

Skyrme interaction with 2-, 3- and 4-body terms

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New developments in nuclear energy-density-functional models
ESNT Saclay – Nov. 24-28, 2014



- Skyrme interactions without density dependent terms
- Requirements v1 and first series of interaction “S3Ly”
- Requirements v2 (stability and pairing)
 - Test case study: SLyMR0
 - The full monty: SLyMR1
- Outlooks

- IPNL (Lyon): K.B., D. Davesne, R. Jodon, J. Meyer
- CENBG (Bordeaux): B. Avez, B. Bally, M. Bender, J. Sadoudy
- IRFU (Saclay): T. Duguet, T. Lesinski
- ULB (Bruxelles): P.H. Heenen, V. Hellemans, A. Pastore
- Many figures from the thesis of R. Jodon

Funded by the ANR and supported by the FIDIPRO programme

How to fit the parameters of an effective interaction ?

It's simple !

- Choose a set relevant observables
- Use constraints to write a penalty function χ^2
- Minimize it...
- ... and, most likely, this will not lead to any useful result

Why ?

- Some parameters can be poorly constrained
- Some constraints may be impossible to satisfy simultaneously
- Problems (which you would not even think¹) can occur

So you need to modify the χ^2

⇒ You don't know the χ^2 before you start to minimize it...

*“Good judgement is the result of experience
and experience the result of bad judgement.”*

– Mark Twain

¹in your worst nightmares

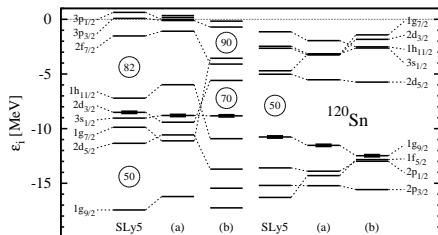
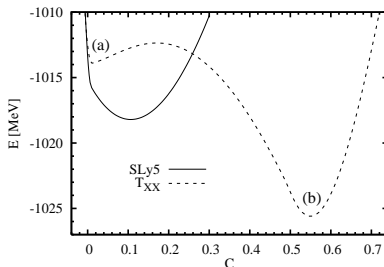
Welcome to my nightmare

Example of source of discontinuity in the penalty function

Competition between different shell structures

$$C = \int \mathbf{J}_n \cdot \nabla \rho_n d^3r$$

Constrained calculation →



$\chi^2(\text{masses, charge radii, ...})$
may not be continuous !

:- (

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The standard (2-body) Skyrme functional

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■ Effective Skyrme *interaction*

$$\begin{aligned} V_{2b} &= t_0 (1 + x_0 \hat{P}^\sigma) \delta(\mathbf{r}) && \text{local} \\ &+ \frac{t_1}{2} (1 + x_1 \hat{P}^\sigma) (\mathbf{k}'^2 \delta(\mathbf{r}) + \delta(\mathbf{r}) \mathbf{k}^2) && \text{non local} \\ &+ t_2 (1 + x_2 \hat{P}^\sigma) \mathbf{k}' \cdot \delta(\mathbf{r}) \mathbf{k} && \text{non local} \\ &+ i W_0 \hat{\boldsymbol{\sigma}} \cdot [\mathbf{k}' \times \delta(\mathbf{r}) \mathbf{k}] && \text{spin-orbit} \\ V_{dd} &= \frac{t_3}{6} (1 + x_3 \hat{P}^\sigma) \rho_0^\alpha \delta(\mathbf{r}) && \text{density dep.} \end{aligned}$$

- Sometimes complemented with tensor, D-wave terms, etc.
- Higher order derivatives ? Other density dependent terms ?
- Different interaction in the pairing channel
- ρ_0^α seems to be the key to succes:
 - Incompressibility
 - Effective mass
 - Stability in the spin channels

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Beyond mean-field calculations

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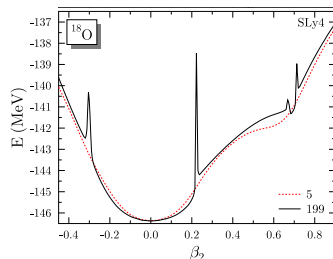
Early attempts

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Outlooks

■ Beyond mean field calculations with a Skyrme EDF



Poles in the
projected energy

See: M. Anguiano *et al.*, NPA 696 (2001) 467,
J. Dobaczewski *et al.*, PRC 76, 054315 (2007),
PRC 79 (2009) 044318, 044319 and 044320.

⇒ The same interaction has to be used for all terms of the energy:
Hartree, Fock and pairing terms

$$E = \langle \hat{T} + \hat{V} \rangle = E_H + E_F + E_P$$

all terms must be kept (even the “**annoying**” ones...)

New strong constraints on the EDF

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The EDF must be derived from an interaction: $E = \langle \hat{T} + \hat{V} \rangle$

- No density dependence
- All terms kept in the functional (Hartree, Fock and pairing)
- Must give attractive pairing

But that's not all:

- First, mean-field calculations must give converged results

See:

A. Pastore, D. Davesne, K.B., J. Meyer and V. Helleman,
Phys. Scr. **2013**, 014014.

A. Pastore, K.B., D. Davesne, J. Meyer,
Int. J. of Modern Phys. E Vol. 21, No. 05, 1250040.

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Finite size instabilities in nuclei

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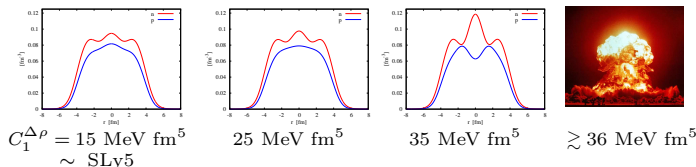
Early attempts

SLyMR0

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Outlooks

- 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



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

- The penalty function may not be continuous everywhere...
it may even **not** be **defined** everywhere !

Linear response – Instabilities in infinite nuclear matter

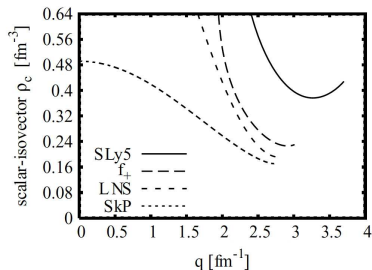
Response of the system to a perturbation given by

$$\mathcal{Q}^{(\alpha)} = \sum_a e^{i\mathbf{q}\cdot\mathbf{r}_a} \Theta_a^{(\alpha)},$$
$$\Theta_a^{\text{ss}} = 1_a, \quad \Theta_a^{\text{vs}} = \boldsymbol{\sigma}_a, \quad \Theta_a^{\text{sv}} = \vec{\tau}_a, \quad \Theta_a^{\text{vv}} = \boldsymbol{\sigma}_a \vec{\tau}_a$$

Response functions are given by

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

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



- Characterizes instabilities in infinite systems
- Easy to implement
- Negligible computation time
- Link with finite nuclei ?

See Phys. Rev. C 88 (2013) 064323

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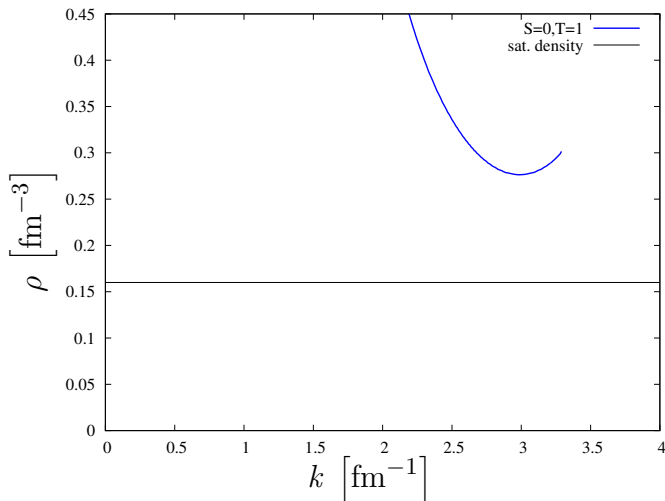
Outlooks

Linear response as a tool for diagnosis

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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: Phys. Rev. C 84, 059904(E) (2011).

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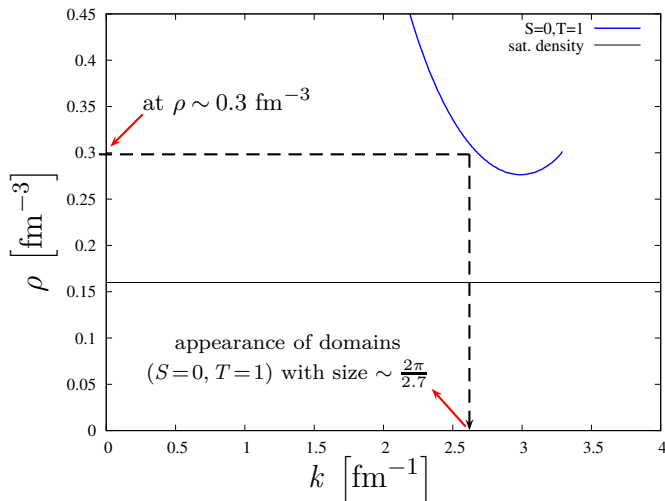
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■ Density dependent term

$$V_{\text{dd}} = \frac{t_3}{6} (1 + x_3 \hat{P}^\sigma) \rho_0^\alpha \delta(\mathbf{r})$$

■ Replaced by

$$\begin{aligned} V_{3b} = & u_0 \delta(\mathbf{r}_{13}) \delta(\mathbf{r}_{23}) \\ & + \frac{u_1}{2} (1 + y_1 \hat{P}_{12}^\sigma) [\mathbf{k}_{12}'^2 \delta(\mathbf{r}_{13}) \delta(\mathbf{r}_{23}) + \delta(\mathbf{r}_{13}) \delta(\mathbf{r}_{23}) \mathbf{k}_{12}^2] \\ & + u_2 [1 + y_{21} \hat{P}_{12}^\sigma + y_{22} (\hat{P}_{13}^\sigma + \hat{P}_{23}^\sigma)] \mathbf{k}_{12}' \cdot \delta(\mathbf{r}_{13}) \delta(\mathbf{r}_{23}) \mathbf{k}_{12} \end{aligned}$$



More terms with gradients,
more chance to encounter instabilities

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Early attempts: “S3Ly” series

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- Interaction with 2- and 3-body terms
- Interaction used for the normal field only
- Penalty function build with constraints on
 - Binding energies of double magic nuclei²
 - Charge radii of double magic nuclei
 - Infinite nuclear matter properties
 - Landau parameters
- Stability controled using empirical considerations and checked afterwards

Results published in J. Sadoudi's thesis:

<https://tel.archives-ouvertes.fr/tel-00653740>

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SLyMR0

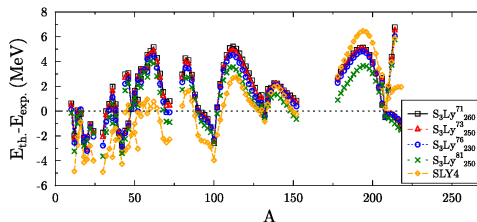
SLyMR1

Outlooks

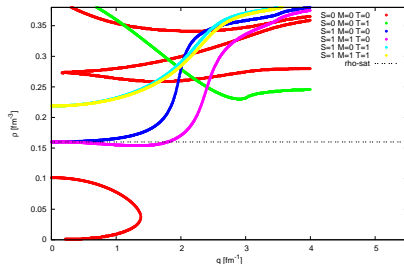
²Interlude: does anybody know where the value for ⁵⁶Ni comes from ?

Early attempts and first judgment

■ Encouraging results



■ No isovector instabilities in finite systems



A 4-body term may help³

☐ good judgment

☐ bad judgment

³Check one box

New constraint and implementation in the codes

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Outlooks

- Linear response code finalized and usable for the fit procedure
- Use of a contact 4-body term
- Use of the same interaction for the normal and pairing fields
with a cut-off $E_{\text{cut}} = E_F \pm 8.5 \text{ MeV}$
- Implementation in existing codes
 - Spherical HFB code (**lenteur**): done
 - 3-D HFB code (**cr8**): done but not fully tested
 - Beyond mean-field code: ask Michael⁴
- Machinery tested with a simpler interaction first...

⁴Prof. Bender

Tentative fit with simplified interaction: SLyMR0

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See: Phys. Scr. 2013 014013

J. Sadoudi, M. Bender, K.B., D. Davesne, R. Jodon, T. Duguet

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Outlooks

- 3- and 4-body terms limited to

$$3 u_0 \delta(\mathbf{r}_{12})\delta(\mathbf{r}_{13}) + v_0 \delta(\mathbf{r}_{12})\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{14})$$

- Infinite nuclear matter properties

- $\rho_{\text{sat}} = 0.152 \text{ fm}^{-3}$
- $E/A = -15.04 \text{ MeV}$
- $K_{\infty} = 264.2 \text{ MeV}$
- $m^*/m = 0.47$
- $J = 23 \text{ MeV}$

- Allows to test the mean-field and beyond mean-field machinery

SLyMR0: Results

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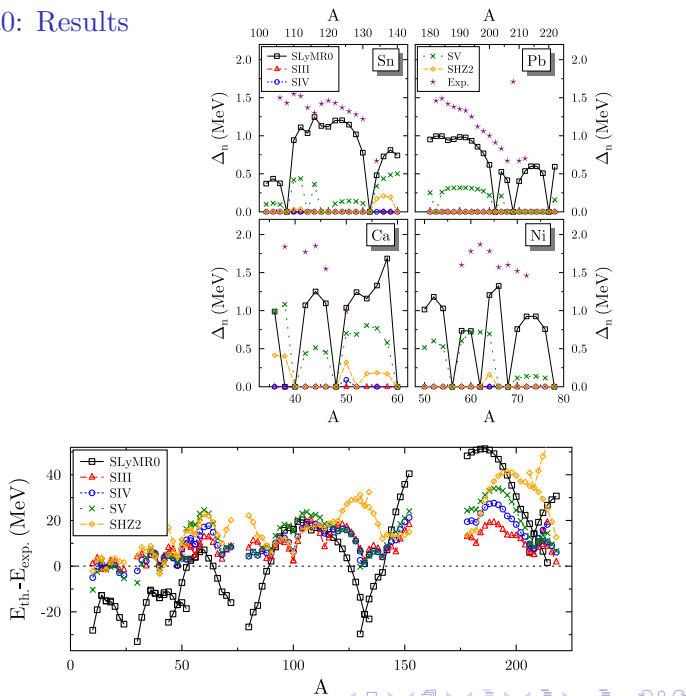
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SLyMR1: the most constrained interaction ever

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Outlooks

- 2- and 3-body terms + 4-body contact term (no ρ_0^α term)
- Used for the normal and pairing fields
- Infinite nuclear matter
 - $\rho_{\text{sat}}, E/A, K_\infty, m^*/m, J, L$
 - Neutron matter equation of state
 - Constraints in spin channels and on the effective mass
- (Double magic) nuclei
 - Binding energy
 - Charge radii
 - Energy difference between 2 spin-orbit partners (in ^{208}Pb)
- Spherical semi-magic nuclei (^{44}Ca and ^{120}Sn)
 - Binding energy
 - Spectral gaps
- Linear response code fully functional
 - $\rho_{\text{crit,min}} \geq 0.26 \text{ fm}^{-3}$ in symmetric and neutron matter

par.	unit	p_i	Δp_i	$\Delta p_i / p_i$
t_0	MeV fm ³	-1229.79	94.95	7.7 %
t_1	MeV fm ⁵	838.80	223.25	26.6 %
t_2	MeV fm ⁵	-1333.04	604.87	45.4 %
u_0	MeV fm ⁶	4017.82	1485.84	37.0 %
u_1	MeV fm ⁸	-3820.19	2293.79	60.0 %
u_2	MeV fm ⁸	14578.51	5322.63	36.5 %
x_0		0.1695	0.2290	135.1 %
x_1		0.6598	0.2686	40.7 %
x_2		-1.1512	0.0999	8.7 %
y_1		1.2941	1.0130	78.3 %
y_{21}		-1.1201	0.0634	5.7 %
y_{22}		-0.0813	0.0212	26.1 %
W_0	MeV fm ⁵	97.780	18.337	18.8 %
v_0	MeV fm ⁹	-9371.16	33266.54	355.0 %

	ρ_{sat}	E/A	K_{∞}	m^*/m	J	$\langle V \rangle_{pp}$
	0.154 fm ⁻³	-16.12 MeV	279 MeV	0.56	33.7 MeV	-2.75 MeV
ρ_{sat}	1.00	-0.24	-0.33	-0.00	0.03	-0.01
E/A		1.00	-0.43	0.18	-0.49	0.17
K_{∞}			1.00	0.29	-0.19	0.13
m^*/m				1.00	-0.17	0.19
J					1.00	-0.33
V_{pp}						1.00

$$K_{\infty} \searrow \Leftrightarrow m^*/m \searrow$$

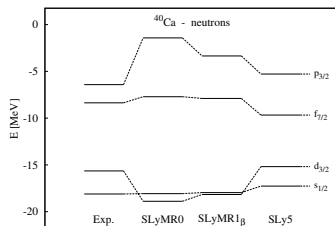
$$m^*/m \searrow \Leftrightarrow \langle V \rangle_{pp} \nearrow$$

Going from $m^*/m = 0.56$ to 0.7 is a change of 25 %

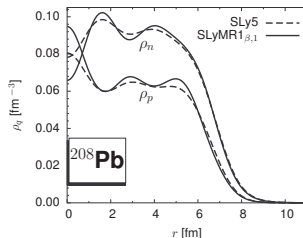
Enlarging the window where pairing is active would help but my colleagues do not want it...

Main problems with SLyMR1 _{β}

- Difficulty to reach the desired effective mass
- Poor spectroscopic properties



- Strong oscillations in densities



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SLyMR1: improved penalty function

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- Constraint on the charge density in ^{208}Pb
- Spin-orbit strength constrained by the binding energy difference between ^{56}Ni and ^{40}Ca
- 4-body term disregarded

■ Parameters

par.	unit	p_i	Δp_i	$\Delta p_i/p_i$	(SLyMR1 $_{\beta}$)
t_0	MeV fm ³	-1249.47	94.95	7.4 %	(7.7 %)
t_1	MeV fm ⁵	943.83	223.25	18.4 %	(26.6 %)
t_2	MeV fm ⁵	-1141.47	604.87	52.3 %	(45.4 %)
u_0	MeV fm ⁶	3436.76	1485.84	37.7 %	(37.0 %)
u_1	MeV fm ⁸	-4471.94	2293.79	14.9 %	(60.0 %)
u_2	MeV fm ⁸	13596.13	5322.63	34.1 %	(36.5 %)
x_0		0.2182	0.2290	102.3 %	(135.1 %)
x_1		0.6306	0.2686	33.7 %	(40.7 %)
x_2		-1.1598	0.0999	7.8 %	(8.7 %)
y_1		0.9880	1.0130	78.7 %	(78.3 %)
y_{21}		-1.1253	0.0634	5.1 %	(5.7 %)
y_{22}		-0.0793	0.0212	26.3 %	(26.1 %)
W_0	MeV fm ⁵	124.647	18.337	18.7 %	(18.8 %)
v_0	MeV fm ⁹				(355.0 %)

■ Infinite nuclear matter

	ρ_{sat} [fm ⁻³]	E/A [MeV]	K_{∞} [MeV]	m^*/m	J [MeV]
SV	0.155	-16.05	305.7	0.38	32.8
SLyMR0	0.152	-15.04	264.2	0.47	23.0
SLyMR1 $_{\beta}$	0.154	-16.12	279.1	0.56	33.7
SLyMR1	0.155	-16.10	276.9	0.53	32.7

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SLyMR1: equations of state

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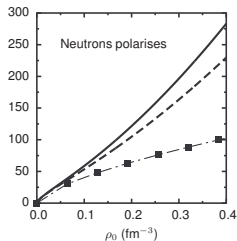
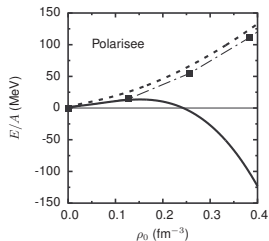
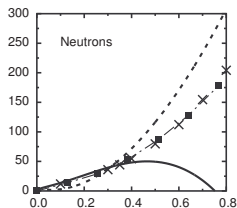
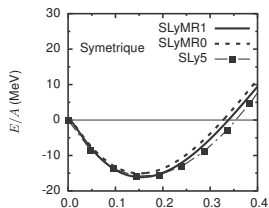
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SLyMR1: critical densities

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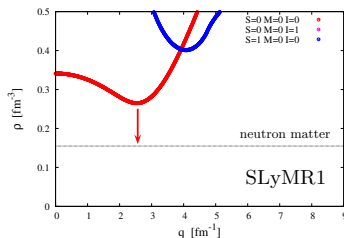
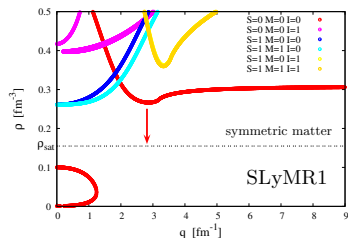
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(Unusual) instabilities in the $S = T = 0$ channel:

- due to the constraint on pairing ?
- responsible for the oscillations in densities ?

SLyMR1: binding energies

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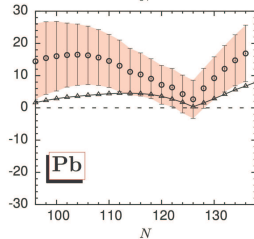
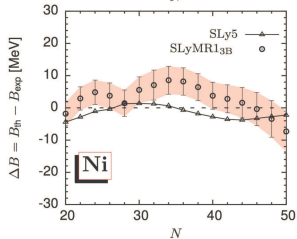
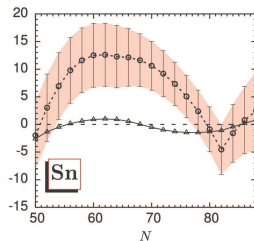
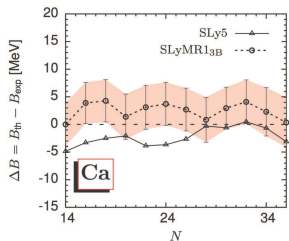
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SLyMR1: gaps

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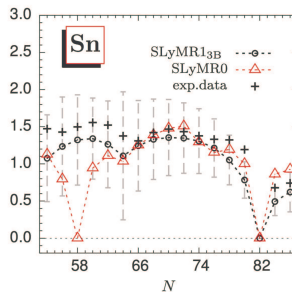
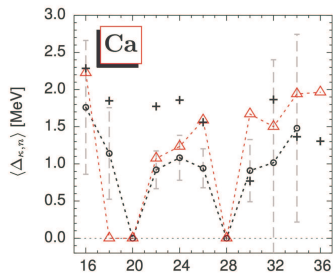
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Outlooks



- Density independent interaction usable at the mean-field level and beyond
- The only fair comparison which can be made is with SV
- Room for improvement...
 - Polarized matter equation of state
 - Correlation between m^*/m and $\langle V \rangle_{pp}$
 - Critical densities in $S = 0$ channels
- ... but how ?
 - Tensor term ? (does not act in $S = 0$ channels...)
 - D wave (N2LO) ?
 - Range ?