

Skyrme N2LO functionals: first results on finite nuclei

D. Davesne, P. Becker, A. Pastore, J. Navarro

Orsay, October 2017

- N2LO/N3LO extensions : physical motivation
- Results in infinite matter
- Extension of Gogny interaction
- Application in astrophysics
- Application to finite nuclei: first results
- Conclusion



N2LO/N3LO extensions : physical motivation

Skyrme N2LO
functionals: first results
on finite nuclei

D. Davesne, P. Becker,
A. Pastore, J. Navarro

Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

Linear response
formalism

- Construction of new effective interactions necessary!
- Instabilities experienced with popular interactions (Skyrme, Gogny)
- Initial idea (Skyrme) : expansion in powers of momentum (k^2)
→ systematic expansion up to k^n ... which n ???
- N2LO : $n = 2$; N3LO : $n = 3$; ...
- Gogny: e^{-r^2/μ^2} , M3Y : $e^{-\mu r}/\mu r$, ... : **SAME** kind of expansion

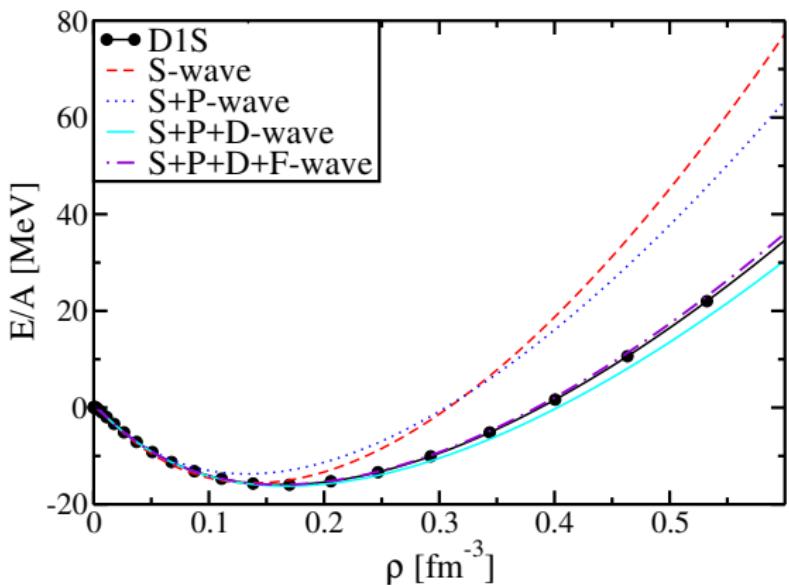
[F. Raimondi et al., Phys.Rev. C84 (2011) 064303]

N2LO/N3LO extensions : physical motivation

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functionals: first results
on finite nuclei

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Finite-range interaction D1S: infinite sum of partial waves.



Only S, P, D and F ($\ell < 4$) waves necessary → **N3LO good enough**

Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

Linear response
formalism

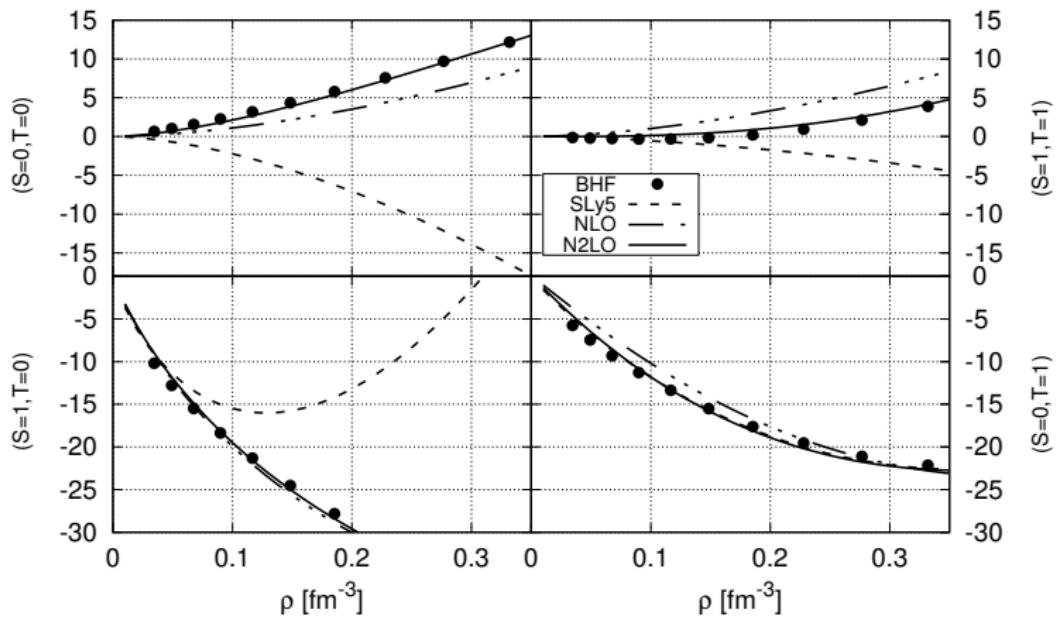
Skyrme pseudo-potential N2LO/N3LO

$$\begin{aligned} \mathcal{V}(\mathbf{r}_1, \mathbf{r}_2) = & t_0 (1 + x_0 P_\sigma) + \frac{1}{6} t_3 (1 + x_3 P_\sigma) \rho^\alpha(R) \\ & + \frac{1}{2} t_1 (1 + x_1 P_\sigma) [\mathbf{k}'^2 + \mathbf{k}^2] + t_2 (1 + x_2 P_\sigma) \mathbf{k}' \cdot \mathbf{k} \\ & + \frac{1}{4} t_1^{(4)} (1 + x_1^{(4)} P_\sigma) [(\mathbf{k}^2 + \mathbf{k}'^2)^2 + 4(\mathbf{k}' \cdot \mathbf{k})^2] \\ & + t_2^{(4)} (1 + x_2^{(4)} P_\sigma) (\mathbf{k}' \cdot \mathbf{k})(\mathbf{k}^2 + \mathbf{k}'^2) \quad \left. \right\} \text{Skyrme N1LO} \\ & + \frac{1}{2} t_1^{(6)} (1 + x_1^{(6)} P_\sigma) (\mathbf{k}'^2 + \mathbf{k}^2) [(\mathbf{k}'^2 + \mathbf{k}^2)^2 + 12(\mathbf{k}' \cdot \mathbf{k})^2] \\ & + t_2^{(6)} (1 + x_2^{(6)} P_\sigma) (\mathbf{k}' \cdot \mathbf{k}) [3(\mathbf{k}'^2 + \mathbf{k}^2)^2 + 4(\mathbf{k}' \cdot \mathbf{k})^2] \quad \left. \right\} \text{Skyrme N2LO} \\ & \quad \left. \right\} \text{Skyrme N3LO} \end{aligned}$$

- D and F partial waves included
- Gauge invariance
- Also includes:
 - spin-orbit term W_0
 - tensor terms

Infinite matter: (S, T) channels N2LO

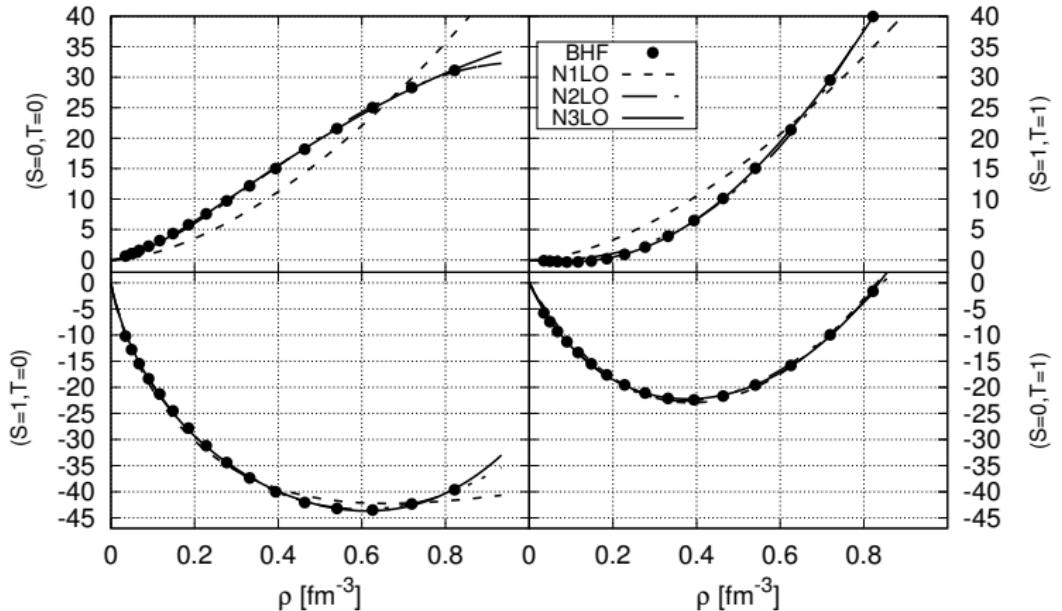
- Used as a preliminary test before dealing with finite nuclei
 - First step: (S, T) channels
 - Results compared to BHF calculations from Baldo *et al.* (1997)



Infinite matter: (S, T) channels N3LO

Skyrme N2LO
functionals: first results
on finite nuclei

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A. Pastore, J. Navarro

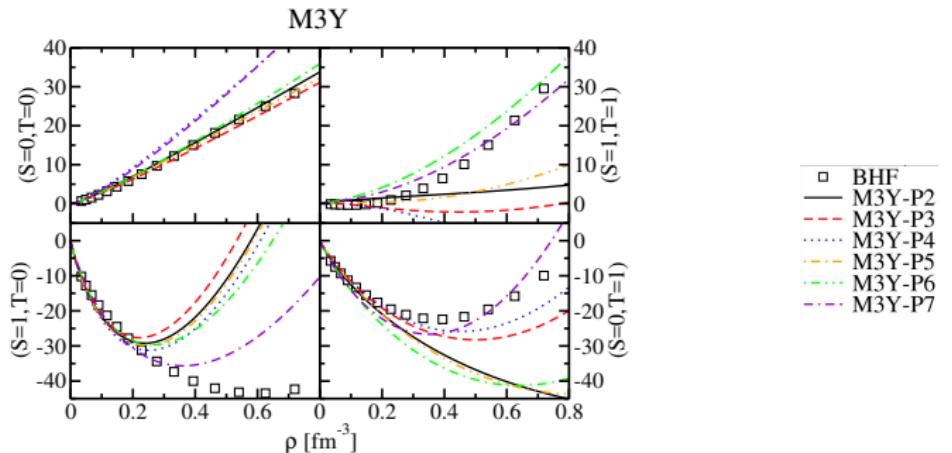


- Agreement up to $\rho = 0.8 \text{ fm}^{-3}$
- Exploration of a new parameter space

Infinite matter: (S, T) channels M3Y

Skyrme N2LO
functionals: first results
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- M3Y takes into account nuclei **and** (S, T) channels: both are **not** incompatible

Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

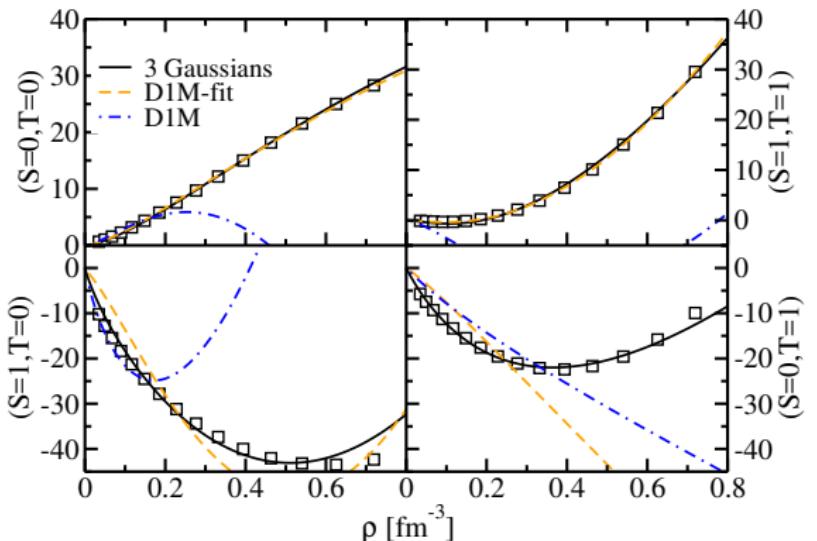
Conclusion and
perspectives

Linear response
formalism

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Not possible...



... except with a third gaussian

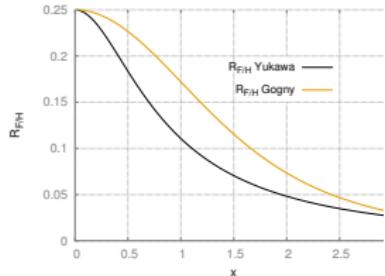
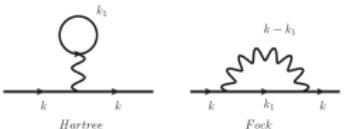
Determination of the three ranges

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Physical meaning of a range :

- Yukawa potential: related to masses (770, 490, 140 MeV)
 - Gaussian potential??? → definition via the self-energy



Example:

$$m_\rho = 770 \text{ MeV}$$

$\rightarrow \mu_Y^{-1} = 0.256$ fm

$$\rightarrow R(\mu_Y^{-1}) = 0.228 = R(\mu_G)$$

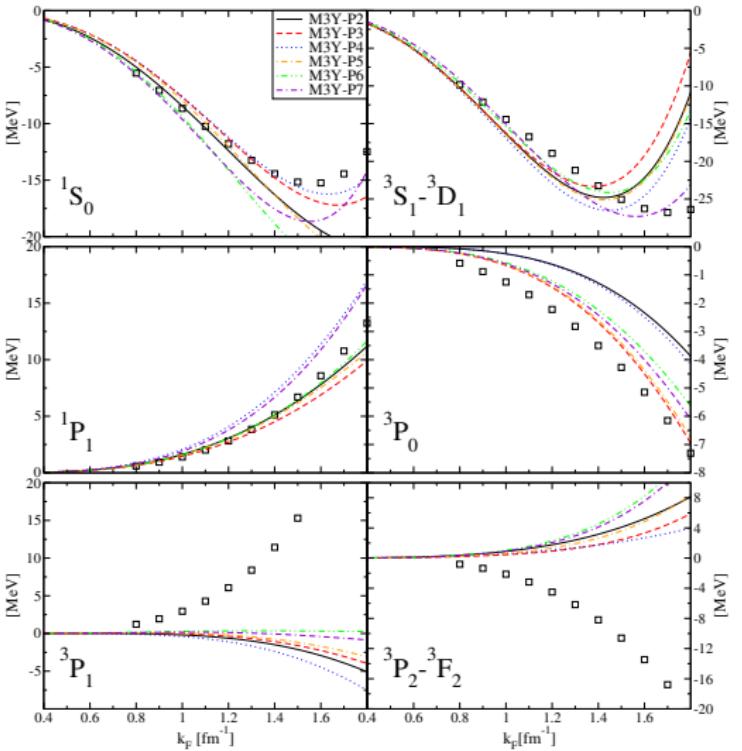
$\rightarrow \mu_G = 0.475$ fm

→ ranges: $\mu_1 = 0.475$ fm, $\mu_2 = 0.746$ fm, $\mu_3 = 1.964$ fm

Partial waves $^{2S+1}L_J$ with M3Y

Skyrme N2LO
functionals: first results
on finite nuclei

D. Davesne, P. Becker,
A. Pastore, J. Navarro



Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

Linear response
formalism

Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

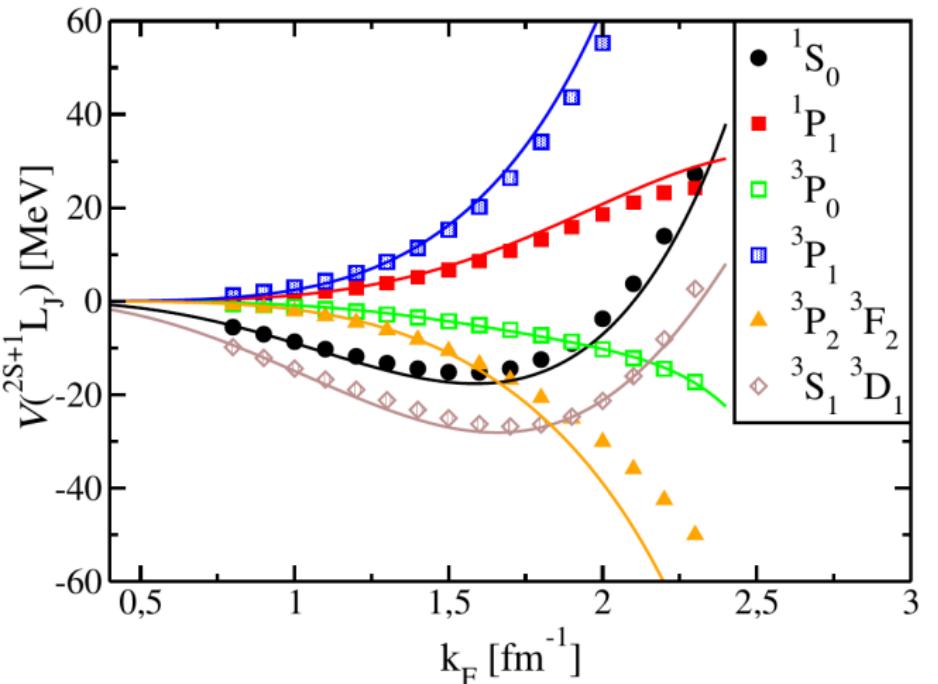
Application to spherical
nuclei

First results

Conclusion and
perspectives

Linear response
formalism

Partial waves with Skyrme N3LO



High degree of flexibility!

Application to astrophysics

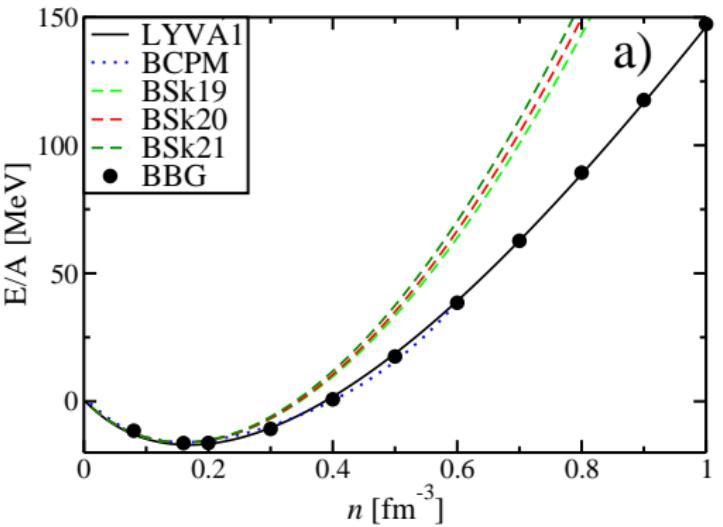
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functionals: first results
on finite nuclei

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A. Pastore, J. Navarro

Goal: only one
parametrisation
for all quantities

BHF calculations
as reference

LYVA1 =
N3LO Skyrme
parametrisation
for astrophysics



Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

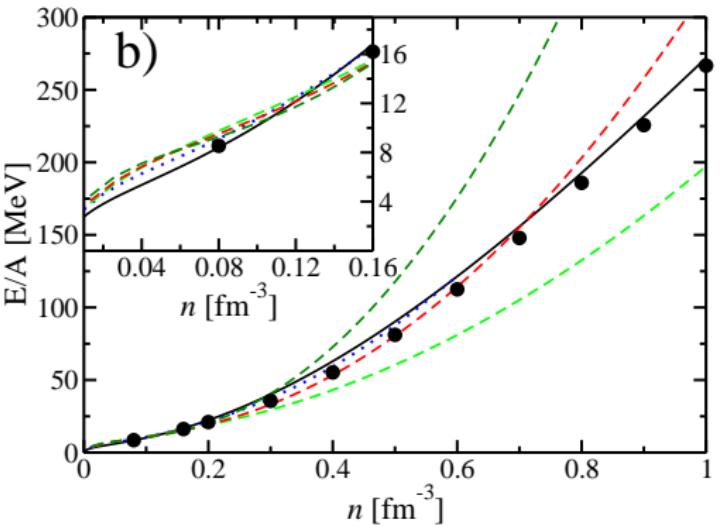
Linear response
formalism

Application to astrophysics

Goal: only one parametrisation for all quantities

BHF calculations as reference

LYVA1 =
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Skyrme N2LO functionals: first results on finite nuclei

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A. Pastore, J. Navarro

Introduction

Infinite matter calculations

Application to astrophysics LYVA1

Application to spherical nuclei

First results

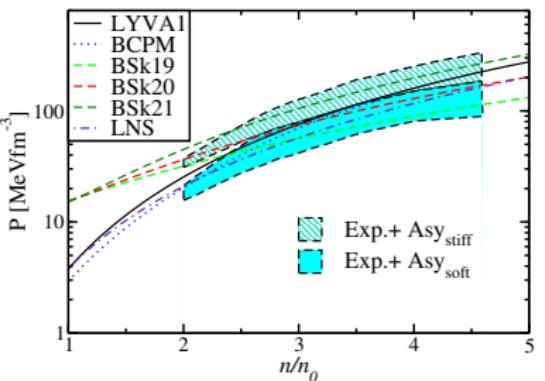
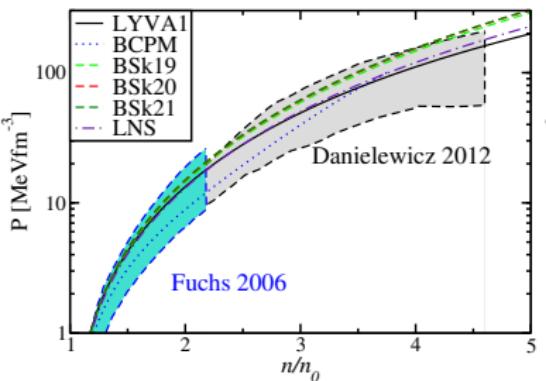
Conclusion and perspectives

Linear response formalism

Application to astrophysics

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$$P = n^2 \frac{\partial(E/A)}{\partial n}$$



Experimental constraints satisfied by **LYVA1**

Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

Linear response
formalism

Application to astrophysics

Skyrme N2LO
functionals: first results
on finite nuclei

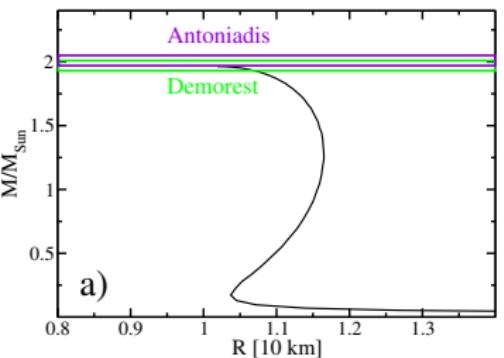
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LYVA1 also reproduces :

- INM properties
- Symmetry energy
- Causality
- Effective masses splitting
- ...

LYVA1 compatible with
a neutron star of $2 M_{\odot}$.
Here, we have $M=1.96 M_{\odot}$.

TOV equations solved



Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

Linear response
formalism

Finite nuclei: N2LO mean-field equation

$$\begin{aligned}\epsilon R &= A_4 R^{(4)} + A_3 R^{(3)} + A_{2R} R^{(2)} + A_{1R} R' + A_{0R} R \\ &+ \frac{\ell(\ell+1)}{r^2} \left[A_{2C} R^{(2)} + A_{1C} R' + A_{0C} R + \frac{\ell(\ell+1)}{r^2} A_{0CC} R \right] \\ &+ C_{jls} \left[W_{2R} R^{(2)} + W_{1R} R' + W_{0R} R + \frac{\ell(\ell+1)}{r^2} W_{0C} R \right]\end{aligned}$$

Introduction

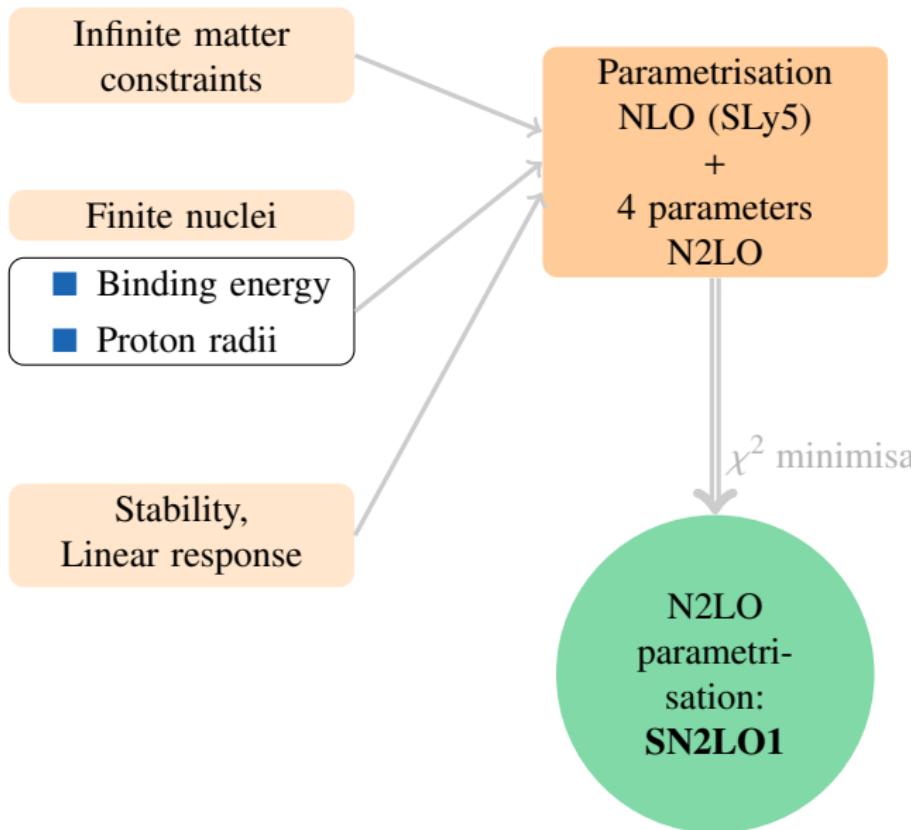
Infinite matter
calculationsApplication to
astrophysics LYVA1Application to spherical
nuclei

First results

Conclusion and
perspectivesLinear response
formalism

- 14 parameters, **4 new**
- New spin-orbit contributions: W_{2R} , W_{1R} , $\frac{\ell(\ell+1)}{r^2} W_{0C}$
- No particular behavior at origin (same as Skyrme)
- New term: $\left(\frac{\ell(\ell+1)}{r^2}\right)^2$ (possible applications)

Fitting protocol



$\rho_0, E/A(\rho_0),$
 $m^*/m, K_{\infty}, J$
Neutron matter

$^{40,48}\text{Ca}$
 ^{56}Ni
 $^{100,132}\text{Sn}$
 ^{208}Pb

Parameter W_0

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Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

Linear response
formalism

First results: infinite matter

Skyrme N2LO
functionals: first results
on finite nuclei

D. Davesne, P. Becker,
A. Pastore, J. Navarro

Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

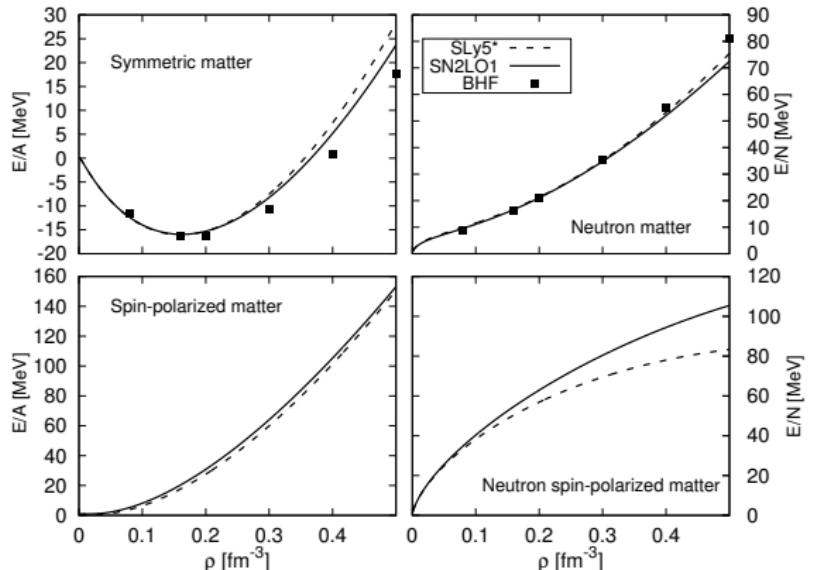
Linear response
formalism

	SN2LO1	SLy5*	Constraint	Error	Result
ρ_0 [fm $^{-3}$]	0.162	0.161	0.16	0.02	✓
E/A(ρ_0) [MeV]	-15.95	-16.02	-16.0	0.1	✓
K_∞ [MeV]	221.9	229.8	230	20	✓
m^*/m	0.709	0.696	0.7	0.02	✓
J [MeV]	31.95	32.03	32.01	2.0	✓

Equation of state of SN2LO1

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functionals: first results
on finite nuclei

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N2LO
interaction
close to
ab initio
calculations

No ferro-
magnetic
transition

Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

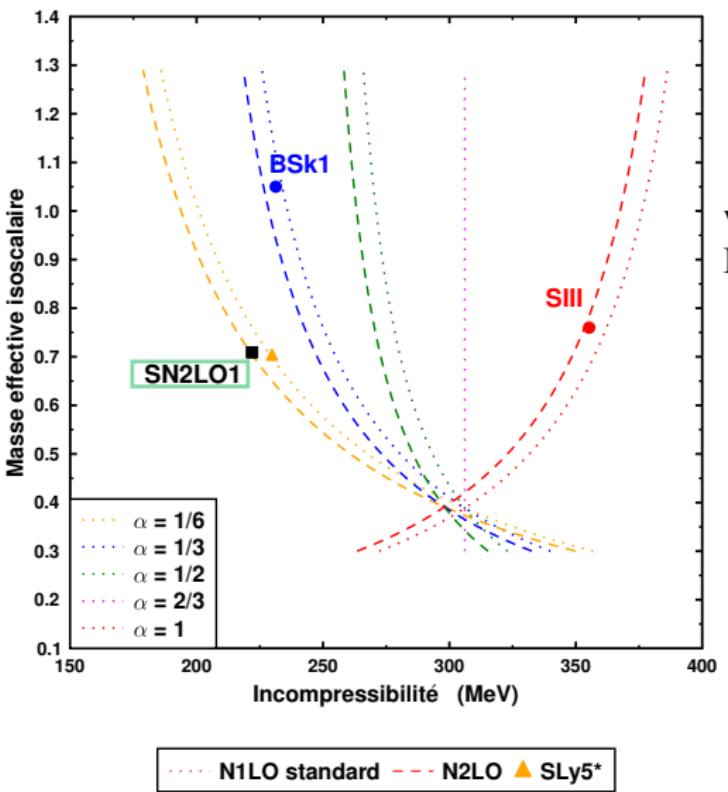
Conclusion and
perspectives

Linear response
formalism

Correlation incompressibility/effective mass

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functionals: first results
on finite nuclei

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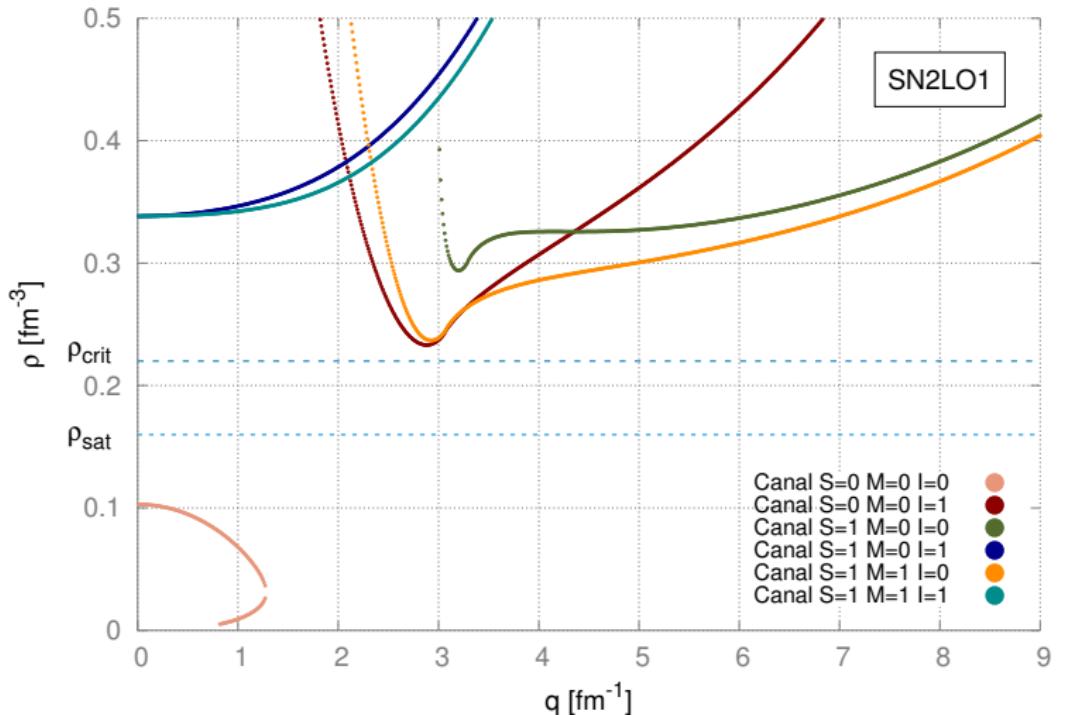
$$K_\infty = A \frac{m}{m^*} + B$$

where

$$\mathbf{B} = B_{N1LO} + B_{N2LO}$$

First results

Stability SN2LO1



$$\rho_{\text{crit}} = 1.4 \rho_{\text{sat}}$$

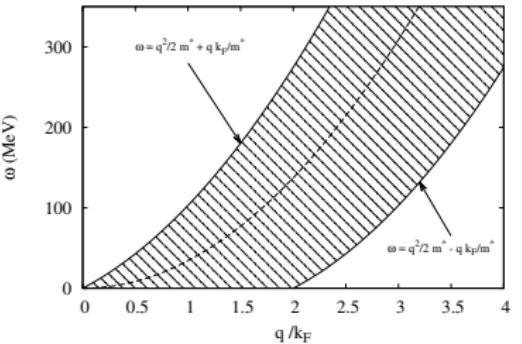
Interaction
N2LO stable

Response function - Formalism

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functionals: first results
on finite nuclei

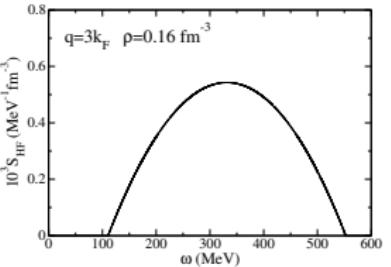
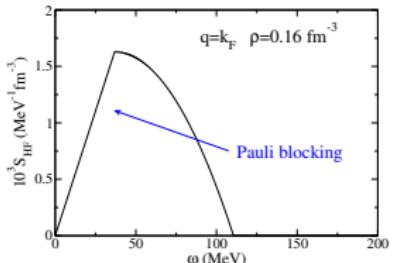
Domain for allowed excitations :

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Response function of a free Fermi gas (at zero temperature):

First results



Response function - Formalism

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functionals: first results
on finite nuclei

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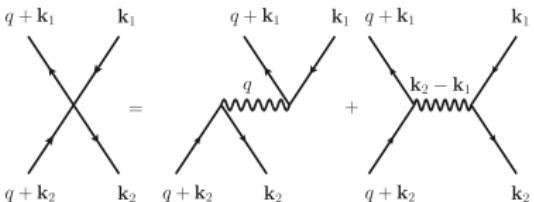
Response function of an interacting gas of nucleons....

The RPA propagator is the solution of Bethe-Salpeter equation :

$$G_{RPA}^{(\text{SMI})}(q, \omega, \mathbf{k}_1) = G_{HF}(q, \omega, \mathbf{k}_1) + G_{HF}(q, \omega, \mathbf{k}_1) \sum_{(\text{S'M'T'})} \int \frac{d^3 k_2}{(2\pi)^3} V_{ph}^{(\text{SMI}; \text{S'M'T'})}(q, \mathbf{k}_1, \mathbf{k}_2) G_{RPA}^{(\text{S'M'T'})}(q, \omega, \mathbf{k}_2)$$

with : $V_{ph}^{(\alpha, \alpha')}(q, \mathbf{k}_1, \mathbf{k}_2) = \langle \mathbf{q} + \mathbf{k}_1, \mathbf{k}_1^{-1}, (\alpha) | V_{eff} | \mathbf{q} + \mathbf{k}_2, \mathbf{k}_2^{-1}, (\alpha') \rangle$

Excitation : $\sum_j \exp^{i\mathbf{qr}} \Theta_\alpha^j \quad \Theta_\alpha^j = 1, \sigma^j, \hat{\tau}^j, \sigma^j \hat{\tau}^j$



Response function - Formalism

Consider the residual interaction in the simplest case :

$$V_{ph}^{(\alpha, \alpha')}(\mathbf{k}_1, \mathbf{k}_2) = \delta(\alpha, \alpha') V_{ph}^{(\alpha)}(q, \omega)$$

→ response function :

$$\chi_{RPA}^{(\alpha)}(q, \omega) = \frac{\chi_{HF}(q, \omega)}{1 - V_{ph}^{(\alpha)}(q, \omega) \chi_{HF}(q, \omega)}$$

→ $\text{Im}\chi_{RPA}(q, \omega) \propto \text{Im}\chi_{HF}(q, \omega)$: **same** domain of definition as the free Fermi gas

→ collective mode $1 - V_{ph}^{(\alpha)} \chi_{HF} = 0$ when $\text{Im}\chi_{HF}(q, \omega) = 0$! (**outside** of the shaded domain!)

Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

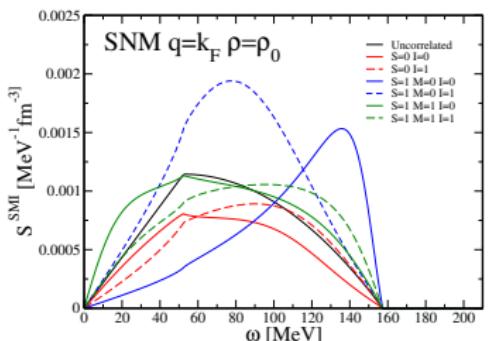
Linear response
formalism

Response function - Formalism

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functionals: first results
on finite nuclei

Effective interaction : Skyrme

$$\begin{aligned}
V_{\text{eff}} = & \color{blue}{t_0} \left(1 + \color{blue}{x_0} \hat{P}_\sigma \right) + \color{blue}{t_3} \left(1 + \color{blue}{x_3} \hat{P}_\sigma \right) \rho_0^\alpha && \text{local} \\
+ \frac{1}{2} \color{blue}{t_1} \left(1 + \color{blue}{x_1} \hat{P}_\sigma \right) \left(\mathbf{k}'^2 + \mathbf{k}^2 \right) + & \color{blue}{t_2} \left(1 + \color{blue}{x_2} \hat{P}_\sigma \right) \mathbf{k}' \cdot \mathbf{k} && \text{non local} \\
& + i \color{blue}{W_0} (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\mathbf{k}' \times \mathbf{k}) && \text{spin-orbit} \\
+ \frac{1}{2} \color{red}{t_e} \left\{ \left[3(\boldsymbol{\sigma}_1 \cdot \mathbf{k}')(\boldsymbol{\sigma}_2 \cdot \mathbf{k}') - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \mathbf{k}'^2 \right] + \text{h.c.} \right\} && \text{tensor} \\
+ \frac{1}{2} \color{red}{t_o} \left\{ \left[3(\boldsymbol{\sigma}_1 \cdot \mathbf{k}')(\boldsymbol{\sigma}_2 \cdot \mathbf{k}) - (\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \mathbf{k}' \cdot \mathbf{k} \right] + \text{h.c.} \right\}
\end{aligned}$$

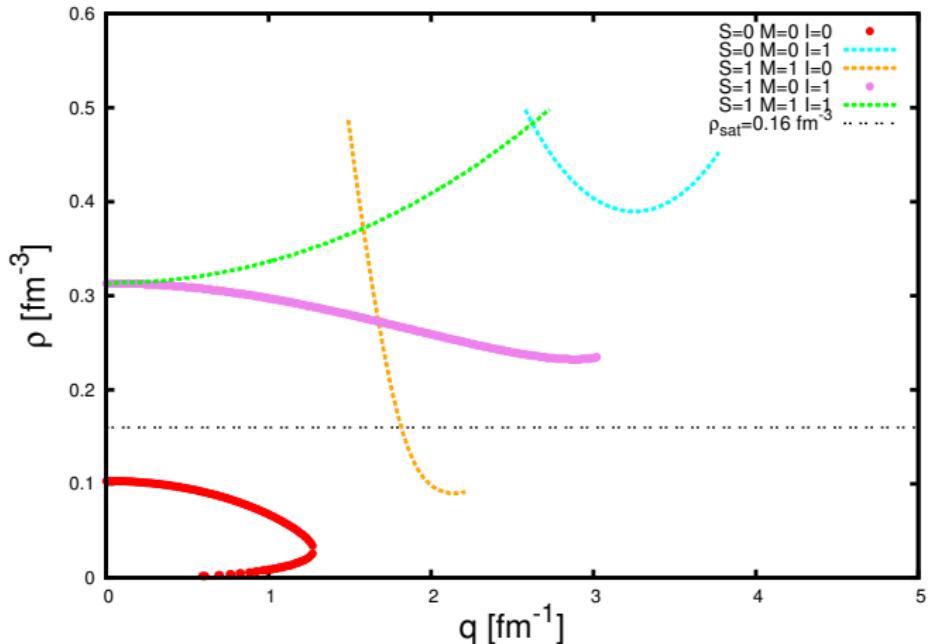


Calculations done : Skyrme/Landau residual interaction, SNM, ASM, PNM, zero and finite temperature

Instabilities

An instability in the functional causes an infinity in the response function :

$$1/\chi^{\text{SMI}}(\omega = 0, q) = 0$$



Instabilities in the different spin/isospin channels (S,M,I) for T22.

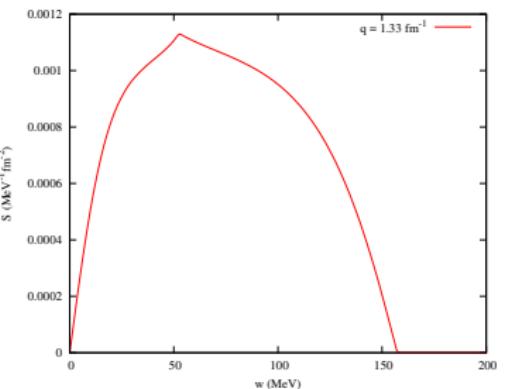
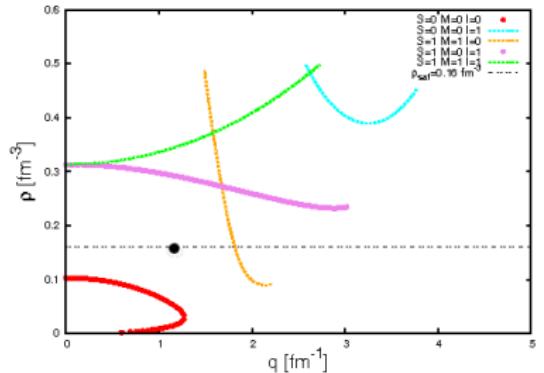
Instabilities

Skyrme N2LO
functionals: first results
on finite nuclei

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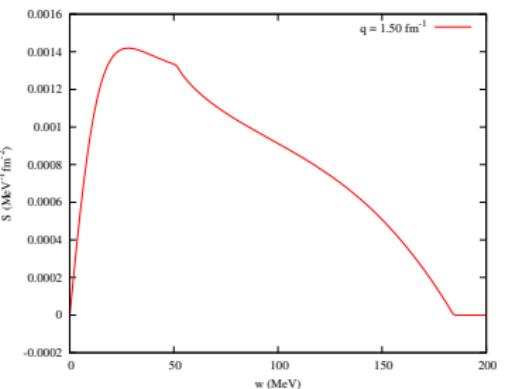
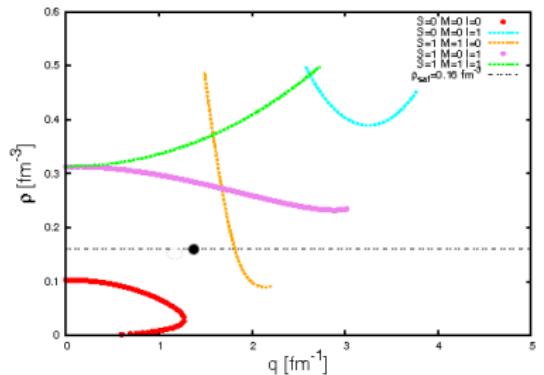
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functionals: first results
on finite nuclei

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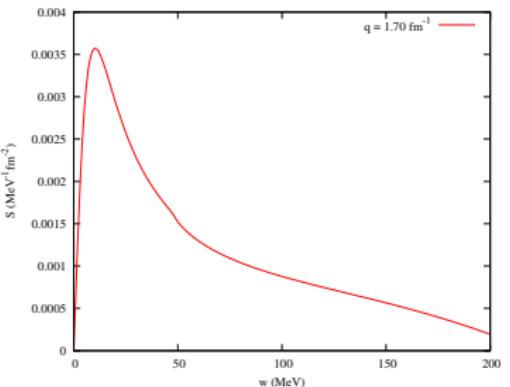
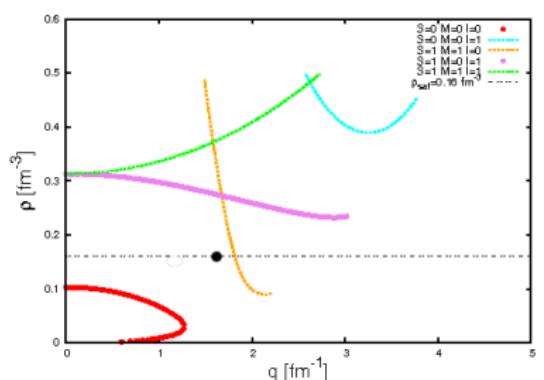
Instabilities

Skyrme N2LO
functionals: first results
on finite nuclei

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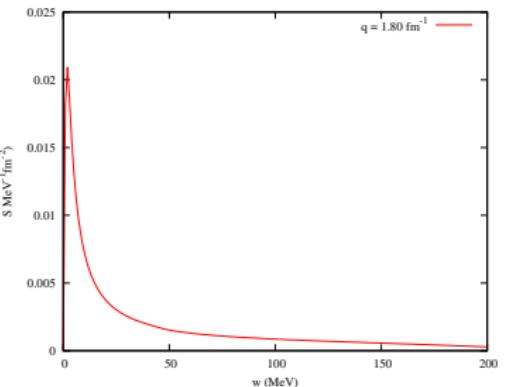
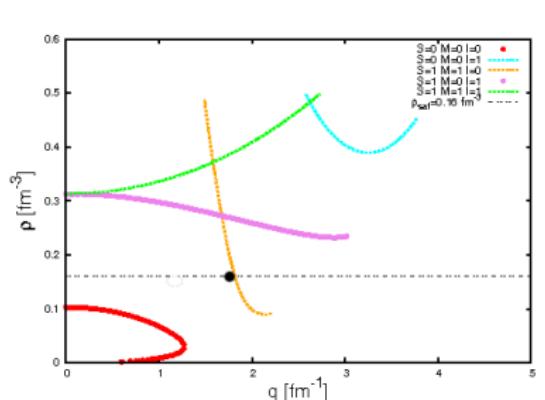
Instabilities

Skyrme N2LO
functionals: first results
on finite nuclei

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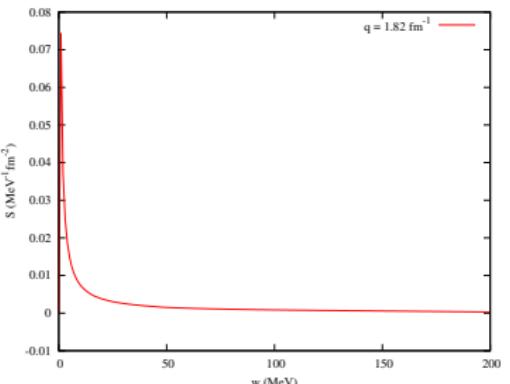
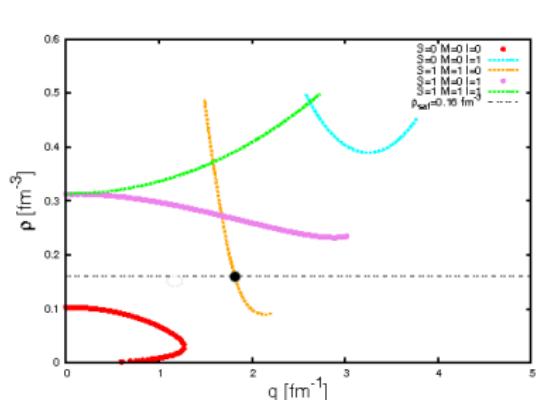
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Skyrme N2LO
functionals: first results
on finite nuclei

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An instability in the functional causes an infinity in the response function :

$$1/\chi^{\text{SMI}}(\omega = 0, q) = 0$$

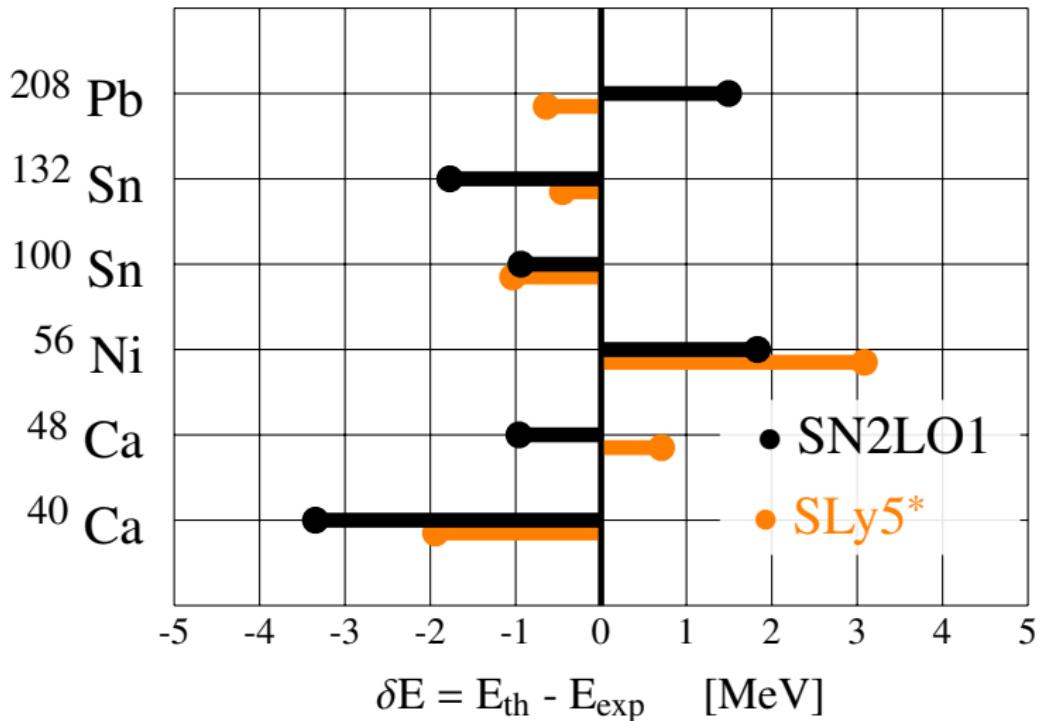


Instabilities in the different spin/isospin channels (S,M,I) for T22.

Binding energies SN2LO1

Skyrme N2LO
functionals: first results
on finite nuclei

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Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

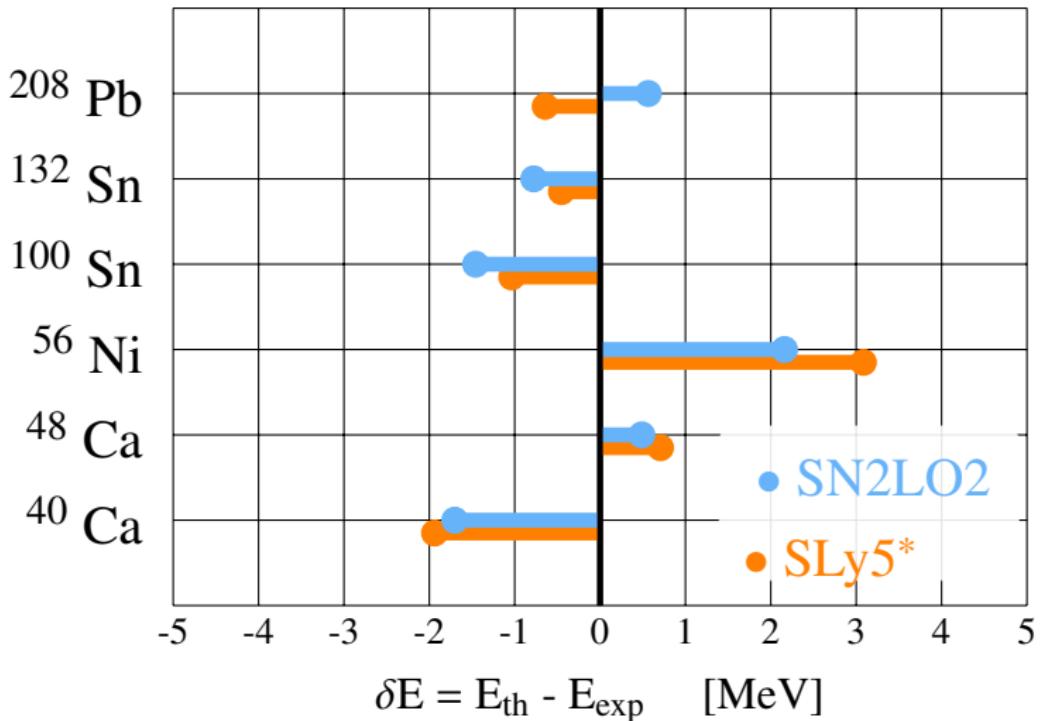
Application to spherical
nuclei

First results

Conclusion and
perspectives

Linear response
formalism

Binding energies SN2LO2



Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

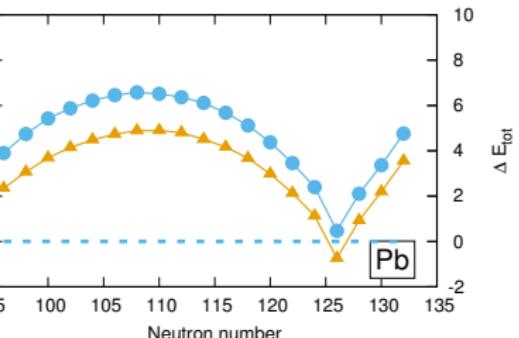
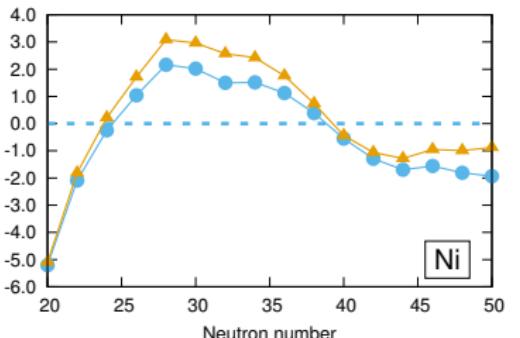
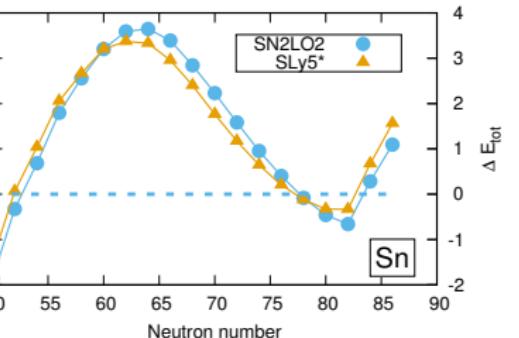
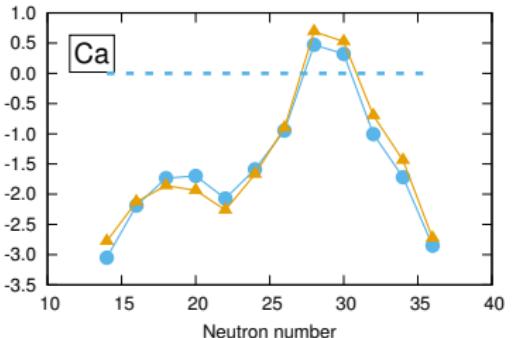
Conclusion and
perspectives

Linear response
formalism

Isotopes with SN2LO2

Skyrme N2LO
functionals: first results
on finite nuclei

D. Davesne, P. Becker,
A. Pastore, J. Navarro



Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

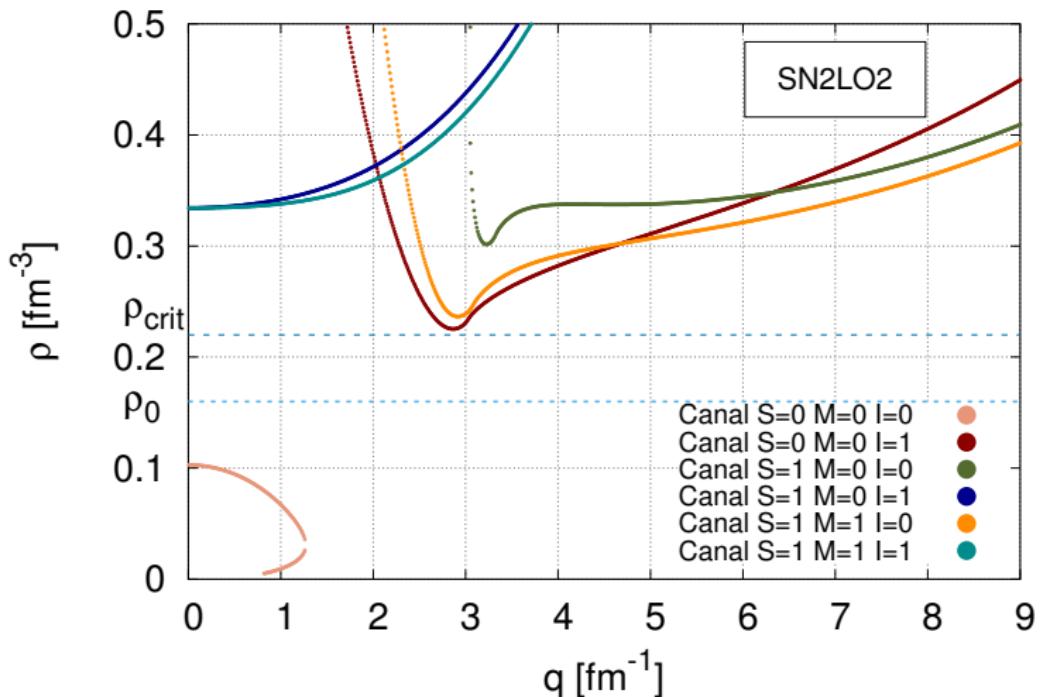
Conclusion and
perspectives

Linear response
formalism

Stability SN2LO2

Skyrme N2LO
functionals: first results
on finite nuclei

D. Davesne, P. Becker,
A. Pastore, J. Navarro



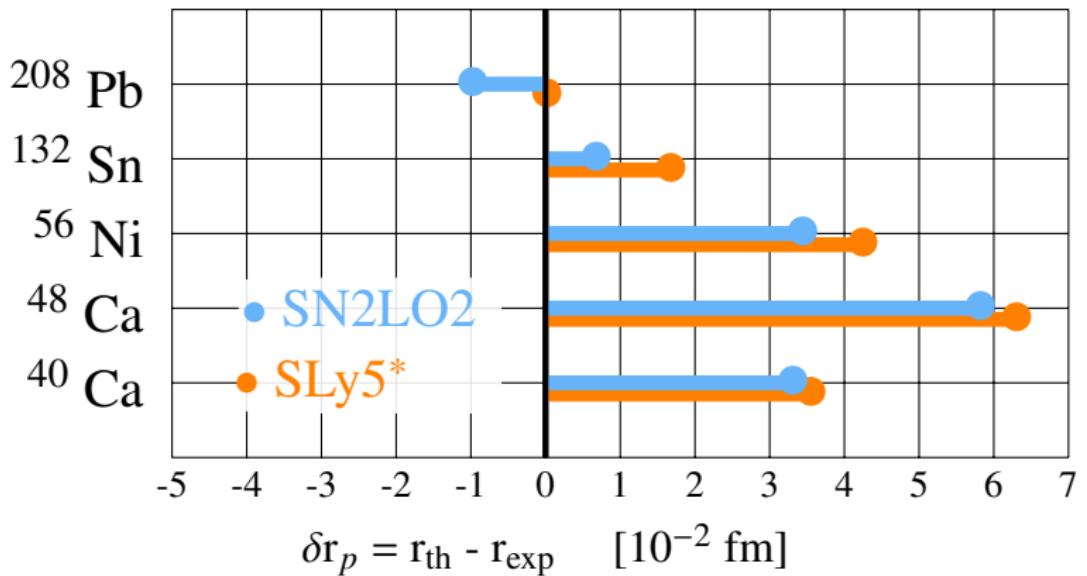
$$\rho_{crit} = 1,4 \rho_{sat}$$

Interaction N2LO stable

Proton radii SN2LO2

Skyrme N2LO
functionals: first results
on finite nuclei

D. Davesne, P. Becker,
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Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

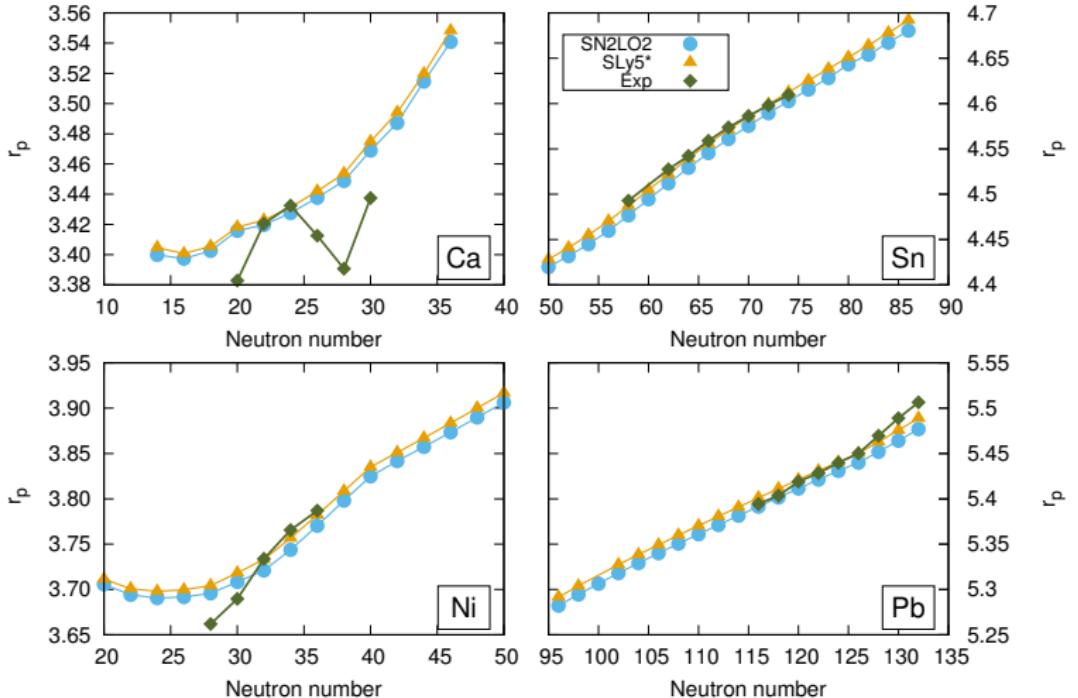
Conclusion and
perspectives

Linear response
formalism

Protons radii SN2LO2

Skyrme N2LO
functionals: first results
on finite nuclei

D. Davesne, P. Becker,
A. Pastore, J. Navarro



Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

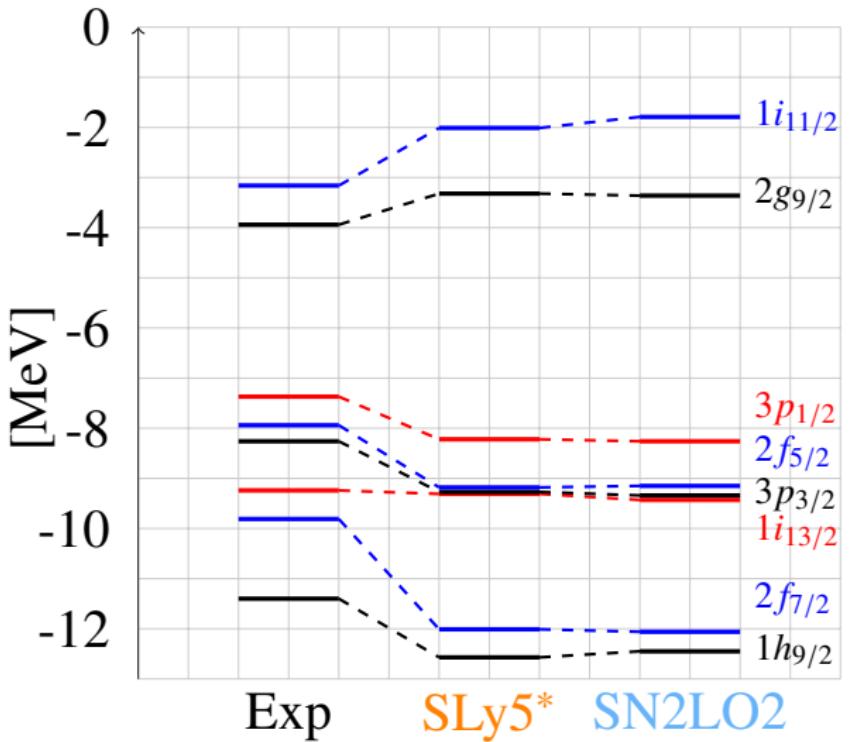
Conclusion and
perspectives

Linear response
formalism

Neutron particle levels for ^{208}Pb

Skyrme N2LO
functionals: first results
on finite nuclei

D. Davesne, P. Becker,
A. Pastore, J. Navarro



Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

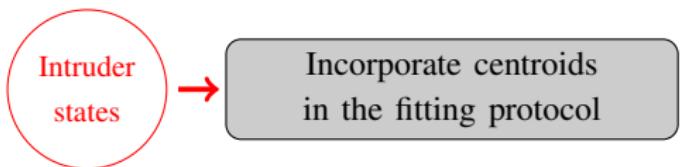
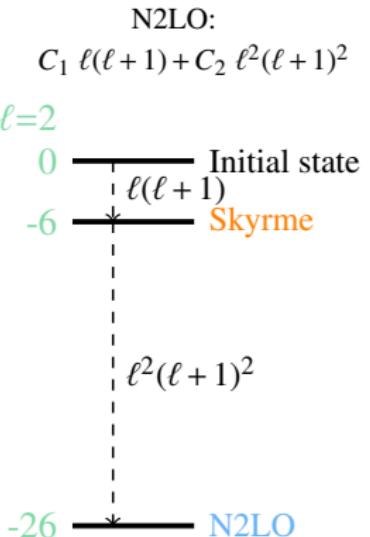
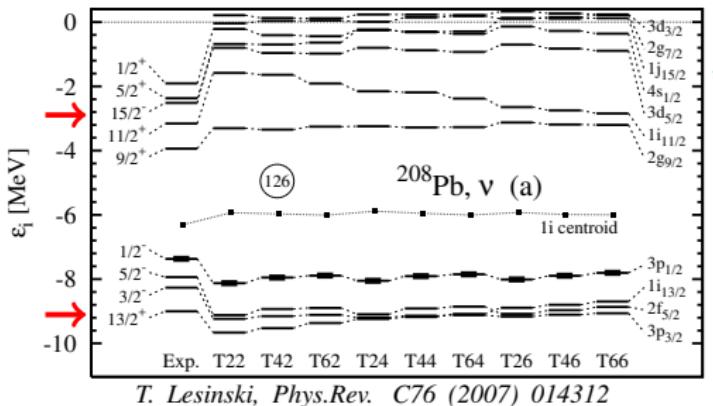
Conclusion and
perspectives

Linear response
formalism

Intruder states problem

Skyrme N2LO
functionals: first results
on finite nuclei

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Conclusion

N2LO

- Numerical code for finite nuclei WHISKY
- Stable parametrisation SN2LO2
- Better results (compared to Skyrme)

Gogny

- Third gaussian
- Optimisation of the numerical part for the nuclei

Future prospects

- Centroids, kink for Pb
- Tensor terms
- N3LO
- Fitting protocol for finite-range potential (Gogny) with linear response

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D.Davesne *et al*, Journal of Physics G, **41** 034001 (2015)
- *Extended Skyrme pseudo-potential deduced from infinite matter properties*
P. Becker *et al*, Phys. Rev. C, **91** 064303 (2015)
- *Partial-wave decomposition of the finite-range effective tensor interaction*
D.Davesne *et al*, Phys.Rev.C, **93** 064001 (2016)
- *Infinite matter properties and zero-range limit of non-relativistic finite-range interactions*
D.Davesne *et al*, Annals Phys., **375** 288-312 (2016)
- *Does the Gogny interaction need a third Gaussian?*
D.Davesne *et al*, Acta Phys.Polon., **B48** 265 (2017)
- *A numerical method for N2LO Hartree-Fock-Bogoliubov calculations*
P.Becker *et al*, Accepted in Phys.Rev.C (2017)
- *Fit of the Gogny interaction with a third gaussian*
P.Becker *et al*, in preparation, (2017)

Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

Linear response
formalism

Acknowledgments

M. Bender, K. Bennaceur, Y. Lallouet, J. Meyer, J. Navarro, A. Pastore, W. Ryssens.

Effective mass in nuclear effective theories

(K. Bennaceur, D. D., J. Meyer, J. Navarro, A. Pastore)

D. Davesne, P. Becker,
A. Pastore, J. Navarro

Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

Linear response
formalism

- Two-body : saturation, effective mass $\simeq 0.4$
- Density-dependent term : effective mass $\simeq 0.7$

Weisskopf's relation (1957): mean field U_i (for a state i) with a quadratic momentum dependance

$$U_i = U_0 + \frac{p_i^2}{p_F^2} U_1 \rightarrow \frac{m^*}{m} = 1 + \frac{U_1}{\varepsilon_F}$$

$$E/A = \frac{3}{5}\varepsilon_F + \frac{1}{2}U_0 + \frac{3}{10}U_1 \rightarrow \frac{\mathbf{m}^*}{\mathbf{m}} = \frac{3}{2} - \frac{5}{2} \frac{E/A}{\varepsilon_F}$$

With $E/A = -16$ MeV and $k_F = 1.33$ fm $^{-1}$, one gets $m^*/m \simeq 0.4$.

Example (SV interaction): $E/A = -16.06$ MeV, $k_F = 1.32$ fm $^{-1}$ and $m^*/m = 0.38$. The relation gives $m^*/m = 0.383$.

N2LO/N3LO/finite-range, no density dependence

Exact relation up to N2LO (first correction: N3LO)

$$\frac{m}{m^*} = \frac{11}{8} + \frac{5}{72} \frac{K_\infty - 21\mathcal{E}_0}{\varepsilon_F} + \frac{1}{90} \frac{C_1^{(6)} \rho_0 k_F^6}{\varepsilon_F}$$

Typical values: 1.375 + 1.033 + 0.012

→ $m^*/m = 0.415$ (N2LO) or **0.413** (N3LO)

Finite-range potential $V(r/\mu)$:

$$\begin{aligned} \frac{m}{m^*} &= \frac{11}{8} + \frac{5}{72} \frac{K_\infty - 21\mathcal{E}_0}{\varepsilon_F} + \frac{12}{\pi} \frac{C_E}{\varepsilon_F} \int dz z^2 V\left(\frac{z}{k_F \mu}\right) \\ &\quad \times \left\{ \mathcal{F}^m(z) + \frac{5}{72} \mathcal{F}^K(z) - \frac{105}{72} \mathcal{F}^\mathcal{E}(z) \right\} \end{aligned}$$

Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

Linear response
formalism

Introduction

Infinite matter
calculations

Application to
astrophysics LYVA1

Application to spherical
nuclei

First results

Conclusion and
perspectives

Linear response
formalism

$$\begin{aligned}\mathcal{F}^{\mathcal{E}}(x) &= \frac{2}{x^2} j_1^2(x) - \frac{2}{3x} j_0(x) j_1(x) \\ \mathcal{F}^K(x) &= 2j_0^2(x) - \frac{12}{x} j_0(x) j_1(x) + \left(\frac{18}{x^2} - 2 \right) j_1^2(x) \\ \mathcal{F}^m(x) &= \frac{1}{3} j_1^2(x)\end{aligned}$$

$$\mathcal{F}^m(x) + \frac{5}{72} \mathcal{F}^K(x) - \frac{105}{72} \mathcal{F}^{\mathcal{E}}(x) \simeq \frac{x^6}{127575} - \frac{8x^8}{9823275} + \frac{x^{10}}{25540515} + \dots$$

Exact cancellation up to x^4 as it should be!

N3LO or finite-range correction to the exact relation: very small!!!

N2LO/N3LO/finite-range, density dependence

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Conclusion and perspectives

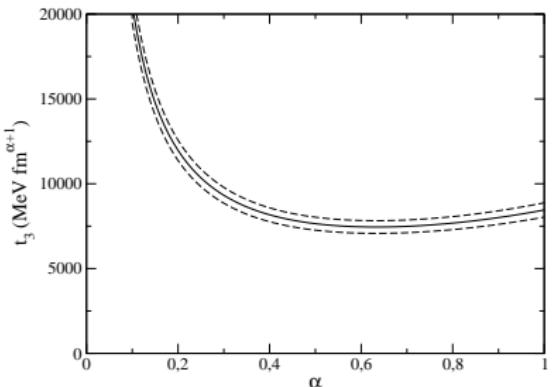
$$\frac{m}{m^*} = \frac{11}{8} + \frac{5}{72} \frac{K_\infty - 21\mathcal{E}_0}{\varepsilon_F} + \Delta_{\text{FR}} - \frac{5}{384} \alpha(10 + 3\alpha) \frac{t_3 \rho_0^{\alpha+1}}{\varepsilon_F}$$

D1: $1.375 + 1.049 + 0.010 \rightarrow 0.411 - 0.934 \rightarrow 0.667$

D1S: $1.375 + 1.002 + 0.029(\rightarrow 0.416) - 0.963(\rightarrow 0.693)$

D1N: $1.375 + 1.067 + 0.033 \rightarrow 0.404 - 1.087 \rightarrow 0.720$

For admitted values of $\frac{m}{m^*}, K_\infty, E/A$: relation between t_3 and $\alpha!$



Curve almost flat: $t_3 \simeq 7500 - 8000$ Mev.fm $^{\alpha+1}$