Nuclear Physics from Scratch

XII Exotic Beam Summer School 2013

July 28 – August 4, 2013

Erich Ormand

Lawrence Livermore
National Laboratory

LLNL-PRES-XXXXXX

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Ab initio approaches to nuclear physics

Goal: Answer the question whether it is possible to describe the basic properties of atomic nuclei (structure and reactions) from the point of view of point-like nucleons with "fundamental" inter-nucleon interactions.

The starting point is more important than you think!

Two major obstacles:

1. Interactions among nucleons are not known precisely

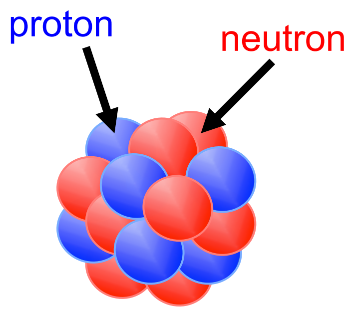
   Nuclear forces governed by quantum chromodynamics (QCD)

   QCD non perturbative at low energies

2. Many-body problem extremely hard to solve:

   << *… many Hottentot tribes do not have in their vocabulary the names for numbers larger than three. Ask a native down there how many sons he has or how many enemies he has slain, and if the number is more than three he will answer "many" …* >>

   From: "*One two three … infinity*" by G. Gamow



A nucleons

The starting point is more important than you think!

Two major obstacles:

1. Interactions among nucleons are not known precisely

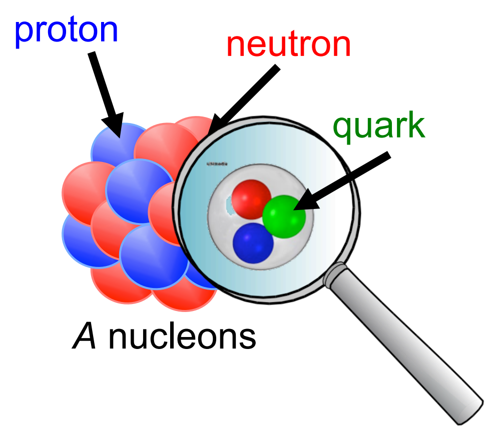
   Nuclear forces governed by quantum chromodynamics (QCD)

   QCD non perturbative at low energies

2. Many-body problem extremely hard to solve:

   << *… many Hottentot tribes do not have in their vocabulary the names for numbers larger than three. Ask a native down there how many sons he has or how many enemies he has slain, and if the number is more than three he will answer "many" …* >>

   From: "*One two three … infinity*" by G. Gamow



The starting point is more important than you think!

Two major obstacles:

1. Interactions among nucleons are not known precisely

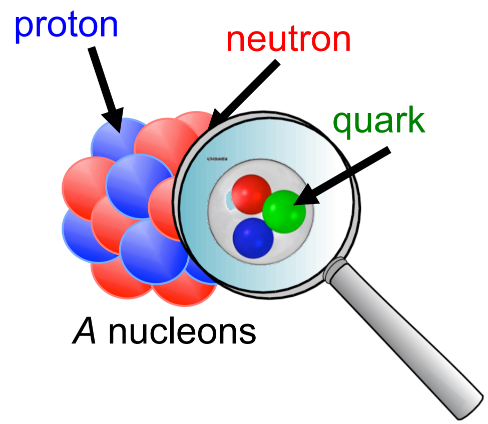
   Nuclear forces governed by quantum chromodynamics (QCD)

   QCD non perturbative at low energies

2. Many-body problem extremely hard to solve:

   << *… many Hottentot tribes do not have in their vocabulary the names for numbers larger than three. Ask a native down there how many sons he has or how many enemies he has slain, and if the number is more than three he will answer "many" …* >>

   From: "*One two three … infinity*" by G. Gamow



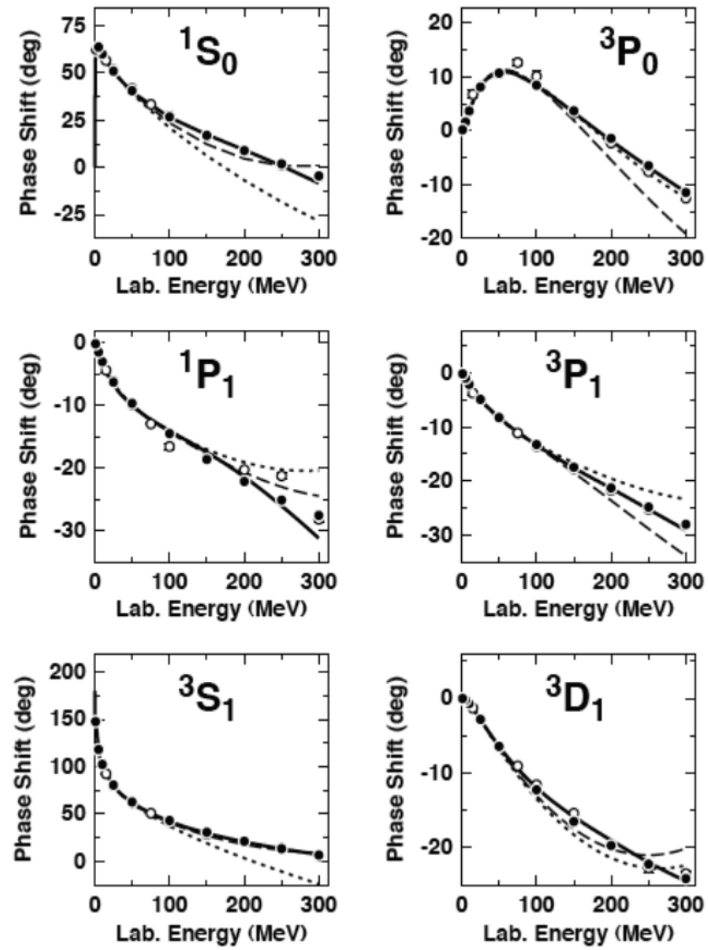
"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!" – Steven Weinberg

“Realistic” Interactions

- There is no **fundamental** NN interaction
  - The underlying physics is QCD – quarks and gluons
  - But we want to treat nuclei as a collection of nucleons and not deal with those pesky quarks and gluons if we don’t have to

- Use an “Effective Interaction”
  - Model the interaction and fit parameters to the deuteron and NN scattering
    - — Meson Exchange
    - — Bonn potentials
    - — Argonne potentials
    - — Chiral Effective Field Theory (EFT)

Experimental Phase Shifts



"Realistic" Interactions – Potential Models

- Long history attempting to model NN-interactions with potentials
- Early on, pion exchange was found to be an important component
  - Yukawa
  - Included in all realistic interactions

$$\langle \vec{p}' | V_{\mathrm{OPEP}} | \vec{p} \rangle = -g^2 \frac{\pi}{E^2} \frac{(\vec{\sigma}_1 \cdot \vec{q})(\vec{\sigma}_2 \cdot \vec{q})}{q^2 + m_\pi^2}$$

$$V_{\mathrm{OPEP}}(r) = g^2 \frac{m_\pi^3}{4M^2} \left[(\vec{\sigma}_1 \cdot \vec{\sigma}_2) + S_{12} \left(1 + \frac{3}{m_\pi r} + \frac{3}{(m_\pi r)^2} \right) \right] \frac{e^{-m_\pi r}}{m_\pi r}$$

$$S_{12} = 3\vec{\sigma}_1 \cdot \vec{r}\, \vec{\sigma}_2 \cdot \vec{r} - \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

Tensor component, S_{12}, explains D-state mixture in the deuteron ground state

“Realistic” Interactions – Potential Models

- Long history of modeling NN-interactions with potentials
- Paris, Reid, etc.,
- CD-Bonn – meson exchange
- Argonne V18 – one-pion exchange with phenomenological intermediate and short-range parts

$$v(NN) = v^{\mathrm{EM}}(NN) + v^{\pi}(NN) + v^{R}(NN)$$

- Very successful potential – one of the most cited papers ever
- Strong short-range repulsion
- Local and extremely useful for Green’s Function Monte Carlo

PHYSICAL REVIEW C VOLUME 51, NUMBER 1 JANUARY 1995

Accurate nucleon-nucleon potential with charge-independence breaking

R. B. Wiringa
Physics Division, Argonne National Laboratory, Argonne, Illinois 60439

V. G. J. Stoks
School of Physical Sciences, The Flinders University of South Australia, Bedford Park, South Australia 5042, Australia

R. Schiavilla
CEBAF Theory Group, Newport News, Virginia 23606
and Department of Physics, Old Dominion University, Norfolk, Virginia 23529
(Received 15 August 1994)

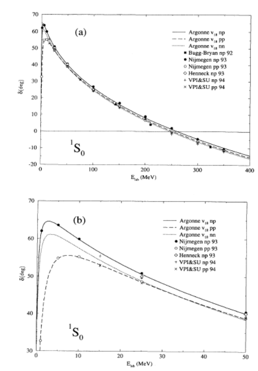


FIG. 2. Phase shifts in the $^1S_0$ channel for *np*, *nn*, and *pp* scattering, compared to various partial-wave phase-shift analyses.

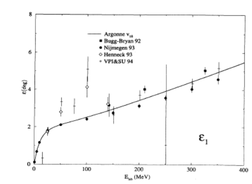


FIG. 4. The ϵ_1 mixing parameter compared to various partial-wave phase-shift analyses.

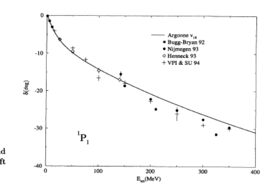


FIG. 5. Phase shifts in the $^1P_1$ channel, compared to various partial-wave phase-shift analyses.

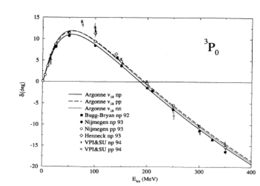


FIG. 3. Phase shifts in the $^3P_0$ channel for *np*, *nn*, and *pp* scattering, compared to various partial-wave phase-shift analyses.

TABLE VIII. Scattering lengths and effective ranges in fm.

	Experiment	Argonne v_{18}	w/o v^{EM}
$^1a_{pp}$	−7.8063±0.0026[a]	−7.8064	−17.164
$^1r_{pp}$	2.794 ± 0.014[a]	2.788	2.865
$^1a_{nn}$	−18.5 ± 0.4[b]	−18.487	−18.818
$^1r_{nn}$	2.80 ± 0.11[b]	2.840	2.834
$^1a_{np}$	−23.749 ± 0.008[c]	−23.732	−23.084
$^1r_{np}$	2.81 ± 0.05[c]	2.697	2.703
$^3a_{np}$	5.424 ± 0.003[c]	5.419	5.402
$^3r_{np}$	1.760 ± 0.005[c]	1.753	1.752

[a] Reference [32].
[b] Reference [28].
[c] Reference [35].

"Realistic" Interactions - χEFT

- The underlying physics is QCD – quarks and gluons
  - Weinberg proposed a mechanism to expand the nuclear interaction in terms of an order parameter $(Q/\Lambda)^n$
  - Leading order, next-to-leading order, etc., N^{n}LO

Cutoff: $\exp(-(Q/\Lambda)^4)$

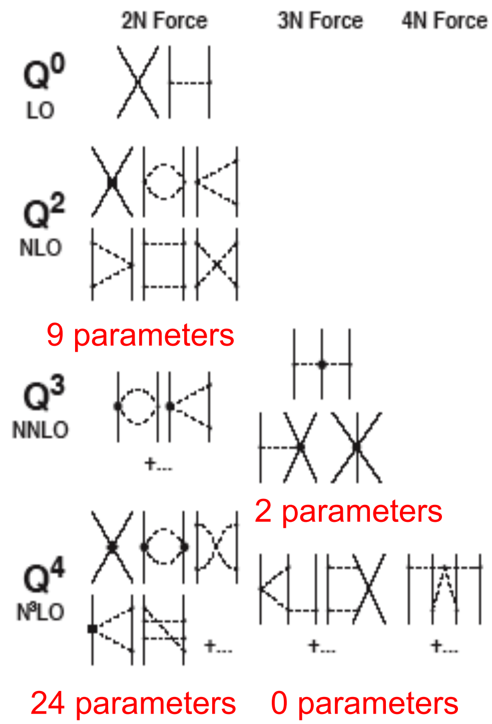
Volume 251, number 2 PHYSICS LETTERS B 15 November 1990

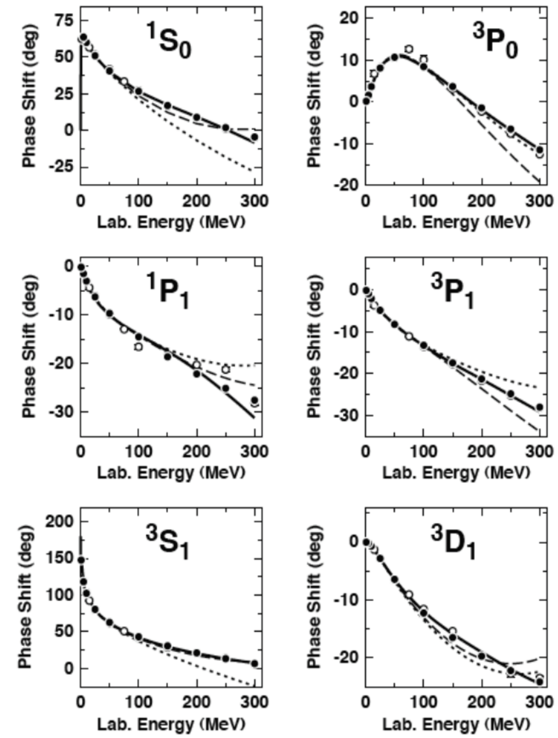
Nuclear forces from chiral lagrangians

Steven Weinberg[1]

Theory Group, Department of Physics, University of Texas, Austin, TX 78712, USA

$$k\cot\left(\delta(k)\right) = -\frac{1}{a} + \frac{1}{2}r_0 k^2 + O\left(k^4\right)$$

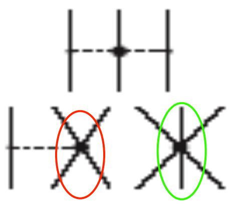




EFT- two-body N^{3}LO, χ^2/ν ~ 1:
Entem et al., PRC **68**, 041001 (2003)

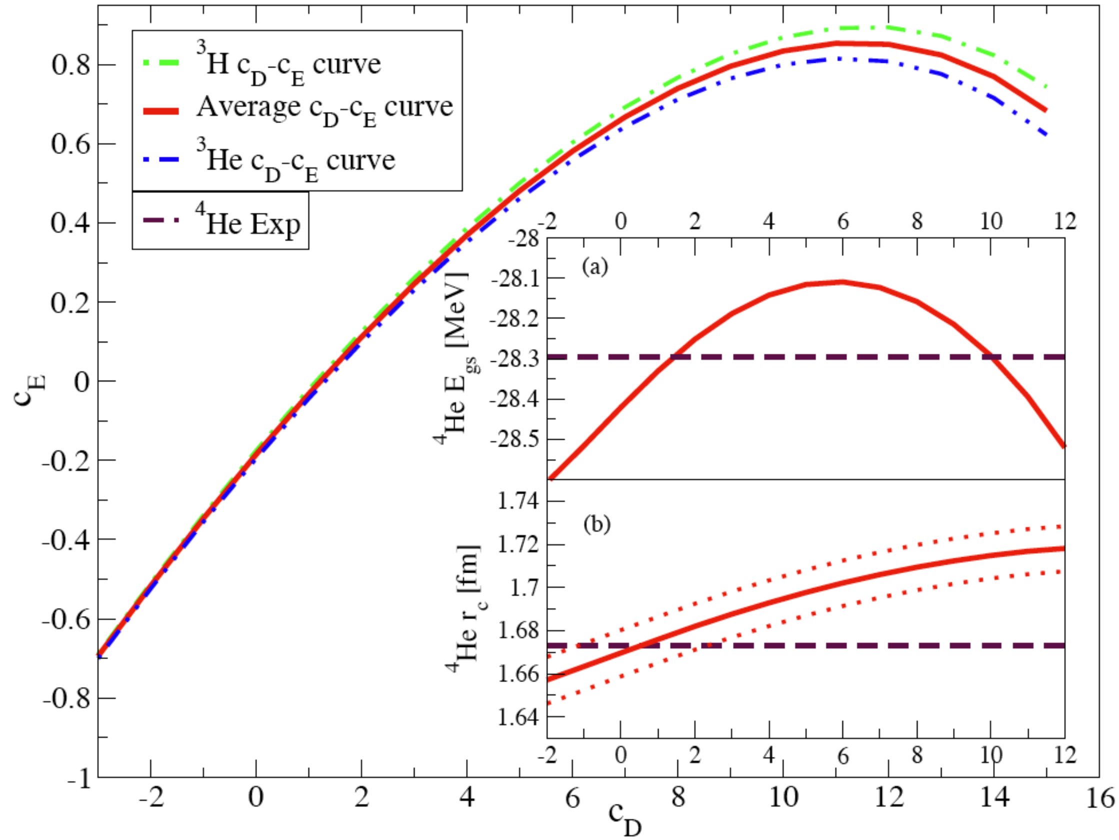
Three-body interactions

- N^{2}LO three-body



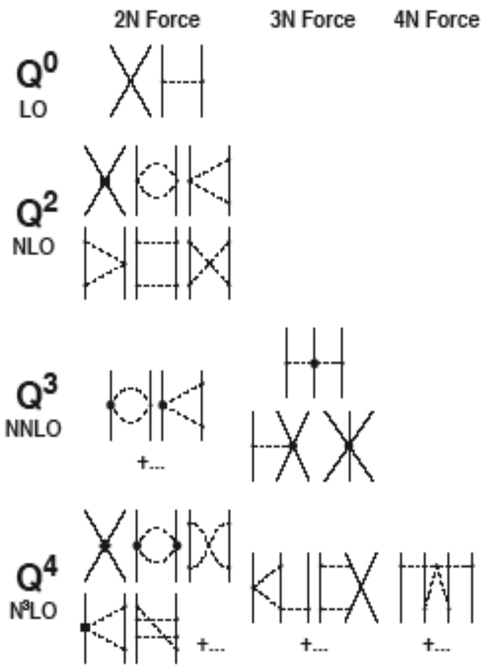
- Fine tune C_D with Tritium beta-decay lifetime (Gazit, Quaglioni, Navratil)

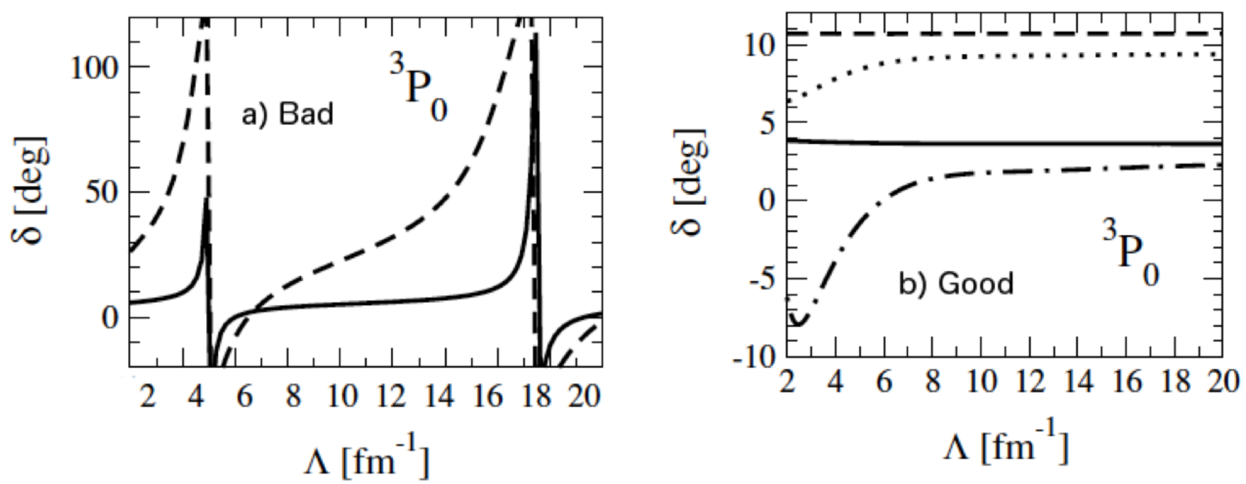
C_D=-0.2, C_E=-0.25



Effective Field theory – cutoff invariance

- Controversy over the counter terms!





Current N3LO formulation is not cutoff independent.

Many-body calculations

- Start with the microscopic *A*-nucleon Hamiltonian

$$H^{(A)} = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j=1}^{A} V^{2b}(\vec{r}_i - \vec{r}_j) + \left(\sum_{i<j<k=1}^{A} V_{ijk}^{3b} \right)$$

  - Nucleons interact with two- and three-nucleon forces: this yields complicated quantum correlations

- Solve the many-body Schrödinger equation

$$H^{(A)}\Psi^{(A)}(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_A) = E\Psi^{(A)}(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_A)$$

  - Negative energies – bound-state boundary conditions
    - — Find eigenfunctions and eigenenergies
  - Continuum of positive energies – scattering boundary conditions
    - — Find elements of the Scattering matrix

Many-body wave functions

- *A* active nucleons – spatial, spin,and isospin degrees of freedom

$$\vec{r}_i \equiv \left\{\vec{r}_i,\ \vec{\sigma}_i,\ \vec{\tau}_i\right\},\ i = 1,2,\cdots,A$$

- Nucleons are fermions – Look for antisymmetric wave function

$$\Psi^{(A)}(\vec{r}_1, \vec{r}_2,\ \ldots\ \vec{r}_k,\ \ldots\ \vec{r}_j,\ \ldots\ \vec{r}_A) = -\Psi^{(A)}(\vec{r}_1, \vec{r}_2,\ \ldots\ \vec{r}_j,\ \ldots\ \vec{r}_k,\ \ldots\ \vec{r}_A)$$

- We are not interested in the motion of the center of mass, but only in the intrinsic motion
  - Look for translationally invariant wave function. Two options:
    - Work with *A* - 1 translational invariant coordinates known as Jacobi coordinates
    - Work with *A* single particle coordinates and aim at exact separation between intrinsic and center of mass motion

$$\Psi^{(A)}(\vec{r}_1,\ \vec{r}_2,\ \ldots\ \vec{r}_A) = \psi^{(A)}(\vec{\xi}_1,\ \vec{\xi}_2,\ \ldots\ \vec{\xi}_{A-1})\Psi_{CM}(\vec{R}_{CM})$$

Many-body calculations

- Few-body calculations can be done by direct solution
  - Two-body: Schrodinger equation
  - Three-body: Feddeev
  - Four-body: Feddeev-Yakubovsky

- Green's Function Monte Carlo
  - Filter states with $e^{-H\tau}$ – imaginary time
  - Limited to A ~ 12

- Basis expansion – Configuration interaction
  - Expand many-body wave function in terms of a convenient basis

$$\Psi_T^{(A)}(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_A) = \sum_{n=1}^{N} c_n \phi_n^{(A)}(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_A)$$

  - Eigenvalue problem to obtain states

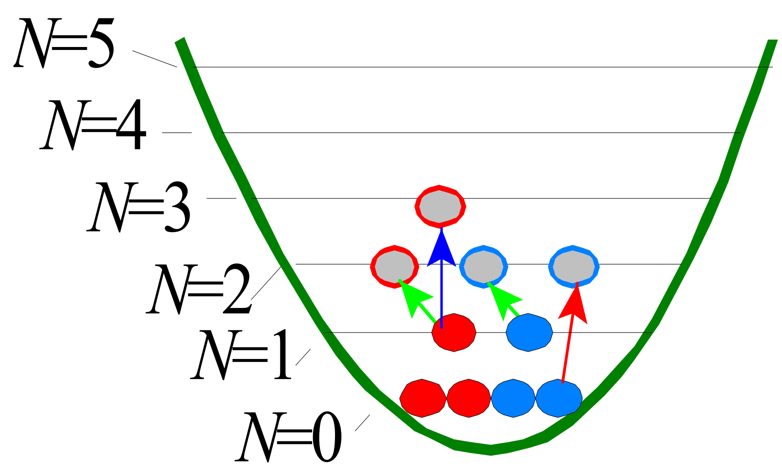
$$\sum_{n=1}^{N} \left[\left\langle \phi_m^{(A)} \middle| H \middle| \phi_n^{(A)} \right\rangle - E\, \delta_{mn} \right] c_n = 0 \ , \ m = 1, \ldots, N$$

Harmonic oscillator as a basis

- Harmonic-oscillator
- Can easily be separated into intrinsic and center-of-mass degrees of freedom – important for light nuclei
- We can separate intrinsic and COM motion in two ways
  - Explicitly, using Jacobi coordinates
  - The Hamiltonian is translationally invariant, so it will happen automatically
    - But add the COM Hamiltonian, and multiply by 100 to push COM states up in energy – Lawson projection

$$H_{HO}^{(A)} = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j=1}^{A} V_{ij}^{2b} + \frac{1}{2} A m \Omega^2 R_{CM}^2$$

$$\sum_{i=1}^{A} \left(\frac{p_i^2}{2m} + \frac{1}{2} m \Omega^2 r_i^2 \right) + \sum_{i<j=1}^{A} \left[V_{ij}^{2b} - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right]$$

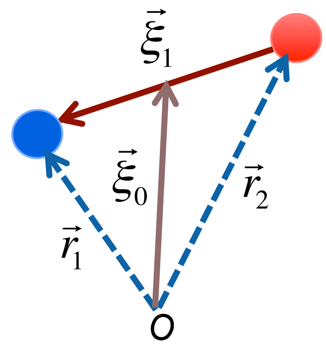


Maximum energy: $N_{\max} \hbar\Omega$

Jacobi Coordinates

- Two body

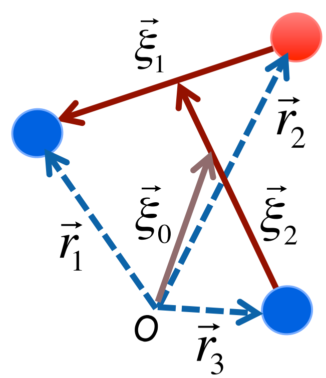
$$\begin{cases} \vec{\xi}_0 = \dfrac{1}{\sqrt{2}}\left(\vec{r}_1 + \vec{r}_2\right) \propto \vec{R}_{CM} \\ \vec{\xi}_1 = \dfrac{1}{\sqrt{2}}\left(\vec{r}_1 - \vec{r}_2\right) \propto \vec{r} \end{cases}$$



$$\begin{cases} \vec{r}_1 = \dfrac{1}{\sqrt{2}}\left(\vec{\xi}_0 + \vec{\xi}_1\right) \\ r_2 = \dfrac{1}{\sqrt{2}}\left(\vec{\xi}_0 - \vec{\xi}_1\right) \end{cases}$$

- Three body

$$\begin{cases} \vec{\xi}_0 = \dfrac{1}{\sqrt{3}}\left(\vec{r}_1 + \vec{r}_2 + \vec{r}_3\right) \\ \vec{\xi}_1 = \dfrac{1}{\sqrt{2}}\left(\vec{r}_1 - \vec{r}_2\right) \\ \vec{\xi}_2 = \sqrt{\dfrac{2}{3}}\left[\dfrac{1}{2}\left(\vec{r}_1 + \vec{r}_2\right) - \vec{r}_3\right] \end{cases}$$



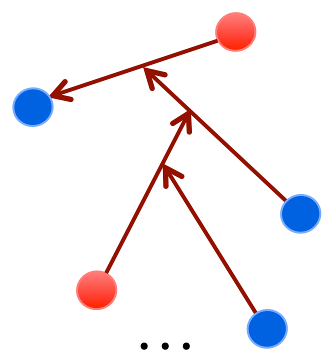
$$\begin{cases} \vec{r}_1 = \dfrac{1}{\sqrt{3}}\vec{\xi}_0 + \dfrac{1}{\sqrt{2}}\vec{\xi}_1 + \dfrac{1}{\sqrt{6}}\vec{\xi}_2 \\ \vec{r}_2 = \dfrac{1}{\sqrt{3}}\vec{\xi}_0 - \dfrac{1}{\sqrt{2}}\vec{\xi}_1 + \dfrac{1}{\sqrt{6}}\vec{\xi}_2 \\ \vec{r}_3 = \dfrac{1}{\sqrt{3}}\vec{\xi}_0 - \sqrt{\dfrac{2}{3}}\vec{\xi}_2 \end{cases}$$

Jacobi Coordinates

- A-body

$$\vec{\xi}_0 = \frac{1}{\sqrt{A}} \sum_{i=1}^{A} \vec{r}_i \qquad \left(\vec{R}_{CM} = \frac{1}{\sqrt{A}} \vec{\xi}_0 \right)$$

$$\begin{cases} \vec{\xi}_1 = \frac{1}{\sqrt{2}} \left(\vec{r}_1 - \vec{r}_2 \right) \\ \vdots \\ \vec{\xi}_k = \sqrt{\frac{k}{k+1}} \left[\frac{1}{k} \sum_{i=1}^{k} \vec{r}_i - \vec{r}_{k+1} \right] \\ \vdots \\ \vec{\xi}_{A-1} = \sqrt{\frac{A-1}{A}} \left[\frac{1}{A-1} \sum_{i=1}^{A-1} \vec{r}_i - \vec{r}_A \right] \end{cases}$$



Jacobi Coordinates

- Harmonic oscillator – three-body

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{p_3^2}{2m} + \frac{1}{2}K\sum_{i<j}\left(\vec{r}_i - \vec{r}_j\right)^2$$

$$= \left(\frac{P_{\xi_1}^2}{2m_{\xi_2}} + \frac{3}{2}K\xi_1^2\right) + \left(\frac{P_{\xi_2}^2}{2m_{\xi_2}} + \frac{3}{2}K\xi_2^2\right) + \frac{P_{\xi_0}^2}{2M}$$

$$m_{\xi_1} = m$$

$$m_{\xi_2} = \frac{m^2}{M}$$

- Jacobi coordinates are most useful for four or fewer particles
- Complication: anti-symmetrizing the wave functions

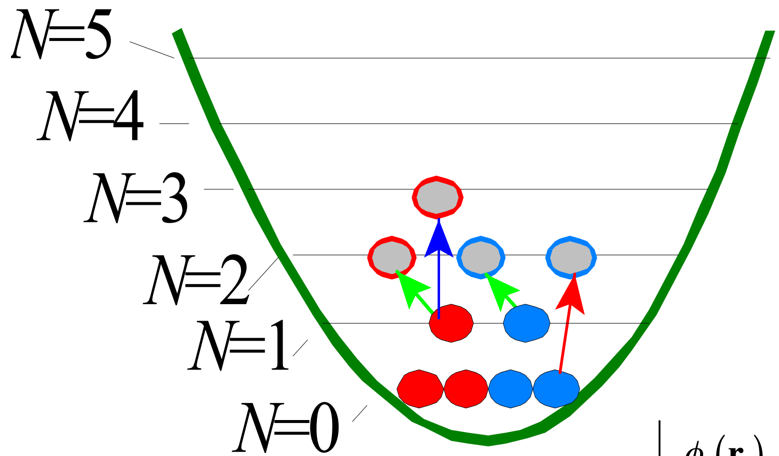
A	N_{max}
2	200
3	38
4	18
5	4

The Harmonic Oscillator in Modern Physics: From Atoms to Quarks, M. Moshinsky, Gordon and Breach, 1969

Harmonic oscillator as a basis

- For A > 4, it is more efficient to use regular coordinates, and standard shell-model technology
  - Single-particle states, with wave function ϕ
  - Slater-determinants using second-quantization

Maximum energy: $N_{\max}\hbar\Omega$



$$\phi = \frac{1}{\sqrt{A!}}\begin{vmatrix} \phi_i(\mathbf{r}_1) & \phi_i(\mathbf{r}_2) & \dots & \phi_i(\mathbf{r}_A) \\ \phi_j(\mathbf{r}_1) & \phi_j(\mathbf{r}_2) & & \phi_j(\mathbf{r}_A) \\ & \vdots & \ddots & \vdots \\ \phi_l(\mathbf{r}_1) & \phi_l(\mathbf{r}_2) & \dots & \phi_l(\mathbf{r}_A) \end{vmatrix}$$

$$= a_l^{+} \dots a_j^{+} a_i^{+} |0\rangle$$

$$H_{ij} = \langle \phi_j | H | \phi_i \rangle \longrightarrow \begin{pmatrix} H_{11} & H_{12} & \cdots & H_{1N} \\ H_{21} & H_{22} & & \\ \vdots & & \ddots & \\ H_{N1} & & \dots & H_{NN} \end{pmatrix} \longrightarrow$$

Shell-model technology

- M-scheme basis
  - Single particle states defined by n, l, j, m, t_z
  - Build many-body wave functions with product Slater determinants with fixed J_z
    - — Angular momentum is restored by diagonalizing the Hamiltonian

$$\phi = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_i(\mathbf{r}_1) & \phi_i(\mathbf{r}_2) & \dots & \phi_i(\mathbf{r}_A) \\ \phi_j(\mathbf{r}_1) & \phi_j(\mathbf{r}_2) & & \phi_j(\mathbf{r}_A) \\ & \vdots & \ddots & \vdots \\ \phi_l(\mathbf{r}_1) & \phi_l(\mathbf{r}_2) & \dots & \phi_l(\mathbf{r}_A) \end{vmatrix}$$

$$= a_l^+ \dots a_j^+ a_i^+ |0\rangle$$

- Second quantization
  - Represent Slater determinants as an integer word

$$a^+_{\frac{5}{2},-\frac{1}{2}} a^+_{\frac{5}{2},\frac{3}{2}} a^+_{\frac{3}{2},-\frac{1}{2}} a^+_{\frac{1}{2},-\frac{1}{2}} |0\rangle$$

	0	0	1	0	1	0	0	1	0	0	1	0
$2j_z$	-5	-3	-1	1	3	5	-3	-1	1	3	-1	1
	$0d_{5/2}$						$0d_{3/2}$				$1s_{1/2}$	

$$2^2 + 2^4 + 2^7 + 2^{10} = 1172$$

Getting the eigenvalues

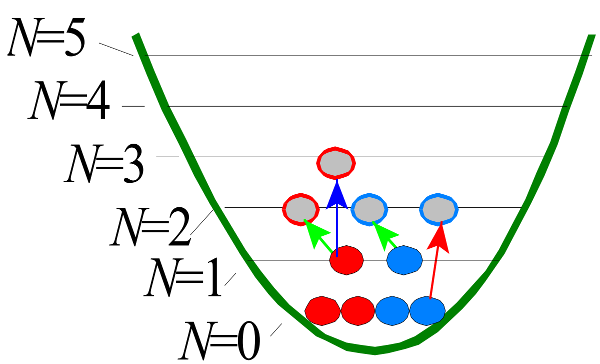
- In general, we only care about the lowest few states
  - We use the Lanczos algorithm to isolate the lowest eigenvalues

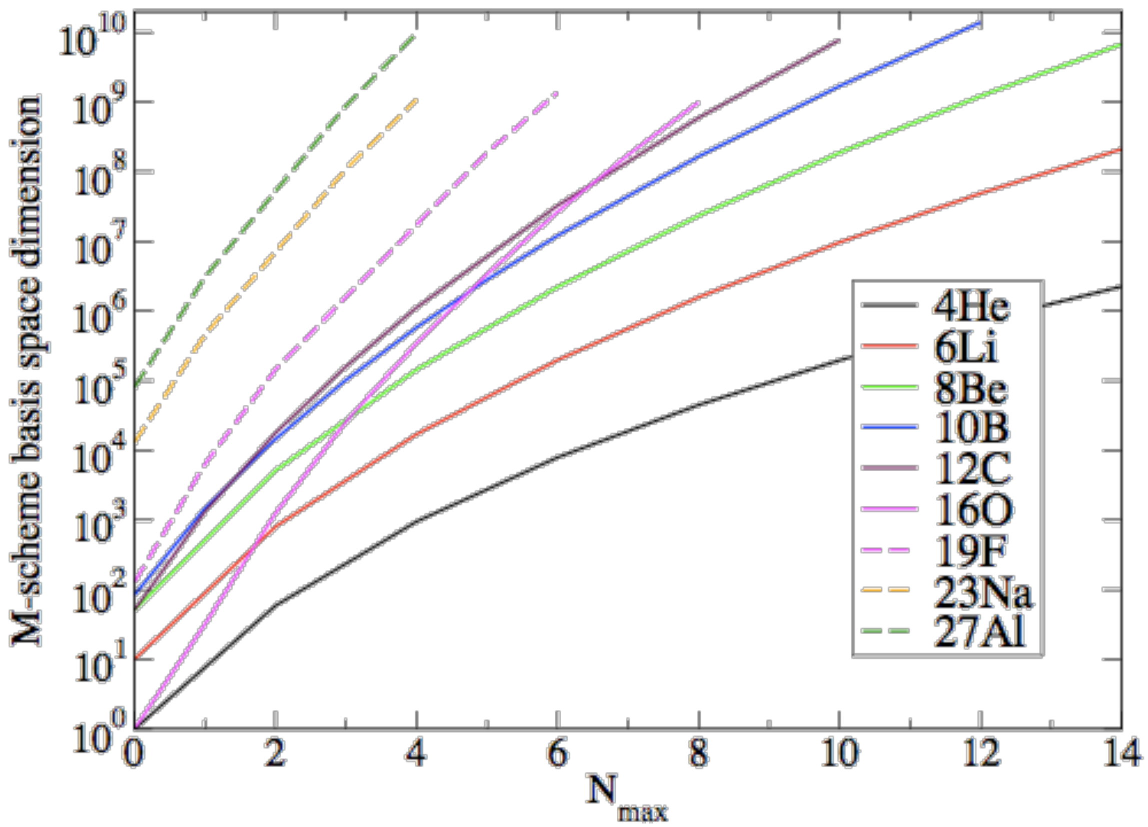
$$
\boxed{
\begin{aligned}
\hat{H}\mathbf{v}_1 &= \alpha_1\mathbf{v}_1 + \beta_1\mathbf{v}_2 \\
\hat{H}\mathbf{v}_2 &= \beta_1\mathbf{v}_1 + \alpha_2\mathbf{v}_2 + \beta_2\mathbf{v}_3 \\
\hat{H}\mathbf{v}_3 &= \beta_2\mathbf{v}_2 + \alpha_3\mathbf{v}_3 + \beta_3\mathbf{v}_4 \\
\hat{H}\mathbf{v}_4 &= \beta_3\mathbf{v}_3 + \alpha_4\mathbf{v}_4 + \beta_4\mathbf{v}_5
\end{aligned}
}
$$

  - Generally, 200 iterations will get us the lowest 10 states, no matter how big the matrix is
  - Numerical issue: we must re-orthogonalize after each iteration
  - Eigenvalues will have symmetries of the Hamiltonian
  - The computational challenge is to store all the information allowing us to to perform $H\mathbf{v}$

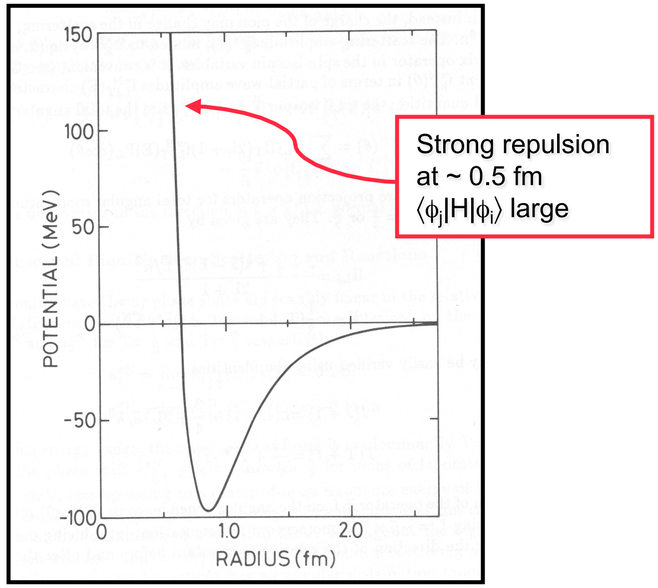
Dimensions as a function of N_{max}

- The basis dimension increases dramatically with increasing oscillator quanta – many are spurious



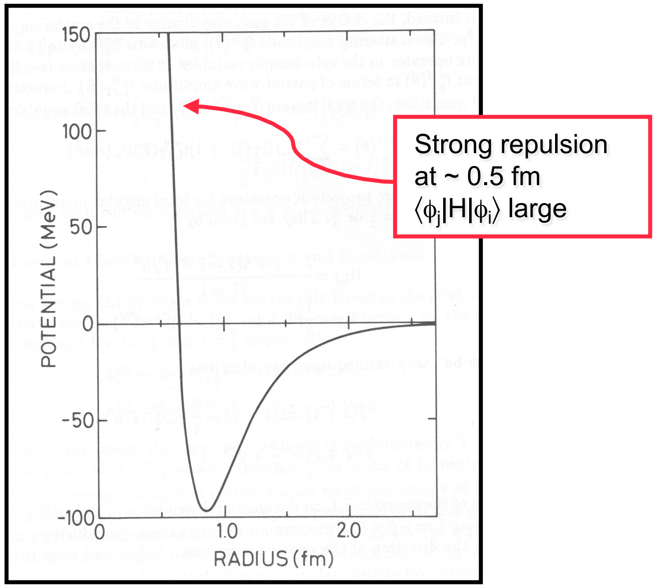


Problem with realistic interactions



Problem: Short-range repulsion requires an infinite space

Problem with realistic interactions



Problem: Short-range repulsion requires an infinite space

We must introduce a renormalization procedure in order to even get started!

Effective Interactions

- Use a formal theory to account for pathologies in the Hamiltonian
  - Bloch-Horowitz
  - Okubo-Lee-Suzuki
  - Low-momentum $V_{low\text{-}k}$
  - Similarity-Renormalization group (SRG)
    - Variational with model space size N_{max}
    - Lots of flexibility to do choice of G_s
      - Can look like $V_{low\text{-}k}$, Lee-Suzuki, or anything. Currently using T_{rel}
    - Study behaviors as a function of λ

$$H_s = U_s H U_s^+ \equiv T_{rel} + V_s$$

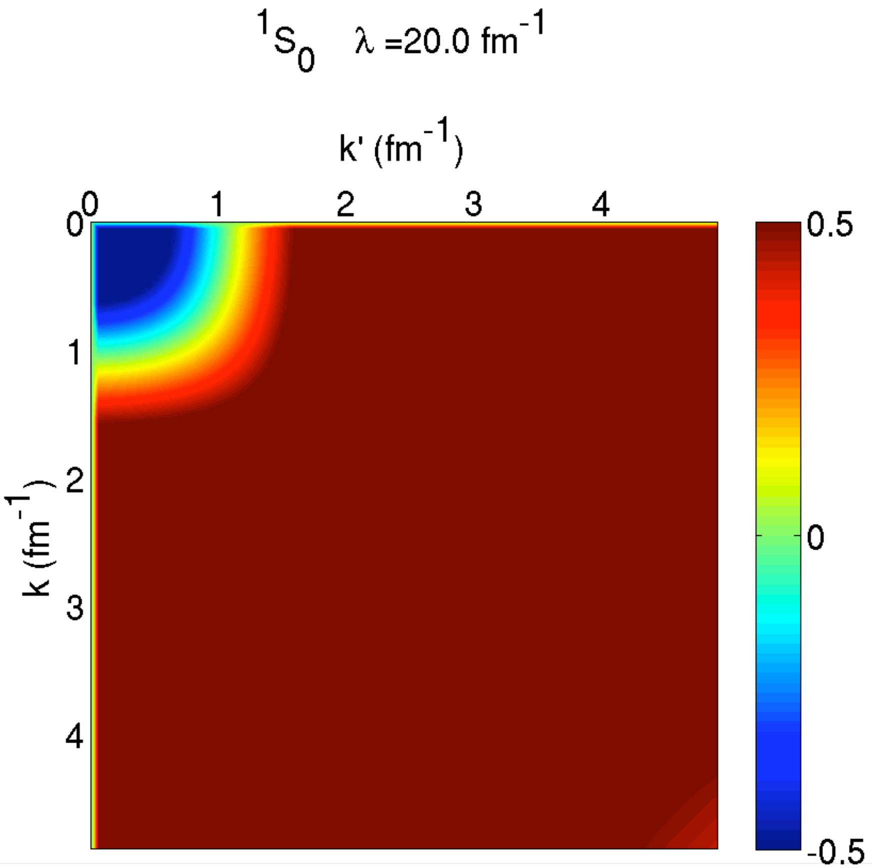
$$\frac{dH_s}{ds} = \left[\left[G_s, H_s\right], H_s\right]$$

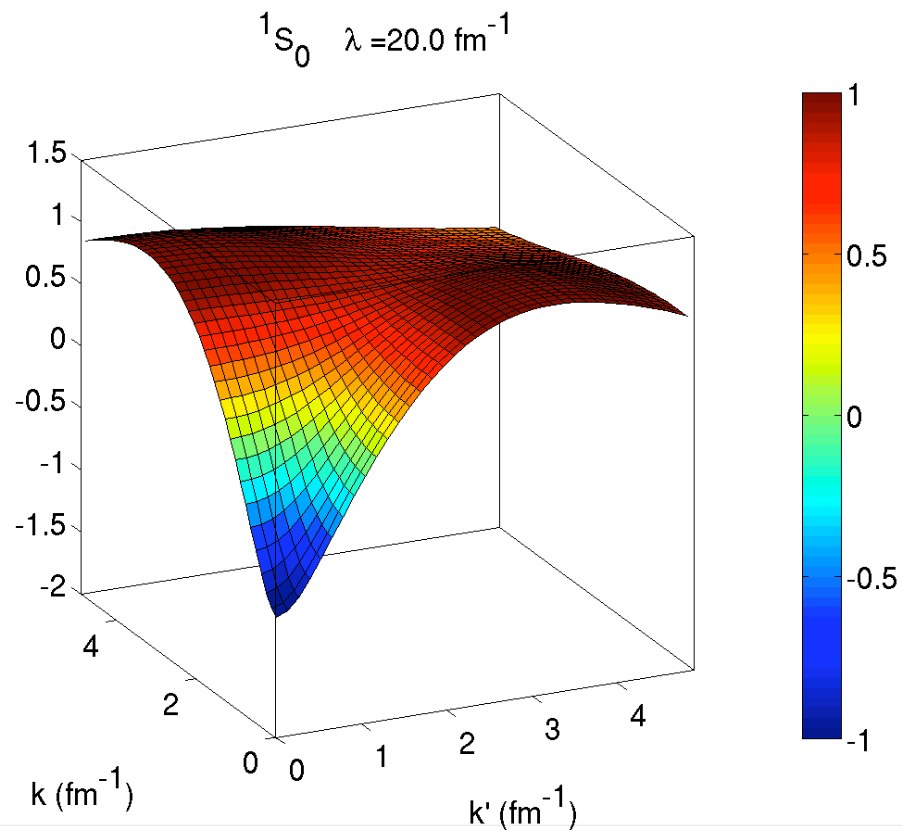
$$G_s = T_{rel}, H_{diag}, H_{BD}, \exp[-T], \cdots$$

Evolution parameter $s=1/\lambda^4$
(so that λ looks like 1/k, units fm^{-1})

SRG evolves Hamiltonians unitarily

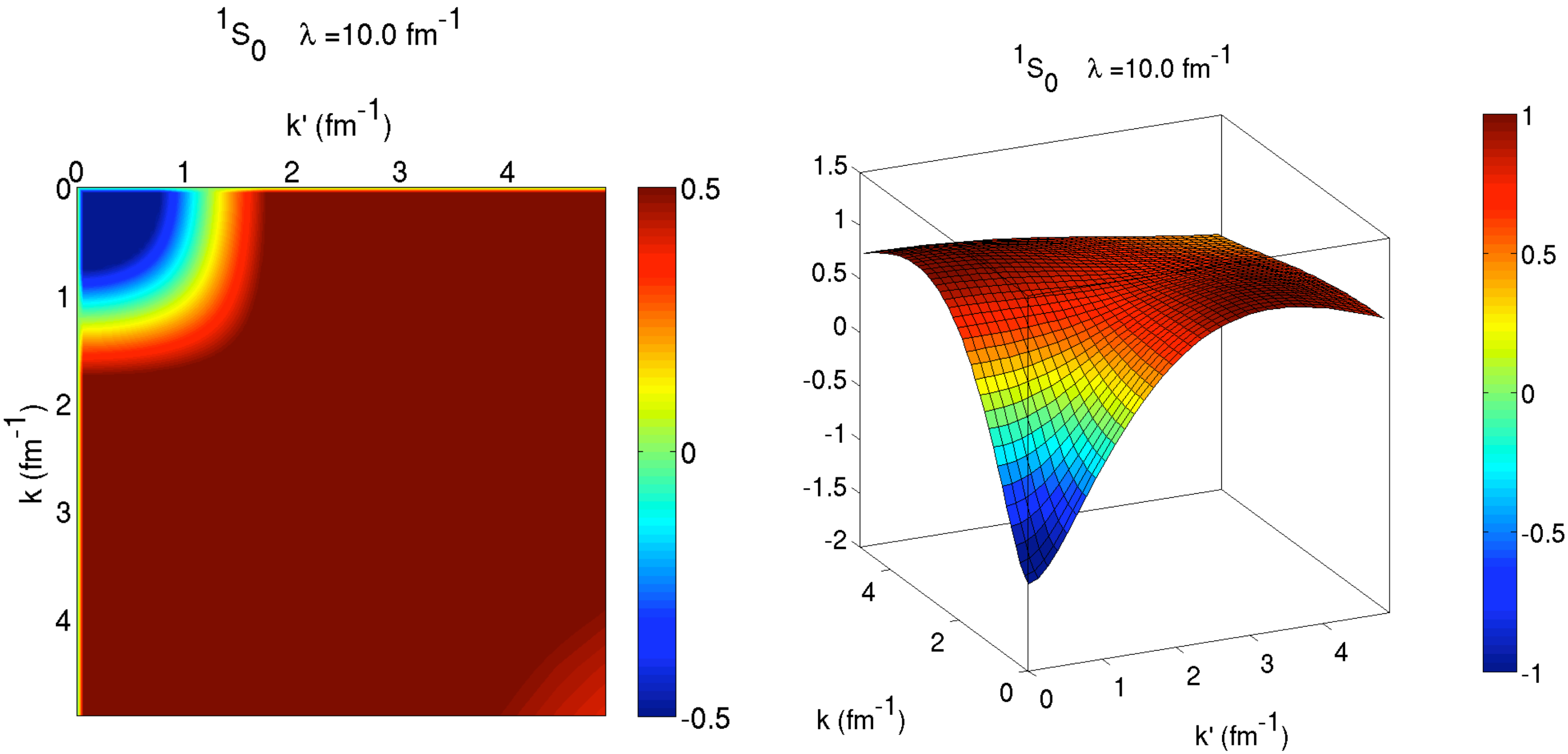
$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = [[T, H_s], H_s] \qquad \left(s = 1/\lambda^4\right)$$





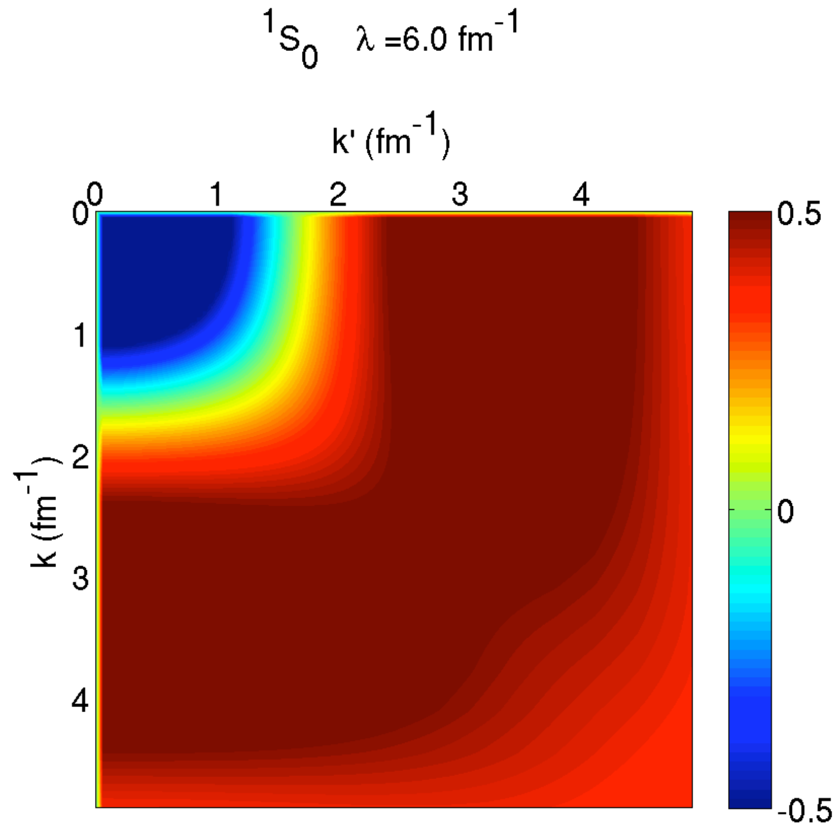
SRG evolves Hamiltonians unitarily

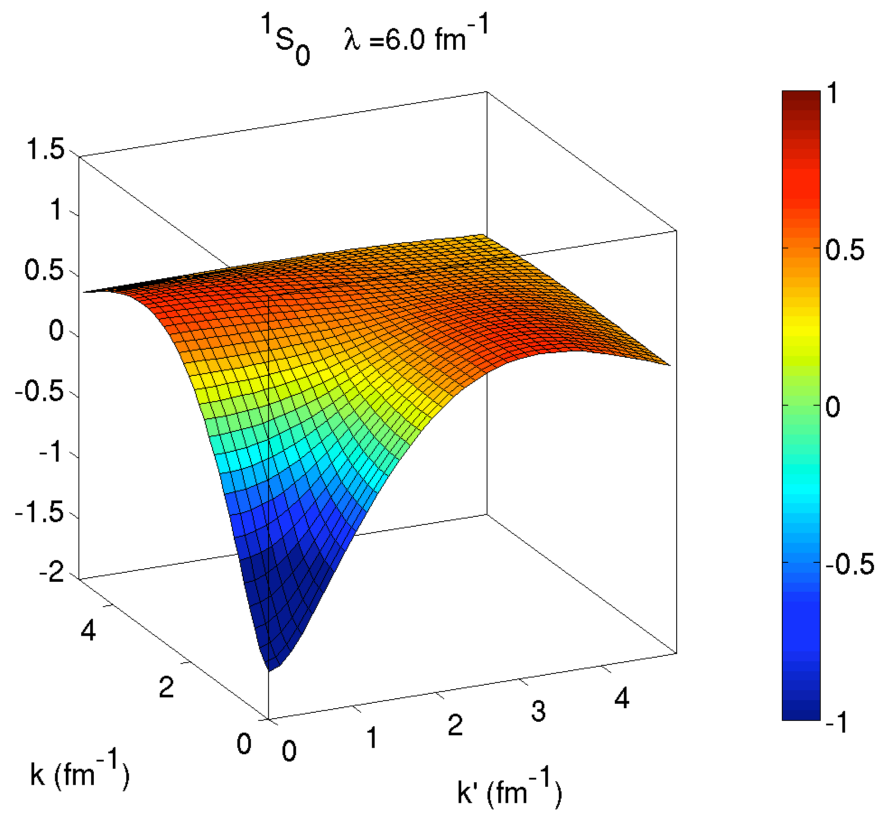
$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = \left[\left[T, H_s\right], H_s\right] \qquad \left(s = 1/\lambda^4\right)$$



SRG evolves Hamiltonians unitarily

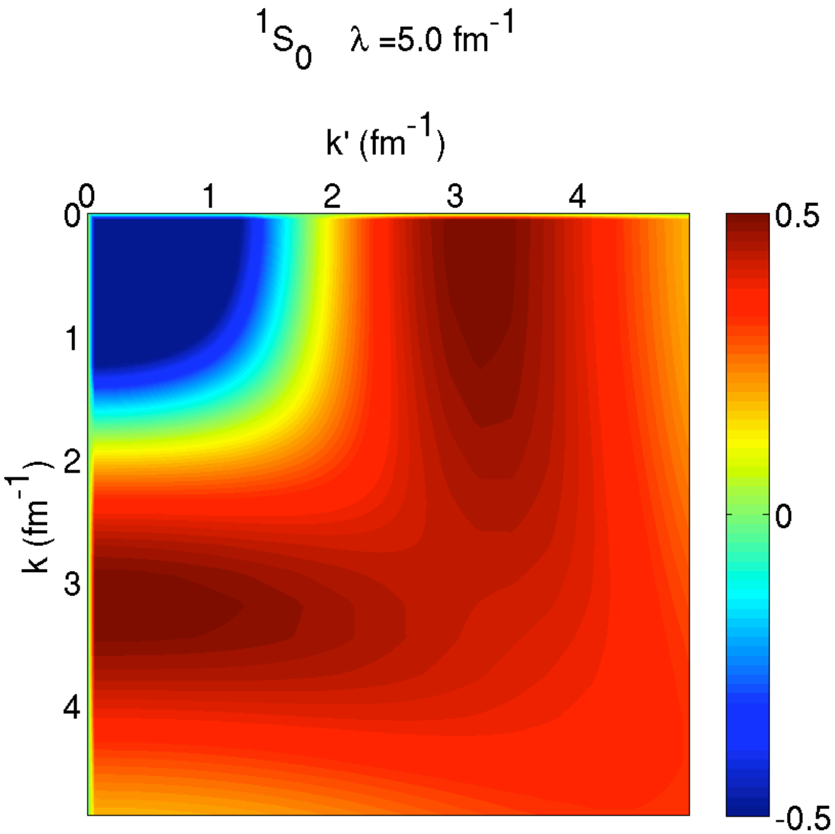
$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = \left[\left[T, H_s\right], H_s\right] \qquad \left(s = 1/\lambda^4\right)$$

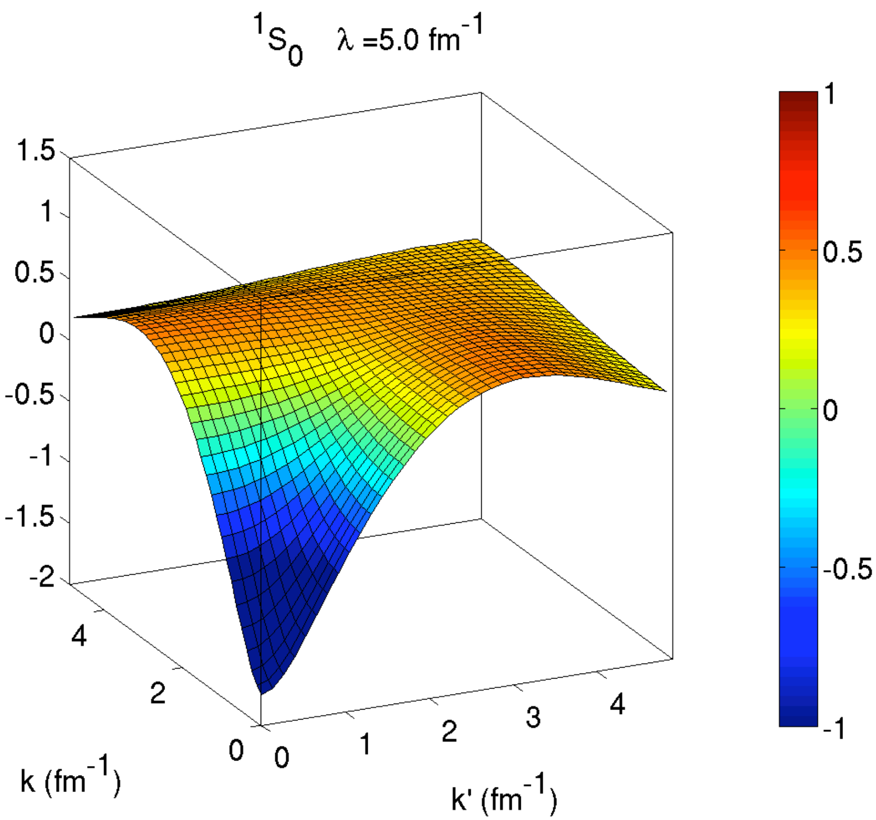




SRG evolves Hamiltonians unitarily

$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = [[T, H_s], H_s] \qquad \left(s = 1/\lambda^4\right)$$

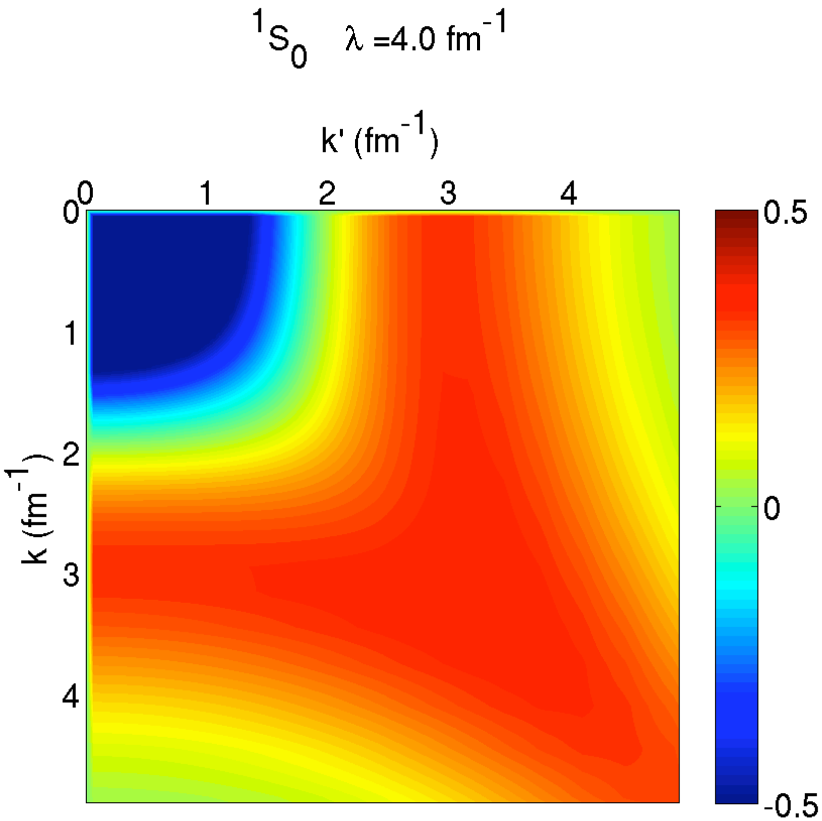


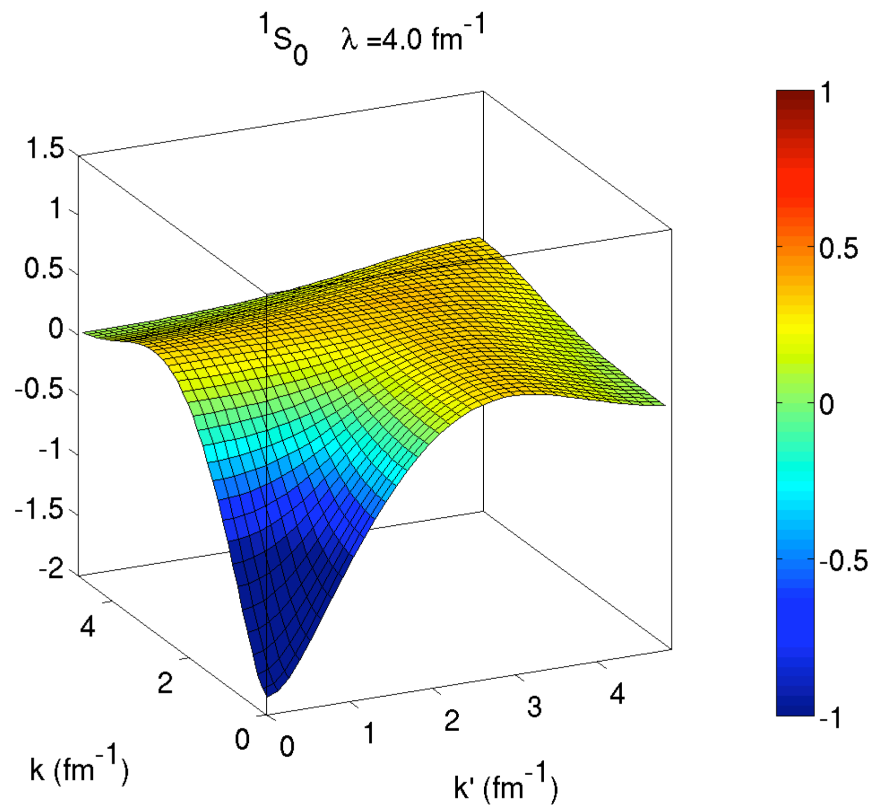


National Nuclear Security Administration

SRG evolves Hamiltonians unitarily

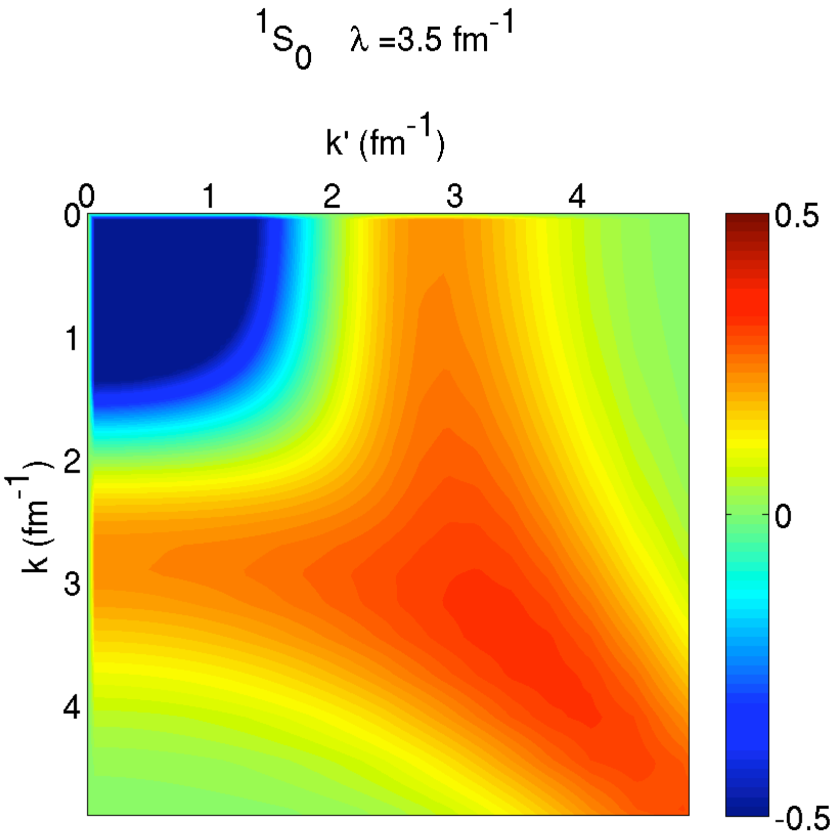
$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = \left[\left[T, H_s\right], H_s\right] \qquad \left(s = \frac{1}{\lambda^4}\right)$$

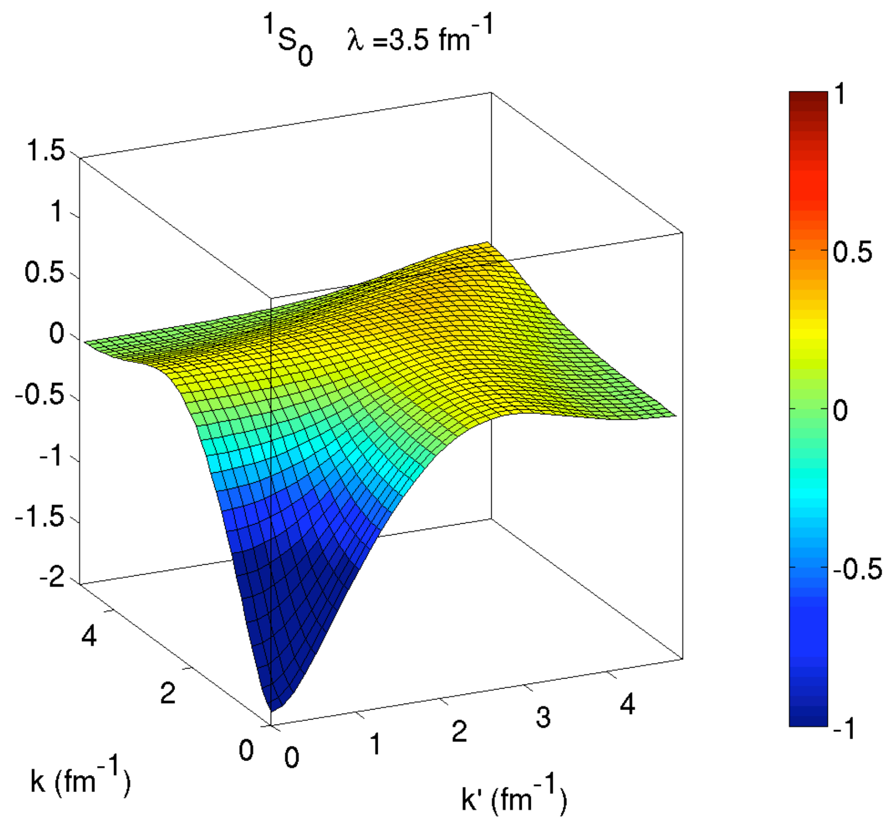




SRG evolves Hamiltonians unitarily

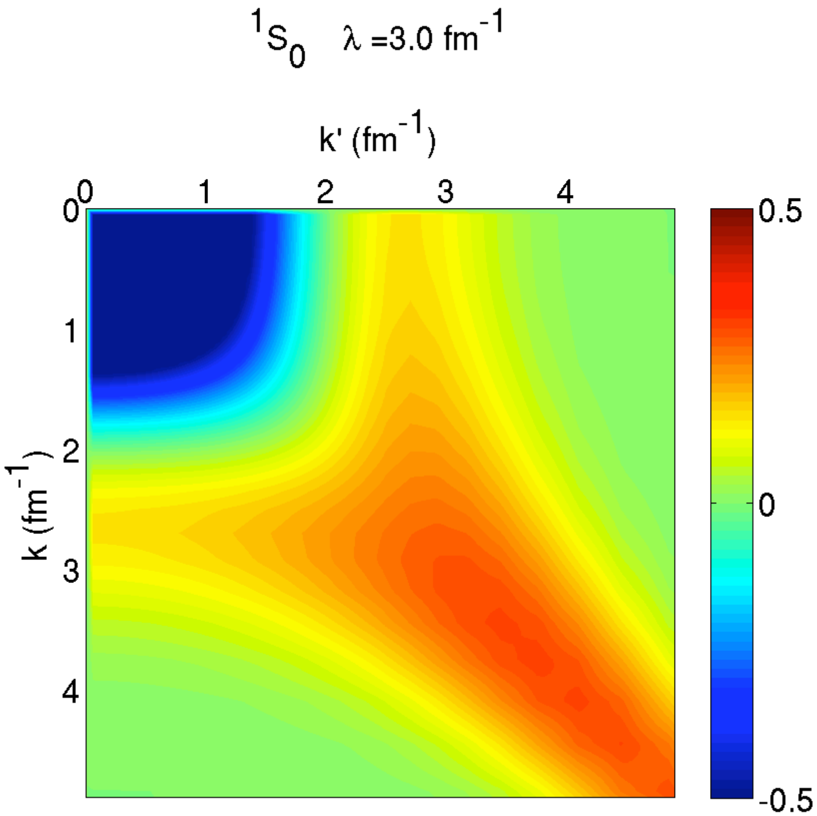
$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = \left[\left[T, H_s\right], H_s\right] \qquad \left(s = 1/\lambda^4\right)$$

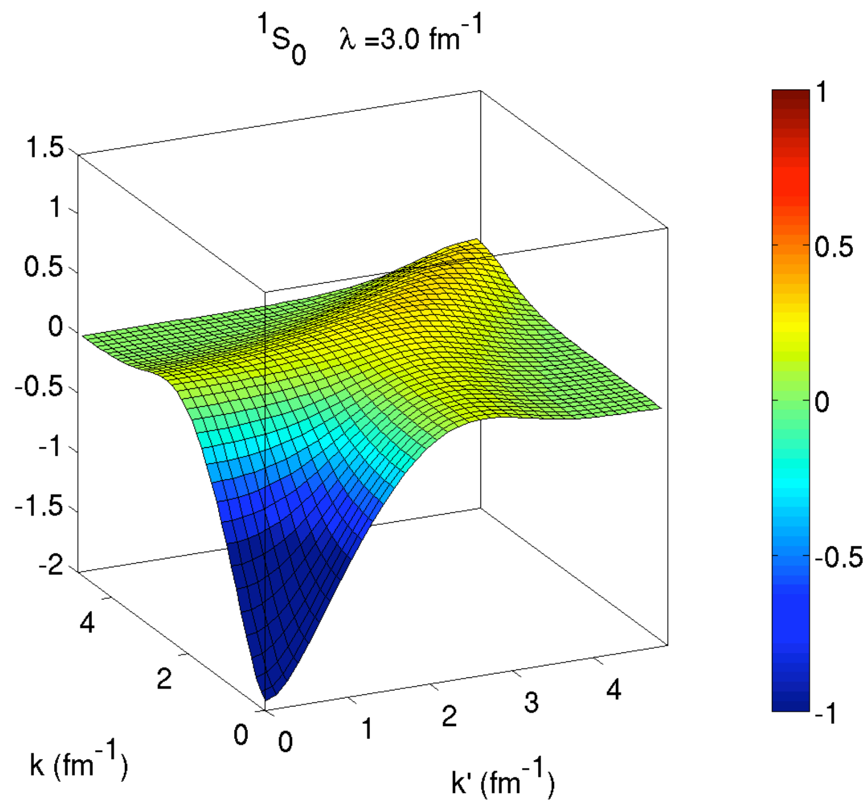




SRG evolves Hamiltonians unitarily

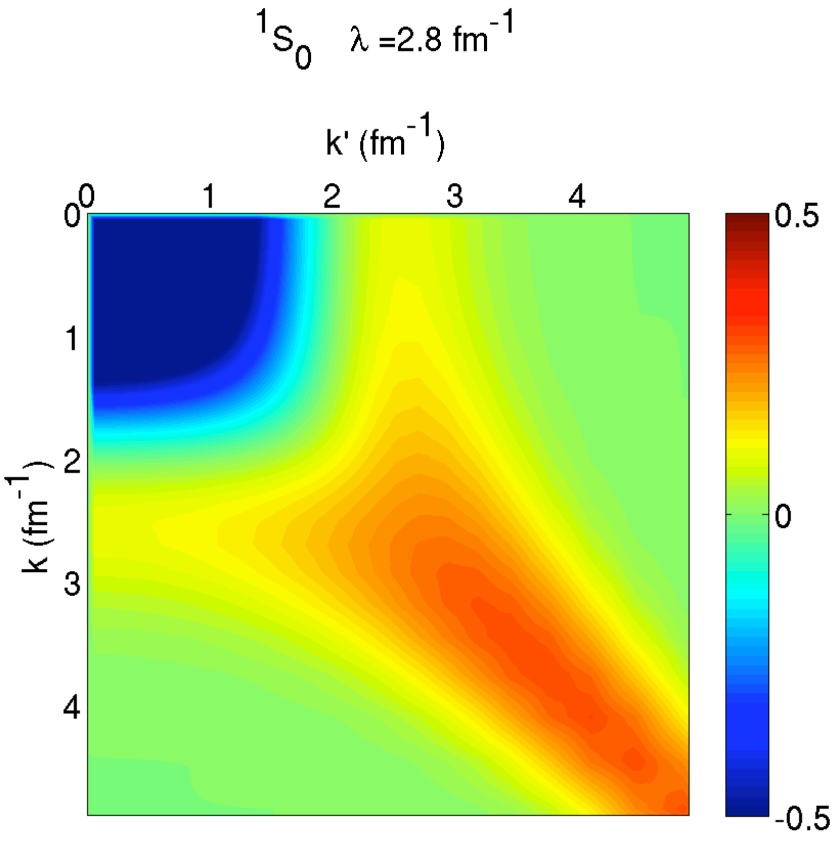
$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = \left[\left[T, H_s\right], H_s\right] \qquad \left(s = 1/\lambda^4\right)$$

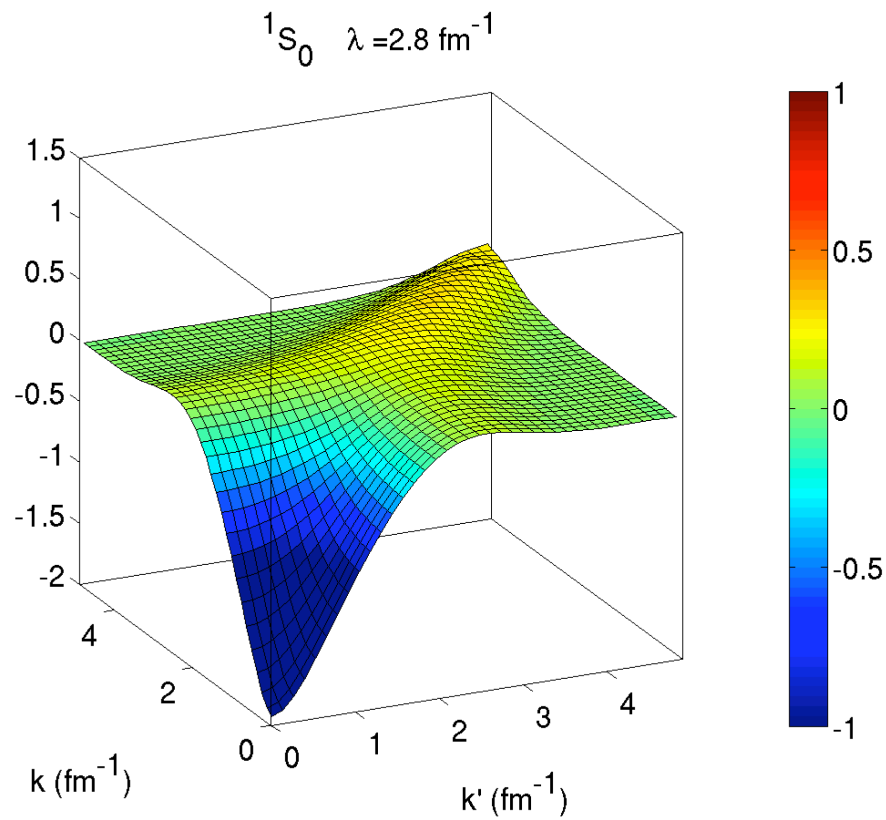




SRG evolves Hamiltonians unitarily

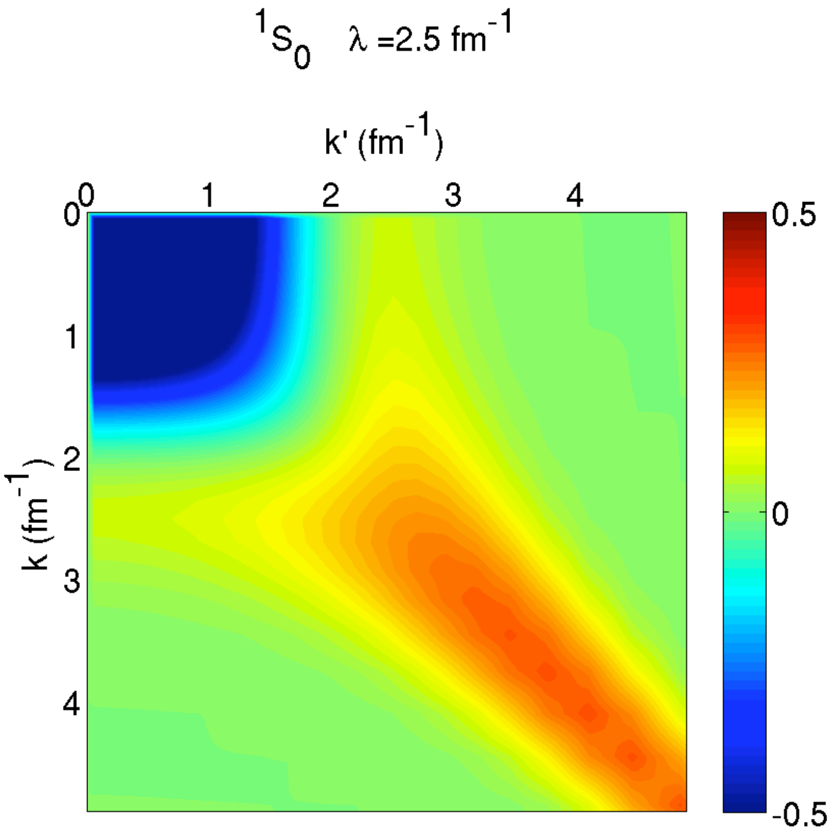
$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = \left[\left[T, H_s\right], H_s\right] \qquad \left(s = 1/\lambda^4\right)$$

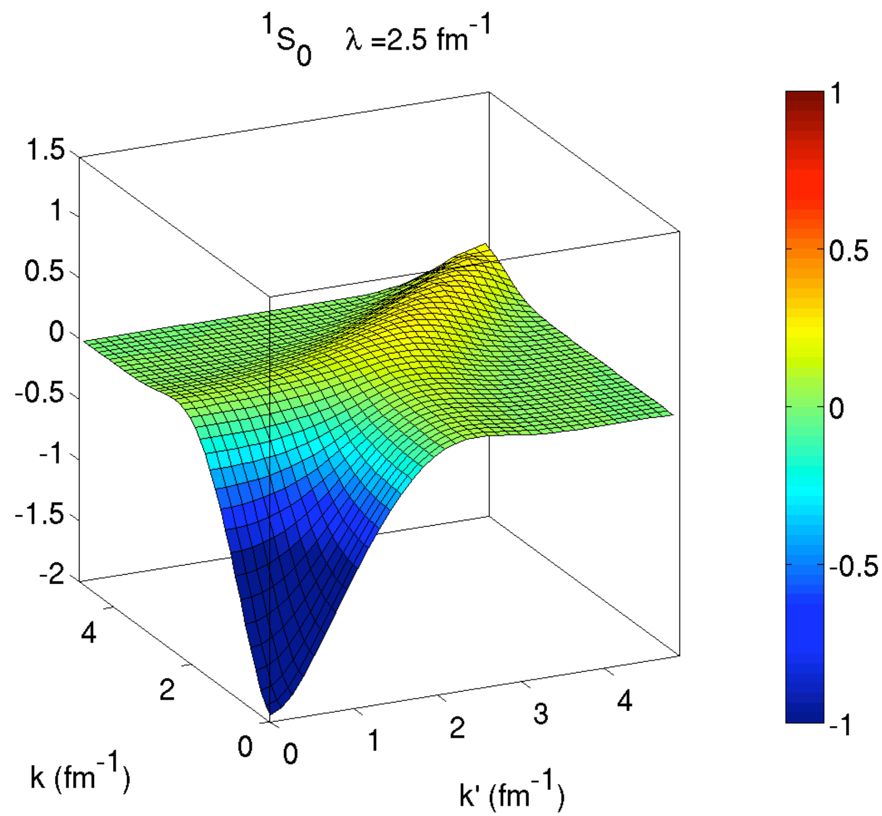




SRG evolves Hamiltonians unitarily

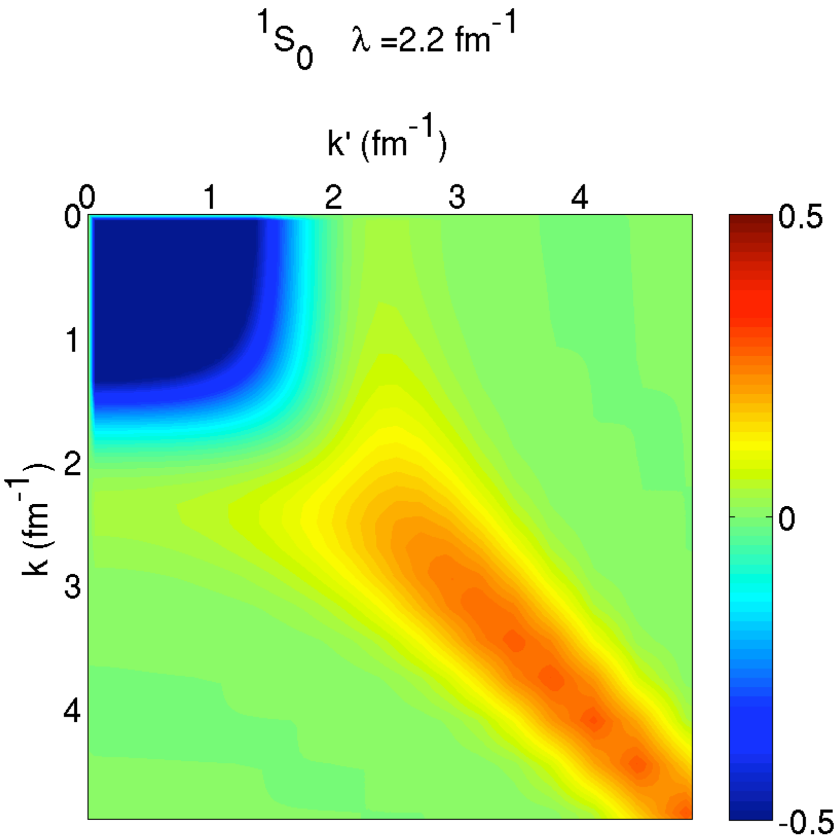
$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = \left[\left[T, H_s\right], H_s\right] \qquad \left(s = 1/\lambda^4\right)$$

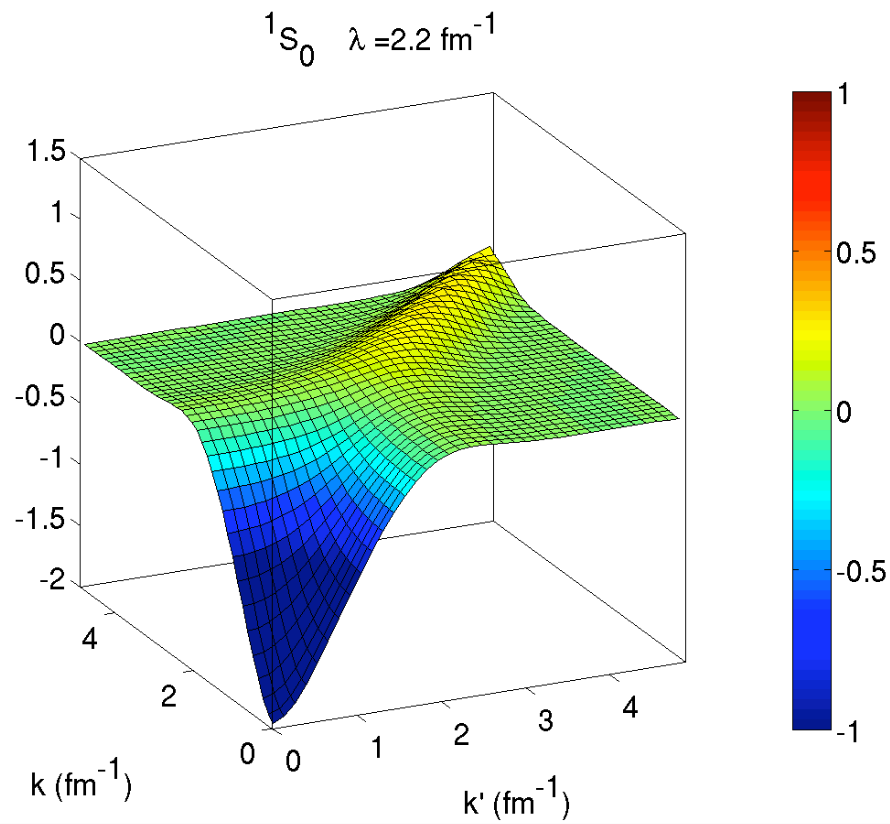




SRG evolves Hamiltonians unitarily

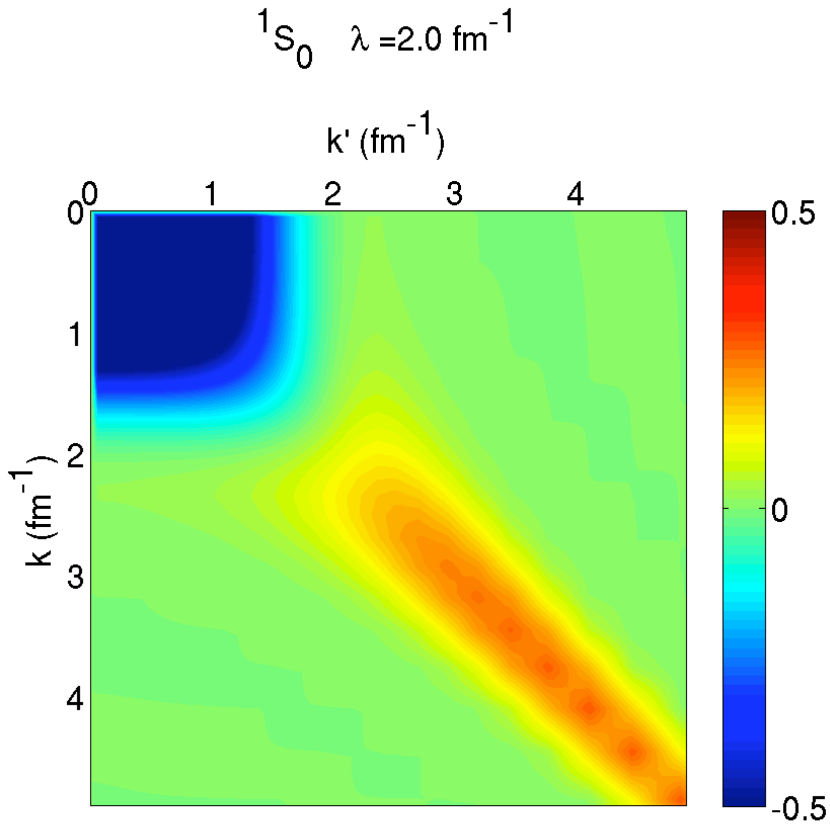
$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = [[T, H_s], H_s] \qquad \left(s = 1/\lambda^4\right)$$

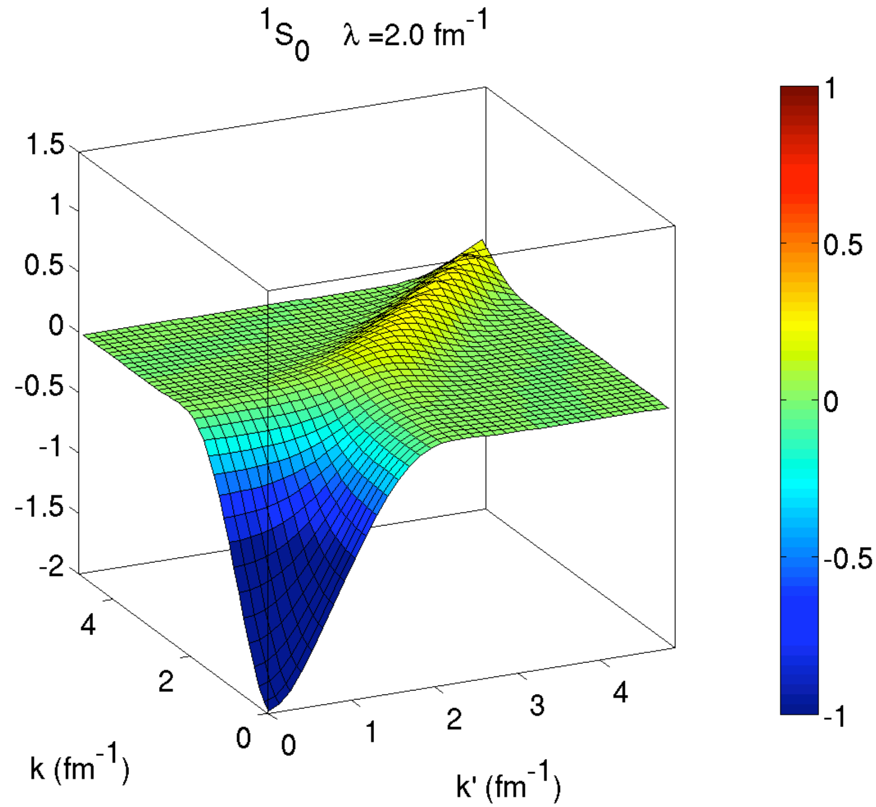




SRG evolves Hamiltonians unitarily

$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = \left[\left[T, H_s\right], H_s\right] \qquad \left(s = 1/\lambda^4\right)$$

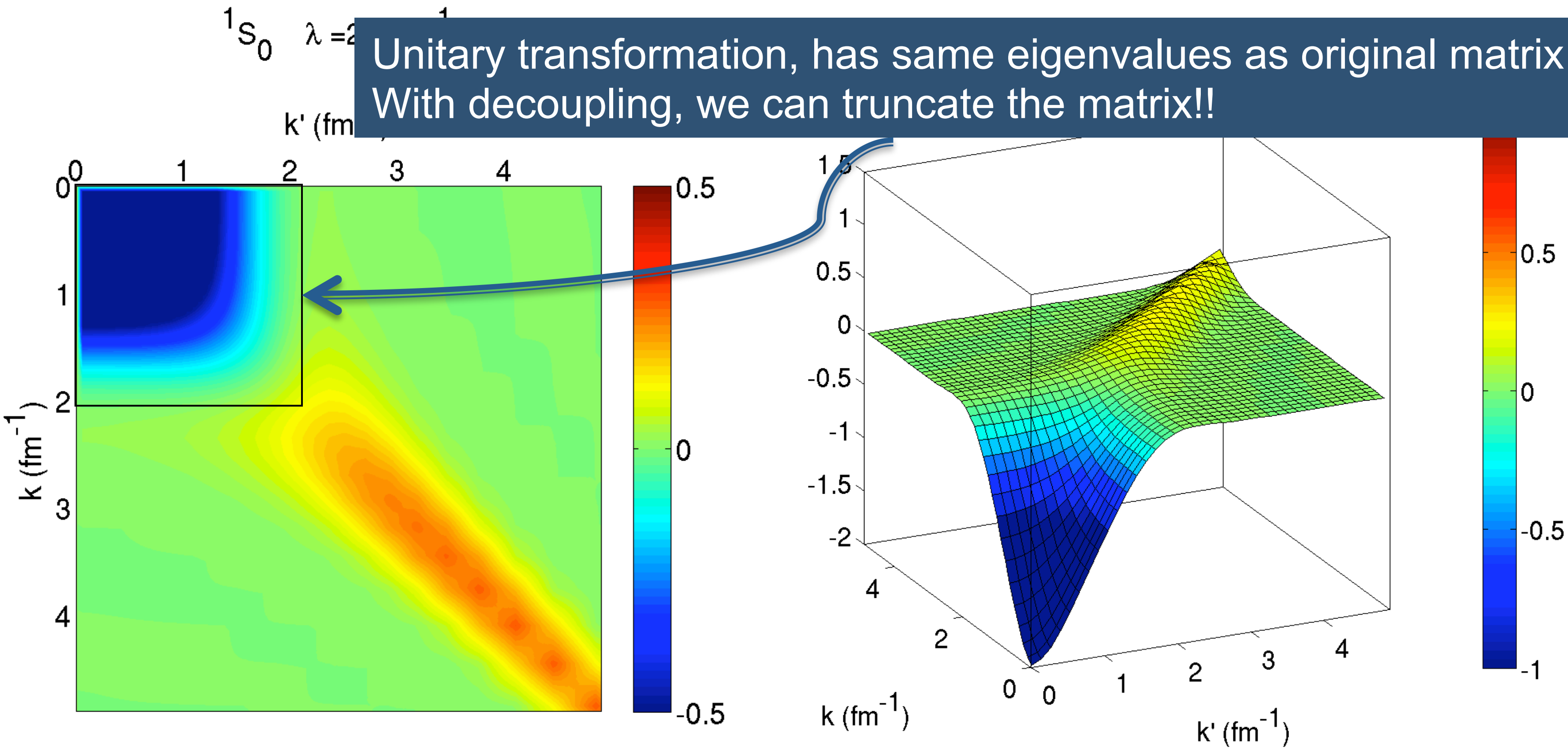




SRG evolves Hamiltonians unitarily

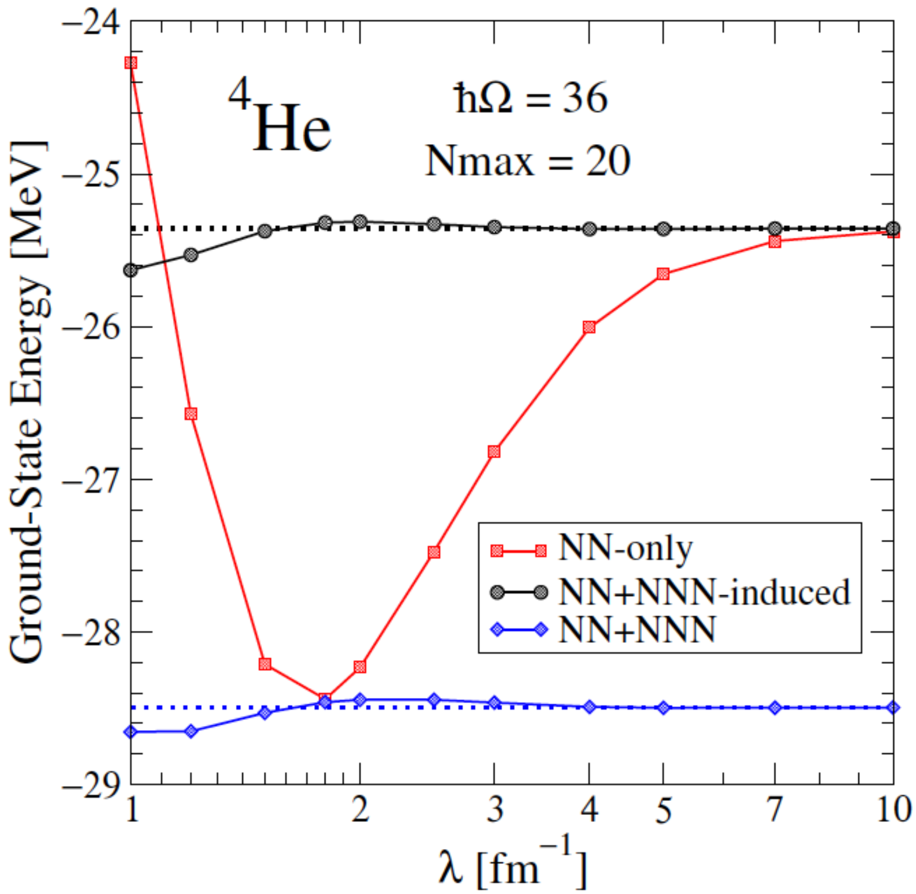
$$H_s = U_s H U_s^+ \Rightarrow \frac{dH_s}{ds} = \left[\left[T, H_s\right], H_s\right] \qquad \left(s = 1/\lambda^4\right)$$

Unitary transformation, has same eigenvalues as original matrix
With decoupling, we can truncate the matrix!!



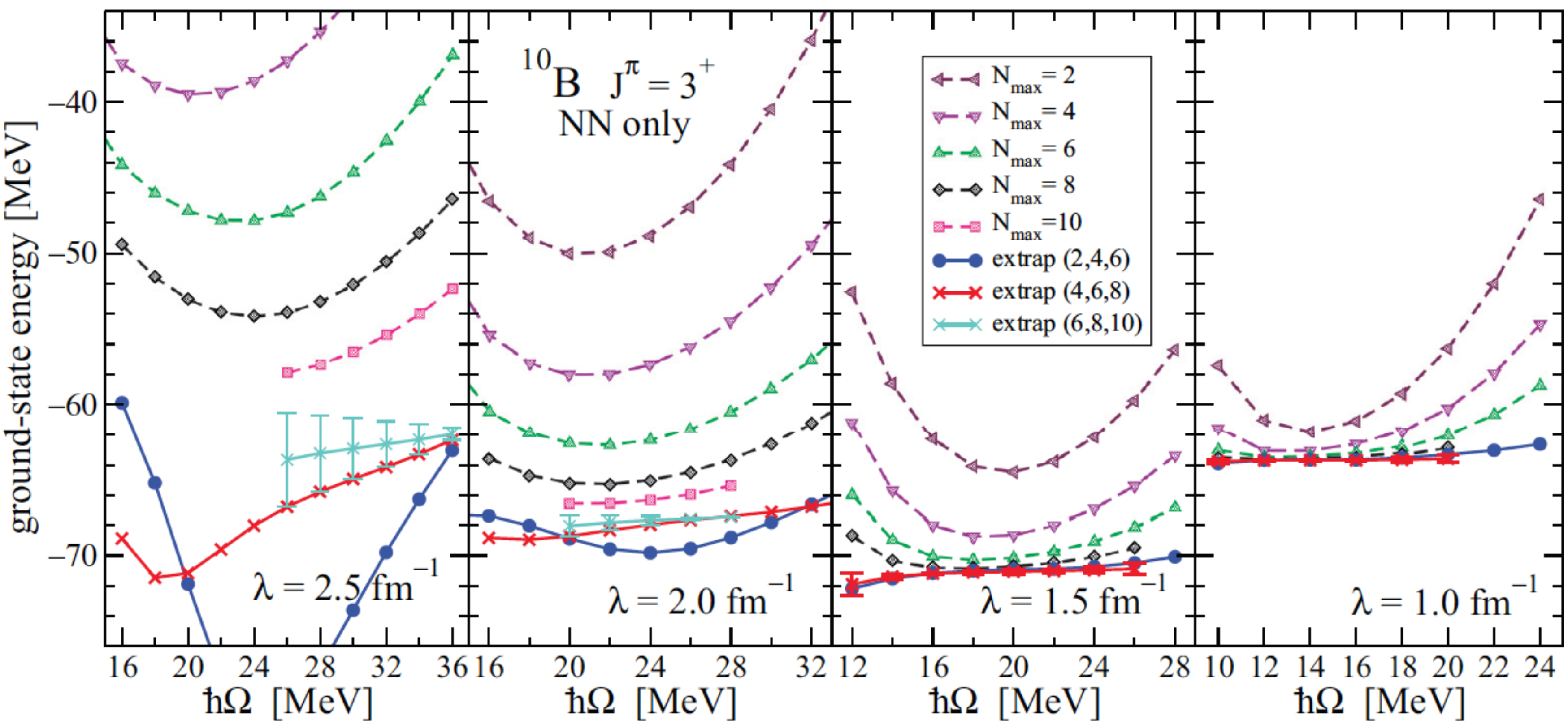
Unitarity behavior of SRG

- Results should be independent of λ
- SRG "softens" the potential making it possible to get converged results
  - BUT, there is no free-lunch
  - SRG procedure induces higher-body terms
  - Are they under control?



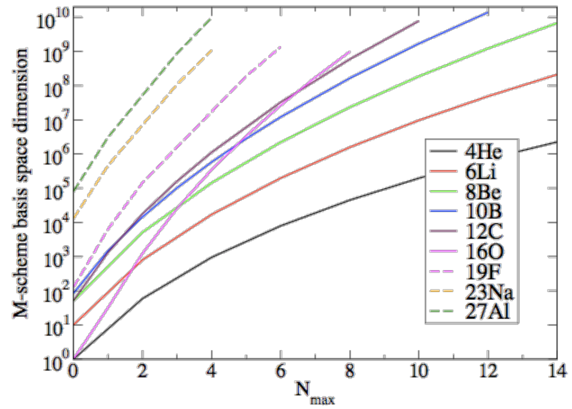
Many-body solutions

- Many-body calculations – calculate for λ, Ω, and N_{max}
  - For fixed N_{max} parabolas in
  - How do we extrapolate to $N_{max} \rightarrow \infty$

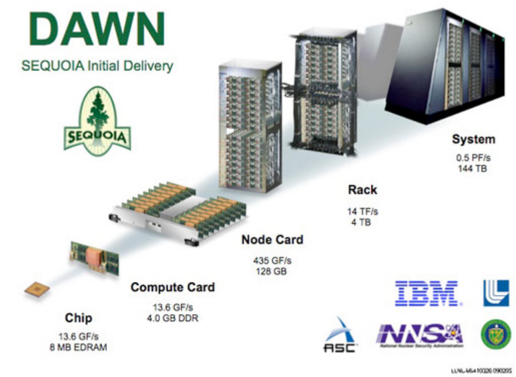


Quantum Many-body problem is fundamental to discovery science

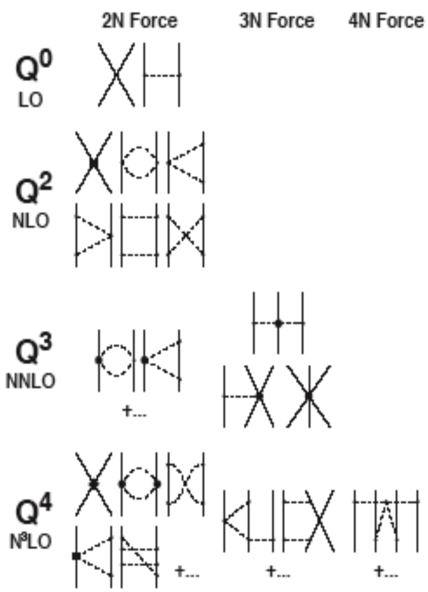
Large dimensions!

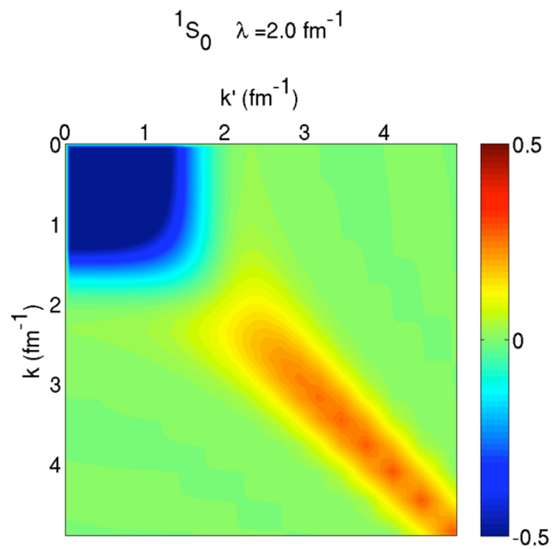


High-performance computing



Unknown interaction!

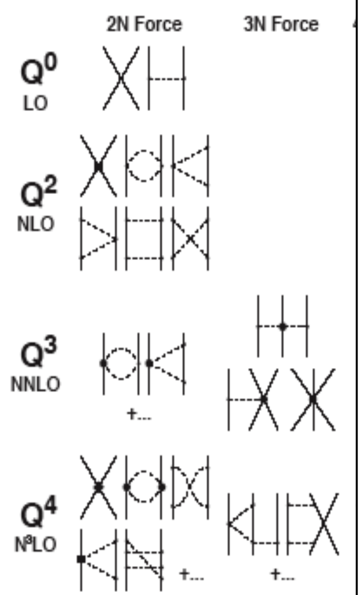


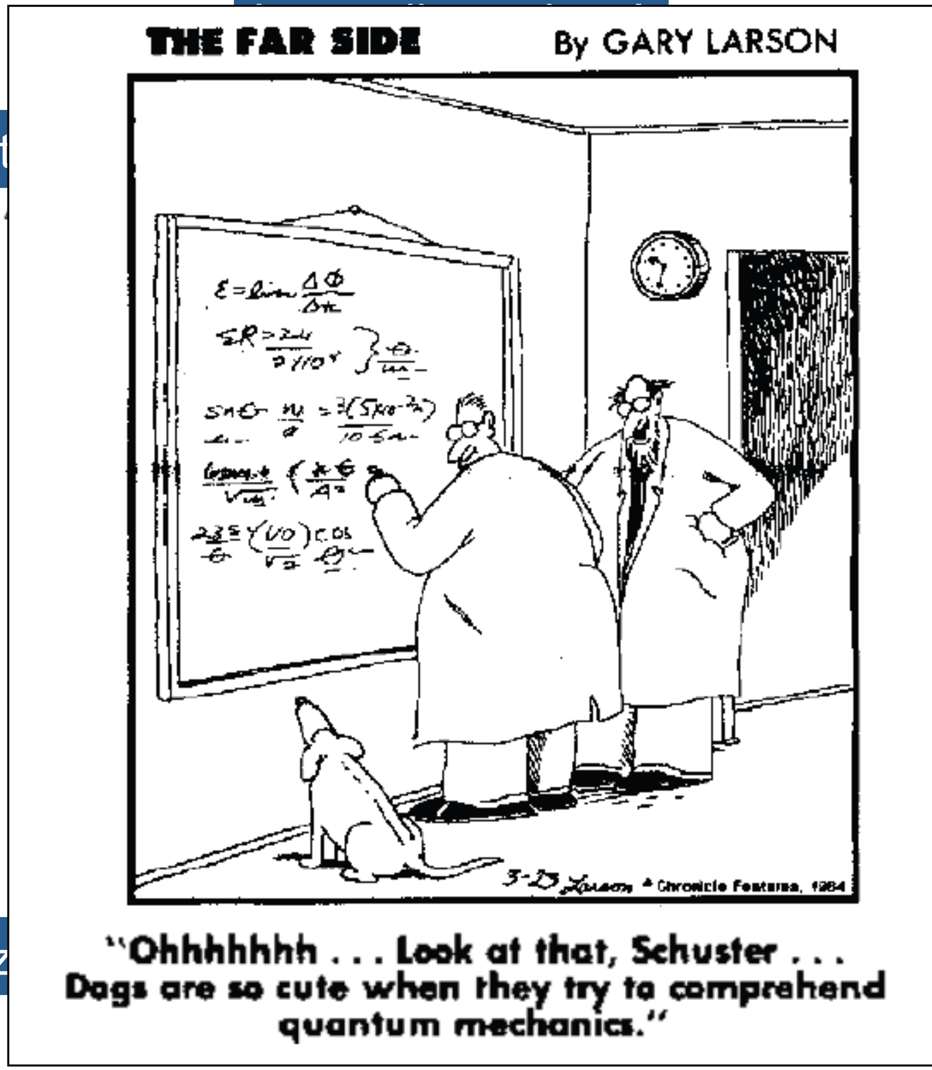


Renormalization

Quantum Many-body problem is fundamental to discovery science

Unknown interact





High-performance
computing

Renormaliz

Convergence – What is the solution?

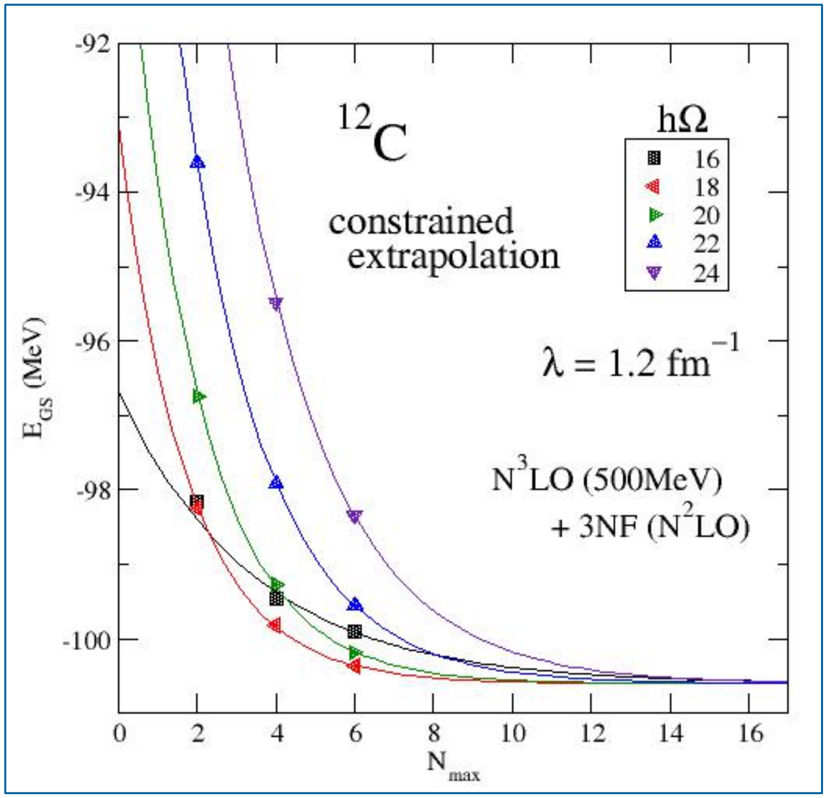
- It is clear that we need to extrapolate to large N_{max} and for hΩ
  - This is clearly a thorny issue and is a source of uncertainty
    - How do we quantify the uncertainty given that we don't know the answer
- Two issues
  - Exponential-like extrapolations to $N_{max} \rightarrow \infty$
  - Calculations to very large N_{max}: Importance truncation

Extrapolating to $N_{max} \rightarrow \infty$

- First approach

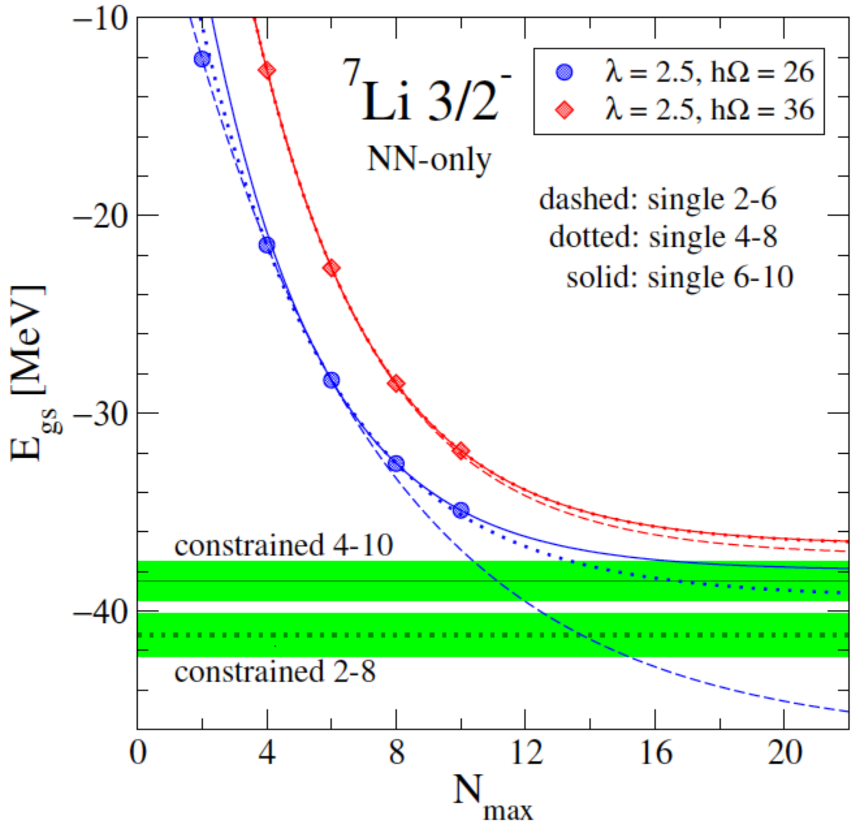
$$E_{\alpha i} = E_{\infty} + A_{\alpha} e^{-b_{\alpha} N_{\alpha i}}$$

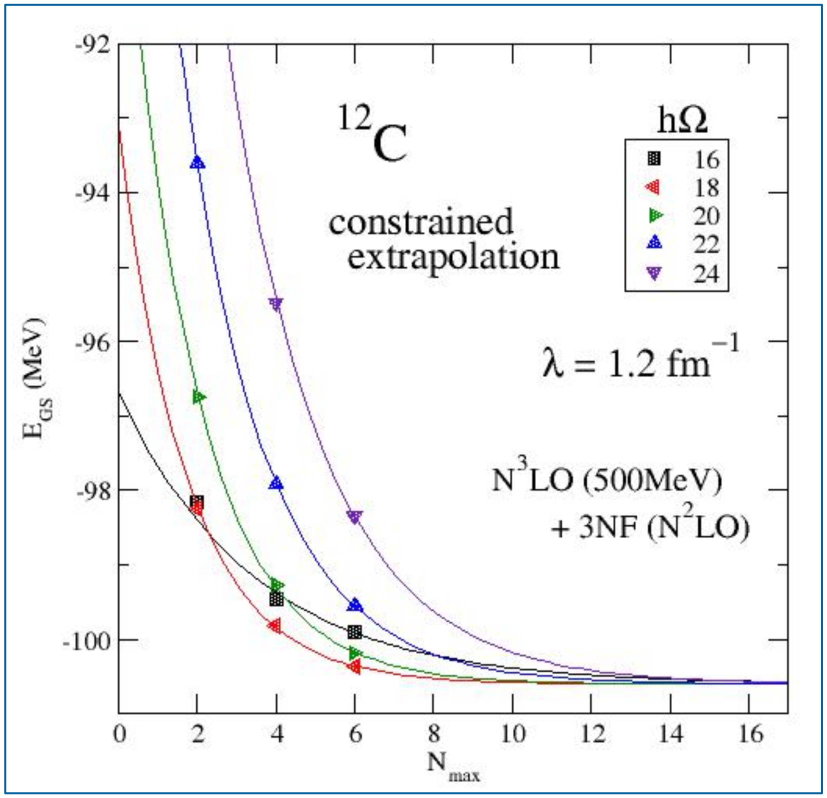
  - Fit to hΩ separately or constrain to same point
  - Fit to clusters of hΩ to estimate uncertainties



Extrapolating

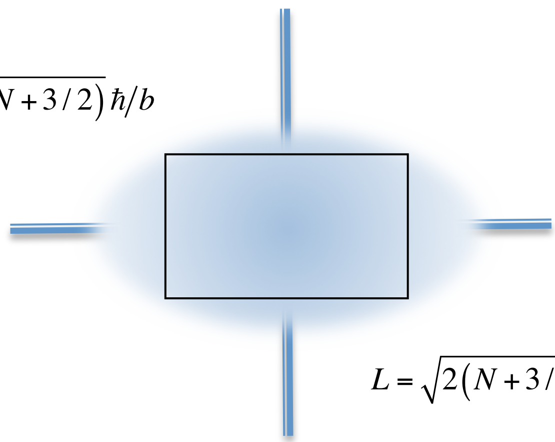
- Constrained fits





Extrapolations

- Large "uncertainty" for large values of λ and hΩ
- Analytic approach

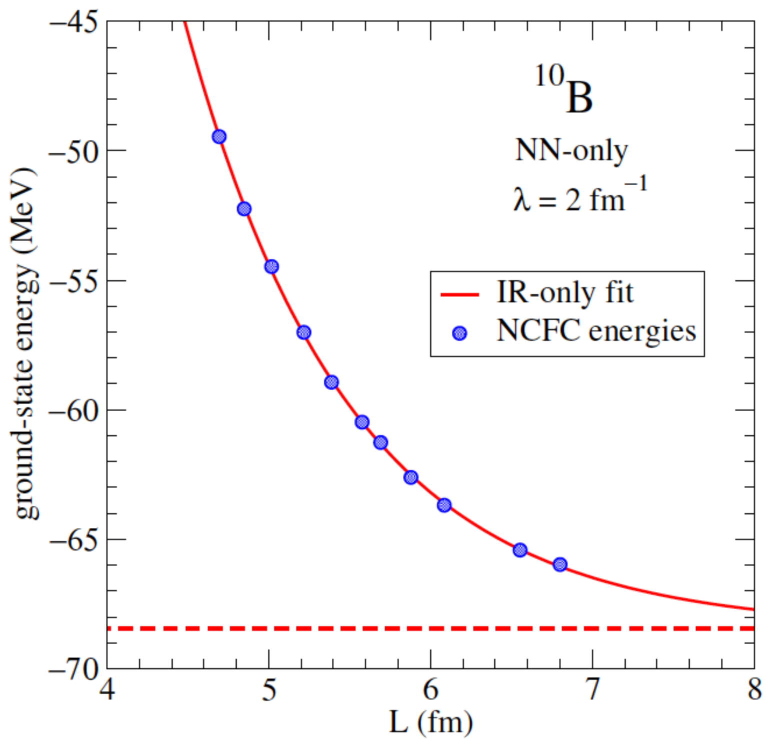


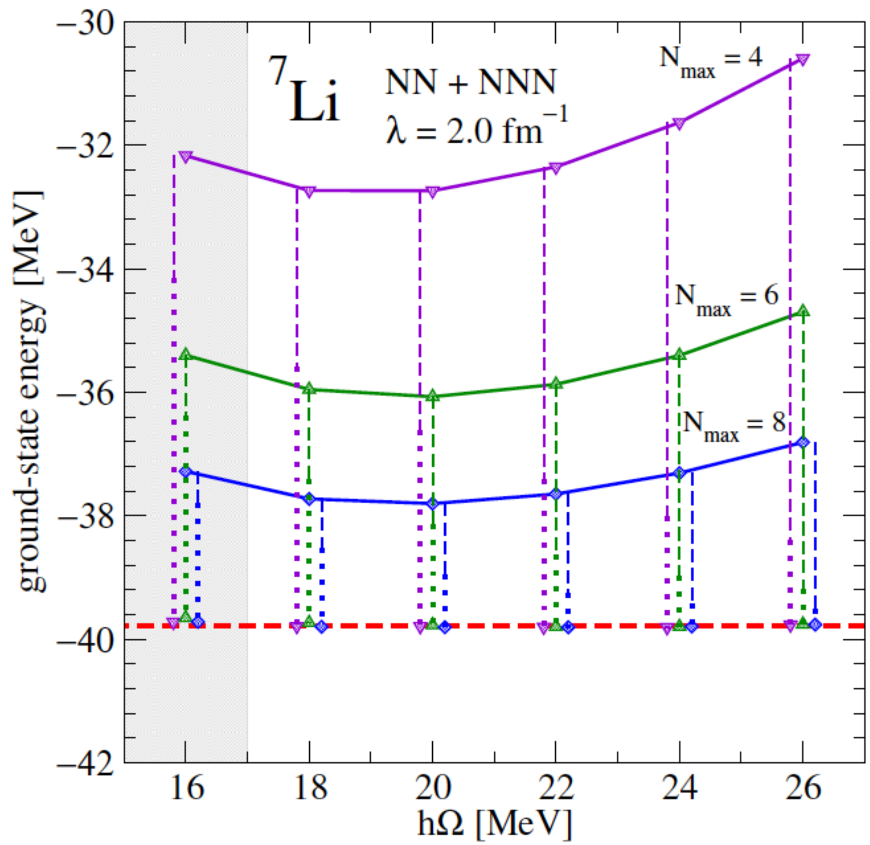
Ansatz for UV limit

$$E(\Lambda_{UV}, L) = E_\infty + B_0 e^{-\Lambda_{UV}^2/B_1^2} + B_2 e^{-k_\infty L}$$

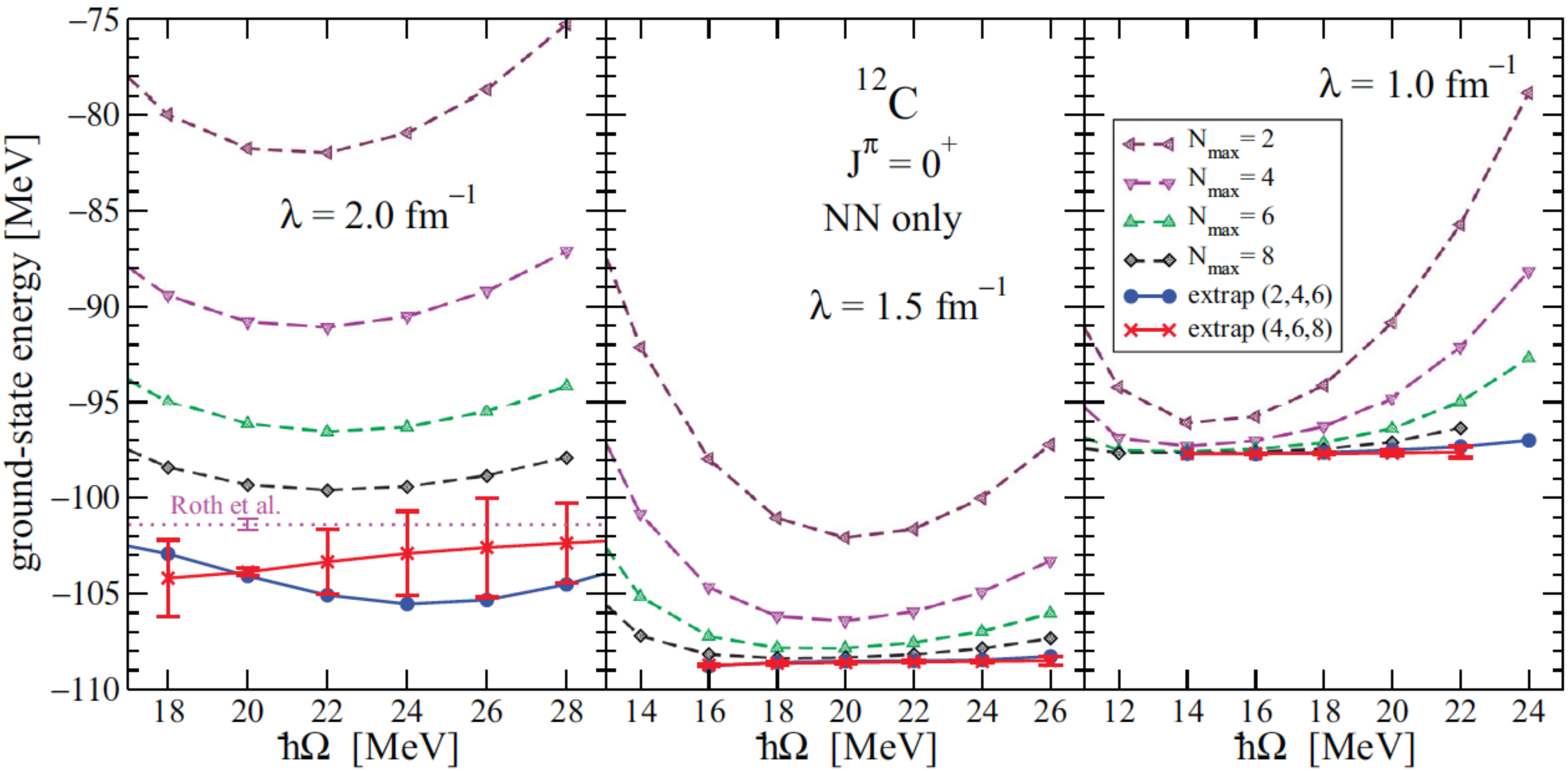
Analytic IR limit

Extrapolations with IR+UV limits

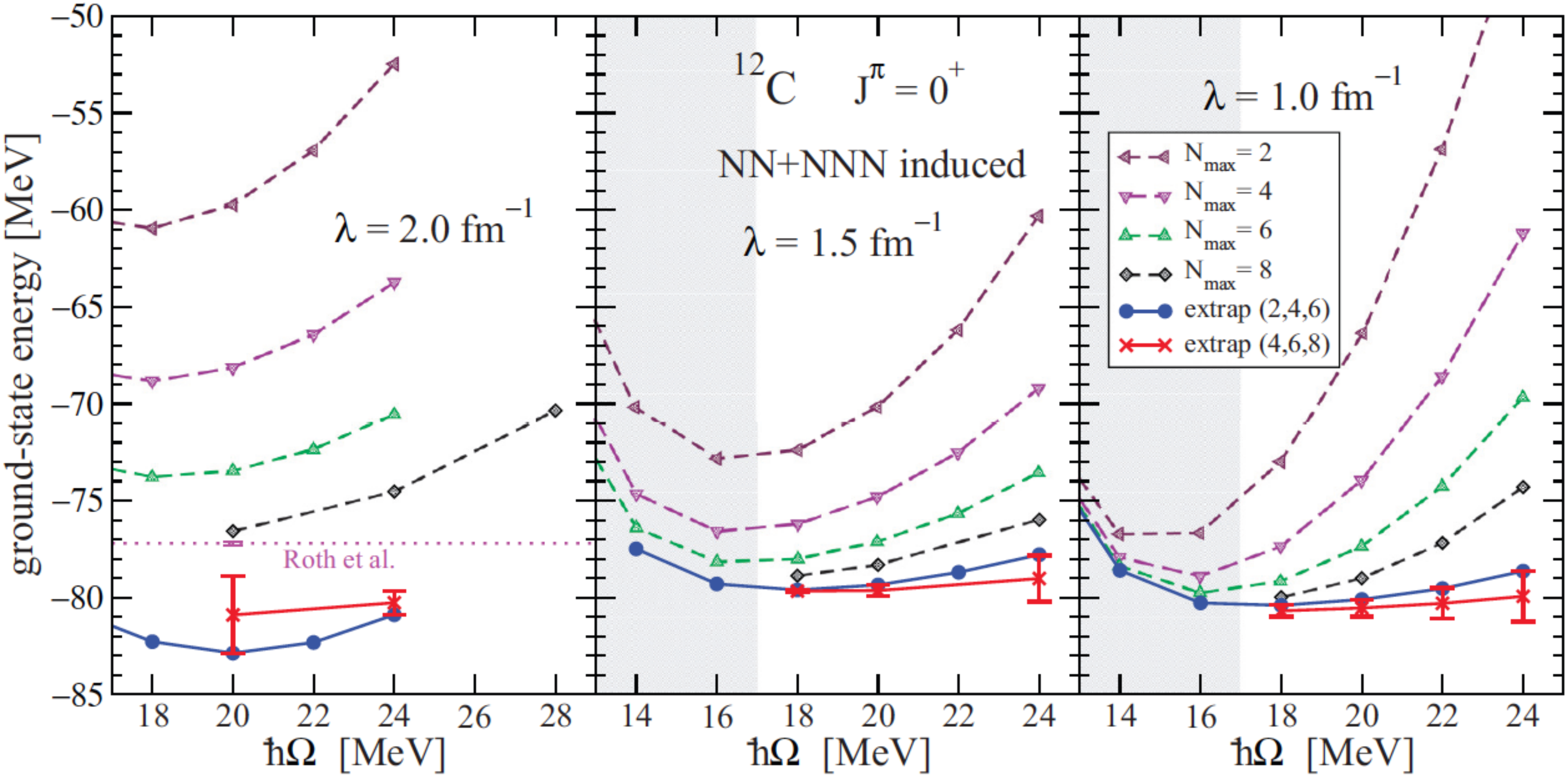




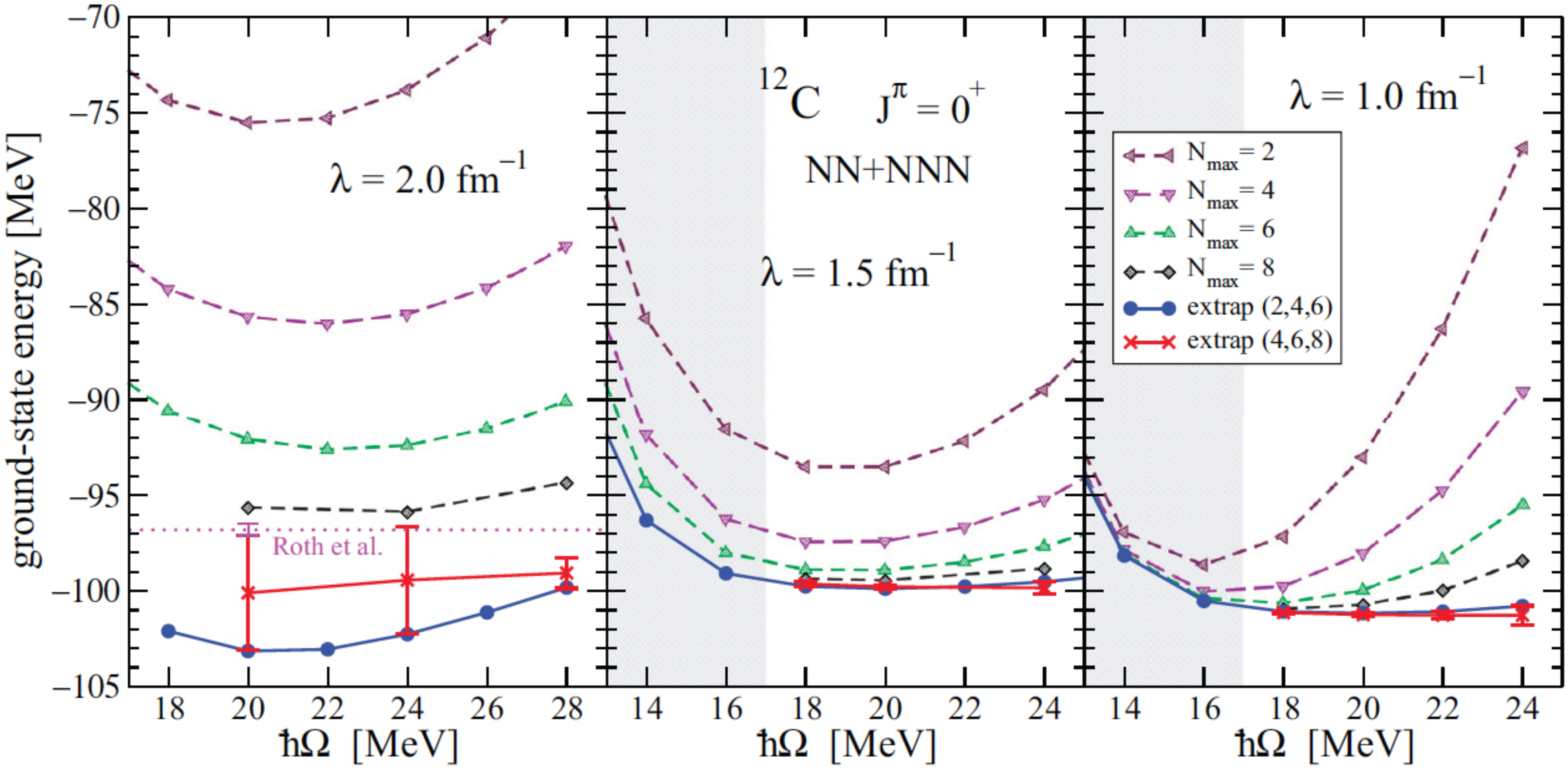
Many-body solutions



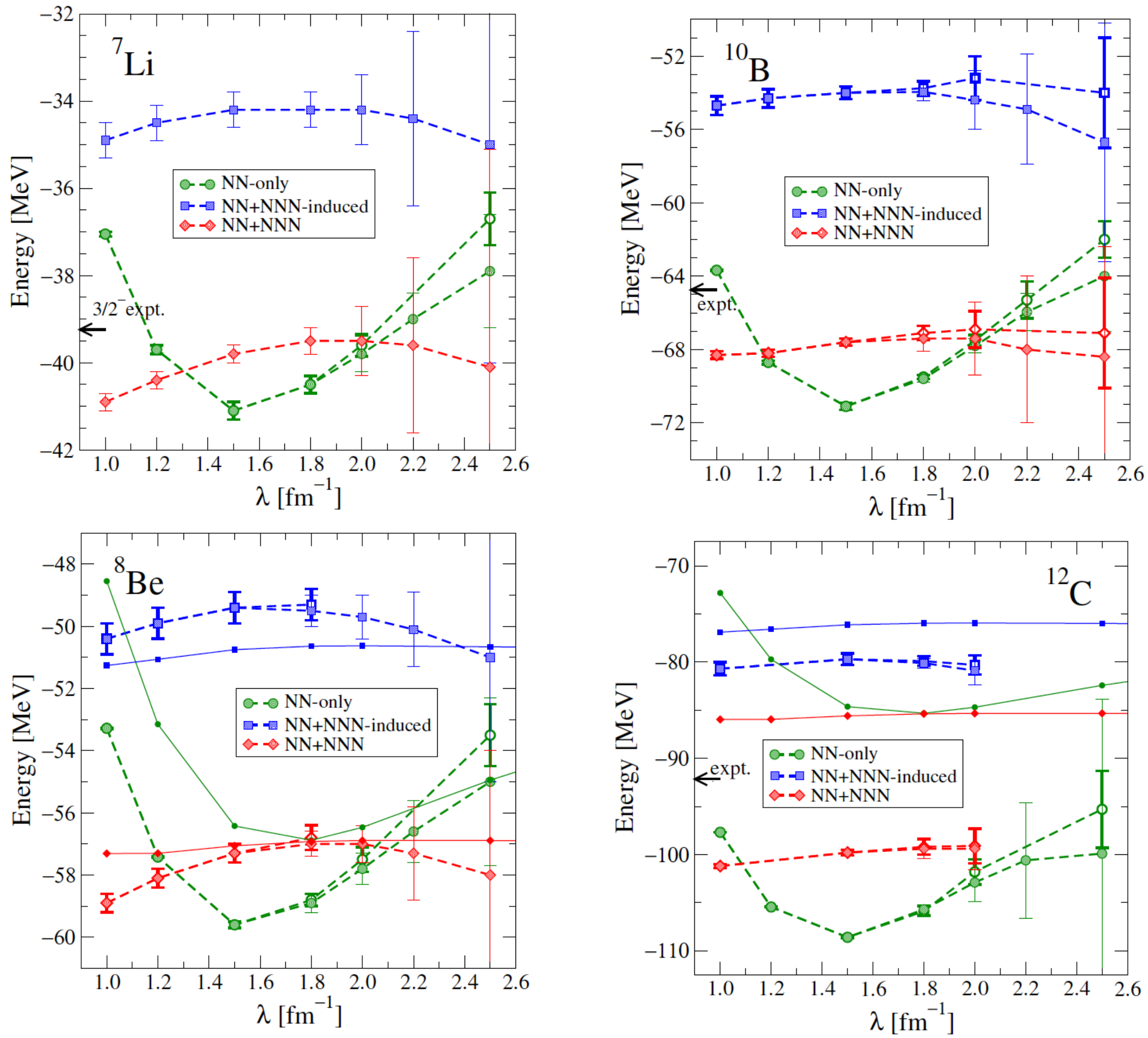
Many-body solutions



Many-body solutions



Full results



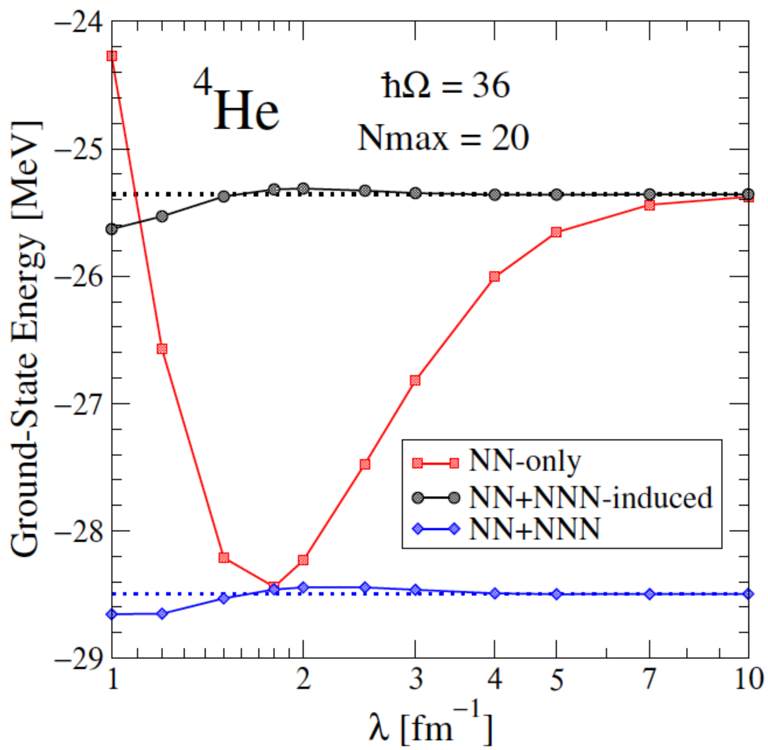
Three-body interaction – what does it do?

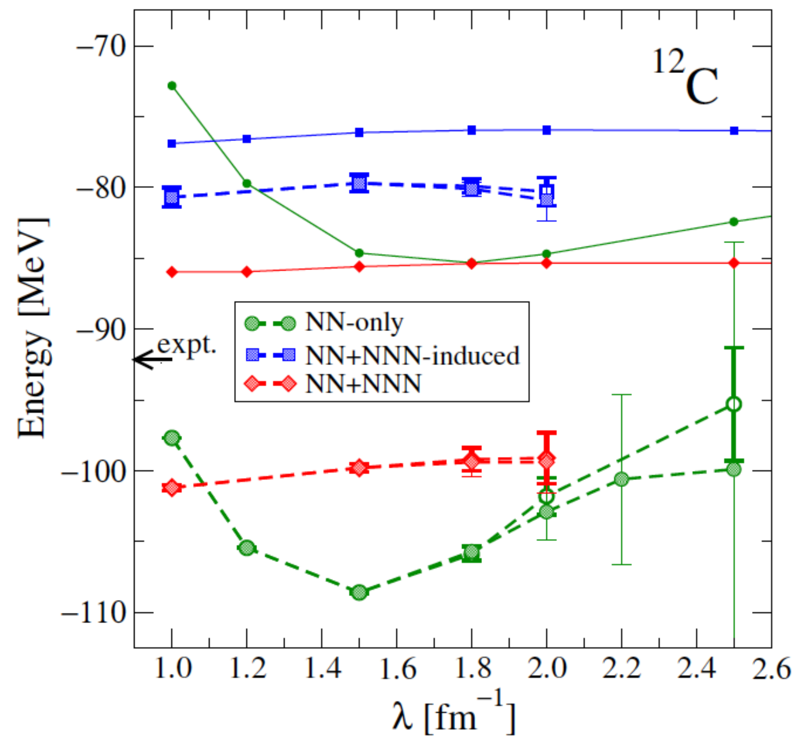
- Need to distinguish between induced and initial
  - Again, note that there is no single three-body interaction
    - Everything is effective
    - It depends on the NN interaction – non-local terms in NN can give more binding, and look like NNN

- NNN interaction
  - More binding
  - Spin-orbit properties

Three-body interaction – what does it do?

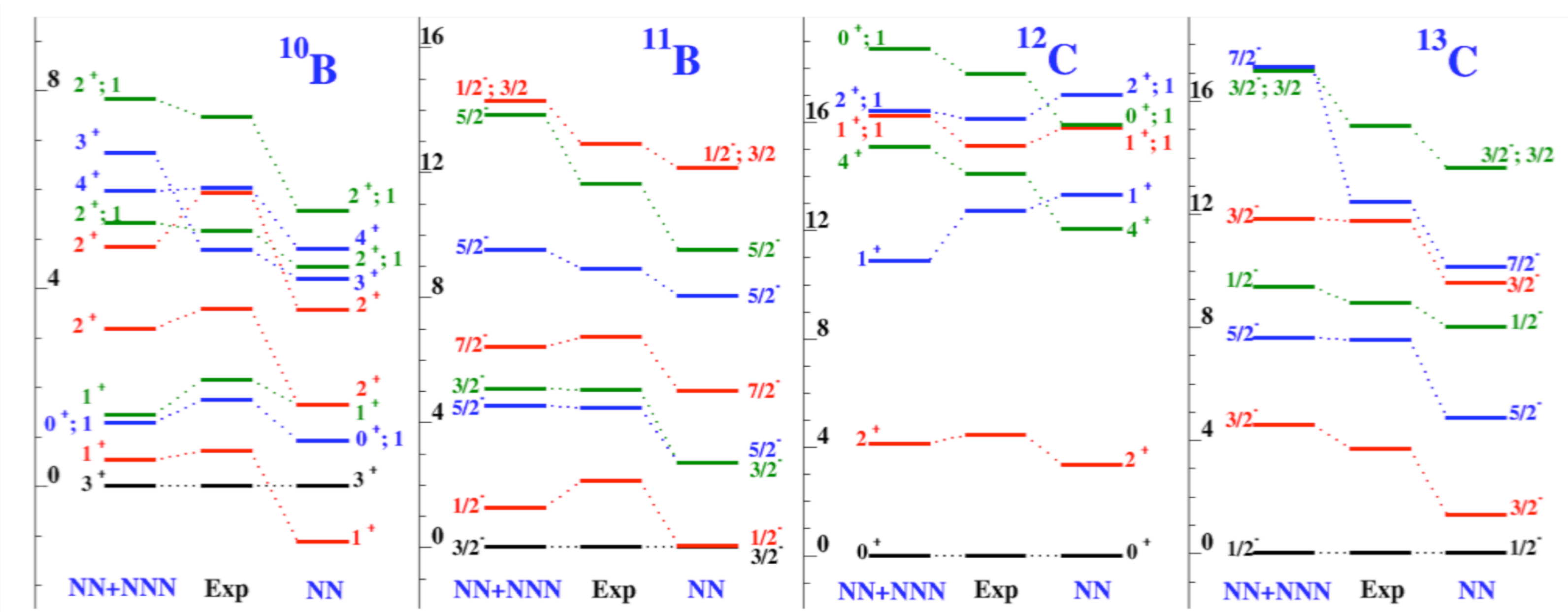
- More binding





Three-body interaction – what does it do?

Excitation energy spectra of ^{10}B, ^{11}B, ^{12}C, and ^{13}C



- Spin-orbit physics is coming from

- While the contact terms prevent collapse

Three-body interaction – what does it do?

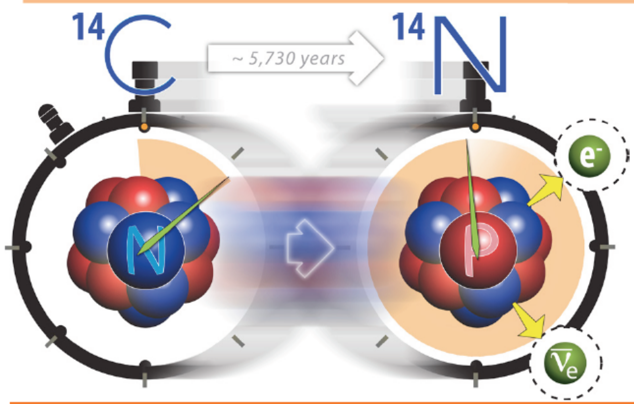
"Anomalous Long Lifetime of Carbon-14"

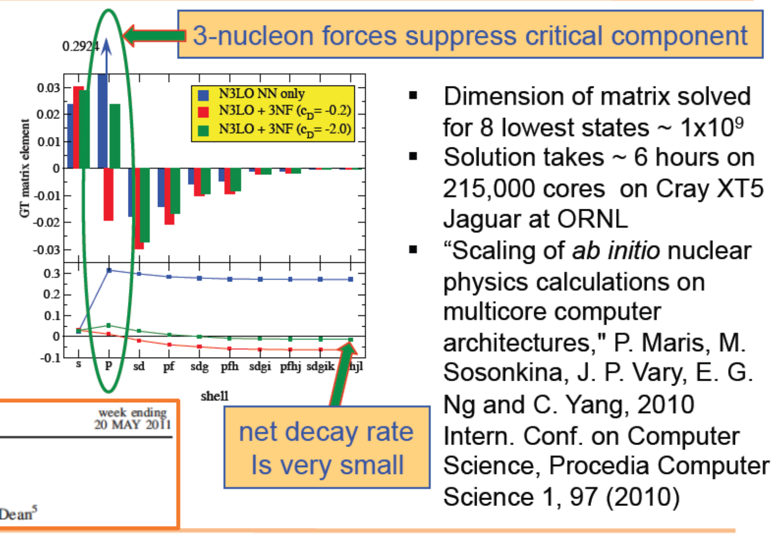
Objectives

- Solve the puzzle of the long but useful lifetime of ^{14}C
- Determine the microscopic origin of the suppressed β-decay rate

Impact

- Establishes a major role for strong 3-nucleon forces in nuclei
- Verifies accuracy of *ab initio* microscopic nuclear theory
- Provides foundation for guiding DOE-supported experiments





- Dimension of matrix solved for 8 lowest states ~ 1×10^9
- Solution takes ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL
- "Scaling of *ab initio* nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97 (2010)

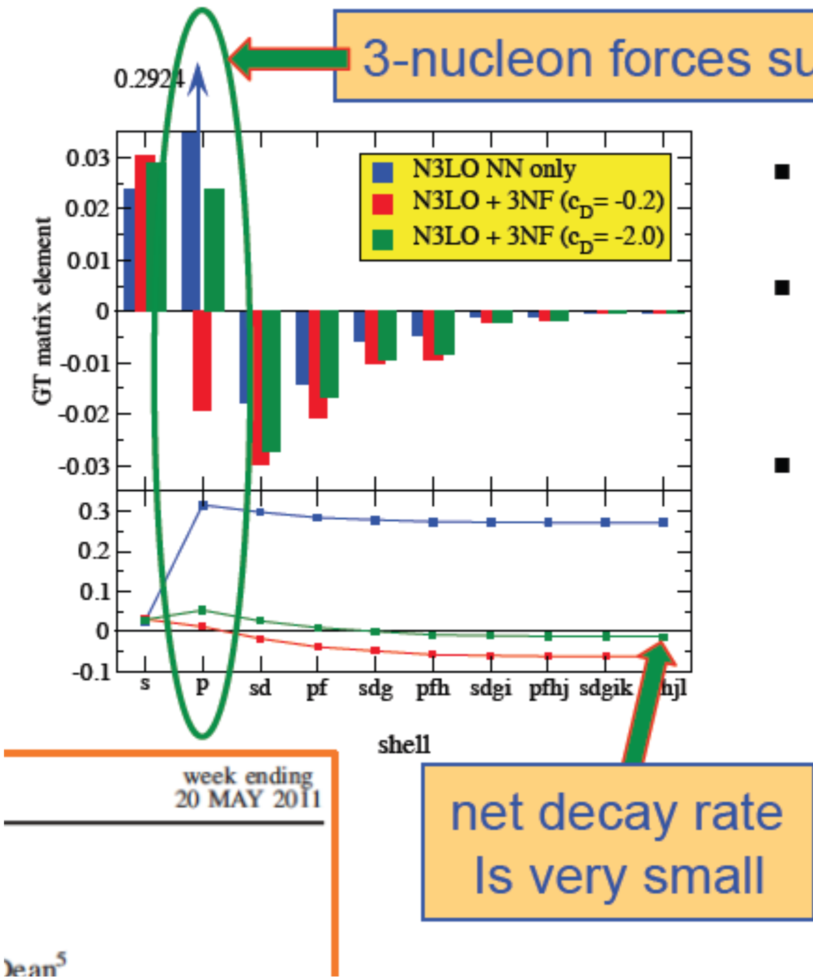
PRL 106, 202502 (2011) PHYSICAL REVIEW LETTERS week ending 20 MAY 2011

Origin of the Anomalous Long Lifetime of ^{14}C

P. Maris,[1] J. P. Vary,[1] P. Navrátil,[2,3] W. E. Ormand,[3,4] H. Nam,[5] and D. J. Dean[5]

U.S. DEPARTMENT OF ENERGY | Office of Science | INCITE | IOWA STATE UNIVERSITY | TRIUMF | UNEDF SciDAC Collaboration – Universal Nuclear Energy Density Functional | NNSA | OAK RIDGE NATIONAL LABORATORY

Three-body interaction – what does it do?



- Dimension of matrix solved for 8 lowest states ~ $1x10^9$
- Solution takes ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL
- "Scaling of *ab initio* nuclear physics calculations on multicore computer architectures," P. Maris, M. Sosonkina, J. P. Vary, E. G. Ng and C. Yang, 2010 Intern. Conf. on Computer Science, Procedia Computer Science 1, 97 (2010)

NCSM is great, but not enough to describe scattering and reactions

- Nuclei exhibit bound states, resonances, scattering states
  - Structure properties affected by many-body continuum of scattering and decay channels
  - Scattering and reaction properties affected by many-body structure of interacting nuclei
- *Ab initio* NCSM

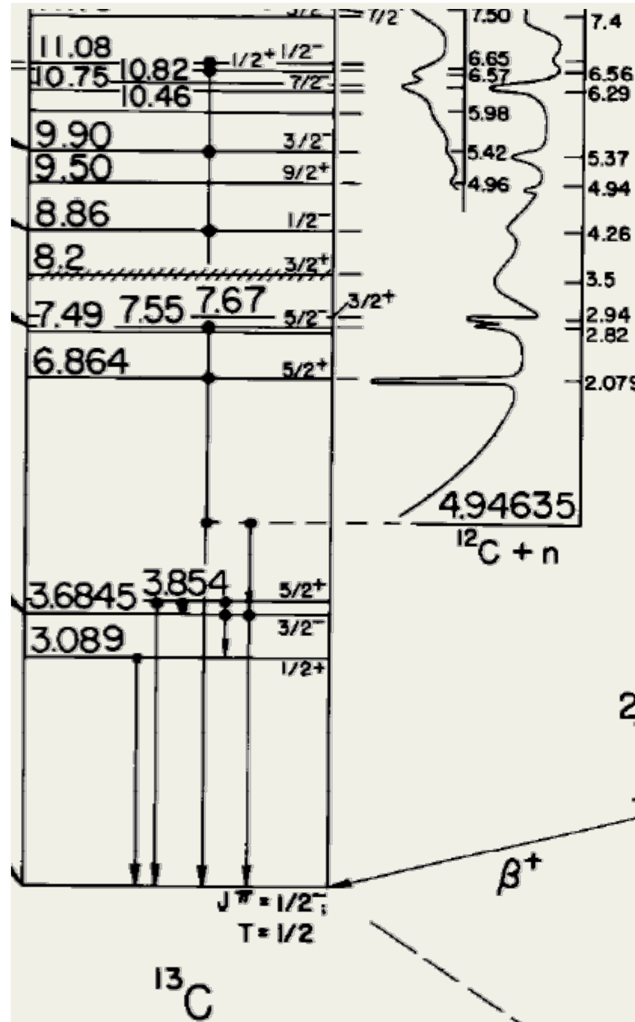
  ☺ Discrete spectrum OK

  — Bound states, narrow resonances

  ☹ No continuum spectrum!

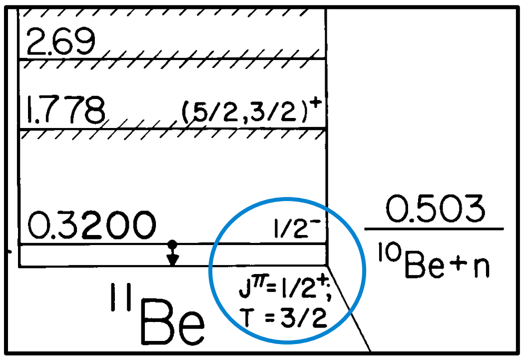
  — Incorrect asymptotic behavior

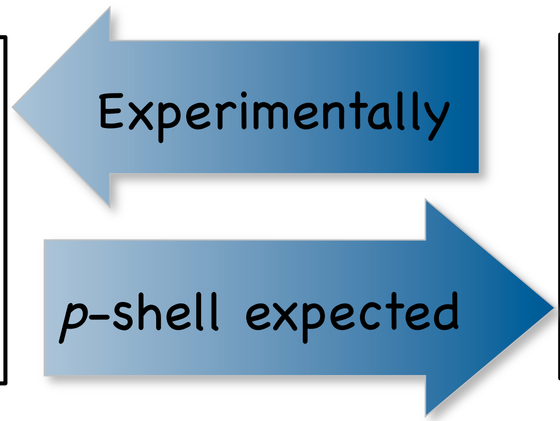
  — No dynamic properties (all states bound)

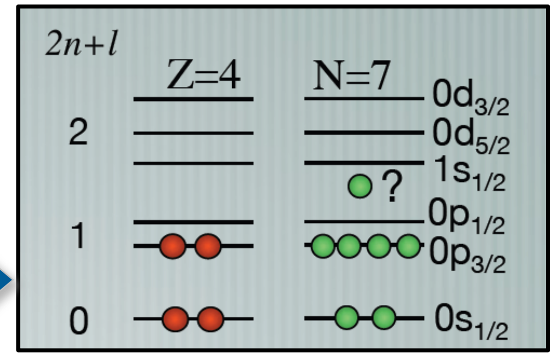


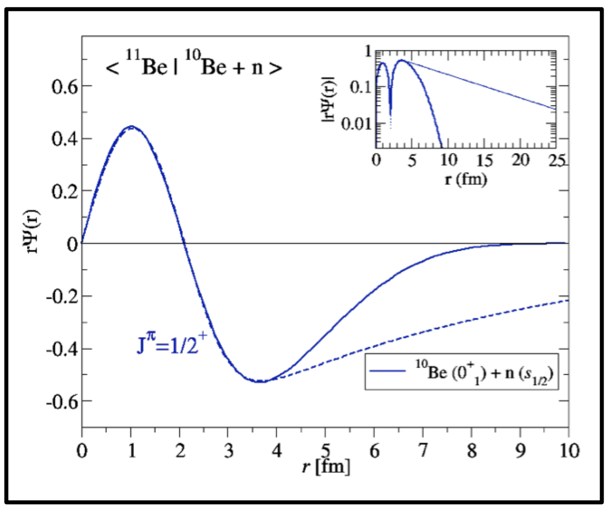
Parity-inverted ground state of ^{11}Be

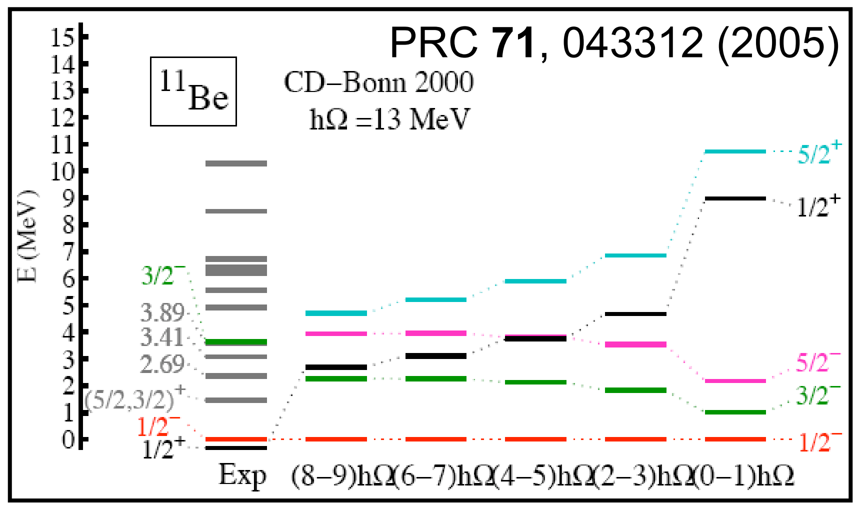
- Disappearance of N=8 magic number with increasing N/Z ratio











Resonating Group Method (RGM) - history

- Proposed in 1937 by Wheeler (following the discovery of the neutron in 1932 and the proposal of the shell model in 1933)
  - Nucleons in nuclei spend fractions of their time in various substructures or clusters
- Physical interpretation in 1958 by Wildermuth & Kanellopoulus (nuclear shell model well established)
  - Because of their on-average attractive nature, nuclear forces give rise to correlations that manifest itself through formation of clusters
  - When clusters overlap, RGM and shell model wave functions can be very similar after antisymmetrization
  - When clusters are separated, RGM wave functions can include correlations not naturally described by shell model wave functions

Resonating Group Method (RGM) - features

Microscopic method which explicitly takes cluster correlations into account

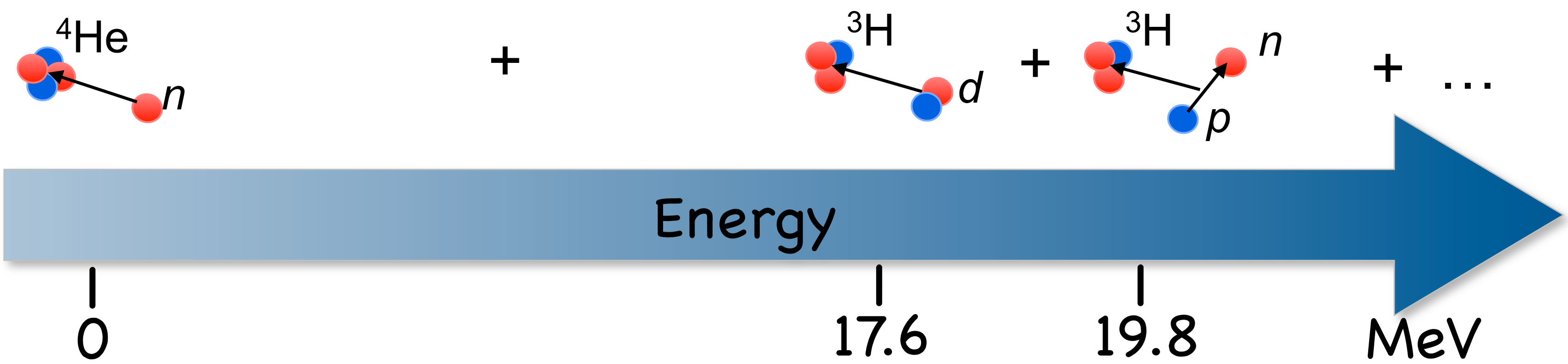
- Solve Schrödinger equation associate with a microscopic Hamiltonian

$$H_{\text{int}}^{(A)} = \frac{1}{A} \sum_{i<j=1}^{A} \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j=1}^{A} V_{ij}^{2b} + \left(\sum_{i<j<k=1}^{A} V_{ijk}^{3b} \right)$$

- Employs totally antisymmetric wave functions: Pauli exclusion principle treated exactly
- Treats nuclear bound states, scattering and reactions within a unified framework
- Can describe reactions with arbitrary composite nuclei in the incoming and outgoing channels

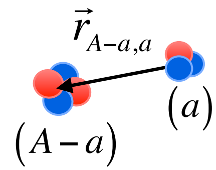
Example: the five-nucleon system

- Consider the T = ½ case: ^{5}He (^{5}Li)
  - Five-nucleon cluster unbound; ^{4}He tightly bound, not easy to deform



- Satisfactory description of *n*-^{4}He (*p*-^{4}He) scattering at low excitation energies within single-channel approximation
- However, both *n*(*p*) + ^{4}He and *d* + ^{3}H(^{3}He) channels needed to describe ^{3}H(*d*,*n*)^{4}He [^{3}He(*d*,*p*)^{4}He] fusion!

Binary cluster Resonating Group Method



- Working in partial waves ($\nu \equiv \{A-a\ \alpha_1 I_1^{\pi_1} T_1; a\ \alpha_2 I_2^{\pi_2} T_2; s\ell\}$)

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{g_\nu^{J^\pi T}(r)}{r} \hat{A}_\nu \left[\left(\underbrace{\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle}_{\text{Target}} \underbrace{\left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle}_{\text{Projectile}} \right)^{(sT)} Y_\ell(\hat{r}) \right]^{(J^\pi T)} \delta(\vec{r} - \vec{r}_{A-a,a})\ r^2 dr\, d\hat{r}$$

- Now introduce partial wave expansion of delta function

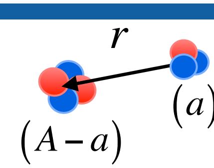
$$\delta(\vec{r} - \vec{r}_{A-a,a}) = \sum_{\lambda\mu} \frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}} Y_{\lambda\mu}^*(\hat{r}) Y_{\lambda\mu}(\hat{r}_{A-a,a})$$

- After integration in the solid angle one obtains:

$$\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{g_\nu^{J^\pi T}(r)}{r} \underbrace{\hat{A}_\nu \left[\left(\left|A-a\ \alpha_1 I_1^{\pi_1} T_1\right\rangle \left|a\ \alpha_2 I_2^{\pi_2} T_2\right\rangle \right)^{(sT)} Y_\ell(\hat{r}_{A-a,a}) \right]^{(J^\pi T)} \frac{\delta(r - r_{A-a,a})}{r r_{A-a,a}}}_{\left|\Phi_{\nu r}^{J^\pi T}\right\rangle \text{ (Jacobi) channel basis}} r^2 dr$$

Binary cluster RGM equations

- Trial wave function: $\left|\psi^{J^\pi T}\right\rangle = \sum_\nu \int \frac{g_\nu^{J^\pi T}(r)}{r} \hat{A}_\nu \left|\Phi_{\nu r}^{J^\pi T}\right\rangle r^2 dr$



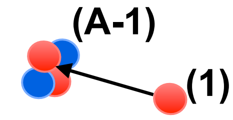
- Projecting the Schrödinger equation on the channel basis yields:

$$\sum_\nu \int \Big[\underbrace{H_{\nu'\nu}^{J^\pi T}(r',r)}_{\left\langle \Phi_{\nu' r'}^{J^\pi T} \left| \hat{A}_{\nu'} H \hat{A}_\nu \right| \Phi_{\nu r}^{J^\pi T} \right\rangle} - E\, \underbrace{N_{\nu'\nu}^{J^\pi T}(r',r)}_{\left\langle \Phi_{\nu' r'}^{J^\pi T} \left| \hat{A}_{\nu'} \hat{A}_\nu \right| \Phi_{\nu r}^{J^\pi T} \right\rangle} \Big] \frac{g_\nu^{J^\pi T}(r)}{r}\, r^2\, dr = 0$$

Hamiltonian kernel

Overlap (or norm) kernel

- Breakdown of approach:
  1. Build channel basis states from input target and projectile wave functions
  2. Calculate Hamiltonian and norm kernels
  3. Solve RGM equations: find unknown relative motion wave functions
     - Bound-state / scattering boundary conditions



Norm Kernel

$$\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) = \delta_{\mu\nu}\,\delta_{\ell'\ell}\frac{\delta(r'-r)}{r'r} - (A-1)\sum_{n'n} R_{n'\ell'}(r')\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle R_{n\ell}(r)$$

$$\langle\Phi^{(A-1,1)JT}_{\mu n'\ell'}|P_{A,A-1}|\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle$$

$$= \sum_{n'_{A-1}\ell'_{A-1}\mathcal{J}'_{A-1}} \langle A-1\,\alpha' I'_1 T'_1|[N_{A-2} i_{A-2} J_{A-2} T_{A-2}; n'_{A-1}\ell'_{A-1}\mathcal{J}'_{A-1}]\, I'_1 T'_1\rangle$$

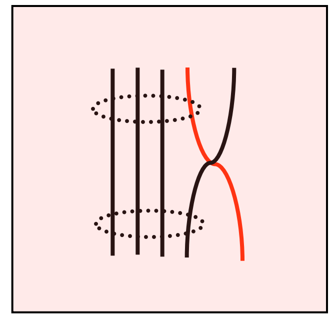
$$\times \sum_{n_{A-1}\ell_{A-1}\mathcal{J}_{A-1}} \langle [N_{A-2} i_{A-2} J_{A-2} T_{A-2}; n_{A-1}\ell_{A-1}\mathcal{J}_{A-1}]\, I_1 T_1|A-1\,\alpha I_1 T_1\rangle$$

$$\times\, \hat{T}'_1\hat{T}_1(-)^{1+T'_1+T_1}\begin{Bmatrix} \frac{1}{2} & T_{A-2} & T_1 \\ \frac{1}{2} & T & T'_1 \end{Bmatrix} \hat{s}'\hat{s}\hat{I}'_1\hat{I}_1\hat{\mathcal{J}}'_{A-1}\hat{\mathcal{J}}_{A-1}(-)^{s'+s+\ell+\ell'_{A-1}}$$

$$\times \sum_{L,Z}\hat{L}^2\hat{Z}^2(-)^L\begin{Bmatrix} \mathcal{J}'_{A-1} & J_{A-2} & I'_1 \\ \mathcal{J}_{A-1} & Z & I_1 \end{Bmatrix}\begin{Bmatrix} \ell'_{A-1} & \frac{1}{2} & \mathcal{J}'_{A-1} \\ I_1 & Z & s \end{Bmatrix}\begin{Bmatrix} \ell_{A-1} & \frac{1}{2} & \mathcal{J}_{A-1} \\ I'_1 & Z & s' \end{Bmatrix}$$

$$\times \begin{Bmatrix} L_2 & \ell'_{A-1} & \ell' \\ \ell_{A-1} & Z & s' \\ \ell & s & J \end{Bmatrix}\langle n'\ell', n'_{A-1}\ell'_{A-1}, L|n_{A-1}\ell_{A-1}, n\ell, L\rangle_{A(A-2)}$$

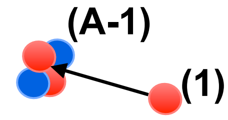
Jacobi coordinate derivation



$A > 3$

$\mu = \{\alpha' I'_1 T'_1 s'\}$

$\nu = \{\alpha I_1 T_1 s\}$



Norm Kernel

$$\mathcal{N}^{(A-1,1)}_{\mu\ell',\nu\ell}(r',r) = \delta_{\mu\nu}\,\delta_{\ell'\ell}\frac{\delta(}{\ldots} \quad \ldots \quad |\Phi^{(A-1,1)JT}_{\nu n\ell}\rangle R_{n\ell}(r)$$

$$\langle\Phi^{(A-1,1}_{\mu n'\ell'} \ldots$$

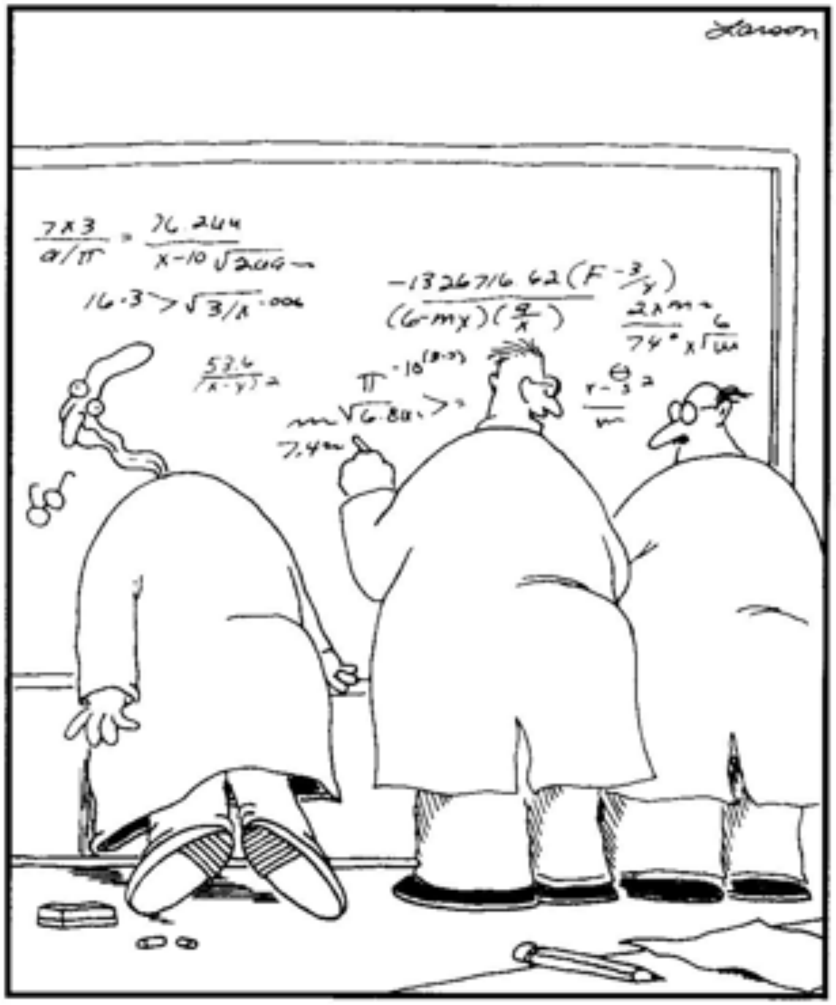
$$= \sum_{n'_{A-1}\ell'_{A-1}\mathcal{J}'_{A-1}} \langle A-1\alpha' I'_1 T \ldots$$

$$\times \sum_{n_{A-1}\ell_{A-1}\mathcal{J}_{A-1}} \langle [N_{A-2} i_{A-2} J \ldots$$

$$\times \hat{T}'_1\hat{T}_1(-)^{1+T'_1+T_1}\begin{Bmatrix}\frac{1}{2} & T_A \ldots \\ \frac{1}{2} & \ldots\end{Bmatrix}$$

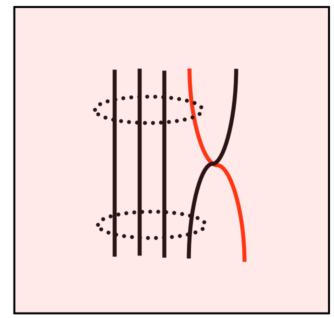
$$\times \sum_{L,Z}\hat{L}^2\hat{Z}^2(-)^L\begin{Bmatrix}\mathcal{J}'_{A-1} & \ldots \\ \mathcal{J}_{A-1} & \ldots\end{Bmatrix}$$

$$\times \begin{Bmatrix} L_2 & \ell'_{A-1} & \ell' \\ \ell_{A-1} & Z & s' \\ \ell & s & J \end{Bmatrix} \langle n'\ell' \ldots$$



"Ha! Webster's blown his cerebral cortex."

Jacobi coordinate derivation



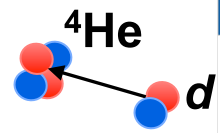
$A > 3$

$\mu = \{\alpha' I'_1 T'_1 s'\}$

$\nu = \{\alpha I_1 T_1 s\}$

Convergence with respect to RGM model space

- NCSM/RGM describes binary reactions (below three-body breakup threshold)

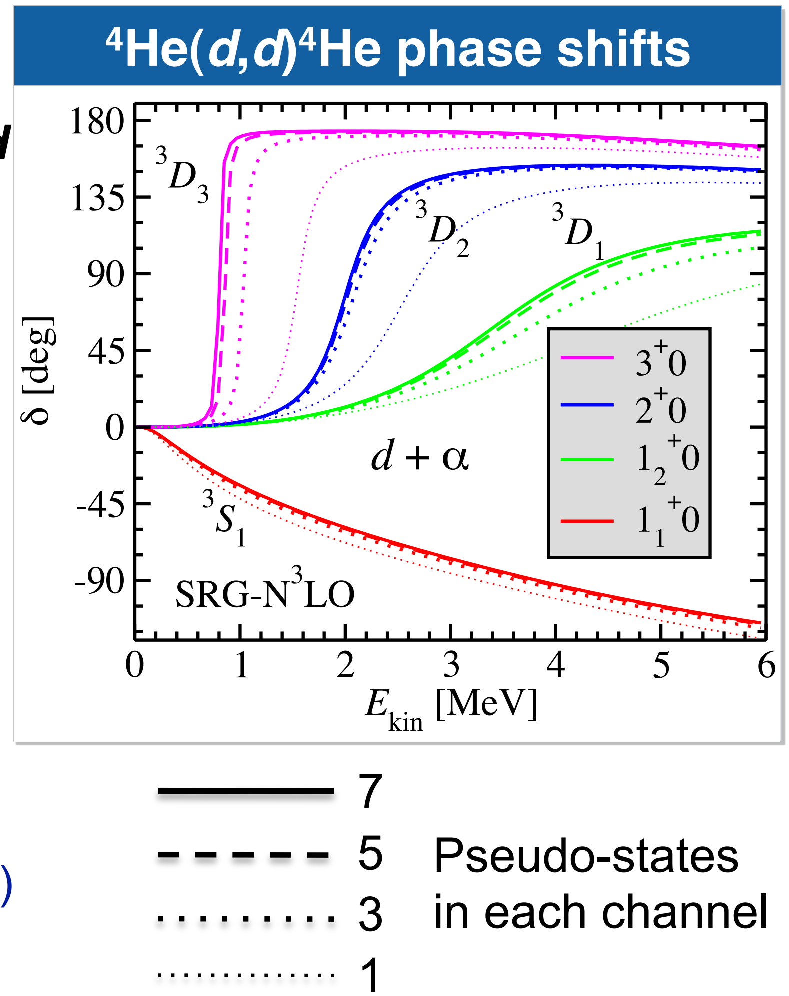


- If projectile (or target) can be easily deformed or broken apart
  - Need to account for virtual breakup
  - Approximate treatment:

    Include multiple excited (pseudo-) states of the clusters
  - Exact treatment:

    1) Inclusion of three-body clusters

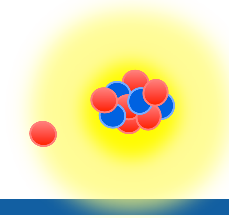
    2) Solution of three-body scattering



- Here:
  - d(g.s.,$^3S_1$-$^3D_1$, $^3D_2$, $^3D_3$-$^3G_3$) + ^{4}He(g.s.)
  - SRG-N^{3}LO NN potential (λ = 1.5 fm^{-1})

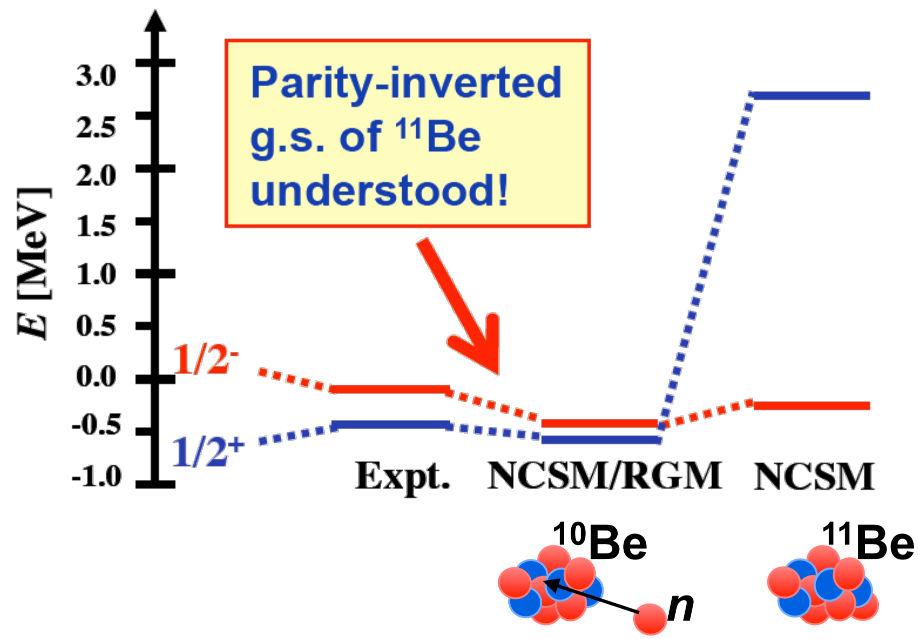
Parity inversion of ^{11}Be ground state

S. Quaglioni and P. Navratil, Phys. Rev. Lett. 101, 092501 (2008)



The ^{11}Be *nucleus offers one of the best examples of phenomena emerging towards the drip lines: vanishing of magic numbers, abnormal spin-parity of ground states*

- Ground state spin-parity
  - Observed : **1/2+**
  - Nuclear Shell model :$1/2^-$
- Despite the use of large bases, *ab initio* NCSM calculations confirm the shell model picture
  - Failure of "static" approaches
- Parity-inversion described for the first time within an *ab initio* framework by means of NCSM/RGM calculations with cluster basis of the type: n + ^{10}Be(g.s.,2_1^+,2_2^+,1_1^+)



Properties of loosely-bound systems can be understood only within a "dynamic" approach that encompasses the continuum

Accurate evaluations for fusion diagnostic

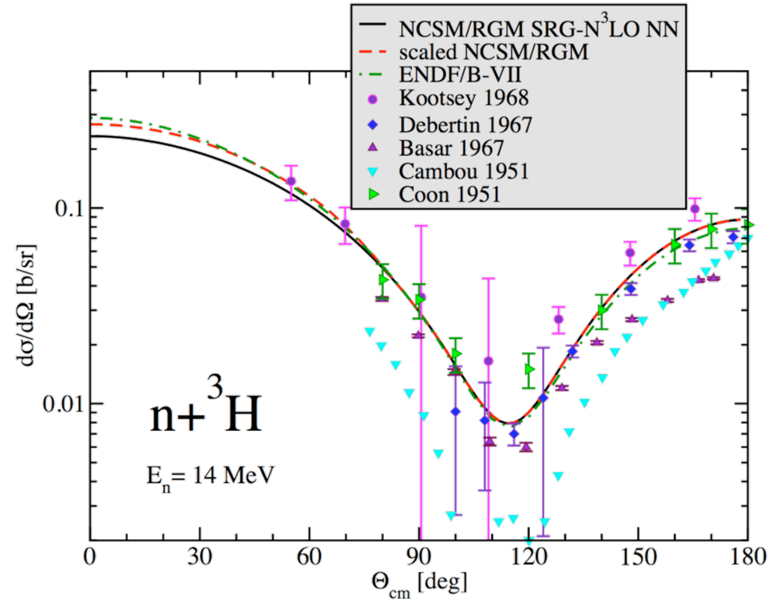
J. A. Frenje *et al.*, Phys. Rev. Lett. 107, 122502 (2011)

The elastic n-^{3}H *cross section for 14 MeV neutrons, important for understanding how the fuel is assembled in an implosion at NIF, was not known precisely enough*

- Nuclear theory was asked to help
- Less than 15% inaccuracy at forward angles due to missing target breakup
- Inaccuracy quantified by comparing accurate *p*-^{3}He data to corresponding NCSM/RGM calculation
- Obtained correction function applied to *n*-^{3}H calculation

Delivered evaluated data with required 5% uncertainty and successfully compared to measurements using an Inertial Confinement Facility

^{3}H(*n*,*n*)^{3}H cross section



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

Accurate evaluations for fusion diagnostic

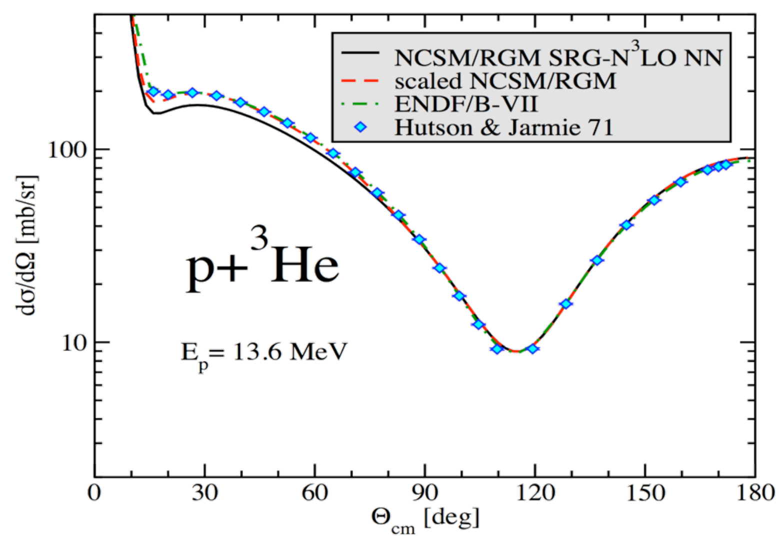
J. A. Frenje *et al.*, Phys. Rev. Lett. 107, 122502 (2011)

The elastic n-^{3}H *cross section for 14 MeV neutrons, important for understanding how the fuel is assembled in an implosion at NIF, was not known precisely enough*

- Nuclear theory was asked to help
- Less than 15% inaccuracy at forward angles due to missing target breakup
- Inaccuracy quantified by comparing accurate *p*-^{3}He data to corresponding NCSM/RGM calculation
- Obtained correction function applied to *n*-^{3}H calculation

Delivered evaluated data with required 5% uncertainty and successfully compared to measurements using an Inertial Confinement Facility

^{3}H(*n*,*n*)^{3}H cross section



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

Accurate evaluations for fusion diagnostic

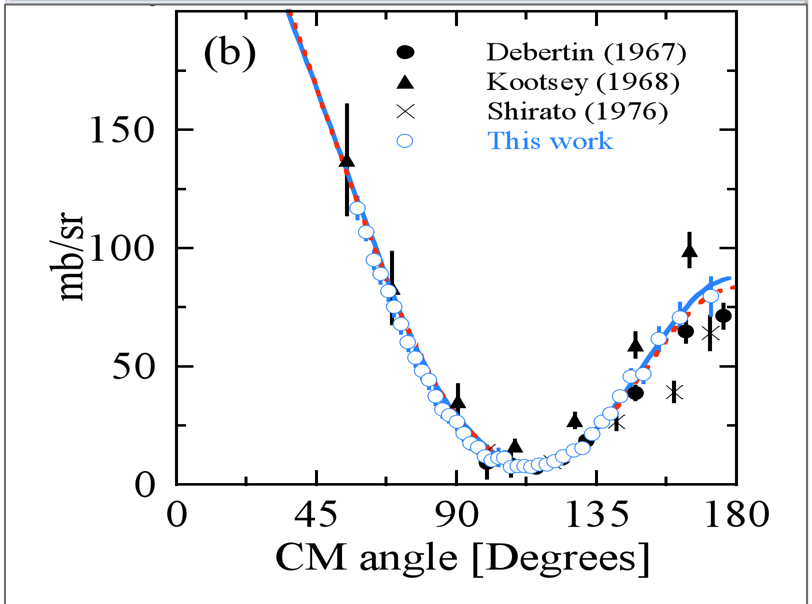
J. A. Frenje *et al.*, Phys. Rev. Lett. 107, 122502 (2011)

The elastic n-^{3}H cross section for 14 MeV neutrons, important for understanding how the fuel is assembled in an implosion at NIF, was not known precisely enough

- Nuclear theory was asked to help
- Less than 15% inaccuracy at forward angles due to missing target breakup
- Inaccuracy quantified by comparing accurate *p*-^{3}He data to corresponding NCSM/RGM calculation
- Obtained correction function applied to *n*-^{3}H calculation

Delivered evaluated data with required 5% uncertainty and successfully compared to measurements using an Inertial Confinement Facility

^{3}H(*n*,*n*)^{3}H cross section



Agreement with new measurements obtained in a deuterium-tritium inertial confinement implosion at the OMEGA laser

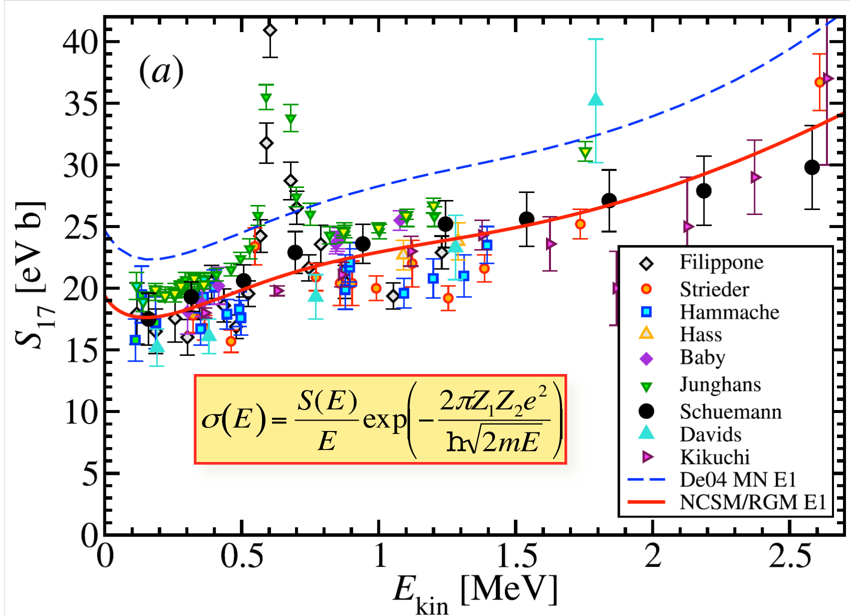
Ab initio many-body calculation of the $^7Be(p,\gamma)^8B$ radiative capture

P. Navrátil, R. Roth, and S. Quaglioni, Phys. Lett. B704, 379 (2011)

The $^7Be(p,\gamma)^8B$ is the final step in the nucleosynthetic chain leading to ^8B and one of the main inputs of the standard model of solar neutrinos

- ~10% error in latest $S_{17}(0)$: dominated by uncertainty in theoretical models
- NCSM/RGM results with largest realistic model space (N_{max} = 10):
  - p+^{7}Be(g.s., 1/2$^-$, 7/2$^-$, 5/2$_1^-$, 5/2$_2^-$)
- Parameter Λ of effective SRG NN interaction chosen to reproduce separation energy: 136 keV (Expt. 137 keV)
- $S_{17}(0)$ = 19.4(7) eV b on the lower side of, but consistent with latest evaluation

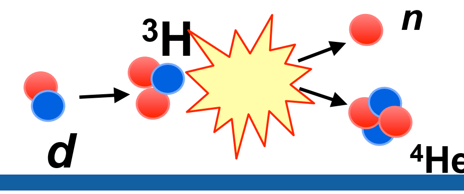
$^7Be(p,\gamma)^8B$ astrophysical S-factor



Ab initio theory predicts simultaneously both normalization and shape of S_{17}. Inclusion of 5/2$_2^-$ state improves S-factor energy dependence above 1.5 MeV.

The $^3H(d,n)^4He$ and $^3He(d,p)^4He$ fusion

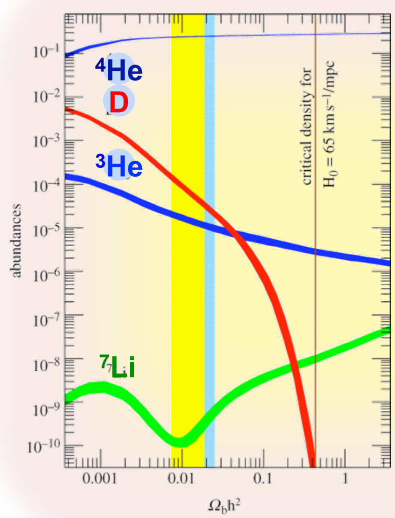
P. Navrátil, S. Quaglioni, arXiv.1110.0460

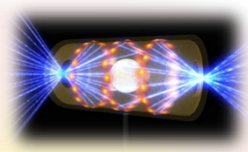


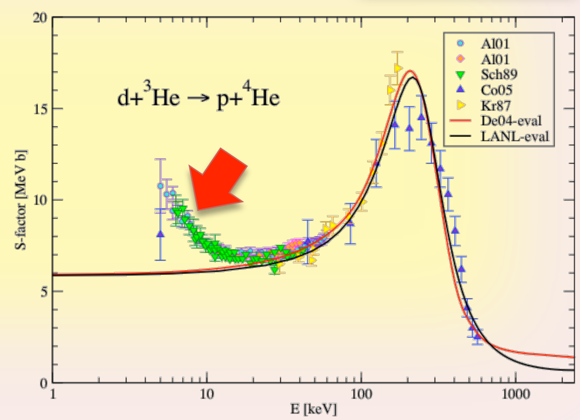
Nuclear astrophysics: Predictions of Big Bang nucleosystesis for light-nucleus abundances

Fusion research and Plasma physics: *d*+T is the easiest fusion to achieve on Earth; $^3H(d,\gamma)^5He$ branch useful for diagnostic, not known well enough

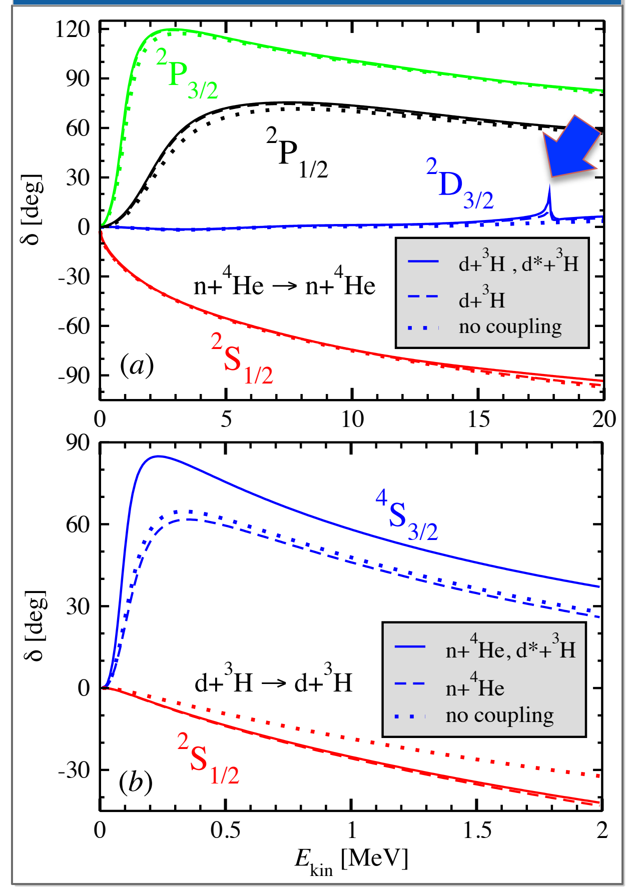
Atomic physics: Considerable electron-screening effects in $d+^3He$ not completely understood







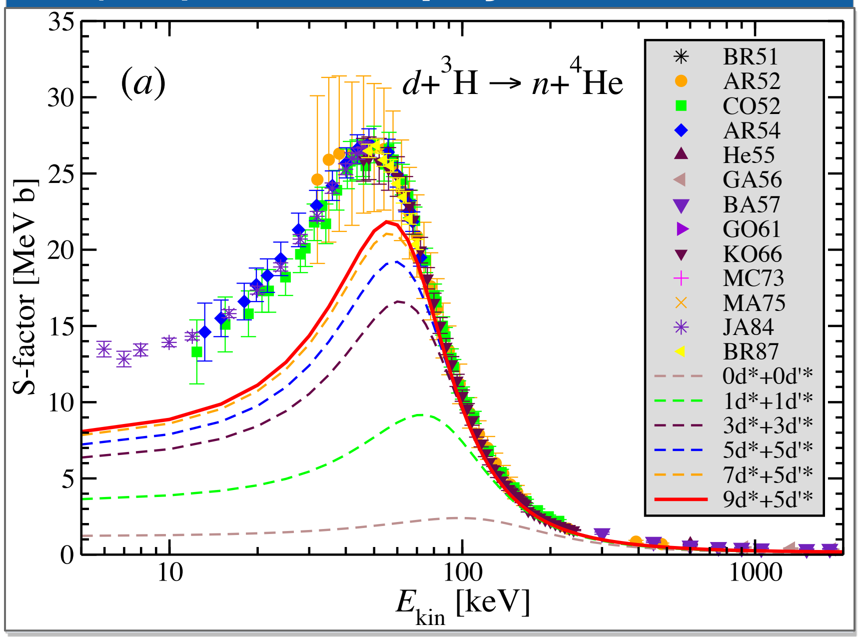
$^4He(n,n)^4He$ & $^3He(d,p)^4He$ elastic phase shifts



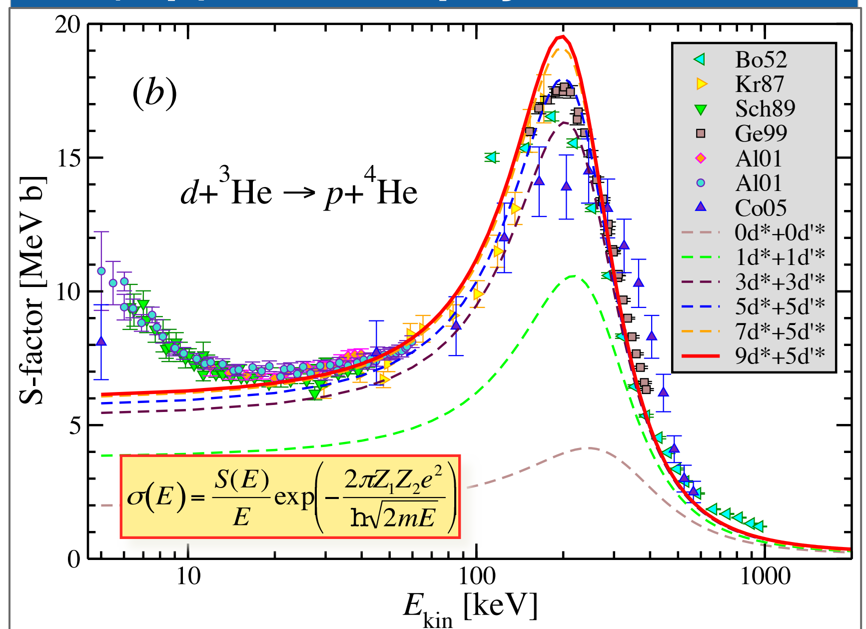
Ab initio many-body calculations of the $^{3}H(d,n)^{4}He$ and $^{3}He(d,p)^{4}He$ fusion

P. Navrátil, S. Quaglioni,
arXiv.1110.0460

$^{3}H(d,n)^{4}He$ astrophysical S-factor



$^{3}He(d,p)^{4}He$ astrophysical S-factor



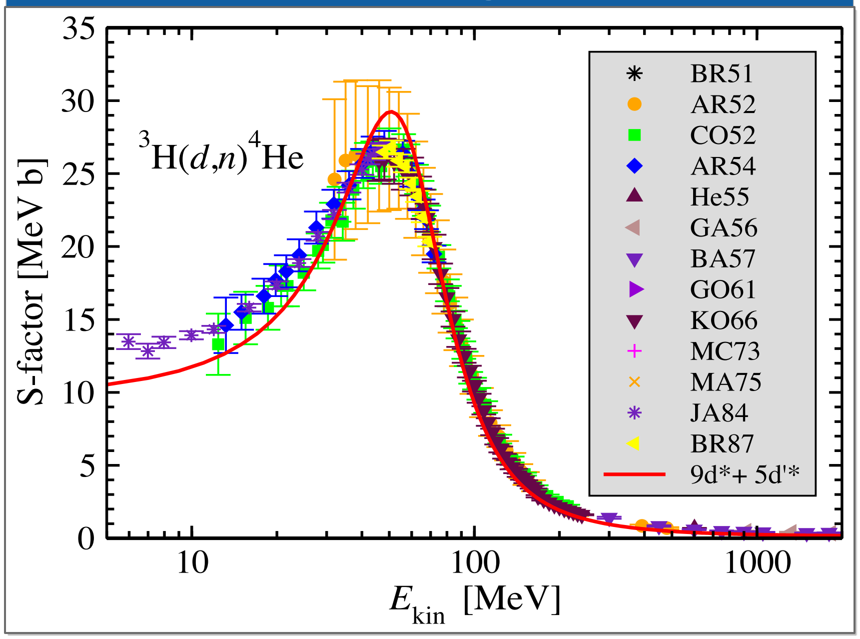
Calculated S-factors improve with the inclusion of the virtual breakup of the deuterium, obtained by means of excited $^{3}S_{1}$-$^{3}D_{1}$ (*d) and $^{3}D_{2}$ (*d'**) pseudo-states.**

NCSM/RGM results for the $^{3}He(d,p)^{4}He$ astrophysical S-factor compared to beam-target measurements. Data curve up and deviate from theoretical results at low energy due to laboratory electron-screening.

Ab initio many-body calculations of the $^3H(d,n)^4He$ and $^3He(d,p)^4He$ fusion

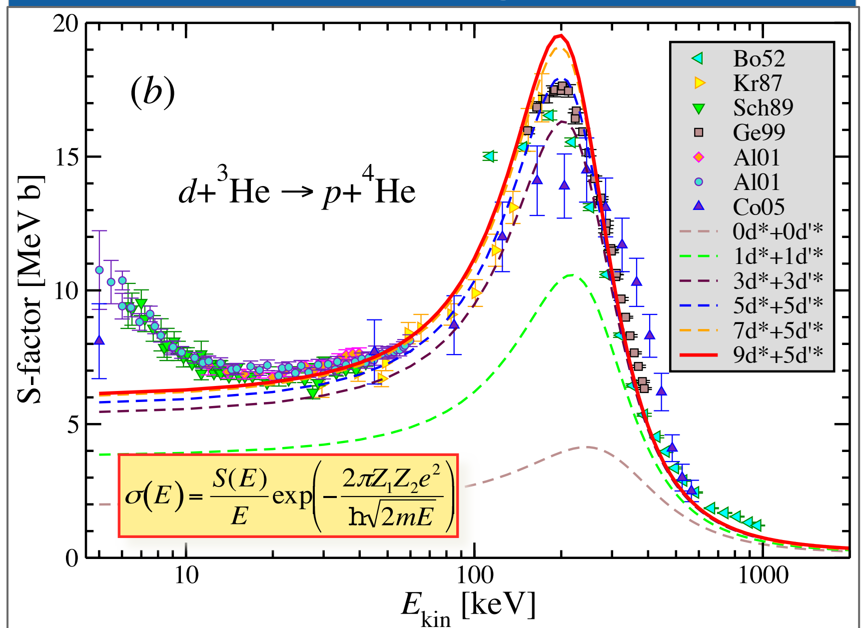
P. Navrátil, S. Quaglioni,
arXiv.1110.0460

$^3H(d,n)^4He$ astrophysical S-factor



Position of the resonance must be obtained with high relative precision. Changing the evolution parameter Λ of the NN effective interaction from 1.5 to 1.45 fm^{-1} improves agreement with data

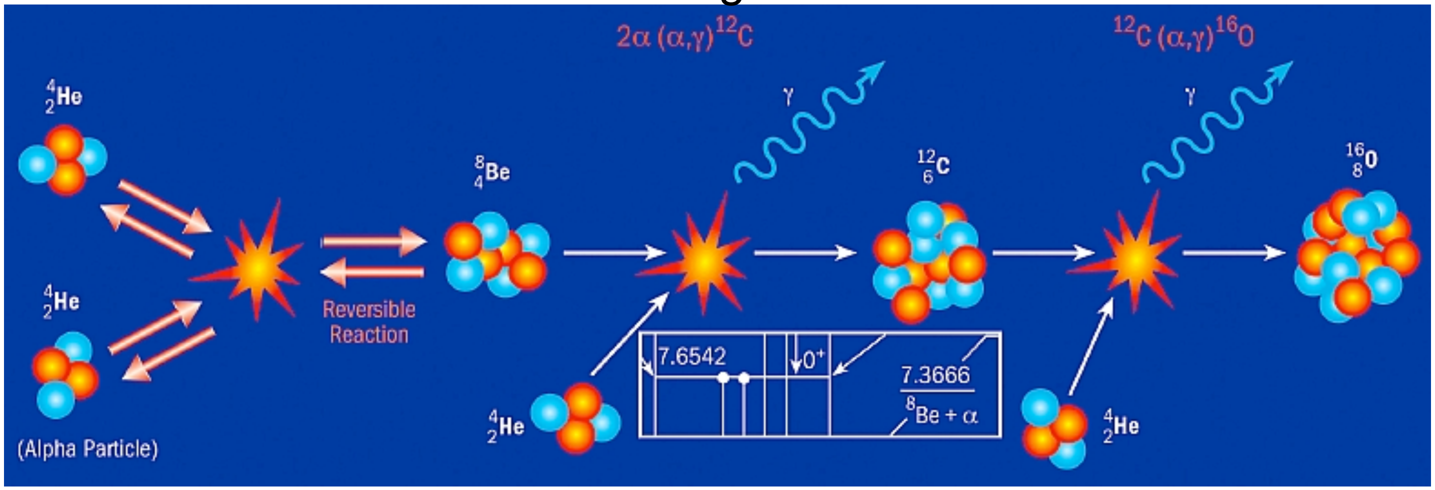
$^3He(d,p)^4He$ astrophysical S-factor



NCSM/RGM results for the $^3He(d,p)^4He$ astrophysical S-factor compared to beam-target measurements. Data curve up and deviate from theoretical results at low energy due to laboratory electron-screening.

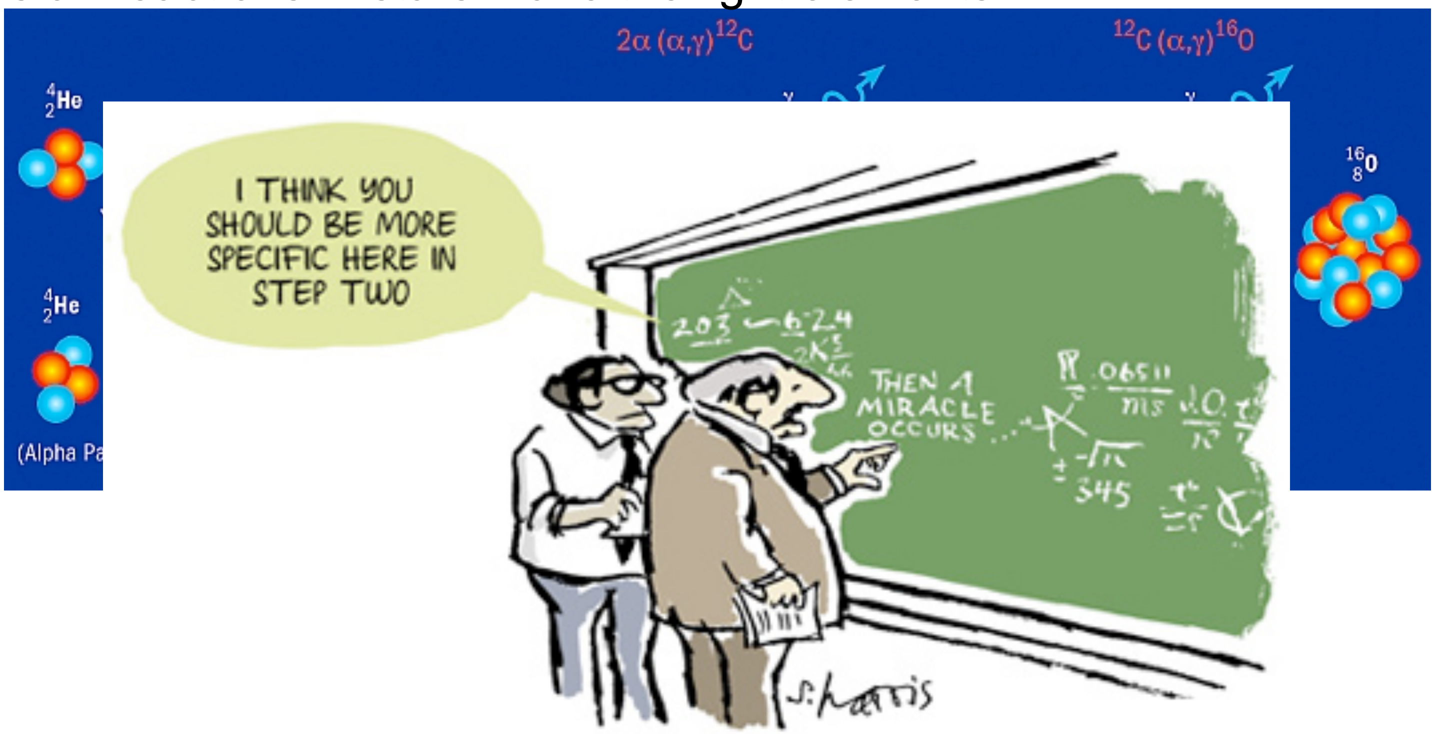
Holy-Grail: How stuff was made?

- The building blocks of life – Carbon and Oxygen, where are they made?
  - Fusion reactions in stars make the light elements

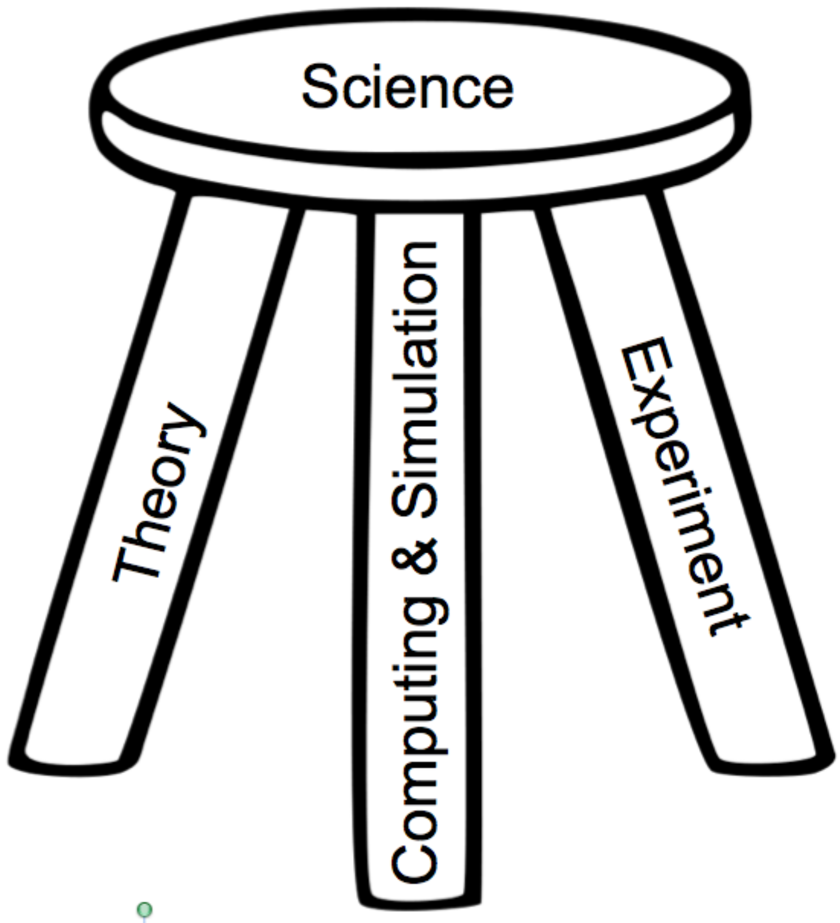


How stuff was made?

- The building blocks of life – Carbon and Oxygen, where are they made?
  - Fusion reactions in stars make the light elements



There are now three components to scientific discovery



Computing enhances theory and
Simulation complements experiment

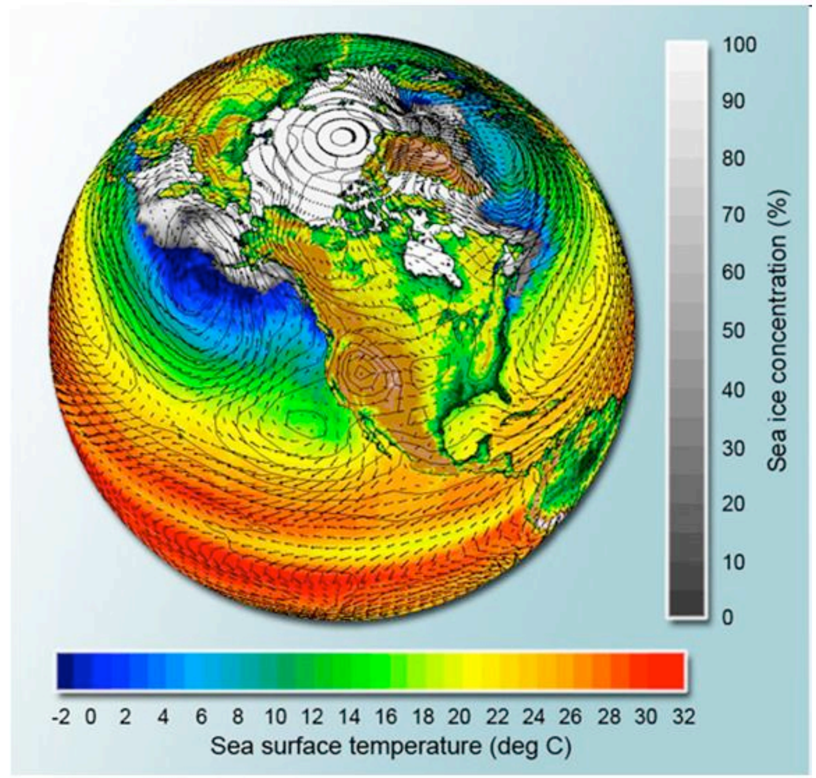
Computing is a new tool in theorist's toolbox

- The computer is a cool tool to solve complex problems!!!

Simulation of events can help understanding

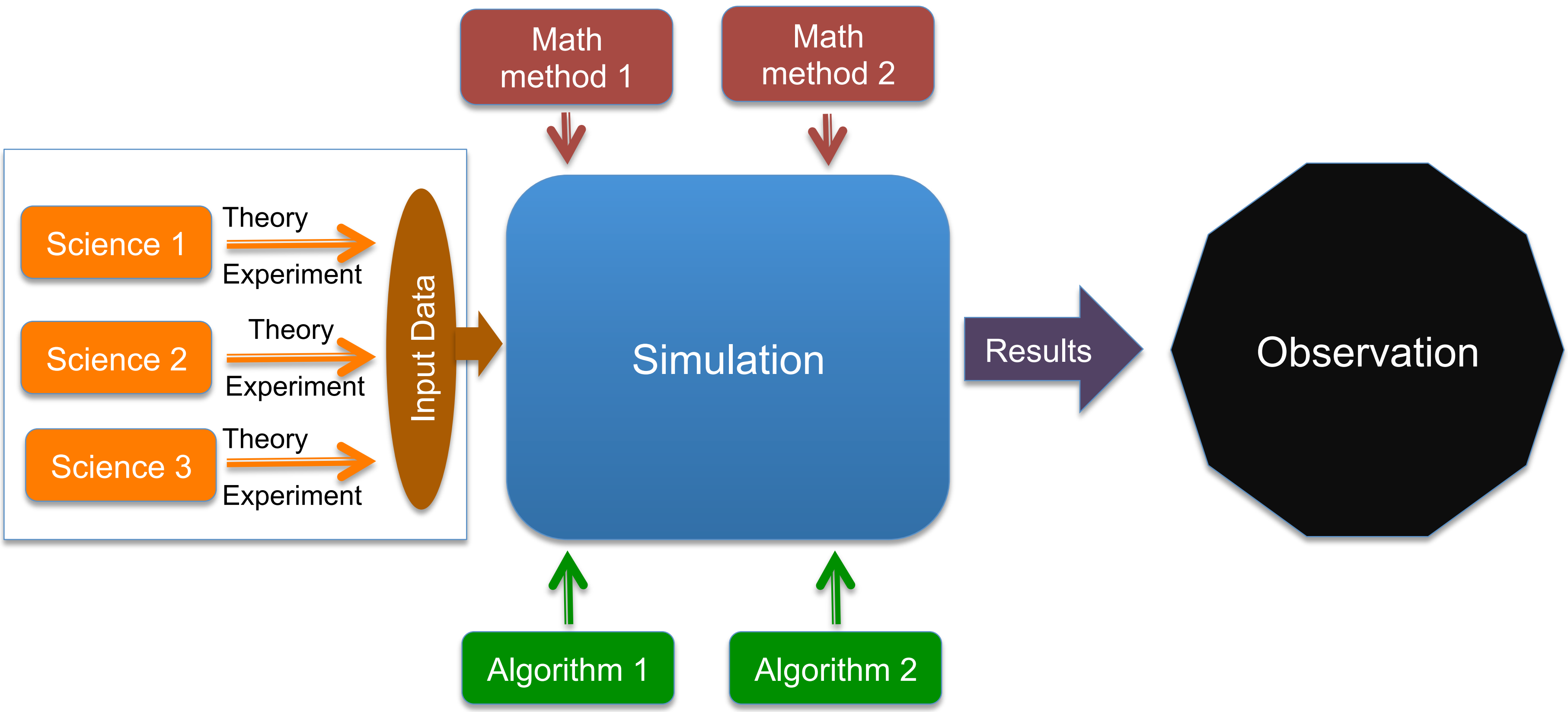
- Sometimes we need to know something when we can make an observation

- Simulations based on sound science and empirical data can provide a critical framework for decision making
  - Climate modeling
  - Drug interactions
  - Economies
  - New materials
  - Supernovae
  - Stockpile stewardship



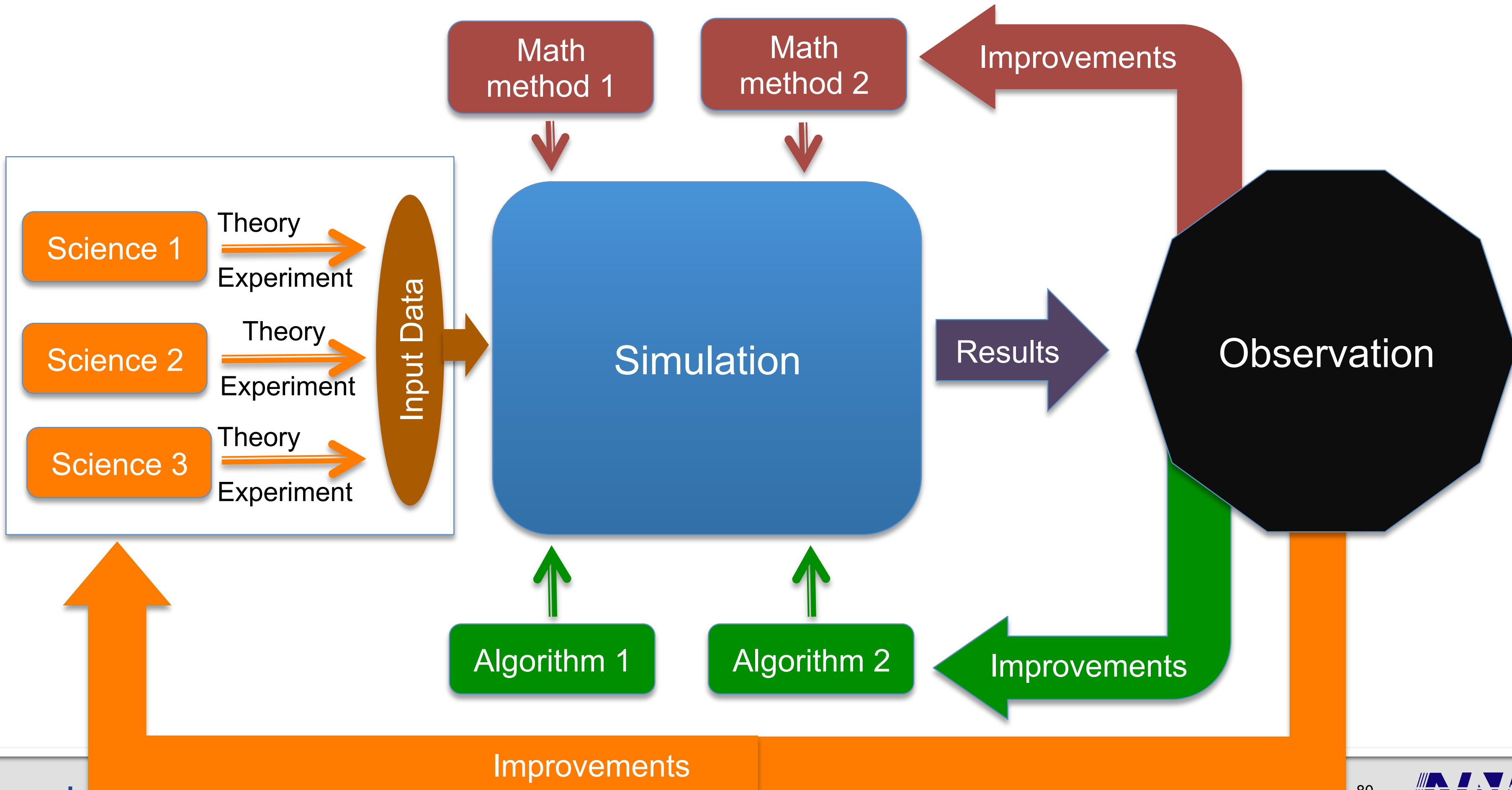
Multi-science simulations

- Beyond pure theory studies, supercomputing, advanced theories, numerical methods, and algorithms will be essential for multi-science simulations



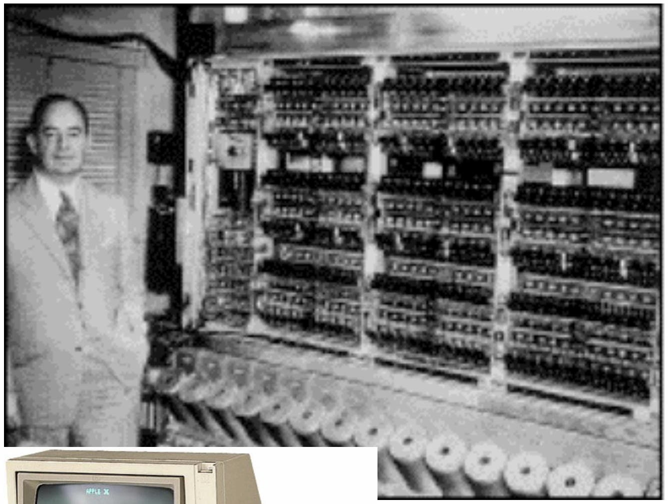
Multi-science simulations

- Beyond pure theory studies, supercomputing, advanced theories, numerical methods, and algorithms will be essential for multi-science simulations

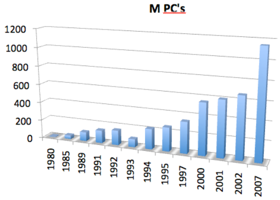


Computing has influenced science for 70+ years

- The utility of computers in theoretical physics has been recognized since the 40's
  - John von Neumann and Architecture of Computer Systems
    - Designed the Electronic Discrete Variable Automatic Computer (EDVAC) in 1945



- Computers for the masses in the 80's
  - They became really personal in 90's
  - More than 1,000,000,000 PC's worldwide



- "Super" computing got to be big starting in the mid 80's
  - But, your laptop is more capable than the Cray-2

Cray-2, 1.9 GFLOPS

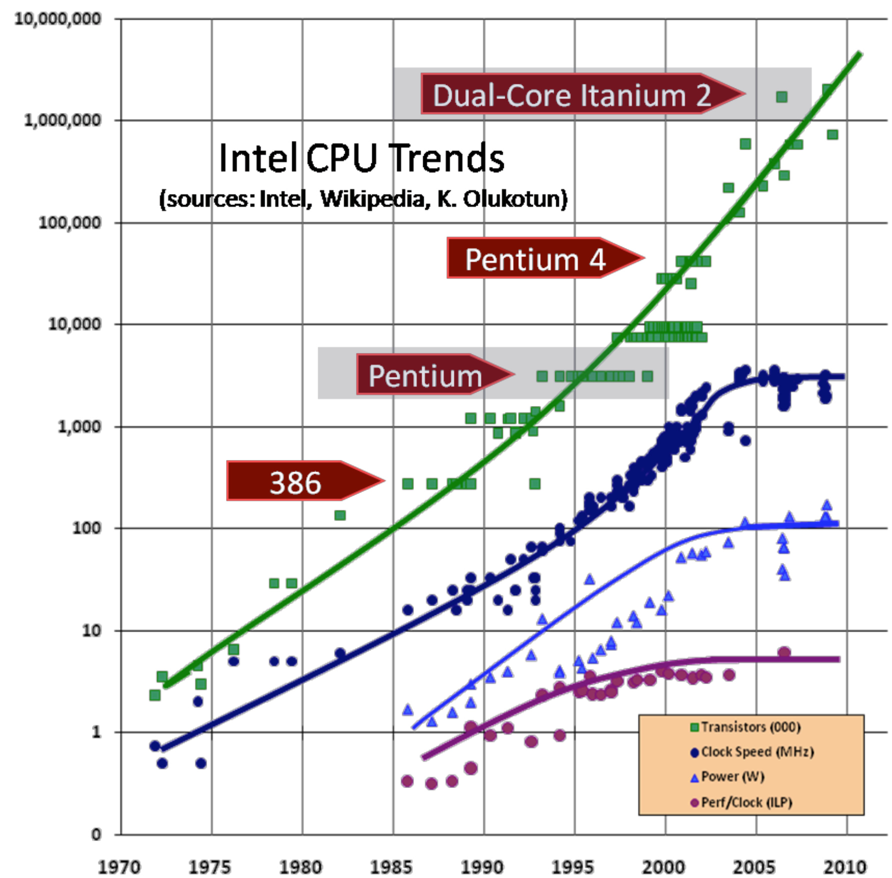
Cray-XMP

Limits to computing with a single CPU

- Moore's law:

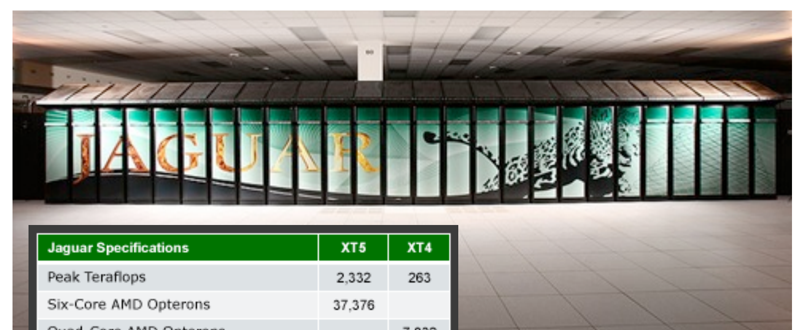
  The number of transistors that can be placed inexpensively on an integrated circuit has doubled approximately every two years

- We are starting to reach limits on the performance of single CPU's
  - Clock speeds are saturating
    - Increasing clock speeds requires more power
    - Physical dimensions are reaching the quantum limit
    - Accessing memory outside the CPU is slow



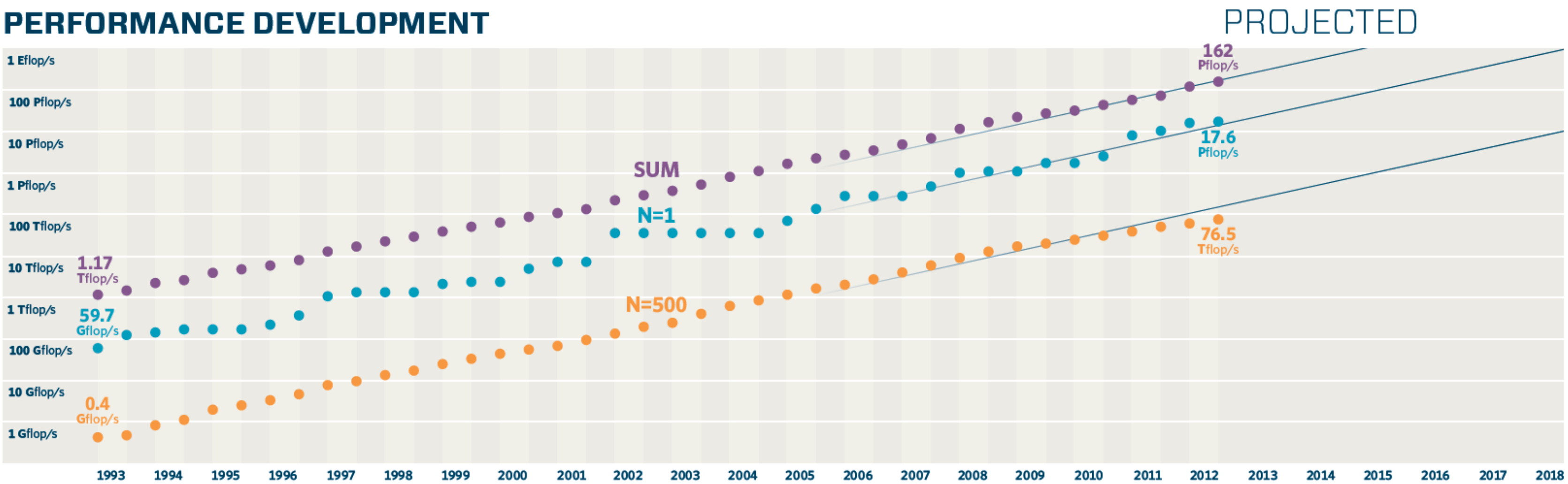
Where to go from here

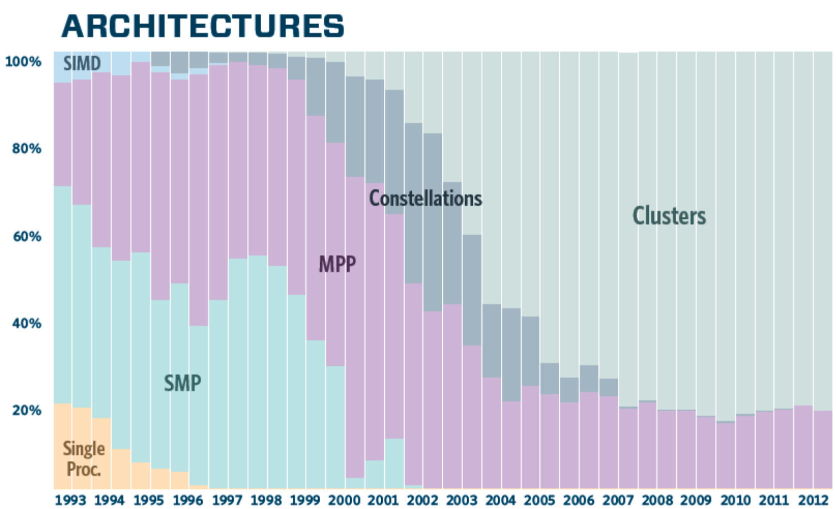
- Throw more CPU's at the problem
- Two ways so far:
  - More CPU's/chip
    - Shared memory with access to common data
    - Distribute work among shared threads
    - Intel Core i7 has eight CPU's
    - OpenMP protocols
  - A "farm" of independent CPU's with high-speed data transfer capability
    - Independent processes with separate memory
    - Message Passage Interface (MPI)

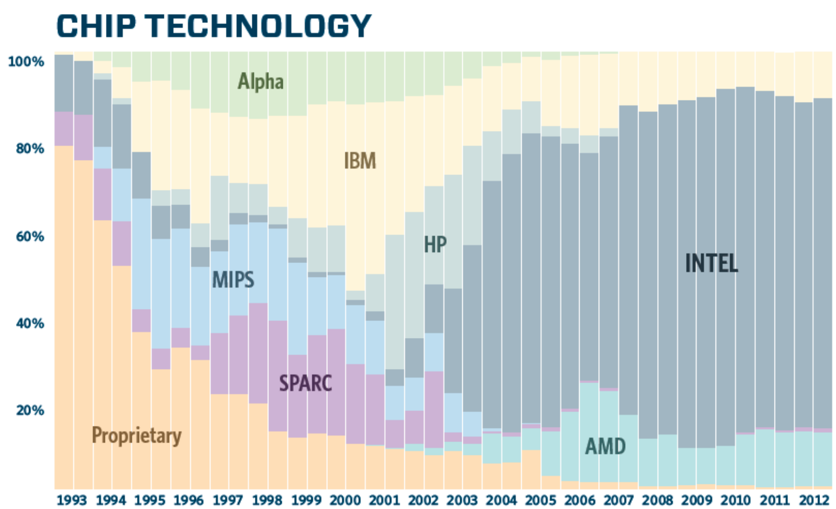


Jaguar Specifications	XT5	XT4
Peak Teraflops	2,332	263
Six-Core AMD Opterons	37,376	
Quad-Core AMD Opterons		7,832
AMD Opteron Cores	224,256	31,328
Compute Nodes	18,688	7,832
Memory (TB)	299	62
Memory Bandwidth (GB/s)	478	100
Disk Space (TB)	10,000	750
Interconnect Bandwidth	374	157
Floor Space (ft²)	4,352	1,344
Cooling Technology	Liquid	Air

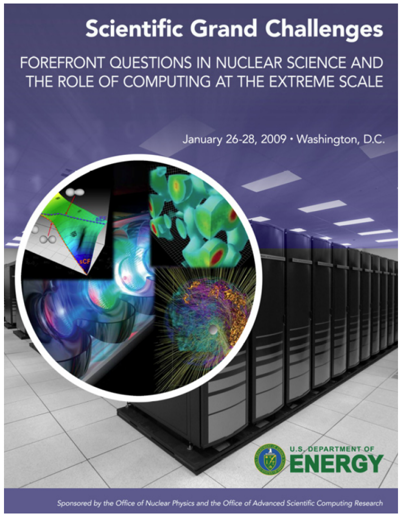
Supercomputing over time

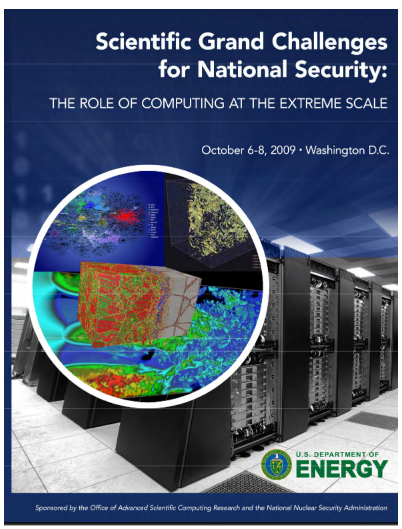


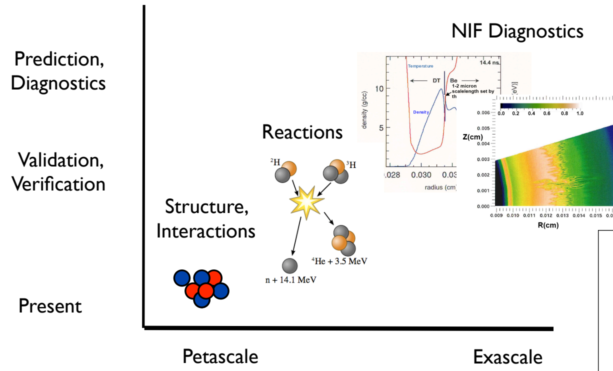


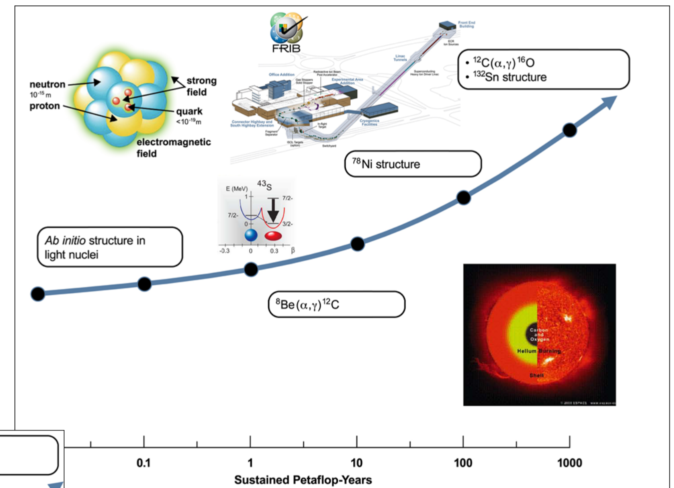


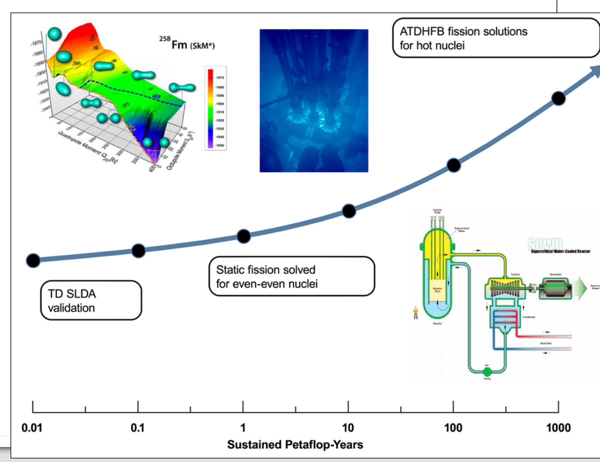
Exascale (10^{15} FLOPS) Computing is seen as the Future of Nuclear Theory



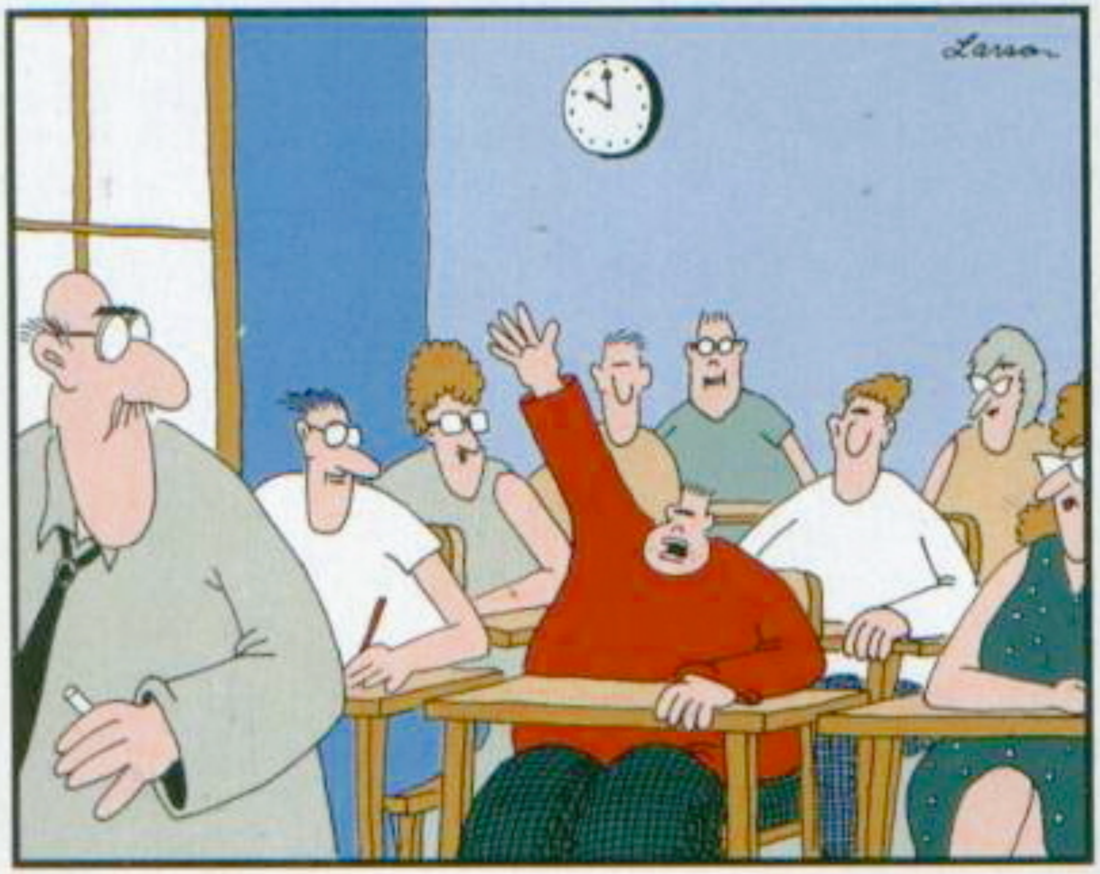








There is much more, but that will do for now



"Mr. Osborne, may I be excused?
My brain is full."

Summary

- *Ab initio* approaches to nuclear structure and reactions are maturing and providing interesting insight into nuclear processes
  - The nature of the three-body interaction in nuclei
  - The strength of electro-weak interactions – C
  - Light-ion reactions
  - Weakly-bound effects, parity inversion in ^{11}Be
- Challenges
  - Convergence for ground-state and “intruder” states
  - Form of three-body interaction
  - Effective operators
  - Complete formulation of bound and unbound states

Summary

- *Ab initio* approaches to nuclear structure and reactions are maturing and providing interesting insight into nuclear processes
  - The nature of the three-body interaction in nuclei
  - The strength of electro-weak interactions – C
  - Light-ion reactions
  - Weakly-bound effects, parity inversion in ^{11}Be

"This is not the end.
It is not even the beginning of the end.
But it is, perhaps, the end of the beginning."
Winston Churchill, Nov. 10, 1942