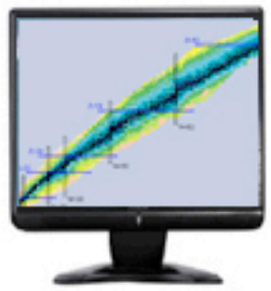
SciDAC

Scientific Discovery through Advanced Computing

understanding our universe

Office of Science



Building a Universal Nuclear Energy Density Functional

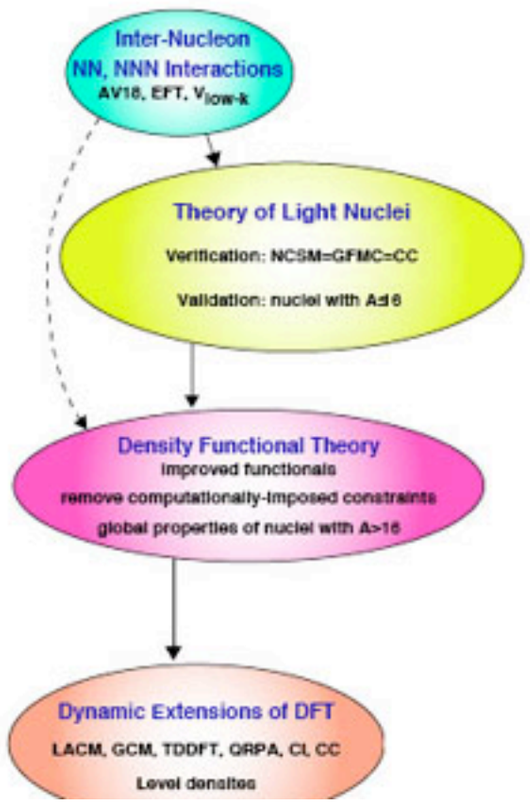
A Low-Energy Nuclear Physics National HPC Initiative

George F. Bertsch (project web page)
University of Washington

There are approximately 3,000 known nuclei, most of them produced in the laboratory. It is estimated that additionally up to approximately 6,000 nuclei could in principle still be created and studied in the foreseeable future. An understanding of the properties of these elements is crucial for a complete nuclear theory, for element formation, for properties of stars, and for present and future energy and defense applications. We plan a comprehensive study of all these nuclei, based on the most accurate knowledge of the strong nuclear interaction, the most reliable theoretical approaches, and a massive use of the computer power available at this moment in time, with the view of scaling to the petaflop computers to become available in the near future.Until recently such an undertaking was hard to imagine, and even at the present time such an ambitious endeavor would be far beyond what a single researcher or a traditional research group could carry out. This project will involve theoretical physicists, computer scientists, and students from universities and national laboratories. Our long-term vision is to arrive at a comprehensive and unified description of nuclei and their reactions, grounded in the fundamental interactions between the constituent nucleons. We seek to replace current phenomenological models of nuclear structure and reactions with a well-founded microscopic theory that delivers maximum predictive power with well-quantified uncertainties.

The Energy Density Functional (EDF) is at the heart of the project. EDF theory has been spectacularly successful in condensed matter physics and chemistry, as was recognized in the Nobel Prize awarded to Walter Kohn in 1998. In fact, it was the combined work of many dedicated researchers that

Universal Nuclear Energy Density Functional



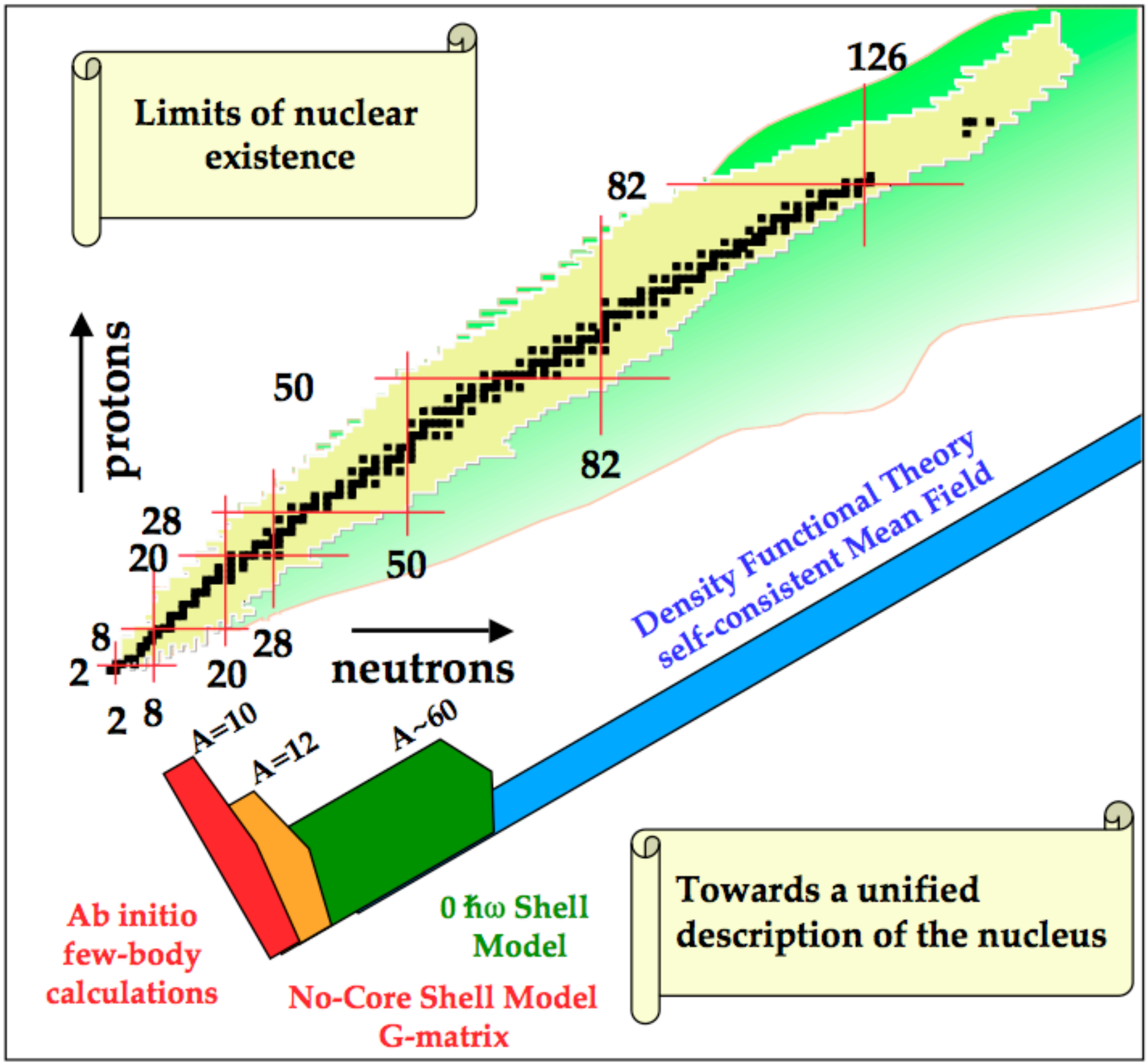
Building a universal nuclear energy density functional

Physics

Physics of nuclei

Density functional theory in chemistry and condensed matter physics

Nuclear physics methodologies


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

What do we want to know?

Binding Energies

Nucleosynthesis

Interactions with neutrons

> Inelastic cross sections: For some intermediate mass nuclei (e.g., ^{23}Na or ^{56}Fe) inelastic scattering cross-section accuracies of the order of 10% are needed. Moreover, there exists a general need to improve the knowledge of inelastic scattering for actinides. Relevant experiments have proven particularly difficult. It would be worthwhile for the basic science community to investigate whether current challenges could be met with new and innovative measurement techniques.

From the report "Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles", 2006

Radioactive decay properties

Fission properties

UNEDF goals

unedf.org/users/project_plan.pdf

The mission of this project is three-fold:

- First, to find an optimal functional using all our knowledge of the nucleonic Hamiltonian and basic nuclear properties.
- Second, to apply the EDF theory and its extensions to validate the functional using all the available relevant nuclear structure data.
- Third, to apply the validated theory to properties of interest that cannot be measured, in particular the transition properties needed for reaction theory.

We have 5 years to make a qualitative improvement in the reliability and accuracy of low-energy nuclear theory

Application to needs in nuclear technology

Leadership-class codes for CI, DFT and DFT extensions

Density Functional Theory--What is it?

Conceptual

A quantum mechanical many-particle system may be characterized by its density distribution, n(r).

There exists a function of that function (a functional) that can be minimized to get the energy of the system and its density distribution (Hohenberg and Kohn, 1964).

$\mathcal{E}(n)$

Practical --Kohn&Sham, 1965

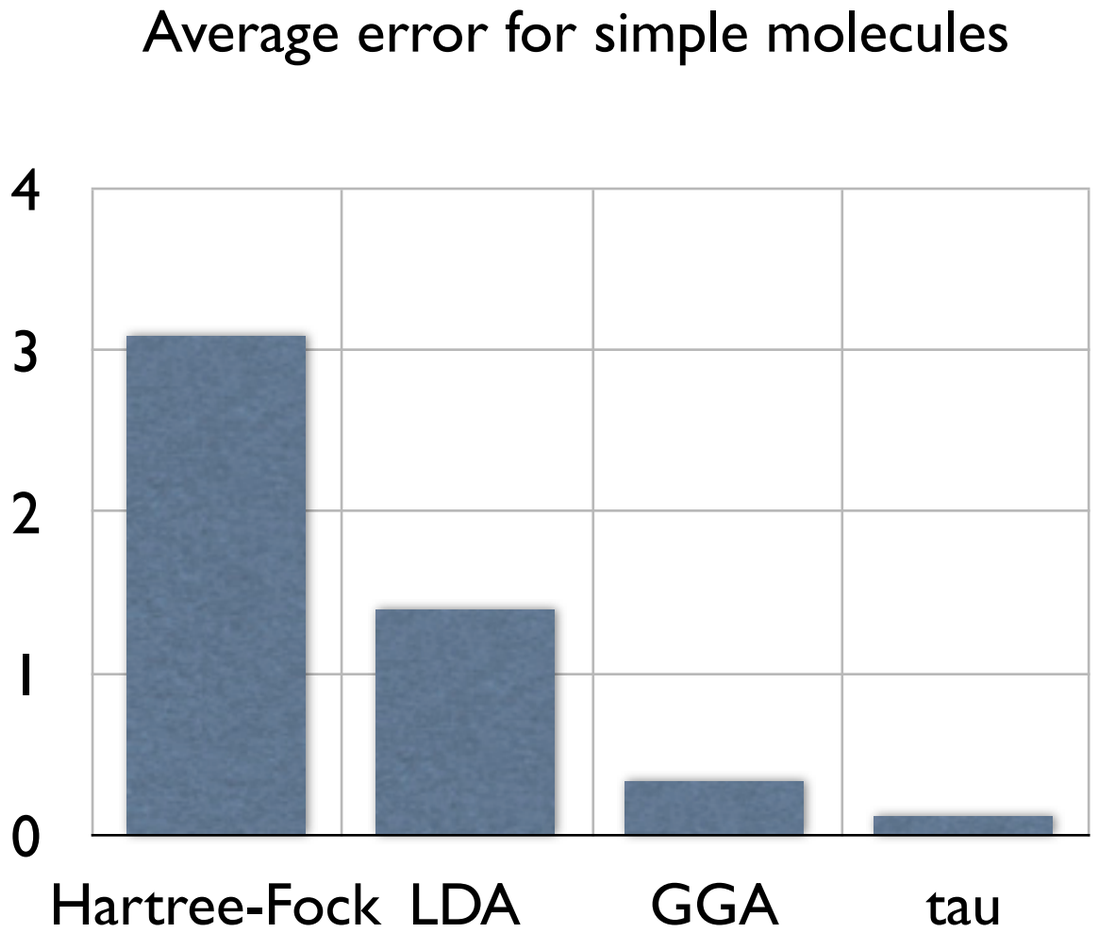
Define a set of N orbitals

$$\phi_i(r);\ i = 1, .., N$$

Minimize with respect to the orbital functions

$$\int \left(\sum_i \frac{|\nabla \phi_i|^2}{2m} + V(\{\phi\}) \right) d^3r \qquad n(r) = \sum_i^N |\phi_i(r)|^2$$

The DFT Success Story



Hartree-Fock	1929
LDA	1965
GGA	1989
tau	1999

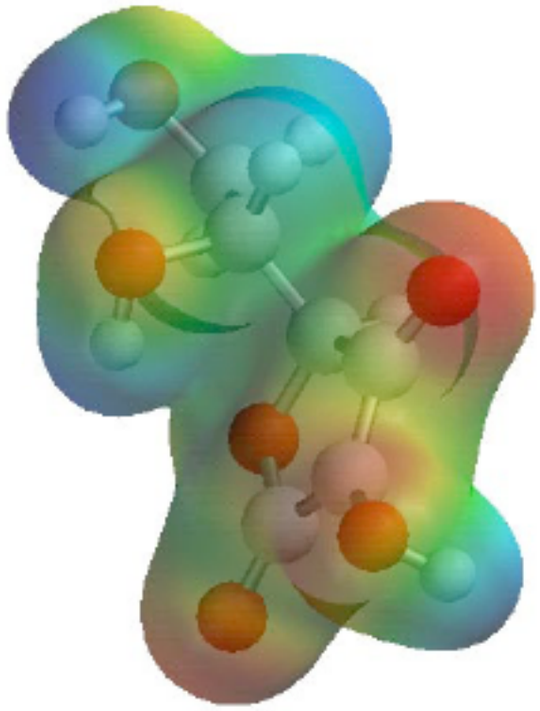


Image of vitamin C from Nobel Foundation website

DFT in nuclear physics

1935

Für die Gesamtenergie erhalten wir

$$E = \int F \, \mathrm{d}\tau = \text{Minimum} \tag{12}$$

mit

$$F = \frac{h^2}{32\,\pi^2\,M}\left[\frac{(\operatorname{grad}\varrho_P)^2}{\varrho_P} + \frac{(\operatorname{grad}\varrho_N)^2}{\varrho_N}\right] + \frac{4\,\pi\,h^2}{5\,M}\left(\frac{3}{8\,\pi}\right)^{5/3}(\varrho_P^{5/3} + \varrho_N^{5/3}) - f(\varrho_P, \varrho_N). \tag{13}$$

Liquid Drop

$$E = a_c A + a_s A^{2/3} + a_C \frac{Z^2}{A^{1/3}} + a_{sym} \frac{N-Z)^2}{A} + \Delta$$

1972

$$F = \text{Polynomial}(\rho_i, \tau_i, \nabla\rho_i, \nabla^2\rho_i, ...)$$

But:

Hardly any systematic studies until the SciDAC

unedf.org --> liquid drop model

Fit Results

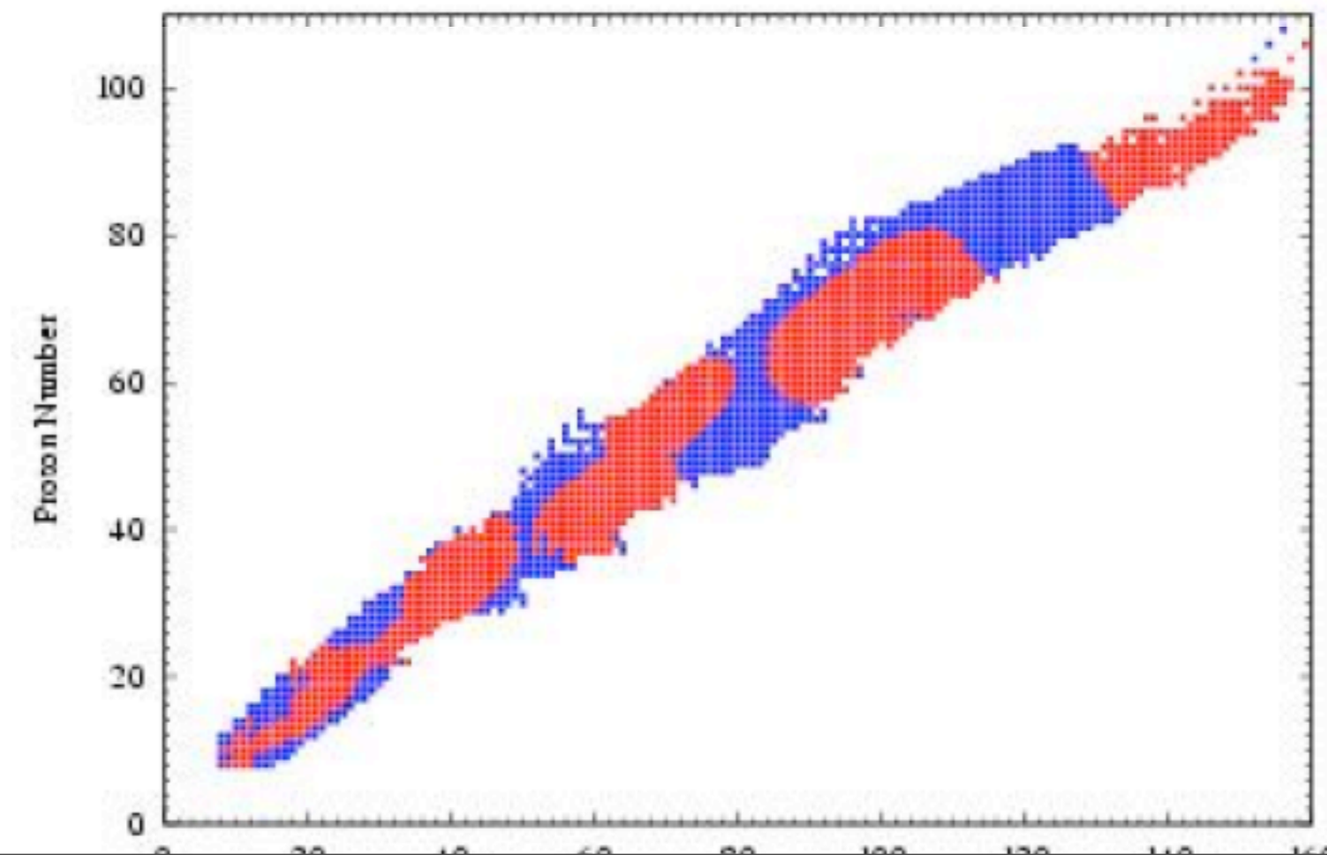
Fitting the nuclear binding energy

0. Number of nuclei fit= 2049 , using the selection criterion 1

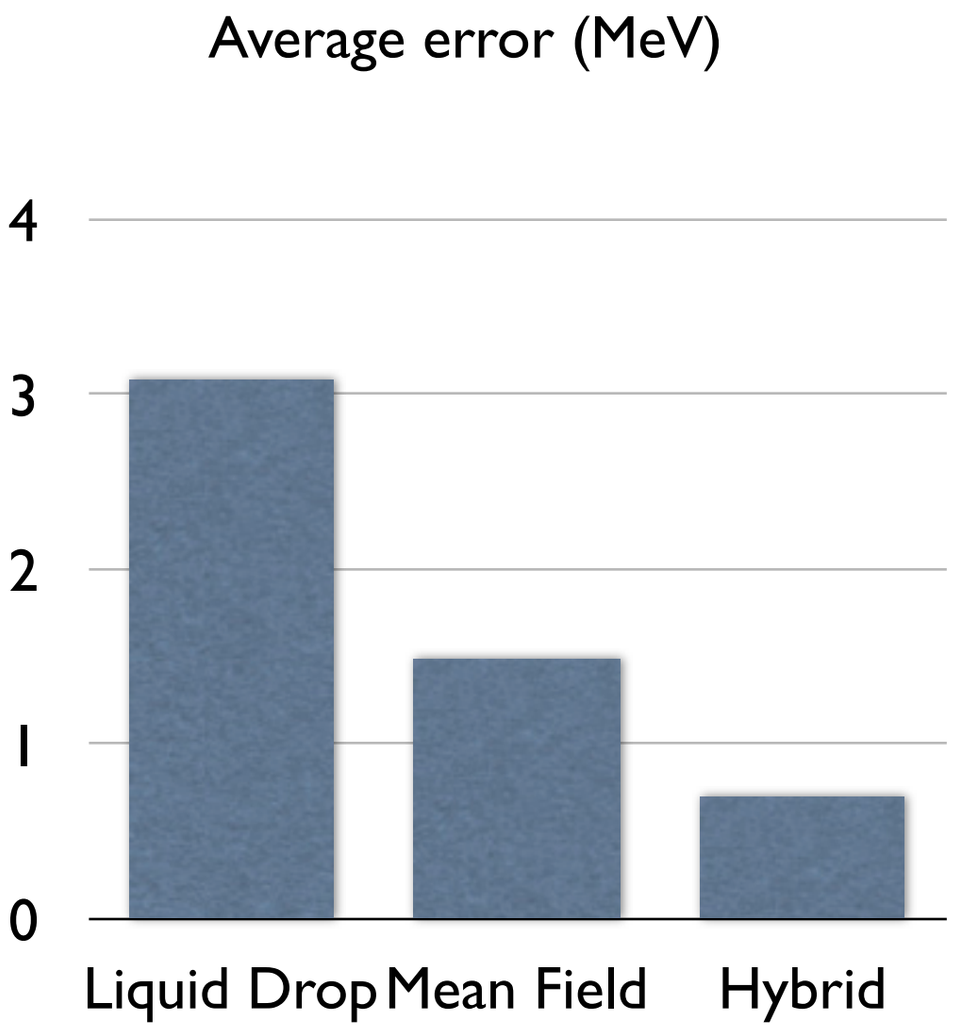
1. The rms error of your fit is 2.82 MeV. Can you do better?
The nucleus with the largest error is N= 82 , Z= 50 for which the error is 13.71 MeV.

2. Chart of nuclides.

The known nuclei are indicated by squares positioned according to N and Z. Blue squares show nuclei that have larger (binding or separation) energy than given by the liquid drop fit. Red squares show nuclei that are less bound.



Present Status--nuclear binding energies

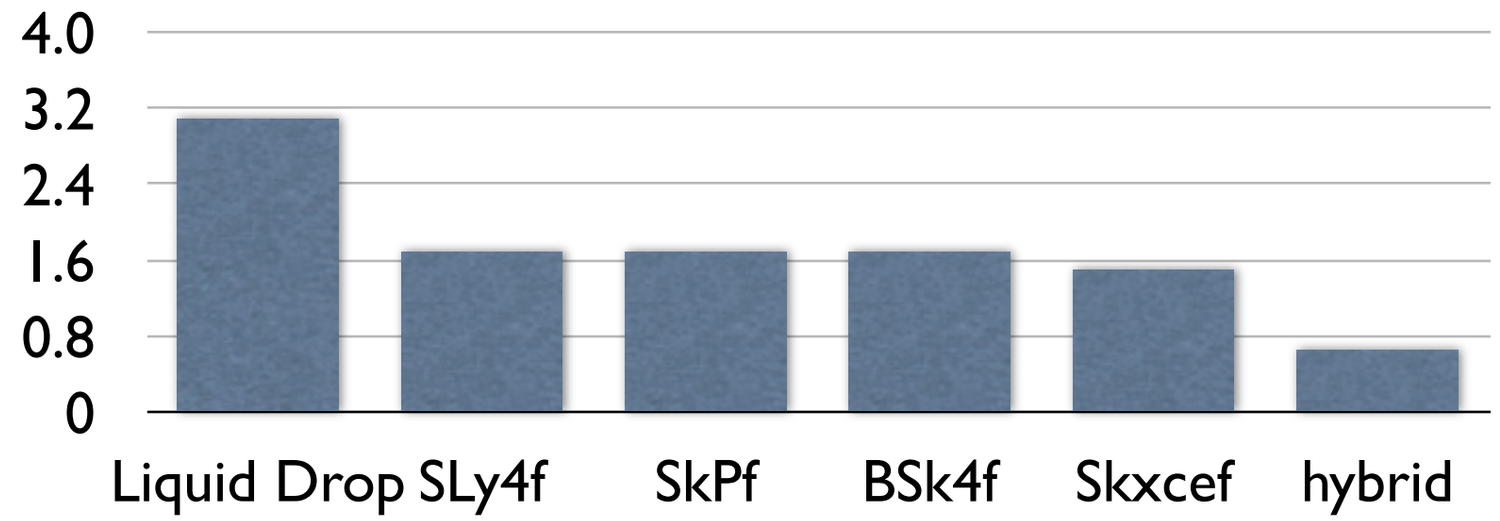


It's a daunting challenge

The liquid drop model is hard to beat.

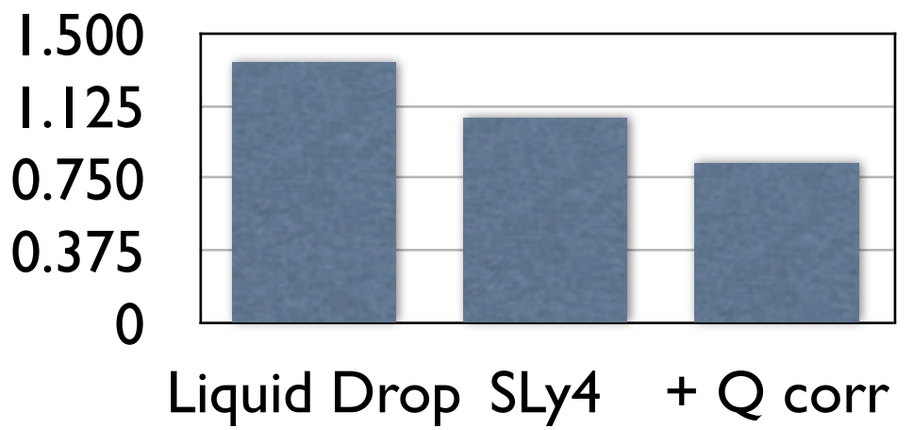
RMS residuals of binding energies

(MeV)



RMS residuals of neutron separation energies

S_2n



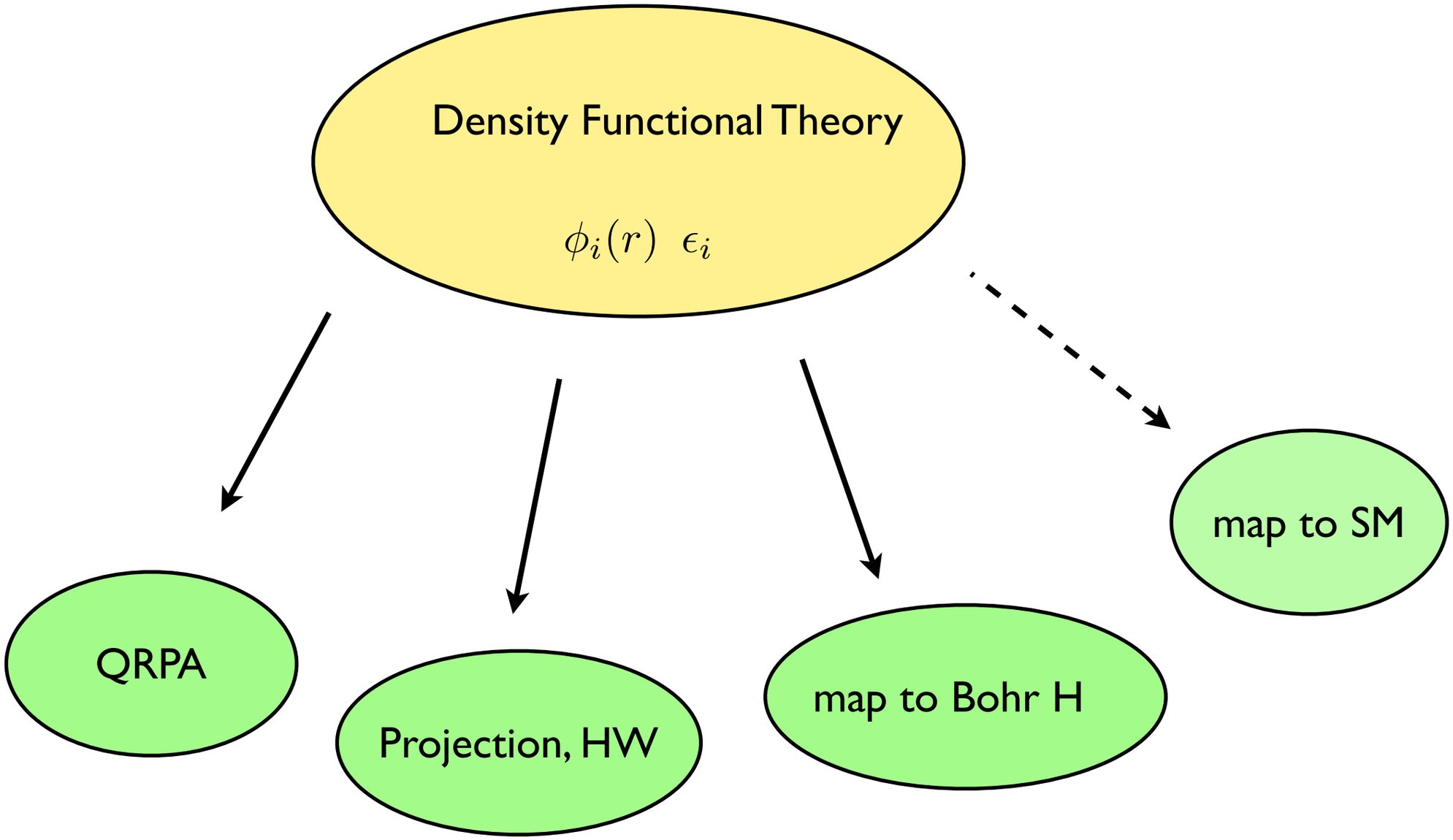
RMS residuals of pairing energies ?

Initial activities

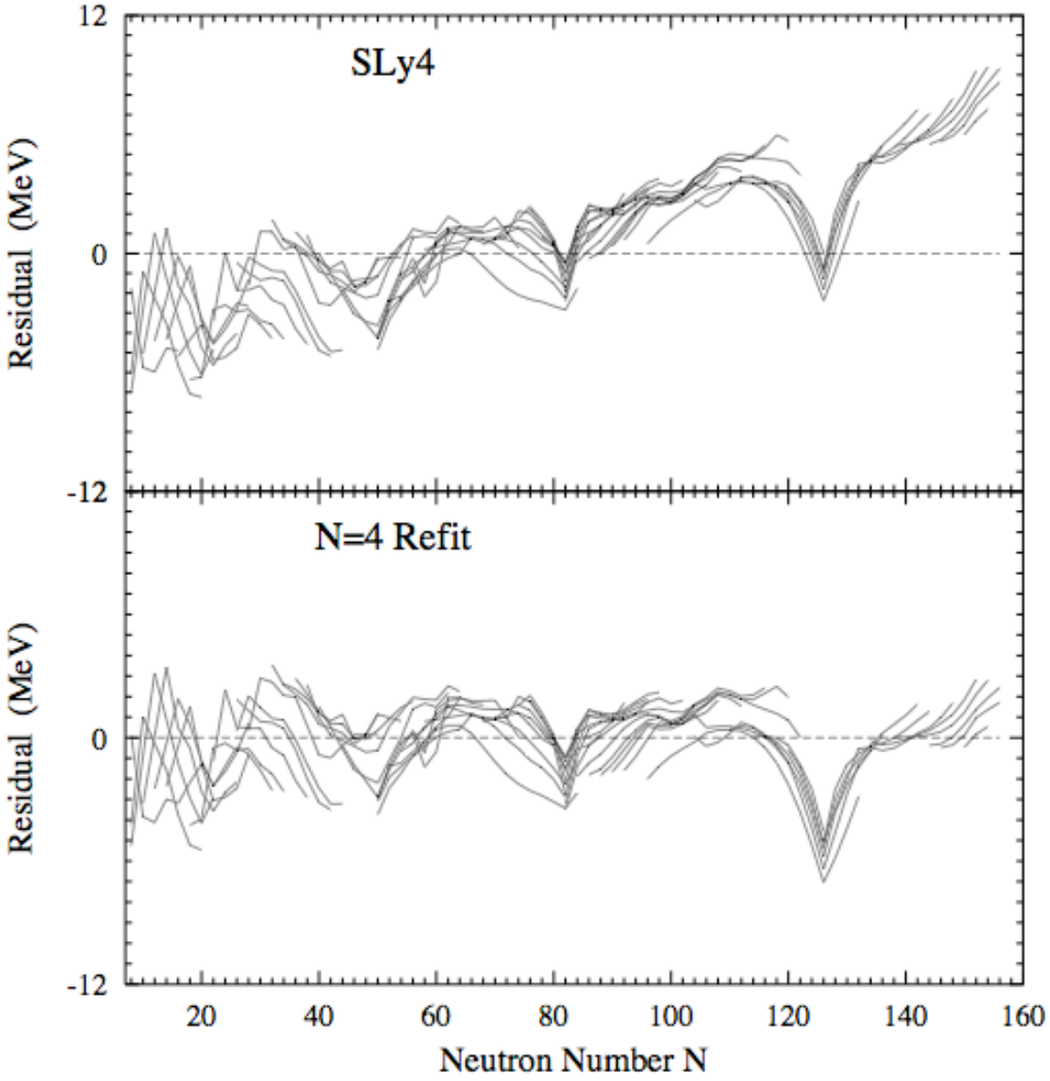
Benchmark present theories and functionals

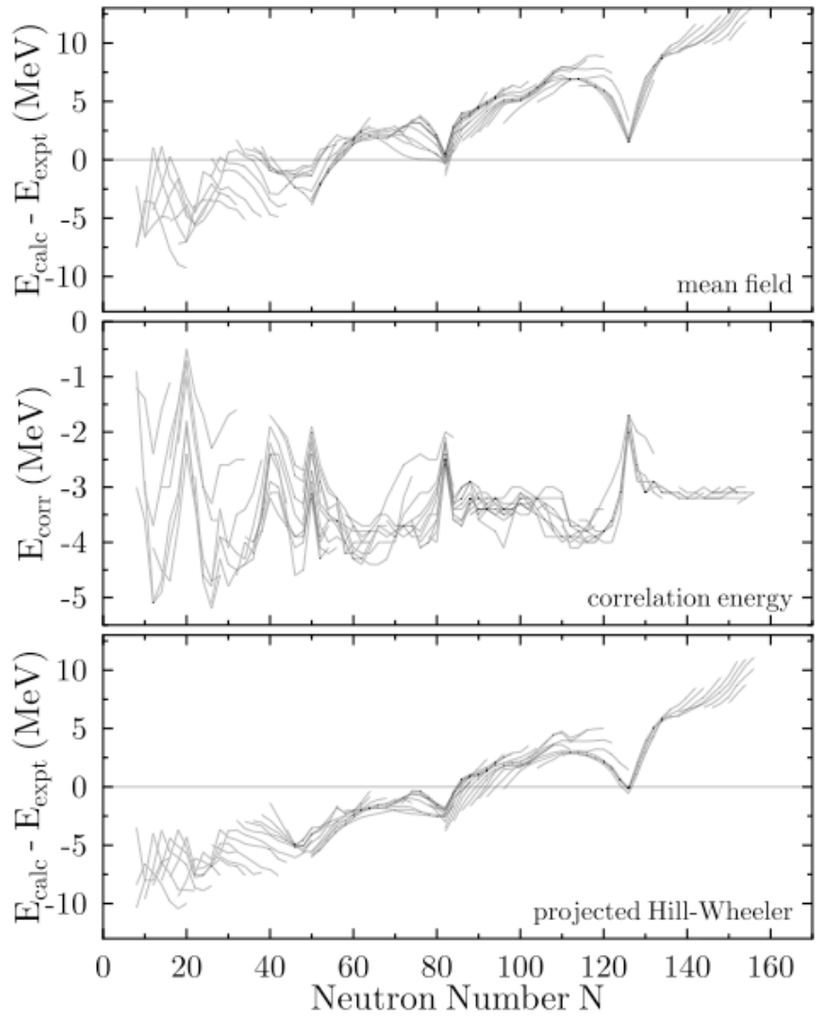
Evaluate numerical representations of the fields $\phi_i(\vec{r})$

Verify methodologies for *ab initio* wave functions


Density Functional Theory
$\phi_i(r)$ ϵ_i
map to SM
QRPA
Projection, HW
map to Bohr H

Example I: role of correlation energy in binding systematics





FPOs=4.10^16

"Global study of qudrupole correlation effects", M. Bender, G.F. Bertsch, and P.-H. Heenen, Phys. Rev. C73 034322 (2006).

Example 2: validating theories of 2+ excitations

Theory I: Sly4 energy functional → axial Q generator + projection

B. Sabbey, et al., Phys. Rev. C75 044305 (2007)

Theory II: Gogny functional → 5-d collective Bohr Hamiltonian

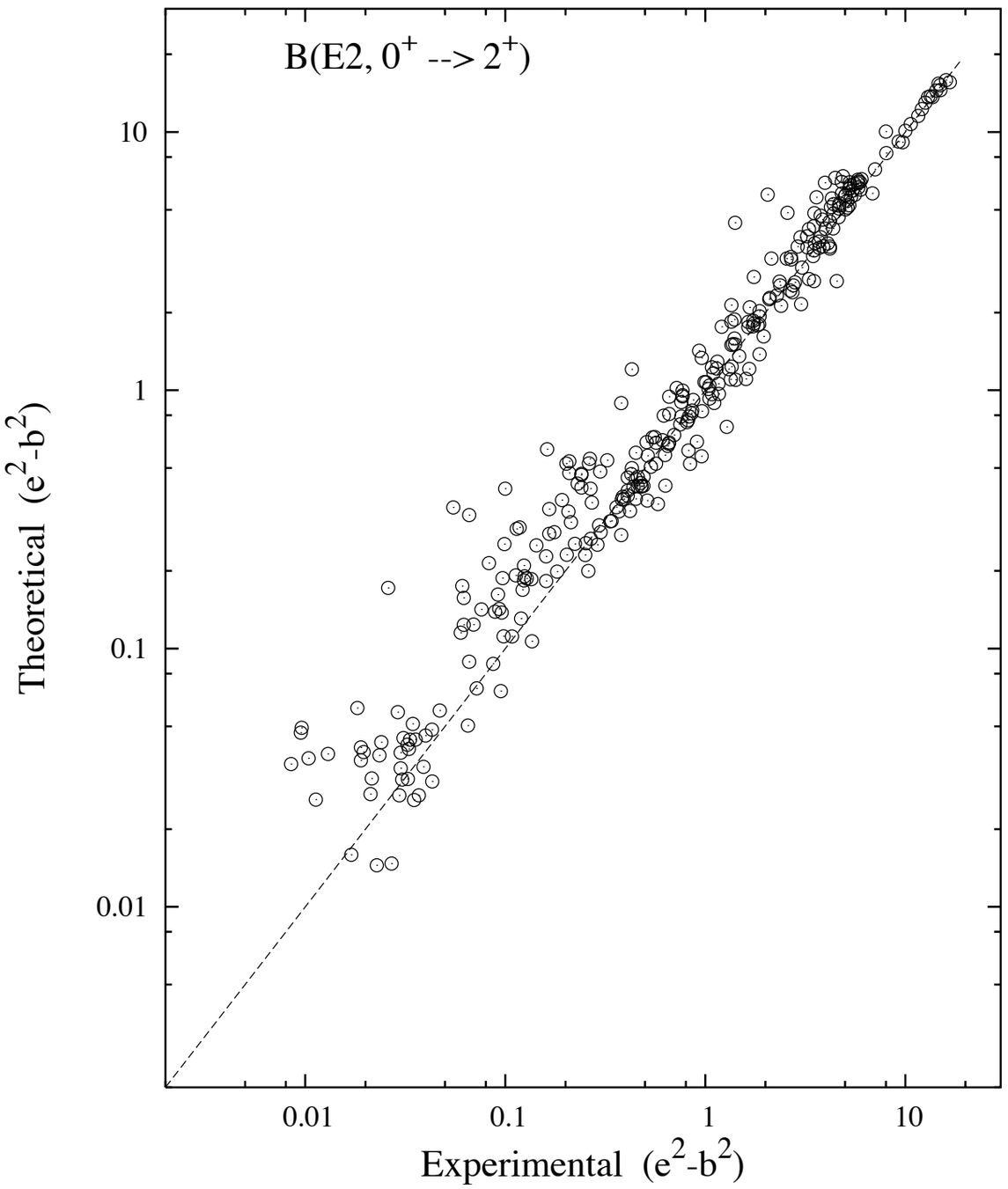
G.F. Bertsch, et al., Phys. Rev. Lett. 99 032502 (2007)

Theory III Sly4 energy functional → QRPA

J. Terasaki, UNEDF workshop (2007)

Comparison should give guidance on methodologies.

Electomagnetic transition strengths of excited states



Another view of the performance on B(E2)

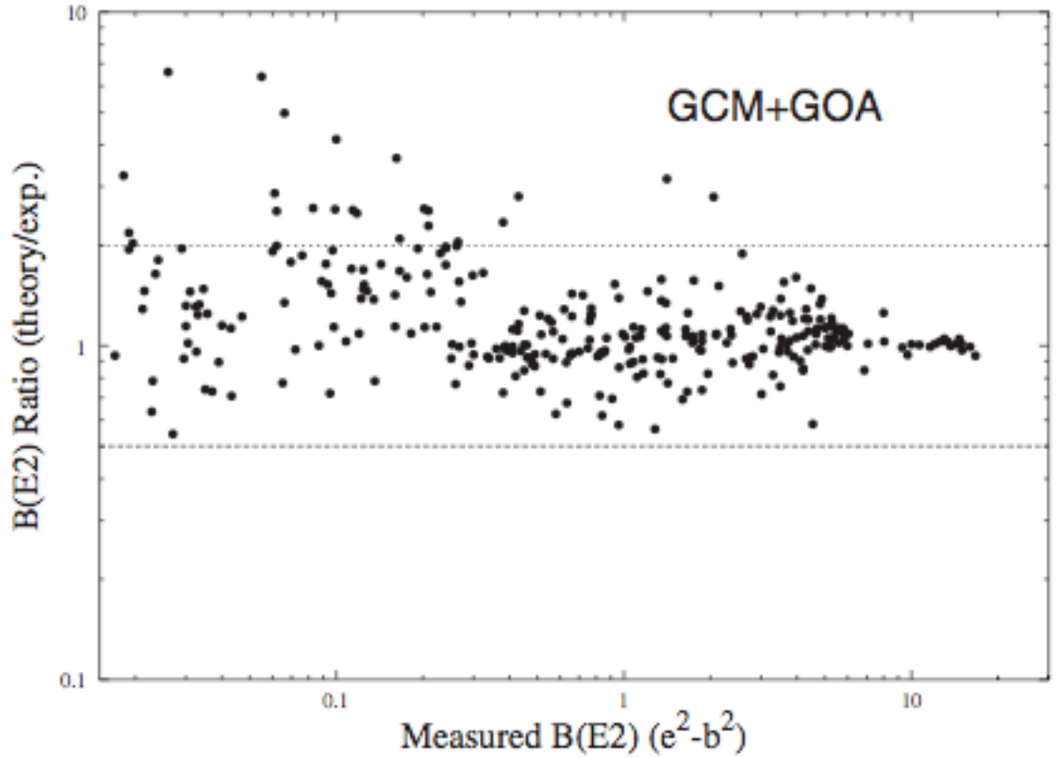
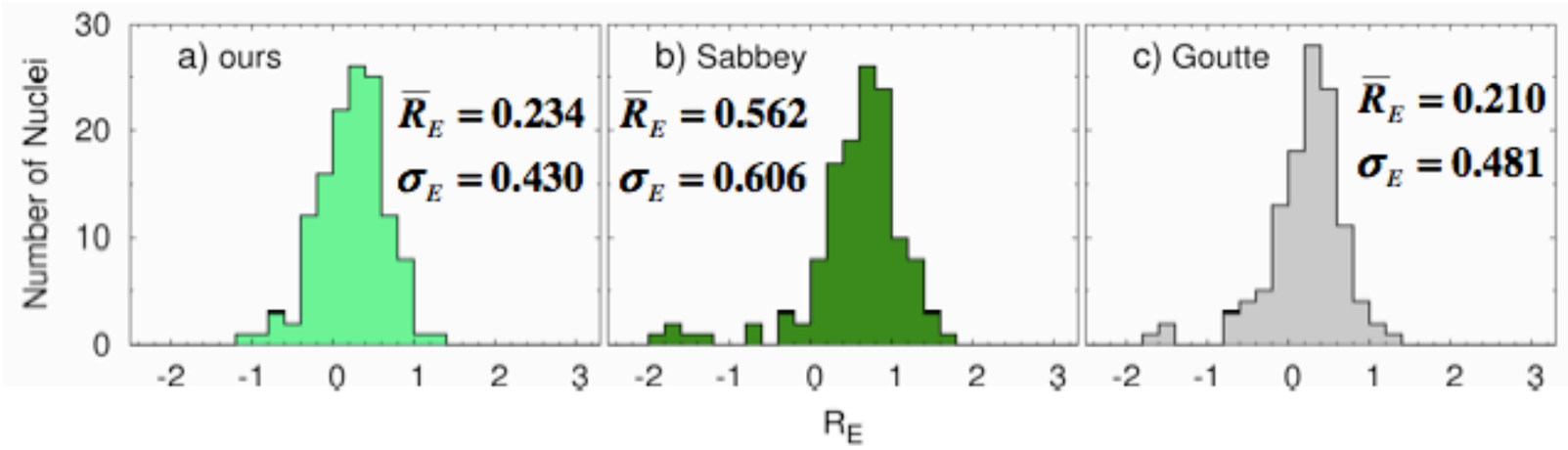


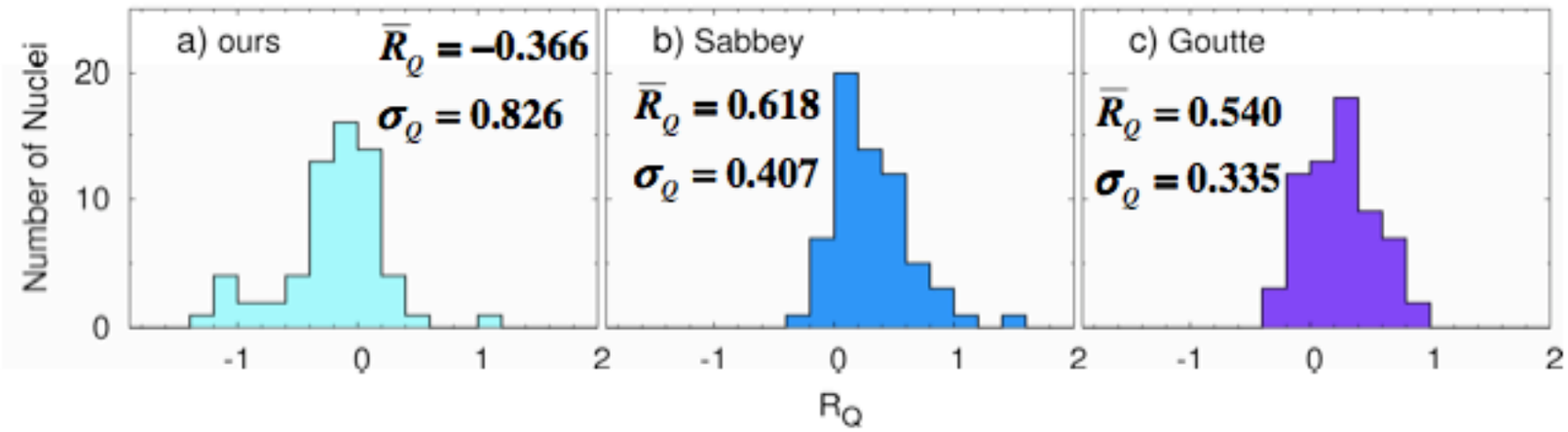
FIG. 3. Experiment compared to theory for the $B(E2, 0^+ \rightarrow 2^+)$ for the nuclei tabulated in Ref. [10]. This graph may be directly compared with their Fig. C. Values within the lines are within a factor of 2 of experiment. Of the 306 cases shown here, 93% are within the error band. This is superior to their "global" phenomenological fit and is much better than the theoretical models they consider.

PRL 99 032502 (2007)

Distribution of $R_E = \log\left(E_{\text{th}}/E_{\text{exp}}\right)$



Distribution of $R_Q = \log\left(\langle 2\|Q\|0\rangle_{\text{th}}/\langle 2\|Q\|0\rangle_{\text{exp}}\right)$



Cf. $\log(2) \cong 0.7,\ \log(1.5) \cong 0.4$

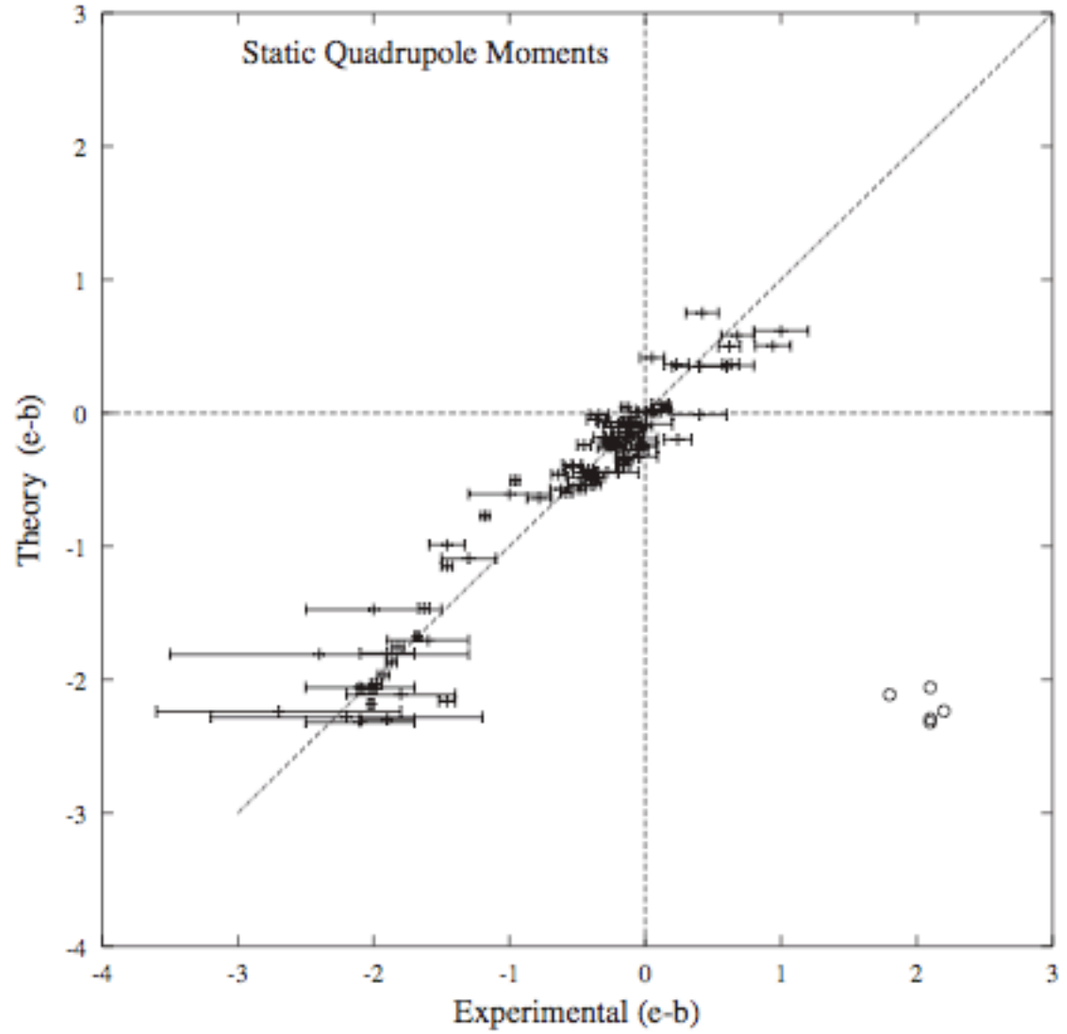
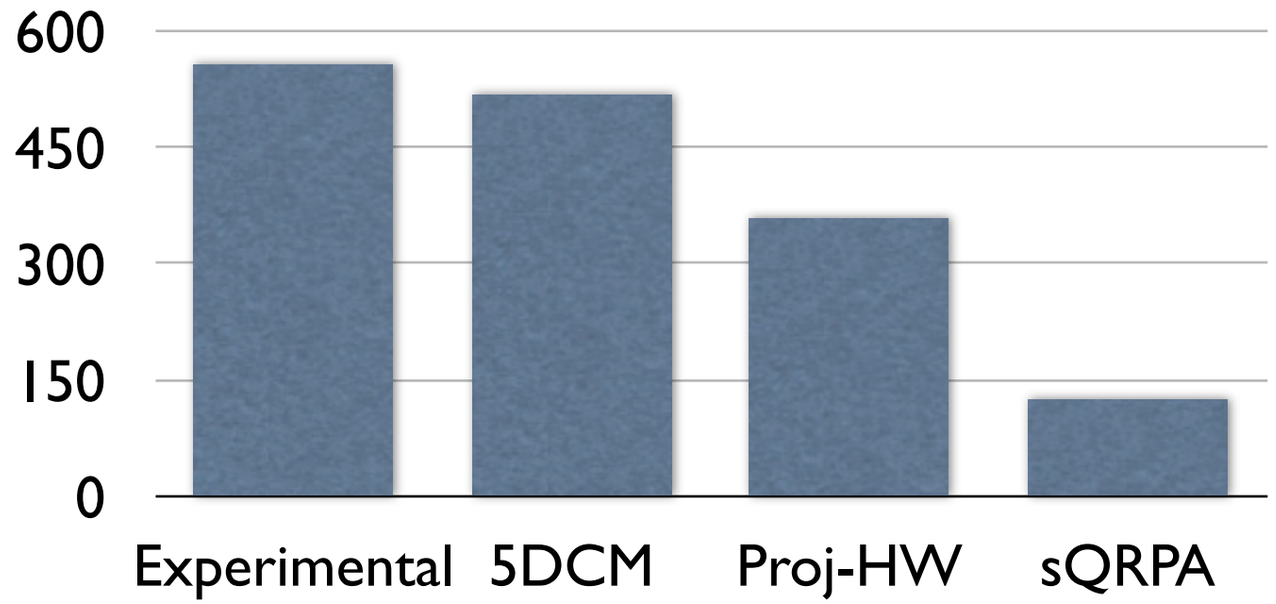


FIG. 4. Experiment compared to theory for the quadrupole moment of 98 excited 2^+ states. Experimental database is from the tabulation in Ref. [12].

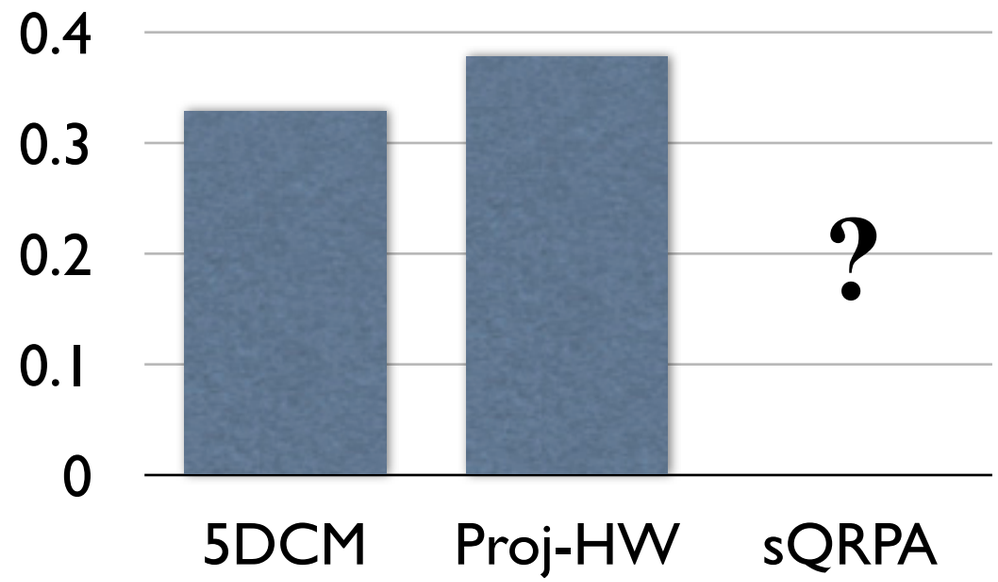
Performance of theories of the first 2+ state

Number of nuclei in data set



Reliability metric for energies

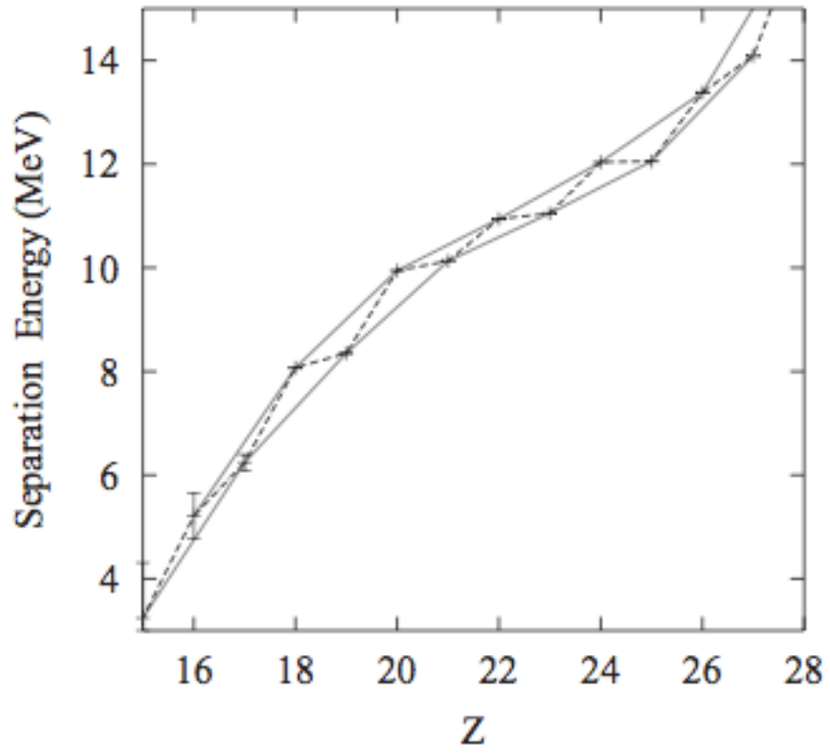
(Smaller is better)



Example 3: neutron-proton pairing

"Neutron-proton pairing reexamined", W.A. Friedman and G.F. Bertsch, Phys. Rev. C in press

[18] Brookhaven Evaluated Nuclear Structure Data File, http://www.nndc.bnl.gov/ensdf/.



Recoupling mechanism tested by 2-particle spectroscopy.

$$\delta_s = \sum_{J=|j_n-j_p|}^{j_n+j_p} (2J+1)E_J/(2j_n+1)(2j_p+1).$$

58Cu from ENSDF

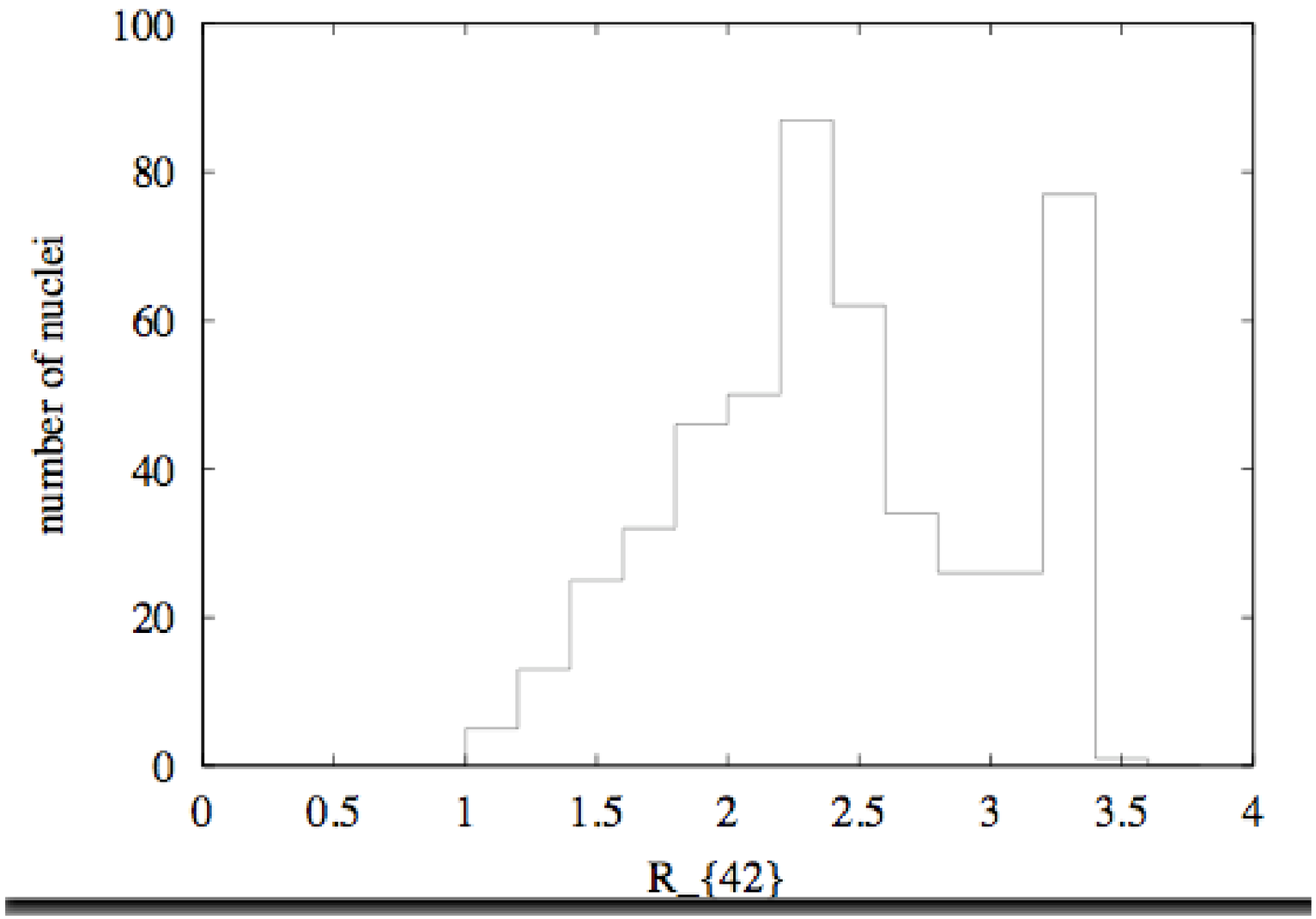
E_{level} #	J^{π} @	$T_{1/2}$ &	XREF	Com
0.0	1+	3.204 s *7*	ABCDEF	%ϵ+%β+=100 T=0 $T_{1/2}$: from 1965Fr06. Other: 3.21 s 2 (1962Mi13). J^{π}: log ft=4.9 to 0+.
202.6 *3*	0+		ABCD	T=1 J^{π}: IAS of ^{58}Ni ground state.
443.7 *2*	(3+)		BCDEF	
1051.0 *3*	(1+)	79 fs *+20-13*	ABCDE	
1427.8 *3*	2+	>670 fs	BCDE	
1549.1 *3*	(4+)	>350 fs	CDEF	
1647.4 *2*	(3+)	>910 fs	BC EF	J^{π}: from spin difference of members in a cascade (1999Ru01).
1651.6 *3*	2+	35 fs *7*	CD	J^{π}: IAS of ^{58}Ni 2+ state.

S_n2p	S_p2n	delta_s
0.81	0.78	0.65 MeV

Work in progress: R_42

$$R_{42} = \frac{E_4 - E_0}{E_2 - E_0}$$

A good indicator of strong deformation; 485 nuclei tabulated by Casten.



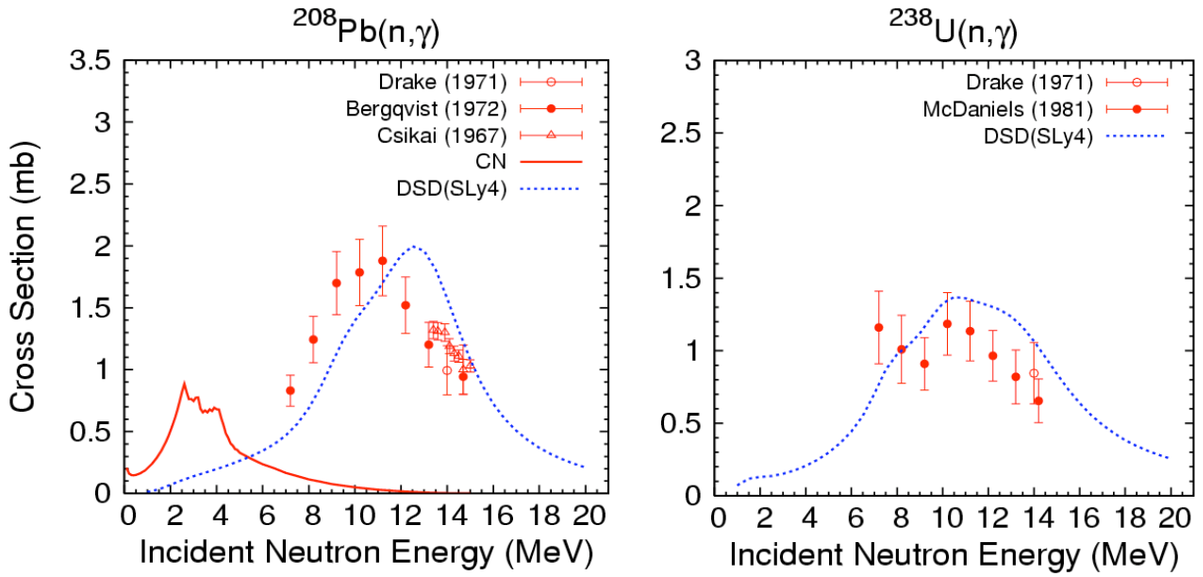
Capture mechanisms:

❖ Compound-Nucleus mechanism: incident energy equally shared among all degrees of freedom (dominant below 5 MeV)

❖ Direct-Semidirect mechanism: projectile scattered into a bound state of the target either directly (direct part) or through the excitation of the giant dipole resonance (semidirect part)

❖ Microscopic single-particle bound states $|b\rangle$ for even-even targets in the Hartree-Fock-BCS model: no input parameters aside from the effective nucleon-nucleon interaction (of the Skyrme type)

Calculated results:



L. Bonneau, T. Kawano, et al., PRC75, 05461 (2007)

DSD Formalism:

$$\sigma_{\mathrm{DSD}} \propto \sum_{b,M,\cdots} \left| \mathcal{M}_{\mathrm{D}} + \mathcal{M}_{\mathrm{SD}} \right|^2$$

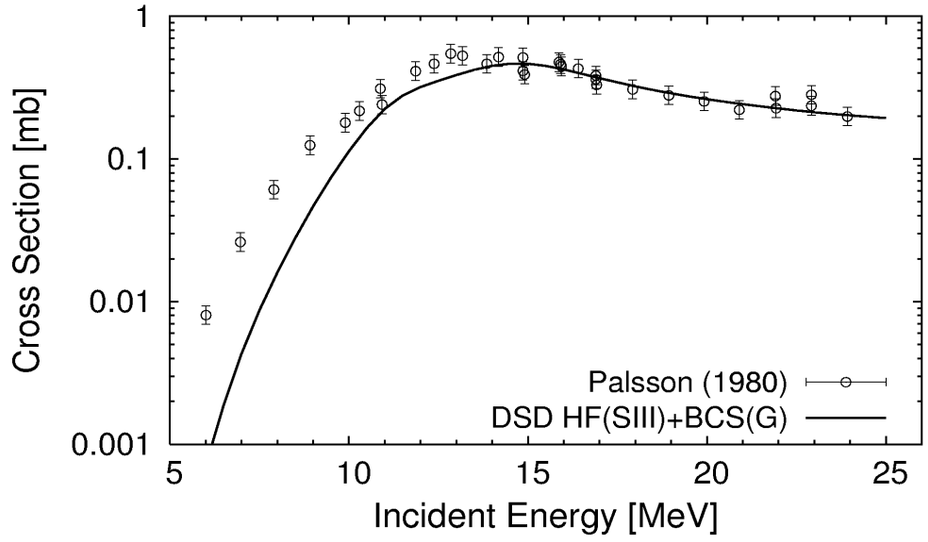
$$\mathcal{M}_{\mathrm{D}} \propto \langle \Psi_f^{(b)} | \hat{O}_{\mathrm{E1}} | \Psi_i \rangle \qquad \mathcal{M}_{\mathrm{SD}} \propto \sum_s \frac{\langle \Psi_f^{(b)} | \hat{O}_{E1} | \Psi_s \rangle \langle \Psi_s | \hat{H}_{p-v} | \Psi_i \rangle}{E_\gamma - E_s + i\Gamma_s/2}$$

$\hat{O}_{E1}$: electric dipole operator $\qquad$ $\hat{H}_{p-v}$: particle-vibration coupling

$$|\Psi_i\rangle \propto \underbrace{|\psi_{00}\rangle}_{\text{GS vibrational core}} \otimes \underbrace{|I_i M_i K_i\rangle}_{\text{rotational state}} \otimes \underbrace{|\Phi_i\rangle}_{\text{scattering state}}$$

$$|\Psi_f^{(b)}\rangle \propto |\psi_{00}\rangle \otimes |I_f M_f K_f\rangle \otimes \underbrace{|b\rangle}_{\text{bound state}}$$

$$|\Psi_s\rangle \propto \underbrace{|\psi_{1\nu}\rangle}_{\text{excited vibrational core}} \otimes |I_s M_s K_s\rangle \otimes |b\rangle$$



Preliminary results

Role of Evaluated Data

"Fitting theories of nuclear binding energies", G.F. Bertsch, B. Sabbey, and M. Uusnakki,
Phys. Rev. C71 054311 (2005)

[10] G. Audi, A. H. Wapstra, and C. Thibault, Nucl. Phys. **A729**, 337 (2003); the data file is available at http://www.nndc.bnl.gov/amdc/masstables/Ame2003/mass.mas03.

"Neutron-proton pairing reexamined", W.A. Friedman and G.F. Bertsch,
Phys. Rev. C in press

[18] Brookhaven Evaluated Nuclear Structure Data File, http://www.nndc.bnl.gov/ensdf/.

"Global study of the spectroscopic properties of the first 2+ state in even-even nuclei", B. Sabbey, M. Bender, G.F. Bersch, and P.-H. Heenen, Phys. Rev. C75 044305 (2007).

"Systematics of the First 2+ Excitation with the Gogny Interaction", G.F. Bertsch, M.Girod, S.Hilaire, J.-P. Delaroche, H. Goutte and S. Peru, Phys. Rev. Lett. 99 032502 (2007).

[10] S. Raman, C. W. Nestor, Jr., and P. Tikkanen, At. Data Nucl. Data Tables **78**, 1 (2001); the 2^+ excitation energy of ^{114}Ru has been corrected to the value given in Ref. [13].

[12] N. J. Stone, At. Data Nucl. Data Tables **90**, 75 (2005).

Suggestions for nndc.bnl.gov

1. Data file for nndc.bnl.gov/be2/

2. Neutron reaction database clickable from index

    2.1 EFT based n+p capture data, with documentation and citations

3. R42 table and histogram

4. Who will update the mass tables?

5. Beta decay table?