Nuclear structure theory

Thomas Papenbrock

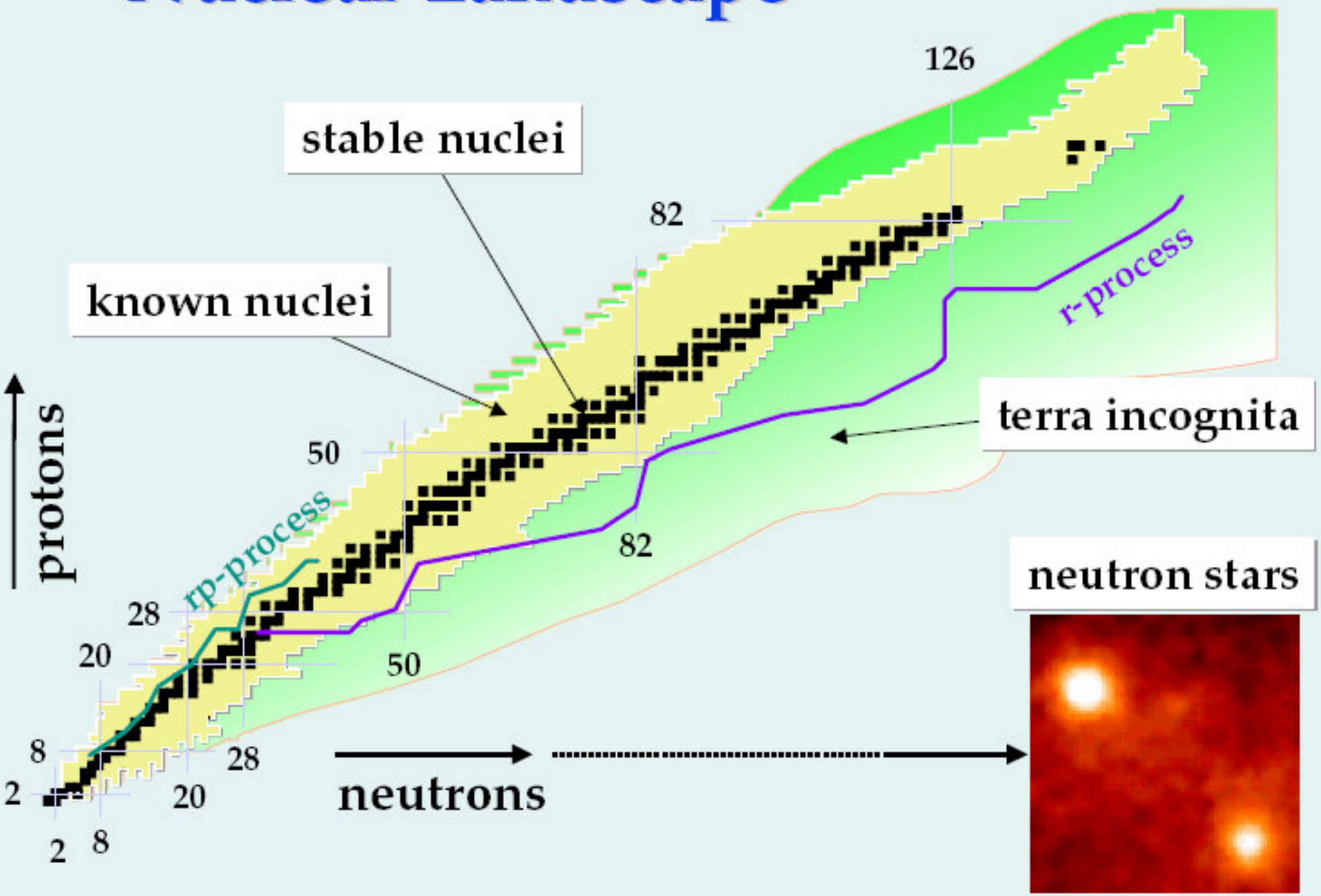
and OAK RIDGE NATIONAL LABORATORY

Aim of these lectures:

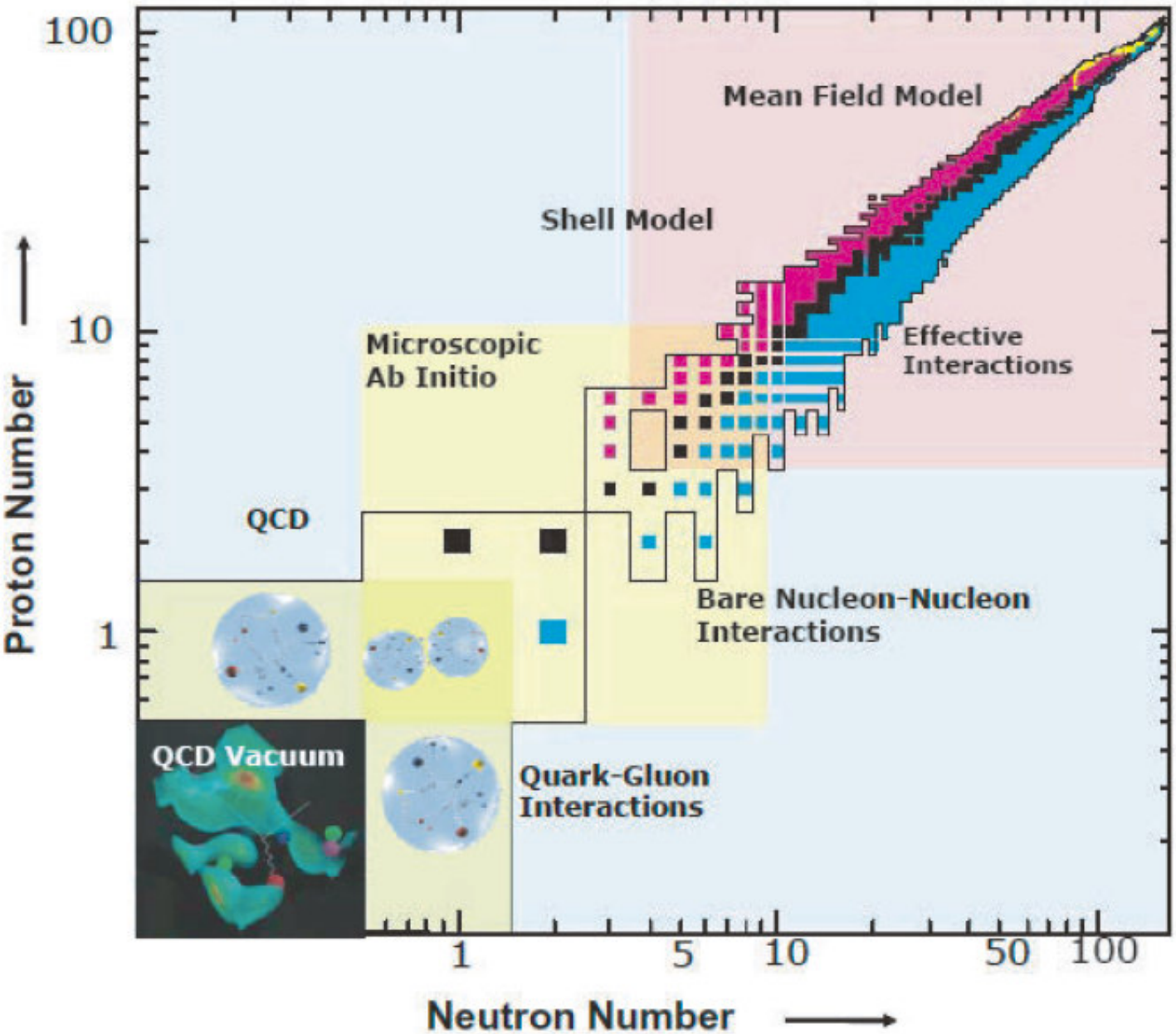
To give an overview of contemporary nuclear structure theory, i. e. effective interactions, methods that solve the quantum many-body problem, and results of such calculations.

RIA 2006 Summer School at Oak Ridge

Nuclear Landscape



Overview: theoretical approaches



What are the properties of nuclei?

What is the effective interaction?

How does one solve the nuclear many-body problem?

Figure from: A. Richter, INPC 2004

Content of lectures

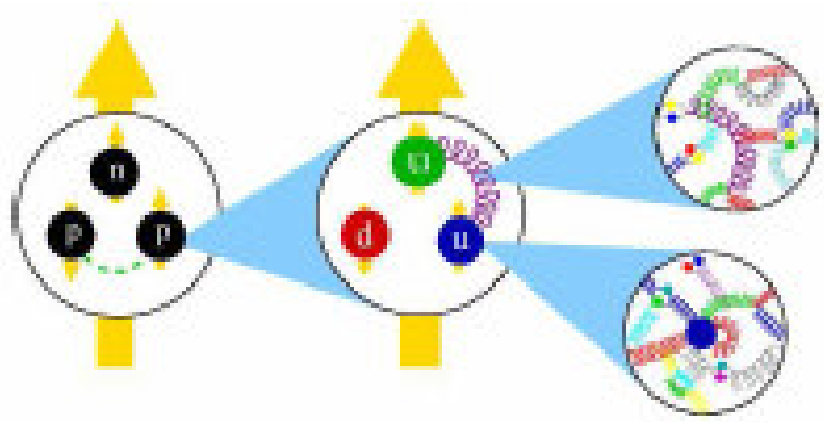
1. Microscopic ab-initio nuclear structure theory
   1. Determination of the effective interaction
   2. Solving the quantum many-body problem

2. Shell model

3. Nuclear density-functional theory & mean field calculations

The effective NN interaction

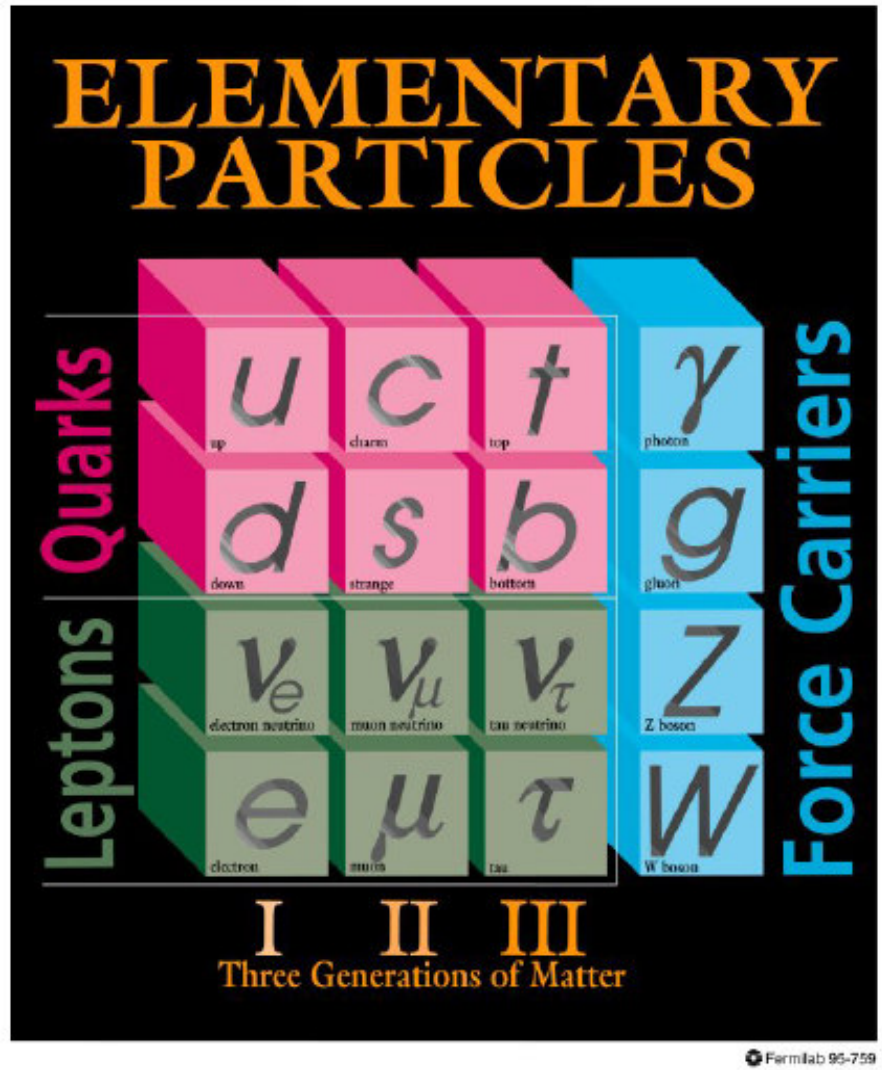
- Nuclei are made of protons and neutrons. These are composite particles



Interplay between nucleonic and sub-nucleonic (quarks and gluons) degrees of freedom in few-body nuclear systems

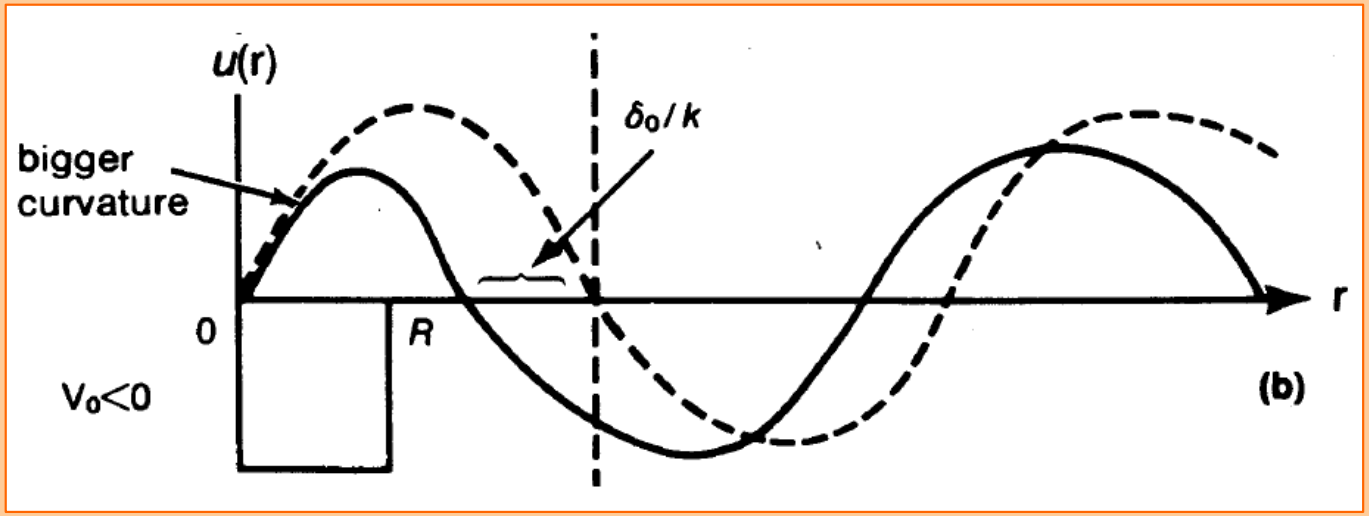
Q: How do we determine the interaction between two nucleons?

A: Study two-nucleon scattering!

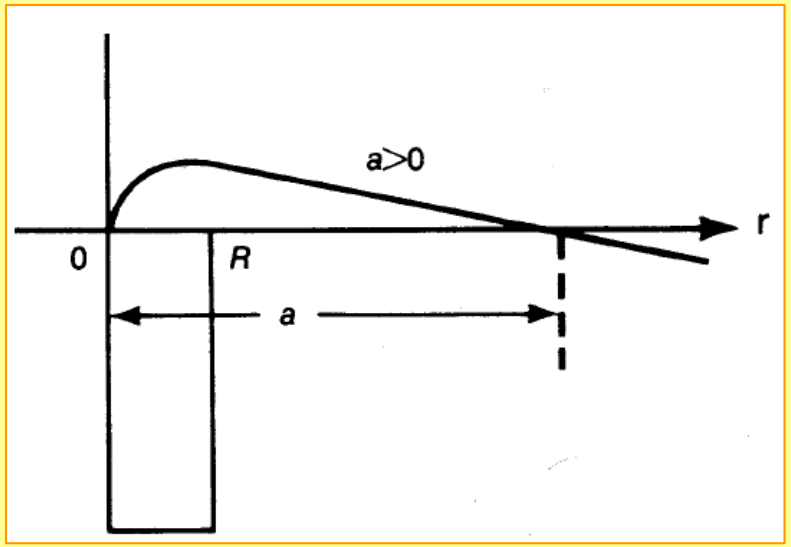


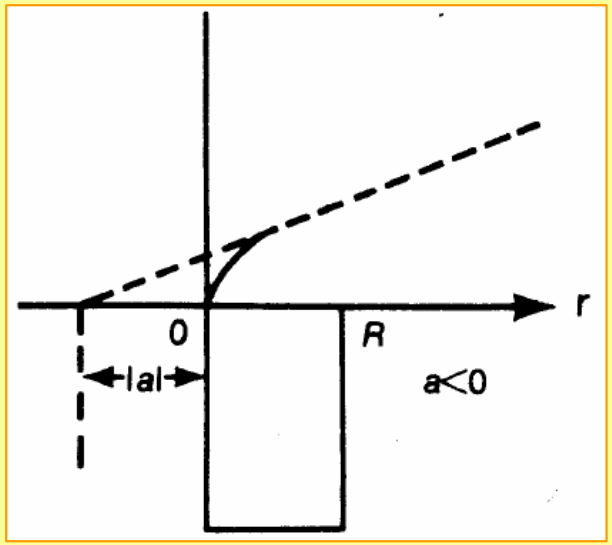
Recapitulation: Scattering theory

Phase shift δ(k) is a function of relative momentum k; Figure shows s-wave.



Scattering length: $k \cot \delta(k) \approx -\frac{1}{a}; \quad \sigma_{\text{tot}} \approx 4\pi a^2 \quad \text{for} \quad k \to 0$

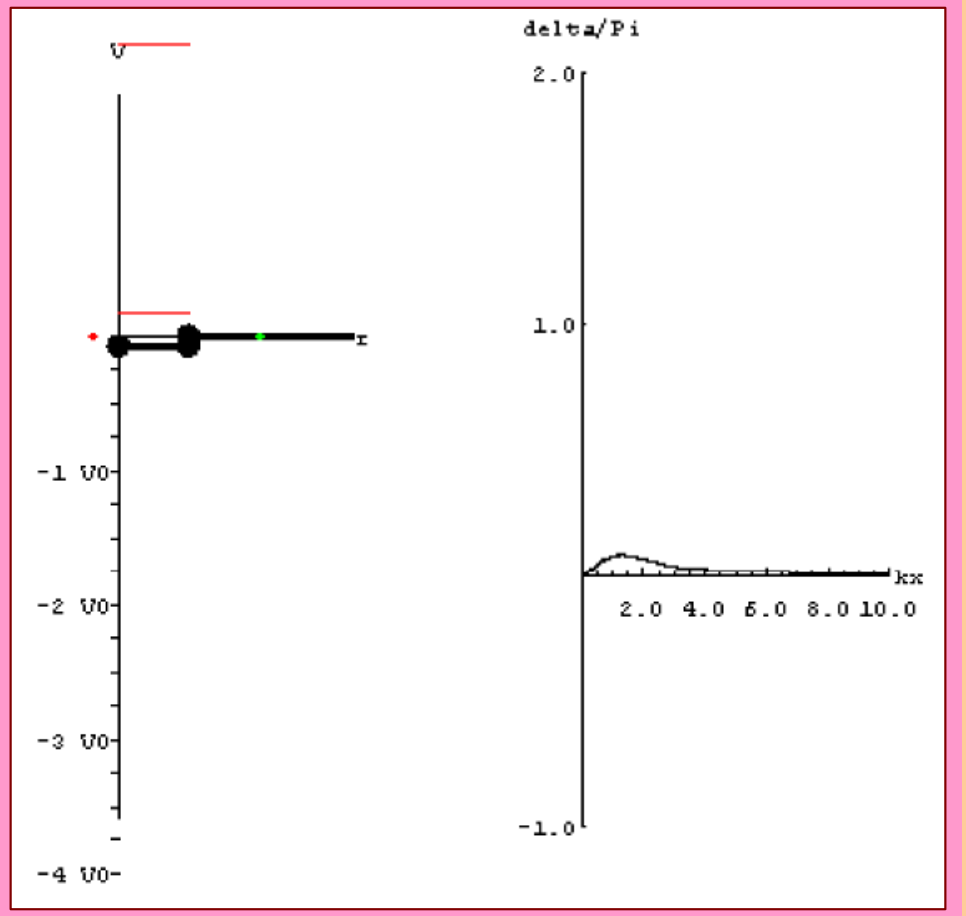




Scattering from a spherical well

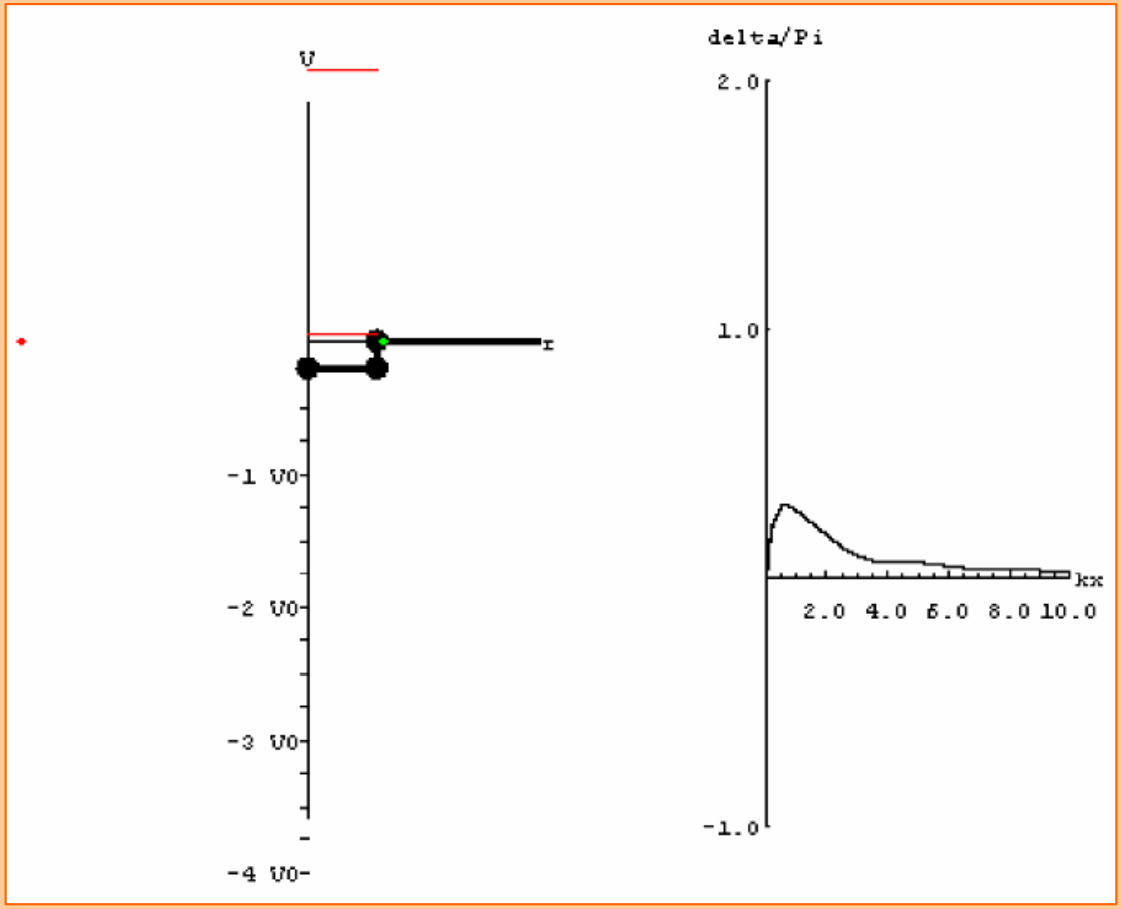
http://people.ccmr.cornell.edu/~emueller/scatter/well.html

System has no bound state



Increase depth of well:

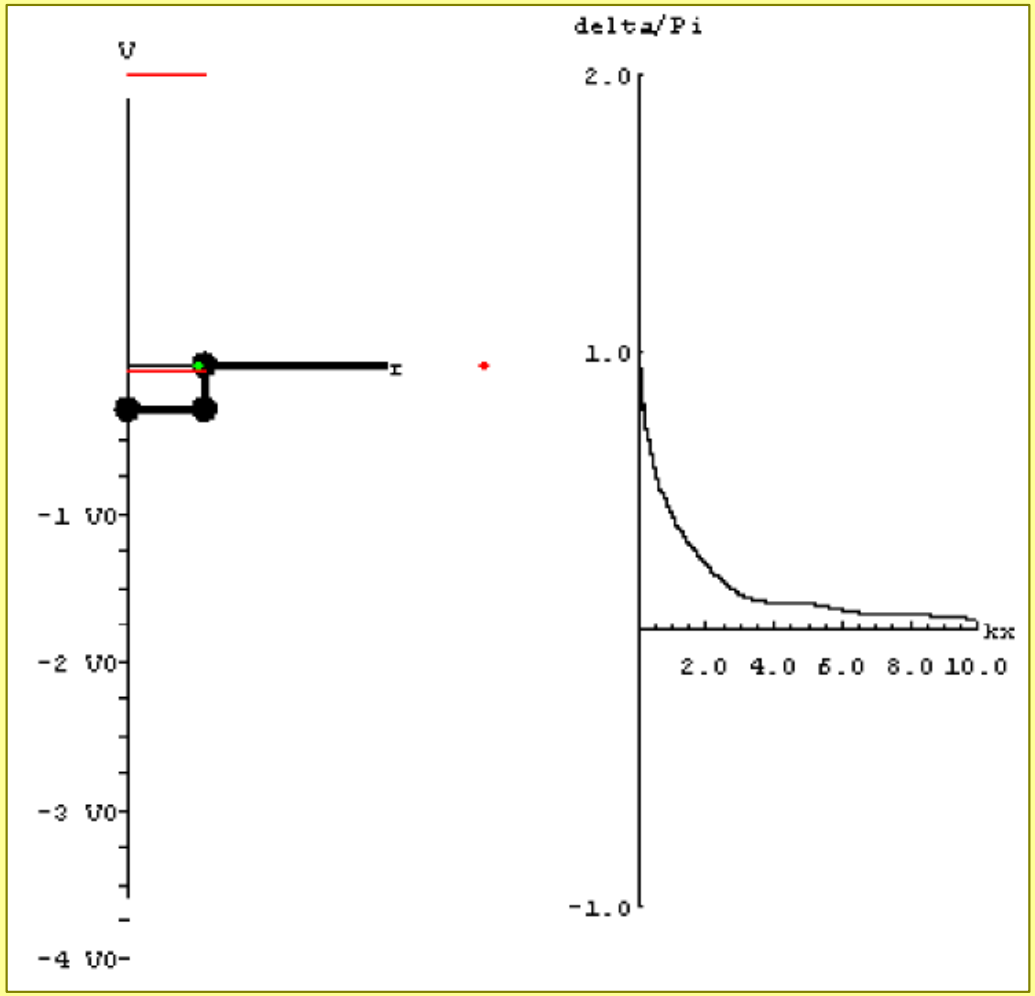
First bound state is about to enter



Scattering from a spherical well

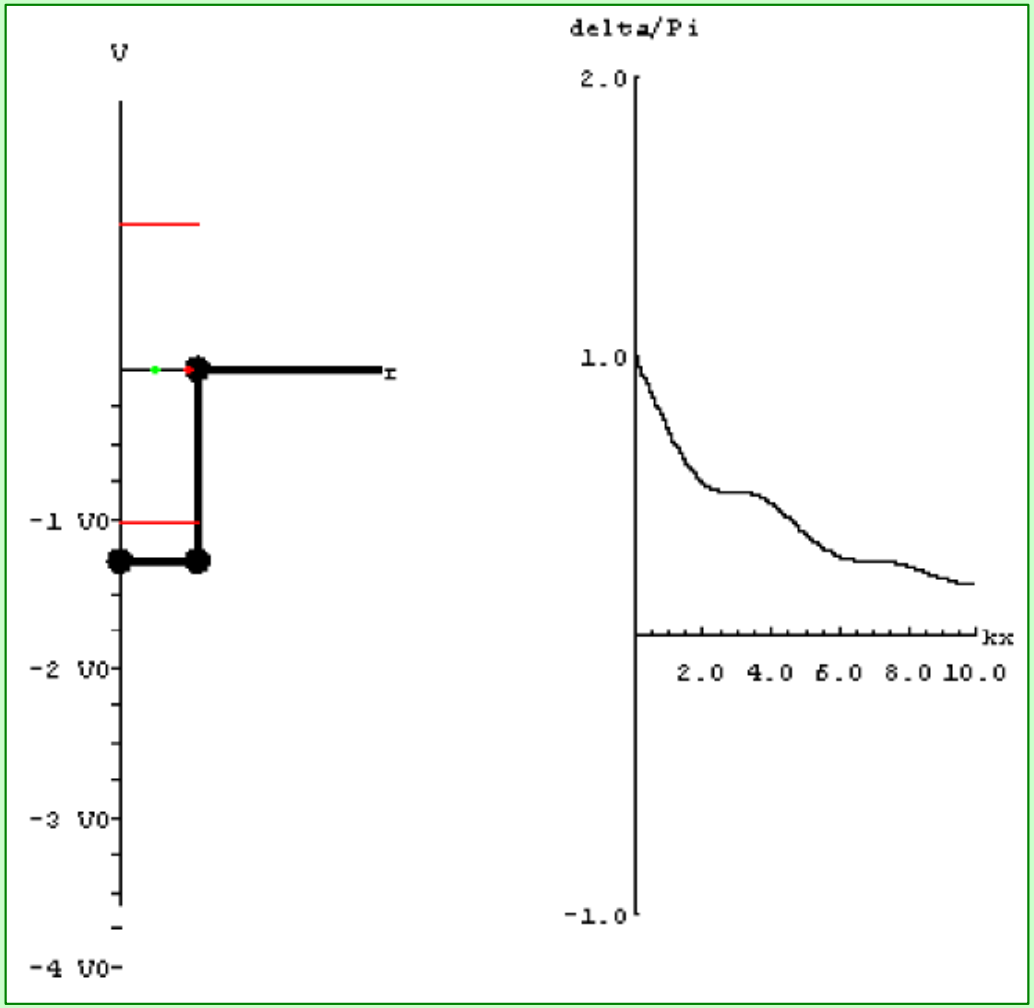
Further increase of depth:

System has one shallow bound state



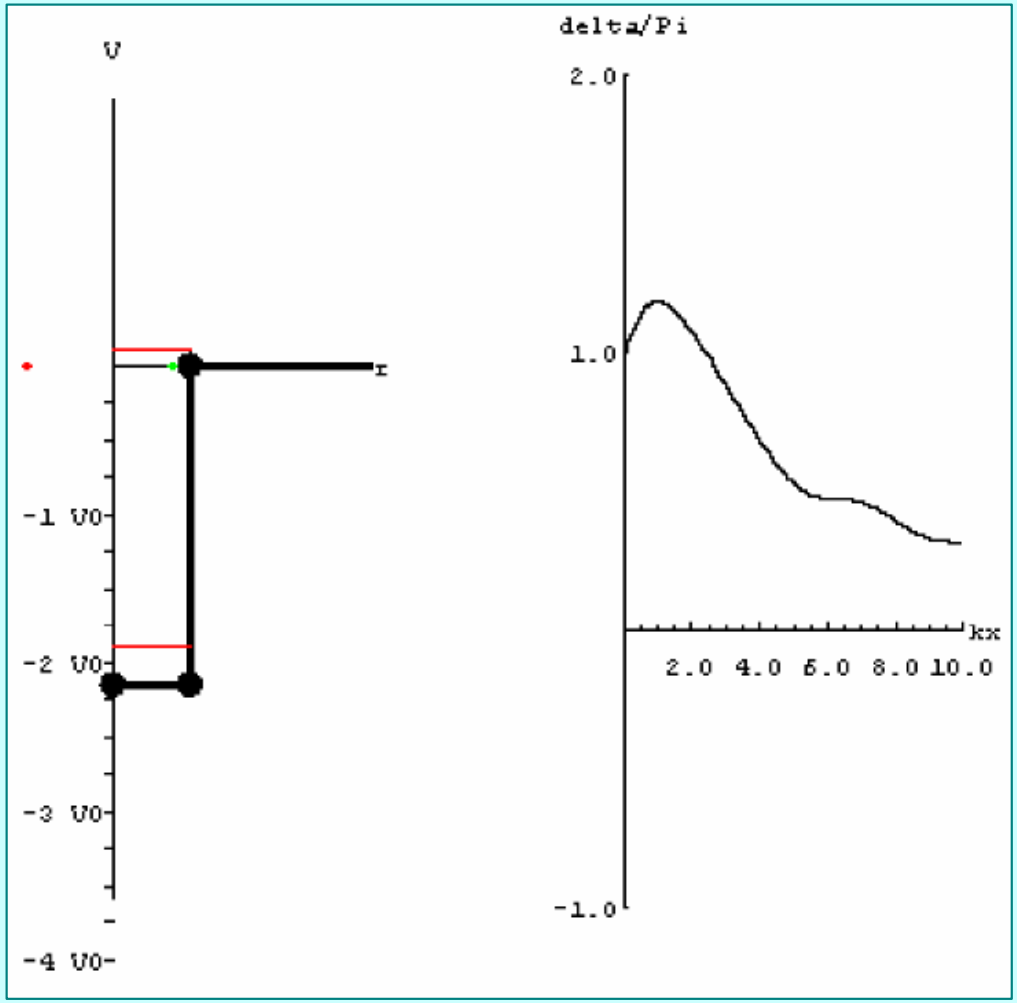
Further increase of depth:

System has one deep bound state

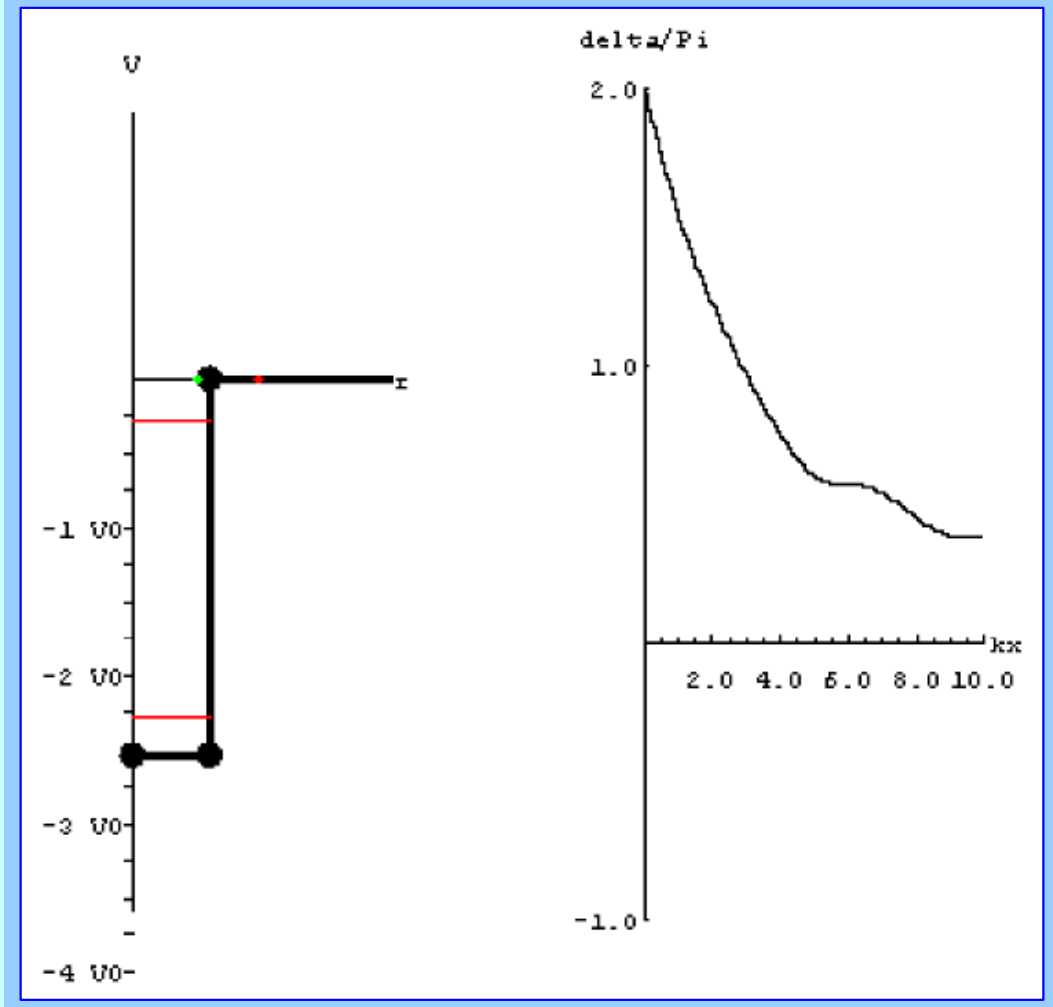


Scattering from a spherical well

Second bound state about to enter

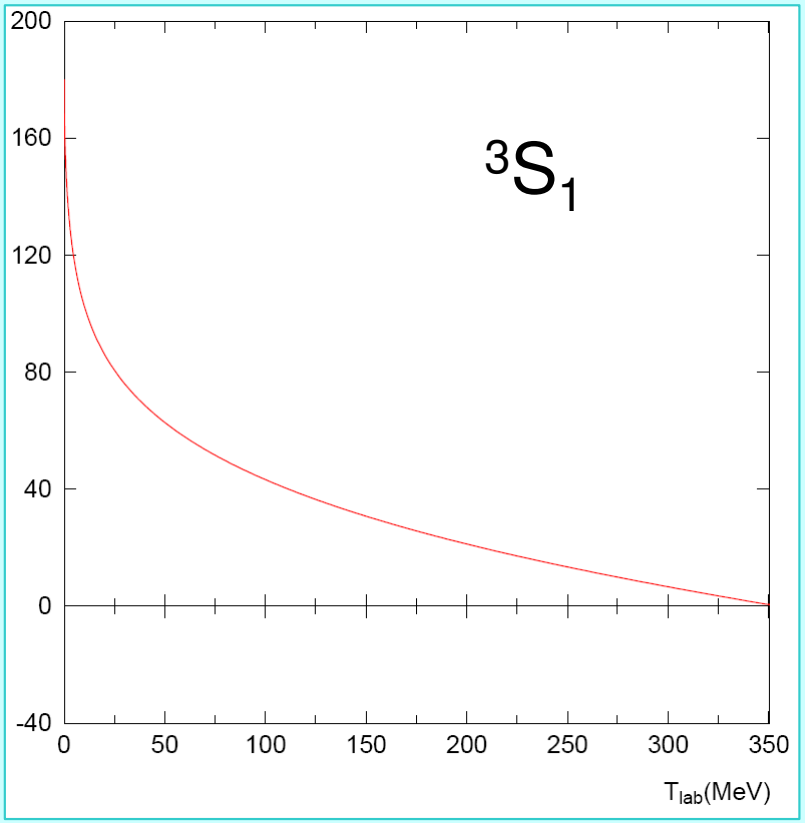


System has two bound state



Nuclear s-wave phase shifts

http://nn-online.org/

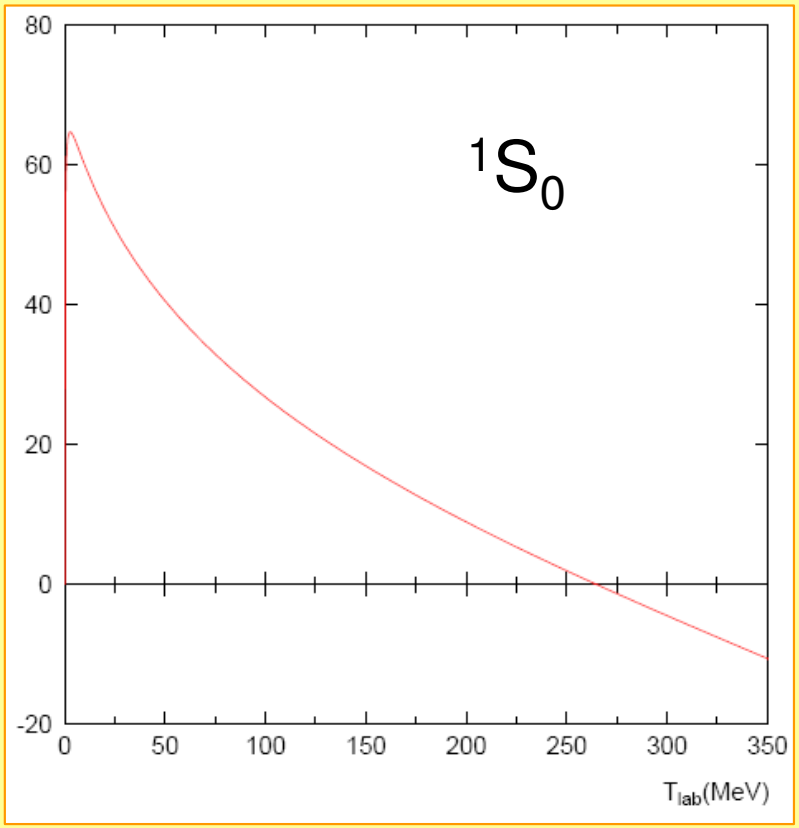


Deuteron is a very weakly bound system!

System has one bound state.

Steep decrease from 180 degrees due to large scattering length a = 5.5 fm.

Acts repulsive due to large (positive) scattering length.



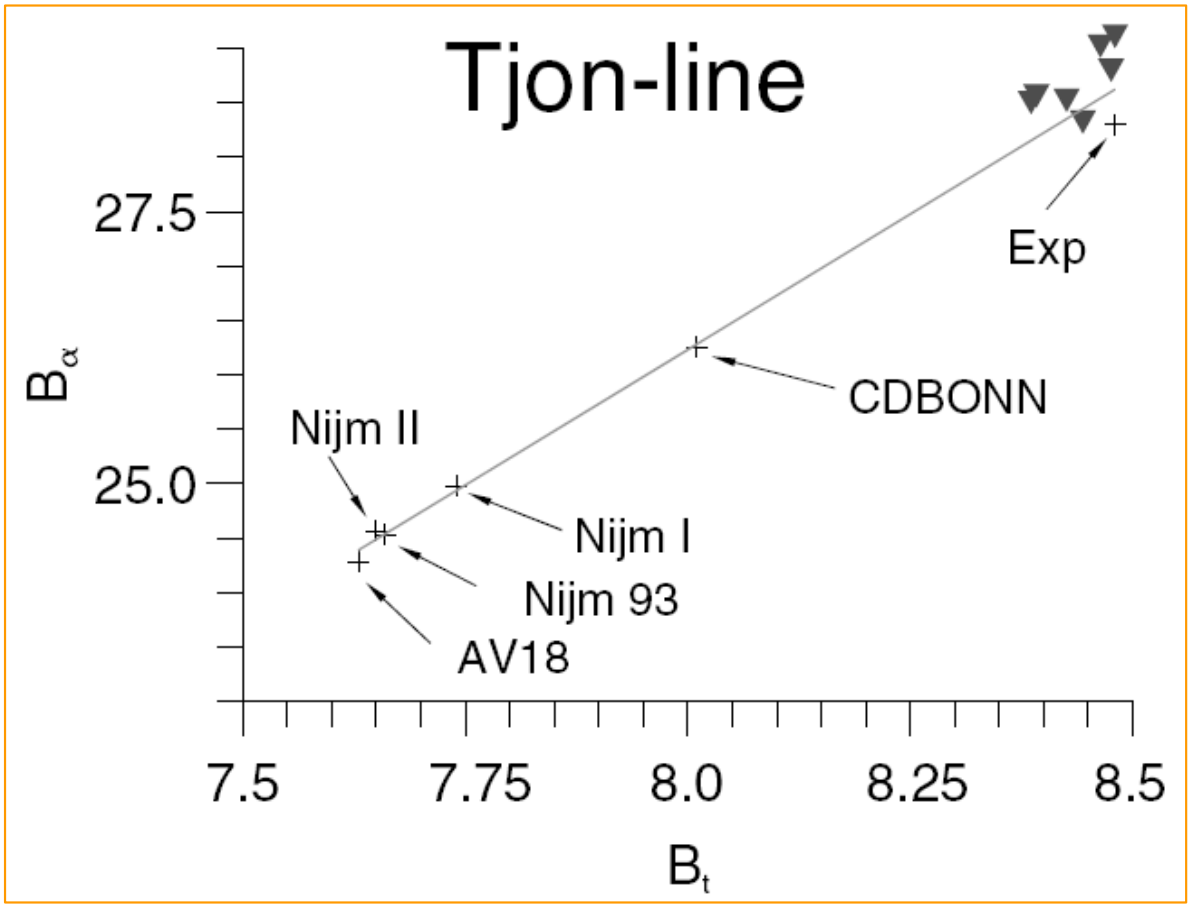
System (barely) fails to exhibit bound state.

Steep rise at 0 due to large scattering length a = -18 fm.

Monotonous decrease due to hard core.

1990s: High precision nucleon-nucleon potential **models**

- Phenomenological models based on meson exchange.
- Contain about 40 parameters; determined by fit to phase shifts/deuteron.
- Reproduce NN phase shifts with a χ^2/datum very close to 1.0.
- "Nearly perfect" two-body physics.



A. Nogga et al, PRL 85 (2000) 944

Different two-body potential models disagree on structure of triton and alpha particle.

With additional **three-nucleon forces**, agreement with experiment is possible.

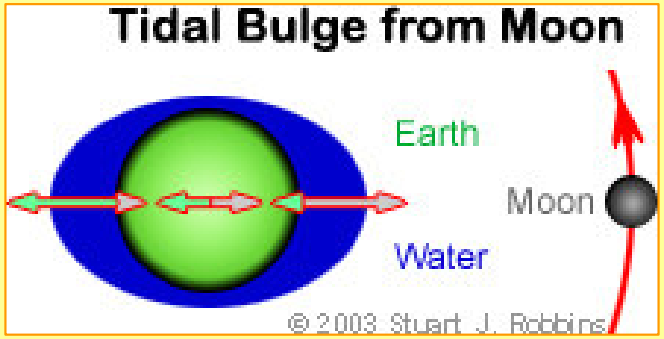
(Three-nucleon force differs for different two-body potentials.)

Four-body forces very small.

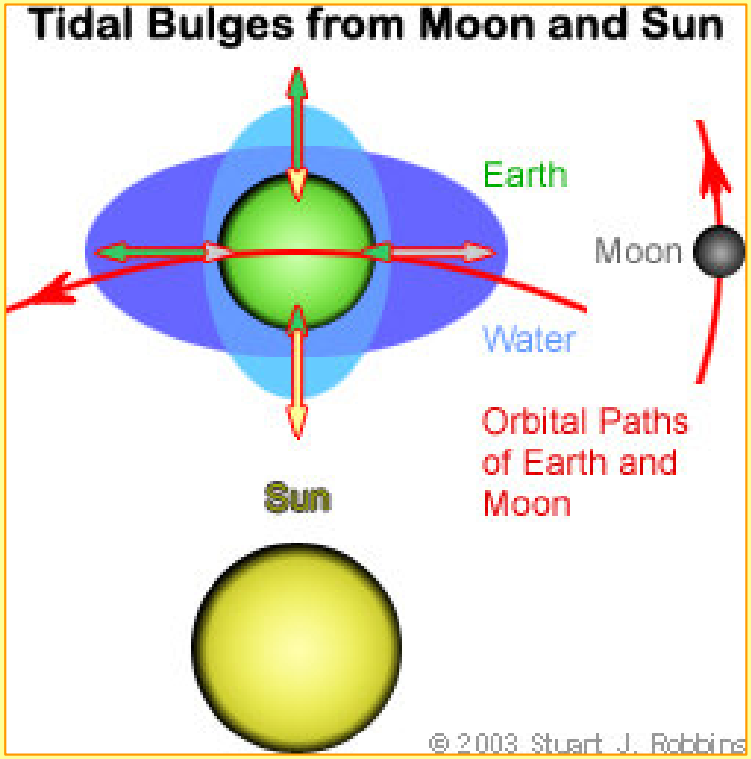
Three nucleon forces: Why?

- Nucleons are not point particles (i.e. elementary).
- We neglected some internal degrees of freedom (e.g. Δ-resonance, "polarization effects", …), and unconstrained high-momentum modes.

Example from celestial mechanics:
Some tidal effects are included in the two-body interaction



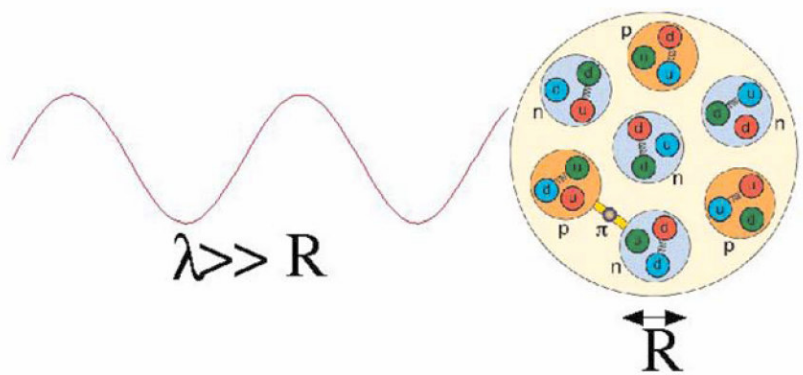
Other tidal effects cannot be included in the two-body interaction! Three-body force unavoidable.



Renormalization group transformation: Removal of "stiff" degrees of freedom at expense of additional forces.

Toward a universal low-momentum potential

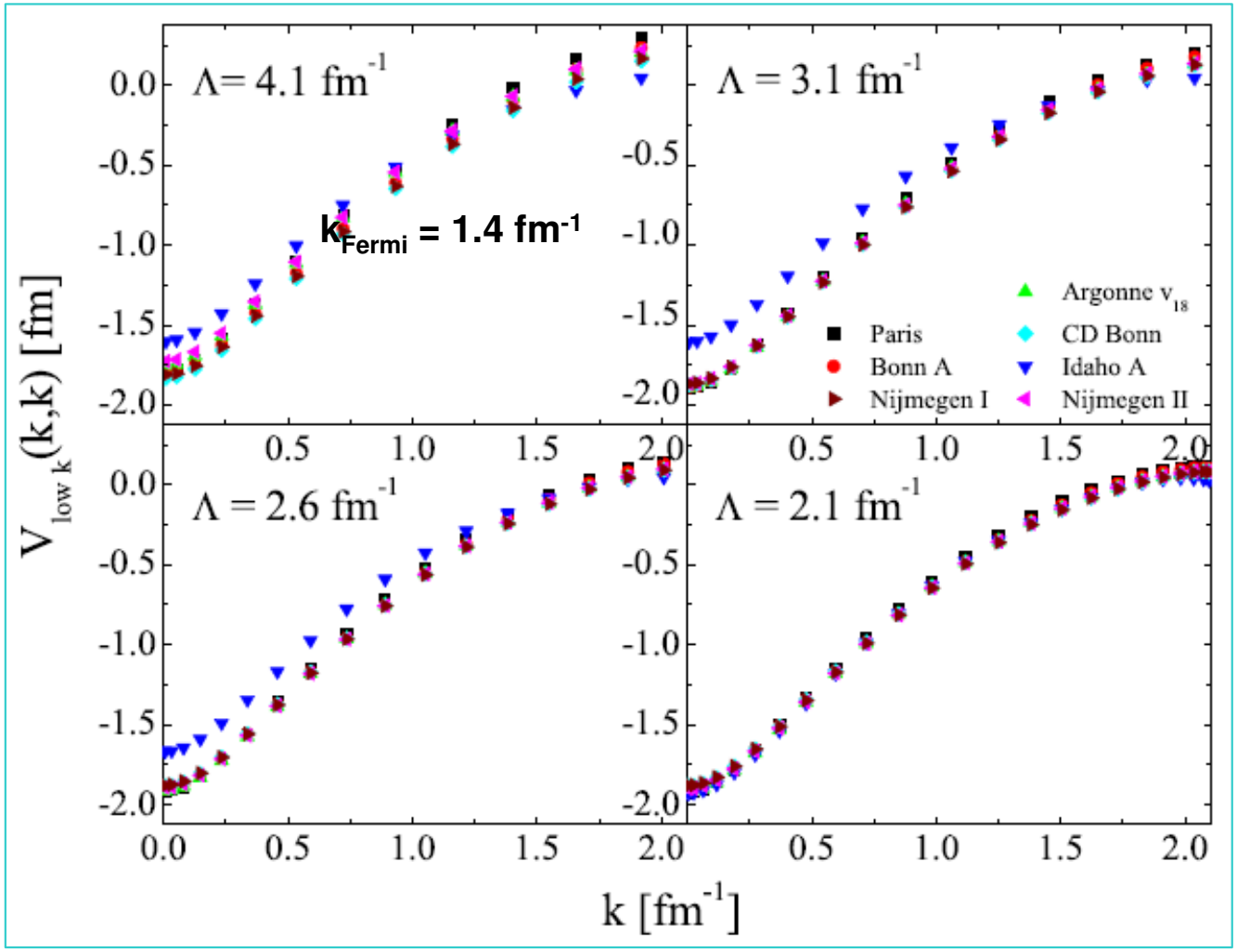
- High-precision potentials contain short-range (high momentum) physics that is not constrained by phase shifts.
- Is it necessary to know the NN interaction at short distances to understand long wavelength physics?



- Introduce momentum cutoff Λ and integrate out high momentum modes such that low-momentum observables are unchanged (Renormalization group transformation).
- Resulting low-momentum potential $V_{low\text{-}k}$.
- Recall: Fermi momentum at saturation density $k_F = 1.4\ fm^{-1}$.

Low momentum potential $V_{low\text{-}k}$

$$\frac{d}{d\Lambda} V_{\mathrm{low\,k}}(k', k) = \frac{2}{\pi} \frac{V_{\mathrm{low\,k}}(k', \Lambda)\, T(\Lambda, k; \Lambda^2)}{1 - (k/\Lambda)^2}$$



Different high-precision potentials

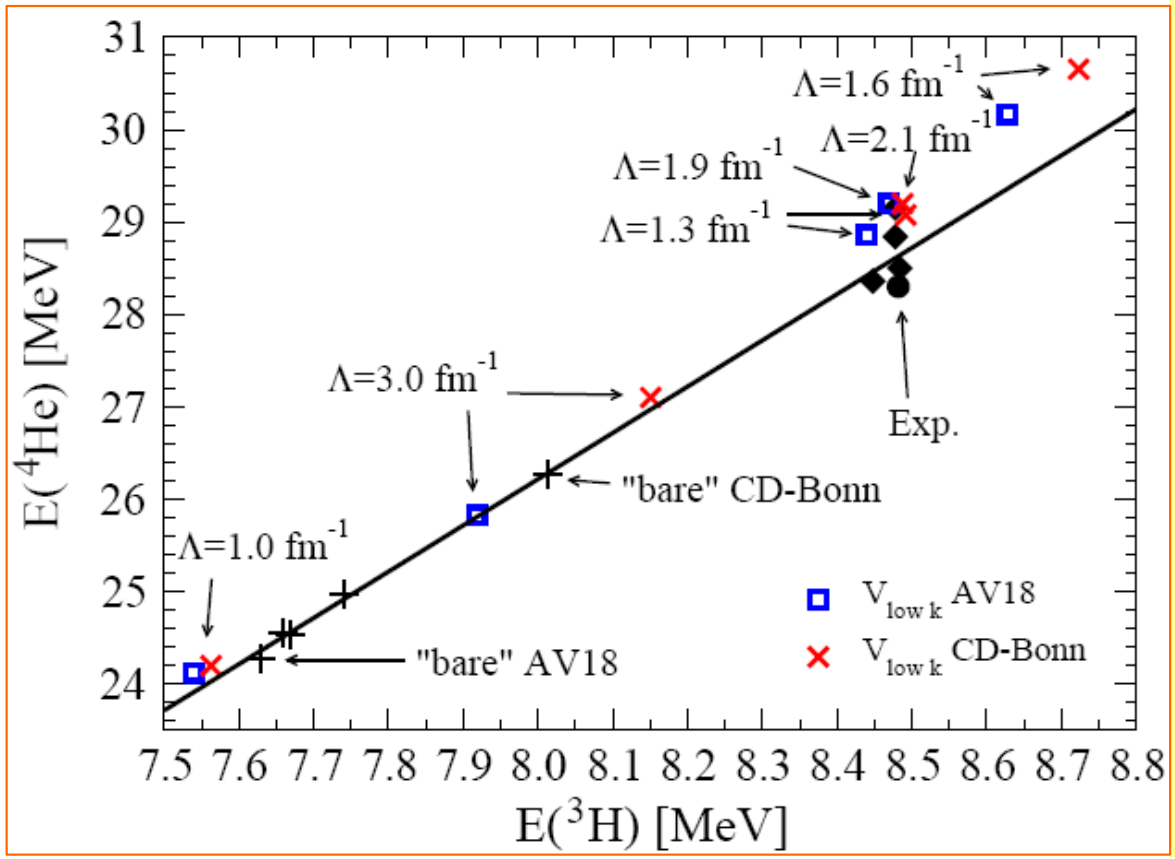
Universal low-momentum potential

Properties of $V_{low\text{-}k}$:

- No hard core
- Nonlocal
- Hartree-Fock already yields bound nuclei.

S. K. Bogner, T. T. S. Kuo, and A. Schwenk, Phys. Rep. 386 (2003) 1

Light nuclei with $V_{low\text{-}k}$



As cutoff Λ is varied, motion along Tjon line.

Addition of Λ-dependent three-nucleon force yields agreement with experiment.

- Three-nucleon force necessary.
- There is no "best" potential & TNF. Choose the most convenient.

A. Nogga, S. K. Bogner, and A. Schwenk, Phys.Rev. C70 (2004) 061002

Q: Can we understand this more systematically?

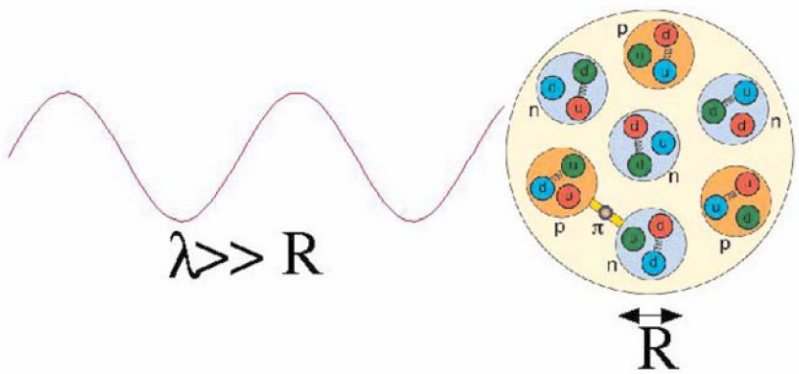
A: Yes, resort to a model-independent approach via effective field theory (EFT).

Vlow-k filters out low-energy physics, while EFT starts from low-energy modes.

Model-independent approach: chiral NN potentials and effective field theory (EFT)

EFT:

- nuclear structure energies Q well below QCD scale of about Λ = 1GeV



- Examples of EFTs:
  - Gravitational potential on Earth $V(h) = -\frac{mMG}{R+h} \approx V(0) + gmh + O\left(\frac{h^2}{R^2}\right)$
  - Multipole expansion of charge distributions.
  - Low-energy potential scattering determined by scattering length alone

$$k \cot \delta(k) \approx -\frac{1}{a}; \quad \sigma_{\text{tot}} \approx 4\pi a^2 \quad \text{for} \quad k \to 0$$

EFT cont'd

- Low energy degrees of freedom:
  - Nucleons
  - Pions (approximate Goldstone bosons of the spontaneously broken chiral symmetry)

- EFT Lagrangian

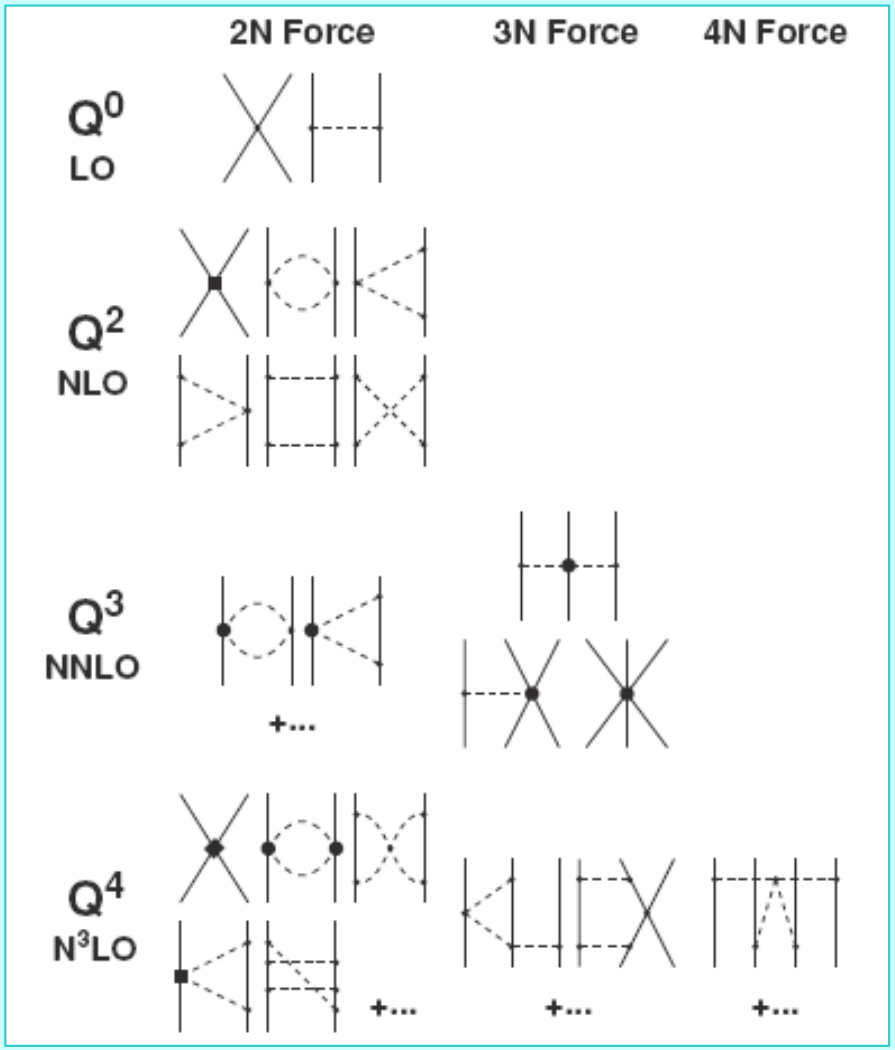
$$\mathcal{L} = \mathcal{L}_{NN} + \mathcal{L}_{N\pi}$$

  - Pion dependence obey rules of broken chiral symmetry
  - Contact terms and derivatives for nucleon fields. (Include effects of short range physics (QCD!) that is not resolved at low energy.)
  - Infinite number of terms
- Order terms of Lagrangian in powers of Q/Λ, and truncate → finite number
- NN-scattering: Feynman diagrams up to given order (finite number)

Refs.: S. Weinberg, Nucl. Phys. B 363 (1991) 3.
C.R.L. Ordenez et al, PRC 53 (1996) 2086.
U. van Kolck, Prog. Part. Nucl. Phys. 43 (1999) 337.

Chiral potential at order N^{3}LO

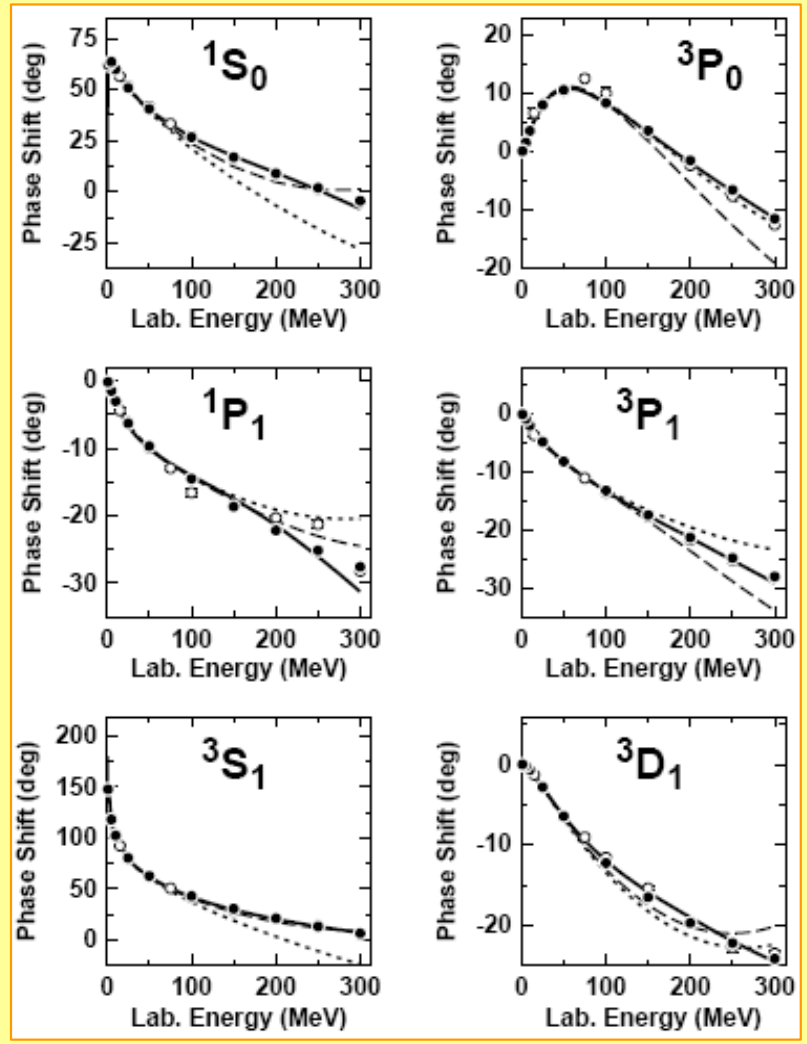
Feynman diagrams



R. Machleidt and D. R. Entem, J. Phys. G 31 (2005) S1235

Phase shifts reproduced to χ^2/datum=1

About 40+ parameters



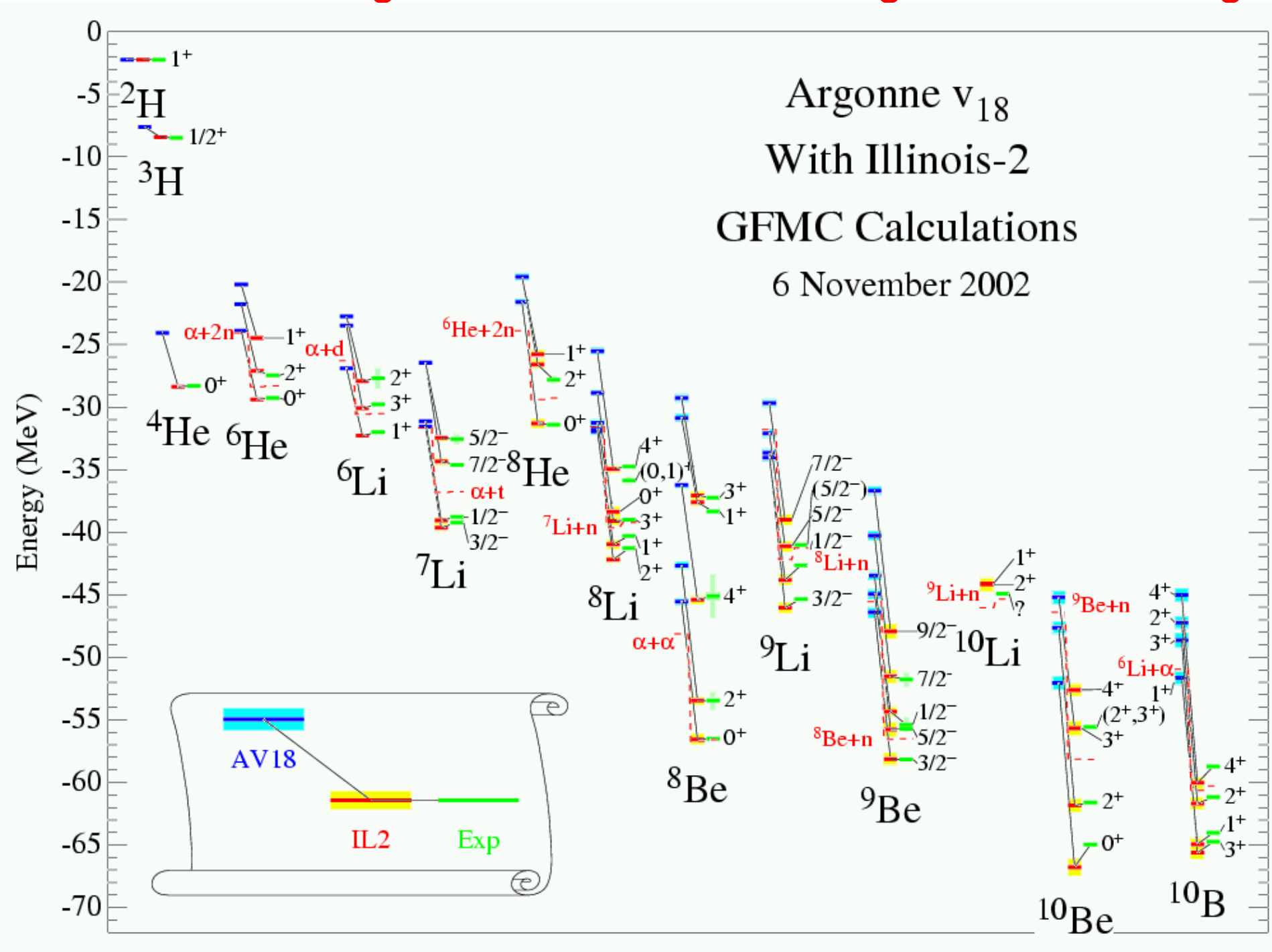
D. R. Entem and R. Machleidt, Phys.Rev. C68 (2003) 041001

Summary on microscopic interactions

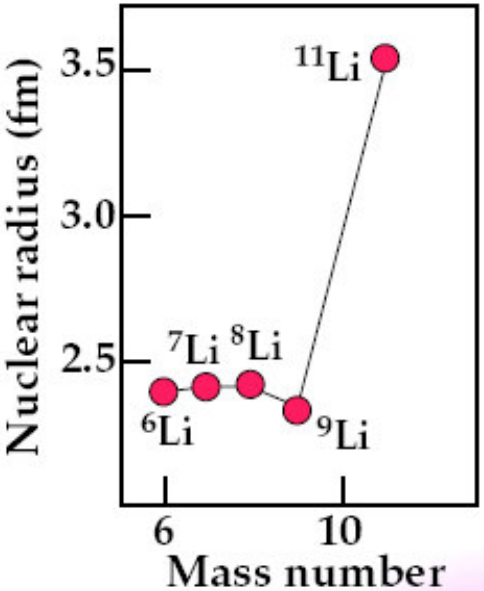
- High precision two-body potential models available
  - Fit two-nucleon scattering data with χ^2/datum close to 1.
  - Yield different results for triton and alpha particle.
- Calculations in light systems require three-nucleon forces
  - No “best” potential.
  - Different TNF for each two-nucleon potential.
- Universal low-momentum potential V low-k emerging
- Chiral effective field theory
  - Based on QCD symmetries.
  - permits systematic construction of nuclear forces (parametrization of our ignorance).
  - TNF arise naturally.

Q: What results do these potential yield for the A-body system?

Role of TNF in light nuclei: overall binding & level ordering

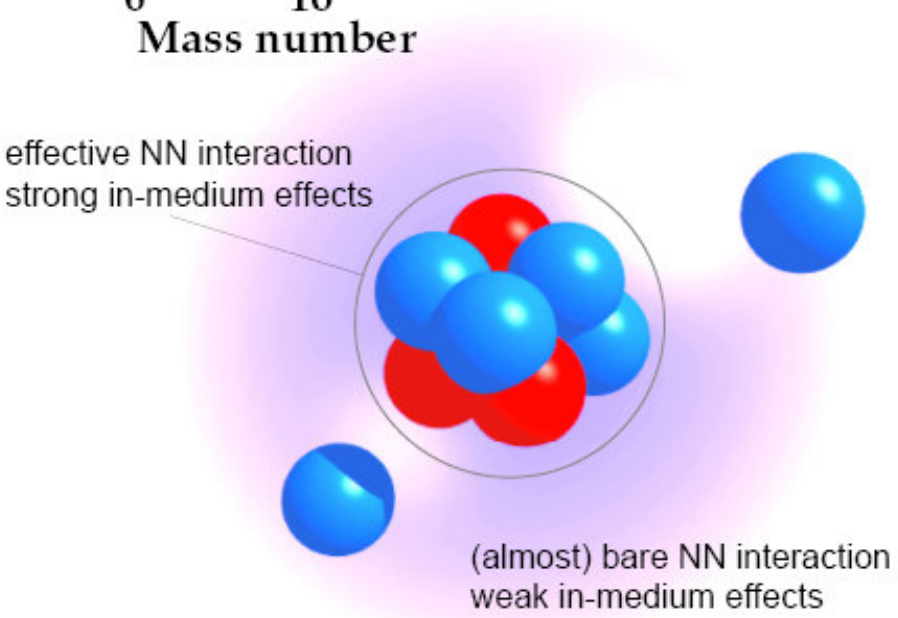


Ab-initio calculations of charge radii of Li isotopes



I. Tanihata et al.
Phys. Rev. Lett. 55, 2676 (1985)

Interaction cross section measurements at Bevalac (790 MeV/u)



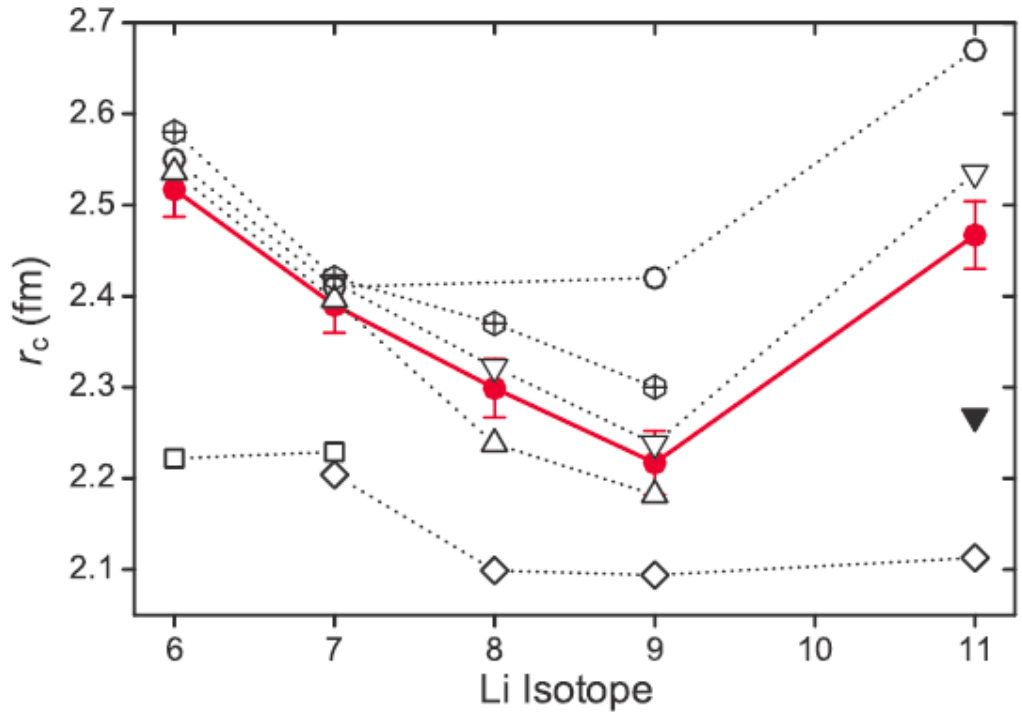


FIG. 2 (color online). Experimental charge radii of lithium isotopes (red, ●) compared with theoretical predictions: △: GFMC calculations [4,22], ▽: SVMC model [27,28] (▼: assuming a frozen ^{9}Li core), ⊕: FMD [26], ○: DCM [19], □ and ◇: *ab initio* NCSM [23,24].

R. Sanchez et al, PRL 96 (2006) 33002.

Solving the ab-initio quantum many-body problem

Exact or virtually exact solutions available for:

- A=3: solution of Faddeev equation.
- A=4: solvable via Faddeev-Yakubowski approach.
- Light nuclei (up to A=12 at present): Green's function Monte Carlo (GFMC); virtually exact; limited to certain forms of interactions.

Highly accurate approximate solutions available for:

- Light nuclei (up to A=16 at present): No-core Shell model (NCSM); truncation in model space.
- Light and medium mass region (A=4, 16, 40 at present): Coupled cluster theory; truncation in model space and correlations.

☺ Theorists agree with each other

PHYSICAL REVIEW C, VOLUME 64, 044001

Benchmark test calculation of a four-nucleon bound state

H. Kamada,* A. Nogga, and W. Glöckle
Institut für Theoretische Physik II, Ruhr-Universität Bochum, D-44780 Bochum, Germany

E. Hiyama
High Energy Accelerator Research Organization, Institute of Particle and Nuclear Studies, Tsukuba 305-0801, Japan

M. Kamimura
Department of Physics, Kyushu University, Fukuoka 812-8581, Japan

K. Varga
Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37380
and Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), Debrecen 4000, PO Box 51, Hunga

Y. Suzuki
Department of Physics, Niigata University, Niigata 950-2181, Japan

M. Viviani and A. Kievsky
INFN, Sezione di Pisa, I-56100 Pisa, Italy

S. Rosati
INFN, Sezione di Pisa, I-56100 Pisa, Italy
and Department of Physics, University of Pisa, I-56100 Pisa, Italy

J. Carlson
Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

Steven C. Pieper and R. B. Wiringa
Physics Division, Argonne National Laboratory, Argonne, Illinois 60439

P. Navrátil
Lawrence Livermore National Laboratory, P. O. Box 808, Livermore, California 94551
and Nuclear Physics Institute, Academy of Sciences of the Czech Republic, 250 68 Řež near Prague, Czech Republic

B. R. Barrett
Department of Physics, P.O. Box 210081, University of Arizona, Tucson, Arizona 85721

N. Barnea
The Racah Institute of Physics, The Hebrew University, 91904 Jerusalem, Israel

W. Leidemann and G. Orlandini
Dipartimento di Fisica and INFN (Gruppo Collegato di Trento), Università di Trento, I-38050 Povo, Italy
(Received 20 April 2001; published 27 August 2001)

In the past, several efficient methods have been developed to solve the Schrödinger equation for four-nucleon bound states accurately. These are the Faddeev-Yakubovsky, the coupled-rearrangement-channel Gaussian-basis variational, the stochastic variational, the hyperspherical variational, the Green's function Monte Carlo, the no-core shell model, and the effective interaction hyperspherical harmonic methods. In this article we compare the energy eigenvalue results and some wave function properties using the realistic AV8′ NN interaction. The results of all schemes agree very well showing the high accuracy of our present ability to calculate the four-nucleon bound state.

TABLE I. The expectation values $\langle T \rangle$ and $\langle V \rangle$ of kinetic and potential energies, the binding energies E_b in MeV, and the radius in fm.

Method	$\langle T \rangle$	$\langle V \rangle$	E_b	$\sqrt{\langle r^2 \rangle}$
FY	102.39(5)	−128.33(10)	−25.94(5)	1.485(3)
CRCGV	102.30	−128.20	−25.90	1.482
SVM	102.35	−128.27	−25.92	1.486
HH	102.44	−128.34	−25.90(1)	1.483
GFMC	102.3(1.0)	−128.25(1.0)	−25.93(2)	1.490(5)
NCSM	103.35	−129.45	−25.80(20)	1.485
EIHH	100.8(9)	−126.7(9)	−25.944(10)	1.486

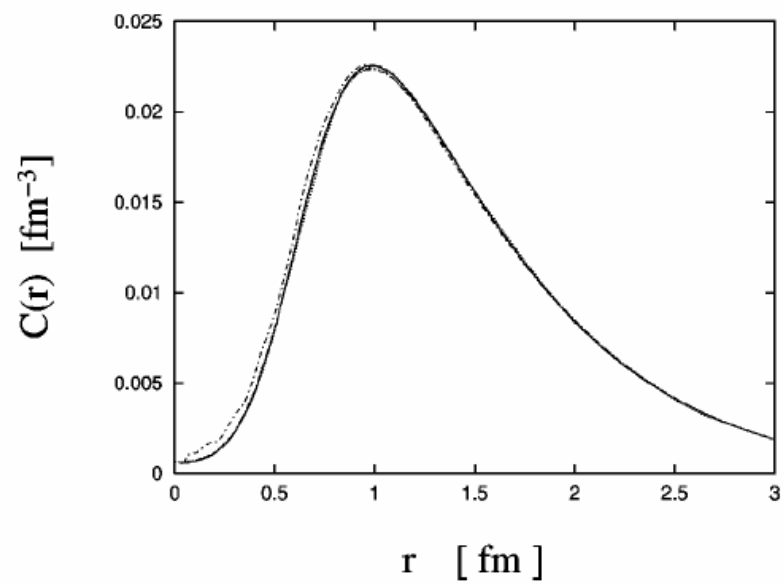


FIG. 1. Correlation functions in the different calculational schemes: EIHH (dashed-dotted curves), FY, CRCGV, SVM, HH, and NCSM (overlapping curves).

Green's Function Monte Carlo

Idea:

1. Determine accurate approximate wave function via variation of the energy (The high-dimensional integrals are done via Monte Carlo integration).

$$E = \frac{\langle \Psi_{\text{trial}} | \hat{H} | \Psi_{\text{trial}} \rangle}{\langle \Psi_{\text{trial}} | \Psi_{\text{trial}} \rangle}$$

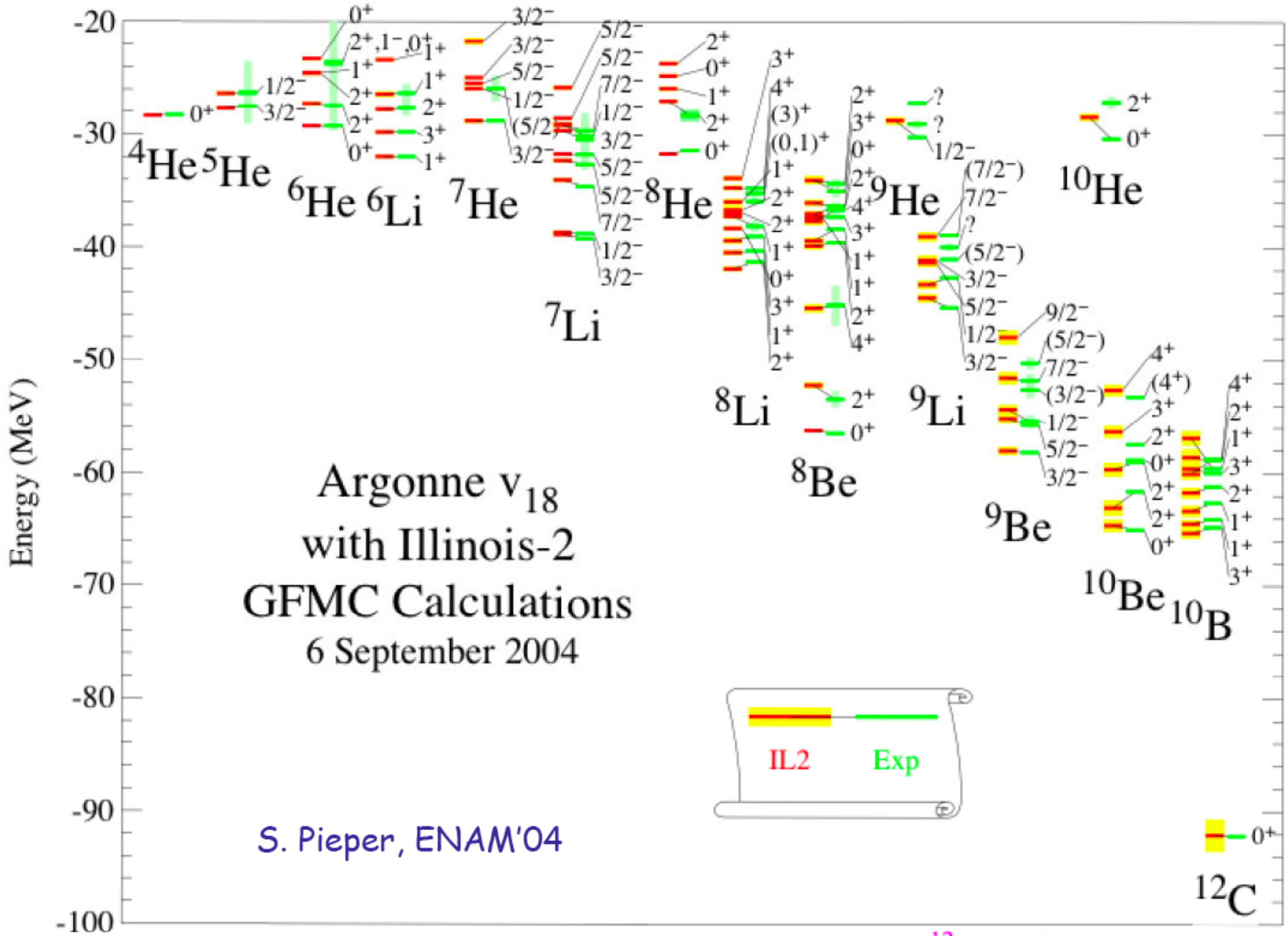
2. Refine wave function and energy via projection with Green's function

$$|\Psi\rangle = \tau \xrightarrow{\lim} \infty \; e^{-\tau(\hat{H}-E)} |\Psi_{\text{trial}}\rangle$$

☺ Virtually exact method.

☹ Limited to certain forms of Hamiltonians; computationally expensive method.

GFMC results for light nuclei



^{12}C results are preliminary.

S. C. Pieper and R. B. Wiringa, Ann.Rev.Nucl.Part.Sci. 51 (2001) 53

Working in a finite model space

NCSM and Coupled-cluster theory solve the Schroedinger equation in a model space with a *finite* (albeit large) number of configurations or basis states.

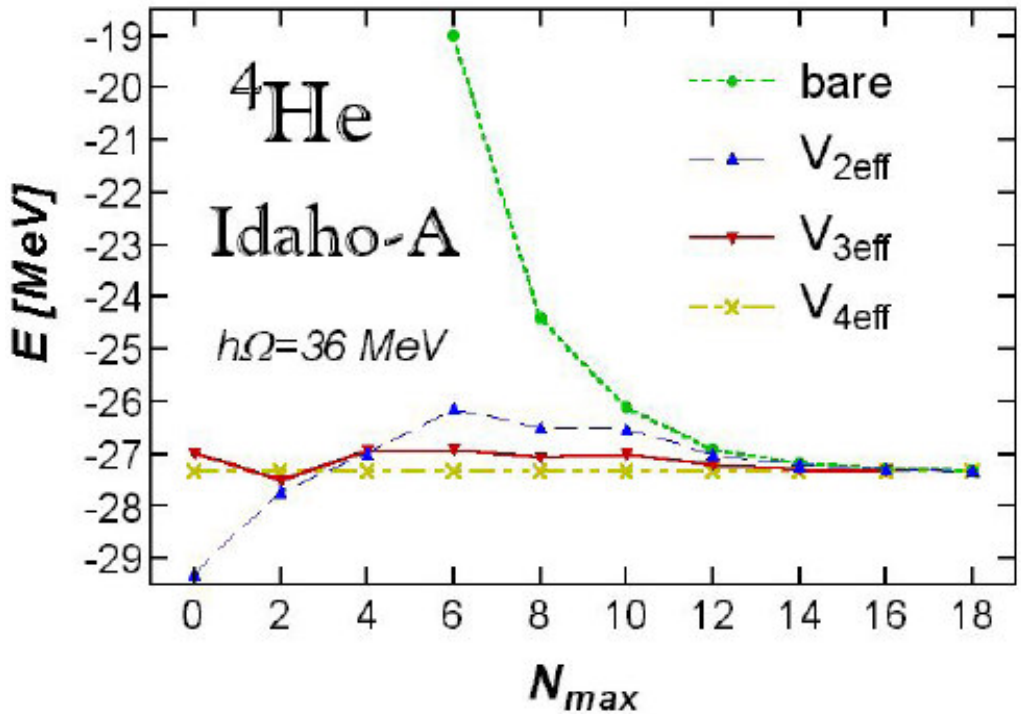
Problem: High-momentum components of high-precision NN interactions require enormously large spaces.

Solution: Get rid of the high-momentum modes via a renormalization procedure. (Vlow-k is an example)

Price tag:

Generation of 3, 4, …, A-body forces unavoidable.

Observables other than the energy also need to be transformed.



E. Ormand
http://www.phy.ornl.gov/npss03/ormand2.ppt

No core shell model

Idea: Solve the A-body problem in a harmonic oscillator basis.

1. Take K single particle orbitals
2. Construct a basis of Slater determinants
3. Express Hamiltonian in this basis
4. Find low-lying states via diagonalization

☺ Get eigenstates and energies

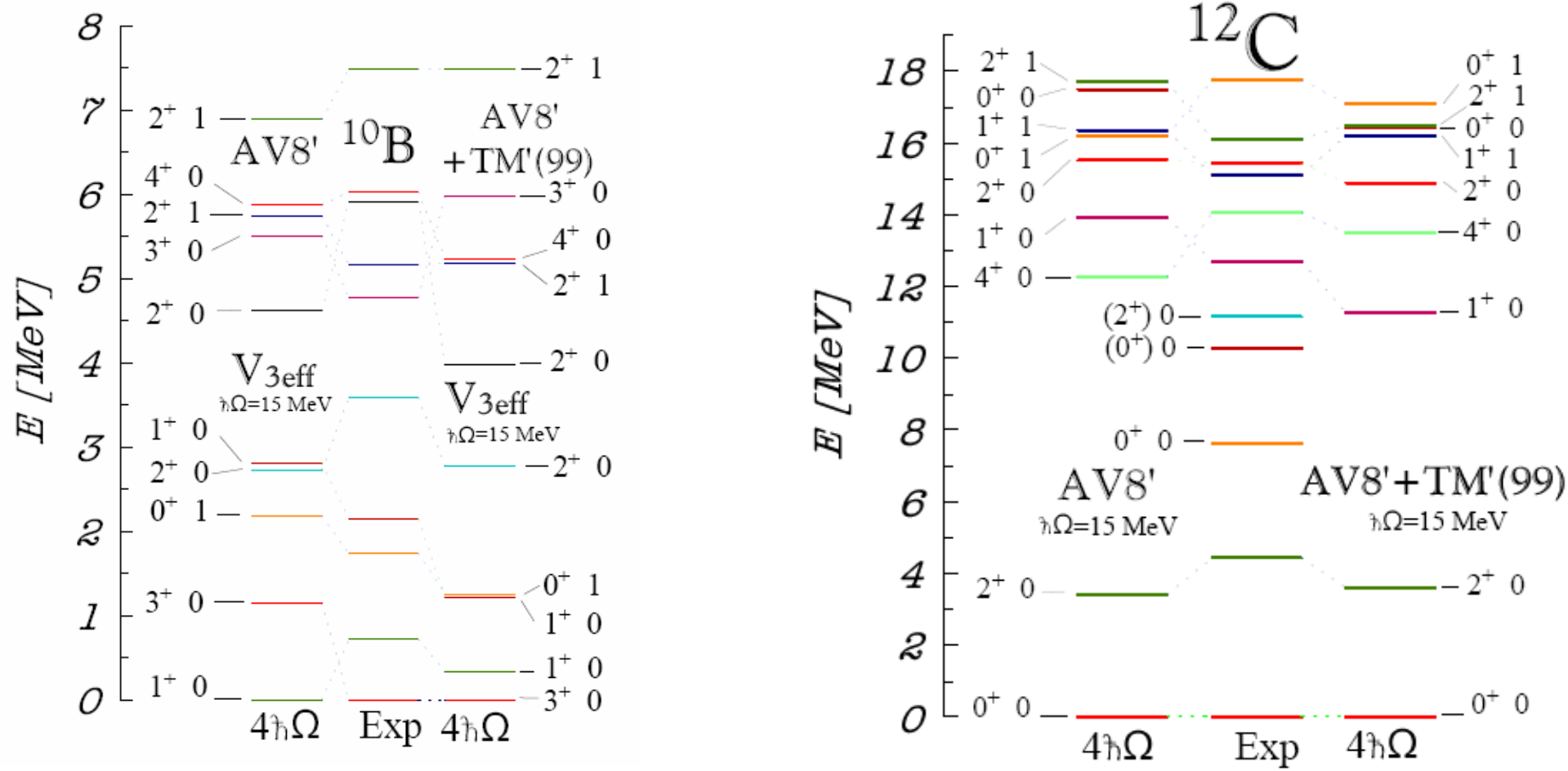
☺ No restrictions regarding Hamiltonian

☹ Number of configurations and resulting matrix very large: There are

$$\binom{K}{A} = \frac{K!}{(K-A)!A!}$$

ways to distribute A nucleons over K single-particle orbitals.

No-core Shell Model results for ^{10}B and ^{12}C



P. Navratil and W. E. Ormand, Phys. Rev. C68 (2003) 034305

Coupled cluster theory

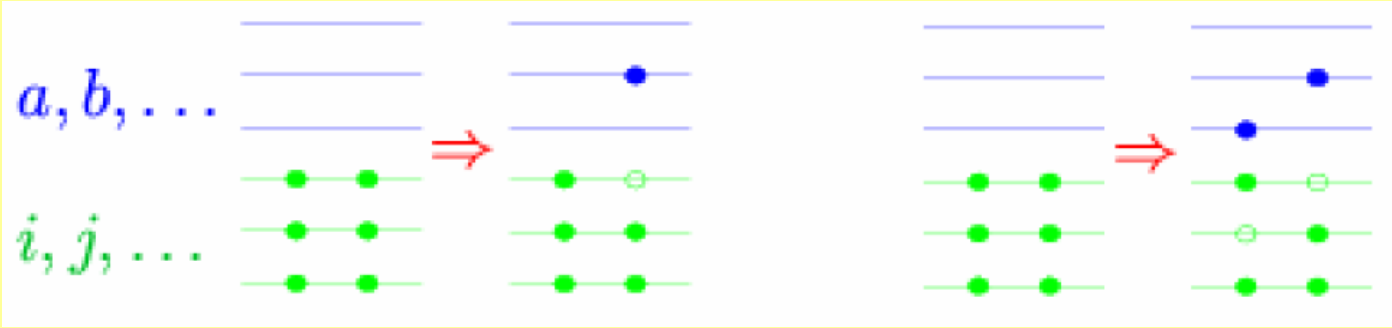
Ansatz:

$$
\begin{aligned}
|\Psi\rangle &= e^{T}|\Phi\rangle \\
T &= 1 + T_1 + T_2 + \ldots \\
T_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\
T_2 &= \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

☺ Scales gently (polynomial, not exponential) with increasing problem size.

☹ Open-shell systems require much more work.

Correlations are exponentiated 1p-1h and 2p-2h excitations. Part of np-nh excitations included!



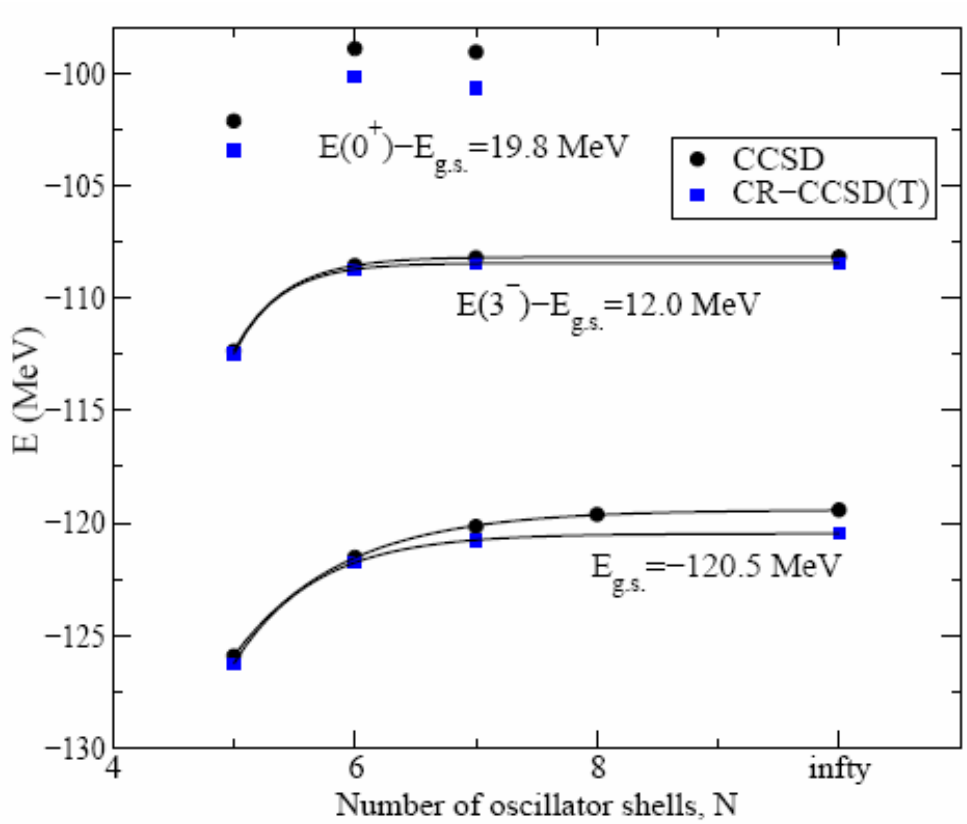
Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle \\
\overline{H} &\equiv e^{-T}He^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \ldots\right)_c
\end{aligned}
$$

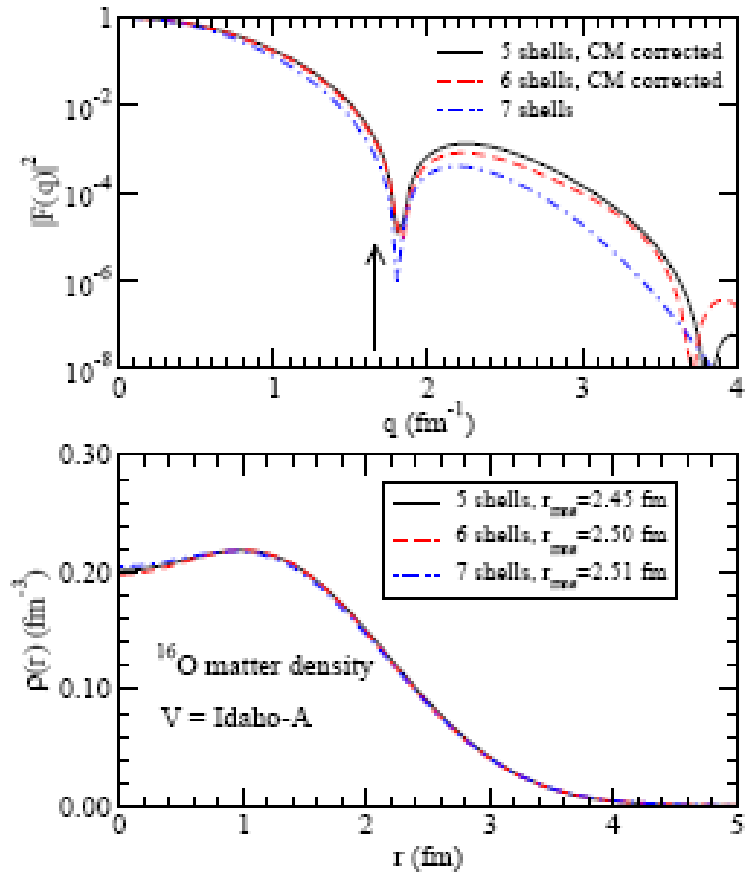
Coupled-cluster calculation for ^{16}O

Interaction: Idaho-A based G-matrix

Model space: Up to 8 oscillator shells



M. Wloch et al, Phys. Rev. Lett. 94, 212501 (2005).



Results converged w.r.t size of model space

Excited 3^- state: 1p-1h, about 6MeV to high

Some deficiencies in form factor.

Three-nucleon force missing.

Summary

- High precision NN interactions now available and understood
  - No “best” potential. Choose one that is most convenient
  - Three nucleon forces natural consequence
  - Interplay between three-body forces and high-momentum modes
- Systematic construction of effective interaction via EFT possible
- Several methods that solve the quantum many-body problem
  - Methods agree with each other in results on light systems.
  - Methods differ in accuracy and expense.
  - Agreement with experiment impressive.
  - Reliable predictions can be made.
- Future:
  - Explore three-nucleon forces
  - Heavier nuclei