Nuclear response for the Skyrme functional with zero-range tensor

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Outline

- The Skyrme Energy density Functional
- Tensor couplings
- Parameters fitting
- Instabilities in finite nuclei
- Linear response formalism
- Conclusion

The standard (2-body) Skyrme functional

- Effective Skyrme *interaction*

$$
\begin{aligned}
V_{\text{eff}} &= t_0\,(1+x_0\,\hat{P}_\sigma)\,\delta && \text{local}\\
&+ \frac{t_1}{2}\,(1+x_1\,\hat{P}_\sigma)\,\left(\mathbf{k}'^2\,\delta+\delta\,\mathbf{k}^2\right) && \text{non local}\\
&+ t_2\,(1+x_2\,\hat{P}_\sigma)\,\mathbf{k}'\cdot\delta\,\mathbf{k} && \text{non local}\\
&+ \frac{t_3}{6}\,(1+x_3\,\hat{P}_\sigma)\,\rho^{\alpha}\,\delta && \text{density dep.}\\
&+ \mathrm{i}\,W_0\;\hat{\boldsymbol{\sigma}}\cdot\left[\mathbf{k}'\times\delta\,\mathbf{k}\right] && \text{spin-orbit}
\end{aligned}
$$

- Energy Density Functional (EDF):

$$E=\int\mathscr{E}[\rho,\tau,\mathbb{J}]\,\mathrm{d}\mathbf{r}$$

functional of the local density $\rho(\mathbf{r}\sigma q,\mathbf{r}\sigma' q')$,

with $\rho(\mathbf{r}\sigma q,\mathbf{r}'\sigma' q')=\sum_{i\leqslant\varepsilon_F}\varphi_i^*(\mathbf{r}\sigma q)\varphi_i(\mathbf{r}'\sigma' q')$

9 or 10 parameters to fit

The standard (2-body) Skyrme functional

- Effective Skyrme *interaction*

$$
\begin{array}{rll}
V_{\text{eff}} = & t_0\,(1+x_0\,\hat{P}_\sigma)\,\delta & \text{local} \\
+ & \frac{t_1}{2}\,(1+x_1\,\hat{P}_\sigma)\,\left(\mathbf{k}'^2\,\delta+\delta\,\mathbf{k}^2\right) & \text{non local} \\
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+ & \frac{t_3}{6}\,(1+x_3\,\hat{P}_\sigma)\,\rho^{\alpha}\,\delta & \text{density dep.} \\
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\end{array}
$$

- Energy Density Functional (EDF):

$$E = \int \mathscr{E}[\rho,\tau,\mathbb{J}]\,\mathrm{d}\mathbf{r}$$

+ other termes if symmetries are broken (deformation, rotation, pairing)

functional of the local density $\rho(\mathbf{r}\sigma q, \mathbf{r}\sigma' q')$,

with $\rho(\mathbf{r}\sigma q, \mathbf{r}'\sigma' q') = \sum_{i \leqslant \varepsilon_F} \varphi_i^*(\mathbf{r}\sigma q)\varphi_i(\mathbf{r}'\sigma' q')$

9 or 10 parameters to fit

Functional of the local energy density ("$\hat{T}$-even" part)

$$\mathscr{H} = \mathscr{K} + \mathscr{H}_0 + \mathscr{H}_3 + \mathscr{H}_{\text{eff}} + \mathscr{H}_{\text{fin}} + \mathscr{H}_{\text{so}} + \mathscr{H}_{\text{sg}} + \mathscr{H}_{\text{coul}}$$

$$\begin{aligned}
\mathscr{H}_0 &= \frac{1}{4} t_0 \left[(2 + x_0)\rho_0^2 - (2x_0 + 1) \sum_q \rho_q^2 \right] && = \sum_{T=0,1} C_T[\rho_0]\,\rho_T^2 \\
\mathscr{H}_3 &= \frac{1}{24} t_3 \rho_0^{\alpha} \left[(2 + x_3)\rho_0^2 - (2x_3 + 1) \sum_q \rho_q^2 \right] && \\
\mathscr{H}_{\text{eff}} &= \frac{1}{8} \left[t_1 (2 + x_1) + t_2 (2 + x_2) \right] \tau_0 \rho_0 && = \sum_{T=0,1} C_T^{\tau}\,\tau_T \rho_T \\
&+ \frac{1}{8} \left[t_2 (2x_2 + 1) - t_1 (2x_1 + 1) \right] \sum_q \tau_q \rho_q && \\
\mathscr{H}_{\text{fin}} &= \frac{1}{32} \left[t_2 (2 + x_2) - 3 t_1 (2 + x_1) \right] \rho_0 \Delta \rho_0 && = \sum_{T=0,1} C_T^{\Delta\rho}\,\rho_T \Delta \rho_T \\
&+ \frac{1}{32} \left[3 t_1 (2x_1 + 1) + t_2 (2x_2 + 1) \right] \sum_q \rho_q \Delta \rho_q && \\
\mathscr{H}_{\text{so}} &= -\frac{W_0}{2} \left[\rho_0 \nabla \cdot \mathbf{J}_0 + \sum_q \rho_q \nabla \cdot \mathbf{J}_q \right] && = \sum_{T=0,1} C_T^{\nabla J}\,\rho_T \nabla \cdot \mathbf{J}_T \\
\mathscr{H}_{\text{sg}} &= -\frac{t_1 x_1 + t_2 x_2}{16} \mathbf{J}_0^2 + \frac{t_1 - t_2}{16} \sum_q \mathbf{J}_q^2 && = \sum_{T=0,1} C_T^{\mathbf{J}}\,\mathbf{J}_T^2
\end{aligned}$$

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&+ \frac{1}{8} \left[t_2(2x_2+1) - t_1(2x_1+1) \right] \sum_q \tau_q \rho_q && \\
\mathscr{H}_{\text{fin}} &= \frac{1}{32} \left[t_2(2+x_2) - 3t_1(2+x_1) \right] \rho_0 \Delta\rho_0 && = \sum_{T=0,1} C_T^{\Delta\rho}\, \rho_T \Delta\rho_T \\
&+ \frac{1}{32} \left[3t_1(2x_1+1) + t_2(2x_2+1) \right] \sum_q \rho_q \Delta\rho_q && \\
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\mathscr{H}_{\text{sg}} &= -\frac{t_1 x_1 + t_2 x_2}{16} \mathbf{J}_0^2 + \frac{t_1 - t_2}{16} \sum_q \mathbf{J}_q^2 && = \cancel{\sum_{T=0,1} C_T^{J}\, \mathbf{J}_T^2} \quad : \textbf{SLy4}
\end{aligned}$$

Functional of the local energy density ("$\hat{T}$-even" part)

$$\mathscr{H} = \mathscr{K} + \mathscr{H}_0 + \mathscr{H}_3 + \mathscr{H}_{\text{eff}} + \mathscr{H}_{\text{fin}} + \mathscr{H}_{\text{so}} + \mathscr{H}_{\text{sg}} + \mathscr{H}_{\text{coul}}$$

$$\mathscr{H}_0 = \frac{1}{4} t_0 \left[(2+x_0)\rho_0^2 - (2x_0+1) \sum_q \rho_q^2 \right] = \sum_{T=0,1} C_T[\rho_0]\, \rho_T^2$$

$$\mathscr{H}_3 = \frac{1}{24} t_3 \rho_0^\alpha \left[(2+x_3)\rho_0^2 - (2x_3+1) \sum_q \rho_q^2 \right]$$

$$\mathscr{H}_{\text{eff}} = \frac{1}{8} \left[t_1(2+x_1) + t_2(2+x_2) \right] \tau_0 \rho_0 + \frac{1}{8} \left[t_2(2x_2+1) - t_1(2x_1+1) \right] \sum_q \tau_q \rho_q = \sum_{T=0,1} C_T^\tau \tau_T \rho_T$$

$$\mathscr{H}_{\text{fin}} = \frac{1}{32} \left[t_2(2+x_2) - 3t_1(2+x_1) \right] \rho_0 \Delta\rho_0 + \frac{1}{32} \left[3t_1(2x_1+1) + t_2(2x_2+1) \right] \sum_q \rho_q \Delta\rho_q = \sum_{T=0,1} C_T^{\Delta\rho} \rho_T \Delta\rho_T$$

$\mathbf{C_0^{\nabla J} \neq 3C_1^{\nabla J}}$ **: SLy10**

$$\mathscr{H}_{\text{so}} = -\frac{W_0}{2} \left[\rho_0 \nabla\cdot\mathbf{J}_0 + \sum_q \rho_q \nabla\cdot\mathbf{J}_q \right] = \sum_{T=0,1} C_T^{\nabla J} \rho_T \nabla\cdot\mathbf{J}_T$$

$$\mathscr{H}_{\text{sg}} = -\frac{t_1 x_1 + t_2 x_2}{16} \mathbf{J}_0^2 + \frac{t_1 - t_2}{16} \sum_q \mathbf{J}_q^2 = \cancel{\sum_{T=0,1} C_T^J \mathbf{J}_T^2}$$

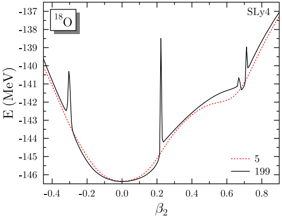
: SLy4

Mean field and beyond

- At the M.F. level: reasons to increase the number of parameters
  - Spectroscopic quality must be improved
  - m^*/m should be ~ 0.8 in the bulk and ~ 1 near the surface
  - *etc.*

$\Rightarrow$ Tensor interaction ? (see PRC 76, 014312; PRC 80, 064302)

- ... and beyond: reasons to change the interaction



(with terms $\propto \rho^\alpha$, $\alpha \notin \mathbb{N}$)

Poles $\rightarrow$ that can be corrected

and steps in the projected energy $\rightarrow$ that can not !

... what about coul-ex ?

See: PRC 79, 044318, 044319 and 044320.

$\Rightarrow$ Three-body interaction ? (see J. Sadoudi thesis, CEA Saclay)

Tensor interaction, tensor couplings

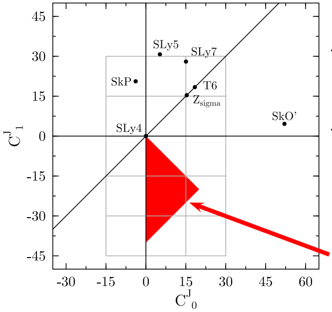
$$v_{\mathrm{T}}(\mathbf{r}) = \tfrac{1}{2}\, t_e \left\{ \left[3\,(\boldsymbol{\sigma}_1 \cdot \mathbf{k}')\,(\boldsymbol{\sigma}_2 \cdot \mathbf{k}') - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)\,\mathbf{k}'^2 \right] \delta(\mathbf{r}) + \text{h.c.} \right\}$$
$$+ t_o \left[3\,(\boldsymbol{\sigma}_1 \cdot \mathbf{k}')\,\delta(\mathbf{r})\,(\boldsymbol{\sigma}_2 \cdot \mathbf{k}) - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)\,\mathbf{k}' \cdot \delta(\mathbf{r})\,\mathbf{k} + \text{h.c.} \right]$$

$$v = v_{\text{loc.}} + v_{\text{non loc.}} + v_{\text{s.o.}} + v_{\text{tens.}}$$

$$\mathscr{E}_T \propto C_T^{\rho} \rho_T^2 \quad C_T^{\tau} \rho_T \tau_T \quad C_T^{\nabla J} \rho_T \nabla \cdot \mathbf{J}_T \quad C_T^{J} \mathbf{J}_T^2$$

$$C_T^{\Delta\rho} \rho_T \Delta \rho_T$$

$T = 0, 1$

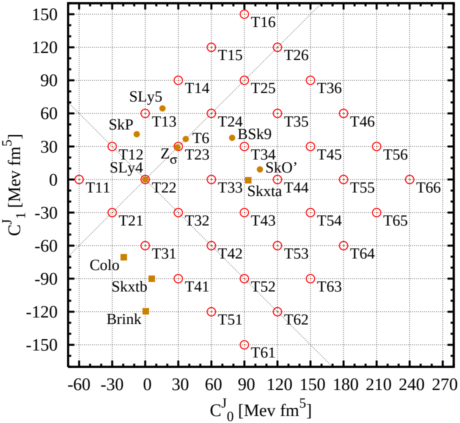


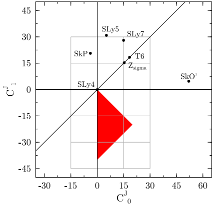
$$C_0^J = \tfrac{1}{8}\, t_1\,(1 - 2x_1) - \tfrac{1}{8}\, t_2\,(1 + 2x_2) + \tfrac{5}{8}\,(3t_o + t_e)$$
$$C_1^J = \tfrac{1}{8}\,(t_1 - t_2) + \tfrac{5}{8}\,(t_o - t_e)$$

Existing forces
(non local contribution)

Region of "reasonable" parameters
(Stancu, Brink, Flocard '77)

Tensor interaction, tensor couplings





"T_{ij}" interactions

- Tensor part of the Skyrme EDF: Spherical nuclei,
  T. Lesinski, M. Bender, K.B., T. Duguet, J. Meyer,
  PRC 76, 014312 (2007).
- Tensor part of the Skyrme EDF: Deformation properties of magic and semi-magic nuclei,
  M. Bender, K.B., T. Duguet, P.-H. Heenen, T. Lesinski, J. Meyer,
  PRC 80, 064302 (2009).

EDF fitting...

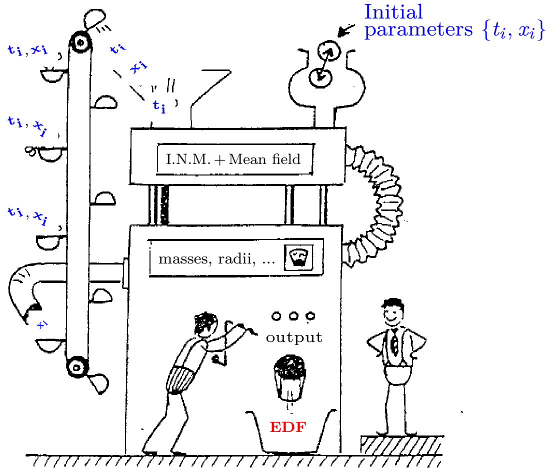
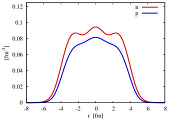


Figure: Adapted from the picture by J. Dechargé, from “Approches de champ moyen et au-delà”, J.-F. Berger, École Joliot-Curie: “Les noyaux en pleine forme”, 1991.

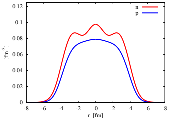
Finite size instabilities in nuclei

- Instabilities often experienced with the skyrme functionals
  - Ferromagnetic instabilities: (spin polarization) $n\uparrow$, $p\uparrow$
  - Isospin instabilities: neutron-proton *segregation*
  - Both: $n\uparrow$, $p\downarrow$

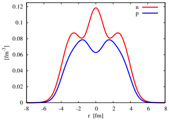
- Example: isospin instability in ^{48}Ca



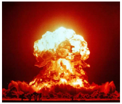
$C_1^{\Delta\rho} = 15$ MeV fm^5
$\sim$ SLy5



25 MeV fm^5



35 MeV fm^5



$\gtrsim 36$ MeV fm^5

T. Lesinski, K.B., T. Duguet, J. Meyer, PRC 74, 044315 (2006).

Linear response – Stability criterium

Response of the system to a perturbation given by

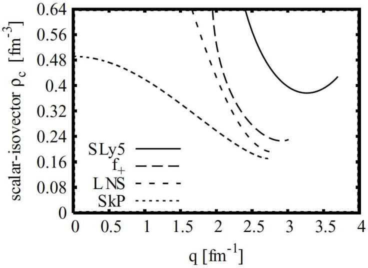
$$\mathscr{Q}^{(\alpha)} = \sum_a e^{i\mathbf{q}\cdot\mathbf{r}_a}\ \Theta_a^{(\alpha)},$$

$$\Theta_a^{\rm SS} = 1_a, \quad \Theta_a^{\rm VS} = \boldsymbol{\sigma}_a, \quad \Theta_a^{\rm SV} = \vec{\boldsymbol{\tau}}_a, \quad \Theta_a^{\rm VV} = \boldsymbol{\sigma}_a \vec{\boldsymbol{\tau}}_a$$

Response functions are given by

$$\chi^{(\alpha)}(\omega, \mathbf{q}) = \frac{1}{\Omega} \sum_n |\langle n|\mathscr{Q}^{(\alpha)}|0\rangle|^2 \left(\frac{1}{\omega - E_{n0} + i\eta} - \frac{1}{\omega + E_{n0} - i\eta} \right)$$

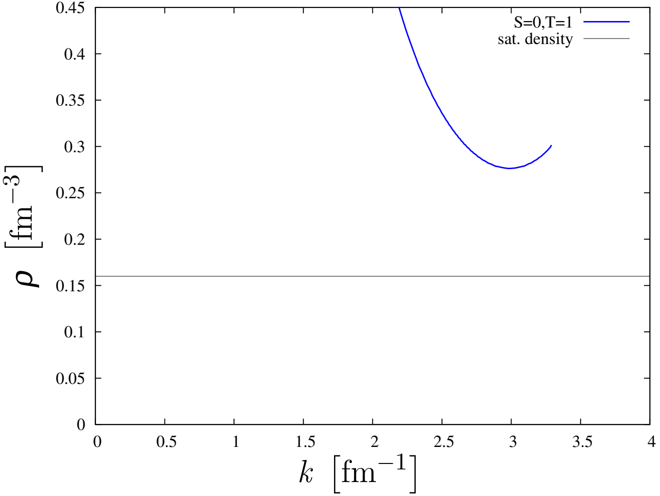
(Cf. C. Garcia–Recio *et al.*, Ann. of Phys. 214 (1992) 293–340)



- Predicts instabilities in finite size systems
- Easy to implement
- Negligible computation time
- Might be crucial with a tensor interaction

Linear response as a tool for diagnosis

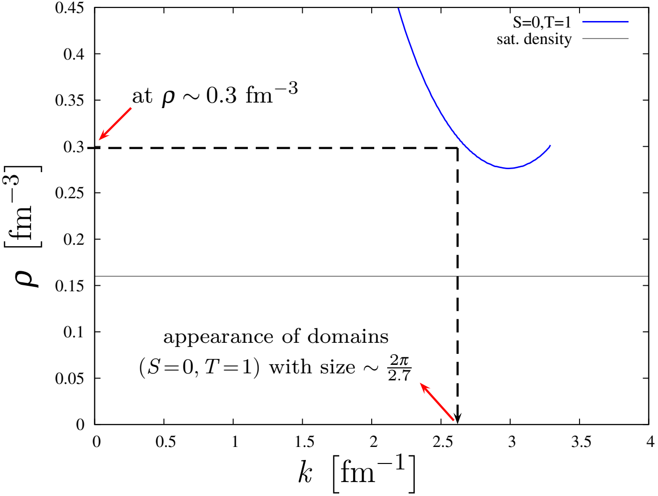
Pole of the response at $E = 0$ $\equiv$ instability



- T. Lesinski, K.B., T. Duguet, J. Meyer, PRC 74, 044315 (2006);
- D. Davesne, M. Martini, K.B., J. Meyer, Phys. Rev. C80, 024314 (2009), **erratum** to be published.

Linear response as a tool for diagnosis

Pole of the response at $E = 0$ $\equiv$ **instability**



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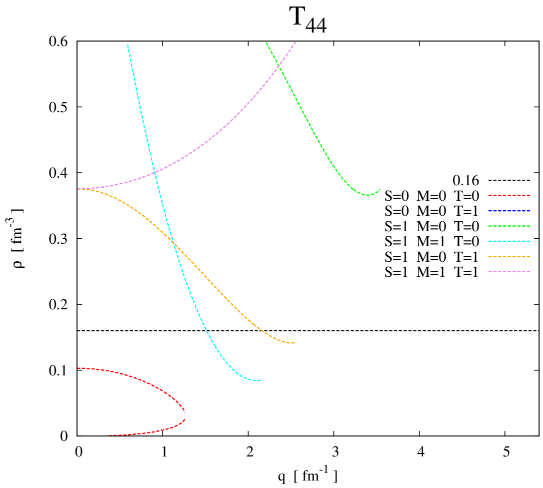
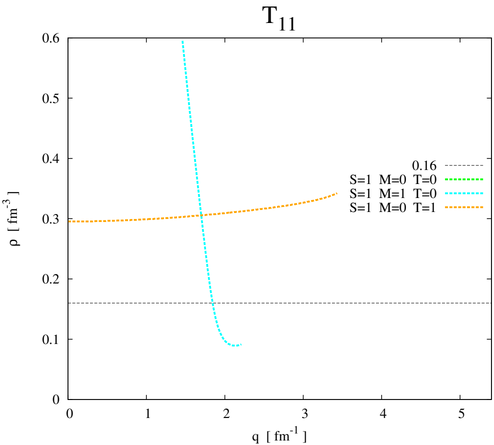
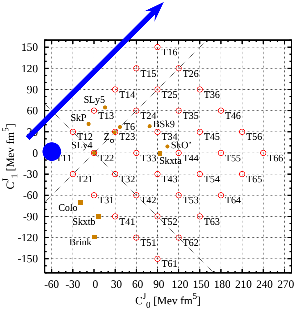
“Standard” EDFs, instabilities and Murphy’s law



“*Anything that can go wrong will go wrong*”, Murphy’s law.

Instabilities in the spin sector





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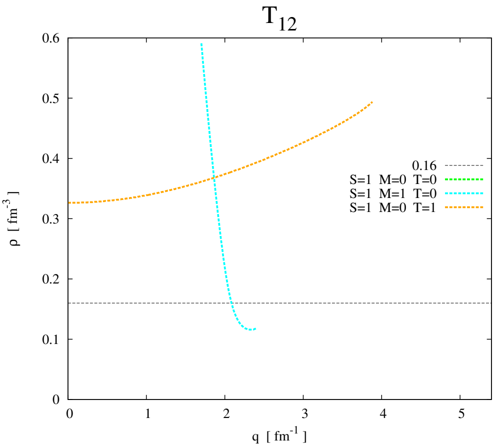

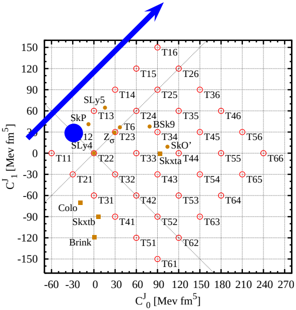

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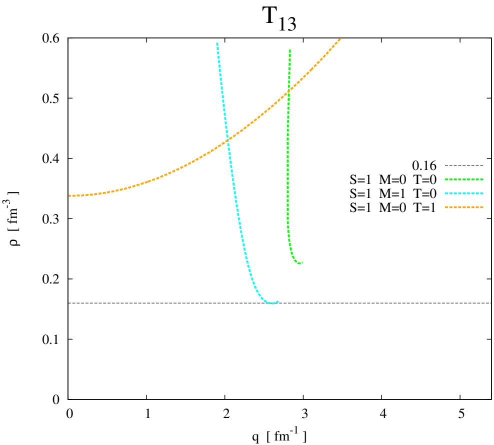

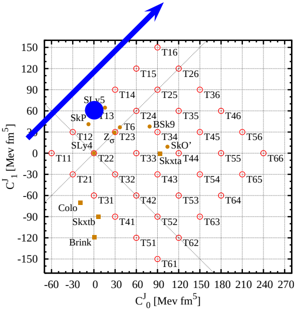

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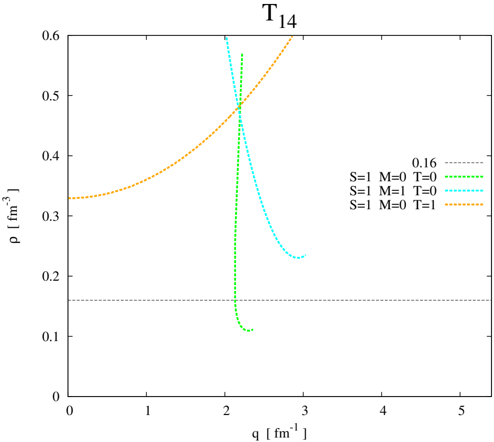

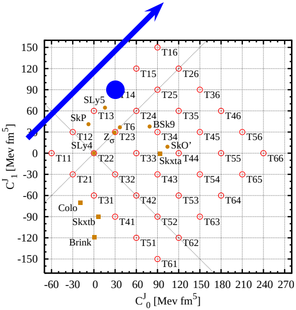

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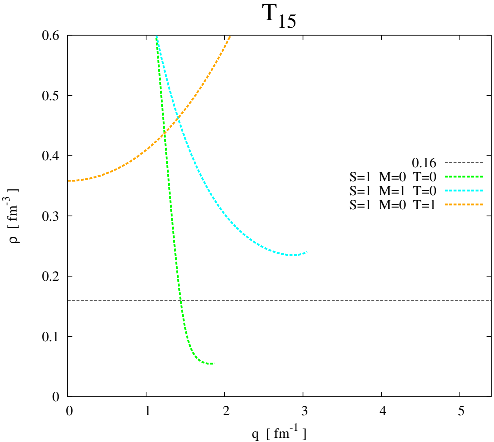

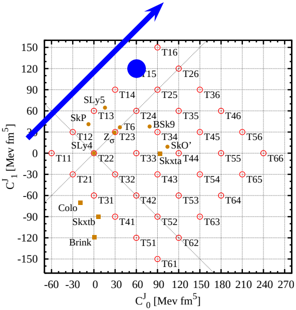

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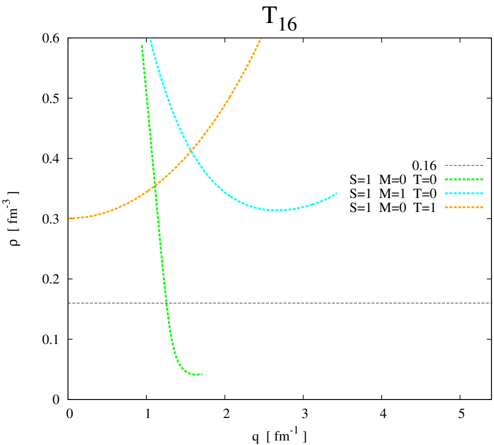

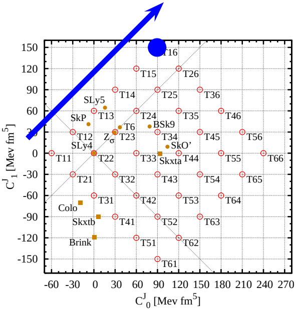

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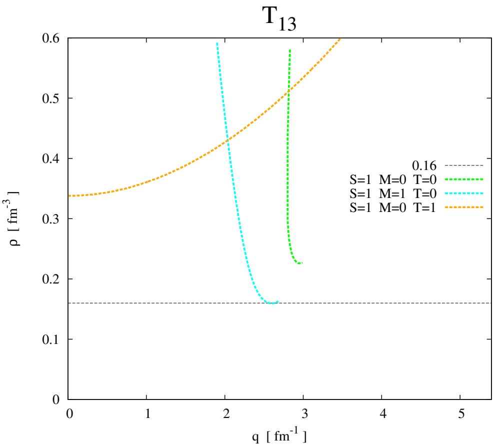

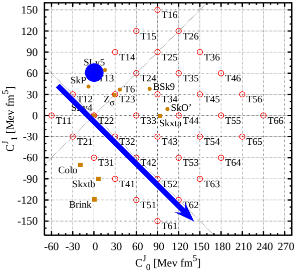

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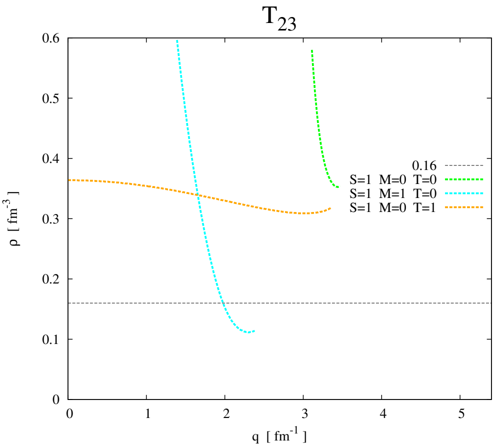

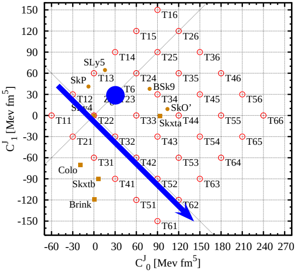

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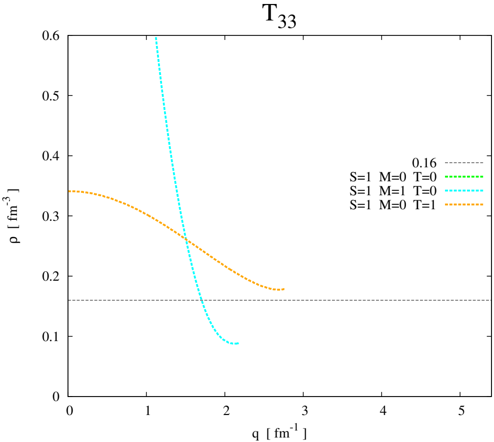
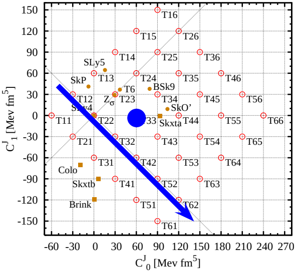
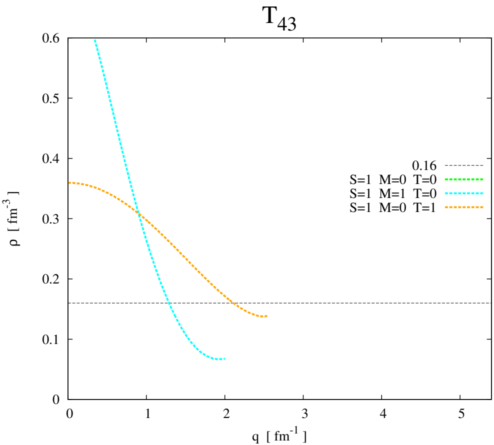
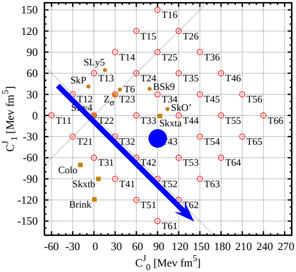


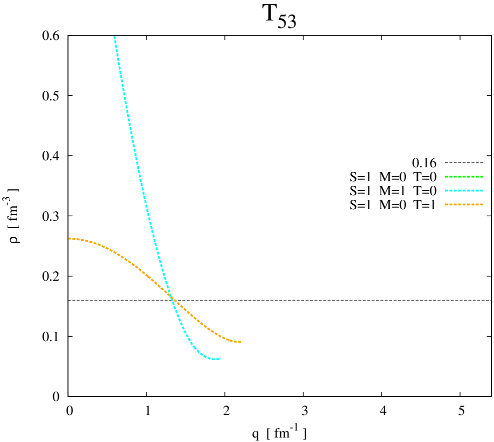


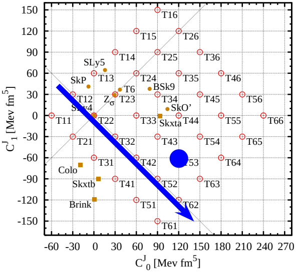
Instabilities in the spin sector



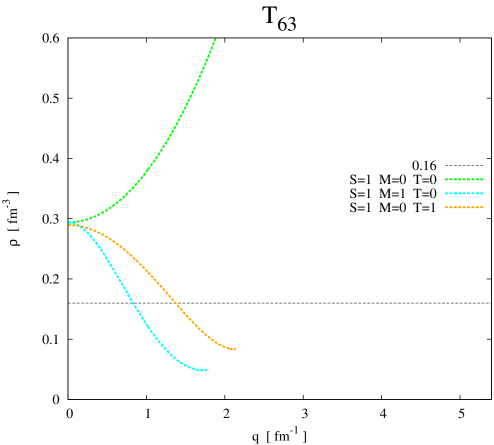


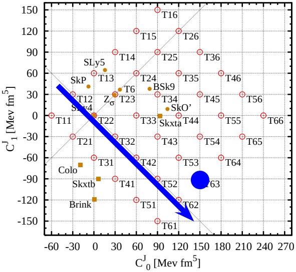
Instabilities in the spin sector



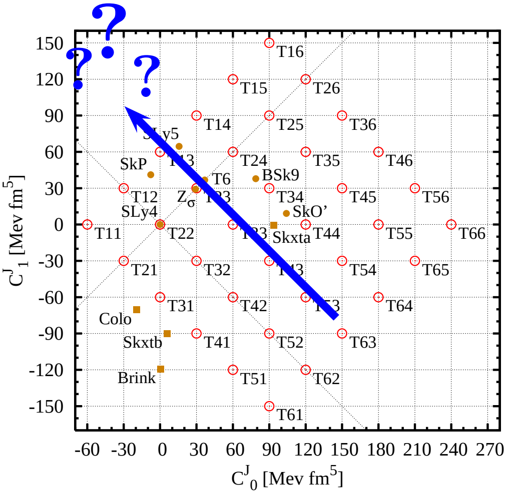


Instabilities in the spin sector

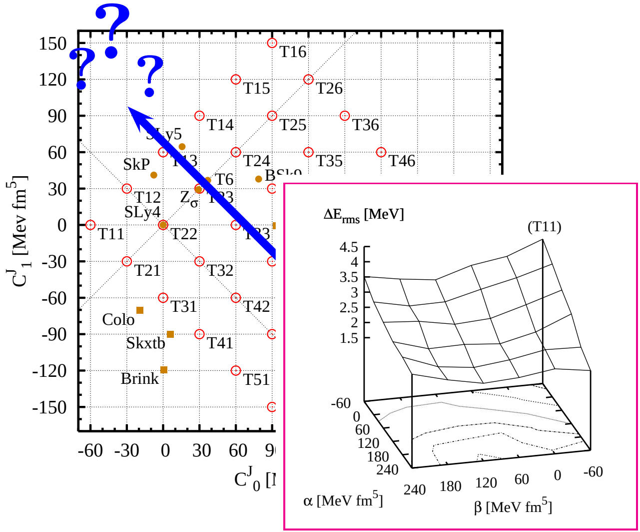




Instabilities in the spin sector



Instabilities in the spin sector



Conclusion

- The "standard" Skyrme EDF needs to be extended and improved
  - at the mean field level
  - for beyond mean field calculations
- Isospin and spin finite size instabilities can easily appear
- The linear response is the tool of choice to detect and avoid these unphysical instabilities
- The code developed in Lyon
  - allows to calculated the linear response from skyrme interactions or functionals
  - implements spin-orbit and tensor contributions
  - implements three body interactions

Collaboration

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