New theoretical methods for nuclear structure/reactions, nuclear matter, and cold atoms

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Basic plan of lectures: [http://www.physics.ohio-state.edu/∼ntg/talks/]

- Overview of physics, Hamiltonians, and what's new
- Highlights of recent applications as examples of new methods

Pictures have been freely borrowed from online sources; I apologize in advance for any omitted citations. Also, inclusion of particular examples does not imply that they are the "best". No animals were harmed in creating these lectures.

Outline

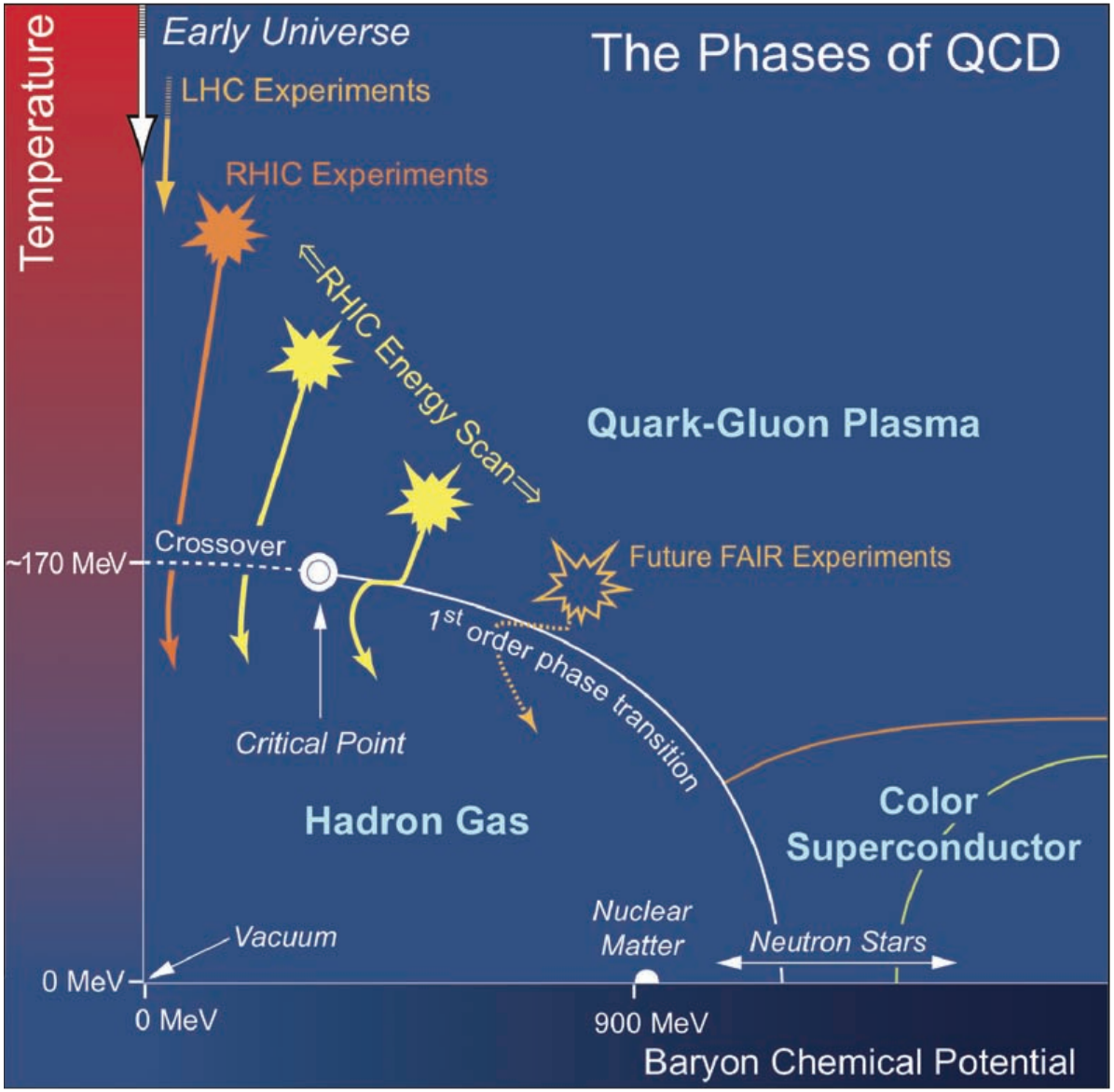
Overview: What is new in low-energy physics?

Background for the inputs and solution methods

Highlights of recent applications: new methods

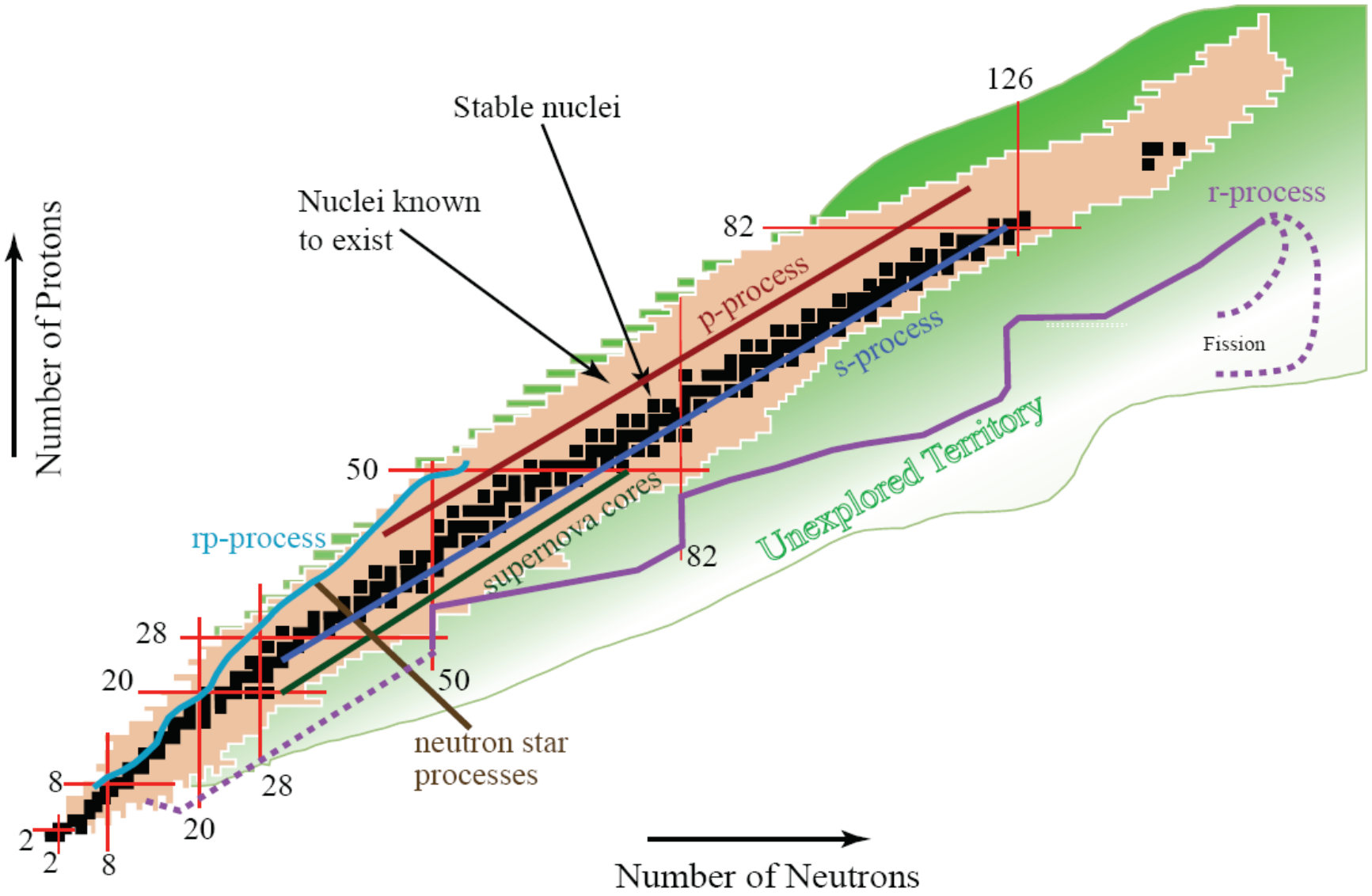
Recap and outlook

Low-energy domain in perspective: QCD phases



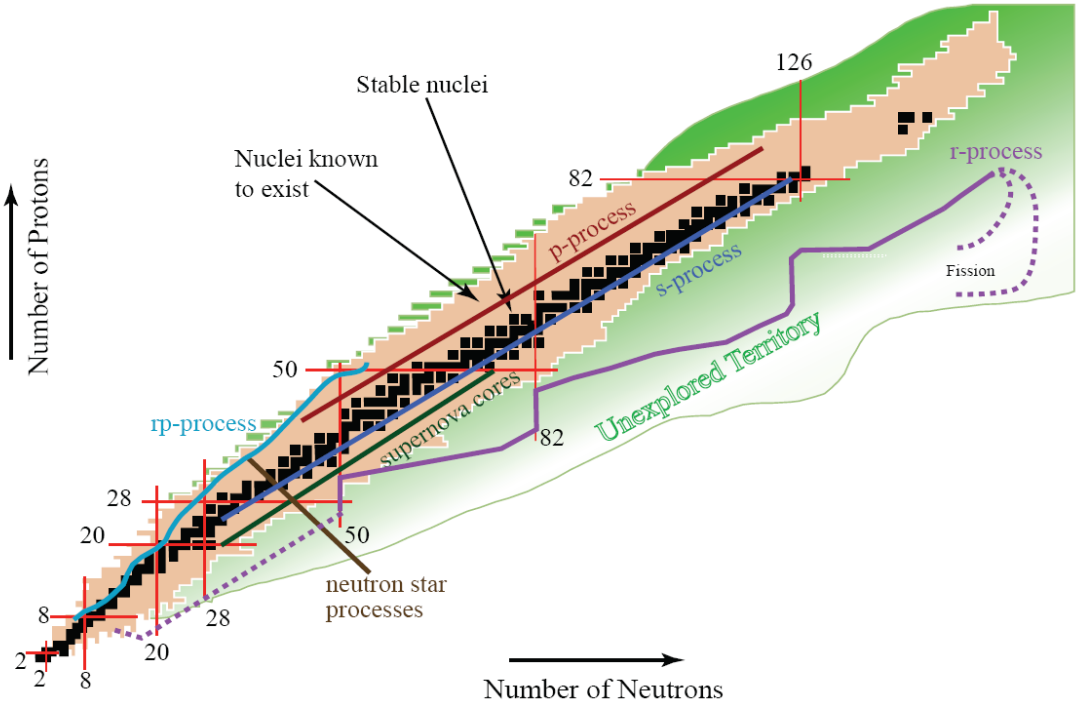
- near the x-axis in the confined phase
- add: isospin axis
- uniform matter: symmetric nuclear matter ($N = Z$) to pure neutron matter
- thermodynamic limit
  $\Longrightarrow$ cf. finite nuclei
- nuclei are self-bound (superfluid) “liquid drops”

Low-energy playground: Table of the nuclides



Questions driving low-energy nuclear physics

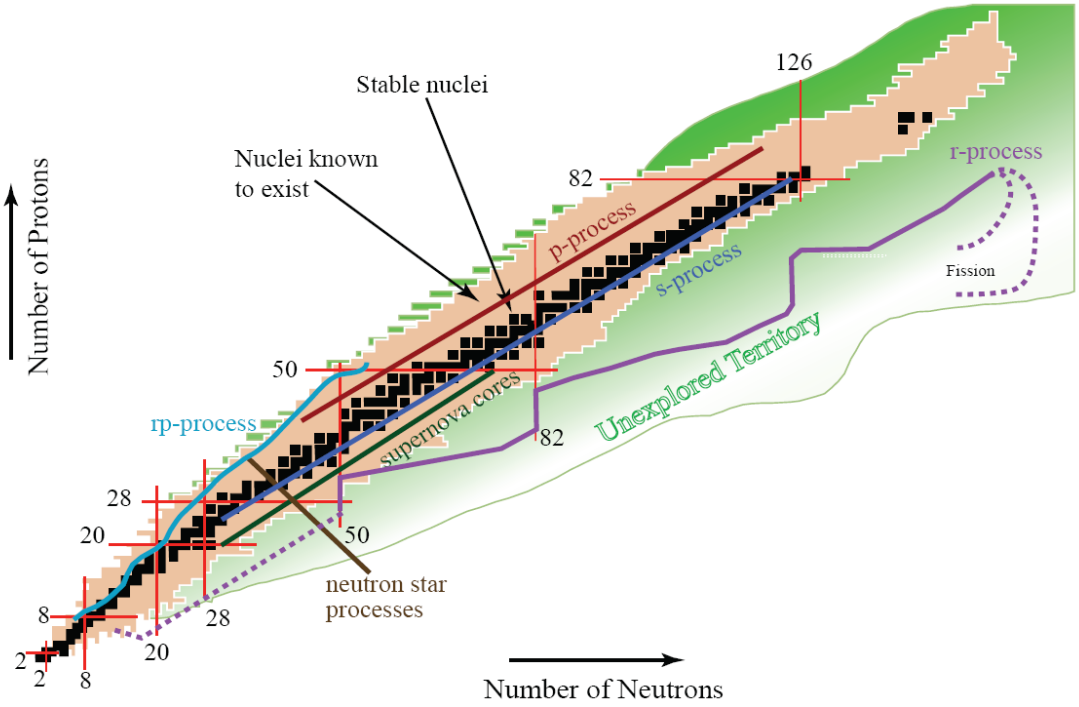
Physics of Nuclei



- How do protons and neutrons make stable nuclei and rare isotopes? Where are the limits?
- What is the equation of state of nucleonic matter?
- What is the origin of simple patterns in complex nuclei?
- How do we describe fission, fusion, reactions, . . . ?

Questions driving low-energy nuclear physics

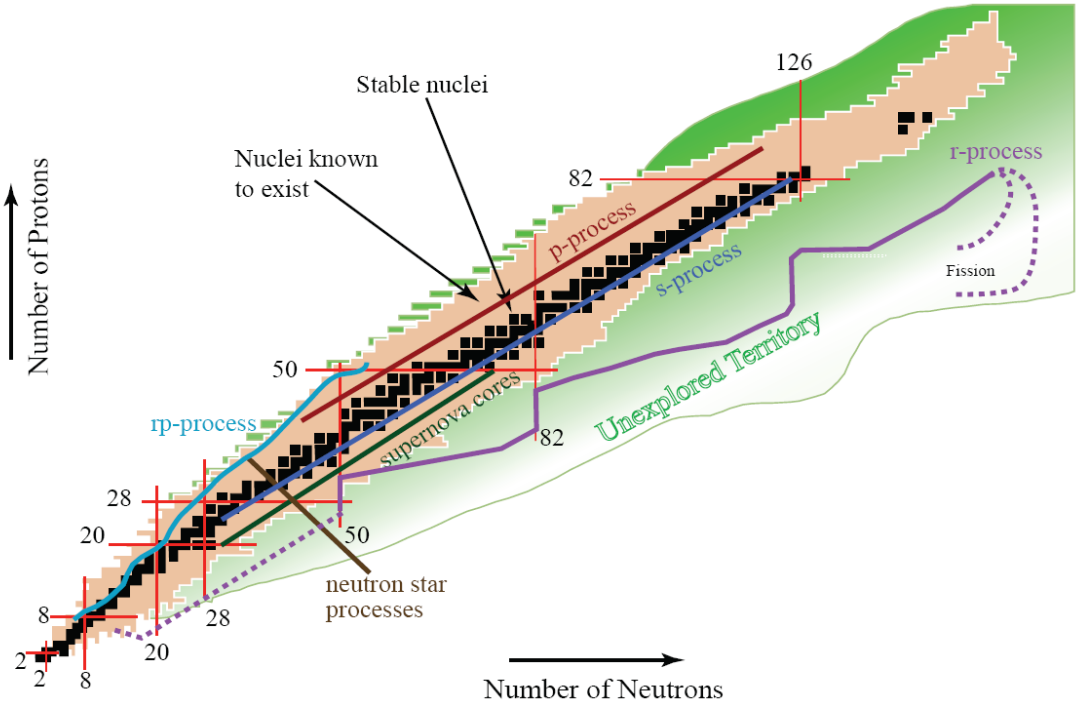
Nuclear Astrophysics



- How did the elements from iron to uranium originate?
- How do stars explode?
- What is the nature of neutron star matter?

Questions driving low-energy nuclear physics

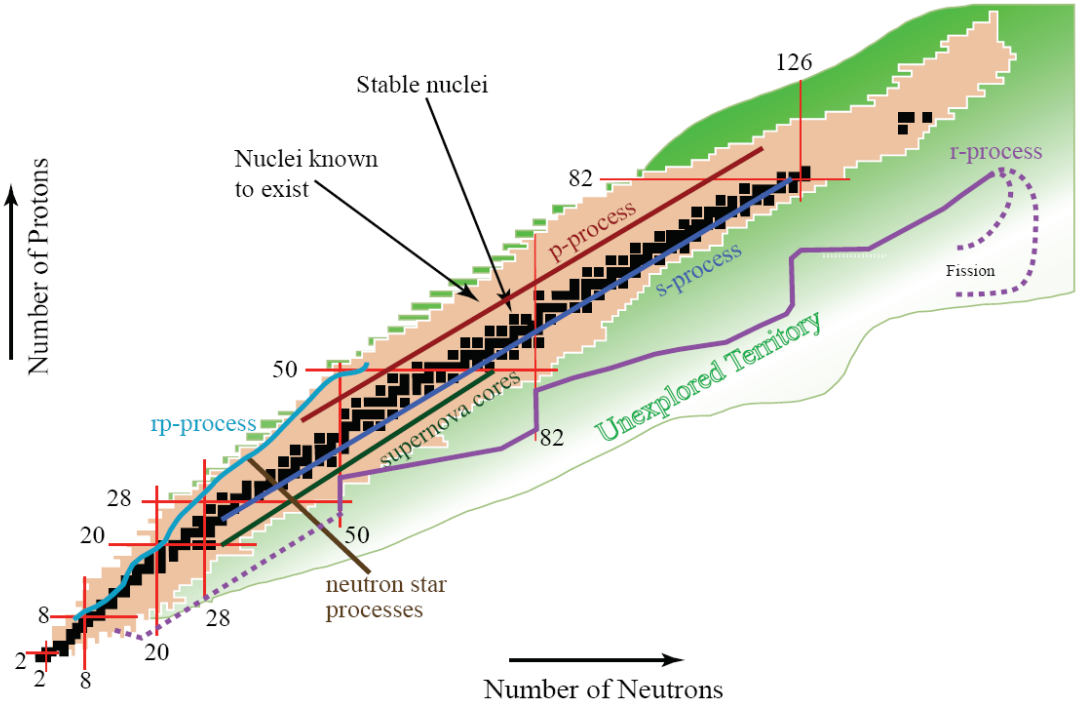
Fundamental Symmetries



- Why is there now more matter than antimatter in the universe?
- What is the nature of the neutrinos and how have they shaped the evolution of the universe?

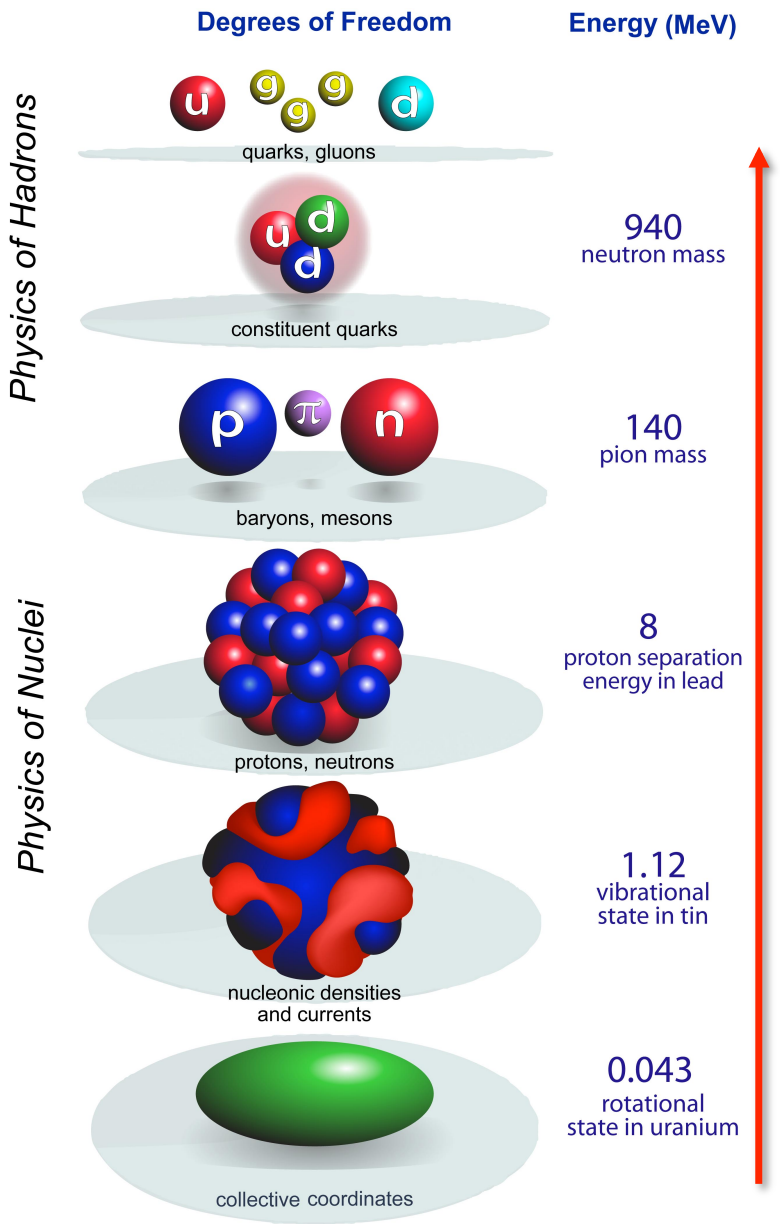
Questions driving low-energy nuclear physics

Applications of Nuclei



- How can our knowledge of nuclei and our ability to produce them benefit humankind? Life Sciences, Material Sciences, Nuclear Energy, Security

Tools to connect degrees of freedom: EFT and RG



Hot and dense quark-gluon matter

Hadron structure

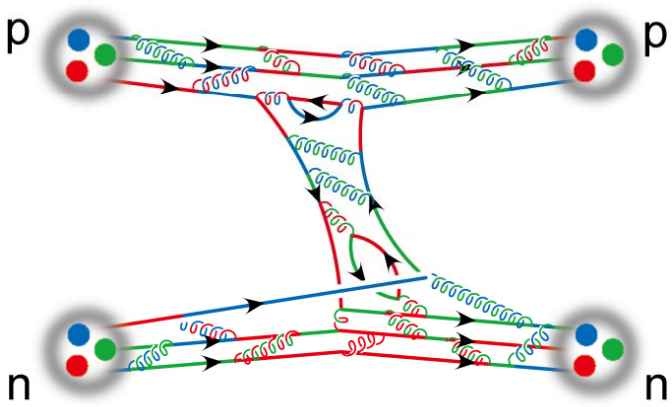
Hadron-Nuclear interface

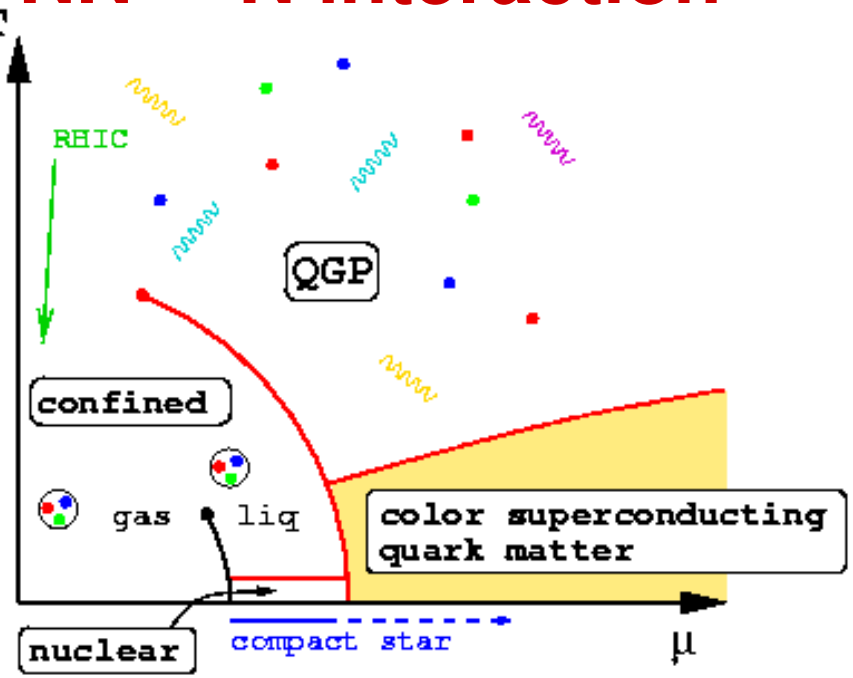
Nuclear structure
Nuclear reactions

Nuclear astrophysics
New standard model

Applications of nuclear science

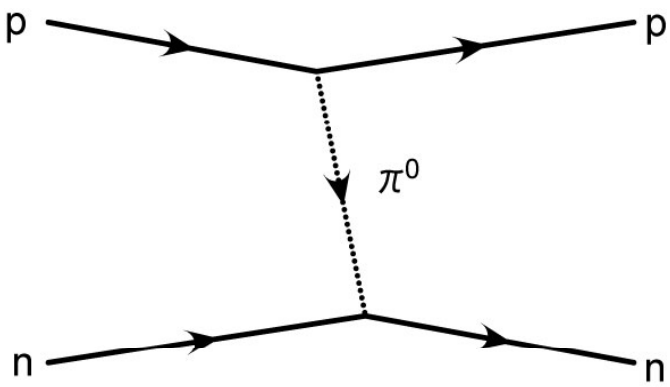
Quark (QCD) vs. hadronic NN$\cdots$N interaction

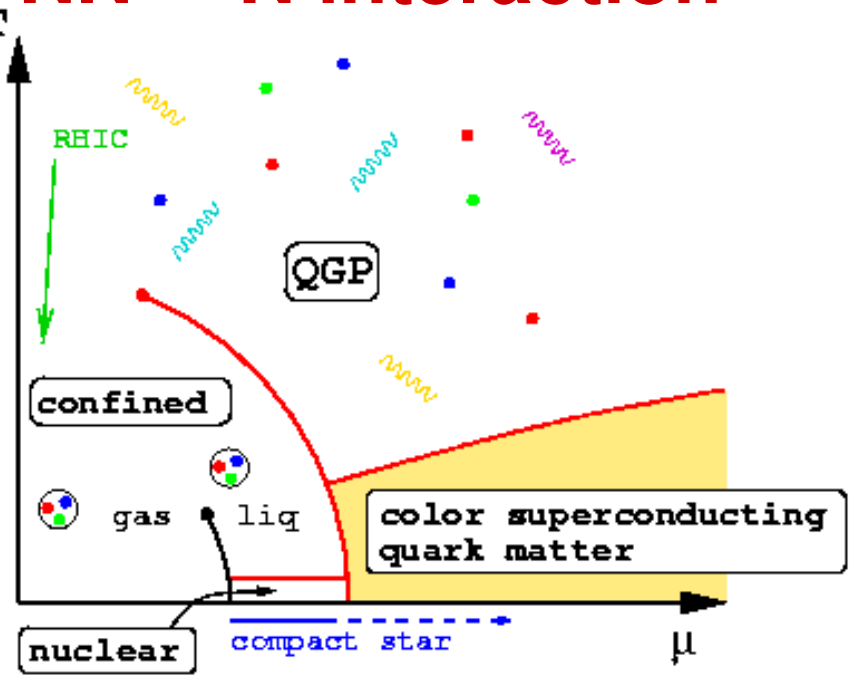




- Old goal: replace hadronic descriptions at ordinary nuclear densities with quark description (since QCD is *the* theory)

Quark (QCD) vs. hadronic NN$\cdots$N interaction



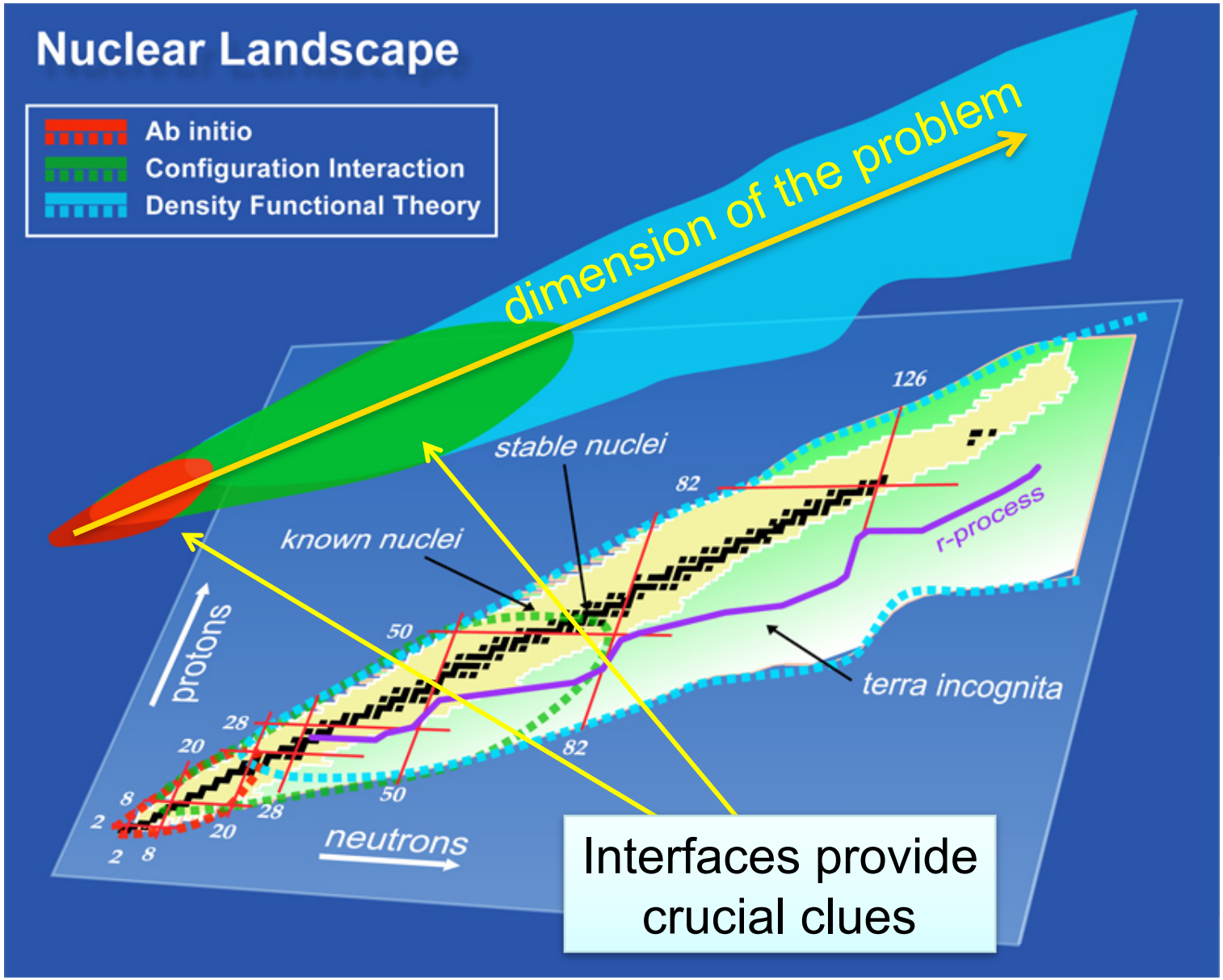


- Old goal: replace hadronic descriptions at ordinary nuclear densities with quark description (since QCD is *the* theory)
- New goal: use effective hadronic dof's *systematically*
  - Seek model independence and theory error estimates
  - Future: Use lattice QCD to match via "low-energy constants"
- Need quark dof's at higher densities (resolutions) where phase transitions happen or at high momentum transfers

What are the theory problems to be solved?

- Solve the many-nucleon Schrödinger equation
  - Focus here on time-independent: $\widehat{H}|\Psi\rangle = E|\Psi\rangle$
  - Time-dependence is an important challenge
- Find appropriate Hamiltonians and consistent operators
  - You mean there is more than one Hamiltonian?
  - What does *consistent* mean in this context?
  - What approximations do we make at this stage?
- We'll restrict ourselves here to non-relativistic approaches
  - How do we justify that? What are the limitations?
  - Doesn't mean ignoring special relativity, but incorporate as an expansion. E.g., $\sqrt{m^2 + p^2} - m = \frac{p^2}{2m} - \frac{p^4}{8m^3} + \cdots \quad (c = 1)$
- Calculate observables using consistent operators
  - Ground state and low-lying energies for sure
  - But what other quantities? Wave functions?

Overlapping theory methods cover all nuclei



What is "new" about theory methods? (examples)

I'll make my task even harder by intepreting "new methods" broadly!

- New methods for theoretical inputs (Hamiltonians and operators)
  - Three-body (and higher) forces (N3LO chiral 3NF, RG methods)
- New extensions of established microscopic techniques
  - e.g., IT-NCSM, MBPT, Berggren basis, LIT
  - Spectroscopic factors, ANCs, . . . (e.g., with GFMC, CC)
- New microscopic many-body techniques
  - e.g., Lattice EFT, IM-SRG, NCSM/RGM
- New analysis methods/philosophy (theory error bars!!)
  - Correlation analysis of energy functionals
  - Power counting, benchmarking, . . .
- New computational reach (e.g., from SciDAC projects)
  - Better scaling: massively parallel codes, load balancing
  - Improved algorithms: e.g., optimization (POUNDERS)

(Partial!) table of acronyms for low-energy nuclear theory

EFT	effective field theory	chEFT	chiral EFT
LO	leading order	NLO	next-to-leading order
LEC	low-energy constant	3NF	three-nucleon force
RG	renormalization group	SRG	similarity RG
$V_{\text{low } k}$	low-momentum potential	IM-SRG	in-medium SRG
MBPT	many-body perturbation theory	LIT	Lorentz integral transform
QMC	quantum Monte Carlo	GFMC	Green's function MC
AFDMC	auxiliary field diffusion MC	HH	hyperspherical harmonics
NCSM	no-core shell model	NCFC	no-core full configuration
IT-NCSM	importance truncated NCSM	CI	configuration interaction
ANC	asymptotic normalization constant	CC	coupled cluster
DFT	density functional theory	EDF	energy density functional
SNM	symmetric nuclear matter	PNM	pure neutron matter
SEMF	semi-empirical mass formula		
UNEDF	universal nuclear EDF	NUCLEI	nuclear computational low-energy initiative

Outline

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Recap and outlook

QM review: $\widehat{H}|\Psi\rangle = E|\Psi\rangle$ in finite matrix form

- Choose (approximately) complete basis: $\{\phi_i\}$, $i = 1, \ldots, N$
  - Very general: discretized coordinate or momentum space, harmonic oscillators, Gaussians (non-orthogonal!), ...
- Then the (Hermitian) matrix eigenvalue problem is

$$H_{ij}\psi_j^{(n)} = E^{(n)}\psi_j^{(n)} \quad \text{where} \quad H_{ij} = \langle\phi_i|\widehat{H}|\phi_j\rangle$$

  - There will be N eigenvalues $E^{(n)}$ and N corresponding eigenvectors (wave functions) $\psi_i^{(n)}$
  - We'll usually be interested here in just the lowest few $E^{(n)}$'s
- At this stage, applies to any number of nucleons
  - E.g., the $\{\phi_i\}$ could be Slater determinants of single-particle wave functions for A nucleons (antisymmetrized!)
- If our table of numbers H_{ij} is not too large, we can give it to Mathematica, MATLAB, LAPACK, ... and get back the eigenvalues and (normalized) eigenvectors. If it is large, do something else!

Scaling of computations

- Dimension of nuclear problem many-body grows very rapidly with A and accuracy desired
  - How a method *scales* with size limits its scope
- Issues that affect scaling:
  - What method is used and choice of algorithms
  - Distribution on parallel cpus (want all processors equally busy without sharing all memory or talking to each other all the time)
  - Something nuclear theorists have to worry about now!
- Example: diagonalization of an $N \times N$ symmetric matrix
  - MATLAB result: when matrix dimension doubles, the `eig` function takes roughly 8 times as long to find eigenvalues
  - Makes sense: full matrix multiplication requires N multiplies for each of N^2 matrix elements $\Longrightarrow \mathcal{O}(N^3)$ operations
  - We'll see that this scaling would eliminate a major method!

Applying $e^{-(H-E_T)\tau}$ to a trial ground state vector

- Consider a vector $|\Psi_{\text{var.}}\rangle$ and its expansion in eigenstates of the Hamiltonian H:

$$|\Psi_{\text{var.}}\rangle = \sum_k C_k |\psi_k\rangle \quad \text{where} \quad H|\psi_k\rangle = E_k|\psi_k\rangle$$

  - E.g., $|\Psi_{\text{var.}}\rangle$ is a variational guess for the ground state

- General: $f(H)|\psi_k\rangle = f(E_k)|\psi_k\rangle$ (where f specified by power series)
  - Later: powers of H (Lanczos method)
- Here, apply imaginary time propagation e^{-iHt} with $\tau = it$:

$$|\Psi(\tau \to \infty)\rangle = \lim_{\tau\to\infty} e^{-(H-E_T)\tau}|\Psi_{\text{var.}}\rangle \overset{\tau\to\infty}{\longrightarrow} C_0 e^{-(E_0-E_T)\tau}|\psi_0\rangle$$

  - We project out the ground state! [MATLAB example available]
  - Note the use of the trial energy E_T. Why? How do I get E_0?
  - In practice, we break up the imaginary time into small intervals to be able to calculate: $e^{-(H-E_T)\tau} = \Pi_{\Delta\tau} e^{-(H-E_T)\Delta\tau}$

Example: coordinate basis for *local* one-body potential

- Discretize $0 \leq r \leq R_{\max}$ with $r_i = i \times h$, where $h = R_{\max}/N$
- We can approximate the Schrödinger equation at point r_k as

$$-\frac{\hbar^2}{2M}\frac{u(r_k+h)-2u(r_k)+u(r_k-h)}{h^2} + V(r_k)u(r_k) = Eu(r_k)\ .$$

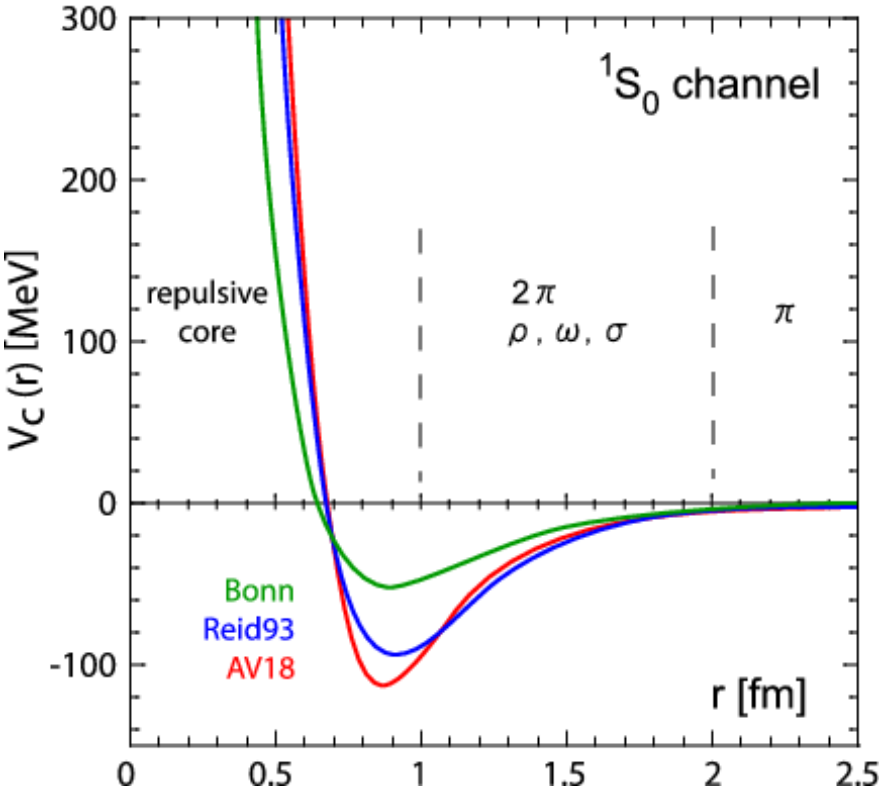
$$\text{or} \qquad -\frac{u_{k+1}-2u_k+u_{k-1}}{h^2} + V_k u_k = Eu_k\ .$$

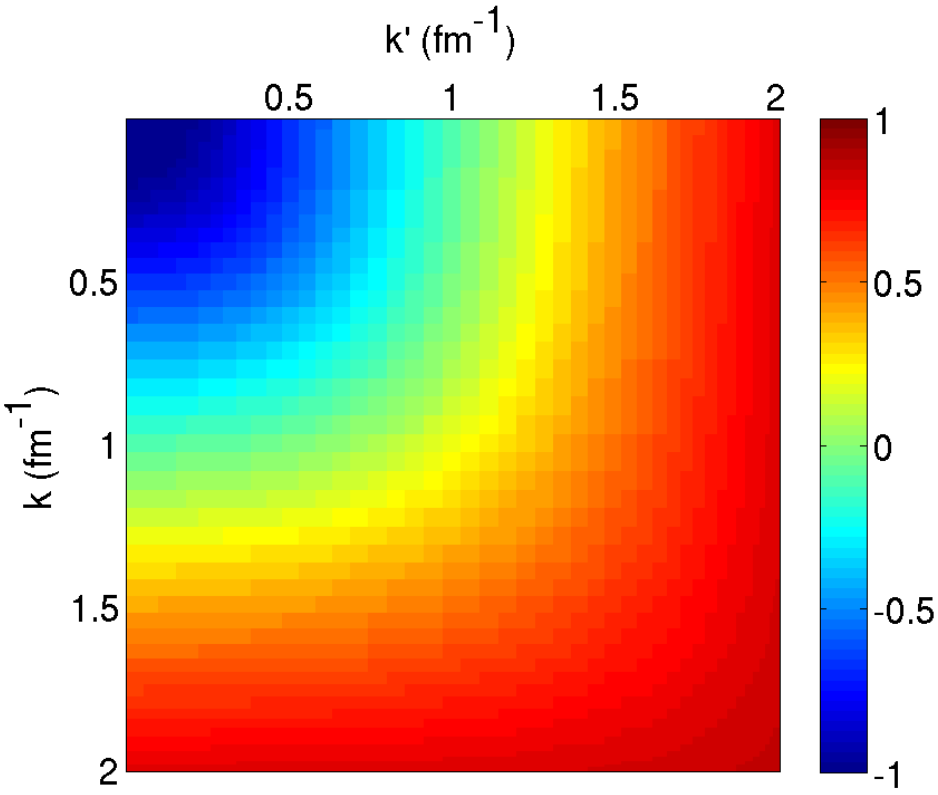
- In matrix form with $u_0 = 0$, $u_N \approx 0$, this is tri-diagonal ($\hbar = 2M = 1$):

$$\begin{pmatrix} \frac{2}{h^2}+V_1 & -\frac{1}{h^2} & 0 & \cdots & 0 \\ -\frac{1}{h^2} & \frac{2}{h^2}+V_2 & -\frac{1}{h^2} & & \vdots \\ 0 & -\frac{1}{h^2} & \ddots & & \vdots \\ \vdots & & & \ddots & -\frac{1}{h^2} \\ 0 & \cdots & \cdots & -\frac{1}{h^2} & \frac{2}{h^2}+V_{N-1} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_{N-1} \end{pmatrix} = E \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ \vdots \\ u_{N-1} \end{pmatrix}$$

- If V is *non-local*, it has off-diagonal matrix elements in this basis

S-wave NN potential as momentum-space matrix





$$\langle k|\, V_{L=0}|k'\rangle = \int d^3r\, j_0(kr)\, V(r)\, j_0(k'r) \implies V_{kk'} \text{ matrix}$$

- Momentum units ($\hbar = c = 1$): typical relative momentum in large nucleus $\approx 1\,\text{fm}^{-1} \approx 200\,\text{MeV}$
- What would kinetic energy look like on right?

Unitary transformations of matrices

- Recall that a unitary transformation can be realized as a unitary matrix with $U_\alpha^\dagger U_\alpha = I$ (where α is just a label)
  - Often used to simplify nuclear many-body problems, e.g., by making them more perturbative
- If I have a Hamiltonian H with eigenstates $|\psi_n\rangle$ and an operator O, then the new Hamiltonian, operator, and eigenstates are

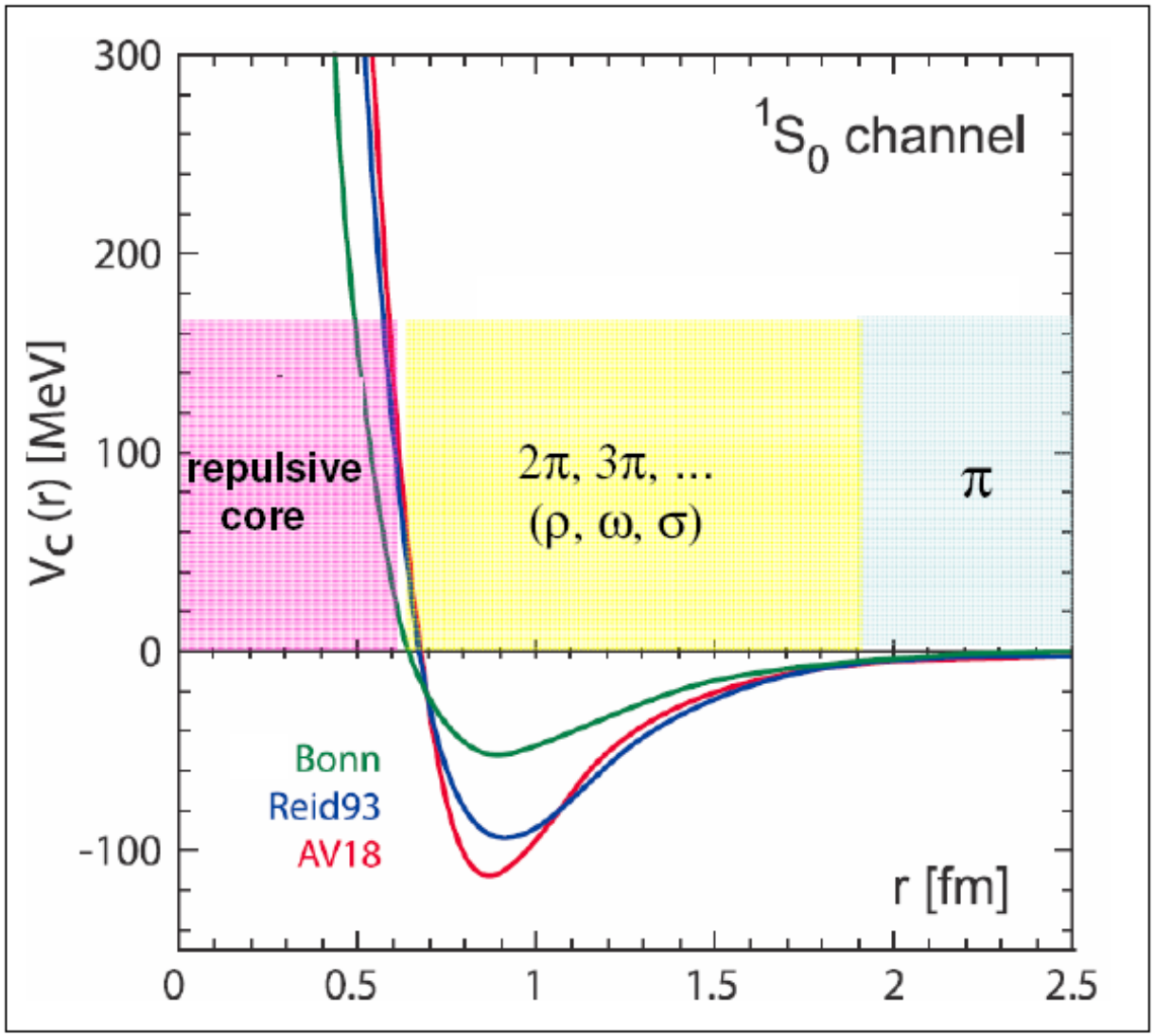
$$\widetilde{H} = UHU^\dagger \qquad \widetilde{O} = UOU^\dagger \qquad |\widetilde{\psi}_n\rangle = U|\psi_n\rangle$$

  - The energy is unchanged: $\langle\widetilde{\psi}_n|\widetilde{H}|\widetilde{\psi}_n\rangle = \langle\psi_n|H|\psi_n\rangle = E_n$
- Furthermore, matrix elements of O are unchanged:

$$O_{mn} \equiv \langle\psi_m|\widehat{O}|\psi_n\rangle = \left(\langle\psi_m|U^\dagger\right) U\widehat{O}U^\dagger \left(U|\psi_n\rangle\right) = \langle\widetilde{\psi}_m|\widetilde{O}|\widetilde{\psi}_n\rangle \equiv \widetilde{O}_{mn}$$

- If the asymptotic (long distance) properties are unchanged, H and $\widetilde{H}$ are equally acceptable physically. What are the observables?
  - Consistency: use O with H and $|\psi_n\rangle$'s but $\widetilde{O}$ with $\widetilde{H}$ and $|\widetilde{\psi}_n\rangle$'s
  - One form may be better for intuition or for calculations

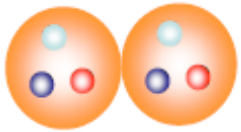
"Traditional" nucleon-nucleon interaction (from T. Papenbrock)



From T. Hatsuda (Oslo 2008)

One-pion exchange
by Yukawa (1935)

Multi-pions
by Taketani (1951)



Repulsive core
by Jastrow (1951)

Local nucleon-nucleon interaction for non-rel S-eqn

- Depends on spins *and* isospins of nucleons; non-central
  - longest-range part is one-pion-exchange potential

$$V_\pi(\mathbf{r}) \propto (\tau_1 \cdot \tau_2) \left[(3\sigma_1 \cdot \hat{\mathbf{r}}\, \sigma_2 \cdot \hat{\mathbf{r}} - \sigma_1 \cdot \sigma_2)(1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2}) + \sigma_1 \cdot \sigma_2 \right] \frac{e^{-m_\pi r}}{r}$$

- Characterize operator structure of shorter-range potential
  - central, spin-spin, non-central tensor and spin-orbit

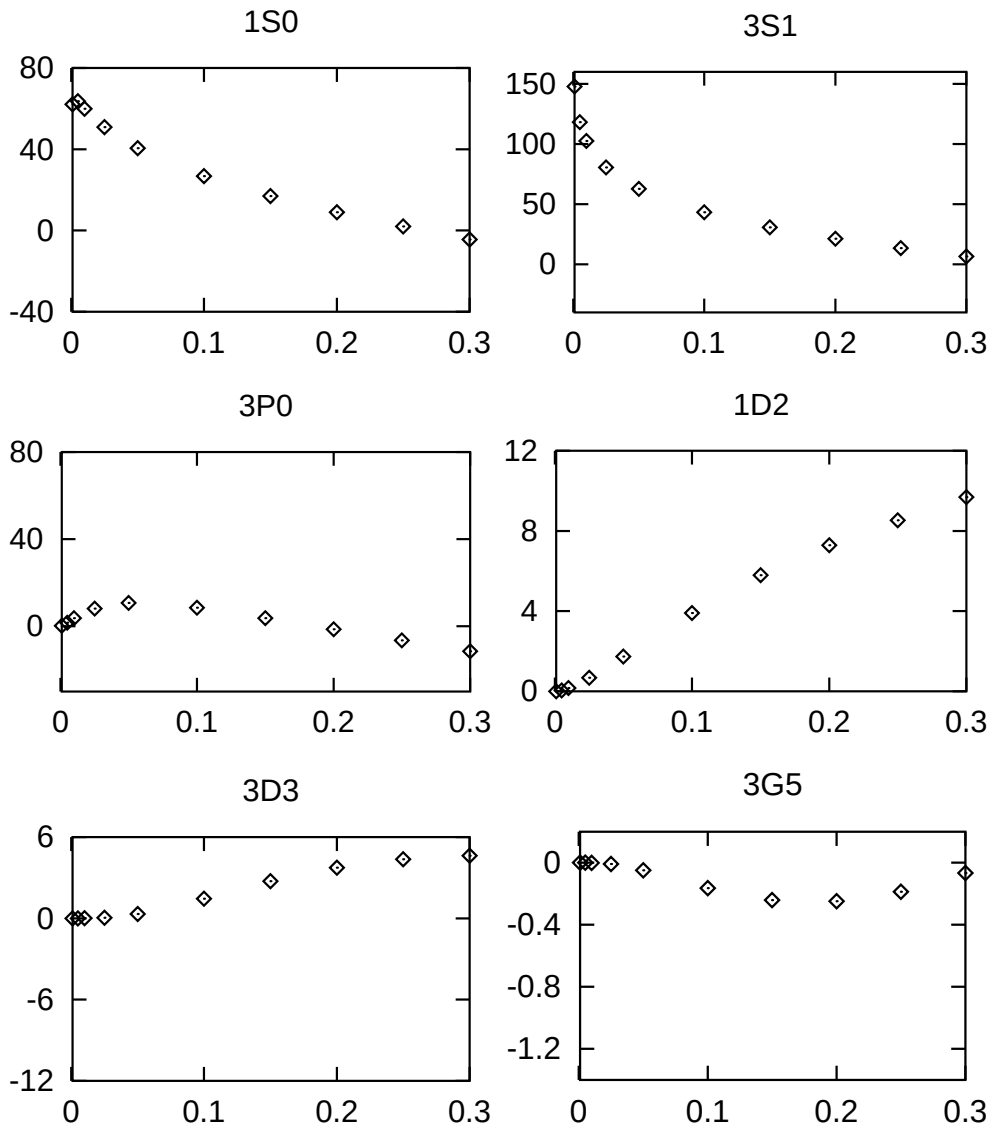
$$\{1, \sigma_1 \cdot \sigma_2, S_{12}, \mathbf{L} \cdot \mathbf{S}, \mathbf{L}^2, \mathbf{L}^2 \sigma_1 \cdot \sigma_2, (\mathbf{L} \cdot \mathbf{S})^2\} \otimes \{1, \tau_1 \cdot \tau_2\}$$

  - Argonne v_{18} is $V_{\rm EM} + V_\pi + V_{\rm short\ range}$ (all cut off at small r)
  - tensor $\Longrightarrow$ deuteron wf is mixed S ($L = 0$) and D ($L = 2$)
- Fit to NN scattering data up to 350 MeV (or $k_{\rm rel} \leq 2.05\,{\rm fm}^{-1}$)
- Alternative characterization is one-boson-exchange
- Systematic treatment: chiral effective field theory (EFT)

Chiral effective field theory for two nucleons

- Epelbaum, Meißner, et al.
- Also Entem, Machleidt
- Organize by $(Q/\Lambda)^\nu$ where $Q = \{\mathbf{p}, m_\pi\}$, $\Lambda \sim 0.5$–1 GeV
- $\mathcal{L}_{\pi N}$ + match at low energy

Q^ν	1π	2π	$4N$



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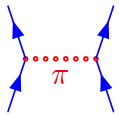
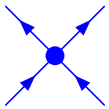
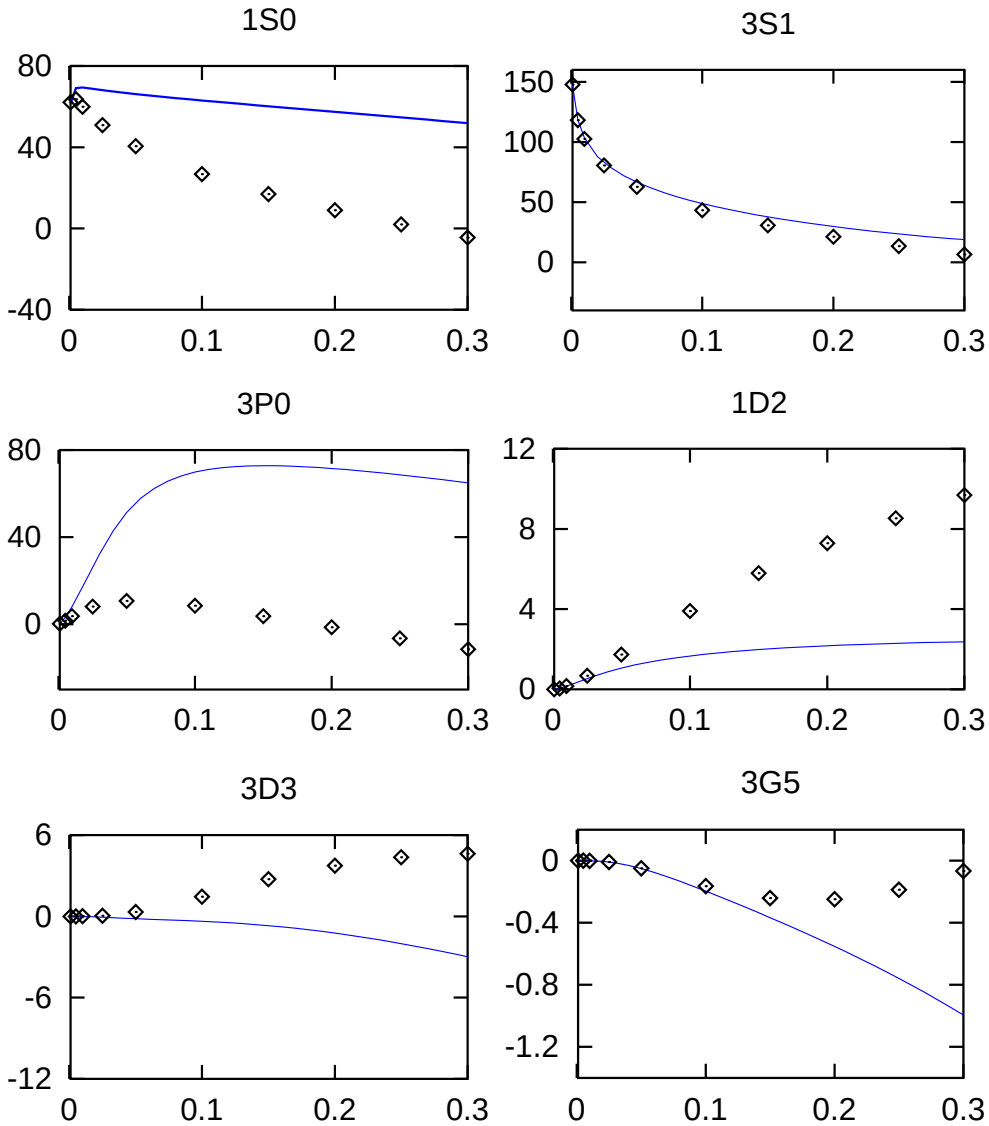
Q^0		—	 (2)



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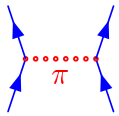
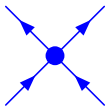
Q^0		—	 (2)
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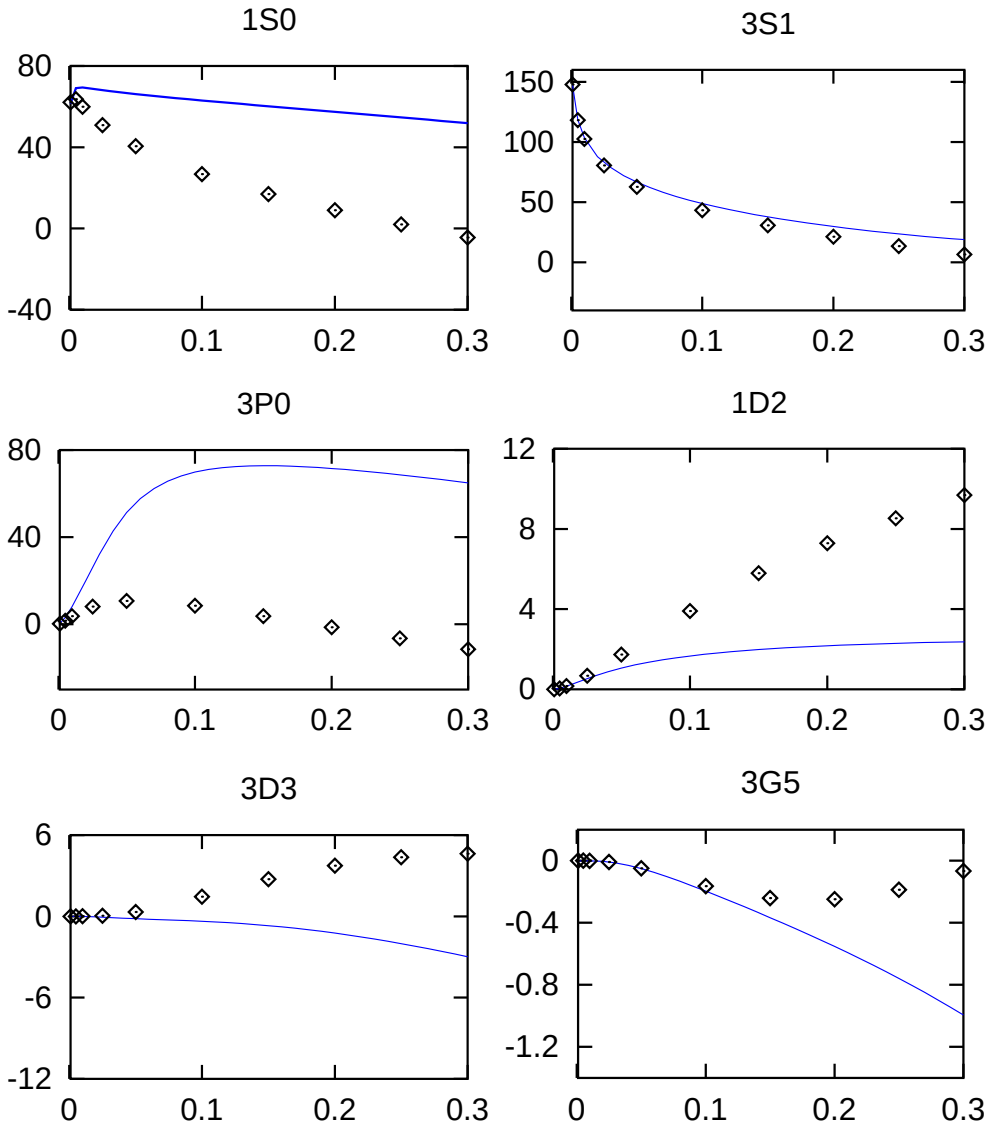

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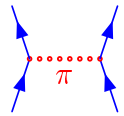
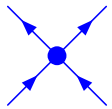
Q^0			 (2)
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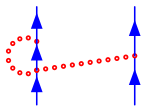
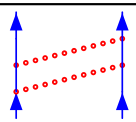
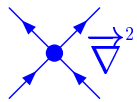
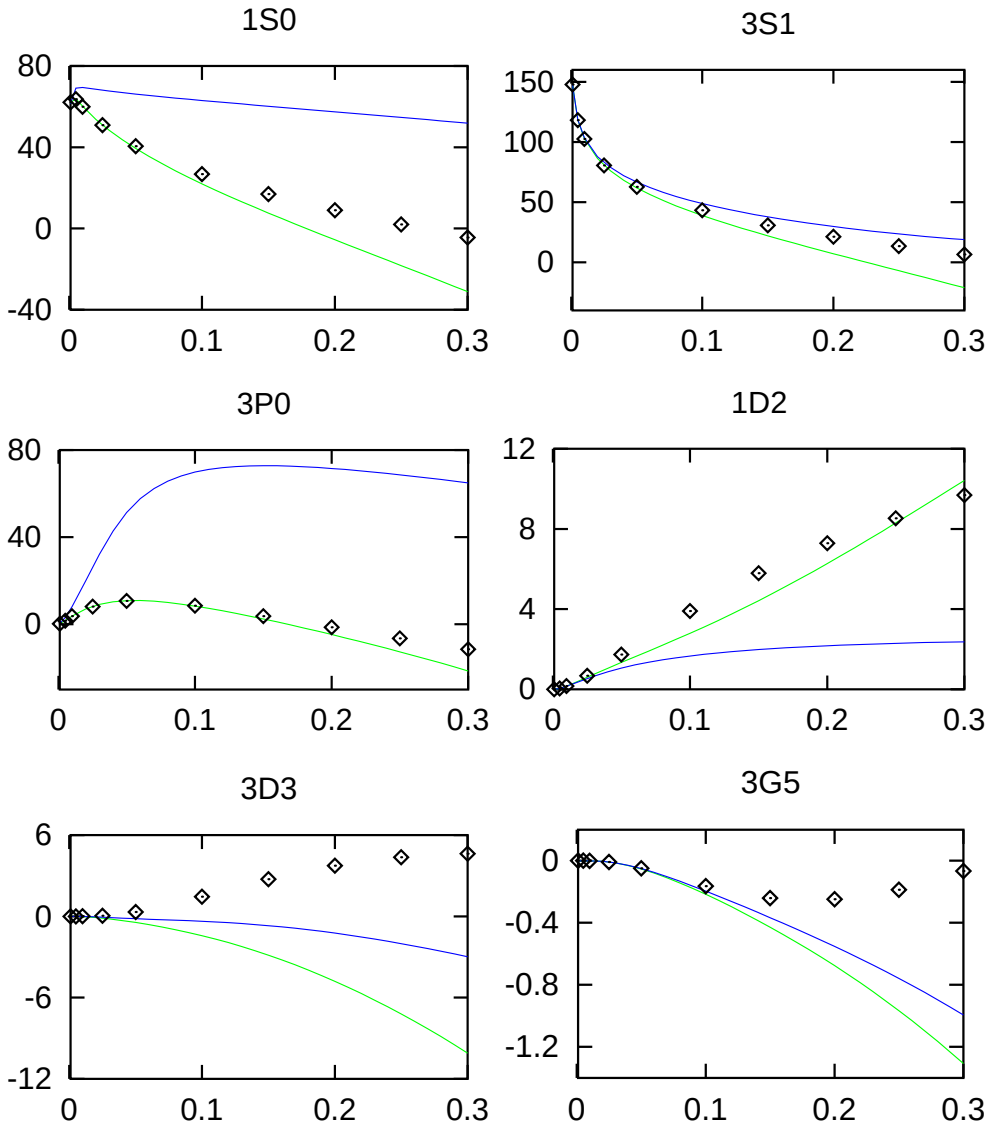
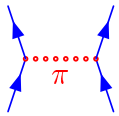
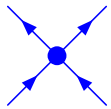
Q^2			 (7)



Chiral effective field theory for two nucleons

- Epelbaum, Meißner, et al.
- Also Entem, Machleidt
- Organize by $(Q/\Lambda)^\nu$ where $Q = \{\mathbf{p}, m_\pi\}$, $\Lambda \sim 0.5$–1 GeV
- $\mathcal{L}_{\pi N}$ + match at low energy

Q^ν	1π	2π	$4N$
Q^0		—	 (2)
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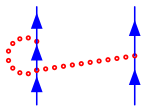
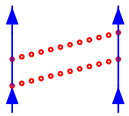
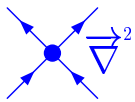
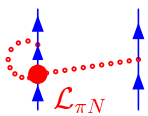
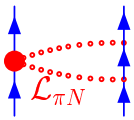
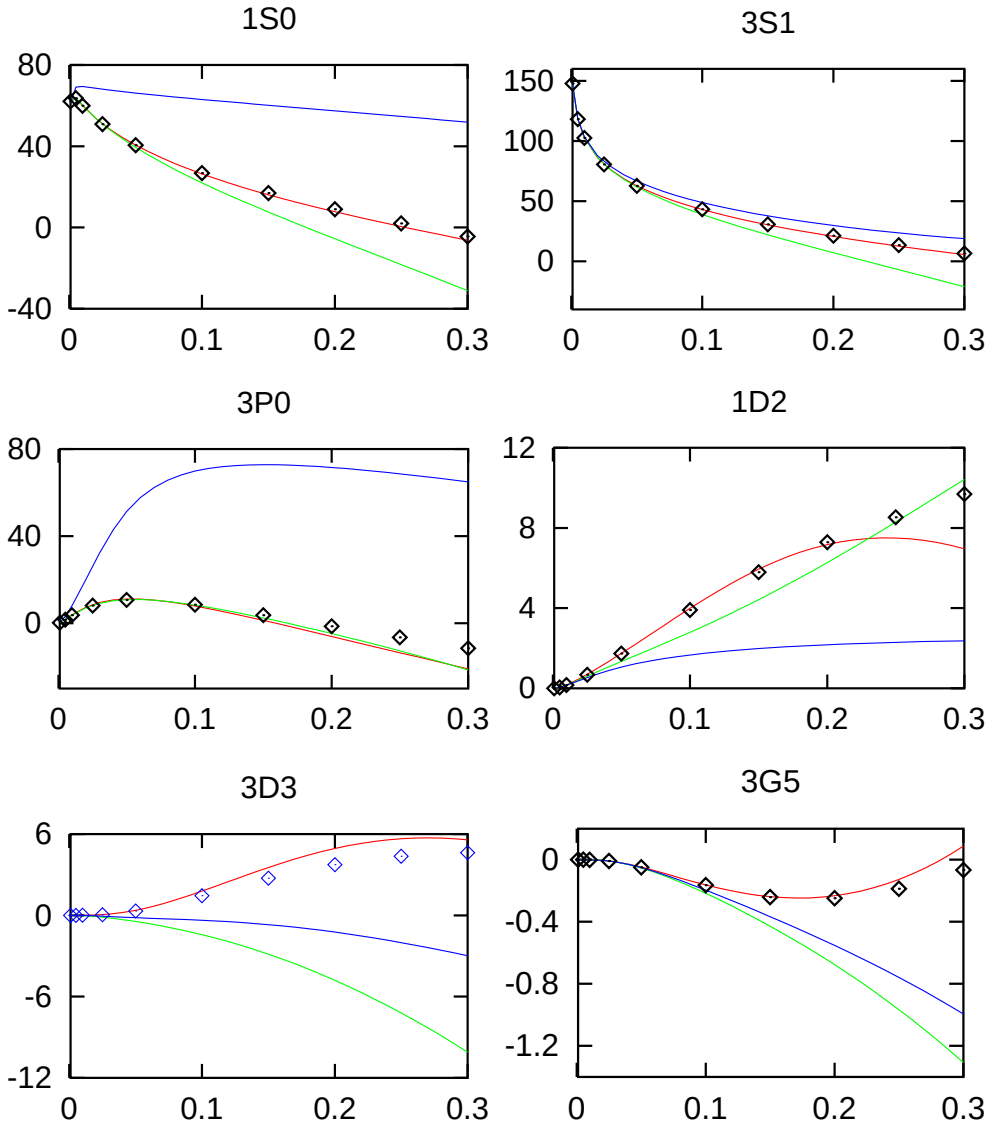
Q^2			 (7)
Q^3			



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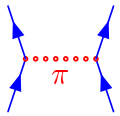
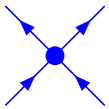
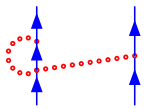
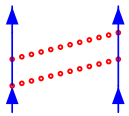
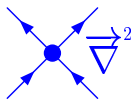
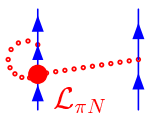
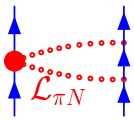
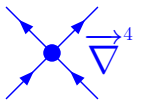
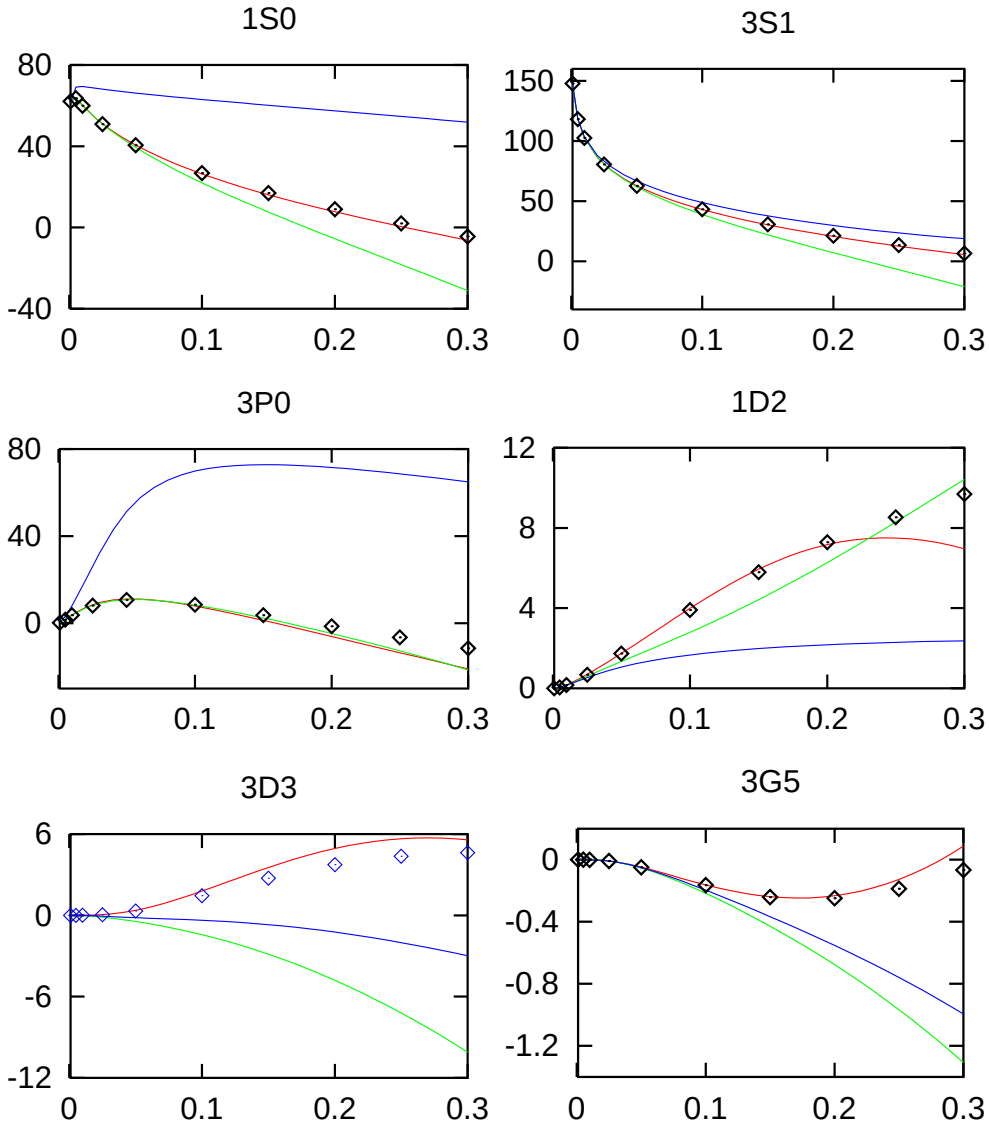
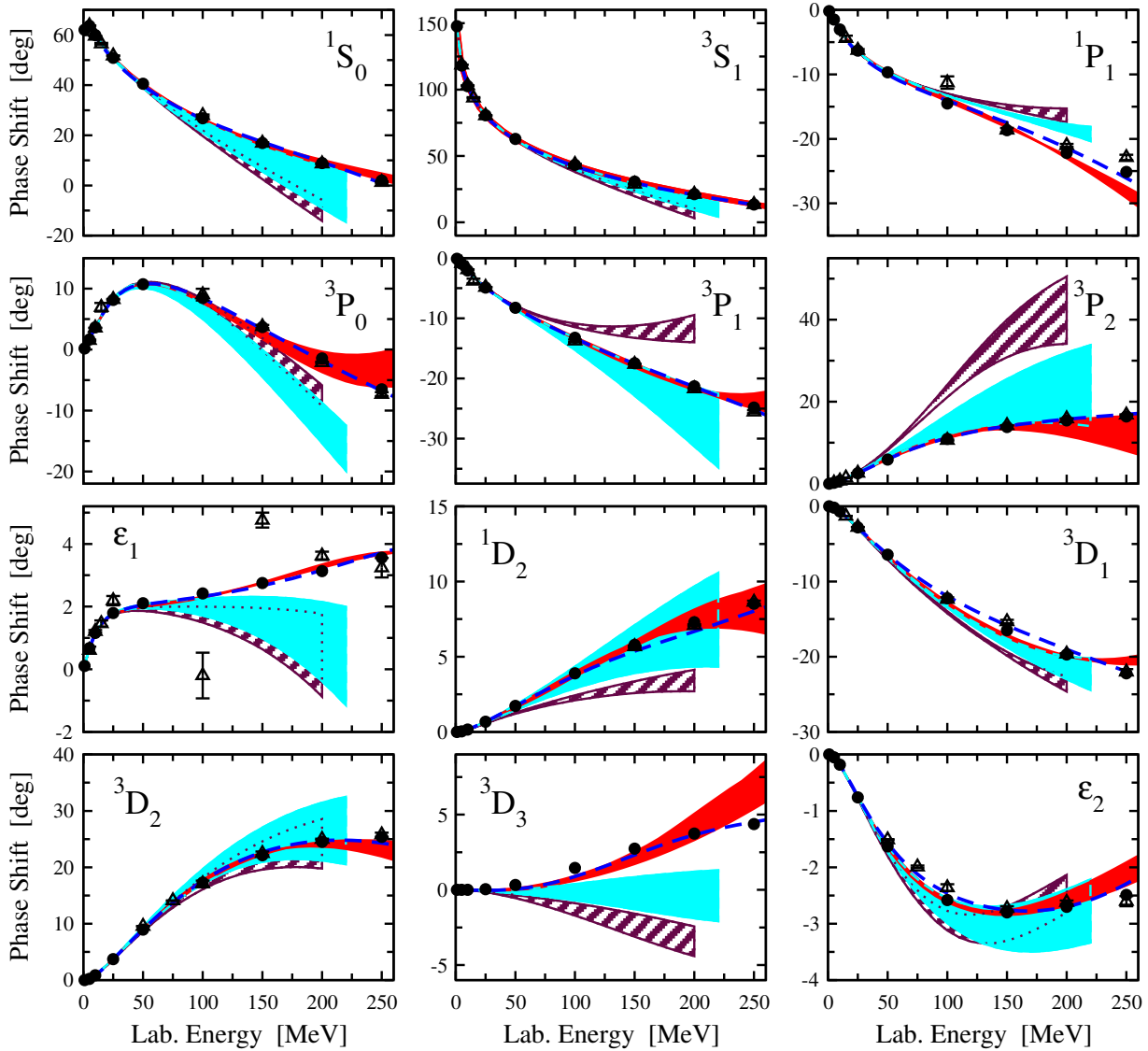
Q^0		—	 (2)
Q^1			
Q^2			 (7)
Q^3			
Q^4	many	many	 (15)



NN scattering up to N^{3}LO (Epelbaum, nucl-th/0509032)



- Theory error bands from varying cutoff over “natural” range

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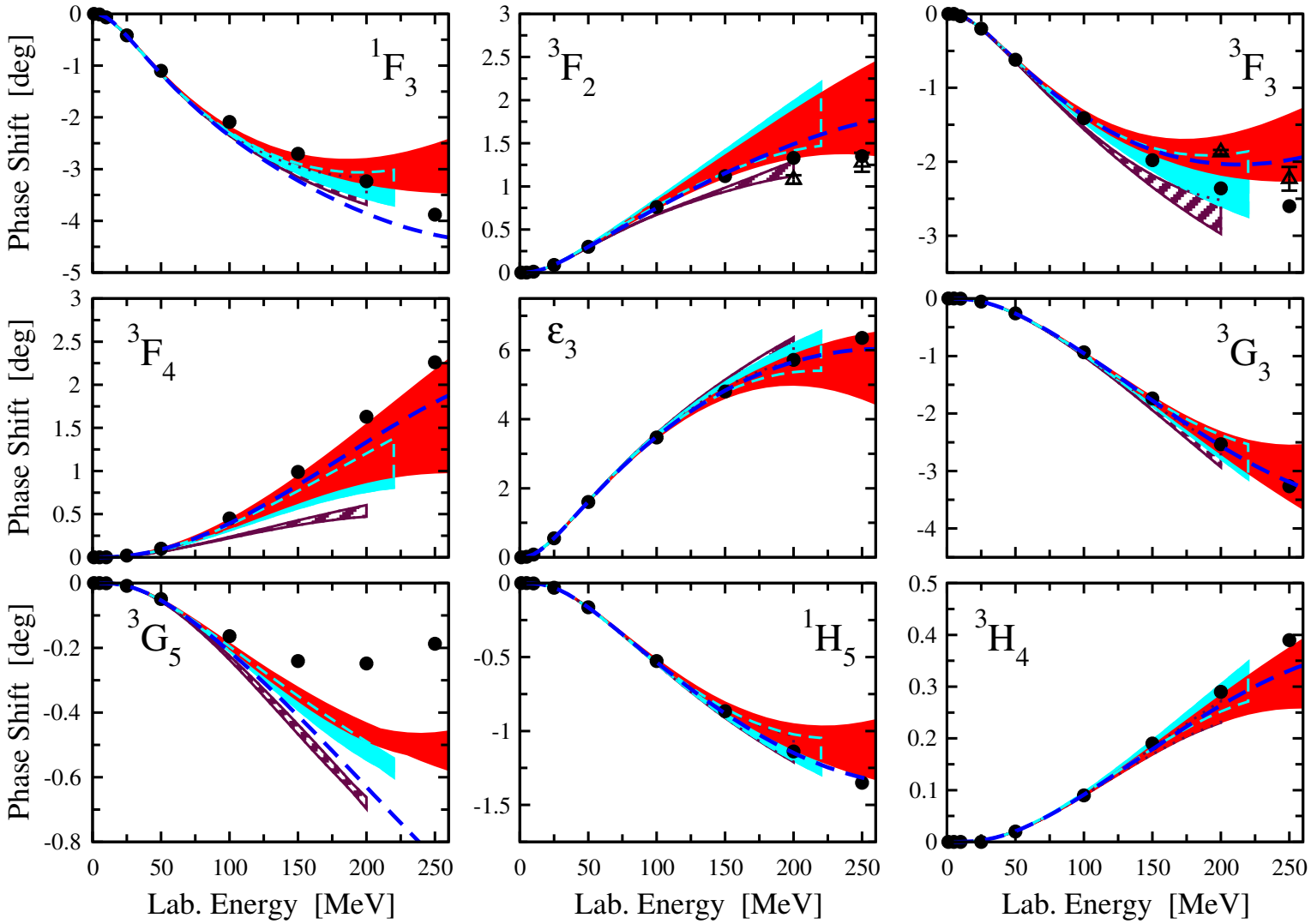
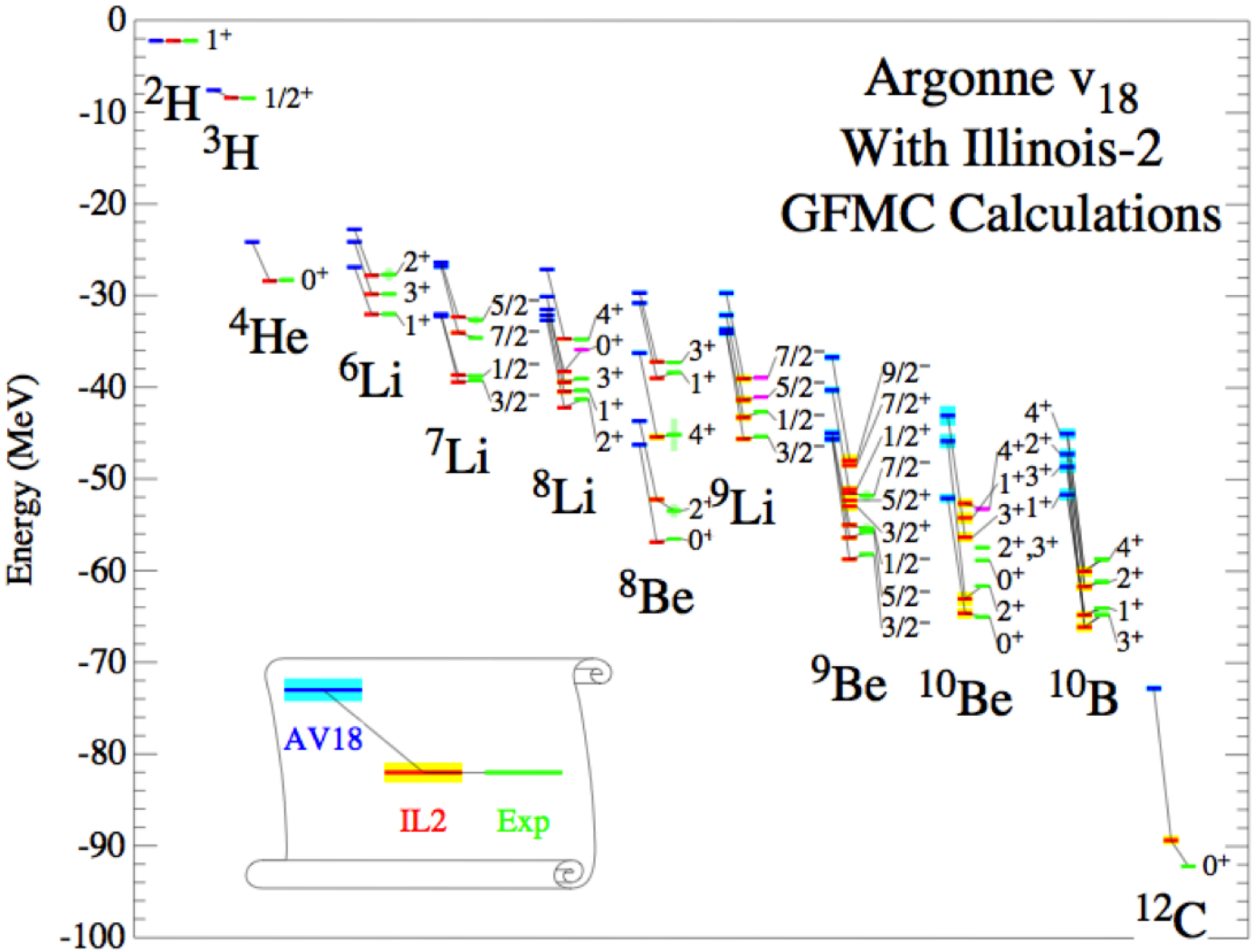


- Theory error bands from varying cutoff over “natural” range

Effective theories [H. Georgi, Ann. Rev. Nucl. Part. Sci. 43, 209 (1993)]

- *One of the most astonishing things about the world in which we live is that there seems to be interesting physics at all scales.*
- *To do physics amid this remarkable richness, it is convenient to be able to isolate a set of phenomena from all the rest, so that we can describe it without having to understand everything. Fortunately, this is often possible. We can divide up the parameter space of the world into different regions, in each of which there is a different appropriate description of the important physics. Such an appropriate description of the important physics is an "effective theory."*
- *The common idea is that if there are parameters that are very large or very small compared to the physical quantities (with the same dimension) that we are interested in, we may get a simpler approximate description of the physics by setting the small parameters to zero and the large parameters to infinity. Then the finite effects of the parameters can be included as small perturbations about this simple approximate starting point.*
- E.g., non-relativistic QM: $c \to \infty$
- E.g., chiral effective *field* theory (EFT): $m_\pi \to 0$, $M_N \to \infty$
- Features: model independence (completeness) and error estimates

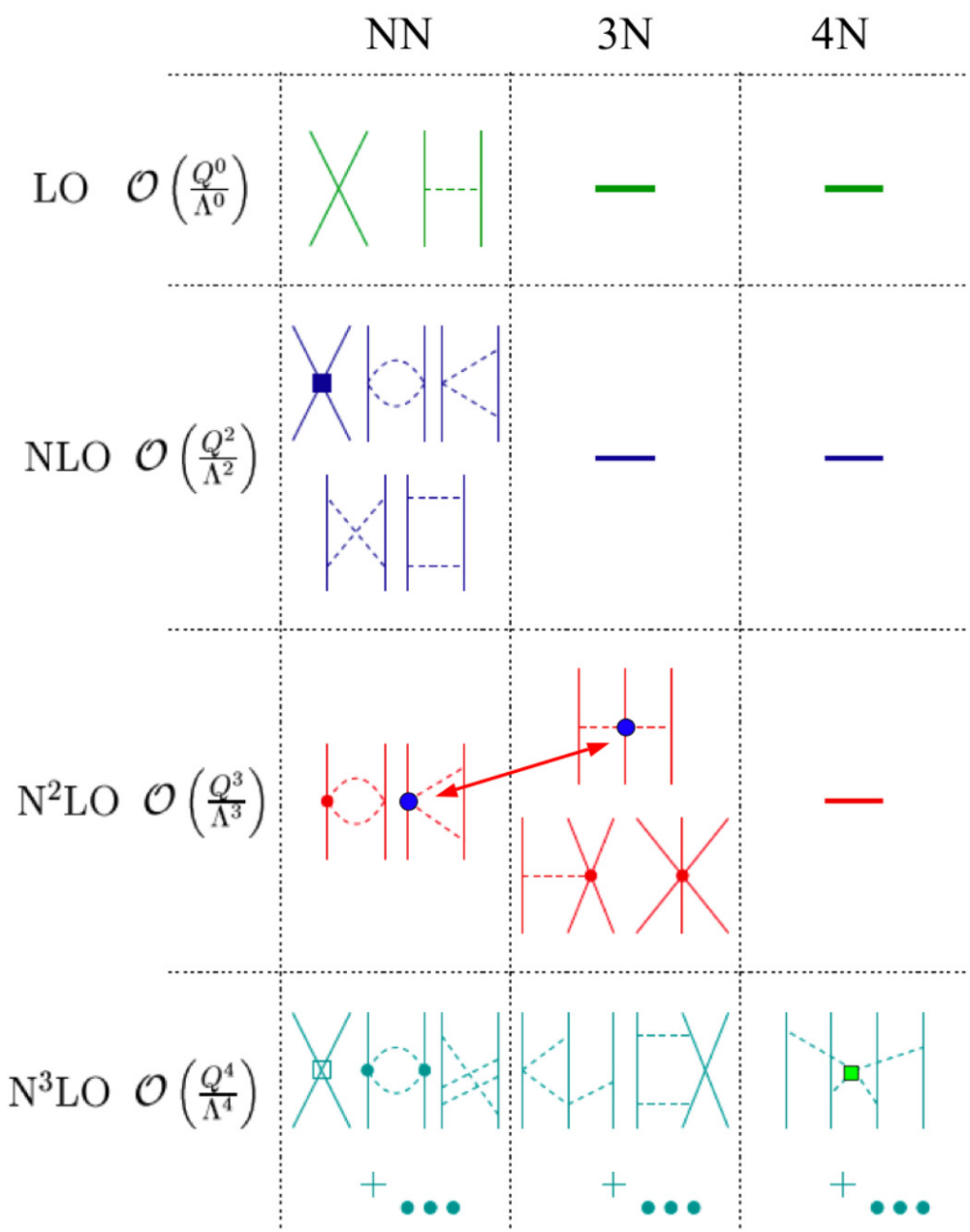
3NF in light nuclei [Pieper/Wiringa (Bonner Prize!)]



- Three-body forces needed for energies, splittings, . . .

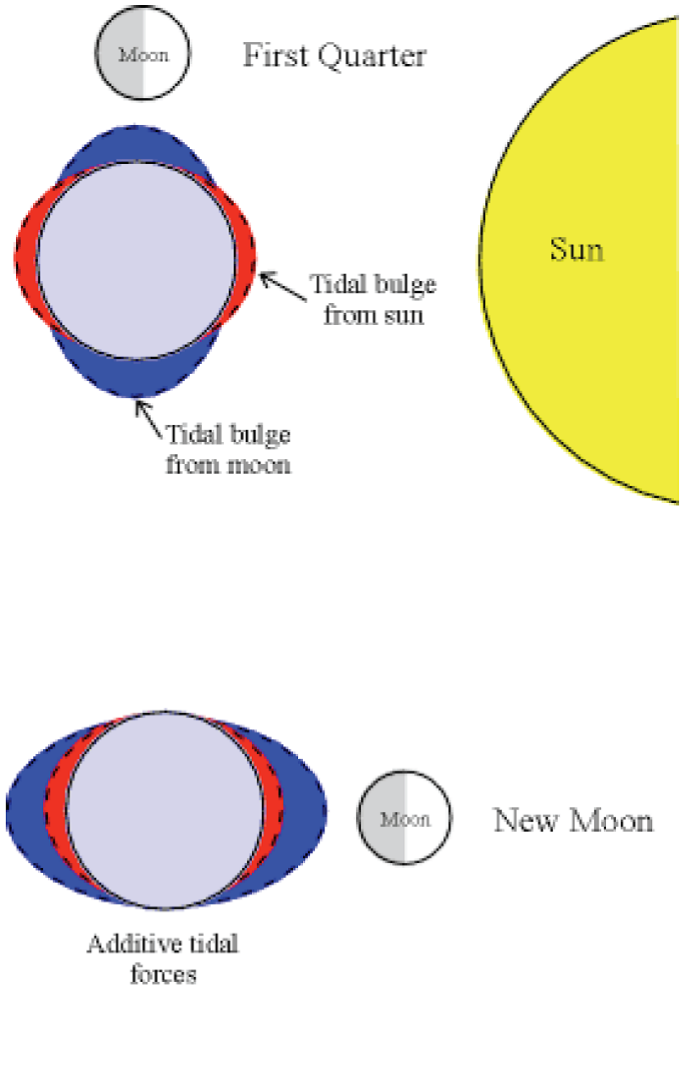
Few-body chiral forces

- At what orders? $\nu = -4 + 2N + 2L + \sum_i (d_i + n_i/2 - 2)$, so adding a nucleon suppresses by Q^2/Λ^2.
- Power counting confirms $2NF \gg 3NF > 4NF$
- NLO diagrams cancel
- 3NF vertices may appear in NN and other processes
- Fits to the c_i's have sizable error bars



Tidal analog to nuclear 3-body forces

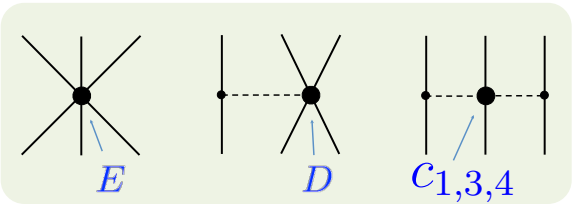
- Three-body forces between pointlike protons and neutrons are not negligible
- Analogous to tidal forces: the gravitational force on the Earth is not just the pairwise sum of the point-like Earth-Moon and Earth-Sun forces



What's new with chiral 3NF [from H. Krebs]

- Three-nucleon forces in chiral EFT start to contribute at NNLO

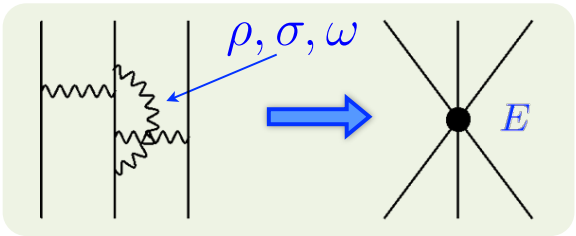
  (U. van Kolck ´94; Epelbaum et al. ´02; Nogga et al. ´05; Navratil et al. ´07)



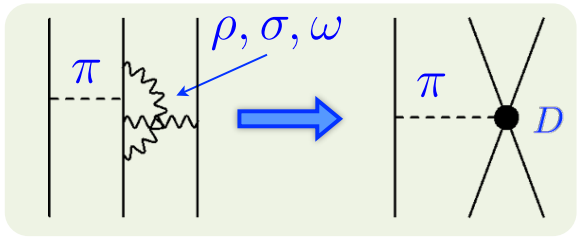
$c_{1,3,4}$ from the fit to πN-scattering data

D, E from ${}^{3}\mathrm{H}, {}^{4}\mathrm{He}, {}^{10}\mathrm{B}$ binding energy + coherent nd - scattering length

- LECs D and E incorporate short-range contr.



Resonance saturation interpretation of LECs



- Delta contributions encoded in LECs

  (Bernard, Kaiser & Meißner '97)

Delta-resonance saturation

$$c_3 = -2c_4 = c_3(\not\Delta) - \frac{4h_A^2}{9\Delta}$$

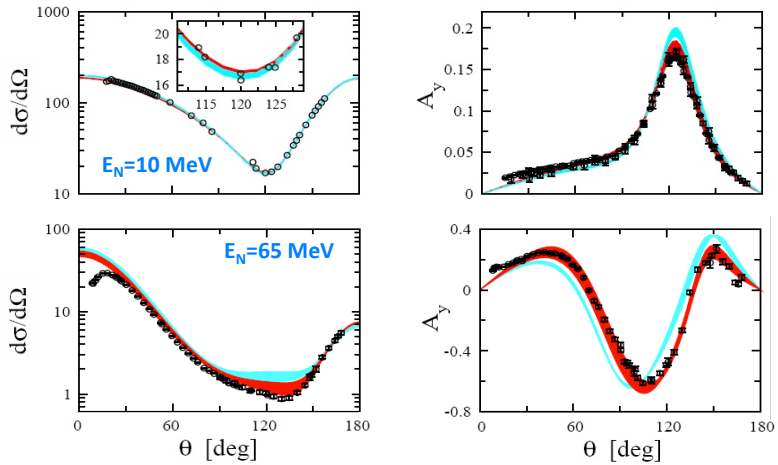
Enlargement due to Delta contribution

What's new with chiral 3NF [from H. Krebs]

Nd elastic scattering

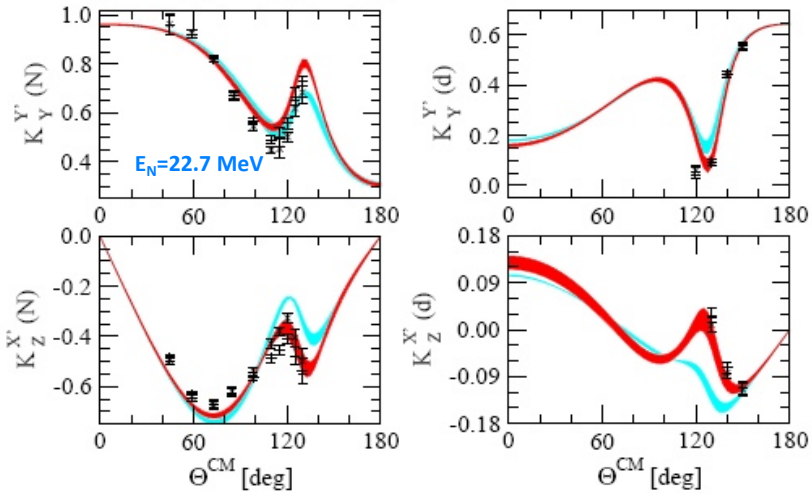
Cross section & vector analyzing power

E.pelbaum, PPNP 57 (2006) 654



Polarization transfer coefficients

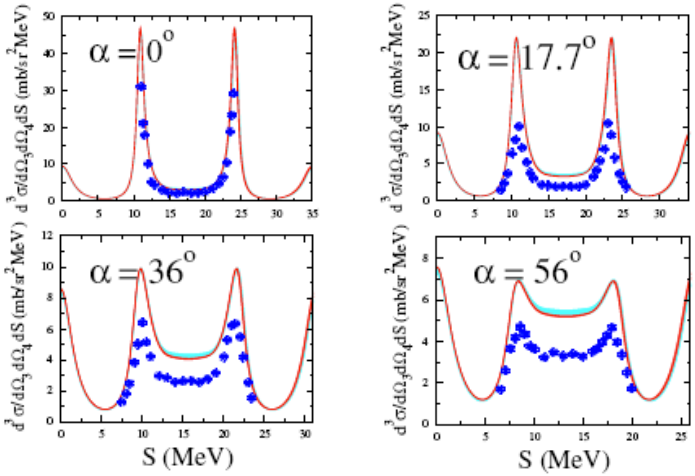
Witała et al., PRC 73 (2006) 044004



Deuteron break-up

SCRE configuration at E_d=19 MeV

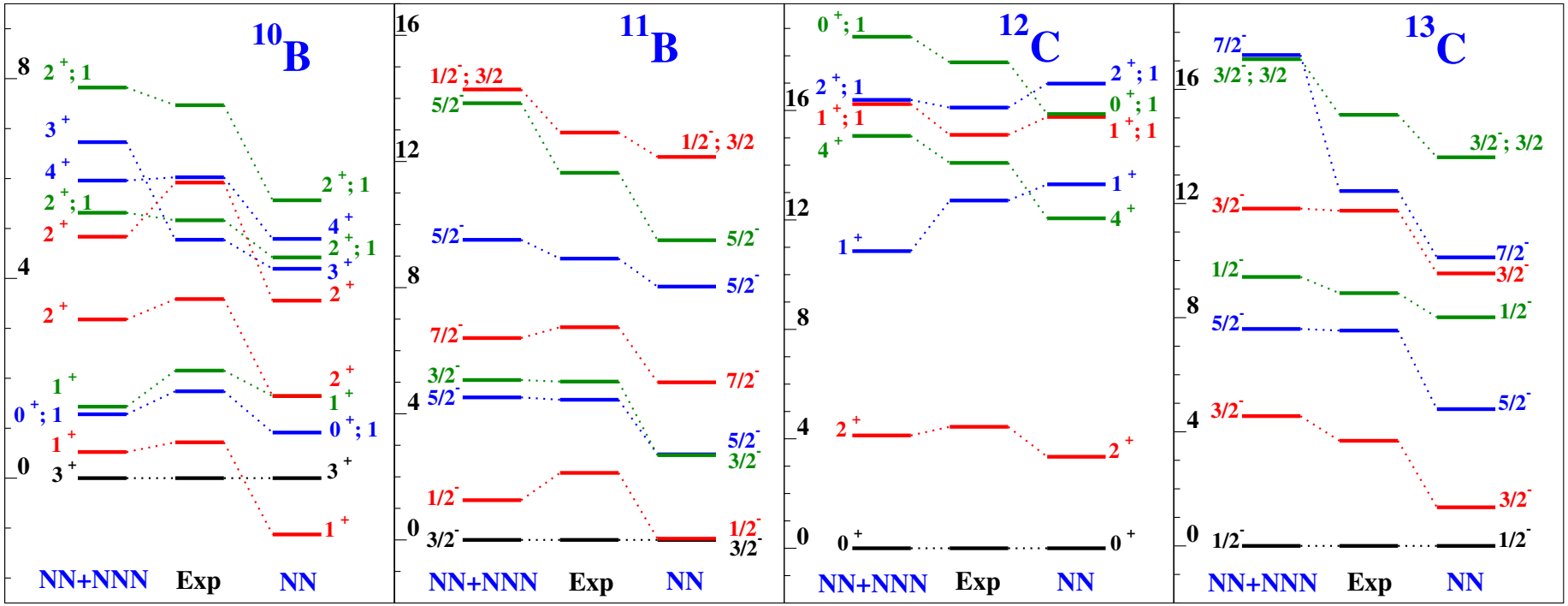
Ley et al., PRC 73 (2006) 064001



- Promising NNLO results for Nd elastic scattering
- Generally good description of break-up observables except for SCRE/SST break-up configuration at low energy
- Hope for improvement at N^{3}LO

No-Core Shell Model (NCSM) with 3NF

- Nuclear structure results point to importance of 3NF
  - Note ^{10}B ground state
  - Note spin-orbit splittings
- Need better convergence (stay tuned!)



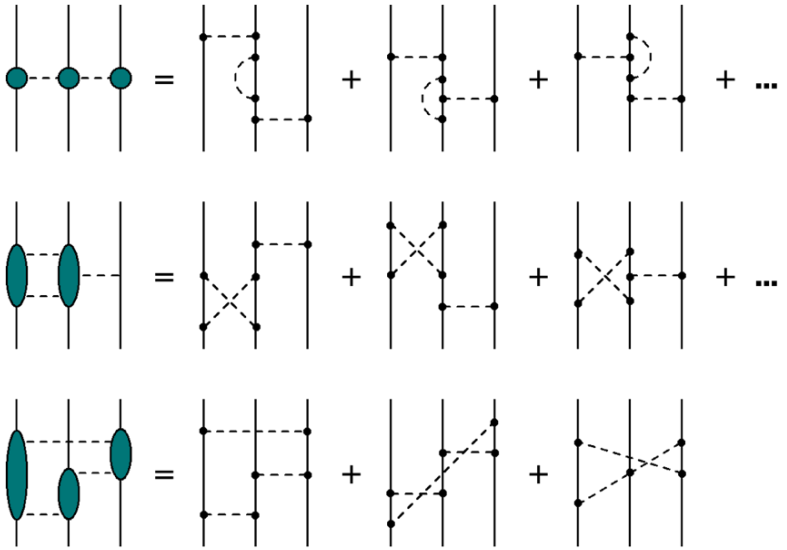
[Navratil et al., (2007)]

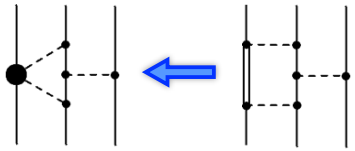
What's new with chiral 3NF [from H. Krebs]

- Three-nucleon forces at N^{3}LO

Long range contributions *Bernard, Epelbaum, H.K., Meißner ´08; Ishikawa, Robilotta ´07*

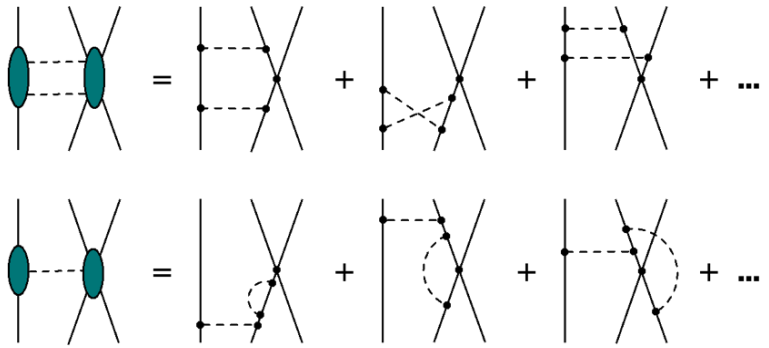
- No additional free parameters
- Expressed in terms of g_A, F_π, M_π
- Rich isospin-spin-orbit structure
- Δ(1232)-contr. are important



Large $c_i \sim$ 

Shorter range contributions *Bernard, Epelbaum, H.K., Meißner ´11*

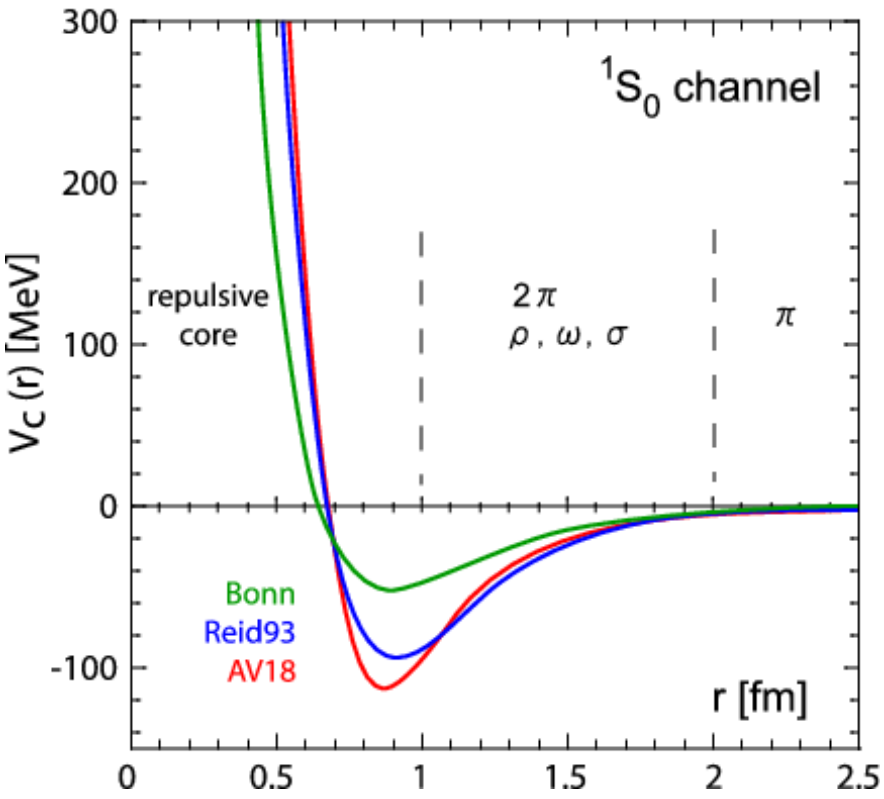
- LECs needed for shorter range contr.
  g_A, F_π, M_π, C_T
- Central NN contact interaction does not contribute
- Unique expressions in the static limit for a renormalizable 3NF

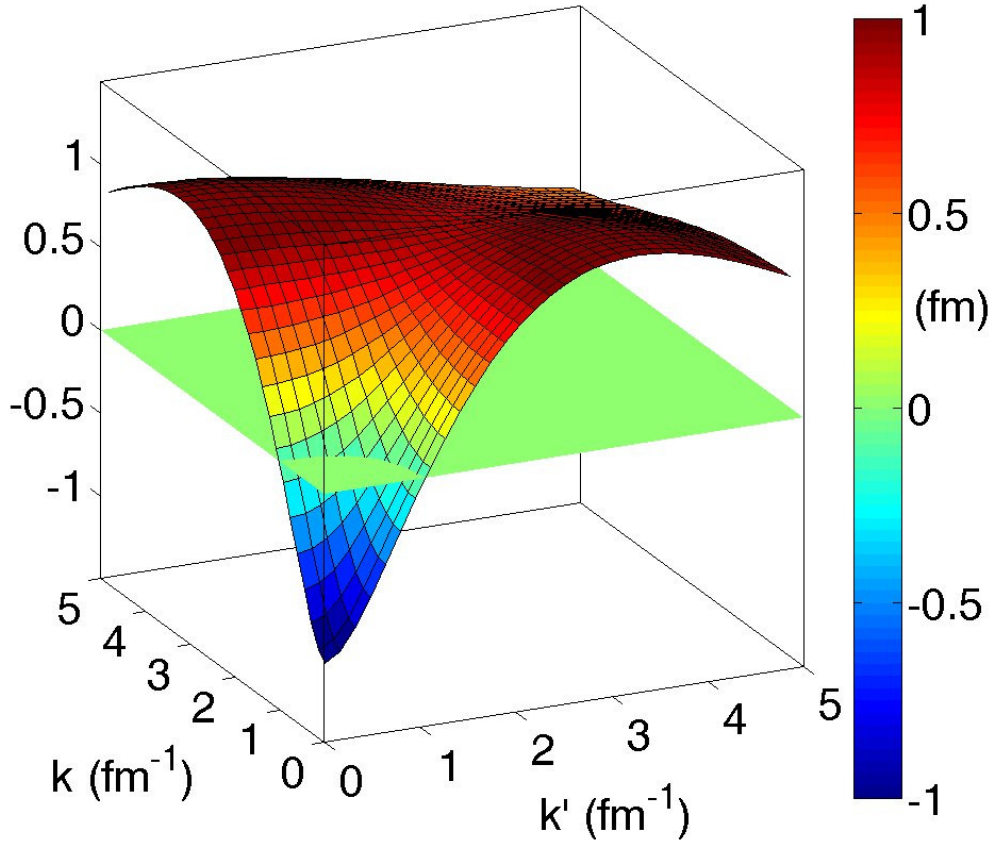


S. Weinberg on the Renormalization Group

- From "Why the Renormalization Group is a good thing"
  "The method in its most general form can I think be understood as a way to arrange in various theories that the degrees of freedom that you're talking about are the relevant degrees of freedom for the problem at hand."
- Improving perturbation theory in high-energy physics
  - Mismatch of energy scales can generate large logarithms
  - Shift between couplings and loop integrals to reduce logs
- Universality in critical phenomena
  - Filter out short-distance degrees of freedom
- Simplifying calculations of nuclear structure/reactions
  - Make nuclear physics look more like quantum chemistry!
  - Like other RG applications, gains can seem like magic
- RG violates the First Law of Progress in Theoretical Physics
  Conservation of Information: "You will get nowhere by churning equations" $\Longrightarrow$ *but with RG you do!*

S-wave NN potential as momentum-space matrix

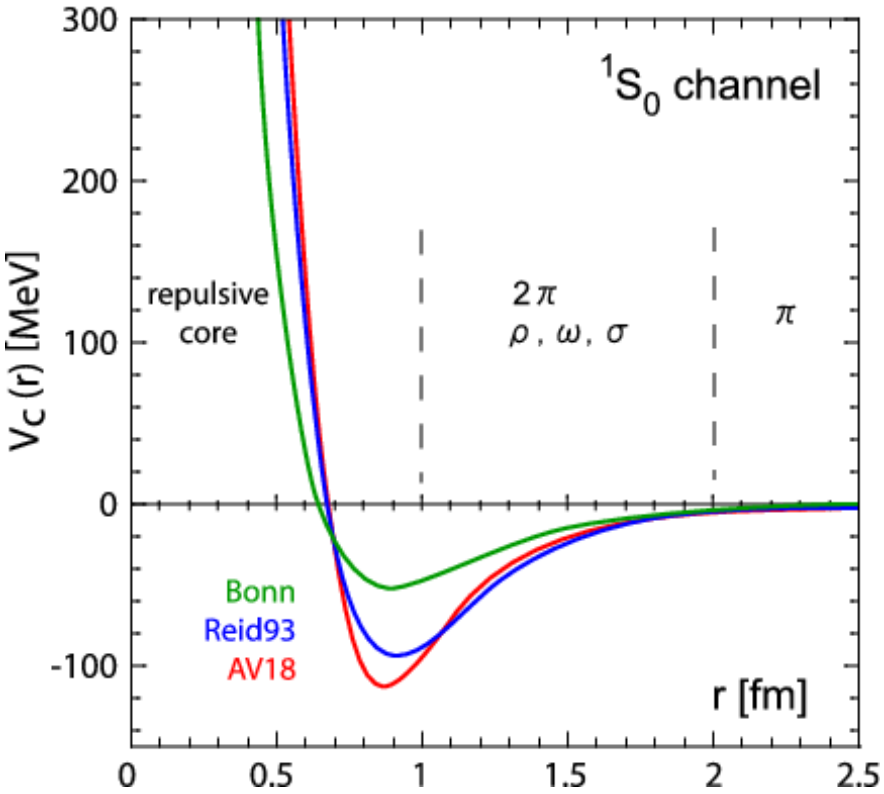


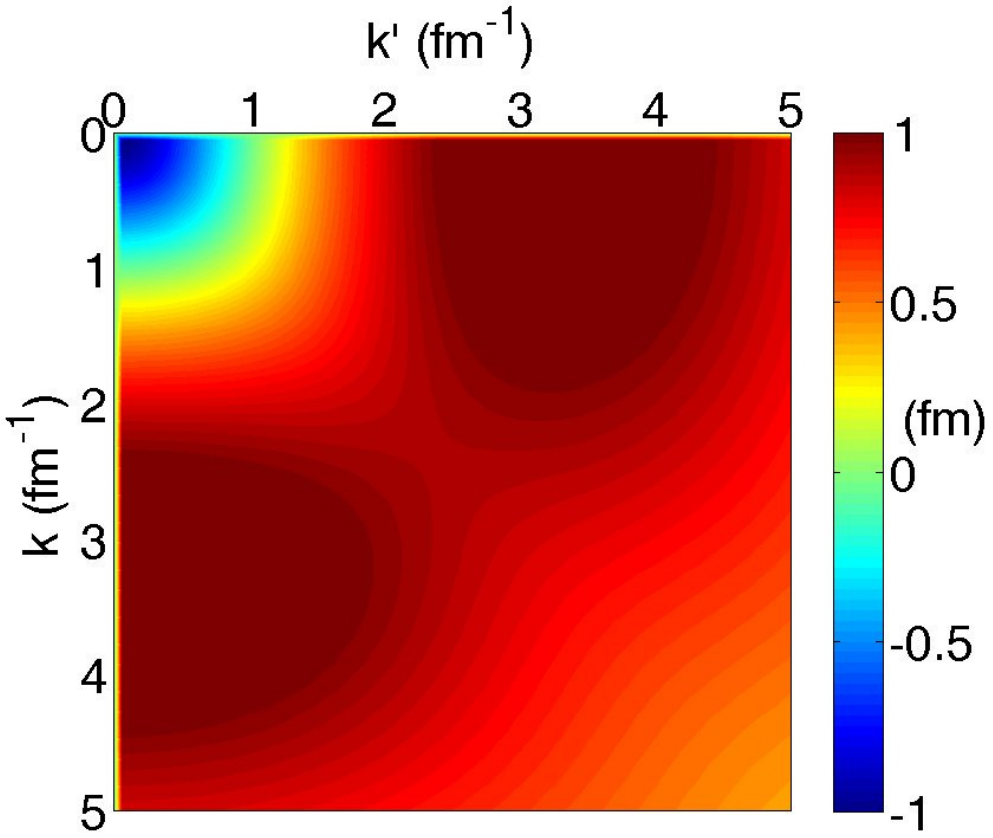


$$V_{L=0}(k,k') = \int d^3r\, j_0(kr)\, V(r)\, j_0(k'r) = \langle k|V_{L=0}|k'\rangle \implies V_{kk'} \text{ matrix}$$

- Momentum units ($\hbar = c = 1$): typical relative momentum in large nucleus $\approx 1\,\text{fm}^{-1} \approx 200\,\text{MeV}$ but ...
- Repulsive core $\implies$ large high-k ($\gtrsim 2\,\text{fm}^{-1}$) components

S-wave NN potential as momentum-space matrix





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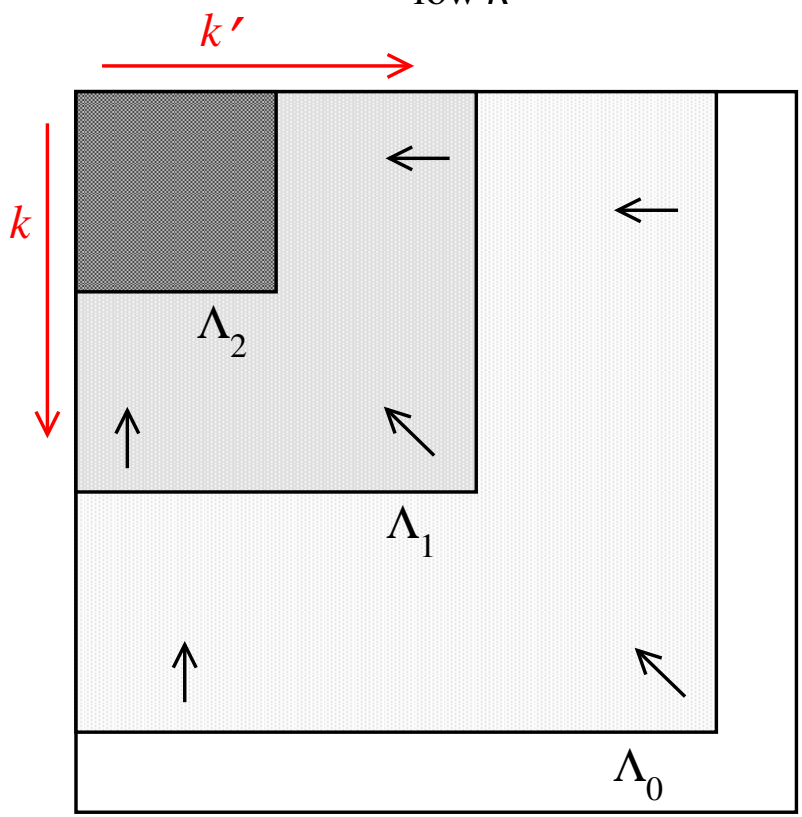
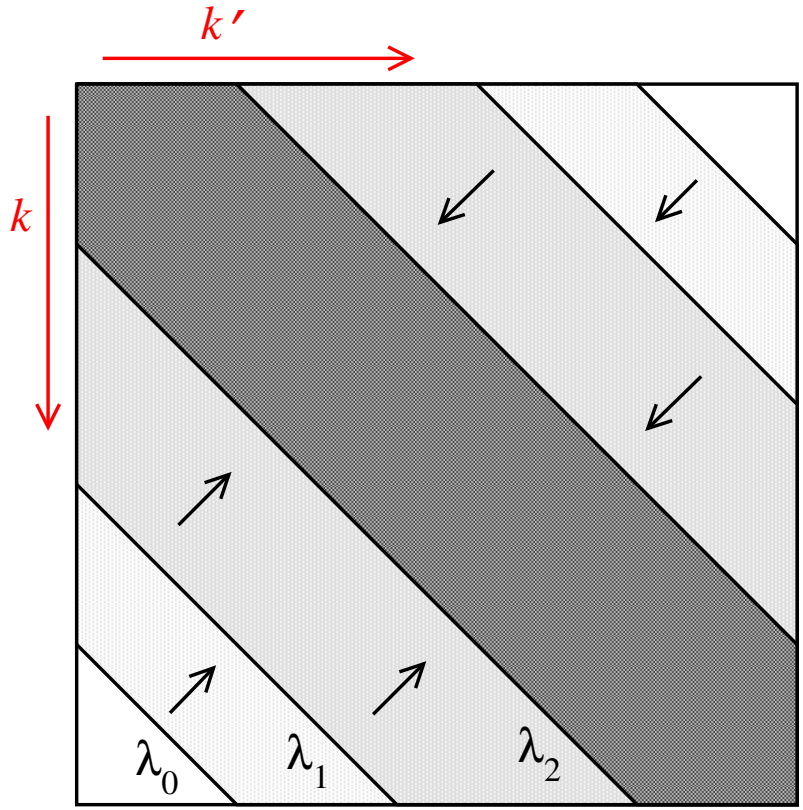
Two ways to use RG equations to evolve Hamiltonians

"$V_{\text{low } k}$"



- Lower a cutoff Λ_i in k, k', e.g., demand $dT(k, k'; k^2)/d\Lambda = 0$

Similarity RG



- Drive the Hamiltonian toward diagonal with "flow equation"

  [Wegner; Glazek/Wilson (1990's)]

$\Longrightarrow$ Both go to soft universal low-momentum interactions!

Basics: SRG flow equations [arXiv:1203.1779]

- Transform an initial hamiltonian, $H = T + V$, with U_s:

$$H_s = U_s H U_s^\dagger \equiv T + V_s \ ,$$

where s is the *flow parameter*. Differentiating wrt s:

$$\frac{dH_s}{ds} = [\eta_s, H_s] \qquad \text{with} \qquad \eta_s \equiv \frac{dU_s}{ds} U_s^\dagger = -\eta_s^\dagger \ .$$

- η_s is specified by the commutator with Hermitian G_s:

$$\eta_s = [G_s, H_s] \ ,$$

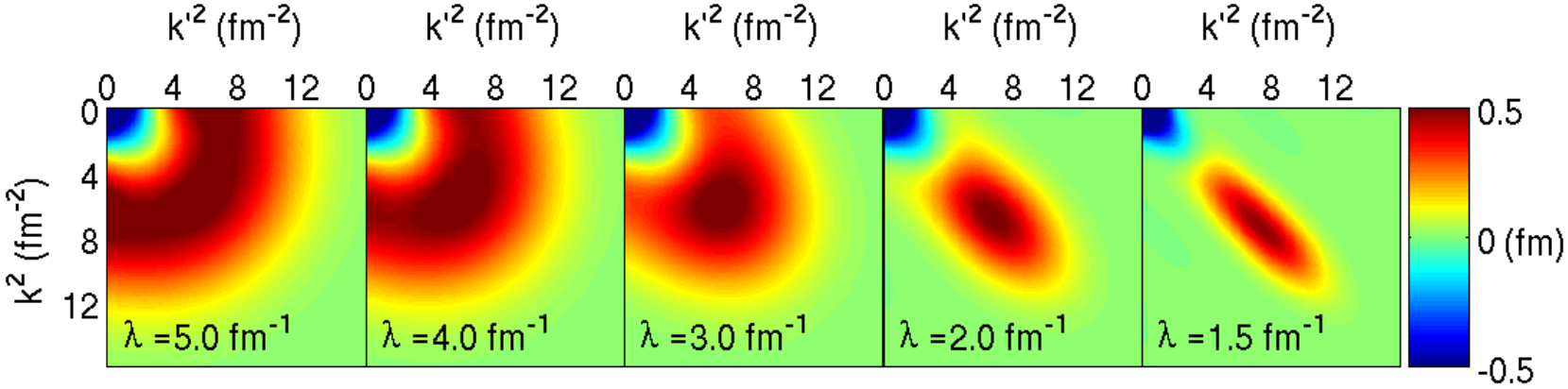
which yields the unitary flow equation (T held fixed),

$$\frac{dH_s}{ds} = \frac{dV_s}{ds} = [[G_s, H_s], H_s] \ .$$

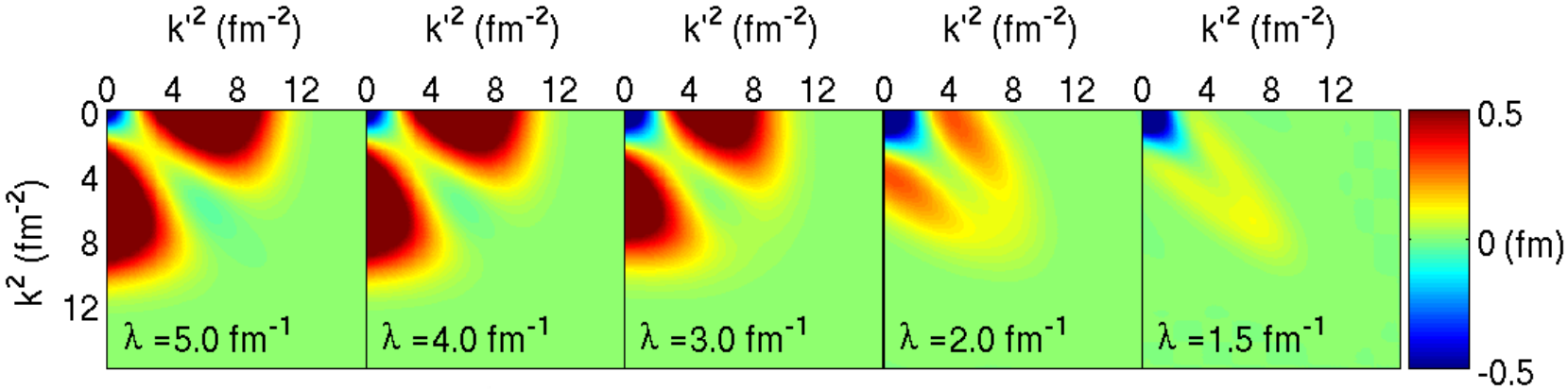
  - Very simple to implement as matrix equation (e.g., MATLAB)
- G_s determines flow $\Longrightarrow$ many choices (T, H_D, H_{BD}, ...)

Flow of different N^{3}LO chiral EFT potentials

- $^1S_0$ from N^{3}LO (500 MeV) of Entem/Machleidt



- $^1S_0$ from N^{3}LO (550/600 MeV) of Epelbaum et al.

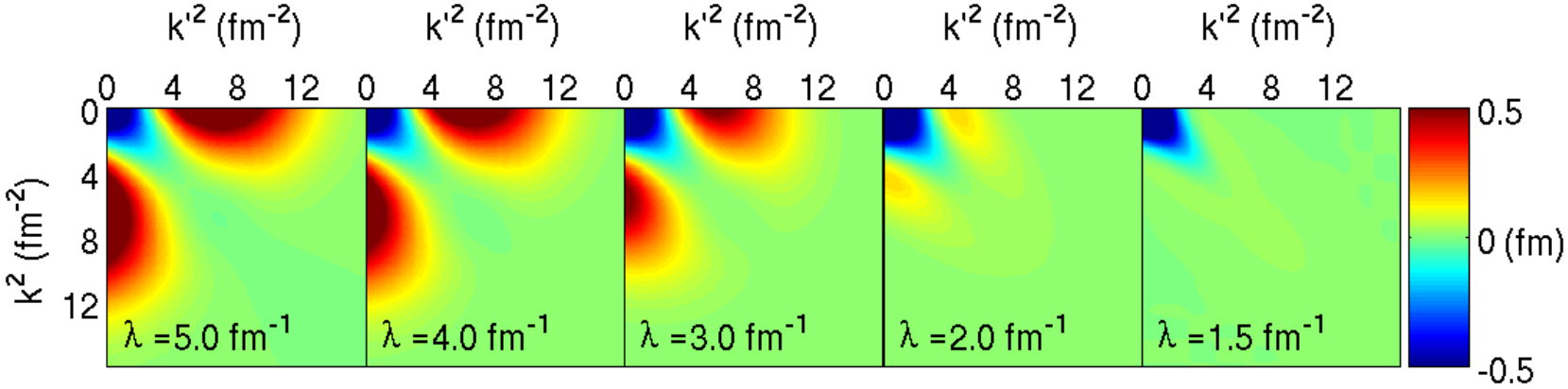


- Decoupling $\Longrightarrow$ perturbation theory is more effective

$$\langle k|V|k\rangle + \sum_{k'} \frac{\langle k|V|k'\rangle\langle k'|V|k\rangle}{(k^2-k'^2)/m} + \cdots \Longrightarrow V_{ii} + \sum_j V_{ij}V_{ji}\frac{1}{(k_i^2-k_j^2)/m} + \cdots$$

Flow of different N^{3}LO chiral EFT potentials

- $^3S_1$ from N^{3}LO (500 MeV) of Entem/Machleidt



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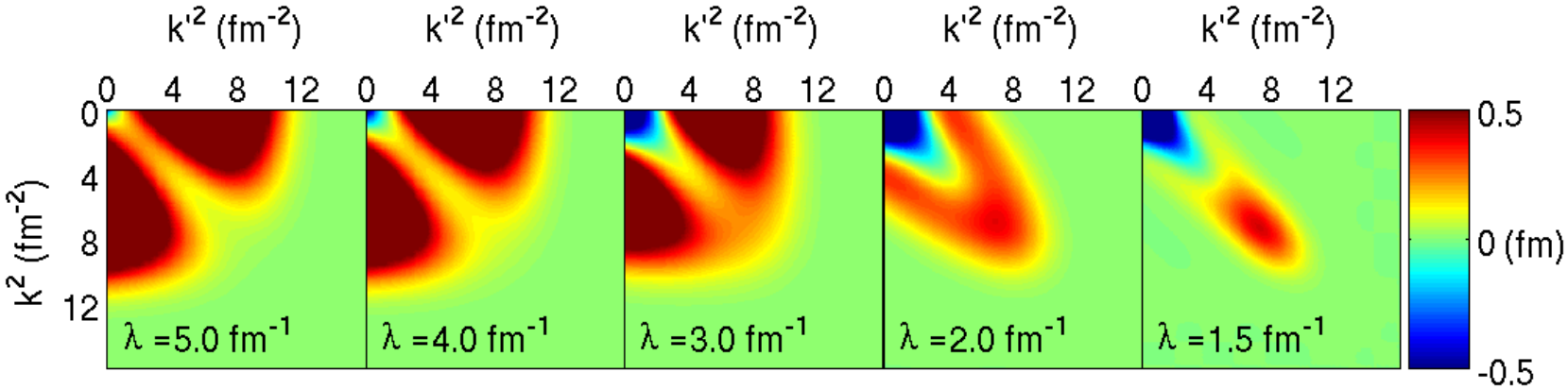

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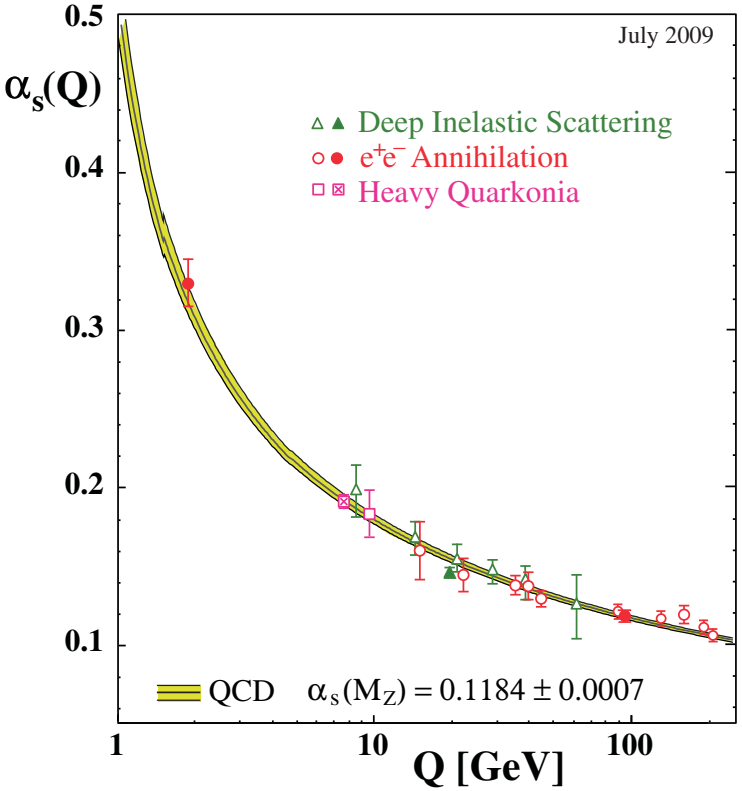
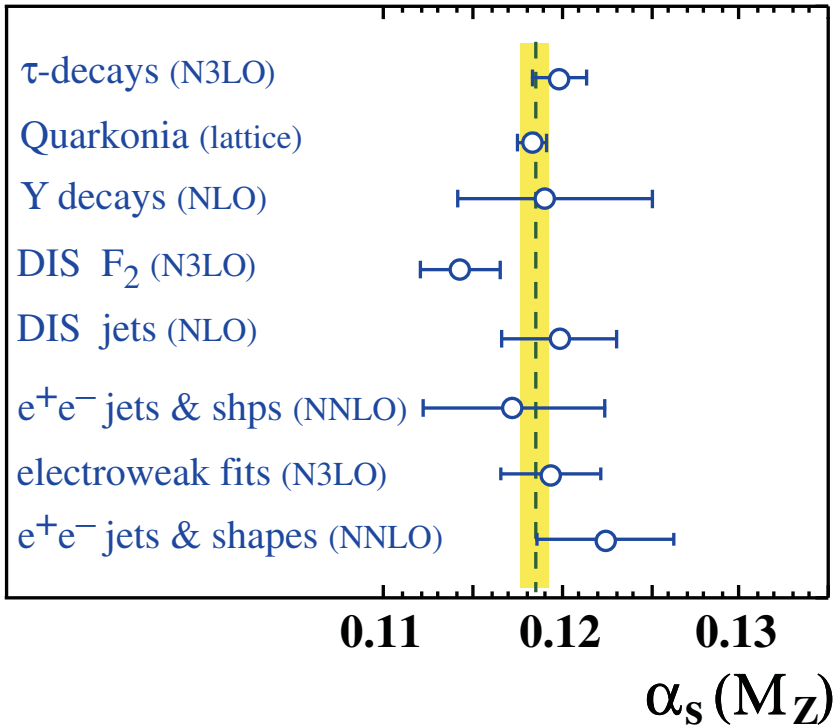
Measuring the QCD Hamiltonian: Running $\alpha_s(Q^2)$



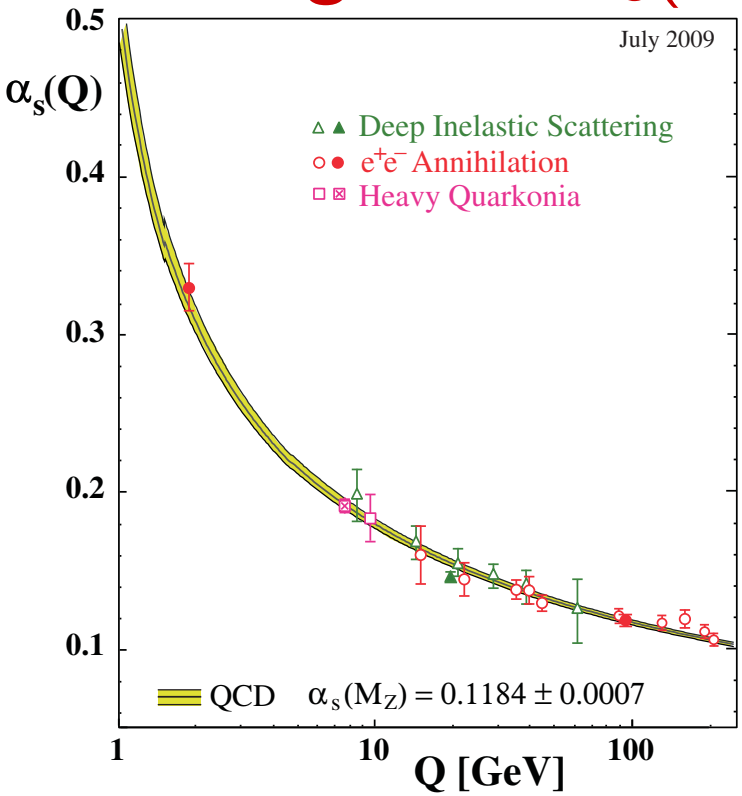
- The QCD coupling is *scale* dependent ("running"):
  $\alpha_s(Q^2) \approx [\beta_0 \ln(Q^2/\Lambda^2_{\rm QCD})]^{-1}$
- The QCD coupling strength α_s is *scheme* dependent (e.g., "V" scheme used on lattice, or $\overline{\rm MS}$)

- Extractions from experiment can be compared (here at M_Z):



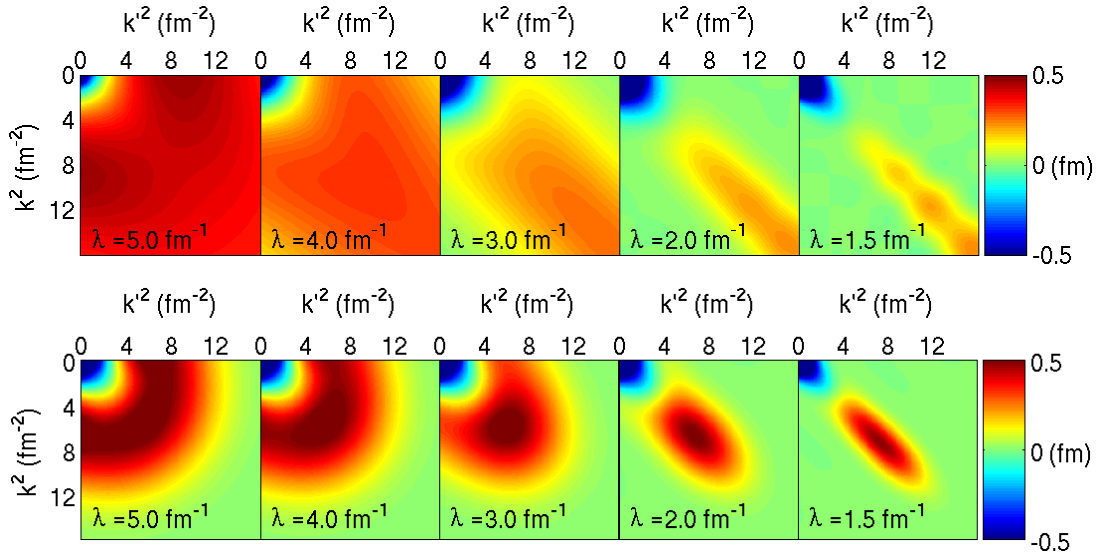
- cf. QED, where $\alpha_{em}(Q^2)$ is effectively constant for soft Q^2:
  $\alpha_{em}(Q^2 = 0) \approx 1/137$
  $\therefore$ fixed H for quantum chemistry

Running QCD $\alpha_s(Q^2)$ vs. running nuclear V_λ



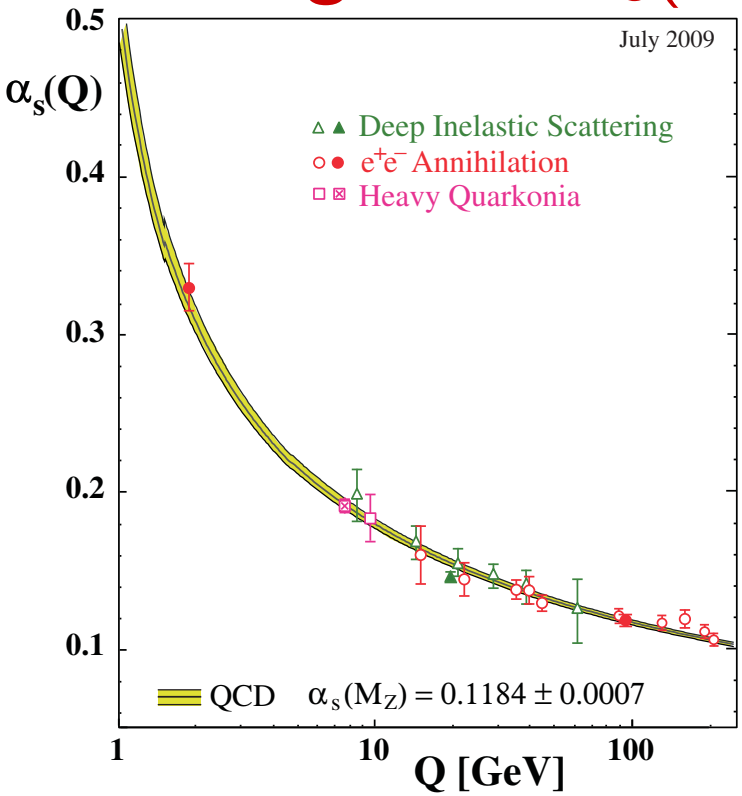
- The QCD coupling is *scale* dependent (cf. low-E QED): $\alpha_s(Q^2) \approx [\beta_0 \ln(Q^2/\Lambda^2_{\rm QCD})]^{-1}$
- The QCD coupling strength α_s is *scheme* dependent (e.g., "V" scheme used on lattice, or $\overline{\rm MS}$)

- Vary scale ("resolution") with RG
- Scale dependence: SRG (or $V_{\rm low\,k}$) running of initial potential with λ (decoupling or separation scale)



- Scheme dependence: AV18 vs. N^{3}LO (plus associated 3NFs)
  - But all are (NN) phase equivalent!
  - Shift contributions between interaction and sums over states

Running QCD $\alpha_s(Q^2)$ vs. running nuclear V_λ



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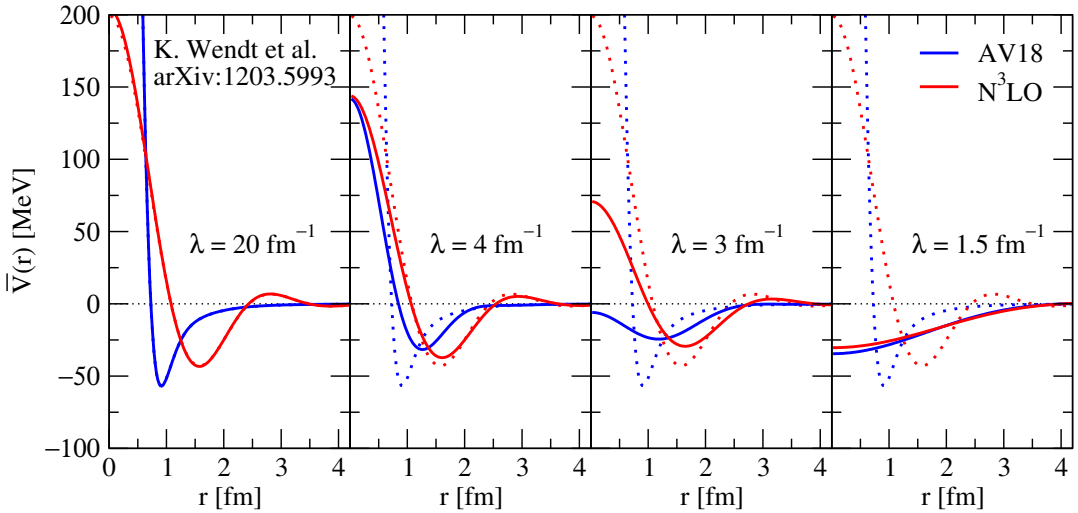
- Vary scale ("resolution") with RG
- Scale dependence: SRG (or $V_{\rm low\,k}$) running of initial potential with λ (decoupling or separation scale)
- Project non-local NN potential to visualize: $\overline{V}_\lambda(r) = \int d^3r'\, V_\lambda(r, r')$



- Scheme dependence: AV18 vs. N^{3}LO (plus associated 3NFs)
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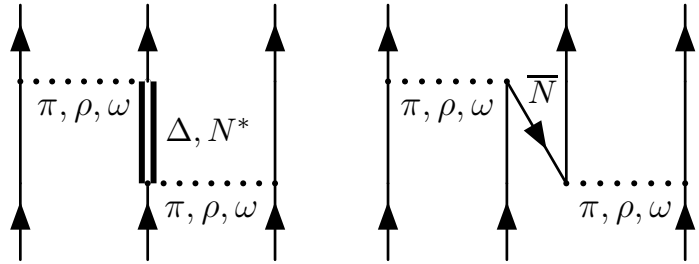
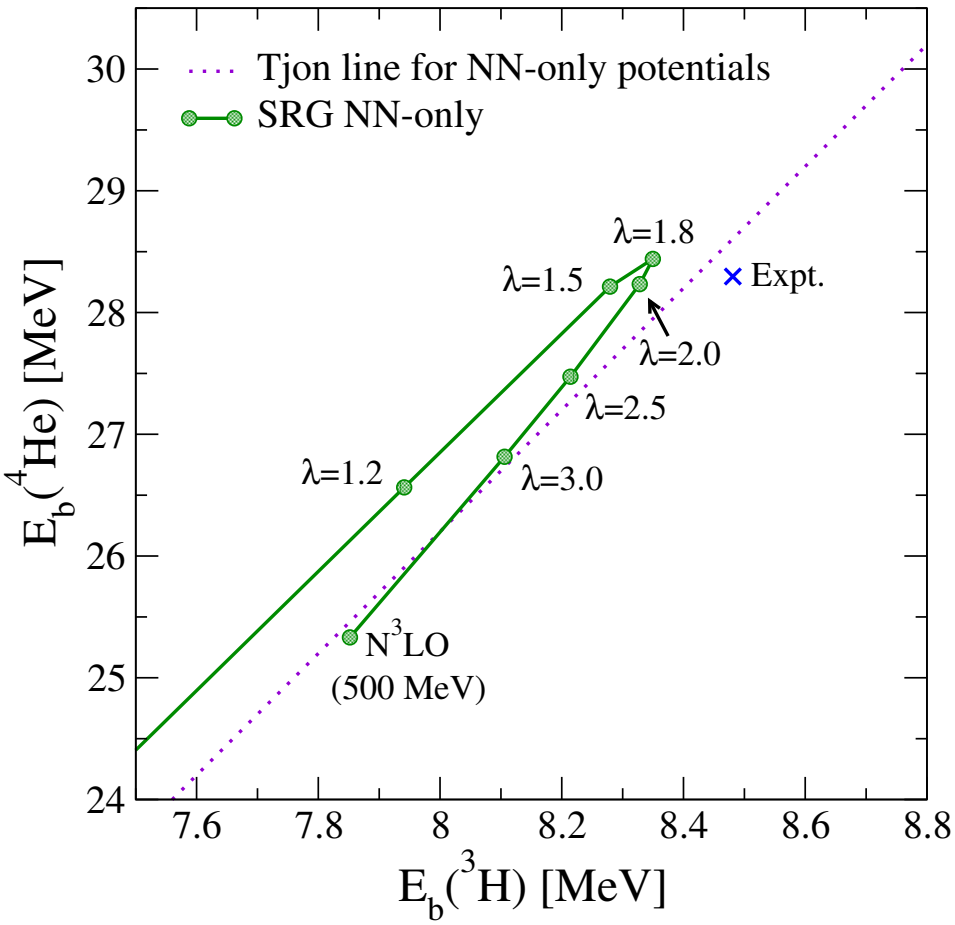
RG running and three-body forces

- Three-body forces change when eliminating/decoupling degrees-of-freedom
  - excited states of nucleon
  - relativistic effects
  - high-momentum intermediate states
- Omitting 3-body forces leads to model dependence
  - observables depend on Λ/λ
  - cutoff dependence as tool





RG running and three-body forces

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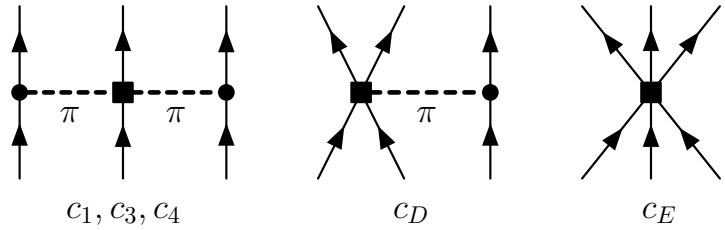
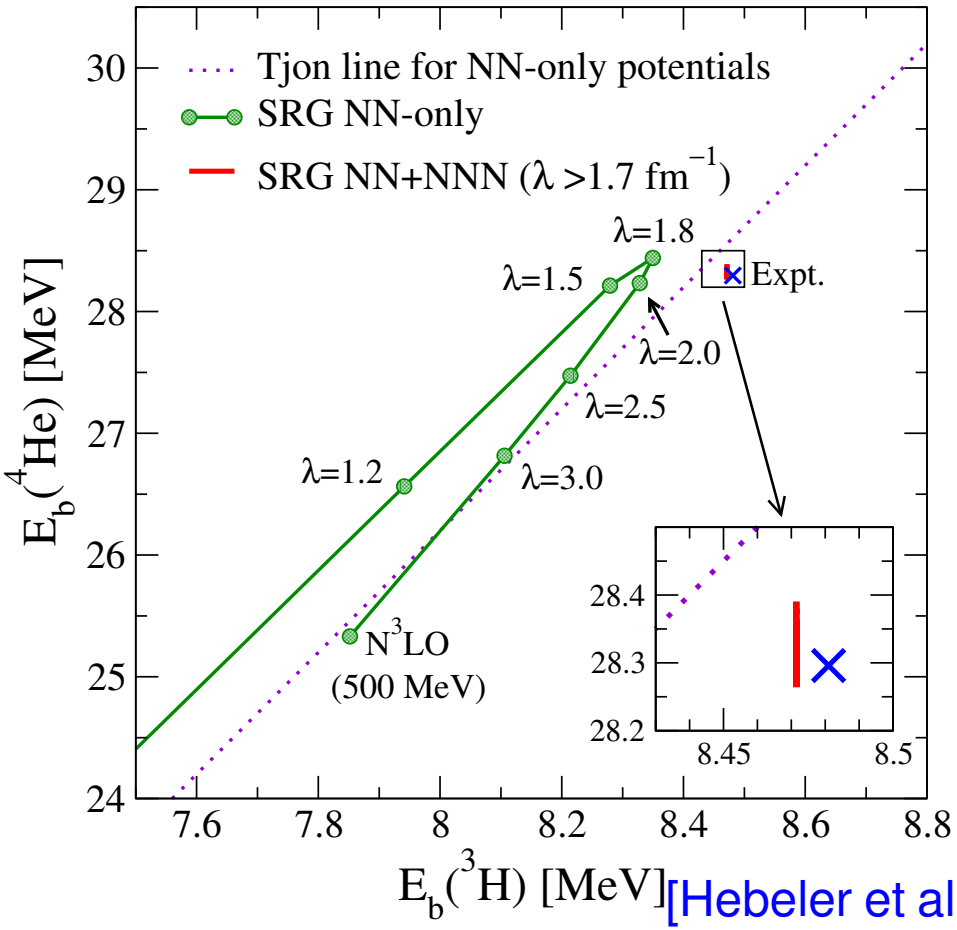
  - excited states of nucleon
  - relativistic effects
  - high-momentum intermediate states
- Omitting 3-body forces leads to model dependence
  - observables depend on Λ/λ
  - cutoff dependence as tool
- NNN at different Λ/λ must be fit or evolved to χEFT
  - Then cutoff dependence of observables greatly reduced. 4-body forces?



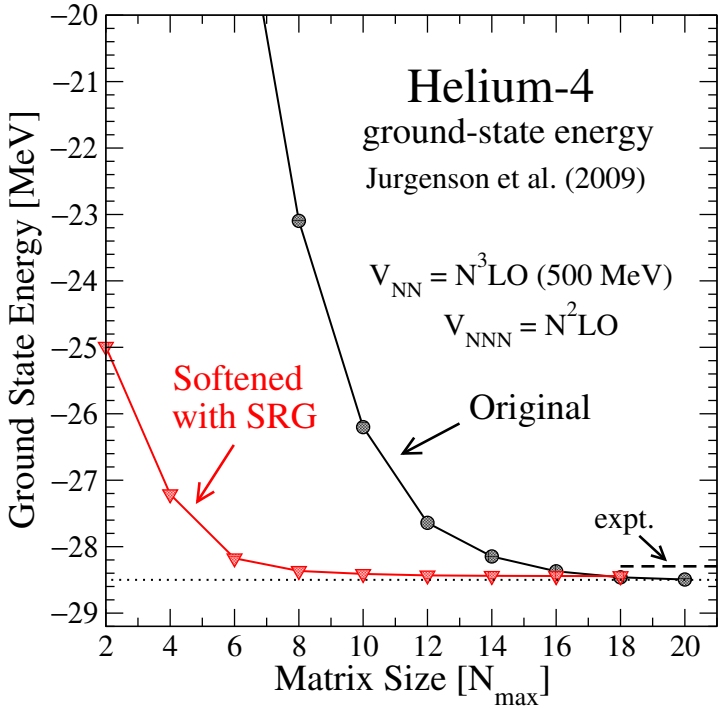


[Hebeler et al.]

RG transformations: Nuclei with *soft* interactions

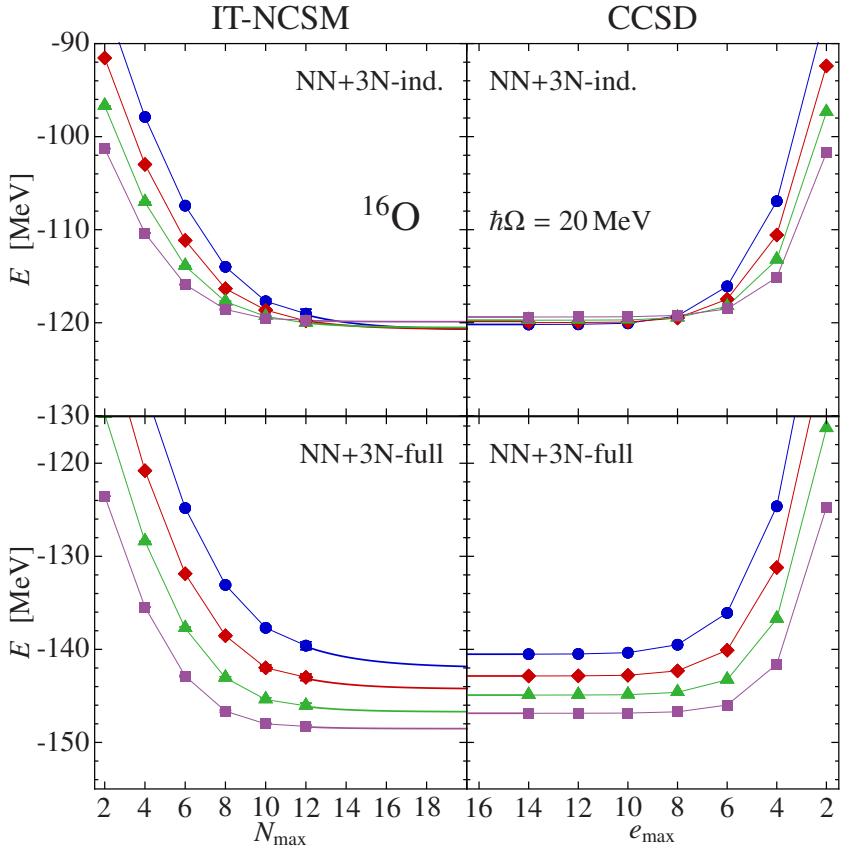
Softened potentials (SRG, $V_{\mathrm{low}\,k}$, UCOM, ...) enhance convergence

- Convergence for no-core shell model (NCSM):



- (Already) soft chiral EFT potential and evolved (softened) SRG potentials, including NNN

- Softening allows importance truncation (IT) and converged coupled cluster (CCSD)

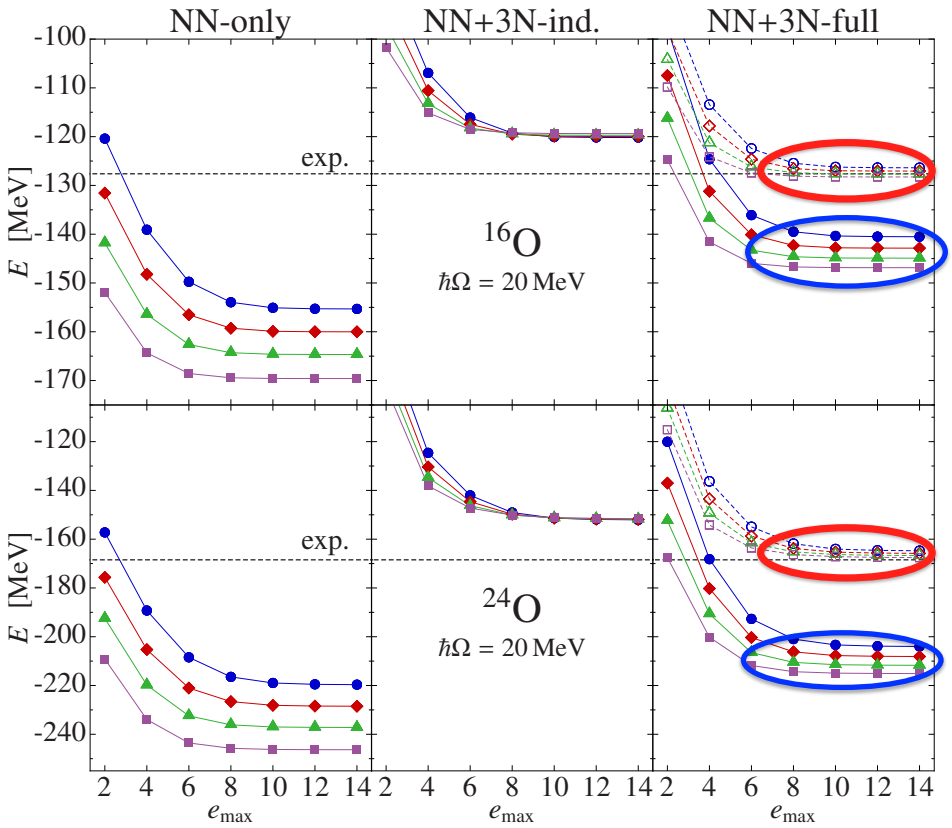


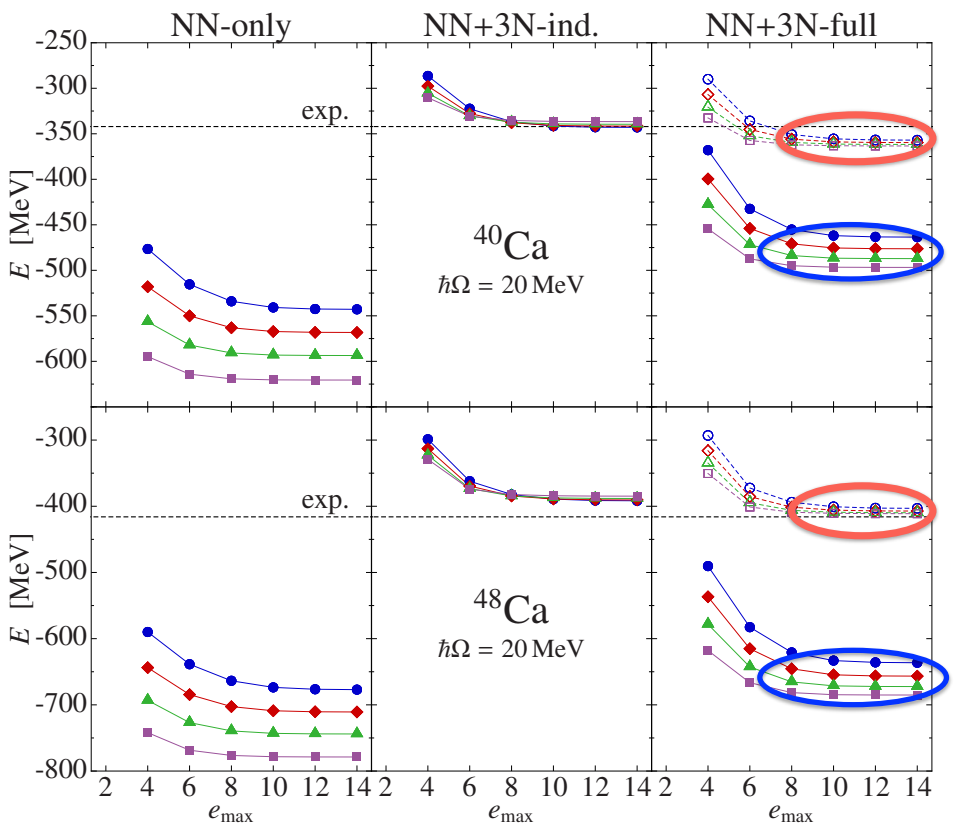
[Roth et al., arXiv:1112.0287]

RG transformations: Nuclei with *soft* interactions

R. Roth et al. SRG-evolved N^{3}LO with NNN [arXiv:1112.0287]

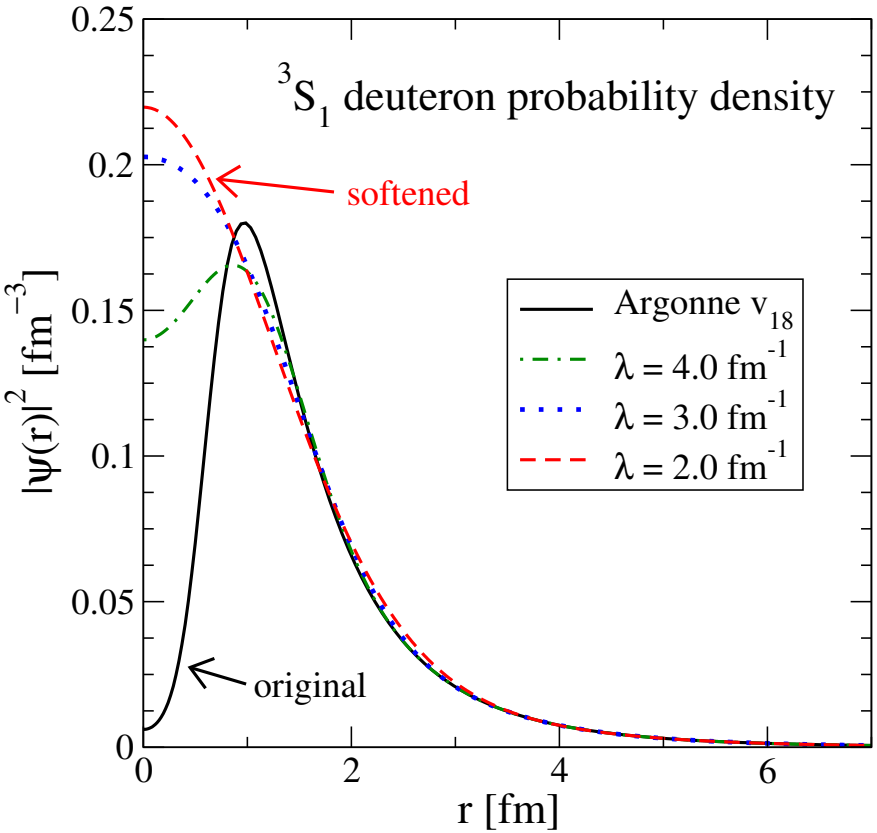
- Coupled cluster with interactions $H(\lambda)$: λ is a decoupling scale
  - NN-only: doesn't include induced NNN $\Longrightarrow$ λ dependent
  - NN+3N-induced: λ independent energies *but different NNN for each* λ
  - NN+3N-full: includes (two) initial NNN fit to $A = 3, 4$ properties

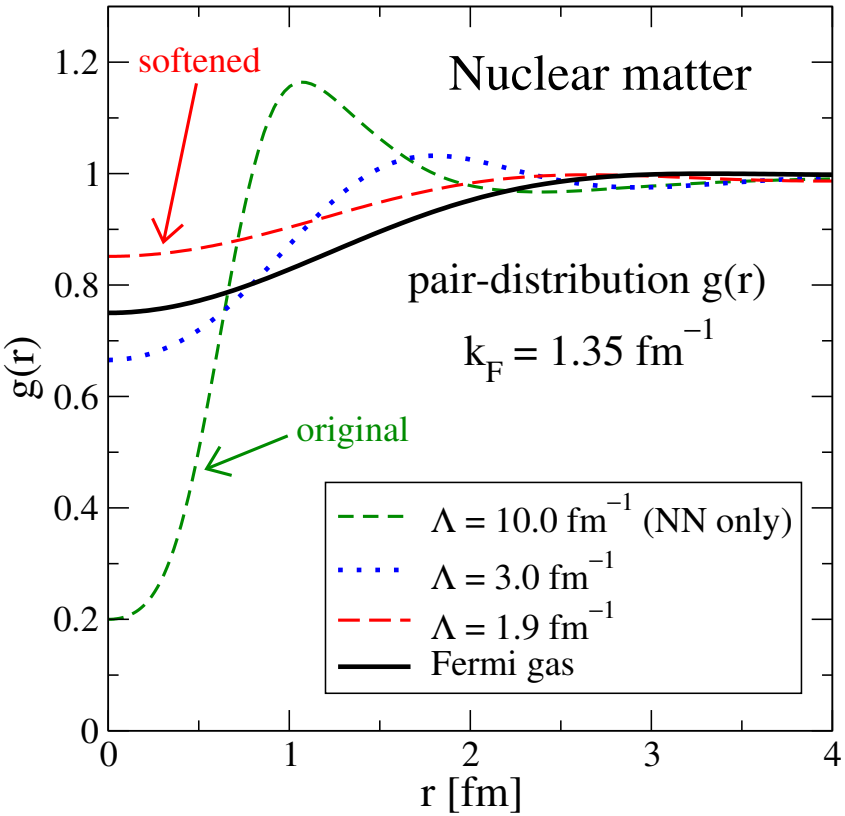




RG transformations: Nuclei with *soft* interactions

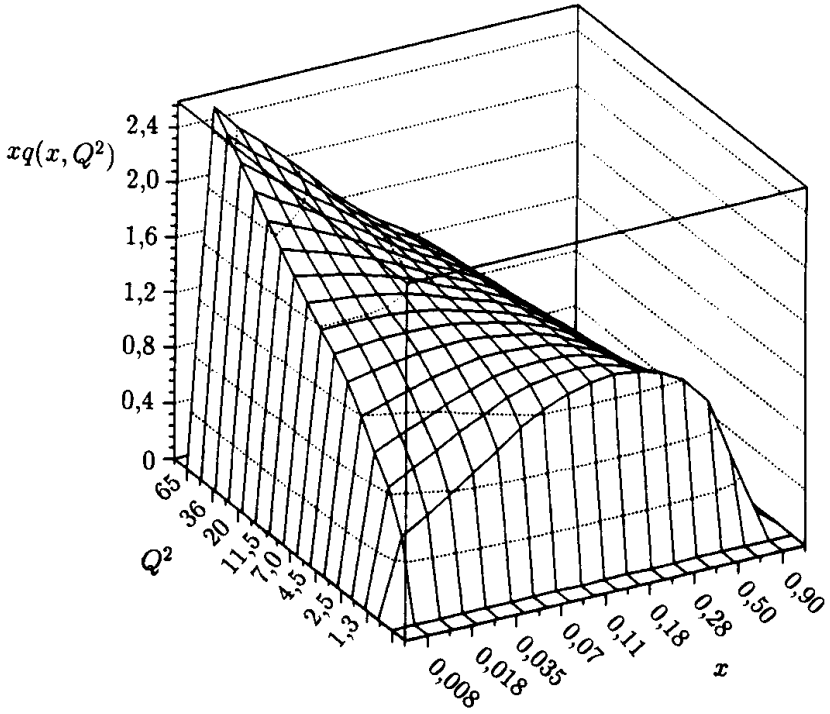
But soft potentials don't lead to short-range correlations (SRC)!



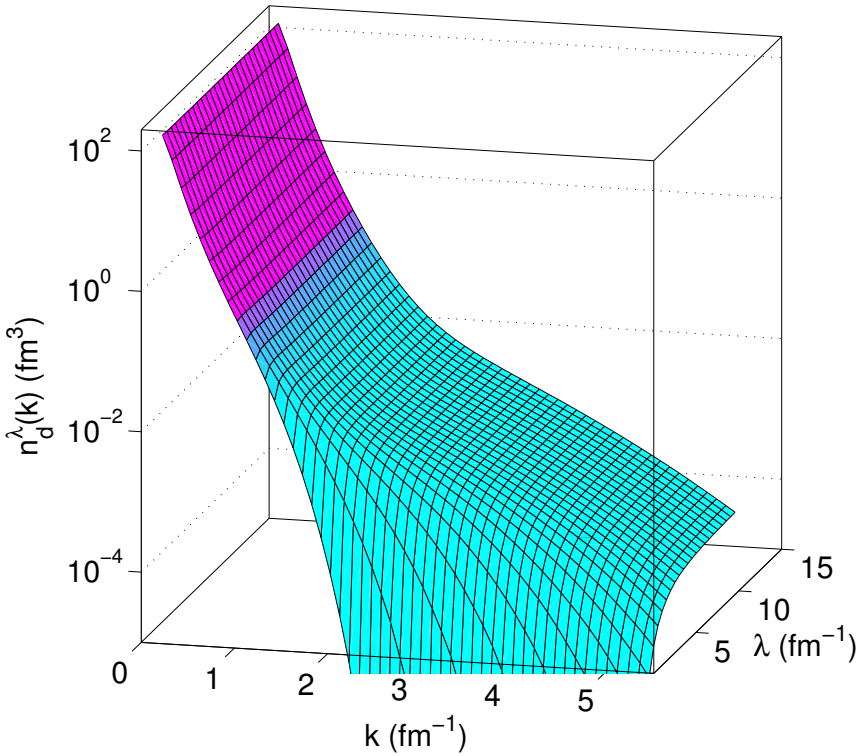


- Continuously transformed potential $\Longrightarrow$ variable SRC's in wf!
- Therefore, it seems that SRC's are *very scale/scheme dependent*
- Analog in high energy QCD: parton distributions

Parton vs. nuclear momentum distributions



- The quark distribution $q(x, Q^2)$ is scheme *and* scale dependent
- $x\ q(x, Q^2)$ measures the share of momentum carried by the quarks in a particular x-interval
- $q(x, Q^2)$ and $q(x, Q_0^2)$ are related by RG evolution equations



- Deuteron momentum distribution is scheme *and* scale dependent
- Initial AV18 potential evolved with SRG from $\lambda = \infty$ to $\lambda = 1.5\,\mathrm{fm}^{-1}$
- High momentum tail shrinks as λ decreases (lower resolution)

Outline

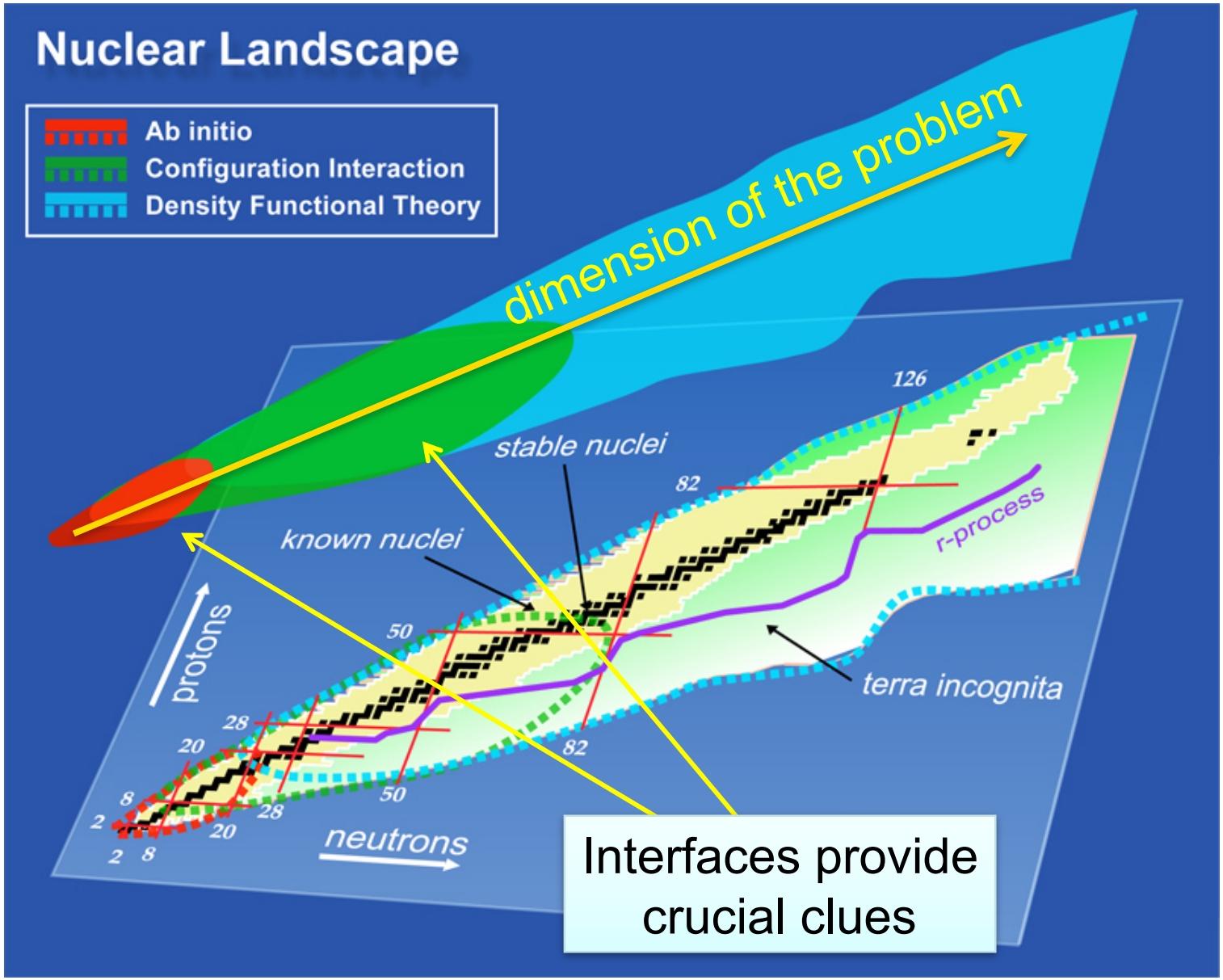
Overview: What is new in low-energy physics?

Background for the inputs and solution methods

Highlights of recent applications: new methods

Recap and outlook

Overlapping theory methods cover all nuclei

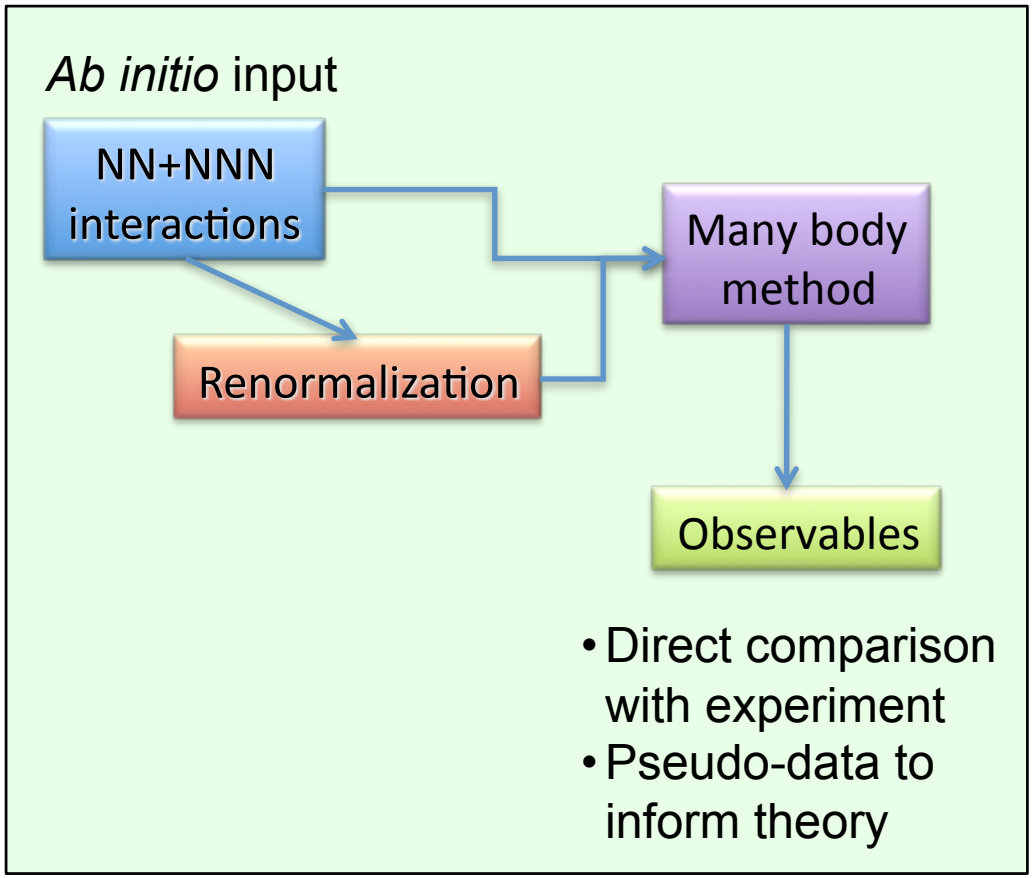


Fully microscopic (from input NN + NNN)

Ab initio theory for light nuclei and uniform matter

Ab initio: QMC, NCSM, CC,…

(nuclei, neutron droplets, nuclear matter)



Input choices:

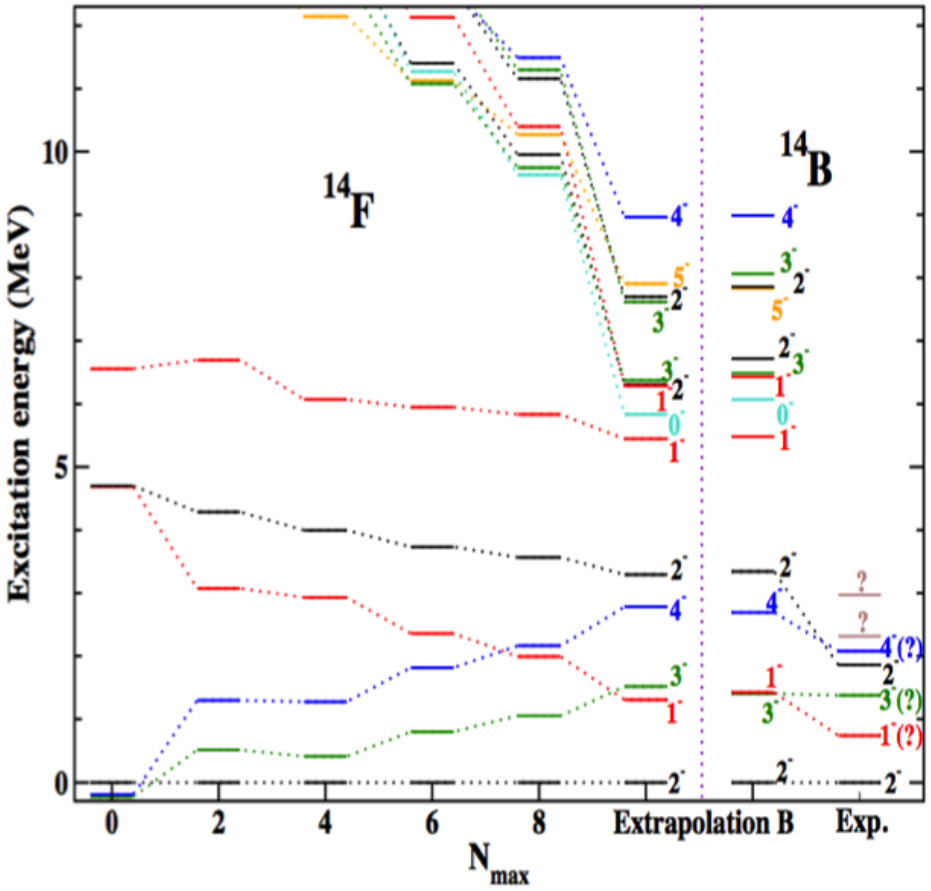
- Accurate forces based on phase shift analysis and few-body data
- EFT-based nonlocal chiral NN and NNN potentials
- RG-softened potentials evolved from NN+NNN interactions

- Quantum Monte Carlo (GFMC, lattice EFT) ^{12}C
- No-Core Shell Model ^{14}F, ^{14}C
- Coupled-Cluster Techniques ^{17}F, ^{56}Ni

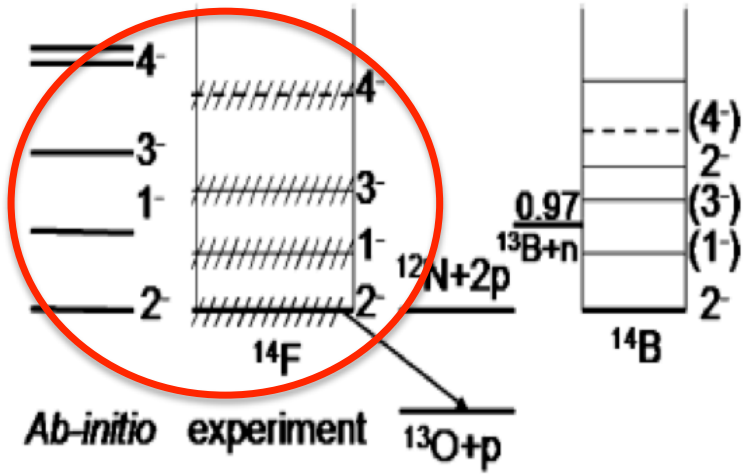
Unstable "proton-dripping" fluorine-14 with NCSM

- Ab initio calculation using "soft" inverse-scattering potential
- New: theory preceded recent experimental measurement!

P. Maris et al., PRC **81**, 021301(R) (2010)

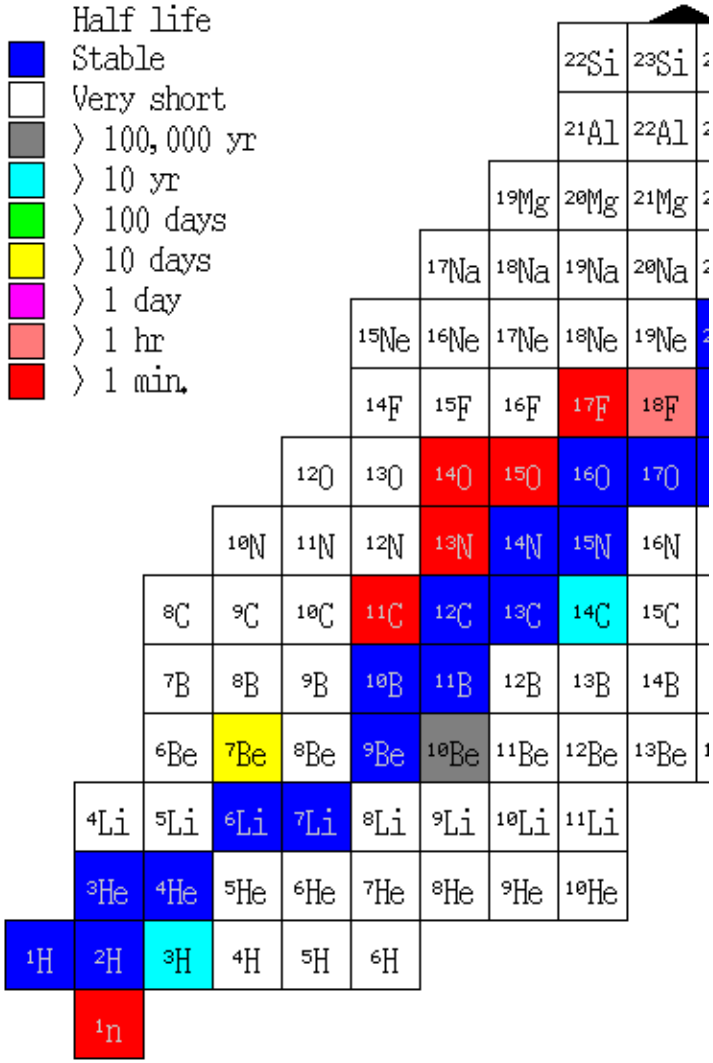


V.Z. Goldberg et al., Phys. Lett. B **692**, 307 (2010)



- Matrix dimension 2×10^9, 2.5 hours on 30,000 cores

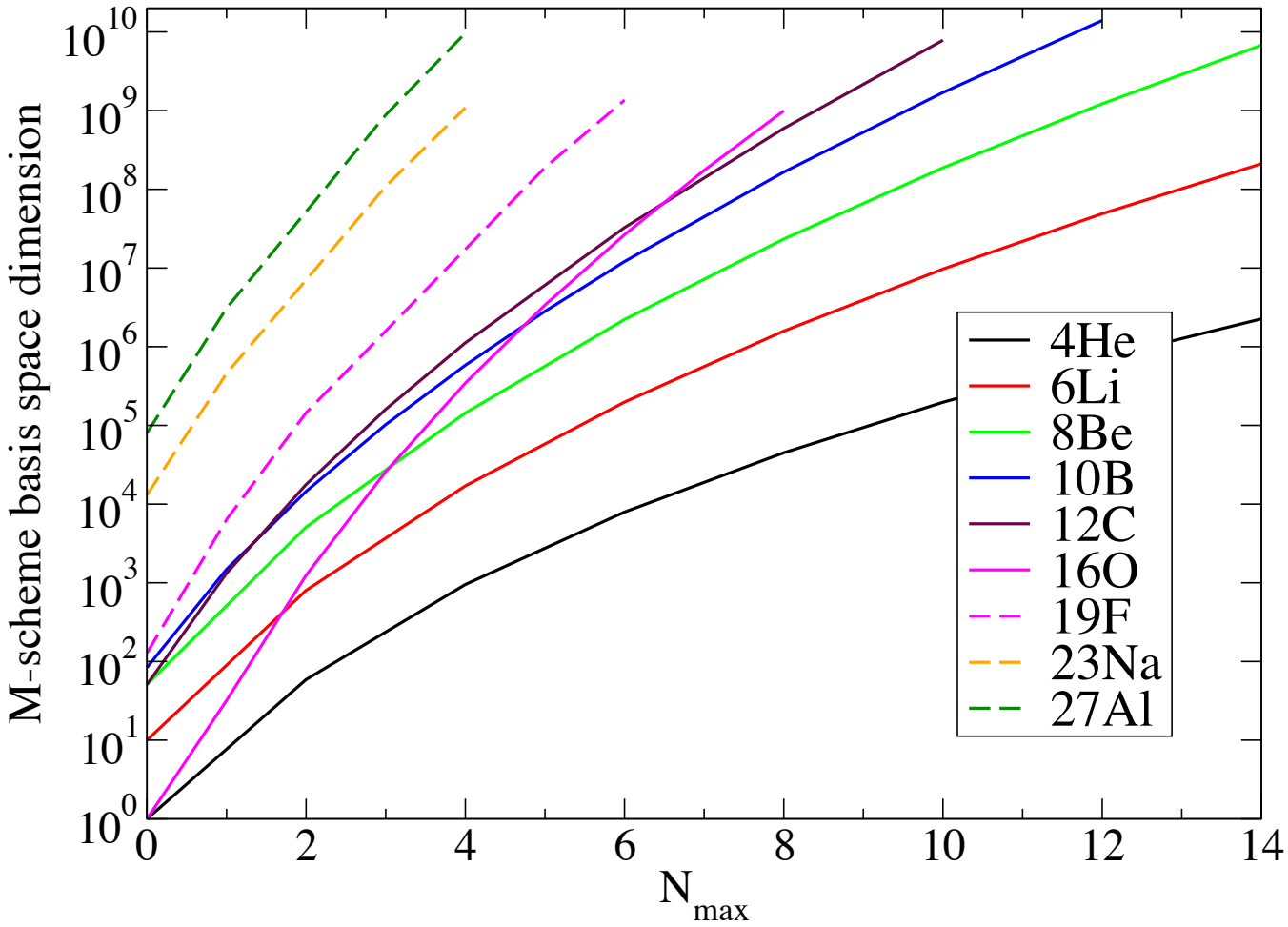
Asides on Fluorine-14 calculation



- ^{14}F decays by proton emission to ^{13}O
  $\Longrightarrow$ "proton drip line"
- What if 2×10^9 dimension matrix full?
  $> 10^{19}$ bytes storage?
  $\Longrightarrow$ obviously *many* matrix elements must be zero! (Sparse)
- Only about 20 out of 2 billion eigenvalues needed
  $\Longrightarrow$ Lanczos method!
- How to scale to 30,000 cores?
  $\Longrightarrow$ work with computer scientists
  $\Longrightarrow$ SciDAC!
- How do you extrapolate $N_{\max} \to \infty$?
  (ask me later!)

Size and sparsity of Hamiltonian matrices [from P. Maris]

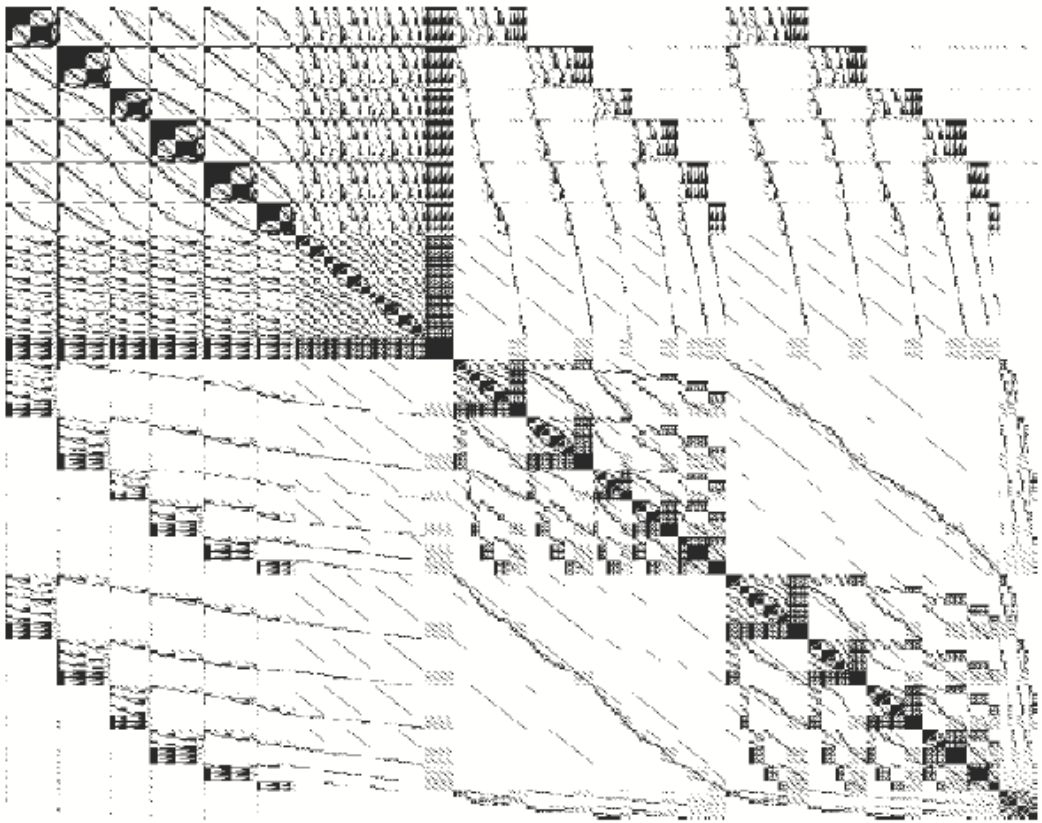
- Hamiltonian matrices grow rapidly with basis size ($N_{\max}$) and $A = N + Z$ from combinatorics:



Size and sparsity of Hamiltonian matrices [from P. Maris]

- But fortunately there are many zero elements so storage is large but feasible. How can we take advantage of sparsity?

Sparsity Structure for ^{6}Li



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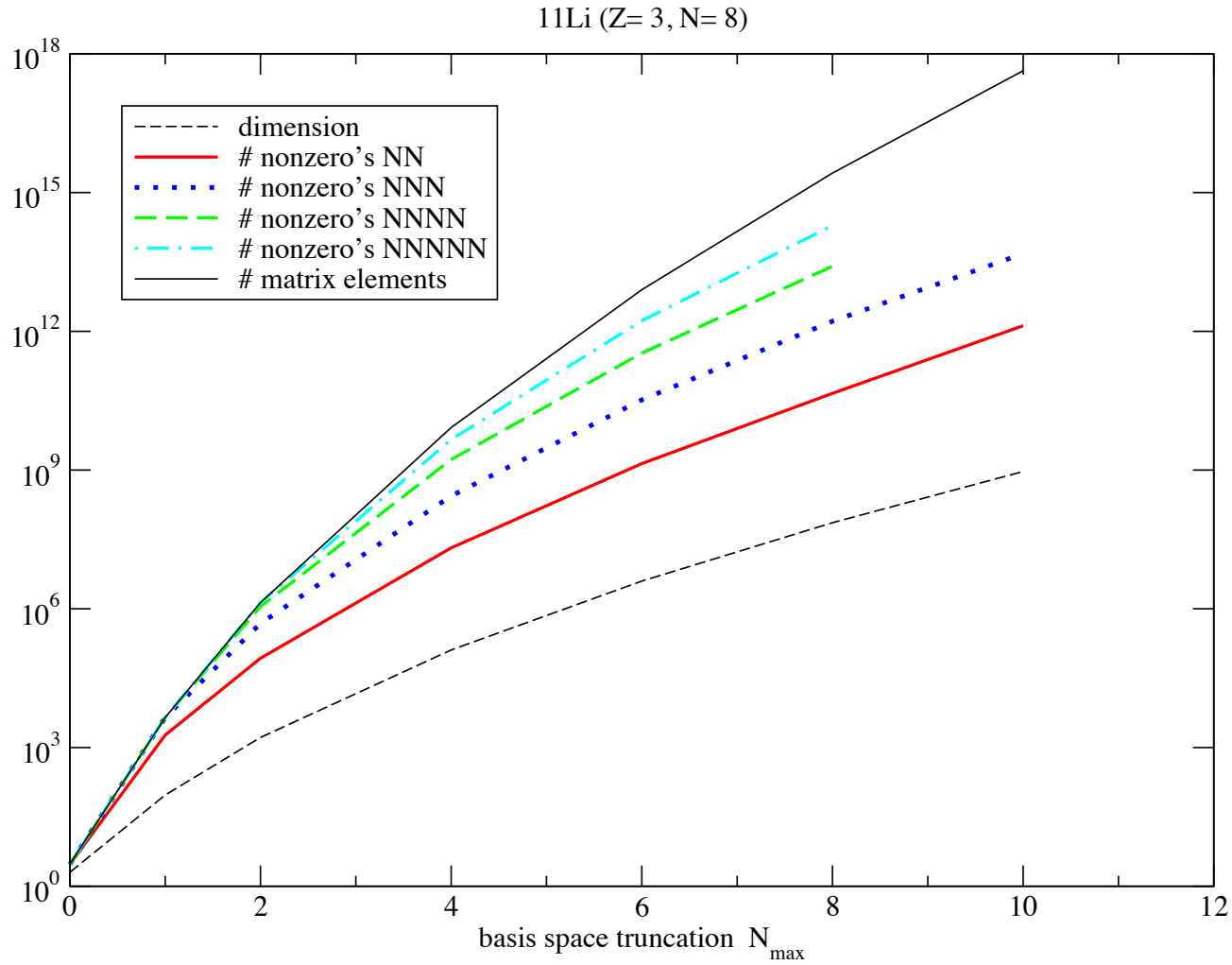


Lanczos method in short

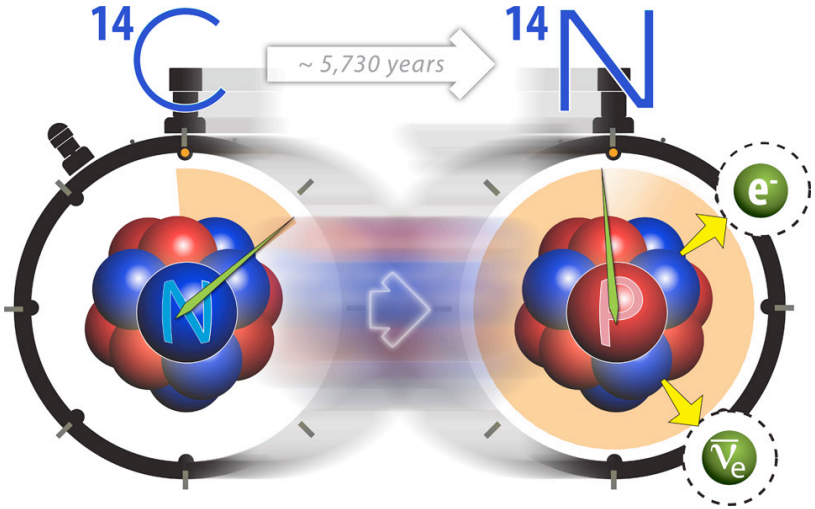
- Consider an arbitrary vector $|\Psi\rangle$ and its expansion in eigenstates of H, where $H|\psi_k\rangle = E_k|\psi_k\rangle$. Then $H^m|\Psi\rangle = \sum_k C_k E_k^m |\psi_k\rangle$
  - If m large enough, largest $|E_k|$ will dominate the sum
    $\Longrightarrow$ project out the corresponding eigenvector
  - To get lowest eigenvalue, use $(H - \sigma I)^m$ with $\sigma > 0$ large enough so that $|E_0 - \sigma| > |E_{\rm max} - \sigma|$
- More efficient to diagonalize H in the basis spanned by $H|\psi_k\rangle$, $H^2|\psi_k\rangle, \ldots, H^m|\psi_k\rangle$
  - Called the "Krylov space"
  - Lanczos: orthogonalize basis states as you go, generating H in tri-diagonal form, which is efficiently diagonalized
  - Re-orthonormalization for numerical stability
- Many computational advantages to treating sparse matrices with Lanczos [see J. Vary et al., arXiv:0907.0209]

U.S. DEPARTMENT OF ENERGY | Office of Science

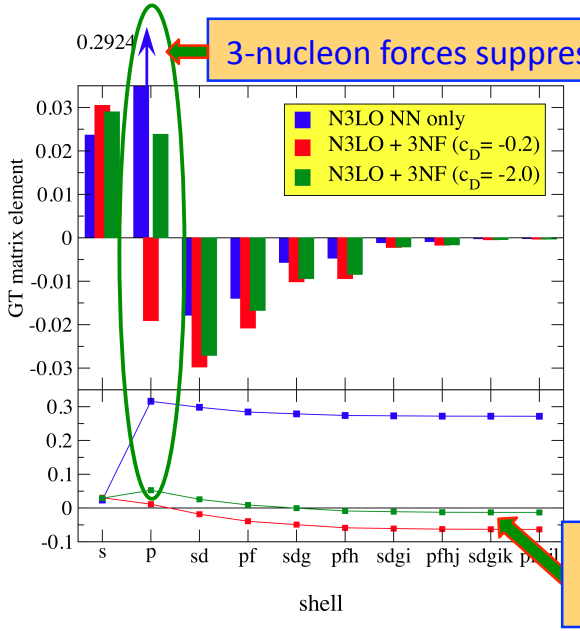
"Why does Carbon-14 live so long?"

Carbon-14 dating relies on ~5,730 year half-life, but other light nuclei undergo similar beta decay with half-lives less than a day!

UNEDF SciDAC Collaboration
Universal Nuclear Energy Density Functional



- Members of UNEDF collaboration made microscopic nuclear structure calculations to solve the puzzle
- Used systematic chiral Hamiltonian from low-energy effective field theory of QCD
- Key feature: consistent *3-nucleon* interactions



3-nucleon forces suppress critical component compared to 2-nucleon forces only

net decay rate is very small

- Solutions of ^{14}C and ^{14}N through Hamiltonian diagonalization
- 100-fold reduction in Gamow-Teller transition matrix element

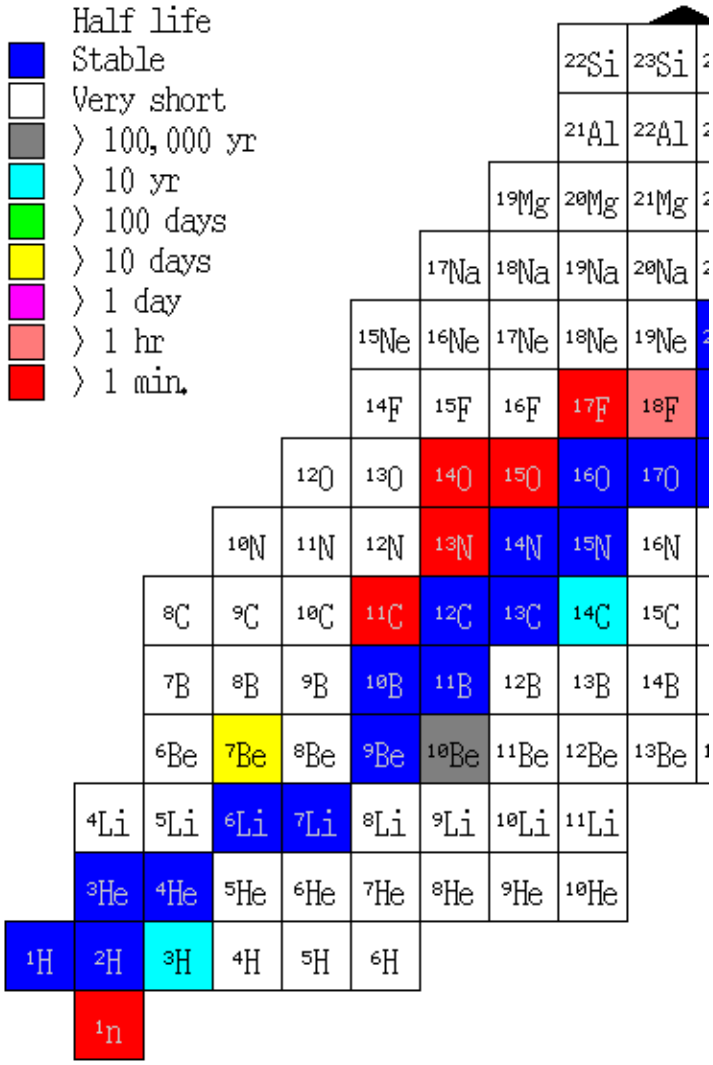
Calculations enabled by high-performance computing through INCITE program

- Dimension of matrix solved for 8 lowest states: ~ 1×10^9
- Solution took ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL

Office of Science INCITE Advancing America's Science and Industrial Competitiveness

Science ref.: Physical Review Letters **106**, 202502 (2011)
Computational ref.: Procedia Computer Science **1**, 97 (2010)

Asides on Carbon-14 decay calculation



- Atomic masses [1 amu = 1/12 mass of ^{12}C]
  ^{14}O: 14.0085953 $\pm$ 0.0000001 amu
  ^{14}N: 14.0030740 $\pm$ 0.0000000 amu
  ^{14}C: 14.0032420 $\pm$ 0.0000000 amu
  (from online “table of nuclides”)
  How does each decay?
- Compare lifetimes: ^{14}C lives long!
- Calculation with NCSM using chiral EFT potentials and operator for β^- decay
  ($^{14}_{6}\mathrm{C} \rightarrow {}^{14}_{7}\mathrm{N} + e^- + \overline{\nu}_e$)
- Scaling enabled by CS/AM collaborations
- Role of 3NF is key
- Determining the contribution of one part of Hamiltonian $\Longrightarrow$ Hellmann-Feynman

Aside: Hellmann-Feynman theorem

- How do you identify the contribution of some part of the Hamiltonian to the energy? E.g., the 3NF: $H = H_2 + g_3 H_3$
  - Could compare energies with and without that part, but only quantitative if perturbative
  - Better to use Hellmann-Feynman (or Feynman-Hellmann):

$$\frac{dE(\lambda)}{d\lambda} = \langle\Psi(\lambda)|\frac{\partial\widehat{H}_\lambda}{\partial\lambda}|\Psi(\lambda)\rangle \text{ where } \widehat{H}_\lambda|\Psi(\lambda)\rangle = E(\lambda)|\Psi(\lambda)\rangle$$

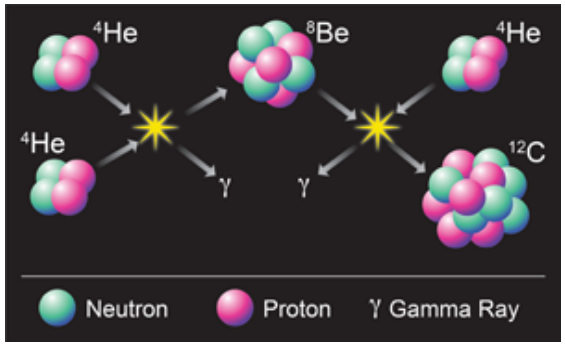
  - So if g_3 is a coupling constant for (part of) the 3NF, calculate $g_3\,(dE/dg_3) \approx g_3[E(g_3+\epsilon/2) - E(g_3-\epsilon/2)]/\epsilon$ for small ϵ
  - Try proving it* (hint: use $\langle\Psi(\lambda)|\Psi(\lambda)\rangle = 1$)
- Hellmann-Feynman with operators: add it to the Hamiltonian

$$\widehat{H} \to \widehat{H}+\lambda\widehat{O} \implies E(\lambda) = E+\lambda\langle\Psi(\lambda)|\widehat{O}|\Psi(\lambda)\rangle \implies \langle\Psi|\widehat{O}|\Psi\rangle = \left.\frac{dE(\lambda)}{d\lambda}\right|_{\lambda=0}$$

- Very general: QCD condensates, energy functionals, ...

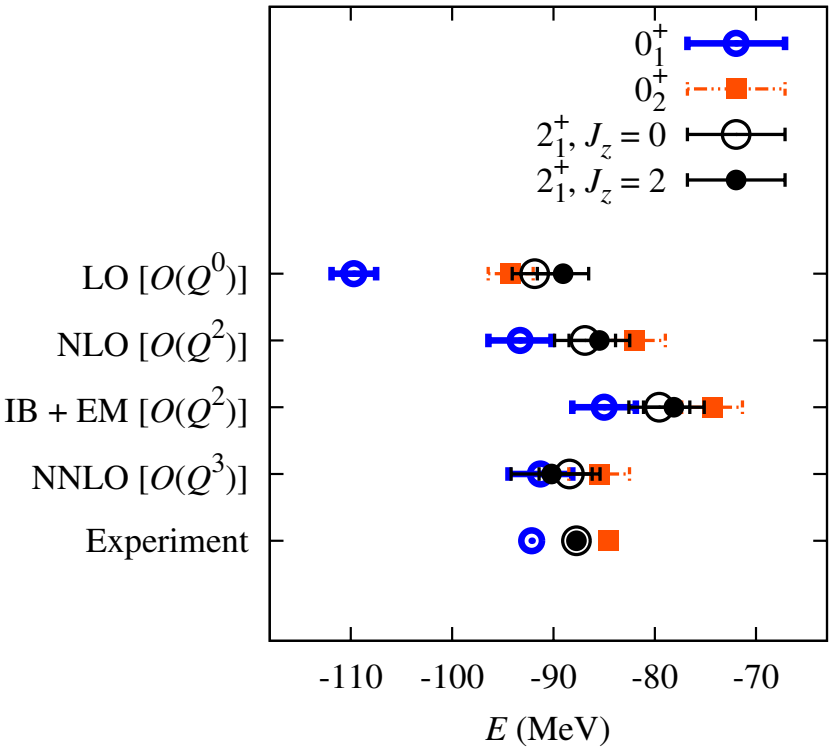
(*Proven by Feynman in his undergraduate thesis at MIT, 1939.)

Hoyle state by complementary QMC methods

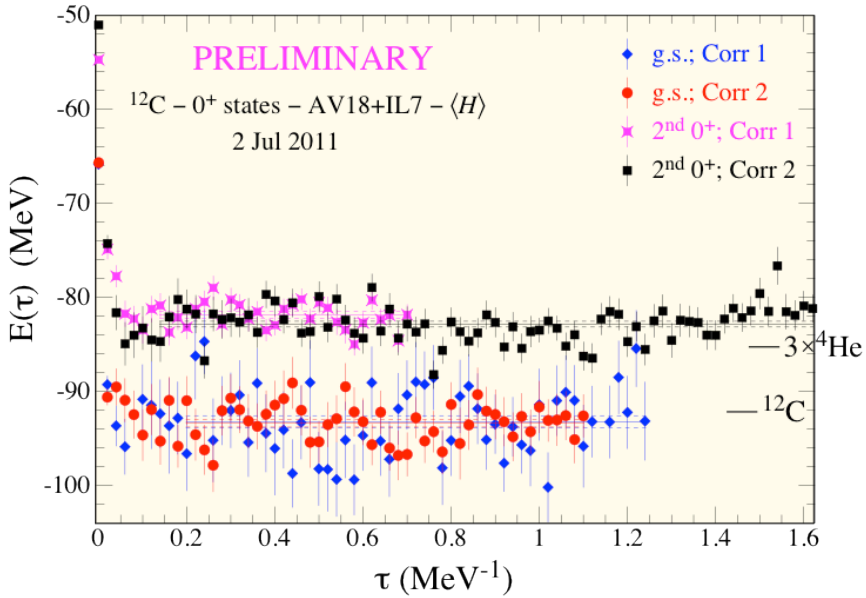


- Triple-α resonance in ^{12}C
- Two distinct Monte-Carlo methods:
  - lattice chiral EFT to N^{2}LO (left)
  - GFMC with AV18+IL7 (right)

Epelbaum et al., PRL **106**, 192501(2011)



S. Pieper et al. (unpublished)



G.s. energy: 93.5(6) MeV [cf. 92.2 MeV]

Radius: 2.35 fm [cf. 2.33 fm]

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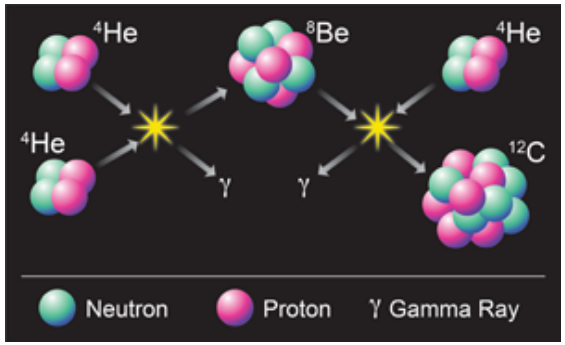

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TABLE I. Lattice results for the ground state energies for ^{4}He, ^{8}Be, and ^{12}C. For comparison we also exhibit the experimentally observed energies. All energies are in units of MeV.

	^{4}He	^{8}Be	^{12}C
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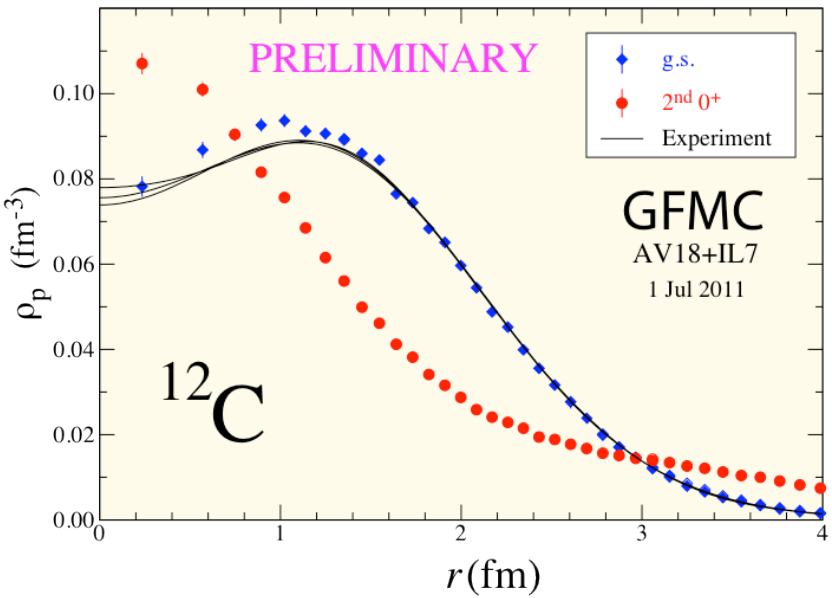

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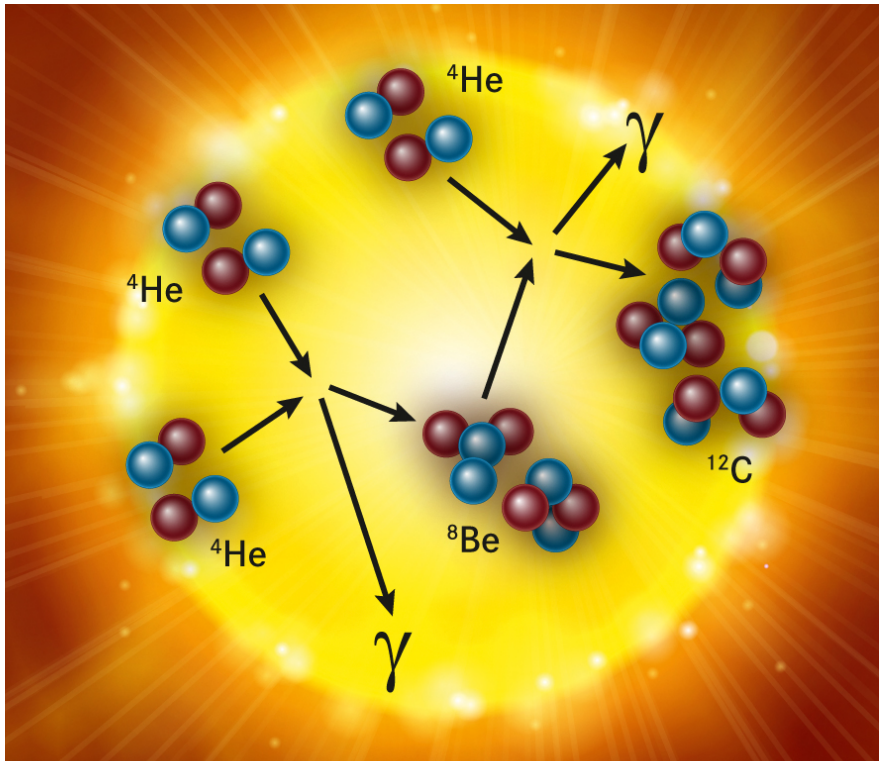
Asides on Hoyle state calculations



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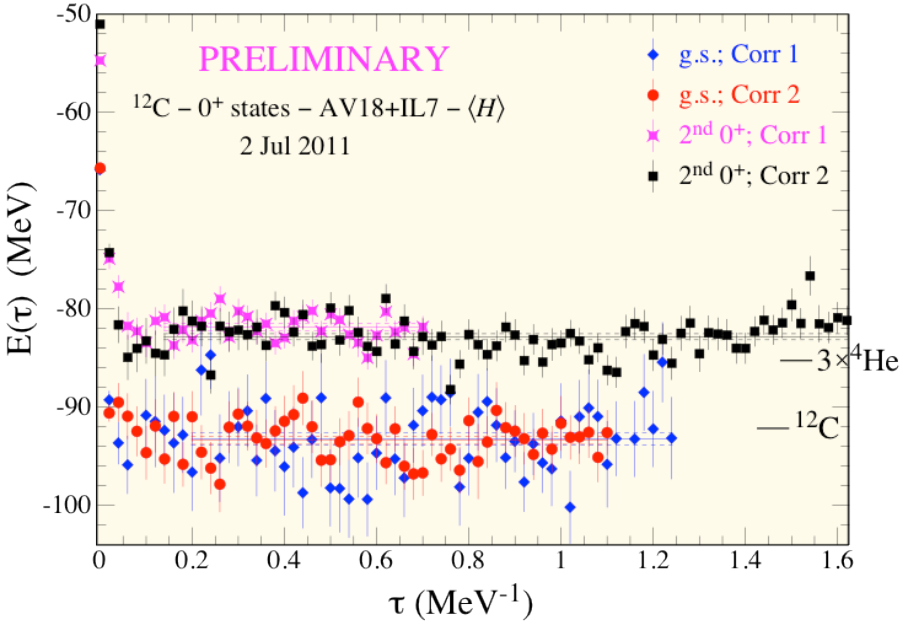
  - Adaptive: can adjust to different structures
  - Favorable scaling of QMC. cf. calculating high-D integral with iterated one-D rules
  - Can refine rough wave function by applying $e^{-H\tau}$
- GFMC implementation
  - shows statistical fluctuations
- Lattice EFT implementation . . .
  - order-by-order refinement

Asides on Hoyle state calculations



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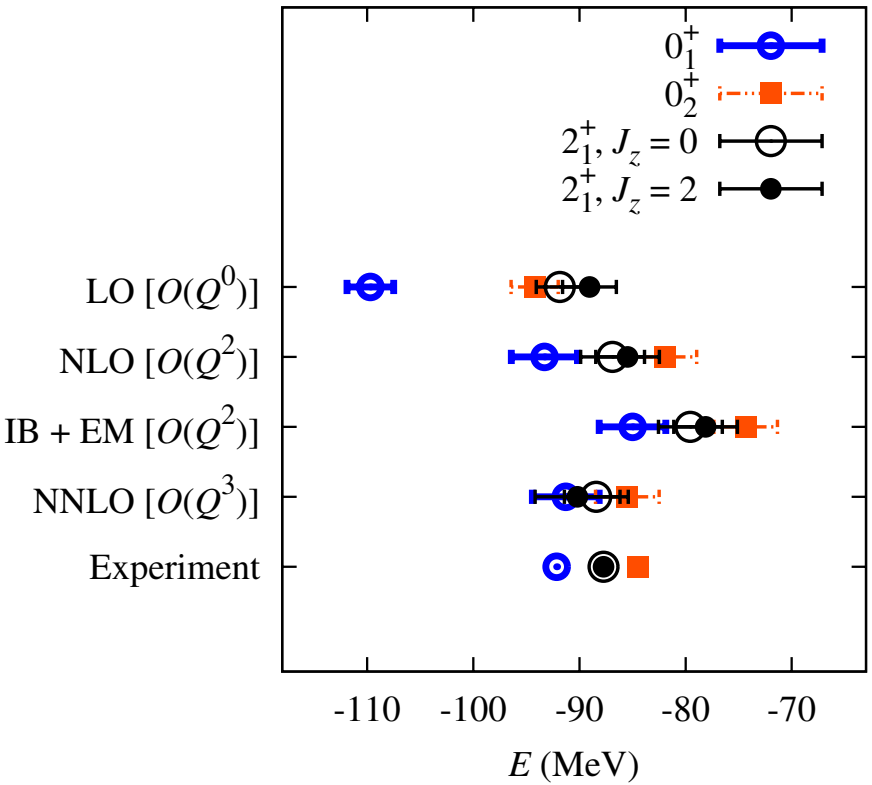

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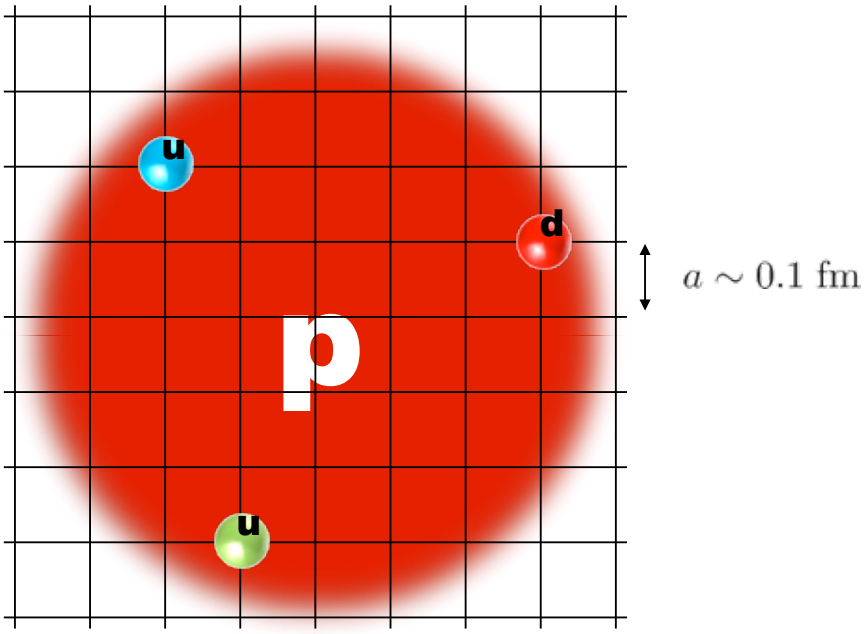
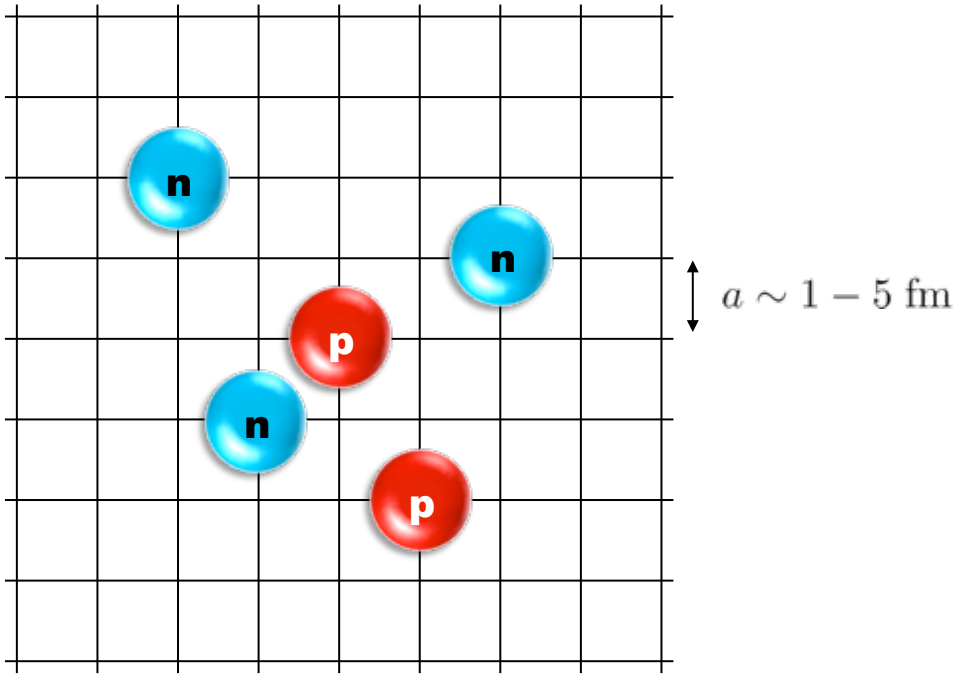
Lattice QCD versus lattice EFT [from Dean Lee]

Compare variables and lattice spacing *a*:

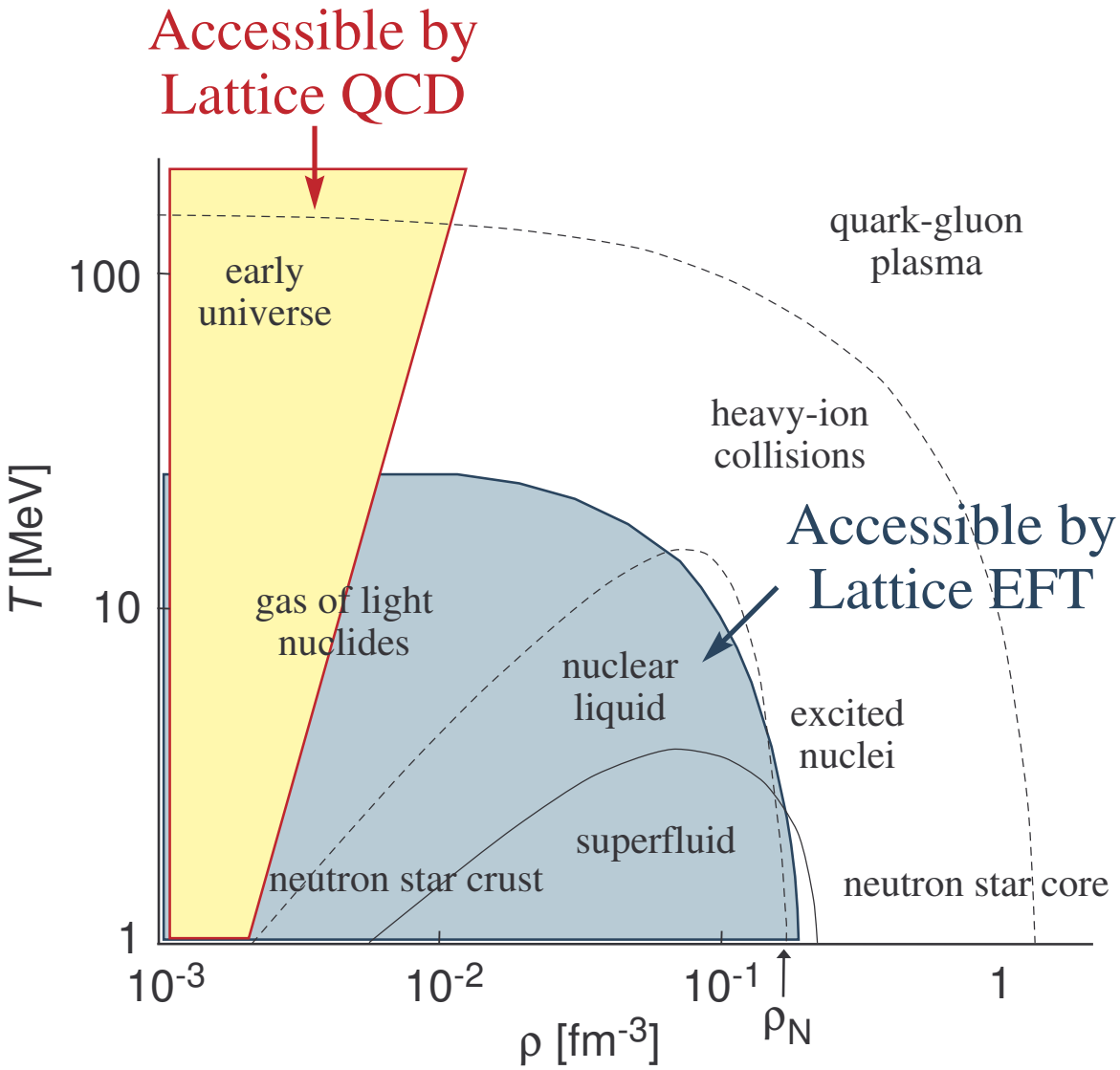
Lattice quantum chromodynamics



Lattice effective field theory



Lattice QCD versus lattice EFT [from U. Meißner]



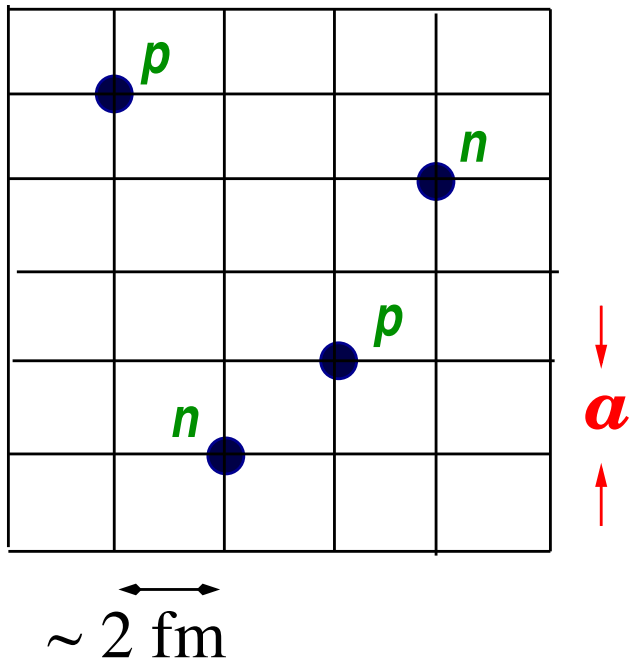
- Note the log scales!

Lattice EFT basics [from U. Meißner]

Frank, Brockmann (1992), Koonin, Müller, Seki, van Kolck (2000) , Lee, Schäfer (2004), . . .
Borasoy, Krebs, Lee, UGM, Nucl. Phys. **A768** (2006) 179; Borasoy, Epelbaum, Krebs, Lee, UGM, Eur. Phys. J. **A31** (2007) 105

- *new method* to tackle the nuclear many-body problem
- discretize space-time $V = L_s \times L_s \times L_s \times L_t$:
  nucleons are point-like fields on the sites
- discretized chiral potential w/ pion exchanges
  and contact interactions
- typical lattice parameters

$$\Lambda = \frac{\pi}{a} \simeq 300\,\text{MeV [UV cutoff]}$$

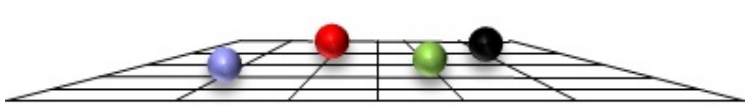
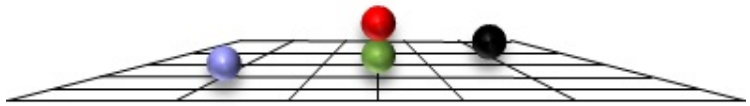


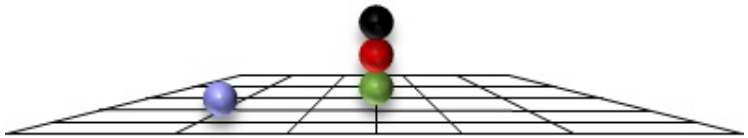
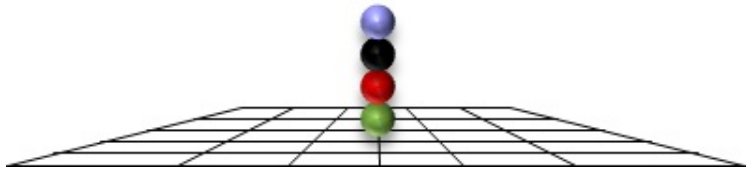
- strong suppression of sign oscillations due to approximate Wigner SU(4) symmetry

J. W. Chen, D. Lee and T. Schäfer, Phys. Rev. Lett. **93** (2004) 242302

- hybrid Monte Carlo & transfer matrix (similar to LQCD)

Lattice EFT basics [from U. Meißner]

$\Rightarrow$ all *possible* configurations are sampled

$\Rightarrow$ *clustering* emerges *naturally*

Lattice EFT basics [from U. Meißner]

- Correlation–function for A nucleons: $Z_A(t) = \langle \Psi_A | \exp(-tH) | \Psi_A \rangle$

  with Ψ_A a Slater determinant for A free nucleons

Euclidean time

- Ground state energy from the time derivative of the correlator

$$E_A(t) = -\frac{d}{dt} \ln Z_A(t)$$

$\longrightarrow$ ground state filtered out at large times: $E_A^0 = \lim_{t\to\infty} E_A(t)$

- Expectation value of any normal–ordered operator $\mathcal{O}$

$$Z_A^{\mathcal{O}} = \langle \Psi_A | \exp(-tH/2)\, \mathcal{O}\, \exp(-tH/2) \, | \Psi_A \rangle$$

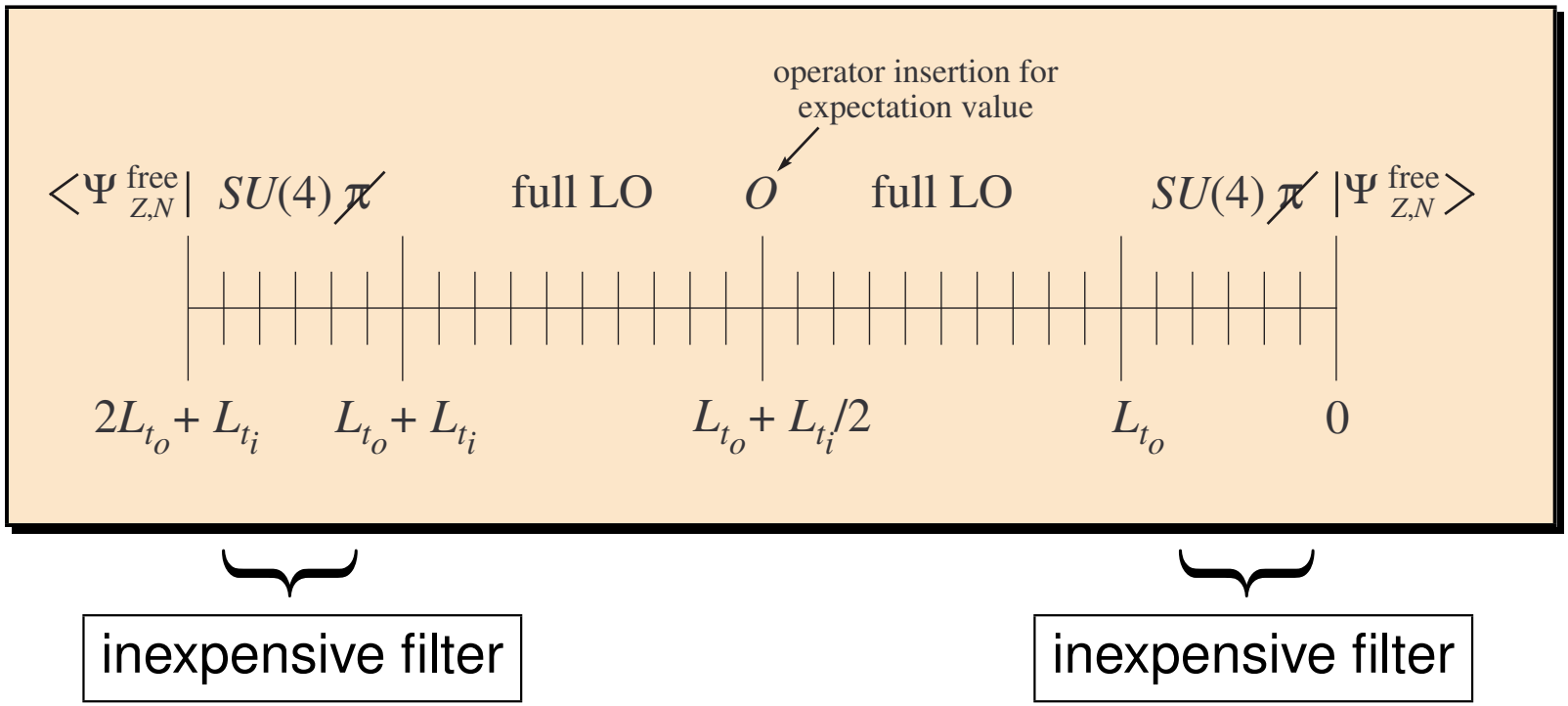
$$\lim_{t\to\infty} \frac{Z_A^{\mathcal{O}}(t)}{Z_A(t)} = \langle \Psi_A | \mathcal{O} \, | \Psi_A \rangle$$

Lattice EFT basics [from U. Meißner]

- Expectation value of any normal–ordered operator $\mathcal{O}$

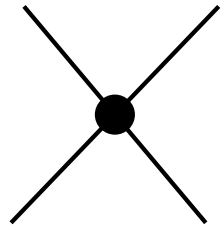
$$\langle \Psi_A | \mathcal{O} | \Psi_A \rangle = \lim_{t\to\infty} \frac{\langle \Psi_A | \exp(-tH/2)\, \mathcal{O}\, \exp(-tH/2) | \Psi_A \rangle}{\langle \Psi_A | \exp(-tH) | \Psi_A \rangle}$$

- Anatomy of the transfer matrix



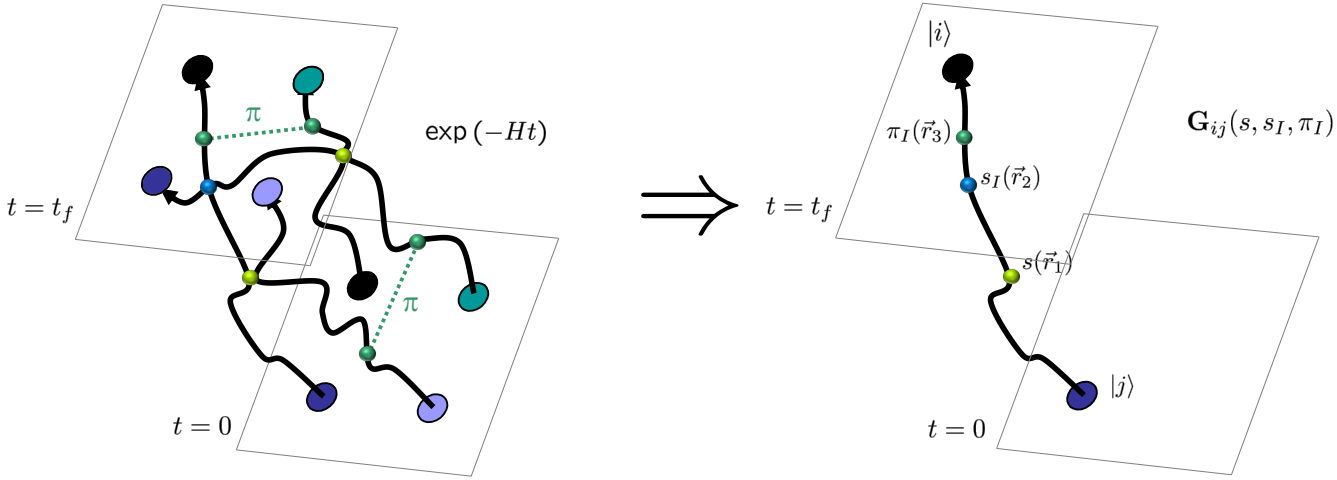
Lattice EFT basics [from U. Meißner]

- Contact interactions represented by auxiliary fields s, s_I



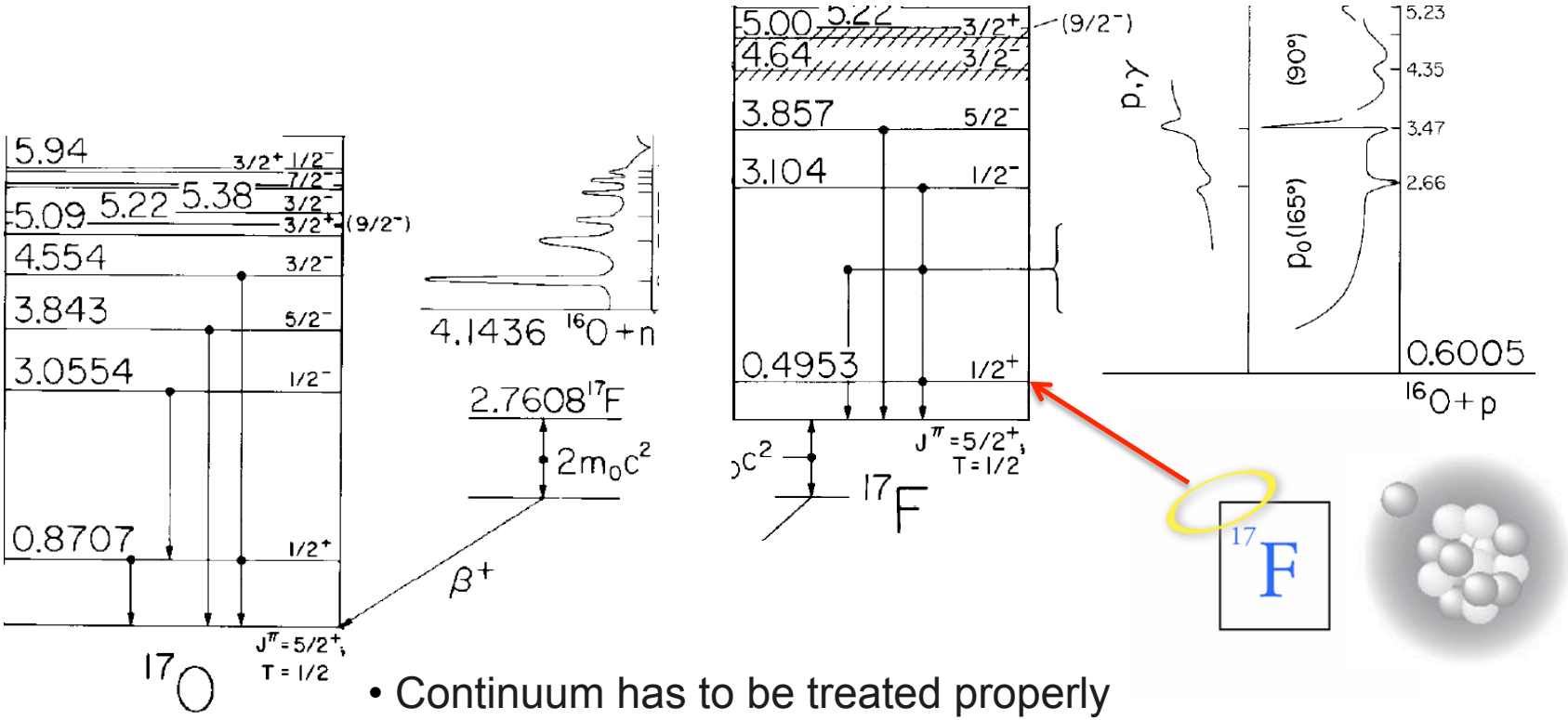
$$\exp(\rho^2/2) \propto \int_{-\infty}^{+\infty} ds \, \exp(-s^2/2 - s\rho) \, , \quad \rho \sim N^\dagger N$$

- Correlation function = path-integral over pions & auxiliary fields



Coupled-Cluster method [G. Hagen et al, PRL 104, 182501 (2010)]

Ab initio description of proton halo state in ^{17}F

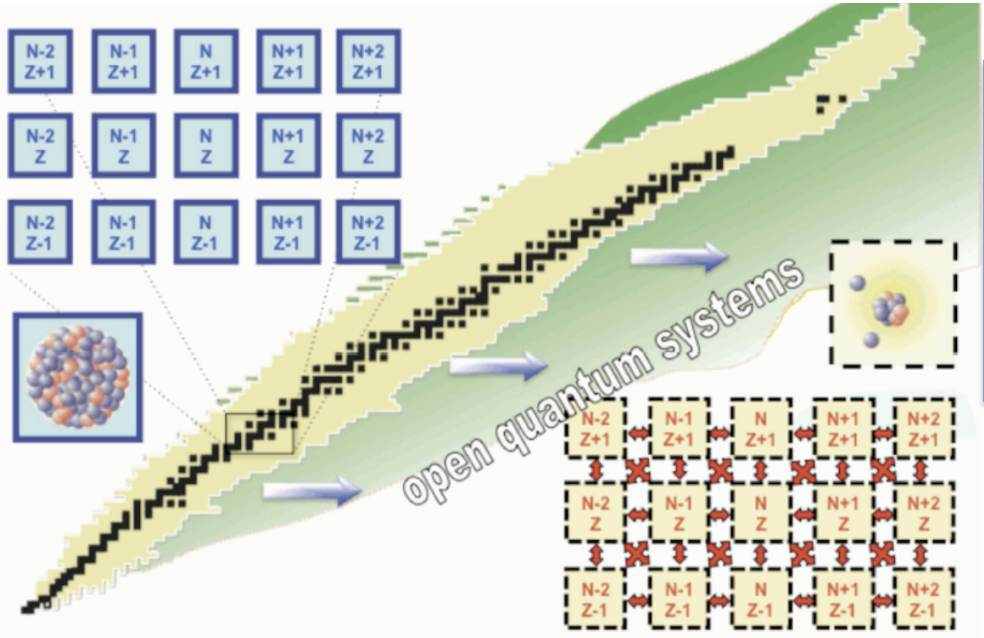


- Continuum has to be treated properly
- Focus is on single-particle states
- Previous study: shell model in the continuum with ^{16}O core

[K. Bennaceur, N. Michel, F. Nowacki, J. Okolowicz, M. Ploszajczak, Phys. Lett. B 488, 75 (2000)]

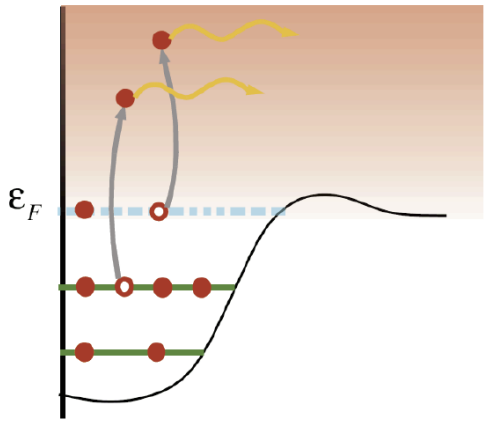
Coupled cluster method [from D. Dean, G. Hagen, T. Papenbrock]

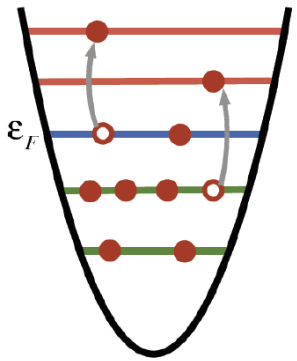
Open Quantum Systems

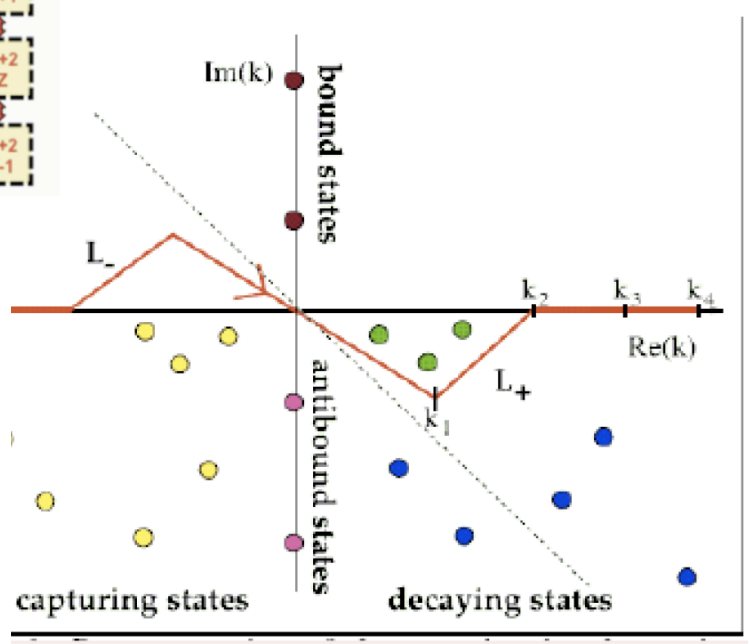


The Berggren completeness treats bound, resonant and scattering states on equal footing.

Has been successfully applied in the shell model in the complex energy plane to light nuclei. For a review see
N. Michel et al J. Phys. G 36, 013101 (2009).







Coupled cluster method [from D. Dean, G. Hagen, T. Papenbrock]

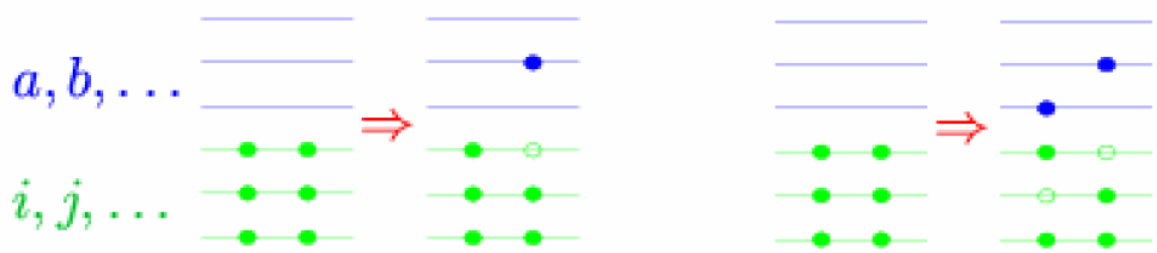
Coupled-cluster method (in CCSD approximation)

Ansatz:

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

- ☺ Scales gently (polynomial) with increasing problem size o^2u^4 .
- ☺ Truncation is the only approximation.
- ☺ Size extensive (error scales with A)
- ☹ Most efficient for doubly magic nuclei

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



Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle
\end{aligned}
$$

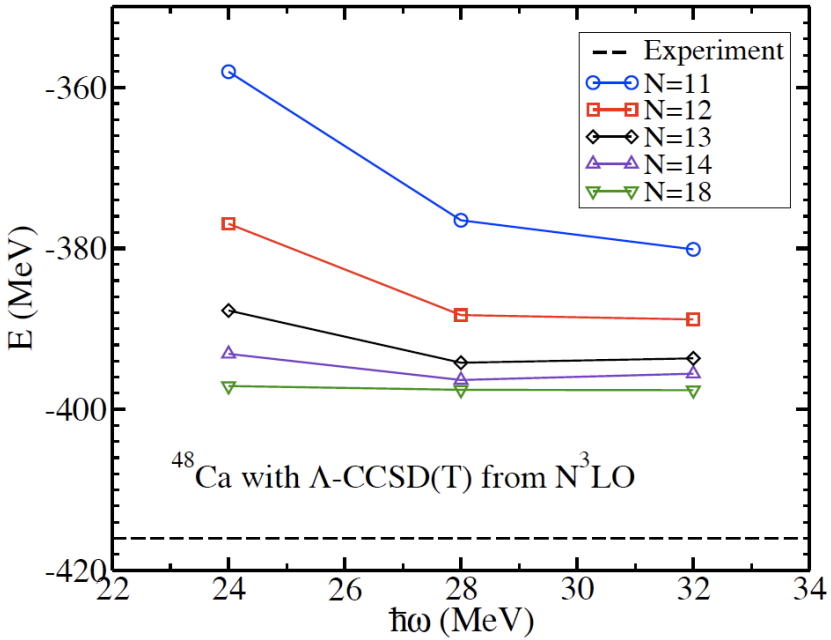
Alternative view: CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations.

$$
\overline{H} \equiv e^{-T} H e^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \dots\right)_c
$$

Coupled cluster method [from D. Dean, G. Hagen, T. Papenbrock]

Toward medium-mass nuclei

Chiral N^{3}LO (500 MeV) by Entem & Machleidt, NN only



Binding energy per nucleon

Nucleus	CCSD	Λ-CCSD(T)	Experiment
^{4}He	5.99	6.39	7.07
^{16}O	6.72	7.56	7.97
^{40}Ca	7.72	8.63	8.56
^{48}Ca	7.40	8.28	8.67

- Chiral NN forces yield saturation, lack about 0.4 MeV per nucleon in binding energy.
- Chiral three-nucleon forces expected to yield 0.4MeV per nucleon?!

Benchmarking different methods:
Our CC results for ^{16}O agree with IT-NCSM (R. Roth et al PRL 107, 072501 (2011)) and UMOA (Fujii et al., Phys. Rev. Lett. 103, 182501 (2009)

	CCM	(IT)-NCSM	UMOA
	E/A	E/A	E/A
^{4}He	-6.39(5)	-6.35	
^{16}O	-7.56(8)	-7.48(4)	-7.47

Coupled cluster method [from D. Dean, G. Hagen, T. Papenbrock]

Asymmetry dependence and spectroscopic factors

- Spectroscopic factors are not observables
- They are extracted from a cross section based on a specific structure and reaction model
- Structure and reaction models needs to be consistent!

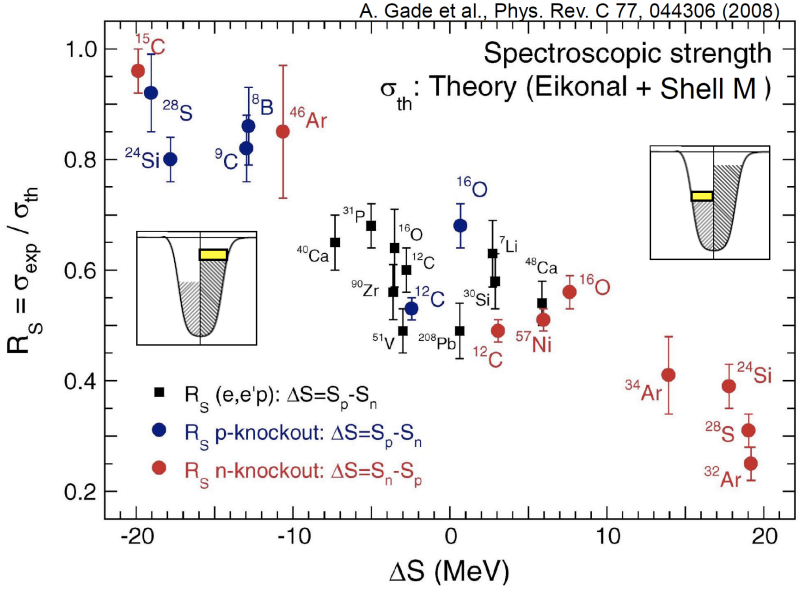
Theoretical cross section:

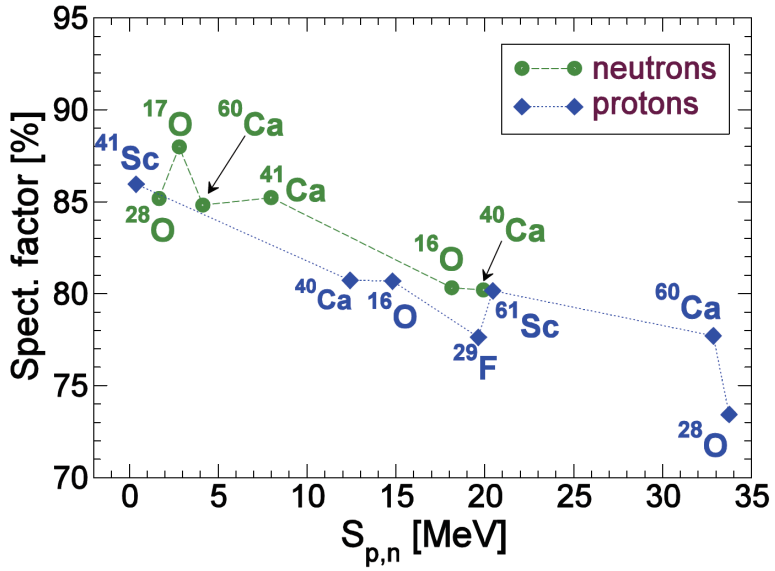
$$\sigma(j^\pi) = \left(\frac{A}{A-1}\right)^N C^2S(j^\pi)\sigma_{sp}(j, S_N + E_x[j^\pi])$$

Reaction theory

Structure theory

A. Gade et al., Phys. Rev. C 77, 044306 (2008)



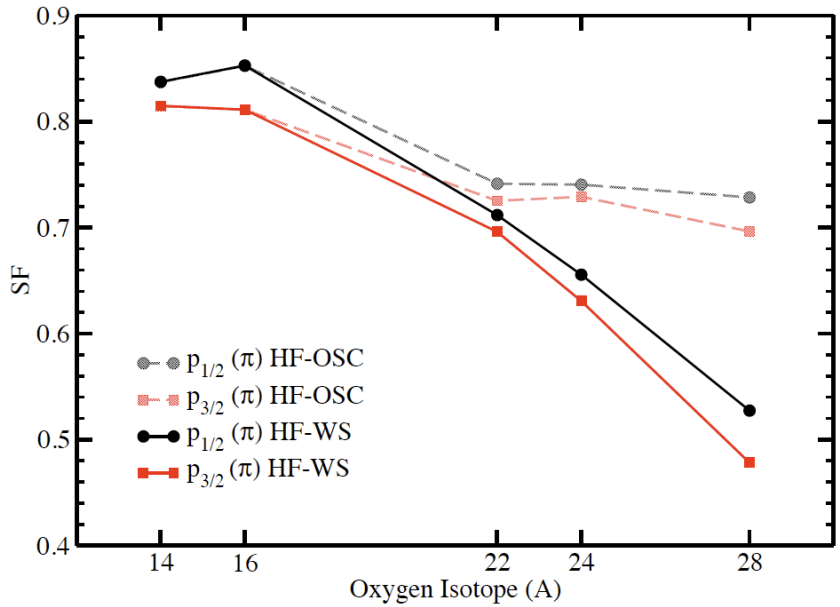


C. Barbieri, W.H.Dickhoff, Int. Jour. Mod. Phys. A24, 2060 (2009).

Self-consistent green's function method show rather weak asymmetry dependence for the spectroscopic factor.

Coupled cluster method [from D. Dean, G. Hagen, T. Papenbrock]

Quenching of spectroscopic factors for proton removal in neutron rich oxygen isotopes

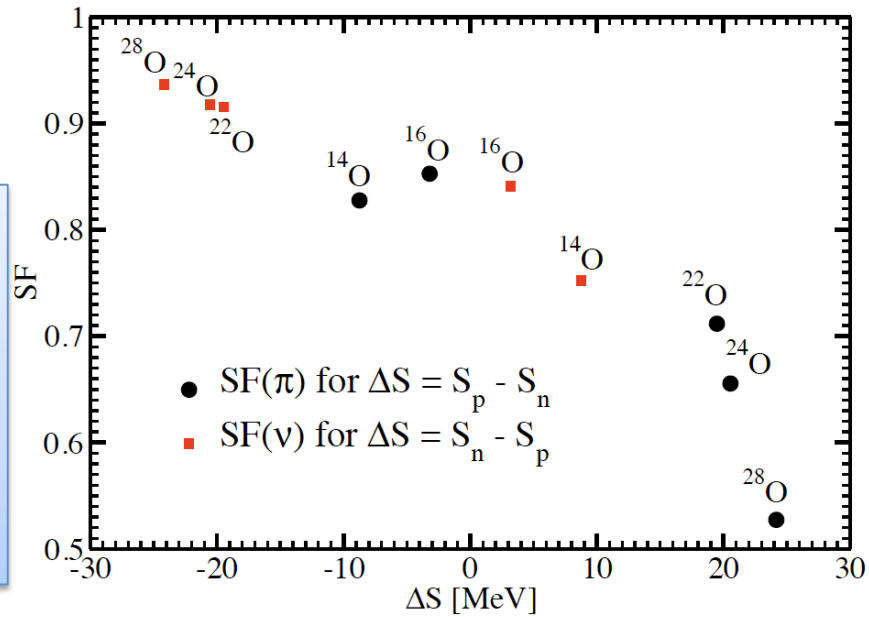


Spectroscopic factor is a useful tool to study correlations towards the dripline.

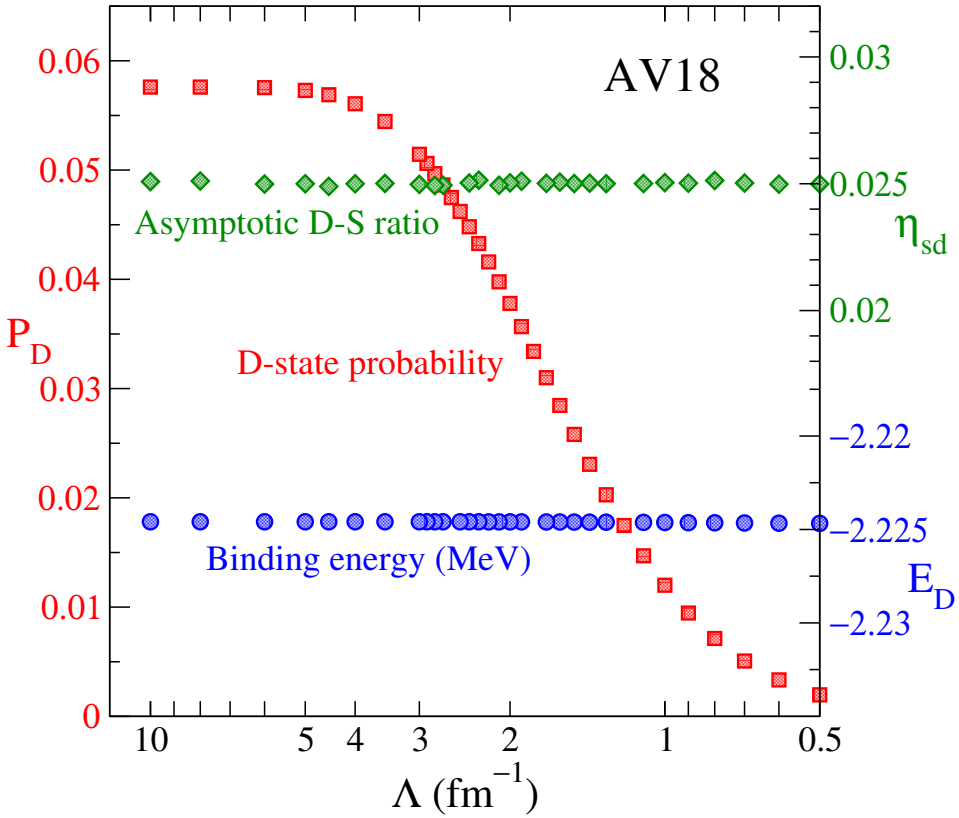
SF for proton removal in neutron rich ^{24}O show strong "quenching" pointing to large deviations from a mean-field like picture.
G. Hagen et al Phys. Rev. Lett. 107, 032501 (2011).

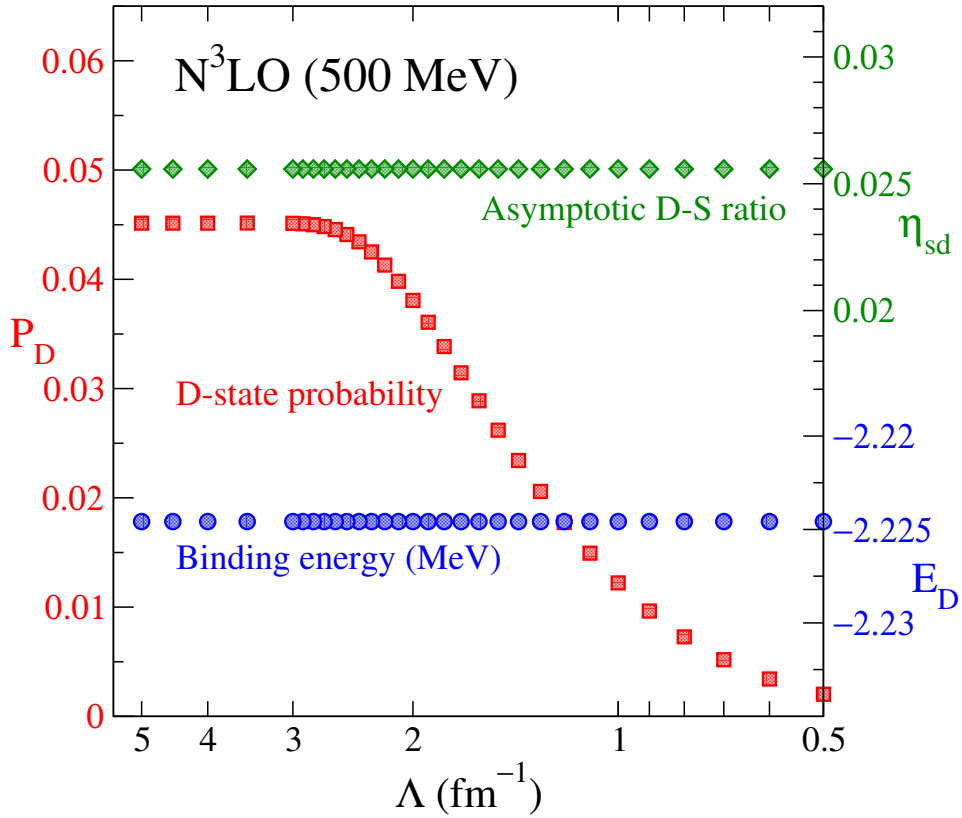
Strong asymmetry dependence on the SF for proton and neutron removal in neutron rich oxygen isotopes.

SF~1 for neutron removal while protons are strongly correlated SF ~0.6-0.7 in ^{22,24,28}O



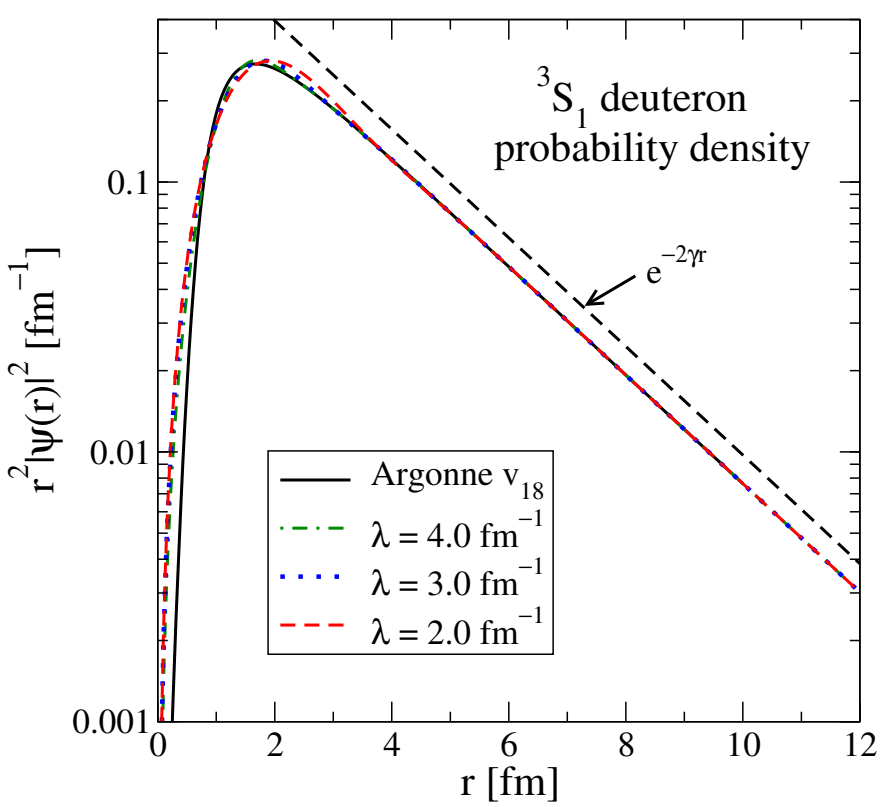
Deuteron scale-(in)dependent observables

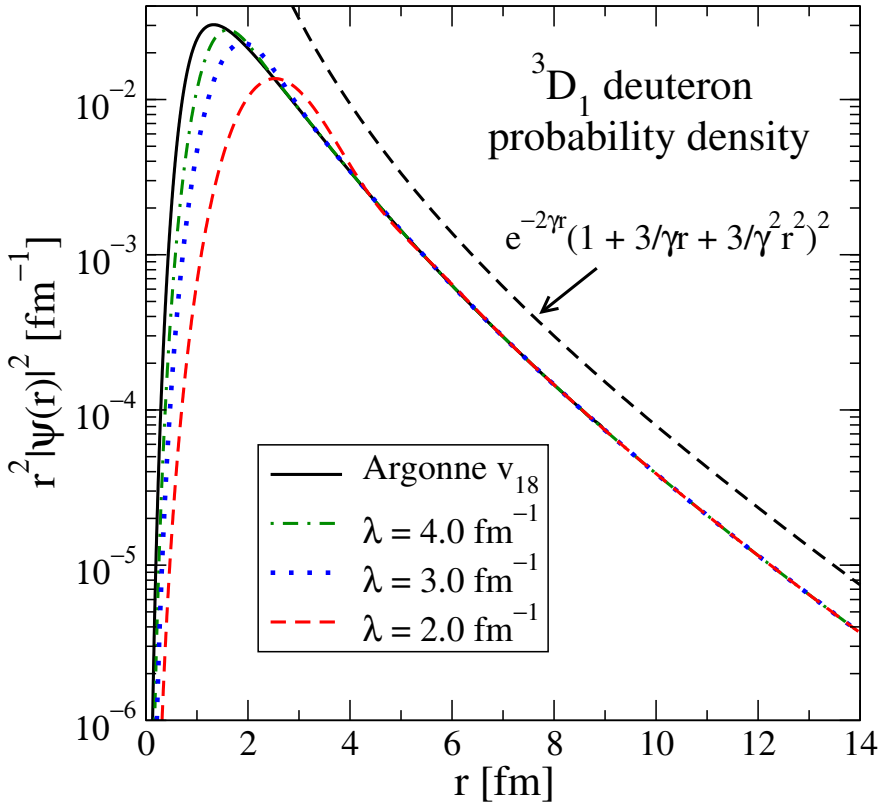




- $V_{\text{low } k}$ RG transformations labeled by Λ (different V_Λ's)
  - $\Longrightarrow$ soften interactions by lowering resolution (scale)
  - $\Longrightarrow$ reduced short-range and tensor correlations
- Energy and asymptotic D-S ratio are unchanged (cf. ANC's)
- But D-state probability changes (cf. spectroscopic factors)

ANCs as wf observables: coordinate space





- ANC's, like phase shifts, are asymptotic properties
  $\Longrightarrow$ short-range unitary transformations do not alter them
  [e.g., see Mukhamedzhanov/Kadyrov, PRC **82** (2010)]
- In contrast, SF's rely on *interior* wave function overlap
- (Note difference in S-wave and D-wave ambiguities)

ANCs as wf observables: momentum space

[based on R.D. Amado, PRC **19** (1979)]

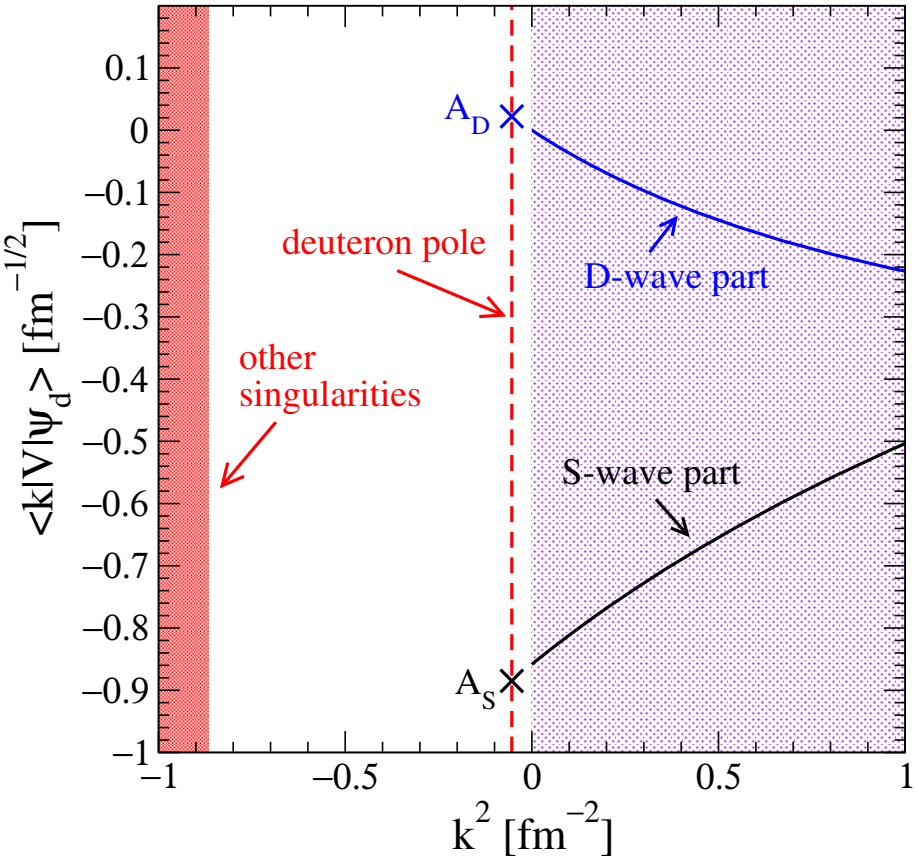
1. $\frac{k^2}{2\mu}\langle \mathbf{k}|\psi_n\rangle + \langle \mathbf{k}|V|\psi_n\rangle = -\frac{\gamma_n^2}{2\mu}\langle \mathbf{k}|\psi_n\rangle$

   $\Longrightarrow \langle \mathbf{k}|\psi_n\rangle = -\frac{2\mu\langle \mathbf{k}|V|\psi_n\rangle}{k^2+\gamma_n^2}$

2. $\langle \mathbf{r}|\psi_n\rangle = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}}\langle \mathbf{k}|\psi_n\rangle$

   $\stackrel{|\mathbf{r}|\to\infty}{\longrightarrow} A_n e^{-\gamma_n r}/r$

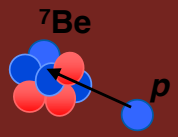
3. integral dominated by pole from 1.
4. extrapolate $\langle \mathbf{k}|V|\psi_n\rangle$ to $k^2 = -\gamma_n^2$



- Or, residue from extrapolating on-shell T-matrix to deuteron pole
  $\Longrightarrow$ invariant under unitary transformations
- How far can we get solely with quantities that are invariant under (short-range) unitary transformations?

Combining structure and reactions [P. Navratil et al.]

TRIUMF



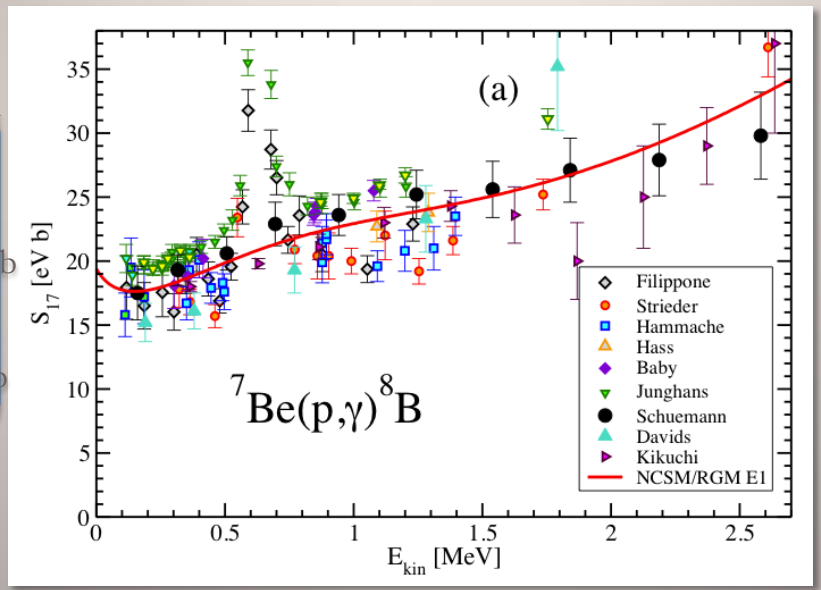
^{7}Be(p,γ)^{8}B radiative capture

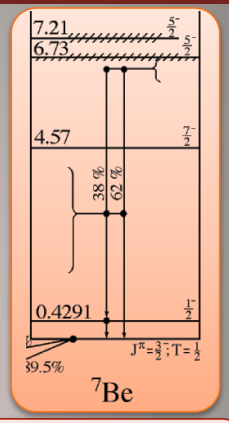
- NCSM/RGM calculation of ^{7}Be(p,γ)^{8}B radiative capture
  - ^{7}Be states 3/2$^-$,1/2$^-$, 7/2$^-$, 5/2$^-_1$, 5/2$^-_2$
  - Soft NN potential (SRG-N^{3}LO with Λ = 1.86 fm^{-1})

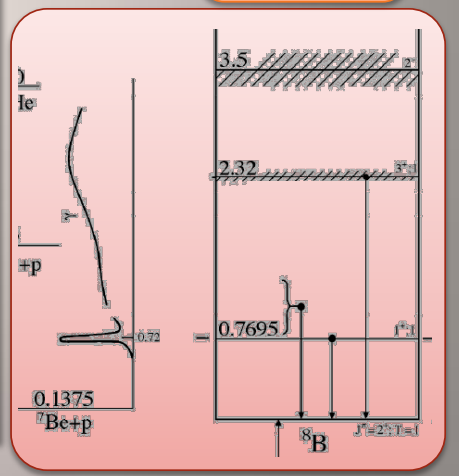
^{8}B 2$^+$ g.s. **bound** by 136 keV (expt. 137 keV)

S(0) ~ 19.4(0.7) eV b

Data evaluation: S(0)=20.8(2.1) eV b







The first ever *ab initio* calculations of ^{7}Be(p,γ)^{8}B

arXiv:1105.5977 [nucl-th]

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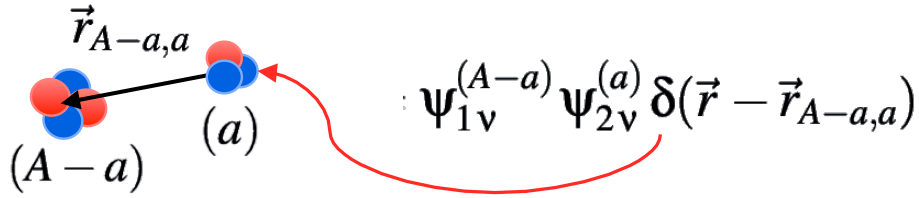
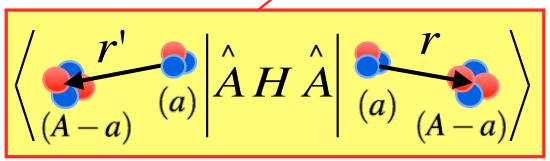
Ab initio NCSM/RGM in a snapshot [from P. Navratil]

- *Ab initio* calculations for reactions and clustering in nuclei
- Constructs integration kernels (≈ projectile-target potentials) starting from
  - NCSM wave functions
  - NN(+NNN) interactions

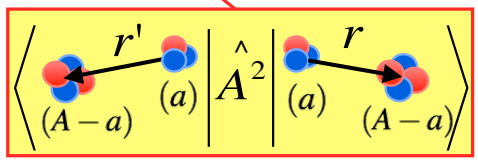


- Solves:

$$\sum_{\nu}\int d\vec{r}\left[\mathcal{H}_{\mu\nu}^{(A-a,a)}(\vec{r}',\vec{r})-E\mathcal{N}_{\mu\nu}^{(A-a,a)}(\vec{r}',\vec{r})\right]\varphi_{\nu}(\vec{r})=0$$



Hamiltonian kernel



Norm kernel

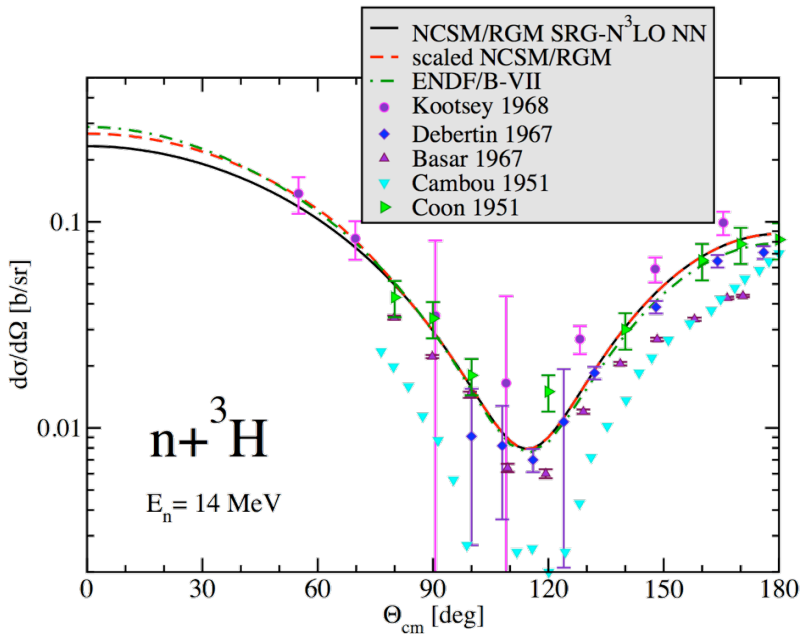
The Resonating Group Method correctly accounts for:
1) the interaction (Hamiltonian kernel) and the Pauli principle (Norm kernel) between clusters and 2) all the available channels

Ultimate Goal: 3α ➔ ^{12}C and ^{12}C(α,γ)^{16}O

Ab initio approach to light-ion reactions

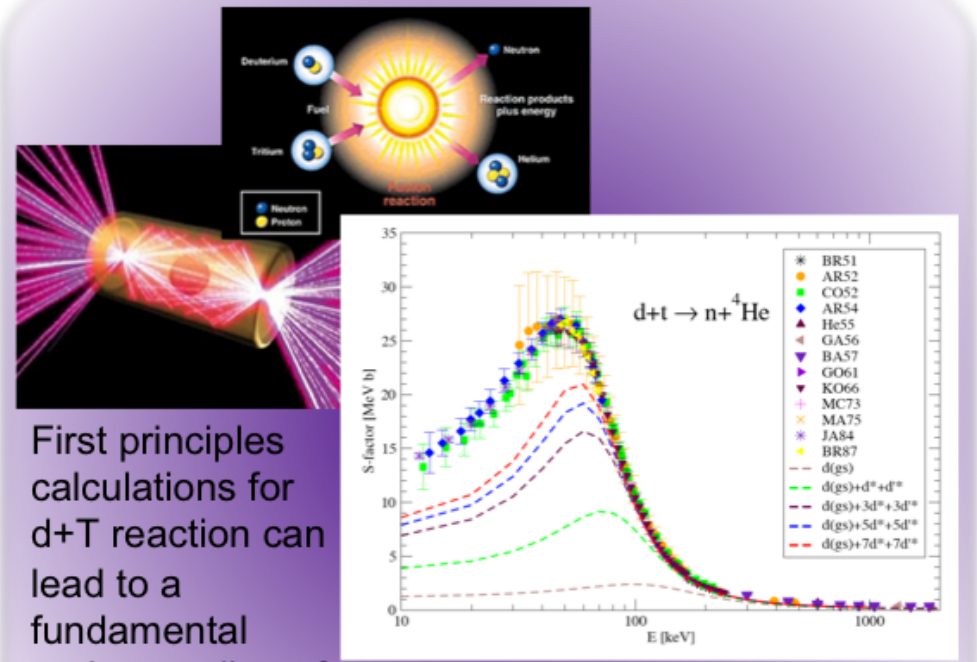
- E.g., applications to fusion energy systems (NIF)

T(*n*,*n*)T cross section



Ab initio theory reduces uncertainty due to conflicting data (•, ◆, ▲, ▼, ▶)

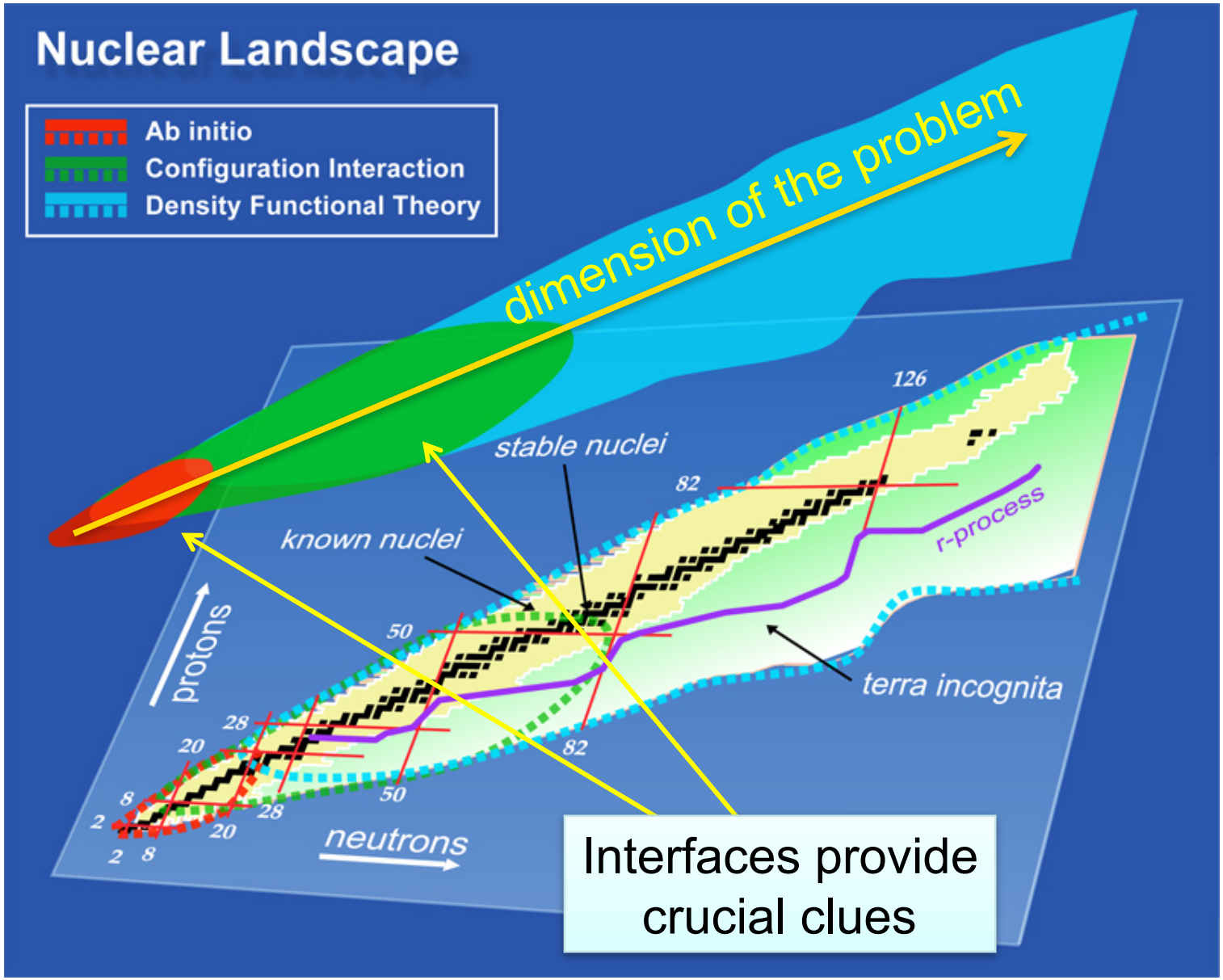
Navrátil *et al.*, LLNL-TR-423504, LLNL-TR-435981, arXiv.1009.3965



First principles calculations for d+T reaction can lead to a fundamental understanding of thermonuclear fusion

- Coming soon: including SRG-evolved NNN interactions

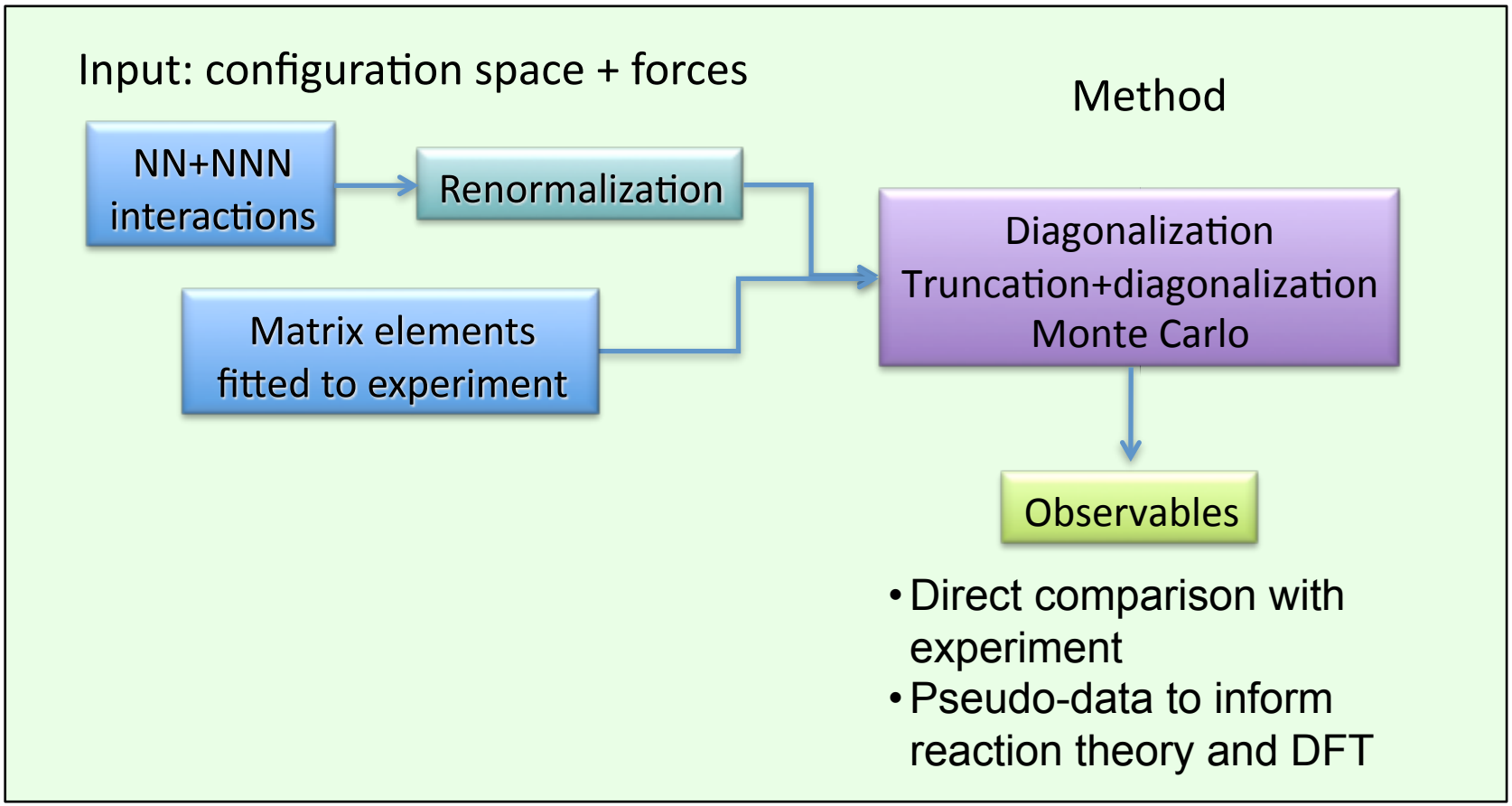
Overlapping theory methods cover all nuclei



The shell model revisited

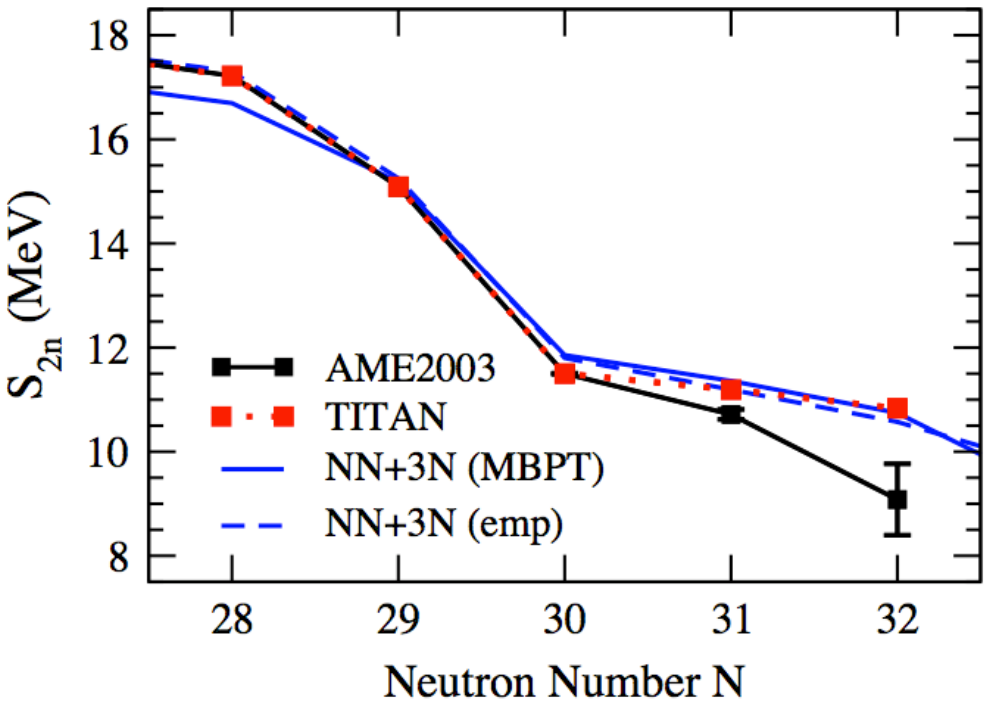
Configuration interaction techniques

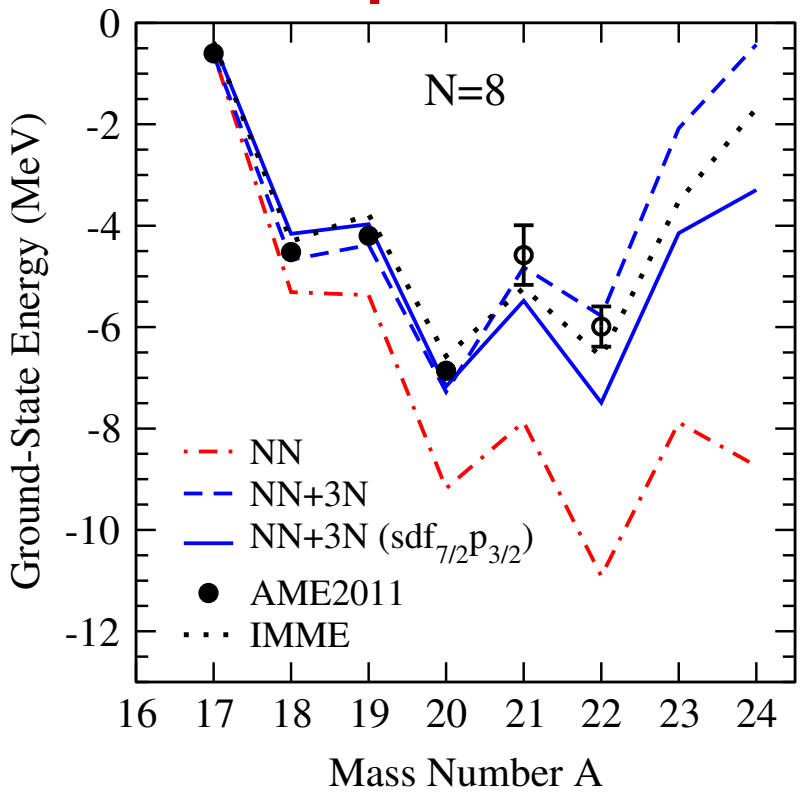
- light and heavy nuclei
- detailed spectroscopy
- quantum correlations (lab-system description)



Confronting theory and experiment to both driplines

- Precision mass measurements test impact of chiral 3NF
- Proton rich [Holt et al., arXiv:1207.1509]
- Neutron rich [Gallant et al., arXiv:1204.1987]
- Many new tests possible!





- Shell model description using chiral potential evolved to $V_{\mathrm{low}\,k}$ plus 3NF fit to $A = 3, 4$
- Excitations outside valence space included in 3rd order MBPT

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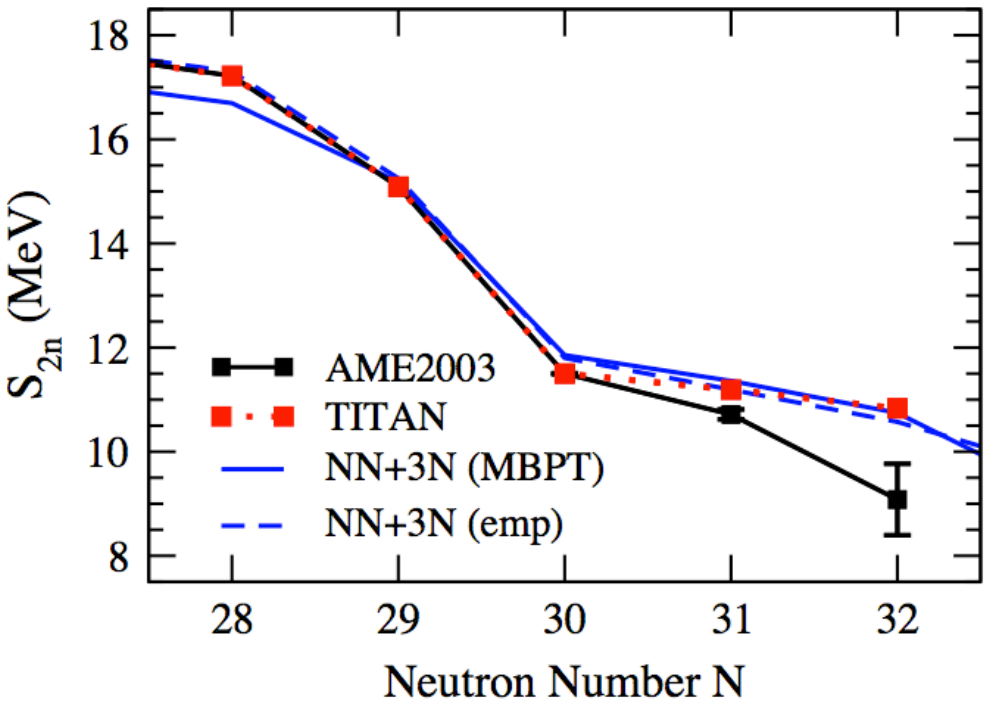

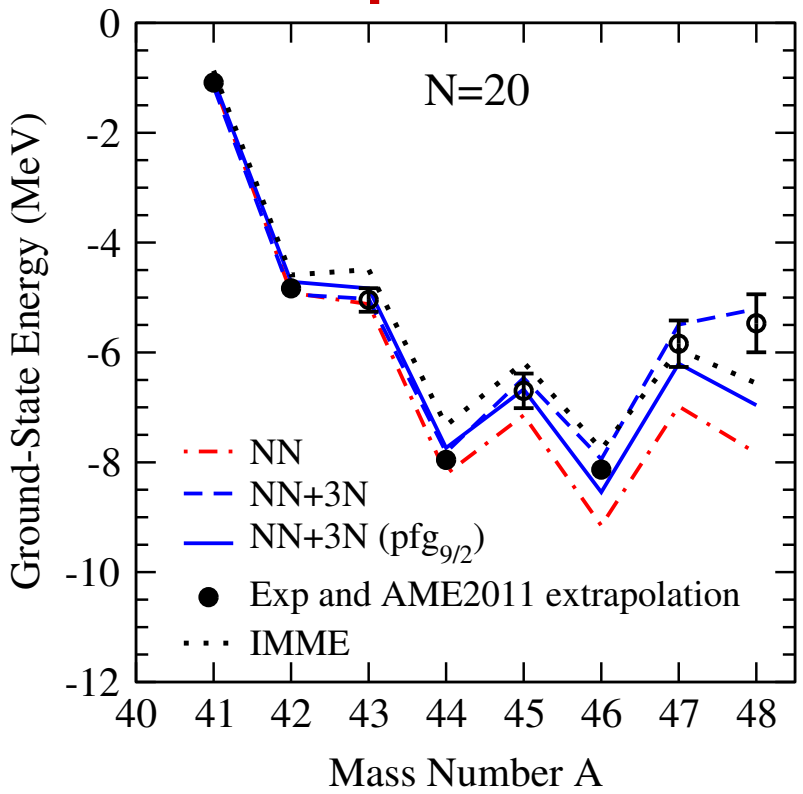

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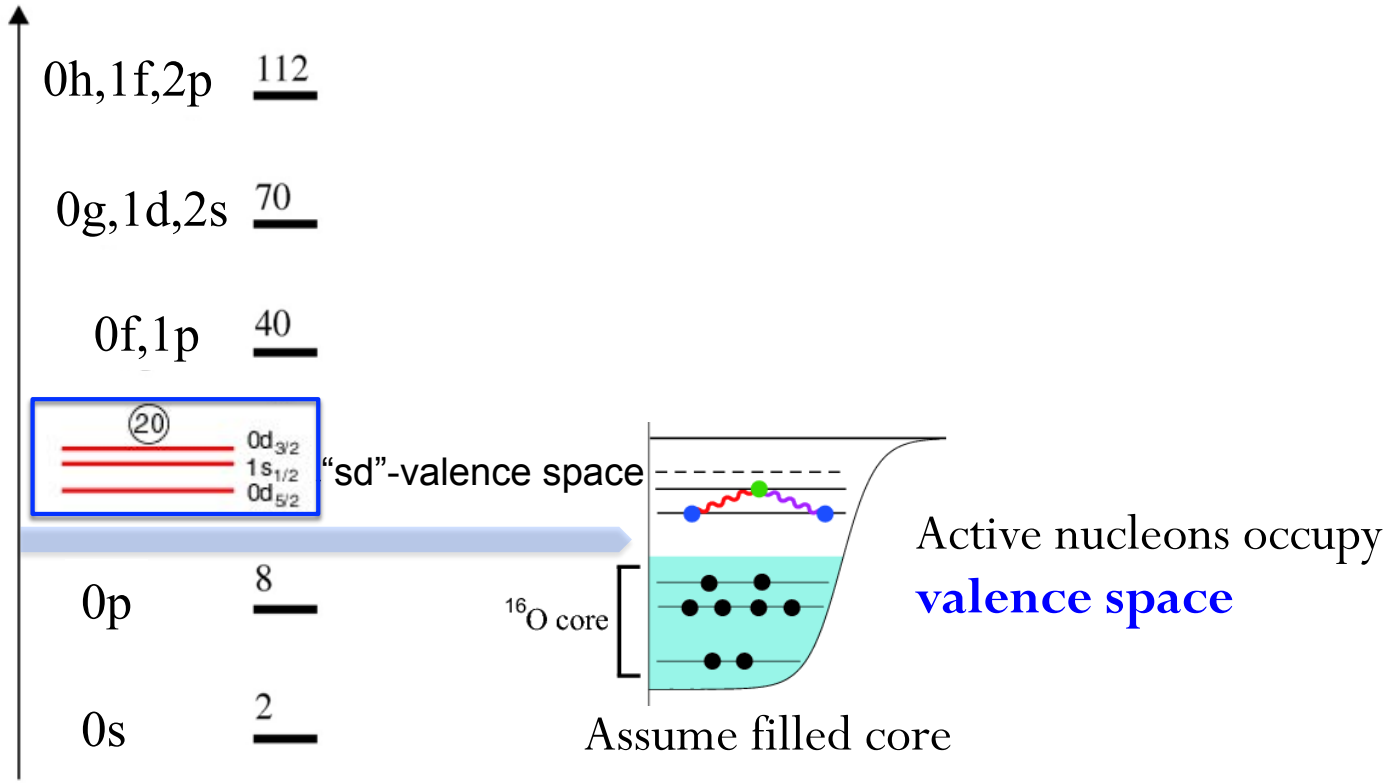
Non-empirical shell model [from J. Holt]

Solving the Nuclear Many-Body Problem

Nuclei understood as many-body system starting from closed shell, add nucleons

Interaction and energies of valence space orbitals from original $V_{\mathrm{low}\,k}$

This alone does not reproduce experimental data



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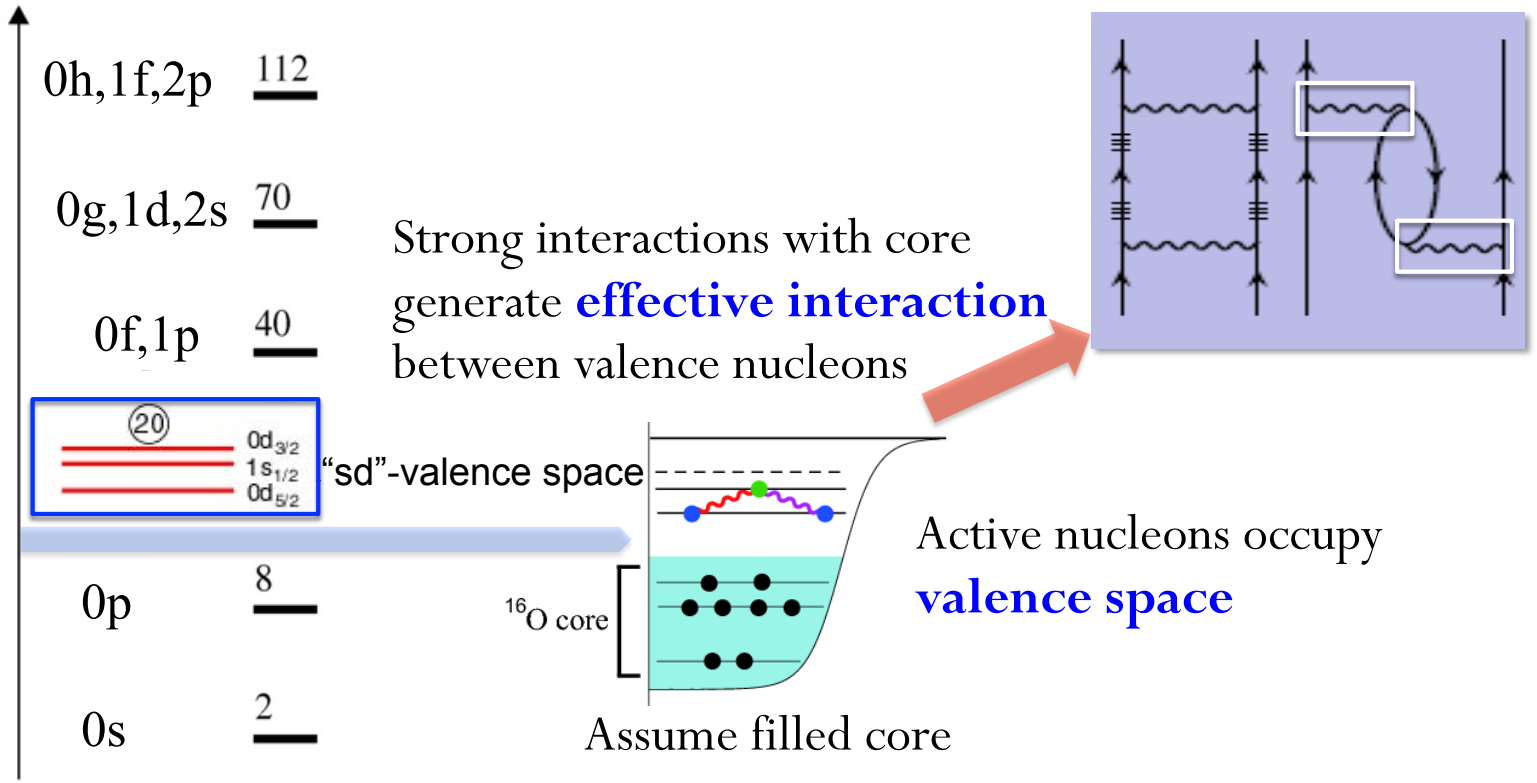

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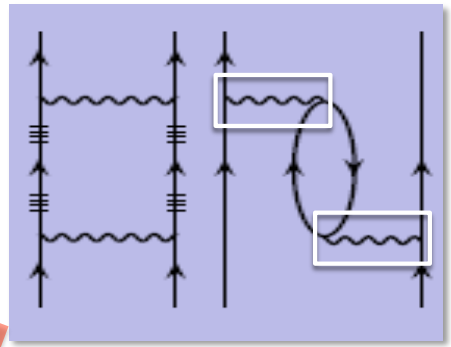
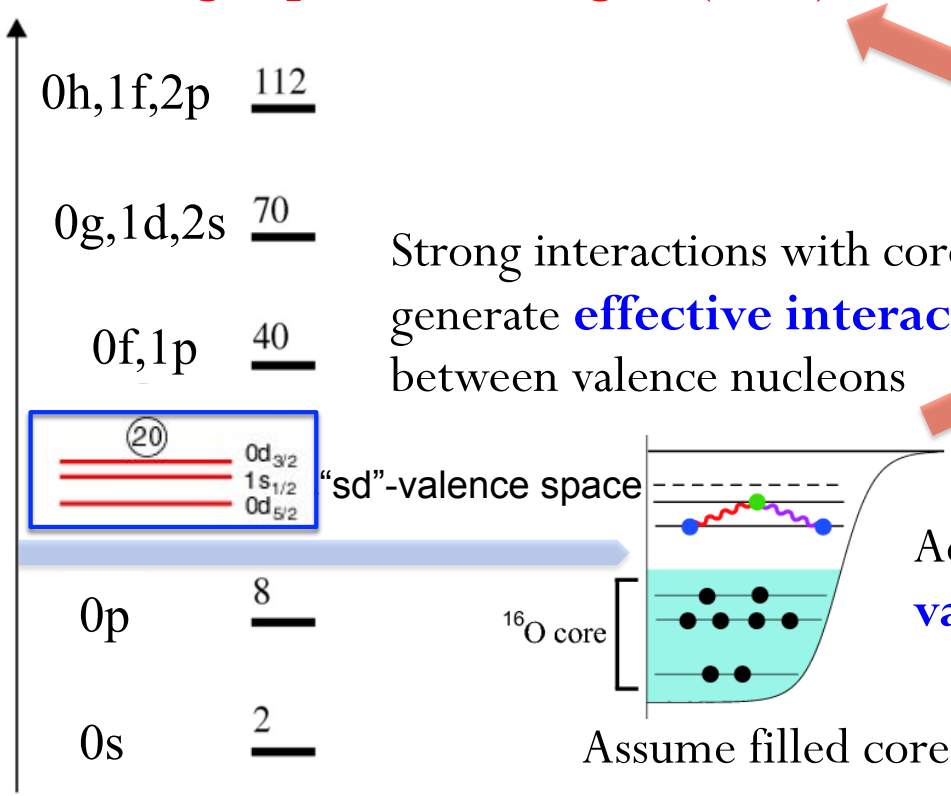
Effective two-body matrix elements

Single-particle energies (SPEs)

Hjorth-Jensen, Kuo, Osnes (1995)





Strong interactions with core generate **effective interaction** between valence nucleons

Active nucleons occupy **valence space**

Assume filled core

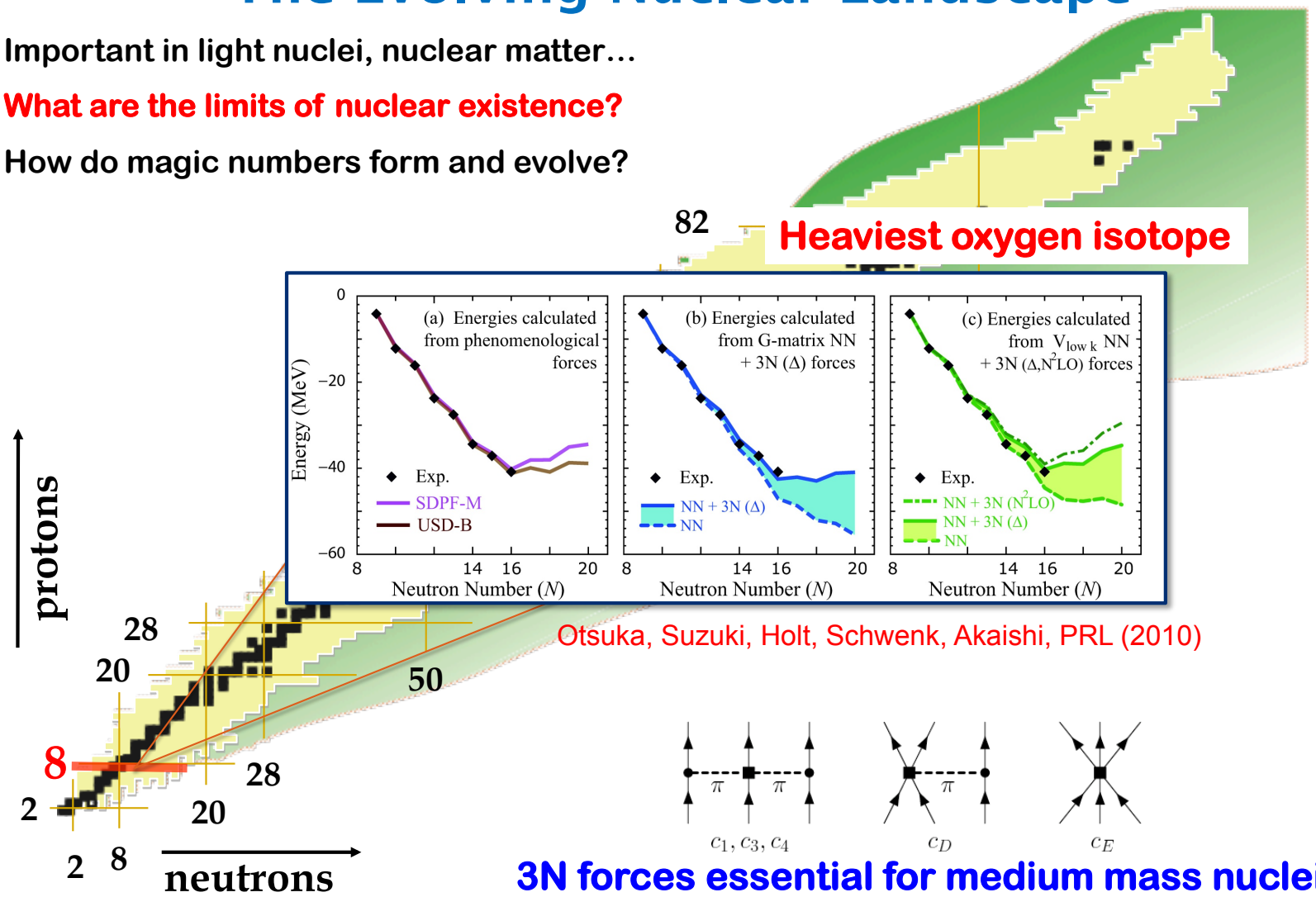
Chiral 3NFs meet the shell model [from J. Holt]

Drip Lines and Magic Numbers: The Evolving Nuclear Landscape

Important in light nuclei, nuclear matter…

What are the limits of nuclear existence?

How do magic numbers form and evolve?

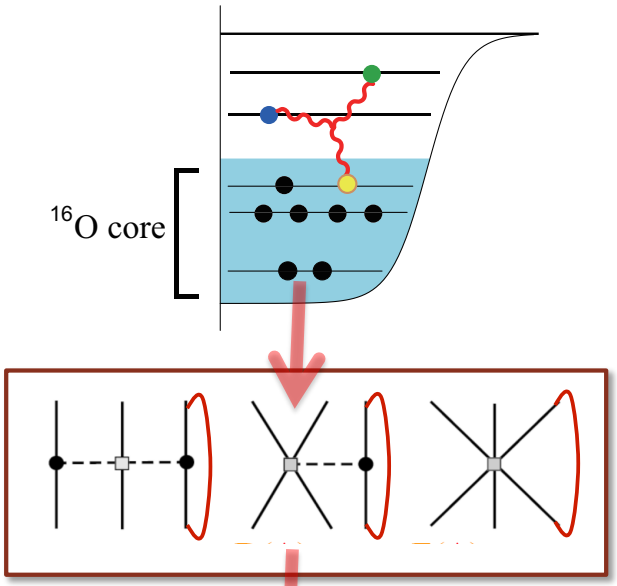


Chiral 3NFs meet the shell model [from J. Holt]

3N Forces for Valence-Shell Theories

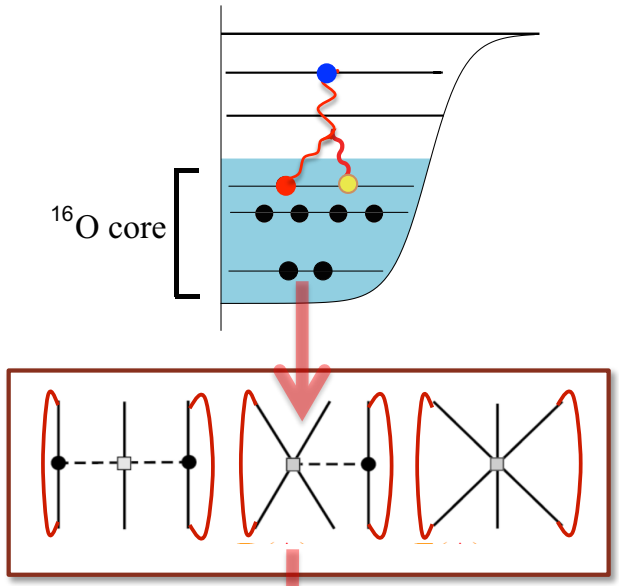
Normal-ordered 3N: contribution to valence neutron interactions

Effective two-body



$$\langle ab|\, V_{3N,\mathrm{eff}}\,|a'b'\rangle = \sum_{\alpha=core}\langle \alpha ab|\, V_{3N}\,|\alpha a'b'\rangle$$

Effective one-body



$$\langle a|\, V_{3N,\mathrm{eff}}\,|a'\rangle = \frac{1}{2}\sum_{\alpha\beta=core}\langle \alpha\beta a|\, V_{3N}\,|\alpha\beta a'\rangle$$

Combine with microscopic NN: eliminate empirical adjustments

Chiral 3NFs meet the shell model [from J. Holt]

Drip Lines and Magic Numbers: 3N Forces in Medium-Mass Nuclei

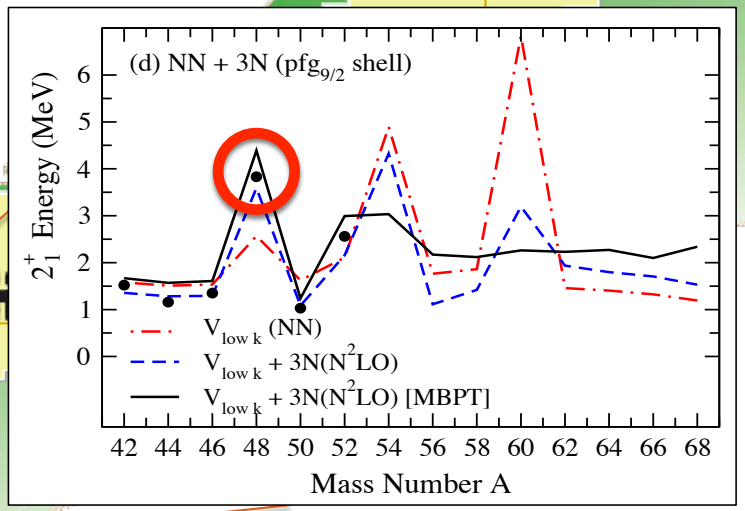
Important in light nuclei, nuclear matter…

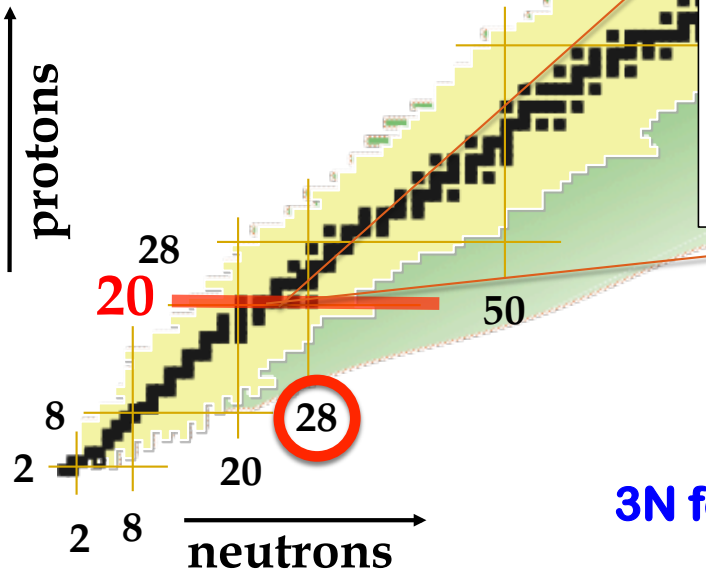
What are the limits of nuclear existence?

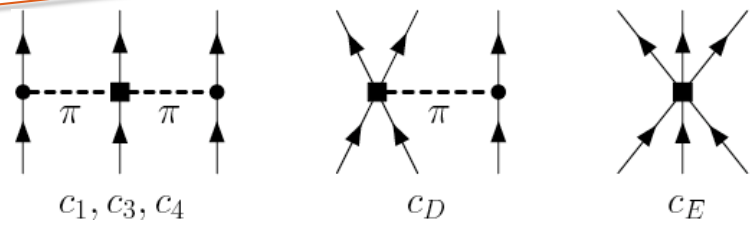
How do magic numbers form and evolve?

N=28 magic number in calcium

Holt, Otsuka, Schwek, Suzuki, arXiv:1009.5984

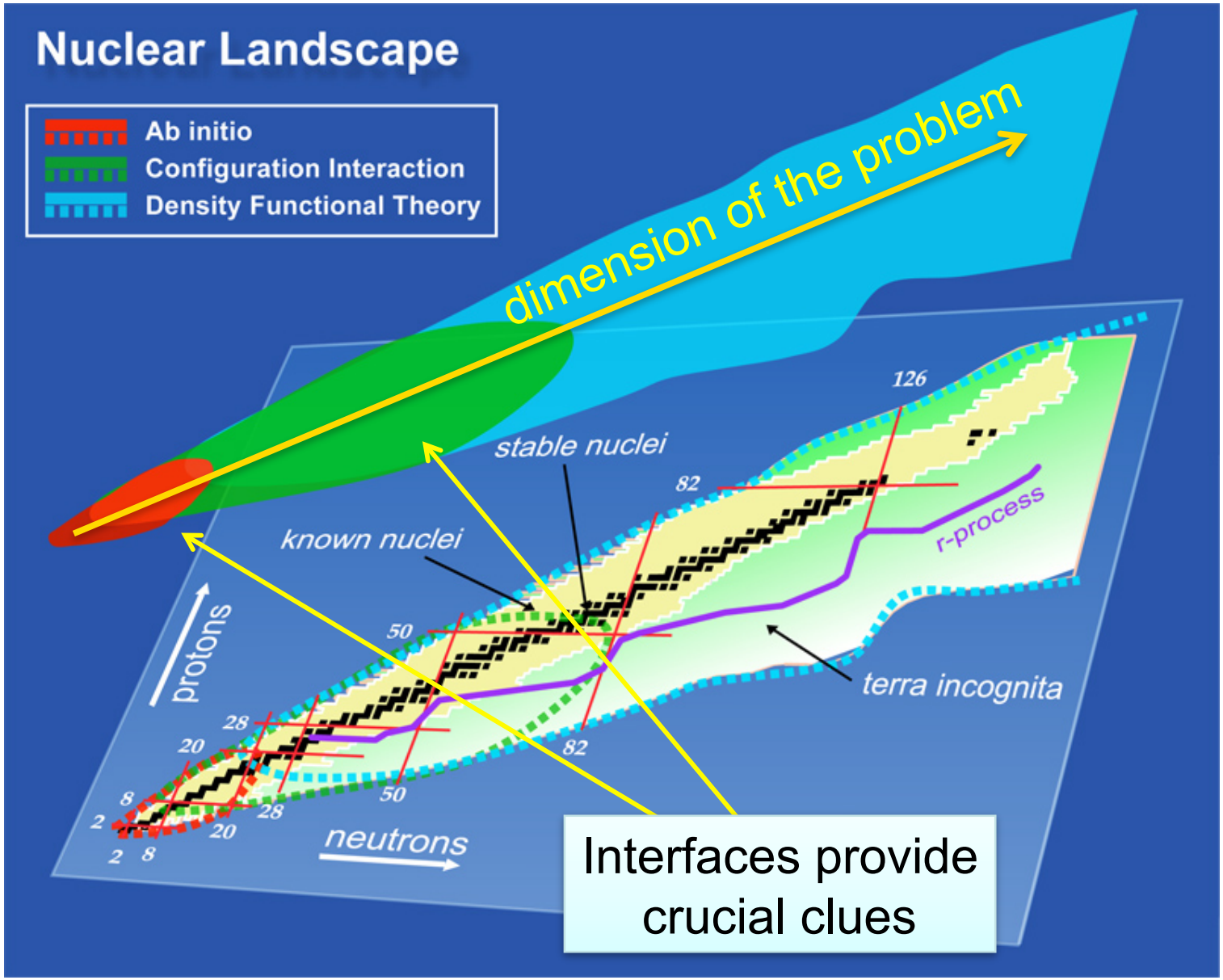






3N forces essential for medium mass nuclei

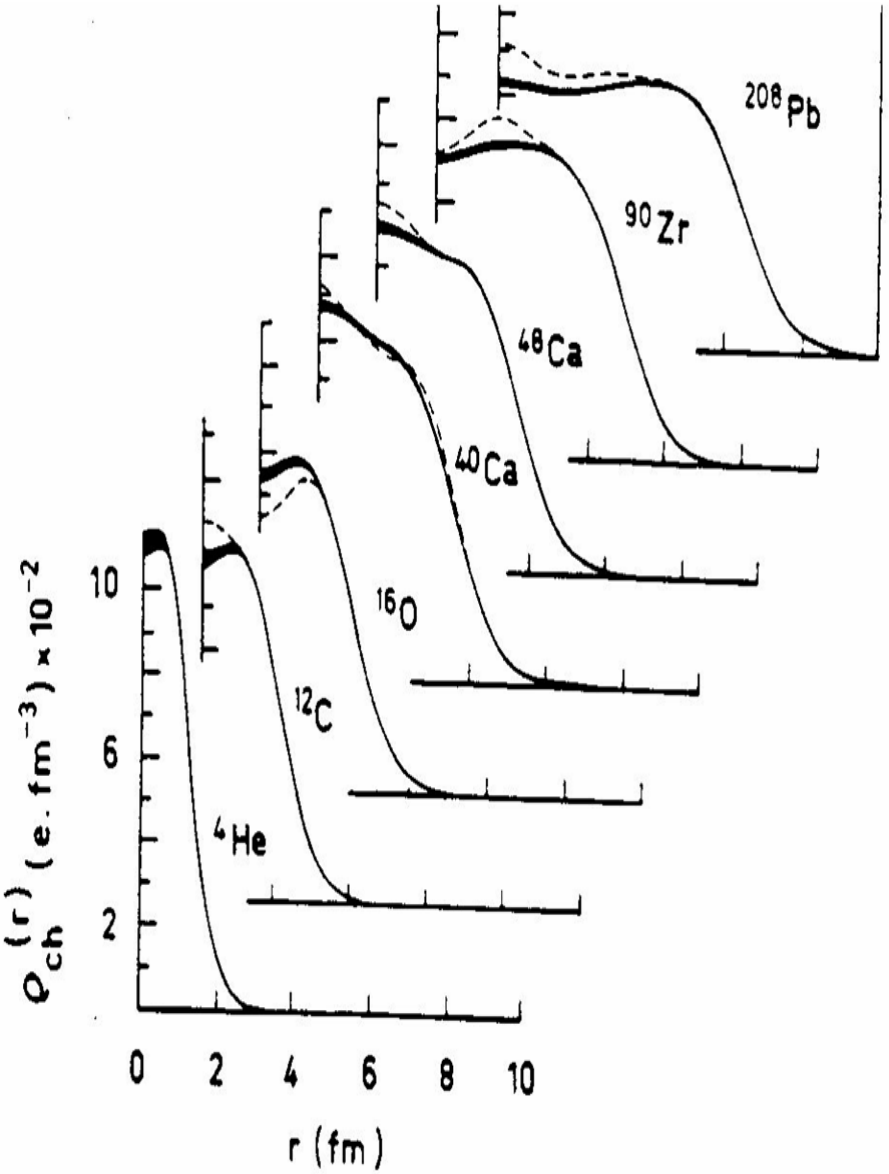
Overlapping theory methods cover all nuclei



What do (ordinary) nuclei look like?

- Charge densities of magic nuclei (mostly) shown
- Proton density has to be "unfolded" from $\rho_{\text{charge}}(r)$, which comes from elastic electron scattering
- Roughly constant interior density with $R \approx (1.1\text{–}1.2\,\text{fm}) \cdot A^{1/3}$
- Roughly constant surface thickness

$\Longrightarrow$ Like a liquid drop!



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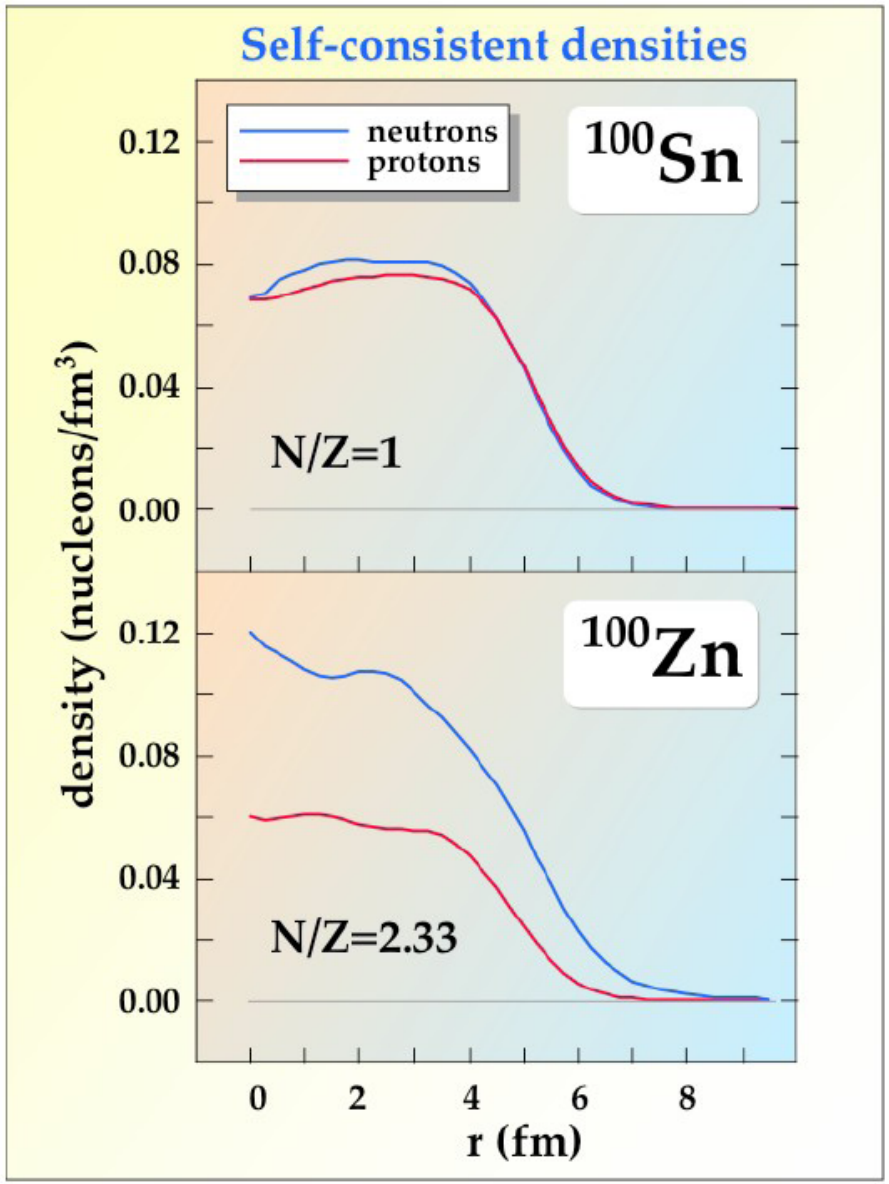
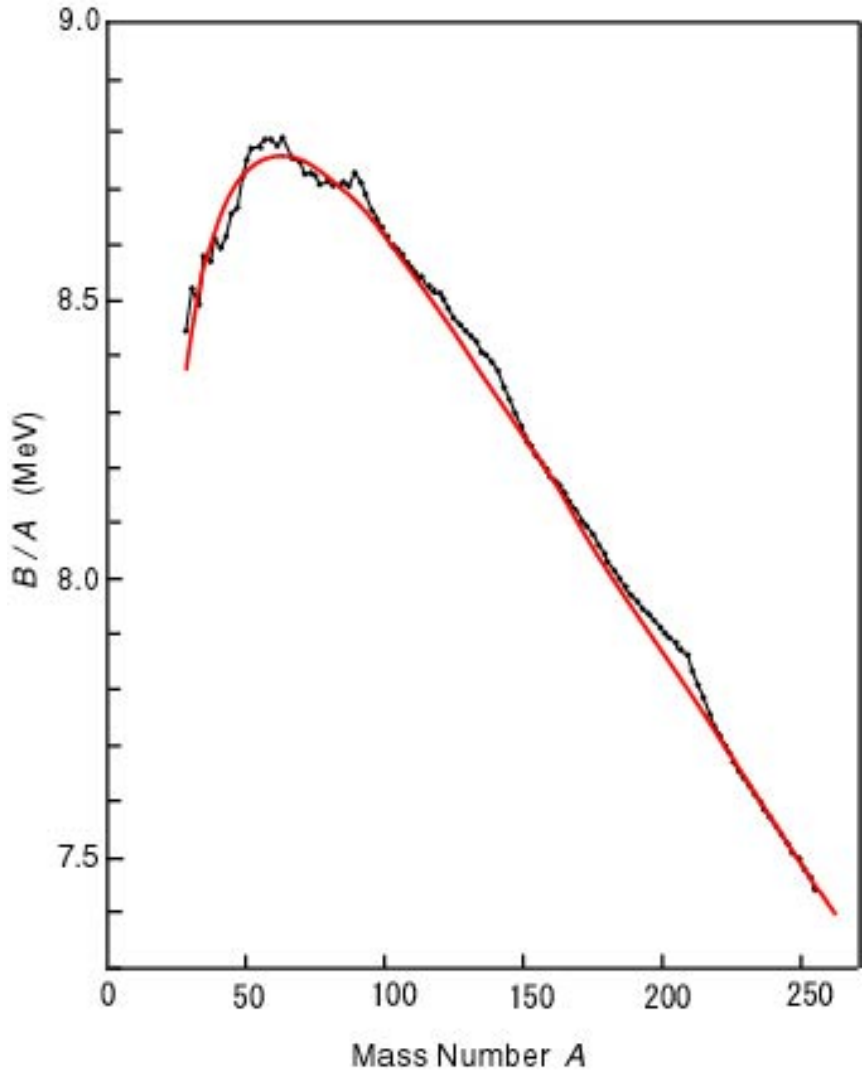


Semi-empirical mass formula ($A = N + Z$)

$$E_B(N,Z) = a_v A - a_s A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_{\rm sym} \frac{(N-Z)^2}{A} + \Delta$$

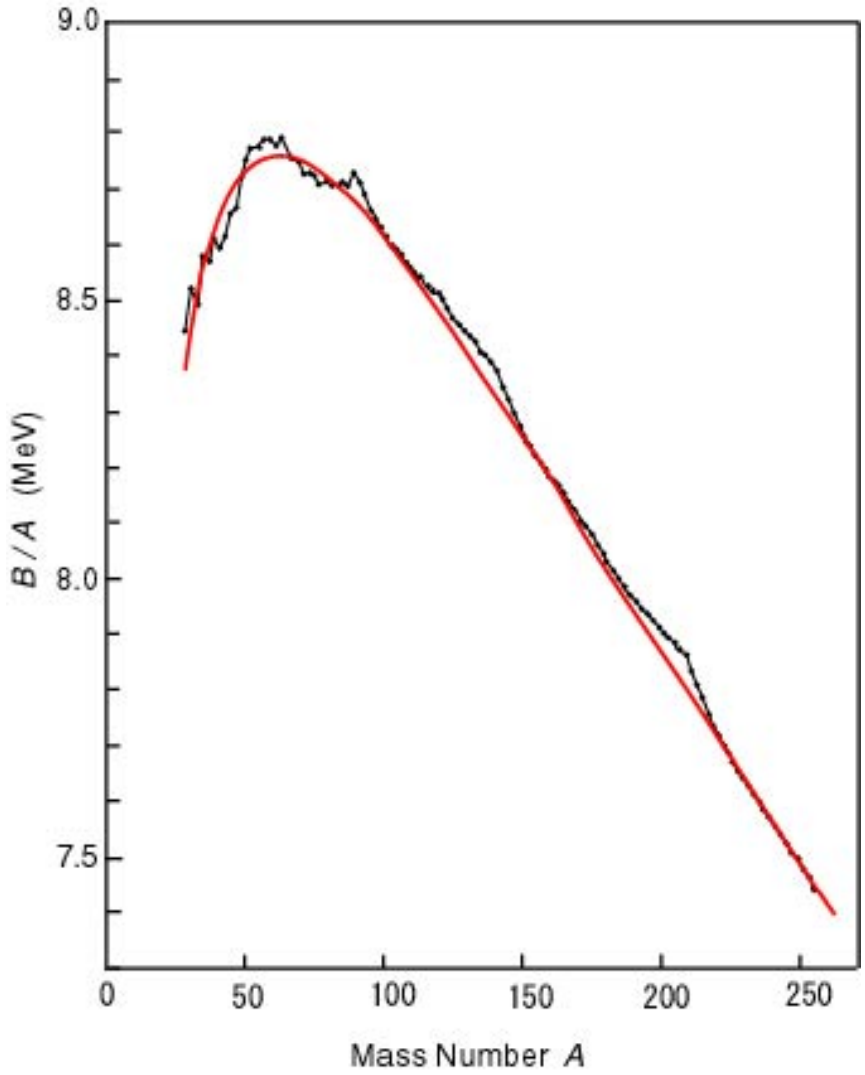
- Many predictions!
- Rough numbers: $a_v \approx 16\,\text{MeV}$, $a_s \approx 18\,\text{MeV}$, $a_C \approx 0.7\,\text{MeV}$, $a_{\rm sym} \approx 28\,\text{MeV}$
- Pairing $\Delta \approx \pm 12/\sqrt{A}\,\text{MeV}$ (even-even/odd-odd) or 0 [or $43/A^{3/4}$ MeV or . . .]
- Surface symmetry energy: $a_{\rm surf\ sym}(N-Z)^2/A^{4/3}$
- Much more sophisticated mass formulas include shell effects, etc.



Semi-empirical mass formula per nucleon

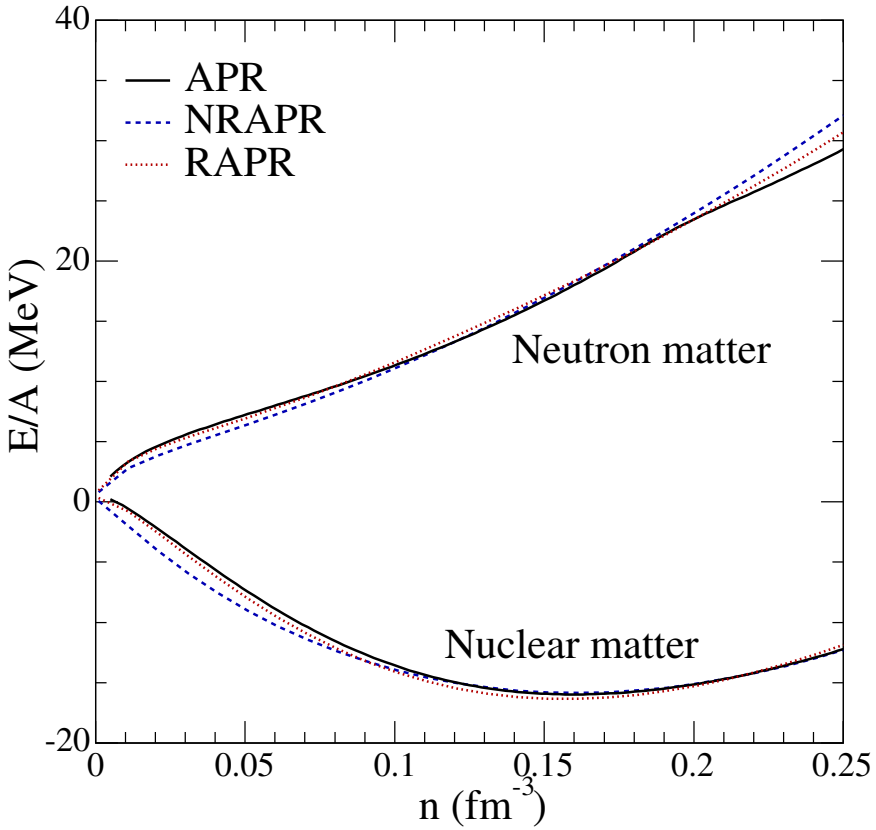
$$\frac{E_B(N,Z)}{A} = a_v - a_s A^{-1/3} - a_C \frac{Z^2}{A^{4/3}} - a_{\rm sym} \frac{(N-Z)^2}{A^2}$$

- Divide terms by $A = N + Z$
- Rough numbers:
  $a_v \approx 16\,\text{MeV}$, $a_s \approx 18\,\text{MeV}$,
  $a_C \approx 0.7\,\text{MeV}$, $a_{\rm sym} \approx 28\,\text{MeV}$
- Surface symmetry energy:
  $a_{\rm surf\ sym}(N-Z)^2/A^{7/3}$
- Now take $A \to \infty$ with Coulomb $\to 0$ and fixed N/A, Z/A
- Surface terms negligible



Nuclear and neutron matter energy vs. density

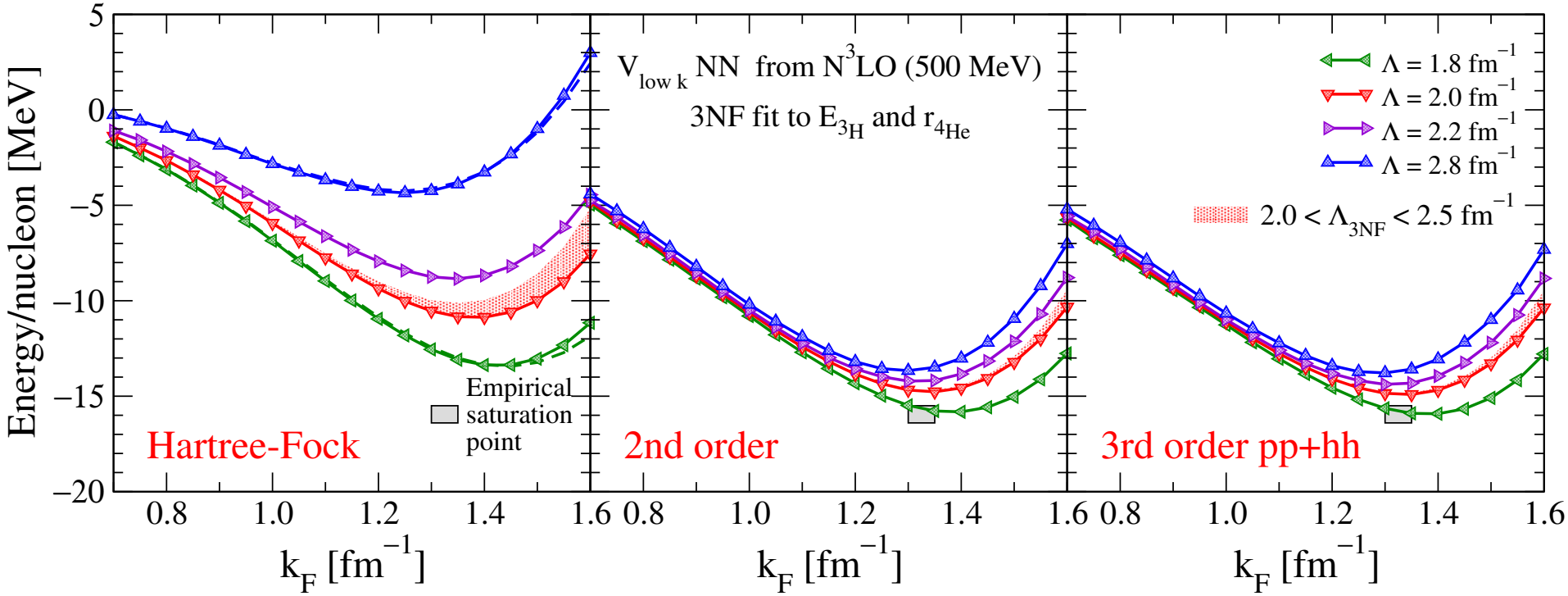
[Akmal et al. calculations shown]



- Uniform with Coulomb turned off
- Density n (or often ρ)
- Fermi momentum $n = (\nu/6\pi^2)k_{\rm F}^3$
- Neutron matter ($Z = 0$) has positive pressure
- Symmetric nuclear matter ($N = Z = A/2$) saturates
- *Empirical* saturation at about $E/A \approx -16\,\text{MeV}$ and $n \approx 0.17 \pm 0.03\,\text{fm}^{-3}$

Low resolution calculations of nuclear matter

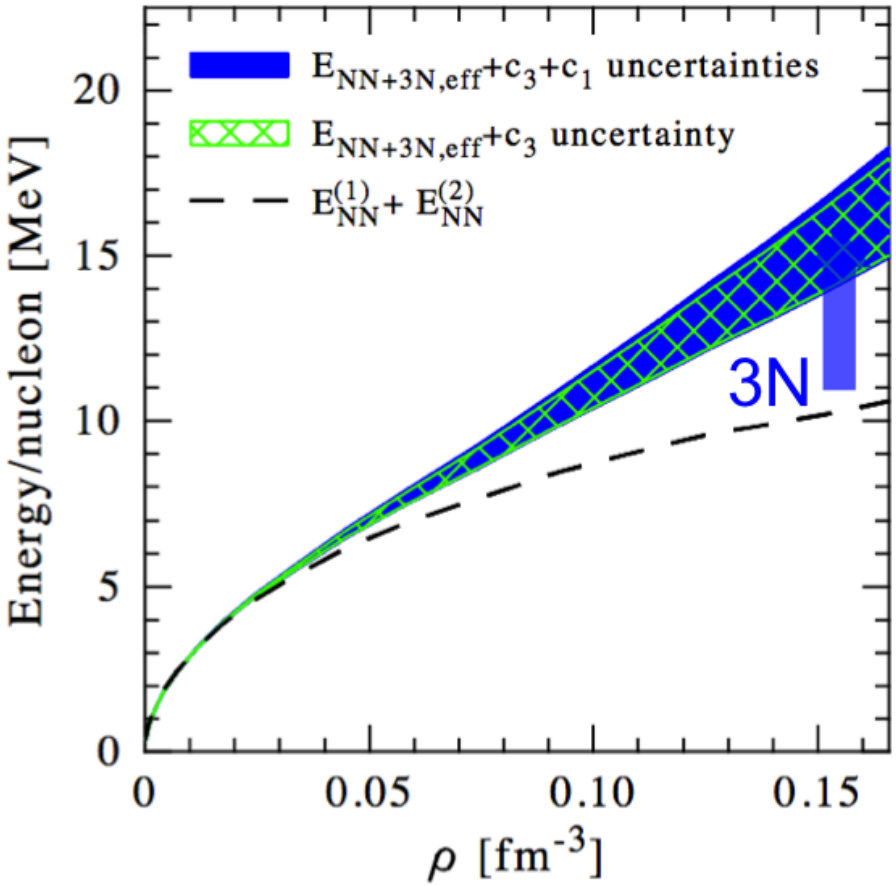
- Evolve NN by RG to low momentum, fit NNN to $A = 3, 4$
- Predict nuclear matter in MBPT [Hebeler et al. (2011)]

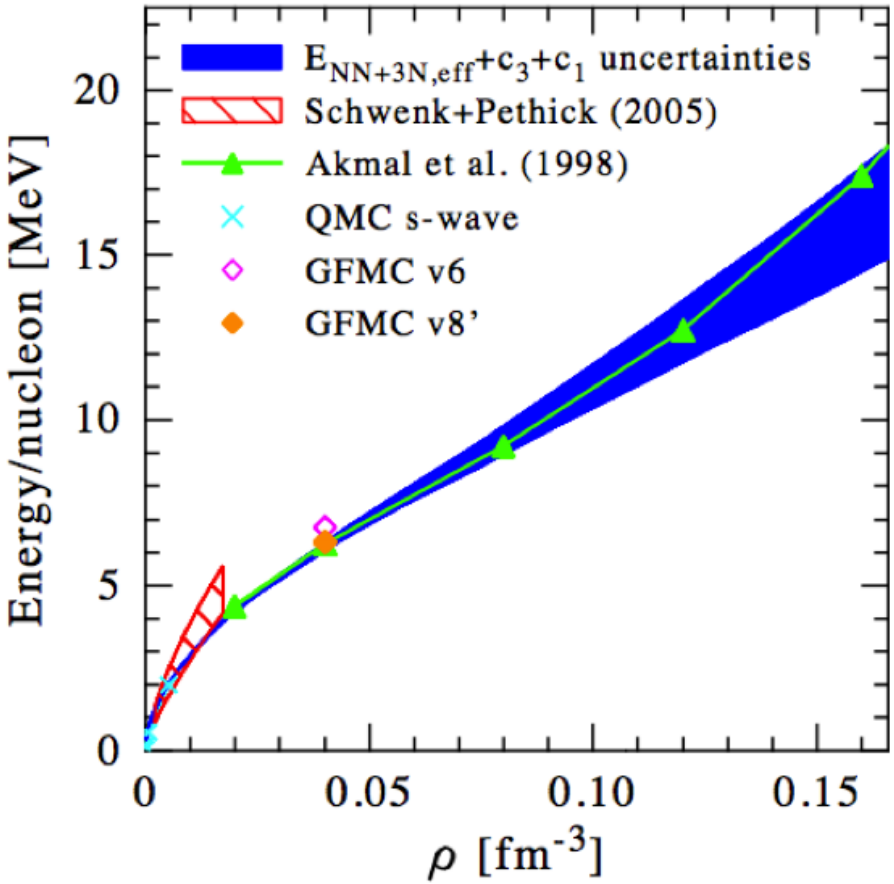


- Cutoff dependence at 2nd order significantly reduced
- 3rd order contributions are small
- Remaining cutoff dependence: many-body corrections, 4NF?

Low resolution calculations of neutron matter

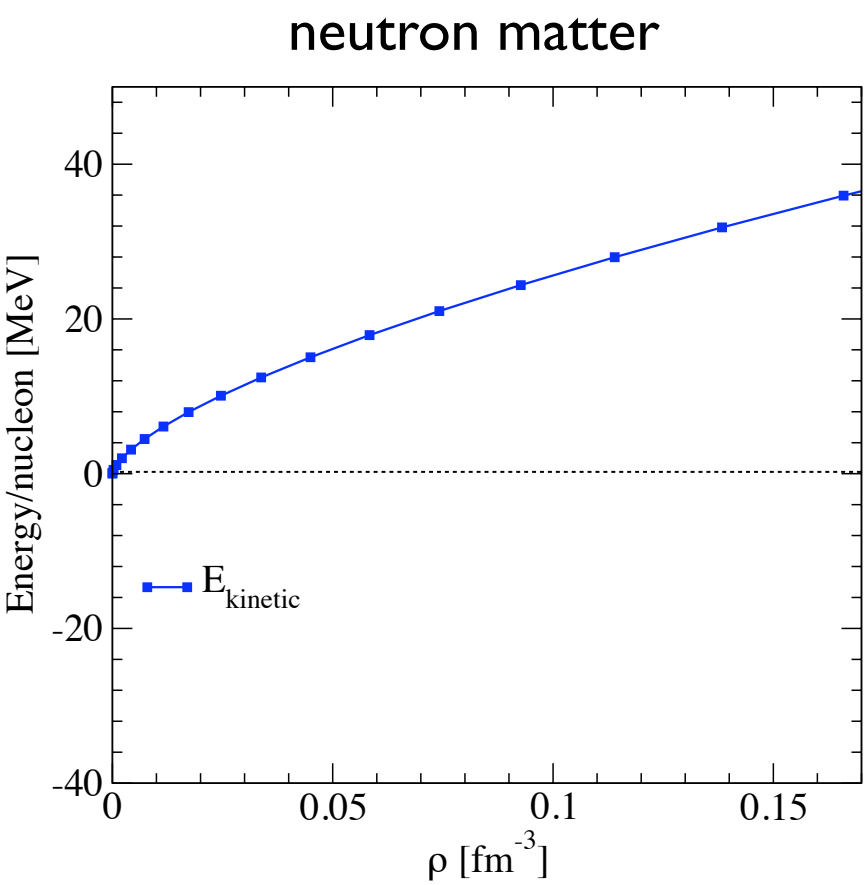
- Evolve NN to low momentum, fit NNN to $A = 3, 4$
- Neutron matter in perturbation theory [Hebeler, Schwenk (2010)]

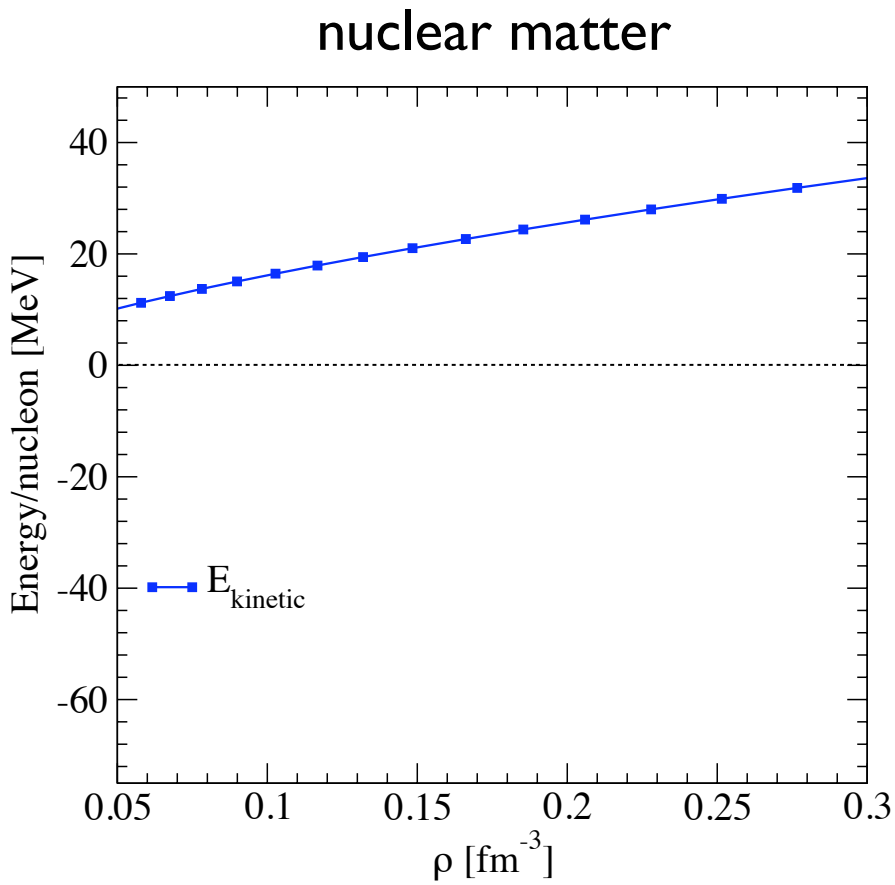




- Use cutoff dependence to estimate many-body uncertainty
- Uncertainties from long-range NNN constants are greatest

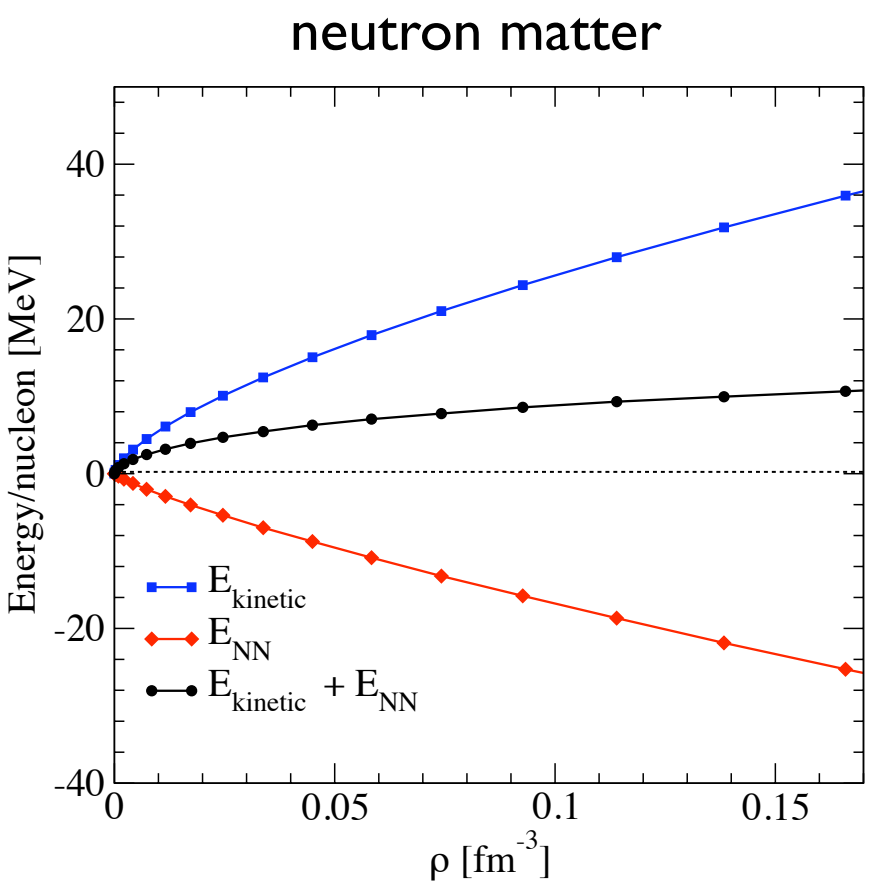
Hierarchy of contributions to infinite matter

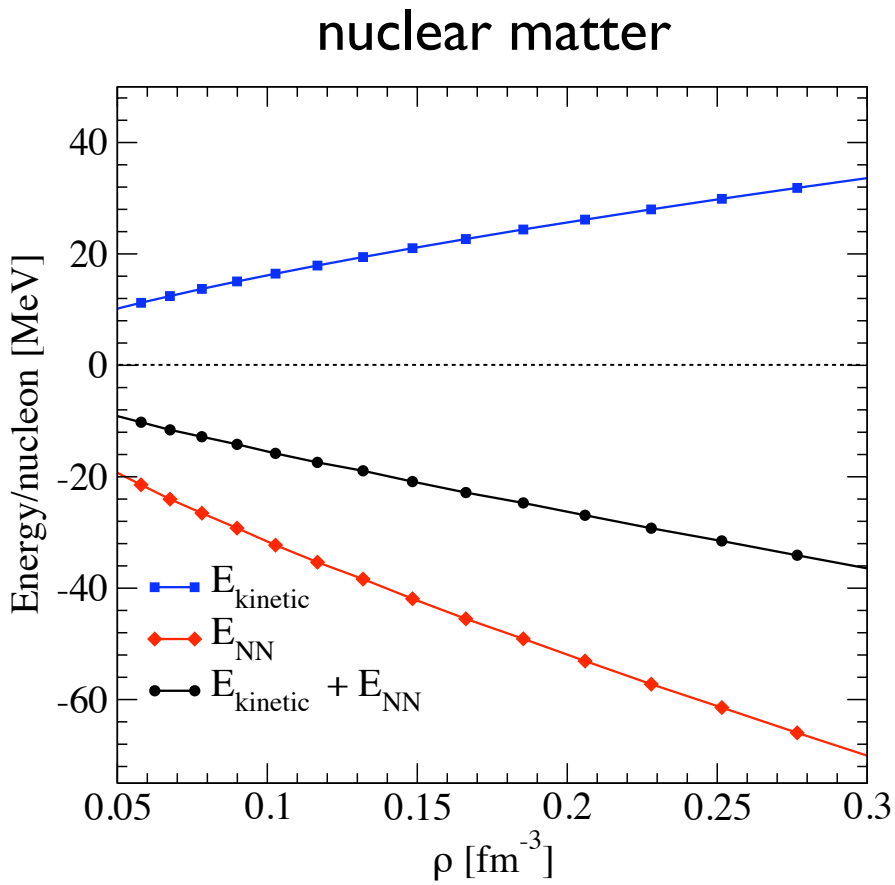




- Large cancellation of kinetic and potential energy
- Chiral hierarchy of 2NF and 3NF up to saturation density

Hierarchy of contributions to infinite matter





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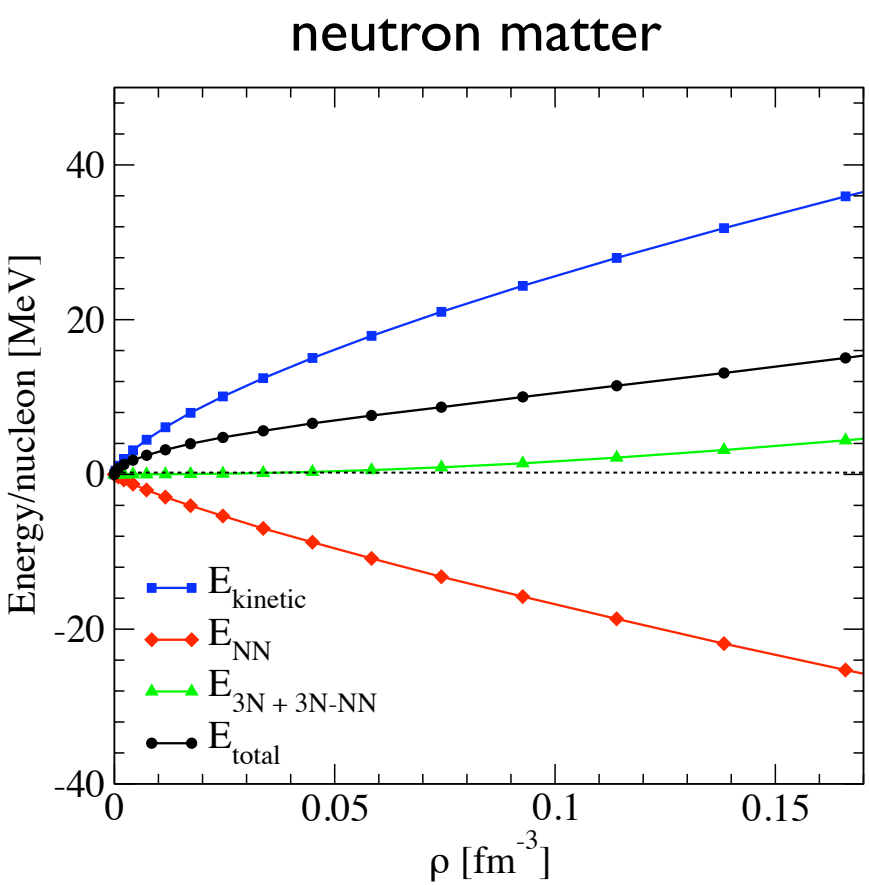

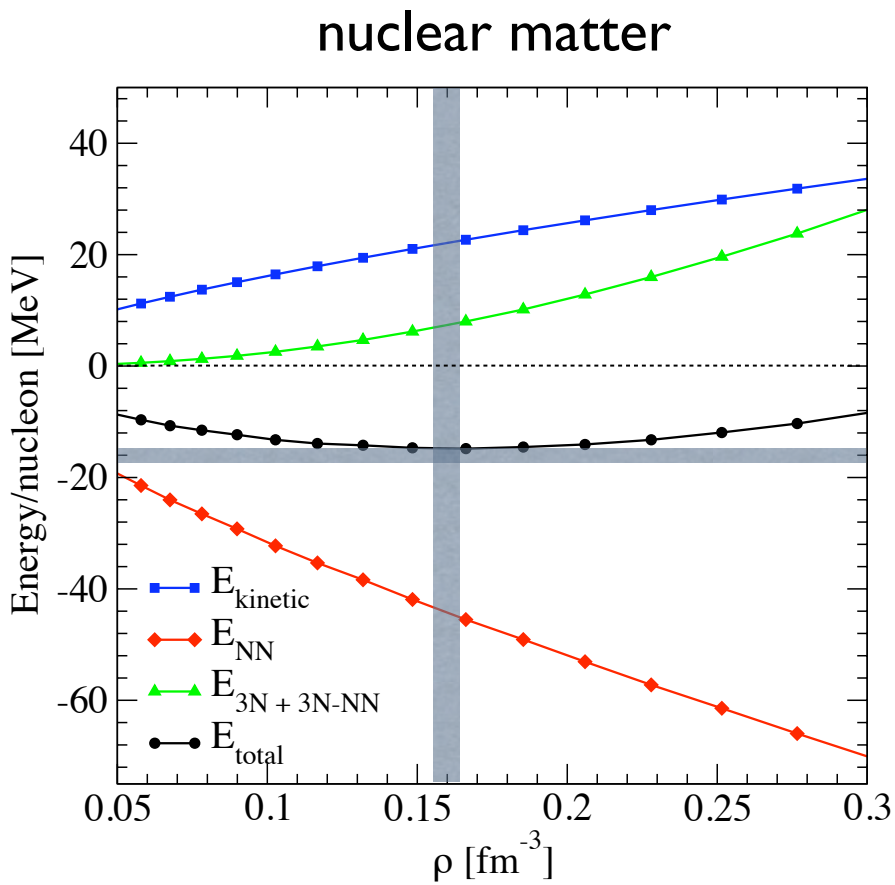

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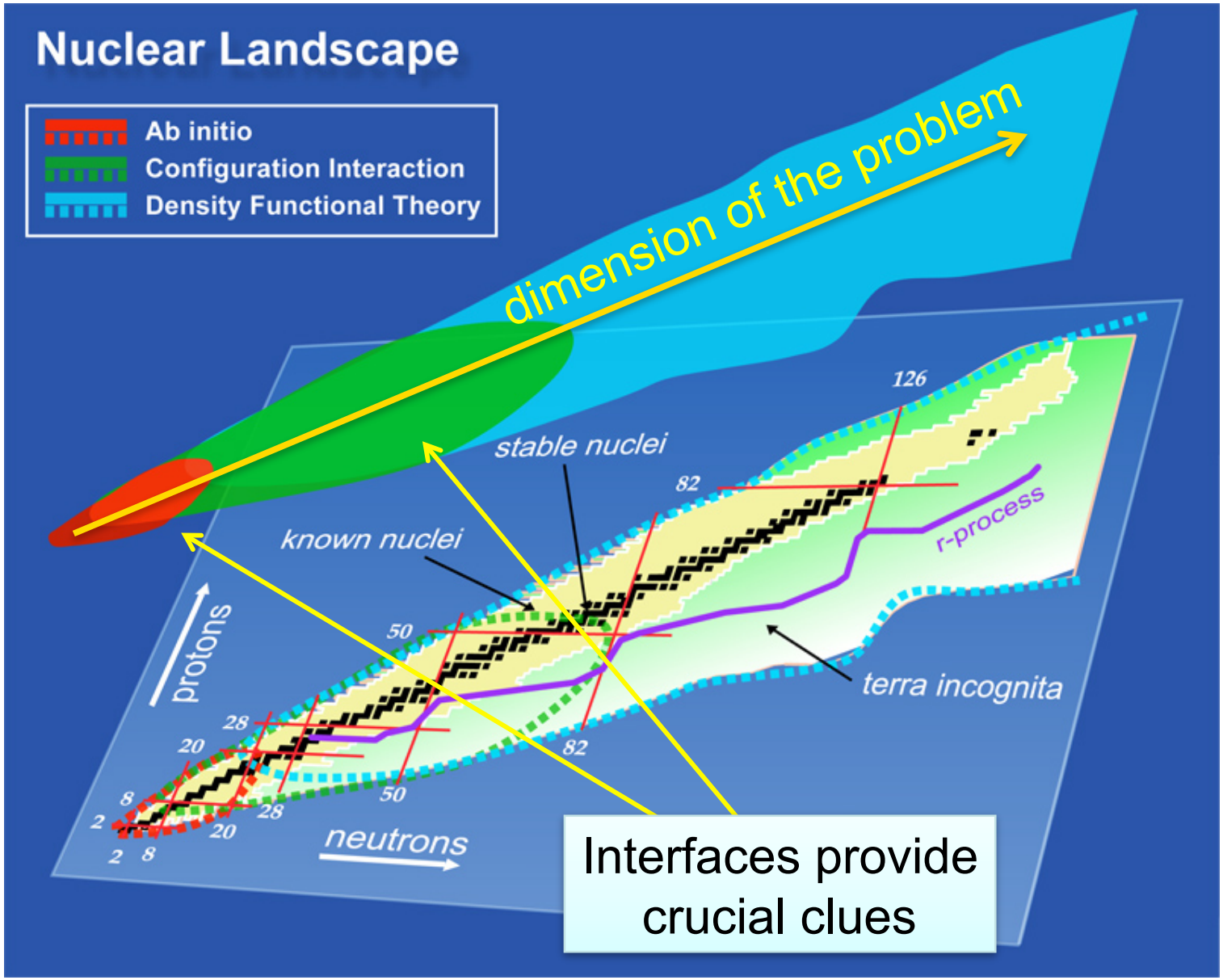
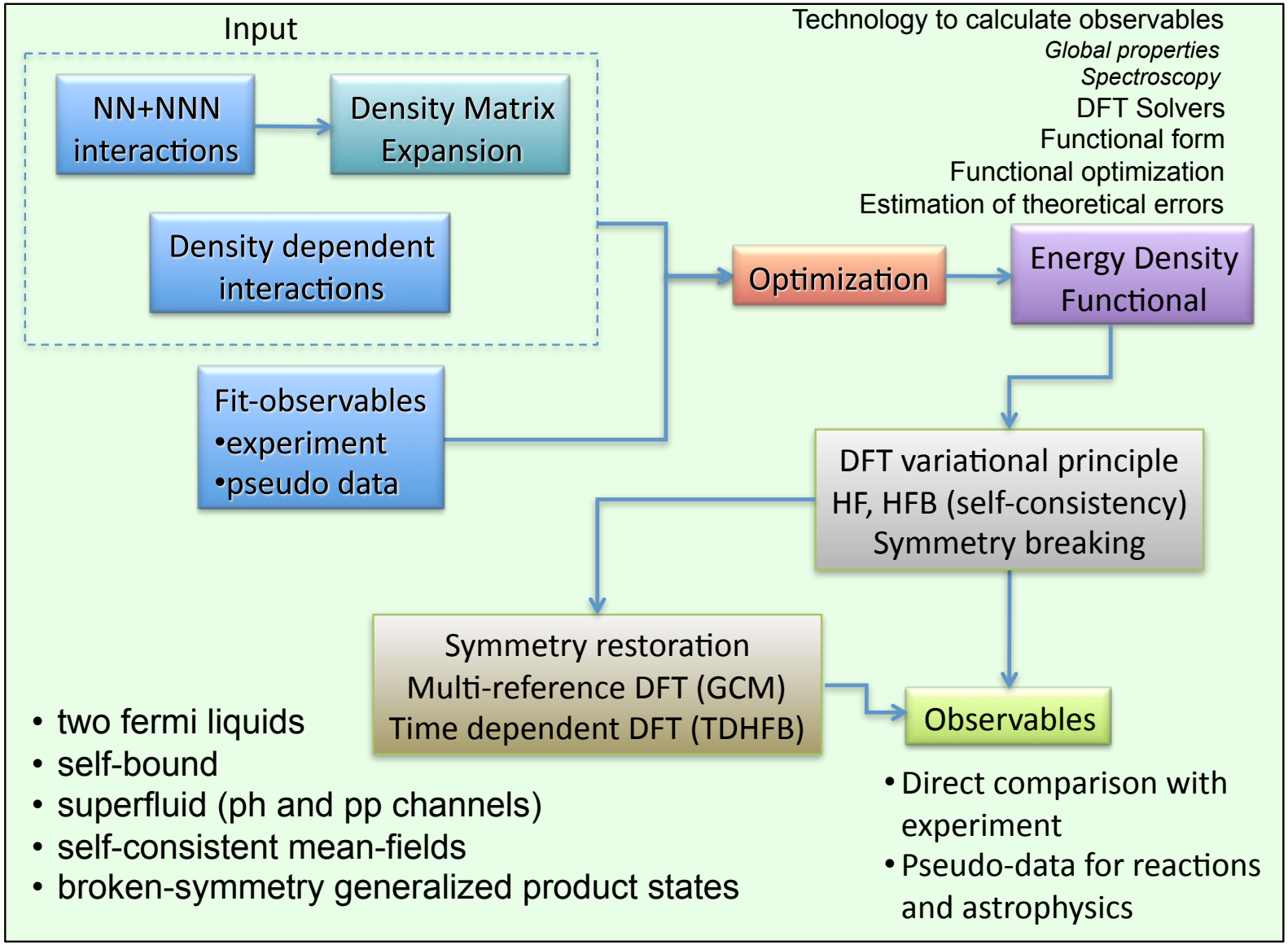
Overlapping theory methods cover all nuclei



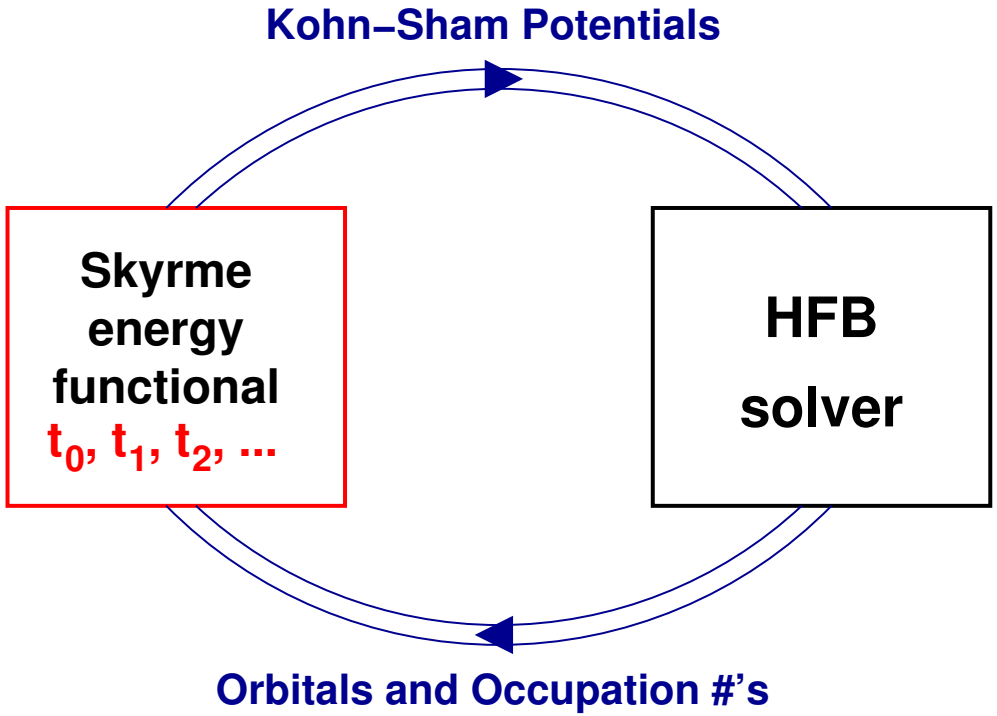
DFT for nuclei [UNEDF and NUCLEI projects]

Nuclear Density Functional Theory and Extensions



Skyrme EDF and beyond

$$\mathcal{E}_{Skyrme} = \frac{\tau}{2M} + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^{2+\alpha} + \frac{1}{16}(3t_1 + 5t_2)\rho\tau + \frac{1}{64}(9t_1 - 5t_2)|\nabla\rho|^2 + \cdots$$



- Kohn-Sham density functional theory $\Longrightarrow$ iterate to self-consistency
- Pairing is critical
- Improve functional with same iteration scheme

Schematic equations to solve self-consistently:

$$V_{\rm KS}(\mathbf{r}) = \frac{\delta E_{\rm int}[\rho]}{\delta\rho(\mathbf{r})} \iff [-\frac{\nabla^2}{2m} + V_{\rm KS}(\mathbf{x})]\psi_\alpha = \varepsilon_\alpha\psi_\alpha \implies \rho(\mathbf{x}) = \sum_\alpha n_\alpha|\psi_\alpha(\mathbf{x})|^2$$

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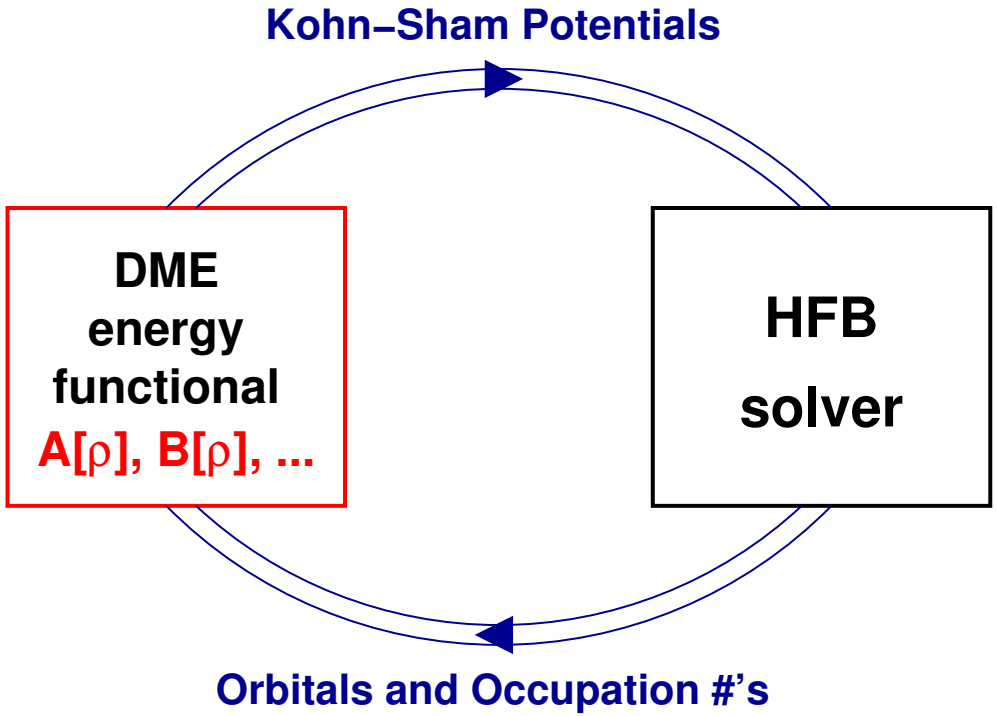

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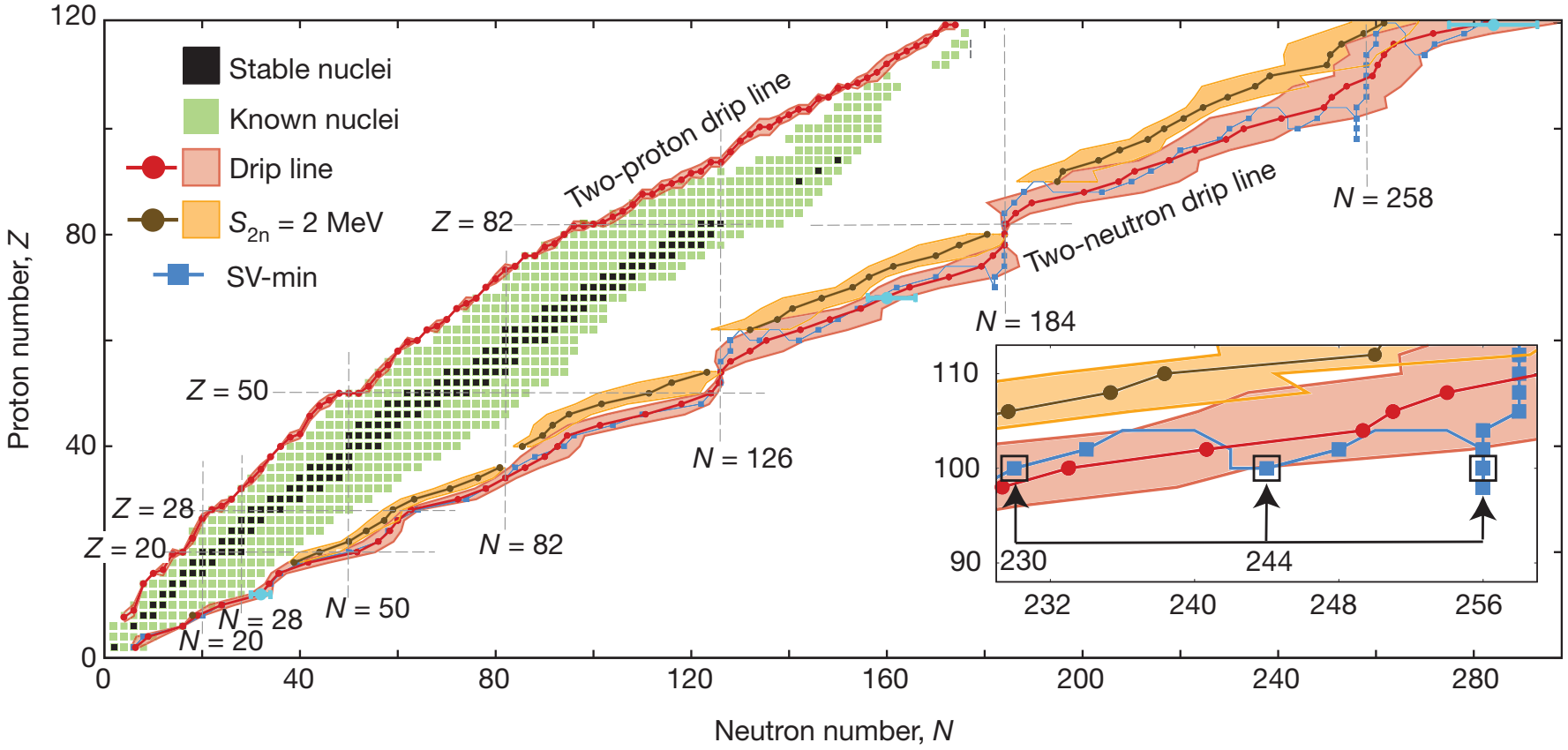
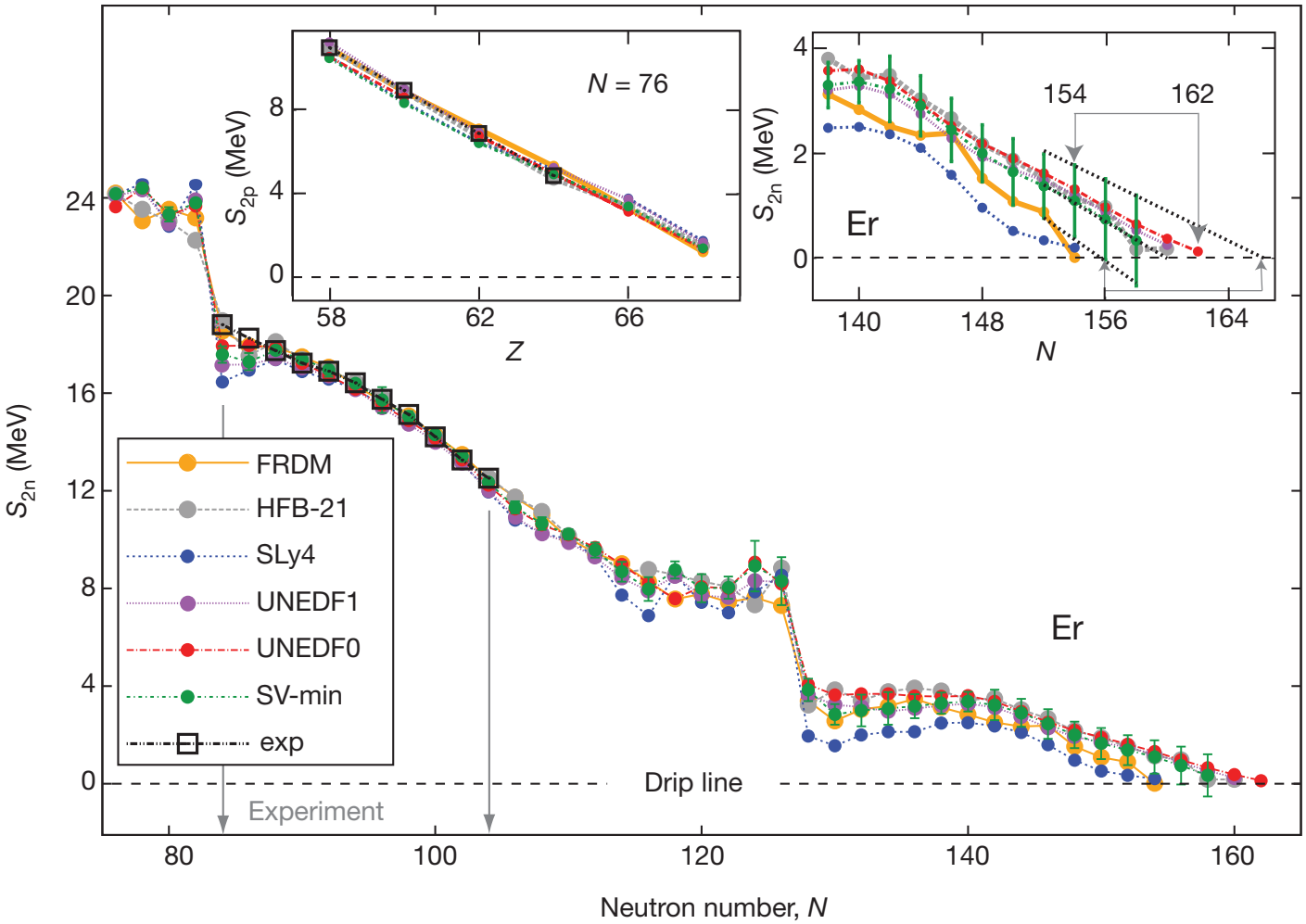
"The limits of the nuclear landscape"

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



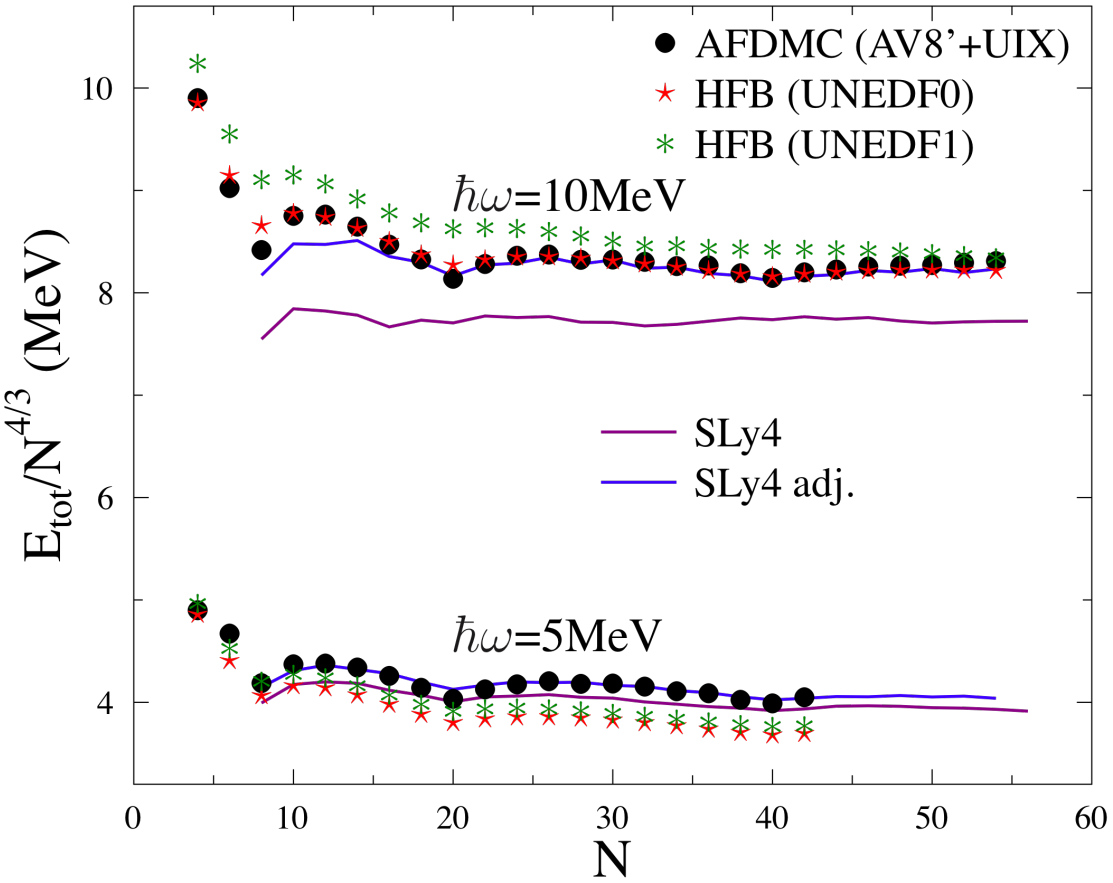
- Proton and neutron driplines predicted by Skyrme EDFs
  - Total: 6900 $\pm$ 500 nuclei with $Z \leq 120$ ($\approx$ 3000 known)
  - Estimate systematic errors by comparing models

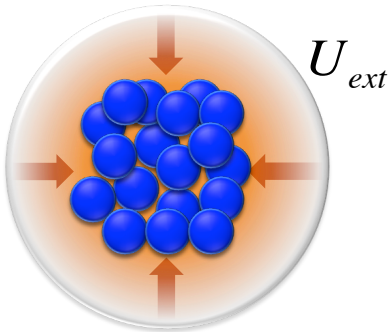
"The limits of the nuclear landscape"



- Two-neutron separation energies of even-even erbium isotopes
  - Compare different functionals, with uncertainties of fits
  - Dependence on neutron excess poorly determined (cf. driplines)

UNEDF Project: Use *ab initio* pseudo-data





- Put neutrons in a harmonic oscillator trap with $\hbar\omega$ (cf. cold atoms!)
- Calculate exact result with AFDMC [S. Gandolfi, J. Carlson, and S.C. Pieper, Phys. Rev. Lett. 106, 012501 (2011)] (or with other methods)
- UNEDF0 and UNEDF1 functionals improve over Skyrme SLy4!

Interaction with applied math experts

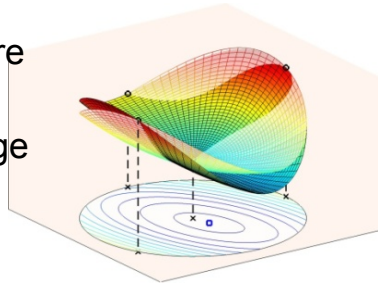
Optimization Algorithms for Calibrating Extreme Scale Simulations

Typical Challenges

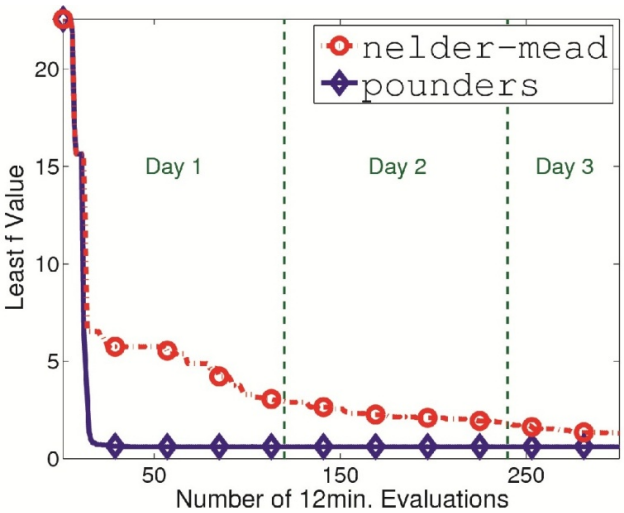
- Computational expense of simulation only allows for evaluating a few sets of parameter values
- Derivatives with respect to parameters can be unavailable or intractable to compute/approximate
- Experimental data incomplete or inaccurate
- Sensitivity analysis/confidence regions desired

New Algorithm POUNDERS

- Exploits mathematical structure in calibration problems
- Benefits from expert knowledge
  - data, weights, uncertainties, etc.
- Obtains good fits in minimal number of simulations



POUNDERS obtains better solutions faster



Energy density functionals (EDFs) for UNEDF

- Enables fitting of complex, state-of-the-art EDFs
  - Optimization previously avoided because too many evaluations required to obtain desirable features
- Substantial computational savings over alternatives
- Using resulting EDF parameterizations, the entire nuclear mass table was computed and is now distributed at **www.massexplorer.org**
  - *Nuclear Energy Density Optimization. Kortelainen et al., Physical Review C **82**, 024313, 2010*
  - *Three joint physics & optimization publications @ SciDAC11!*

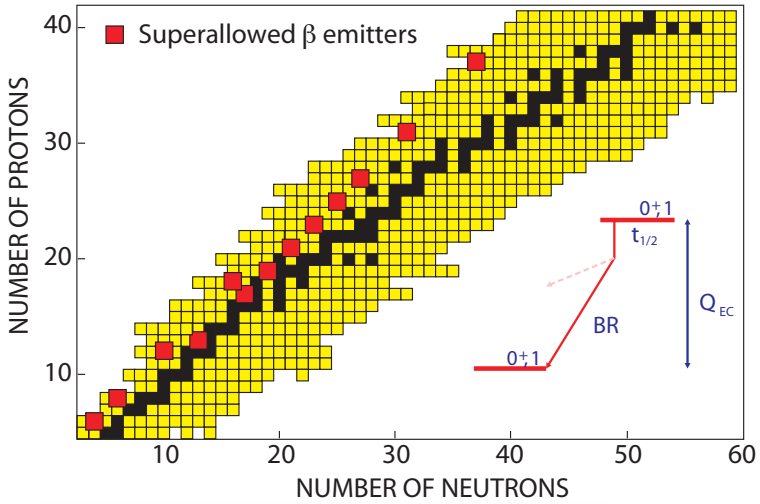
Application of DFT to beta decay

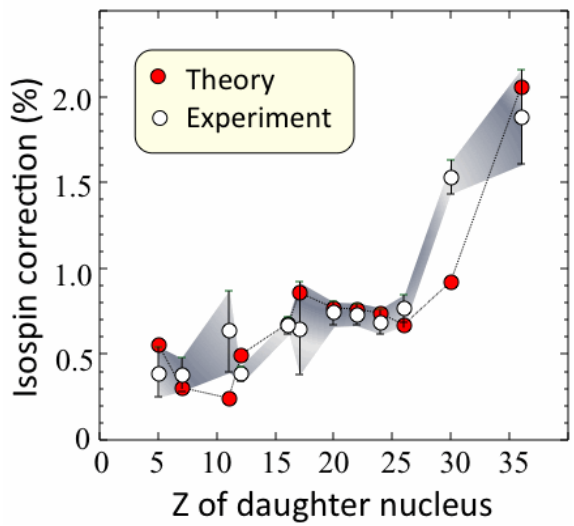
Microscopic calculations of isospin-breaking corrections to superallowed β-decay

W. Satuła et al.,Phys. Rev. Lett 106, 132502 (2011)

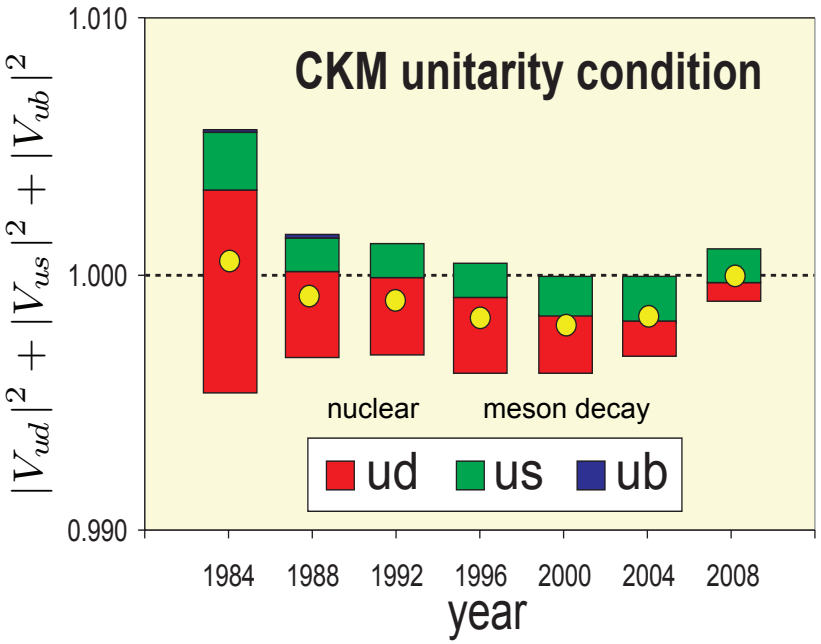
Superallowed Fermi $0^+ \rightarrow 0^+$ β-decay studies

Impressive experimental effort worldwide





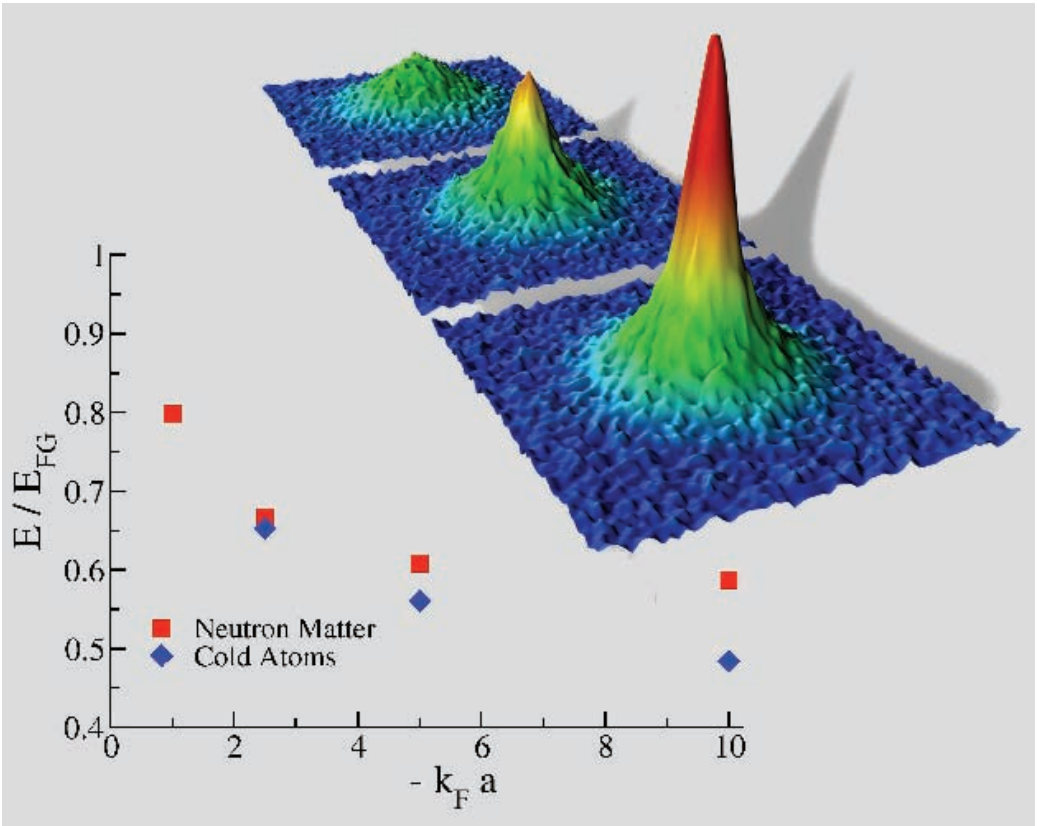
Kobayashi and Maskawa: … for "the discovery of the origin of broken symmetry, which predicts the existence of at least three families of quarks in nature."



Towner and Hardy 2010

$$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.9999(6)$$

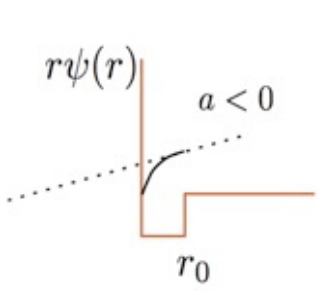
Neutron matter vs. cold atoms

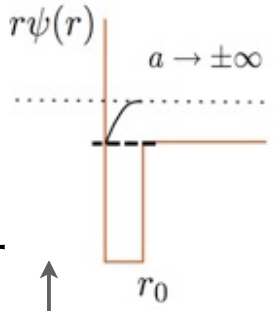


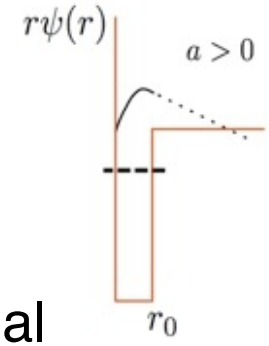
[Gezerlis/Carlson (2008)]

- Energy relative to free Fermi gas versus dimensionless $k_{\mathrm{F}}a$
- Physics overlap at low density because of large *nn* scattering length $a_{nn} \Longrightarrow$ universality
- Testbed for many-body methods!

Cold atoms: The BCS-BEC crossover [from J. Drut]







T

Normal

T_c

Normal

T_c

?

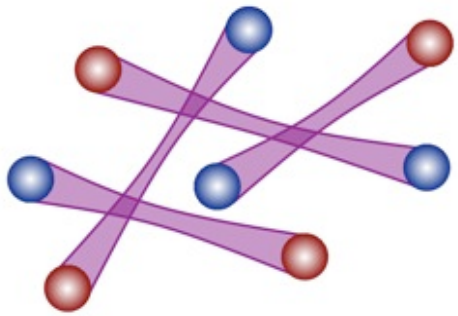
?

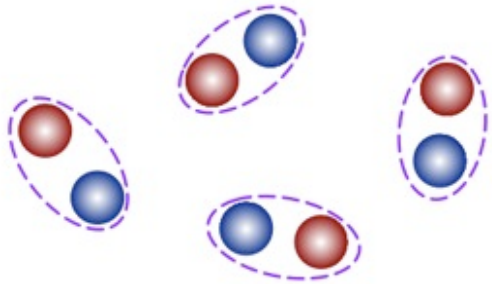
BCS
Superfluid

BEC
Superfluid

$1/k_F a$

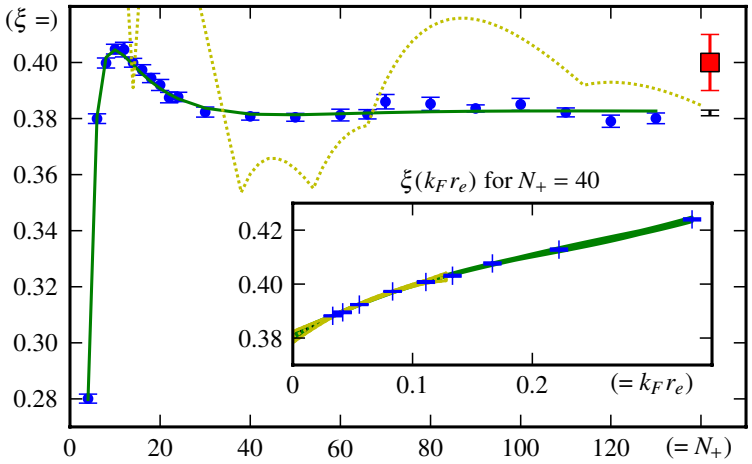
$1 \ll k_F|a|$
Unitary regime





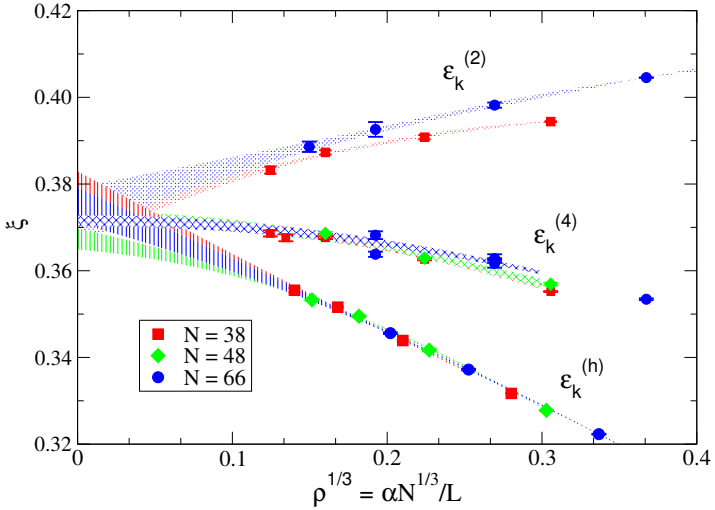
(Some) new results for cold atomic gases at unitarity

M. Forbes et al., PRL **106**, 235303 (2011)



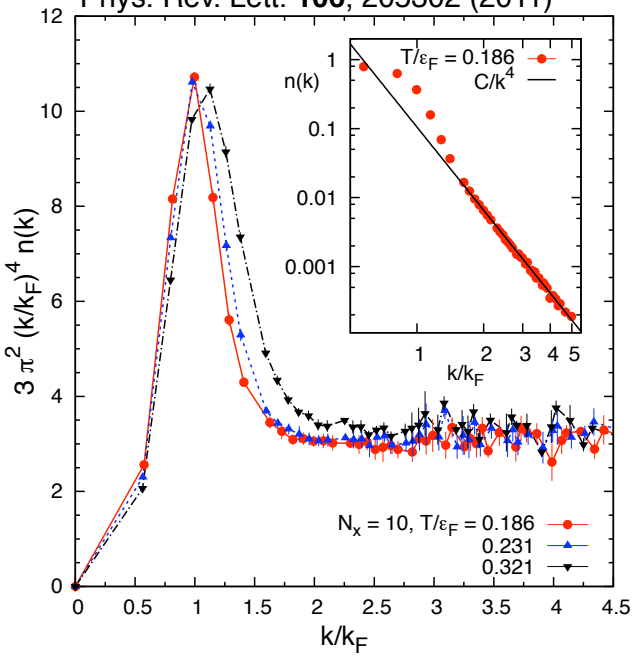
SLDA

J. Carlson et al., PRA **84**, 061602(R) (2011)



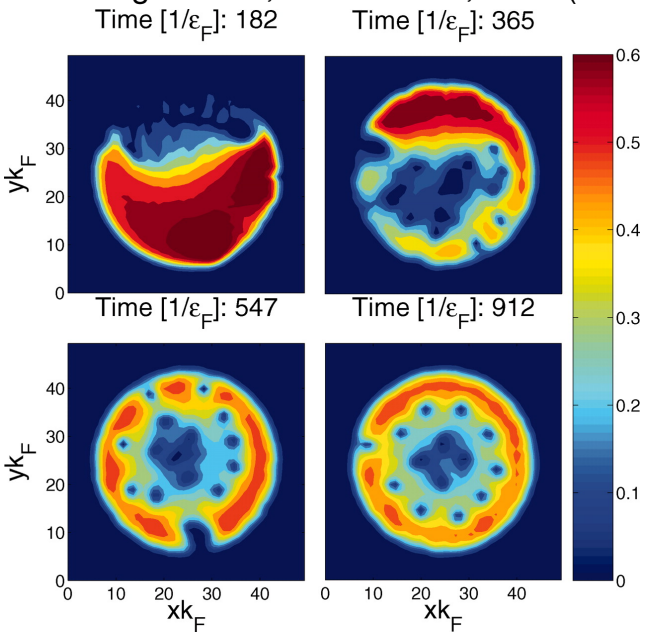
AFQMC

J. E. Drut, T. A. Lähde, T. Ten
Phys. Rev. Lett. **106**, 205302 (2011)



lattice QMC

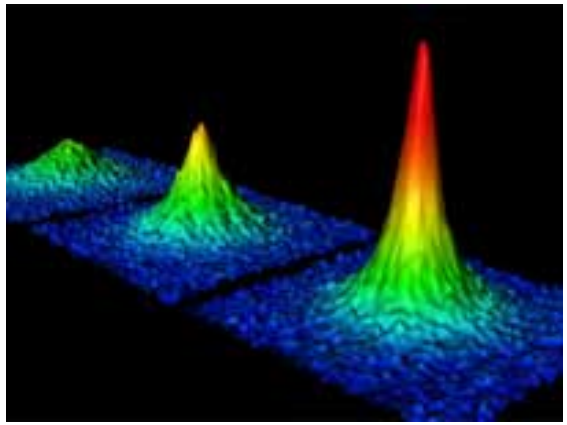
A. Bulgac et al., Science **332**, 1288 (2011)

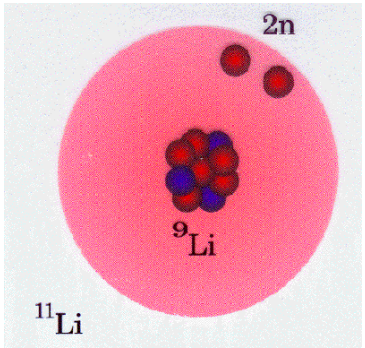


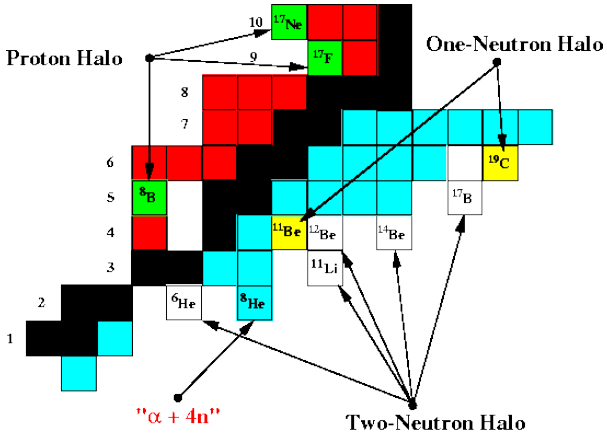
TD-DFT
TD-SLDA

Nuclei at *very* low resolution

- If separation of scales is sufficient, then EFT with pointlike interactions is efficient (e.g., $kR \ll 1$)
- Universal properties (large a_s)
  - connect to cold atom physics
  - low-density neutron matter
  - e.g., Efimov physics (3-body)
- Pionless EFT
  - e.g., $np \to d\gamma$ with $E_{\rm typ} \approx 0.02$–$0.2\,{\rm MeV}$
- Halo EFT
  - $B_{\rm valence} \ll B_{\rm core}, E_{ex}$
  - $n\alpha$-system (Bedaque et al.) or $\alpha\alpha$-system (Higa et al.) or ...







Outline

Low-energy nuclear theory is exploding with new stuff!

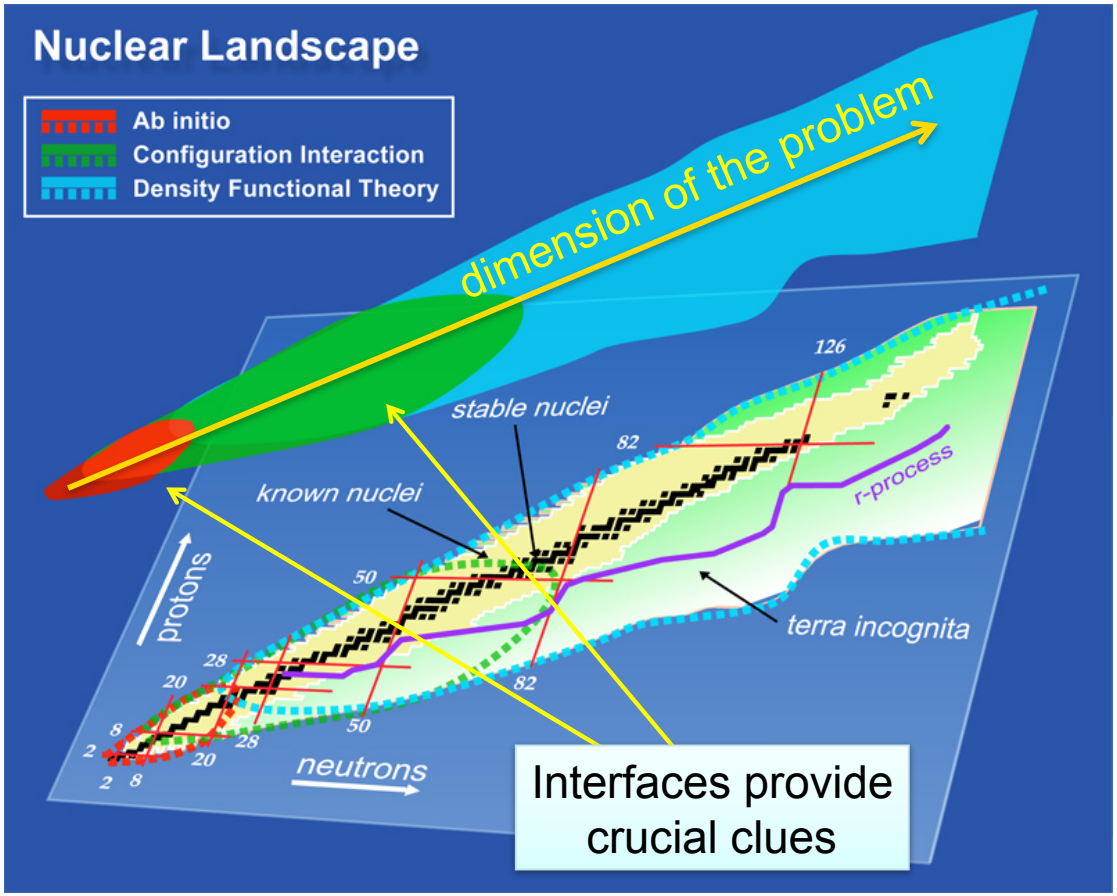
- New methods for theoretical inputs (Hamiltonians and operators)
  - Three-body (and higher) forces (N3LO chiral 3NF, RG methods)
- New extensions of established microscopic techniques
  - e.g., IT-NCSM, MBPT, Berggren basis, LIT
  - Spectroscopic factors, ANCs, . . . (e.g., with GFMC, CC)
- New microscopic many-body techniques
  - e.g., Lattice EFT, IM-SRG, NCSM/RGM
- New analysis methods/philosophy (theory error bars!!)
  - Correlation analysis of energy functionals
  - Power counting, benchmarking, . . .
- New computational reach (e.g., from SciDAC projects)
  - Better scaling: massively parallel codes, load balancing
  - Improved algorithms: e.g., optimization (POUNDERS)

Sermon: Doing good (low-energy) theory

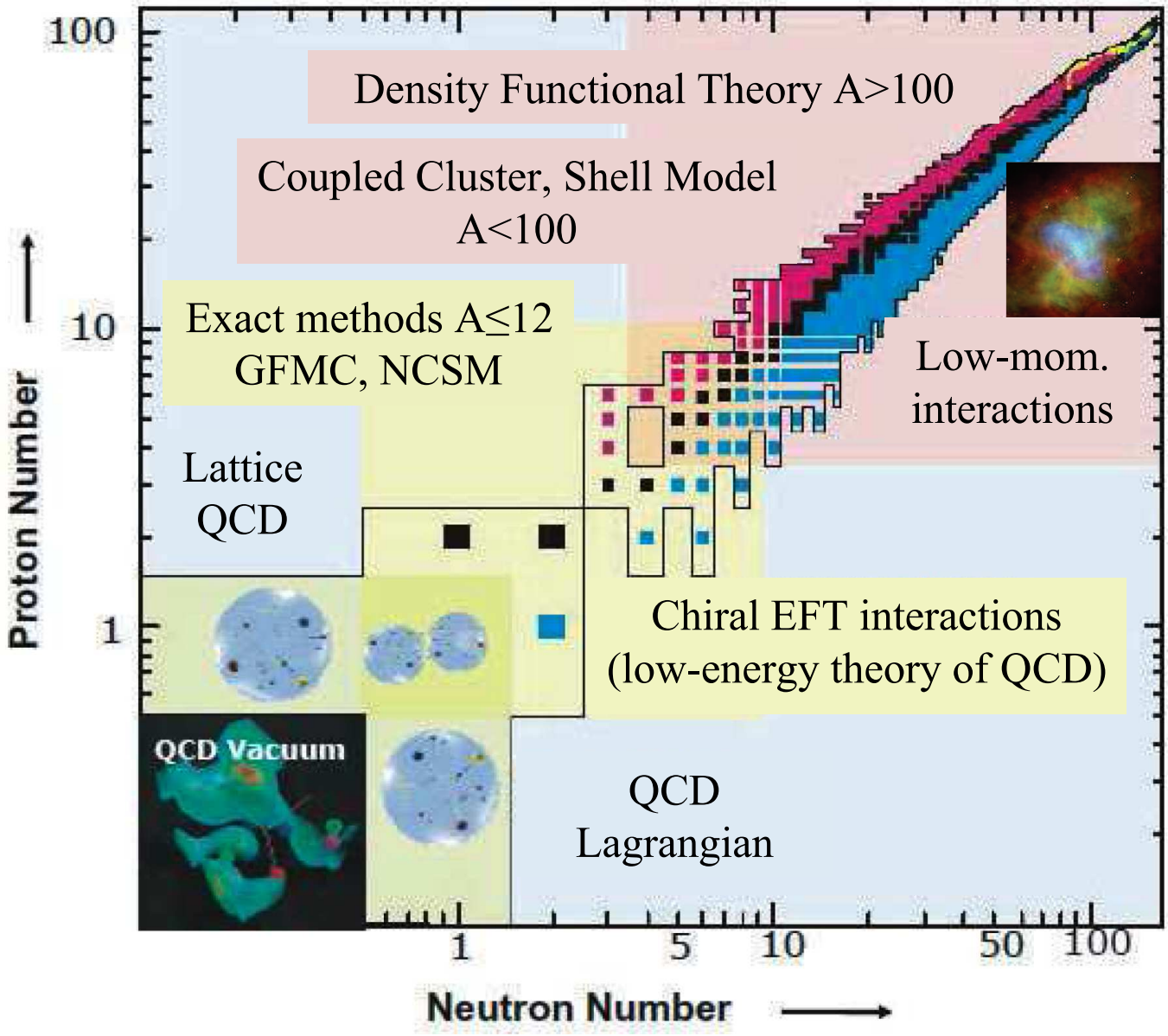
- Experiment must be the guide and the arbiter for theory
  - But be aware of scheme-dependent observables
  - "Just because it works, doesn't mean it's right!"
- Other maxims:
  - "Do the easy problems first!"
  - Weinberg's Three Laws of Progress in Theoretical Physics
    - Conservation of information: "You will get nowhere by churning equations." [context: RG apparently violates it!]
    - "Do not trust arguments based on the lowest order of perturbation theory."
    - "You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry."
- Find ways to validate your results (method, algorithm, physics, . . .)
  - e.g., multiple methods: benchmark!
  - e.g., use cold atom systems to test methods
- Strive for robust theory error bars (cf. model dependence)

Why do we need so many different methods?

- Each method has strengths and limitations
- Need to cross-check results
- Exploit overlapping domains
- Superior scaling vs. accuracy or more microscopic



Long-term gameplan: connected descriptions

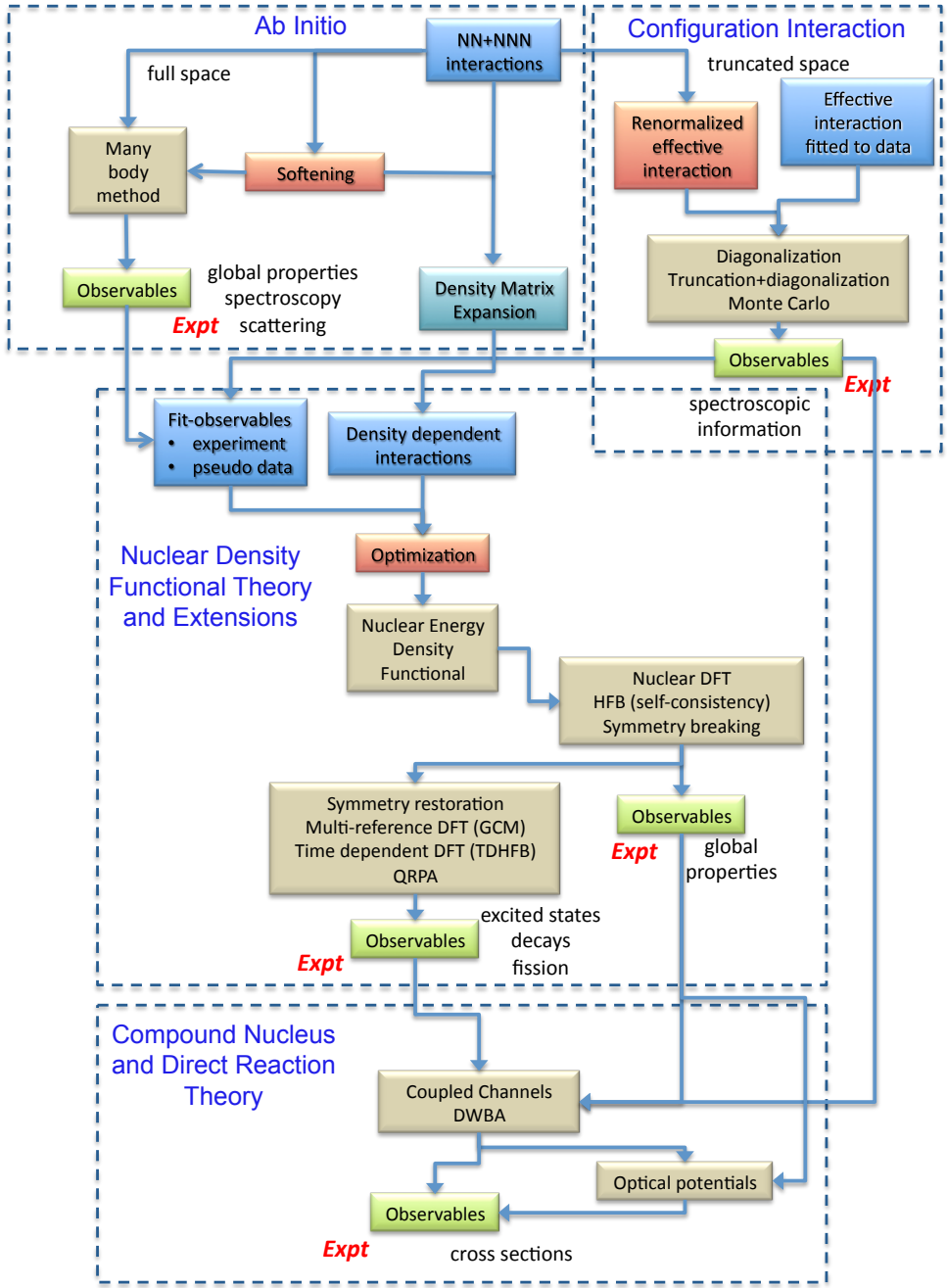


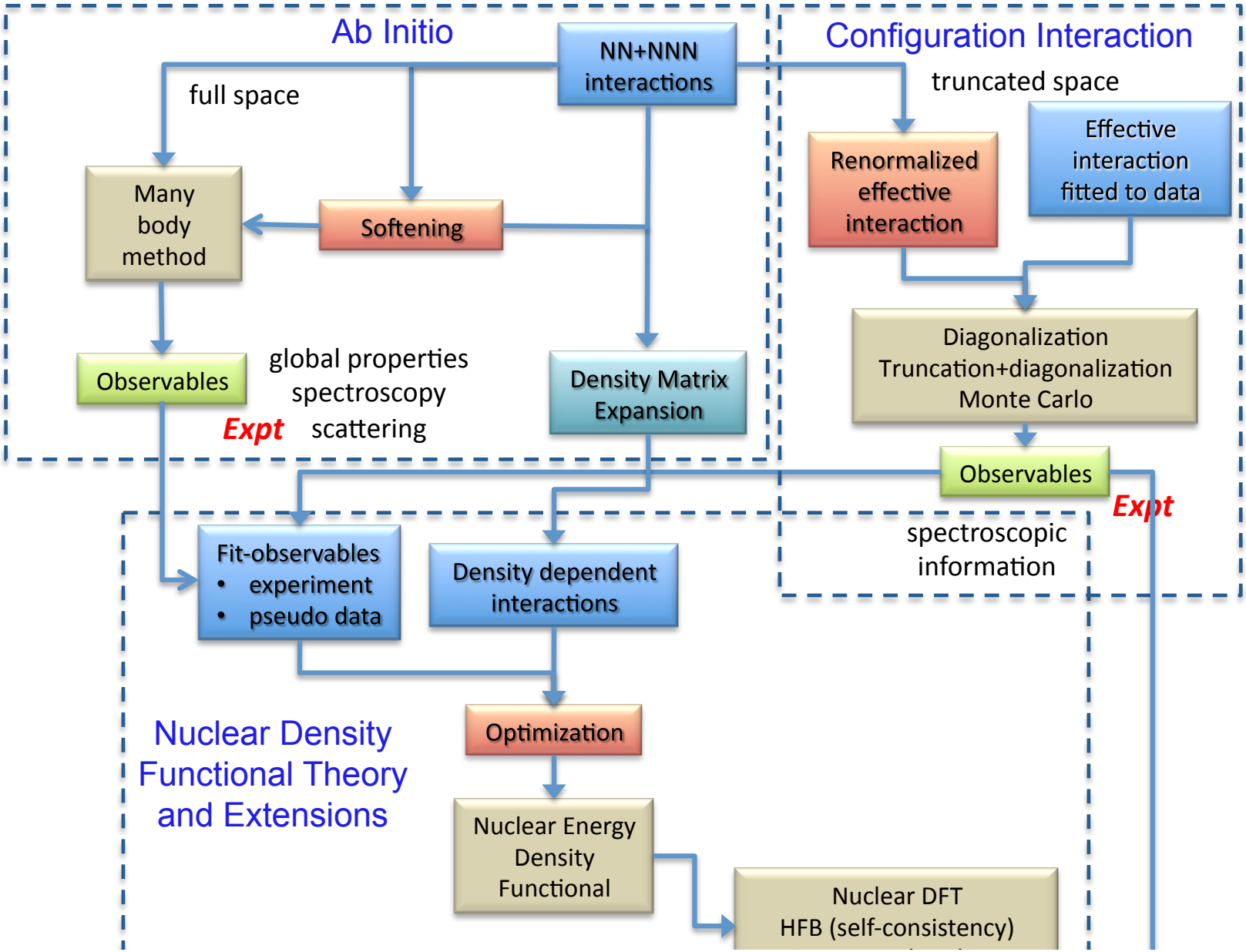
HPC motto

"High performance computing (HPC) provides answers to questions that neither experiment nor analytic theory can address; hence it becomes a third leg supporting the field of nuclear physics."

- SciDAC-2 UNEDF project
- Universal Nuclear Energy Density Functional
- Collaboration of physicists, applied mathematicians, and computer scientists
- US funding but international collaborators also
- See unedf.org for highlights!

New SciDAC-3 NUCLEI project:
NUclear Computational Low-Energy Initiative




Ab Initio
NN+NNN interactions
full space
Many body method
Softening
Observables
global properties
spectroscopy
scattering
Expt
Density Matrix Expansion
Configuration Interaction
truncated space
Renormalized effective interaction
Effective interaction fitted to data
Diagonalization
Truncation+diagonalization
Monte Carlo
Observables
Expt
spectroscopic information
Fit-observables
• experiment
• pseudo data
Density dependent interactions
Optimization
Nuclear Density Functional Theory and Extensions
Nuclear Energy Density Functional
Nuclear DFT
HFB (self-consistency)

Interaction with computer science experts

"Load Balancing at Extreme Scale" – Ewing Lusk, Argonne National Laboratory

ASCR- SciDAC UNEDF Computer Science Highlight

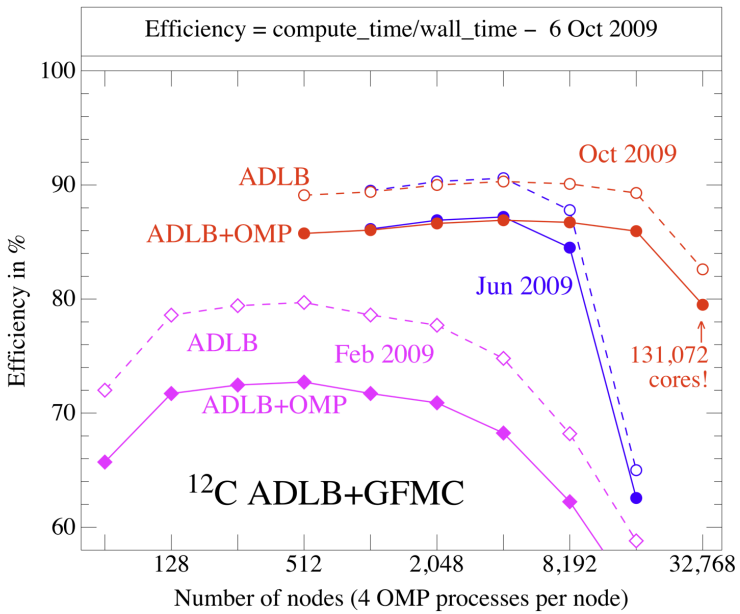
Objectives

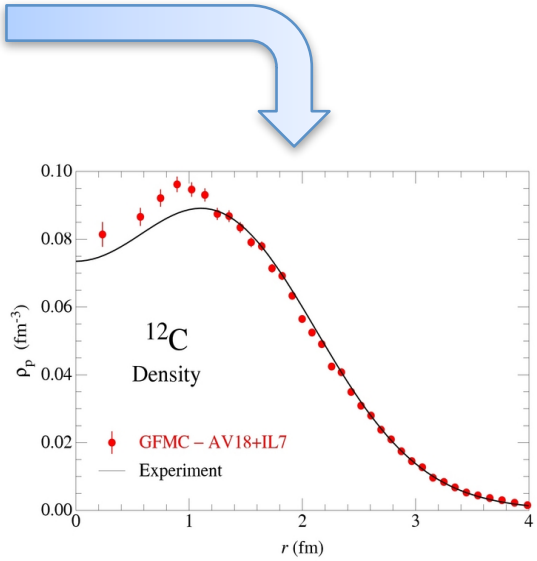
- **Enable Green's Function Monte Carlo calculations for ^{12}C on full BG/P as part of UNEDF project**
- **Simplify programming model**
- **Scale to leadership class machines**

Impact

- **Demonstrate capabilities of simple programming models at petascale and beyond**
- **Show path forward with hybrid programming models in library implementation**

Improved Efficiency (compute time/wall time) with more nodes





Progress

- **Initial load balancing was of CPU cycles**
- **Next it became necessary to balance memory utilization as well**
- **Finally ADLB acquired the capability to balance message flow**
- **"More Scalability, Less Pain" by E. Lusk, S.C. Pieper and R. Butler published in SciDAC Review 17, 30 (2010)**

SciDAC-3 NUCLEI Project