Recent progress on extended Skyrme functionals

(and it works!)

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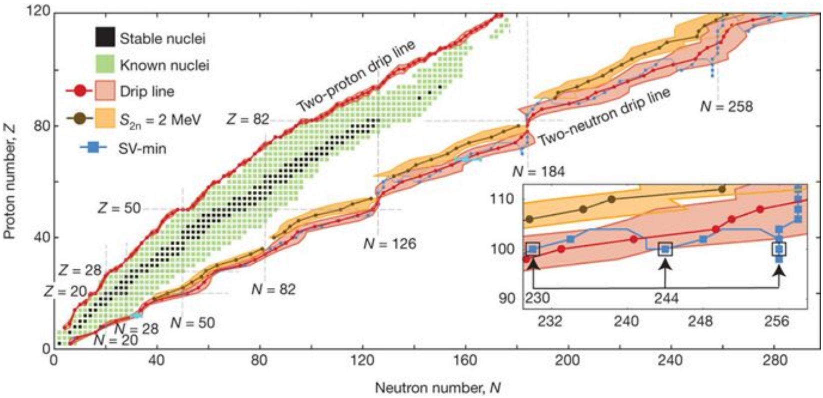
Introduction: the nuclear chart

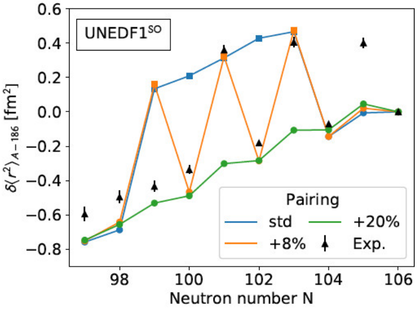


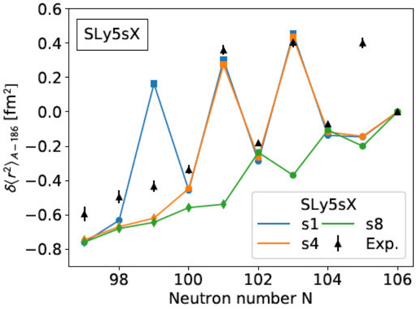
Nuclear chart

Atomic nucleus is the best example for *strange* quantum phenomena
[J. Erler et al. (2012); Nature, 486(7404), 509.]

A *simple* model: Skyrme Nuclear-DFT

Global description of nuclear properties with ≈ 10 parameters.





Odd-even staggering in Hg nuclei

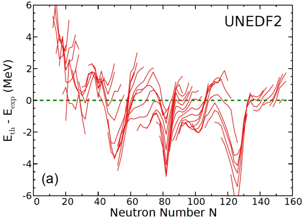
A sudden change in the potential energy surface (oblate/prolate)
[B. Marsh,. . . ,J.Dobaczewski, AP et al.; Nature Physics (accepted)]
[S. Sels,. . . ,J.Dobaczewski,AP et al. PRC (in preparation)]

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. C89, 054314 (2014)]



Observable	UNEDF0	UNEDF1	UNEDF2	No.
E	1.428	1.912	1.950	555
E $(A < 80)$	2.092	2.566	2.475	113
E $(A \geq 80)$	1.200	1.705	1.792	442
S_{2n}	0.758	0.752	0.843	500
S_{2n} $(A < 80)$	1.447	1.161	1.243	99
S_{2n} $(A \geq 80)$	0.446	0.609	0.711	401
S_{2p}	0.862	0.791	0.778	477
S_{2p} $(A < 80)$	1.496	1.264	1.309	96
S_{2p} $(A \geq 80)$	0.605	0.618	0.572	381
$\tilde{\Delta}_n^{(3)}$	0.355	0.358	0.285	442
$\tilde{\Delta}_n^{(3)}$ $(A < 80)$	0.401	0.388	0.327	89
$\tilde{\Delta}_n^{(3)}$ $(A \geq 80)$	0.342	0.350	0.273	353
$\tilde{\Delta}_p^{(3)}$	0.258	0.261	0.276	395
$\tilde{\Delta}_p^{(3)}$ $(A < 80)$	0.346	0.304	0.472	83
$\tilde{\Delta}_p^{(3)}$ $(A \geq 80)$	0.229	0.248	0.194	312
R_p	0.017	0.017	0.018	49
R_p $(A < 80)$	0.022	0.019	0.020	16
R_p $(A \geq 80)$	0.013	0.015	0.017	33

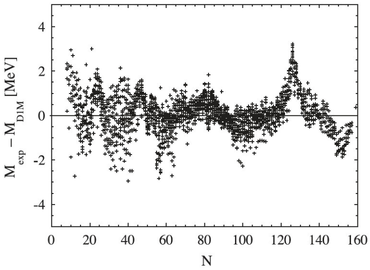
Result

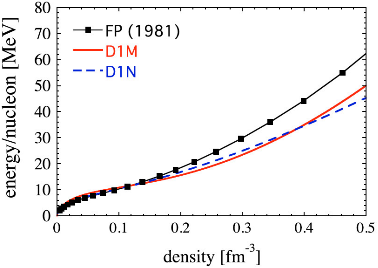
Skyrme functional can not further improved: need to go *beyond*. How?

Option 1: multi-reference calculations

Change many-body method!

Gogny D1M $\rightarrow$ parameters adjusted using 5D collective Hamiltonian





[S. Goriely et al. Physical Review letters, 102(24), 24250]

Result

Major improvement on masses $\sigma_{mass} \approx 0.8$ MeV.... but still not perfect!

Option 2... back to the Skyrme idea...

$$t_{12} = \delta(\mathbf{r}_1 - \mathbf{r}_2) t(\mathbf{k}', \mathbf{k}) \qquad (3)$$

where $\mathbf{k}$ is the operator corresponding to the relative wave-number,

$$\mathbf{k} = \tfrac{1}{2} i (\nabla_1 - \nabla_2); \qquad (4)$$

placed on the *right* of the delta-function $\mathbf{k}'$ denotes the same operator placed on the *left*; this form was used in an earlier discussion [8]) of the spin-orbit potential. An ordinary static (Wigner) interaction would then be described by a t dependent only on $\mathbf{k}' - \mathbf{k}$.

It is generally believed that the most important part of the two-body interaction can be represented by a contact potential, i.e. by constant $t(\mathbf{k}', \mathbf{k})$; this suggests an expansion in powers of $\mathbf{k}'$ and $\mathbf{k}$. If this expansion

Why 2nd order only?

We can remove the approximation of Skyrme and make the expansion beyond 2nd order

Taylor expansion of Gogny interaction

We can make a Taylor expansion of a finite range interaction

$$v^c_G(\mathbf{k},\mathbf{k}') = \sum_{n=1}^{2} \left[W^n + B^{(n)}P_\sigma - H^{(n)}P_\tau - M^{(n)}P_\sigma P_\tau\right] \pi^{3/2}(\mu_n^{c,G})^3 e^{-(\mathbf{k}-\mathbf{k}')^2/4(\mu_n^{c,G})^2},$$

Mapping to N3LO by a formal Taylor expansion of a scalar function $F(\mathbf{k}-\mathbf{k}')$

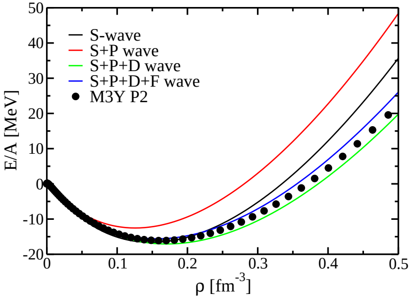
$$\begin{aligned} F(\mathbf{k}-\mathbf{k}') &= C_0 + C_2(\mathbf{k}-\mathbf{k}')^2 + C_4(\mathbf{k}-\mathbf{k}')^4 + \cdots \\ &= C_0 + C_2\left[\mathbf{k}^2 + \mathbf{k}'^2 - 2\mathbf{k}'\cdot\mathbf{k}\right] \\ &\quad + C_4\left[(\mathbf{k}^2+\mathbf{k}'^2)^2 + 4(\mathbf{k}'\cdot\mathbf{k})^2 - 4(\mathbf{k}'\cdot\mathbf{k})(\mathbf{k}^2+\mathbf{k}'^2)\right] + \cdots \end{aligned}$$

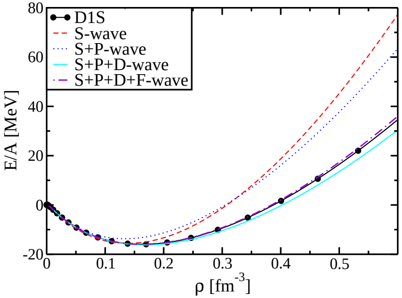
Skyrme N2LO: Skyrme has more freedom than Gogny!!!

$$\begin{aligned} V^c_{\text{N2LO}} &= t_0(1+x_0P_\sigma) + \frac{1}{2}t_1(1+x_1P_\sigma)(\mathbf{k}^2+\mathbf{k}'^2) + t_2(1+x_2P_\sigma)(\mathbf{k}\cdot\mathbf{k}') \\ &\quad + \frac{1}{4}t_1^{(4)}(1+x_1^{(4)}P_\sigma)\left[(\mathbf{k}^2+\mathbf{k}'^2)^2 + 4(\mathbf{k}'\cdot\mathbf{k})^2\right] \\ &\quad + t_2^{(4)}(1+x_2^{(4)}P_\sigma)(\mathbf{k}'\cdot\mathbf{k})(\mathbf{k}^2+\mathbf{k}'^2) \end{aligned}$$

Partial wave expansion

A finite range interaction can be decomposed into an infinite sum of partial waves



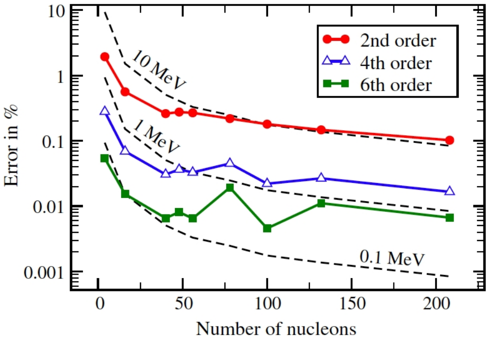


Fast convergence!

Including D-wave we reproduce the same physics at saturation

Density Matrix Expansion (DME)

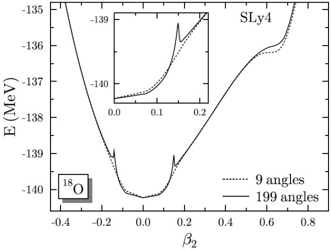
[G. Carlsson and J. Dobaczewski; Phys. Rev. Lett. (2013)]



Results

DME converges quite well at 4th order!!

Role of density-dependent term



[D. Lacroix et al; Physical Review C 79.4 (2009): 044318.]

- Density dependent (DD) term are used in *all* current pseudo-potential
- Multi-reference is OK for interactions with no DD terms:
  1. SV → 2-body force ($m^* = 0.4$)
  2. SLYMR0 → 2- and 3-body force [J. Sadoudi et al. Phys. Rev. C 88.6 (2013): 064326.]

Important result

To have $m^* \approx 0.7$ (or more) we <u>need</u> a 3-body term (or density dependent one!)

[D. Lacroix et al; Physical Review C 79.4 (2009): 044318.]

$$
\begin{aligned}
\mathcal{V}_{Ex}(\mathbf{r}_1,\mathbf{r}_2) = \; & t_0\,(1+x_0\,P_\sigma) + \frac{1}{6}\,t_3\,(1+x_3P_\sigma)\rho^\alpha(R) \\
& + \frac{1}{2}\,t_1\,(1+x_1\,P_\sigma)\left[\mathbf{k}'^2+\mathbf{k}^2\right] + t_2\,(1+x_2\,P_\sigma)\,\mathbf{k}'\cdot\mathbf{k} \\
& + \frac{1}{4}\,t_1^{(4)}(1+x_1^{(4)}P_\sigma)\left[(\mathbf{k}^2+\mathbf{k}'^2)^2+4(\mathbf{k}'\cdot\mathbf{k})^2\right] \\
& + t_2^{(4)}(1+x_2^{(4)}P_\sigma)(\mathbf{k}'\cdot\mathbf{k})(\mathbf{k}^2+\mathbf{k}'^2) \\
& + \frac{1}{2}\,t_1^{(6)}\left(1+x_1^{(6)}P_\sigma\right)(\mathbf{k}'^2+\mathbf{k}^2)\left[(\mathbf{k}'^2+\mathbf{k}^2)^2+12(\mathbf{k}'\cdot\mathbf{k})^2\right] \\
& + t_2^{(6)}\left(1+x_2^{(6)}P_\sigma\right)(\mathbf{k}'\cdot\mathbf{k})\left[3(\mathbf{k}'^2+\mathbf{k}^2)^2+4(\mathbf{k}'\cdot\mathbf{k})^2\right].
\end{aligned}
$$

Skyrme NLO (first two lines)

Skyrme N2LO (third and fourth lines)

Skyrme N3LO (last two lines)

D and F partial waves included

Gauge invariant

18 parameters, **8 new**

Also includes

- a spin-orbit term W_0
- tensor terms (4 new)

[F. Raimondi et al; Physical Review C 83.5 (2011): 054311]

N2LO in finite nuclei

A 4th order equation in spherical symmetry

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

14 parameters,
4 new

Doubly centrifugal term

$\left(\frac{\ell(\ell+1)}{r^2}\right)^2$

New spin-orbit contributions

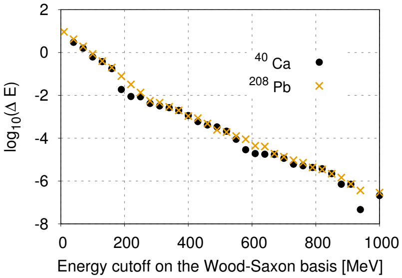
$W_{2R},\ W_{1R},\ \frac{\ell(\ell+1)}{r^2} W_{0C}$

Same behaviour at the origin than Skyrme NLO

Numerical solver in coordinate space: fast and accurate!

[P .Becker et al.; Physical Review C 96.4 (2017): 044330.]

WHISKY: 2 basis methods HFB code



^{208}Pb		
[MeV]	WHISKY	LENTEUR
Total Energy	-1636.1**06**	-1636.1**05**
Kinetic energy	3874.7**89**	3874.7**95**
Field energy	-6209.6**42**	-6209.6**50**
Spin-orbit	-99.081	-99.081
Direct Coulomb	829.143	829.143
Exchange Coulomb	-31.314	-31.314

^{208}Pb		
[MeV]	WHISKY	MOCCA
Total Energy	-1539.2**53**	-1539.2**63**
Total energy N2LO	89.**278**	89.**360**
E$[(\Delta\rho)^2]$	4.39**4**	4.39**5**
E$[\rho Q]$	37.4**77**	37.4**88**
E$[\tau^2]$	27.2**12**	27.2**21**
E$[\tau_{\mu\nu}\tau_{\mu\nu} - \tau_{\mu\nu}\nabla_\mu\nabla_\nu\rho]$	19.8**55**	19.8**61**
E$[K_{\mu\nu\kappa}K_{\mu\nu\kappa}]$	0.0546**0**	0.0546**1**
E$[J_{\mu\nu}V_{\mu\nu}]$	0.3385**0**	0.3385**8**

Fitting protocol

Infinite nuclear matter			
ρ_{sat}	0.1600	0.001	fm^{-3}
E/A (ρ_{sat})	-16.0000	0.2	MeV
m^*/m	0.7000	0.02	
K_∞	230.00	10.00	MeV
J	32.00	2.00	MeV
EoS PNM			
E/N (ρ=0.1)	11.88	2.0	MeV
E/N (ρ=0.3)	35.94	7.0	MeV
E/N (ρ=0.35)	44.14	9.0	MeV
Stability			
INM(S,M,T)	$\rho_{crit} \geq 0.24$	asymmetric constraint	fm^{-3}
Finite nuclei			
Binding energies			
^{40}Ca	-342.02300	1.5	MeV
^{48}Ca	-415.98300	1.0	MeV
^{56}Ni	-483.95300	1.5	MeV
^{100}Sn	-825.13000	1.5	MeV
^{132}Sn	-1102.67300	1.0	MeV
^{208}Pb	-1635.86100	1.0	MeV
Proton radii			
^{40}Ca	3.38282	0.03	fm
^{48}Ca	3.39070	0.02	fm
^{56}Ni	3.66189	0.03	fm
^{132}Sn	4.64745	0.02	fm
^{208}Pb	5.45007	0.02	fm
Parameter W_0	120.0	2.0	MeV fm^5

Introducing SN2LO1

Valencia-Lyon-York fitting protocol

- Double magic nuclei
- Infinite matter properties
- Finite-size instabilities
- W_0 fixed (for the moment)

Natural Units

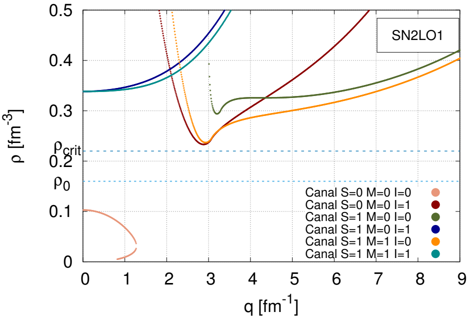
C_0^{ρ}	-1.06	C_1^{ρ}	0.754
$C_0^{\rho}[\rho^{\alpha}]$	13.0	$C_1^{\rho}[\rho^{\alpha}]$	-12.1
C_0^{τ}	0.892	C_1^{τ}	0.00624
$C_0^{\Delta\rho}$	-1.06	$C_1^{\Delta\rho}$	0.382
$C_0^{\nabla J}$	-1.22	$C_1^{\nabla J}$	-0.406
C_0^{T}	-0.0882	C_1^{T}	-0.816
$C_0^{(\Delta\rho)^2}$	-0.115	$C_1^{(\Delta\rho)^2}$	0.0396
$C_0^{M\rho}$	-0.288	$C_1^{M\rho}$	0.143
C_0^{Ms}	0.117	C_1^{Ms}	-0.0162

Important remarks

- The coupling constants look *natural* (Grain of salt!!)
- We need further studies on naturalness

[Kortelainen, M., Furnstahl, R. J., Nazarewicz, W., Stoitsov, M. V. (2010). Phys. Rev. C, 82(1), 011304.

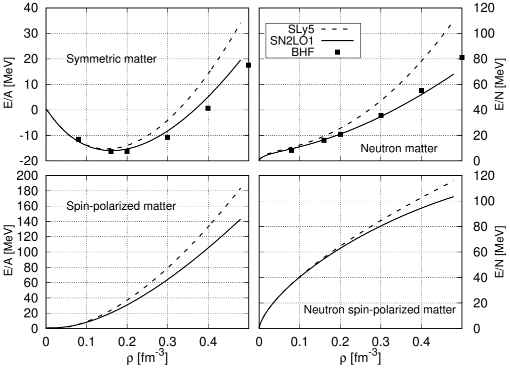
Finite-size instabilities



An *empirical solution*

- Use Linear Response to detect instabilities [Lesinski, T., et al. ; Phys. Rev. C 74.4 (2006): 044315.] [PA et al. Physics reports 563 (2015): 1-67.]
  [De Pace, A., and M. Martini; Physical Review C 94.2 (2016): 024342.]
- Impose $\rho_{pole} > 1.2\rho_{sat}$

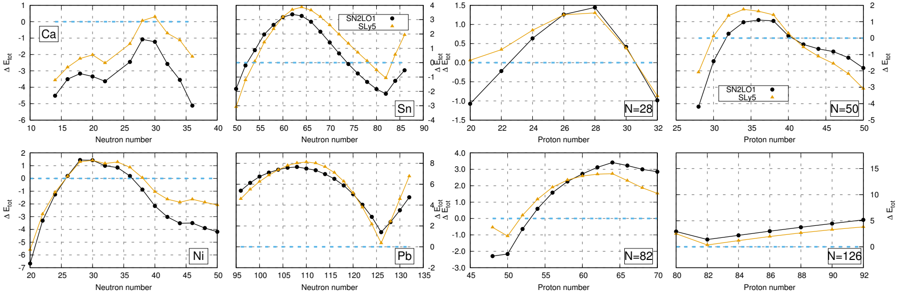
Infinite nuclear matter properties



	SN2LO1	SLy5
ρ_0 [fm^{-3}]	0.162	0.1603
E/A(ρ_0) [MeV]	-15.948	-15.98
K_∞ [MeV]	221.9	229.92
J [MeV]	31.95	32.03
L [MeV]	48.9	48.15
m^*/m	0.709	0.696

Masses

Systematic comparison of binding energies for isotopic (isotonic) chains calculated with SN2LO1 and SLy5 parametrisation



Only even-even nuclei!

SN2LO1 gives slightly worst results than SLy5.

Error analysis

	SN2LO1	SN2LO2	SLy5*	*Last fit*	%	
INM Properties	1.40	0.85	0.07	1.17		
Neutron matter	0.19	0.21	0.05	0.2		
Stability	5.04	6.72	5.32	3.09		
Nuclei	236.82	57.44	64.20	18.36	- 71 %	✓
Proton radii	8.81	13.44	17.31	8.57	- 51 %	✓
W_0 Parameter	1.10	0.66	0.02	1.22		
Total χ^2	8.77	2.77	3.03	1.15	- 62 %	✓

What new constraints ?

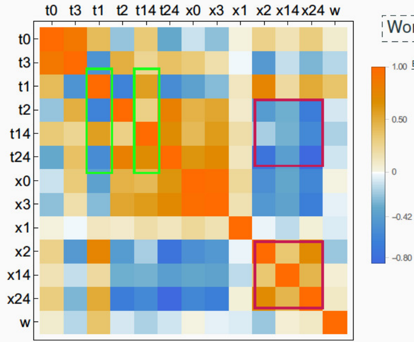
- Nuclear channels
- Landau parameters
- s.p. levels
- New nuclei, maybe with pairing or deformation

Covariance matrix

- Different correlation structure
- Net terms NOT compatible with 0

Results

- *Special* observables for higher order terms
- New statistical tools (Bootstrap/Gaussian Process Emulator)
- New interesting terms $C_1 l(l+1) + C_2 l^2 (l+1)^2 \rightarrow$ Candidate to change position high l states



Work in progress

Errors :

- t0=-2477.48 +/- 5.88
- t3 =13660.68 +/- 54.95
- t1=507.81 +/- 6.64
- t2=-421.48 +/- 23.07
- **t14=-29.68 +/- 4.67**
- **t24= 4.69 +/- 0.63**
- x0= 0.77 +/- 0.01
- x3= 1.17 +/- 0.02
- **x1= 0.0014 +/- 0.0035**
- x2= -0.92 +/- 0.01
- x14= 0.353 +/- 0.006
- x24= 2.14 +/- 0.06
- w = 122.30 +/- 6.72

Summary and Conclusions

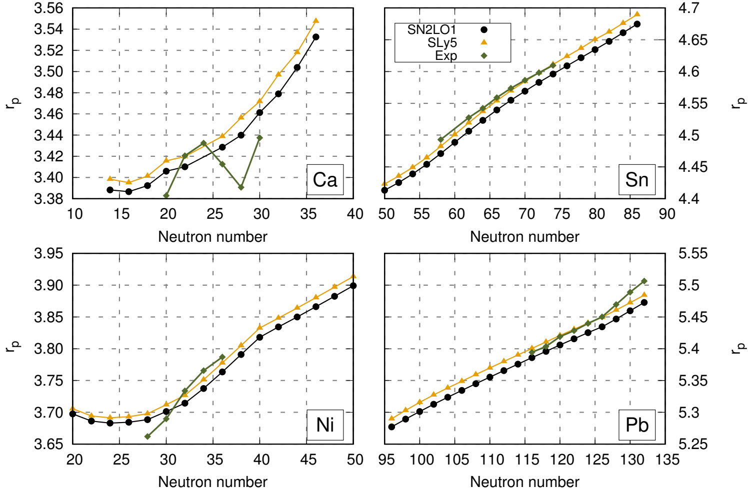
- We have produced the first N2LO parametrisation
- Very difficult fit higher order:
  - use of RPA in IM to avoid instabilities
  - need $ad-hoc$ observables
  - understand the role of new fields/densities
  - N3LO is also ready spherical/deformed
- New numerical code

The next step...

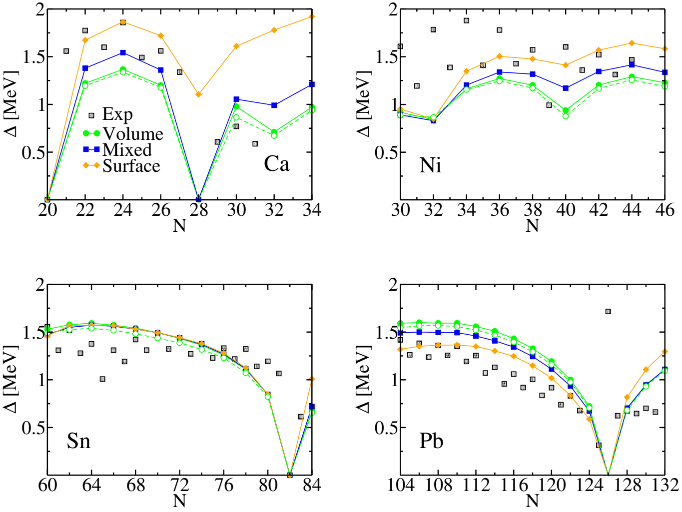
- Need new fitting protocol beyond modified Saclay-Lyon $\rightarrow$ ideas for χ^2???
- Improving super-heavy nuclei spectroscopy
- Exploring excited states (joint PhD student York/Lyon/CEA)

THANK YOU

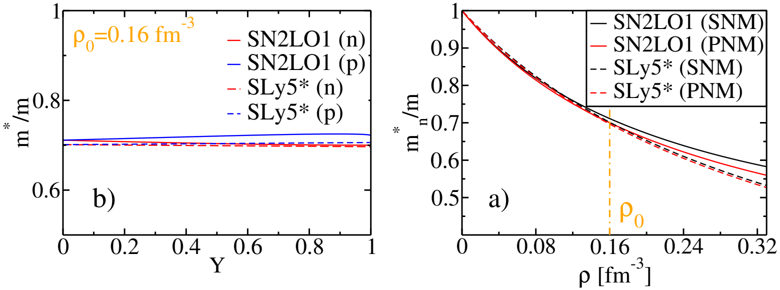
Charge radii



Pairing gaps



Effective mass



Better to compare with SLy5*

SN2LO1 $\rightarrow$ **same** fitting protocol SLy5* (and same results!)

[Pastore, A., Davesne, D., Bennaceur, K., Meyer, J., and Hellemans, V. (2013); Phys. Scrip., 2013(T154), 014014.]