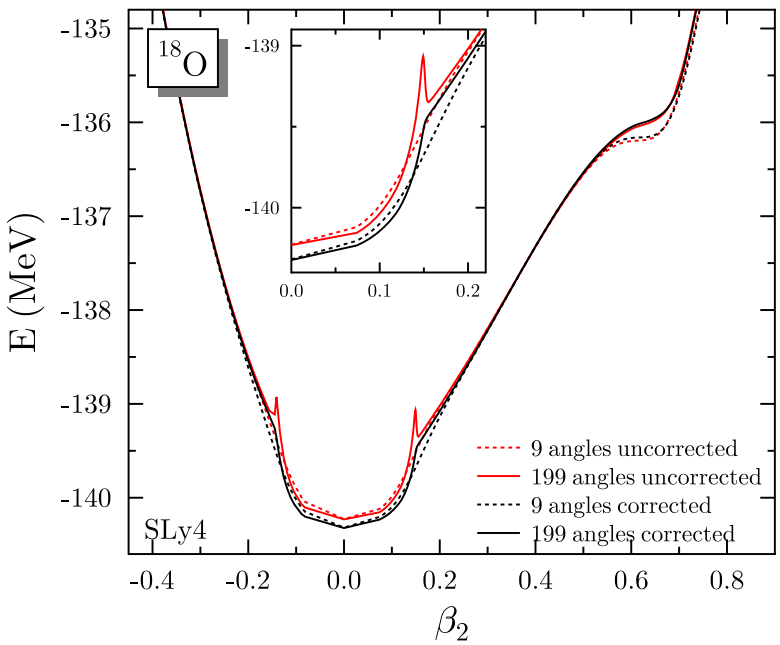
The origin of the problem in a nutshell

- 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

Using non-analytical density dependences

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 (strategy currently used by L. Egido and collaborators).
  - Difficult to justify formally.
  - Does not bypass the problem anymore when using time-reversal-invariance breaking reference states.

What to do?

1. constructing the EDF as expectation value of a strict Hamiltonian. Numerically very costly due to Coulomb exchange & pairing; no available parameterisations of high quality (the difficulties to construct such parametrisations was the main motivation to use more general EDFs in the 1970s).
2. construct the EDF from a density-dependent Hamiltonians with special treatment of the density entering density dependent terms for which numerically efficient high-quality parameterisations can be easily constructed. Problem: cannot be defined for all possible configuration mixing [Robledo, J. Phys. G 37 (2010) 064020].
3. introduce a physics-motivated regularisation scheme of the EDF that allows for the use of (almost) standard functionals [Lacroix, Duguet, & Bender, PRC 79 (2009) 044318] for which numerically efficient high-quality parameterisations can be easily constructed. Works for particle-number projection, but not for angular-momentum projection or GCM mixing. Alternative mathematics-motivated regularisation [Satuła & Dobaczewski, PRC 90 (2014) 054303] has problems too when applied in realistic calculations [Dobaczewski, private communication].
4. Construct symmetry-conserving functionals from projected density (matrices). [Hupin, Lacroix, Bender, PRC 84 (2011) 014309; Hupin, Lacroix, PRC86 (2012) 024309]. Difficult to apply to spatial projection and GCM mixing for conceptual and numerical reasons, and also potential problems with nuclear saturation [Robledo, J. Phys. G 37 (2010) 064020].

- In general, (non-normalised) projected matrix elements of an operator $\hat{T}$ read

$$\langle q|\hat{P}^{J}_{KM}\,\hat{T}\,\hat{P}^{J'}_{M'K'}|q'\rangle\,. \tag{8}$$

- If the operator is an irreducible tensor operator $\hat{T}^{\lambda}_{\mu}$, then the commutator $[\hat{T}^{\lambda}_{\mu}\,\hat{P}^{J'}_{M'K'}]$ is known from the general properties of the rotational group. For the special case of a scalar tensor operator $\hat{T}^{0}_{0}$ (i.e. a tensor operator of rank 0 like the Hamiltonian), one has $[\hat{T}^{0}_{0},\hat{P}^{J'}_{M'K'}]=0$.
- Using $\hat{P}^{J}_{KM}\hat{P}^{J'}_{M'K'}=\hat{P}^{J}_{KK'}\,\delta_{JJ'}\,\delta_{MM'}$, it follows that

$$\langle q|\hat{P}^{J}_{KM}\,\hat{T}^{0}_{0}\,\hat{P}^{J'}_{M'K'}|q'\rangle=\langle q|\hat{P}^{J}_{KK'}\,\hat{T}^{0}_{0}|q'\rangle\,\delta_{JJ'}\,\delta_{MM'}\,. \tag{9}$$

- It is sufficient to rotate one state to calculate matrix elements

$$\langle q|\hat{P}^{J}_{KK'}\hat{H}|q'\rangle=\frac{2J+1}{16\pi^2}\int_0^{4\pi}d\alpha\int_0^{\pi}d\beta\,\sin(\beta)\int_0^{2\pi}d\gamma\,\mathcal{D}^{*J}_{KK'}(\alpha,\beta,\gamma)\langle q|\hat{R}^{\dagger}(\alpha,\beta,\gamma)\hat{H}|q'\rangle\,. \tag{10}$$

- Using the example of a *linear* density dependence of the mixed density $\rho^{LR}(\mathbf{r})$

$$\langle q|\hat{P}^J_{KK'}\hat{H}[\rho]|q'\rangle = \frac{2J+1}{16\pi^2}\int_0^{4\pi}d\alpha\int_0^{\pi}d\beta\,\sin(\beta)\int_0^{2\pi}d\gamma\,\mathcal{D}^{*J}_{KK'}(\alpha,\beta,\gamma) \times\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)\hat{H}|q'\rangle\frac{\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)\hat{\rho}|q'\rangle}{\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)|q'\rangle}\,. \quad (11)$$

  it has been argued that density-dependent Hamiltonians are invariant under rotations [Rodríguez-Guzmán et al., NPA709 (2002) 201].

- But a density dependent term uses [Note: α represents two different things here]

$$\langle q|\hat{P}^J_{KK'}\hat{H}[\rho]|q'\rangle = \frac{2J+1}{16\pi^2}\int_0^{4\pi}d\alpha\int_0^{\pi}d\beta\,\sin(\beta)\int_0^{2\pi}d\gamma\,\mathcal{D}^{*J}_{KK'}(\alpha,\beta,\gamma) \times\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)\hat{H}|q'\rangle\left(\frac{\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)\hat{\rho}|q'\rangle}{\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)|q'\rangle}\right)^{\alpha}\,. \quad (12)$$

- Is $\left[\rho^{LR}(\mathbf{r})\right]^{\alpha}$ an irreducible scalar tensor operator for $\alpha \neq 1$?

In case of combined angular-momentum and particle-number projection one has for a Hamiltonian

$$\begin{aligned}\langle q|\hat{P}^J_{KK'}\hat{H}\hat{P}_N|q'\rangle &= \frac{1}{2\pi}\int d\phi_N\, e^{+iN\phi}\frac{2J+1}{16\pi^2}\int_0^{4\pi}d\alpha\int_0^{\pi}d\beta\ \sin(\beta)\int_0^{2\pi}d\gamma\ \mathcal{D}^{*J}_{KK'}(\alpha,\beta,\gamma)\\ &\quad\times\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)\hat{H}e^{-i\hat{N}\phi}|q'\rangle\,.\end{aligned}$$

The arguments brought forward above lead for density-dependent Hamiltonians to

$$\begin{aligned}\langle q|\hat{P}^J_{KK'}\hat{H}[\rho]|q'\rangle &= \frac{1}{2\pi}\int d\phi_N\, e^{+iN\phi}\frac{2J+1}{16\pi^2}\int_0^{4\pi}d\alpha\int_0^{\pi}d\beta\ \sin(\beta)\int_0^{2\pi}d\gamma\ \mathcal{D}^{*J}_{KK'}(\alpha,\beta,\gamma)\\ &\quad\times\int d^3r\,\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)\hat{H}e^{-i\hat{N}\phi}|q'\rangle(\mathbf{r})\left[\frac{\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)\hat{\rho}e^{-i\hat{N}\phi}|q'\rangle}{\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)e^{-i\hat{N}\phi}|q'\rangle}(\mathbf{r})\right]^\alpha\end{aligned}$$

The Madrid group started to use a density that is projected on particle number (but still mixed in all other degrees of freedom) for the density dependence

$$\begin{aligned}\langle q|\hat{P}^J_{KK'}\hat{H}[\rho]|q'\rangle &= \frac{2J+1}{16\pi^2}\int_0^{4\pi}d\alpha\int_0^{\pi}d\beta\ \sin(\beta)\int_0^{2\pi}d\gamma\ \mathcal{D}^{*J}_{KK'}(\alpha,\beta,\gamma)\\ &\quad\times\int d^3r\left[\frac{1}{2\pi}\int d\phi_N\, e^{+iN\phi}\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)\hat{H}e^{-i\hat{N}\phi}|q'\rangle(\mathbf{r})\right]\\ &\quad\times\left[\frac{1}{2\pi}\int d\phi'_N\, e^{+iN\phi'}\frac{\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)\hat{\rho}e^{-i\hat{N}\phi}|q'\rangle}{\langle q|\hat{R}^\dagger(\alpha,\beta,\gamma)e^{-i\hat{N}\phi'}|q'\rangle}(\mathbf{r})\right]^\alpha.\end{aligned}$$

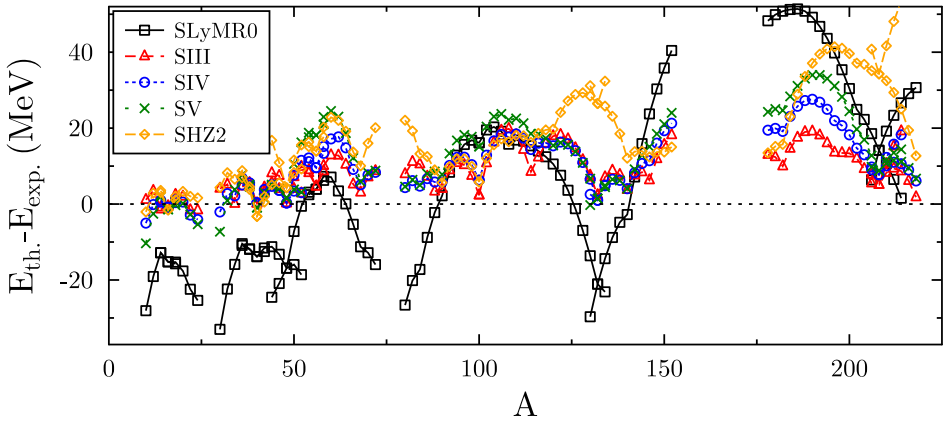
For non-paired Slater determinants this becomes the standard recipe again.

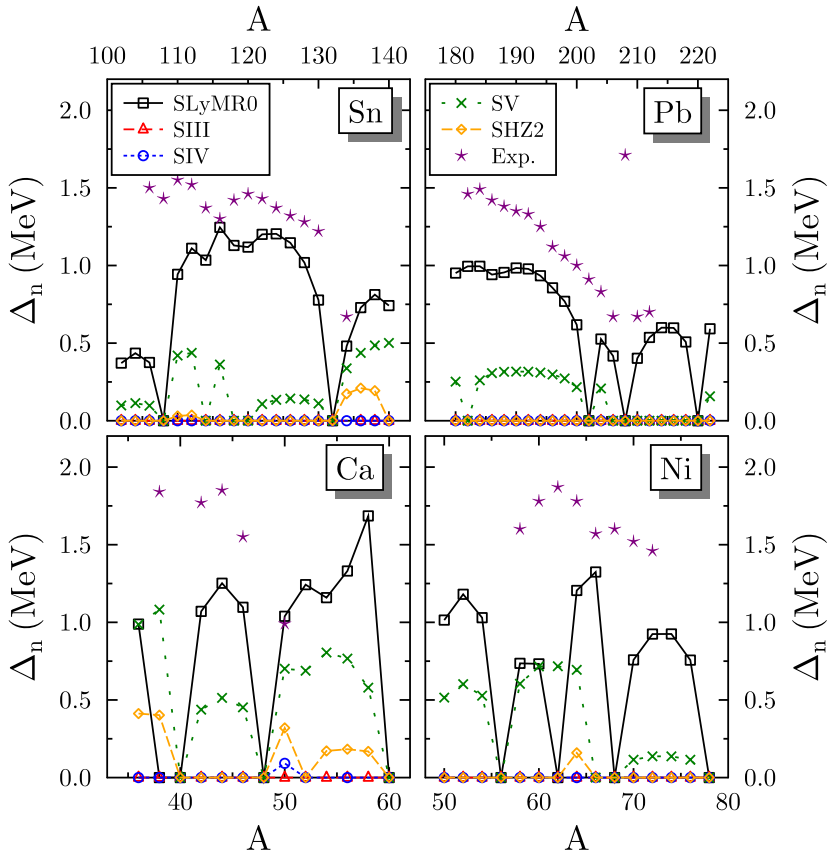
Effective interaction used throughout this talk: SLyMR0

$$
\begin{aligned}
\hat{v} = & \; t_0 \left(1 + x_0 \hat{P}_\sigma\right) \hat{\delta}_{r_1 r_2} \\
& + \frac{t_1}{2} \left(1 + x_1 \hat{P}_\sigma\right) \left(\hat{\mathbf{k}}_{12}'^{\,2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12}^{\,2}\right) \\
& + t_2 \left(1 + x_2 \hat{P}_\sigma\right) \hat{\mathbf{k}}_{12}' \cdot \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12} \\
& + \mathrm{i}\, W_0 \left(\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2\right) \cdot \hat{\mathbf{k}}_{12}' \times \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12} \\
& + u_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1}\right) \\
& + v_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \hat{\delta}_{r_3 r_4} + \hat{\delta}_{r_1 r_2} \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_2 r_4} + \cdots\right)
\end{aligned}
$$

J. Sadoudi, M. Bender, K. Bennaceur, D. Davesne, R. Jodon, and T. Duguet, Physica Scripta T154 (2013) 014013

Pseudo-potentials for MR EDF. First try: SLyMR0

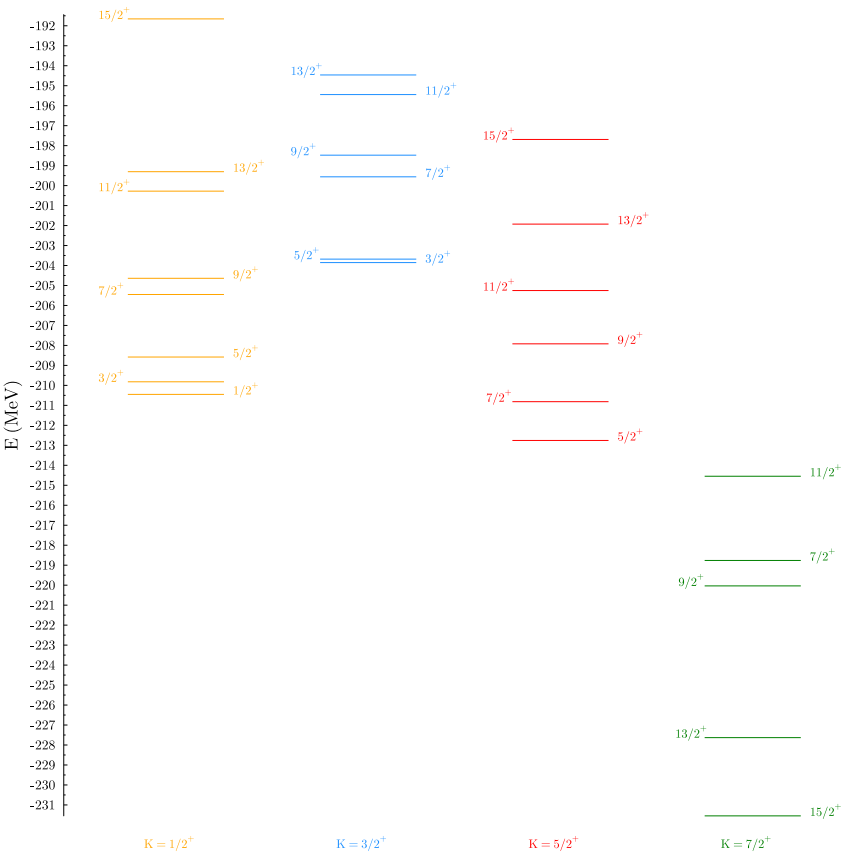




- it is impossible to fulfill the usual nuclear matter constraints , to have stable interactions and attractive pairing
- no "best fit" possible
- very bad performance compared to standard general functionals

J. Sadoudi, M. Bender, K. Bennaceur, D. Davesne, R. Jodon, and T. Duguet, Physica Scripta T154 (2013) 014013

Density dependence with particle-number projected density



^{25}Mg

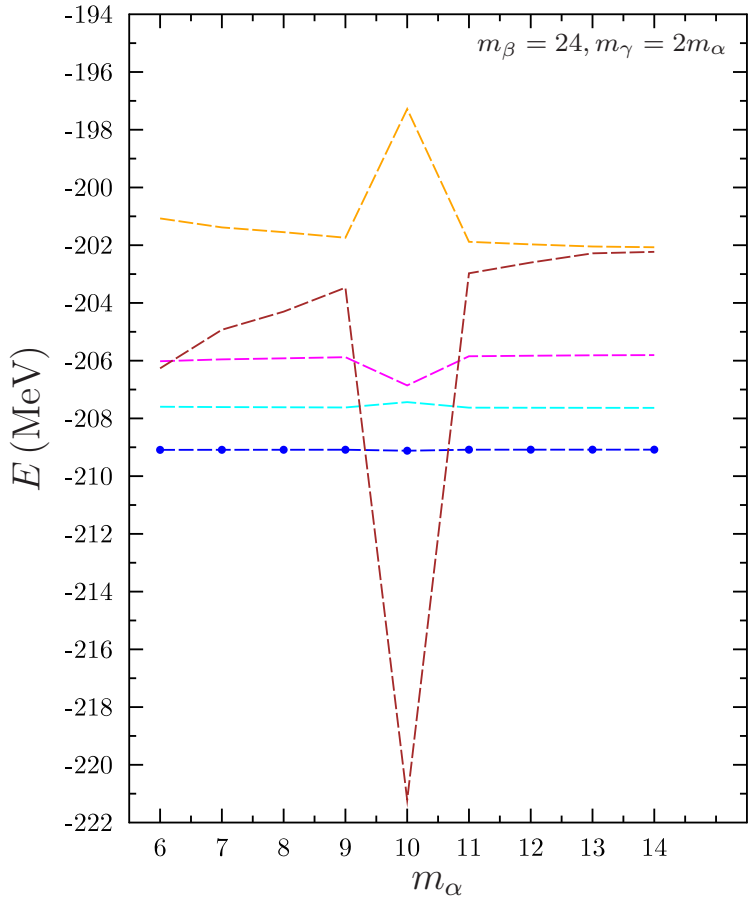
B. Bally, B. Avez, M. Bender, unpublished (2012).

- effective interaction: standard density-dependent Skyrme 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 discretisation points and sum-rules 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*)

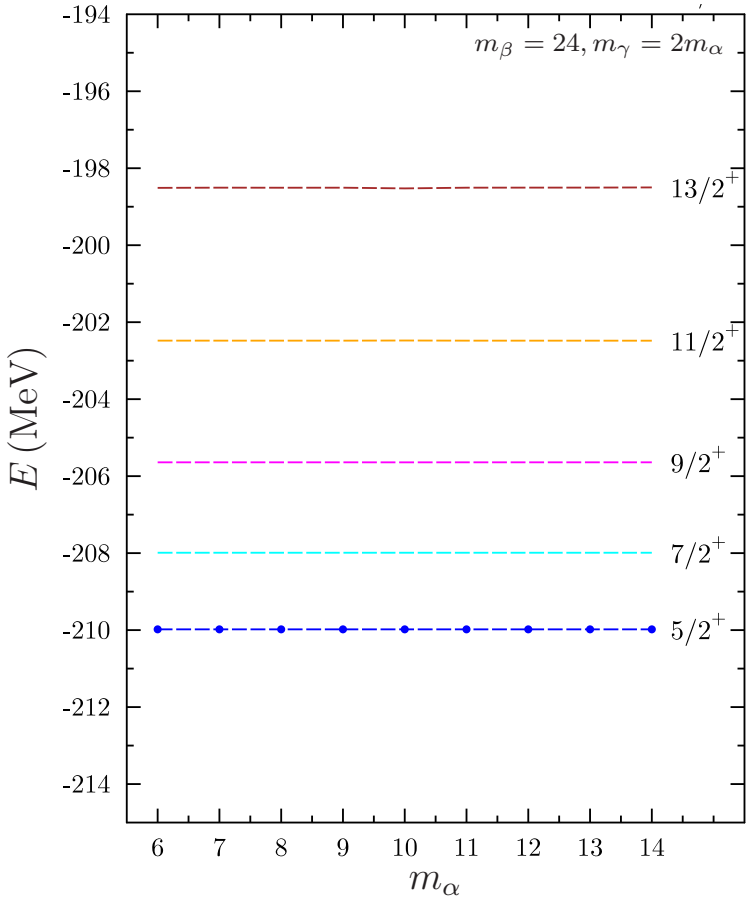
Discretisation dependence

Dependence on the number of discretisation 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.

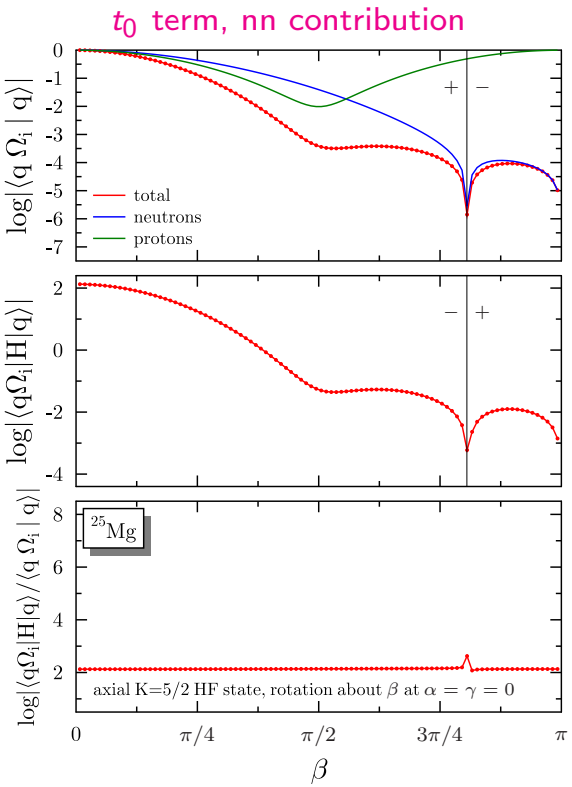
SLy5sp$_2$

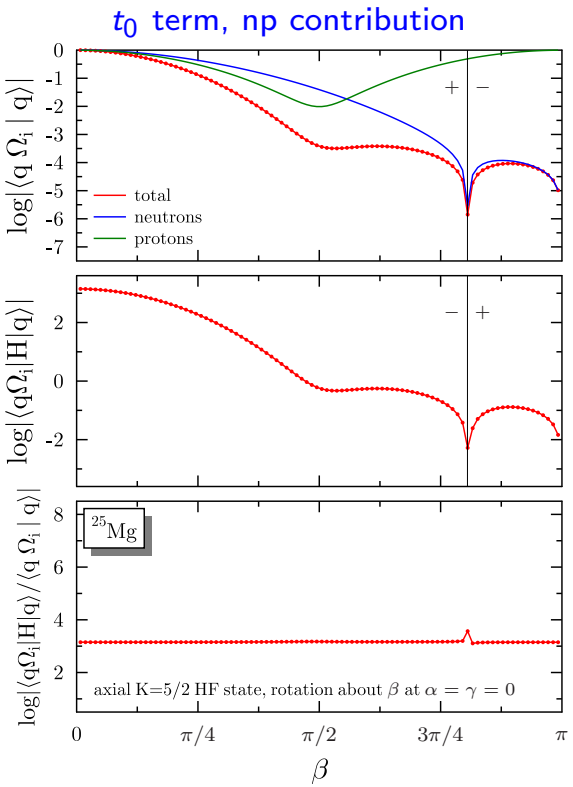


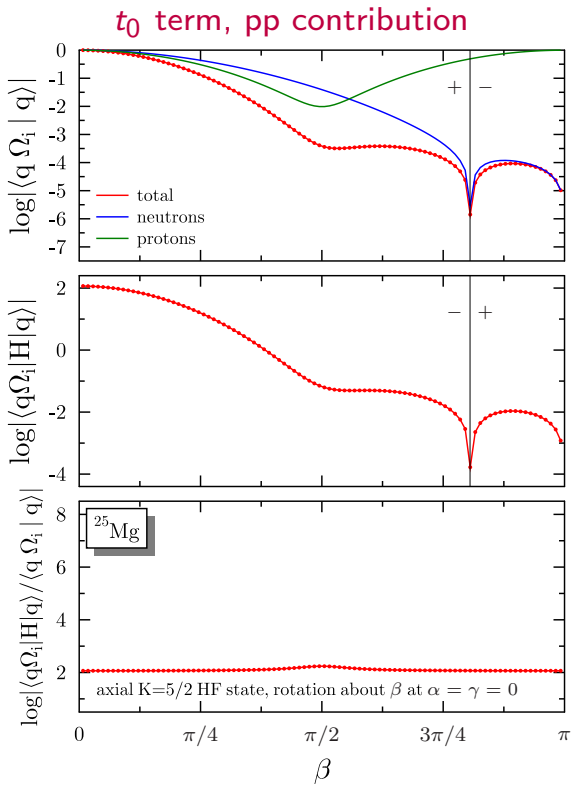
SLyMR0



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



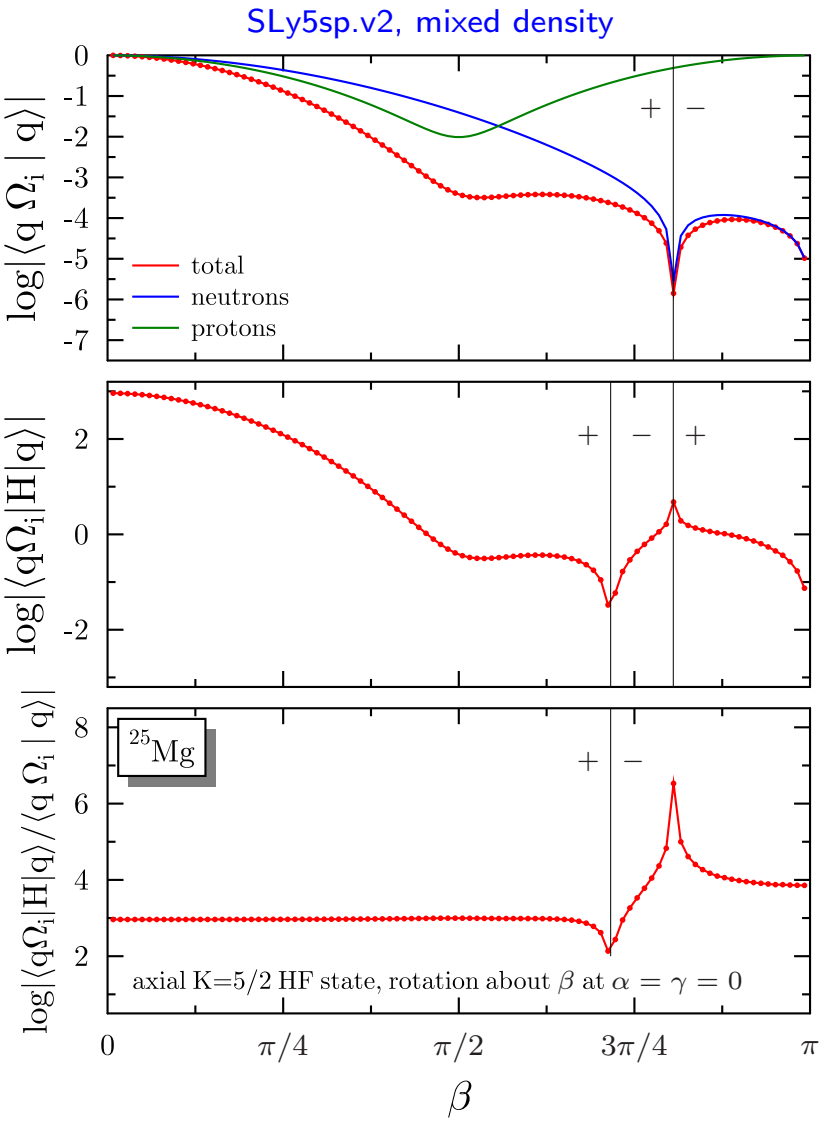




$$
\begin{aligned}
E^{LR}_{t_0} &= \langle \mathsf{L}|t_0\,(1+x_0\hat{P}_\sigma)\,\hat{\delta}^{\mathbf{r}}|\mathsf{R}\rangle \\
&= \tfrac{1}{4}t_0(1-x_0)\int d^3r\left[\rho^{LR}_n(\mathbf{r})\,\rho^{LR}_n(\mathbf{r}) - \mathbf{s}^{LR}_n(\mathbf{r})\cdot\mathbf{s}^{LR}(\mathbf{r}) + \tilde{\rho}^{RL*}_n(\mathbf{r})\,\tilde{\rho}^{LR}_n(\mathbf{r})\right]\langle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

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

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

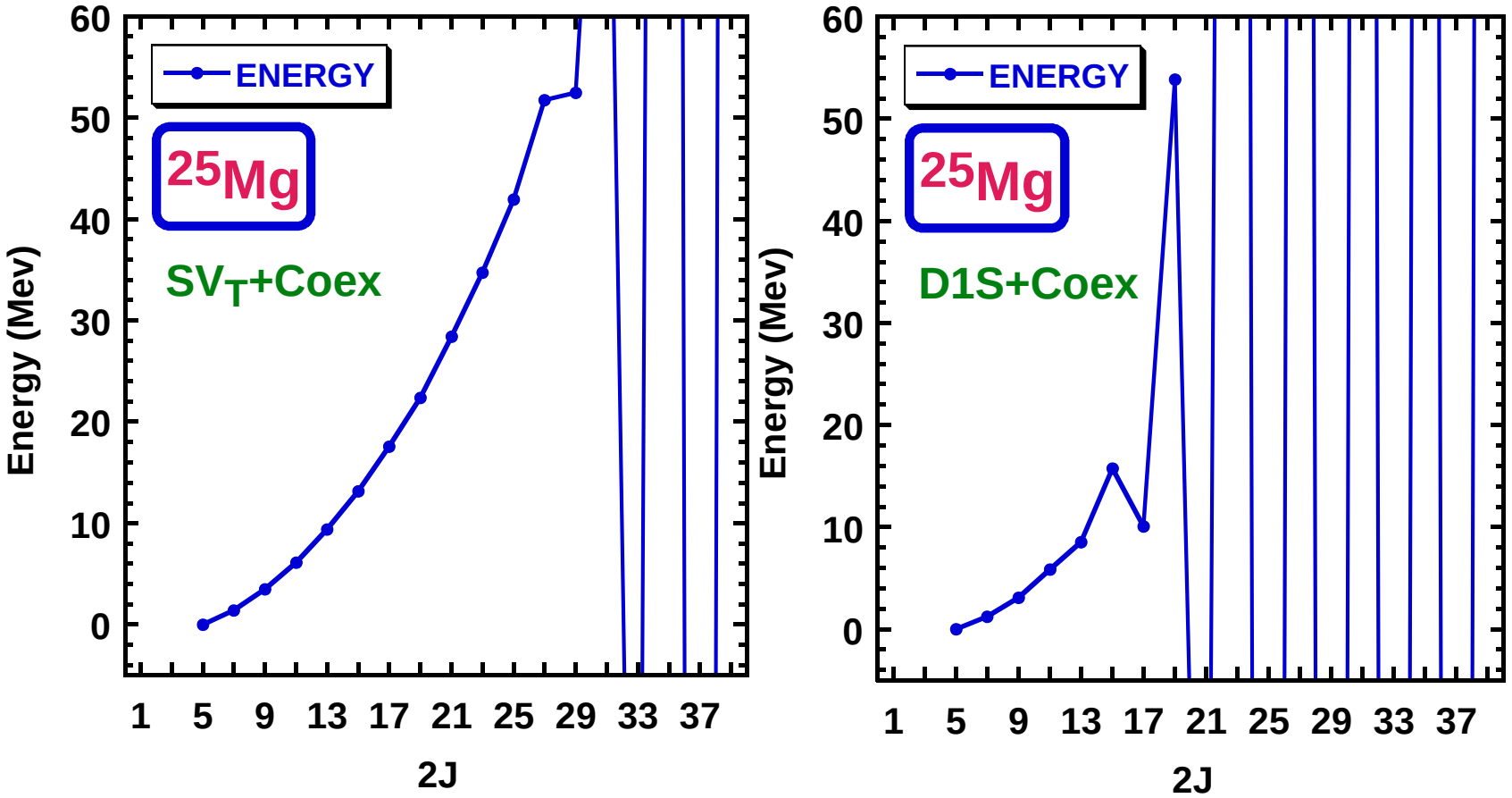


For a parameteriation with $x_3 = 1$ and in the limit of Slater determinants, the energy kernel of the density-dependent part of the Skyrme interaction reads

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

Same in HFODD

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

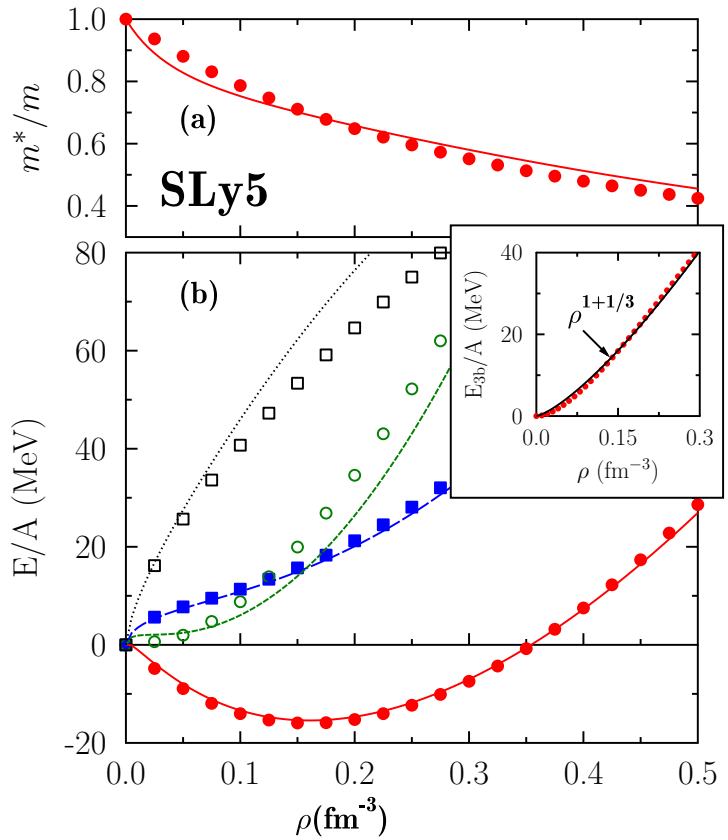


A dead end (unfortunately)

$(v_{ijk} + v_{ikj} + v_{kij})/3$, with

$$v_{ijk} = \{V_0(r) + V_\sigma(r)P_\sigma + V_\tau(r)P_\tau + V_{\sigma\tau}(r)P_\sigma P_\tau\} \times \delta\left(\mathbf{r}_k - \left[\frac{\mathbf{r}_i + \mathbf{r}_j}{2}\right]\right), \quad (1)$$

where the short-hand notation $r = |\mathbf{r}_i - \mathbf{r}_j|$ is used, while P_σ (P_τ) exchanges the projections of spin (isospin) of particles i and j. Note that the interaction can be used without isospin



Lacroix & Bennaceur, PRC91 (2015) 011302r

Construction of new forms of effective interactions

- Skyrme-type interactions with higher-order terms in derivatives

  (not aiming at true Hamiltonians so far, though)

  Carlsson, Dobaczewski, Kortelainen, PRC 78 (2008) 044326

  Raimondi, Carlsson, Dobaczewski, PRC 83 (2011) 054311

  Davesne, Pastore, Navarro, JPG 40 (2013) 095104

  Becker, Davesne, Meyer, Pastore, Navarro, JPG 42 (2015) 034001

- Skyrme-type interactions with explicit three-body interactions

  Sadoudi, thèse, Université de Paris-Sud XI (2011)

  Sadoudi, M. Bender, Bennaceur, Davesne, Jodon, Duguet, Phys Scr T154 (2013) 014013

  Sadoudi, Duguet, Meyer, M. Bender, PRC 88 (2013) 064326

- regularised contact interactions (replacing the delta function in Skyrme with Gaussians)

  Raimondi, Bennaceur, Dobaczewski, JPG 41 (2014) 055112

  Bennaceur, Idini, J. Dobaczewski, P. Dobaczewski, Kortelainen, Raimondi, JPG44 (2017) 045106

- non-local three-body forces simulating density dependences

  Gezerlis, Bertsch, PRL 105 (2010) 212501

  Lacroix, Bennaceur, PRC 91 (2015) 011302(R)

- or try a different strategy: explicit in-medium correlations from MBPT

  Duguet, M. Bender, Ebran, Lesinski, Somà, EPJA 51 (2015) 162

Ongoing improvements: 3-body terms of 2nd order in gradients

the most general central Skyrme-type 3-body force up to 2nd order in gradients has been constructed by J. Sadoudi with a dedicated formal algebra code

$$
\begin{aligned}
\hat{v}_{123} \;=\; & u_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \right) \\
& + \frac{u_1}{2} \left[1 + y_1 P^\sigma_{12} \right] \left(\hat{\mathbf{k}}_{12} \cdot \hat{\mathbf{k}}_{12} + \hat{\mathbf{k}}'_{12} \cdot \hat{\mathbf{k}}'_{12} \right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\
& + \frac{u_1}{2} \left[1 + y_1 P^\sigma_{31} \right] \left(\hat{\mathbf{k}}_{31} \cdot \hat{\mathbf{k}}_{31} + \hat{\mathbf{k}}'_{31} \cdot \hat{\mathbf{k}}'_{31} \right) \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} \\
& + \frac{u_1}{2} \left[1 + y_1 P^\sigma_{23} \right] \left(\hat{\mathbf{k}}_{23} \cdot \hat{\mathbf{k}}_{23} + \hat{\mathbf{k}}'_{23} \cdot \hat{\mathbf{k}}'_{23} \right) \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \\
& + u_2 \left[1 + y_{21} P^\sigma_{12} + y_{22} (P^\sigma_{13} + P^\sigma_{23}) \right] \left(\hat{\mathbf{k}}_{12} \cdot \hat{\mathbf{k}}'_{12} \right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\
& + u_2 \left[1 + y_{21} P^\sigma_{31} + y_{22} (P^\sigma_{32} + P^\sigma_{12}) \right] \left(\hat{\mathbf{k}}_{31} \cdot \hat{\mathbf{k}}'_{31} \right) \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} \\
& + u_2 \left[1 + y_{21} P^\sigma_{23} + y_{22} (P^\sigma_{21} + P^\sigma_{31}) \right] \left(\hat{\mathbf{k}}_{23} \cdot \hat{\mathbf{k}}'_{23} \right) \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1}
\end{aligned}
$$

Sadoudi, Duguet, Meyer, M. Bender, PRC 88 (2013) 064326

Take-away messages

Why density dependences are needed

- Density dependences are a shortcut to in-medium correlations
- Without them it is difficult to model phenomenology.
- Use of density dependences instead of 3-body forces solves problems with K_∞, spin-stability, sign of pairing matrix elements, ...

Why density dependences should not be used

- Source of self-interaction and self-pairing that might spoil results.
- MR calculations become mathematically ill-defined and might/will give surprising/non-physical results.
- Some doubts about their use in diagrammatic beyond-mean-field models have been voiced too.

Where does this contradiction come from?

- In one way or the other, density dependences are meant to approximately describe the in-medium correlation energy from summing diagrams in a "vertical" expansion.
- The key problem concerning multi-reference calculations is that approximations are made in the wrong order when expressing the k_F dependence of "vertical" correlation energies by a density dependence in local-density approximation of infinite nuclear matter and then using it to calculate "horizontal" correlation energies. That final step is ill-defined conceptually (as the densities entering a "horizontal calculation" are not related to k_F) and mathematically (as densities are functions in the complex plane).

Acknowledgements

The work presented here would have been impossible without my collaborators

founding fathers

Paul Bonche	SPhT, CEA Saclay
Hubert Flocard	CSNSM Orsay
Paul-Henri Heenen	Université Libre de Bruxelles

formal aspects of the big picture

Thomas Duguet	Irfu/CEA Saclay
Denis Lacroix	IPN Orsay

design and implementation of code extensions

Benoît Avez	CEN Bordeaux Gradignan
Benjamin Bally	CEN Bordeaux Gradignan, now SPhN, CEA Saclay
Veerle Hellemans	Université Libre de Bruxelles
Jiangming Yao	Université Libre de Bruxelles
Wouter Ryssens	IPN Lyon

development and benchmarking of new functionals

Karim Bennaceur	IPN Lyon & Jyväskylä
Dany Davesne	IPN Lyon
Robin Jodon	IPN Lyon
Jacques Meyer	IPN Lyon
Alessandro Pastore	formerly IPN Lyon, now University of York
Jeremy Sadoudi	Irfu/CEA Saclay first, then CEN Bordeaux Gradignan

color code: active (past) member of the collaboration