Nuclear structure

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1. Nuclear theory – selection of starting point
2. What can be done ‘exactly’ (*ab-initio* calculations) and why we cannot do that systematically?
3. Effective interactions
4. Density functional theory
5. Shell structure and shell effects. Their consequences.
6. Nuclear landscape: what we know and how well we extrapolate
7. Superheavy nuclei: successes and challenges

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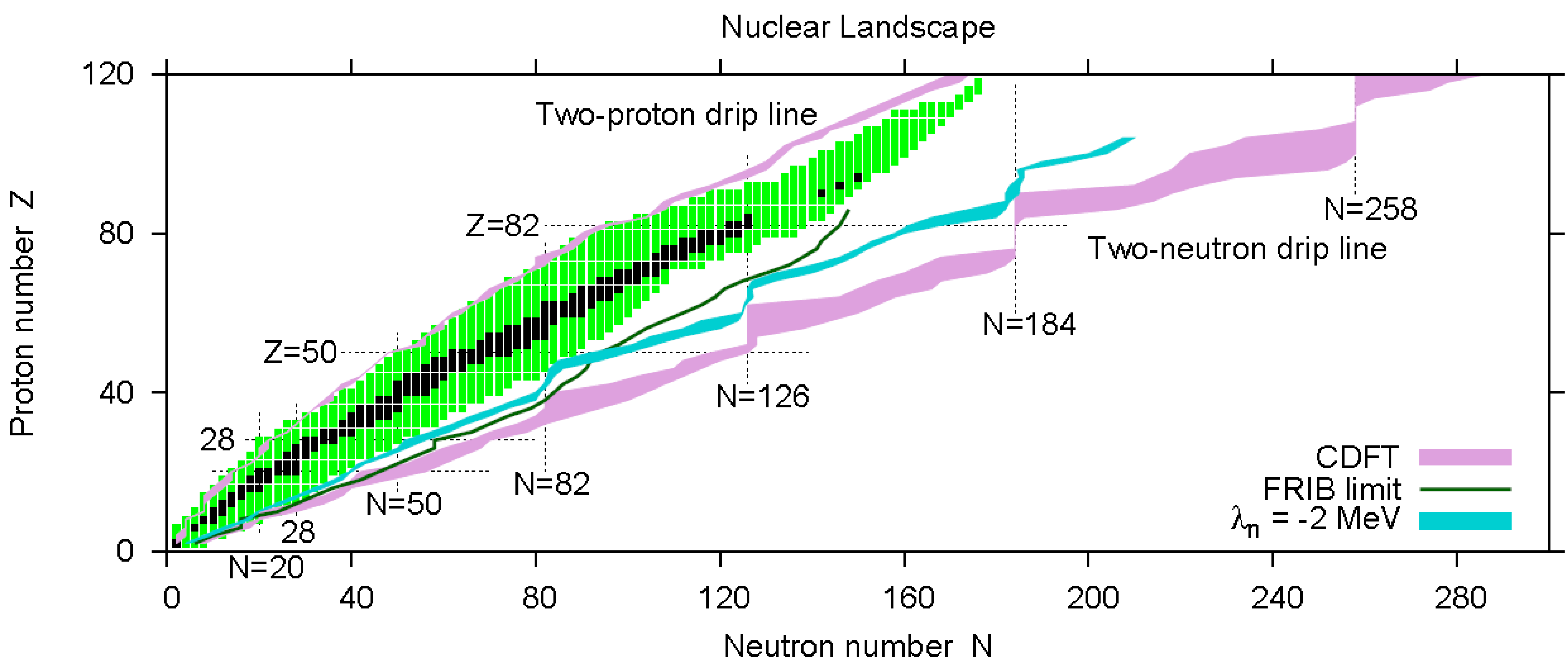
The improvement in theory is critical:
FRIB will allow to explore
only some part of nuclear chart



1. Nuclear theory –
selection of starting point

Building blocks of nuclear matter

FERMIONS matter constituents spin = 1/2, 3/2, 5/2, ...

Leptons spin = 1/2			Quarks spin = 1/2		
Flavor	Mass GeV/c^2	Electric charge	Flavor	Approx. Mass GeV/c^2	Electric charge
ν_e electron neutrino	$<1\times10^{-8}$	0	u up	0.003	2/3
e electron	0.000511	−1	d down	0.006	−1/3
ν_μ muon neutrino	<0.0002	0	c charm	1.3	2/3
μ muon	0.106	−1	s strange	0.1	−1/3
ν_τ tau neutrino	<0.02	0	t top	175	2/3
τ tau	1.7771	−1	b bottom	4.3	−1/3

BOSONS force carriers spin = 0, 1, 2, ...

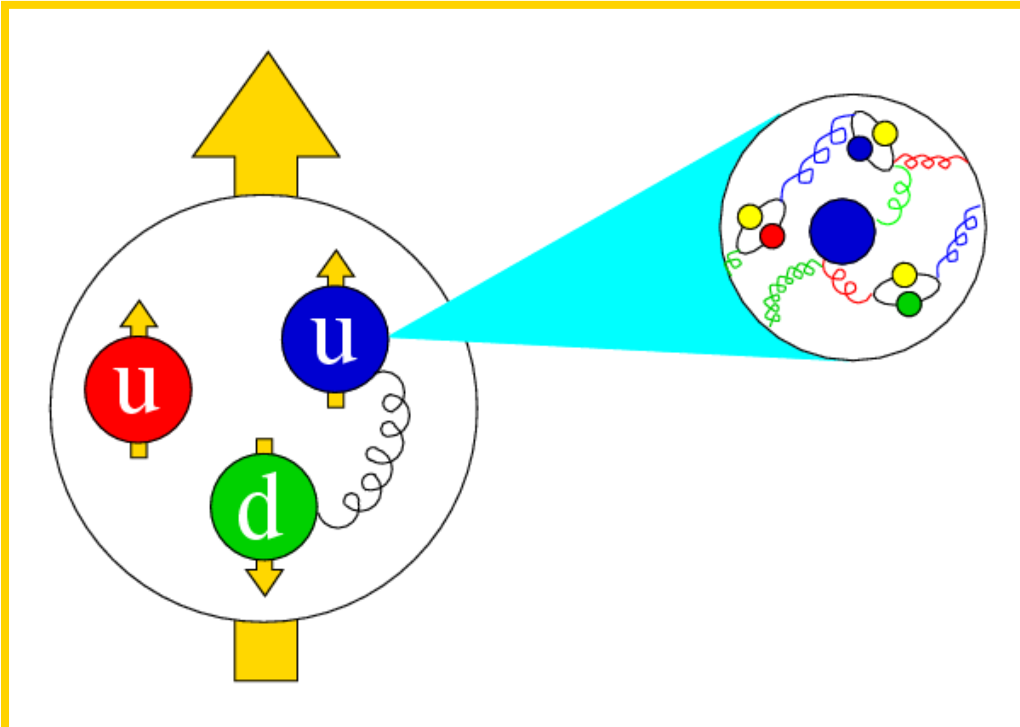
Unified Electroweak spin = 1		
Name	Mass GeV/c^2	Electric charge
γ photon	0	0

The complete QCD Lagrangian

$$\Lambda = -\frac{1}{4} F^{\alpha}_{\mu\nu} F^{\mu\nu}_{\alpha} - \sum_n \overline{\Psi}_n \gamma^{\mu} [\delta_{\mu} - ig A^{\alpha}_{\mu} t_{\alpha}] \Psi_n - \sum_n m_n \overline{\Psi}_n \Psi_n$$

6 quark fields: n=1,…,6

8 SU(3) matrices numbered by the gluon-color index α=1,2,...,8



Proton = uud

Neutron = ddu

Mesons: built from quark and anti-quark

Example: pion π^0

Quark-meson coupling models

Quark degrees of freedom can be neglected and the description of low-energy nuclear systems can be based on the hadrons interacting by the exchange of different mesons

Physics is an art of approximations

Challenges of description of many-body nuclear systems

Start from Schrodinger equation

$$E = \sum_i \frac{\vec{p}^{\,2}}{2m} + \sum_{i<j} V(\vec{r}_{ij}, t_{ij}, s_{ij}, \ldots)$$

- Nuclear forces inside of finite nuclei are poorly known
  Example: the need for 3-body forces

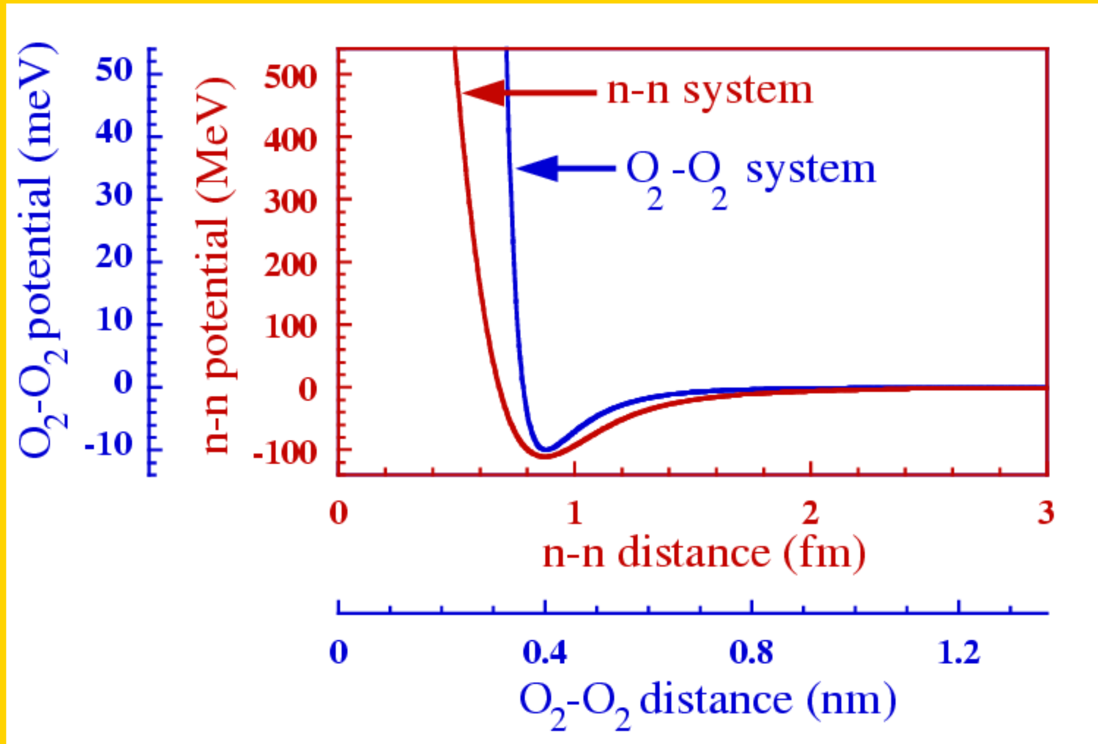
- Many-body aspect of the problem
  Example: 'exact' multi-particle wave function methods

  - exponential wall (# of Slater determinants up to 10^9) A_{max}~12
  - improvements of analytical and computational methods will lead only to modest increase of A_{max}

- Relativistic effects are PARAMETRIZED: for example, spin-orbit interaction

$$V_{LS} = W(r)\vec{l}\,\vec{s}$$

The description of the interaction of particles at short distances is extremely complicated → HARD CORE problem



Polarization effects at short distances – fermionic constituents do not like being put close to one another --- the Pauli exclusion principle creates additional polarization and repulsion effects

if 3 particles → polarization effects depends on explicit positions of each of them

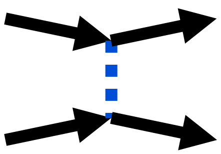
THREE-BODY EFFECTS

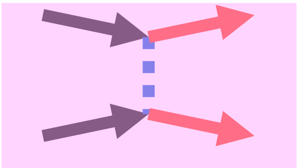
Use EFFECTIVE FORCES which truncate momenta above ~ 500-1000 MeV

Effective forces according to Brueckner theory (1958):

Brueckner,Gammel, Phys. Rev. 109, 1023 (1958)

- The nucleons in the interior of the nuclear medium do not feel the same bare force V, as the nucleons feel in free space.





- They feel an effective force G.
- The Pauli principle prohibits the scattering into states, which are already occupied in the medium → the force $G(\rho)$ depends on the density
- This force G is much weaker than bare force V.
- Nucleons move nearly free in the nuclear medium and feel only a strong attraction at the surface (shell model)

THREE-BODY EFFECTS

4- body ???

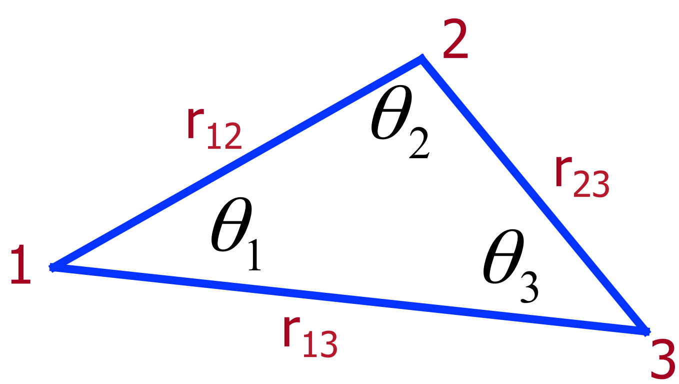
$$V(\vec{r}^{\,N}) = \sum_{i \neq j=1}^{N} V_{ij}(\vec{r}_{ij}) + \sum_{i,j,l}^{N} V_{ijl}(\vec{r}_{ij}, \vec{r}_{il}, \vec{r}_{jl}) + \ldots$$

2-body

3-body

Axilrod-Teller potential

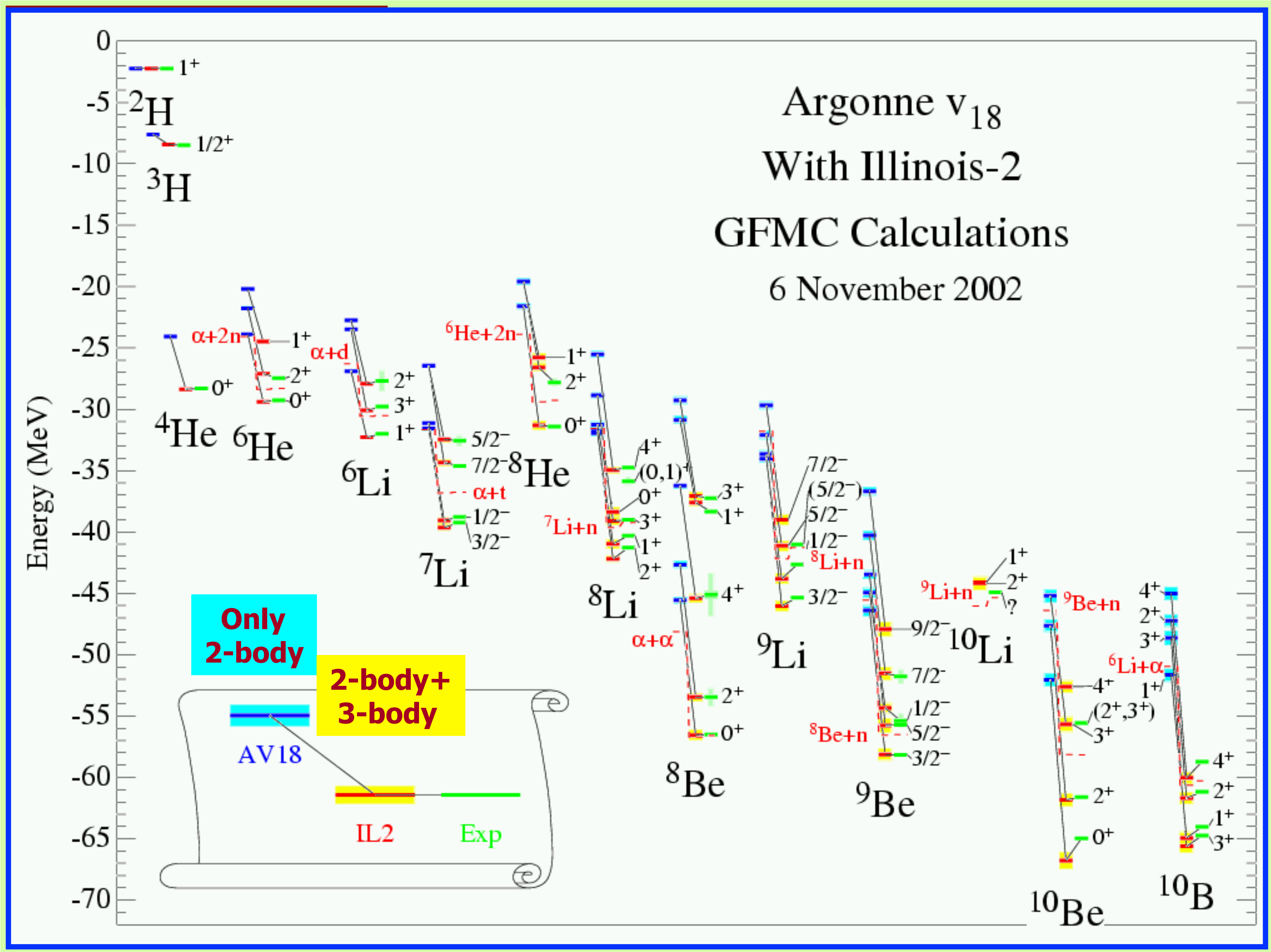
$$V^{(3)}(\vec{r}_1, \vec{r}_2, \vec{r}_3) = A\left[\frac{3\cos(\theta_1)\cos(\theta_2)\cos(\theta_3)+1}{\vec{r}_{12}^{\,3}\vec{r}_{13}^{\,3}\vec{r}_{23}^{\,3}}\right]$$



3-body effects in liquid argon:

- 10% effect on partition function
- 40% effects on transport coefficients

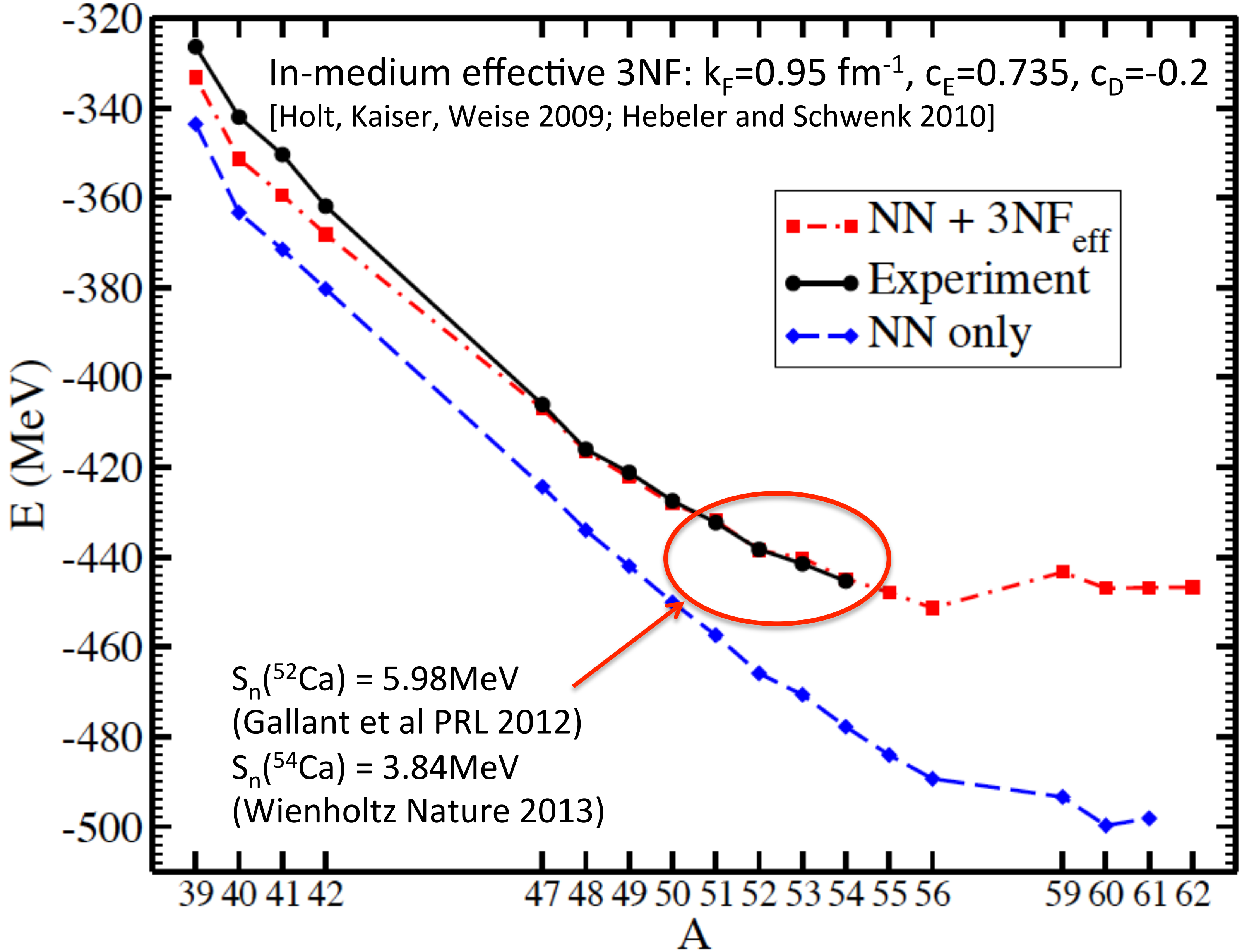
2. What can be done ‘exactly’ (*ab initio* calculations) and why we cannot do that systematically



Argonne v18
With Illinois-2
GFMC Calculations
6 November 2002
Energy (MeV)
0
-5
-10
-15
-20
-25
-30
-35
-40
-45
-50
-55
-60
-65
-70
2H
3H
4He
6He
6Li
7Li
8He
8Li
8Be
9Li
9Be
10Li
10Be
10B
α+2n
α+d
α+t
6He+2n
7Li+n
α+α
8Li+n
8Be+n
9Li+n
9Be+n
6Li+α
Only 2-body
2-body+ 3-body
AV18
IL2
Exp

Calcium isotopes from chiral interactions

[Hagen et al, Phys. Rev. Lett. 109, 032502 (2012).]



The description of heavy nuclei is still a problem.

S. Binder et al, arXiV: 1312.5685v1 (2013)

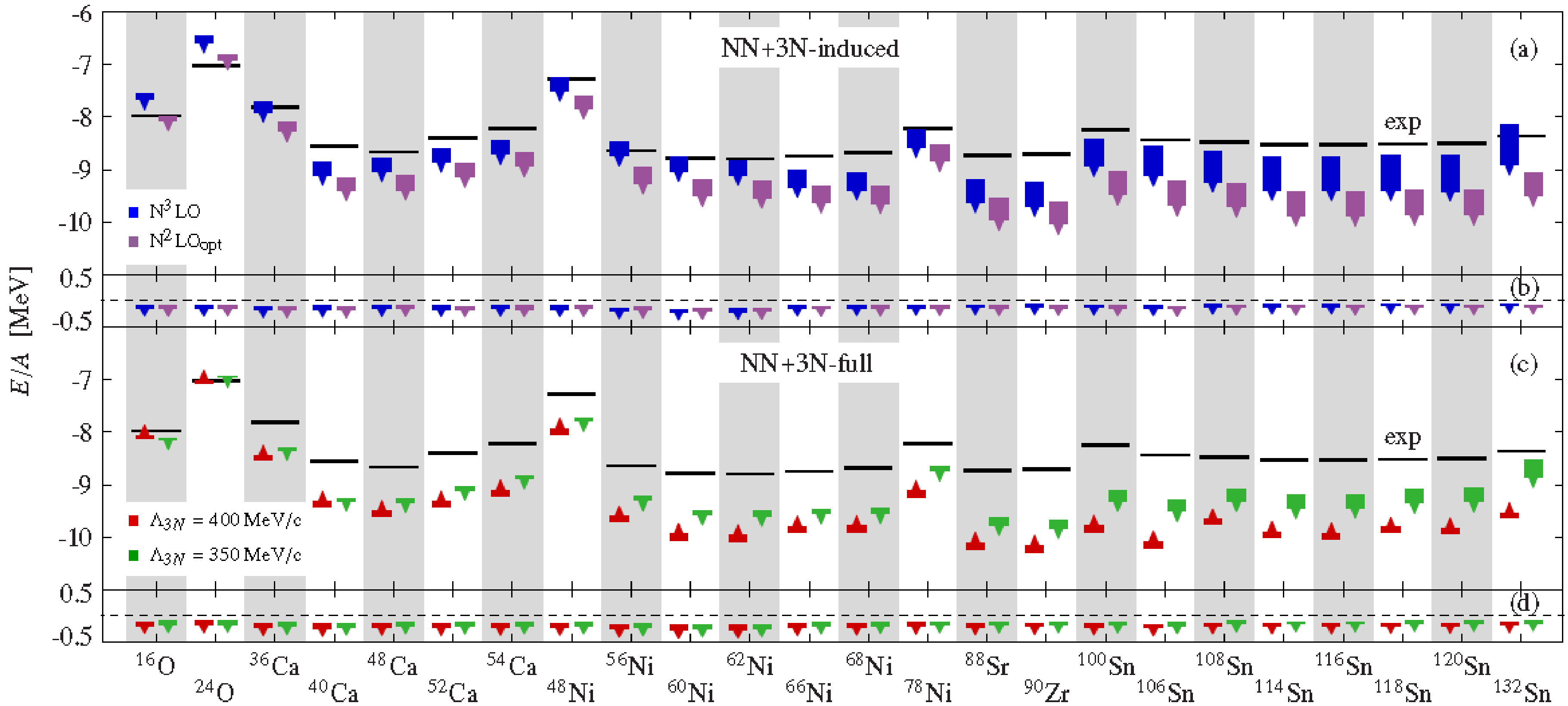


FIG. 5: (Color online) Ground-state energies from CR-CC(2,3) for (a) the $NN+3N$-induced Hamiltonian starting from the N^3LO and N^2LO-optimized NN interaction and (c) the $NN+3N$-full Hamiltonian with $\Lambda_{3N} = 400$ MeV/c and $\Lambda_{3N} = 350$ MeV/c. The boxes represent the spread of the results from $\alpha = 0.04\ \mathrm{fm}^4$ to $\alpha = 0.08\ \mathrm{fm}^4$, and the tip points into the direction of smaller values of α. Also shown are the contributions of the CR-CC(2,3) triples correction to the (b) $NN+3N$-induced and (d) $NN+3N$-full results. All results employ $\hbar\Omega = 24$ MeV and $3N$ interactions with $E_{3\max} = 18$ in NO2B approximation and full inclusion of the $3N$ interaction in CCSD up to $E_{3\max} = 12$. Experimental binding energies [32] are shown as black bars.

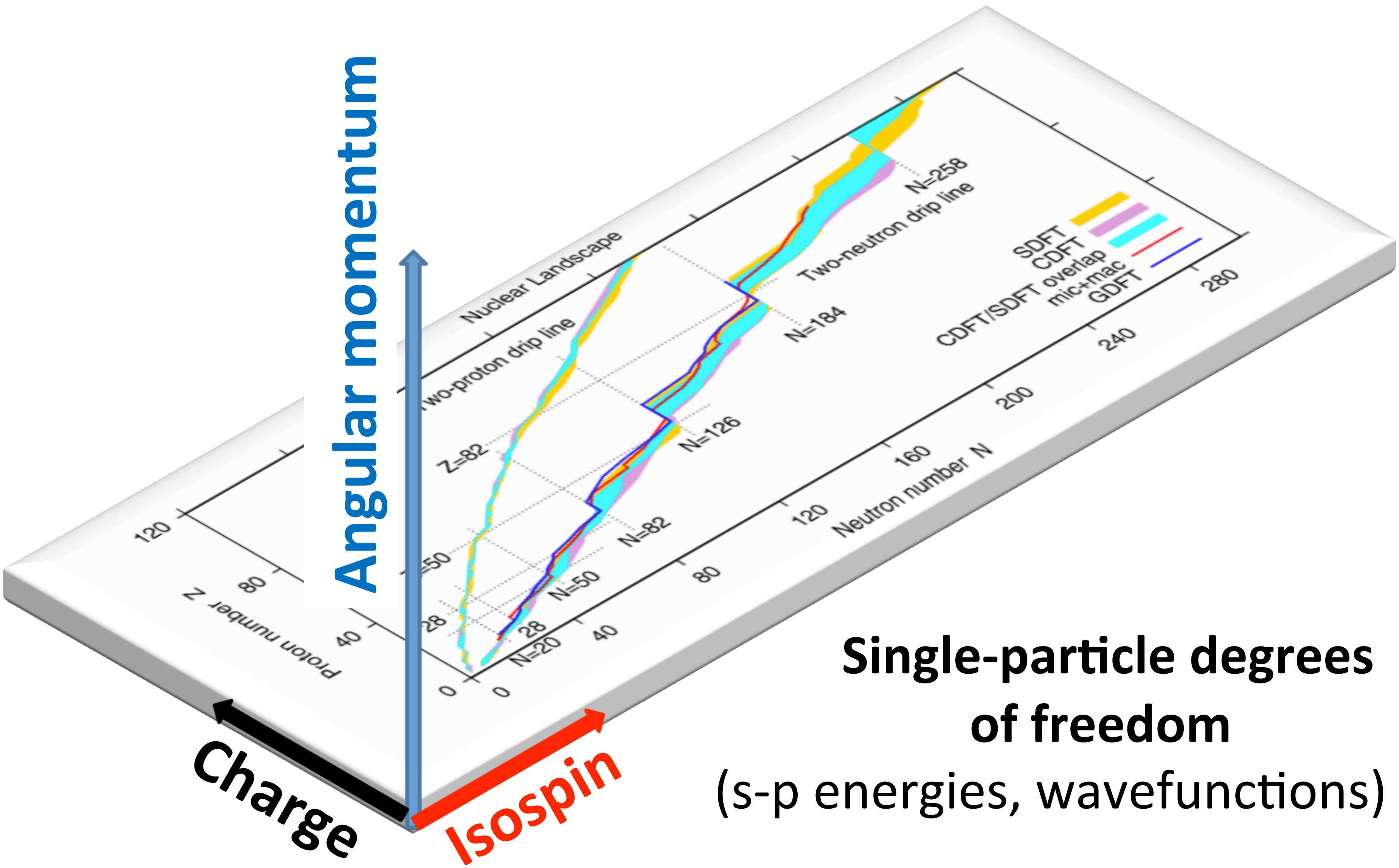
Even if these problems are resolved in future

- it is not clear whether *ab initio* calculations will be more accurate as compared with experiment than other approaches

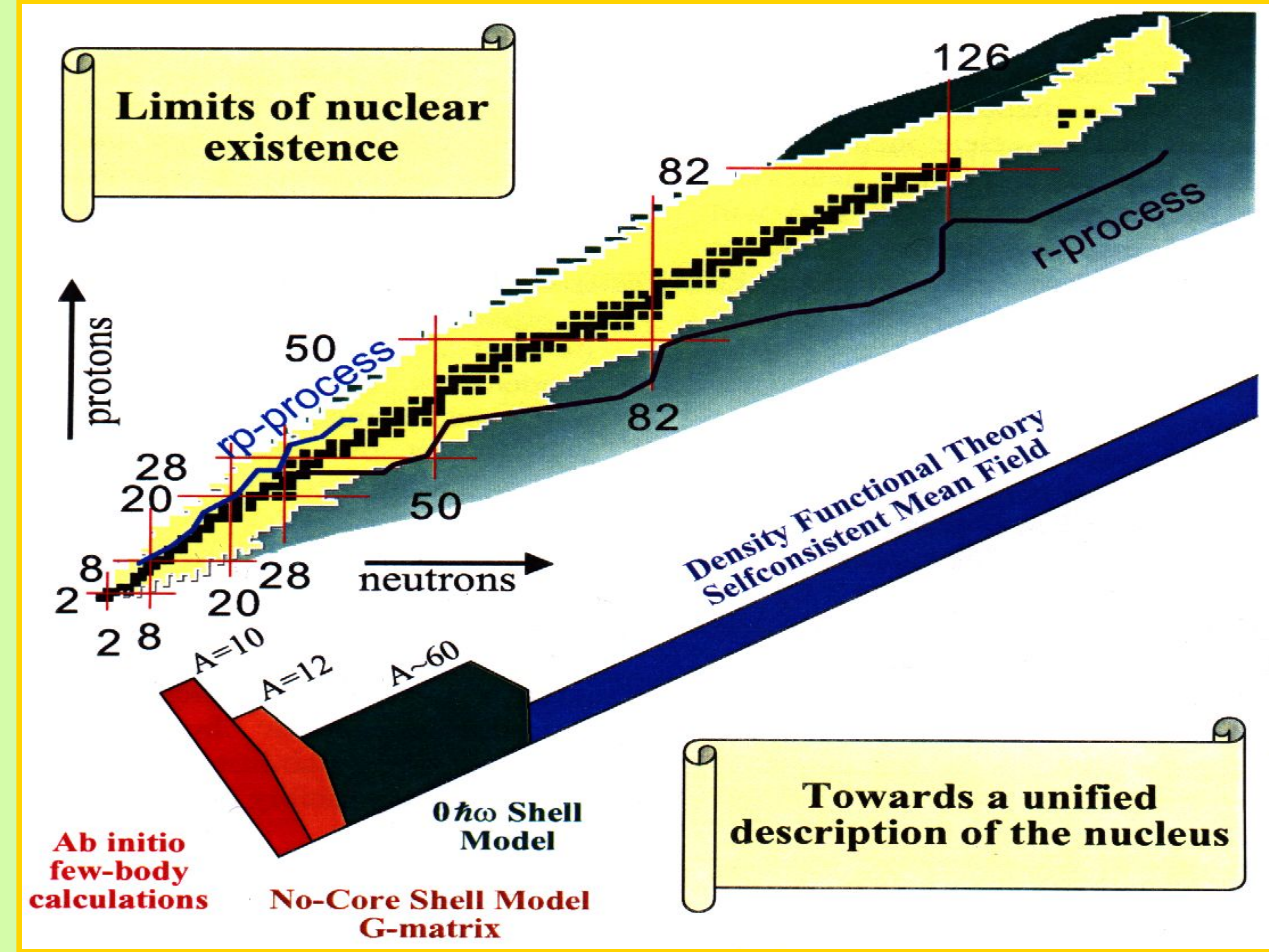
- numerically, *ab initio* calculations are significantly more expensive than in other approaches

Density functional theory

Collective degrees of freedom (deformation, rotation, fission)

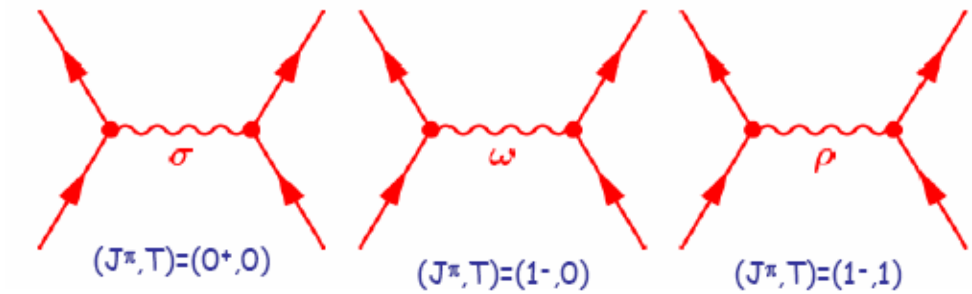


Single-particle degrees of freedom
(s-p energies, wavefunctions)


Limits of nuclear existence
protons
neutrons
rp-process
r-process
2
8
20
28
50
82
126
2 8
20
28
50
82
Density Functional Theory
Selfconsistent Mean Field
A=10
A=12
A~60
0ℏω Shell Model
Ab initio few-body calculations
No-Core Shell Model G-matrix
Towards a unified description of the nucleus

Covariant density functional theory (CDFT)

The nucleons interact via the exchange of effective mesons → → **effective Lagrangian**



Long-range attractive scalar field

Short-range repulsive vector field

Isovector field

$$E_{\mathrm{RMF}}[\hat{\rho},\phi_m] = \mathrm{Tr}[(\boldsymbol{\alpha p} + \beta m)\hat{\rho}] \pm \int \left[\frac{1}{2}(\nabla\phi_m)^2 + U(\phi_m)\right] \mathrm{d}^3r + \mathrm{Tr}[(\Gamma_m\phi_m)\hat{\rho}]$$

density matrix $\hat{\rho}$

$\phi_m \equiv \{\sigma, \omega^\mu, \vec{\rho}^\mu, A^\mu\}$ - meson fields

$$\boxed{\hat{h} = \frac{\delta E}{\delta\hat{\rho}}}$$ **Mean field**

$$\boxed{\hat{h}|\varphi_i\rangle = \varepsilon_i|\varphi_i\rangle}$$ **Eigenfunctions**

Non-relativistic mean field and density functional theories

1. Macroscopic + microscopic method

Bulk properties → liquid drop

Single-particle properties → single-particle potential (Woods-Saxon, Nilsson, folded Yukawa)

Very flexible but no self-consistency → extrapolation to unknown regions of nuclear chart maybe unreliable

2. Density functional theories starting from 2 - and 3 - nucleon effective interactions

Finite range Gogny force

$$
\begin{aligned}
V_{12} \;=\; & \sum_{i=1}^{2} \left(W_i + B_i \hat{P}_\sigma - H_i \hat{P}_\tau - M_i \hat{P}_\sigma \hat{P}_\tau\right) e^{-\frac{(\vec{r}_1 - \vec{r}_2)^2}{\mu_i^2}} \\
& + \; i\, W_{\mathrm{LS}}\, (\overleftarrow{\nabla_1 - \nabla_2}) \times \delta(\vec{r}_1 - \vec{r}_2)(\overrightarrow{\nabla_1 - \nabla_2}) \cdot (\vec{\sigma}_1 + \vec{\sigma}_2) \\
& + \; t_0\, (1 + x_0 \hat{P}_\sigma)\, \delta(\vec{r}_1 - \vec{r}_2) \left[\rho\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right)\right]^{\gamma} + V_{\mathrm{Coul}}\;,
\end{aligned}
$$

Central finite range force

Spin-orbit 0-range

Density-dependent 0-range + Coulomb

Zero-range (contact) Skyrme forces

Effective interactions

Realistic 2-body forces

Local:
1. Central force
2. Tensor force

$$V(r) = -V_0 e^{-r^2/r_0^2}$$

$$V_T(1,2) = [V_{T_0}(r) + V_{T_\tau}\tau^{(1)}\tau^{(2)}]S_{12}$$

Non-local (velocity-dependent)
Example, 2-body spin-orbit interaction

Many-body techniques (Bruckner G-matrix, …)

Effective nucleon-nucleon forces

1. well-behaved at short distances (no hard core problem)

Hard core can be neglected: nucleons move through the nucleus most of the time as independent particles because of Pauli exclusion principle (Weisskopf, 1950)

2. Include some part of many body correlations
3. Possible to apply many-body techniques

Nucleons within a nucleus do not feel the bare nn-interaction !!!

FIT TO EXP. DATA → PHENOMENOLOGICAL EFFECTIVE FORCES

Mean field and Hartree+Fock(+Bogoliubov) approaches

MEAN FIELD – nucleons move independently in an average potential produced by all the nucleons ➔

$$V(1 \ldots A) = \sum_{i>j=1}^{A} V(i,j) \approx \sum_{i=1}^{A} V(i)$$

$$H|\Psi> = E|\Psi> \quad \equiv \quad \delta E[\Psi] = 0$$

Exact Schrodinger eq. Variational eq.

Transition to single-particle levels

$$H^{HF} = \sum_{i=1}^{A} h(i)$$

$$h(i)\varphi_k(i) = \varepsilon_k \varphi_k(i)$$

$$i = \{\vec{r}_i, s_i, t_i\}$$

Total HF wave function= = Slater determinant

$$\Phi_{k_1 \ldots k_A}(1,\ldots,A) = \begin{vmatrix} \varphi_{k_1}(1) & \ldots. & \varphi_{k1}(A) \\ \vdots & & \vdots \\ \varphi_{k A}(1) & \ldots. & \varphi_{k_A}(A) \end{vmatrix}$$

The Hartree-Fock energy

$$E^{HF} = <\Phi|H^{HF}|\Phi>$$

$$\boxed{h = t + \Gamma}$$

$$\boxed{\Gamma_{kk'} = \sum_{ll'} \bar{u}_{kl'k'l}\,\rho_{ll'}}$$

Single-particle kinetic energy

Self-consistent field

Single-particle density matrix

ME of 2-body interaction

Pairing correlations can be accounted by BCS method or in the Hartree+Fock+Bogoliubov (HFB) method

$$\boxed{\begin{pmatrix} h & \Delta \\ -\Delta^{*} & -h^{*} \end{pmatrix}\begin{pmatrix} U_k \\ V_k \end{pmatrix} = \begin{pmatrix} U_k \\ V_k \end{pmatrix}\cdot E_k}$$

Pairing field

$$\boxed{\Delta_{kk'} = \frac{1}{2}\sum_{qq'} \bar{u}_{ll'qq'}\,\kappa_{qq'}}$$

Wave function of quasi-particles

Energy

$$\boxed{\rho_{ll'} =< \Phi \,|\, c_{l'}^{+} c_l \,|\, \Phi >}$$ **Density matrix** ph-

$$\boxed{\kappa_{ll'} =< \Phi \,|\, c_{l'} c_l \,|\, \Phi >}$$ **Pairing tensor** pp-

pp- and ph- channels of interaction are taken into account simultaneously

Density functional theory: Hohenberg-Kohn-Sham approach

- Starting point – energy functional E of local densities ρ and currents j

$$\rho = \sum_k v_k^2 \Psi_k^*(\ldots)\Psi_k(\ldots)$$

- Maps the nuclear many-body problem for the 'real' highly correlated many-body wave function on a system of independent particles is so-called Kohn-Sham orbitals $\Psi_k(\ldots)$

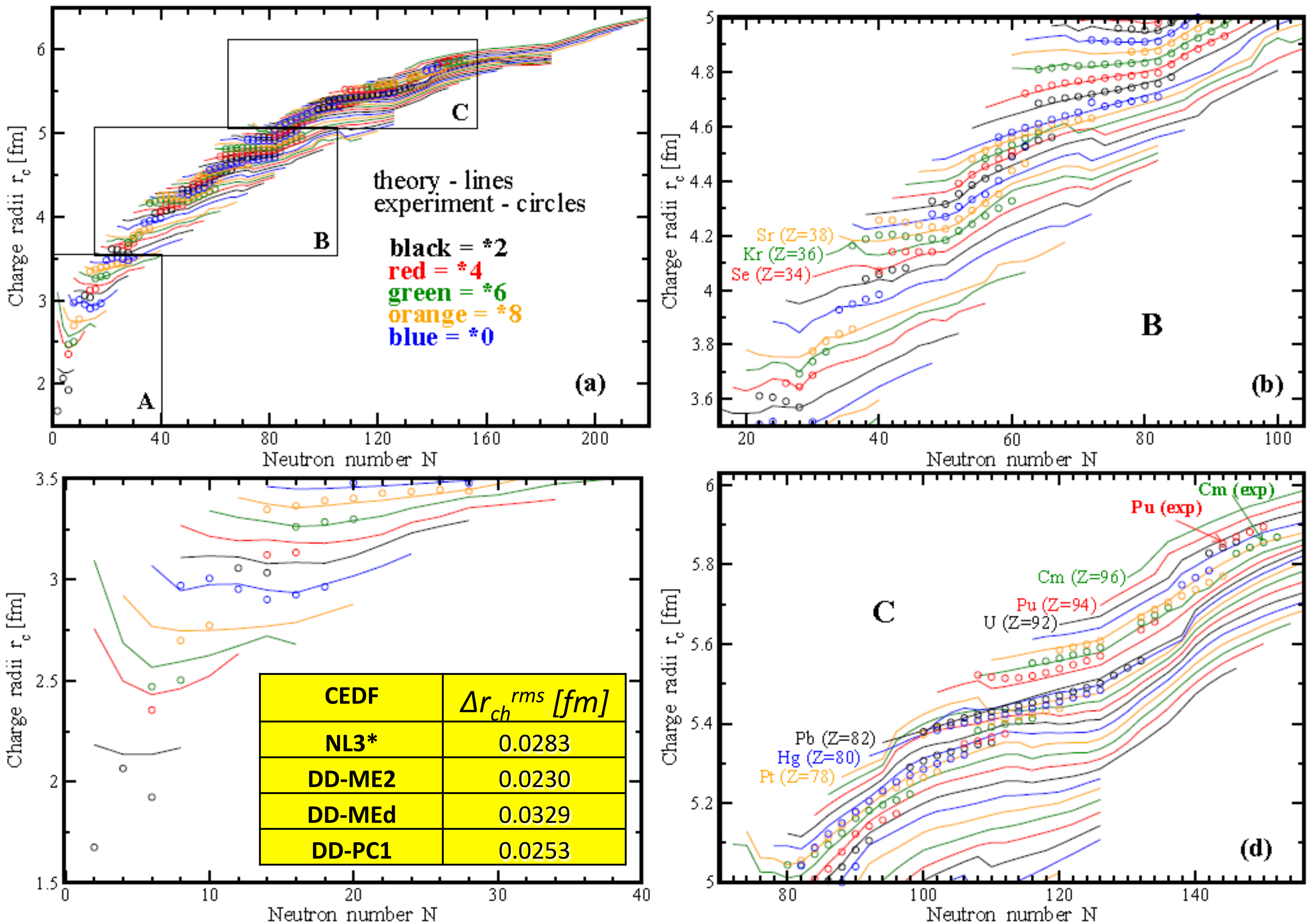
- **Variational** principle → equations of motion for $\Psi_k(\ldots)$

$$\delta E = 0 \quad \rightarrow \quad H\Psi_k(\ldots) = e_k\Psi_k(\ldots) \quad \rightarrow \quad H = \frac{\delta E}{\delta \rho}$$

- The existence theorem for the effective energy functional makes no statement about its structure.

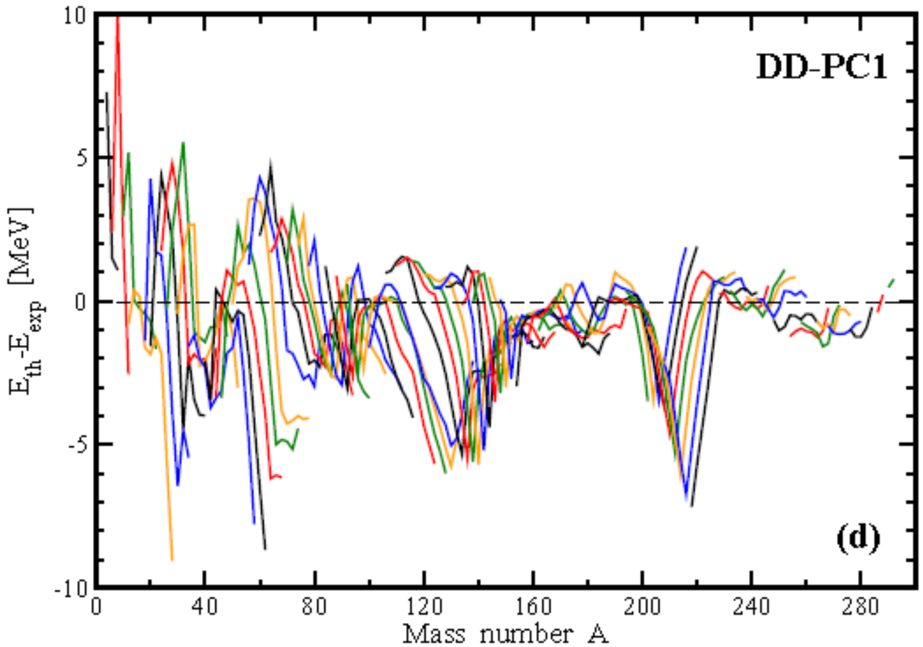
Its form is motivated by 'ab initio' theory, but the actual parameters are adjusted to nuclear structure data.

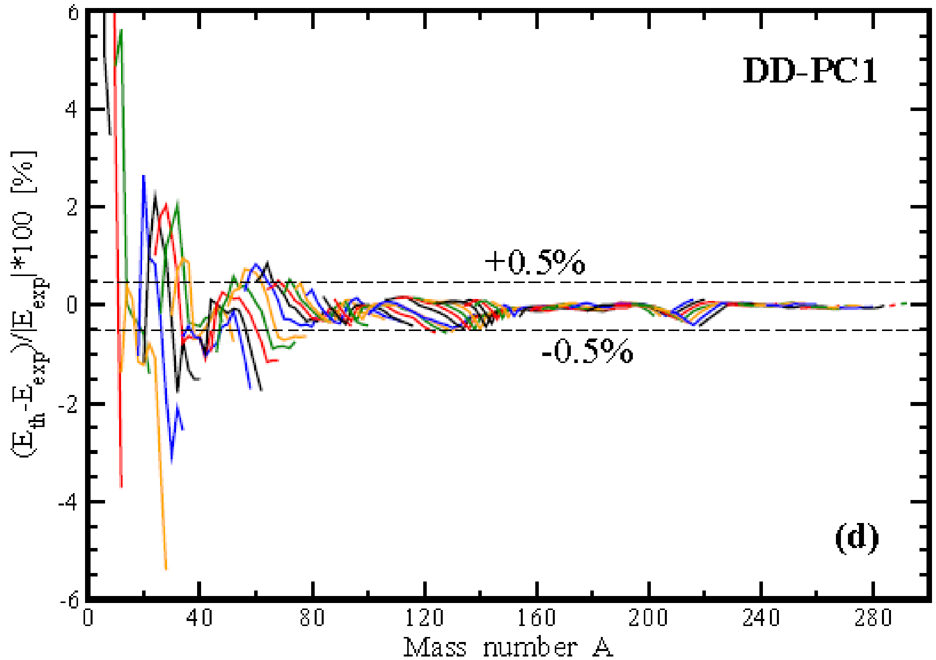
In Coulombic systems the functional is derived *ab initio*



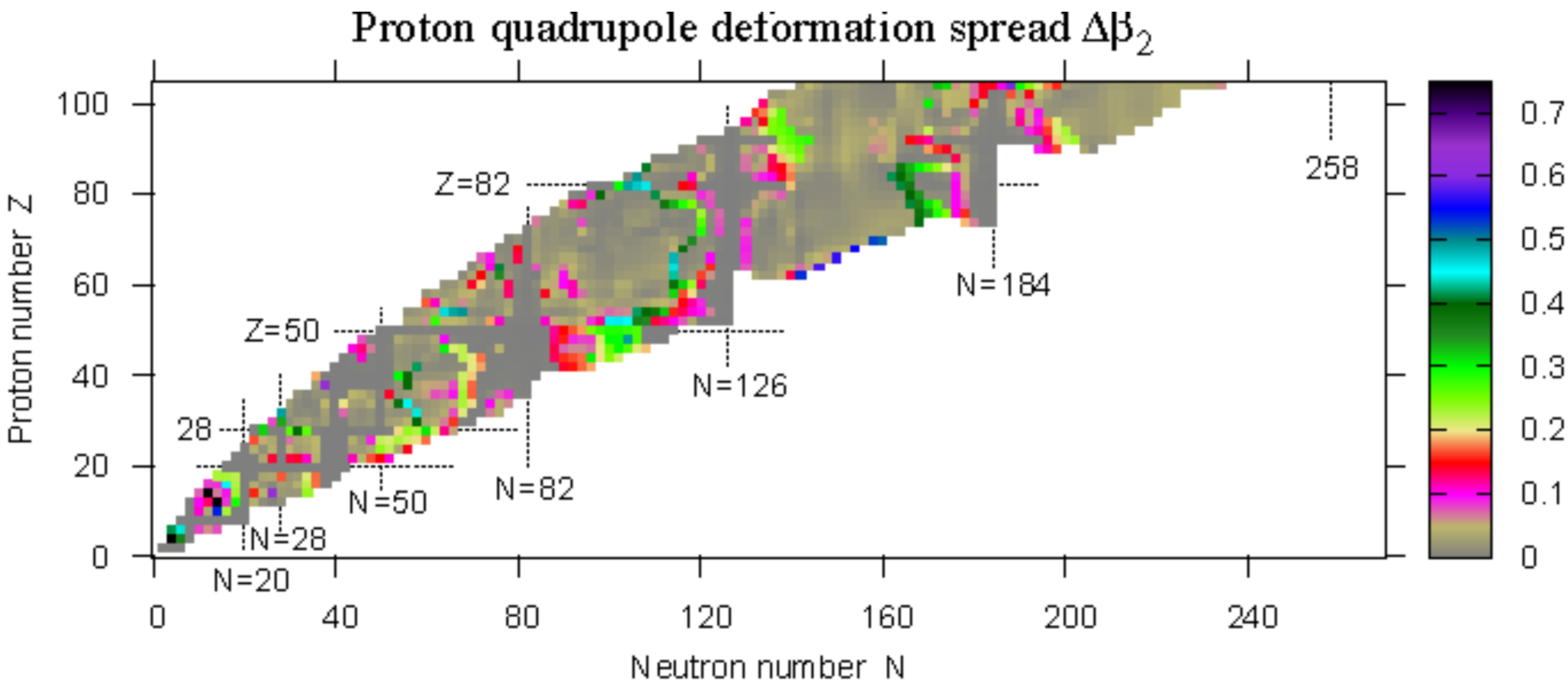
CEDF	Δr_{ch}^{rms} [fm]
NL3*	0.0283
DD-ME2	0.0230
DD-MEd	0.0329
DD-PC1	0.0253

Theoretical uncertainties in the description of masses





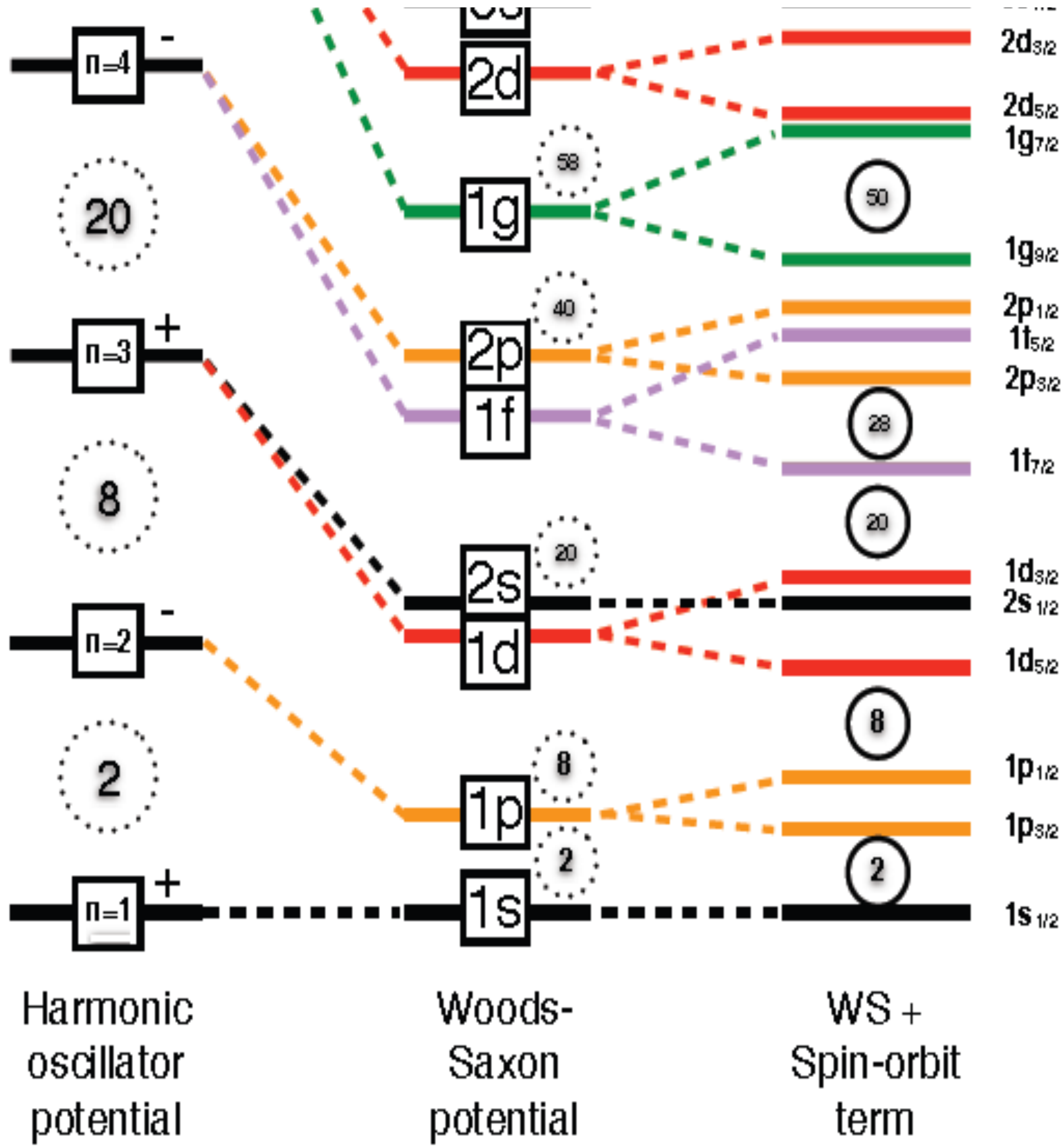
EDF	measured	measured+estimated		
	$\Delta E_{\rm rms}$	$\Delta E_{\rm rms}$	$\Delta(S_{2n})_{\rm rms}$	$\Delta(S_{2p})_{\rm rms}$
NL3*	2.96	3.00	1.23	1.29
DD-ME2	2.39	2.45	1.05	0.95
DD-MEδ	2.29	2.40	1.09	1.09
DD-PC1	2.01	2.15	1.16	1.03



Theoretical uncertainties are most pronounced for transitional nuclei (due to soft potential energy surfaces) and in the regions of transition between prolate and oblate shapes. Details depend of the description of single-particle states

Shell structure and shell effects

Single-particle states and shell structure in spherical nuclei



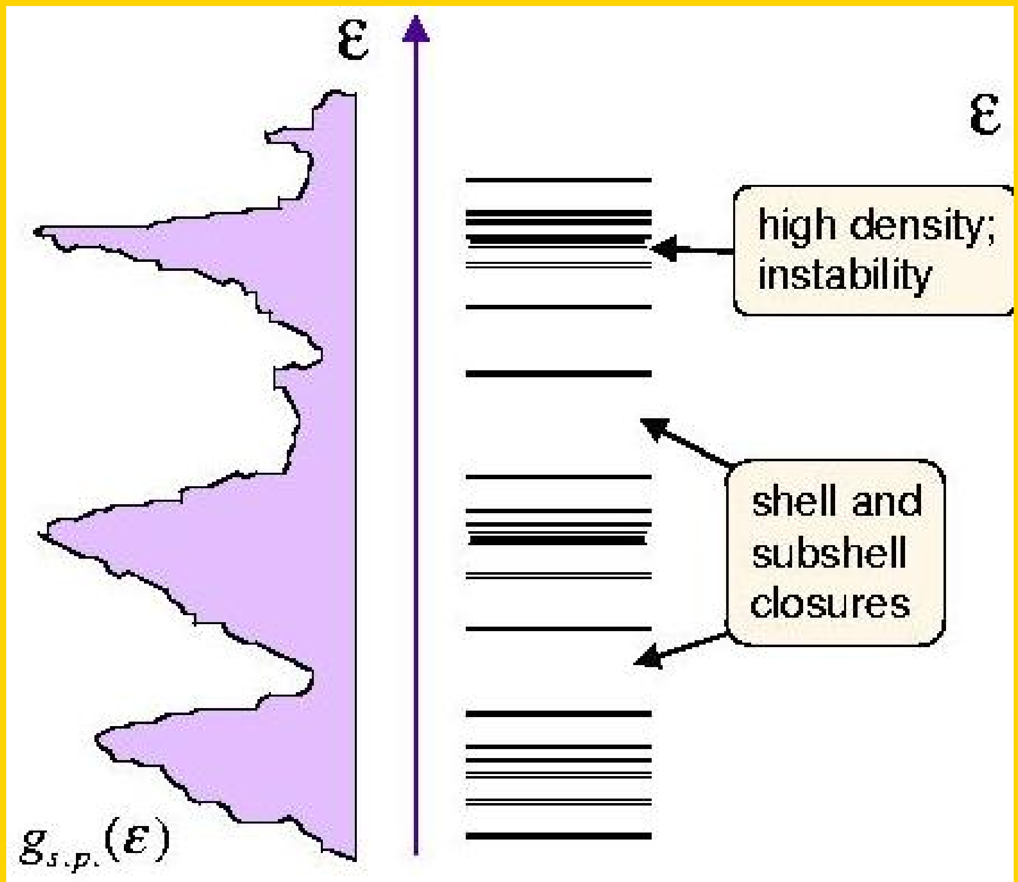
Shell structure and shell correction energies

$$\delta E_{shell} = 2\sum_{\nu} e_{\nu} - 2\int e\tilde{g}(e)de$$ **shell correction energy**

e_{ν} - single-particle energies

$\tilde{g}(e)$ - smeared level density

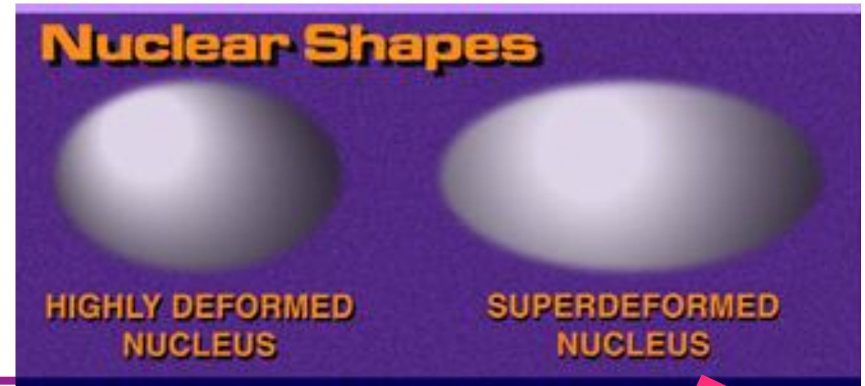
$$E_{tot} = E_{LD} + \delta E_{sh}(p) + \delta E_{sh}(n)$$

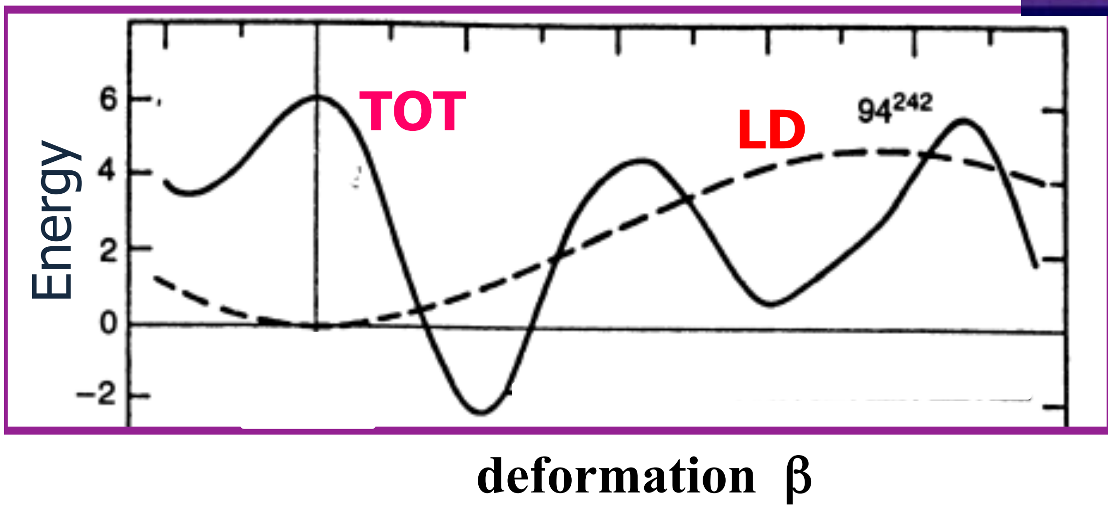


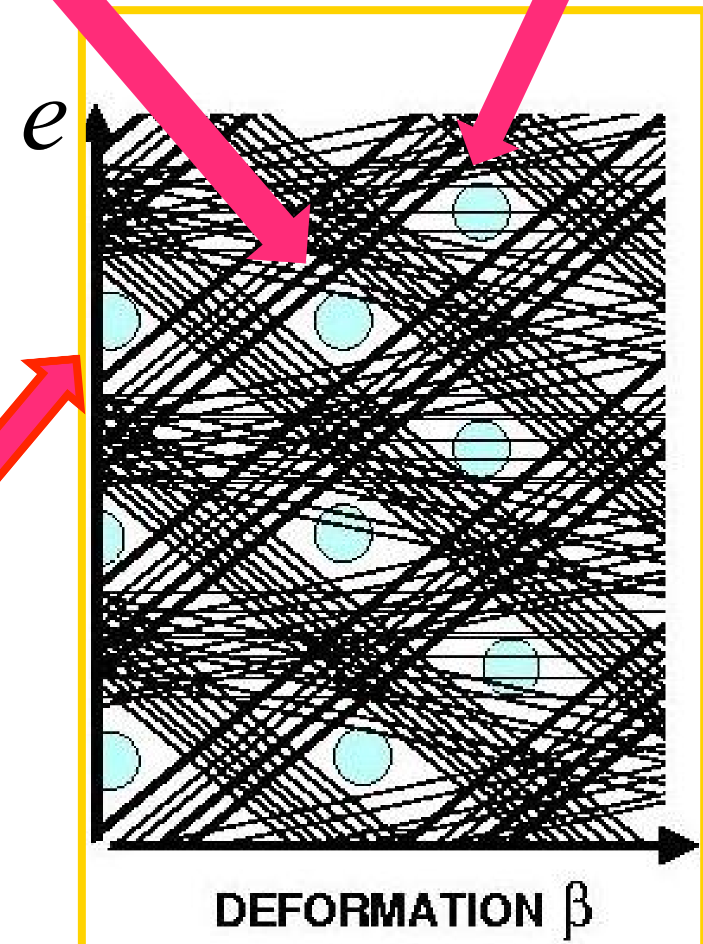
$\delta E_{shell} > 0$

$\delta E_{shell} < 0$

Shell effects as a function of deformation





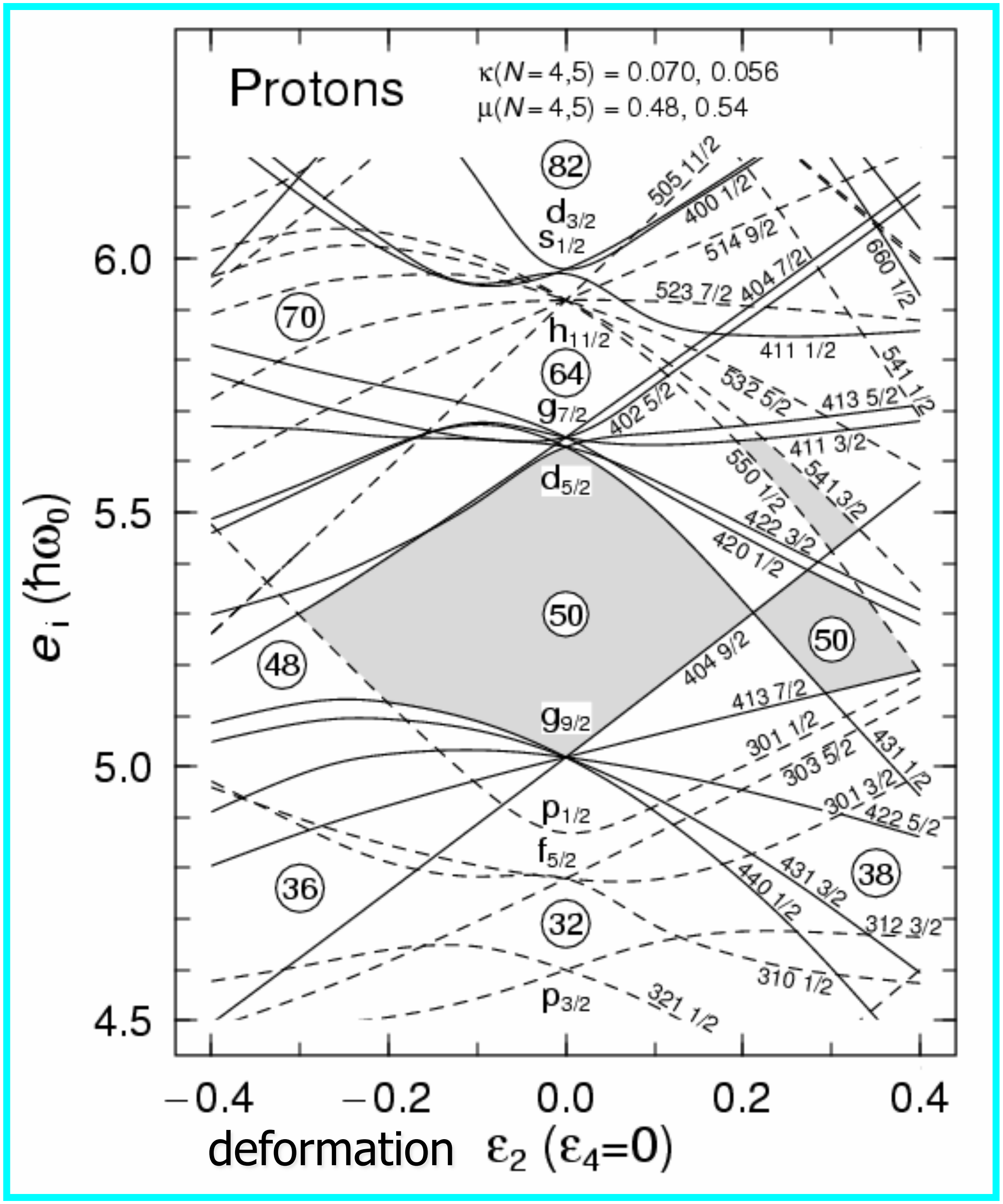


Deformation dependence of the single-particle energies in a realistic Nilsson potential

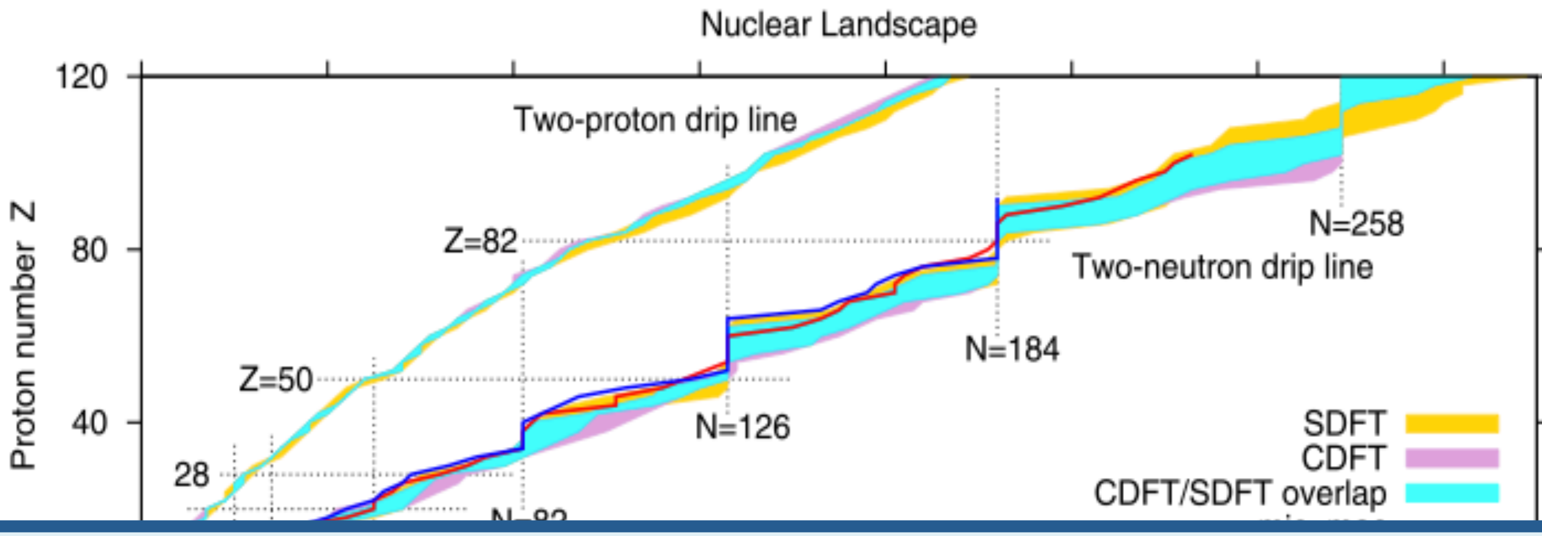
1. removing of the 2j+1 degeneracy of single-particle state seen at spherical shape

2. single-particle states at deformation ε_2 not equal 0 are only two-fold degenerate

3. creation of deformed shell gaps



Nuclear landscape: what we know and how well we extrapolate?



Sources of uncertainties in the prediction of two-neutron drip line

--- **poorly known isovector properties of energy density functionals**

--- **inaccurate description of the energies of single-particle states**

--- **shallow slope of two-neutron separation energies**

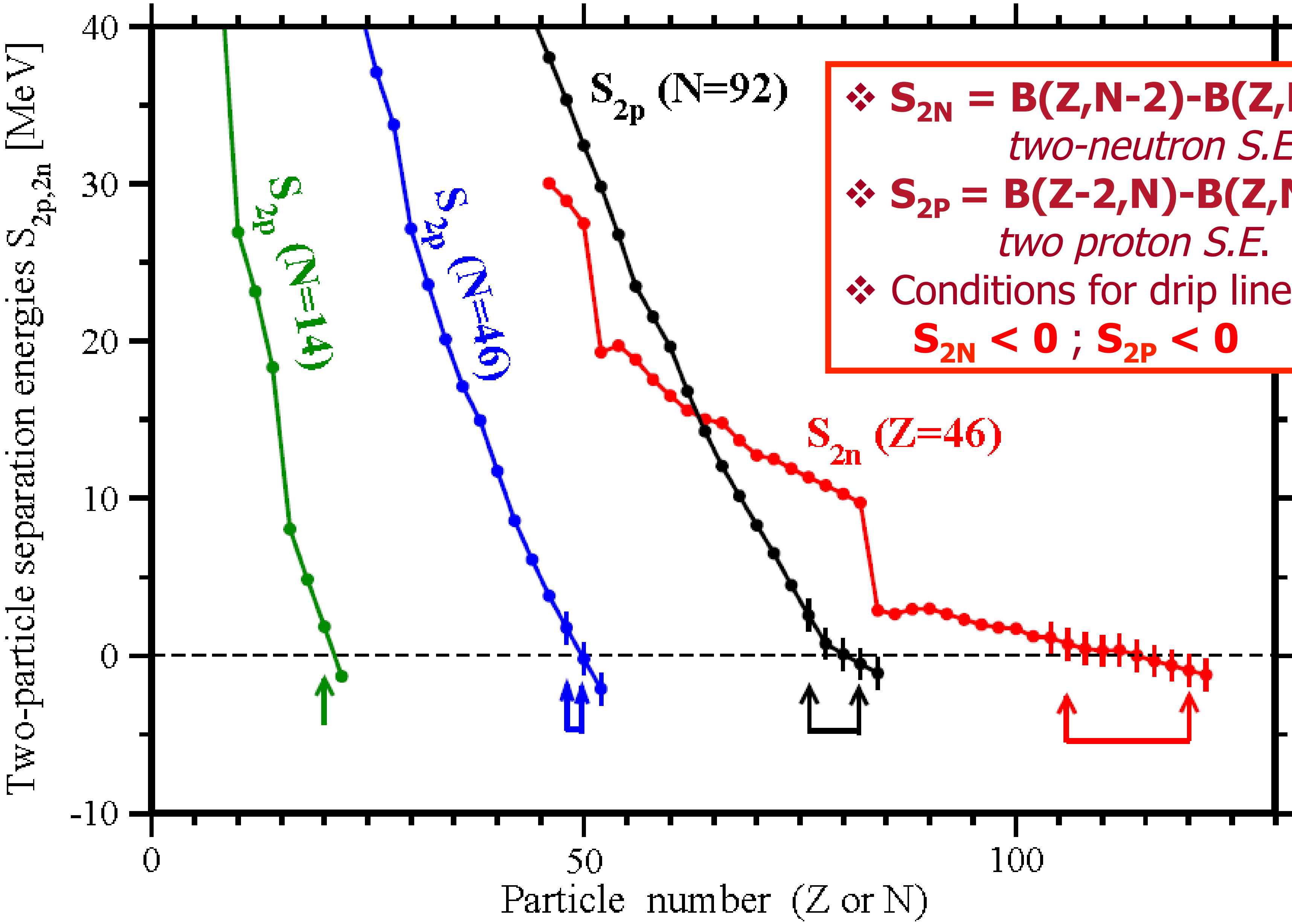
Position of two-neutron drip line does not correlate with nuclear matter properties of the energy density functional

AA, S. Agbemava, D. Ray and P. Ring, PLB 726, 680 (2013)

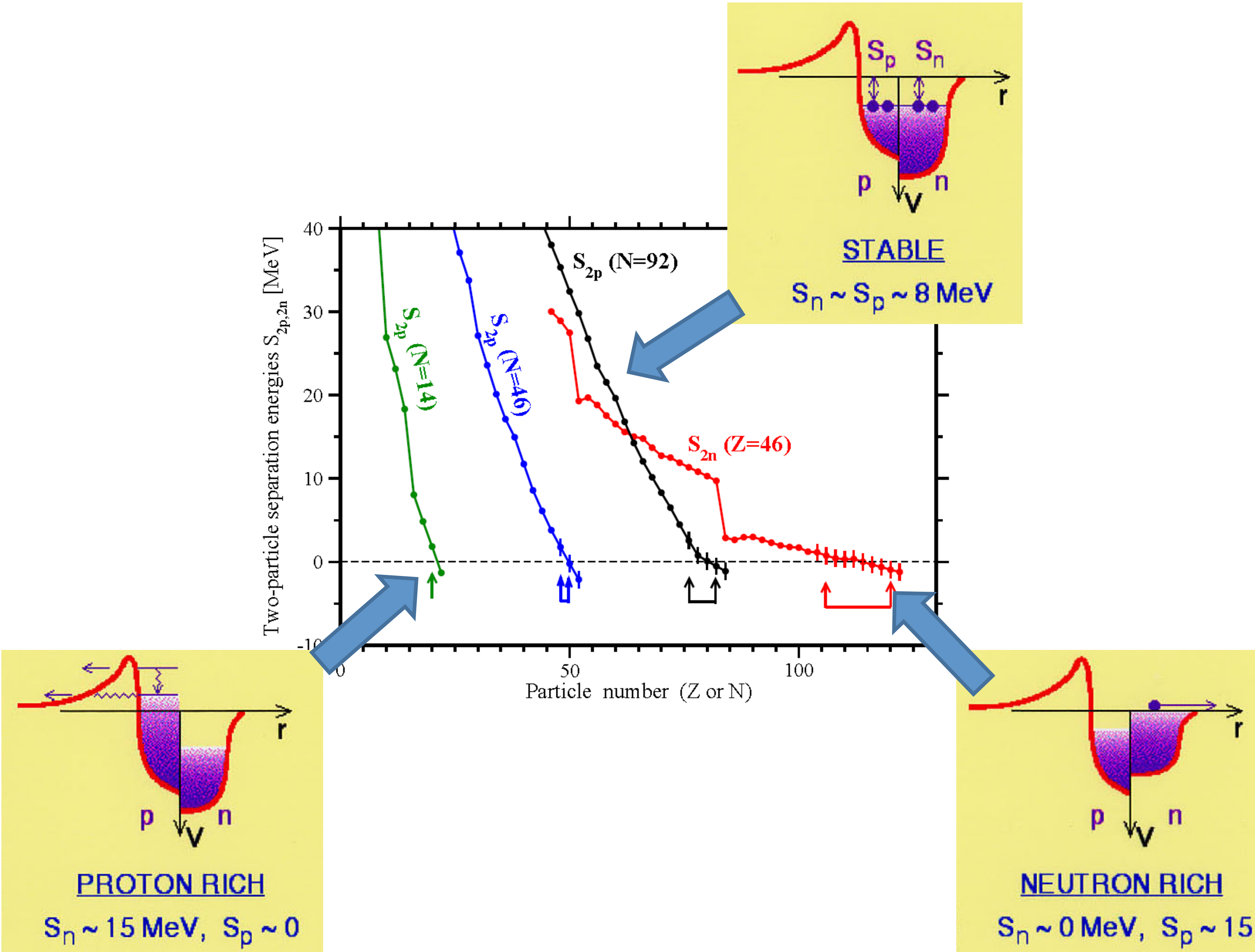
S. Agbemava, AA, D. Ray and P. Ring, PRC 89, 054320 (2014)

J.Erler et al et al, Nature 486 (2012) 509

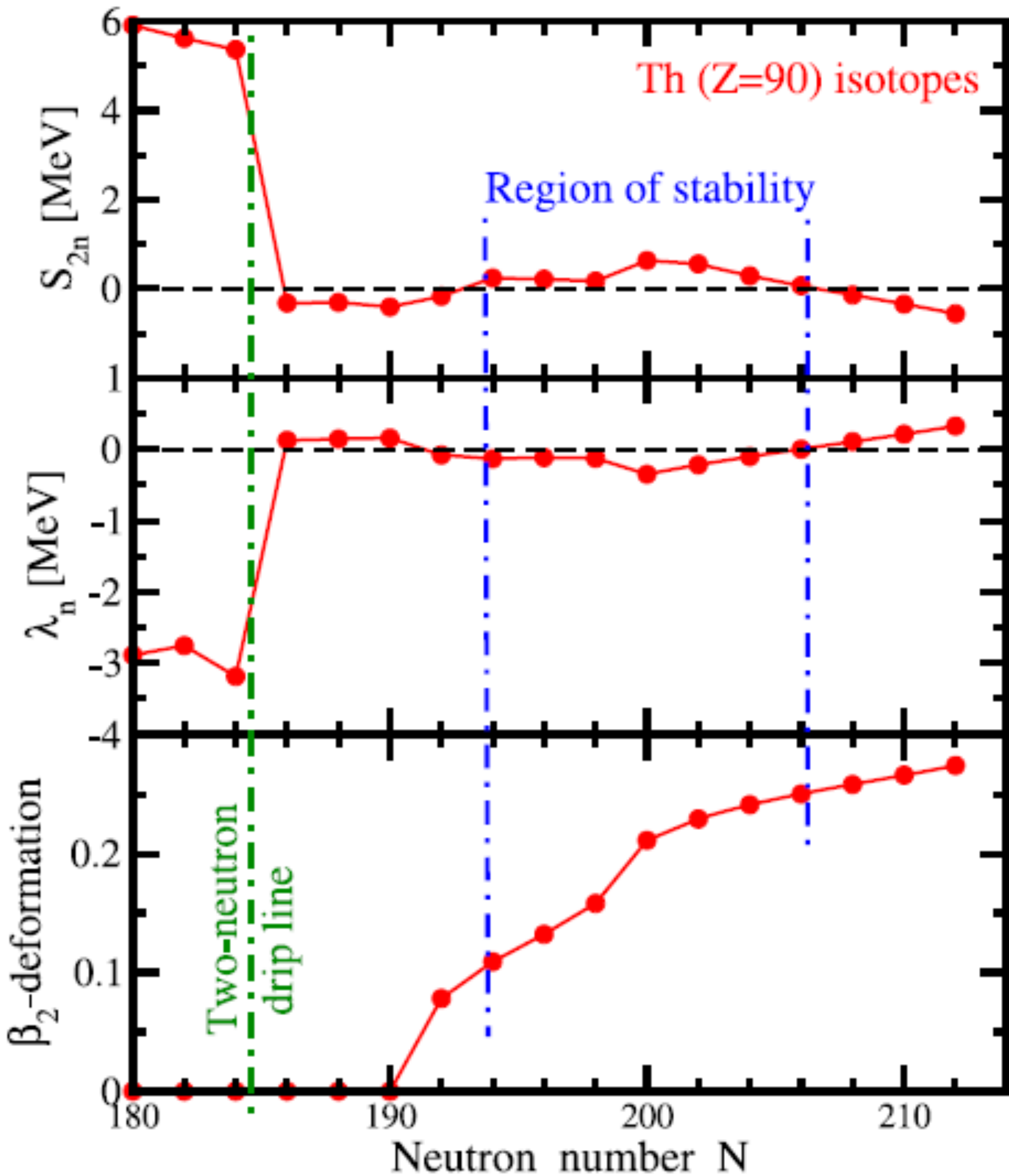
Two-neutron drip lines: the impact of slope of two-particle separation energies



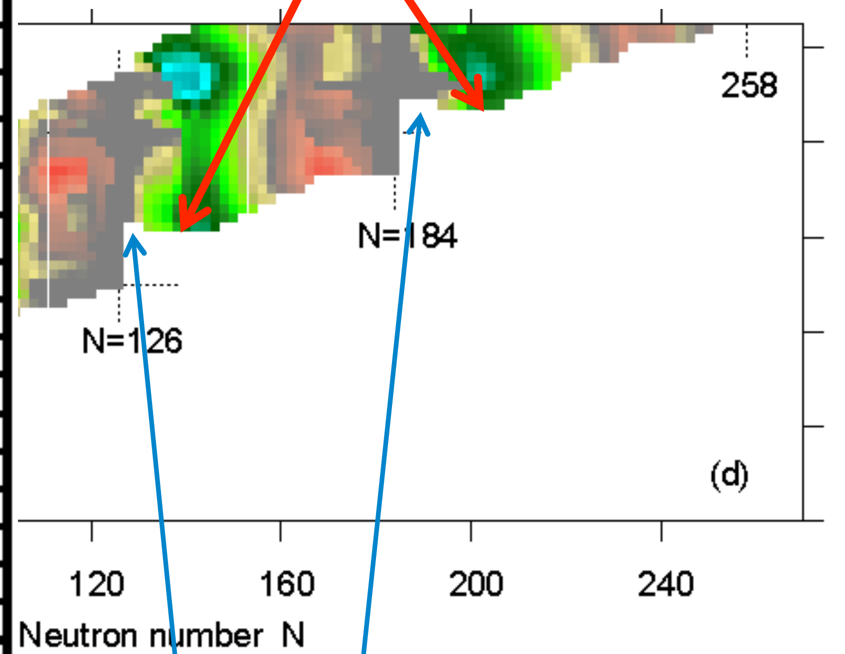
- S_{2N} = B(Z,N-2)-B(Z,N) *two-neutron S.E.*
- S_{2P} = B(Z-2,N)-B(Z,N) *two proton S.E.*
- Conditions for drip lines $S_{2N} < 0$; $S_{2P} < 0$



Sp Sn
r
p
n
V
STABLE
Sn ~ Sp ~ 8 MeV
Two-particle separation energies S2p,2n [MeV]
40
30
20
10
0
-10
0
50
100
Particle number (Z or N)
S2p (N=14)
S2p (N=46)
S2p (N=92)
S2n (Z=46)
r
p
n
V
PROTON RICH
Sn ~ 15 MeV, Sp ~ 0
r
p
n
V
NEUTRON RICH
Sn ~ 0 MeV, Sp ~ 15

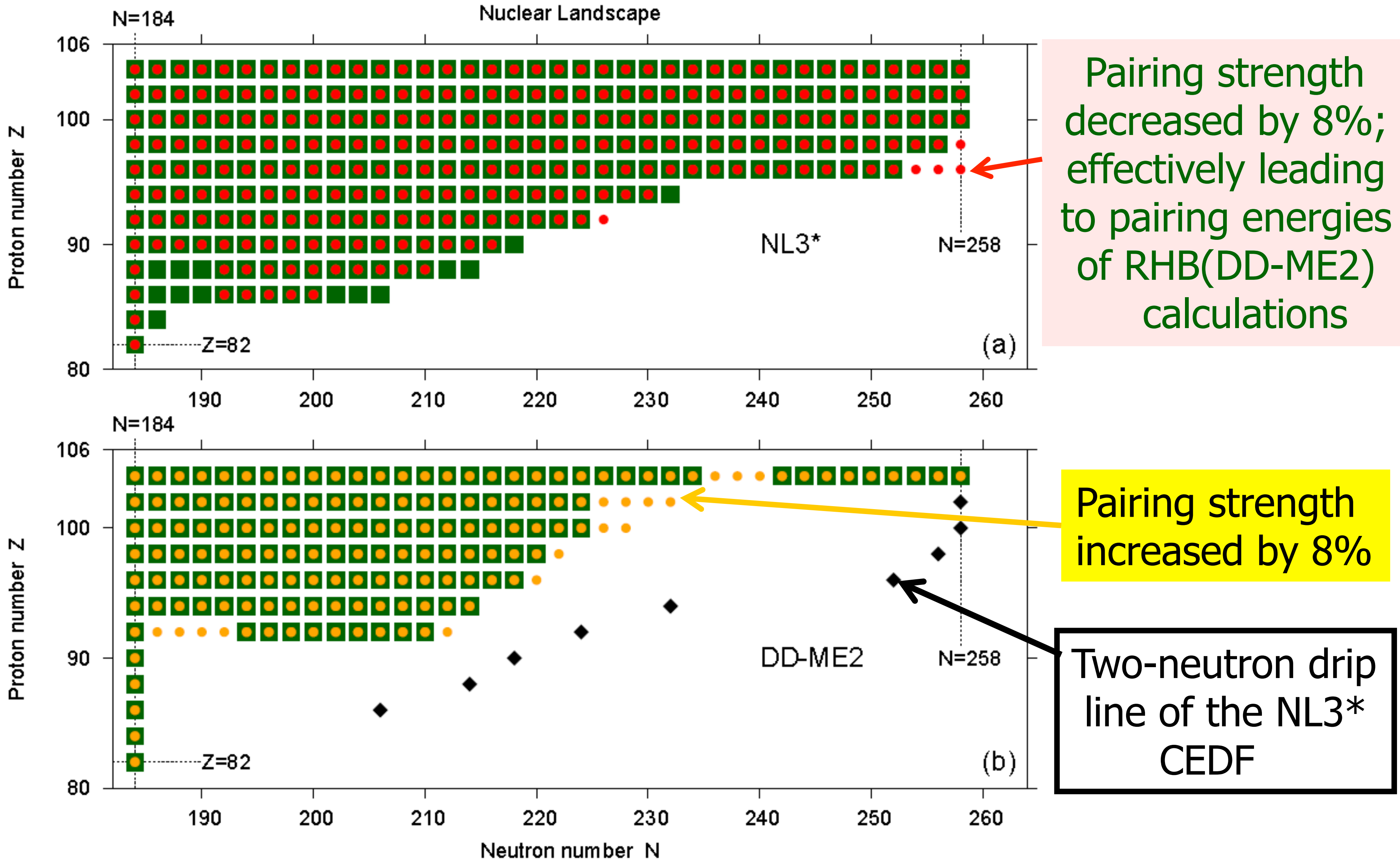


Peninsulas

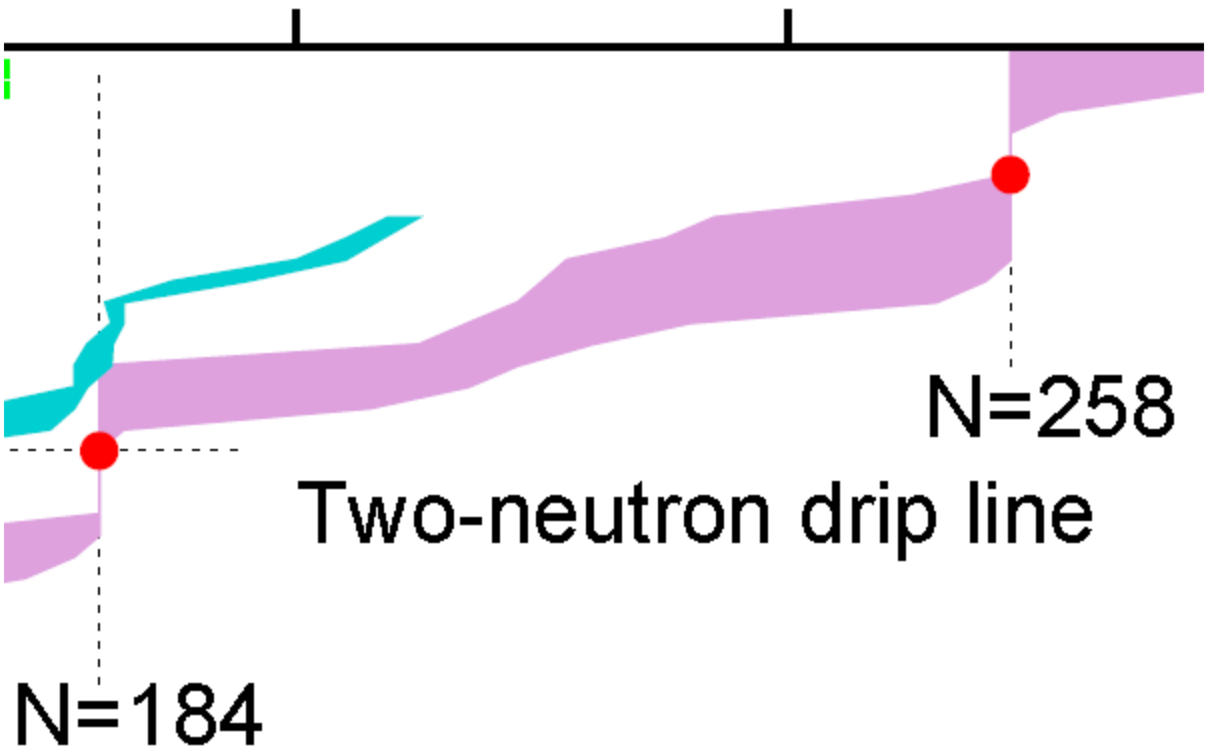


The presence of these gaps leading to the formation of peninsulas may be a consequence of the model limitations in some cases

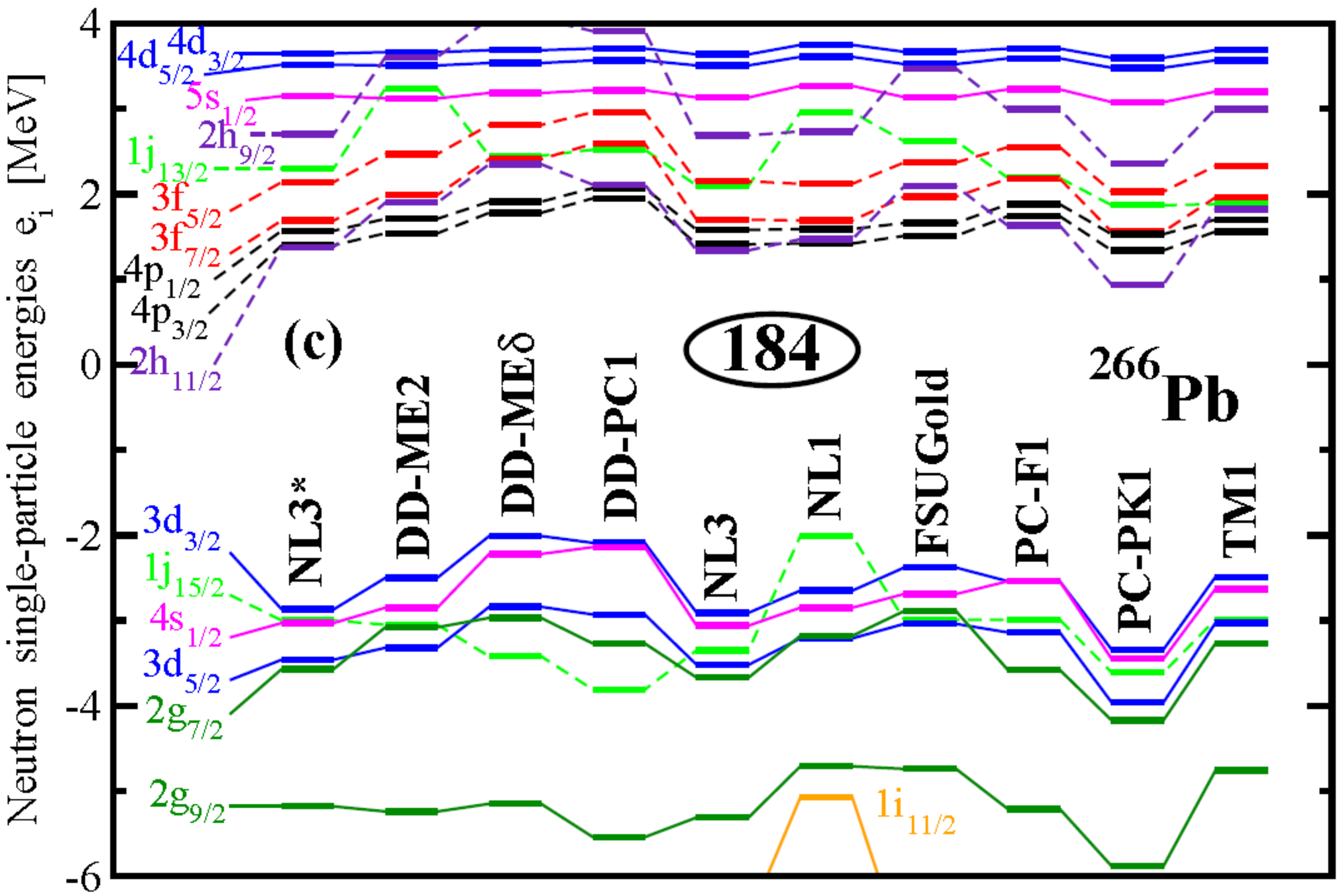
Two-neutron drip lines: the impact of uncertainties in pairing



The impact of single-particle states on the position of two-neutron drip line



The impact of single-particle states on the position of two-neutron drip line



The impact of single-particle states on the position