

# **FRIB science (lecture 2)**

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## Lecture 1:

- basic concepts and language
- big science questions
- cool phenomena
- production of the exotic stuff
- what is FRIB?

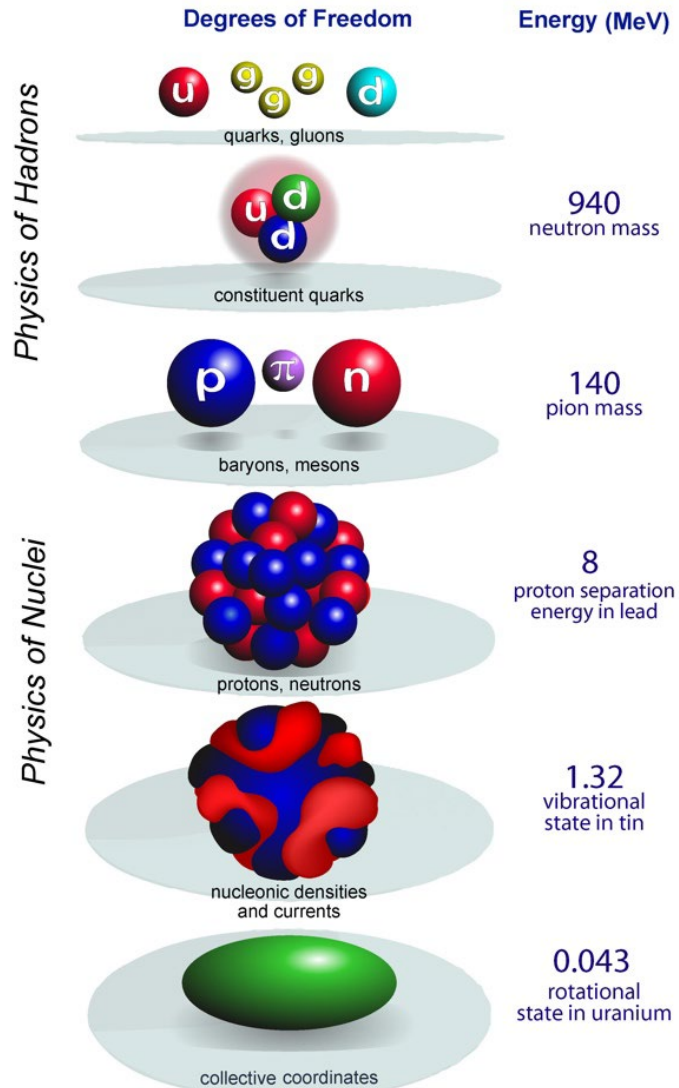
## Lecture 2

- connection to QCD
- the many-body problem
- forces and EFT
- various applications
- current status for nuclear structure

## Lecture 3

- nuclear reactions as a tool
- basics concepts in nuclear reactions
- some examples from my research

# Multiple scales in nuclear physics



Our building blocks are nucleons

# nuclei: a tough many-body problem

$$H_A = - \sum_{i=1}^A \frac{\hbar^2}{2m_i} \nabla_{\mathbf{r}_i}^2 + \frac{\hbar^2}{2M} \nabla_{\mathbf{S}}^2 + \sum_{i>j}^A V^{(2)}(\mathbf{r}_i - \mathbf{r}_j) + \sum_{i>j>k}^A V^{(3)}(\mathbf{r}_i - \mathbf{r}_j, \mathbf{r}_i - \mathbf{r}_k),$$

$$H_A \Phi_{I\mu}(\boldsymbol{\rho}_1, \dots, \boldsymbol{\rho}_{A-1}) = E_I \Phi_{I\mu}$$

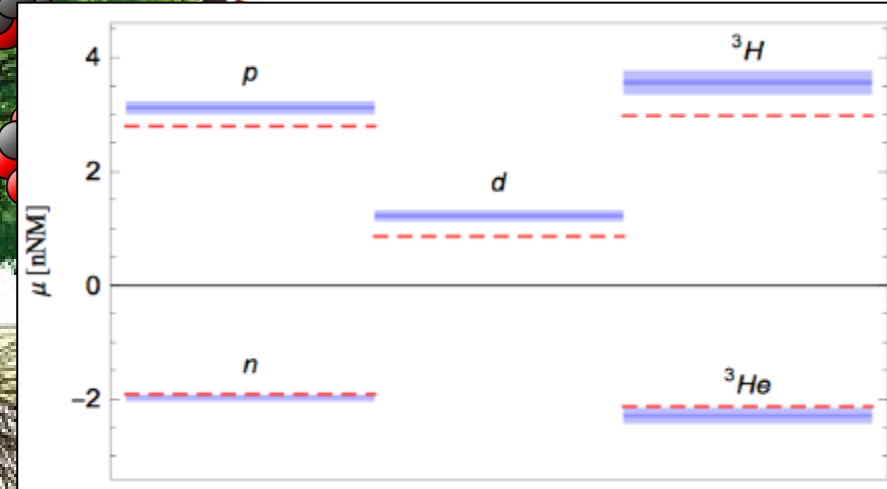
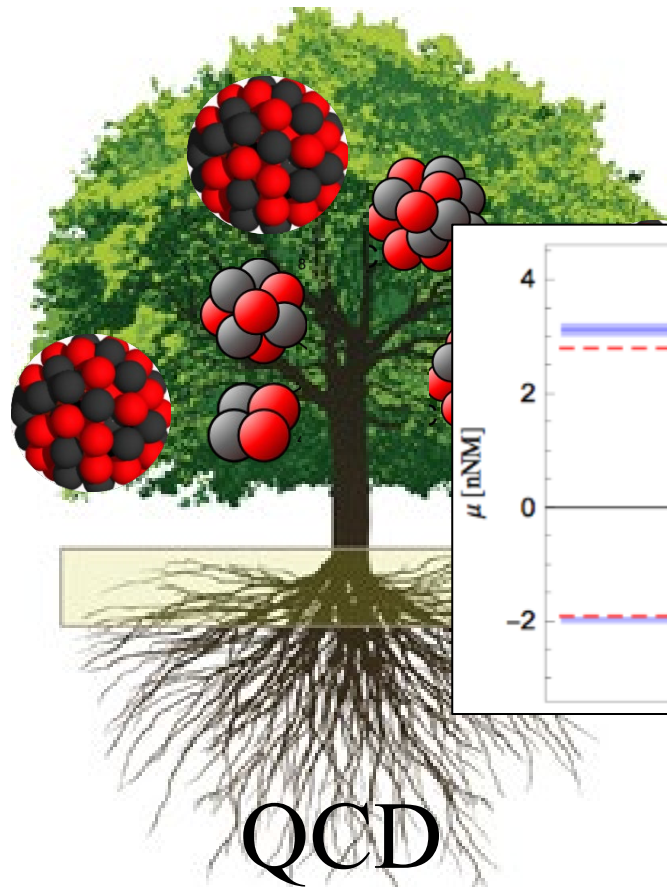
$$\lim_{\boldsymbol{\rho}_i \rightarrow \infty} \Phi_{I\mu}(\dots, \boldsymbol{\rho}_i, \dots) = 0$$

$$\int d\boldsymbol{\rho}_1 \dots \int d\boldsymbol{\rho}_{A-1} |\Phi_{I\mu}(\boldsymbol{\rho}_1, \dots, \boldsymbol{\rho}_{A-1})|^2 = 1$$

non-relativistic!

# The fundamental theory: QCD

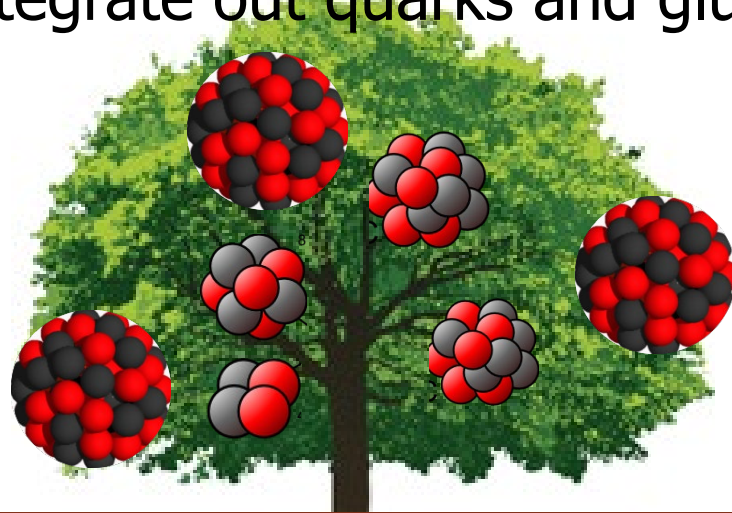
A reliable theory for nuclei needs to be rooted in QCD!



*LQCD predictions for  
magnetic moments  $A < 4$*

# The fundamental theory: QCD

QCD may one day calculate the lightest nuclei  
but what about  $^{238}\text{U}$ ?  
we need to integrate out quarks and gluons...

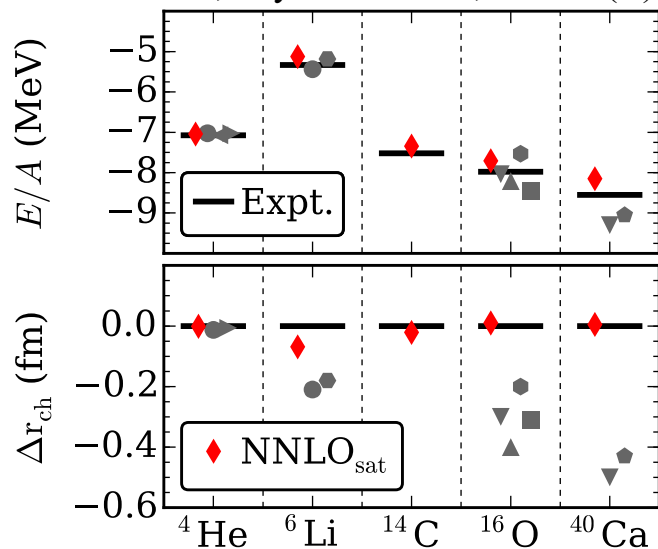


This is where effective field theory comes in

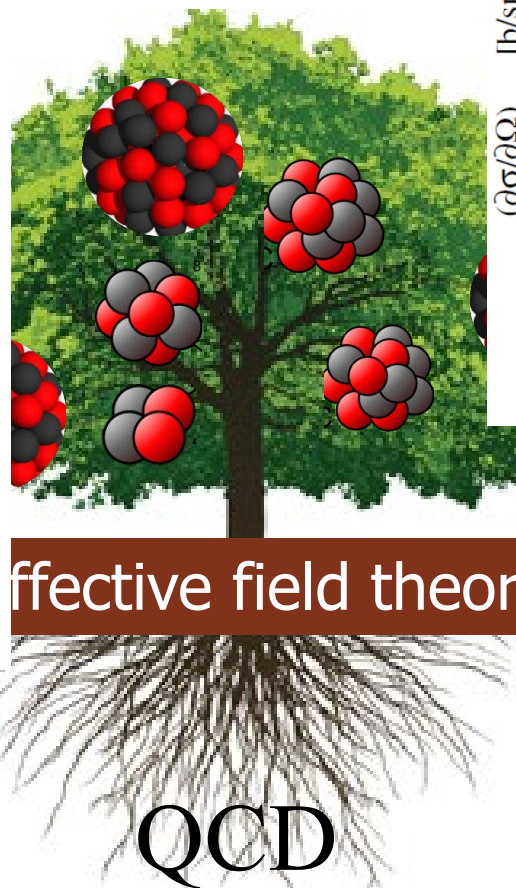
QCD

# Rooting nuclei in QCD

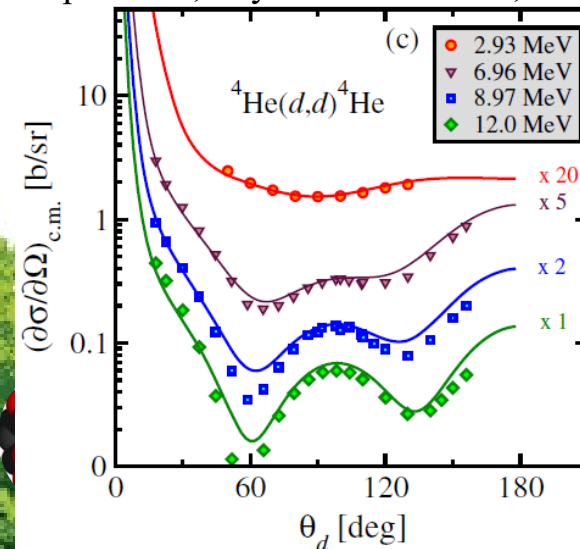
Ekstrom et al, Phys. Rev. C **91**, 051301(R)



*Coupled cluster  
predictions of binding  
energies and radii*



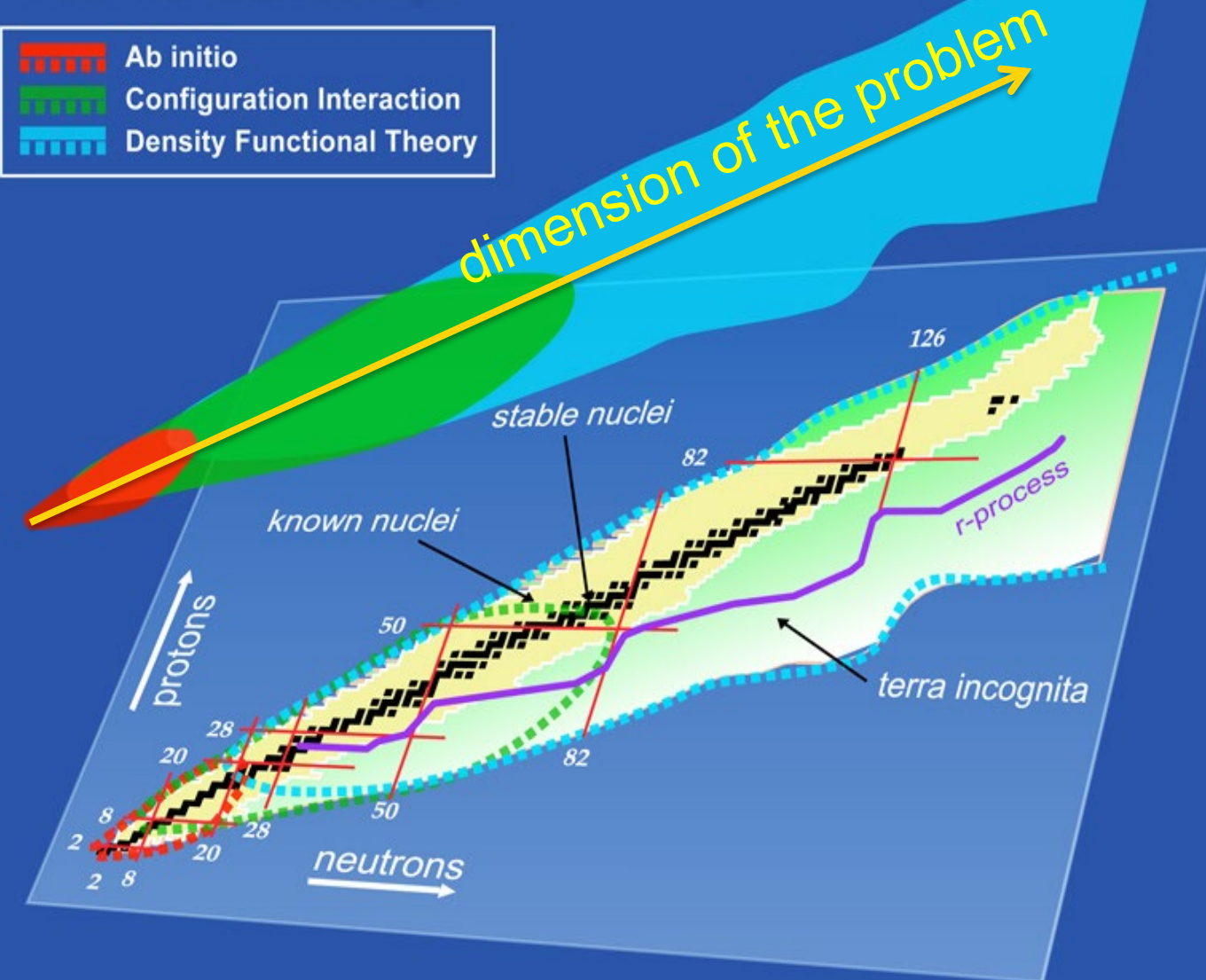
Hupin et al., Phys. Rev. Lett. **114**, 212502



*No Core Shell Model  
with continuum  
predictions for d- $\alpha$   
elastic scattering*

# The nuclear many-body problem

## Nuclear Landscape



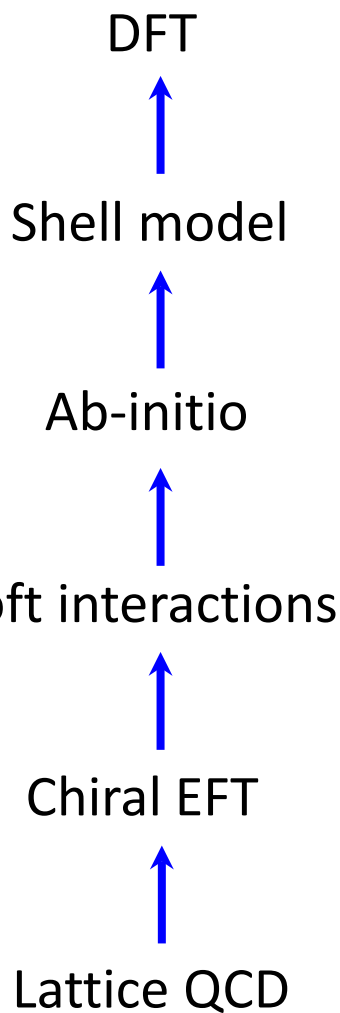


# Interactions and methods

Poorly known



Well known

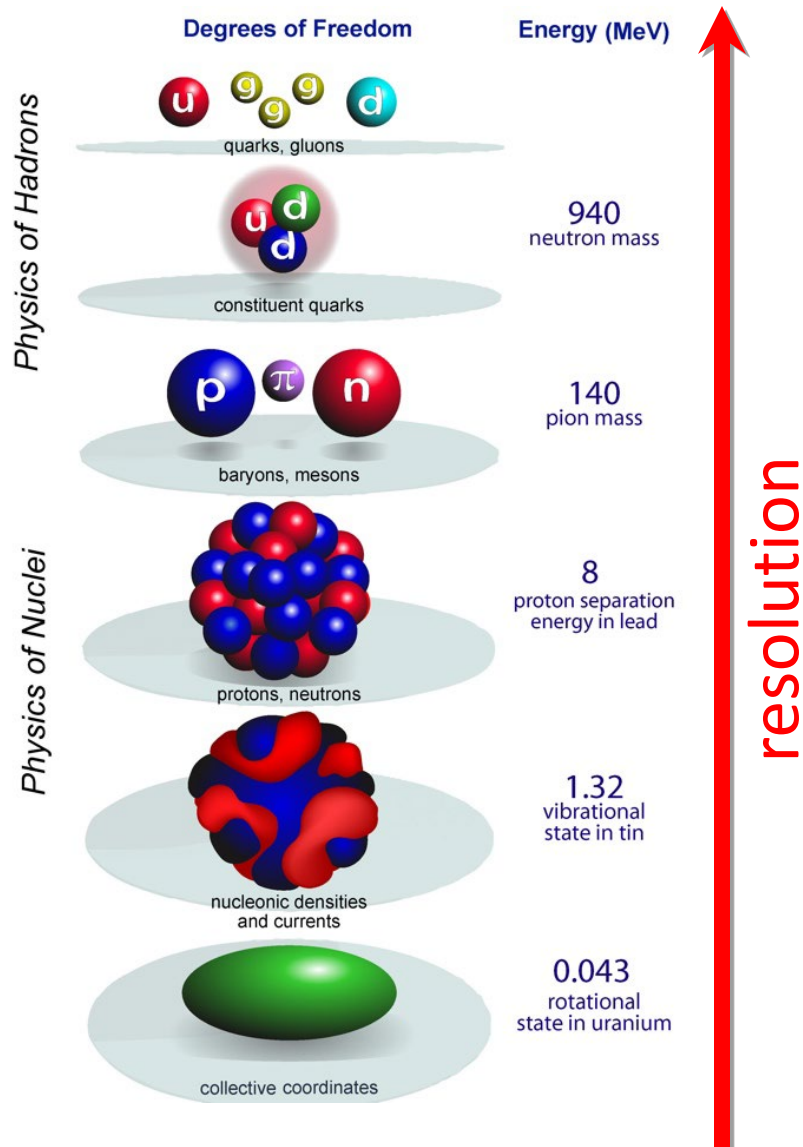


easy to solve



hard to solve

# Multiple scales and resolution



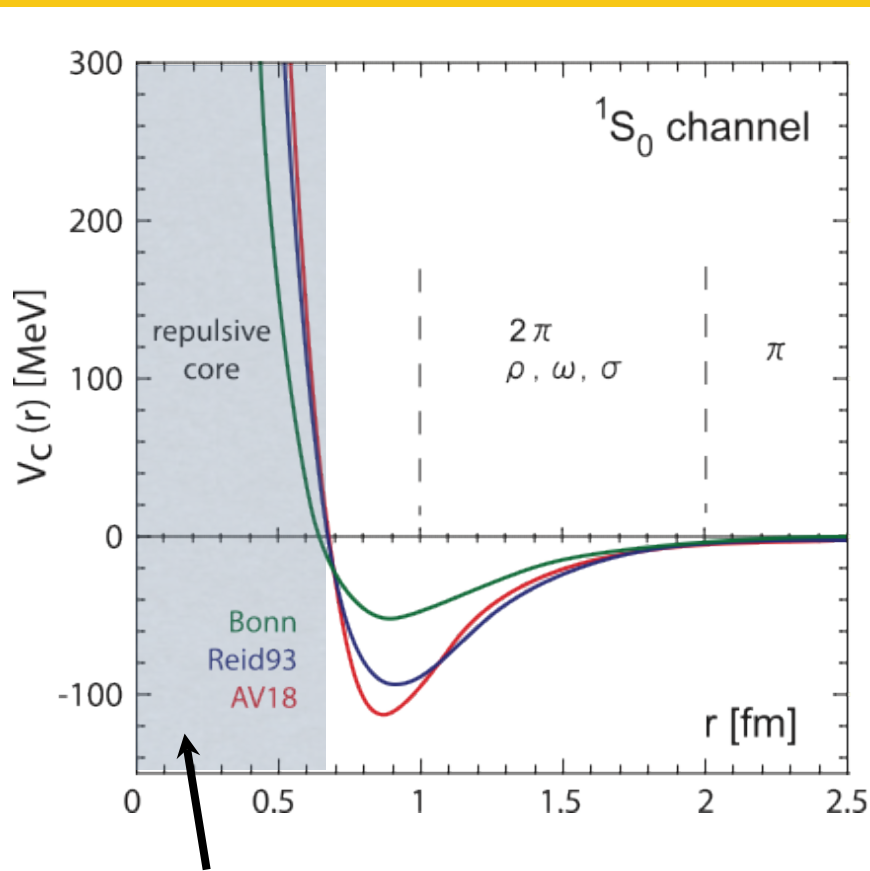
Ratio of scales => small parameters!

- Effective theories at each scale connected by renormalization group

$$V(\Lambda) = V_{2N}(\Lambda) + V_{3N}(\Lambda) + \dots$$

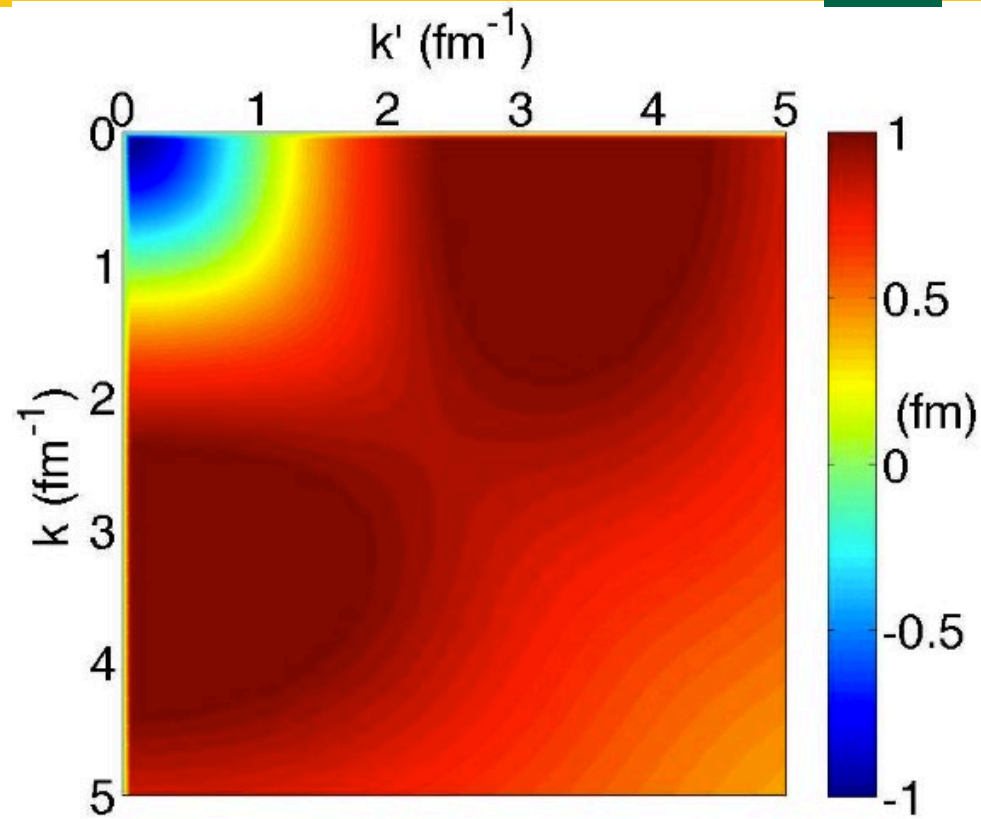
Use RG to pick a convenient  $\Lambda$  "resolution scale"

# Why are nuclear many-body problems hard?



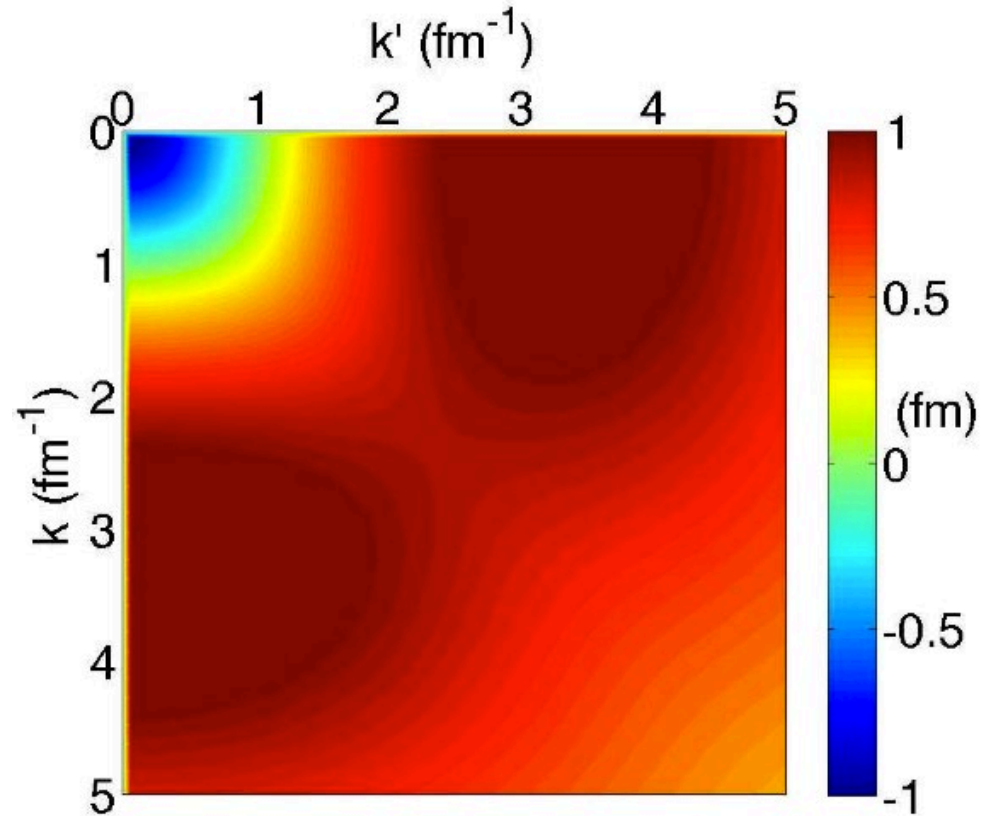
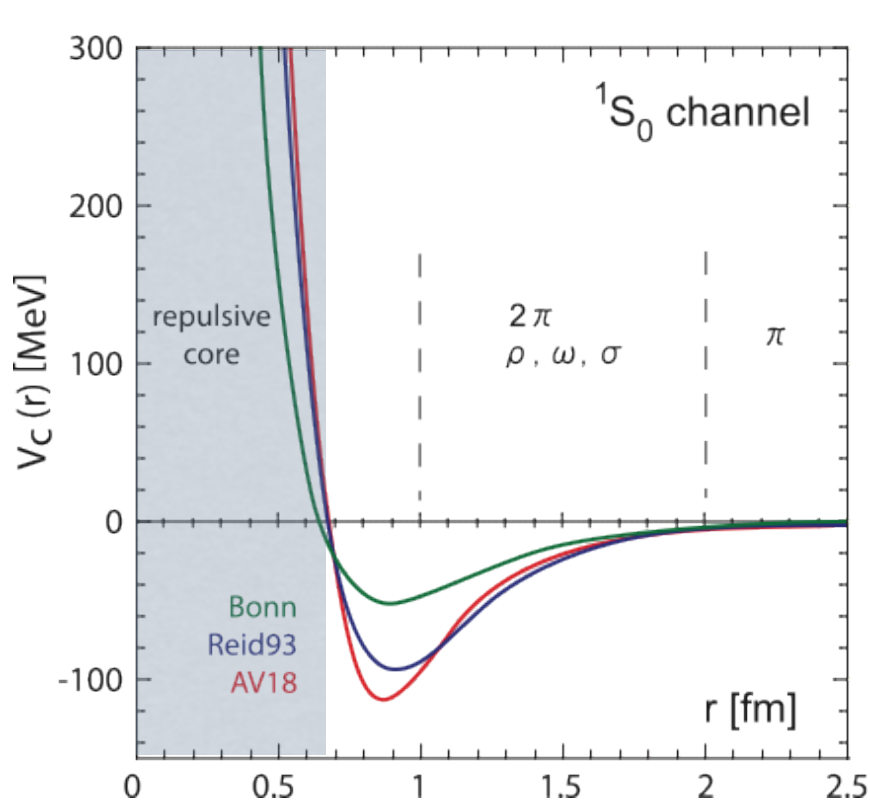
“hard-core” of  $V(r)$   $\Rightarrow$  strong offdiagonal  $V(k, k')$

$$V_{l=0}(k, k') = \int d^3r j_0(kr) V(r) j_0(k'r')$$



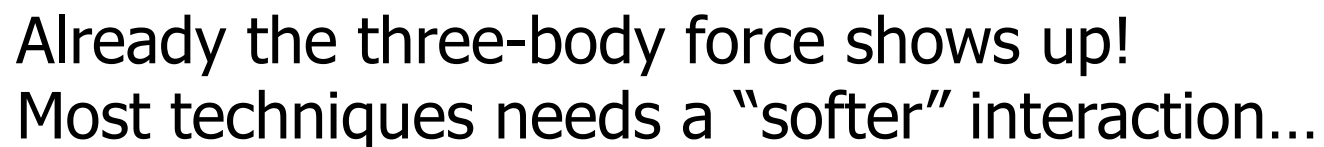
Characteristic  $k_F \sim 1 \text{ fm}^{-1}$

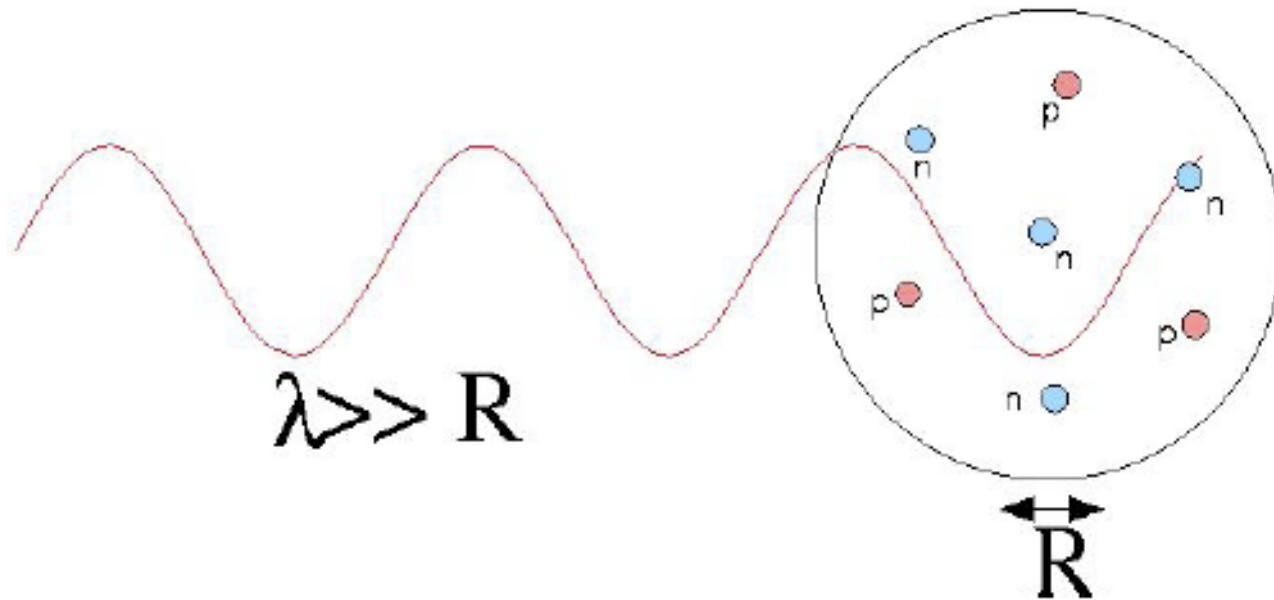
# Why are nuclear many-body problems hard?



**Complications:** strong correlations, non-perturbative, poorly convergent basis expansions, ...

Characteristic  $k_F \sim 1 \text{ fm}^{-1}$





- If a system is probed at low energies, fine details not resolved
- Use convenient dof to describe low-energy processes
- Complicated short-distance structure **replaced** by something simpler without distorting low-E observables

# Low energy effective theories



Generic form of  
the effective theory

$$V_{eff} = V_L + \delta V_{c.t.}(\Lambda)$$

$$\delta V_{ct} = C_0(\Lambda) \delta^3(\mathbf{r}) + C_2(\Lambda) \nabla^2 \delta^3(\mathbf{r}) + \dots$$

encodes the  
effects of integrated  
dof on low-E physics

universal form; depends  
only on symmetries

The complicated short-distance structure of the “true” theory is encoded in a few numbers that can be **calculated** from the underlying theory

OR

in cases where the short-distance structure is unknown or too complicated, can be **extracted** from low energy data








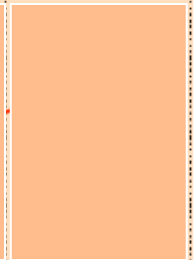


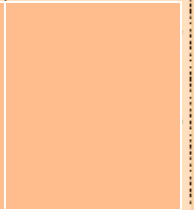
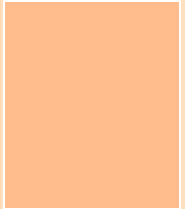
**Effective Field Theory (EFT) is based on these ideas**

# Nuclear forces from Chiral EFT

Separation of scales: low momenta  $Q \ll \Lambda_b$  (breakdown scale)

- Include long-range pion physics explicitly
- Short-distance **details** not resolved, Encoded in short-range couplings fit to data once
- Systematic: can work to desired accuracy

$$\Delta \mathcal{O}_\nu \sim \left( \frac{Q}{\Lambda} \right)^{\nu+1}$$

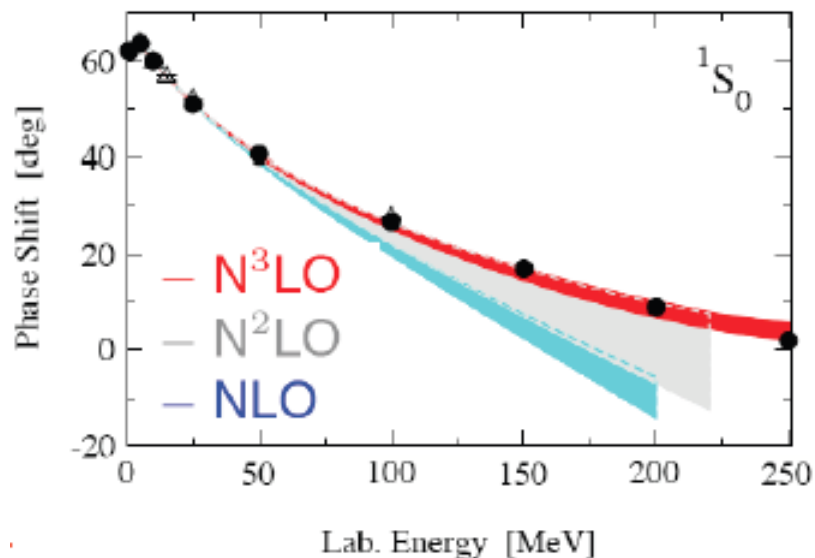
|   | NN  | 3N  | 4N  |
|---|---|---|---|
| LO $\mathcal{O}\left(\frac{Q^0}{\Lambda^0}\right)$                |    |    |    |
| NLO $\mathcal{O}\left(\frac{Q^2}{\Lambda^2}\right)$               |    |    |    |
| N <sup>2</sup> LO $\mathcal{O}\left(\frac{Q^3}{\Lambda^3}\right)$ |   |   |    |
| N <sup>3</sup> LO $\mathcal{O}\left(\frac{Q^4}{\Lambda^4}\right)$ |  |  |  |



# Nuclear forces from Chiral EFT

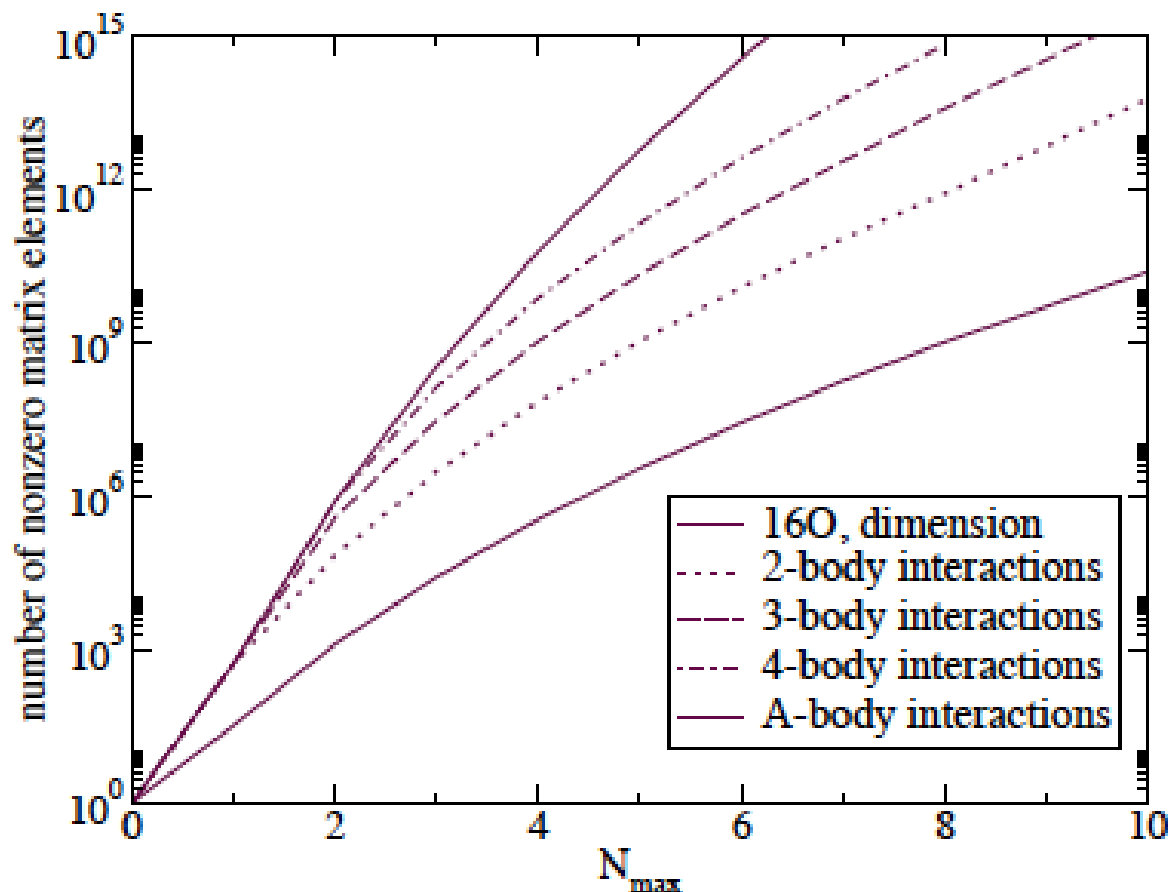
Separation of scales: low momenta  $Q \ll \Lambda_b$  breakdown scale

- Explains why  $2N > 3N > 4N$
- Error determined from  $\Lambda$  variation



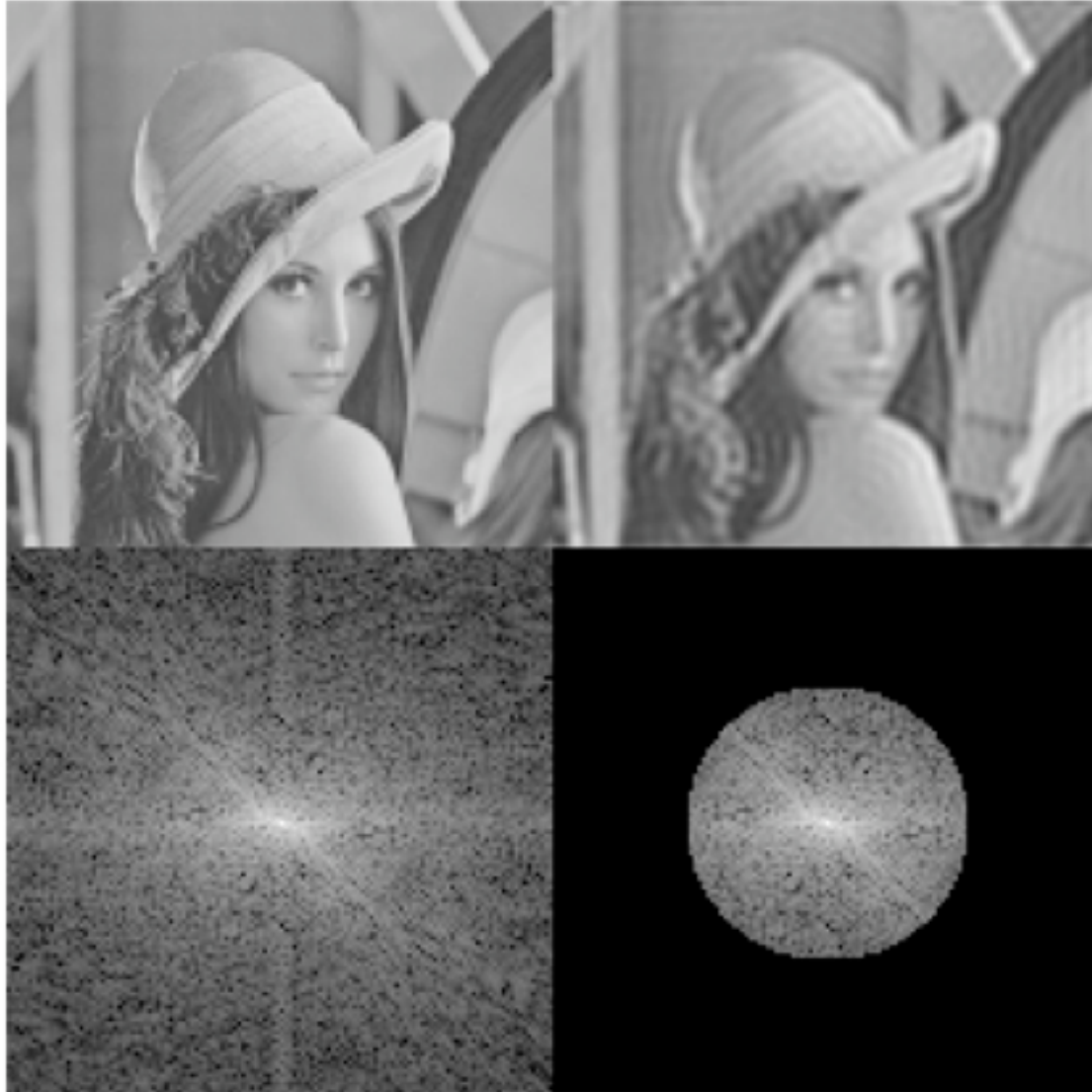
|   | NN | 3N | 4N |
|---|----|----|----|
| LO $\mathcal{O}\left(\frac{Q^0}{\Lambda^0}\right)$      |    | —  | —  |
| NLO $\mathcal{O}\left(\frac{Q^2}{\Lambda^2}\right)$     |    | —  | —  |
| $N^2LO$ $\mathcal{O}\left(\frac{Q^3}{\Lambda^3}\right)$ |    |    | —  |
| $N^3LO$ $\mathcal{O}\left(\frac{Q^4}{\Lambda^4}\right)$ |    |    |    |

# No free lunch: beyond two-body forces



Higher-order forces are a computational nightmare!

# Ex: Low-pass filter on fourier transform of a 2d-image

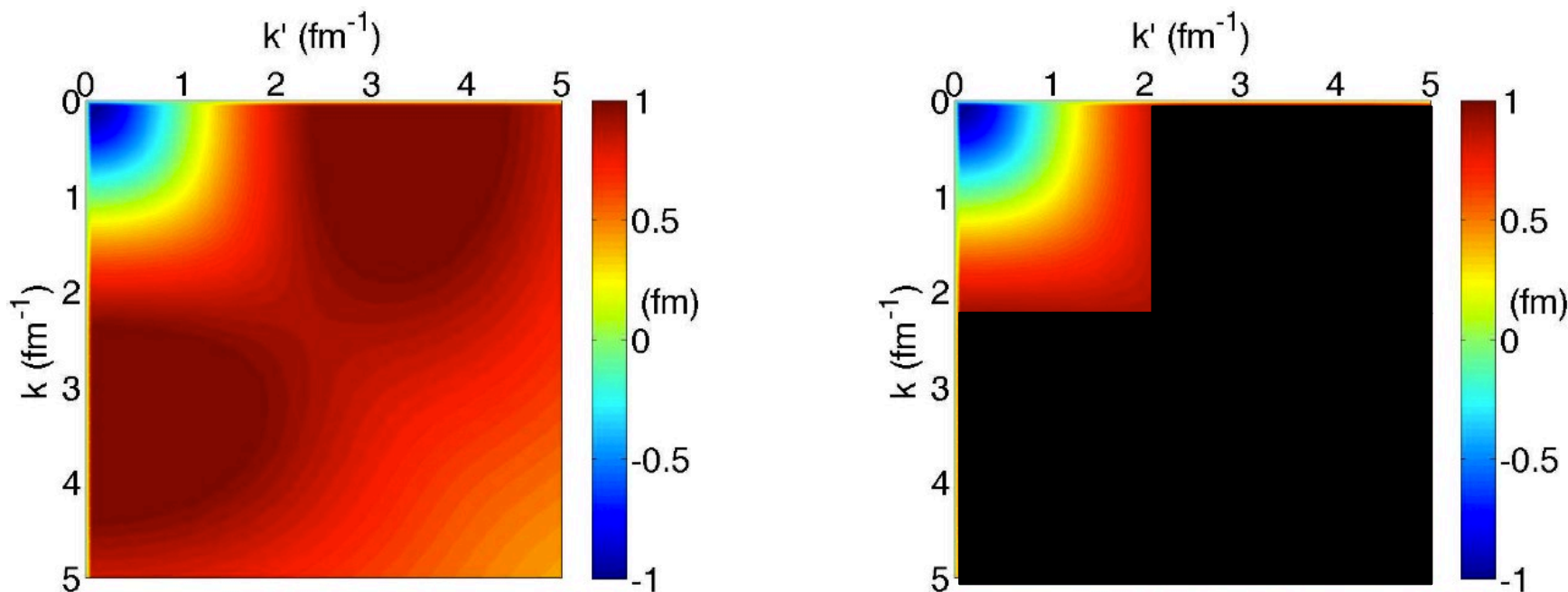


filtered image contains  
much less information

BUT

Long-wavelength info  
preserved

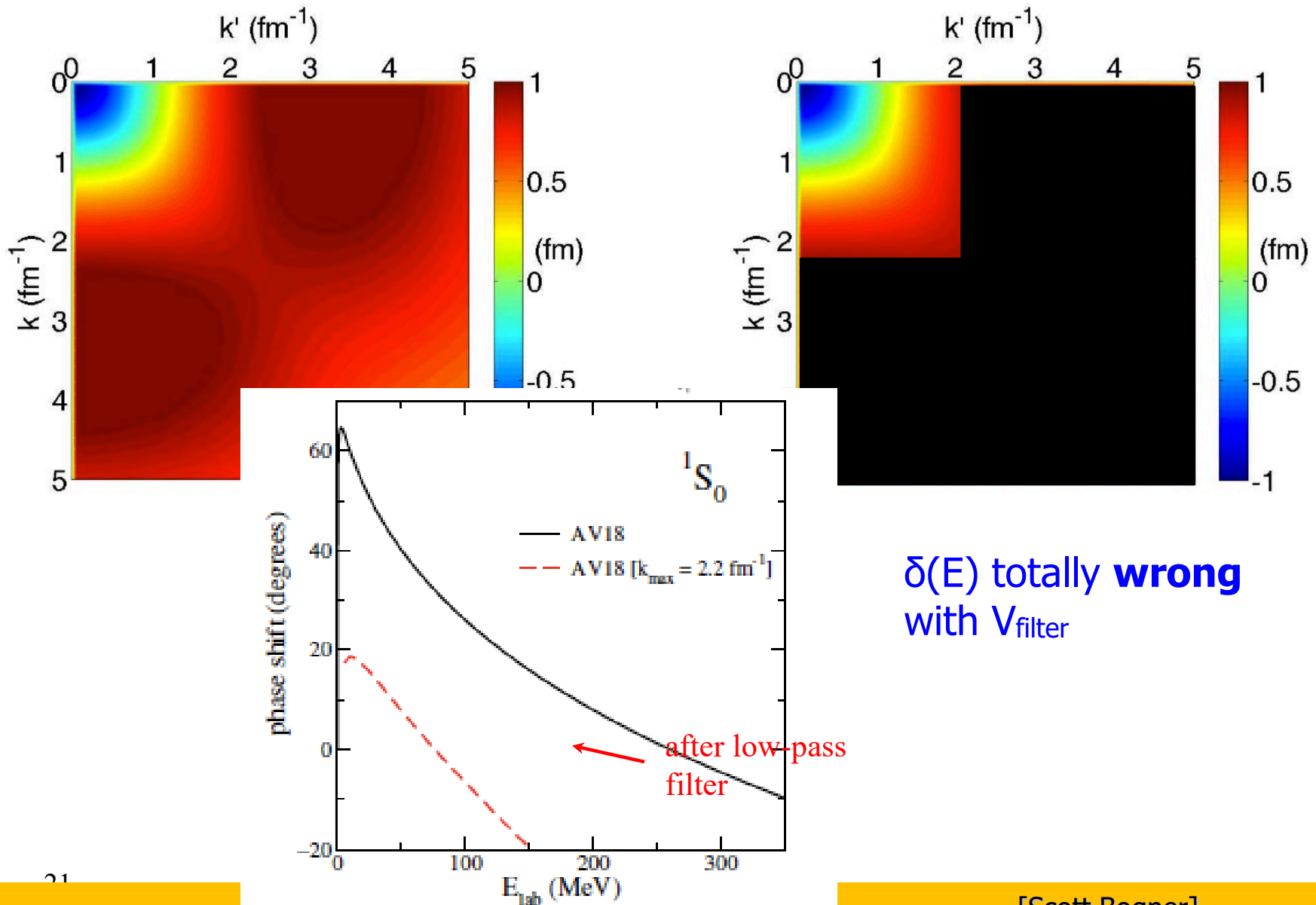
# Try a naive “low-pass” filter on V:



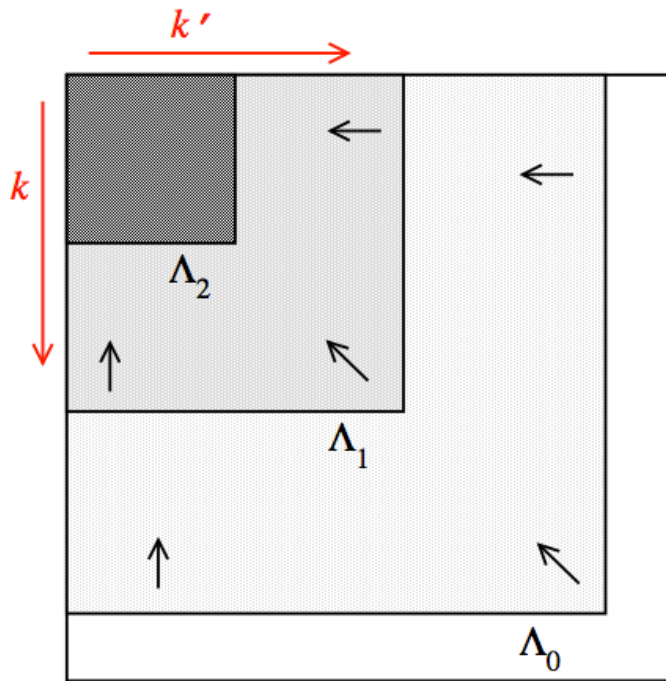
$$V_{filter}(k', k) \equiv 0 \quad k, k' > 2.2 \text{ fm}^{-1}$$

Now calculate low E observables (e.g., NN scattering) and see what happens...

# Try a naive “low-pass” filter on V:



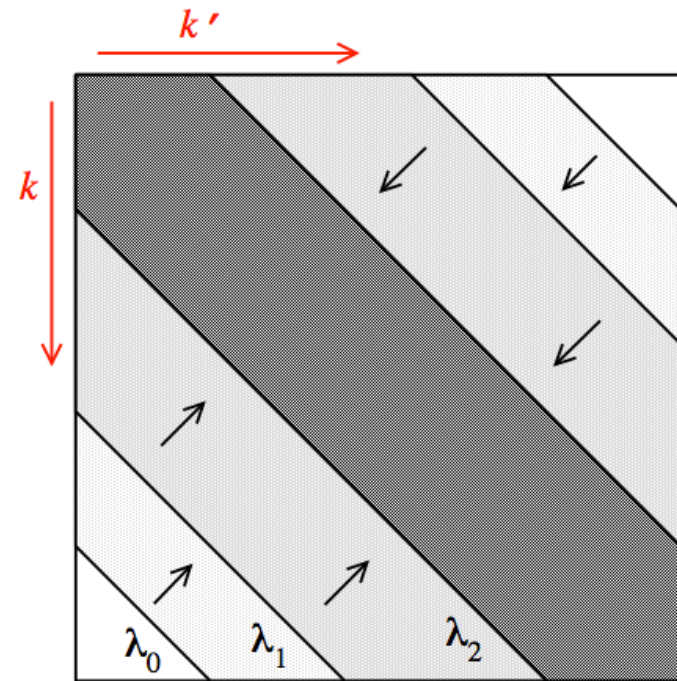
# 2 Types of Renormalization Group Transformations



“ $V_{\text{low } k}$ ”

integrate-out high  $k$  states

preserves observables for  $k < \Lambda$



“Similarity RG”

eliminate far off-diagonal coupling

preserves “all” observables

Identical simplifications despite differences in appearance!

Bogner, Furnstahl, Schwenk, Prog. Part. Nucl. Phys. **65** (2010)

# nuclei: a tough many-body problem

$$H_A = - \sum_{i=1}^A \frac{\hbar^2}{2m_i} \nabla_{\mathbf{r}_i}^2 + \frac{\hbar^2}{2M} \nabla_{\mathbf{S}}^2 + \sum_{i>j}^A V^{(2)}(\mathbf{r}_i - \mathbf{r}_j) + \sum_{i>j>k}^A V^{(3)}(\mathbf{r}_i - \mathbf{r}_j, \mathbf{r}_i - \mathbf{r}_k),$$

$$H_A \Phi_{I\mu}(\boldsymbol{\rho}_1, \dots, \boldsymbol{\rho}_{A-1}) = E_I \Phi_{I\mu}$$

$$\lim_{\boldsymbol{\rho}_i \rightarrow \infty} \Phi_{I\mu}(\dots, \boldsymbol{\rho}_i, \dots) = 0$$

$$\int d\boldsymbol{\rho}_1 \dots \int d\boldsymbol{\rho}_{A-1} |\Phi_{I\mu}(\boldsymbol{\rho}_1, \dots, \boldsymbol{\rho}_{A-1})|^2 = 1$$

soft forces make it more like quantum chemistry  
lead to approximations/controlled truncations

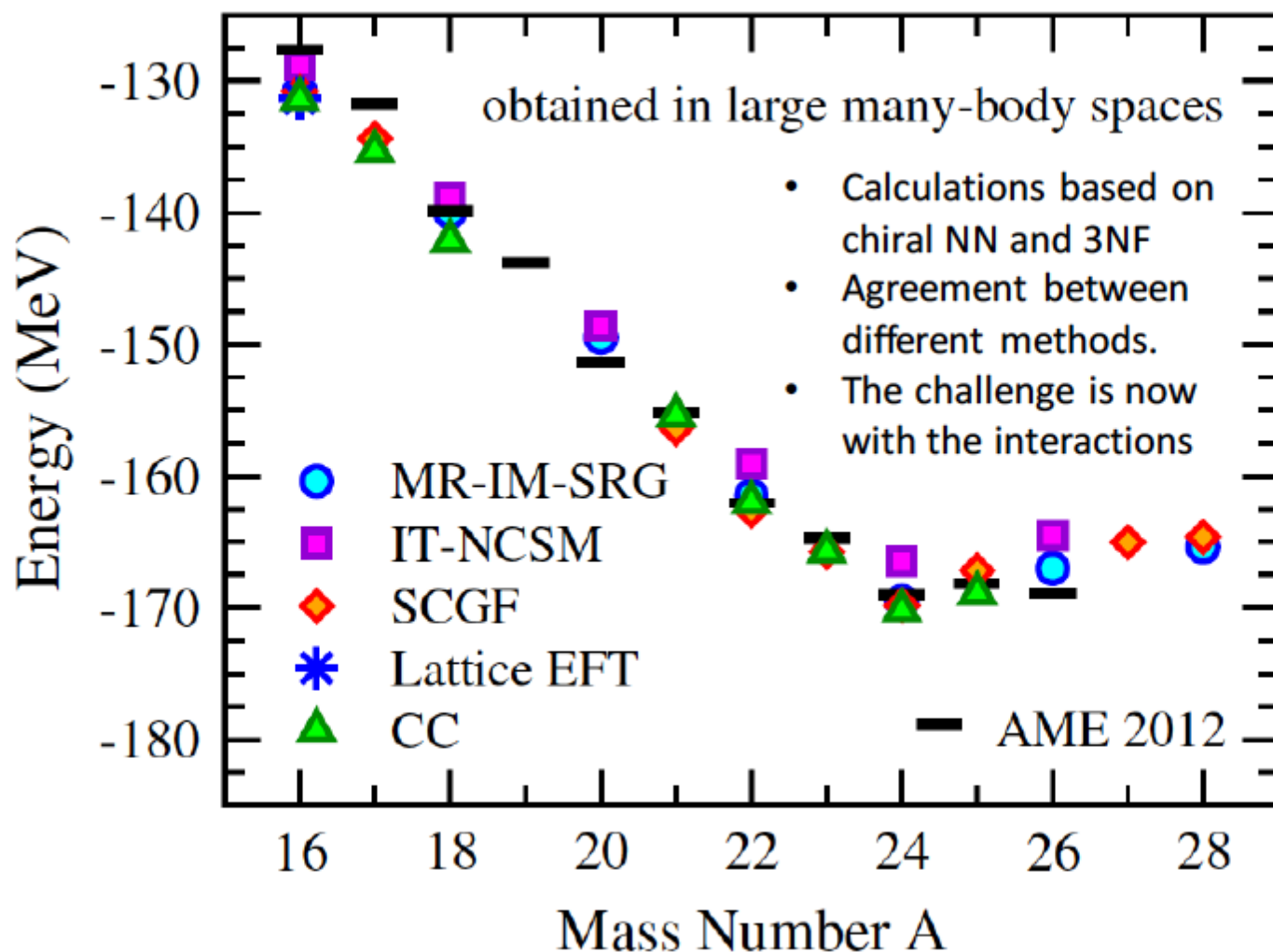
# Exciting developments in ab-initio methods



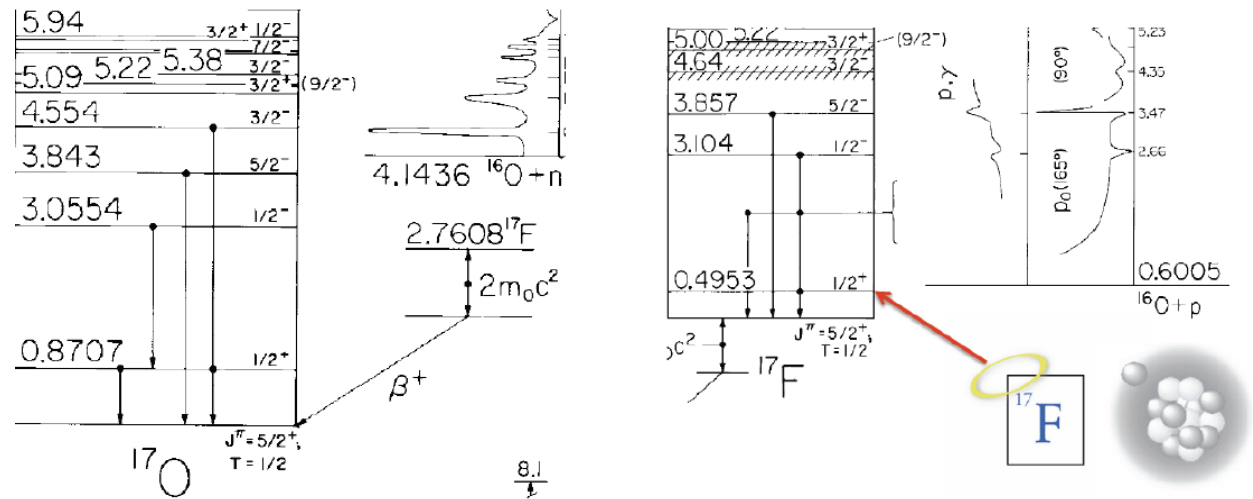
- no core shell model (NCSM)
  - based on harmonic oscillators
  - good for energies, not so good for other observables
  - up to  $A=16$
  - extension to include continuum and specific reaction channels
- green's function monte carlo (GFMC)
  - need a good starting variational wavefunction
  - implemented for specific forces
  - computationally demanding: hard limit  $A=12$
- coupled cluster method (CC)
  - widely used in quantum chemistry
  - ansatz contains correlations in the exponential
  - scaling better than NCSM
  - implemented with the gamow basis (continuum)
  - applications up to 2 nucleons away from closed sub-shell
- in medium Similarity Renormalization Group method (IMSRG)
  - applies a flow equation to obtain a diagonal matrix
  - scaling similar to coupled cluster
  - extension to ab-initio type shell model



## Oxygen chain with interactions from chiral EFT



# Ab-initio methods: coupled cluster for halos

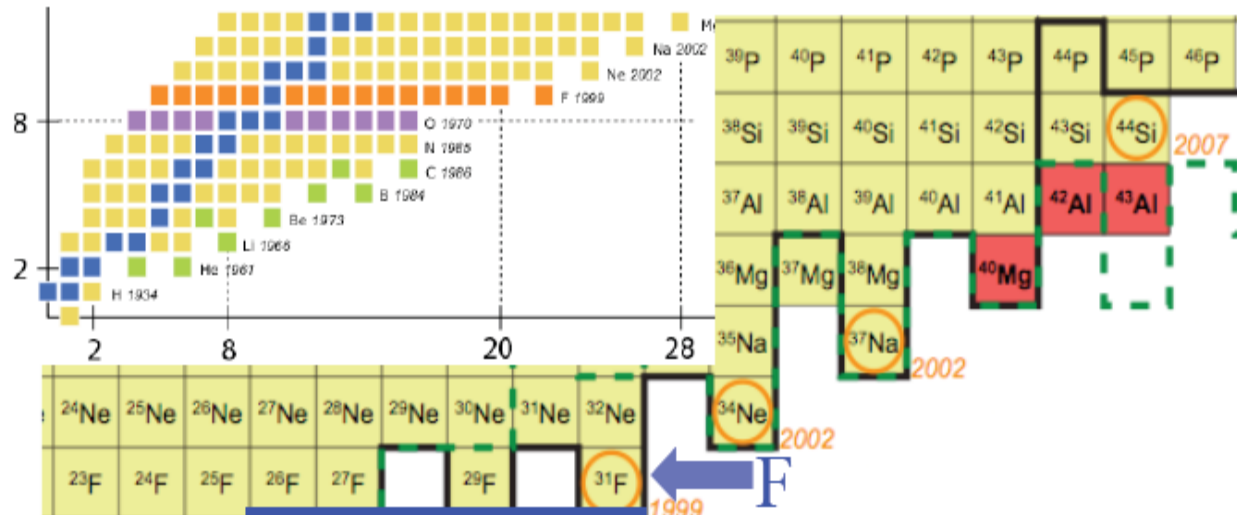


| $^{17}\text{O}$ |             |             |                   | $^{17}\text{F}$ |             |                   |
|-----------------|-------------|-------------|-------------------|-----------------|-------------|-------------------|
|                 | $(1/2)_1^+$ | $(5/2)_1^+$ | $E_{\text{s.o.}}$ | $(1/2)_1^+$     | $(5/2)_1^+$ | $E_{\text{s.o.}}$ |
| OHF             | -1.888      | -2.955      | 4.891             | 0.976           | 0.393       | 4.453             |
| GHF             | -2.811      | -3.226      | 4.286             | -0.082          | 0.112       | 3.747             |
| Exp.            | -3.272      | -4.143      | 5.084             | -0.105          | -0.600      | 5.000             |

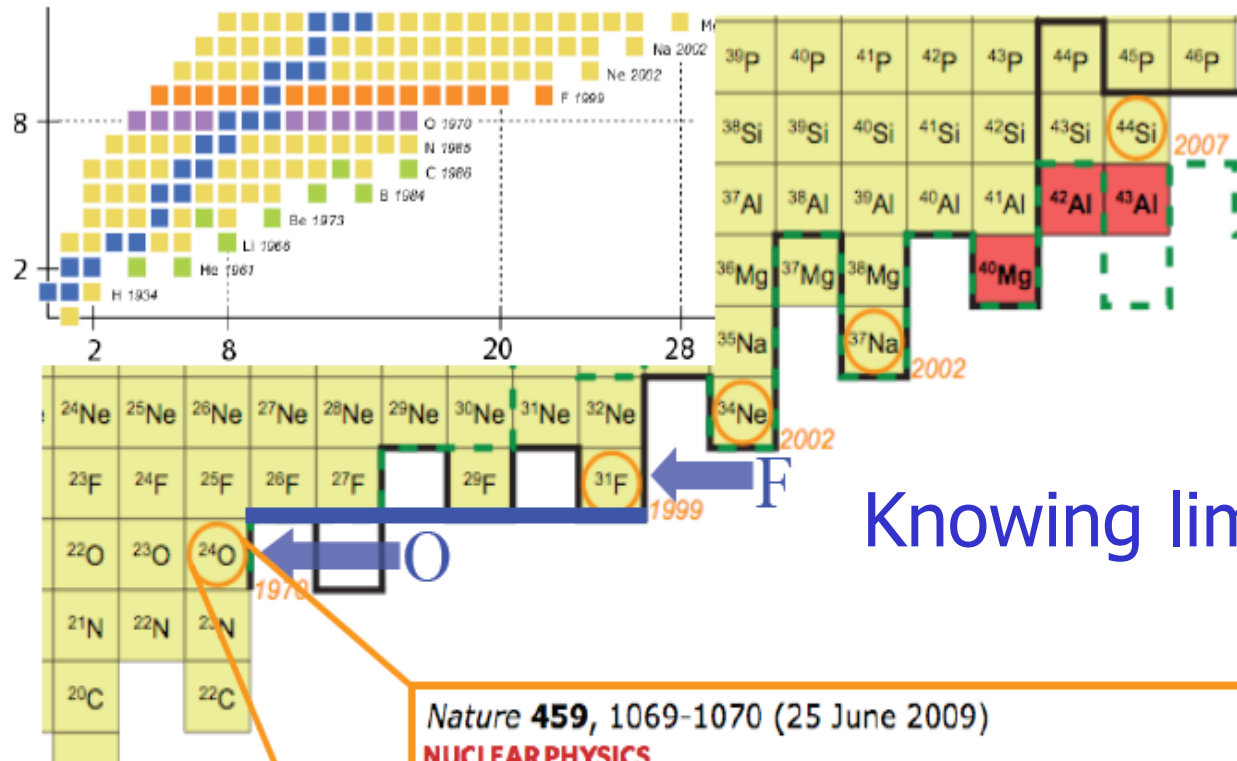
| $^{17}\text{O} (3/2)_1^+$ |                            |          | $^{17}\text{F} (3/2)_1^+$  |          |
|---------------------------|----------------------------|----------|----------------------------|----------|
|                           | $\text{Re}[E_{\text{sp}}]$ | $\Gamma$ | $\text{Re}[E_{\text{sp}}]$ | $\Gamma$ |
| PA-EOMCCSD                | 1.059                      | 0.014    | 3.859                      | 0.971    |
| Experiment                | 0.942                      | 0.096    | 4.399                      | 1.530    |

# QUESTION TIME

1. When solving the many-nucleon problem, what is the price you pay in using RG techniques to soften NN forces?
2. What is the dripline of  $Z=8$  isotopes? First have a guess using only the nuclear chart provided below. Then you can google...



# understanding nuclei



Knowing limits of stability

*Nature* **459**, 1069-1070 (25 June 2009)

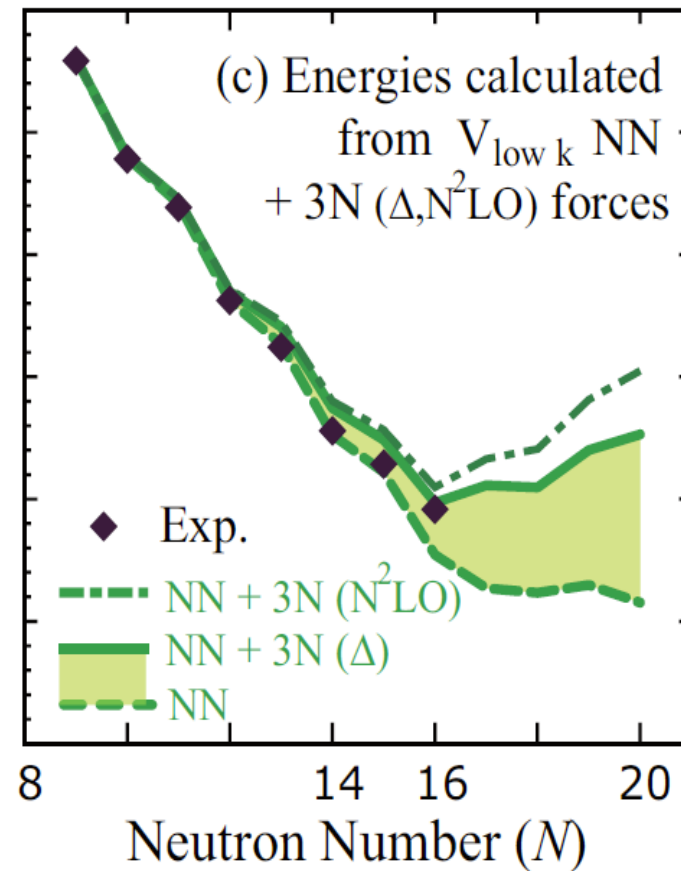
**NUCLEAR PHYSICS**

## Unexpected doubly magic nucleus

Robert V. F. Janssens

Nuclei with a 'magic' number of both protons and neutrons, dubbed doubly magic, are particularly stable. The oxygen isotope  $^{24}\text{O}$  has been found to be one such nucleus — yet it lies just at the limit of stability.

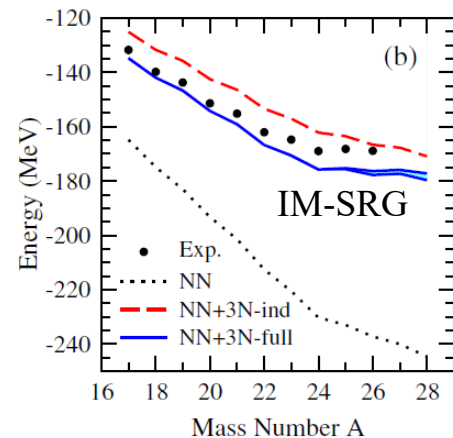
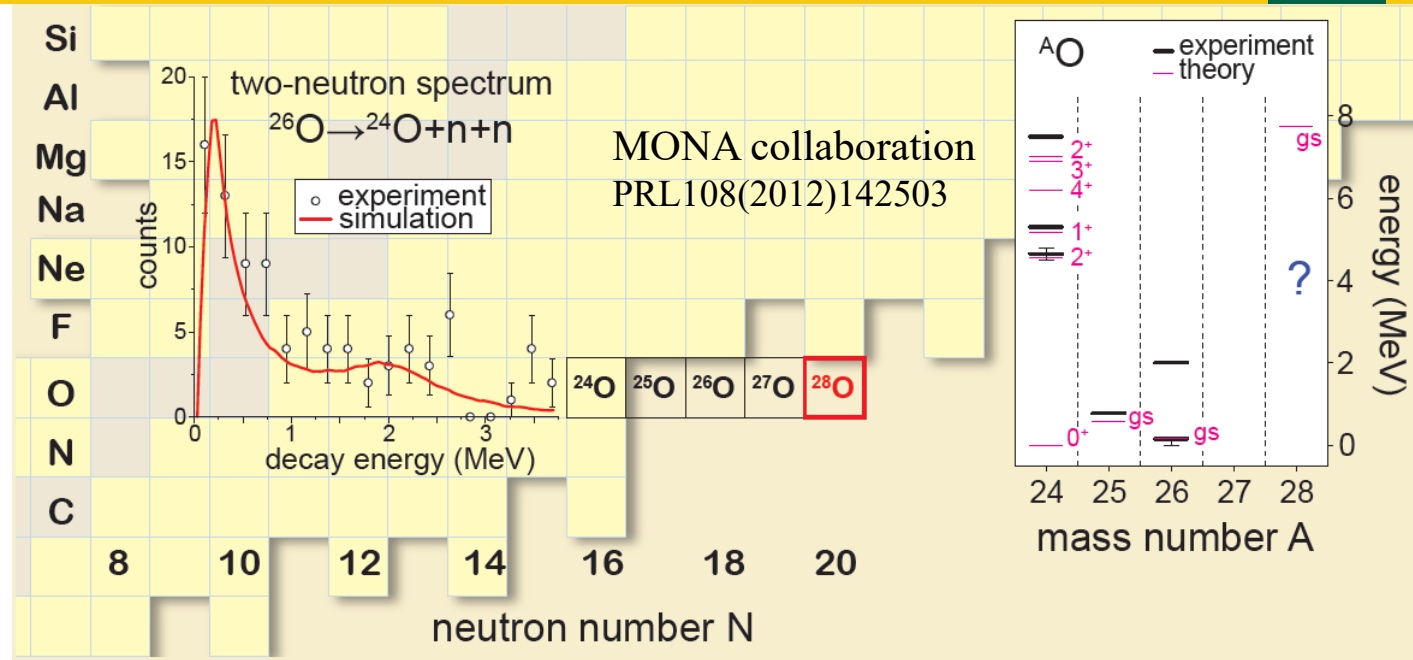
# three-body force for Oxygen isotopes



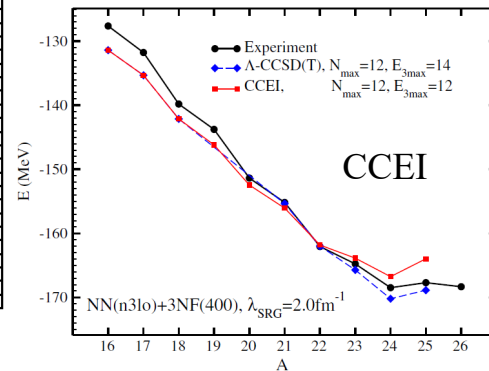
Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL (2009)

# Exotic nuclei impose stringent tests on theory

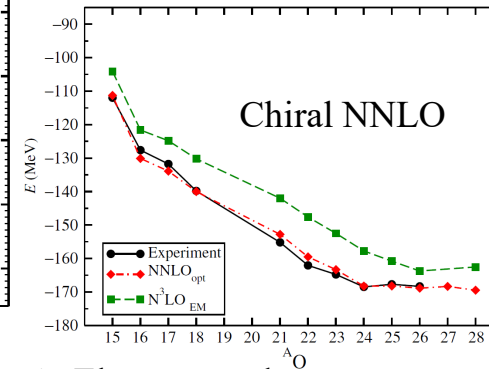
Surprises with the Oxygen isotopes, at and beyond stability, have provided crucial information to constrain the effective nuclear force!



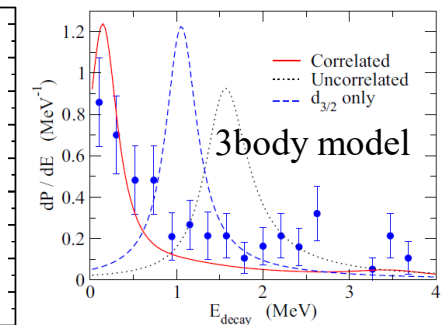
S.K. Bogner et al.  
PRL113(2014)142501



G.R. Jansen et al.  
PRL113(2015)142502

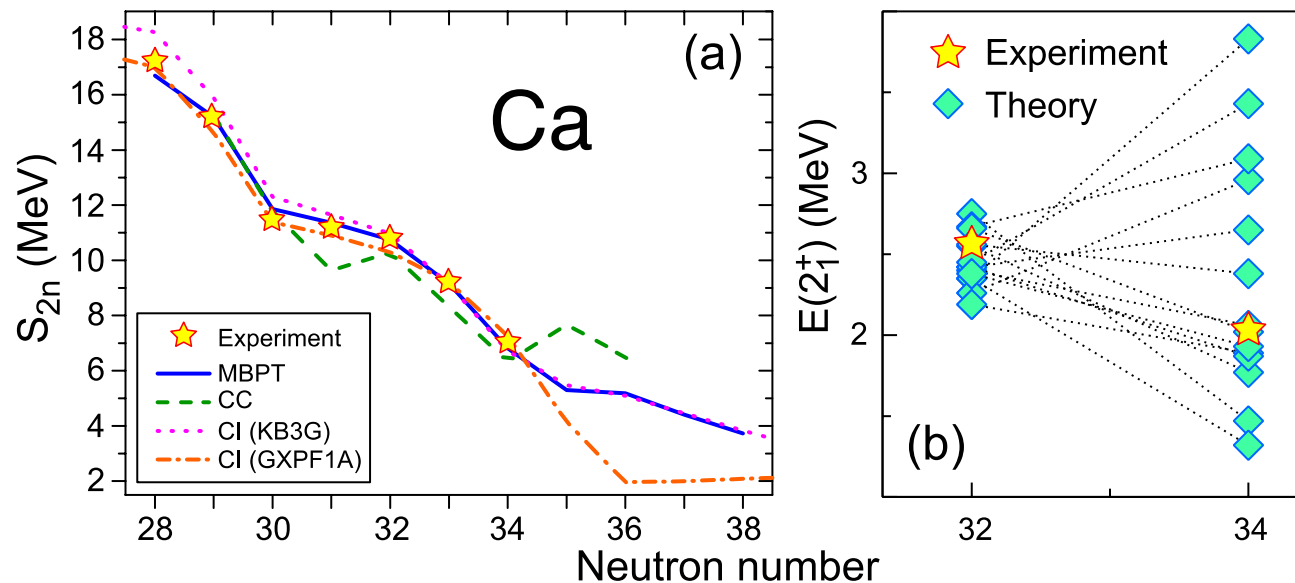


A. Ekström et al.  
PRL110(2013)192502



K. Hagino and H. Sagawa  
PRC89(2014)014331

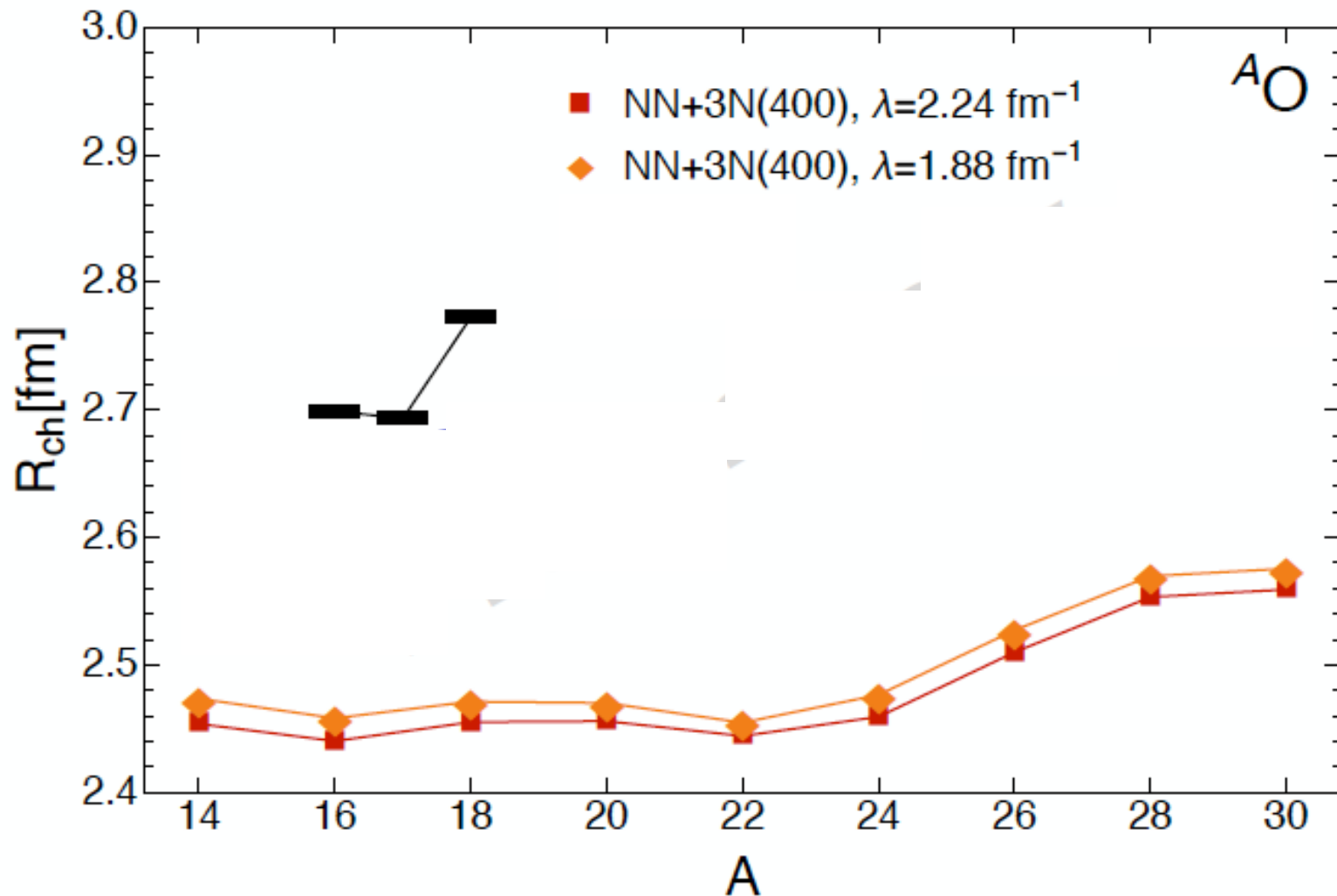
- Theory and experiment work hand-in-hand:  
experiment guides theory --- theory guides experiment
- Need to integrate theory and experiment to exploit FRIB's full potential and optimize its research.



F. Wienholtz *et al.*, *Nature* **498**, 346 (2013).  
D. Steppenbeck *et al.*, *Nature* **502**, 207 (2013)

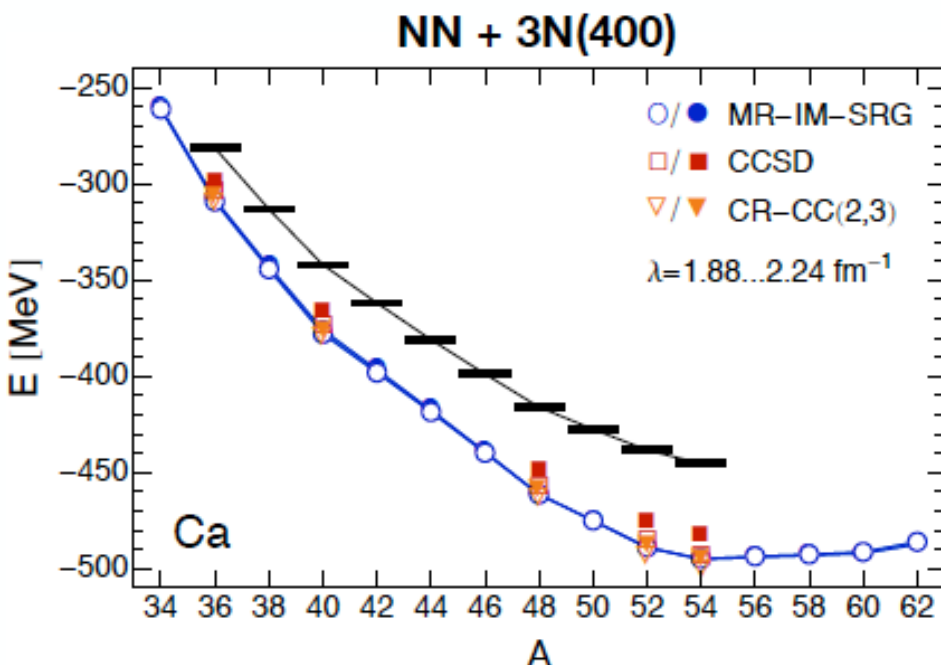
# problems with our forces? radii for Oxygen

*V. Lapoux, V. Somà, C. Barbieri, H. H., J. D. Holt, and S. R. Stroberg,*

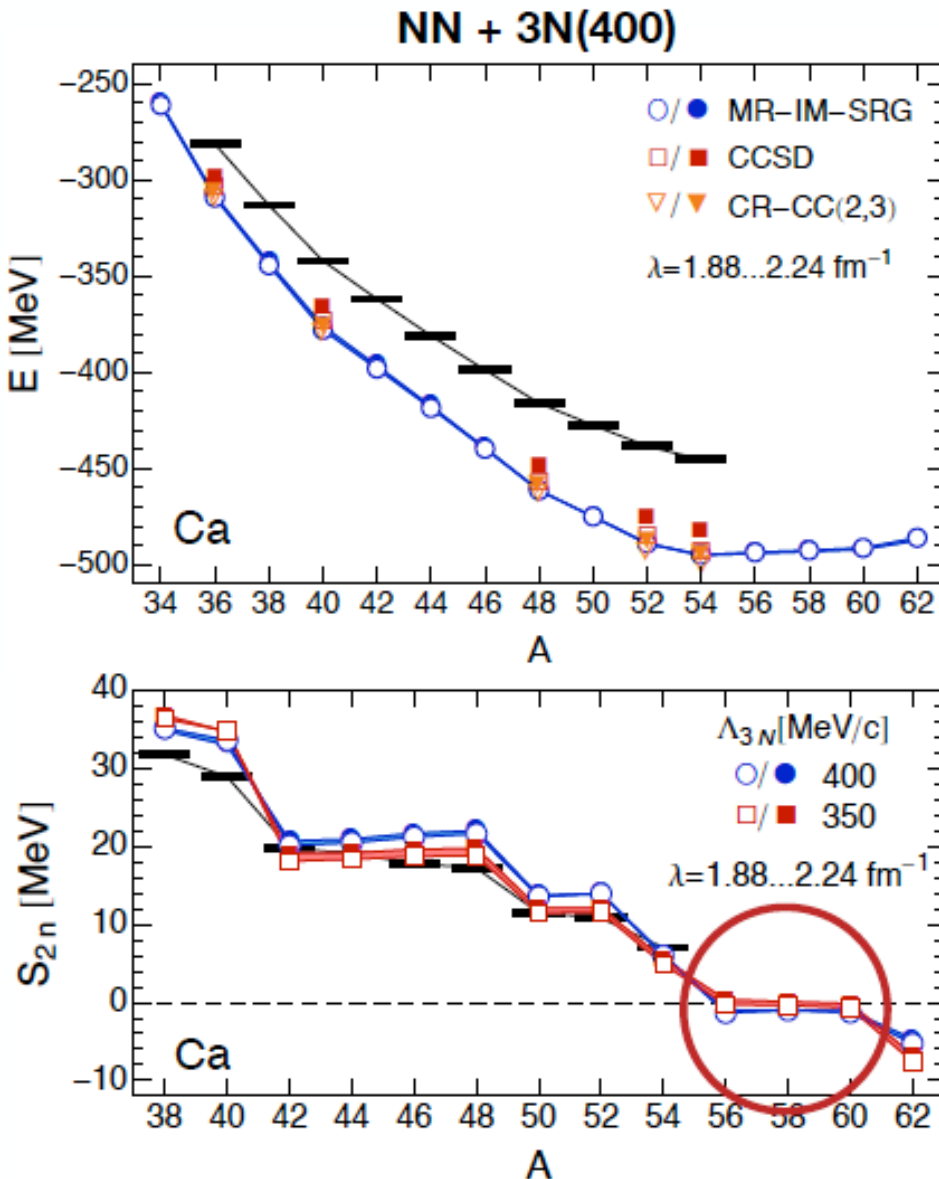




# Other issues with Chiral EFT forces



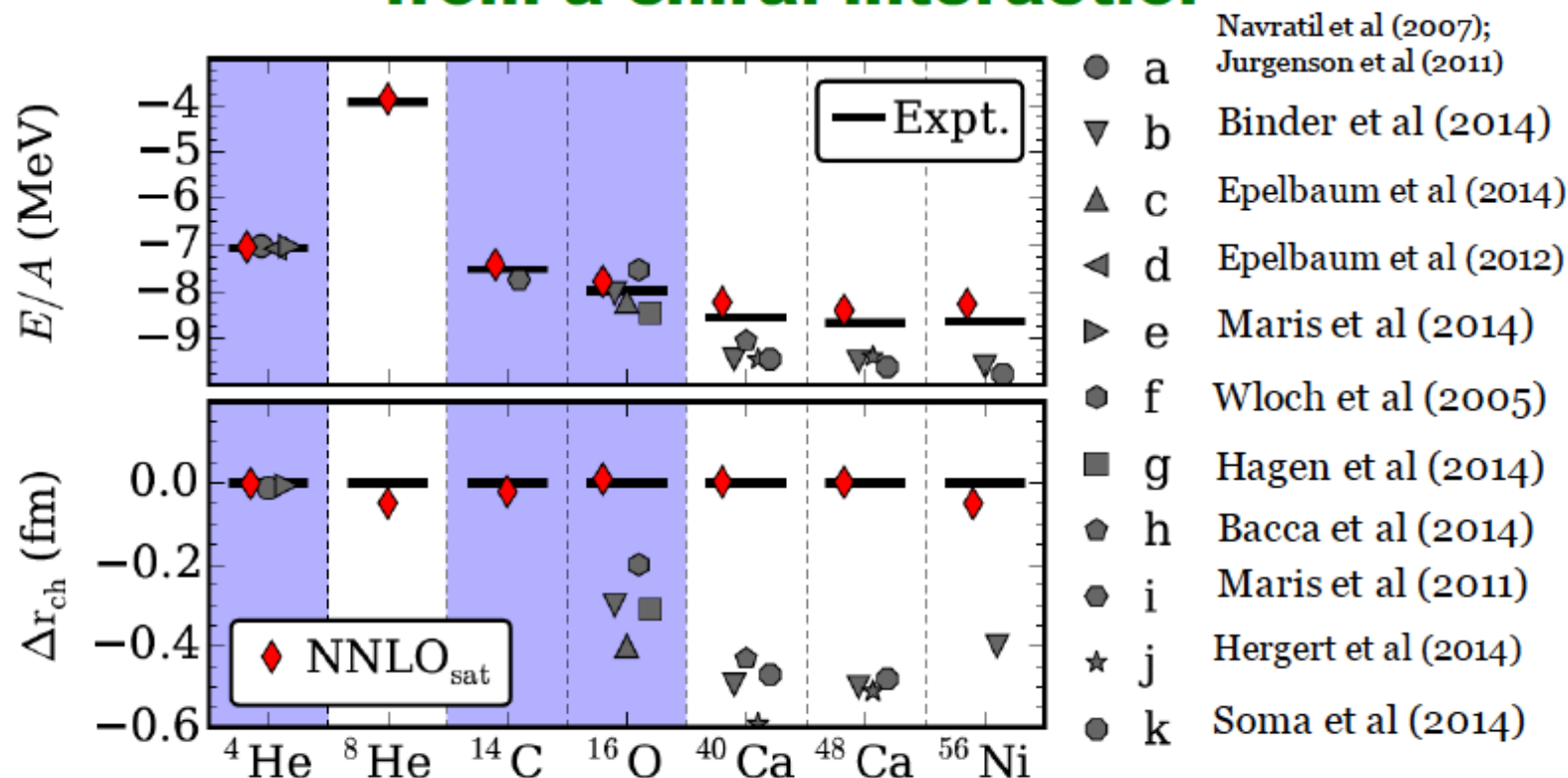
# Other issues with Chiral EFT forces



- differential observables ( $S_{2n}$ , spectra,...) filter out interaction components that cause overbinding
- predict flat trends for g.s. energies/ $S_{2n}$  beyond  $^{54}\text{Ca}$  - await experimental data
- $^{52}\text{Ca}$ ,  $^{54}\text{Ca}$  magic for these NN+3N interactions
- no continuum coupling yet, other  $S_{2n}$  uncertainties  $< 1\text{MeV}$

# Refitting EFT parameters to include nuclei

## Accurate nuclear binding energies and radii from a chiral interaction



Simultaneous optimization of NN and 3NFs  
Include charge radii and binding energies of  $^3\text{H}$ ,  $^3,4\text{He}$ ,  $^{14}\text{C}$ ,  $^{16}\text{O}$  in the optimization ( $\text{NNLO}_{\text{sat}}$ )

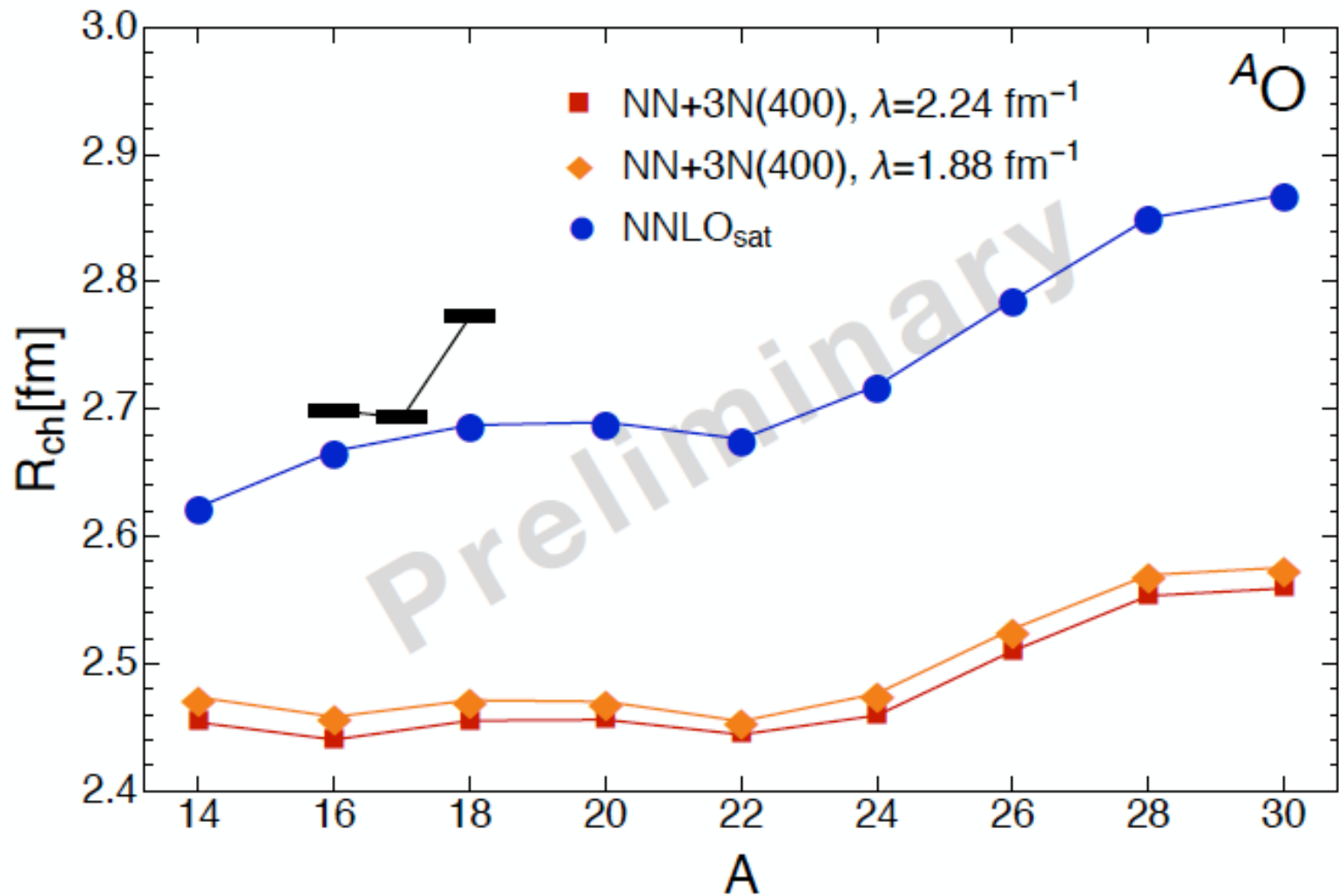
A. Ekström et al, Phys. Rev. C **91**, 051301(R) (2015).

G. Hagen et al, arXiv:1601.08203 (2016).

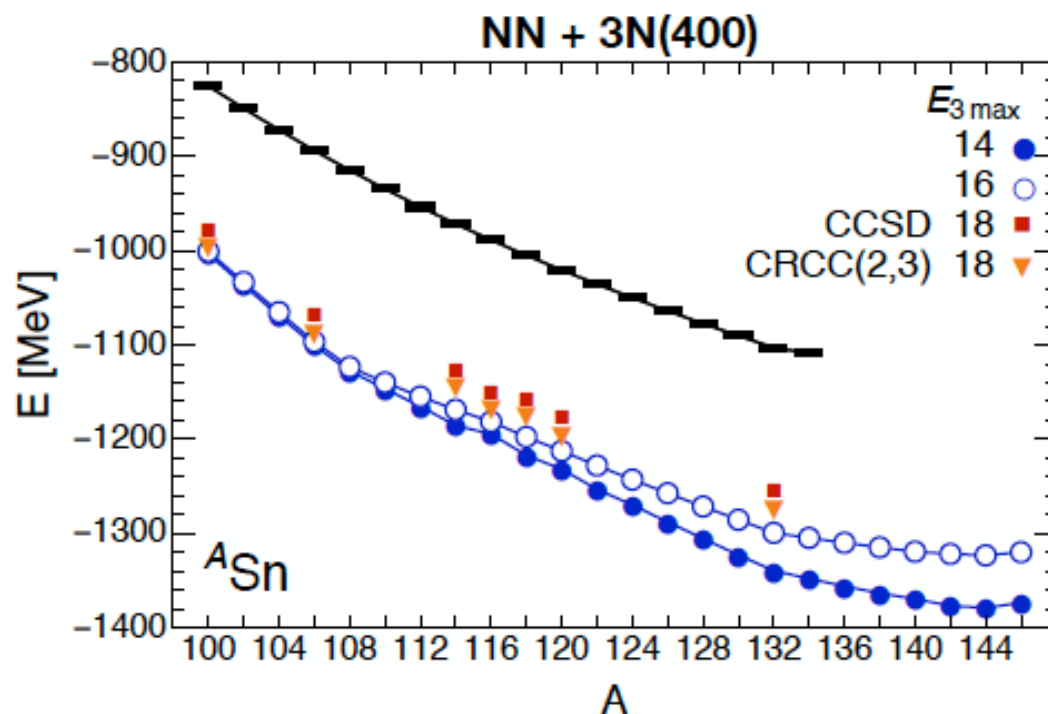
**Critical ingredient:**  
Three-nucleon forces  
with non-local  
regulators

# problems with our forces? radii for Oxygen

*V. Lapoux, V. Somà, C. Barbieri, H. H., J. D. Holt, and S. R. Stroberg,*



# The mass frontier with ab-initio: Tin



| $E_{3\text{max}}$ | memory (float) [GB] |
|-------------------|---------------------|
| 14                | 5                   |
| 16                | ~20                 |
| 18                | 100+                |

- systematics of overbinding similar to Ca/Ni
- not converged with respect to 3N matrix element truncation:

$$e_1 + e_2 + e_3 \leq E_{3\text{max}}$$

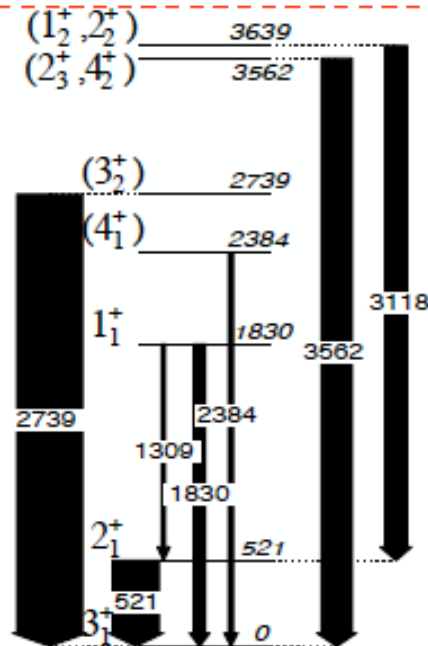
( $e_{1,2,3}$  : SHO energy quantum numbers)

- need technical improvements to go further

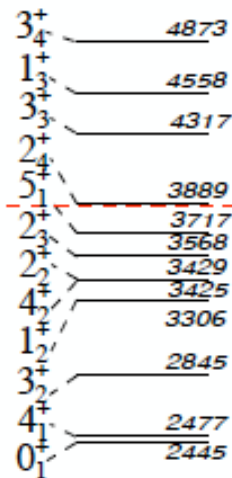
# Detailed spectroscopy with ab-initio theories

**$^{24}\text{F}$**

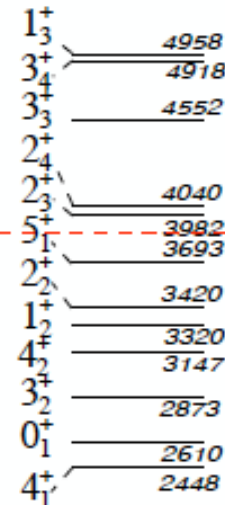
$S_n = 3840(110) \text{ keV}$



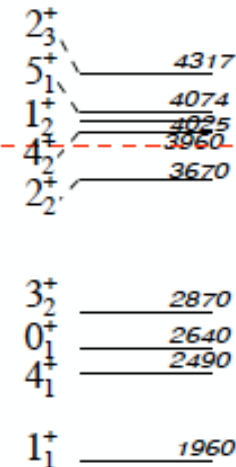
Exp.



USDA



USDB



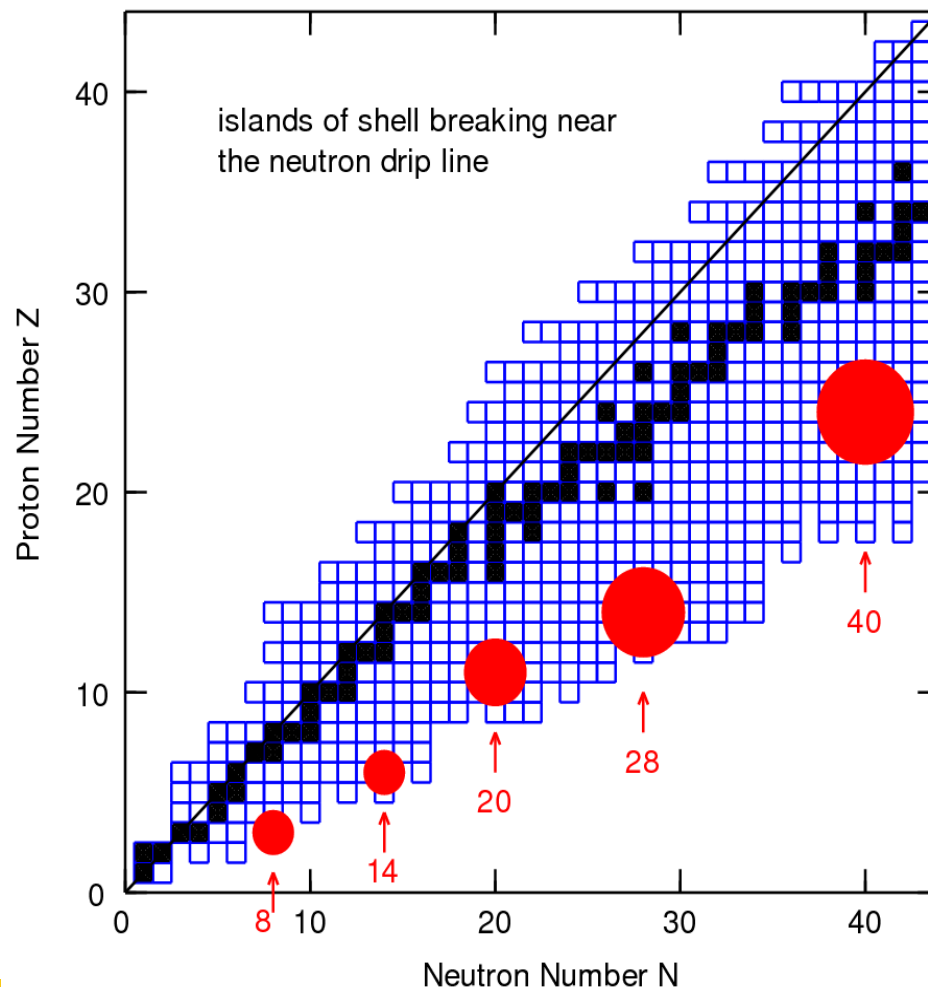
IM-SRG  
NN+3N-full

L. Caceres et al., PRC92, 014327 (2015)

# shell structure away from stability

*what happened to our magic numbers?*

Brown, Viewpoint 2010

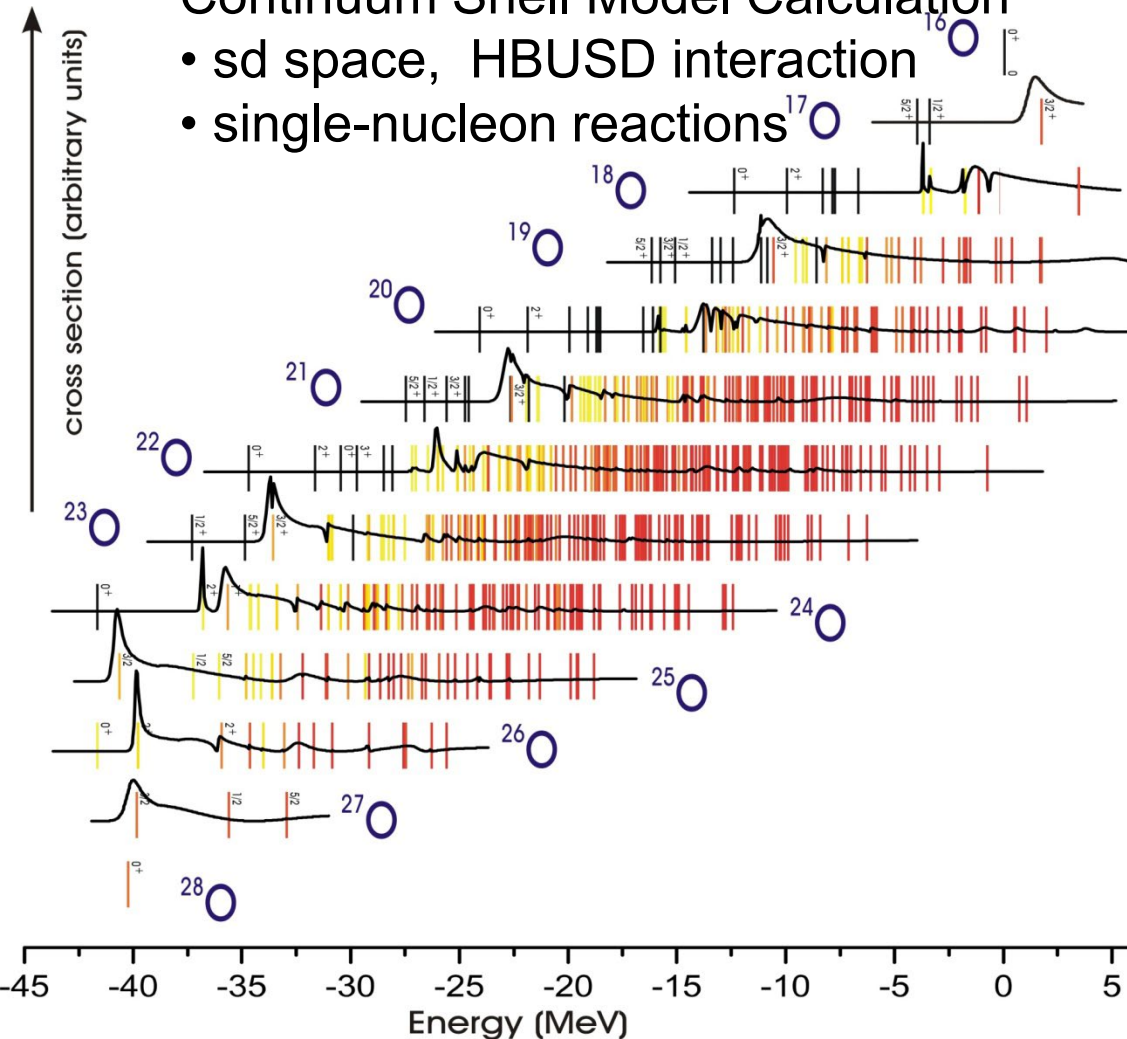


# Continuum shell model

## Oxygen Isotopes

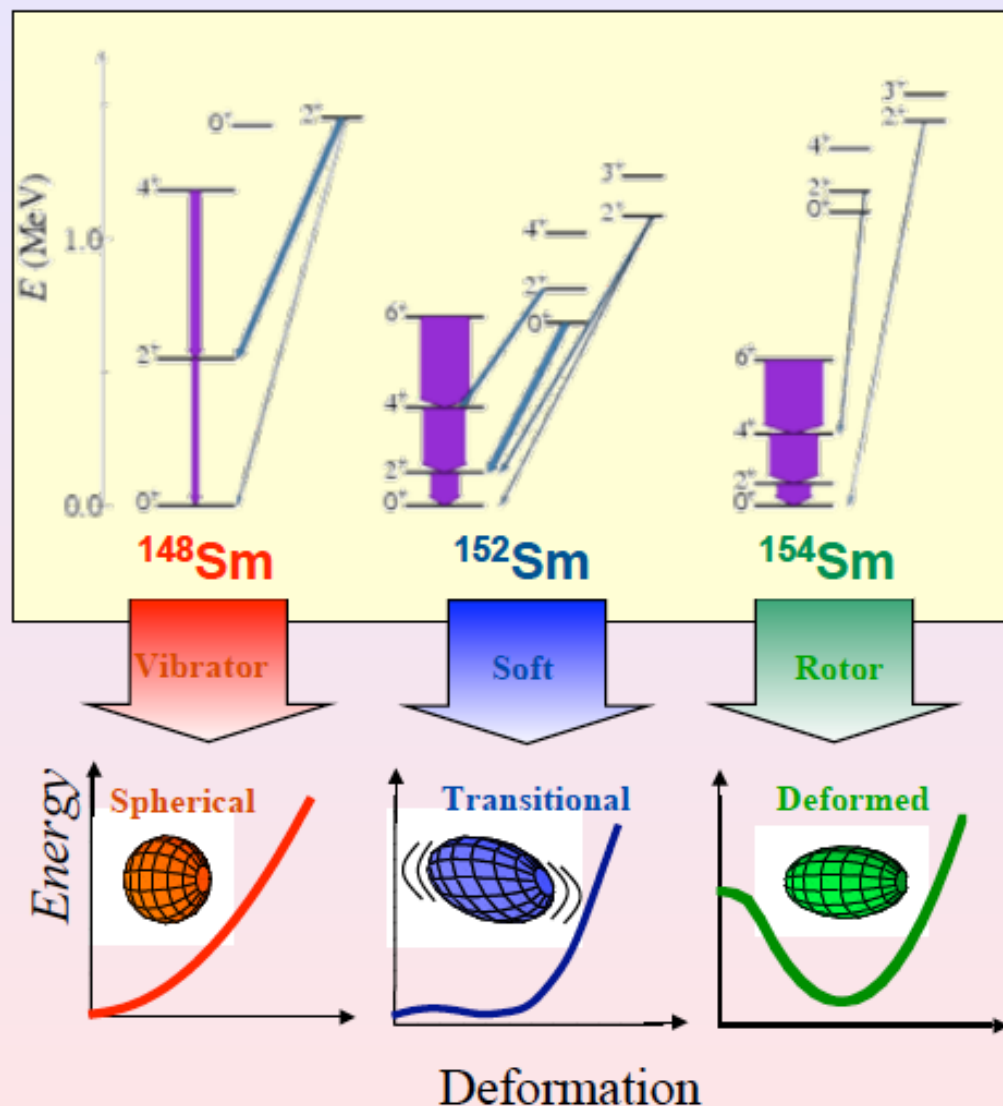
### Continuum Shell Model Calculation

- sd space, HBUSD interaction
- single-nucleon reactions





# Collective effects are a real challenge for ab-initio



## Challenges for theory

- Possible shape transitions, huge spaces needed to describe properly.
- Theory: need to marry *ab initio* methods with density functional theories in order to describe such systems
- Need a large wealth of experimental data to constrain theory

# Density functional approach

- Hohenberg-Kohn: there exists a universal energy functional
- approximate the energy functional
- introduce orbitals and minimize energy functional
- self-consistent

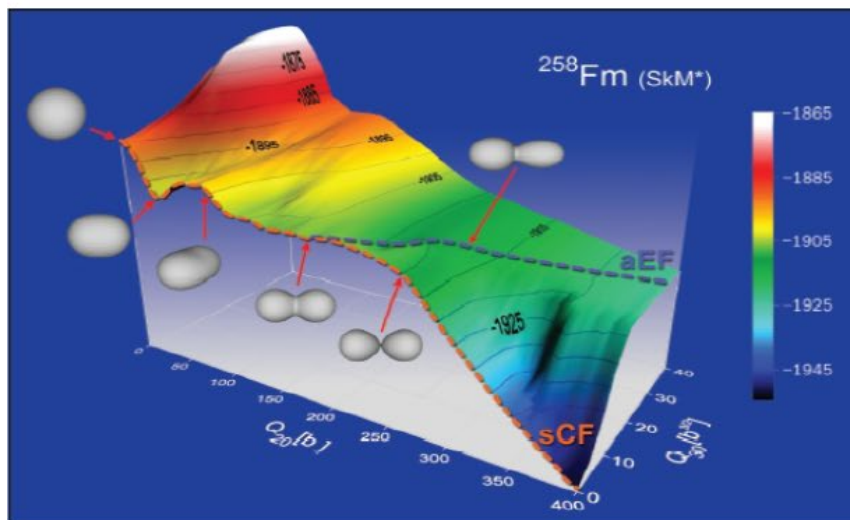
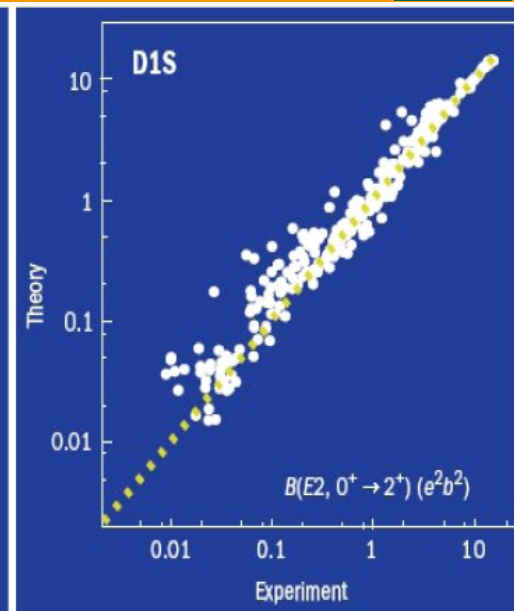
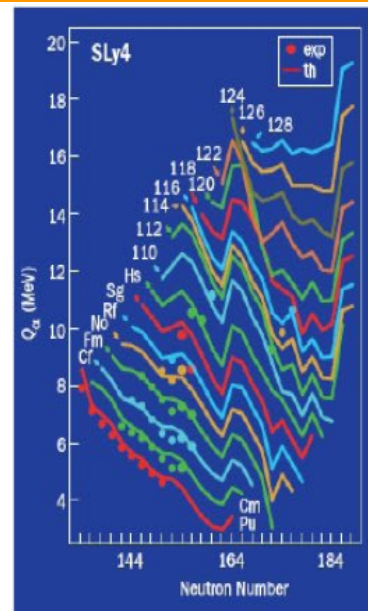
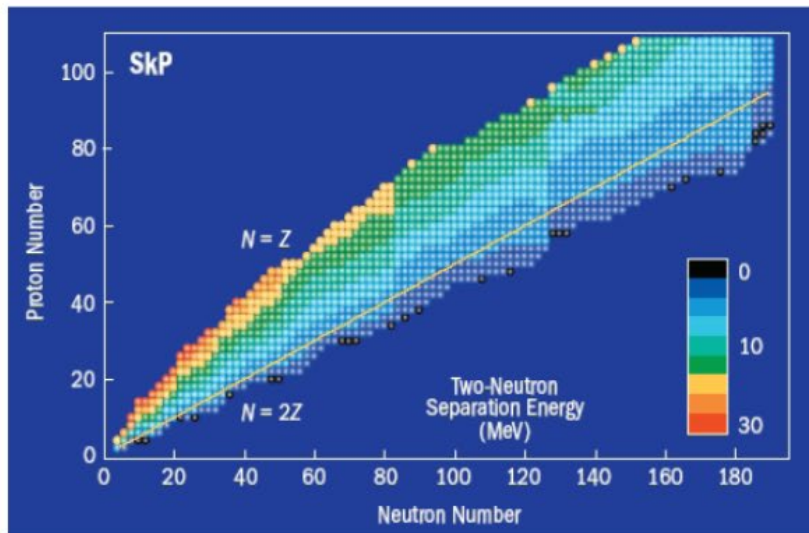
## Phenomenological Skyrme Functionals

- Minimize  $E = \int d\mathbf{x} \mathcal{E}[\rho(\mathbf{x}), \tau(\mathbf{x}), \mathbf{J}(\mathbf{x}), \dots]$  (for  $N = Z$ ):

$$\begin{aligned} \mathcal{E}[\rho, \tau, \mathbf{J}] = & \frac{1}{2M} \tau + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} t_3 \rho^{2+\alpha} + \frac{1}{16} (3t_1 + 5t_2) \rho \tau \\ & + \frac{1}{64} (9t_1 - 5t_2) (\nabla \rho)^2 - \frac{3}{4} W_0 \rho \nabla \cdot \mathbf{J} + \frac{1}{32} (t_1 - t_2) \mathbf{J}^2 \end{aligned}$$

- where  $\rho(\mathbf{x}) = \sum_i |\phi_i(\mathbf{x})|^2$  and  $\tau(\mathbf{x}) = \sum_i |\nabla \phi_i(\mathbf{x})|^2$  (and  $\mathbf{J}$ )

# Density functional approach



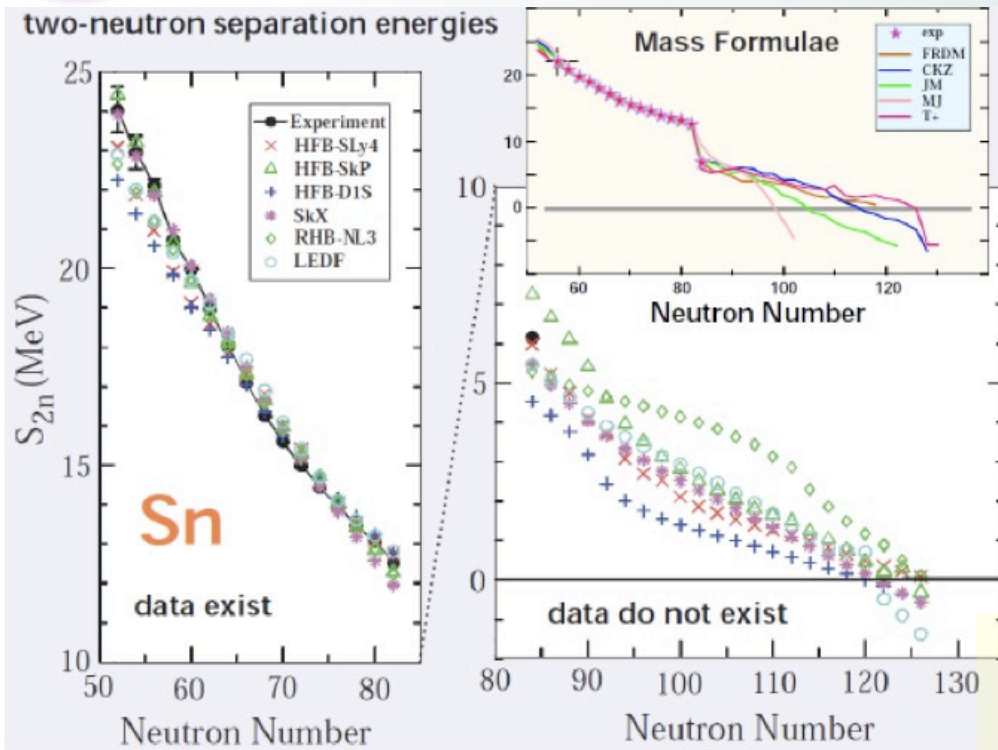
2N separation energies, Quadrupole and BE2 values, Fission energy surfaces, mass tables in a day, plus many other impressive feats

**BUT...**

# Density functional approach



## UNEDF SciDAC Collaboration Universal Nuclear Energy Density Functional



What is missing from Skyrme?

- Simplistic density dependence
- No connection to pion-exchange (NN+NNN)
- Does not capture different spin-orbit NN and NNN mechanisms (short versus long range)

Turn to underlying  
NN+NNN forces +  
microscopic many-body  
theories for guidance

# Why exotic stuff?

Nuclear forces constrained in the valley of stability

predict diverging properties away from stability

need exotic nuclei for reliability

feeds back into our understanding of stable matter

Moving along an isotopic line: provides sensitivity to isospin

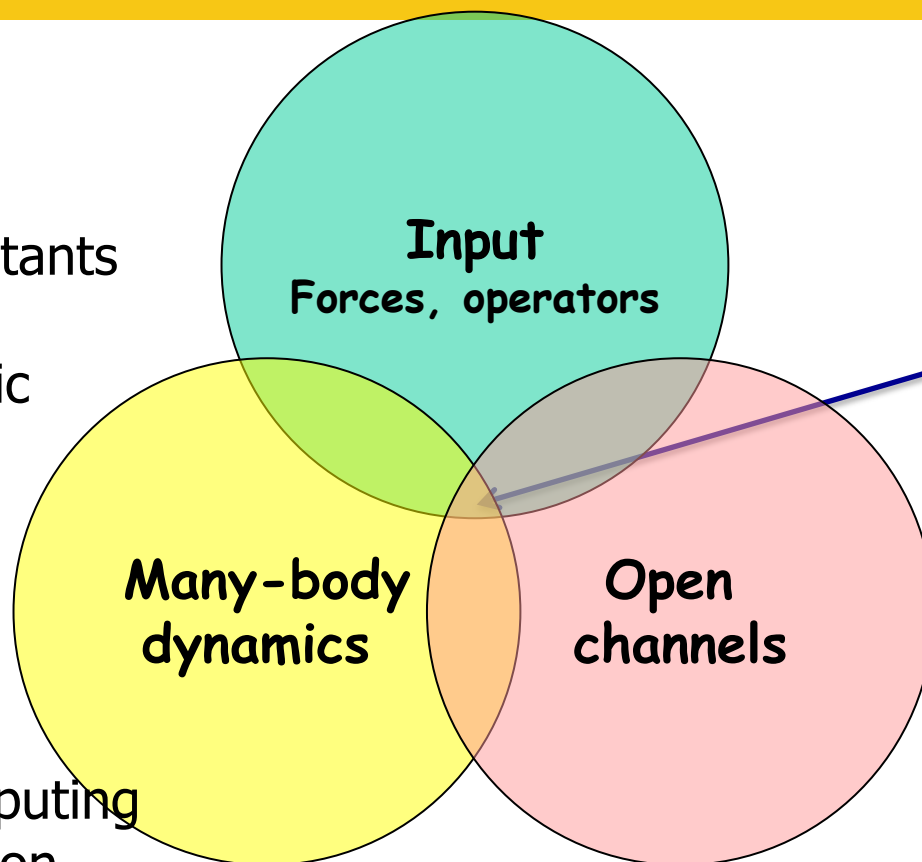
Moving to low binding energies: sensitivity to  $3N$  (or higher)

Moving toward nuclear dripline: probes density dependence

Wider variety of nuclear phenomena away from stability

# Physics of nuclei is demanding

- rooted in QCD – EFT expansions
- many-body interactions
- low-energy coupling constants optimized to NN data
- crucial insights from exotic nuclei



$^{11}\text{Li}$   
 $^{240}\text{Pu}$   
 $^{298}\text{U}$

- many-body techniques
- high-performance computing
- uncertainty quantification
- interdisciplinary connections

- nuclear structure impacted by couplings to reaction and decay channels
- clustering, alpha decay, and fission still remain major challenges for theory
- unified picture of structure and reactions

## QUESTION TIME

Go and explore DFTs  
[massexplorer.frib.msu.edu](http://massexplorer.frib.msu.edu)

Compare the predictions of binding energy for  $^{40}\text{Ca}$  and  $^{60}\text{Ca}$  for a number of different functionals.

Where is the Ca dripline for these various functionals?

Questions?



# Reaching towards the FRIB benchmark $^{60}\text{Ca}$

G. Hagen *et al*, arXiv:1601.08203 (2016).

