Time-odd terms in nuclear energy density functionals

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Prospects on the microscopic description of odd mass nuclei
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with beyond-mean-field and related methods

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Formal aspects
For the sake of compact and comprehensible notation, the following abuse of vocabulary will be systematically made throughout the following presentation:

- HF state $\equiv$ Slater determinant $\iff$ product state of single-particle states $\prod_k \hat{a}_k^\dagger |\!-\rangle$
- HFB state $\equiv$ Bogoliubov quasiparticle state $\iff$ product state of Bogoliubov-type one-quasiparticle state $\prod_k \hat{\beta}_k |\!-\rangle$
  (indifferently on if it was obtained solving HF+BCS or HFB equations)
- HF(B) $\equiv$ product state of either “HF” or “HFB” type

I apologize to those whose feelings might be hurt.
The Skyrme energy density functional at NLO

\[ E = E_{\text{kin}} + E_{\text{Skyrme}} + E_{\text{Coul}} + E_{\text{pair}} + E_{\text{corr}} \]

\[ E_{\text{Skyrme}} = \int d^3 r \sum_{t=0,1} \sum_{t_3=-t}^{+t} \left\{ C_{t}^{\rho \rho} \rho_{tt_3} \rho_t - t_3 + C_{t}^{\rho \tau} (\rho_{tt_3} \tau_t - t_3 - j_{tt_3} \cdot j_t - t_3) \right. \]

\[ \left. + C_{t}^{\rho \Delta \rho} \rho_{tt_3} \Delta \rho_t - t_3 + C_{t}^{ss} s_{tt_3} \cdot s_t - t_3 + C_{t}^{s \Delta s} s_{tt_3} \cdot \Delta s_t - t_3 \right. \]

\[ \left. + C_{t}^{sT} (s_{tt_3} \cdot T_t - t_3 - \sum_{\mu, \nu=x,y,z} J_{\mu \nu;tt_3} J_{\mu \nu;t - t_3}) \right. \]

\[ \left. + C_{t}^{\rho \nabla J} (\rho_{tt_3} \nabla \cdot J_t - t_3 + s_{tt_3} \cdot \nabla \times j_t - t_3) \right. \]

\[ \left. + C_{t}^{sF} (s_{tt_3} \cdot F_t - t_3 - \frac{1}{2} \sum_{\mu, \nu=x,y,z} J_{\mu \nu;tt_3} J_{\nu \mu;t - t_3} - \frac{1}{2} \sum_{\mu, \nu=x,y,z} J_{\mu \mu;tt_3} J_{\nu \nu;t - t_3}) \right. \]

\[ \left. + C_{t}^{\nabla s \nabla s} (\nabla \cdot s_{tt_3}) (\nabla \cdot s_{t-t_3}) \right\} \]

Some combinations required by Galilean invariance.
Some of these densities are even under time-reversal $\hat{T}$

\[
\begin{align*}
\hat{T} \rho(r) \hat{T}^\dagger &= \rho(r) & \text{density} \\
\hat{T} \tau(r) \hat{T}^\dagger &= \tau(r) & \text{kinetic density} \\
\hat{T} J_{\mu\nu}(r) \hat{T}^\dagger &= J_{\mu\nu}(r) & \text{spin current tensor density}
\end{align*}
\]

while others are time-odd

\[
\begin{align*}
\hat{T} s(r) \hat{T}^\dagger &= -s(r) & \text{spin density} \\
\hat{T} T(r) \hat{T}^\dagger &= -T(r) & \text{spin kinetic density} \\
\hat{T} F(r) \hat{T}^\dagger &= -F(r) & \text{some other spin kinetic density} \\
\hat{T} j(r) \hat{T}^\dagger &= -j(r) & \text{current density}
\end{align*}
\]

The expectation values of the components of angular momentum can be calculated from the local spin density and the current

\[
\langle \hat{J} \rangle = \int d^3 r \left[ r \times j(r) + \frac{1}{2} s(r) \right]
\]

- finite angular momentum of a system implies that time-odd densities are non-zero
- In such systems there will be contributions from time-odd terms to the energy
General remarks on time-odd terms

- Galilean invariance (of a non-relativistic system): the internal energy of the system is independent on the inertial frame it is described in.
  - In a boosted frame moving with some total momentum $P = \langle \hat{P} \rangle$ relative to the frame of the observer the current $j(r)$ (and other time-odd densities) are non-zero.
  - As the internal energy has to be invariant under such boost, part of the energy of the time-even terms is shifted to the time-odd terms.
  - (At least part of) the time-odd terms have to be internally consistent with the time-even ones.
  - In relativistic models, Lorentz invariance plays the same role.

- Time-reversal invariance: scalar many-body observables of stationary states cannot distinguish the direction of time. Observables measuring the movement of particles in the system change their sign.
FIG. 1. The c.m. energy of a single free nucleus moving through the grid for three different test cases as indicated. The nearly constant lines correspond to the full Skyrme treatment, while the other results were calculated omitting the odd-odd l*’s coupling.

FIG. 3. Artist’s view of the spin excitation generated in a central collision of two $^{16}$O nuclei. Closely based on the numerical spin-density vectors produced in the calculations.

Omitting the odd-odd coupling thus leads to a spurious excitation of a ring-like spin density, which with the full Skyrme force is suppressed by the odd-odd terms.

The spurious dissipation is caused by the intrinsic excitation of a spin-twist mode. For a nucleus moving with constant velocity $\vec{v}$, the coupling term contains

$$\nabla \times \vec{j} = (\nabla \rho) \times \vec{v} = \frac{d\rho}{dr} \frac{\vec{r} \times \vec{v}}{r},$$

where spherical symmetry was assumed for simplicity. This is an azimuthal vector field which thus couples to a spin field of the same character. Omitting the odd-odd coupling thus leads to unacceptable physical behavior.

At this point we can already conclude that the omission of these terms leads to unacceptable physical behavior.
What is impacted by time-odd terms?

Self-consistent mean-field calculations

- Spin-polarized nuclear matter
- HF(B) states where some single-(quasi-)particle states cannot be paired up
  - odd-A nuclei
  - odd-odd nuclei
  - non-collective states in even-even nuclei (K isomers etc)

Note: there are tricks to describe such states as a statistical mixing that cancels the time-odd terms (equal filling). Such statistically mixed ensembles cannot be used as starting point for the (Q)PRA, TDHF, projection on good quantum numbers, GCM without disentangling the statistical mixing.

- rotational states calculated by the cranked HF(B) method

\[ \delta (\mathcal{E} - \omega \cdot \langle \mathbf{J} \rangle) \]

- time-dependent HF(B). Time dependence of the HF(B) state implies \( \partial_t \rho(r) \neq 0 \). For local interactions, one has the continuity equation

\[ \partial_t \rho(r, t) = -\frac{\hbar}{m} \nabla \cdot \mathbf{j}(r, t) \]

and a similar one for the time-evolution of the spin density [Raimondi et al, PRC85 (2012) 014326 and references therein] (for non-local interactions there are additional terms).
Response properties

- Landau parameters $g_\ell$, $g'_\ell$
- (Q)RPA [the linear response limit of TDHF(B)]. In particular, excitations like M1 and GT only depend on time-odd terms [see my talk at the ECT* on 23/05/2017 for some results on GT response]

- adiabatic TDHF(B) for large-scale collective motion
- Projection on good angular momentum
- Most configuration mixings in a GCM
- Diagrammatic expansion of correlations

The list of self-consistent mean-field calculations not affected by time-odd terms is in fact shorter

- Spherical HF and HFB calculations
- Deformed HF and HFB calculations of "ground states" of even-even nuclei
What is impacted by time-odd terms?

- The ground-states of all known even-even nuclei are $0^+$ states
- Nucleons favour pairwise coupling to states with seniority 0
- This minimises the time-odd terms (in the intrinsic frame) (in many models even puts them to zero)
- The net effect of time-odd terms of the effective in-medium NN (and NNN etc) interaction is repulsive

This is not a universal property of any interaction. The electromagnetic interaction has different preferences:

- Hund’s first rule: the lowest energy atomic state is the one that maximises the total spin quantum number for the electrons in the open sub-shell.
Case 1: Skyrme

The standard Skyrme energy density functional at NLO

\[ E = E_{\text{kin}} + E_{\text{Skyrme}} + E_{\text{Coul}} + E_{\text{pair}} + E_{\text{corr}} \]

\[ E_{\text{Skyrme}} = \int d^3r \sum_{t=0,1} \sum_{t_3=-t}^t \left\{ C_{t}^{\rho \rho} \rho_{tt3} \rho_{t-t_3} + C_{t}^{\rho \tau} (\rho_{tt3} \tau_{t-t_3} - j_{tt3} \cdot j_{t-t_3}) \right. \]

\[ + C_{t}^{\rho \Delta \rho} \rho_{tt3} \Delta \rho_{t-t_3} + C_{t}^{ss} s_{tt3} \cdot s_{t-t_3} + C_{t}^{s \Delta s} s_{tt3} \cdot \Delta s_{t-t_3} \]

\[ + C_{t}^{s T} (s_{tt3} \cdot T_{t-t_3} - \sum_{\mu, \nu=x,y,z} J_{\mu \nu;tt3} J_{\mu \nu;t-t_3}) \]

\[ + C_{t}^{\rho \nabla J} (\rho_{tt3} \nabla \cdot J_{t-t_3} + s_{tt3} \cdot \nabla \times j_{t-t_3}) \]

\[ + C_{t}^{s F} (s_{tt3} \cdot F_{t-t_3} - \frac{1}{2} \sum_{\mu, \nu=x,y,z} J_{\mu \nu;tt3} J_{\nu \mu;t-t_3} - \frac{1}{2} \sum_{\mu, \nu=x,y,z} J_{\mu \mu;tt3} J_{\nu \nu;t-t_3}) \]

\[ + C_{t}^{\nabla s \nabla s} (\nabla \cdot s_{tt3})(\nabla \cdot s_{t-t_3}) \right\} \]

Some combinations are required by Galilean invariance as indicated by terms in parentheses having a common coupling constant. The other terms are Galilean-invariant on their own.
Energy functional from a "density-dependent Skyrme force"

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

- **central**
  \[
  \hat{v}^{\text{central}} = t_0 (1 + x_0 \hat{P}_\sigma) \delta + \frac{1}{6} t_3 (1 + x_3 \hat{P}_\sigma) \rho^\alpha \delta \\
  + \frac{1}{2} t_1 (1 + x_1 \hat{P}_\sigma) (\hat{k}'^2 \delta + \delta \hat{k}^2) \\
  + t_2 (1 + x_2 \hat{P}_\sigma) \hat{k}' \cdot \delta \hat{k} \\
  + \frac{1}{6} t_3 (1 + x_3 \hat{P}_\sigma) \rho_0^\alpha \delta
  \]

- **spin-orbit**
  \[
  \hat{v}^{\text{LS}} = i W_0 (\hat{\sigma}_1 + \hat{\sigma}_2) \cdot \hat{k}' \times \delta \hat{k}
  \]

- **tensor**
  \[
  \hat{v}^{\text{tensor}} = \frac{1}{2} t_e \left\{ 3(\hat{\sigma}_1 \cdot \hat{k}') (\hat{\sigma}_2 \cdot \hat{k}') - (\hat{\sigma}_1 \cdot \hat{\sigma}_2) (\hat{k}')^2 \right\} \delta \\
  + \delta \left\{ 3(\hat{\sigma}_1 \cdot \hat{k}) (\hat{\sigma}_2 \cdot \hat{k}) - (\hat{\sigma}_1 \cdot \hat{\sigma}_2) (\hat{k})^2 \right\} \\
  + \frac{1}{2} t_o \left\{ 3(\hat{\sigma}_1 \cdot \hat{k}') \delta (\hat{\sigma}_2 \cdot \hat{k}) + 3(\hat{\sigma}_2 \cdot \hat{k}') \delta (\hat{\sigma}_1 \cdot \hat{k}) - 2(\hat{\sigma}_1 \cdot \hat{\sigma}_2) \hat{k}' \cdot \hat{k} \right\}
  \]
When the Skyrme EDF is calculated as $\mathcal{E}_{\text{Skyrme}} \equiv \langle \text{HF} | v_{\text{Skyrme}} | \text{HF} \rangle$, its coupling constants read

$$
\begin{align*}
C_0^{\rho\rho} &= \frac{3}{8} t_0 + \frac{3}{48} t_3 \rho_0^\alpha \\
C_1^{\rho\rho} &= -\frac{1}{4} t_0 \left( \frac{1}{2} + x_0 \right) - \frac{1}{24} t_3 \left( \frac{1}{2} + x_3 \right) \rho_0^\alpha \\
C_0^{\rho\tau} &= \frac{3}{16} t_1 + \frac{1}{4} t_2 \left( \frac{5}{4} + x_2 \right) \\
C_1^{\rho\tau} &= -\frac{1}{8} t_1 \left( \frac{1}{2} + x_1 \right) + \frac{1}{8} t_2 \left( \frac{1}{2} + x_2 \right) \\
C_0^{\rho\Delta\rho} &= -\frac{9}{64} t_1 + \frac{1}{16} t_2 \left( \frac{5}{4} + x_2 \right) \\
C_1^{\rho\Delta\rho} &= \frac{3}{32} t_1 \left( \frac{1}{2} + x_1 \right) + \frac{1}{32} t_2 \left( \frac{1}{2} + x_2 \right) \\
C_0^{\rho\nabla J} &= -\frac{3}{4} W_0 \\
C_1^{\rho\nabla J} &= -\frac{1}{4} W_0 \\
C_0^{ss} &= -\frac{1}{4} t_0 \left( \frac{1}{2} - x_0 \right) - \frac{1}{24} t_3 \left( \frac{1}{2} - x_3 \right) \rho_0^\alpha \\
C_1^{ss} &= -\frac{1}{8} t_0 - \frac{1}{48} t_3 \rho_0^\alpha
\end{align*}
$$

$$
\begin{align*}
C_0^{sT} &= -\frac{1}{8} t_1 \left( \frac{1}{2} - x_1 \right) + \frac{1}{8} t_2 \left( \frac{1}{2} + x_2 \right) \\
&\quad -\frac{1}{8} (t_e + 3t_o) \\
C_1^{sT} &= -\frac{1}{16} t_1 + \frac{1}{16} t_2 + \frac{1}{8} (t_e - t_o) \\
C_0^{s\Delta s} &= \frac{3}{32} t_1 \left( \frac{1}{2} - x_1 \right) + \frac{1}{32} t_2 \left( \frac{1}{2} + x_2 \right) \\
&\quad + \frac{3}{32} (t_e - t_o) \\
C_1^{s\Delta s} &= \frac{3}{64} t_1 + \frac{1}{64} t_2 - \frac{1}{32} (3t_e + t_o) \\
C_0^{sF} &= \frac{3}{8} (t_e + 3t_o) \\
C_1^{sF} &= -\frac{3}{8} (t_e - t_o) \\
C_0^{\nabla s \nabla s} &= \frac{9}{32} (t_e - t_o) \\
C_1^{\nabla s \nabla s} &= -\frac{3}{32} (3t_e + t_o)
\end{align*}
$$

Otherwise, the $C_t$ can, in principle, be chosen as independent parameters.
Landau-Migdal interaction (from second derivative of the EDF)

\[
f_0 = N_0 \left[ 2 C_0^{\rho \rho} [\rho_0] + 4 \frac{\partial C_0^{\rho \rho} [\rho_0]}{\partial \rho_0} \rho_0 + \frac{\partial^2 C_0^{\rho \rho} [\rho_0]}{\partial \rho_0^2} \rho_0^2 + 2 C_0^{\rho \tau} k_F^2 \right],
\]

\[
f_1 = -2 N_0 C_0^{\rho \tau} k_F^2,
\]

\[
f_0' = N_0 \left[ 2 C_1^{\rho \rho} [\rho_0] + 2 C_1^{\rho \tau} k_F^2 \right],
\]

\[
f_1' = -2 N_0 C_1^{\rho \tau} k_F^2,
\]

\[
g_0 = 2 N_0 \left[ C_0^{ss} + (C_0^{sT} + \frac{1}{3} C_0^{sF}) k_F^2 \right],
\]

\[
g_0' = 2 N_0 \left[ C_1^{ss} + (C_1^{sT} + \frac{1}{3} C_1^{sF}) k_F^2 \right],
\]

\[
g_1 = -2 N_0 \left( C_0^{sT} + \frac{1}{3} C_0^{sF} \right) k_F^2,
\]

\[
g_1' = -2 N_0 \left( C_1^{sT} + \frac{1}{3} C_1^{sF} \right) k_F^2,
\]

\[
h_0 = \frac{1}{3} N_0 C_0^{sF} k_F^2,
\]

\[
h_0' = \frac{1}{3} N_0 C_1^{sF} k_F^2.
\]

- Normalisation \( N_0 \equiv 2 k_F m_0^* / \hbar^2 \pi^2 \) at the Fermi momentum \( k_F = (\frac{3}{2} \pi^2 \rho_0)^{1/3} \), in which \( m_0^* \) is the isoscalar effective mass associated with a given parameterisation.

- For a force-generated functional, the contribution of the tensor forces to \( g_0, g_1, g_0', \) and \( g_1' \) cancels. For a general functional, it does not.
Case 1: Skyrme 3-body force vs. density-dependence

- 3-body contact force

\[ \nu^{3b} = u_0 \left( \delta_{r_1 r_3} \delta_{r_2 r_3} + \delta_{r_3 r_2} \delta_{r_1 r_2} + \delta_{r_2 r_1} \delta_{r_3 r_1} \right) . \]

\[ \mathcal{E}^{3b} = \frac{3}{4} u_0 \int d^3r \left[ \rho_n (\rho_p^2 - s_p^2) + \rho_p (\rho_n^2 - s_n^2) \right] \]


- This as one of the major motivations to replace the contact gradientless 3-body force by a density-dependent 2-body force that for \( \alpha = 1, x_3 = +1 \) gives the same time-even terms but time-odd spin-spin terms of different isospin structure that turned out to be stable

\[ \nu^{2b, dd} = \frac{1}{3} t_3 \left( 1 + x_3 \hat{P}_\sigma \right) \left[ \rho_n(R) + \rho_p(R) \right]^\alpha \delta_{r_1 r_2} \]

\[ \mathcal{E}_{t_3} = \int d^3r \left\{ \frac{1}{12} t_3 (1 - x_3) \left[ (\rho_n^2 - s_n^2) + (\rho_p^2 - s_p^2) \right] (\rho_n + \rho_p)^\alpha \right. \]

\[ + \left. \frac{1}{6} t_3 \left( 1 + \frac{x_3}{2} \right) \rho_n \rho_p (\rho_n + \rho_p)^\alpha + \frac{1}{12} t_3 s_n \cdot s_p (\rho_n + \rho_p)^\alpha \right\} . \]

[The other motivations were the too large incompressibility of interactions with trilinear terms that can be made realistic by choosing \( \alpha \approx 1/3 \). \( x_3 \neq +1 \) enriches structure of the functional.]
Case 1: Skyrme – single-particle Hamiltonian

\[ \hat{h}_q = - \nabla \cdot B_q(r) \nabla + U_q(r) + S_q(r) \cdot \hat{\sigma} \]

\[ - \frac{i}{2} \sum_{\mu, \nu = x}^z \left[ W_{q,\mu\nu}(r) \nabla_\mu \sigma_\nu + \nabla_\mu \sigma_\nu W_{q,\mu\nu}(r) \right] \]

\[ - \frac{i}{2} [A_q(r) \cdot \nabla + \nabla \cdot A_q(r)] \]

\[ - \nabla \cdot [\hat{\sigma} \cdot C_q(r)] \nabla - \nabla \cdot D_q(r) \hat{\sigma} \cdot \nabla \]

\[ \neq \hat{T} \hat{h}_q \hat{T}^\dagger \]

**time-even fields:**

\[ U_q = \frac{\delta \mathcal{E}}{\delta \rho_q} \]

\[ B_q = \frac{\delta \mathcal{E}}{\delta \tau_q} \]

\[ W_{q,\mu\nu} = \frac{\delta \mathcal{E}}{\delta J_{q,\mu\nu}} \]

**time-odd fields:**

\[ A_q = \frac{\delta \mathcal{E}}{\delta j_q} \]

\[ S_q = \frac{\delta \mathcal{E}}{\delta q} \]

\[ C_q = \frac{\delta \mathcal{E}}{\delta T_q} \]

\[ D_q = \frac{\delta \mathcal{E}}{\delta F_q} \]
Virtually every group has a different logic when choosing time-odd terms in their calculations with the Skyrme EDF. Some examples:

- $\langle \text{HF}|v_{\text{Skyrme}}|\text{HF}\rangle$ with explicit tensor force

\[
E_{\text{Skyrme}} = \int d^3 r \sum_{t=0,1} \left[ - C_t^{\rho T} \mathbf{j}_t \cdot \mathbf{j}_t + C_t^{\rho \nabla J} \mathbf{s}_t \cdot \nabla \times \mathbf{j}_t + C_t^{s T} \mathbf{s}_t \cdot \mathbf{T}_t + C_t^{s F} \mathbf{s}_t \cdot \mathbf{F}_t \\
+ C_t^{s s} \mathbf{s}_t \cdot \mathbf{s}_t + C_t^{s s \rho} \mathbf{s}_t \cdot \mathbf{s}_t \rho_0^\alpha + C_t^{s \Delta s} \mathbf{s}_t \cdot \Delta \mathbf{s}_t + C_t^{\nabla s \nabla s} (\nabla \cdot \mathbf{s}_t)(\nabla \cdot \mathbf{s}_t) \right]
\]

- $\langle \text{HF}|v_{\text{Skyrme}}|\text{HF}\rangle$ without explicit tensor force (SLy5*, SLy5s1, ..., SLy5s8)

\[
E_{\text{Skyrme}} = \int d^3 r \sum_{t=0,1} \left[ - C_t^{\rho T} \mathbf{j}_t \cdot \mathbf{j}_t + C_t^{\rho \nabla J} \mathbf{s}_t \cdot \nabla \times \mathbf{j}_t + C_t^{s T} \mathbf{s}_t \cdot \mathbf{T}_t \\
+ C_t^{s s} \mathbf{s}_t \cdot \mathbf{s}_t + C_t^{s s \rho} \mathbf{s}_t \cdot \mathbf{s}_t \rho_0^\alpha + C_t^{s \Delta s} \mathbf{s}_t \cdot \Delta \mathbf{s}_t \right]
\]
Case 1: Skyrme - uses in the literature

How to handle EDFs where time-even terms do not correspond to $\langle HF|v_{\text{Skyrme}}|HF\rangle$? The most popular example are parameterisations like SLy4, SkM* etc where the "tensor terms" $\sim J_{\mu\nu}J_{\mu\nu}$ are omitted. The time-odd term $\sim s \cdot T$ then have be removed as well to conserve Galilean invariance. What about the other time-odd terms that are Galilean-invariant on their own?

- Bonche/Heenen/Flocard et al: keep time-odd terms from $\langle HF|v_{\text{Skyrme}}|HF\rangle$ but remove everything with two nablas and two Pauli matrices

$$E_{\text{Skyrme}} = \int d^3r \sum_{t=0,1} \left[ - C_t^{\rho\tau} j_t \cdot j_t + C_t^{\rho\nabla J} s_t \cdot \nabla \times j_t \\
+ C_t^{ss} s_t \cdot s_t + C_t^{ss\rho} s_t \cdot s_t \rho_0^\alpha \right]$$

- Dobaczewski et al keep time-odd terms from $\langle HF|v_{\text{Skyrme}}|HF\rangle$ but the $s \cdot T$ term that violates Galilean invariance when the $J_{\mu\nu}J_{\mu\nu}$ term is absent

$$E_{\text{Skyrme}} = \int d^3r \sum_{t=0,1} \left[ - C_t^{\rho\tau} j_t \cdot j_t + C_t^{\rho\nabla J} s_t \cdot \nabla \times j_t \\
+ C_t^{ss} s_t \cdot s_t + C_t^{ss\rho} s_t \cdot s_t \rho_0^\alpha + C_t^{s\Delta s} s_t \cdot \Delta s_t \right]$$

- keep only terms needed as complement of the time-even terms to ensure Galilean-invariance

$$E_{\text{Skyrme}} = \int d^3r \sum_{t=0,1} \left[ - C_t^{\rho\tau} j_t \cdot j_t + C_t^{\rho\nabla J} s_t \cdot \nabla \times j_t \right]$$
Exploit the freedom provided by nuclear DFT: terms needed as complement of the time-even terms to ensure Galilean-invariance + phenomenologically adjusted spin-terms with independent coupling constants $D$ (often parametrised through Landau parameters)

$$\mathcal{E}_{\text{Skyrme}} = \int d^3 r \sum_{t=0,1} \left[ - C_t^\rho \tau j_t \cdot j_t + C_t^\rho \nabla J_t s_t \cdot \nabla \times j_t ight. \\
+ D_t^{ss} s_t \cdot s_t + D_t^{ss\rho} s_t \cdot s_t \rho_0^\alpha + D_t^{s\Delta s} s_t \cdot \Delta s_t \right]$$

similar rescaling of the spin-terms have also been done when ”tensor terms” are present

$s_t \cdot \Delta s_t$ often dropped for reasons of (in-)stability (I’ll come back to that below).

When the ”tensor terms” bilinear in $J_{\mu \nu}$ are also treated in the DFT spirit with independent coupling constants, there is even larger freedom for time-odd terms.

Sometimes all time-odd terms are dropped.
Scientists ignorant of these subtleties are prone to use Skyrme parameterisations "wrongly" [by adding terms dropped during the fit, etc] or radically reinterpret them in disagreement with the original authors' intentions.

Recent fits tend to the two extremes:

1. define all time-odd terms strictly through $\langle HF|v_{\text{Skyrme}}|HF \rangle$ (Lyon)
2. lift all internal constraints from $\langle HF|v_{\text{Skyrme}}|HF \rangle$ (which also affect time-even spin-orbit and tensor terms), leaving all time-odd terms not fixed by Galilean invariance to an independent adjustment (UNEDF).

But what about pairing, then?

Note that other energy density functionals defined in the DFT spirit (Fayans, BCPM) have no \textit{a priori} fixed time-odd terms.
Case 2: Gogny

\[ \mathcal{V}_{\text{loc}}^{(0)}(\mathbf{r}_1, \mathbf{r}_2; \mathbf{r}_3, \mathbf{r}_4) = (W_1^{(0)} \hat{\sigma} \hat{T} + B_1^{(0)} \hat{T} \hat{P}^\sigma - H_1^{(0)} \hat{T} \hat{P}^T - M_1^{(0)} \hat{P}^\sigma \hat{P}^T) \times \delta(\mathbf{r}_{13}) \delta(\mathbf{r}_{24}) g_a(\mathbf{r}_{12}). \]

\[ \langle V_0^L \rangle = \sum_{T=0,1} \int d^3r_1 \ d^3r_2 \ g_a(\mathbf{r}_{12}) [A_0^{\rho_T} \rho_T(\mathbf{r}_1) \rho_T(\mathbf{r}_2) \]
\[ + A_0^{s_T} s_T(\mathbf{r}_1) \cdot s_T(\mathbf{r}_2)], \]

\[ \langle V_0^N \rangle = \sum_{T=0,1} \int d^3r_1 \ d^3r_2 \ g_a(\mathbf{r}_{12}) [B_0^{\rho_T} \rho_T(\mathbf{r}_2, \mathbf{r}_1) \rho_T(\mathbf{r}_1, \mathbf{r}_2) \]
\[ + B_0^{s_T} s_T(\mathbf{r}_2, \mathbf{r}_1) \cdot s_T(\mathbf{r}_1, \mathbf{r}_2)], \]

\[ \langle V_0^P \rangle = \sum_{t=n,p} \int d^3r_1 \ d^3r_2 \ g_a(\mathbf{r}_{12}) [C_0^{\tilde{\rho}_t}(\mathbf{r}_1, \mathbf{r}_2) \tilde{\rho}_t(\mathbf{r}_1, \mathbf{r}_2) \]
\[ + C_0^{\tilde{s}_t} \tilde{s}_t^*(\mathbf{r}_1, \mathbf{r}_2) \cdot \tilde{s}_t(\mathbf{r}_1, \mathbf{r}_2)]. \]


Time-reversal-breaking calculations using the Gogny force are done in Bruyères-le-châtel, Madrid, and by various japanese groups for a long time.
Case 3: Relativistic mean fields

We start from the Lagrangian of the RMF model,

\[ \mathcal{L} = \sum_k v_k^2 \bar{\psi}_k \left( i \gamma - m_B \right) \psi_k \]

\[ - \sum_k v_k^2 \bar{\psi}_k \left( g_\sigma \Phi + g_\omega \phi + g_\rho \phi \cdot \tau + e A \frac{1+\gamma_5}{2} \right) \psi_k \]

\[ + \frac{1}{2} \partial_\mu \Phi \partial^\mu \Phi - \mathcal{U}_{\sigma} [\Phi] - \frac{1}{2} \left( \frac{1}{2} \Omega_{\mu\nu} \Omega^{\mu\nu} - m_\omega^2 \omega_\mu \omega^\mu \right) \]

\[ - \frac{1}{2} \left( \frac{1}{2} R_{\mu\nu} \cdot R^{\mu\nu} - m_\rho^2 \rho_\mu \cdot \rho^\mu \right) - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}, \]

were \( \Omega_{\mu\nu}, R_{\mu\nu}, \) and \( F_{\mu\nu} \) are the field tensors of the \( \omega-, \rho-, \) and the electromagnetic field, e.g. \( \Omega_{\mu\nu} = \partial_\mu \omega_\nu - \partial_\nu \omega_\mu. \) For the non-linear self-coupling \( \mathcal{U}_\sigma \) of the scalar field we use the alternative, stabilized form described in Ref. [13].

Assuming stationarity and isotopic purity for the nucleon states, standard techniques lead to Dirac equations for the nucleons,

\[ \varepsilon_k \gamma_0 \psi_k = \left( \gamma \cdot \left( -i \nabla - g_\omega \omega \right) + m_B + g_\sigma \Phi + g_\omega \gamma_0 \omega_0 \right) \psi_k, \]

and Klein–Gordon equations for the mesons,

\[ - \Delta \Phi + \mathcal{U}' [\Phi] = -g_\sigma \rho_s, \]

\[ (-\Delta + m_\omega^2) \omega_0 = g_\omega \rho_0, \]

\[ (-\Delta + m_\omega^2) \omega = g_\omega \mathbf{j}, \quad \nabla \cdot \omega = 0, \]

where

\[ \rho_s = \sum_k v_k^2 \bar{\psi}_k \psi_k, \quad \rho_0 = \sum_k v_k^2 \bar{\psi}_k \gamma_0 \psi_k, \quad \mathbf{j} = \sum_k v_k^2 \bar{\psi}_k \gamma \psi_k \]

Case 3: Relativistic mean fields

For cranked RMF, see

W. Koepf and P. Ring, NPA 493 (1989) 61
Non-relativistic limit of relativistic Hartree

\[ \mathcal{L}_c = \mathcal{L}_{\text{free}} + \frac{c_s}{2} \mathcal{Q}_s^2 + \frac{c_v}{2} \mathcal{Q}_\mu \mathcal{Q}^\mu, \quad (2) \]

with

\[ \mathcal{Q}_s = \sum_\alpha \bar{\psi}_\alpha \psi_\alpha = \sum_\alpha [\varphi_\alpha^{(u)} \varphi_\alpha^{(u)} - \varphi_\alpha^{(d)} \varphi_\alpha^{(d)}], \quad (3a) \]

\[ \mathcal{Q}_0 = \sum_\alpha \bar{\psi}_\alpha \gamma_0 \psi_\alpha = \sum_\alpha [\varphi_\alpha^{(u)} \varphi_\alpha^{(u)} + \varphi_\alpha^{(d)} \varphi_\alpha^{(d)}], \quad (3b) \]

\[ \mathcal{E} = \sum_\alpha \bar{\psi}_\alpha \gamma \psi_\alpha = \sum_\alpha [\varphi_\alpha^{(u)} \varphi_\alpha^{(d)} + \varphi_\alpha^{(d)} \varphi_\alpha^{(u)}]. \quad (3c) \]


The scalar density shows the wanted Galilean-invariant combinations and the vector density reproduces the correct invariance property, \( \mathcal{Q}_\mu \mathcal{Q}^\mu = \mathcal{E}_0^2 - \mathcal{E}^2 \approx \rho^2 \), up to terms of second order, of course. We thus insert the mapped scalar and vector densities \((16)\) into the interaction Lagrangian density \((2)\), getting (up to second-order)

\[ \mathcal{L}_c = \frac{c_s}{2} \rho^2 - 2c_s B_0^2 \left[ \rho \tau - \mathbf{j}^2 \right. \]

\[ - \left. \left[ \rho \nabla \cdot \mathbf{j} + \mathbf{j} \cdot (\nabla \times \mathbf{\sigma}) \right] - \frac{1}{4} (\nabla \times \mathbf{\sigma})^2 \right]. \quad (17) \]

That result is manifestly Galilean invariant.

- there are no \( s^2(\mathbf{r}) \) terms (= \( \mathbf{\sigma}^2(\mathbf{r}) \) terms in that paper’s notation)
- Note that \( \int d^3 r \left[ \nabla \times \mathbf{s}(\mathbf{r}) \right]^2 = - \int d^3 r \left\{ [\nabla \cdot \mathbf{s}(\mathbf{r})]^2 + \mathbf{s}(\mathbf{r}) \Delta \mathbf{s}(\mathbf{r}) \right\} \)
Spin-spin terms such as $s^2(r)$ would emerge as exchange terms in relativistic Hartree-Fock.

Various possible consequences of the absence of spin-spin interaction terms in the standard RMF for the calculation of quasiparticle states and cranked states are discussed in

A. V. Afanasjev and H. Abusara, PRC 81, 014309 (2010)
A. V. Afanasjev and H. Abusara, PRC 82, 034329 (2010)

In QRPA for spin excitations, a pion term and a phenomenological Landau-Migdal interaction are added to the RMF Lagrangian

Non-nuclear time-odd terms

- **magnetic interaction**

\[
H_{e.m.} = e_1 e_2 / r_{12}
\]  
\[=- \frac{e_1 e_2}{2 m_1 m_2 c^2} \left[ \frac{1}{r_{12}} \mathbf{p}_1 \cdot \mathbf{p}_2 + \frac{1}{r_{12}^3} (\mathbf{r}_{12} \cdot (\mathbf{r}_{12} \cdot \mathbf{p}_1) \mathbf{p}_2) \right]
\]  
\[=- \frac{e_2}{m_2 c} \mu_1 \mathbf{\sigma}_1 \cdot \frac{\mathbf{r}_{12} \times \mathbf{p}_2}{r_{12}^3} - \frac{e_1}{m_1 c} \mu_2 \mathbf{\sigma}_2 \cdot \frac{\mathbf{r}_{12} \times \mathbf{p}_1}{r_{12}^3}
\]  
\[=- \mu_1 \mu_2 \left[ 3 \frac{(\mathbf{\sigma}_1 \cdot \mathbf{r}_{12}) (\mathbf{\sigma}_2 \cdot \mathbf{r}_{12})}{r_{12}^5} - \frac{\mathbf{\sigma}_1 \cdot \mathbf{\sigma}_2}{r_{12}^3} + \frac{8 \pi}{3} (\mathbf{\sigma}_1 \cdot \mathbf{\sigma}_2) \delta(r_{12}) \right]
\]  
\[=- \frac{e_2 \hbar}{2 m_1 c} \left( 2 \mu_1 - \frac{e_1 \hbar}{2 m_1 c} \right) \mathbf{\sigma}_1 \cdot \frac{\mathbf{r}_{12} \times \mathbf{p}_1}{r_{12}^3} - \frac{e_1 \hbar}{2 m_2 c} \left( 2 \mu_2 - \frac{e_2 \hbar}{2 m_2 c} \right) \mathbf{\sigma}_2 \cdot \frac{\mathbf{r}_{21} \times \mathbf{p}_2}{r_{12}^3}
\]  
\[=- \left[ \frac{e_2 \hbar}{4 m_1 c} \left( 2 \mu_1 - \frac{e_1 \hbar}{2 m_1 c} \right) + \frac{e_1 \hbar}{4 m_2 c} \left( 2 \mu_2 - \frac{e_2 \hbar}{2 m_2 c} \right) \right] 4 \pi \delta(r_{12})
\]

where \( r_{ij} = r_i - r_j \), \( r_{ij} = |r_{ij}| \) and \( \mathbf{p}_i \) is the linear momentum of the \( i \)th particle. The physical interpretation of the terms in (1) are the following: the first term (1a) is the Coulomb interaction between point particles of charges \( e_1 \) and \( e_2 \), (1b) corresponds to the interaction of the magnetic field arising from the orbital motion of one particle with the orbital motion of the other, known also as the Breit interaction [12]. The term (1c) describes the interaction of the spin magnetic moment of one particle with the magnetic field produced by the orbital motion of the other, (1d) is the mutual interaction between spin magnetic moments, (1e) is the well known spin-orbit interaction, and (1f) is known as the Darwin interaction.

S. Shlomo, PLB 6 (1976) 244

- usually/always ignored in non-relativistic EDF approaches
- (automatically) partially included in RMF through Lorentz-invariance, but with ”wrong” (i.e. the free) \( g \) factors of protons and neutrons
Typical Results
"Single-particle states" in even-even nuclei

K. Rutz, M. Bender, P.-G. Reinhard, J. A. Maruhn, and W. Greiner, NPA
634 (1998) 67


Fig. 14. Excitation neutron spectra in $^{207}$Pb for the parameterizations SkI3 (a), SLy6 (b), and SV-bas (c). In every panel, the experimental data [52,53] are compared with the SHF results for the options (10)-(12). Also, the simple one-hole (1h) and one-particle--two-hole (1p2h) estimates from the single-neutron spectrum of $^{208}$Pb are exhibited. The dotted horizontal line marks energy of the lowest collective state 4$^-$ in $^{208}$Pb. For better view, results for one and the same level are connected by dash lines. See text for more details.

K. J. Pototzky: Properties of doubly neutron-deficient nuclei and their impact to time-odd mean field... TOMF effects. These effects are illustrated in fig. 14 for the options even, mean, and min +s2 where the TOMF are added.
Energy gain from time-odd terms in 1qp states of odd nuclei

![Graph showing energy gain from time-odd terms in nuclei](image)

**FIG. 2.** (Color online) Impact of NM on binding energies of light odd-mass nuclei. Calculations were performed with the NL3 parametrization of the RMF Lagrangian. They cover nuclei from the proton drip line up to the neutron drip line.

A. V. Afanasjev and H. Abusara, PRC 81, 014309 (2010)
Here, we discuss several versions of the functional, depending on how the time-odd coupling constants are determined.

(i) Native version, which corresponds to all time-odd coupling constants being determined by the underlying Skyrme interaction [18].

(ii) Gauge version, which corresponds to the subset of time-odd coupling constants being determined through the gauge-invariance conditions [18,21], namely, $C_i^t = -C_i^T$, $C_i^t = -C_i^J$, and $C_i^{\Delta J} = C_i^{\Delta J}$, with all other time-odd coupling constants set to zero.

(iii) Landau version, which is based on the gauge version, where the subset of time-odd coupling constants $C_i^s$ and $C_i^T$ is reset through the Landau parameters [23]:

$$
\begin{align*}
g_0 &= N_0(2C_0^s + 2C_1^T \beta \rho_0^{2/3}), \\
g_1 &= -2N_0C_0^T \beta \rho_0^{2/3}, \\
g_0' &= N_0(2C_1^s + 2C_1^T \beta \rho_0^{2/3}), \\
g_1' &= -2N_0C_1^T \beta \rho_0^{2/3},
\end{align*}
$$

where $\beta = (3\pi^2/2)^{2/3}$, $1/N_0 = \pi^2h^2/2m^*k_F$, and, additionally, $C_i^{\Delta s} = 0$ for $t = 0, 1$. Because the Landau prescription only sets $C_i^T$, the gauge condition is broken because $C_i^T \neq -C_i^J$ anymore.

(iv) Time-even version, in which all time-odd coupling constants in Eq. (6) are set equal to zero.

There is a complication: imposing "triaxial" symmetry in a code, the energy gain depends on the relative orientation of the nucleus in the box.

This degree of freedom has been dubbed "alispin" by Dobaczewski et al.

This does not mean that the time-odd terms are orientation dependent (which is incompatible with rotational symmetry) but that the spatial symmetries in a "triaxial code" are not plane reflections and mirror symmetries as one might naively think.

⇒ see talks by Jacek Dobaczewski and Wouter Ryssens on tuesday.

FIG. 5. Cumulative histogram of deviations $\Delta E^j = E_{qp}^j - E_{qp}^{\perp}$ between energies of one-quasiproton states calculated in the noncollective-rotation (∥) and collective-rotation (⊥) variants. Dot-dashed open bins, native variants; filled bins, Landau variants. The bin size is 5 keV.

Energy gain from time-odd terms in 1qp states of odd nuclei

Convergence problems:

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

We come back to that later on . . .

... noting that other groups faced similar difficulties:

\( \tilde{b}_i' \) uniquely related to the \( b_i, b'_i \), see appendix A. Following our experience, the term \( H_{Sk}^{(s \Delta s)} \) leads to unstable ground states for many medium and heavy nuclei. This is a common problem in most Skyrme parameterizations [36,37]. Thus, we include in the option \( H_{Sk}^{(\text{min} + s^2)} \) only the simple spin term \( H_{Sk}^{(s^2)} \). The comparison of results for \( H_{Sk}^{(\text{even})} \)

Finally, note that time-conjugate states are easily obtained in even-even nuclei ... of Emin +s^2 − Eexp for SkI3 and SLy6 in panels c) of figs. 1 and 2, where we see similar SkI3 and SLy6 trends for

Time-odd terms in nuclear energy density functionals
ECT*, 25 September 2017 34 / 51

Energy gain from time-odd terms in 1qp states of odd nuclei
M. Bender, IPN Lyon (IPN Lyon)

K. J. Pototzky et al.: Properties of odd nuclei and their impact to time-odd mean field...

Fig. 1. The energy differences E_{even} − E_{min} (a), E_{even} − E_{min+s^2} (b), and E_{min+s^2} − E_{exp} (c), in odd Sn isotopes for the parameterizations SkI3, SLy6, and SV-bas.

Fig. 3. The binding energy difference E_{even} − E_{min+s^2}^{\ast} for the Skyrme parameterizations SkI3, SLy6 and SV-bas, drawn in the N-Z plane. All available neutron and proton odd nuclei with the charge 16 ≤ Z ≤ 92 are included.

Self-interaction in a nut-shell:

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

  early papers by Hartree and Fock

  S. Stringari and D. M. Brink, NPA 304, 307 (1978)
  P. Perdew and A. Zunger, PRB 23, 5048 (1981)
  D. Lacroix, T. Duguet, and M. Bender, PRC 79, 044318 (2009); M. Bender, T. Duguet, and D. Lacroix, PRC 79, 044319 (2009)

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

  \[
  \lim_{A \rightarrow 1} \mathcal{E} \rightarrow \mathcal{E}_{\text{kin}} \quad \Leftrightarrow \quad \lim_{A \rightarrow 1} \mathcal{E}_{\text{Skyrme}} \rightarrow 0
  \]

- Similarly, the 3-body contribution to the EDF has to vanish in the 2-body limit

- Automatically fulfilled for HF-expectation values of true operators

- Similar concept ("self-pairing") for paired systems: "A correlated pair shall not gain energy by pair-interaction with itself", automatically fulfilled for HFB-expectation values of true operators

  M. Bender, T. Duguet, and D. Lacroix, PRC 79, 044319 (2009)
This can be summarized in the form of polarization corrections to energies of odd states $\delta E$, 

$$E^{A \pm 1} = E^A \pm e_\lambda + \delta E,$$  

(20)

or polarization corrections to s.p. energies $\delta e_\lambda$, 

$$E^{A \pm 1} = E^A \pm (e_\lambda + \delta e_\lambda),$$  

(21)

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

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

(46)

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

$$\text{SI} \equiv \text{self-interaction}$$

$$\text{SIF} \equiv \text{self-interaction-free}$$
FIG. 6. (Color online) The SIF and SI contributions to the polarization corrections of Eq. (46), calculated in $^{100}$Sn for the Skyrme EDF SLy5.

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

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

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

\[
\hat{J}_z \Psi_1(r) = K_1 \Psi_1(r) \quad \text{with} \quad K_1 = \langle \Psi_1 | \hat{L}_z | \Psi_1 \rangle + \langle \Psi_1 | \hat{S}_z | \Psi_1 \rangle \\
\hat{J}_z \Psi_2(r) = K_2 \Psi_2(r) \quad \text{with} \quad K_2 = \langle \Psi_2 | \hat{L}_z | \Psi_2 \rangle + \langle \Psi_2 | \hat{S}_z | \Psi_2 \rangle
\]

to a two-particle state with good $j_z$

\[
\hat{J}_z \Psi_1(r) \Psi_2(r') = (K_1 + K_2) \Psi_1(r) \Psi_2(r') \\
\hat{J}_z \Psi_1(r) \Psi_2(r') = (K_1 - K_2) \Psi_1(r) \Psi_2(r')
\]

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

- [C. J. Gallagher, PR 126 (1962) 1525]: For the lower 2qp state in well-deformed even-even nuclei $|\langle \Psi_1 | \hat{S}_z | \Psi_1 \rangle + \langle \Psi_2 | \hat{S}_z | \Psi_2 \rangle|$ is minimal (anti-parallel spins)
- [C. J. Gallagher and S. A. Moszkowski, PR 111 (1958) 1282]: For the lower 2qp state in odd-odd nuclei $|\langle \Psi_1 | \hat{S}_z | \Psi_1 \rangle + \langle \Psi_2 | \hat{S}_z | \Psi_2 \rangle|$ is maximal (parallel spins)

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

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

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

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

1. Superdeformed rotational band of $^{194}$Hg
2. Skyrme SLy4, T22, T44
3. surface pairing, HFB+LN

V. Hellemans, P.-H. Heenen and M. Bender, PRC 85 (2012) 014326
Time-odd terms in rotational bands – dynamical moment of inertia

\[ \mathcal{J}^2 = \frac{\partial \langle J_z \rangle}{\partial \omega} = \frac{1}{\omega} \frac{\partial \mathcal{E}}{\partial \omega} \]

V. Hellemans, P.-H. Heenen and M. Bender, PRC 85 (2012) 014326
Time-odd terms in rotational bands – total energy

- Superdeformed rotational band of $^{152}$Dy
- Skyrme SLy4, T22, T44
- surface pairing, HFB+LN

V. Hellemans, P.-H. Heenen and M. Bender, PRC 85 (2012) 014326
(a) Dependence of the $C_0^{Δs}s_0 \cdot Δs_0$ term of a variant of the T22 parameterisation on the value of $C_0^{Δs}$ for the $⟨\hat{J}_z⟩ = 54\hbar$ state in the yrast superdeformed rotational band of $^{194}$Hg.

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

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

V. Hellemans, P.-H. Heenen and M. Bender, PRC 85 (2012) 014326
FIGURE 1. Left: Dependence of the \( C_{\Delta s_0} \) term of a modified T22 parameterization (see text) on the value of its coupling constant \( C_{\Delta s_0} \) for the \( J_z = 54\hbar \) state in the ground superdeformed band of \(^{194}\text{Hg}\). Variation of the \( C_s t_s^2 t_e \), \( t_e = 0, 1 \) terms relative to their values at \( C_{\Delta s_0} = 0 \) in the same calculation.

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

Finite-size spin instabilities

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

**FIGURE 3.** (color online) Cut through the spin density $s_0$ at $x = 4.4$ fm for the $J_z = 54\hbar$ state in the ground superdeformed band of $^{194}$Hg as obtained with a modified T22 parameterization (see text) with $C_0^{\Delta s} = 40$ MeV fm$^5$ at the onset of the instability (left panel) and at few iterations before the crash of the code (right panel).

Finite-size spin instabilities – linear response

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

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

Finite-size spin instabilities can be correlated to linear response in infinite matter.

Infinite nuclear matter

In this section, we present the formalism of the linear response theory in infinite nuclear matter. This method has been the subject of a recent review article, where all the details of the formalism are presented and discussed. We limit ourselves to sketching the basic ingredients of the formalism.

The first ingredient is the Hartree-Fock retarded propagator of a noninteracting particle pair. Because for the present study we ignore the charge-exchange process, the particle and the hole in the same pair share the same isospin number \( \tau = p, n \):

\[
G(\tau)_{\text{HF}}(k, p, \omega) = \theta(k_{\tau F} - k) - \theta(k_{\tau F} - |k + q|) \omega + \epsilon_{\tau}(k) - \epsilon_{\tau}(k + q) + i\eta,
\]

where \( \theta(\cdot) \) is the standard step-function, \( \epsilon_{\tau}(k) = \hbar^2 k^2 / 2 m^* \tau + U_{\tau} \) is the single-particle energy, and \( m^* \) and \( U_{\tau} \) represent the effective mass and the single-particle potential, respectively, while \( k \) is the moment of the hole and \( q \) is the external momentum transferred by the probe we use to excite the system. The latter can be taken along the \( z \) axis without loss of generality. For simplicity, we illustrate the case of SNM, but the formalism has been already generalized to the more general case of isospin asymmetric nuclear matter.

Because the two Fermi surfaces are equal in SNM, we can...

FIG. 7. (Color online) Instabilities in SNM for the functionals considered in the present article. The dashed-dotted horizontal line stands for the saturation density of the functional. See text for details.
Cranked HFB and calculation of odd nuclei seems to be more sensitive to instabilities than RPA response in finite nuclei.

The computationally-friendly RPA response in infinite matter can be used as criterion in the parameter fit to obtain parameterisations that are safe to use as "HF"-like functionals.

- SLy5s1, . . . , SLy5s8, [R. Jodon, M. Bender, K. Bennaceur, and J. Meyer, PRC 94 (2016) 024335]
Phenomena impacted by time-odd terms that I will not discuss

- Many-body matrix elements entering projection and/or GCM
- Mass parameters entering the Bohr Hamiltonian
- Mass parameters entering ATDHF(B)
Take-away messages

- Time-odd terms are ubiquitous
- They are often, but not necessarily, small
- They are not well fixed by today’s fit protocols
- Advocates of nuclear DFT see them as additional free terms (unless fixed by a symmetry (other than exchange symmetry))
- In the Skyrme community, it is hence popular to tweak time-odd terms
- For Skyrme-HF and the RMF, there are coexisting recipes how to use them
- Time-odd terms are sometimes inconsistently used in the literature
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