

# Determination of Energy Density Functionals from Brueckner-Hartree-Fock calculations

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# Outline of talk:

1. Motivation of the investigation
2. Brueckner-HF with effects of 3-body forces
3. How to determine Skyrme energy functionals from BHF equation of state
4. Applications to ground states of closed shell nuclei and Sn isotopes
5. Giant resonances in  $^{208}\text{Pb}$
6. Summary

# 1. Motivations

- The Skyrme-type Energy Density Functionals (**EDF**) are very successful for describing many nuclear phenomena.
- The 8 parameters are generally adjusted directly on (mostly empirical) properties of nuclear matter.
- It is desirable to build EDF on the basis of microscopic calculations of nuclear matter.
- An earlier attempt (**Cao, Lombardo, Shen, NVG, Phys. Rev. C 73, 014313 (2006)**) has proposed the **LNS** parametrization based on Brueckner-HF (**BHF**) calculations.
- Can one improve this result?

# Brueckner-HF with 3-body forces (1)

Brueckner-Bethe-Goldstone (BBG) equation:

$$G(\omega) = v_{\text{NN}} + v_{\text{NN}} \sum_{k_1 k_2} \frac{|k_1 k_2\rangle Q_{k_1, k_2} \langle k_1 k_2|}{\omega - \epsilon_{k_1} - \epsilon_{k_2}} G(\omega)$$

$$\epsilon_k = k^2/2m + U_k$$

$$U_k = \sum_{k'} \langle k, k' | G(\epsilon_k + \epsilon_{k'}) | k, k' \rangle_A \theta(k_F - k')$$

$$v_{\text{NN}} = V_2^{\text{bare}} + V_3^{\text{eff}}$$

$V_2(\text{bare})$ : Bonn B potential

# Brueckner-HF with 3-body forces (2)

effective two-body force obtained from the three-body force  $W_3$

$$\begin{aligned} \langle \vec{r}_1 \vec{r}_2 | V_3^{\text{eff}} | \vec{r}'_1 \vec{r}'_2 \rangle &= \frac{1}{4} \text{Tr} \sum_n \int d\vec{r}_3 d\vec{r}'_3 \phi_n^*(\vec{r}'_3) \psi(r'_{13}) \psi(r'_{23}) \\ &\times W_3(\vec{r}'_1 \vec{r}'_2 \vec{r}'_3 | \vec{r}_1 \vec{r}_2 \vec{r}_3) \phi_n(r_3) \psi(r_{13}) \psi(r_{23}). \end{aligned}$$

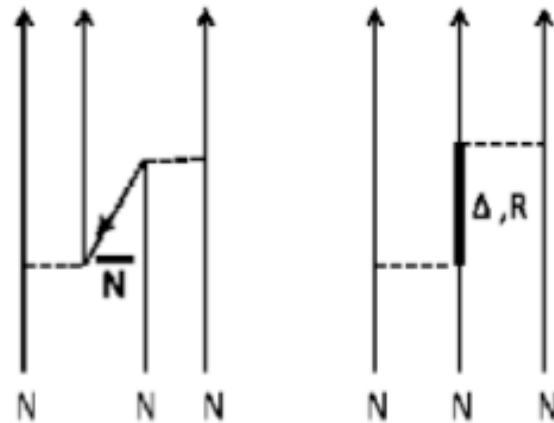
$\psi(r) = 1 - \eta(r)$  : correlated two body wave function

$\eta(r)$  : the defect function

$$\eta_{12} = \langle \vec{r} | \frac{Q}{H_0 - \epsilon_{k_1} - \epsilon_{k_2}} G | k_1, k_2 \rangle$$

Z.H. Li, U. Lombardo, and H.J. Schulze and W. Zuo,  
Phys. Rev. **C 77**, 034316 (2008).

# Brueckner-HF with 3-body forces (3)



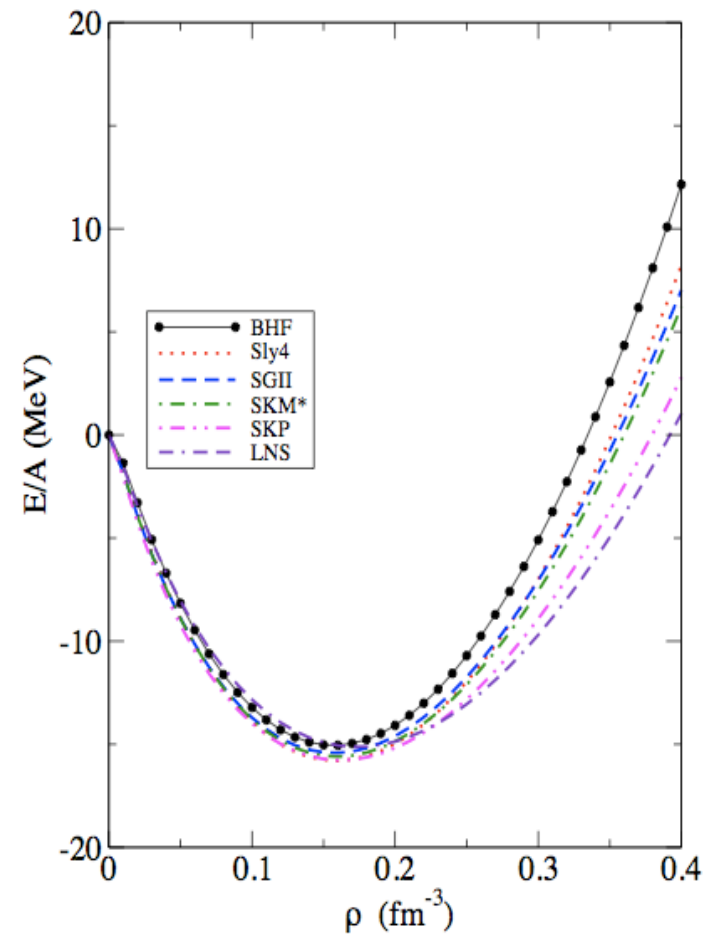
Three body force diagrams included in the BHF calculations. On the left:  $N\bar{N}$  virtual excitations. On the right:  $\Delta(1232)$  and  $N^*(1440)$  (Roper) resonances.

Same meson exchange parameters as in Bonn B  
P. Grangé et al., Phys. Rev. C 40, 1040 (1989)

# How to determine Skyrme energy functionals from BHF equation of state

BHF results of  $E/A$  are reasonably well reproduced in general by Skyrme parametrizations, at least up to saturation density

Fitting only  $E/A$  leads to large indetermination



Energy per particle of symmetric nuclear matter calculated in BHF and with various Skyrme forces.

## U(T,S) components of potential energy in symmetric nuclear matter

$$U_{00}^{(Skyrme)}(\rho) = \frac{3}{160} \left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} t_2 (1 - x_2) \rho^{\frac{5}{3}}, \quad (\text{A2})$$

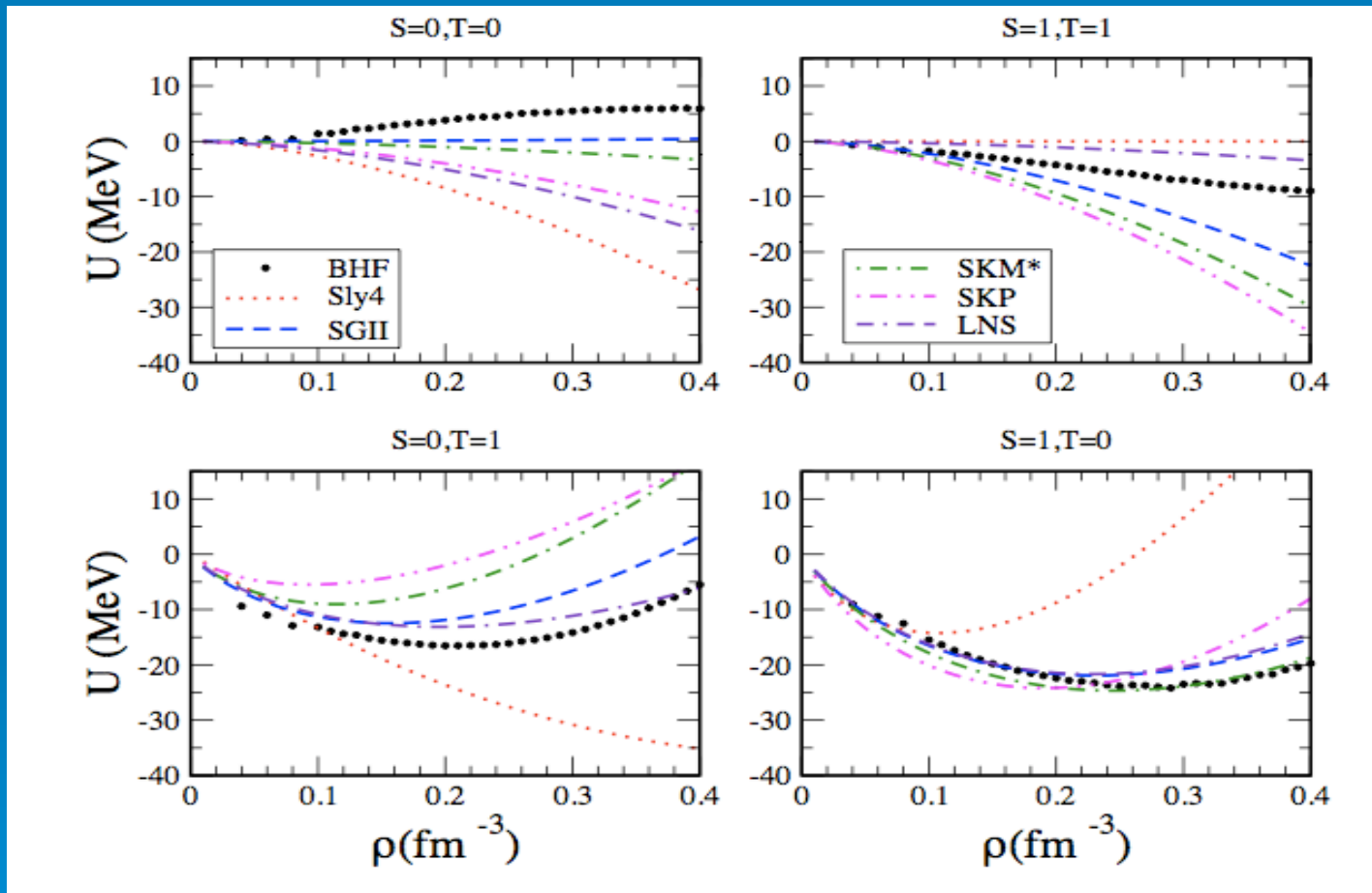
$$U_{11}^{(Skyrme)}(\rho) = \frac{27}{160} \left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} t_2 (1 + x_2) \rho^{\frac{5}{3}}, \quad (\text{A3})$$

$$U_{10}^{(Skyrme)}(\rho) = \frac{3}{16} t_0 (1 - x_0) \rho + \frac{9}{160} \left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} t_1 (1 - x_1) \rho^{\frac{5}{3}} + \frac{1}{32} t_3 (1 - x_3) \rho^{\sigma+1}, \quad (\text{A4})$$

$$U_{01}^{(Skyrme)}(\rho) = \frac{3}{16} t_0 (1 + x_0) \rho + \frac{9}{160} \left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} t_1 (1 + x_1) \rho^{\frac{5}{3}} + \frac{1}{32} t_3 (1 + x_3) \rho^{\sigma+1}. \quad (\text{A5})$$



# contradictory results in separate spin-isospin channels



(S,T) components of potential energy

# LNS parametrization

(Cao, Lombardo, Shen, NVG, Phys. Rev. C 73, 014313 (2006))

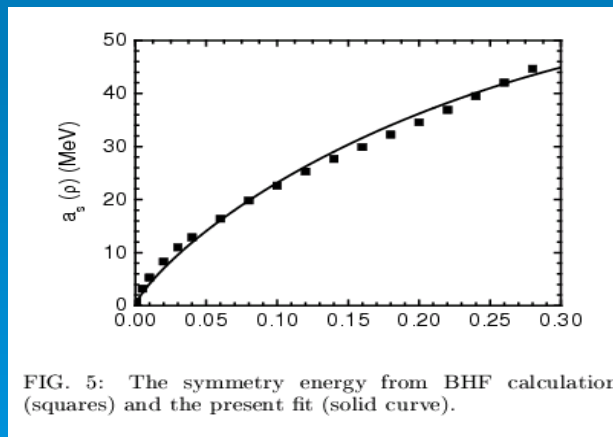
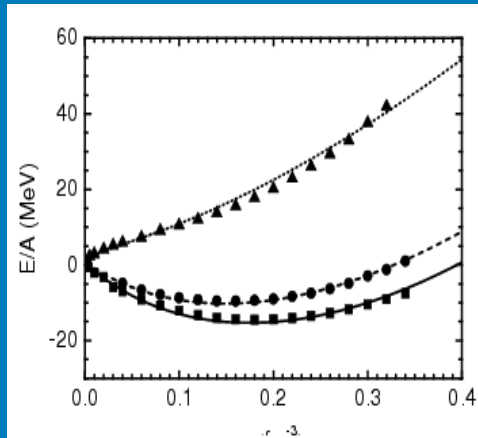


FIG. 5: The symmetry energy from BHF calculations (squares) and the present fit (solid curve).

TABLE I: The Skyrme parameter set and the corresponding bulk properties of infinite nuclear matter.

LNS	
$t_0(\text{MeV fm}^3)$	-2484.97
$t_1(\text{MeV fm}^5)$	266.735
$t_2(\text{MeV fm}^5)$	-337.135
$t_3(\text{MeV fm}^{3+3\sigma})$	14588.2
$x_0$	0.06277
$x_1$	0.65845
$x_2$	-0.95382
$x_3$	-0.03413
$\sigma$	0.16667
$W_0(\text{MeV fm}^5)$	96.00
$\rho_0(\text{fm}^{-3})$	0.1746
$E/A(\text{MeV})$	-15.32
$K_\infty(\text{MeV})$	210.85
$\frac{m^*}{m}(\text{isoscalar})$	0.825
$\frac{m^*}{m}(\text{isovector})$	0.727
$a_s(\text{MeV})$	33.4

# Finite Nuclei with LNS

➤ Density profiles

➤ Energies and Radii

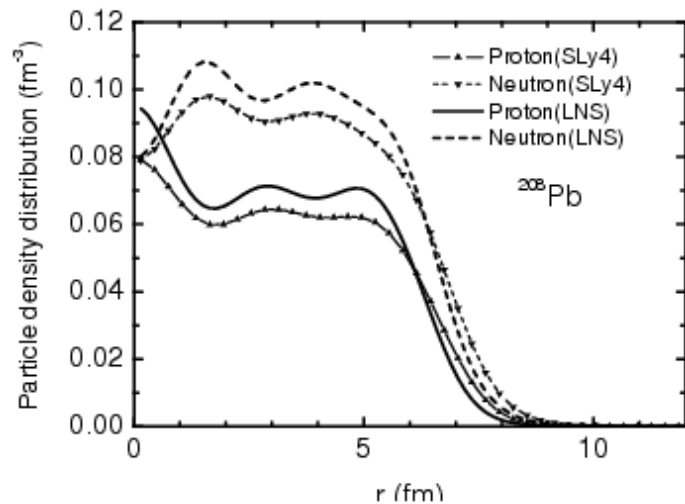
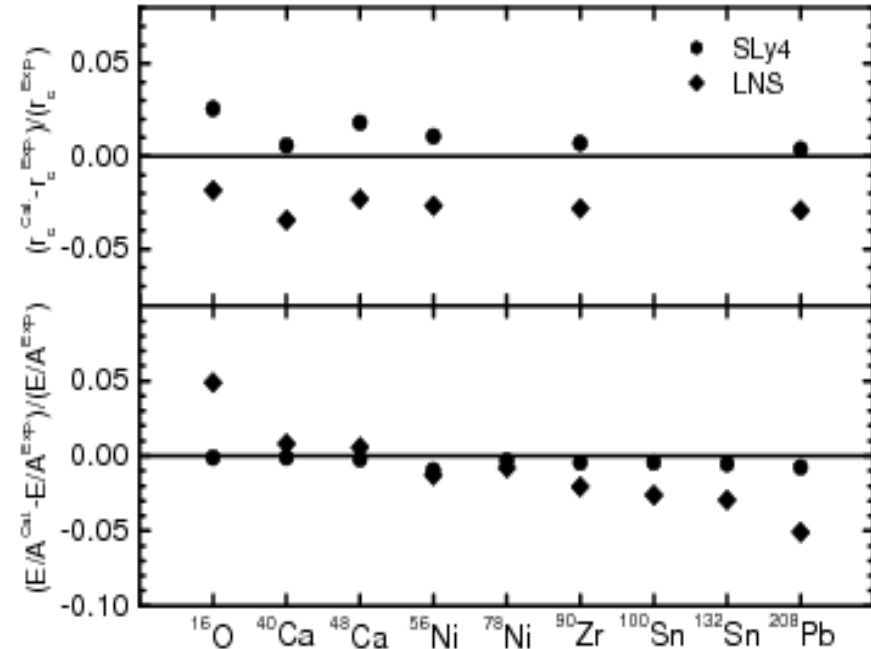


FIG. 7: Neutron and proton densities in <sup>208</sup>Pb, calculated with LNS and SLy4 parametrizations.



# Strategy for parameter fitting

Minimization of

$$\chi^2 = \sum_{i=1}^{N_p} \left( \frac{U_{TS}^{(BHF)}(i) - U_{TS}^{(Skyrme)}(i, t, \mathbf{x})}{\delta_U(i)} \right)^2 +$$

$$\sum_{i=1}^N \left( \frac{E^{(Exp)}(i) - E^{(SHF)}(i, t, \mathbf{x})}{\delta_E(i)} \right)^2 +$$

$$\sum_{i=1}^N \left( \frac{r_c^{(Exp)}(i) - r_c^{(SHF)}(i, t, \mathbf{x})}{\delta_r(i)} \right)^2 + (P(t, \mathbf{x})|_{\rho=\rho_0})/\delta_P)^2$$

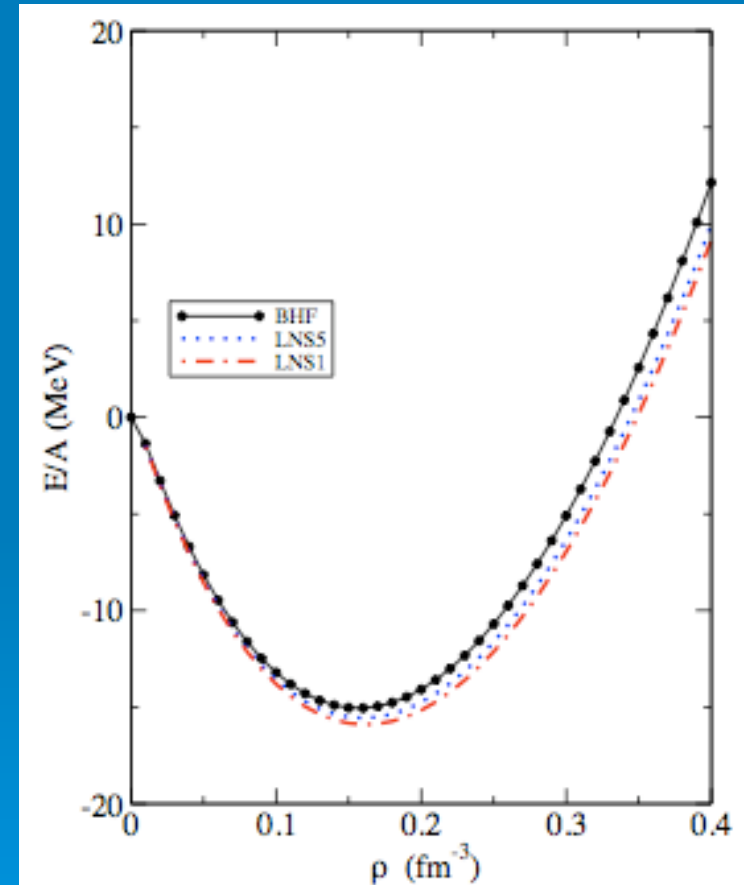
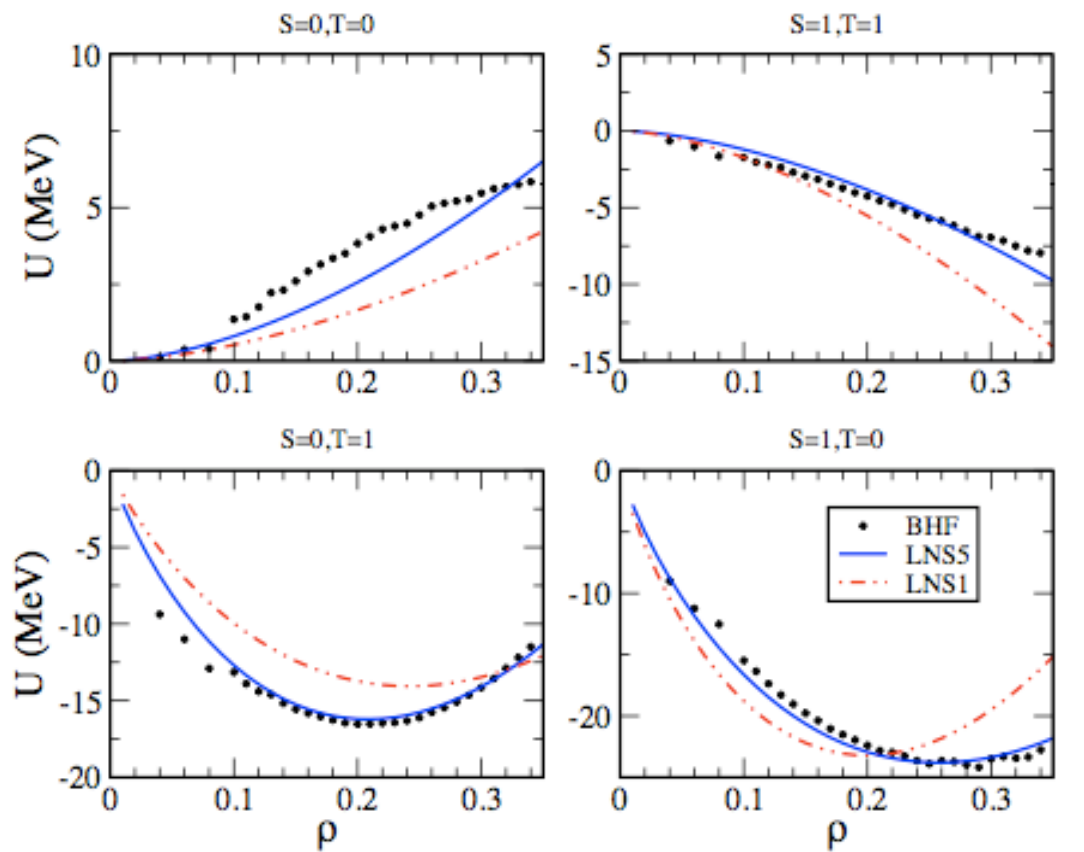
$N_p$ : 10 values for each (S,T)  
 $N$ : 8 magic nuclei  
 Impose  $P=0$  at saturation point

$\text{fm}^{-3}$	$\rho \leq 0.10$	$0.10 \leq \rho \leq 0.25$	$0.25 \leq \rho \leq 0.32$
$\delta_U$	10%	5%	1%

$$\delta_E = 0.5 \text{ MeV (LNS5)}$$

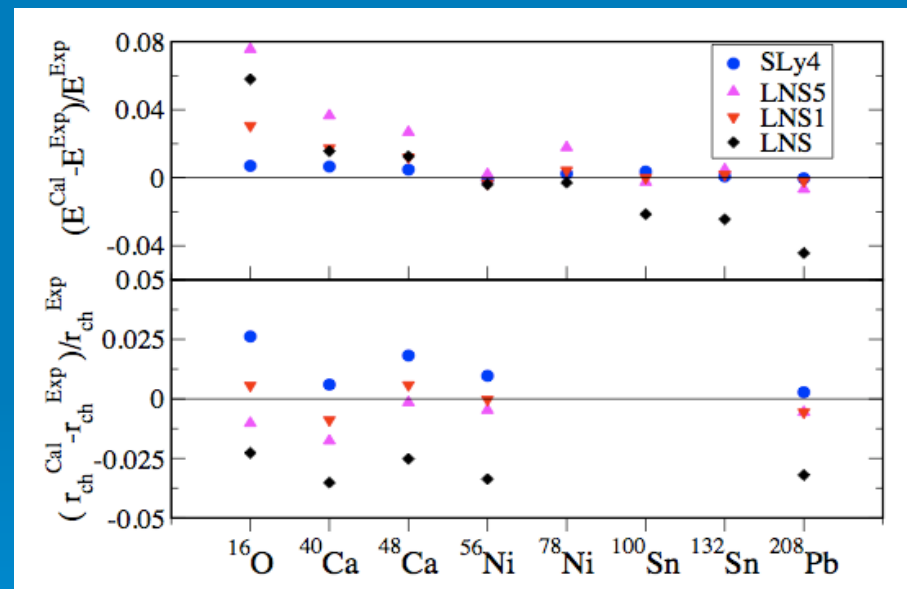
$$\delta_E = 0.1 \text{ MeV (LNS1)}$$

# Nuclear matter results of the 2 new parametrizations

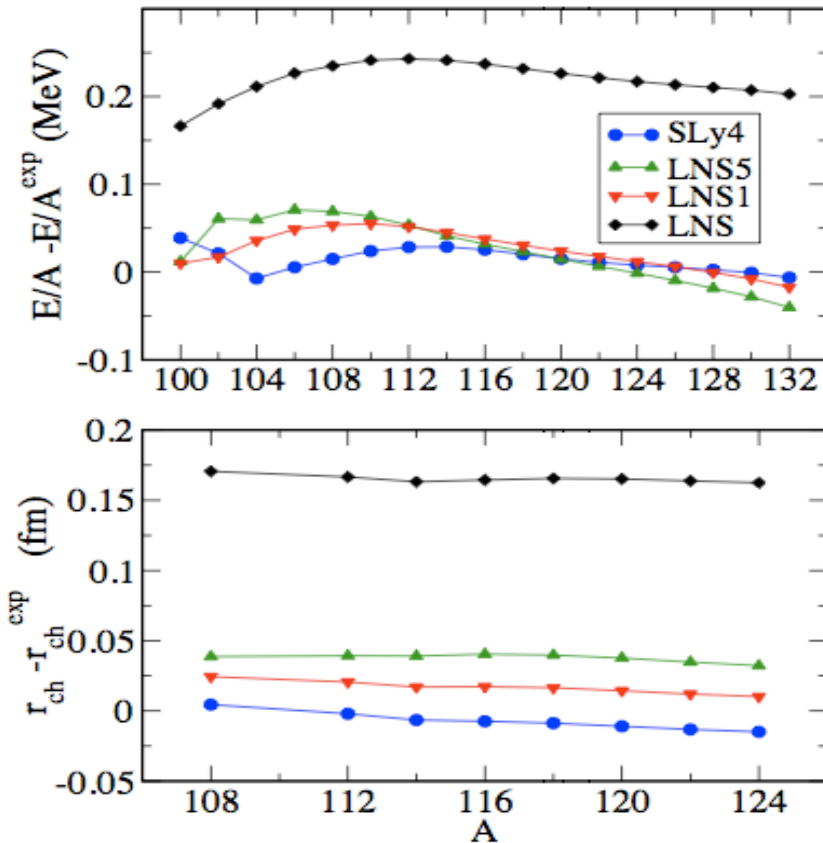


# Closed-shell nuclei with new parametrizations

	Exp	LNS5	LNS1
$^{16}\text{O}$	-127.62 2.73	-137.27 2.758	-131.52 2.745
$^{40}\text{Ca}$	-342.05 3.49	-354.55 3.551	-348.00 3.521
$^{48}\text{Ca}$	-415.99 3.48	-427.13 3.485	-421.03 3.500
$^{56}\text{Ni}$	-483.99 3.75	-484.97 3.768	-482.41 3.751
$^{78}\text{Ni}$	-642.40	-653.81 3.961	-645.24 3.973
$^{100}\text{Sn}$	-825.78	-823.69 4.446	-825.81 4.457
$^{132}\text{Sn}$	-1102.90	-1108.23 4.694	-1104.9 4.700
$^{208}\text{Pb}$	-1636.44 5.50	-1625.41 5.531	-1633.41 5.531



# Nuclei not included in the fit: the Sn chain



Energies

Radii

# A further test: giant resonances

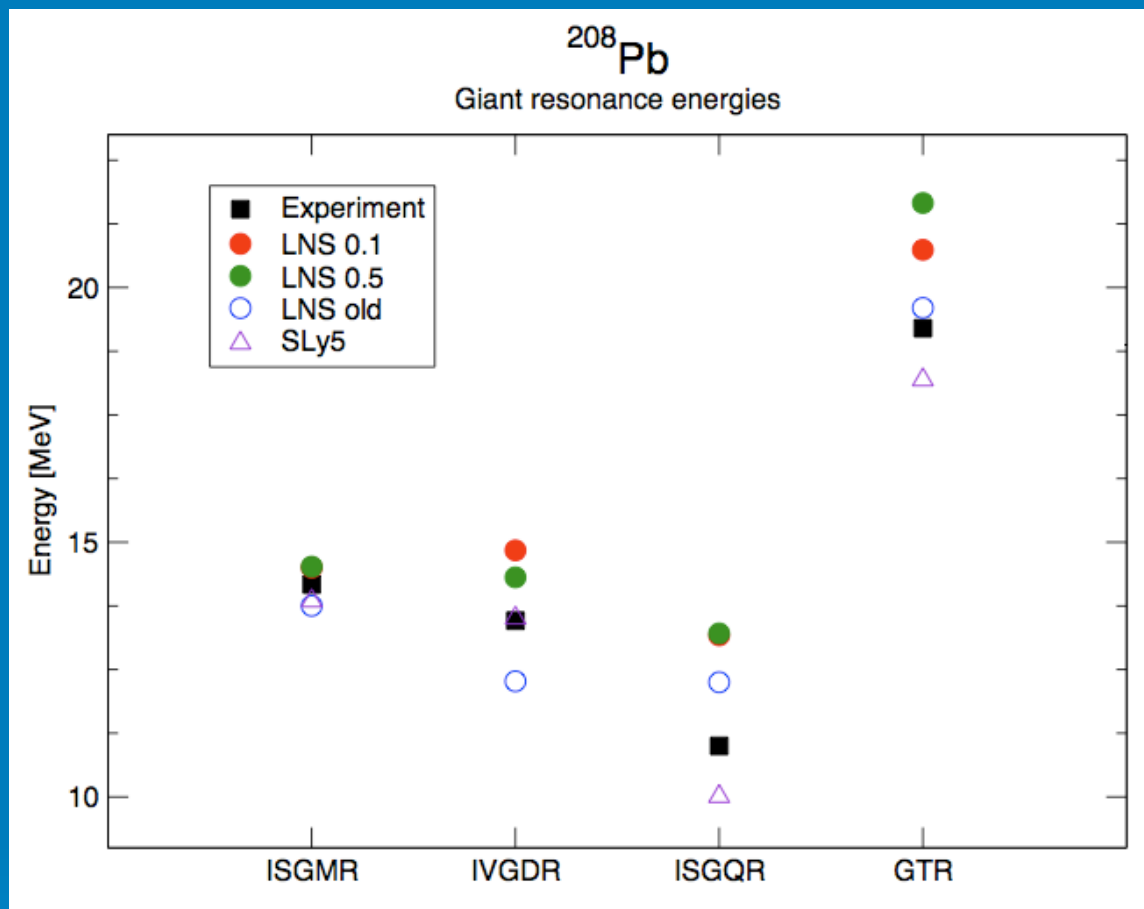
We calculate as a check, using RPA,  
some collective excitations in  $^{208}\text{Pb}$

Isoscalar:  $0+$ ,  $2+$

Isovector:  $1-$ , Gamow-Teller ( $1+$ )

Mode	Operator $F$
Isoscalar monopole	$\sum_{i=1}^A r_i^2$
isovector dipole	$\frac{Z}{A} \sum_{n=1}^N r_n Y_{10}(\hat{r}_n) - \frac{N}{A} \sum_{p=1}^Z r_p Y_{10}(\hat{r}_p)$
Isoscalar quadrupole	$\sum_i r_i^2 Y_{2M}(\hat{r}_i)$
Gamow-Teller	$\sum_i \vec{\sigma}_i \tau_i^{(-)}$
Sum rules	$m_k = \sum_{\alpha} E_{\alpha}^k  \langle \tilde{o}   F   \alpha \rangle ^2$





Mode	Energy	Energy range
Isoscalar monopole	$E_1 = (m_1/m_{-1})^{1/2}$	complete range
isovector dipole	$E_0 = m_1/m_0$	(10 - 17.5) MeV
Isoscalar quadrupole	$E_0 = m_1/m_0$	(10 - 17.5) MeV
Gamow-Teller	$E_0 = m_1/m_0$	...

Advances in Nuclear Many-Body  
Theory, Primosten

The 2 new Skyrme  
parameter sets  
LNS1 and LNS5

	LNS5	LNS1
$t_0$ (MeV fm <sup>3</sup> )	-2194.776	-2215.322
$t_1$ (MeV fm <sup>5</sup> )	482.518	532.536
$t_2$ (MeV fm <sup>4</sup> )	138.137	67.761
$t_3$ (MeV fm <sup>3(1+<math>\sigma</math>)</sup> )	10784.169	10931.718
$x_0$	0.134	0.463
$x_1$	-0.097	0.128
$x_2$	-1.399	-2.174
$x_3$	0.171	0.615
$W_0$ (MeV fm <sup>5</sup> )	105.674	116.789
$\rho_0$ (fm <sup>-3</sup> )	0.1599	0.1604
$E/A$ (MeV)	-15.57	-15.86
$K_\infty$ (MeV)	240.06	241.42
$a_s$ (MeV)	29.21	29.63
$\frac{m^*}{m}$	0.603	0.615
$\chi^2$ per point	1.76	0.38

# Summary

- BHF with 3-body effects can describe correctly the EOS
- Skyrme functionals can only reproduce approximately BHF results in nuclear matter
- One has to impose additional constraints on finite nuclei
- It is then possible to determine parameter sets (LNS1,LNS5) which give satisfactory results in nuclear matter and in nuclei
  - The analytical form of Skyrme parametrization puts constraints on results

# Thank You!

and Happy Birthday  
to you, Peter !