Connecting microscopic NN interactions with heavy nuclei through DFT

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MSU. June 20th, 2018

FRIB-TA Workshop. From bound states to the continuum

Outline

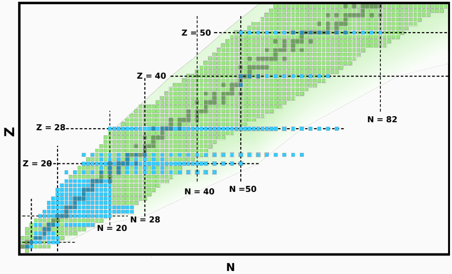
- Density Functional Theory:
  - Motivation
  - Overview of self-consistent mean field
  - Implementing a Microscopic Functional
  - Validation calculations

- Elastic Nucleus-Nucleus scattering
  - Coulomb threshold "anomaly"
  - ^{6}Li + ^{209}Bi with uncertainties

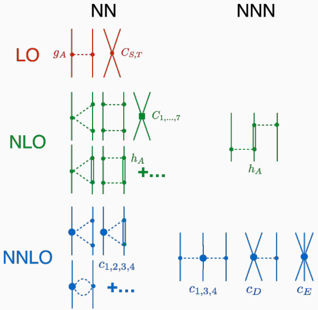
- Summary and Outlook

Microscopic DFT

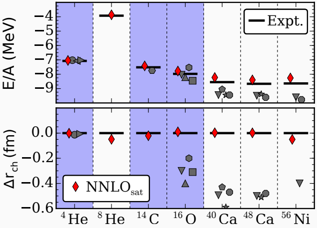
Ab-initio methods with χ-EFT



[Hergert et al. Phys. Rept. 621 (2016) 165]



[Ekström et al. arXi:1707.09028]



[Hagen et al. Phys. Scr. 91 (2016) 063006]

- Systematic, order by order
- Light and medium nuclei ✓
- Heavy nuclei out of reach
    - A problem of scaling

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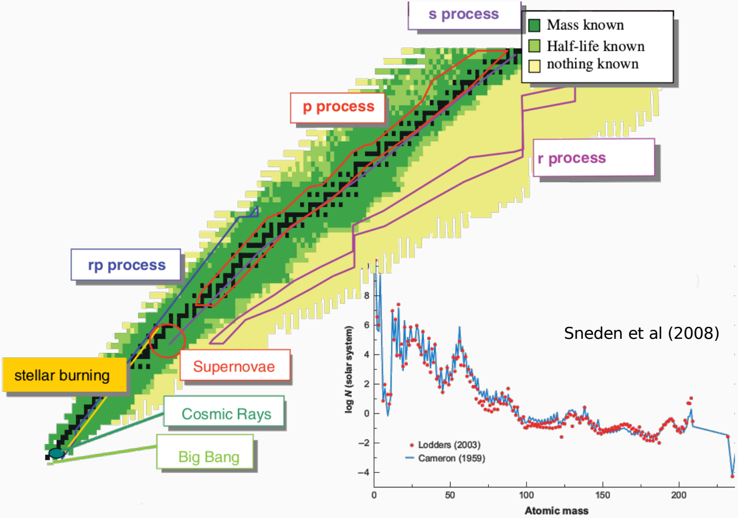
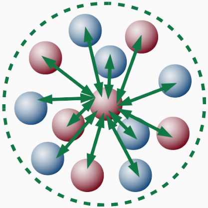
FRIB and astrophysical processes



[Grawe et al. Rept. Prog. Phys. 70 (2007) 1525]

Phenomenological DFT

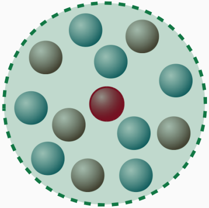
Ab-initio



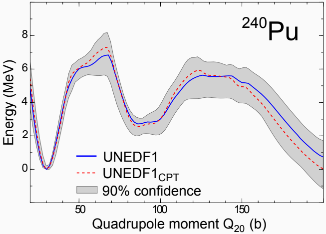
$$(T + \sum_{ij}^{A} V_{ij})\Psi = E\Psi$$

- Good computational scaling
- Static and dynamic properties of nuclei
- Can go “beyond mean field”
- No systematic improvement

Mean field



$$(T + \sum_{i}^{A} \tilde{V}_{i})\Psi = E\Psi$$



[McDonnell et al. PRL114 (2015) 122501]

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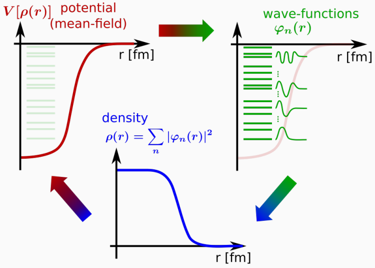
Self-Consistent Mean Field

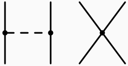
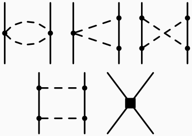
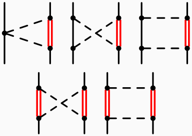
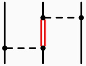
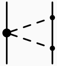
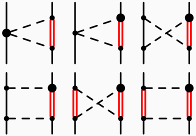
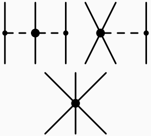
- DFT, based on HFB theory
- Non-linear eigenvalue problem
- Iterative solutions
- Phenomenological interactions
    - Fitted to hundreds of nuclear data
    - Contact interactions: Skyrme
    - Finite range: Gogny



Self-consistent mean-field theory

[https://commons.wikimedia.org/]

Microscopically constrained EDF: Chiral expansion

	NN force		$3N$ force	
	Δ-less EFT	Δ contributions	Δ-less EFT	Δ contributions
LO		—	—	—
NLO			—	
N^{2}LO				—

[A. Dyhdalo, et al. PRC95 (2017) 054314]

Structure of the potential and the EDF

- (Extremely) schematic 2 body chiral potential

$$\hat{V}_{NN}(r_1, r_2) = \underbrace{\delta(r_1 - r_2)}_{\text{yields Skyrme-like}} + \underbrace{V_F(r_1 - r_2)}_{\text{sum of Yukawas}}$$

- Yukawas expanded as a sum of Gaussians
    - Treat Hartree term of the EDF like a Gogny force
- 3N force has similar structure but:
    - Hartree term is zero in time-reversal invariant systems
    - Fock term induced by finite range has non-local densities
- Use density matrix expansion for all exchange terms
    - Recast V_{NN} and V_{3N} into Skyrme-like terms
    - Reduces computational cost significantly
    - Also reduces numerical stability issues

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The best of both worlds

DFT Component

- Contact terms for short range physics
- Adjusted to nuclear properties
- Encodes many body correlations

+

Microscopic Component

- Derived from χ-EFT
- Long range physics, pions
- Order by order
- Non-Local density!

A scalable framework with systematic improvements

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Microscopically constrained DFT

- Non-local densities for finite range potentials

$$E_H^{NN} \sim \int dR dr \langle r|V^{NN}|r\rangle \rho_1\left(R+\frac{r}{2}\right)\rho_2\left(R-\frac{r}{2}\right)$$

$$E_F^{NN} \sim \int dR dr \langle r|V^{NN}|r\rangle \rho_1\left(R-\frac{r}{2}, R+\frac{r}{2}\right)\rho_2\left(R+\frac{r}{2}, R-\frac{r}{2}\right)\hat{P}_{12}$$

- Density Matrix Expansion (DME)

$$\rho\left(R+\frac{r}{2}, R-\frac{r}{2}\right) \approx \Pi_0^\rho(k_F r)\rho(R) + \frac{r^2}{6}\Pi_2^\rho(k_F r)\left[\frac{1}{4}\Delta\rho(R) - \tau(R) + \frac{3}{5}k_F^2\rho(R)\right]$$

Like a Taylor expansion for the non-local density

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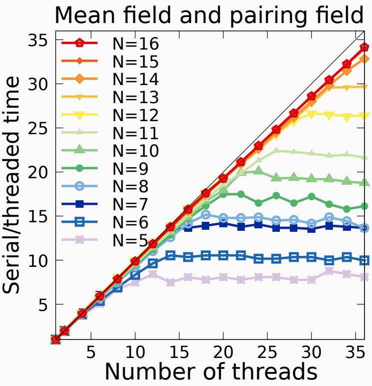
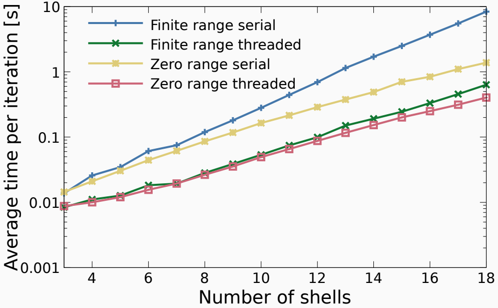
HFBTHO v3 takes advantage of current HPC architectures





- Finite-range calculation not much more expensive that zero-range when threading

[RNP, Schunck, Lasseri, Zhang CPC220 (2017) 363]

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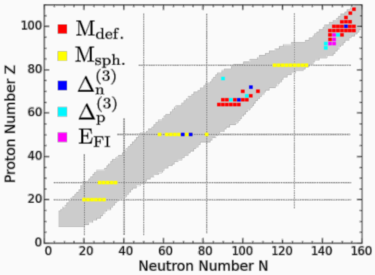
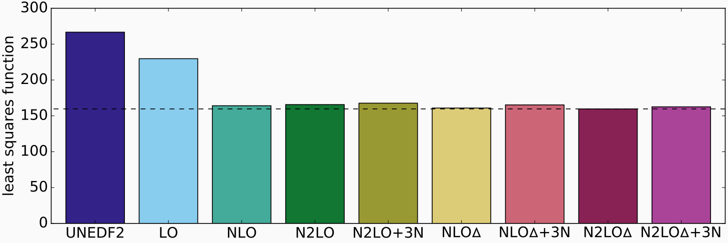
Optimizing DFT component

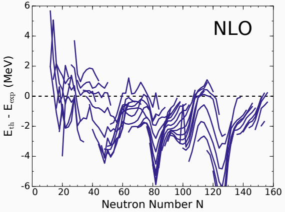
- UNEDF2 optimization protocol
- 130 data, 14 parameters
- Masses, radii, fission isomers, spin-orbit splittings, nuclear matter

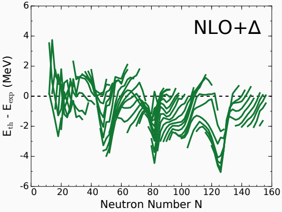


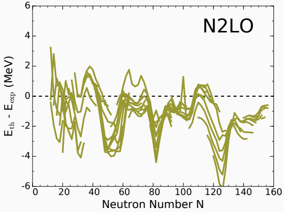
[Schunck et al. EPJA51 (2015) 169]

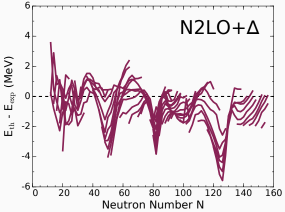


Mass Tables







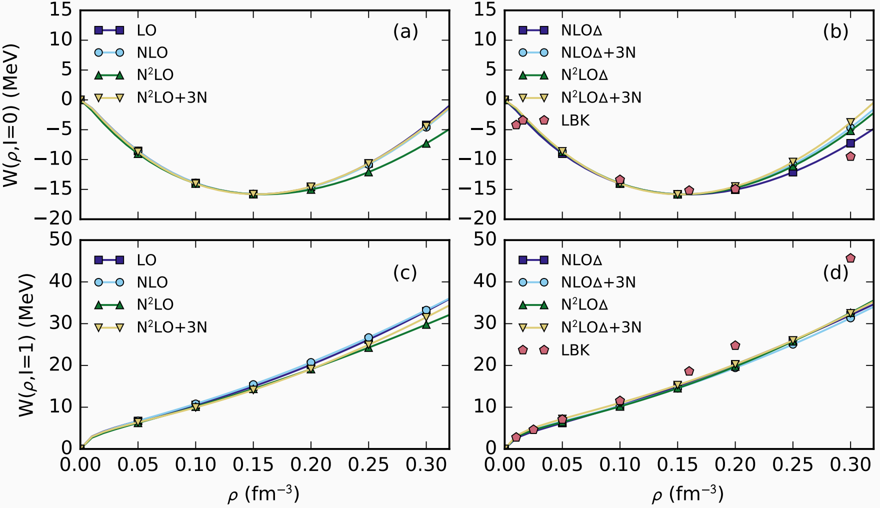


Order by order improvement

EDF	r.m.s. deviation
UNEDF2	1.98
LO	1.99
NLOΔ	1.41
N2LOΔ	1.26

[RNP, Schunck, Dyhdalo, Furnstahl, Bogner. PRC97 (2018) 05430]

Nuclear Matter and Neutron Matter



[RNP, Schunck, Dyhdalo, Furnstahl, Bogner. PRC97 (2018) 05430]

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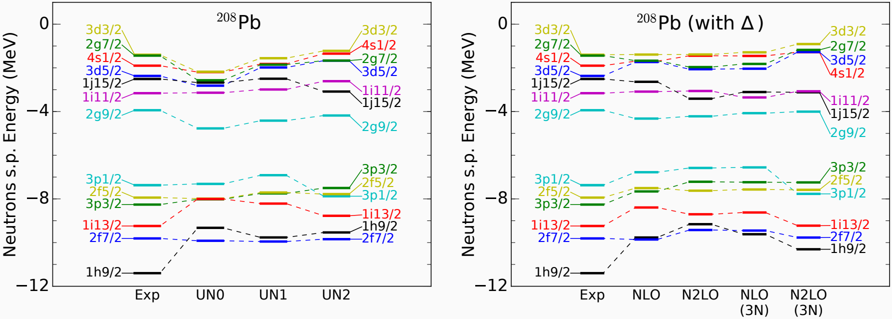
Single-Particle Spectra

Quantitatively comparable to UNEDF results

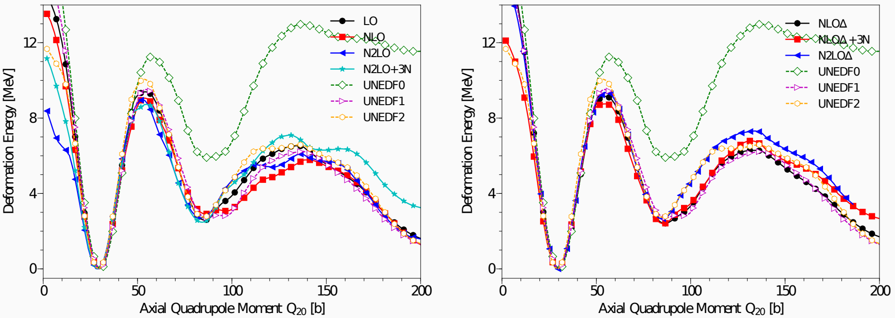


[RNP, Schunck, Dyhdalo, Furnstahl, Bogner. PRC97 (2018) 05430]

- Single-particle energies from blocking calculations
- Exactly the same conditions for all EDFs

Deformation Properties

Quality of fission barriers is comparable to other EDFs



[RNP, Schunck, Dyhdalo, Furnstahl, Bogner. PRC97 (2018) 05430]

- Inclusion of fission isomers in fitting protocols constrains fission barriers
- Variations up to 2 MeV in height of fission barriers

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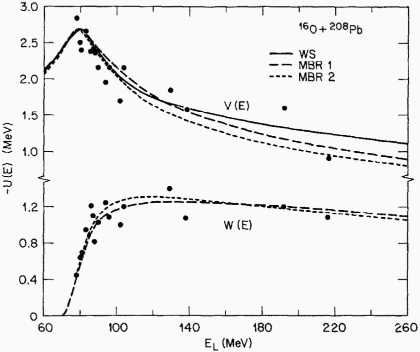
Elastic Nucleus-Nucleus scattering

Elastic Nucleus-Nucleus scattering

- Near the Coulomb barrier
- Energy dependence of the effective (optical) potential
- Imaginary part decreases with energy
- Real part shows an "anomaly"
- A consequence of causality
  - Dispersion relation

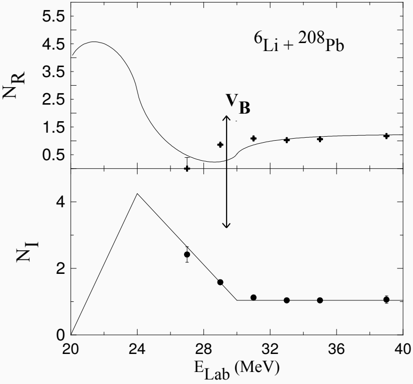
$$V(r;E) = V_0(r) + \frac{P}{\pi}\int_0^{\infty} \frac{W(r;E')}{E'-E} dE'$$



[Mahaux et al. NPA449 (1986) 354]

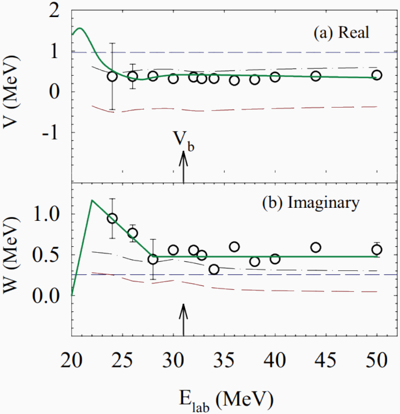
Looking at weakly bound Nuclei

New manifestation of the dispersion relation: Breakup threshold anomaly



[Hussein et al. PRC 73 (2006) 044610]

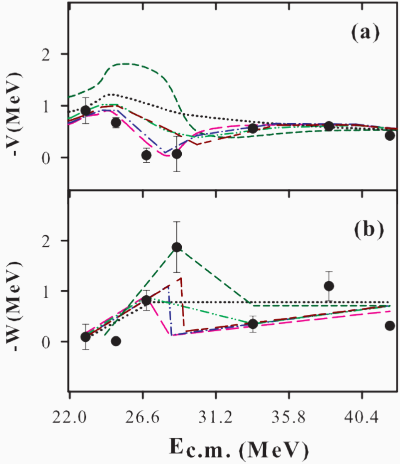
Reaction mechanisms involving weakly bound ^{6}Li and ^{209}Bi at energies near the Coulomb barrier



[Santra et al. PRC 83 (2011) 034616]

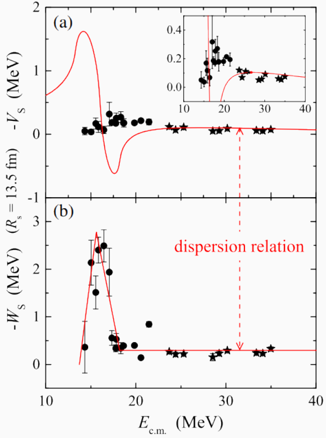
Looking at weakly bound Nuclei

Investigation of the threshold anomaly for the ^{7}Li + ^{159}Tb system



[Patel et al. PRC 91 (2015) 054614]

Is the Dispersion Relation Applicable for Exotic Nuclear Systems? The Abnormal Threshold Anomaly in the ^{6}He + ^{209}Bi System



[L. Yang et al. PRL 119 (2017) 042503]

Looking at weakly bound Nuclei

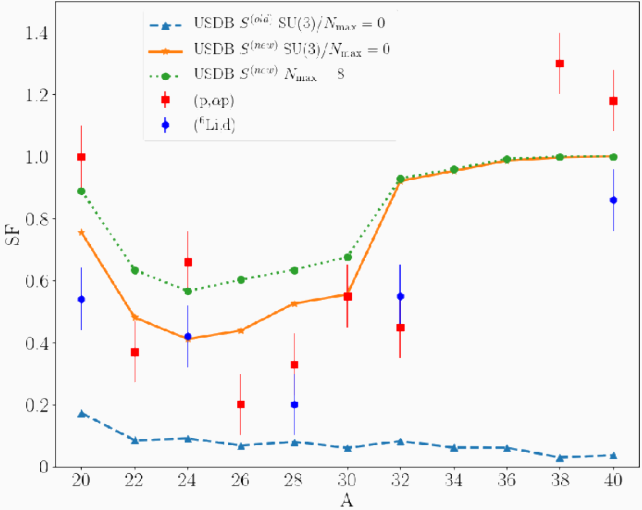
- This is a cautionary tale in:
  - Underestimated experimental uncertainties
  - Misunderstood theoretical uncertainties
  - Good software used as a black box
  - Ignoring the underlying physics
- Let's focus on one of these four examples
  - Elastic $^{6}Li + ^{209}Bi$ cross sections
  - Measured at energies from 24 to 50 MeV
  - Use an effective potential with Woods Saxon shape

$$V(r;E) = -\frac{V_E}{1+e^{(r-R_v)/a_v}} - i\frac{W_E}{1+e^{(r-R_W)/a_W}}$$

  - Integrate with Numerov and match to Coulomb WF

Incompatible experimental data

During Heiko's talk …



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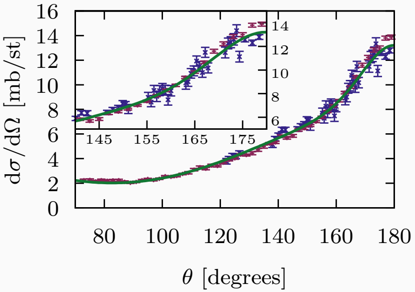
Incompatible experimental data

- Fits NEVER give $\chi^2/\mathrm{d.o.f.} \lesssim 1$
  - Restrictive model ? $\rightarrow$ Improve model
  - Mutually incompatible data ? $\rightarrow$ Reject data
- np $d\sigma/d\Omega$ at 162 MeV
- Statistical and systematic errors over or underestimated

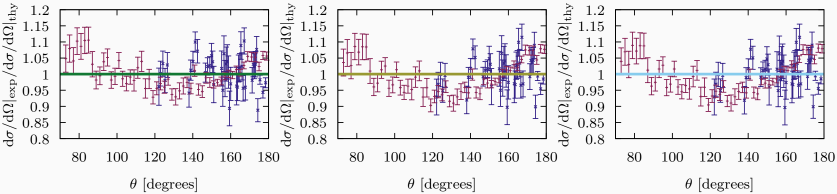
- 3σ criterion
  - Fit to all data ($\chi^2/\mathrm{d.o.f.} > 1$)
  - Remove data sets with improbably high or low χ^2
  - Refit parameters



[RNP, Amaro, Arriola PRC88 (2013) 064002]

Incompatible experimental data

- Mutually incompatible data
  - Which experiment is correct?
  - Is any of the two correct?
- Maximization of experimental consensus
  - Fit to all data ($\chi^2/\mathrm{d.o.f.} > 1$)
  - Apply 3σ criterion
  - Refit parameters
  - Re-apply 3σ criterion to all data
  - Repeat until no more data is excluded or recovered

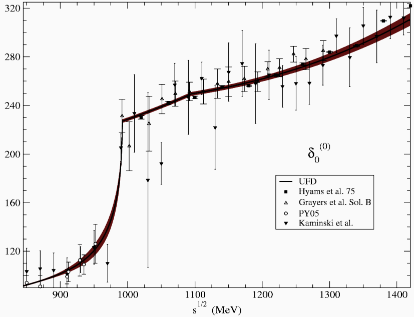


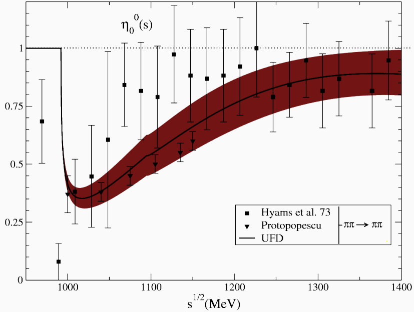
[RNP, Amaro, Arriola PRC88 (2013) 064002]

Incompatible experimental data

π - π scattering data analysis

Elastic and inelastic data





[RNP, Arriola, Ruiz de Elvira, PRD91 (2015) 074014]

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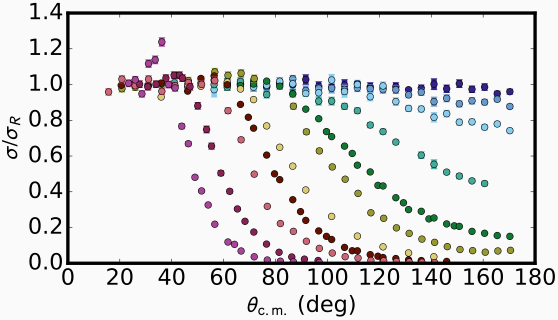
Incompatible experimental data

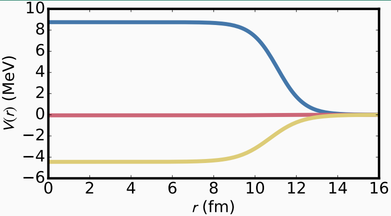
$^{6}Li + ^{209}Bi$ data

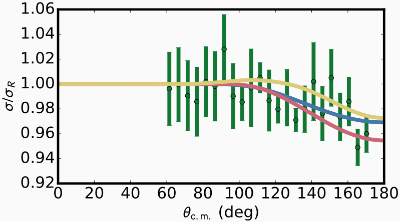


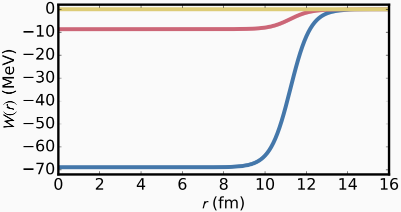
One single experiment at different energies

3σ criterion still applicable

Large uncertainties at low energies (24 MeV)







3 different effective potentials

$V(r,E) = -V_E/(1+e^{(r-r_v)/a_v}) - iW_E/(1+e^{(r-r_w)/a_w})$

- No constrains
- Attractive potentials
- Small imaginary part

Fit simultaneously at different energies and “Bootstrap” data

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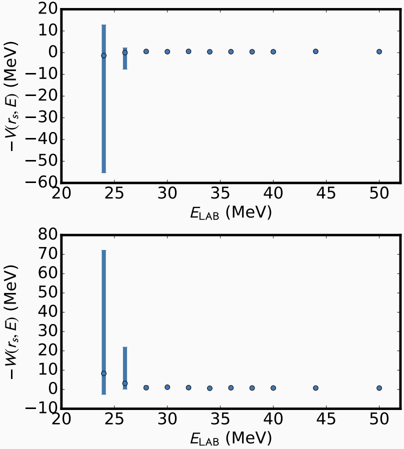
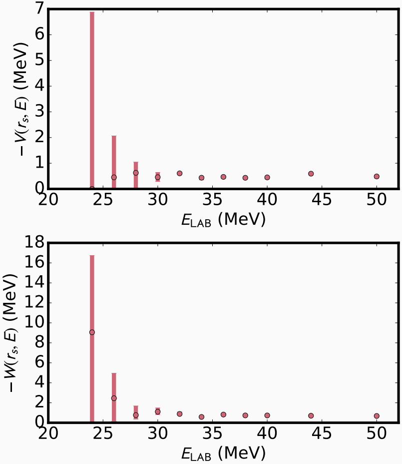
3 Types of analysis

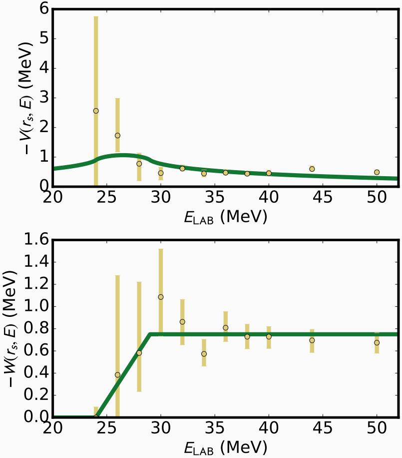
Unconstrained fits



Attractive potentials



3 Types of analysis



- Constraining some parameters
- Penalty function
- $\chi^2 \to \chi^2 + (W_{24})^2 + (W_{26})^2 + (W_{28})^2$
- This is a prior from the Bayesian point of view
- Results are compatible with dispersion relation

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Summary

Microscopic DFT

- New family of EDFs constrained by χ-EFT
  - Up to N2LO with/o 3N and Δ-excitations
- Quality EDFs with global predictive power and microscopic underpinning
- Surprising improvement in mass calculations

Elastic Nucleus-Nucleus scattering

- UQ has meaningful consequences
- Physics needs to be included in any analysis

Outlook

Microscopic DFT

- Effect of 3N forces
  - Δ's improve performance, 3N terms don't
- Quantification and propagation of uncertainties
  - Truncation, fitting bias, sensitivity to LEC's
- Use the same EDF in pairing channel

Elastic Nucleus-Nucleus scattering

- Propagate uncertainty to dispersion relation
- Include dispersion relation by construction
- Analyze other reactions with weakly bound nuclei