Some new developments in relativistic point-coupling models

T. J. Buervenich[1], D. G. Madland[1], J. A. Maruhn[2], and P.-G. Reinhard[3]

[1]Los Alamos National Laboratory
[2]University of Frankfurt
[3]University of Erlangen-Nuernberg

INT03 workshop on Theories of Nuclear Forces & Nuclear Systems

December 3, 2003

Outline

- The relativistic mean-field point-coupling (RMF-PC) approach to nuclear ground states
- Current issues, puzzles, questions, ...
- Extensions of the model

Status

additional nonlinear terms

observables

binding energy, radii, surface, single-particle energies, shell structure, ... for the whole nuclear chart
further (on top of the mean field): excitations, collective states, ...

naturalness

Motivation

Successful models with point couplings

- Fermi theory
- NJL model
- Skyrme-Hartree-Fock
- Effective Field Theories

$$\frac{1}{m^2-q^2} \approx \frac{1}{m^2} + \frac{q^2}{m^4} + \dots$$

low momentum:
derivative expansion
should work

does work

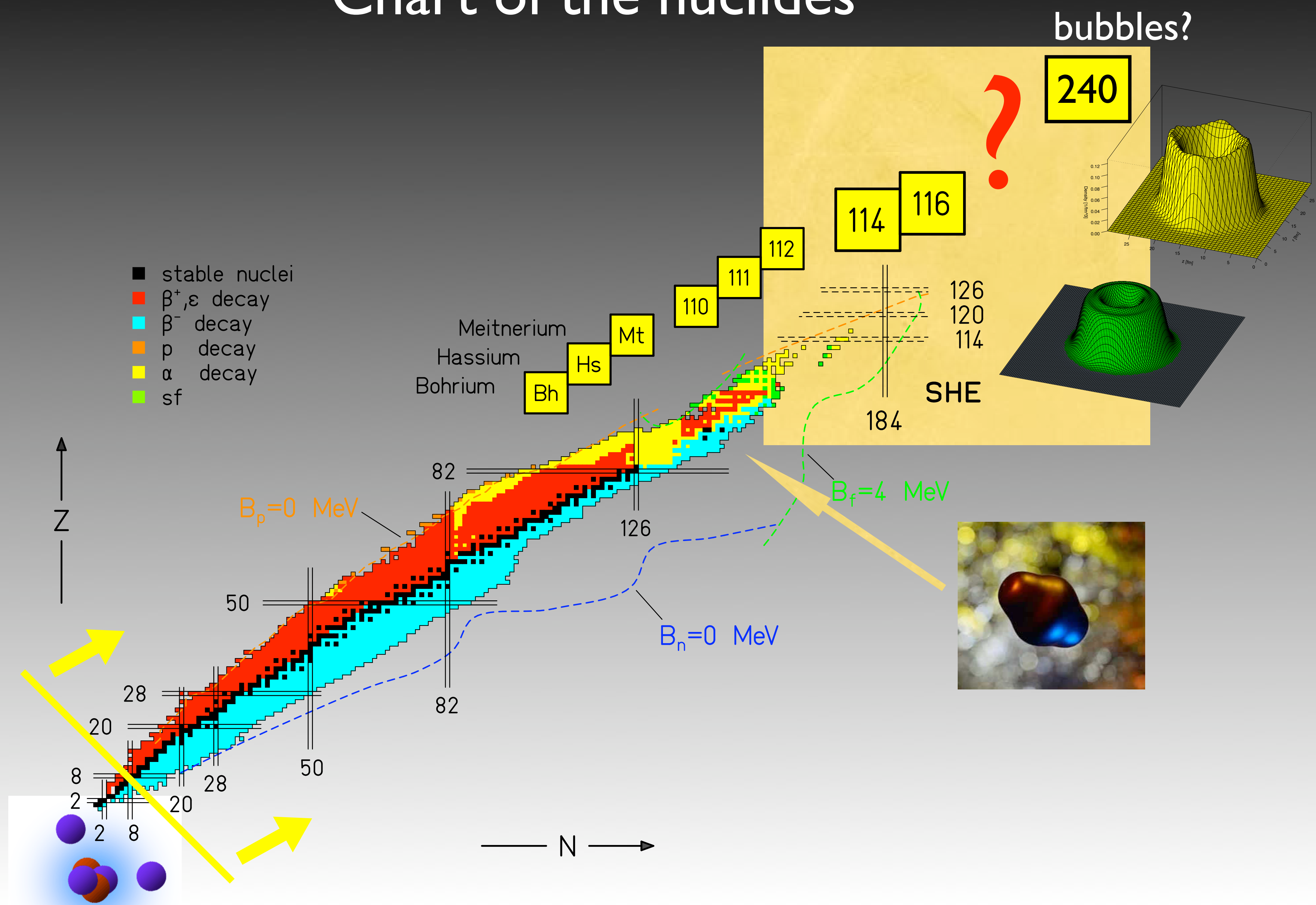
Predictive power comparable to Walecka-type relativistic mean-field (RMF) models with "meson exchange"

Features

- Hartree and Hartree-Fock
- Link to relativistic "meson" models
- Link to nonrelativistic Skyrme-Hartree-Fock point-coupling models
- Test of power counting in finite nuclei
- EFT / DFT

covariant framework:
large scalar and vector potentials:
saturation
spin-orbit for free!

Chart of the nuclides



Philosophy of self-consistent mean-field models for nuclei

(to set the stage)

Construct an Effective Interaction (or an Energy Functional) between point-like nucleons

Introduce approximations and solve the reduced problem numerically

Adjust the coupling constants introduced through the interaction (6 to10, 2 for pairing): a *force* is born (biased, thus there are many forces)

There is no *'best force'*: the adjustment procedure determines the predictive power for various observables

Predict nuclear ground-state observables throughout the nuclear chart and extrapolate

The relativistic mean-field (RMF) model

nucleons interact with each other through the exchange of various mesons (scalar, vector, isovector-vector, ...)

historic view

covariant Lagrangian

Hartree approximation (no exchange terms)

mean-field (field operators can be replaced by their expectation values)

no-sea (vacuum polarization is ignored)

RMF approximates the exact density functional of strongly interacting fermions [Hartree + exchange-correlation functional] - Effective Field Theory

modern view

interaction due to mean meson fields or point-like (contact) interactions and derivatives

Building blocks

in principle all possible Lorentz invariants
(isoscalar, isovector) should be there

Phenomenology, Symmetries, Approximations:

- large scalar and vector potentials $(\bar{\psi}\psi)^2,\ (\bar{\psi}\gamma_\mu\psi)^2$
- density dependence $(\bar{\psi}\psi)^3,\ (\bar{\psi}\psi)^4,\ (\bar{\psi}\gamma_\mu\psi)^4$
- derivatives (~ finite range) $(\partial_\mu\bar{\psi}\psi)^2,\ (\partial_\mu\bar{\psi}\gamma_\nu\psi)^2$
- isovector channel $(\bar{\psi}\gamma_\mu\vec{\tau}\psi)^2,\ (\partial_\mu\bar{\psi}\gamma_\nu\vec{\tau}\psi)^2$
- Coulomb force
- pairing

The RMF-PC Lagrangian

$$\mathcal{L} = \mathcal{L}^{\rm free} + \mathcal{L}^{\rm 4f} + \mathcal{L}^{\rm hot} + \mathcal{L}^{\rm der} + \mathcal{L}^{\rm em}$$

$$\begin{aligned}
\mathcal{L}^{\rm free} &= && \bar\psi(i\gamma_\mu\partial^\mu - m)\psi \\
\mathcal{L}^{\rm 4f} &= &-& \frac{1}{2}\alpha_{\rm S}(\bar\psi\psi)(\bar\psi\psi) - \frac{1}{2}\alpha_{\rm V}(\bar\psi\gamma_\mu\psi)(\bar\psi\gamma^\mu\psi) - \frac{1}{2}\alpha_{\rm TV}(\bar\psi\vec\tau\gamma_\mu\psi)\cdot(\bar\psi\vec\tau\gamma^\mu\psi) \\
\mathcal{L}^{\rm hot} &= &-& \frac{1}{3}\beta_{\rm S}(\bar\psi\psi)^3 - \frac{1}{4}\gamma_{\rm S}(\bar\psi\psi)^4 - \frac{1}{4}\gamma_{\rm V}[(\bar\psi\gamma_\mu\psi)(\bar\psi\gamma^\mu\psi)]^2 \\
\mathcal{L}^{\rm der} &= &-& \frac{1}{2}\delta_{\rm S}(\partial_\nu\bar\psi\psi)(\partial^\nu\bar\psi\psi) - \frac{1}{2}\delta_{\rm V}(\partial_\nu\bar\psi\gamma_\mu\psi)(\partial^\nu\bar\psi\gamma^\mu\psi) \\
& &-& \frac{1}{2}\delta_{\rm TV}(\partial_\nu\bar\psi\vec\tau\gamma_\mu\psi)\cdot(\partial^\nu\bar\psi\vec\tau\gamma^\mu\psi) \\
\mathcal{L}^{em} &= &-& eA_\mu\bar\psi[(1-\tau_3)/2]\gamma^\mu\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}
\end{aligned}$$

$$+BCS + \delta - force(volume)pairing$$

BCS pairing

standard BCS formalism
proton-proton / neutron-neutron pairing only

The assumption of a local δ-like interaction leads to a contribution to $\mathcal{E}$ of the form

$$\mathcal{E}_{pair} = \frac{1}{4} \int d^3r \; G(\vec{r}) \; \chi^2(\vec{r})$$

with the *pairing density*

$$\chi(\vec{r}) = -2 \sum_{k>0} u_k \; v_k \; |\psi_k(\vec{r})|^2 .$$

δ-force pairing

$$G(\vec{r}) = constant = V_0 .$$

$$\mathcal{E}^{\delta}_{pair} = \frac{V_0}{4} \int d^3r \; \chi^2(\vec{r}) .$$

The *pairing potential*

+ cutoff

$$\Delta_q = \frac{V_0}{2} \; \chi_q$$

is mainly located inside the nucleus.

Adjustment of forces

binding energy [all forces]

diffraction radius [NL-Z2, PC-F1, SkI3/4]

surface thickness [NL-Z2, PC-F1, SkI3/4]

rms radius [NL-Z2, NL3, PC-F1, SkI3/4, SkP, SLy6]

neutron radius [NL3]

spin-orbit splitting [Skyrme forces]

isotope shift in lead [SkI3/4]

nuclear matter [NL3]

neutron matter [SLy6]

form factor

chisquared adjustment to magic and doubly-magic nuclei

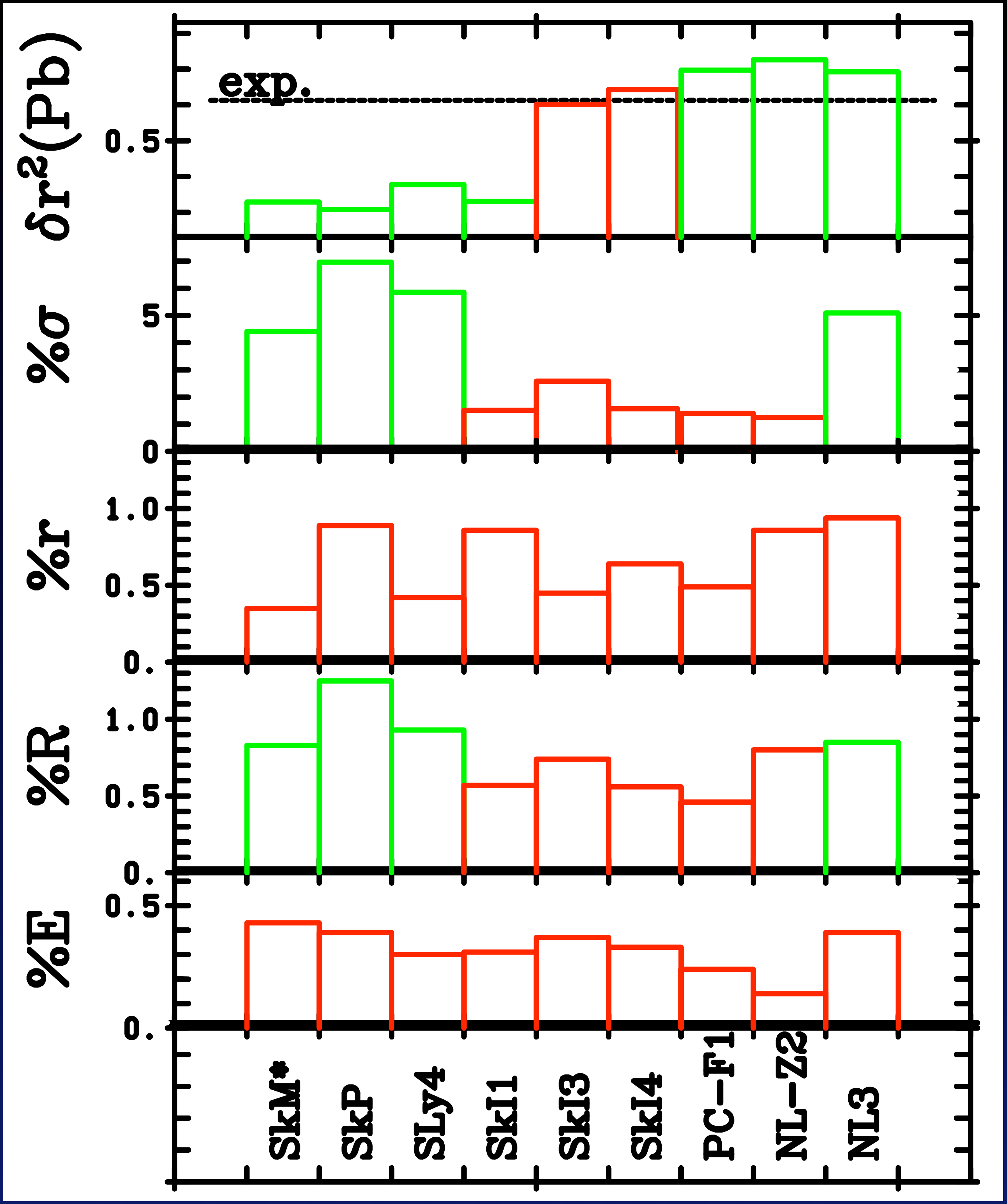
Adjusting the parameters of the RMF model

observable	error	^{16}O	^{40}Ca	^{48}Ca	^{56}Ni	^{58}Ni	^{88}Sr	^{90}Zr	^{100}Sn	^{112}Sn	^{120}Sn	^{124}Sn	^{132}Sn	^{136}Xe	^{144}Sm	^{202}Pb	^{208}Pb	^{214}Pb
E_B	0.2 %	+	+	+	+	+	+	+	+	+	+	+	+	+	+	−	+	+
R_{dms}	0.5 %	+	+	+	−	+	+	+	−	+	+	+	−	−	−	−	+	−
σ	1.5 %	+	+	+	−	−	−	+	−	−	−	−	−	−	−	−	+	−
r_{rms}^{ch}	0.5 %	−	+	+	+	+	+	+	−	+	−	+	−	−	−	+	+	+
Δ_p	0.05 MeV	-	-	-	-	-	-	-	-	-	-	-	-	+	+	-	-	-
Δ_n	0.05 MeV	-	-	-	-	-	-	-	-	+	+	+	-	-	-	-	-	-

magic and doubly-magic (spherical) nuclei are chosen

adjustment to both binding energy and form factor

pairing strengths are adjusted simultaneously with the mean-field parameters



prediction

adjusted

surface thickness

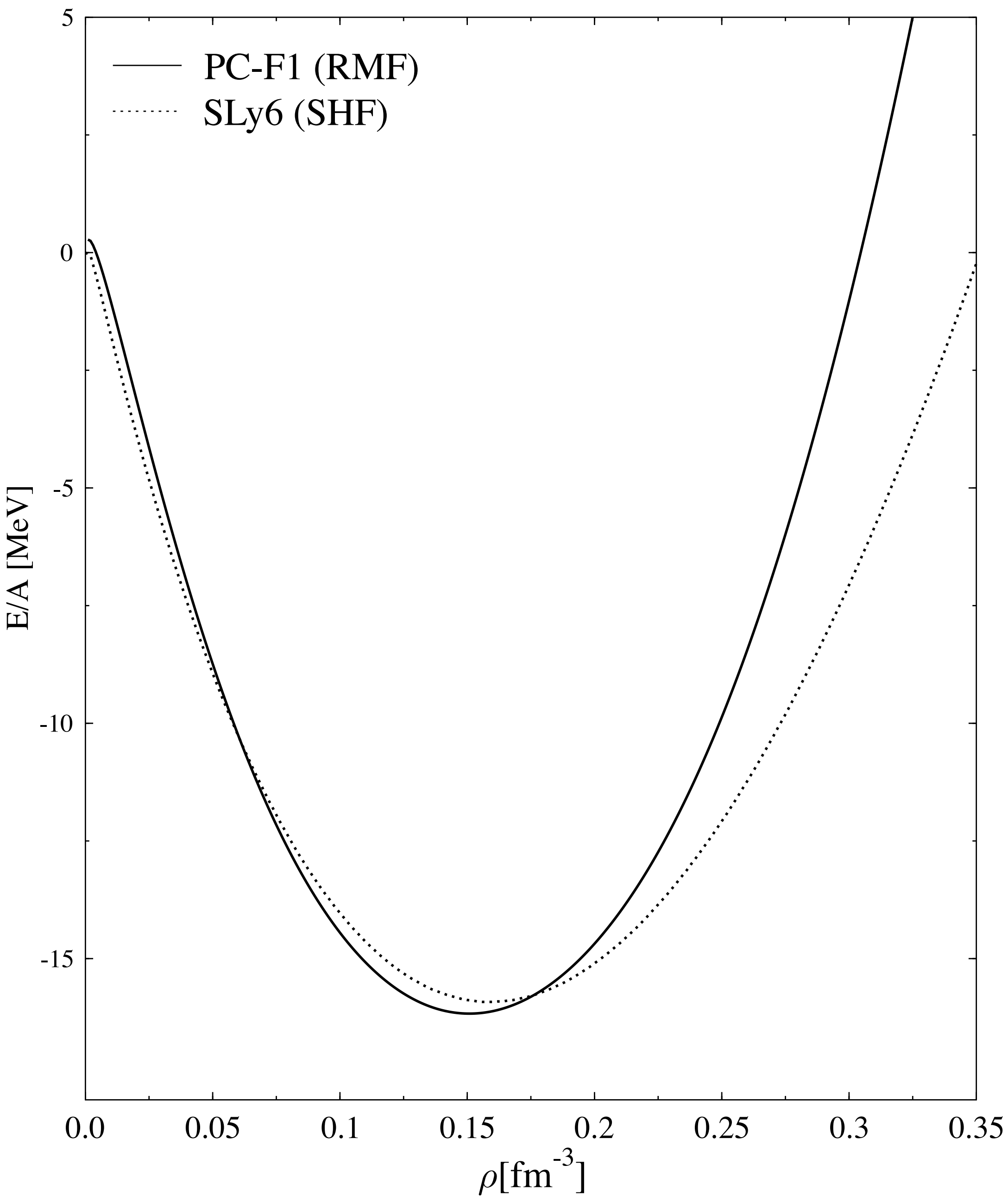
rms radius

diffraction radius

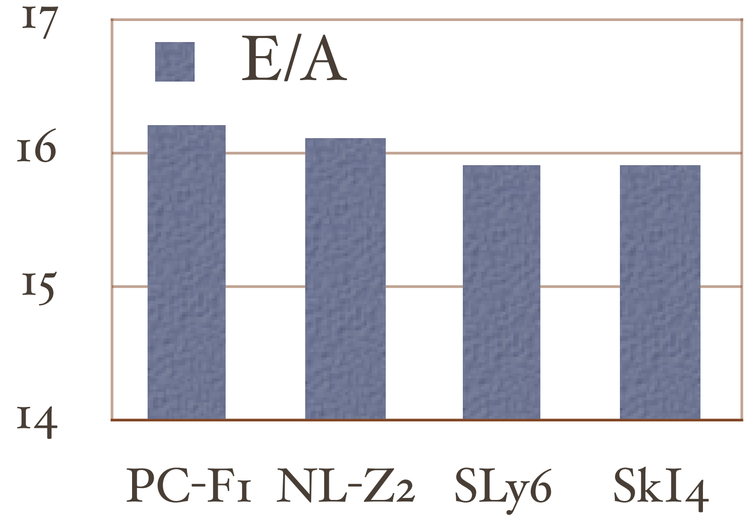
binding energy

Current puzzles

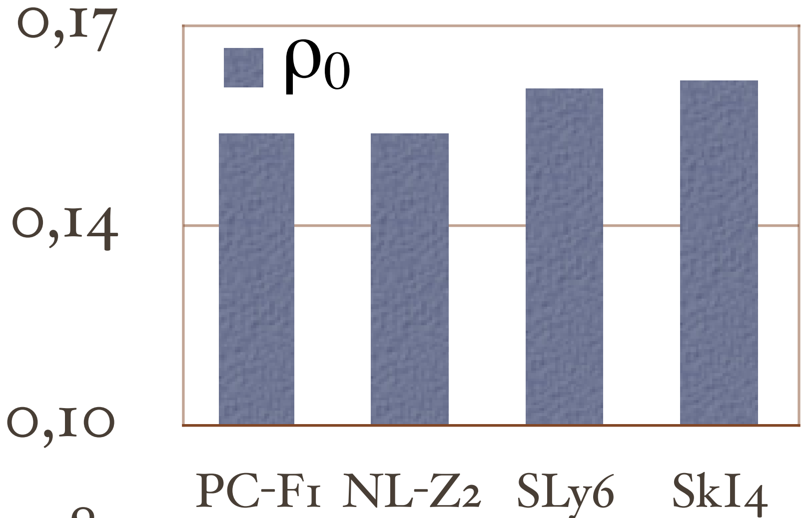
- nuclear matter bulk properties differ in RMF and Skyrme-Hartree-Fock (SHF)
- wrong trends in binding energies
- asymmetry energy appears to be too large (~ 38 MeV) compared to empirical values of ~ 32 MeV
- surface thicknesses are too small (~ 5 %)
- compressibility does not seem to be determined by ground-state observables
- axial fission barriers in RMF and SHF differ by up to factor of two for superheavies (trends already visible in actinides)
- . . .



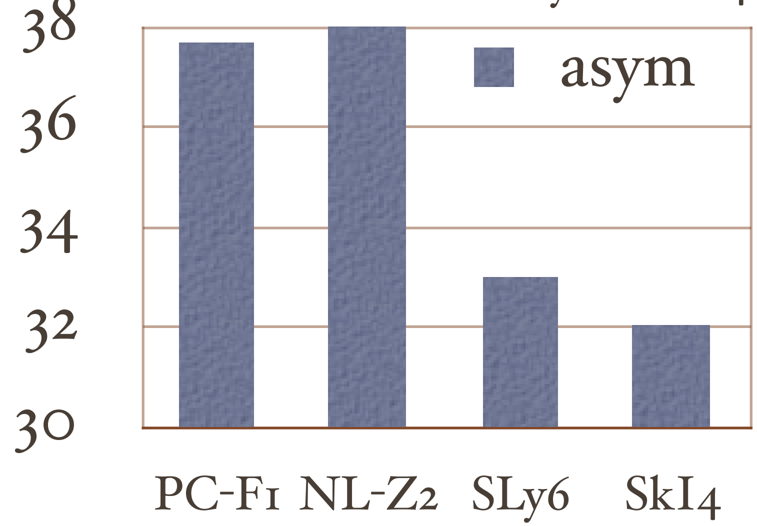
PC-F1 (RMF)
SLy6 (SHF)
E/A [MeV]
ρ[fm^-3]



E/A
PC-F1 NL-Z2 SLy6 SkI4



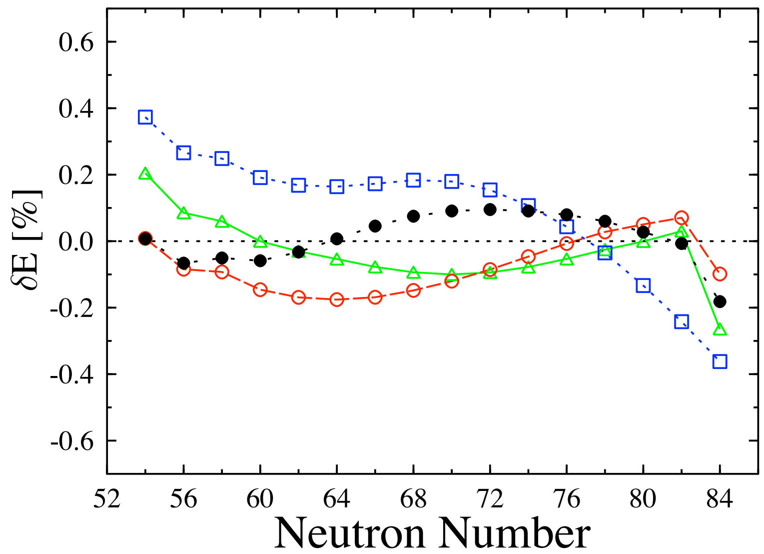
ρ0
PC-F1 NL-Z2 SLy6 SkI4



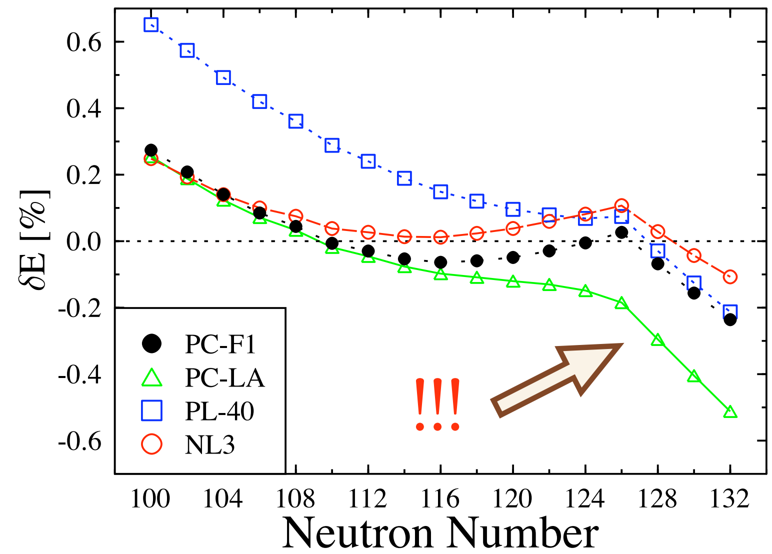
asym
PC-F1 NL-Z2 SLy6 SkI4

T=0: attraction
T=1: repulsion

Sn

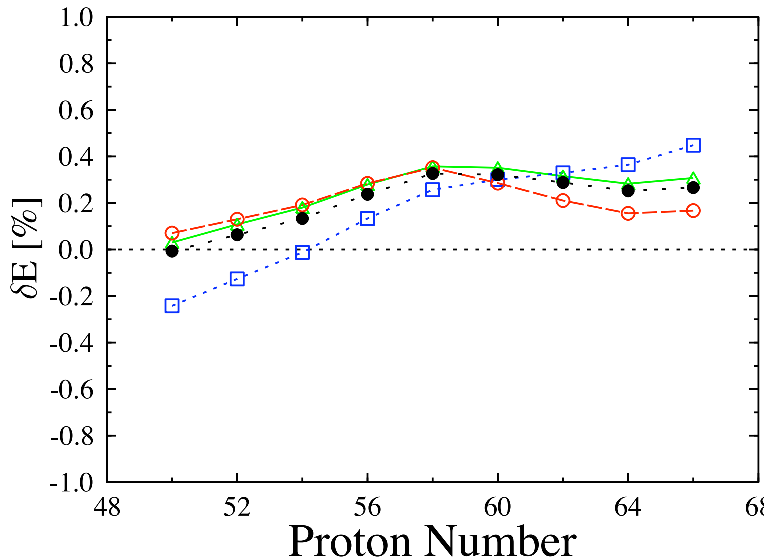


Pb

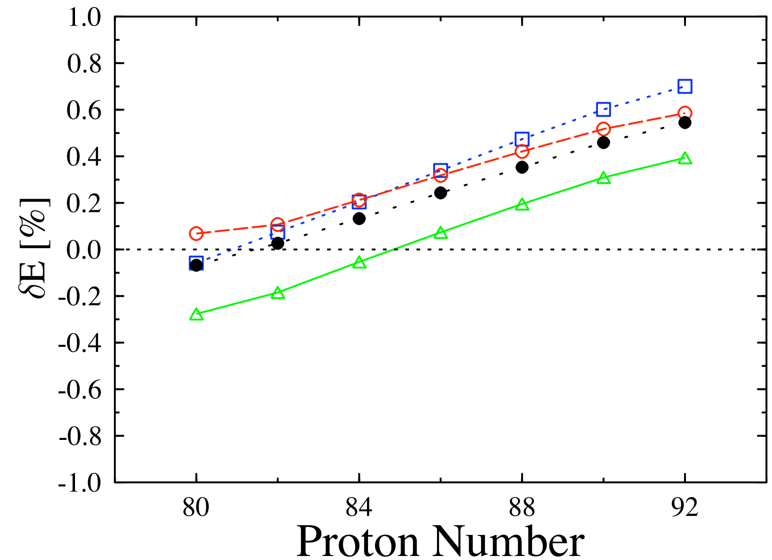


T=0: attraction
T=1: attraction
Coulomb: repulsion

N = 82



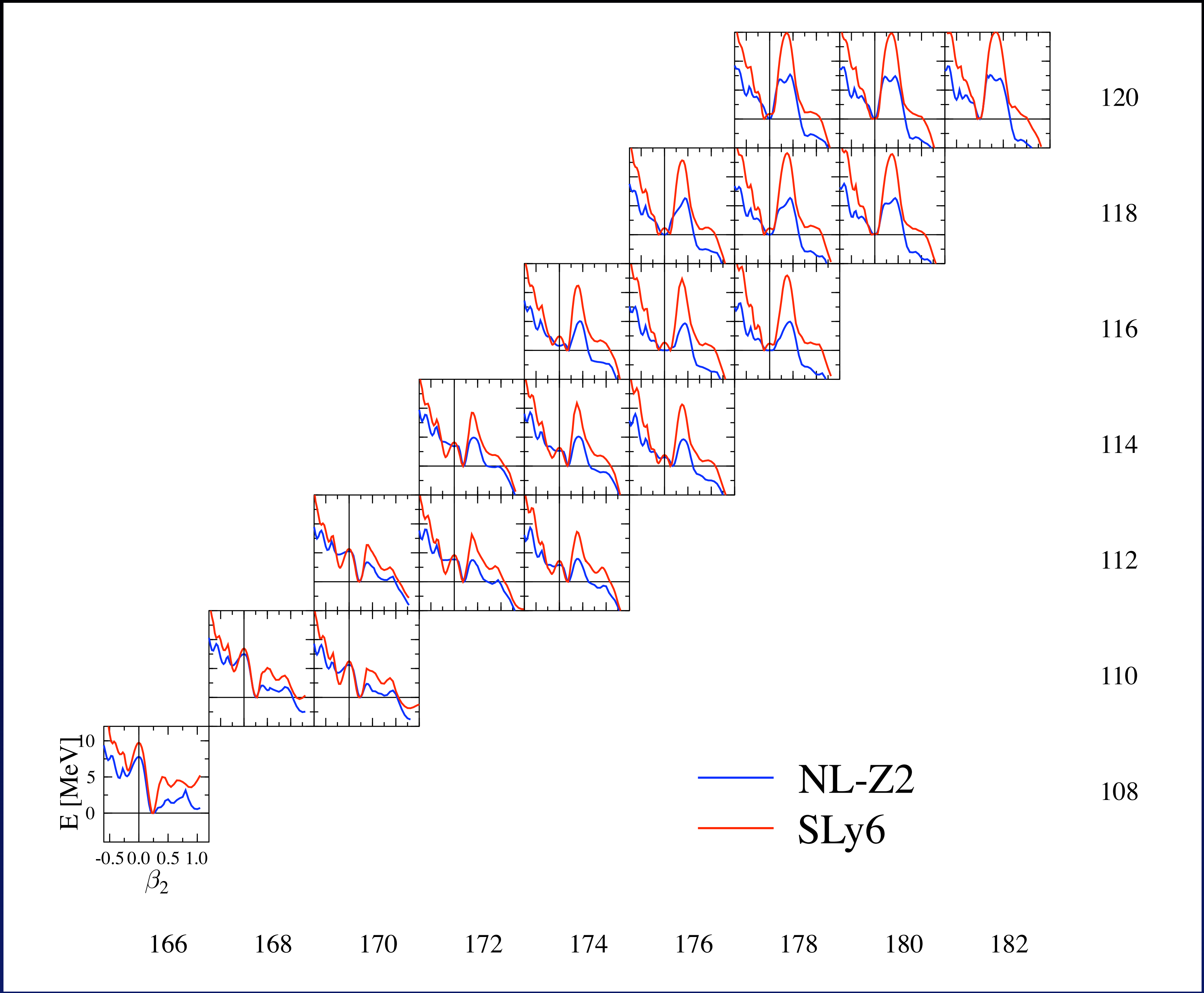
N = 126



SHE

axial
symmetry

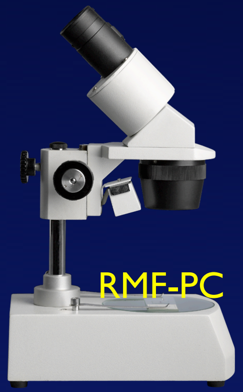
reflection
asymmetry



TJB, M. Bender, J.A. Maruhn, P.-G. Reinhard, to appear in PRC

Some observations and findings

- both the isovector and the isoscalar channel need further adjustment
- in both channels the density dependence is not optimal
- energies and form factor compete in the adjustment procedure as do light and heavy systems
- isovector channel possibly absorbs mismatch of the isoscalar channel

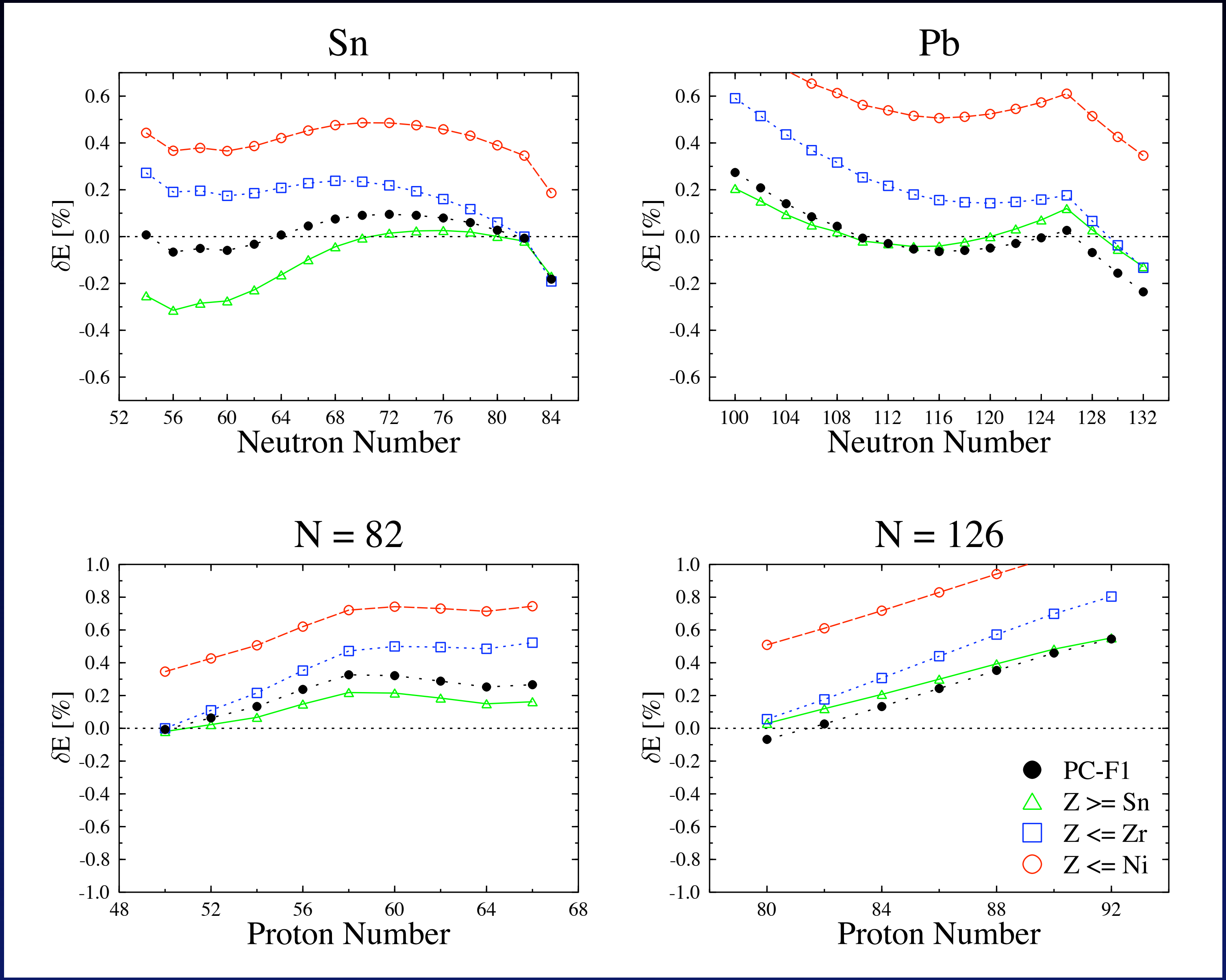


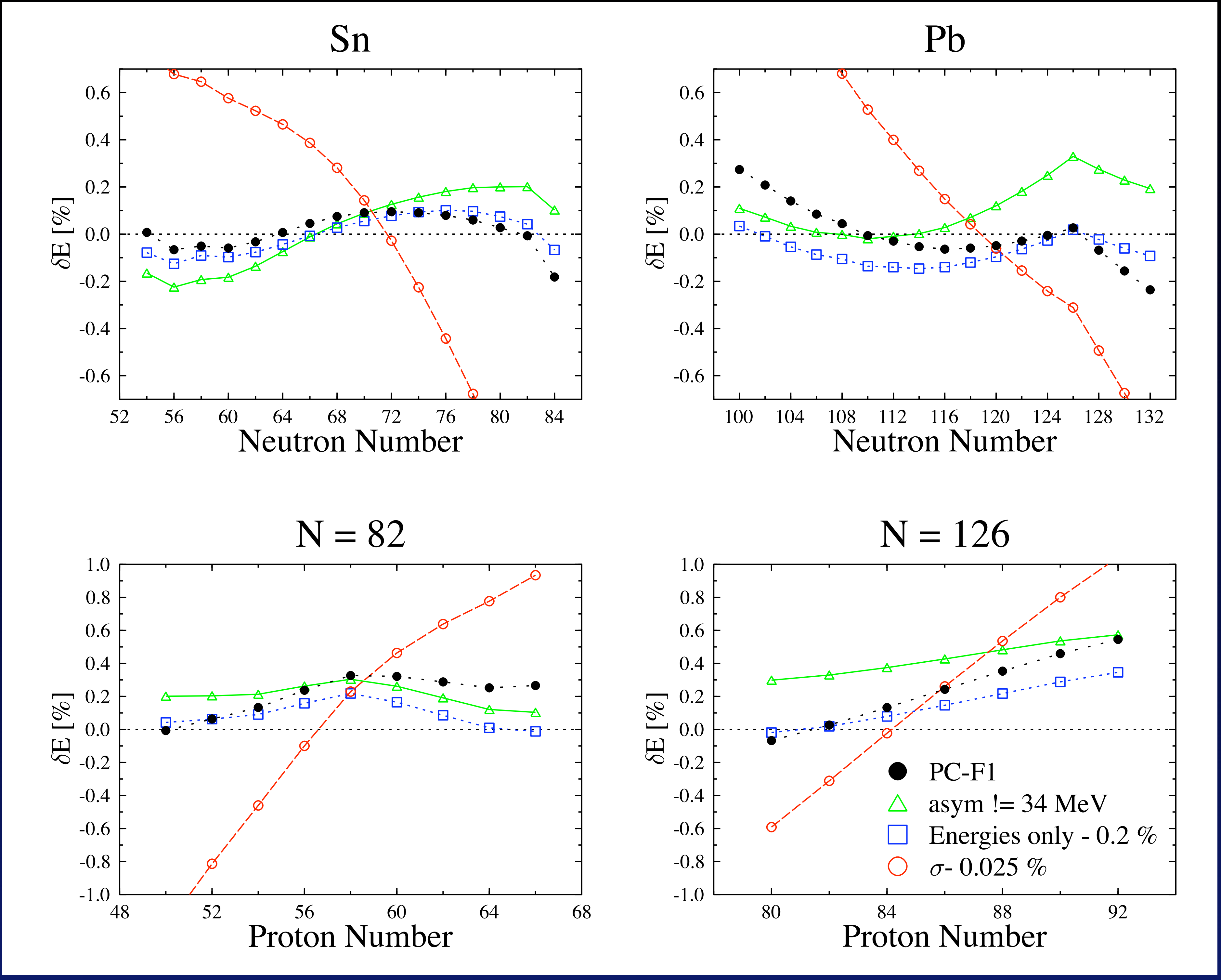
Bulk properties of nuclear matter

modified fitting protocols

Type of adjustment	ρ_0 [fm^{-3}]	E/A [MeV]	K [MeV]	m^*/m	a_4 [MeV]
$\{Z \vert Z \leq Ni\}$	0.151	16.25	280	0.61	36.7
$\{Z \vert Z \leq Zr\}$	0.150	16.22	281	0.61	38.0
$\{Z \vert Z \leq Sn\}$	0.151	16.18	272	0.61	38.2
$\{Z \vert Z \leq Zr \; or \; Z = Pb\}$	0.151	16.22	277	0.61	38.4
$\{Z \vert Z \geq Sn\}$	0.152	16.24	267	0.61	37.8
no T=1 terms	0.152	15.35	246	0.61	17.8
a_4 ! = 34 MeV	0.151	16.12	268	0.61	33.2
only E - error 0.2 %	0.150	16.03	237	0.61	33.9
only E - error 0.5 MeV	0.150	16.02	272	0.61	33.6
σ error 0.025 %	0.147	16.28	238	0.62	40.6

Different selections of nuclei





Sn
Pb
N = 82
N = 126
δE [%]
Neutron Number
Proton Number
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
52
56
60
64
68
72
76
80
84
100
104
108
112
116
120
124
128
132
1.0
0.8
-0.8
-1.0
48
80
88
92
PC-F1
asym != 34 MeV
Energies only - 0.2 %
σ- 0.025 %

Where to go from here?

- an accurate and well adjusted mean-field is desirable for ground-states and all correlations on top of it (pairing, ground-state correlations, excited states, …)
- drip lines , superheavy nuclei, ...
- extend / modify the current models
- force for the complete nucleus - force only for energies / for the geometry / ...
- guidance for important / physical terms ?

QCD scaling

scale the Lagrangian using two scales:

- $f_\pi = 93.5$ MeV   pion decay constant
- $\Lambda = 770$ MeV   QCD mass scale

$$\mathcal{L} = c_{lmn} \left(\frac{\bar{\psi}\psi}{f_\pi^2 \Lambda}\right)^l \left(\frac{\vec{\pi}}{f_\pi}\right)^m \left(\frac{\partial^\mu, m_\pi}{\Lambda}\right)^n f_\pi^2 \Lambda^2$$

$\Delta = l + n - 2 \geq 0.$

i) c_{lmn} of order unity (*natural*) if of physical significance

ii) in principle this should involve a complete set of Lorentz invariants $\{1, \gamma_\mu, \gamma_5, \gamma_5\gamma_\mu, \sigma_{\mu\nu}\}$ and the same coupled to isospin

iii) maybe only a subset is needed

with QCD scaling so far successful for the best forces

RMF-PC force PC-F1

C. Const.	Magnitude	Dim.	Order	c_{lmn}
α_S	$-3.836 \cdot 10^{-4}$	MeV^{-2}	Λ^0	-1.64
β_S	$+7.688 \cdot 10^{-11}$	MeV^{-5}	Λ^{-1}	1.44
γ_S	$-2.899 \cdot 10^{-17}$	MeV^{-8}	Λ^{-2}	2.69
δ_S	$-4.202 \cdot 10^{-10}$	MeV^{-4}	Λ^{-2}	-1.07
α_V	$+2.593 \cdot 10^{-4}$	MeV^{-2}	Λ^0	1.11
γ_V	$+3.908 \cdot 10^{-18}$	MeV^{-8}	Λ^{-2}	-0.36
δ_V	$+1.173 \cdot 10^{-10}$	MeV^{-4}	Λ^{-2}	-0.30
α_{TV}	$+3.456 \cdot 10^{-5}$	MeV^{-2}	Λ^0	0.59
δ_{TV}	$-5.237 \cdot 10^{-11}$	MeV^{-4}	Λ^{-2}	-0.53

TJB, D. G. Madland, J. A. Maruhn, and P.-G. Reinhard,
PRC 65 (2002) 044308

Extended relativistic point-coupling models

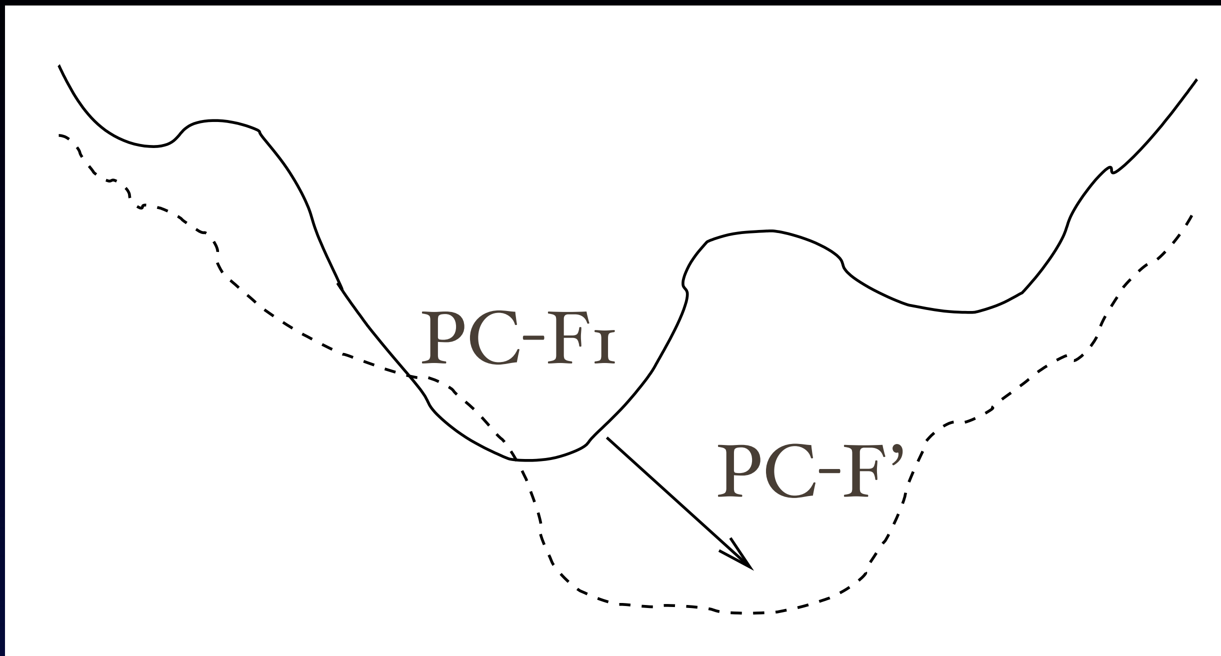
- add new terms and adjust them with the standard adjustment protocols but with various algorithms
- complement adjustment protocols by additional observables (single-particle energies, spin-orbit and/or pseudo-spin splittings, energies / radii / neutron radii , ...)
- guidance: power counting (QCD scaling)
- . . .

TJB, D. G. Madland, J. A. Maruhn, and P.-G. Reinhard, in preparation

compare also to work by Furnstahl et al., M. A. Huertas, ...

“nearest” minimum is found

Bevington (downhill)

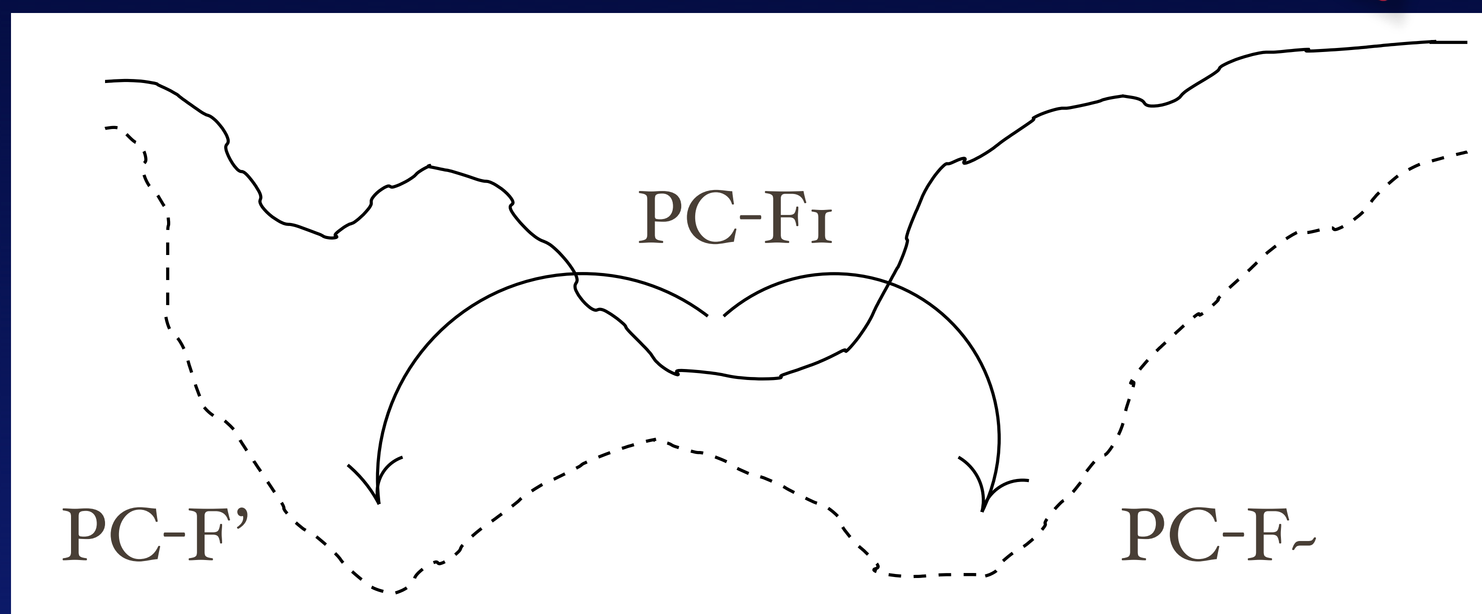


for each new force:
downhill plus MC runs
with max. of 30 walkers
and slow cooling

many walkers (diffusion Monte Carlo)

large region of the parameter space is explored

Simulated annealing (Monte Carlo)



Extending RMF-PC

mixed terms contribute to two potentials simultaneously

$$\mathcal{L} = \rho_S^2 + \rho_V^2 + \rho_S^2\rho_V^2$$

$$V_S = 2\rho_S + 2\rho_V^2\rho_S = (2 + 2\rho_V^2)\rho_S$$

$$V_V = 2\rho_V + 2\rho_S^2\rho_V = (2 + 2\rho_S^2)\rho_V$$

'density dependent' coupling constants

(isoscalar / isovector) scalar / vector potentials become interdependent

various effects on energies and the form factor (geometry of the nucleus)

Symbolic notation

$$\mathcal{L} = \mathcal{L}^{\rm free} + \mathcal{L}^{\rm 4f} + \mathcal{L}^{\rm hot} + \mathcal{L}^{\rm der} + \mathcal{L}^{\rm em},$$

$$\begin{aligned}
\mathcal{L}^{\rm free} &= \bar\psi(\mathrm{i}\gamma_\mu\partial^\mu - m)\psi, \\
\mathcal{L}^{\rm 4f} &= -\frac{1}{2}\,\alpha_{\rm S}(\bar\psi\psi)(\bar\psi\psi) - \frac{1}{2}\,\alpha_{\rm V}(\bar\psi\gamma_\mu\psi)(\bar\psi\gamma^\mu\psi) \\
&\quad -\frac{1}{2}\,\alpha_{\rm TS}(\bar\psi\vec\tau\psi)\cdot(\bar\psi\vec\tau\psi) - \frac{1}{2}\,\alpha_{\rm TV}(\bar\psi\vec\tau\gamma_\mu\psi)\cdot(\bar\psi\vec\tau\gamma^\mu\psi), \\
\mathcal{L}^{\rm hot} &= -\frac{1}{3}\,\beta_{\rm S}(\bar\psi\psi)^3 - \frac{1}{4}\,\gamma_{\rm S}(\bar\psi\psi)^4 - \frac{1}{4}\,\gamma_{\rm V}[(\bar\psi\gamma_\mu\psi)(\bar\psi\gamma^\mu\psi)]^2, \\
\mathcal{L}^{\rm der} &= -\frac{1}{2}\,\delta_{\rm S}(\partial_\nu\bar\psi\psi)(\partial^\nu\bar\psi\psi) - \frac{1}{2}\,\delta_{\rm V}(\partial_\nu\bar\psi\gamma_\mu\psi)(\partial^\nu\bar\psi\gamma^\mu\psi) \\
&\quad -\frac{1}{2}\,\delta_{\rm TS}(\partial_\nu\bar\psi\vec\tau\psi)\cdot(\partial^\nu\bar\psi\vec\tau\psi) - \frac{1}{2}\,\delta_{\rm TV}(\partial_\nu\bar\psi\vec\tau\gamma_\mu\psi)\cdot(\partial^\nu\bar\psi\vec\tau\gamma^\mu\psi), \\
\mathcal{L}^{\rm em} &= -eA_\mu\bar\psi[(1-\tau_3)/2]\gamma^\mu\psi - \frac{1}{4}\,F_{\mu\nu}F^{\mu\nu}.
\end{aligned}$$

We can rewrite it using symbolic notation:

$$\begin{aligned}
\mathcal{L} &= S^2 + V^2 + S_{\rm T}^2 + V_{\rm T}^2 + S^3 + S^4 + V^4 \\
&\quad + \text{derivative terms} \ + \ \text{Coulomb force}
\end{aligned}$$

inverse Order in Λ

(yet) no tensor terms, no isovector-scalar terms

0	$s^2, v^2, v_T^2, \ldots$
1	$s^3, sv^2, sv_T^2, \ldots$
2	$s^4, v^4, s^2v^2, s^2v_T^2, v^2v_T^2, \ldots$
3	$s^5, \ldots$
4	$s^6, v^6, \ldots$
…	…

'organizing scheme perspective' ⇄ 'phenomenology perspective'

$$
\begin{aligned}
\mathcal{L}(1) &= \mathcal{L} - S^3 \\
\mathcal{L}(2) &= \mathcal{L}(1) + S^6 + V^6 \\
\mathcal{L}(2‘) &= \mathcal{L} + S^5 + S^6 + V^6 \\
\mathcal{L}(3) &= \mathcal{L}(1) - V^4 + S^6 \\
\mathcal{L}(3‘) &= \mathcal{L} - V^4 + S^5 + S^6 \\
\mathcal{L}(3“) &= \mathcal{L} - V^4 + S^5 \\
\mathcal{L}(4) &= \mathcal{L} + S^5 \\
\mathcal{L}(5) &= \mathcal{L} + S^5 + S^6 \\
\mathcal{L}(6) &= \mathcal{L}(1) + S^2V^2 \\
\mathcal{L}(6‘) &= \mathcal{L} + S^2V^2 \\
\mathcal{L}(7) &= \mathcal{L}(1) + V^2V_{\mathrm{T}}^2 \\
\mathcal{L}(7‘) &= \mathcal{L} + V^2V_{\mathrm{T}}^2 \\
\mathcal{L}(8) &= \mathcal{L}(1) + S^2V^2 + V^2V_{\mathrm{T}}^2 \\
\mathcal{L}(8‘) &= \mathcal{L} + S^2V^2 + V^2V_{\mathrm{T}}^2 \\
\mathcal{L}(9) &= \mathcal{L}(1) + S^2V^2 + S^2V_{\mathrm{T}}^2 + V^2V_{\mathrm{T}}^2 \\
\mathcal{L}(9‘) &= \mathcal{L} + S^2V^2 + S^2V_{\mathrm{T}}^2 + V^2V_{\mathrm{T}}^2 \\
\mathcal{L}(10) &= \mathcal{L} + SV^2 + SV_{\mathrm{T}}^2 \\
\mathcal{L}(11) &= \mathcal{L} - V^4 + SV^2 + SV_{\mathrm{T}}^2 \\
\mathcal{L}(12) &= \mathcal{L} - V^4 - S^4 + SV^2 + SV_{\mathrm{T}}^2 \\
\mathcal{L}(13) &= \mathcal{L}(1) + S^2V^2 + S^2V_{\mathrm{T}}^2 + V^2V_{\mathrm{T}}^2 + S^6 \\
\mathcal{L}(13‘) &= \mathcal{L} + S^2V^2 + S^2V_{\mathrm{T}}^2 + V^2V_{\mathrm{T}}^2 + S^5 + S^6 \\
\mathcal{L}(14) &= \mathcal{L}(1) + S^2V^2 + S^2V_{\mathrm{T}}^2 + V^2V_{\mathrm{T}}^2 + S^6 + V^6 \\
\mathcal{L}(14‘) &= \mathcal{L} + S^2V^2 + S^2V_{\mathrm{T}}^2 + V^2V_{\mathrm{T}}^2 + S^5 + S^6 + V^6
\end{aligned}
$$

Extensions

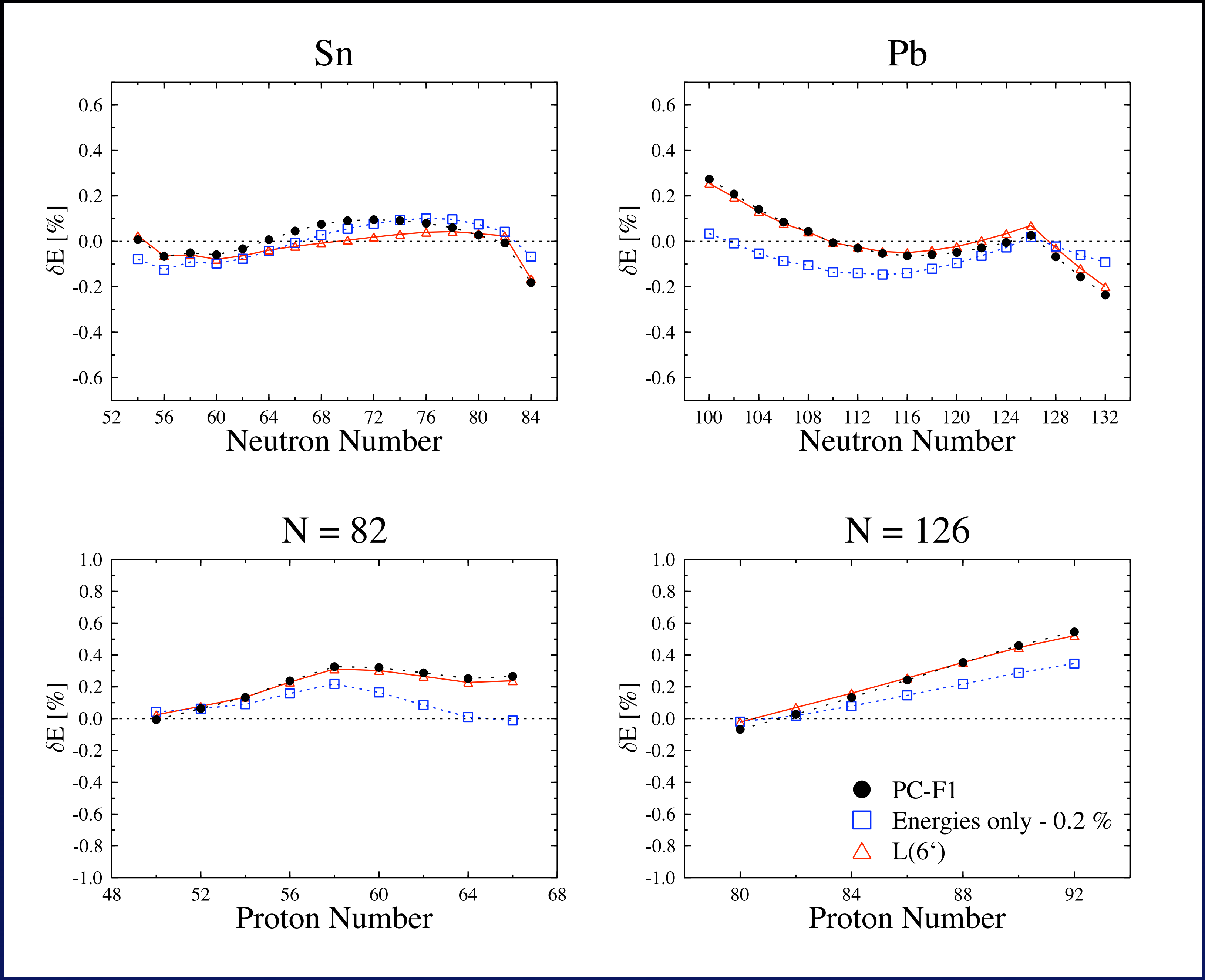
- 3rd and 4th order mixed terms

- mixings include isoscalar/ isovector and scalar/vector terms

- 5th and 6th order scalar and vector (6th only) terms

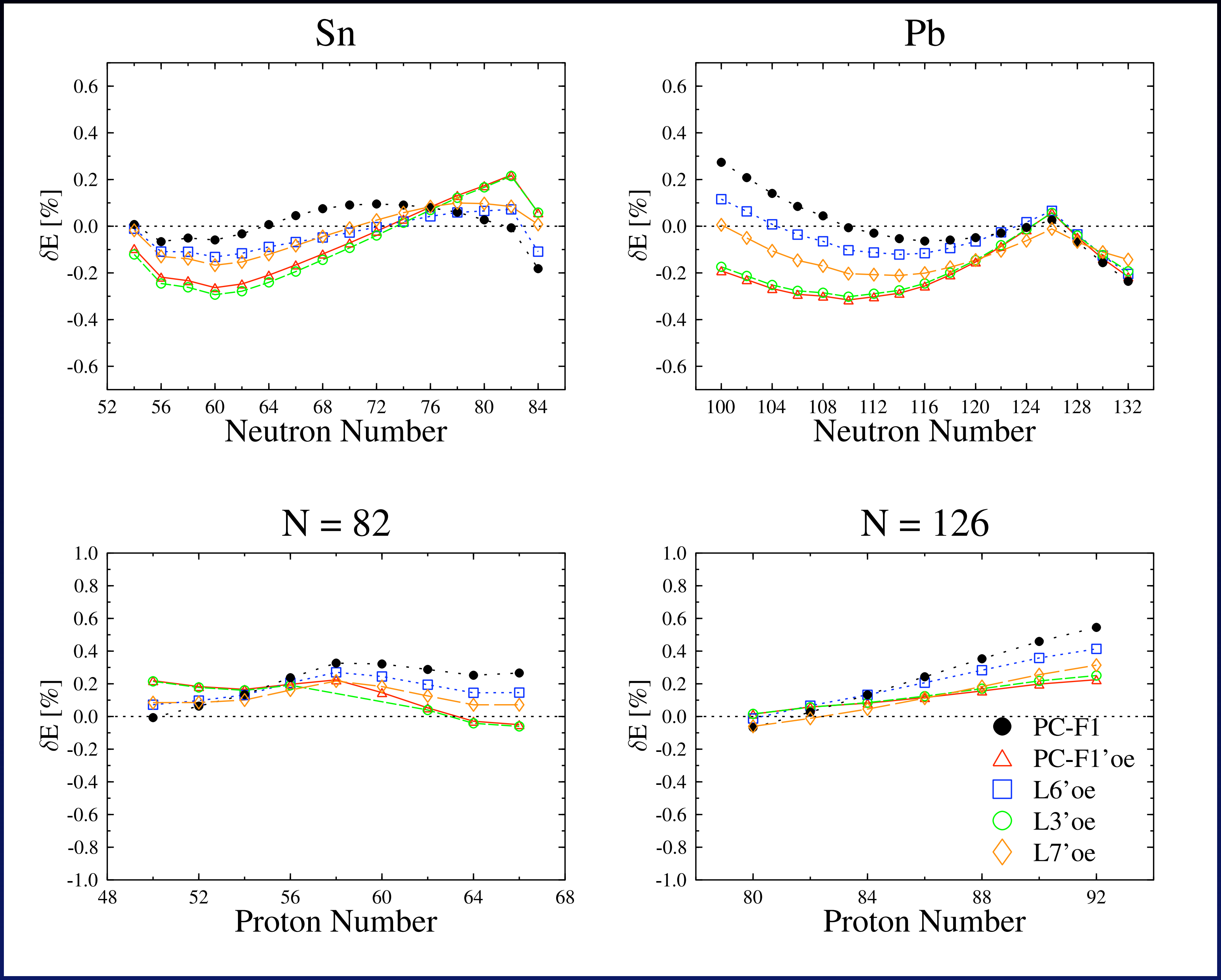
- no isovector-scalar terms since nuclear ground-state observables only determine the sum of (linear) isovector-vector and isovector-scalar terms

force	# cc (mf)	# w.d.	χ^2_{dof}	χ^2_{pt}	χ^2_{tot}	χ^2_{BE}	χ^2_{ff}	adjustment
PC-F1	9	8	2.75	2.11	99	62	35	MC+B
PC-F1‘	9	7	2.28	1.74	82	40	41	ISO
L(4)	10	8	2.34	1.74	82	40	41	B (sP1‘)
L(5)	11	8	2.4	1.74	82	40	41	B (sP1‘)
L(6‘)	10	8	2.71	2.02	95	57	36	B (sP1)
L(6‘)	10	8	2.26	1.68	79	40	38	B+C (sP1‘)
L(6‘)	10	7	2.23	1.66	78	35	42	MC 1
L(7‘)	10	10	2.26	1.68	79	42	37	B+C (sP1‘)
L(7‘)	10	10	2.54	1.89	89			B (sP1)
L(8’)	11	10	2.68	1.94	91			B (sP1)
L(8‘)	11	8	2.2	1.6	77	35	41	B+C (sP1p
L(9‘)	12	7	2.42	1.70	80	41	39	B (sP1‘)
L(9‘)	12	5	2.97	2.09	99	50	49	MC 1
L(10)	11	10	2.56	1.85	87	51	35	B (sP1)
L(10‘)	11	9	2.24	1.62	76	37	37	B (sP1‘
L(11)	10	9	5.7	4.3	202	58	139	B (sP1)
L(11)	10	9	2.80	2.09	98	46	46	B (sP1‘)
L(13‘)	14	7	2.52	1.6	78	39	39	B (sP1‘)
L(14‘)	15	7	2.63	1.68	79	39	40	B (sP1‘)



excellent for tin! (but never only consider one chain alone ...)

Fitting to energies only



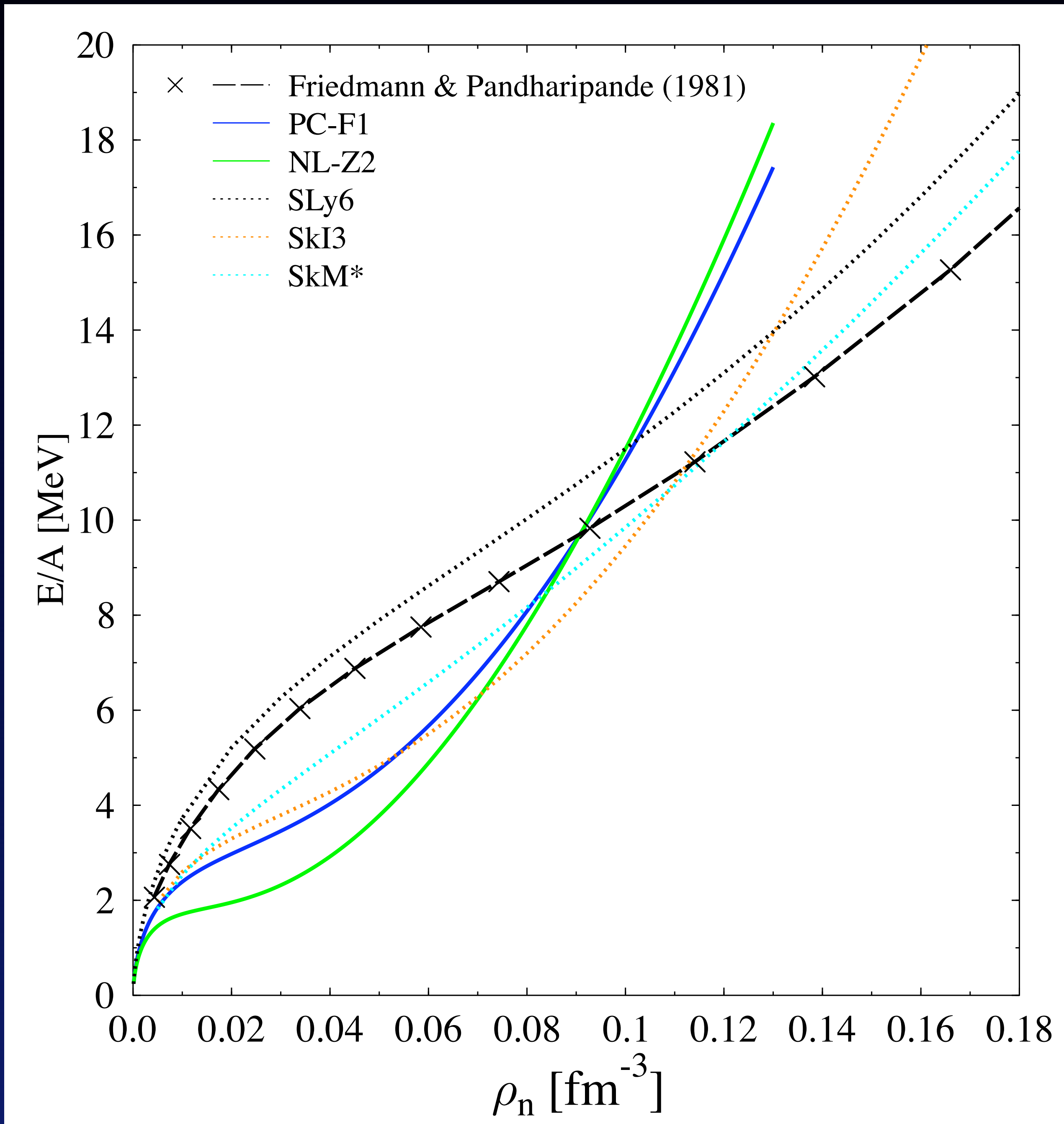
L6': $+ S^2V^2$

L3': $- V^4 + S^{5,6}$

L7': $+ V^2 V_T{}^2$

improvements so far result from increased compatibility of energy and form factor

Neutron matter

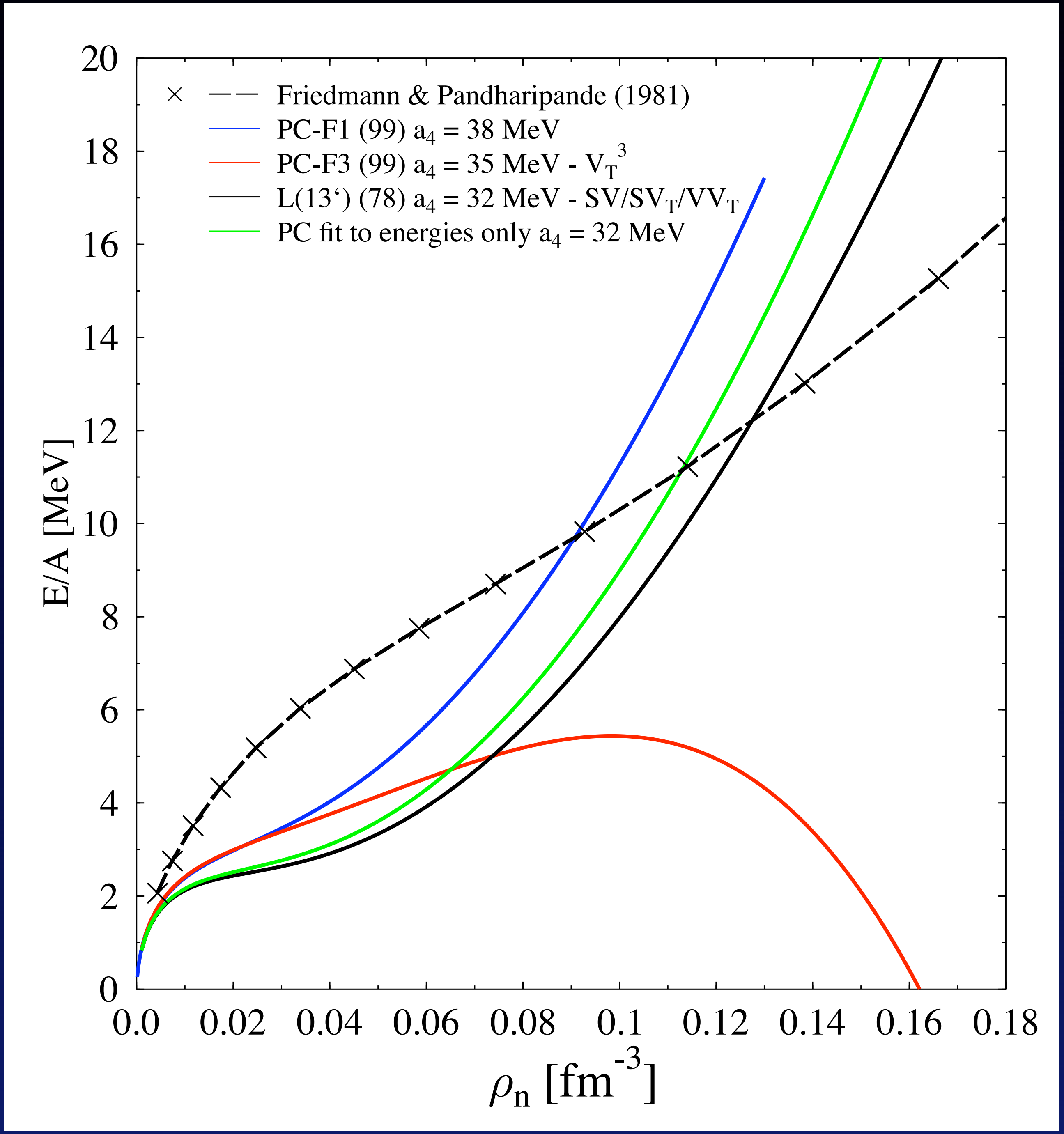


wrong curvature: generic feature of RMF forces

SLy6 has been adjusted to the neutron matter EOS

density dependence of asymmetry energy

neutron star poperties



neutron matter EOS not determined by nuclear ground-state observables

extended models may provide enough freedom to simultaneously describe neutron matter and finite nuclei

some of them: better chisquared at the cost of smaller (and too small) a_4

possible next steps:
adjustment to both nuclei and neutron matter calculations / isovector-sensitive observables

- with a few additional parameters enhancements are possible

- (yet) no dramatic improvements have been obtained so far

- form factor vs. binding energies

- neutron matter description may be possible
- isovector properties are still an issue

- new freedom demands more (new / different) observables

- density dependence - powers of k_F vs. powers of density ?

- isovector-scalar terms in nuclear ground states (effective mass splittings, ls-, pseudo-spin splittings) ?