Linear response theory as a tool to detect intabilities

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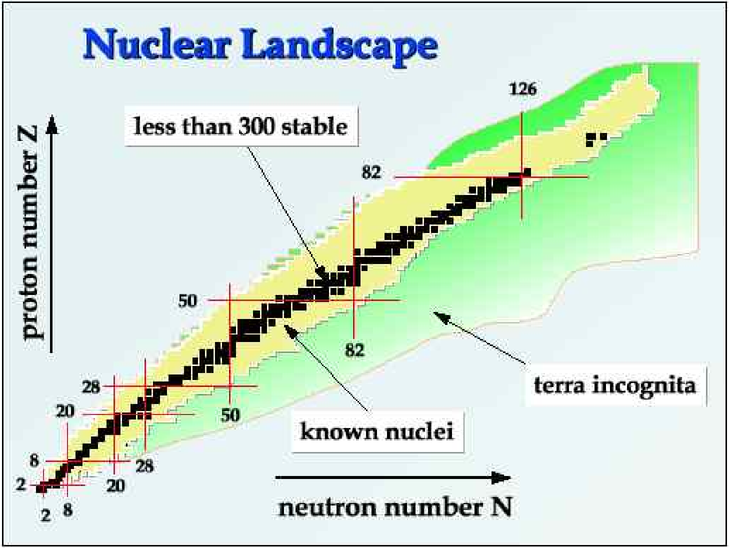
Outline

1. Introduction
2. Linear Response in IM
3. RPA Results
4. RPA Instabilities

Introduction



Skyrme functionals

We can write the total energy of the system for a general Skyrme functional

$$\mathcal{E} = \mathcal{E}_{kin} + \mathcal{E}_{Skyrme} + \mathcal{E}_{pairing} + \mathcal{E}_{Coulomb} + \mathcal{E}_{corr.}$$

Skyrme functional

$$\begin{aligned}\mathcal{E}_{Skyrme} \quad = \quad & \sum_{t=0,1} \int d^3\mathbf{r} \left\{ C_t^{\rho}\left[\rho_0\right]\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}\rho_t\tau_t + C_t^{j}\mathbf{j}_t^2 + C_t^{s}\left[\rho_0\right]s_t^2 \right. \\ & + C_t^{\nabla s}(\nabla\cdot s_t)^2 + C_t^{\Delta s}s_t\cdot\Delta s_t + C_t^{T}s_t\cdot\mathbf{T}_t + C_t^{F}s_t\cdot\mathbf{F}_t + C_t^{\nabla J}\rho_t\nabla\cdot\mathbf{J}_t \\ & \left. + C_t^{\nabla j}s_t\cdot(\nabla\times\mathbf{j}_t) + C_t^{J^{(0)}}(J_t^{(0)})^2 + C_t^{J^{(1)}}(\mathbf{J}_t^{(1)})^2 + C_t^{J^{(2)}}\sum_{\mu\nu=x}^{z} J_{t\mu\nu}^{(2)}J_{t\mu\nu}^{(2)} \right\}\end{aligned}$$

[E . Perlinska et al. Phys. Rev C 69, 014316 (2004))]

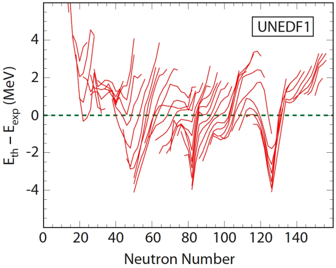
The coupling constants are fitted on data.

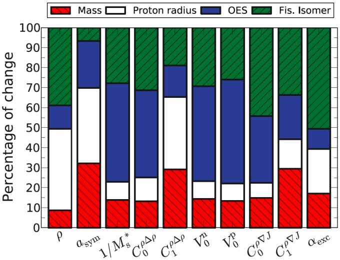
How to determine the coupling constants?

We impose a fitting protocol (observables and pseudo-observables)

- IM properties ($i.e.\ E/A, K_\infty, m^*, ...$)
- Ground state of some nuclei ($i.e.$ ^{40}Ca, ^{48}Ca,^{208}Pb, ...)
- Charge radii
- Spin orbit splitting
- ...

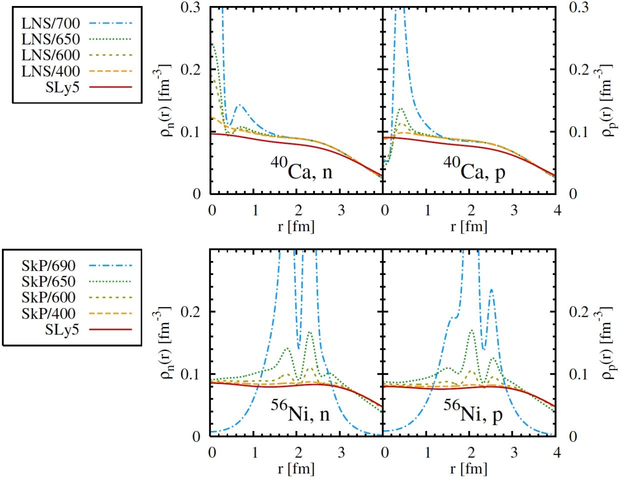
[M . Kortelainen et al. Phys. Rev C 85 (2012)024304]





Good description of masses $\sigma_{rms} = 0.582$ MeV. [S . Goriely et al. Phys. Rev Lett. 112 (2009), 152503]

... unexpected results ...



[T. Lesinski et al. Phys. Rev. C 76, 014312 (2007)]

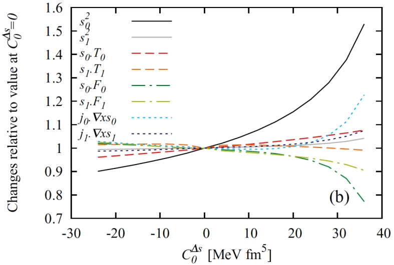
Instabilities

Instabilities can be very difficult to detect. A good way could be to run 3D - codes to test *all* the coupling constant

- Talk of N. Schunck
- Talk of V. Hellemans

Cranking of ^{194}Hg at $J_z = 54\hbar$ with T22 ($C_0^{\Delta s} = 67.2908$ MeV fm^5)

[T. Lesinski et al. Phys. Rev C 76, 014312 (2007)]

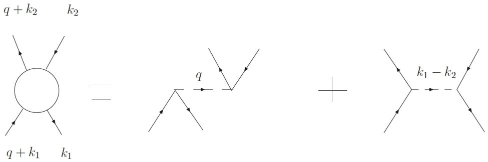


... time consuming calculations!! [V. Hellemas et al. Phys. Rev C 85, 014326 (2012)]

Outline

We consider an in infinite medium in the Hartree-Fock formalism (T=0). We act with an external field

$$\sum_j \exp^{i\mathbf{q}\mathbf{r}} \Theta_\alpha^j \quad \Theta_\alpha^j = 1, \boldsymbol{\sigma}^j, \hat{\tau}^j, \boldsymbol{\sigma}^j \hat{\tau}^j$$



Within the Green function formalism we have for non interacting system

$$G_{HF}(q,\omega,\mathbf{k}_1) = \frac{\theta(k_F - k_1) - \theta(k_F - |\mathbf{k}_1 + \mathbf{q}|)}{\omega + \varepsilon(\mathbf{k}_1) - \varepsilon(|\mathbf{k}_1 + \mathbf{q}|) + i\eta\omega}$$

[C . Garcia-Recio , Ann. Phys. 214, 293-340, 1992]

RPA formalism II

The residual interaction among ph pairs reads

$$V_{\text{ph}}^{(\alpha,\alpha')}(q,\mathbf{k}_1,\mathbf{k}_2) \equiv \langle \mathbf{q}+\mathbf{k}_1,\mathbf{k}_1^{-1},(\alpha)|V|\mathbf{q}+\mathbf{k}_2,\mathbf{k}_2^{-1},(\alpha')\rangle.$$

Second functional derivative of the Skyrme functional

[E . Perlinska et al. Phys. Rev C 69, 014316 (2004))]

$$\begin{aligned}
V_{\text{ph}} &= \frac{1}{4}W_1^{00} + \frac{1}{4}W_1^{01}\hat{\tau}_a\circ\hat{\tau}_b + \frac{1}{4}W_1^{10}\boldsymbol{\sigma}_a\cdot\boldsymbol{\sigma}_b + \frac{1}{4}W_1^{11}\boldsymbol{\sigma}_a\cdot\boldsymbol{\sigma}_b\hat{\tau}_a\circ\hat{\tau}_b \\
&+ \frac{1}{4}\left(W_2^{00} + W_2^{01}\hat{\tau}_a\circ\hat{\tau}_b + W_2^{10}\boldsymbol{\sigma}_a\cdot\boldsymbol{\sigma}_b + W_2^{11}\boldsymbol{\sigma}_a\cdot\boldsymbol{\sigma}_b\hat{\tau}_a\circ\hat{\tau}_b\right) \\
&\times \left[q_1^2 + q_2^2 - \frac{8\pi}{3}q_1 q_2 \sum_{\mu=-1,0,1} Y_\mu^{(1)*}(\hat{q}_1)Y_\mu^{(1)}(\hat{q}_2)\right] \\
&+ \left[+2\vec{\rho}C_1^{\rho,\gamma}\gamma\rho_0^{\gamma-1}\circ(\hat{\tau}_a+\hat{\tau}_b) + 2\gamma C_0^{s\gamma}\rho_0^{\gamma-1}\mathbf{s}_0\cdot(\boldsymbol{\sigma}_a+\boldsymbol{\sigma}_b) + 2\gamma C_1^{s\gamma}\rho_0^{\gamma-1}\vec{\mathbf{s}}\cdot(\boldsymbol{\sigma}_a\circ\hat{\tau}_a+\boldsymbol{\sigma}_b\circ\hat{\tau}_b)\right] \\
&+ 2\left(C_0^{\nabla s} + C_1^{\nabla s}\hat{\tau}_a\circ\hat{\tau}_b\right)\mathbf{q}\cdot\boldsymbol{\sigma}_a\mathbf{q}\cdot\boldsymbol{\sigma}_b + \left(C_0^F + C_1^F\hat{\tau}_a\circ\hat{\tau}_b\right)\left\{\mathbf{k}_{12}\cdot\boldsymbol{\sigma}_a\mathbf{k}_{12}\cdot\boldsymbol{\sigma}_b - \frac{1}{2}\mathbf{q}\cdot\boldsymbol{\sigma}_a\mathbf{q}\cdot\boldsymbol{\sigma}_b\right\} \\
&- i\left(C_0^{\nabla J} + C_1^{\nabla J}\hat{\tau}_a\circ\hat{\tau}_b\right)(\boldsymbol{\sigma}_a+\boldsymbol{\sigma}_b)\cdot[\mathbf{q}\times\mathbf{q}_1 - \mathbf{q}\times\mathbf{q}_2]
\end{aligned}$$

RPA formalism III

The RPA correlated Green function is the solution of Bethe-Salpeter equation

$$\begin{aligned} G_{RPA}^{(\mathrm{S,M,I})}(q,\omega,\mathbf{k}_1) &= G_{HF}(q,\omega,\mathbf{k}_1) \\ &+ G_{HF}(q,\omega,\mathbf{k}_1)\sum_{\mathrm{S',M',I'}}\int\frac{d^3k_2}{(2\pi)^3}V_{ph}^{\mathrm{S,M,I;S',M',I'}}(q,\mathbf{k}_1,\mathbf{k}_2)G_{RPA}^{\mathrm{S',M',I'}}(q,\omega,\mathbf{k}_2) \end{aligned}$$

The response function is now defined as

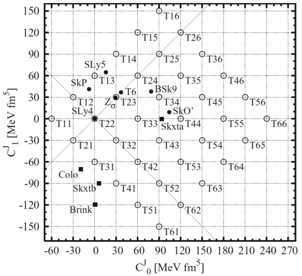
$$\chi_{RPA}^{\alpha}(q,\omega) = g\int\frac{d^3k_1}{(2\pi)^3}G_{RPA}^{\alpha}(q,\omega,\mathbf{k}_1)$$

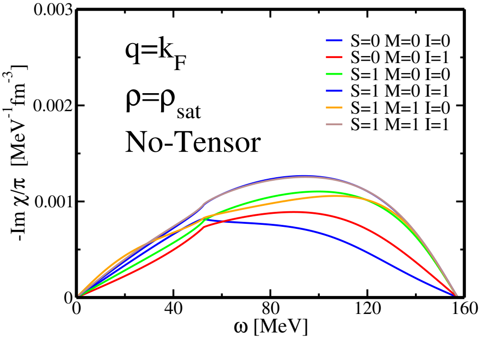
$g=4$ is the degeneracy of SNM.

Outline

An example: T22

T22 has a zero tensor in the spherical g.s.





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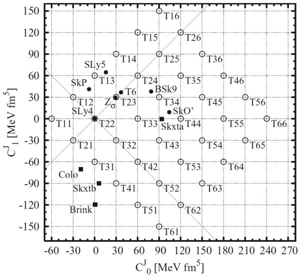
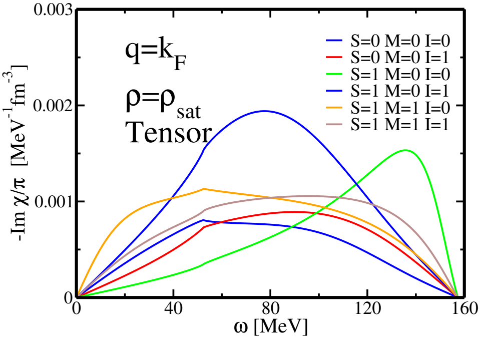




Sum Rules

We can define the k-moments per particle in infinite matter

$$M_k(\mathbf{q})^{(\mathsf{S,M,I})} = -\frac{1}{\pi}\int_0^{+\infty} d\omega \omega^k \Im\left[\chi^{(\mathsf{S,M,I})}(\mathbf{q},\omega)\right]$$

or through the expansions

- for $\omega \rightarrow +\infty$, the positive odd order moments read (M_1,M_3,...)

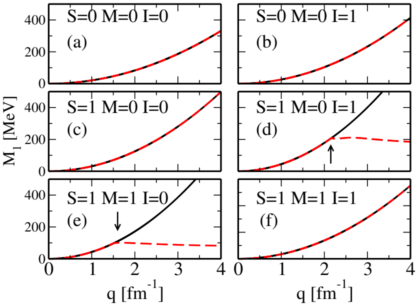
$$\chi^{(\mathsf{S,M,I})}(\omega,\mathbf{q}) \approx \quad 2\rho\sum_{p=0}^{+\infty}(\omega)^{-(2p+2)} M_{2p+1}^{(\mathsf{S,M,I})}(\mathbf{q}),$$

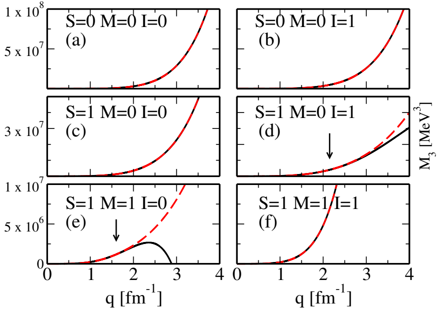
- for $\omega \rightarrow 0$, the negative odd order moments read (M_{-1})

$$\chi^{(\mathsf{S,M,I})}(\omega,\mathbf{q}) \approx -2\rho\sum_{p=0}^{+\infty}(\omega)^{2p} M_{-(2p+1)}^{(\mathsf{S,M,I})}(\mathbf{q}),$$

Results Sum Rules I

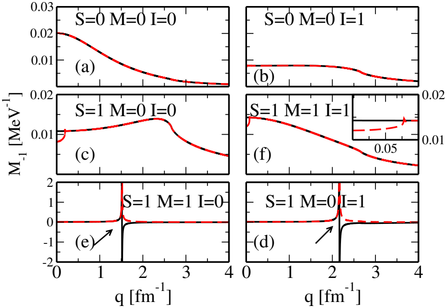
We take T44 as an example and we calculate the odd power sum rules [A . Pastore , Phys. Rev. C 85, 054317 (2012)]

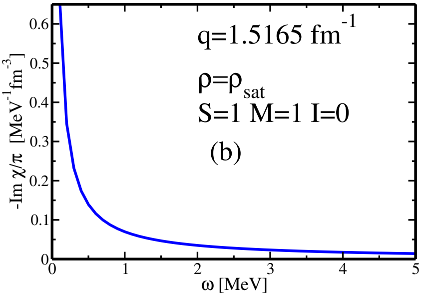




Results Sum Rules II

The M_{-1} sum rule is sensitive to the poles of the response function

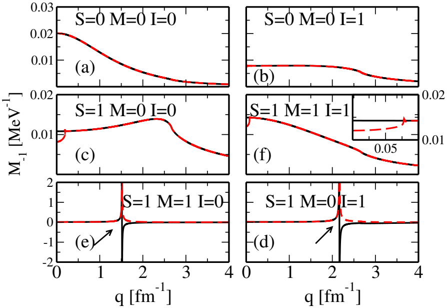


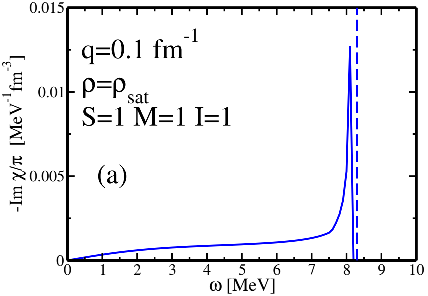


$$1/M_{-1}(q) = 0 \quad \longrightarrow 1/\chi(\omega = 0, q) = 0$$

Results Sum Rules III

When a zero-sound mode appears we loose some strength in the integrated some rules, but it is not an instability.





A single ph transition not damped.

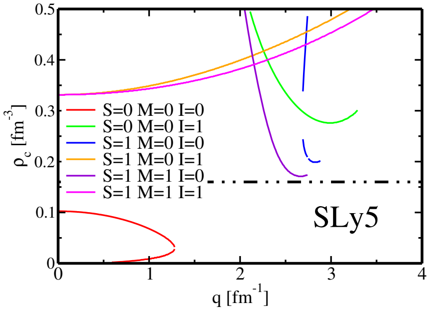
Outline

Instabilities in SNM

Poles

We solve the equation for different values of $\rho \in [0, 0.5]\text{fm}^{-3}$

$$1/M_{-1}^{(\mathsf{S,M,I})}(q) = 0$$



Relations with finite nuclei

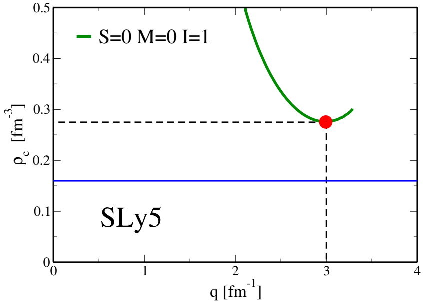
Can we relate a pole in SNM with an instability in a finite nucleus?

Some remarks

- Instabilities of SNM have different origin: spinodal (bound state in EoS), ferromagnetic, ...
- Not all instabilities in SNM have to be related to *problem* of the functional
- Not all the instabilities of finite nuclei can be found in IM (surface effects??) ($\rightarrow$ Hellemans's talk)
- RPA is the quickest method to improve the quality of Skyrme functionals ($\rightarrow$ Schunck's talk)

Example $C_1^{\rho\Delta\rho}$ instability

We Calculate the RPA poles in the S=0, M=0, I=1 channel for SLy5 functional

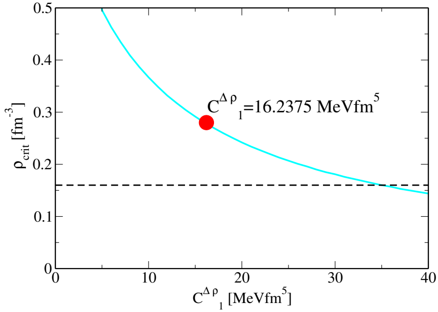


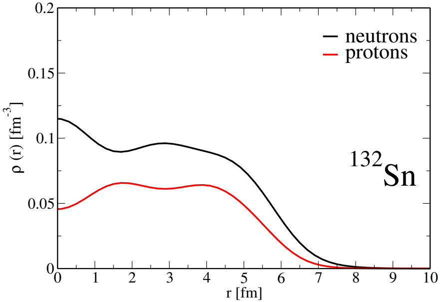
The $C_1^{\rho\Delta\rho} = 16.375$ MeVfm^5 do not contribute to the Landau parameter

$$
\begin{aligned}
N_0^{-1} F_0 &= 2C_0^{\rho 0} + (2+\gamma)(1+\gamma)C_0^{\rho\gamma}\rho_0^{\gamma} + 2k_F^2\,[C_0^{\tau}] \\
N_0^{-1} F_0' &= 2C_1^{\rho 0} + 2C_1^{\rho,\gamma}\rho_0^{\gamma} + 2k_F^2\,[C_1^{\tau}] \\
N_0^{-1} F_1 &= -2k_F^2\,(C_0^{\tau}) \\
N_0^{-1} F_1' &= -2k_F^2\,(C_1^{\tau})
\end{aligned}
$$

Example $C_1^{\rho\Delta\rho}$ instability

In the functional spirit we change $C_1^{\rho\Delta\rho}$ and we use a spherical HFB code





[A. Pastore et al., IJME 21, vol.5 1250040 (2012)]

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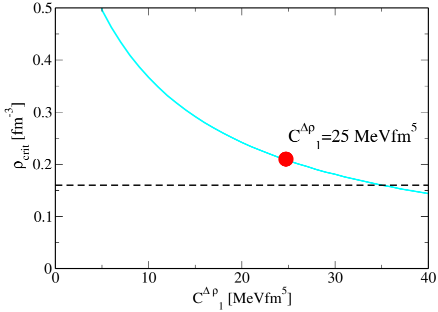

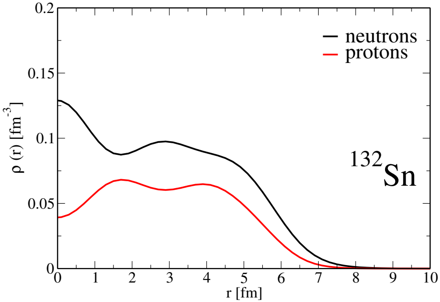

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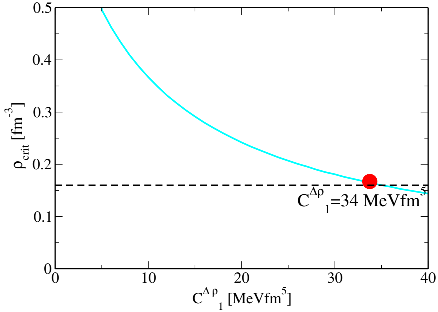

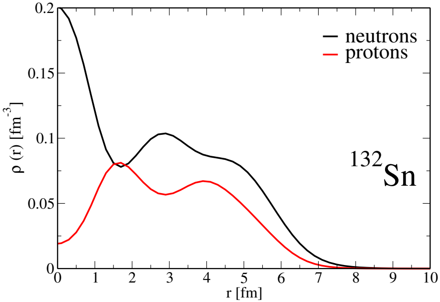

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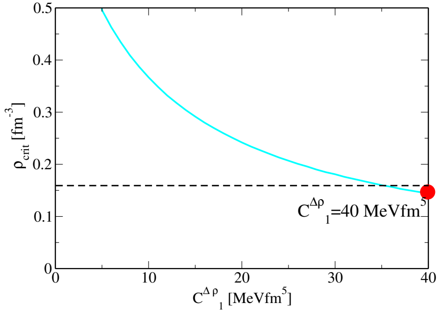

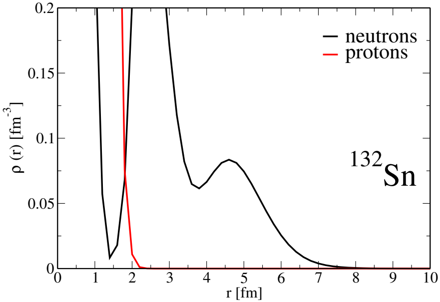

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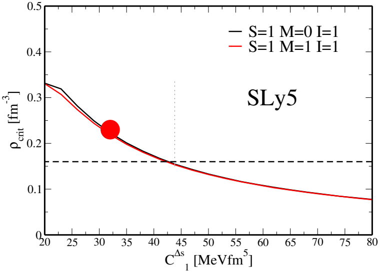
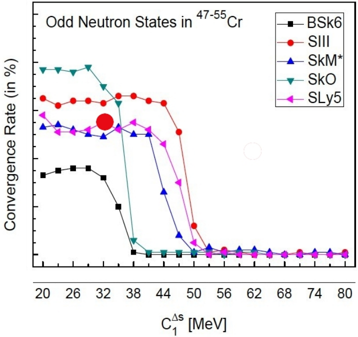
Example $C_1^{s\Delta s}$ instability

Blocking calculations with SLY5 *modified* ($i.e.$ $C_0^{s\Delta s} = 0$)





[N Schunck, T Duguet et al. (in preparation)]

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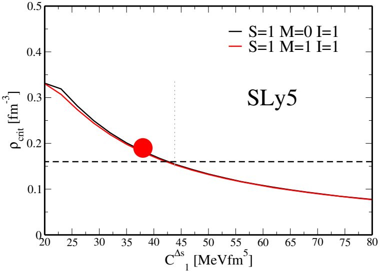

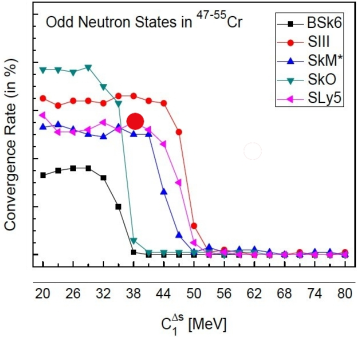

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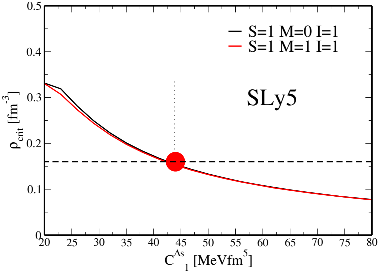

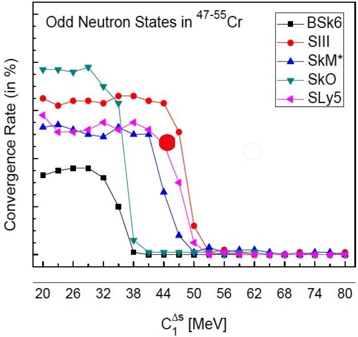

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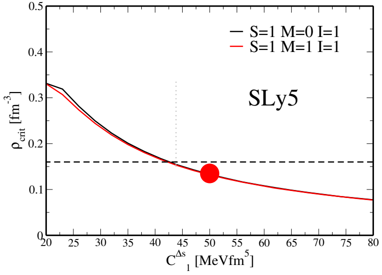

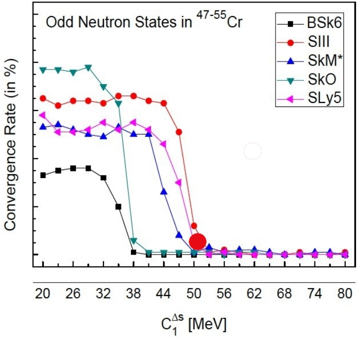

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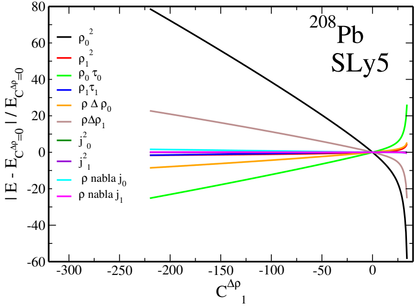
Some conclusions

A tool to detect instabilities

- We found a relation among the two systems
- 1. Systematic calculations with HFB codes (spherical and 3D...)
  2. Determine the *sensitivity* of the RPA code
- We can find instabilities although Landau parameters are reasonable ($long - wavelength$ limit)

Spherical calculations I

It is not easy to detect an instability in a finite nucleus. Example: ^{208}Pb using *Lenteur* [spherical HFB code] K. Bennaceur, private

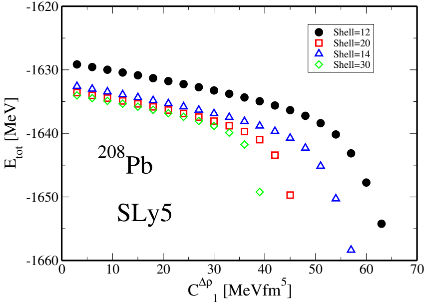


What is an instability?

- The code stops converging (explosion $\rightarrow right - side$)
- The code oscillates among two minima (possible deformation$\rightarrow left - side$)

Spherical calculations II

Example II: ^{208}Pb using *HOSPHE* [spherical HFB code] J. Toivanen et al. Comp. Phys. Com.181, 1641 (2010)

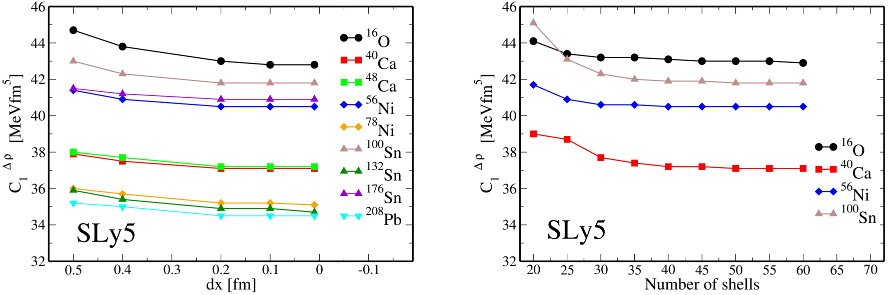


Model dependent!!

We have to be very careful since using small basis can hide the problem!

Comparing two basis

We observe that the *critical* value of $C_1^{\rho\Delta\rho}$ depends on: the nucleus, the basis type, the basis size...



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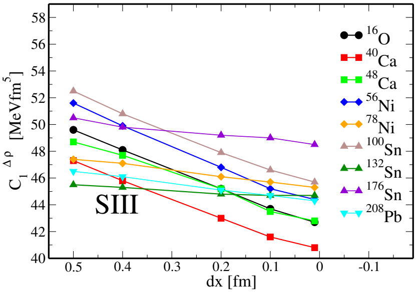
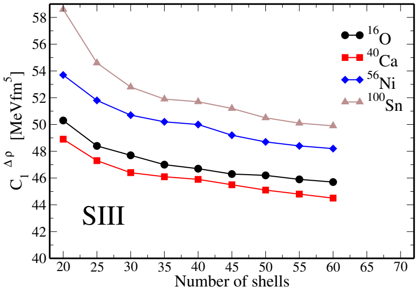
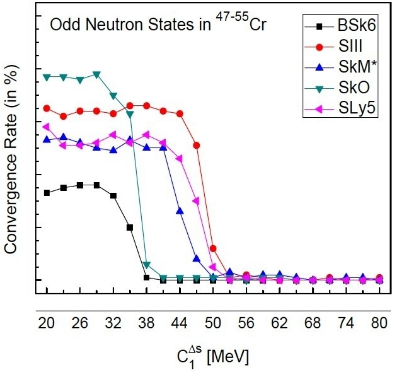


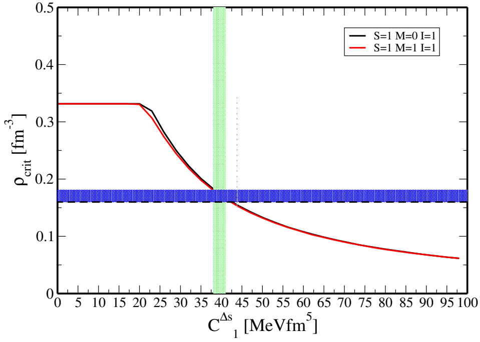


Safe region: SLY5 functional

We want to build a functional without pathologies

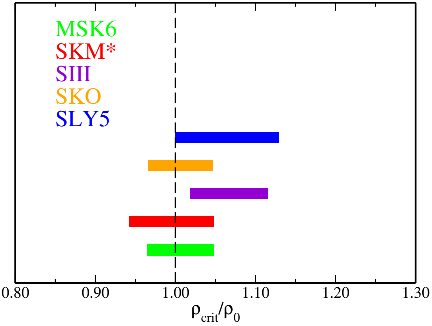
- We can define a *dangerous* region in SNM
- We do not want to remove *all* the instabilities





[T Duguet , private communication]

Safe region: SLY5 functional



Safe region

Although the critical vale of the coupling constant strongly depends on the functional, the *band* is quite similar!

- The band allows us to see if a functional is stable or not using the RPA code!

Conclusions

Status of the work

- We derived the RPA formalism for the most general 2-body Skyrme functional
- 3-body terms have been added [J. Sadoudi et al. , private communication]
- D-wave term has been added [K. Bennaceur et al. , private communication]
- We extended the formalism to Pure Neutron Matter
- We found the relation among IM and finite nuclei's instabilities

... and future development

- Asymmetric nuclear matter
- Finite temperature calculations
- Fitting new forces without instabilities

Thank you!!!

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