Spuriousities in the multi-reference energy density functional formalism

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how to efficiently grasp collective correlations in mesoscopic many-body systems?"
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Glossary of frequently used terms

- **E**nergy **D**ensity **F**unctional: Expression for the energy given in terms of one-body density matrices (or local one-body densities).
- Instead of calculating the energy from an effective interaction, there is the (frequently used) possibility to postulate directly the form of the energy functional.
- **S**ingle-**R**eference EDF: Method where the EDF is calculated from the one-body density matrices of a variationally optimized single product state ("HF", "HFB").
- **M**ulti-**R**eference EDF: Method where the EDF is calculated from off-diagonal one-body density matrices $\rho^{LR}(x,x') \equiv \langle \mathrm{L}|\hat{a}_x^\dagger, \hat{a}_x|\mathrm{R}\rangle / \langle \mathrm{L}|\mathrm{R}\rangle$, covering the beyond-mean-field techniques "symmetry restoration" and "Generator Coordinate Method" in the EDF context (see lecture by L. Robledo)
- **pseudo-potential-based EDF**: EDF derived from a generating operator ("effective Hamiltonian")
- **pseudo-potential**: operator used to generate an EDF. Note: the notion of pseudo potential is also used for completely different concepts in quantum chemistry, nuclear physics, and other subfields of quantum physics.
- **Skyrme EDF**: Local energy density functional depending on local densities and currents containing gradients and simple density dependences.
- **Skyrme pseudo-potential**: momentum-dependent two-body + three-body + 4-body + ... pseudo-potential that is used as generator of the EDF.

The Skyrme energy density functional at NLO

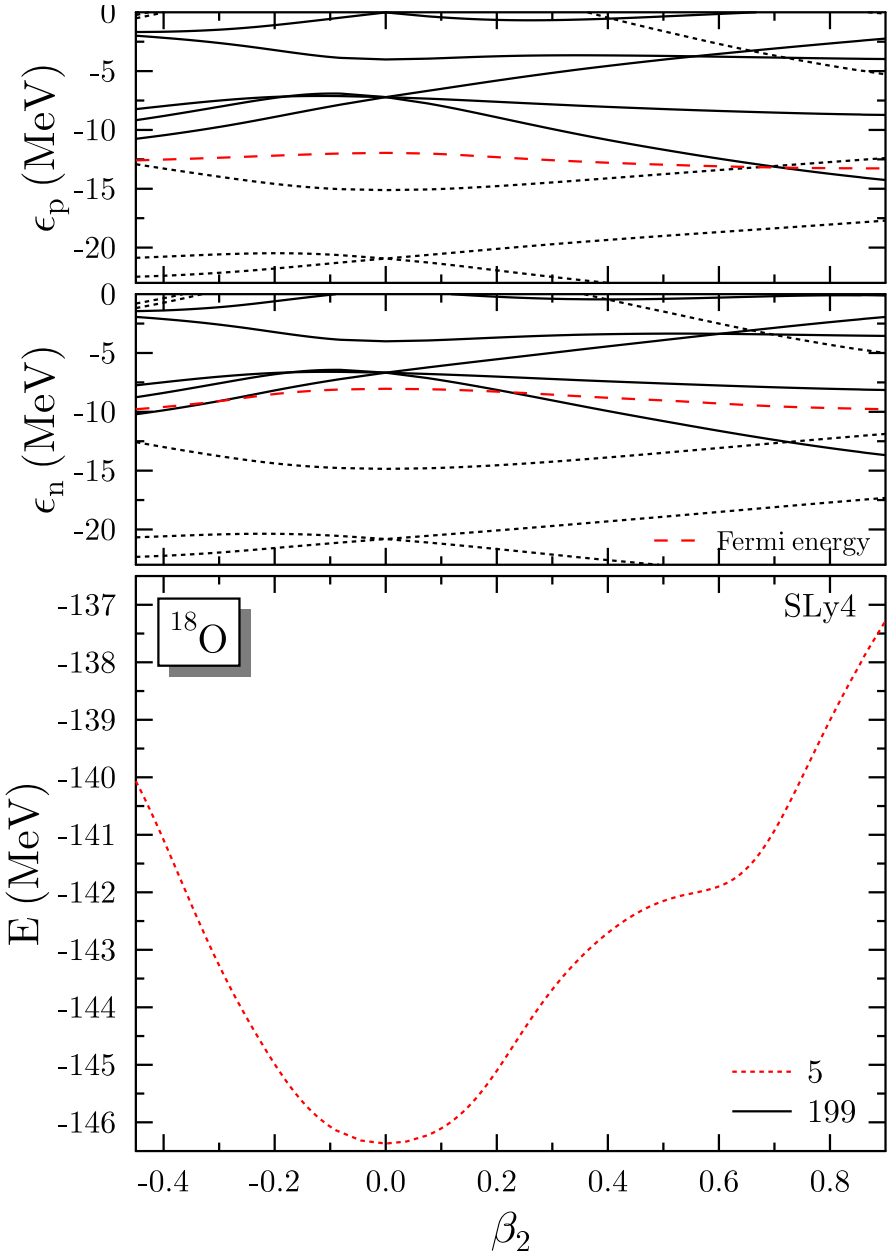
In Skyrme-EDF jargon, NLO means "next-to-leading order in gradients", i.e. the terms in the EDF contain zero (LO) or two (NLO) gradients. There are efforts to construct extended EDFs with four (N2LO) and six (N3LO) gradients. There is no reason to expect that this refers to a strict hierarchy in physical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

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

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

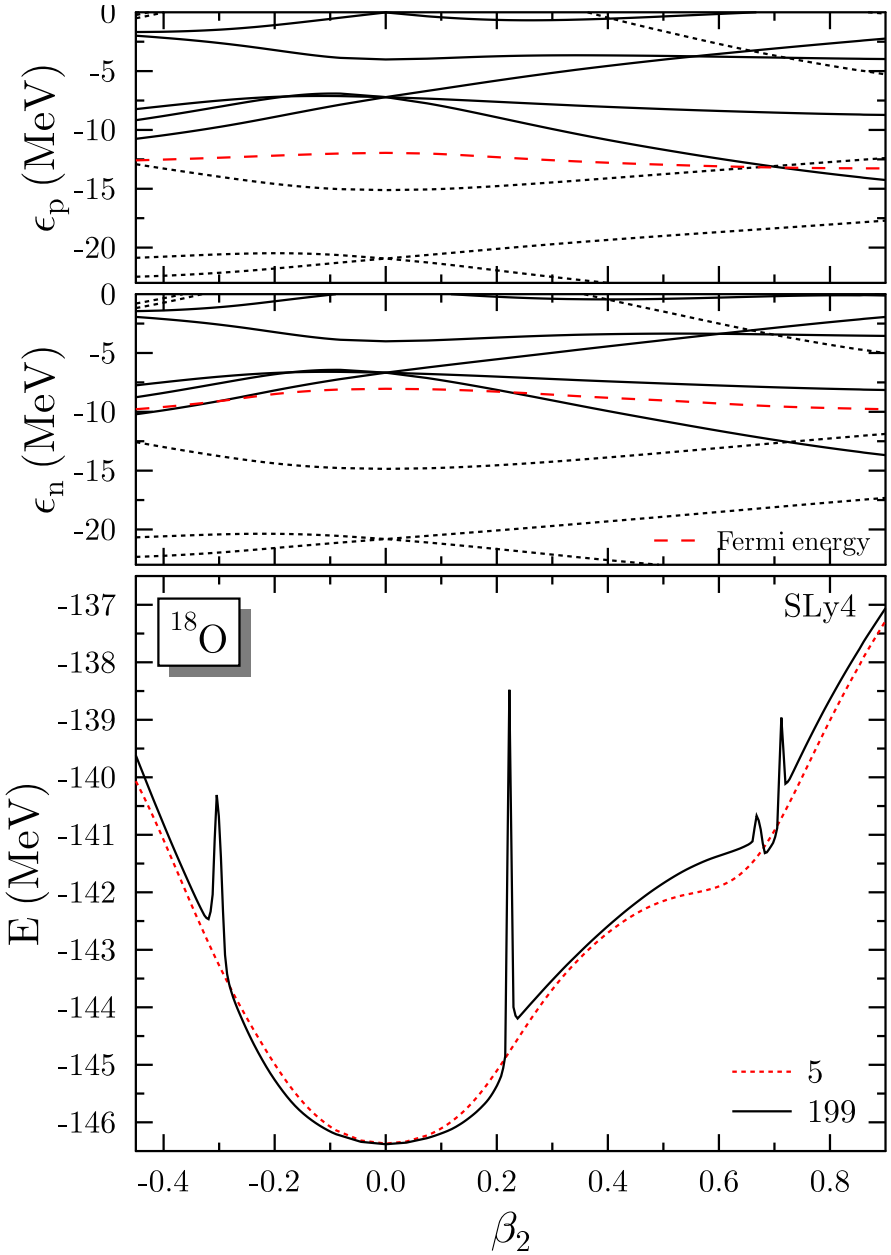
$$
\begin{aligned}
\rho_q(\mathbf{r}) &= \rho_q(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}\,, \\
\tau_q(\mathbf{r}) &= \nabla\cdot\nabla'\,\rho_q(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}\,, \\
J_{q,\mu\nu}(\mathbf{r}) &= -\tfrac{i}{2}\left(\nabla_\mu-\nabla'_\mu\right)s_{q,\nu}(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}\,,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

Problems with standard Skyrme



- pure particle-number projection

Problems with standard Skyrme



- 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*
- A different manifestation of the same problem is discussed by Tajima, Flocard, Bonche, Dobaczewski and Heenen, NPA542 (1992) 355 for EDF kernels between HFB vacua and two-quasiparticle states.

The origin of the problem in a nutshell

- All (present) standard EDFs do not correspond to the expectation value of a Hamiltonian for at least one of the following reasons:
  - the use of density-dependent coupling constants
  - the use of different effective interactions in the particle-hole and pairing parts of the energy functional (exceptions: Gogny and very few non-standard parameterizations of the Skyrme EDF)
  - the omission, approximation or modification of specific exchange terms

  that are all introduced for phenomenological reasons and/or the sake of numerical efficiency.

Consequences:

- 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. ["self-interaction", Stringari & Brink NPA307 (1978) 307; Perdew & Zunger PRB23 (1981) 5048] or of non-physical interactions of a given pair of nucleons with itself ["self-pairing", Bender, Duguet, Lacroix, PRC 79 (2009) 044319].
- The EDF might not be representable as a sum of irreps of the symmetry groups of the "true" nuclear Hamiltonian [Duguet & Sadoudi, JPG 37 (2010) 064009].
- the resulting self-interactions and self-pairing-interactions might spoil mean-field calculations, but there is no obviously "large" non-physical behaviour caused by them.
- in the extension to symmetry-restored GCM, these terms cause
  - discontinuities and divergences in symmetry-restored energy surfaces
  - violation of sum rules in symmetry restoration
  - density dependences are multivalued complex functions with branch cuts in most MR-type calculations.

The poles are a consequence of using the Generalized Wick theorem of Balian and Brézin

$$\frac{\langle \mathrm{L}|\hat{H}^{(2)}|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} = \frac{\langle \mathrm{L}|\sum_{ijmn}\hat{H}^{(2)}_{ijmn}a^\dagger_i a^\dagger_j a_n a_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle}$$

$$= \sum_{ijmn}\hat{H}^{(2)}_{ijmn}\Big[\frac{\langle \mathrm{L}|\hat{a}^\dagger_i\hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle}\frac{\langle \mathrm{L}|\hat{a}^\dagger_j\hat{a}_n|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} - \frac{\langle \mathrm{L}|\hat{a}^\dagger_i\hat{a}_n|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle}\frac{\langle \mathrm{L}|\hat{a}^\dagger_j\hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} + \frac{\langle \mathrm{L}|\hat{a}^\dagger_i\hat{a}^\dagger_j|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle}\frac{\langle \mathrm{L}|\hat{a}_n\hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle}\Big]\langle \mathrm{L}|\mathrm{R}\rangle$$

to *postulate* an MR EDF *that does not corespond to an operator*.

$$\begin{aligned}\mathcal{E} \quad = \quad & \Big[\sum_{ijmn}\hat{v}^{\rho\rho}_{ijmn}\frac{\langle \mathrm{L}|\hat{a}^\dagger_i\hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle}\frac{\langle \mathrm{L}|\hat{a}^\dagger_j\hat{a}_n|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} - \hat{v}'^{\rho\rho}_{ijmn}\frac{\langle \mathrm{L}|\hat{a}^\dagger_i\hat{a}_n|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle}\frac{\langle \mathrm{L}|\hat{a}^\dagger_j\hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle} \\ & + \hat{v}^{\kappa\kappa}_{ijmn}\frac{\langle \mathrm{L}|\hat{a}^\dagger_i\hat{a}^\dagger_j|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle}\frac{\langle \mathrm{L}|\hat{a}_n\hat{a}_m|\mathrm{R}\rangle}{\langle \mathrm{L}|\mathrm{R}\rangle}\Big]\langle \mathrm{L}|\mathrm{R}\rangle\end{aligned}$$

as the $\frac{1}{\langle \mathrm{L}|\mathrm{R}\rangle}$ divergence for orthogonal states $\langle \mathrm{L}|\mathrm{R}\rangle \to 0$ does not cancel out anymore.

$$\int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, c_N^2} \, \mathcal{E}_{GWT}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0\,*}] \, \langle \Phi_0 | \Phi_\varphi \rangle$$

$$= \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, c_N^2} \Bigg[\sum_\mu t_{\mu\mu} \, \frac{v_\mu^2 \, e^{2i\varphi}}{u_\mu^2 + v_\mu^2 \, e^{2i\varphi}}$$

$$+ \frac{1}{2} \sum_{\mu\nu} \bar{v}^{\rho\rho}_{\mu\nu\mu\nu} \, \frac{v_\mu^2 \, e^{2i\varphi}}{u_\mu^2 + v_\mu^2 \, e^{2i\varphi}} \, \frac{v_\nu^2 \, e^{2i\varphi}}{u_\nu^2 + v_\nu^2 \, e^{2i\varphi}}$$

$$+ \frac{1}{4} \sum_{\mu\nu} \bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\nu\bar{\nu}} \, \frac{u_\mu v_\mu}{u_\mu^2 + v_\mu^2 \, e^{2i\varphi}} \, \frac{u_\nu v_\nu \, e^{2i\varphi}}{u_\nu^2 + v_\nu^2 \, e^{2i\varphi}} \Bigg] \prod_{\lambda>0} \left(u_\lambda^2 + v_\lambda^2 \, e^{2i\varphi} \right)$$

there are terms with $\mu = \nu$ which diverge for $u_\mu^2 = v_\mu^2 = 0.5 \Leftrightarrow \frac{|u_\mu|}{|v_\mu|} = 1$ and $\varphi = \pi/2$

Anguiano, Egido, Robledo, NPA696 (2001) 467

Translating to coordinate space representation

$$\begin{aligned}\int d^3r\ \rho^2(\mathbf{r}) &= \int d^3r \left[\sum_{ik} \rho_{ki}\psi_i^\dagger(\mathbf{r})\psi_k(\mathbf{r})\right]\left[\sum_{lj} \rho_{lj}\psi_j^\dagger(\mathbf{r})\psi_l(\mathbf{r})\right] \\ &= \sum_{ijkl} \underbrace{\int d^3r\ \psi_i^\dagger(\mathbf{r})\psi_j^\dagger(\mathbf{r})\psi_k(\mathbf{r})\psi_l(\mathbf{r})}_{\bar{v}^{\rho\rho}_{ijkl}}\ \rho_{ki}\ \rho_{lj}\end{aligned}$$

and similar for other terms.

Pseudo-potential-generated EDFs vs. "general" EDFs

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

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

Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC 76 (2007) 054315
Bender, T. Duguet, and D. Lacroix, PRC 79 (2009) 044319

substitute $z = e^{i\varphi}$ $\Rightarrow$ contour integrals in the complex plane

Projected energy functional

$$\mathcal{E}_N = \oint_{C_1} \frac{dz}{2i\pi c_N^2} \frac{\mathcal{E}[z]}{z^{N+1}} \prod_{\mu>0}(u_\mu^2 + v_\mu^2 z^2)$$

norm

$$c_N^2 = \oint_{C_1} \frac{dz}{2i\pi} \frac{1}{z^{N+1}} \prod_{\mu>0}(u_\mu^2 + v_\mu^2 z^2),$$

transition density matrix and pairing tensor

$$\rho_{\mu\nu}^{0z} = \frac{v_\mu^2 z^2}{u_\mu^2 + v_\mu^2 z^2}\delta_{\nu\mu} \quad \kappa_{\mu\nu}^{0z} = \frac{u_\mu v_\mu}{u_\mu^2 + v_\mu^2 z^2}\delta_{\nu\bar{\mu}}, \quad \kappa_{\mu\nu}^{z0\,*} = \frac{u_\mu v_\mu z^2}{u_\mu^2 + v_\mu^2 z^2}\delta_{\nu\bar{\mu}}$$

Complex plane analysis II

- Contour integrals can be evaluated using Cauchy's residue theorem [Bayman, NP15 (1960) 33]
- the norm and all operator matrix elements have a pole at $z = 0$

$$c_N^2 = 2i\pi\,\mathcal{R}es(0)\left[\frac{1}{z^{N+1}}\prod_{\mu>0}\left(u_\mu^2 + v_\mu^2\,z^2\right)\right]$$

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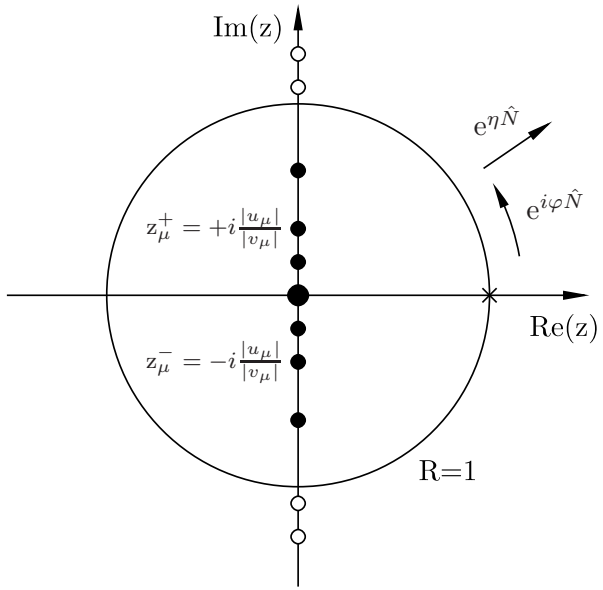
- A non-pseudo-potential-based EDF has poles at $z = 0$ and $z^\pm = \pm\frac{u_\mu}{v_\mu}$

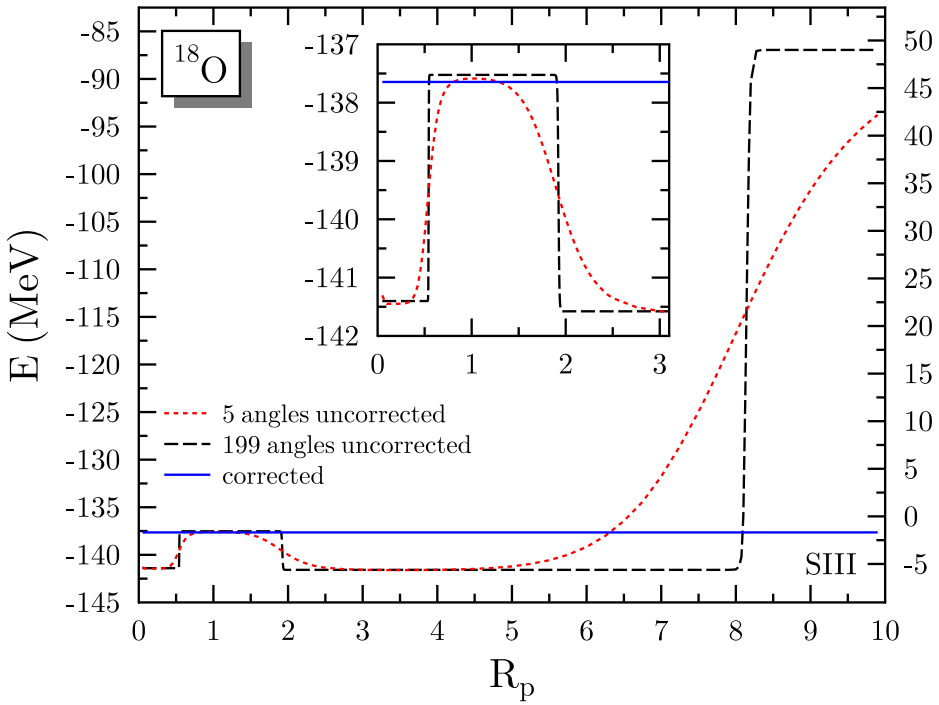
$$\mathcal{E}_N = \sum_{\substack{z_i=0\\ |z_\mu^\pm|<1}} \frac{2i\pi}{c_N^2}\,\mathcal{R}es(z_i)\left[\frac{\mathcal{E}[z]}{z^{N+1}}\prod_{\mu>0}\left(u_\mu^2 + v_\mu^2 z^2\right)\right]$$

- poles entering or leaving the integration contour might generate divergences, steps, or discontinuities



- poles of the particle number restored EDF
- filled (open) circles: poles inside (outside) the standard integration contour at $R = 1$
- cross: SR energy functional at $\varphi = 0$.

Complex plane analysis II



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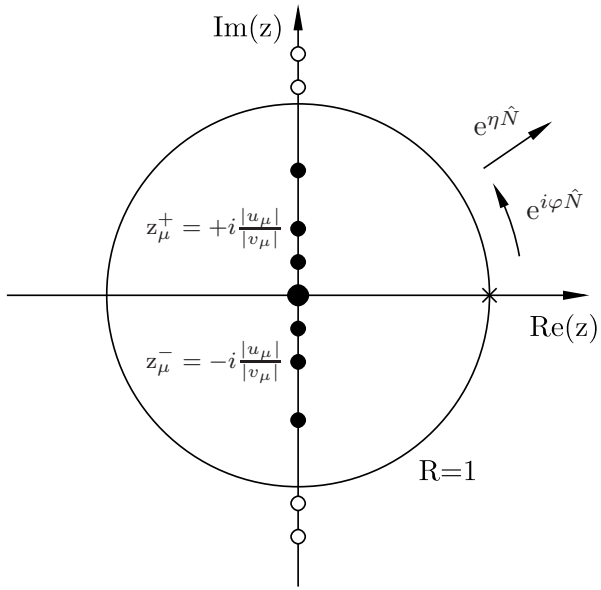

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Second problem: non-analytical density dependences

- Given a complex number z that in rectangular representation reads $z = x + \mathrm{i}y$ and in polar representation is given by $z = r\,e^{\mathrm{i}\varphi}$ with $r > 0$. A priori, φ is only determined up to integer multiples of 2π.
- The principal value of φ, which lies in the interval $-\pi < \varphi \leq \pi$, is

$$\varphi = \begin{cases} \arctan(\frac{y}{x}) & \text{if } x > 0 \\ \arctan(\frac{y}{x}) + \pi & \text{if } x < 0 \text{ and } y \geq 0 \\ \arctan(\frac{y}{x}) - \pi & \text{if } x < 0 \text{ and } y < 0 \\ \frac{\pi}{2} & \text{if } x = 0 \text{ and } y > 0 \\ -\frac{\pi}{2} & \text{if } x = 0 \text{ and } y < 0 \\ \text{indeterminate} & \text{if } x = 0 \text{ and } y = 0 \end{cases} \tag{1}$$

  where the principal value for $-\frac{\pi}{2} < \arctan(x) < \frac{\pi}{2}$ is assumed. In FORTRAN, the principal value for φ is conveniently provided by the atan2(y, x) function.
- The n-th roots of z are given by

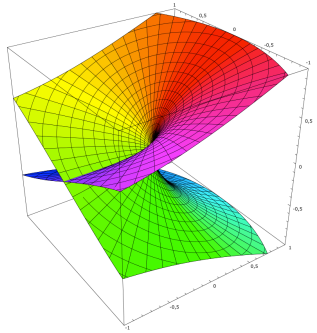
$$z^{1/n} = \sqrt[n]{z} = r^{1/n} \exp\left\{\mathrm{i}\frac{\varphi + 2k\pi}{n}\right\} \tag{2}$$

  with $0 \leq k \leq n-1$ and $r^{1/n}$ the nth positive root of r.
- The principal value of z^α, $0 < \alpha < 1$ can be obtained as

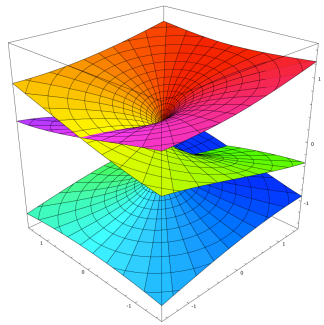
$$(x + \mathrm{i}y)^\alpha = R\,e^{\mathrm{i}\Phi} \quad \text{with} \quad \begin{cases} R = (x^2 + y^2)^{2\alpha} \\ \Phi = \text{atan2}(y, x) \times \alpha \end{cases} \tag{3}$$

  including values of α different from $1/n$.

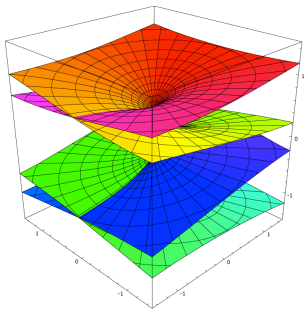
$z^{1/2}$



$z^{1/3}$

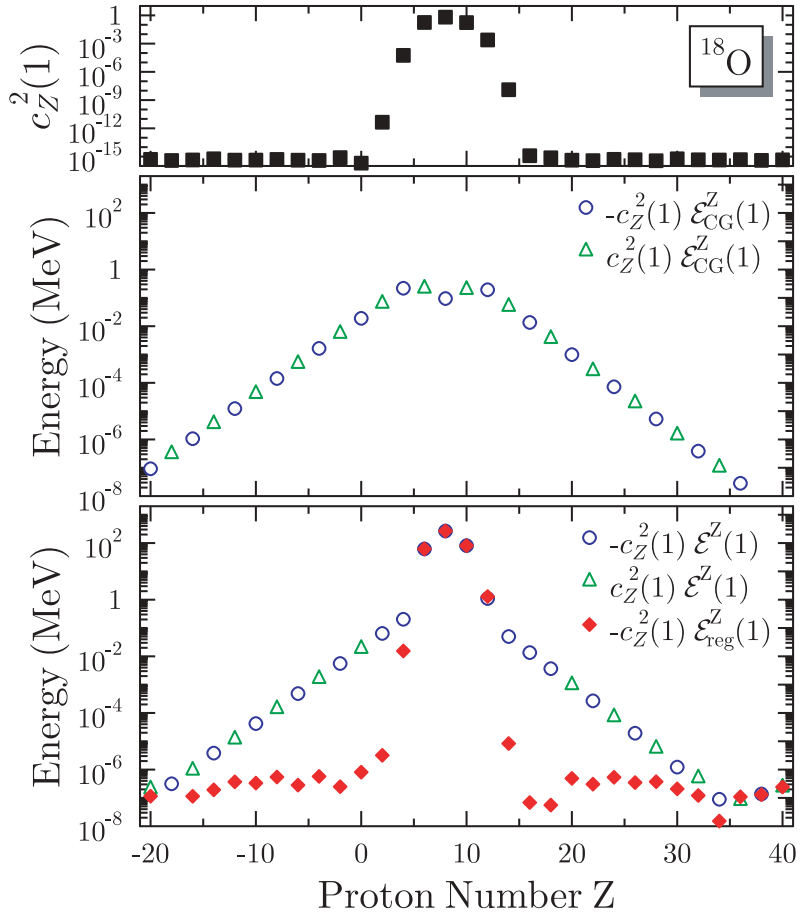


$z^{1/4}$



Sum rules

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



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For any scalar operator $\hat{O}$, one has

$$\langle\Theta|\hat{O}\hat{P}^{\lambda}_{jj}|\Theta\rangle = \sum_{\epsilon=1}^{n_\lambda}\sum_{\epsilon'=1}^{n_\lambda}\left(c^{\lambda j}_{\epsilon}\right)^{*} c^{\lambda j}_{\epsilon'}\langle\Psi^{\lambda j}_{\epsilon}|\hat{O}|\Psi^{\lambda j}_{\epsilon'}\rangle$$

Norm as special case

$$\langle\Theta|\hat{P}^{\lambda}_{jj}|\Theta\rangle = \sum_{\epsilon=1}^{n_\lambda}|c^{\lambda j}_{\epsilon}|^2$$

These relations imply that zero norm implies zero (non-normalized) operator matrix element.

$\Rightarrow$ a general EDF might not correspond to the sum over irreps of the physical group of the nuclear Hamiltonian.
$\Rightarrow$ "projection" does not make sense for such objects

Bally & Bender, to be submitted

Why using density dependences?

- 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 $\rho_{\rm sat}$ 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?

Density dependence vs. three-body force

Skyrme's simple gradientless contact three-body force

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

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

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

Density-dependent two-body "force" [Köhler, NPA258 (1976) 301]

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

which leads to the EDF

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

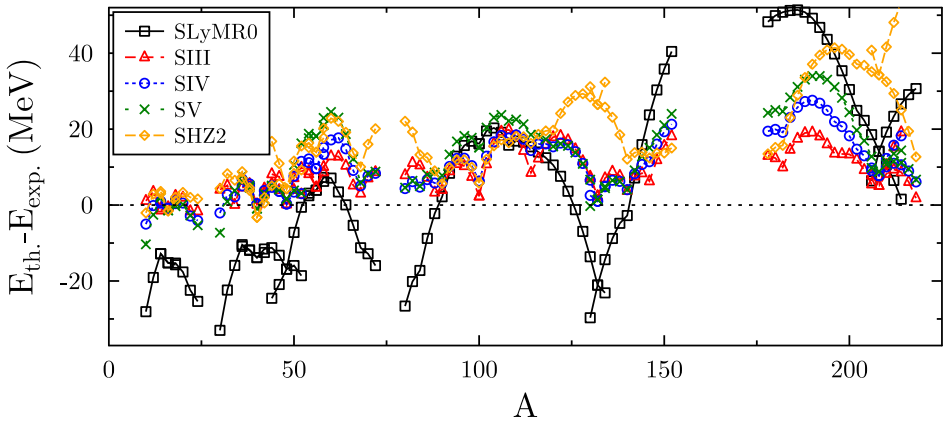
- different isospin structure in spin terms $\Rightarrow$ suppresses possible spin instbility
- $\alpha \approx 1/3 \Rightarrow$ empirical incompressibility
- Works very well on SR EDF level

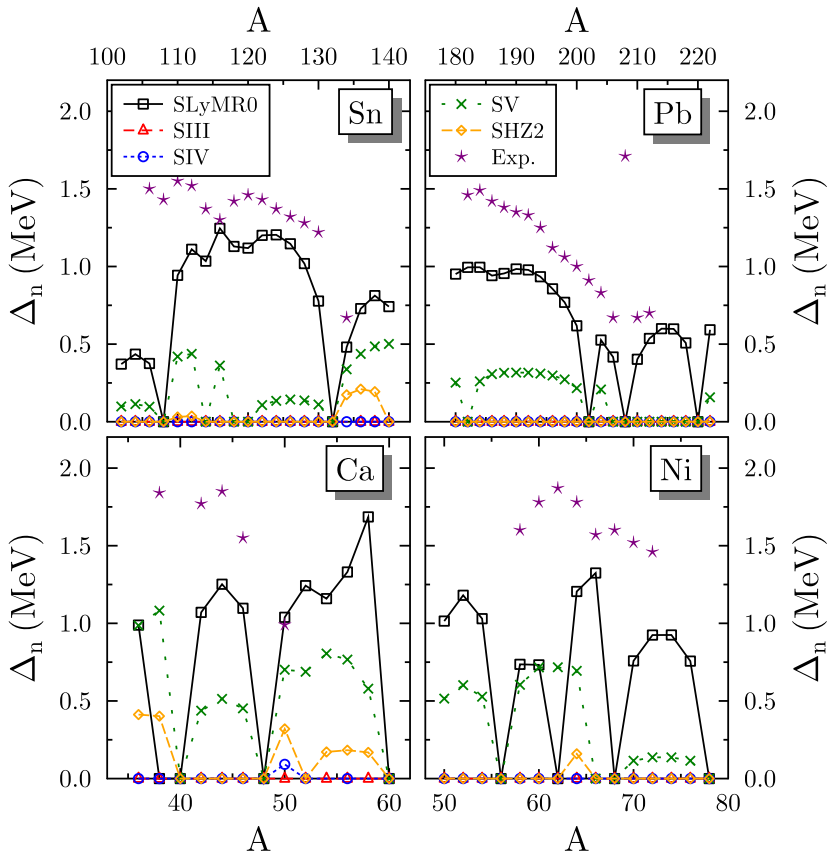
Minimal form: SLyMR0

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

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

Pseudo-potentials for MR EDF. First try: SLyMR0





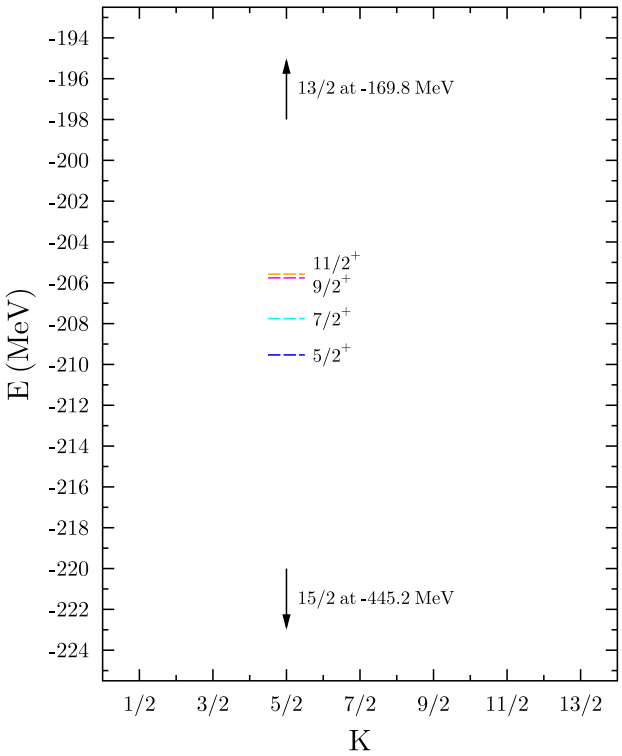
- it is impossible to fulfill the usual nuclear matter constraints , to have stable interactions and attractive pairing
- no "best fit" possible
- very bad performance compared to standard general functionals

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

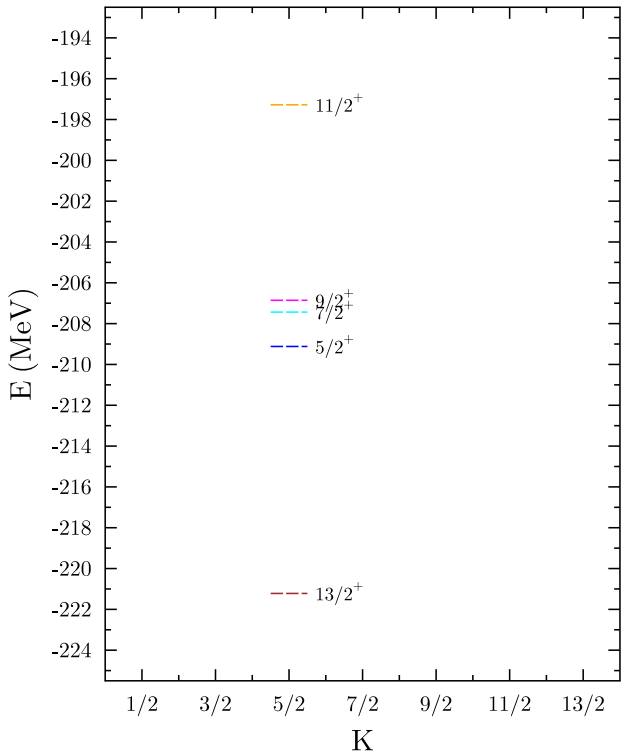
Odd nuclei: density dependence ⇔ Hamiltonian

Decomposition of the energy of the blocked HFB state of ^{25}Mg with $q_1 = 80\,\mathrm{fm}^2$, $q_2 = 0$ that is practiacally pure $K = 5/2$ for a given discretization of the integrals over Euler angles

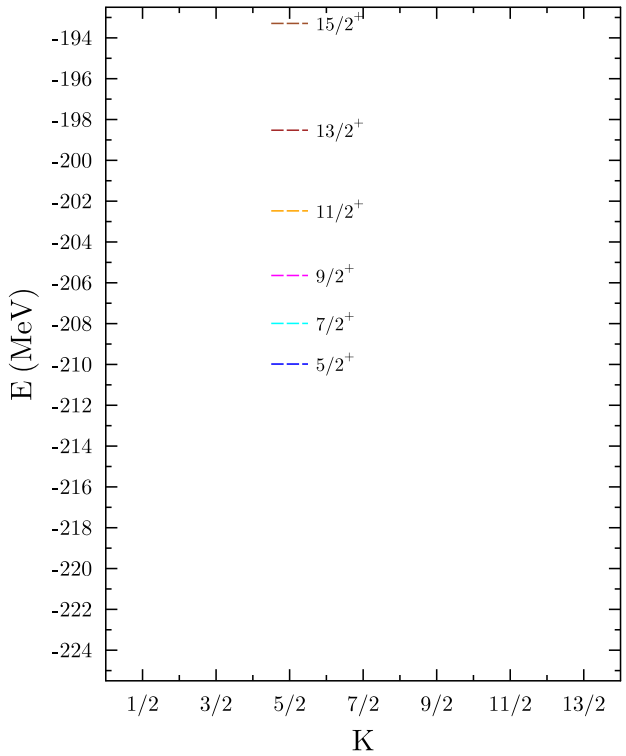
JyLy, mixed density



JyLy, PNP density



SLyMR0, mixed density

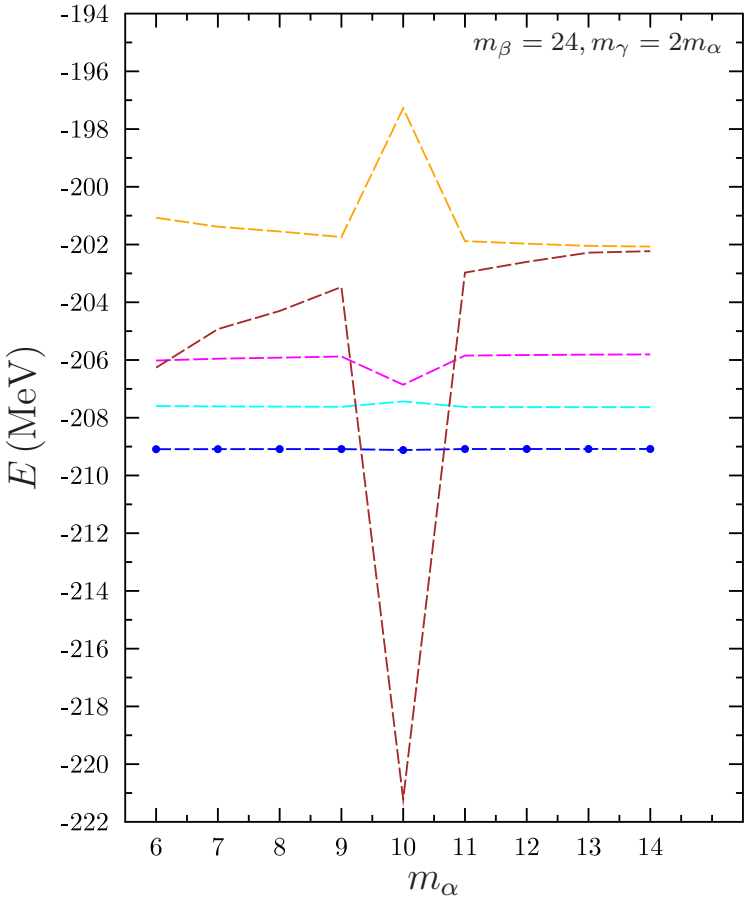


- Jyly: unpublished (density-dependent) Skyrme interaction whose only source of spurious energies is the density dependence
- exact Coulomb exchange and pairing (in the MR calculation)
- either the mixed density or the particle-number-projected (PNP) density is used in the density dependence.

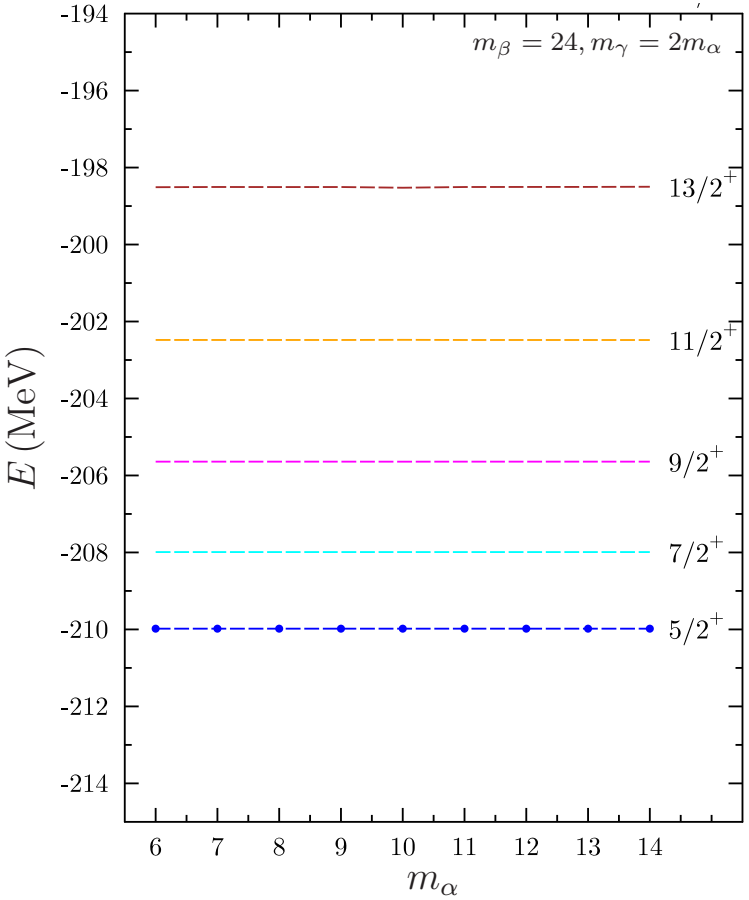
Discretisation dependence

Dependence on the number of discretisation points chosen for Euler angles when projecting the blocked HFB state of ^{25}Mg with $q_1 = 80\,\mathrm{fm}^2$, $q_2 = 0$ that is practiacally pure $K = 5/2$.

JyLy



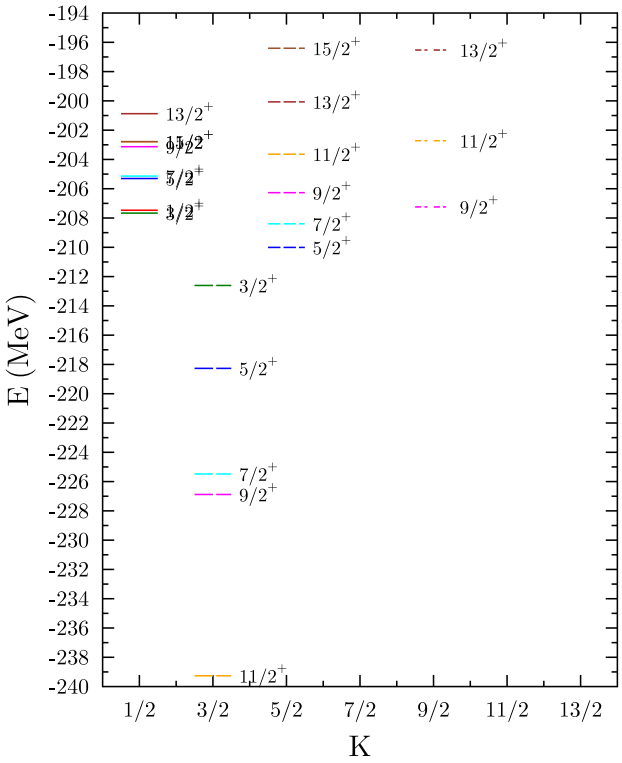
SLyMR0



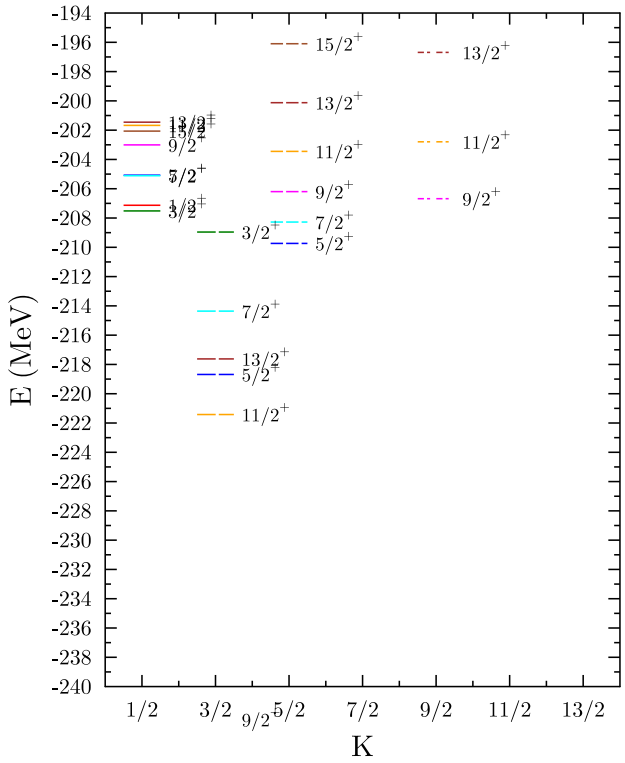
Odd nuclei: density dependence ⇔ Hamiltonian

Decomposition of the energy of the blocked HFB state with $q_1 = 80\,\mathrm{fm}^2$, $q_2 = 20\,\mathrm{fm}^2$ for na.nb.ng = 10.24.20 and using the parameterizations and recipes as indicated.

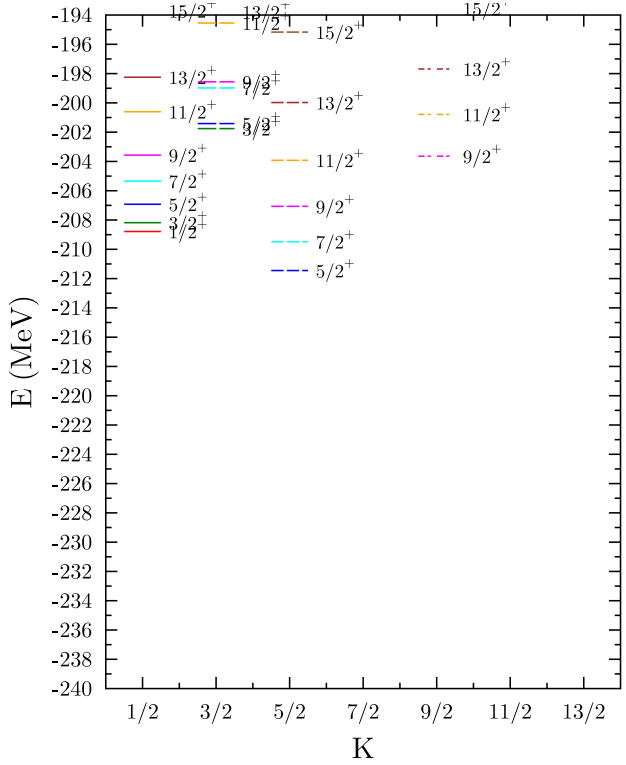
JyLy, mixed density



JyLy, PNP density

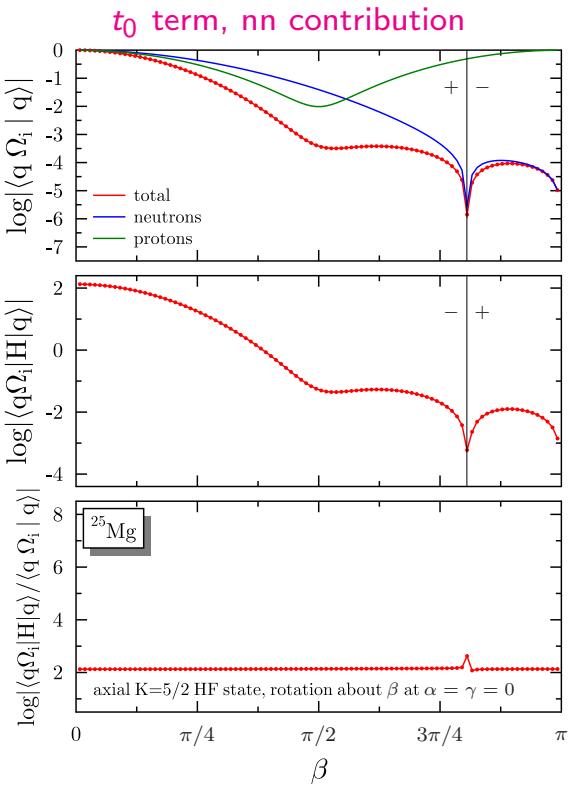


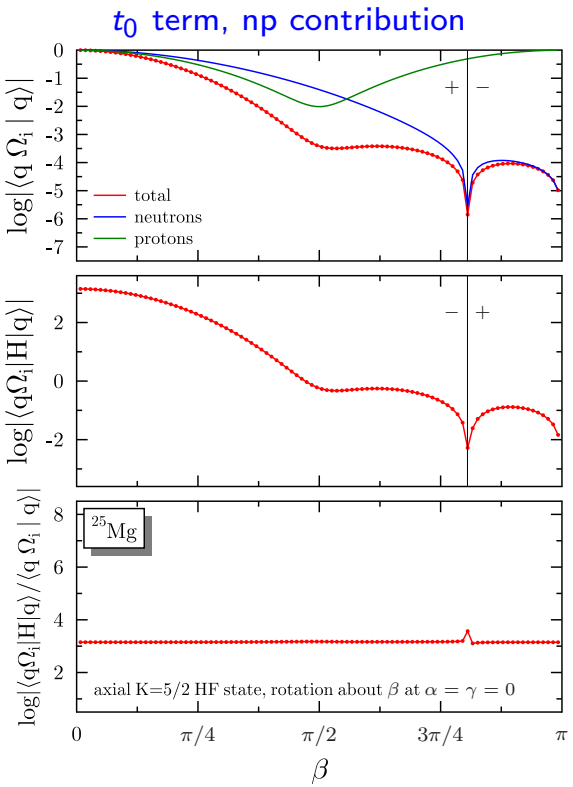
SLyMR0, mixed density

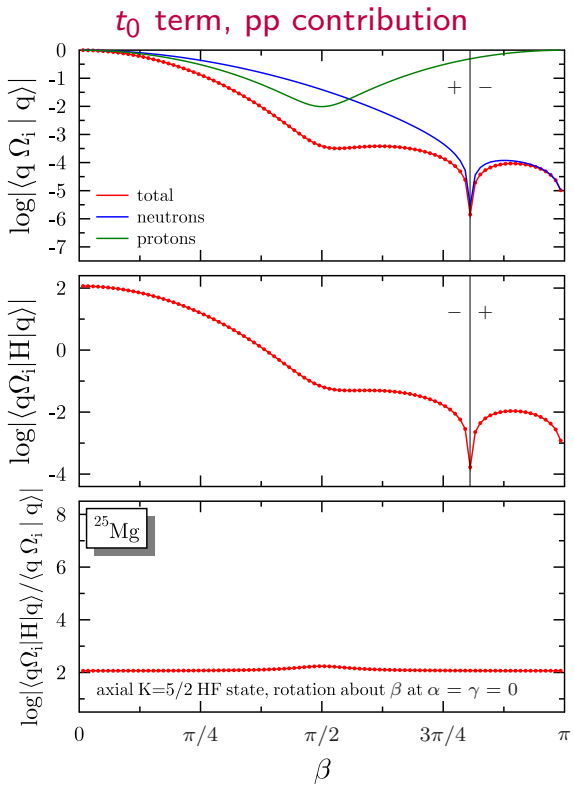


- JyLy: standard density-dependent Skyrme taking all exchange and pairing terms into account, courtesy of K. Bennaceur (unpublished, 2016).
- mixed density: standard recipe to handle density dependence
- PNP: using the particle-number projected density in the density dependence
- SLyMR0: true Skyrme Hamiltonian (see below)

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



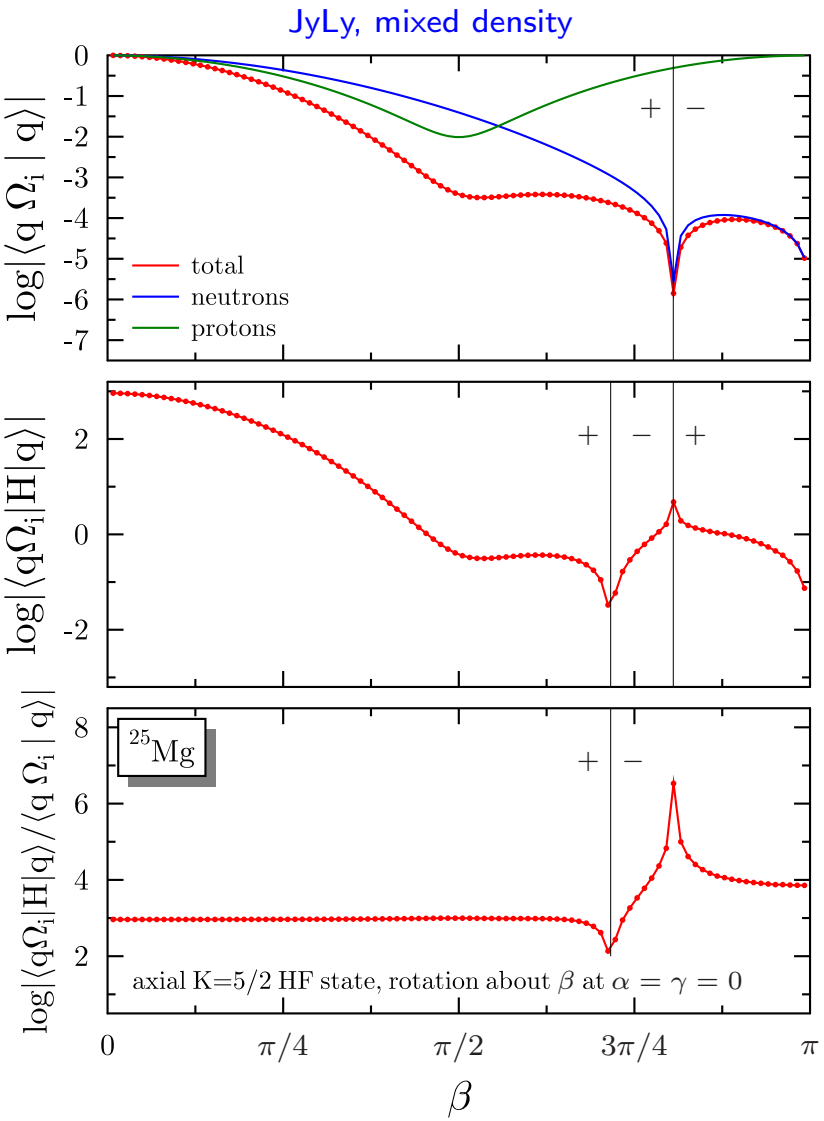




$$
\begin{aligned}
E^{LR}_{t_0} &= \langle \mathsf{L}|t_0\,(1+x_0\hat{P}_\sigma)\,\hat{\delta}^{\mathbf{r}}|\mathsf{R}\rangle \\
&= \tfrac{1}{4}t_0(1-x_0)\int d^3r\left[\rho^{LR}_n(\mathbf{r})\,\rho^{LR}_n(\mathbf{r}) - \mathbf{s}^{LR}_n(\mathbf{r})\cdot\mathbf{s}^{LR}(\mathbf{r}) + \tilde{\rho}^{RL*}_n(\mathbf{r})\,\tilde{\rho}^{LR}_n(\mathbf{r})\right]\langle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

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



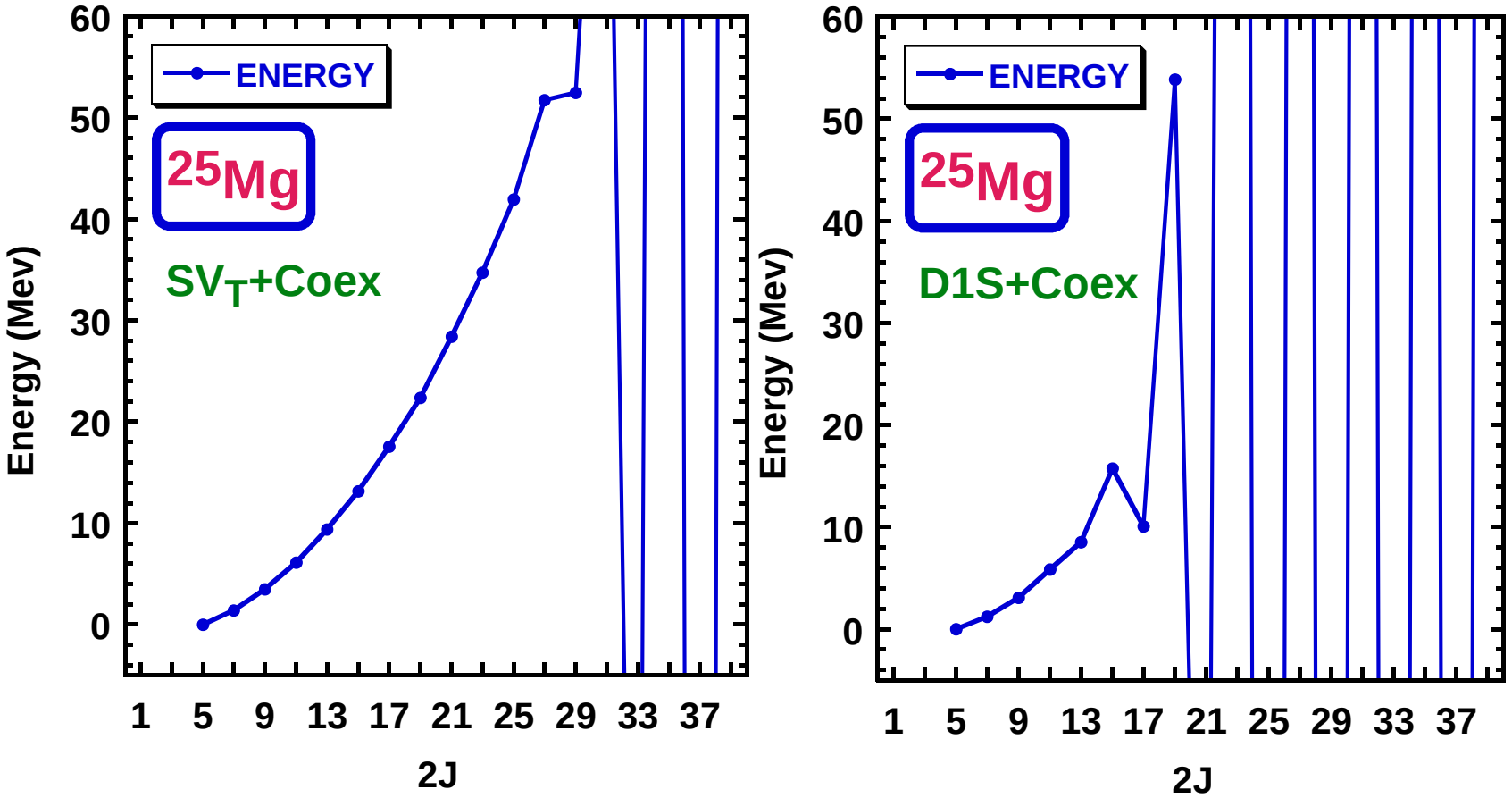
For a parameteriation with $x_3 = 1$ and in the limit of Slater determinants, the energy kernel of the density-dependent part of the Skyrme interaction reads

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

- kernel from density-dependent terms has an (Euler) angular dependence that is qualitatively different from the one of the norm kernel
- density-dependent terms will decompose into J, K components quite differently from the norm kernel

Same in HFODD

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



Are there tricks to use general EDFs in MR calculations?

- 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 mixings of interest [Robledo, J. Phys. G 37 (2010) 064020].
- 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]. Works for particle-number projection, but not for angular-momentum projection or GCM mixing.
- introduce a mathematics-motivated regularisation [Satuła & Dobaczewski, PRC 90 (2014) 054303]. Has problems too when applied in realistic calculations [Dobaczewski, private communication].
- 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].

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

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

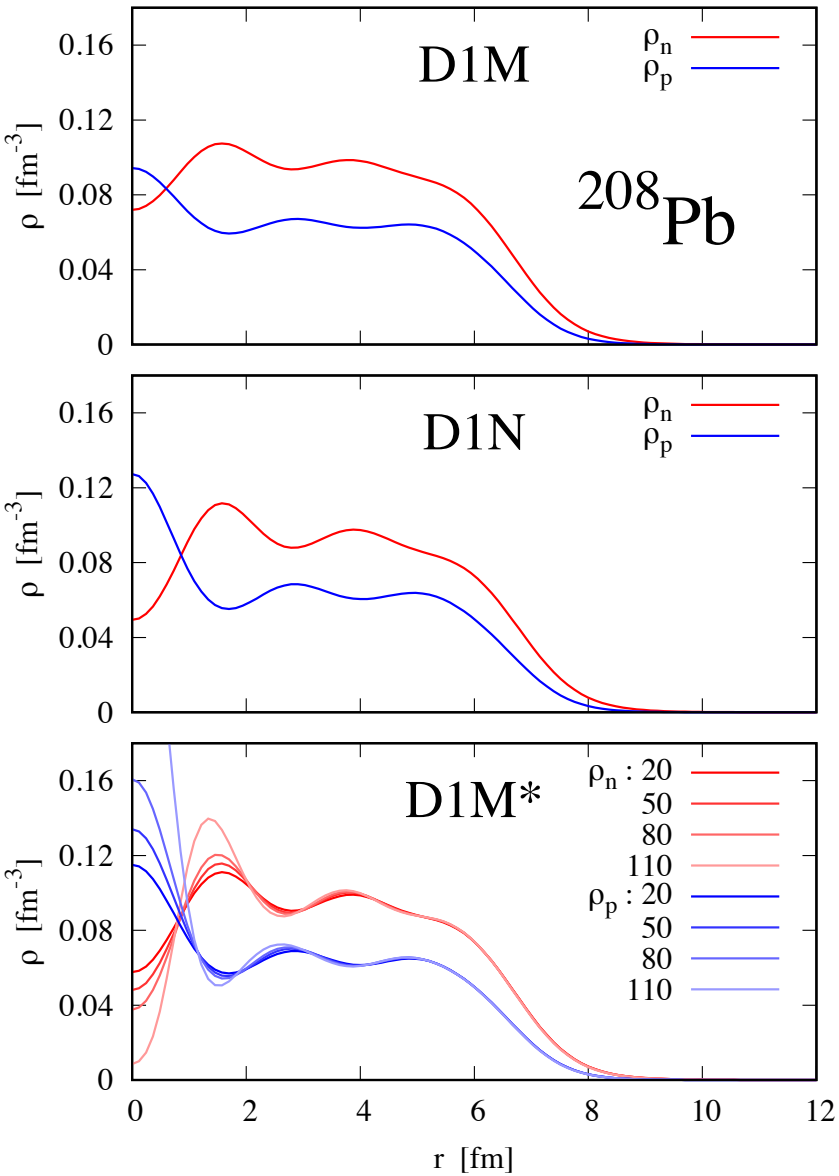
MR-EDF also suffers from possible spuriosities of the SR EDF

Many present parameterizations of the nuclear EDF exhibit spurious non-physical *finite-size* instabilities of the EDF, which correspond to the transition of homogeneous infinite nuclear matter to an inhomogeneous phase.

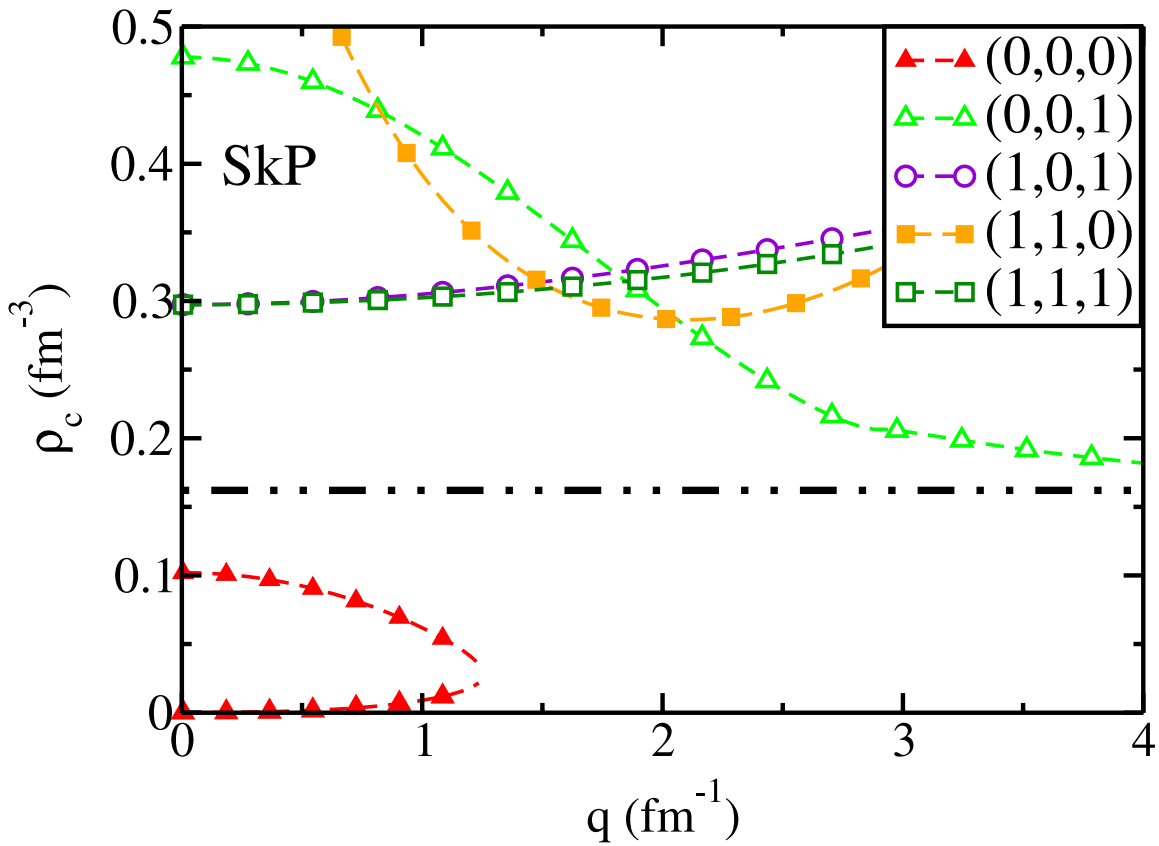
- Lesinski et al, PRC74 (2006) 044315
- Hellemans et al, PRC85 (2012) 014326
- Hellemans et al, PRC88 (2013) 064323
- Hellemans et al, AIP Conf. Proc. 1491 (2012) 242
- Pastore et al, PRC 92 (2015) 024305
- Pastore et al, Phys Rep 563 (2015) 1
- Martini et al, arXiv:1806.02080

- These need to be distinguished from the instabilities signalled by certain values of the Landau parameters and that correspond to the transition of a homogeneous phase of infinite nuclear matter to a different homogeneous phase.
- In the $S = 0$, $T = 0$ channel there is a *physical* instability that corresponds to the formation of finite nuclei in nuclear matter at sub-saturation density.

Martini, DePace, Bennaceur, arXiv:1806.02080



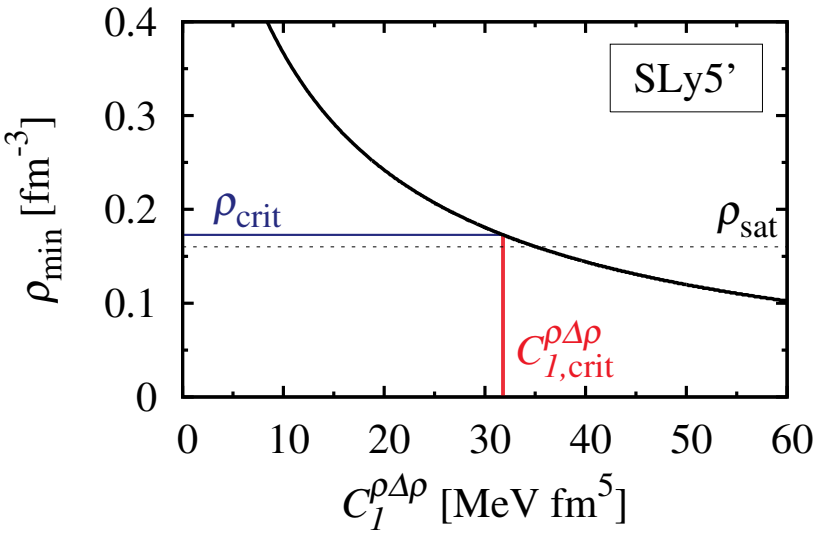
Pastore et al, Phys Rep 563 (2015) 1



Pole in the response function of symmetric homogeneous infinite nuclear matter in the (S, M, T) channel as indicated and calculated in linear response, as a function of density.

Finite-size spin instabilities

Hellemans et al, PRC88 (2013) 064323

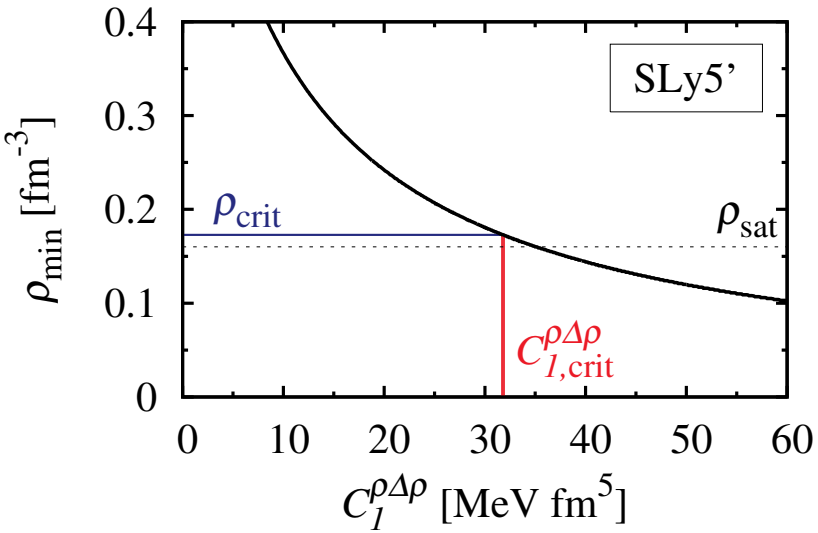


density of lowest pole in infinite nuclear matter in the $(0,0,1)$ channel as a function of the coupling constant of the

$$C_1^{\rho\Delta\rho} \int \mathrm{d}^3 r \rho_1(\mathbf{r}) \Delta\rho_1(\mathbf{r})$$

term

Finite-size spin instabilities

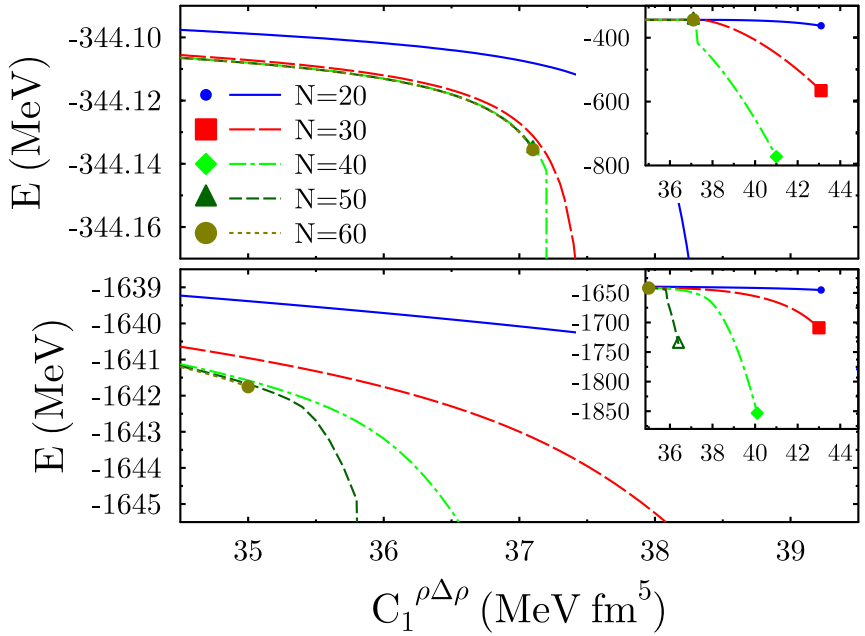


density of lowest pole in infinite nuclear matter in the $(0,0,1)$ channel as a function of the coupling constant of the

$$C_1^{\rho\Delta\rho}\int \mathrm{d}^3 r \rho_1(\mathbf{r})\,\Delta\rho_1(\mathbf{r})$$

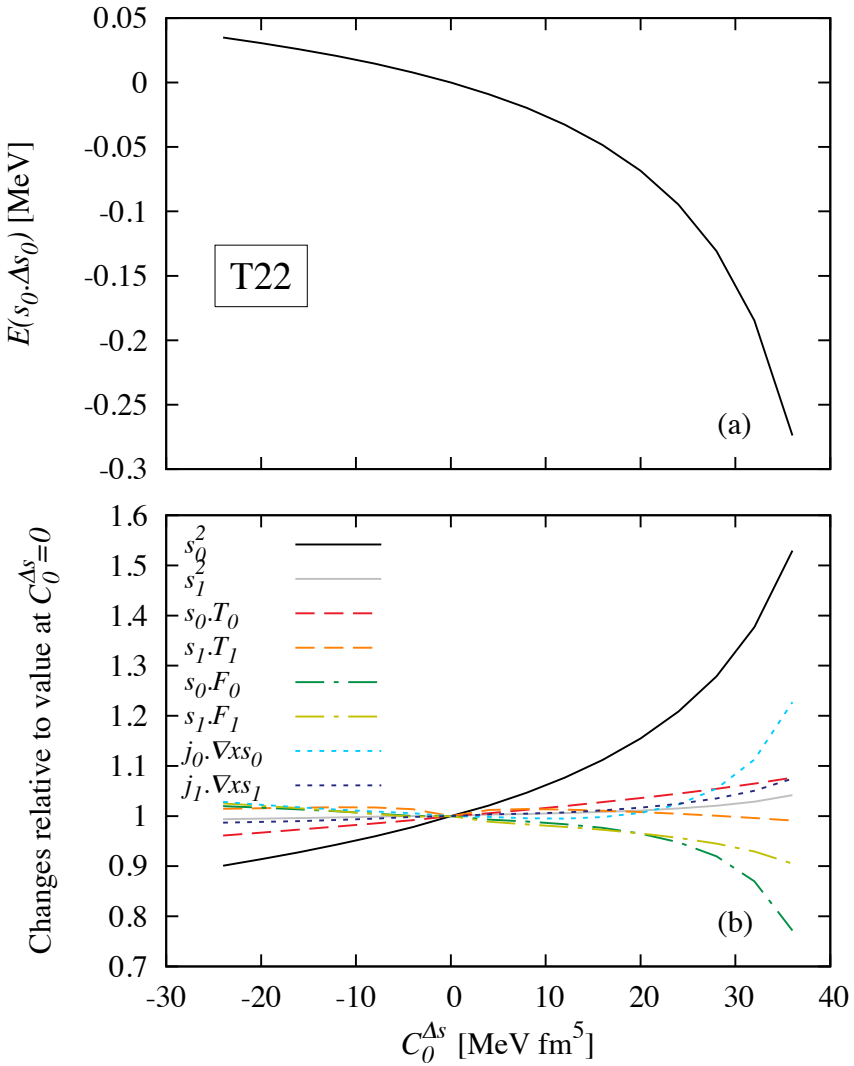
term

Hellemans et al, PRC88 (2013) 064323



Harmonic-oscillator codes usually have problems to resolve the instabilities, and find irregular convergence with increasing basis size instead.

Finite-size spin instabilities



(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.

In response calculations of infinite nuclear matter, there is a pole approaching saturation density when increasing $C_0^{\Delta s}$ analogous to what has been explained the other day by Karim Bennaceur.

V. Hellemans, P.-H. Heenen and M. Bender, PRC 85 (2012) 014326

Finite-size spin instabilities – linear response

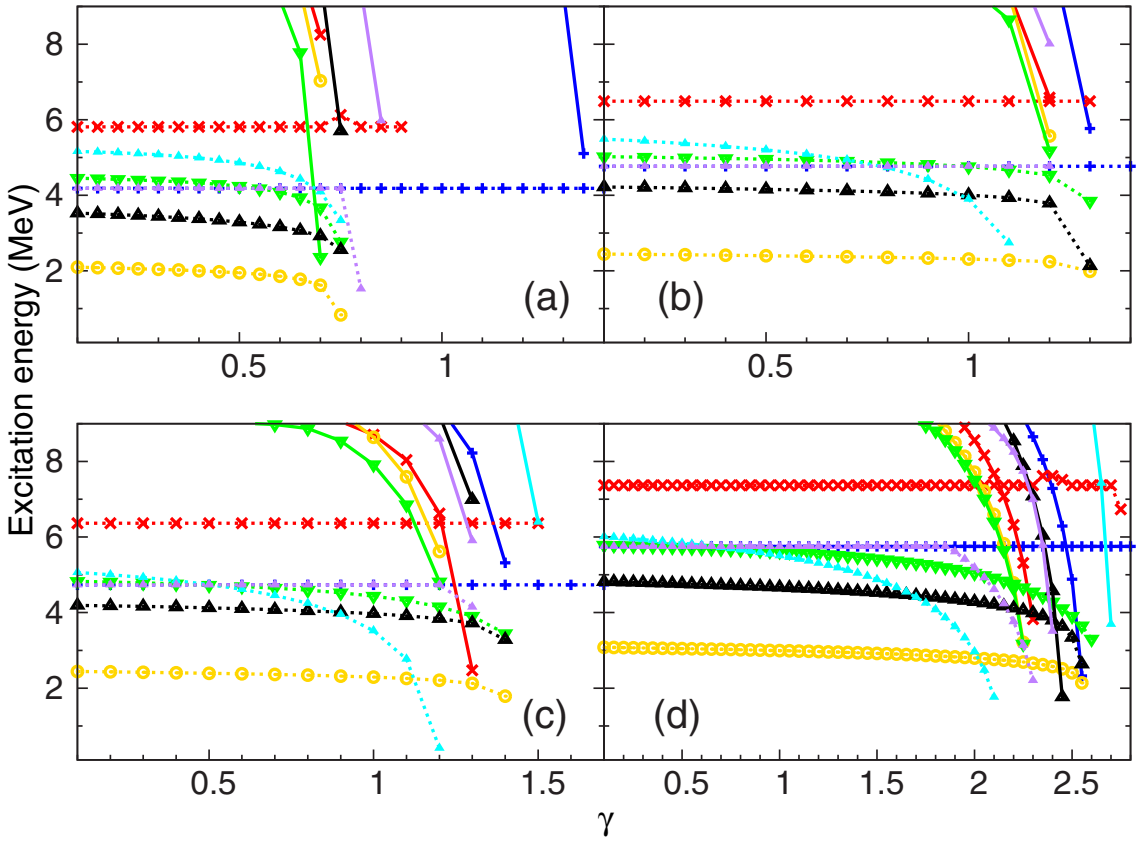


FIG. 3. (Color online) Evolution phonons in ^{56}Ni as a function of the multiplicative factor γ for T44 (a), SLy5 (b), BSk27 (c), and SIII (d). The caption is the same as that for Fig. 2.

- RPA calculation of lowest state of various 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, Navarro, PRC 92, 024305 (2015)

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/meaningless 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).

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formal aspects of the big picture

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color code: active (past) member of the collaboration

back-up slides

Reminder: Self-interaction

- related to broken antisymmetry of vertices in the functional
- The presence of self-interaction in the functionals used in DFT has been pointed out by J. P. Perdew and A. Zunger, Phys. Rev. B23, 5048 (1981).
- violation of the exchange symmetry in nuclear effective interactions has also been discussed from a different perspective and using different vocabulary by S. Stringari and D. M. Brink, *Constraints on effective interactions imposed by antisymmetry and charge independence*, Nucl. Phys. A304, 307 (1978).
- the interaction energy of a particle with itself should be zero
- One-particle limit of the interaction energy divided by the probability to occupy this state

$$\frac{\mathcal{E}_\mu - t_{\mu\mu}}{v_\mu^2} = \frac{1}{2}\,\bar{v}^{\rho\rho}_{\mu\mu\mu\mu}\,v_\mu^2\,.$$

  In a composite system, the particle-number of other particle species is left untouched.
- complete correction for self-interaction requires so-called orbital-dependent energy functional; approximate corrections have been proposed for DFT

- self-pairing comes from an incomplete combination of vertices
- Direct interaction energy: remove self-interaction and divide by the probability $P^{\Phi}_{\mu\bar{\mu}}$ to occupy the pair

$$\frac{\mathcal{E}_{\mu\bar{\mu}} - \mathcal{E}_{\mu} - \mathcal{E}_{\bar{\mu}}}{P^{\Phi}_{\mu\bar{\mu}}} = \tfrac{1}{2}\left(\bar{v}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}} + \bar{v}^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu}\right) v^2_{\mu} + \bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}}\, u^2_{\mu}\,.$$

Probability $P^{\Phi}_{\mu\bar{\mu}}$ to occupy the pair $P^{\Phi}_{\mu\bar{\mu}} = \dfrac{\langle\Phi_{\varphi}|a^{\dagger}_{\mu}a^{\dagger}_{\bar{\mu}}a_{\bar{\mu}}a_{\mu}|\Phi_{\varphi}\rangle}{\langle\Phi_{\varphi}|\Phi_{\varphi}\rangle} = v^2_{\mu}$

For a Hamiltonian $\bar{v}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}} = \bar{v}^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu} = \bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}} \equiv \bar{v}_{\mu\bar{\mu}\mu\bar{\mu}}$, the terms recombine

$$\frac{E_{\mu\bar{\mu}} - E_{\mu} - E_{\bar{\mu}}}{P^{\Phi}_{\mu\bar{\mu}}} = \bar{v}_{\mu\bar{\mu}\mu\bar{\mu}}\,,$$

into the HF interaction energy without pairing.

- The energy from scattering a pair of particles onto themselves should be equal to the no-pairing value
- To the best of our knowledge, self-pairing was never considered in the published literature so far.