Recent Developments in Nuclear Energy Functionals

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in collaboration with

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Outline

- framework
- adjustment
- input from DBHF
- applications
- outlook

Strings ?

E

effective field theory

EFT

QCD

density functional theory

DFT

low energy degrees of freedom

symmetries, power counting, scales, truncation

many-body approximations (mean field), parameters, ...

Hohenberg-Kohn Theorem: non-degenerate ground-state energy of a many-body system is a unique functional of the local density

can go beyond literal mean field

relativistic/non-relativistic Kohn-Sham scheme

goal: universal functional for finite, self-bound nuclei

Considerations for finite nuclei:

- spin
- relativistic systems (scalar/vector density)
- self-bound systems
- intrinsic density
- broken symmetries
- pairing, long-range effects
- ...

$$\left[\frac{-\hbar}{2m}\nabla^2 + V_{int} + V_{ext} + V_{xc}\right]\psi_i = \varepsilon_i \psi_i$$

$$\rho = \sum_i |\psi_i|^2$$

looks like mean-field, but can go beyond literal mean field

EFT + DFT = 'MF' (B. Serot)

correlation effects are present in energy and density (not in the wave function)

Extensions of the Hohenberg-Kohn theorem:

- QHD-I: C. Speicher, R. M. Dreizler, and E. Engel, Annals of Physics 213 (1992) 312

- intrinsic density: J. Engel, nucl-th/0610043

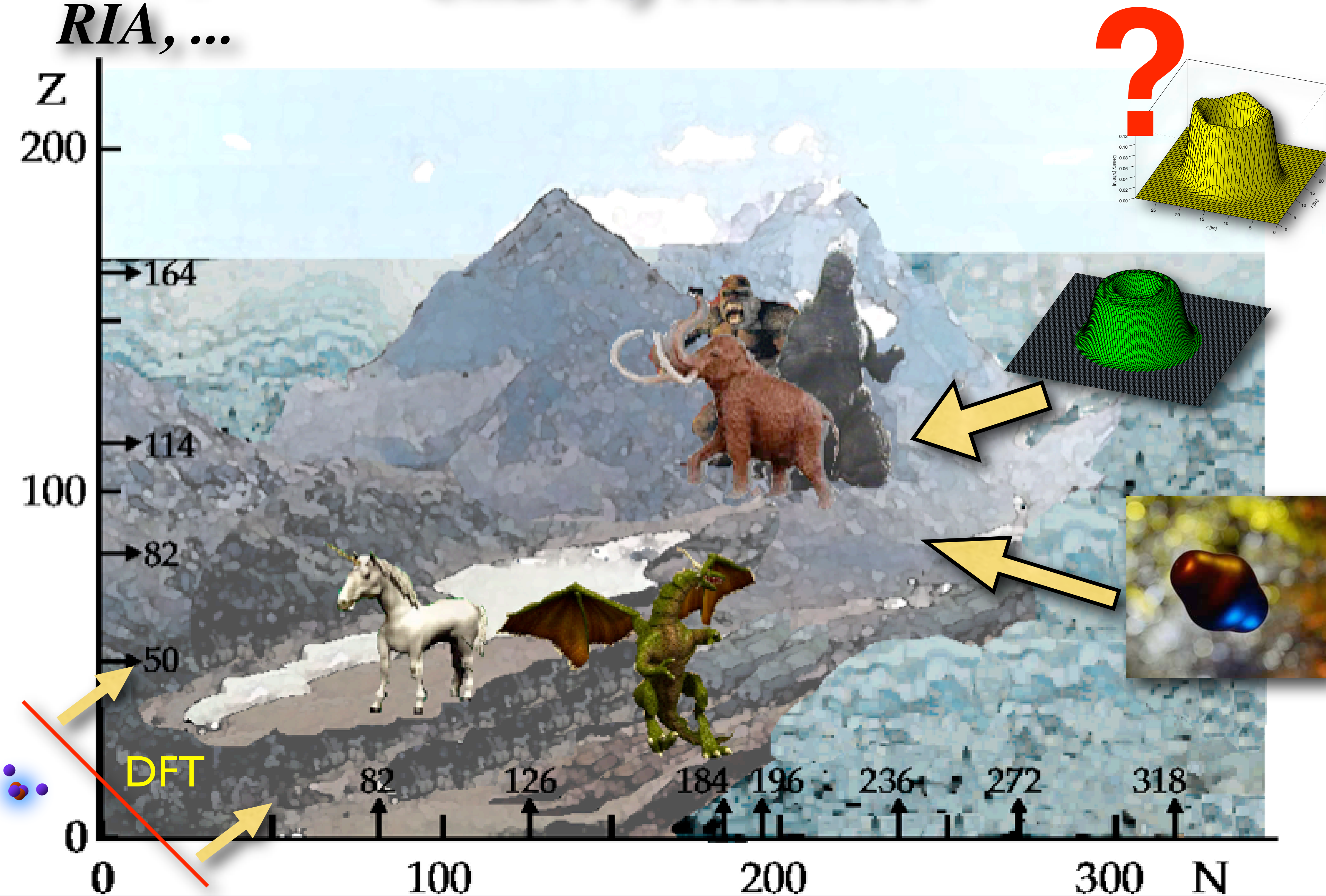
- functionals for other observables can be constructed as well (momentum space: Englert, Henderson, ...)

problems:

- true functional is probably very complicated, nonlocal, ...
- Hohenberg-Kohn theorem is non-constructive (practice → LDA)
- problems are not of principal but of practical nature

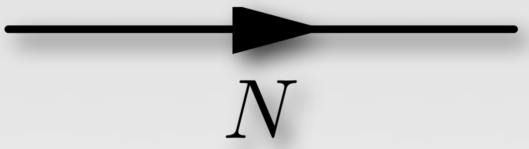
GSI,
RIA, ...

Chart of Nuclides



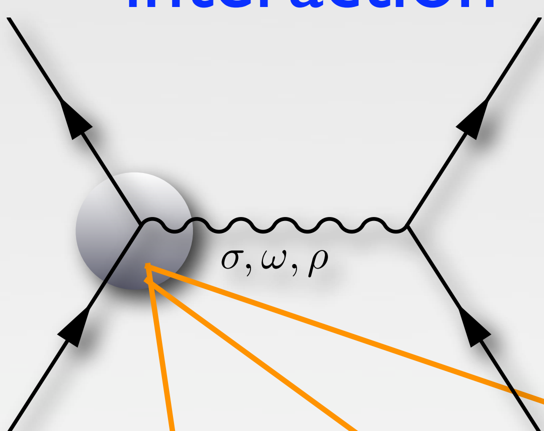
relativistic mean-field (RMF) model

free nucleons

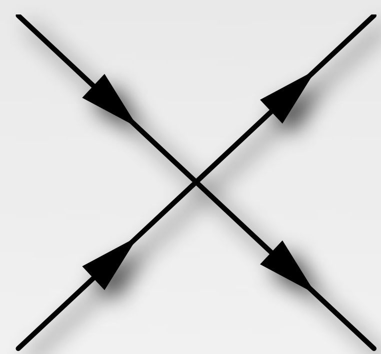


$$\mathcal{L} = \bar{\psi}(i\gamma_\mu \partial^\mu - m)\psi$$

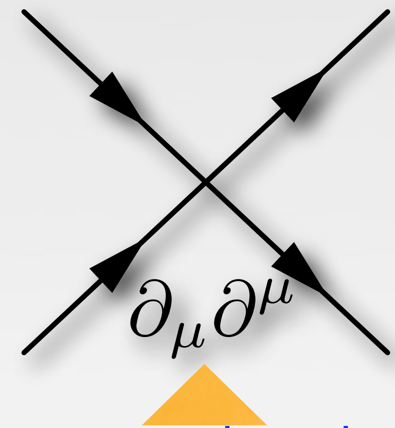
+ interaction



or



+



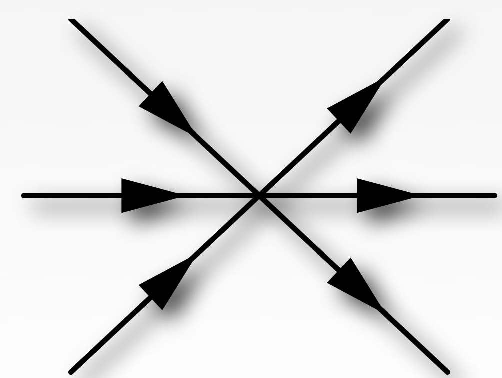
+ Coulomb force

momentum dependence

$$\mathcal{L} = \underline{g_\sigma} \sigma \bar{\psi}\psi + \underline{g_\omega} \omega_\mu \bar{\psi}\gamma^\mu \psi + \underline{g_\rho} \vec{\rho}_\mu \cdot \bar{\psi}\vec{\tau}\gamma^\mu \psi$$

+ free mesons

+ nonlinear interaction:



or self-interaction of scalar field

pion: $\langle \pi \rangle = 0, \; 2\pi \approx \sigma$

mean-field approximation in stationary ground states:

$$\sigma \rightarrow \langle \sigma \rangle$$
$$\omega \rightarrow \langle \omega_0 \rangle \quad \text{classical fields}$$
$$\vec{\rho} \rightarrow \langle \rho_{0,3} \rangle$$

potential:

$$V = g_\sigma \sigma + g_\omega \omega_0 \gamma^0 + g_\rho \rho_{0,3} \gamma^0 \tau_3 + e A_0 \frac{1+\tau_3}{2} \quad \sim -50 \text{ MeV}$$

isovector-vector

Coulomb

scalar potential, ~ -350 MeV

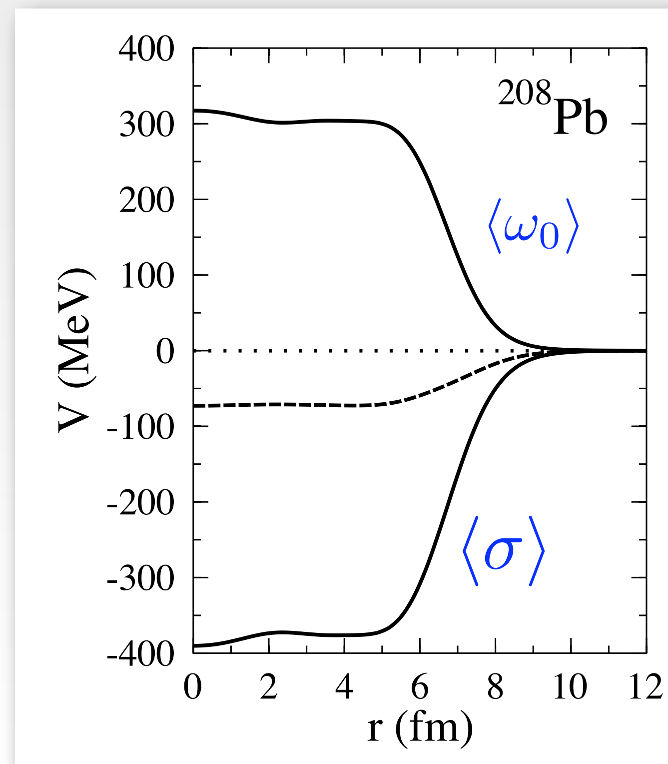
vector potential, ~ +300 MeV

relativity

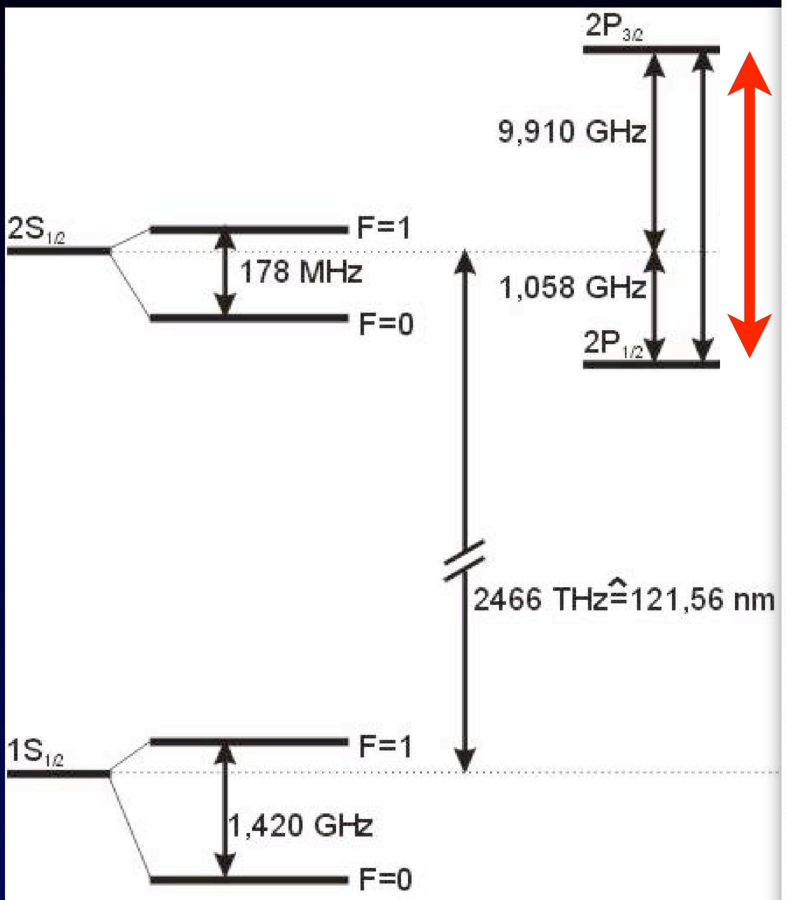
spin-orbit potential:

$$V_{s.p.} \propto \frac{d}{dr} \left(g_\sigma \sigma - g_\omega \omega_0 \gamma^0 \right) \vec{l} \cdot \vec{s}$$

~ -650 MeV

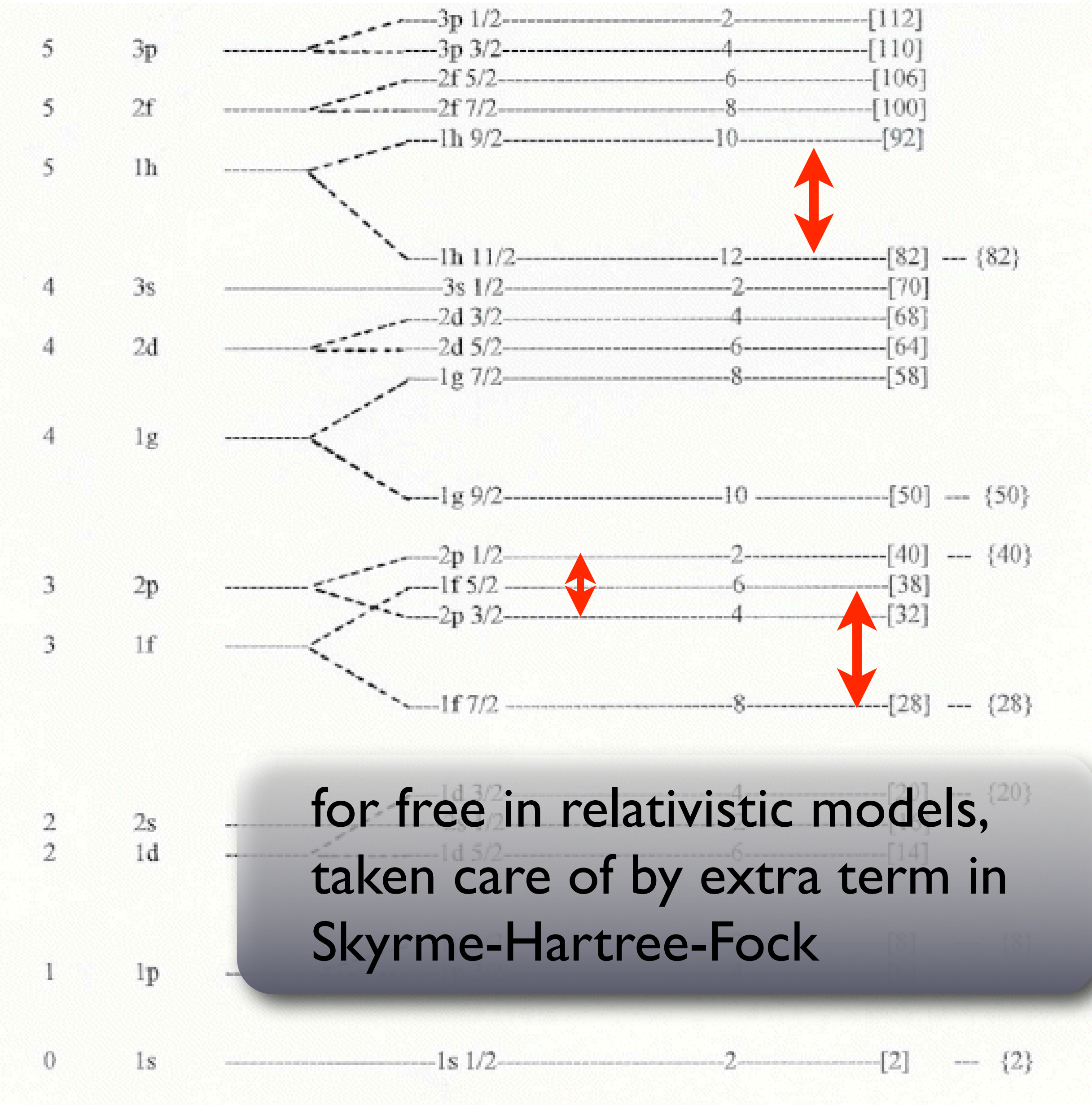


atomic case



spin-orbit force much stronger and with opposite sign in nuclei

nuclear case



for free in relativistic models, taken care of by extra term in Skyrme-Hartree-Fock

Adjusting the parameters of RMF/SHF models

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^{ch}_{rms}	0.5 %	−	+	+	+	+	+	+	−	+	−	+	−	−	−	+	+	+
Δ_p	0.05 MeV	-	-	-	-	-	-	-	-	-	-	-	-	+	+	-	-	-
Δ_n	0.05 MeV	-	-	-	-	-	-	-	-	+	+	+	-	-	-	-	-	-

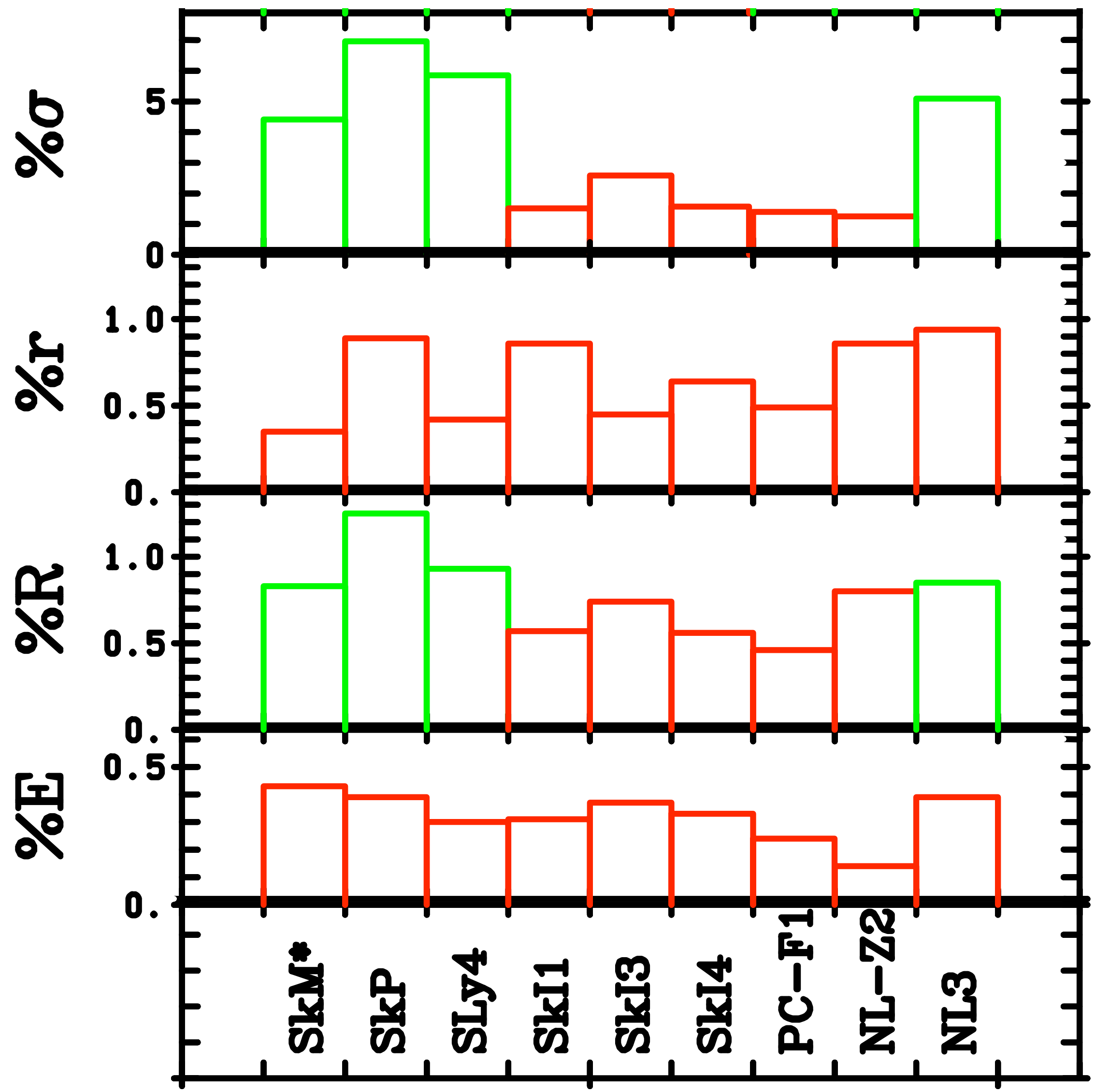
NL-Z2
PC-F1
SkI3,4

(one possibility)

- 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

Overall performance



prediction

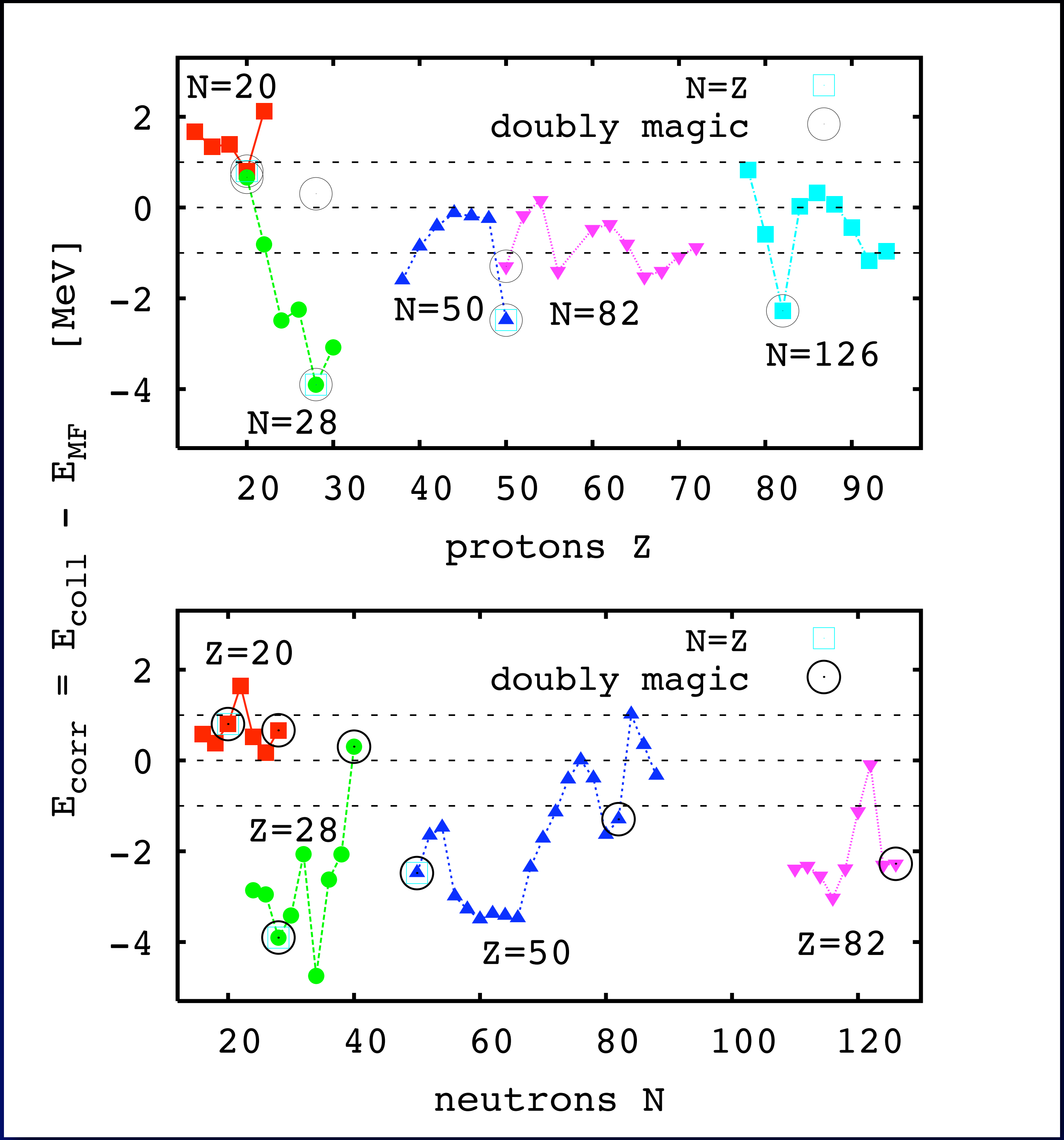
adjusted

surface thickness

rms radius

diffraction radius

binding energy



- reconsideration of suitable fit nuclei
- consider ground-state correlation energies

- isotone chains (except N=28) appear to be favorable over isotope

- selection / availability of nuclear data is important

- new data from NUSTAR@FAIR.GSI

P.-G. Reinhard et al.

in progress

Relativistic and non-relativistic energy functionals with DBHF input

DBHF → LDA fit → fit of gradient term / spin-orbit term

$\frac{E}{A}(\rho)$

nuclear matter at various p/n ratios

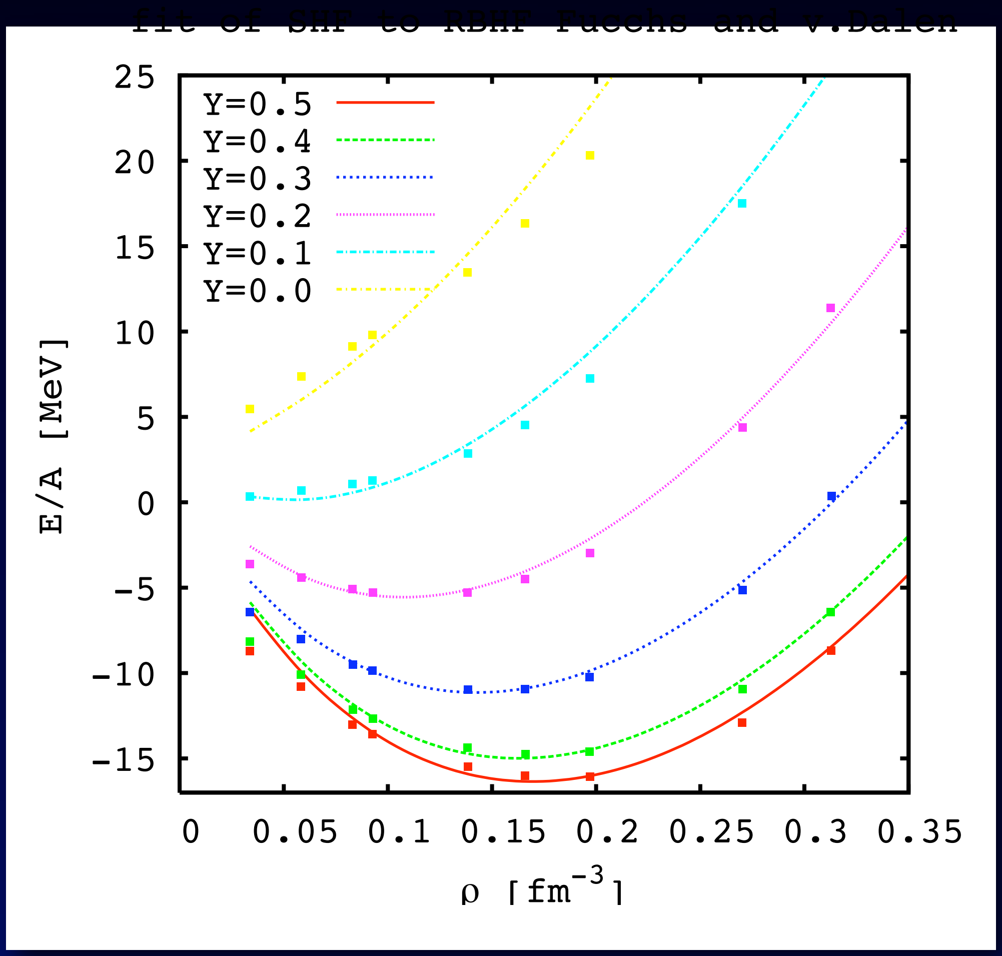
7 parameters

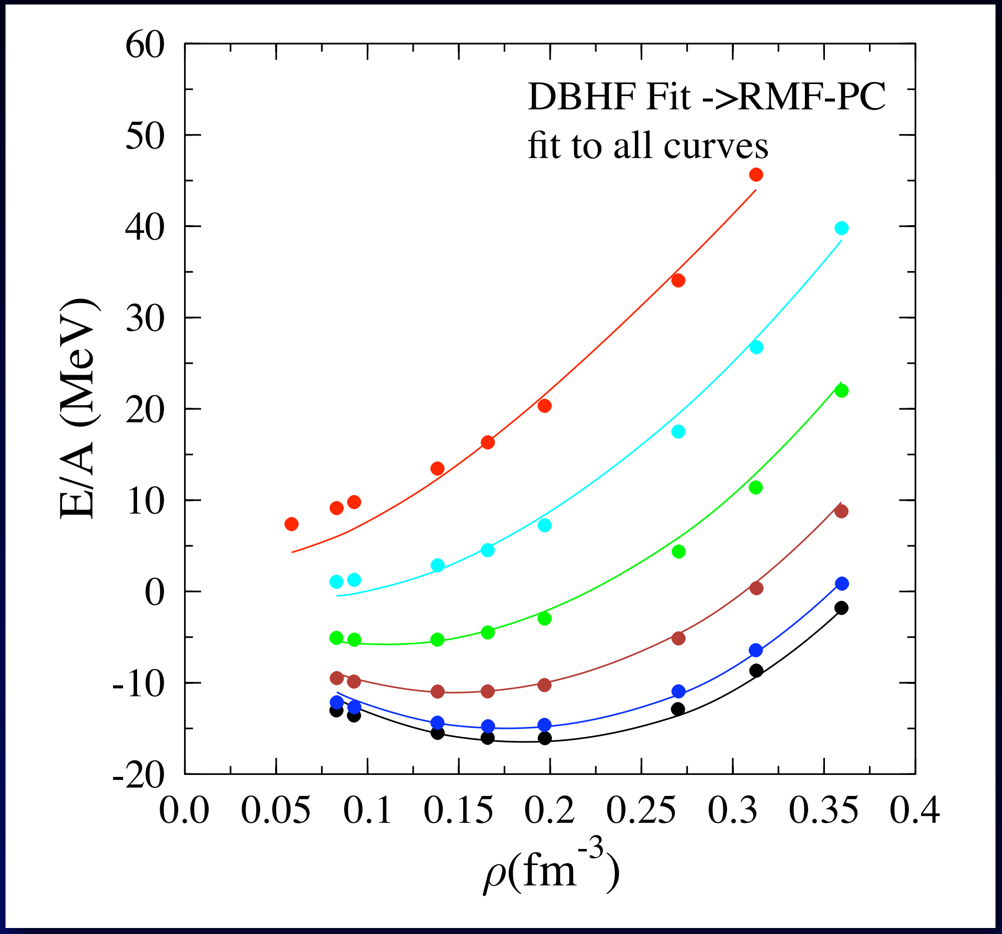
-1 free parameter (RMF-PC)
[gradient]

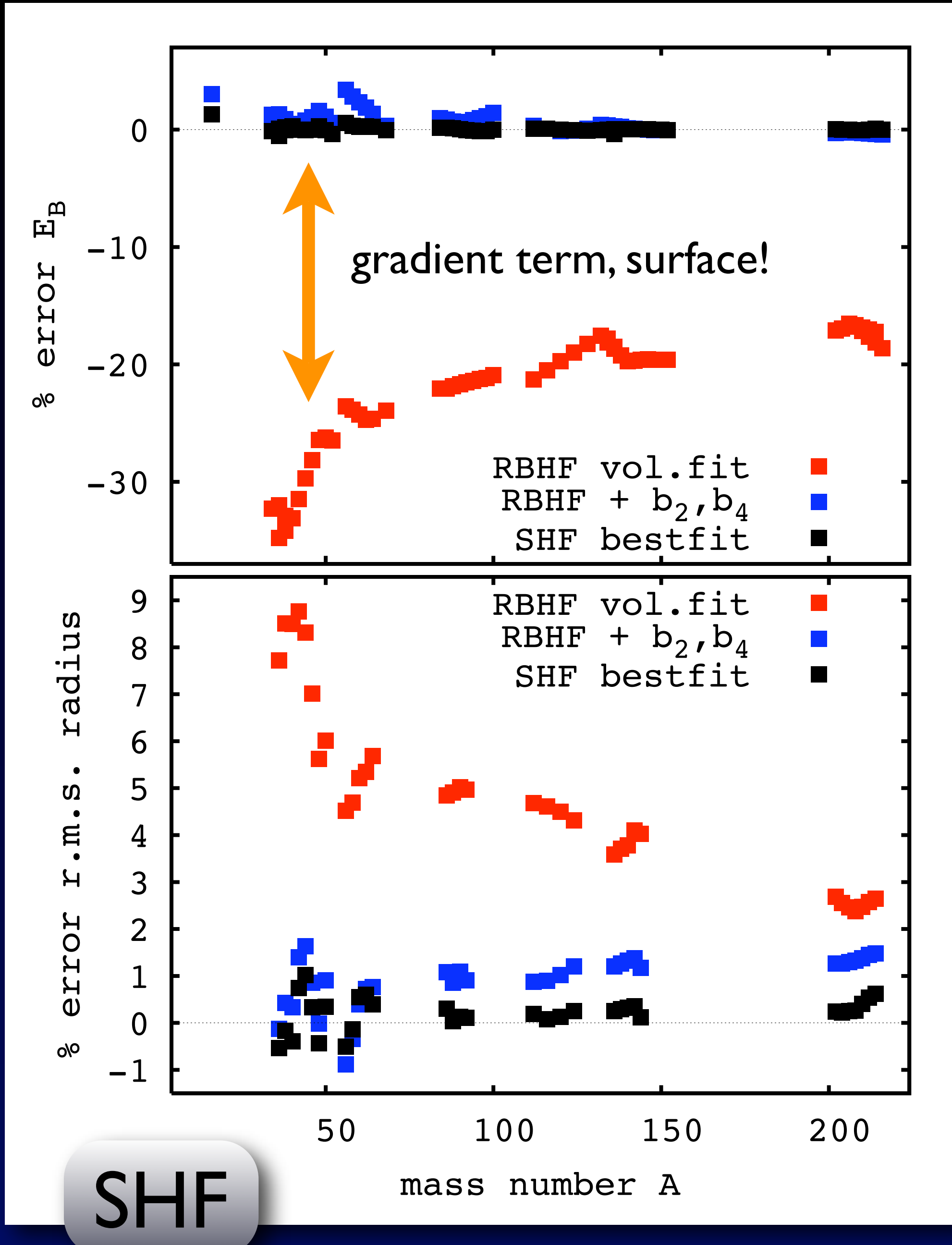
-2 free parameters (SHF)
[gradient + spin-orbit]

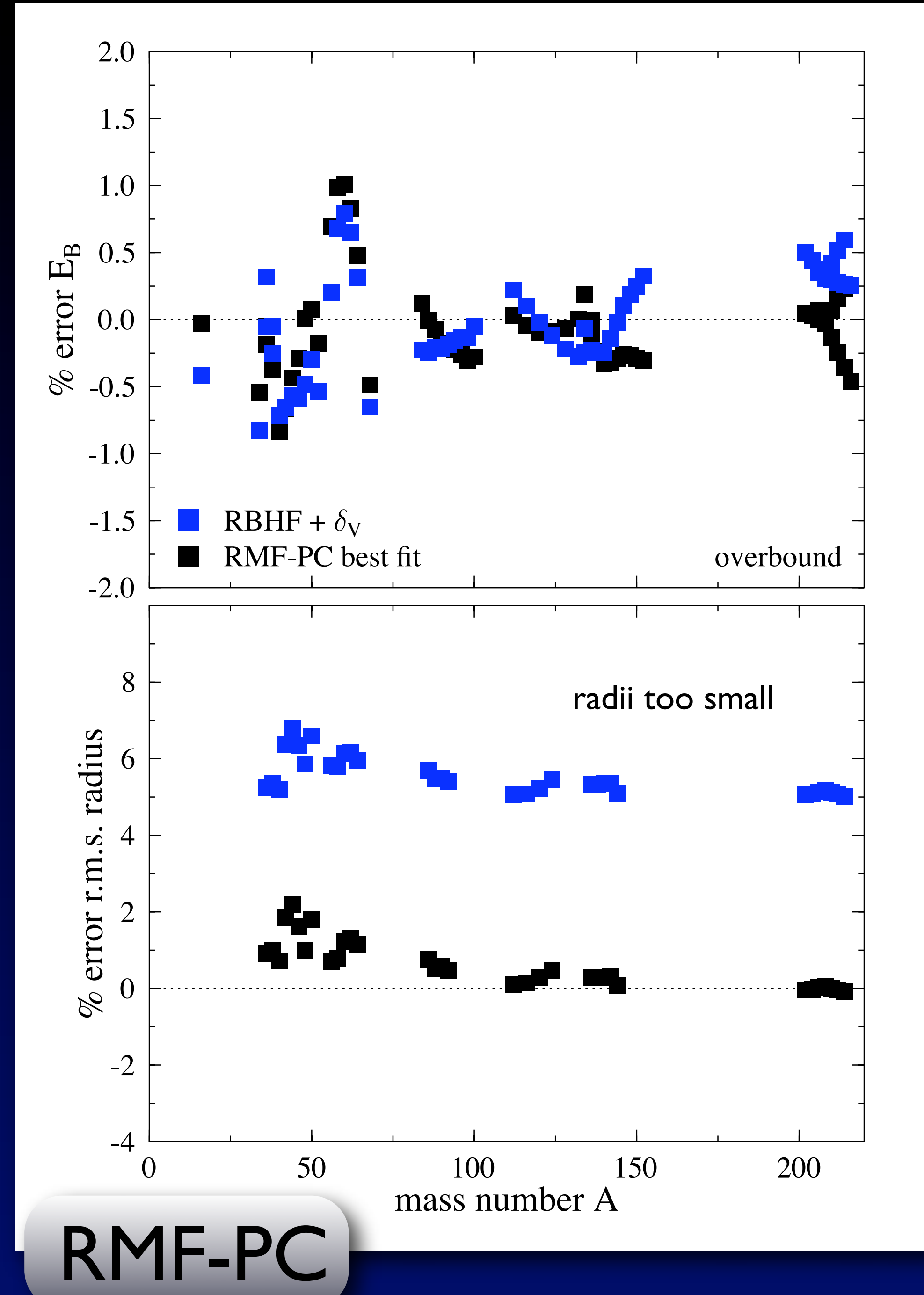
DBHF calculations by C. Fuchs, E. v. Dalen et al.

Fit to various asymmetries

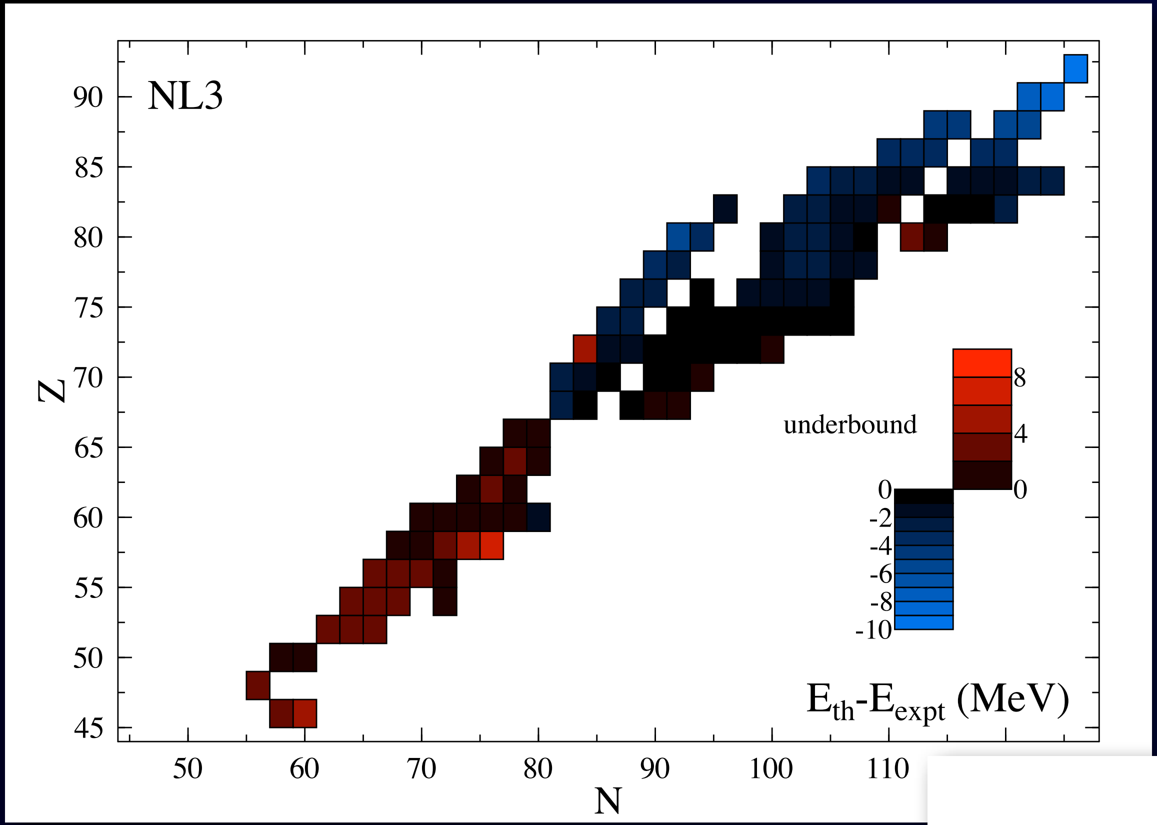




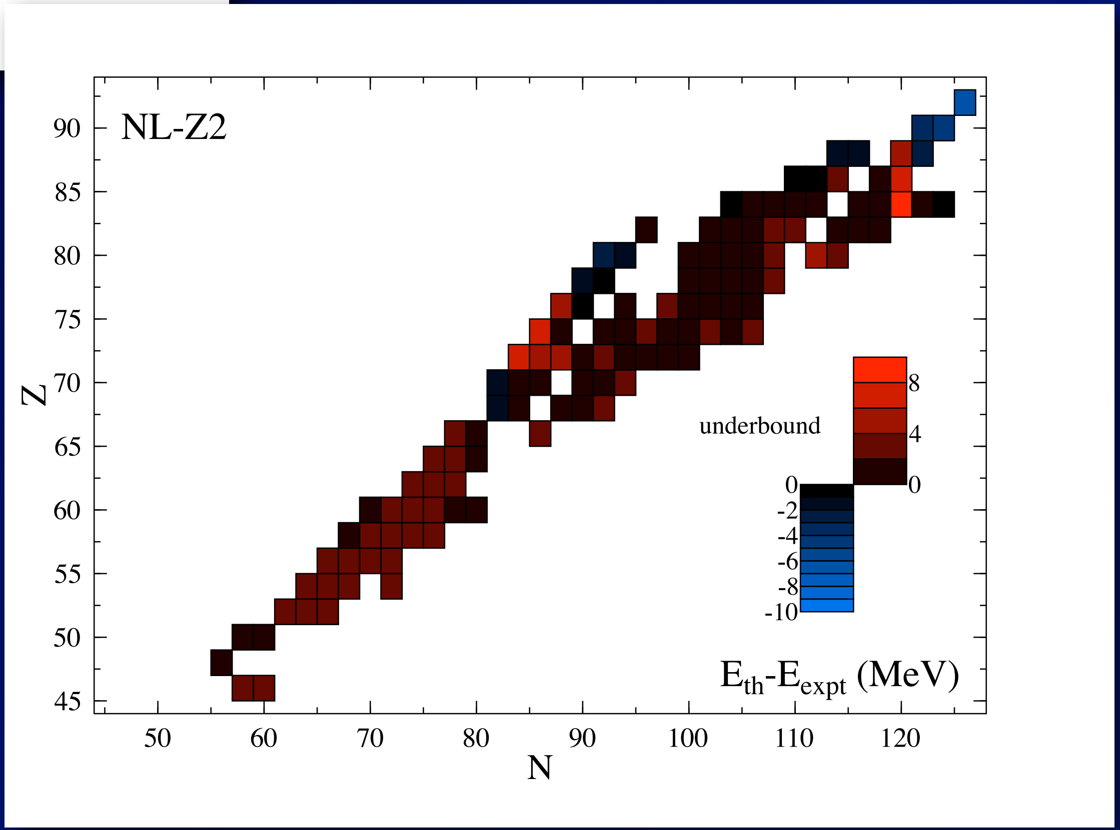




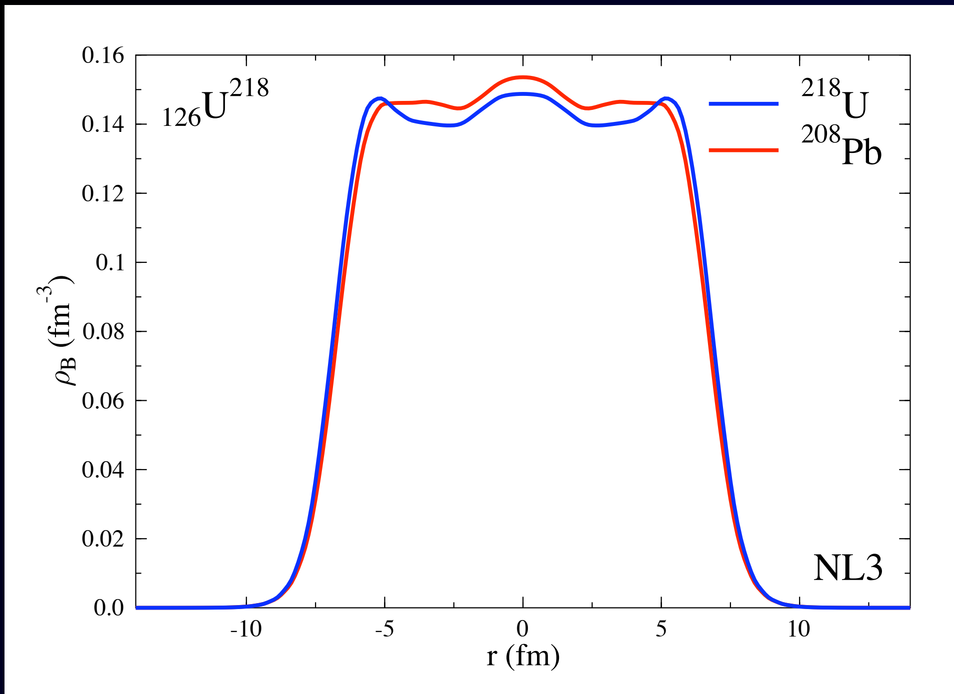
DBHF + gradient + spin-orbit =
high-quality model



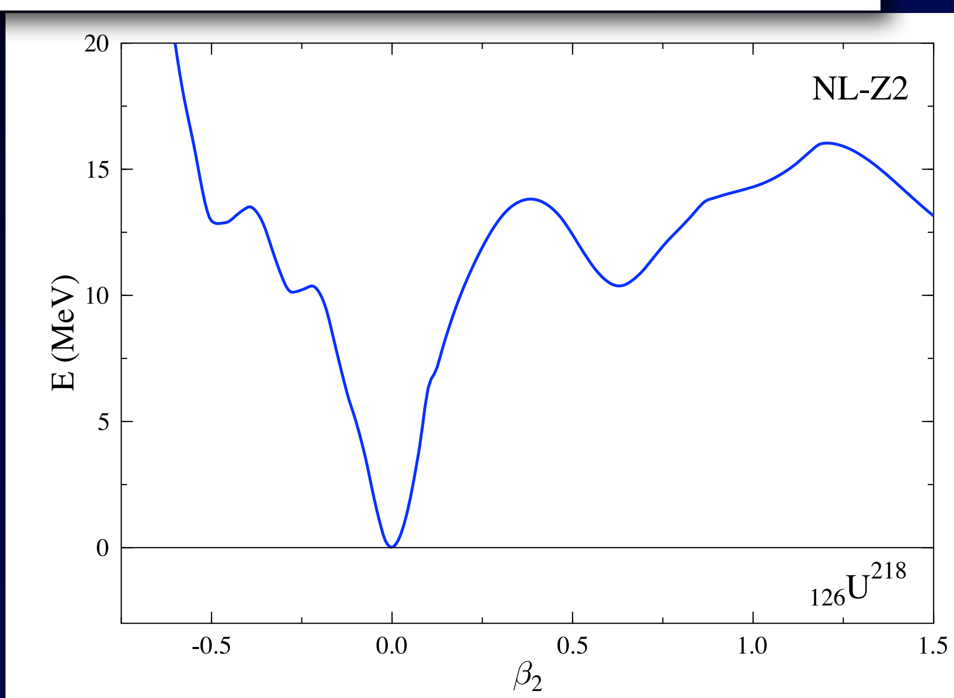
masses reveal model trends



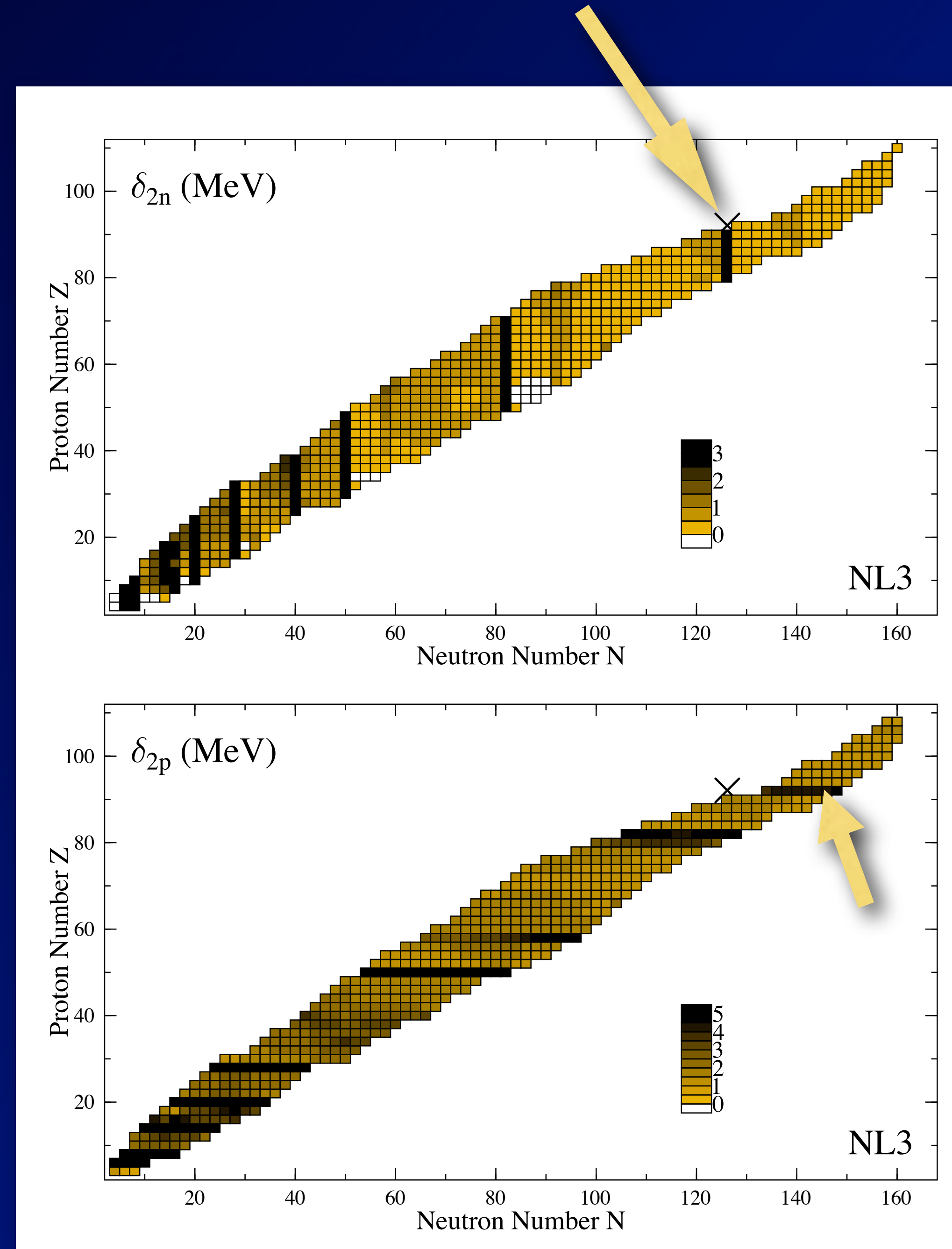
$^{218}U_{126}$



0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0.0
$_{126}U^{218}$
^{218}U
^{208}Pb
ρ_B (fm^{-3})
NL3
-10
-5
0
5
10
r (fm)

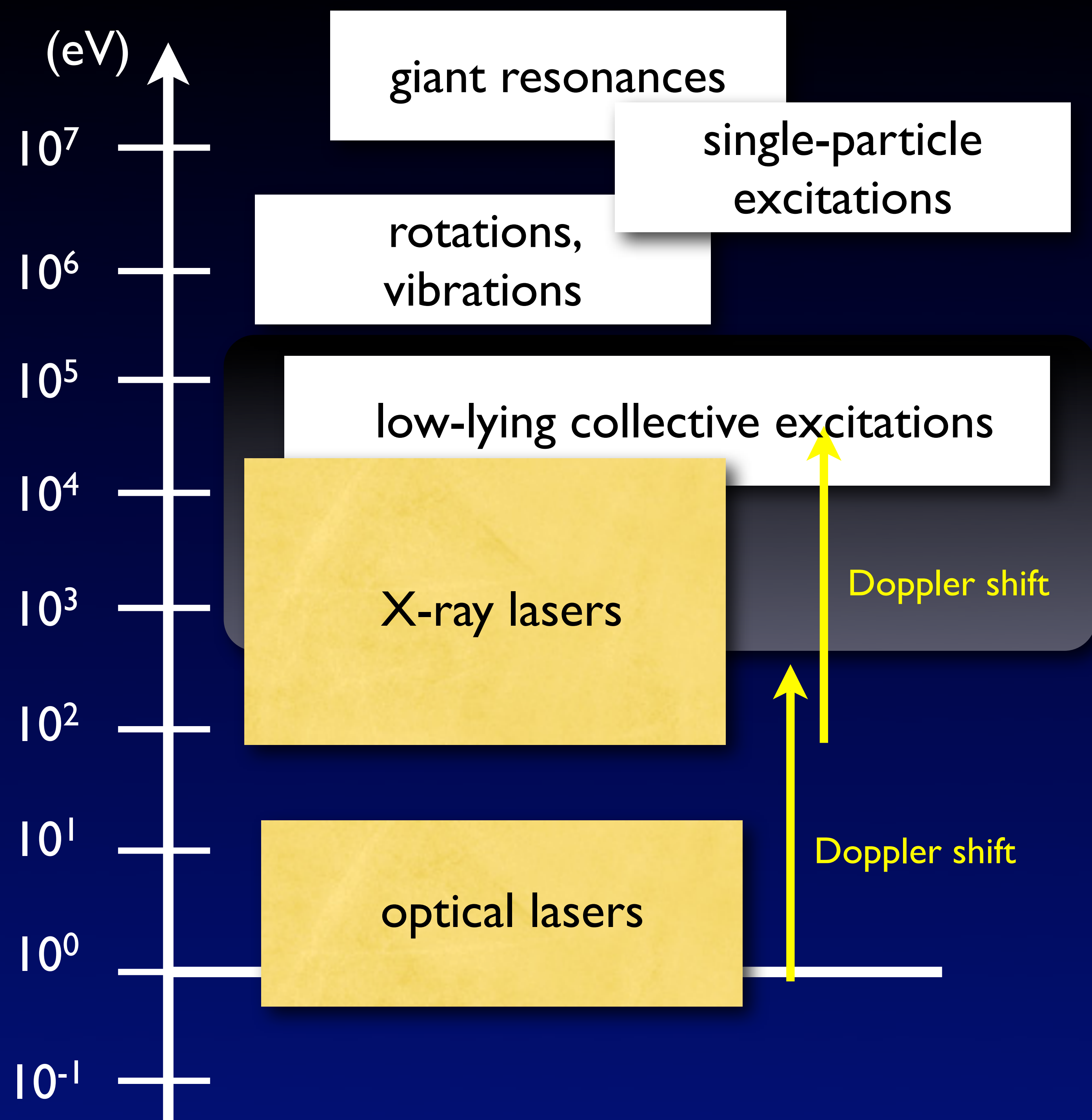


20
15
10
5
0
E (MeV)
NL-Z2
$_{126}U^{218}$
-0.5
0.0
0.5
1.0
1.5
β_2

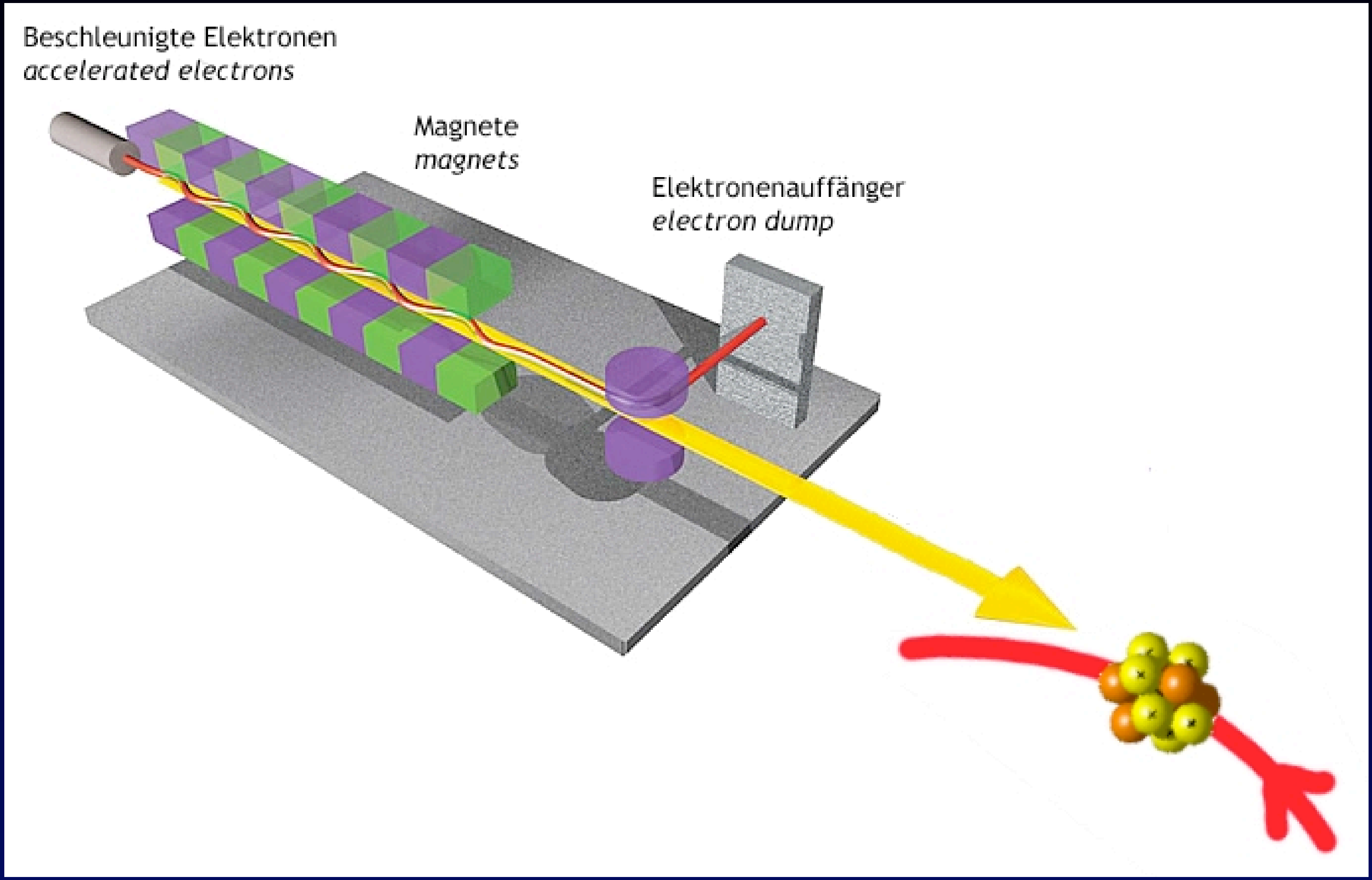


δ_{2n} (MeV)
100
80
60
40
20
Proton Number Z
3
2
1
0
NL3
20
40
60
80
100
120
140
160
Neutron Number N
δ_{2p} (MeV)
100
80
60
40
20
Proton Number Z
5
4
3
2
1
0
NL3
20
40
60
80
100
120
140
160
Neutron Number N

Where nuclear excitations and lasers meet



Direct laser-nucleus interactions



$$E_N = \sqrt{(1+\beta)/(1-\beta)}E_L = (1+\beta)\gamma E_L$$

$$\nu_N = \sqrt{(1+\beta)/(1-\beta)}\nu_L = (1+\beta)\gamma \nu_L$$

combination of laser and beam facilities

The dynamical AC Stark shift in nuclei

- analogy to electronic dynamical Stark shift
- consider laser pulses at optical frequencies
- head-on collision of nuclei and laser pulses to achieve high intensities
- small interaction matrix elements $R \approx 2 - 10\ \mathrm{fm}, \quad \langle m|z|n\rangle = \mathcal{O}(\mathrm{fm})$
- mean-field model for description of nuclear structure

laser-nucleus interaction $H_I = e\mathcal{E}(t)z$

electric dipole approximation

$\mathcal{E}(t) = \mathcal{E}_0 \sin(\nu t)$ c.w.

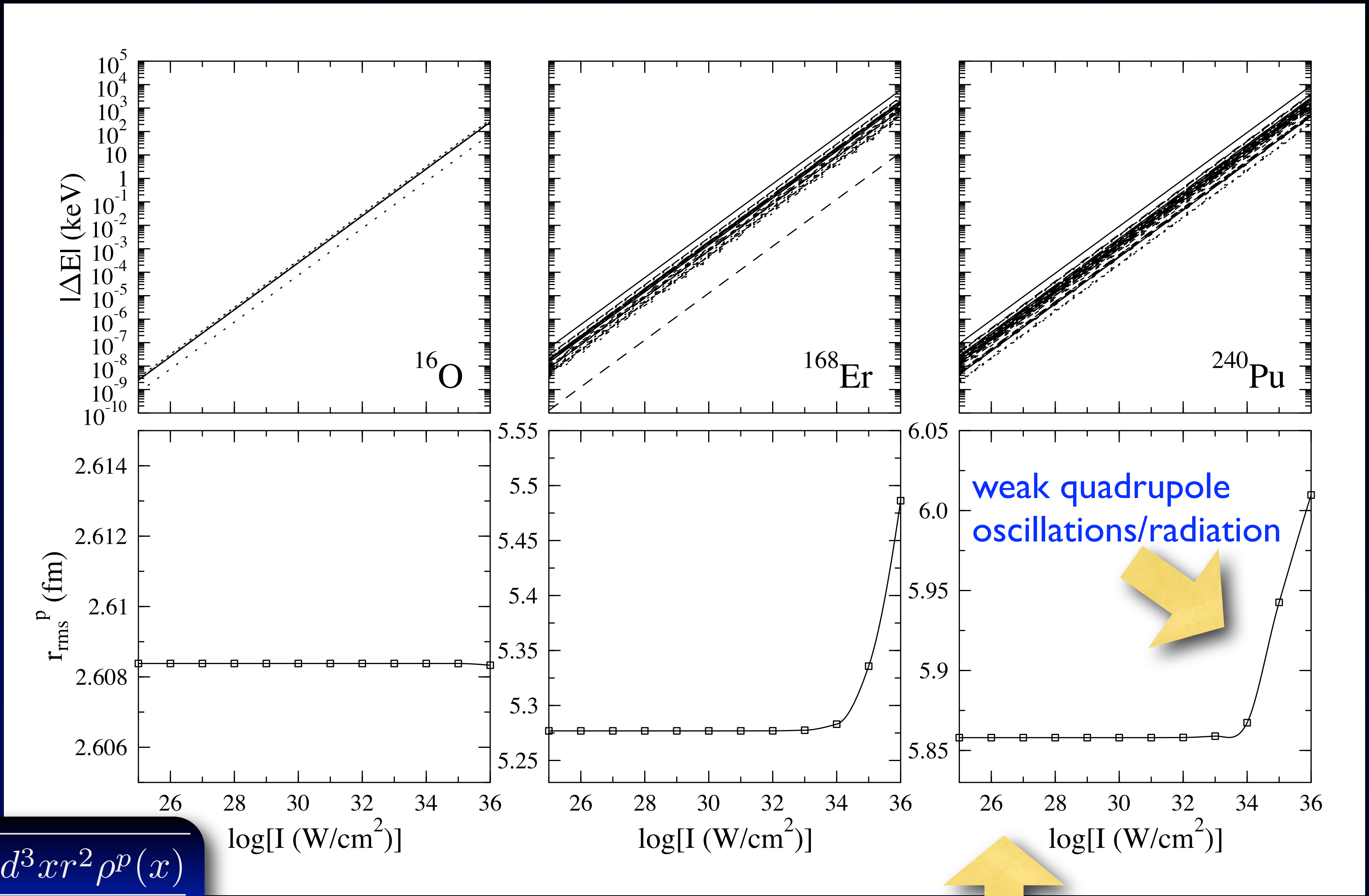
2nd order PT
$$\Delta E_n = \frac{1}{4} \sum_{m,\pm} \frac{\langle n|H_I|m\rangle\langle m|H_I|n\rangle}{\epsilon_n - \epsilon_m \pm \hbar\nu + i\hbar\epsilon}$$

$\hbar\nu \ll \epsilon_n - \epsilon_m$ optical laser frequencies

$$\Delta E_n^{<<} = \frac{1}{2} \sum_{m\neq n} \frac{\langle n|H_I|m\rangle\langle m|H_I|n\rangle}{\epsilon_n - \epsilon_m}$$

proton single-particle wave-functions; input from the relativistic mean-field model

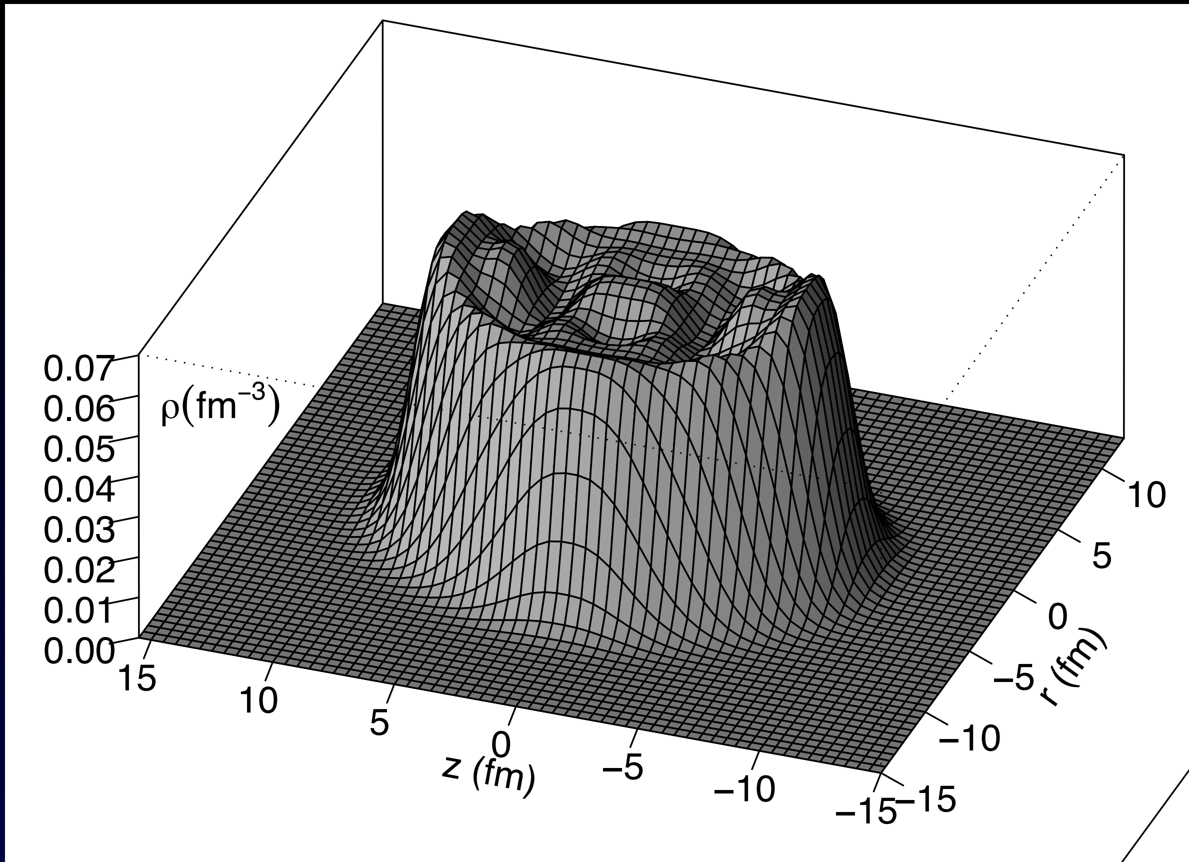
AC Stark shifts



$$r^p_{rms} = \sqrt{\frac{\int d^3x r^2 \rho^p(x)}{\int d^3x \rho^p(x)}}$$

$$\Delta E \propto \mathcal{E}^2 \propto I$$

~ relation as in atomic situations

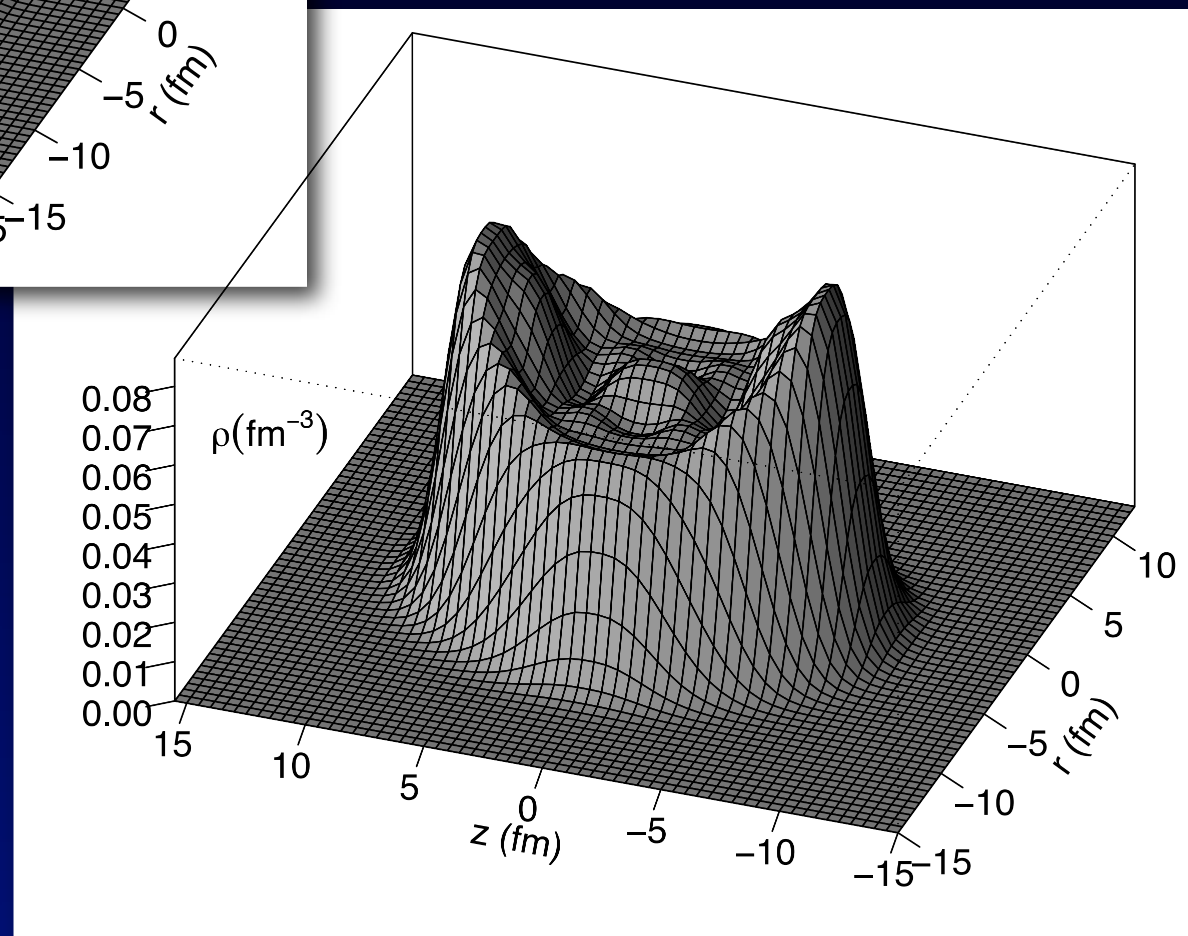


$I = 10^{25}$ W/cm^2

^{240}Pu

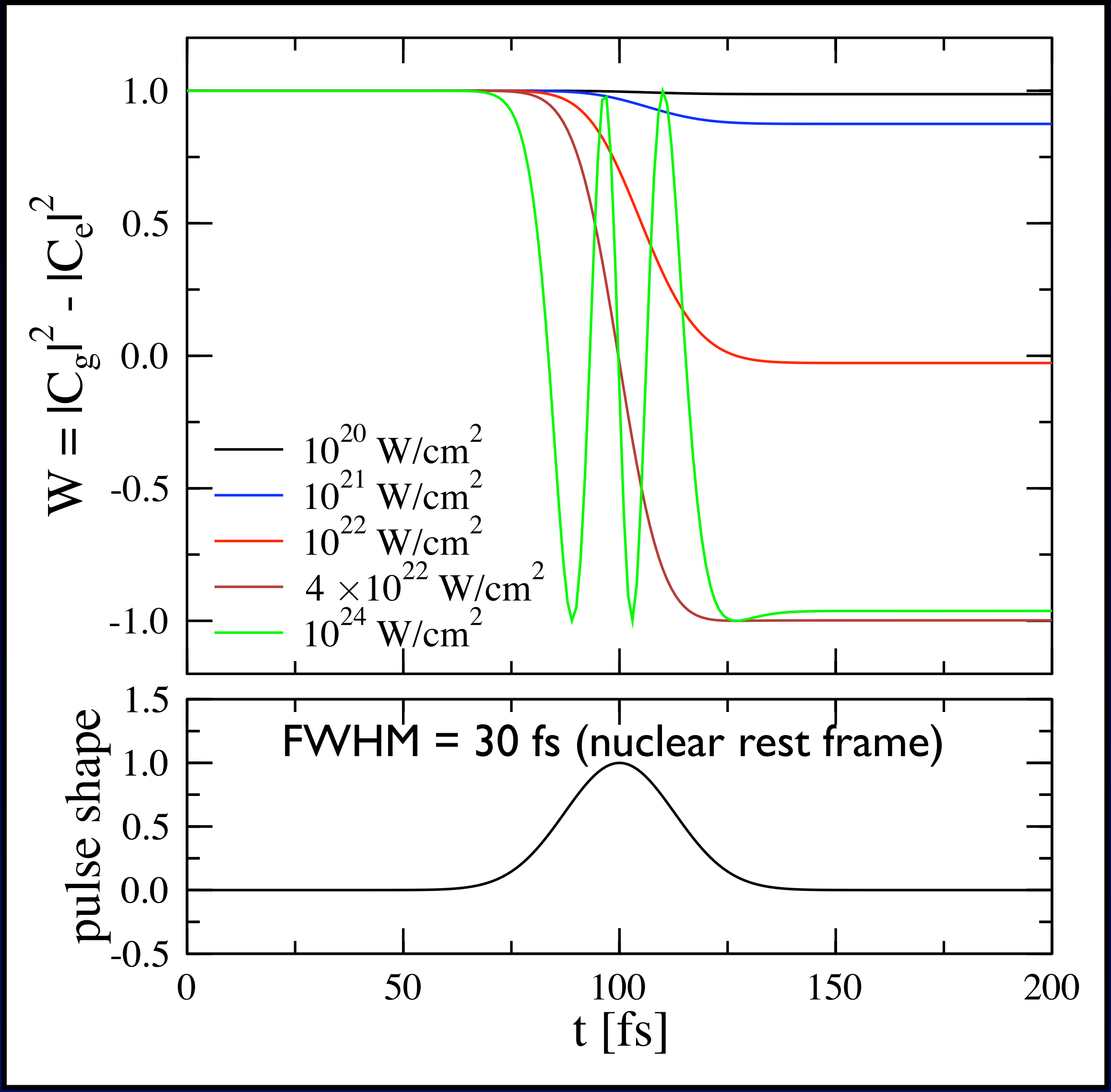
$I = 10^{35}$ W/cm^2

proton densities built from
(2nd order PT) single-particle proton
wave-functions



Rabi oscillations between ground and excited states

$$\Omega^{-1} \ll \tau(e)$$



π pulse at I = 4 * 10^{22} W/cm^2

^{223}Ra

$$\Delta E = 50.1 \text{ keV}$$
$$\tau(e) = 730 \text{ ps}$$
$$\mu = 0.12 \text{ e fm}$$

- measure excitation function as the response of the nucleus with respect to laser parameters

- optical and model-independent determination of nuclear transition frequency and dipole moment

- many nuclear systems available

Outlook

- mean-field models/nuclear density functional theory have reached high predictive power and increase our understanding of exotic nuclei
- laser-nucleus interactions: input from mean-field models
- systematic and controlled model developments combined with new experimental data are desirable
- an exciting future lies ahead of us