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

Nguyen Van Giai
Institut de Physique Nucléaire
Université Paris-Sud, Orsay

Collaboration:
D. Gambacurta, U. Lombardo (Università di Catania)
G. Colò (Università di Milano)
L. Li (PKU), W. Zuo (IMP Lanzhou)

Phys. Rev. C 84, 024301 (2011)

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 208Pb
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:

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

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

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

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

V_2(bare): Bonn B potential

Brueckner-HF with 3-body forces (2)

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

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

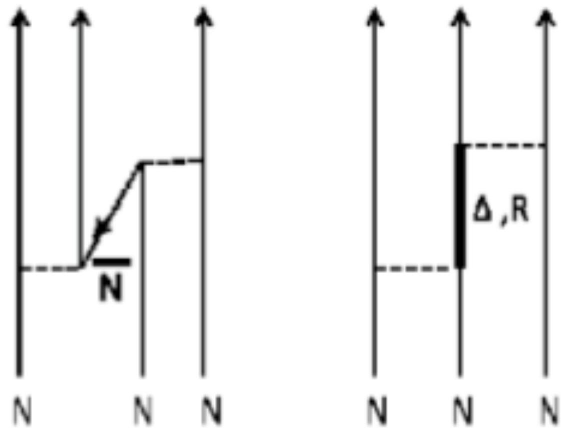
$\psi(r) = 1 - \eta(r)$: correlated two body wave function

$\eta(r)$: 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)



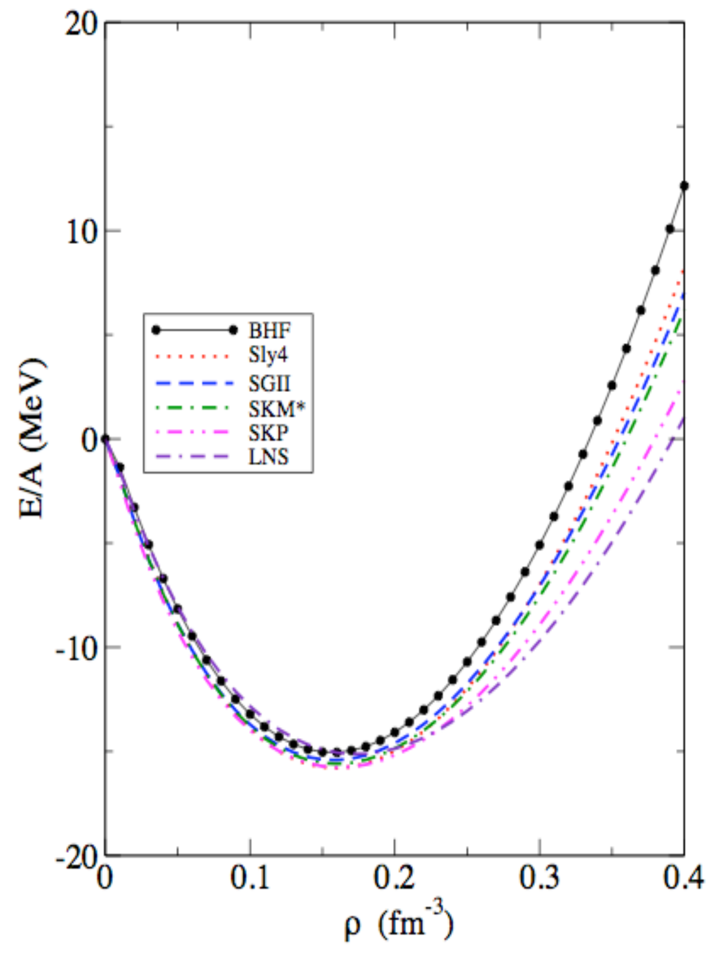
Three body force diagrams included in the BHF calculations. On the left: $N\overline{N}$ virtual excitations. On the right: $\Delta(1232)$ and $N^*(1440)$ (Roper) resonances.

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

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

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

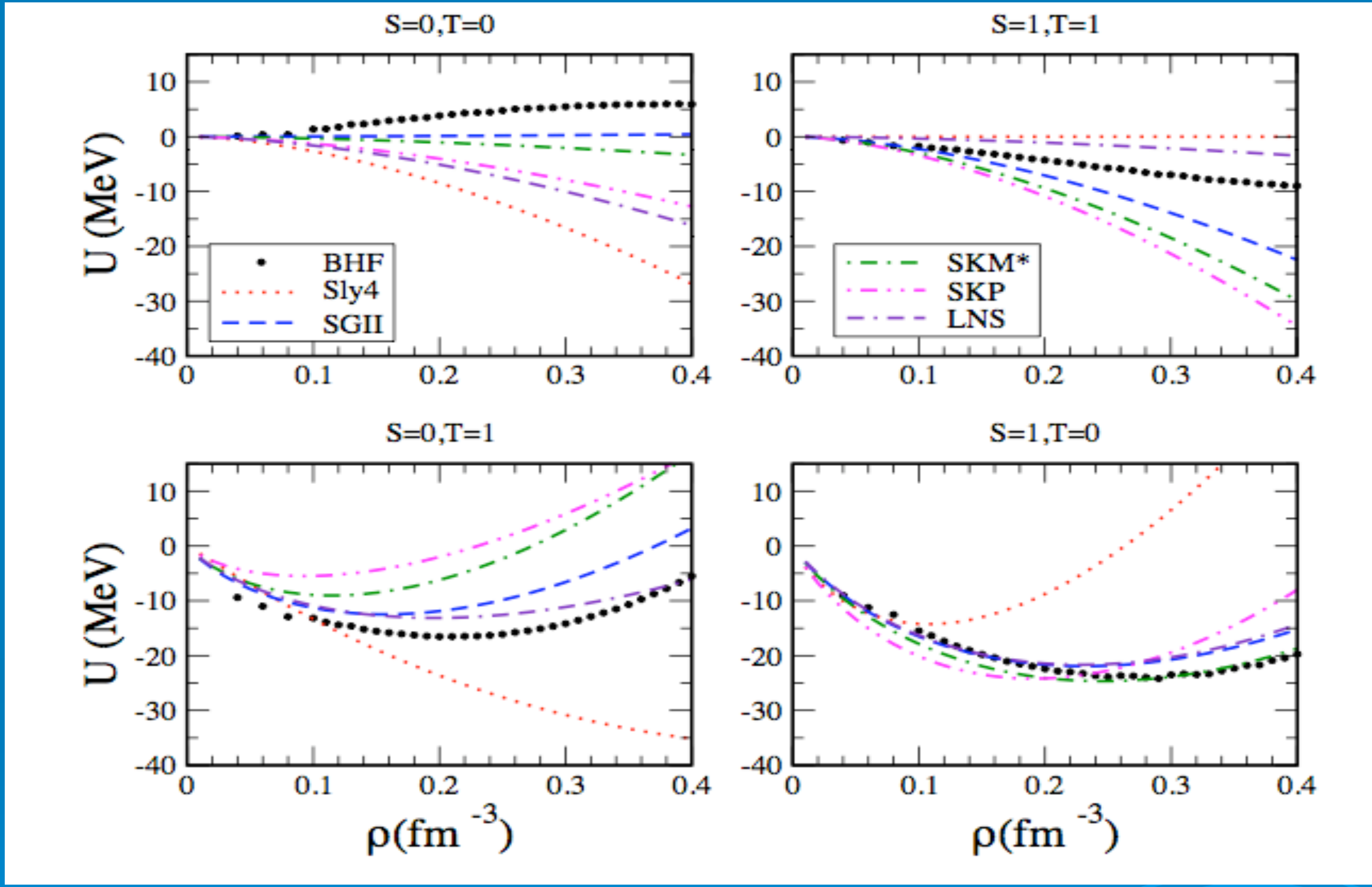
$$U_{10}^{(Skyrme)}\rho) = \frac{3}{16} t_0(1 - x_0)\rho \frac{9}{160}(\frac{3\pi^2}{2})^{\frac{2}{3}} t_1(1 - x_1)\rho^{\frac{5}{3}} +$$

$$+\frac{1}{32} t_3(1 - x_3)\rho^{\sigma+1}, \qquad \text{(A4)}$$

$$U_{01}^{(Skyrme)}(\rho) = \frac{3}{16} t_0(1 + x_0)\rho + \frac{9}{160}(\frac{3\pi^2}{2})^{\frac{2}{3}} t_1(1 + x_1)\rho^{\frac{5}{3}},$$

$$+\frac{1}{32} t_3(1 + x_3)\rho^{\sigma+1}. \qquad \text{(A5)}$$

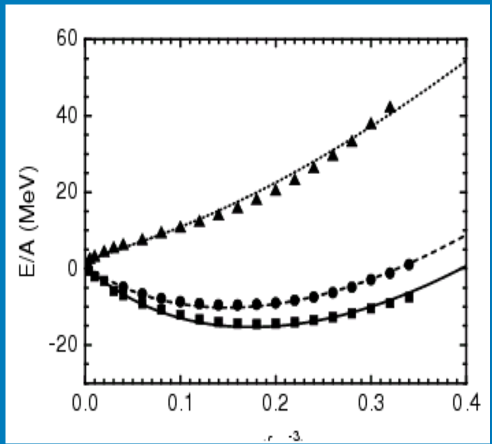
contradictory results in separate spin-isospin channels



(S,T) components of potential energy

LNS parametrization

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



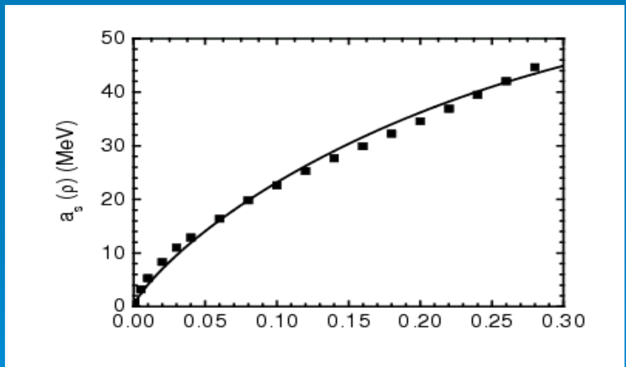


FIG. 5: The symmetry energy from BHF calculations (squares) and the present fit (solid curve).

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

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

Finite Nuclei with LNS

- Density profiles
- Energies and Radii

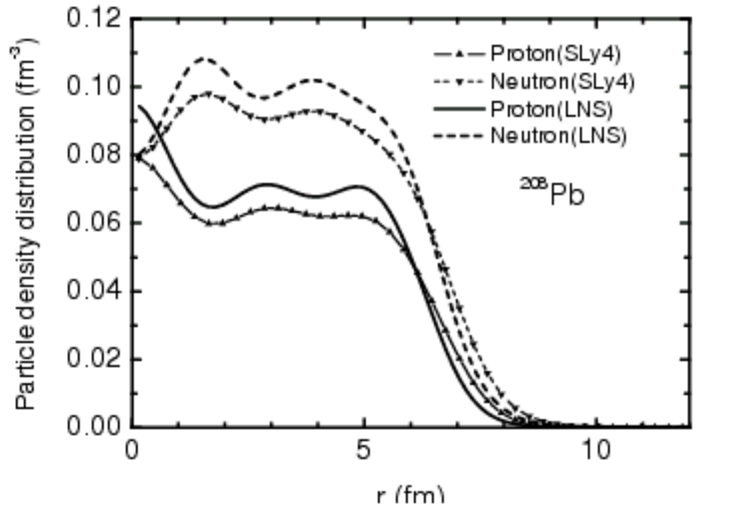
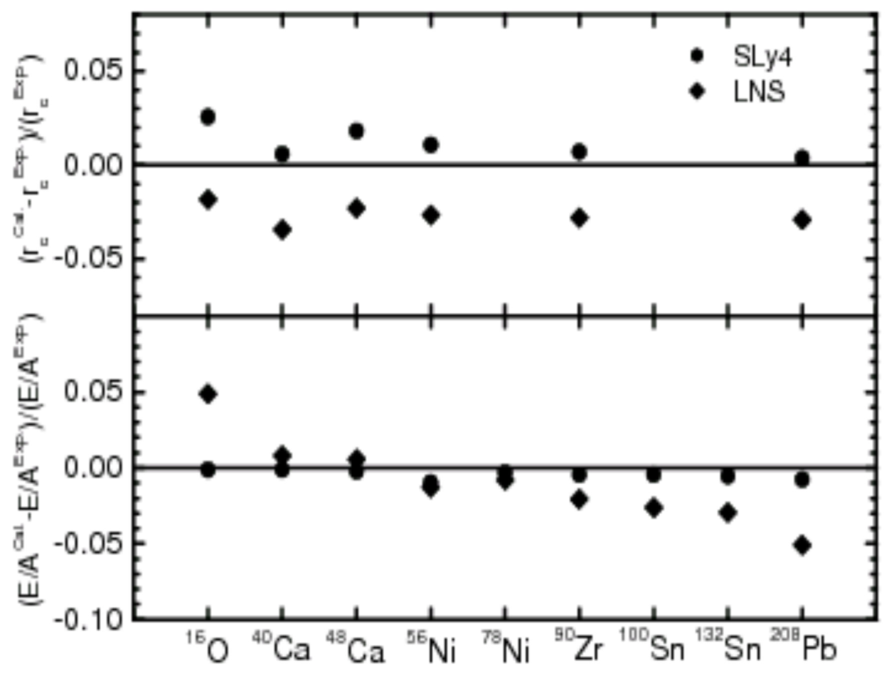


FIG. 7: Neutron and proton densities in ^{208}Pb, calculated with LNS and SLy4 parametrizations.



Strategy for parameter fitting

Minimization of

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

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

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

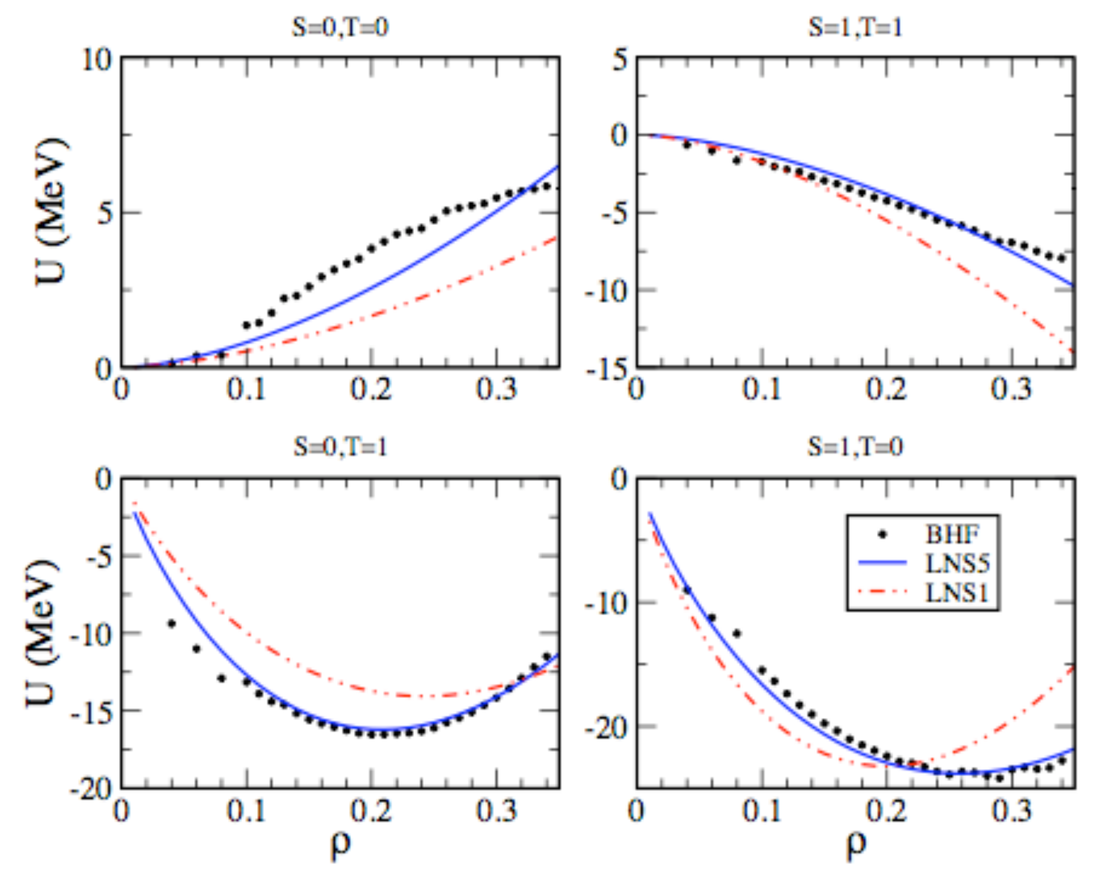
Np: 10 values for each (S,T)
N: 8 magic nuclei
Impose P=0 at saturation point

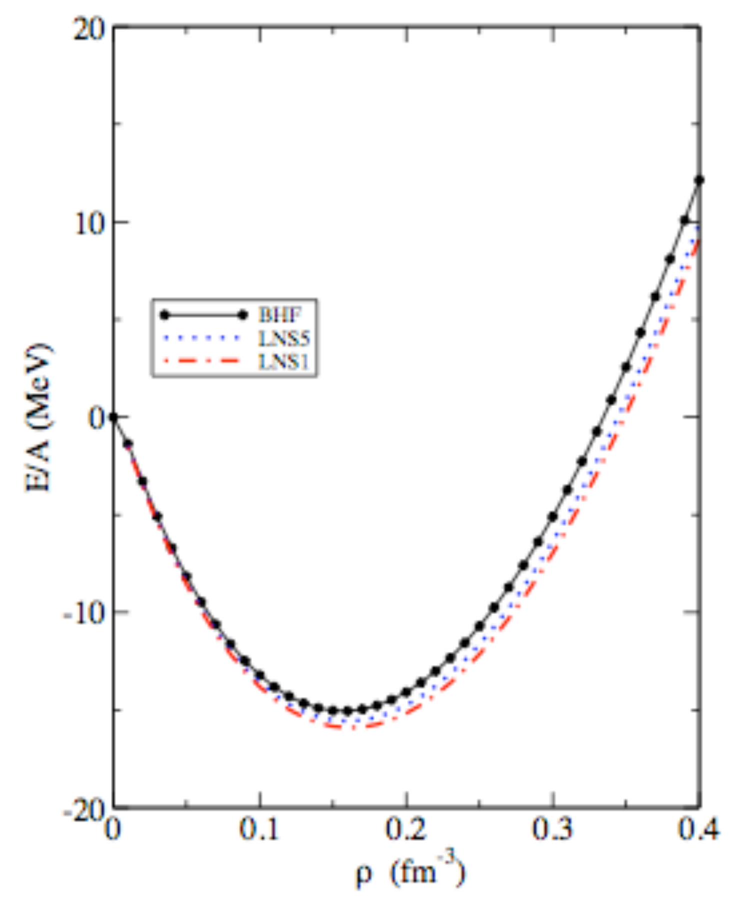
fm^{-3}	$\rho \leq 0.10$	$0.10 \leq \rho \leq 0.25$	$0.25 \leq \rho \leq 0.32$
δ_U	10%	5%	1%

$\delta_E = 0.5$ MeV (LNS5)

$\delta_E = 0.1$ MeV (LNS1)

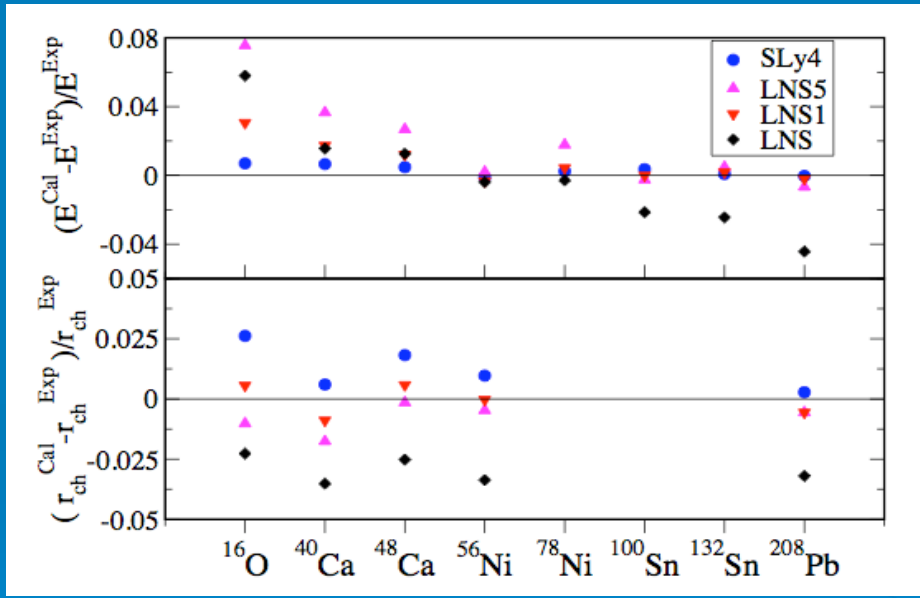
Nuclear matter results of the 2 new parametrizations



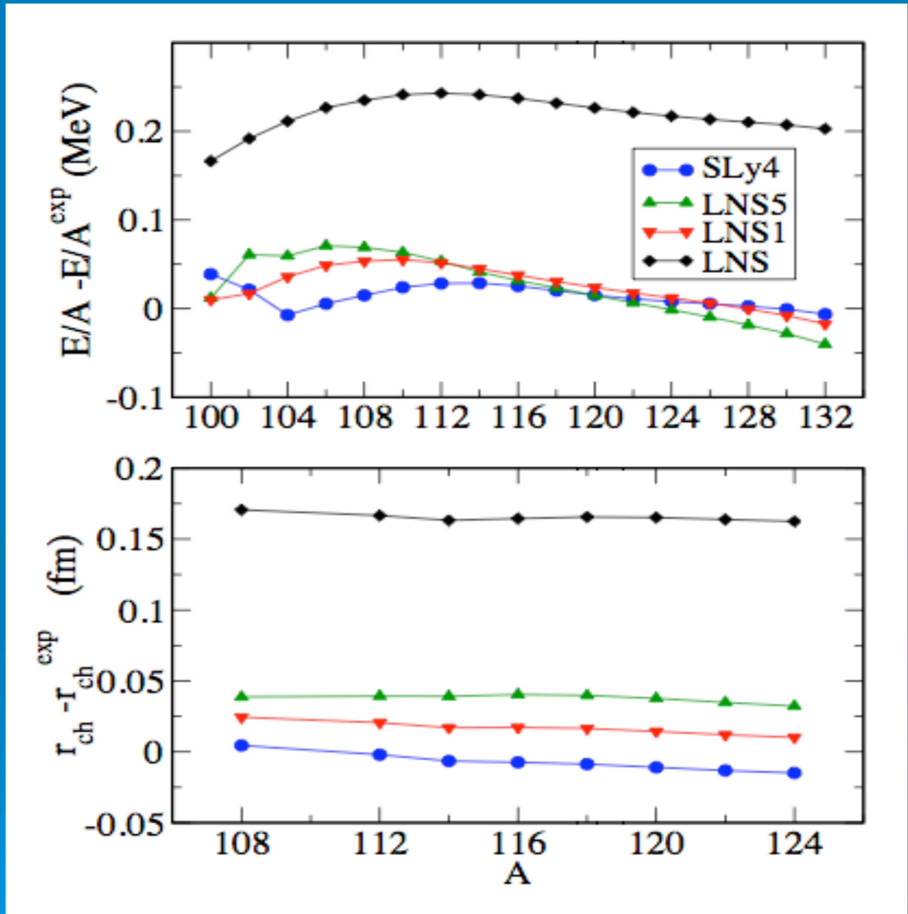


Closed-shell nuclei with new parametrizations

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



Nuclei not included in the fit: the Sn chain



Energies

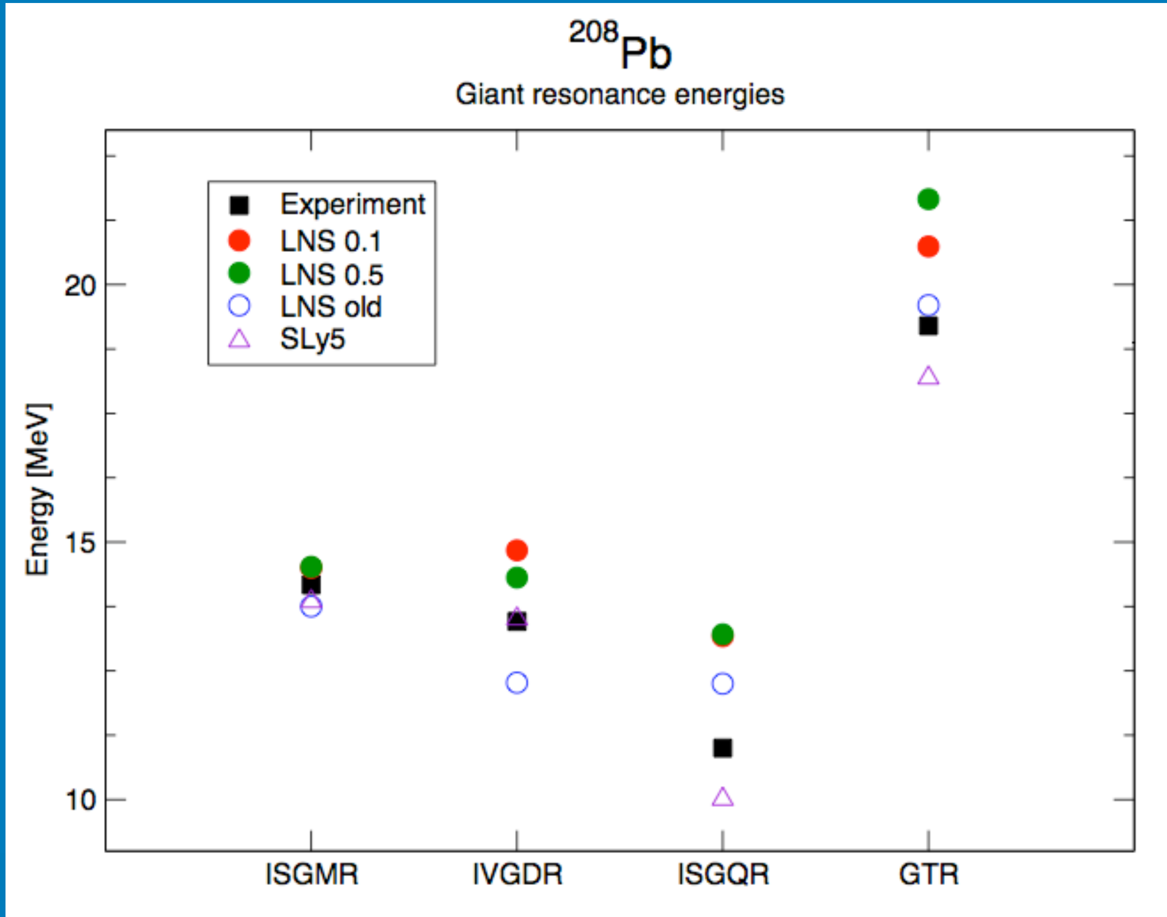
Radii

A further test: giant resonances

We calculate as a check, using RPA, some collective excitations in 208Pb

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	$\mathrm{m}_k = \sum_\alpha E_\alpha^k \lvert\langle\tilde{o}\lvert F\rvert\alpha\rangle\rvert^2$



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	$E_0 = m_1/m_0$	...

The 2 new Skyrme parameter sets LNS1 and LNS5

	LNS5	LNS1
t_0 (MeV fm^3)	-2194.776	-2215.322
t_1 (MeV fm^5)	482.518	532.536
t_2 (MeV fm^4)	138.137	67.761
t_3 (MeV fm$^{3(1+\sigma)}$)	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^5)	105.674	116.789
ρ_0 (fm^{-3})	0.1599	0.1604
E/A (MeV)	-15.57	-15.86
K_∞ (MeV)	240.06	241.42
a_s (MeV)	29.21	29.63
$\frac{m*}{m}$	0.603	0.615
χ^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