Applications of Renormalization Group Methods in Nuclear Physics – 4

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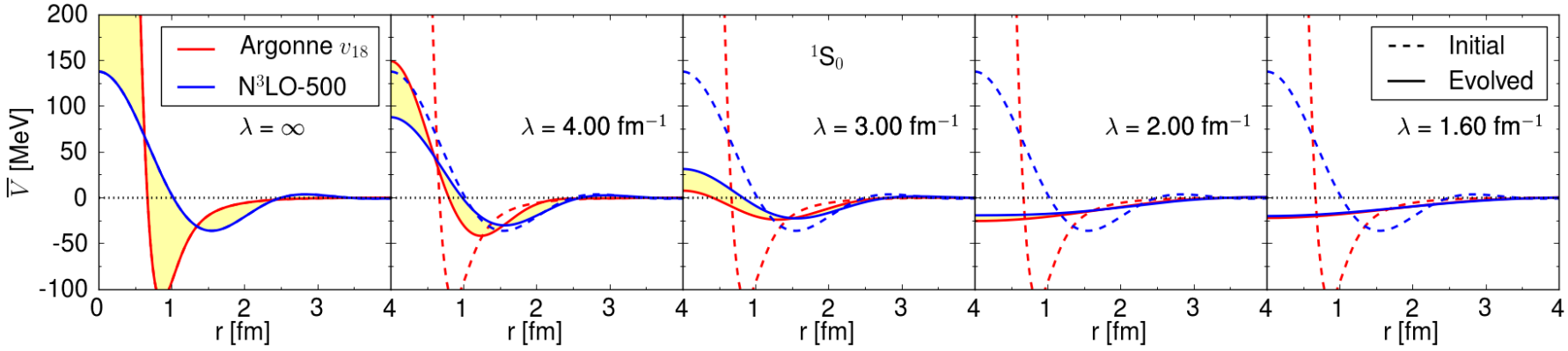
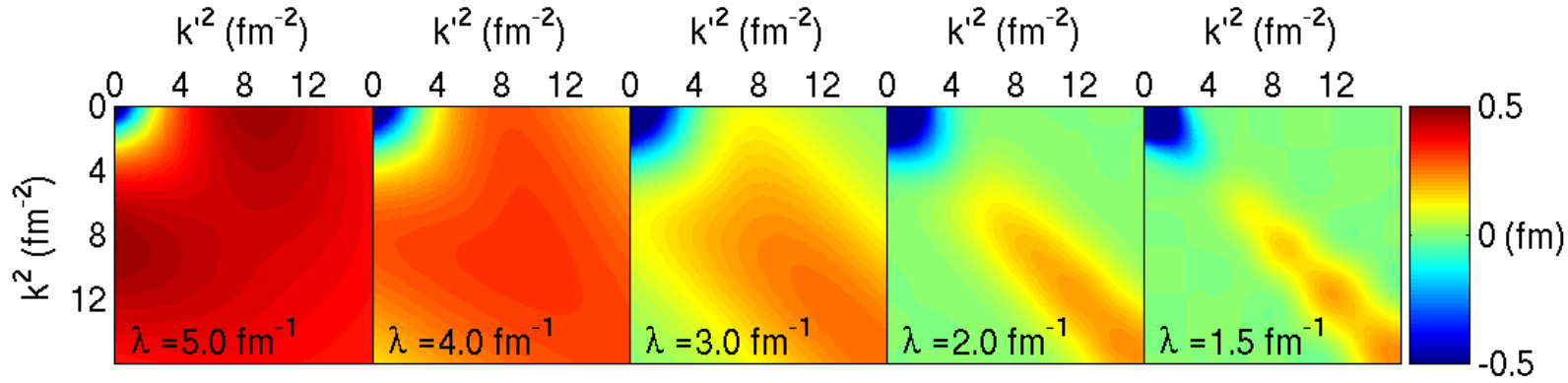
HUGS 2014





Outline: Lecture 4

Lecture 4: 3NF and applications

- RG-induced many-body forces
- Some places where the 3NF matters
- Results for infinite matter
- Future trends for chiral 3NF

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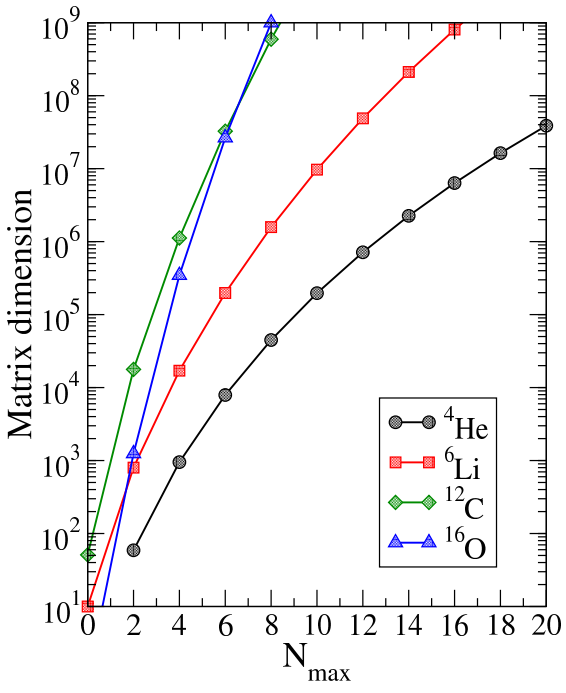
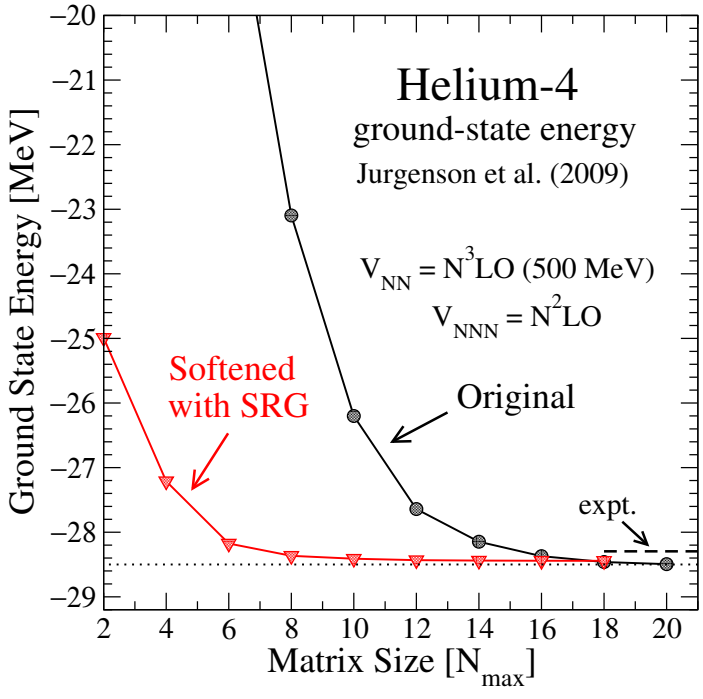
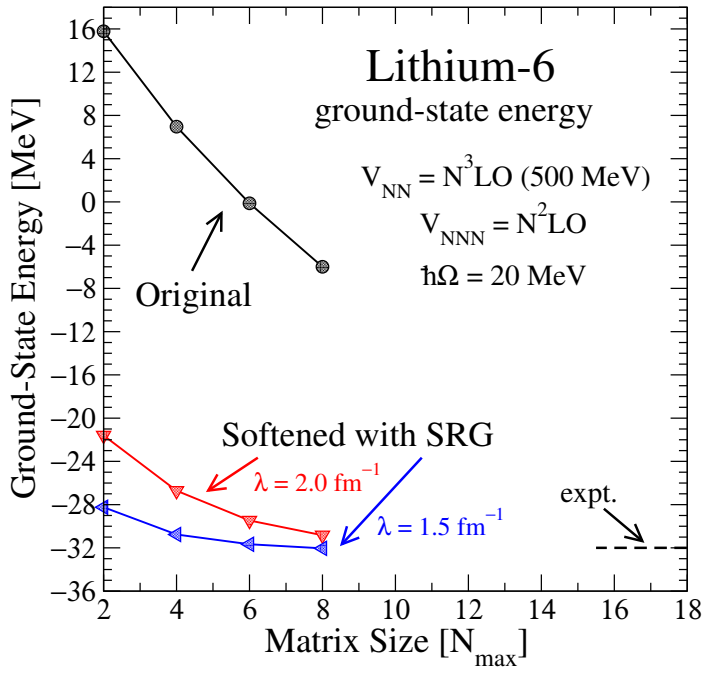
Recap: Evolving to lower resolution *seems* to be a big win

- Harmonic oscillator basis with N_{max} shells for excitations

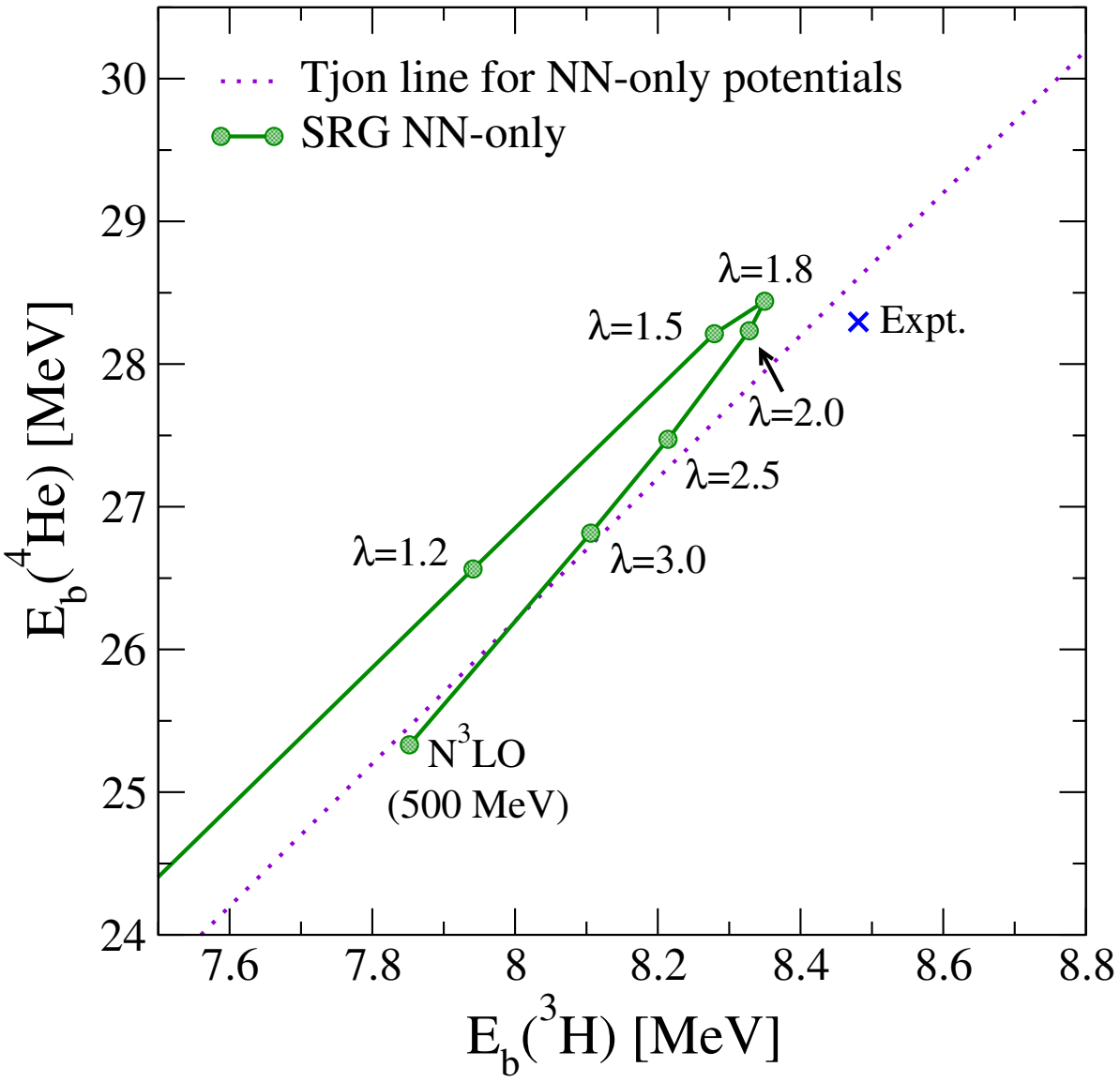






- Graphs show that convergence for *soft* chiral EFT potential is accelerated for evolved SRG potentials
- But we've jumped ahead here. Calculate just with NN.

Calculate triton and α masses at different λs

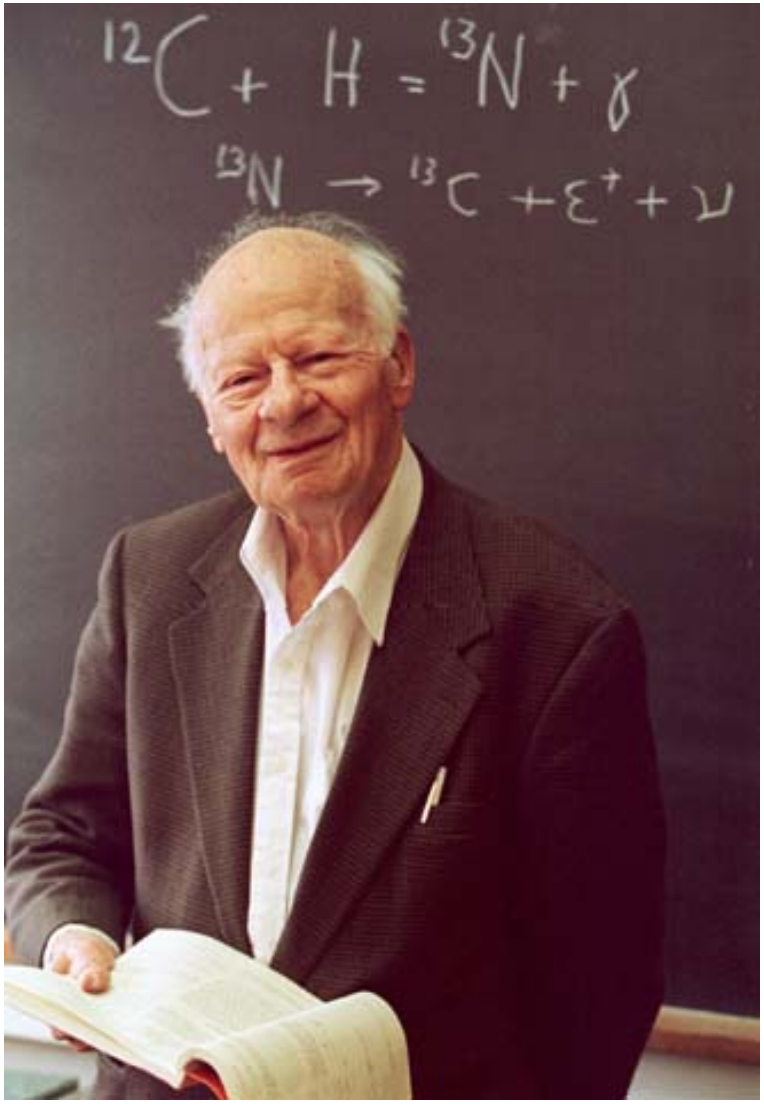


- Unitary transformation $\Longrightarrow$ energy unchanged
- Plot calculated binding energies ^{4}He vs. ^{3}H
- Oh, no! The energies change with λ!
- They follow a trajectory; cf. “Tjon line”

Symmetric infinite matter E/A vs. ρ is also a disaster $\Longrightarrow$ no equilibrium

Deja vu all over again?

- There were active attempts to transform away hard cores and soften the tensor interaction in the late sixties and early seventies.
- But the requiem for soft potentials was given by Hans Bethe (1971):
  "Very soft potentials must be excluded because they do not give saturation; they give too much binding and too high density. In particular, a substantial tensor force is required."
- Next 30+ years struggling to solve accurately with "hard" potential



Deja vu all over again?

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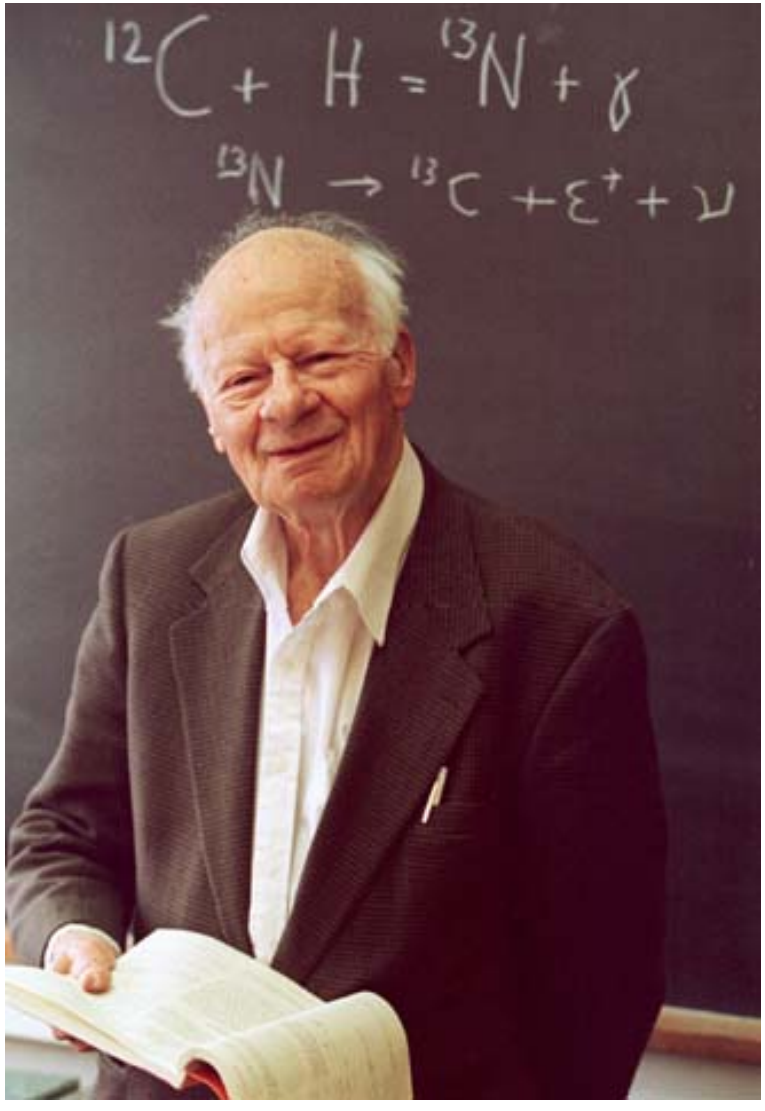
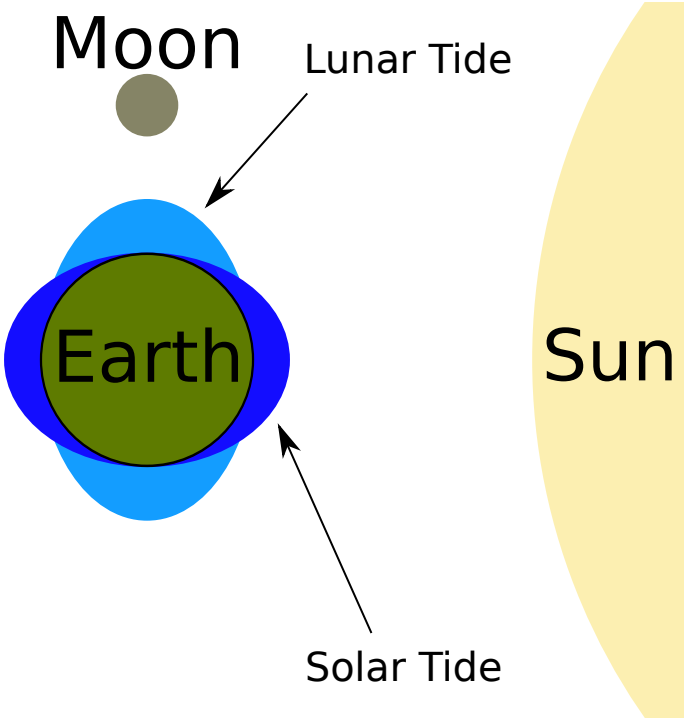
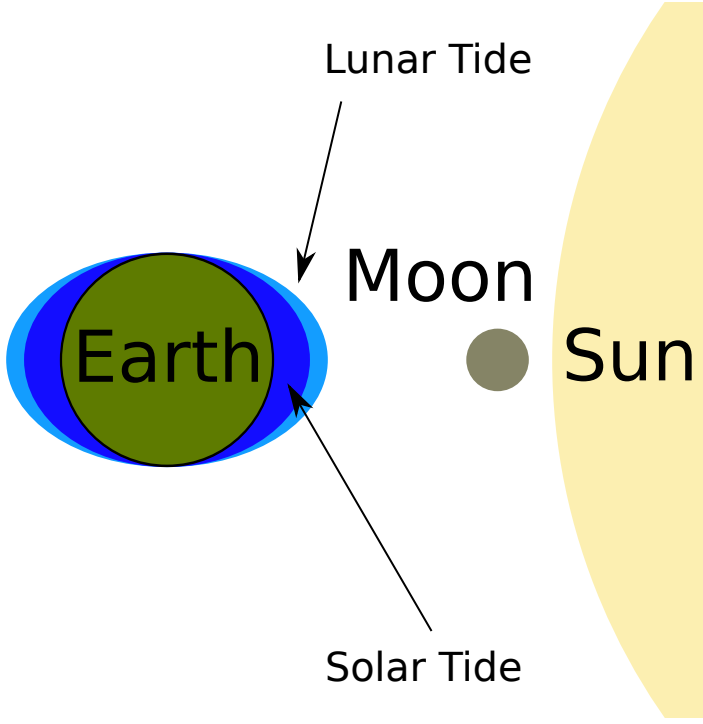
  "Very soft potentials must be excluded because they do not give saturation; they give too much binding and too high density. In particular, a substantial tensor force is required."
- Next 30+ years struggling to solve accurately with "hard" potential
- But the story is not complete: three-nucleon forces (3NF)!



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

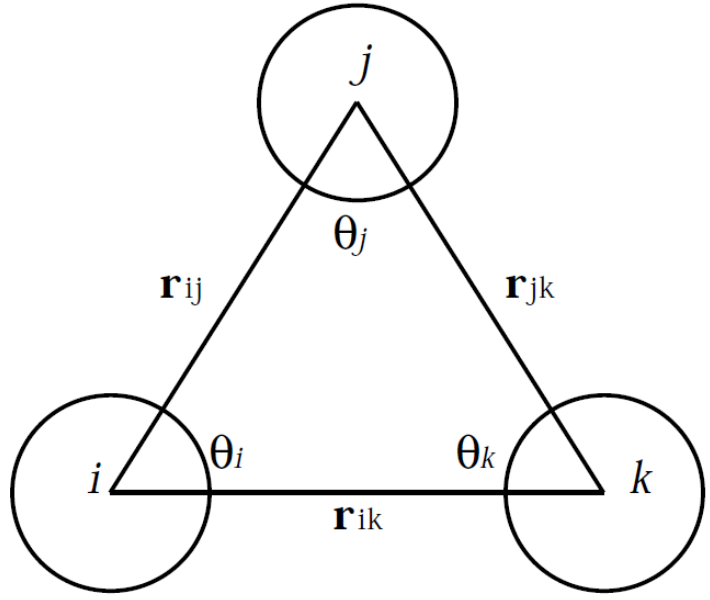




Atomic 3-body forces: Axilrod-Teller term (1943)

- Three-body potential for atoms/molecules from triple-dipole mutual polarization (3rd-order perturbation correction)

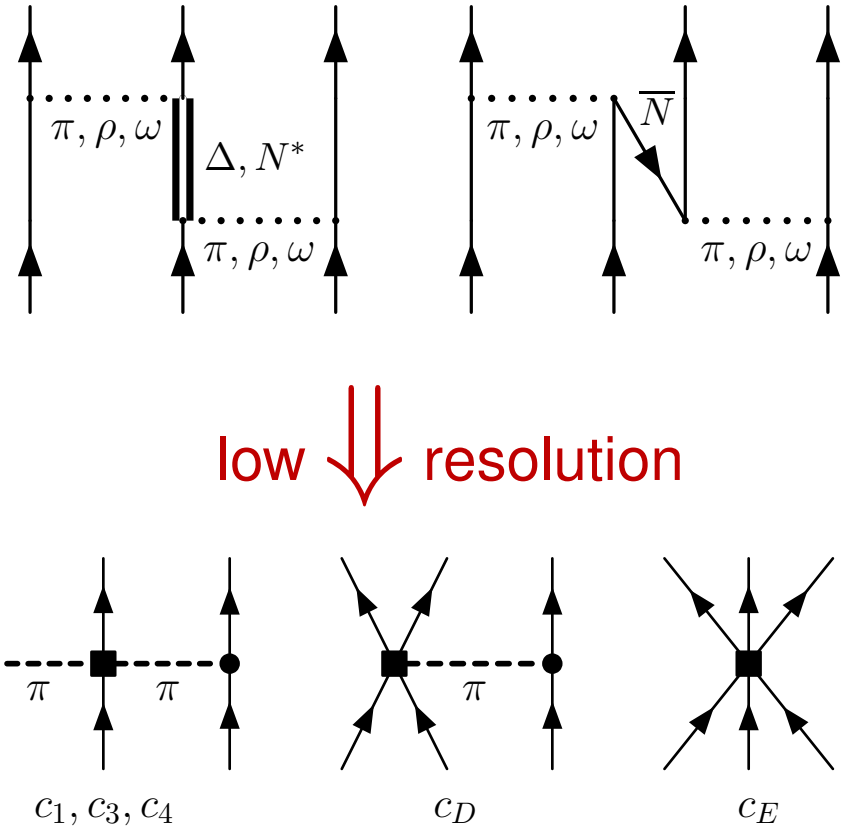
$$V(i,j,k) = \frac{\nu(1 + 3\cos\theta_i \cos\theta_j \cos\theta_k)}{(r_{ij} r_{ik} r_{jk})^3}$$



- Usually negligible in metals and semiconductors
- Can be important for ground-state energy of solids bound by van der Waals potentials
- Bell and Zuker (1976): 10% of energy in solid xenon

Origin of nuclear three-body forces

- Three-body forces arise from eliminating/decoupling dof's
  - excited states of nucleon
  - relativistic effects
  - high-momentum intermediate states
- Omitting 3-body forces leads to model dependence
  - observables depend on λ
  - cutoff dependence as tool
- NNN at different λ must be evolved like NN
  - NNN contribution is critical at low resolution



Flow equations lead to many-body operators

- Consider a's and $a^\dagger$'s wrt given s.p. basis and reference state:

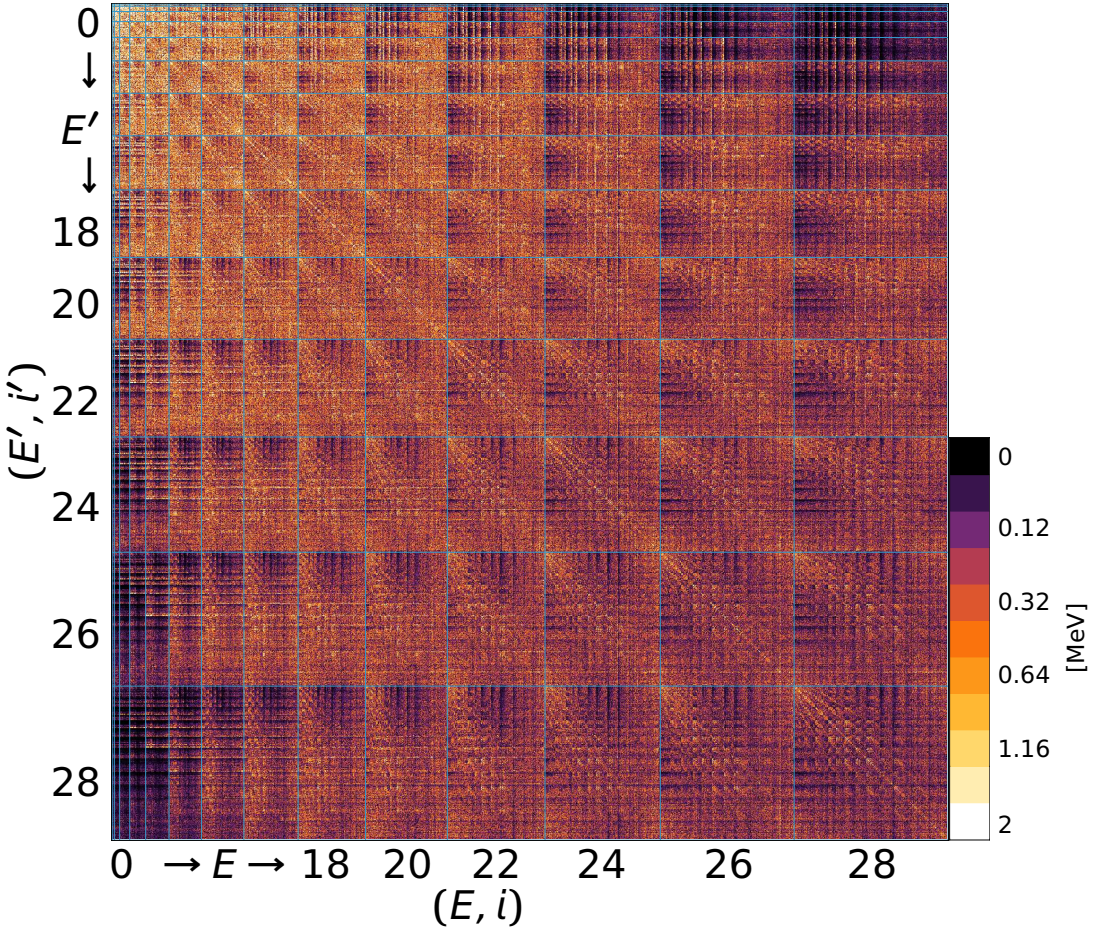
$$\frac{dV_s}{ds} = \Big[\Big[\sum \underbrace{a^\dagger a}_{\text{1-body}}, \sum \underbrace{a^\dagger a^\dagger aa}_{\text{2-body}}\Big], \sum \underbrace{a^\dagger a^\dagger aa}_{\text{2-body}}\Big] = \cdots + \sum \underbrace{a^\dagger a^\dagger a^\dagger aaa}_{\text{3-body!}} + \cdots$$

  so there will be A-body forces (and operators) generated!

- Is this a problem?
  - Ok if "induced" many-body forces are same size as natural ones
- Nuclear 3-body forces already needed in unevolved potential
  - In fact, there are A-body forces (operators) initially!
  - Natural hierarchy from chiral EFT
    $\Longrightarrow$ stop flow equations before unnaturally large
- SRG is a tractable method to evolve many-body operators

3NF evolution in Jacobi HO basis [Angelo Calci, Trento, 2013]

3B-Jacobi HO matrix elements

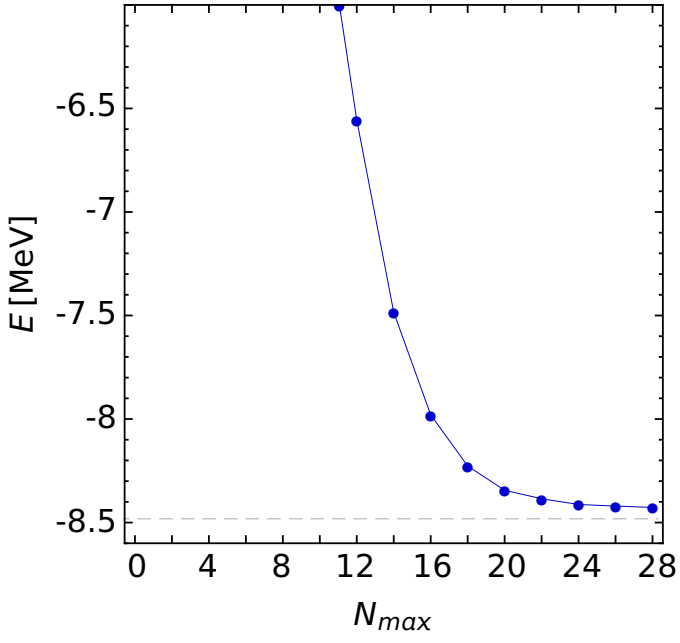


$$\alpha = 0.00\,\mathrm{fm}^4$$
$$\lambda = \infty\,\mathrm{fm}^{-1}$$

$$\langle E'i'JT \left| \tilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} \right| EiJT \rangle$$

$$J^\pi = \tfrac{1}{2}^+, T = \tfrac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$$

NCSM ground state ^{3}H



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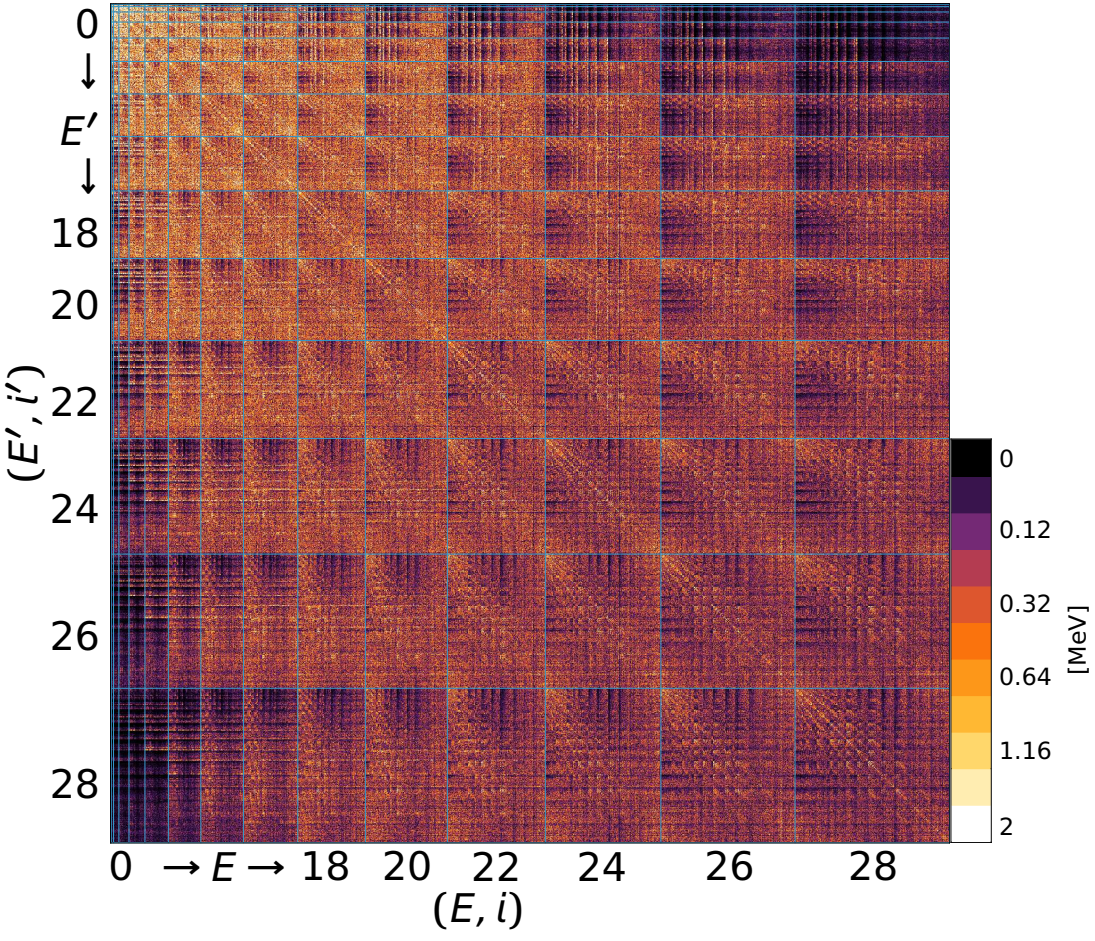

$$\alpha = 0.0025\,\mathrm{fm}^4$$

$$\lambda = 4.47\,\mathrm{fm}^{-1}$$

$$\langle E' i' J T \left| \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} \right| E i J T \rangle$$

$$J^\pi = \tfrac{1}{2}^+, T = \tfrac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$$

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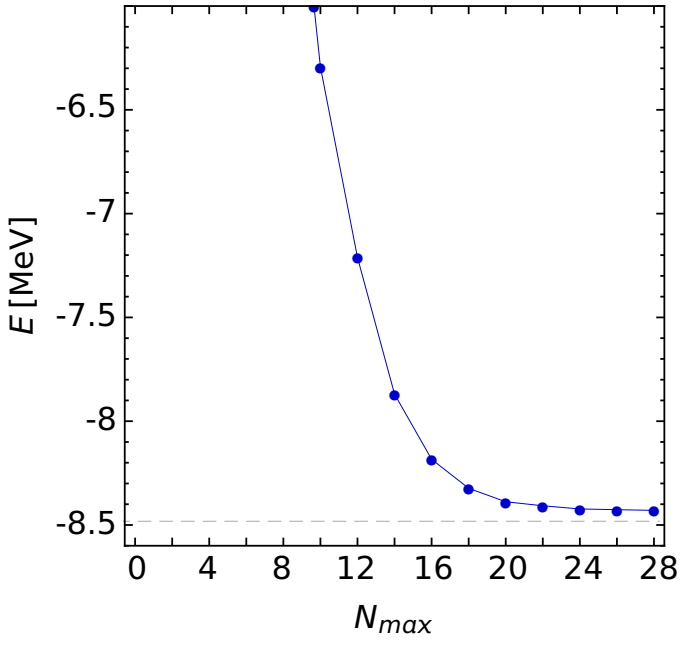

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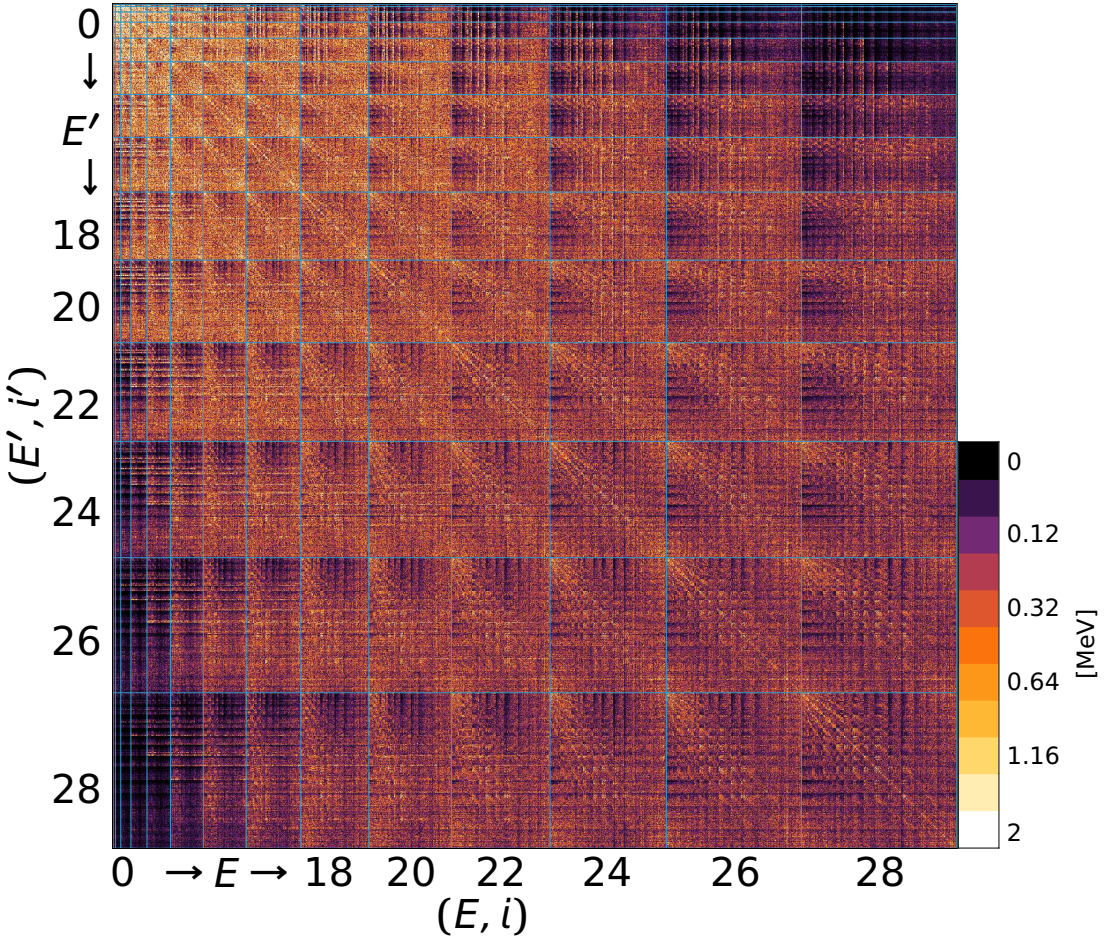

$$\alpha = 0.005\,\mathrm{fm}^4$$
$$\lambda = 3.76\,\mathrm{fm}^{-1}$$

$$\langle E'i'JT \left| \tilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} \right| EijT \rangle$$

$$J^\pi = \tfrac{1}{2}^+, T = \tfrac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$$

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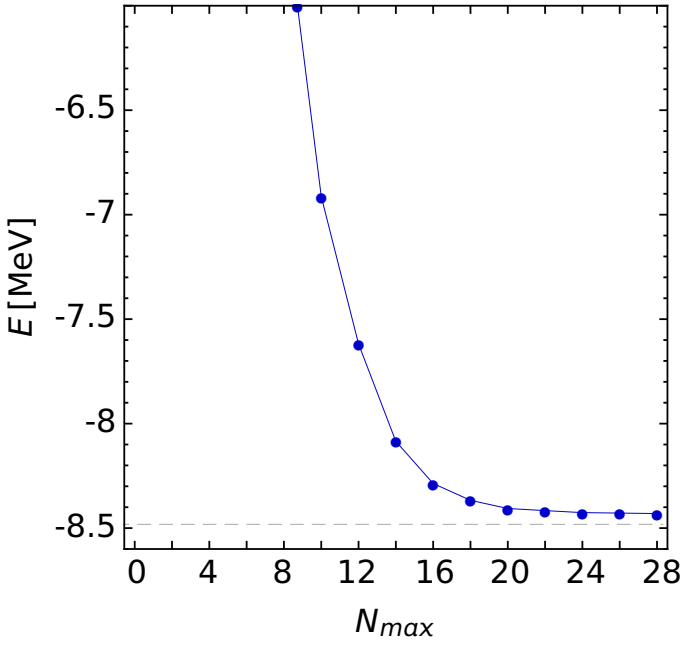

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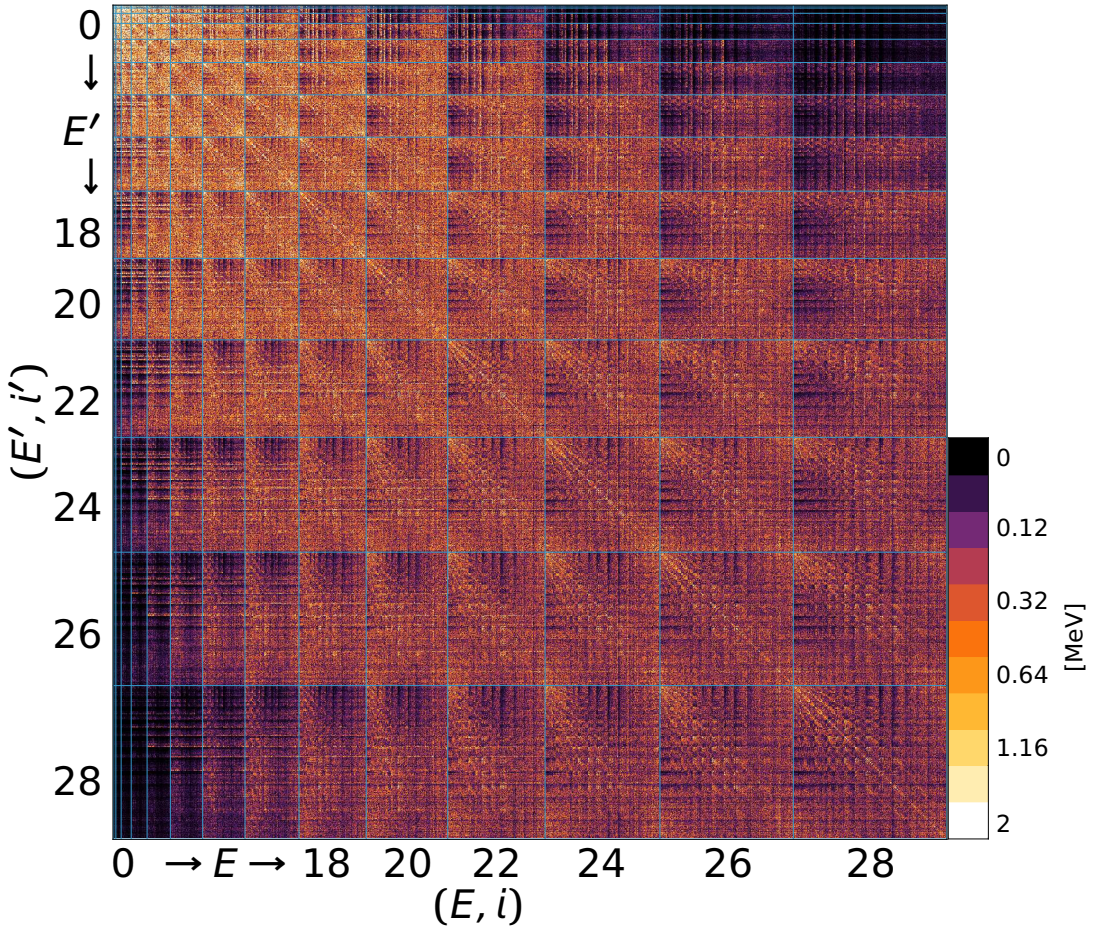

$$\alpha = 0.01\,\mathrm{fm}^4$$

$$\lambda = 3.16\,\mathrm{fm}^{-1}$$

$$\langle E'i'JT \left| \tilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} \right| EijT \rangle$$

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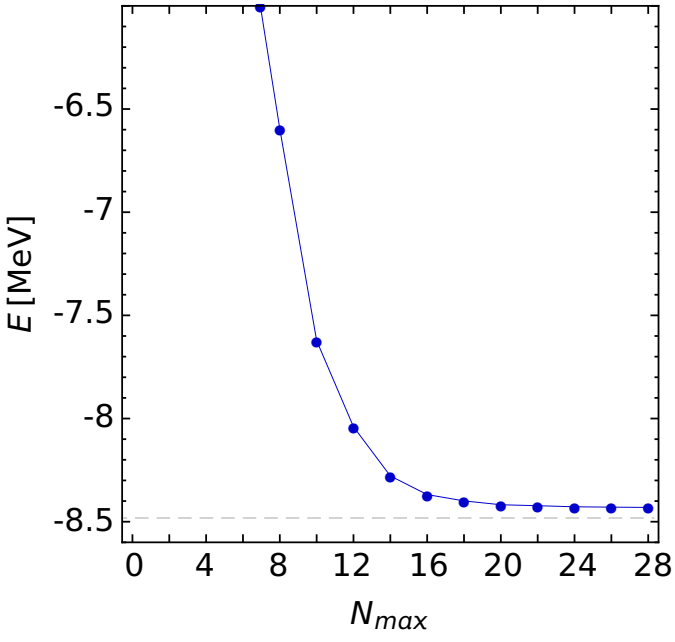

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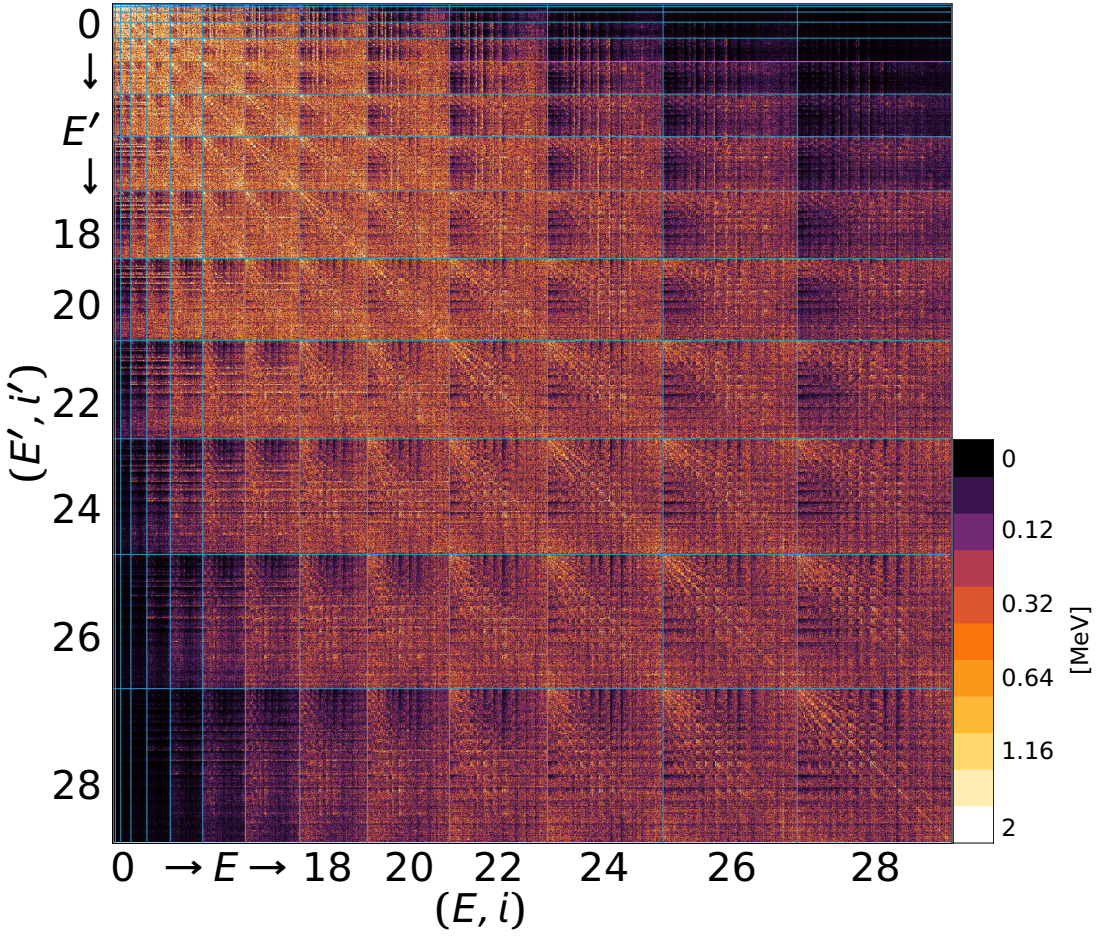

$$\alpha = 0.02\,\mathrm{fm}^4$$

$$\lambda = 2.66\,\mathrm{fm}^{-1}$$

$$\langle E'i'JT \left| \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} \right| EijT \rangle$$

$$J^\pi = \tfrac{1}{2}^+, T = \tfrac{1}{2}, \hbar\Omega = 24\,\mathrm{MeV}$$

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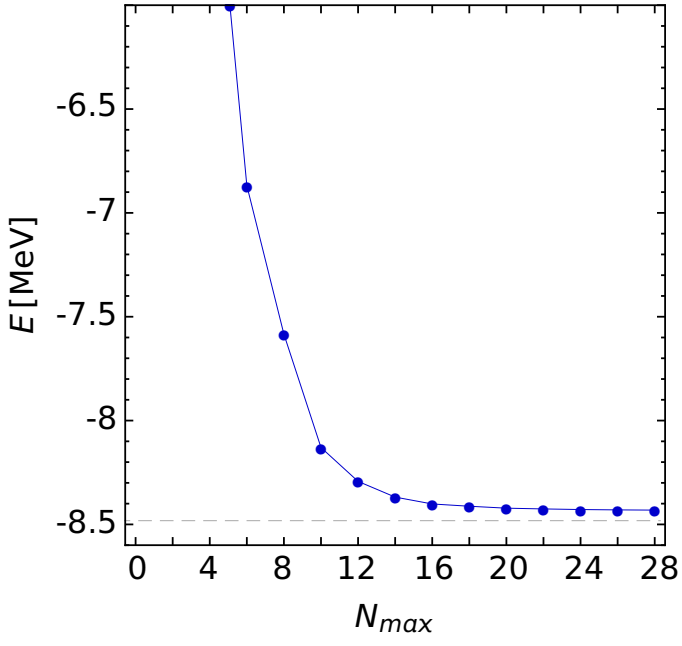

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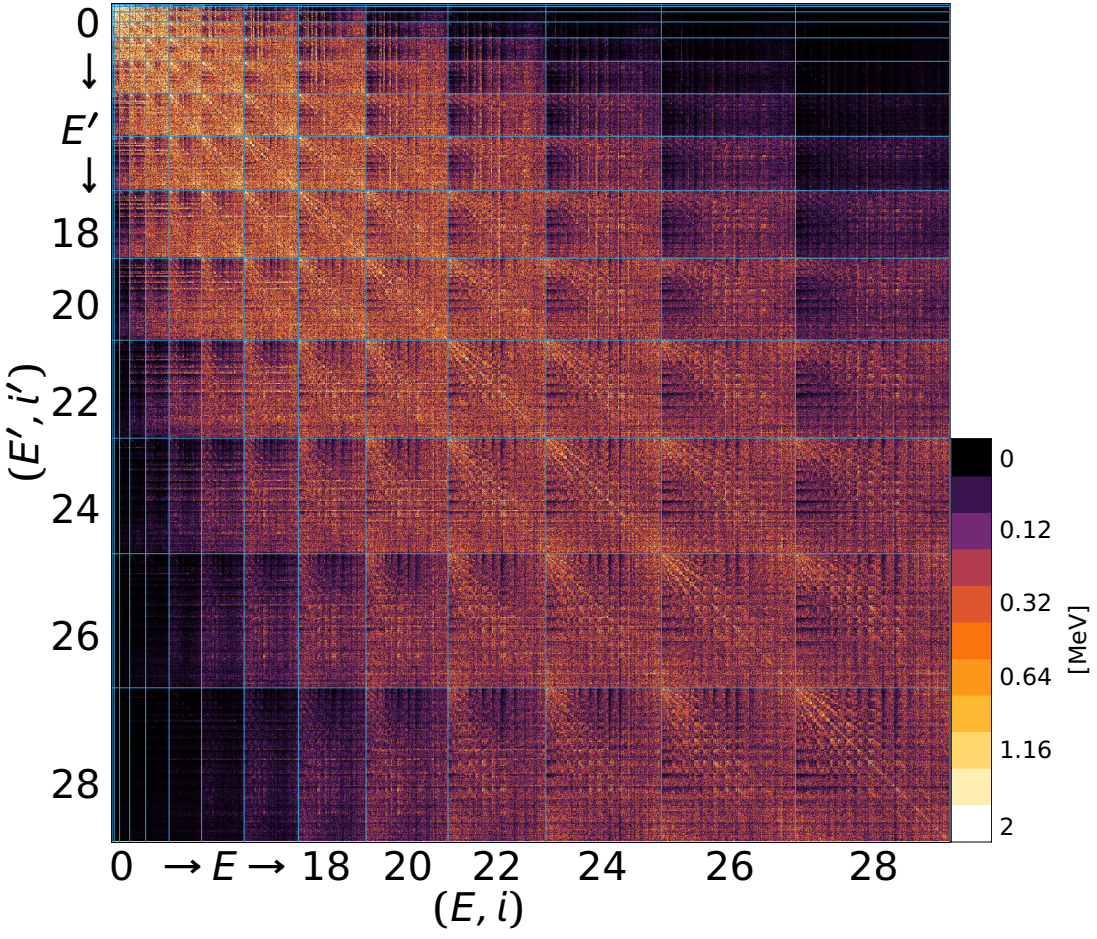

$$\alpha = 0.04\,\mathrm{fm}^4$$

$\lambda = 2.24\,\mathrm{fm}^{-1}$

$$\langle E'i'JT \left| \tilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} \right| EijT \rangle$$

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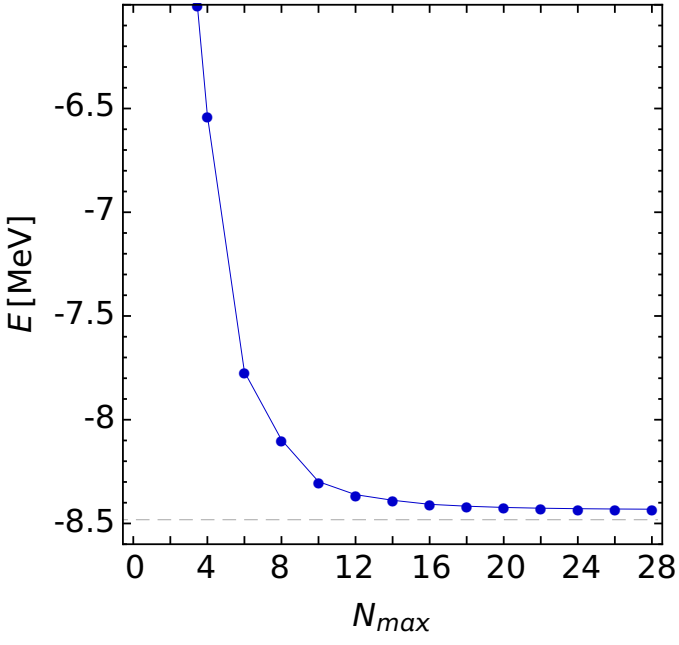

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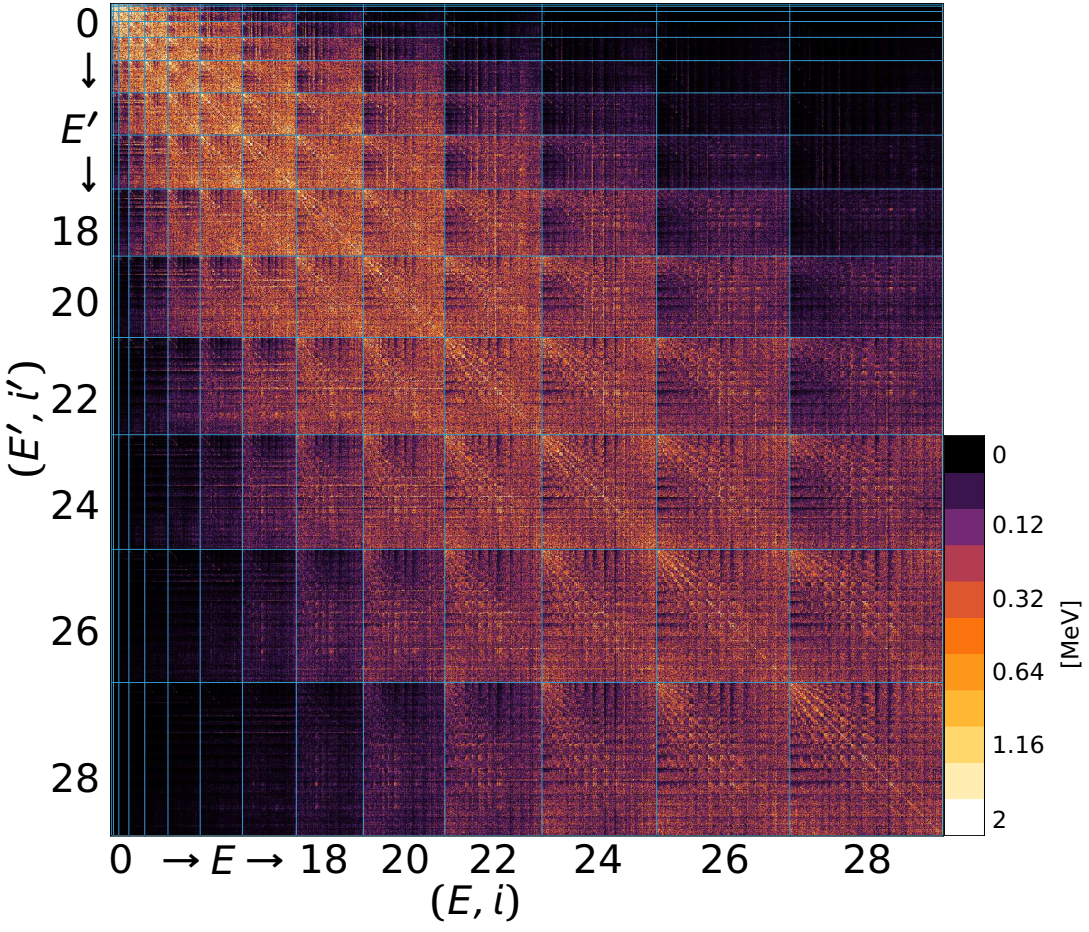

$$\alpha = 0.08\,\mathrm{fm}^4$$

$$\lambda = 1.88\,\mathrm{fm}^{-1}$$

$$\langle E'i'JT \left| \tilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} \right| EijT \rangle$$

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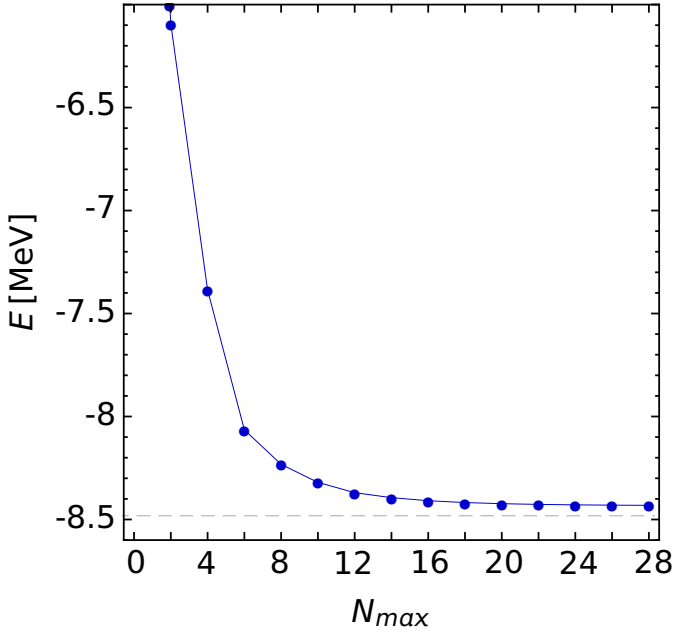

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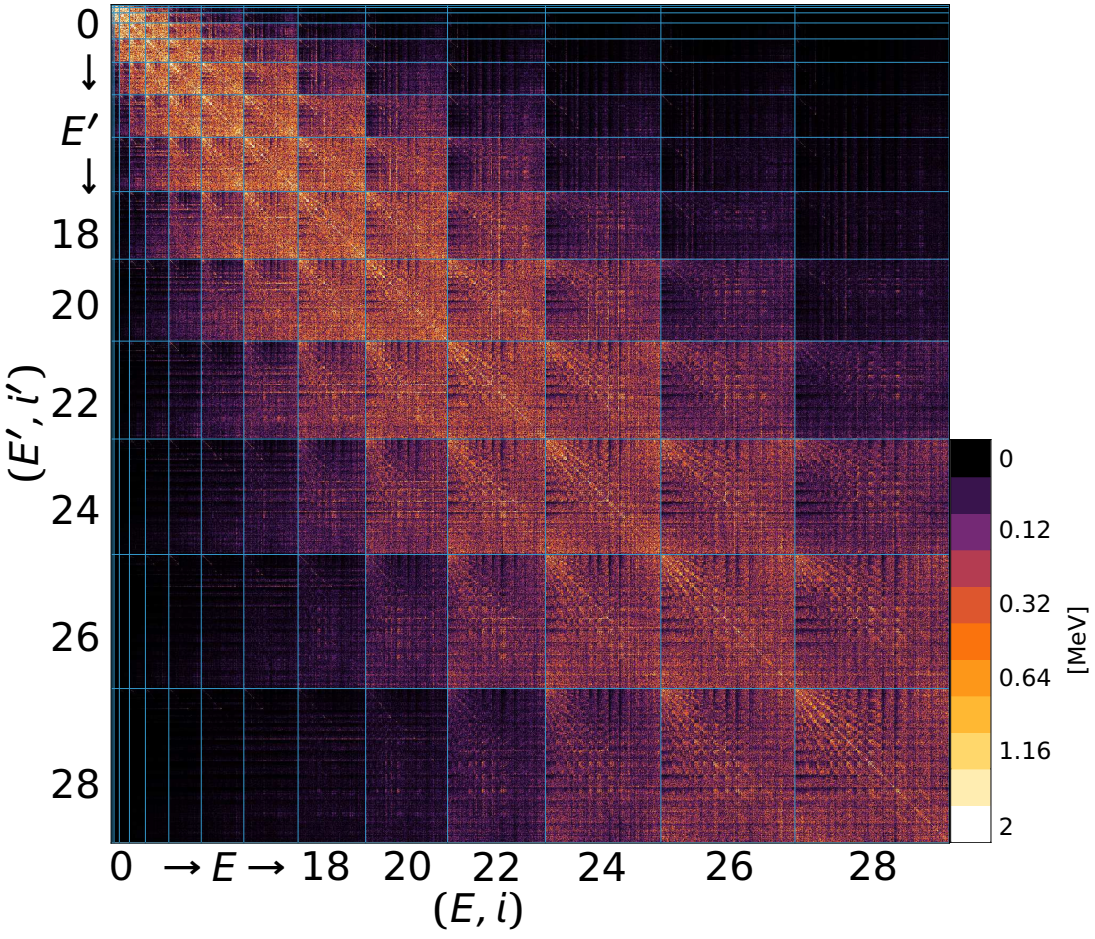

$$\alpha = 0.16\,\mathrm{fm}^4$$

$$\lambda = 1.58\,\mathrm{fm}^{-1}$$

$$\langle E'i'JT \left| \tilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} \right| EijT \rangle$$

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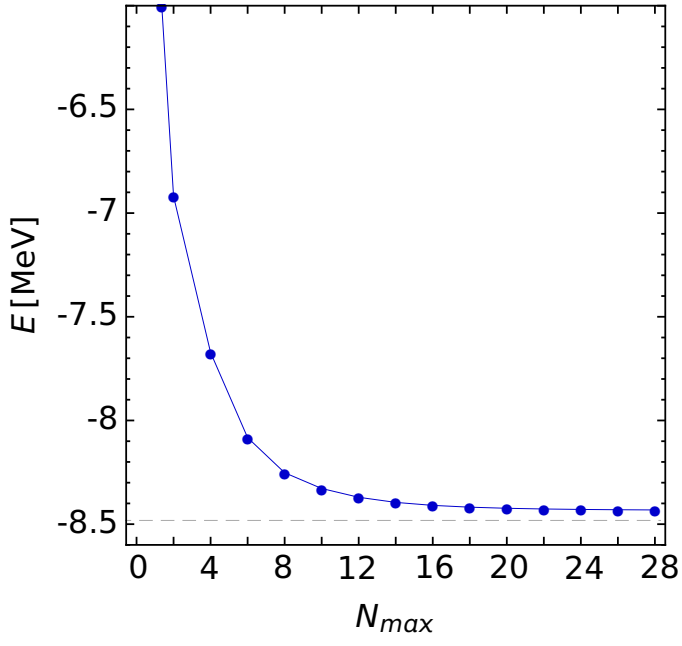

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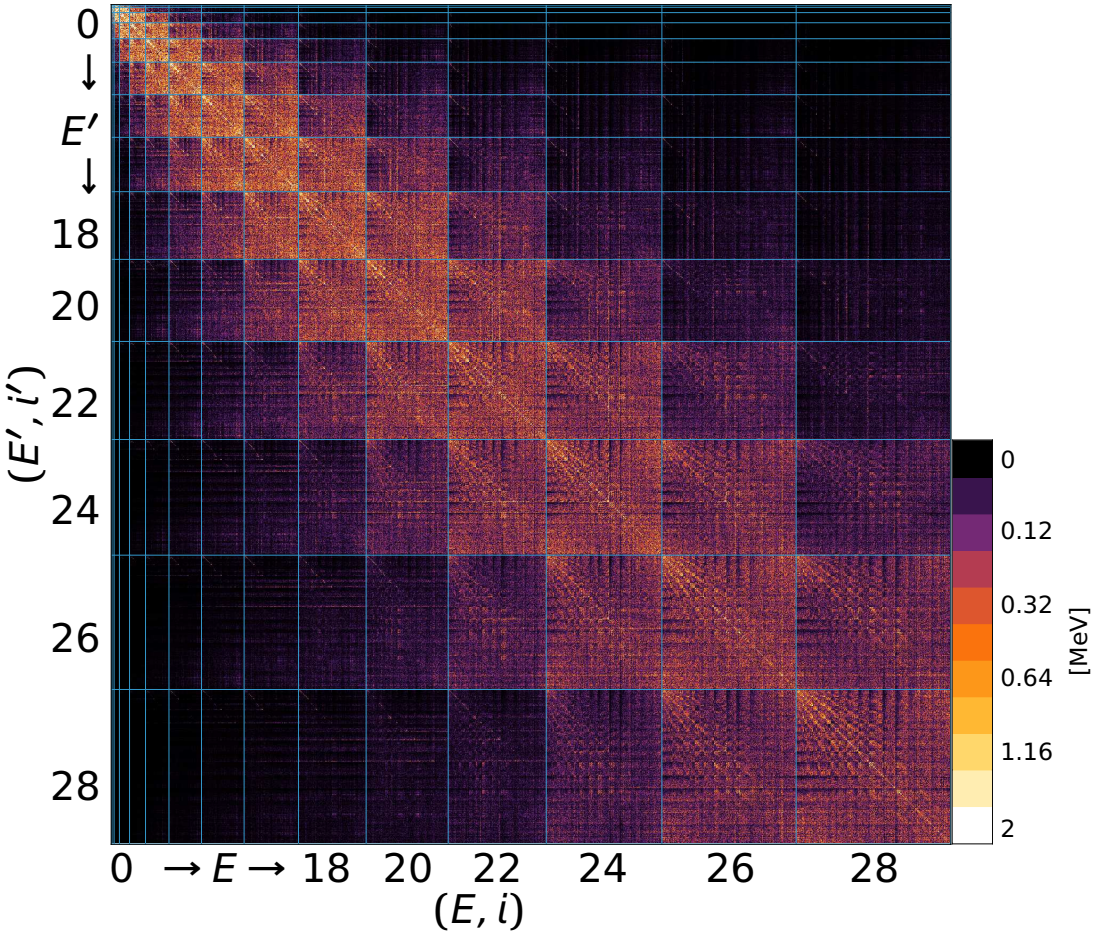

$$\alpha = 0.32\,\mathrm{fm}^4$$

$\lambda = 1.33\,\mathrm{fm}^{-1}$

$$\langle E'i'JT \left| \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} \right| EijT \rangle$$

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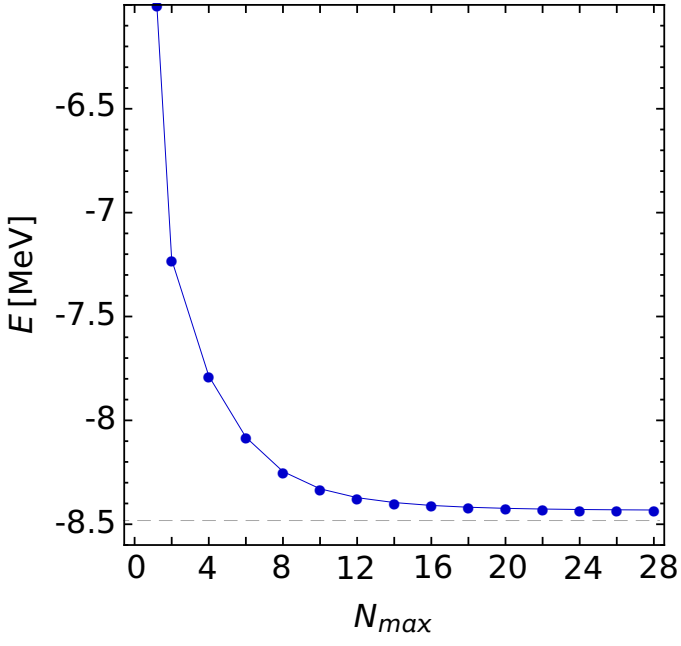

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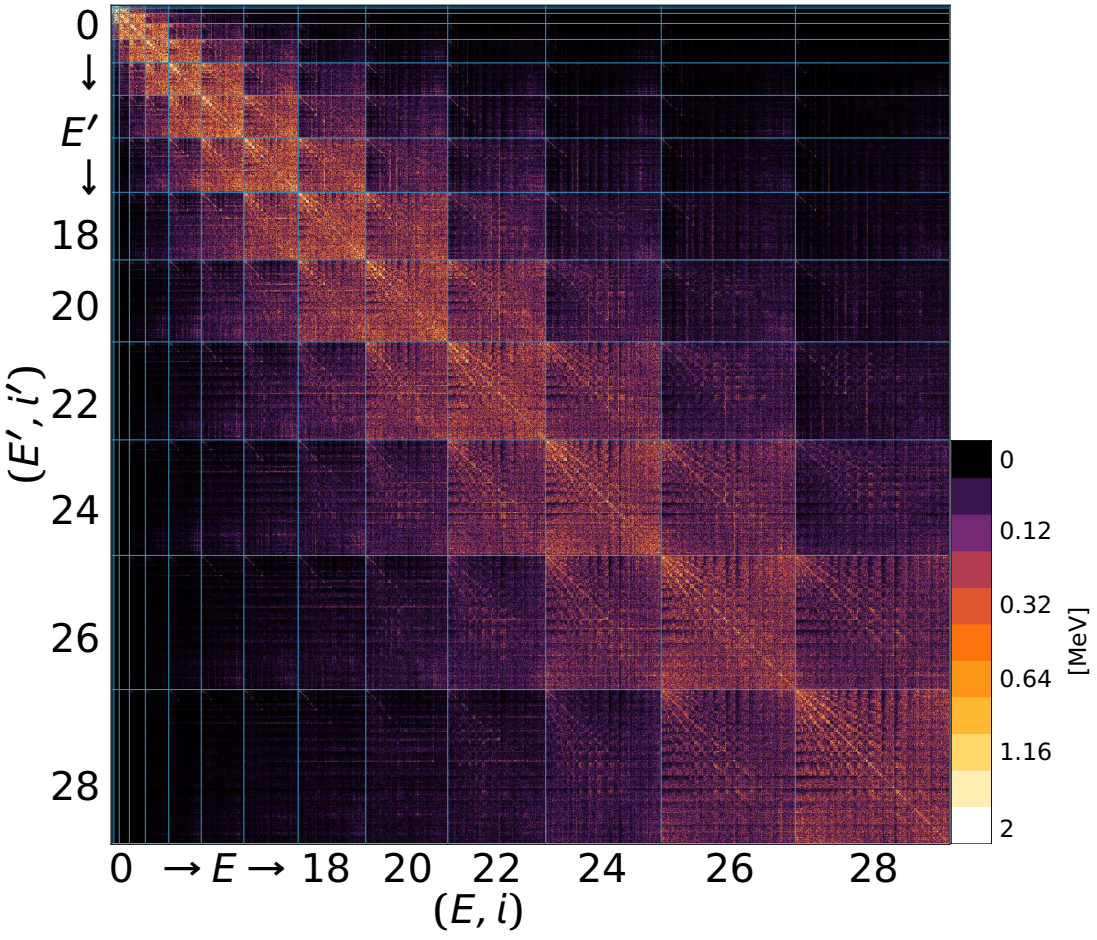

$$\alpha = 0.64\,\mathrm{fm}^4$$

$\lambda = 1.12\,\mathrm{fm}^{-1}$

$$\langle E'i'JT \left| \widetilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} \right| EijT \rangle$$

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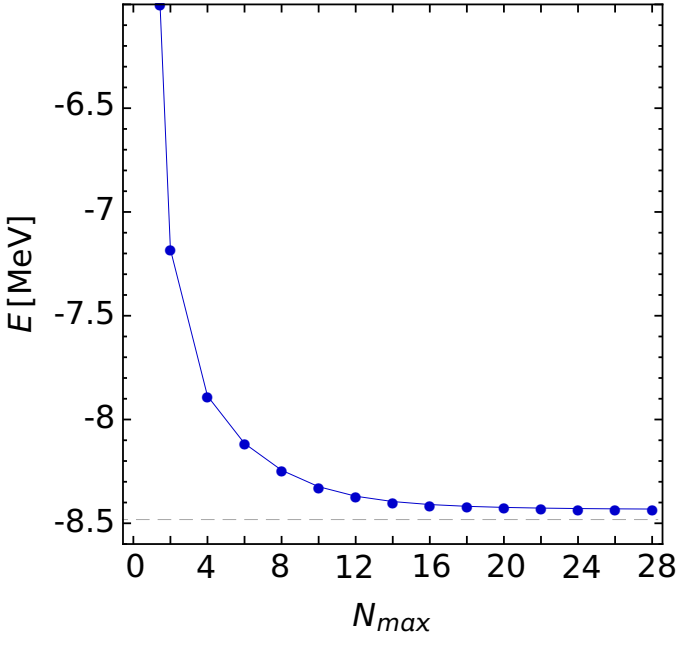
NCSM ground state ^{3}H



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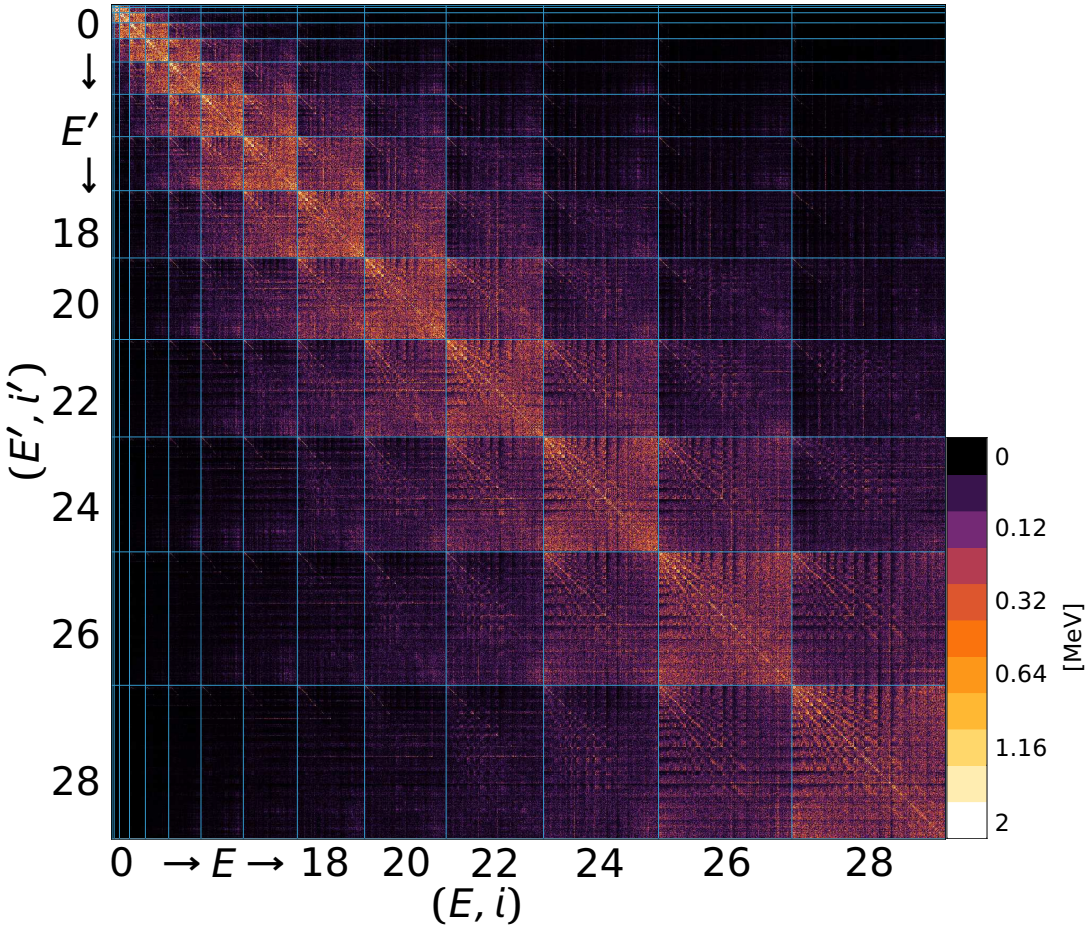

$$\alpha = 1.28\,\mathrm{fm}^4$$

$$\lambda = 0.94\,\mathrm{fm}^{-1}$$

$$\langle E'i'JT \left| \tilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} \right| EijT \rangle$$

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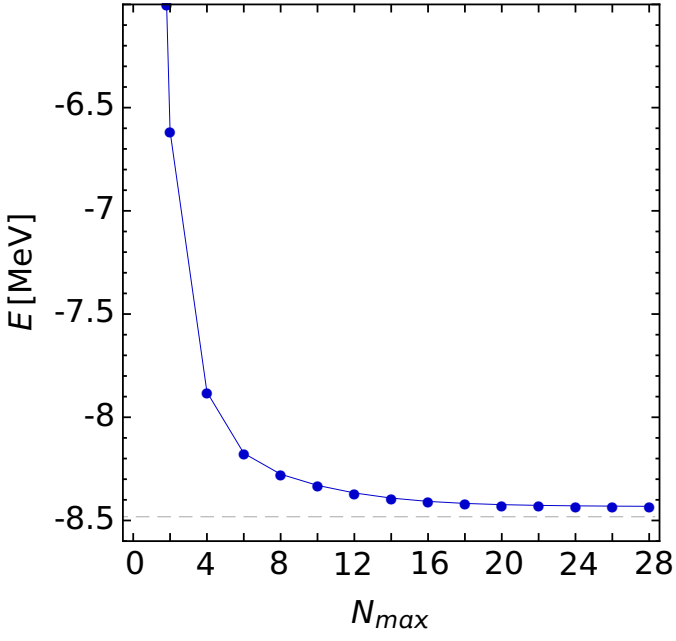
NCSM ground state ^{3}H



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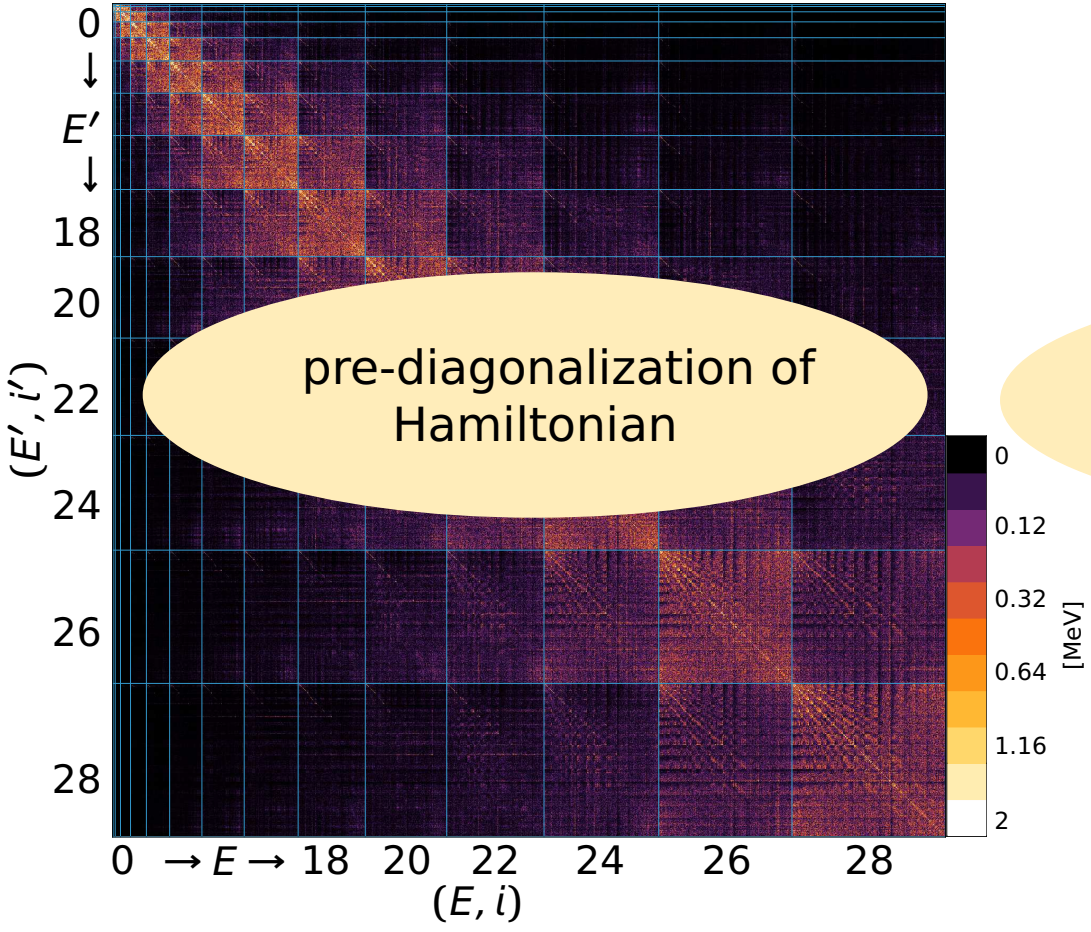

pre-diagonalization of Hamiltonian

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$$\lambda = 0.94\,\mathrm{fm}^{-1}$$

$$\langle E'i'JT \left| \tilde{\mathrm{H}}_\alpha - \mathrm{T}_{\mathrm{int}} \right| EijT \rangle$$

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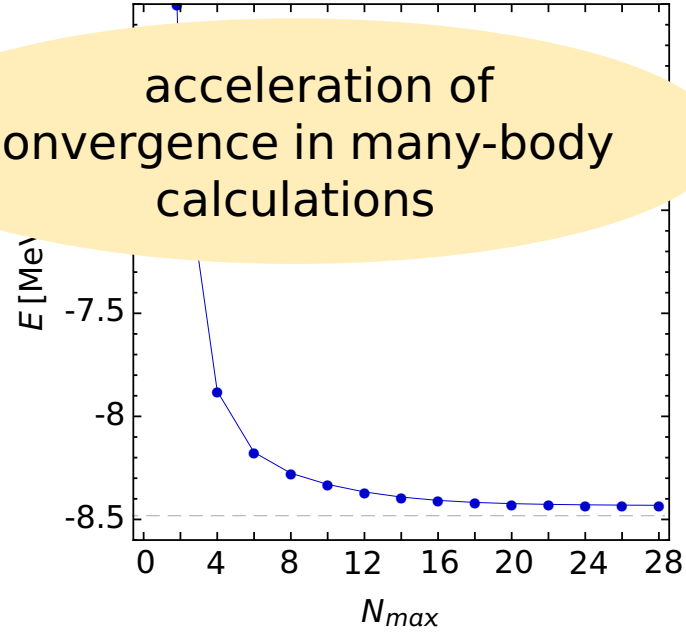
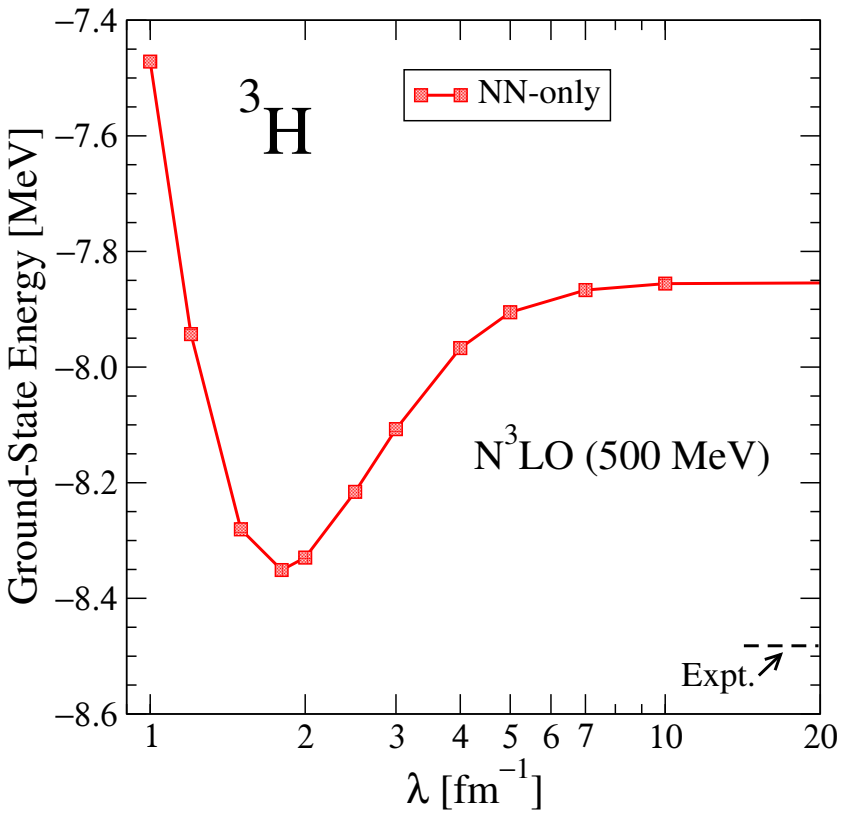
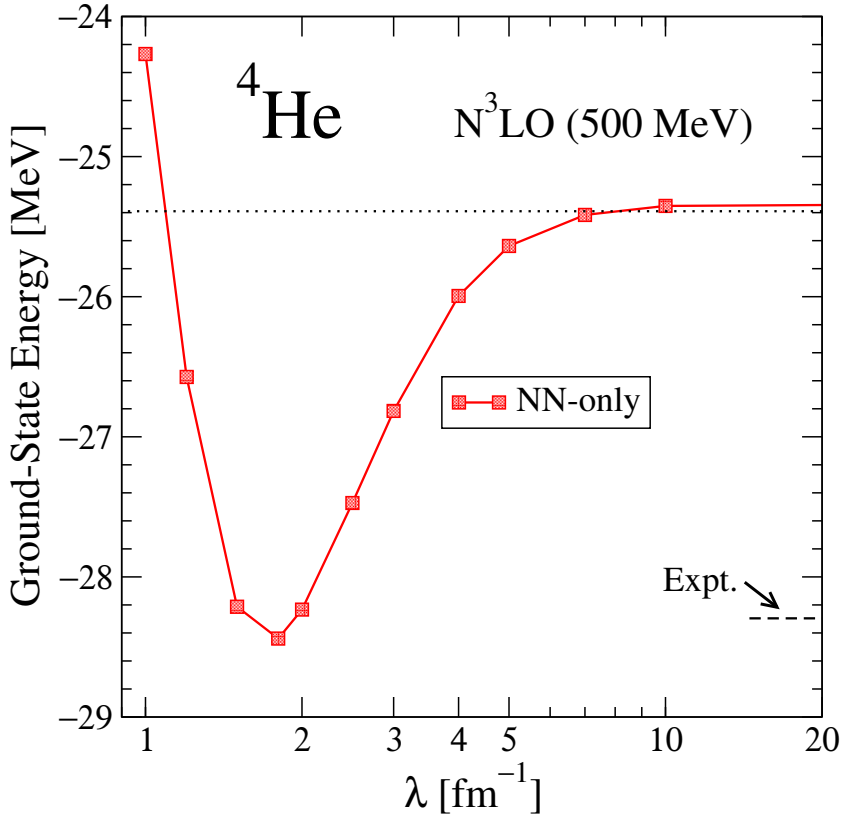


acceleration of convergence in many-body calculations

SRG evolution of NN *and* NNN

- Can evolve in *any* basis [E. Jurgenson, P. Navrátil, rjf (2009)]
  - first in anti-symmetric Jacobi HO basis from NCSM
  - directly obtain SRG matrix elements in HO basis
  - more recently: evolution in k-space [Hebeler (2012)] and in hyperspherical harmonics basis [Wendt (2013)]
- Compare 2-body only to full 2 + 3-body evolution:





SRG evolution of NN *and* NNN

- Can evolve in *any* basis [E. Jurgenson, P. Navrátil, rjf (2009)]
  - first in anti-symmetric Jacobi HO basis from NCSM
  - directly obtain SRG matrix elements in HO basis
  - more recently: evolution in *k*-space [Hebeler (2012)] and in hyperspherical harmonics basis [Wendt (2013)]
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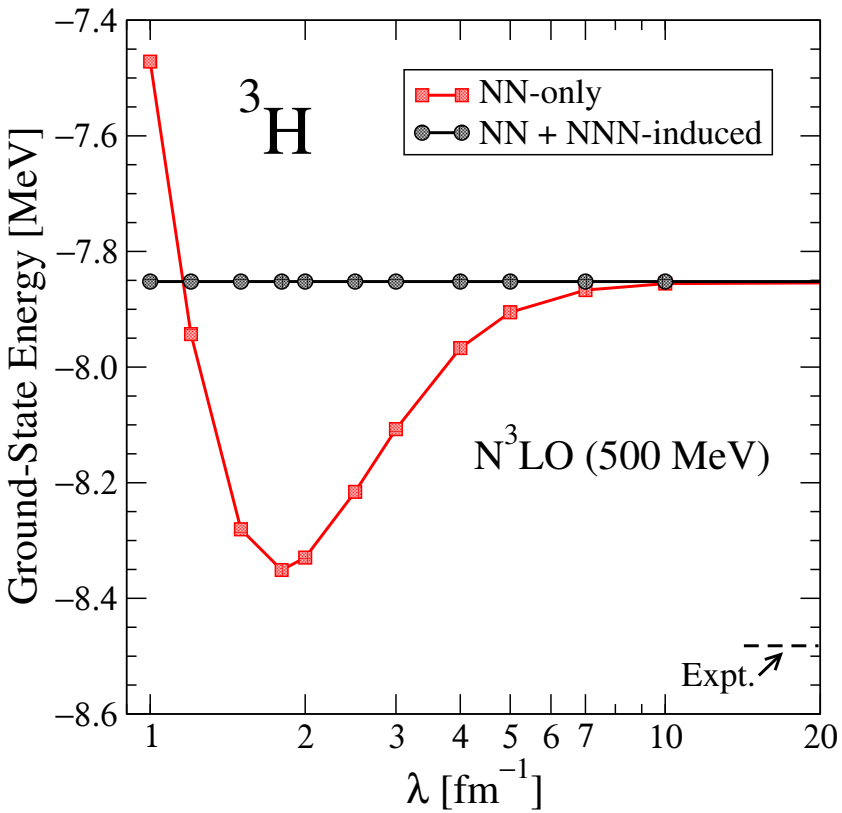

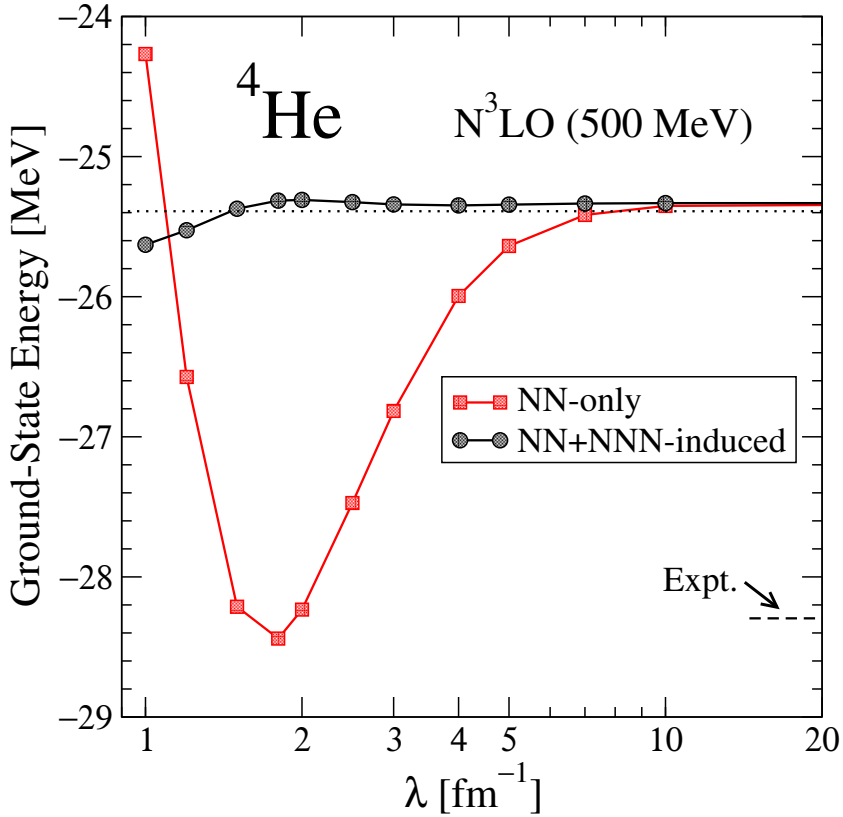

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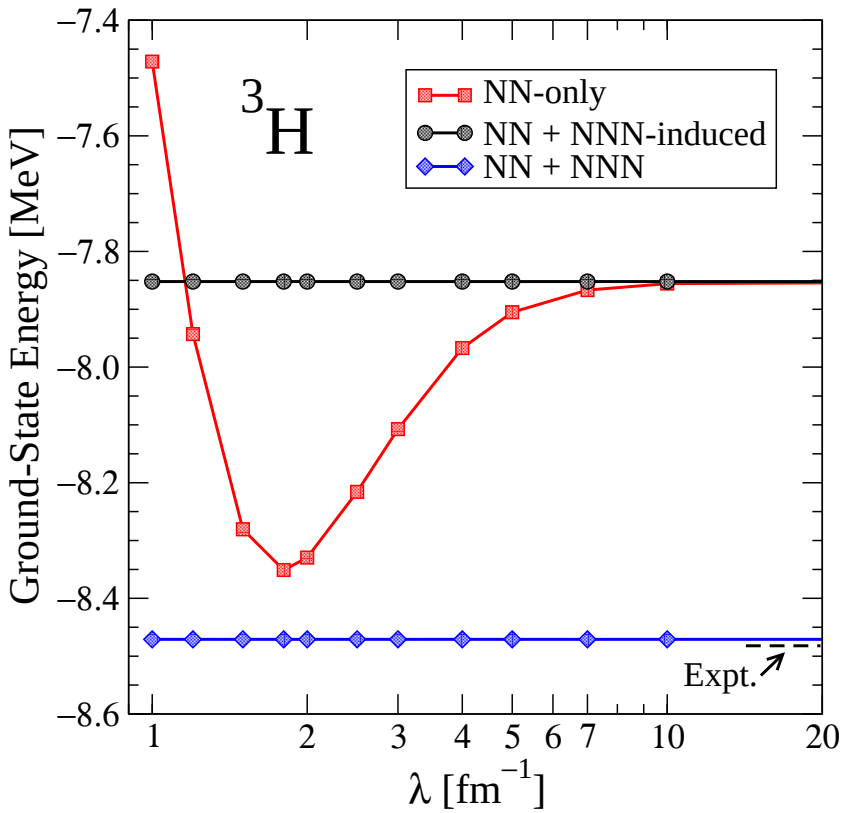
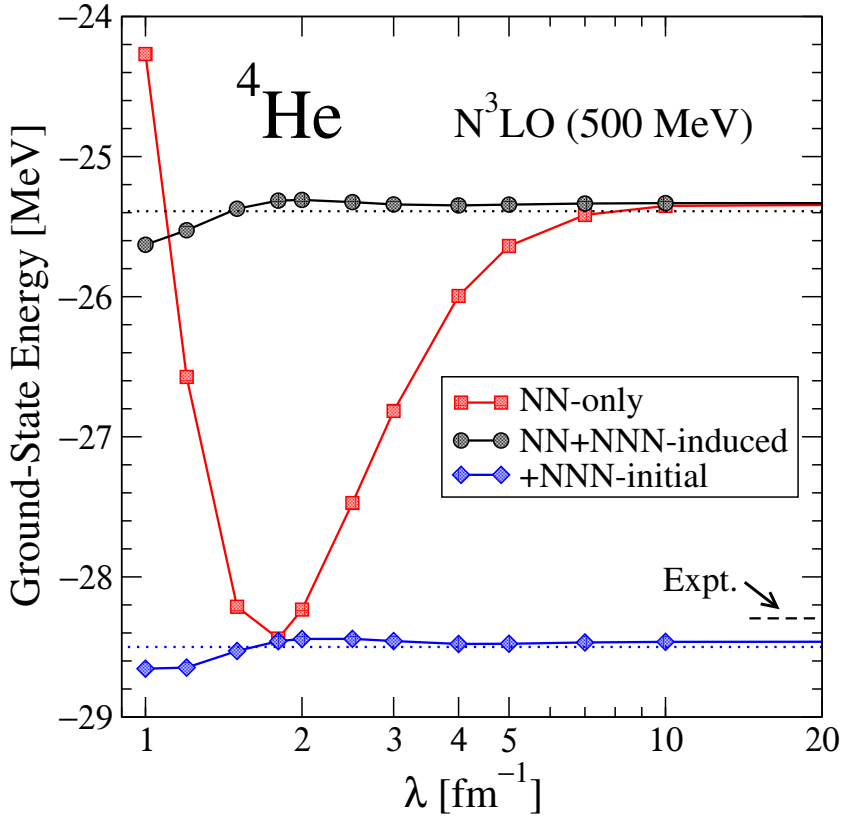
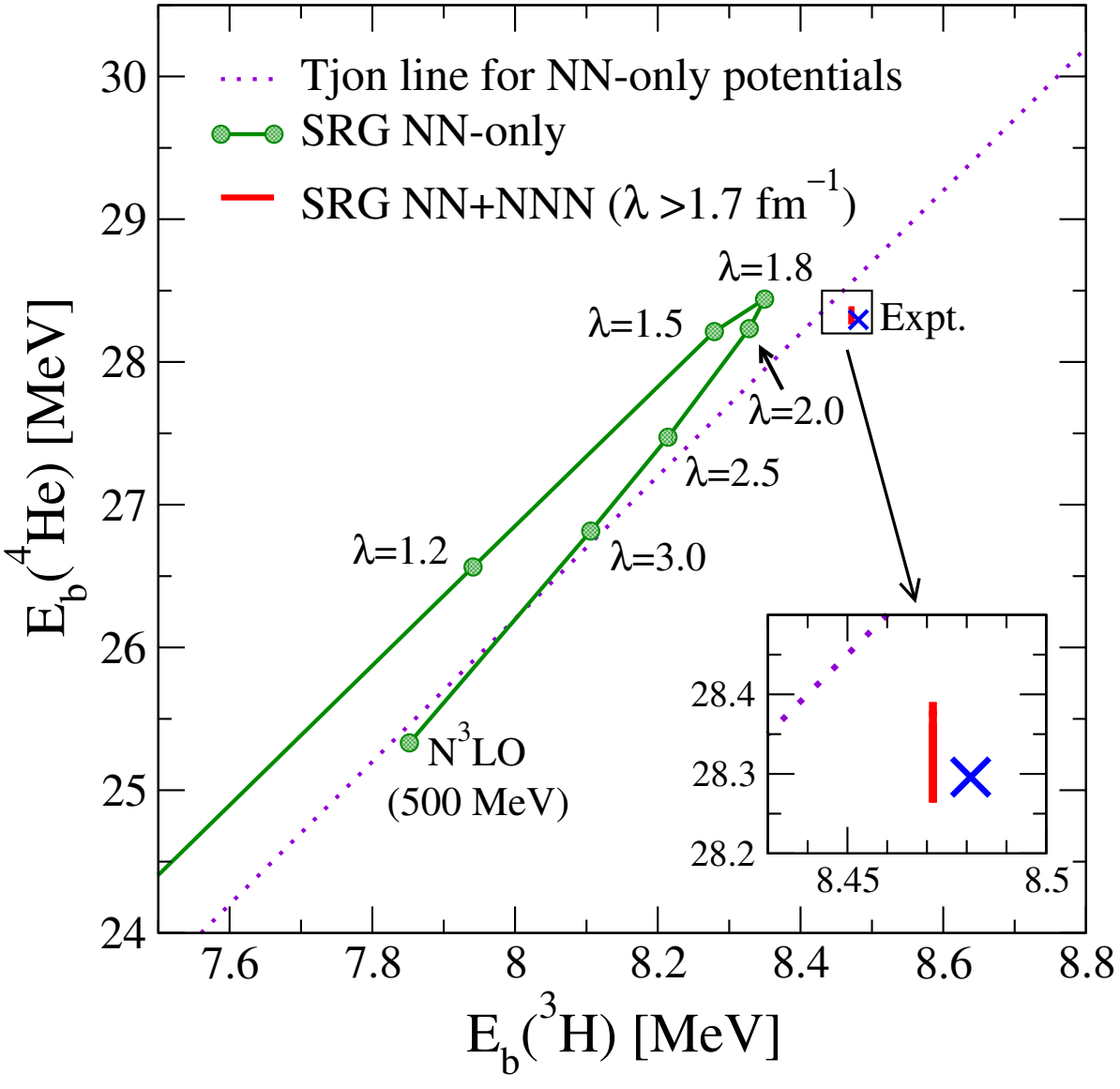




Tjon line revisited

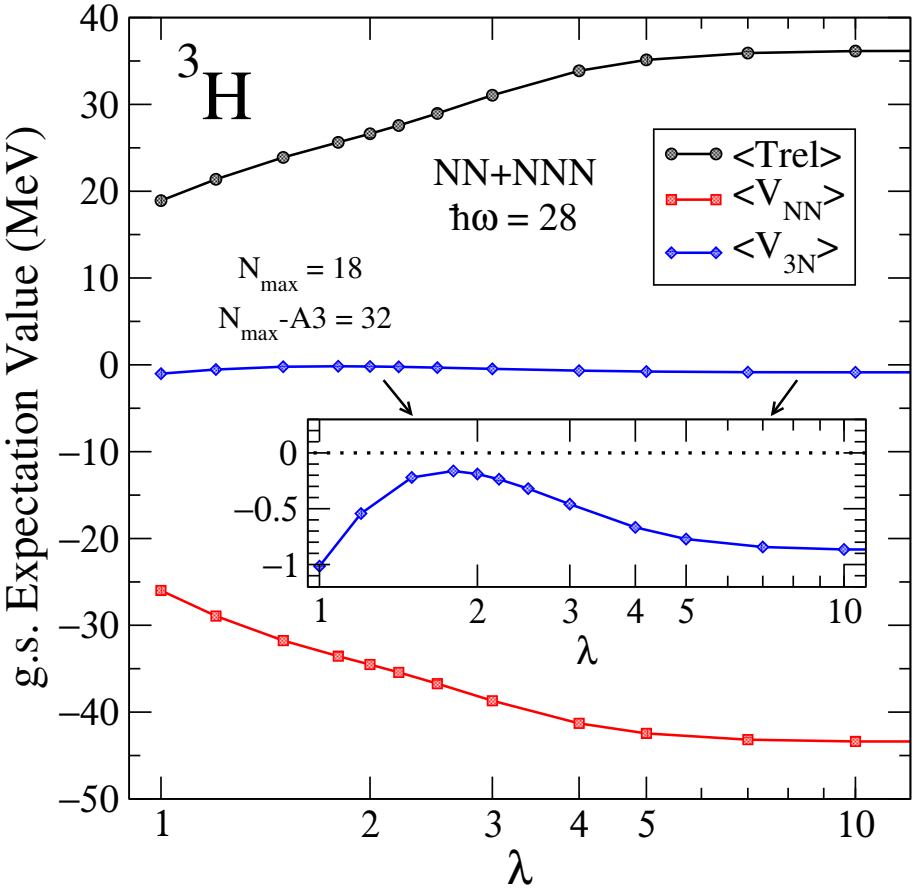


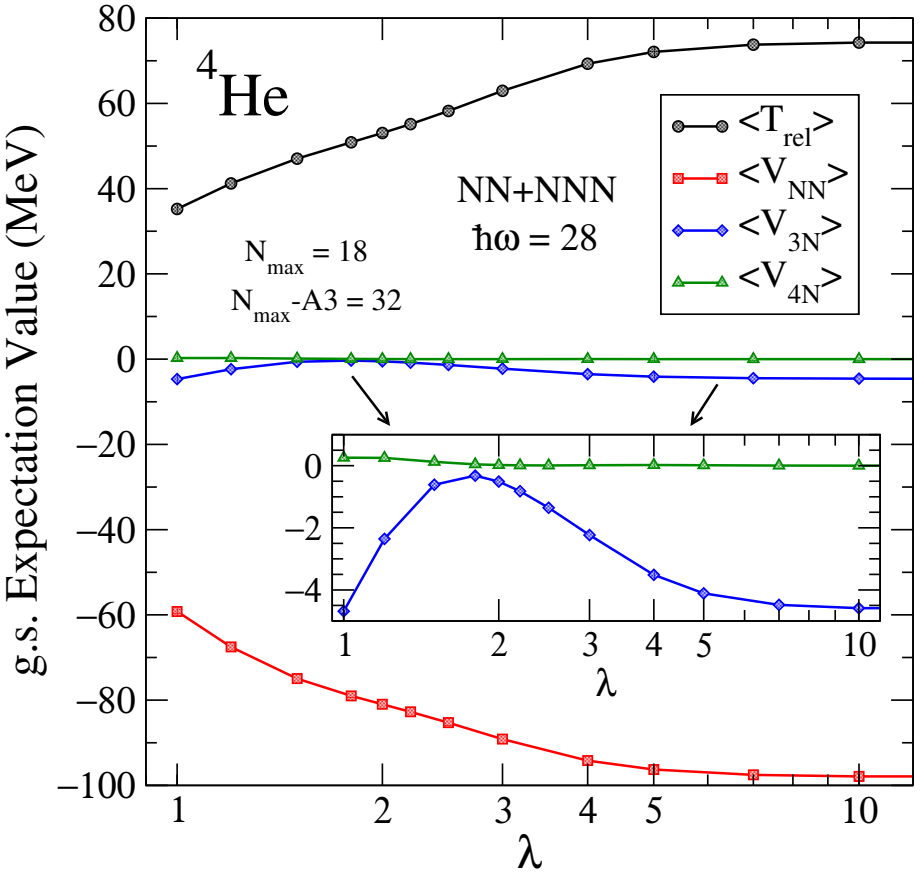
- Unitary transformation $\Longrightarrow$ energy unchanged
- Plot calculated binding energies ^{4}He vs. ^{3}H
- Now include initial and evolved three-body force
- Energies barely change! (see inset)
- Residual λ dependence $\Longrightarrow$ theory error bars

- Is the growth of 3+ body forces under control?

Contributions to the ground-state energy

- Look at ground-state matrix elements of KE, NN, 3N, 4N



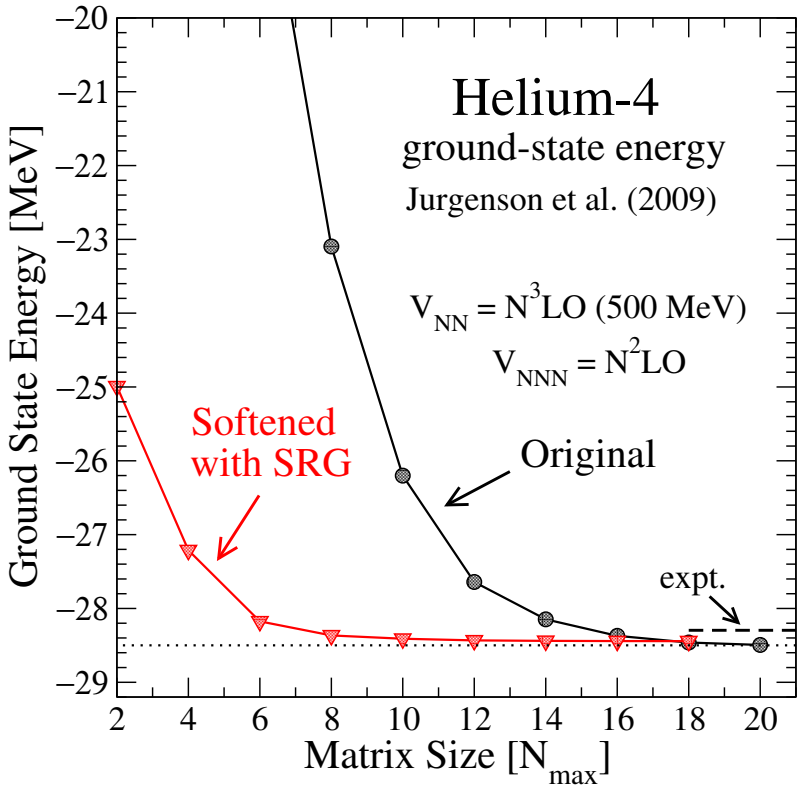


- Clear hierarchy, but also strong cancellations at NN level
- What about the *A* dependence? We can test it now!

RG softening $\Longrightarrow$ quantum chemistry methods work!

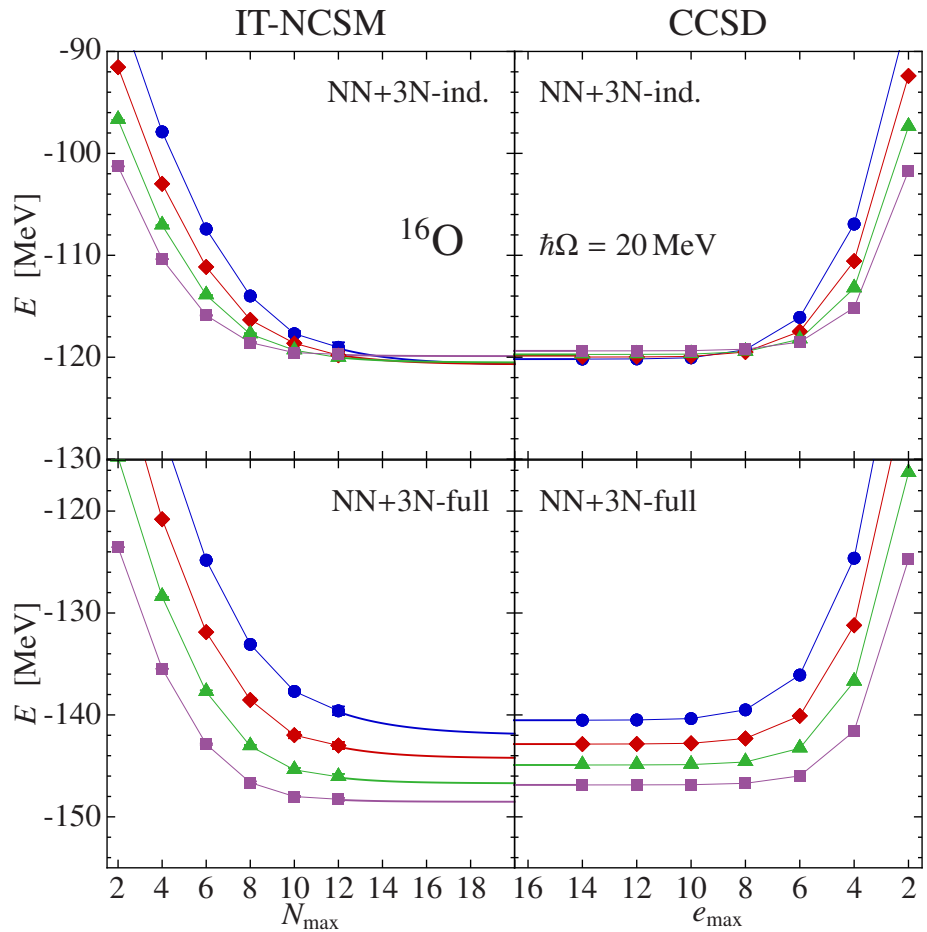
Softened potentials (SRG, $V_{\mathrm{low}\,k}$, UCOM, ...) enhance convergence

- 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)

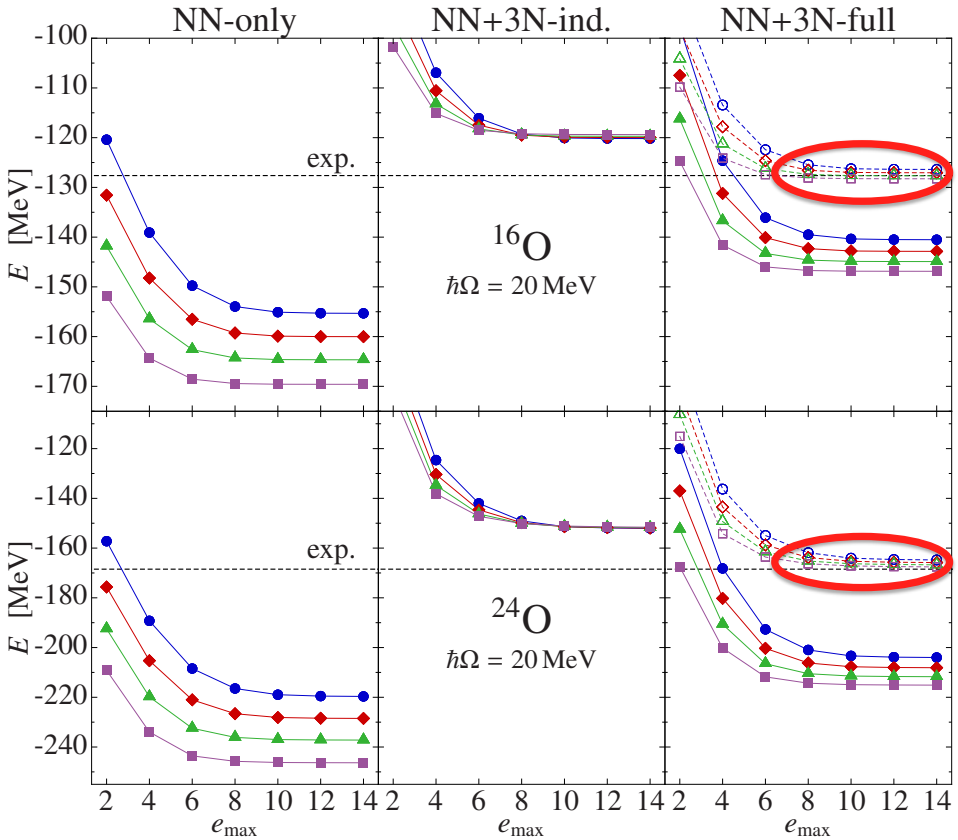


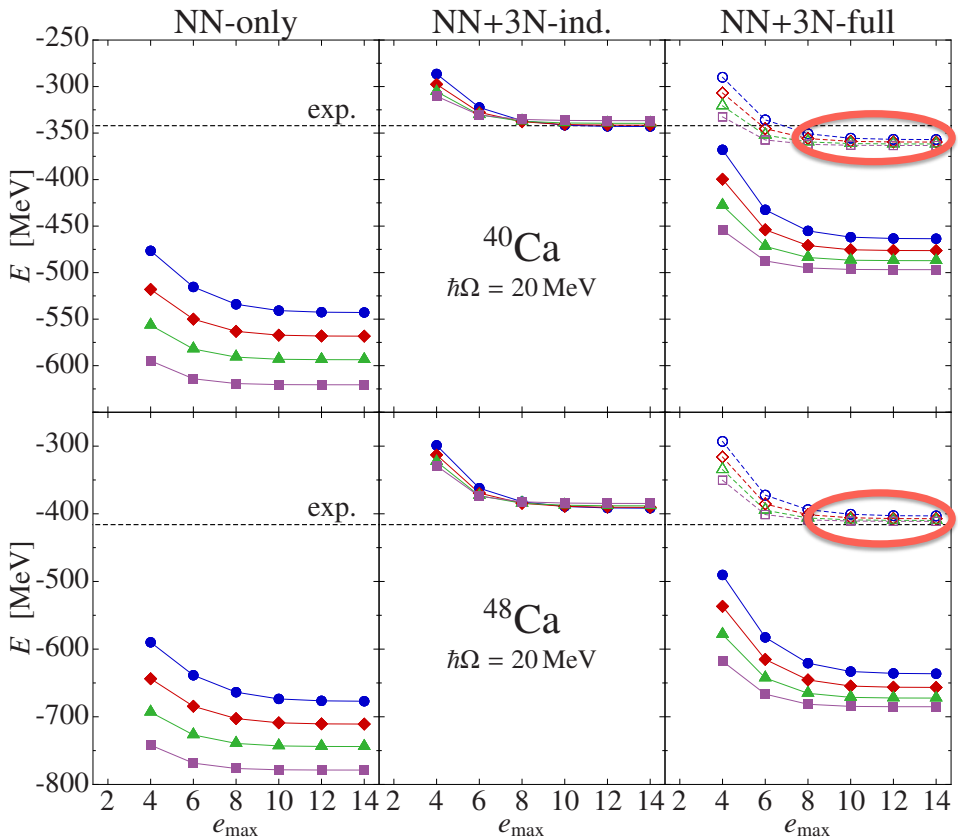
[Roth et al. (2012)]

SRG-evolved N^{3}LO(500) with NNN [R. Roth et al. (2012)]

Use dependence on SRG λ to test evolved Hamiltonian!

- NN-only: doesn't include induced NNN $\Longrightarrow$ λ dependent
- NN+3N-induced: λ independent but doesn't match experiment
- NN+3N-full: includes (two) initial NNN fit to $A = 3, 4$ properties

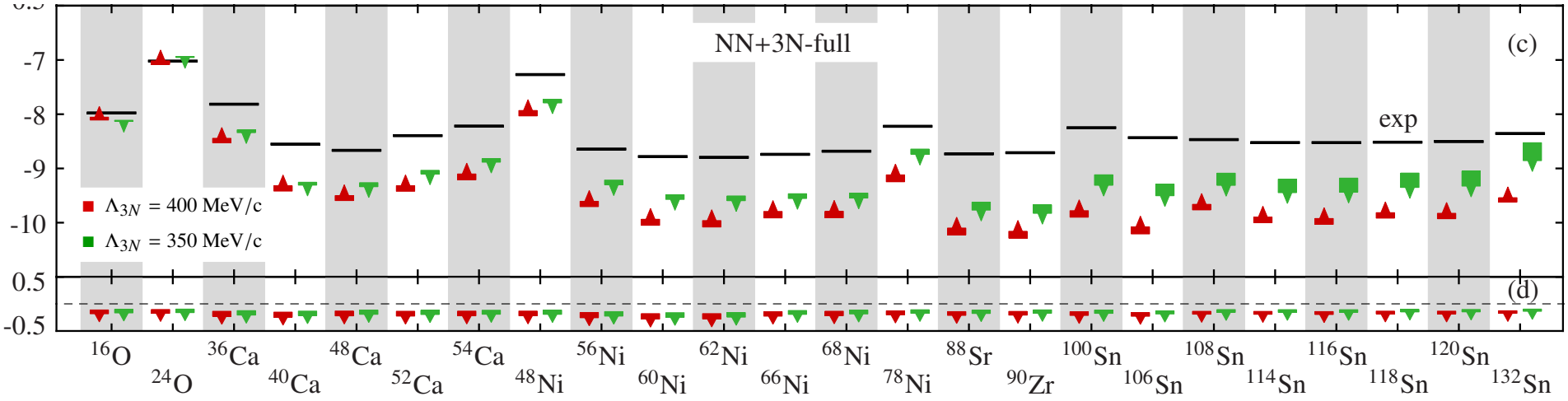




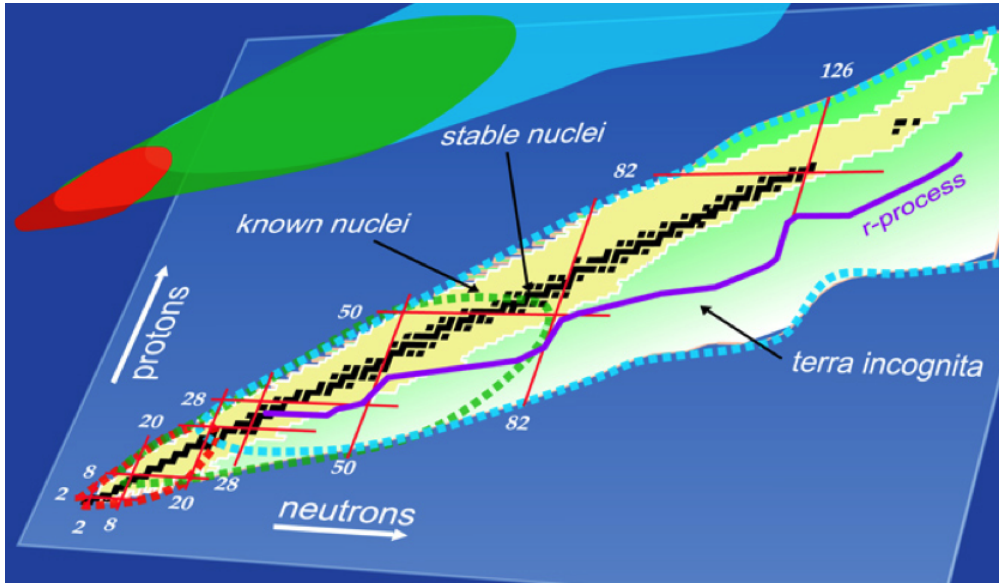
- Coupled cluster method $\Longrightarrow$ Pure predictions!

What is feasible for *ab initio* structure with SRG today?

- Similarity-RG-evolved Hamiltonians with coupled-cluster method
  - Figure from Binder et al., arXiv:1312.5685 (Dec. 2013)
  - Energy/particle (in MeV) from oxygen to tin ($A = 132$!)



- Use *cutoff dependence* as tool
- Uncertainty quantification (theory error bars)
- Test and refine nuclear EFT Hamiltonians (NN+NNN)
- Status: precise but not accurate



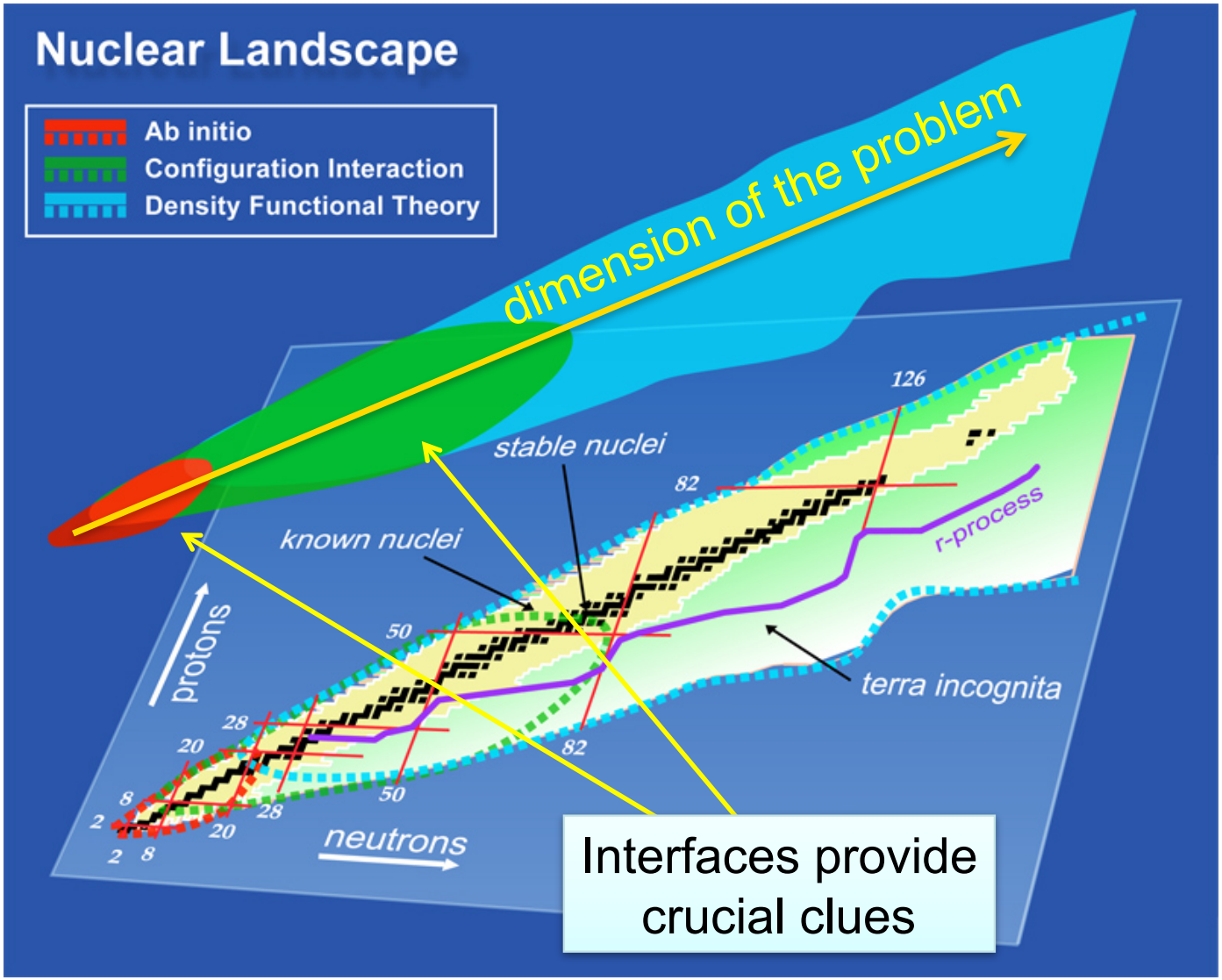
Outline: Lecture 4

Lecture 4: 3NF and applications

- RG-induced many-body forces
- Some places where the 3NF matters
- Results for infinite matter
- Future trends for chiral 3NF

Historical perspective: ab initio structure 10–15 years ago

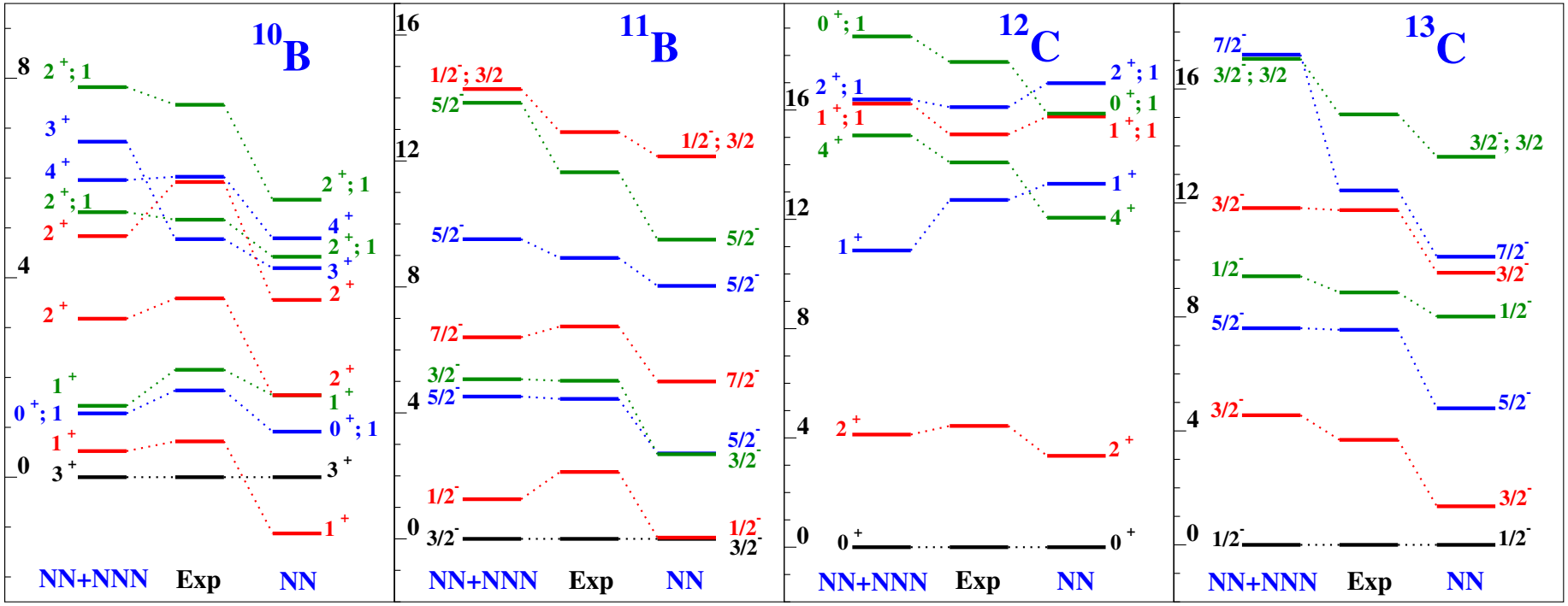
- From the start of the SciDAC UNEDF project (2007)



- Ab initio: Where did details of 3NF forces make a difference?

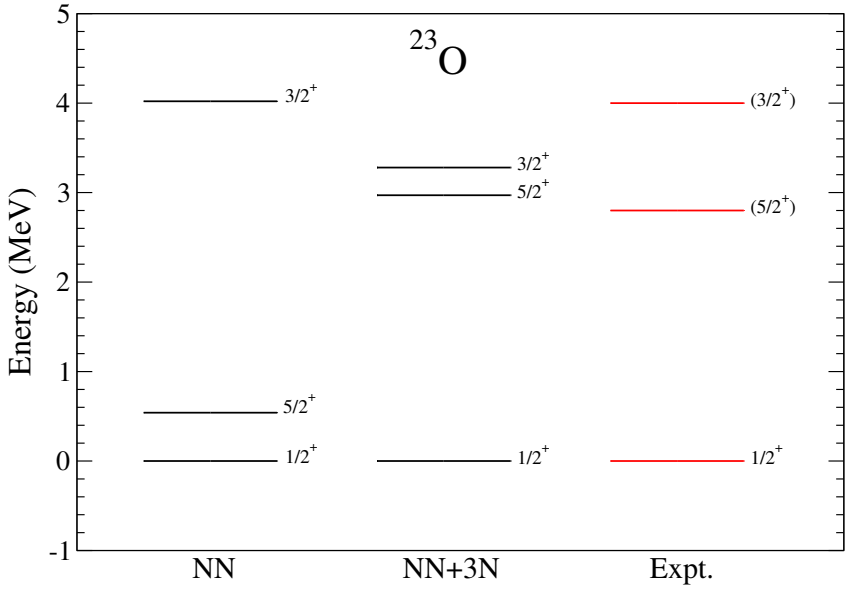
No-Core Shell Model (NCSM) with 3NF in 2007

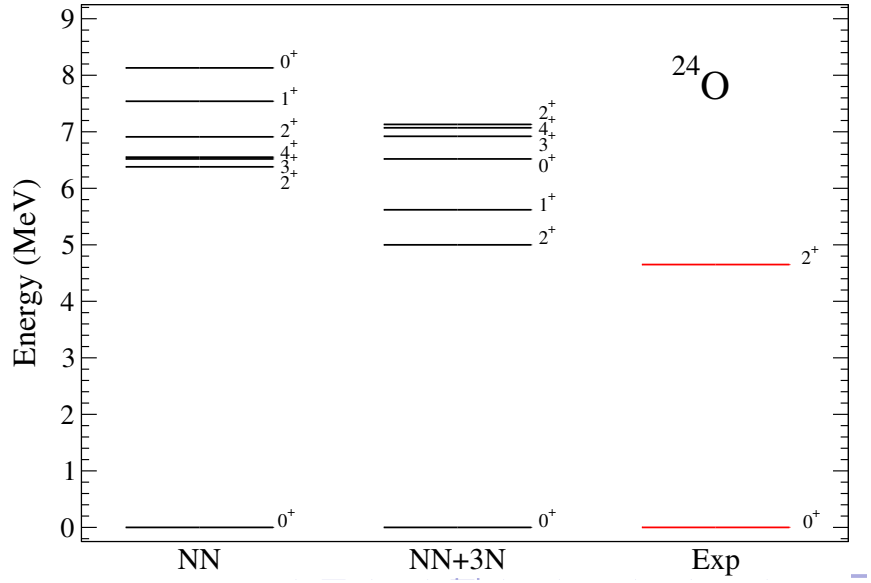
- Nuclear structure results point to importance of 3NF
  - Note ^{10}B ground state
  - Note spin-orbit splittings
- Needed better convergence (which we now have!)



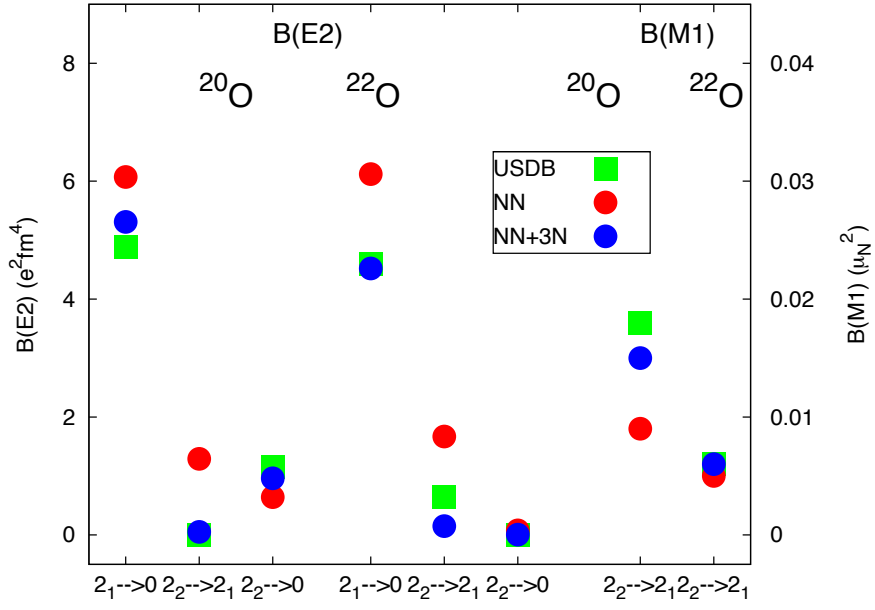
[Navratil et al., (2007)]

Oxygen spectra and transitions from MPBT





- J. Menendez et al.
- Many-body perturbation theory (MBPT)
- Enabled by RG softening
- Chiral EFT interaction with NN and 3N forces
- Needs error bands!



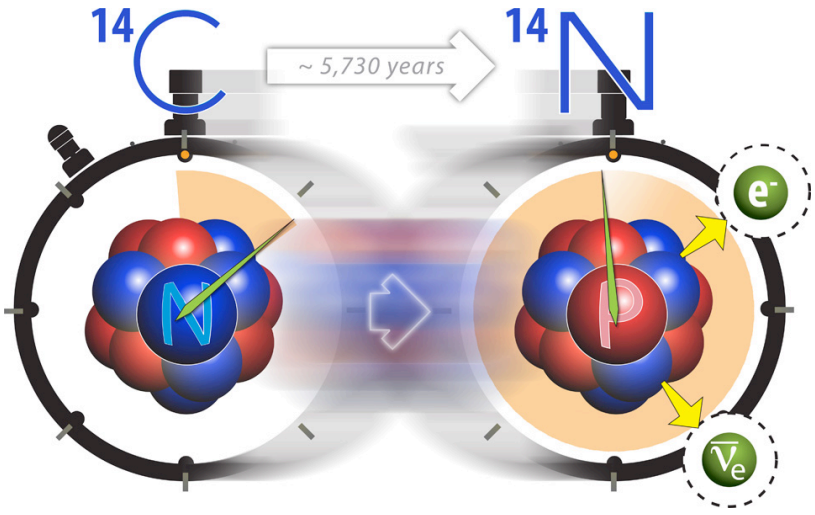
Electromagnetic transitions (decay lifetimes)

B(E2) transitions in 2_2^+ states, ^{20}O and ^{22}O

U.S. DEPARTMENT OF ENERGY | Office of Science

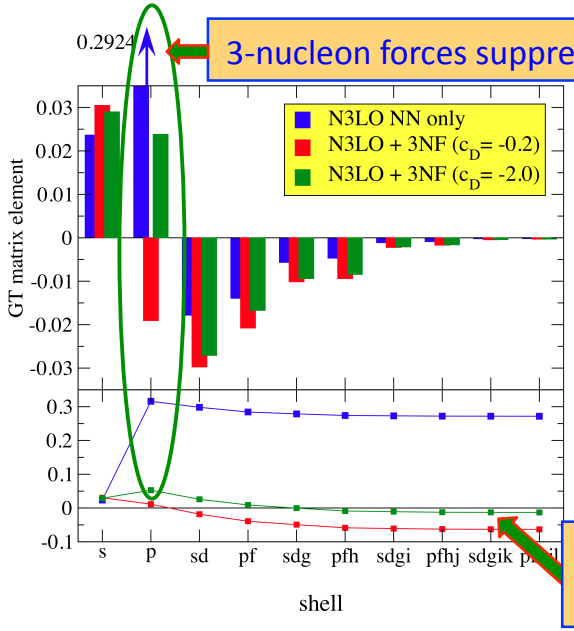
"Why does Carbon-14 live so long?"

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

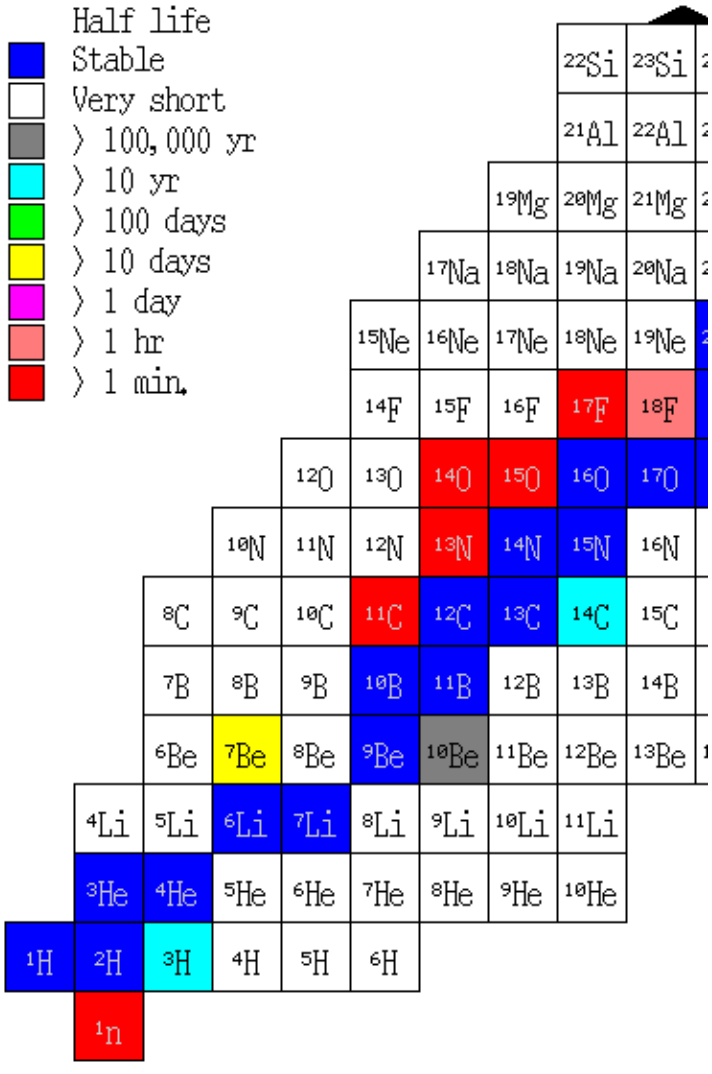
Calculations enabled by high-performance computing through INCITE program

- 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

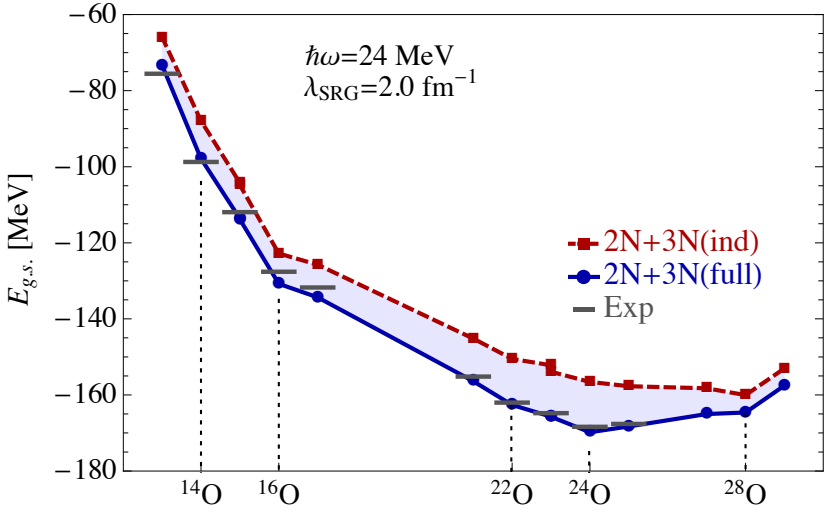
Science ref.: Physical Review Letters **106**, 202502 (2011)
Computational ref.: Procedia Computer Science **1**, 97 (2010)

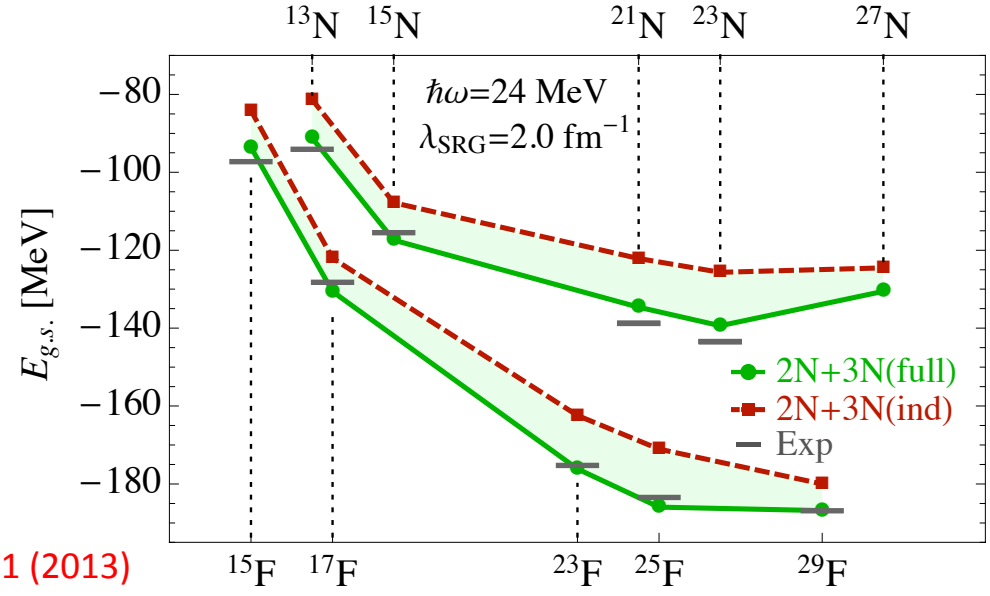
Asides on Carbon-14 decay calculation



- 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

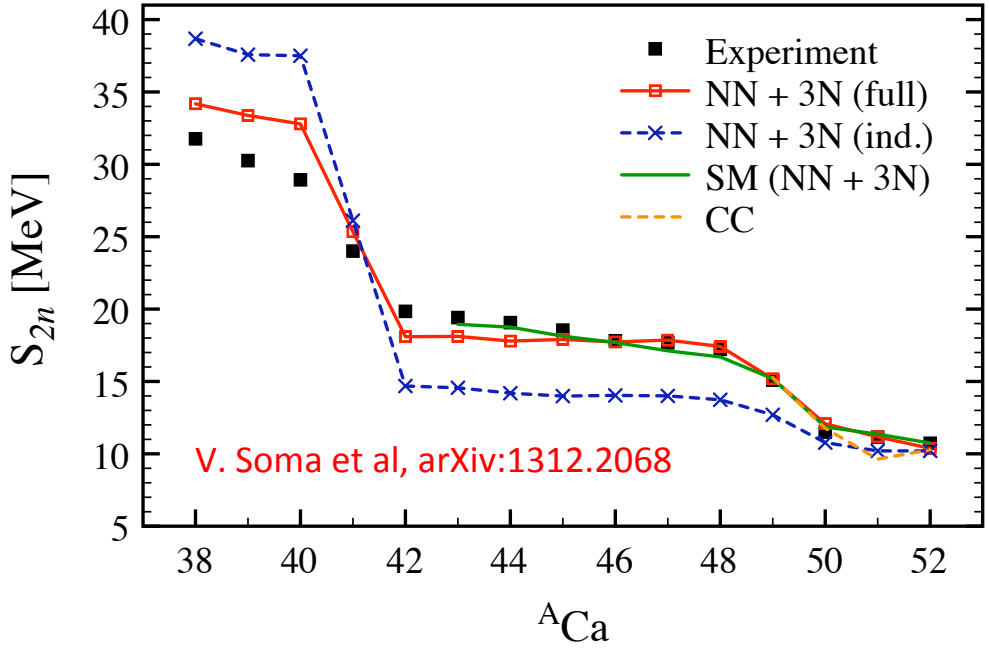
3NF improves descriptions along isotope chains





Cipollone et al., PRL **111**, 062501 (2013)

- Self-consistent Green's function (SCGF) approach
- Chiral EFT interaction with NN and 3N forces
- Evolved by SRG to $\lambda = 2\,\mathrm{fm}^{-1}$
- Compare NN-only (ind) to full
- Needs error bands!



Outline: Lecture 4

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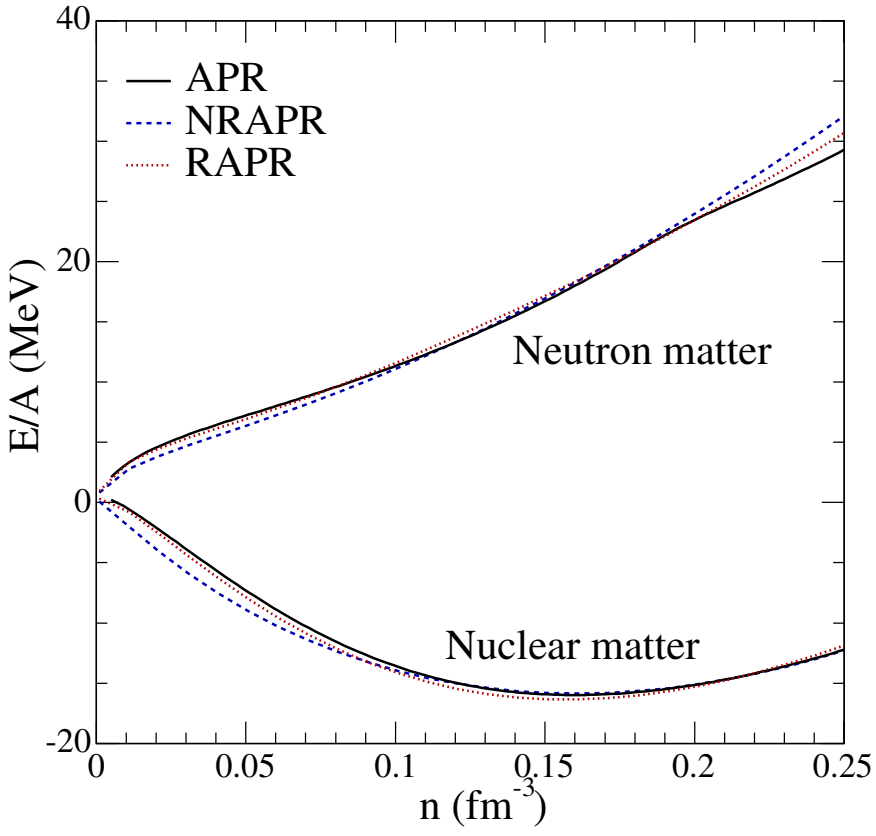
Nuclear and neutron matter energy vs. density

[Akmal et al. calculations shown]



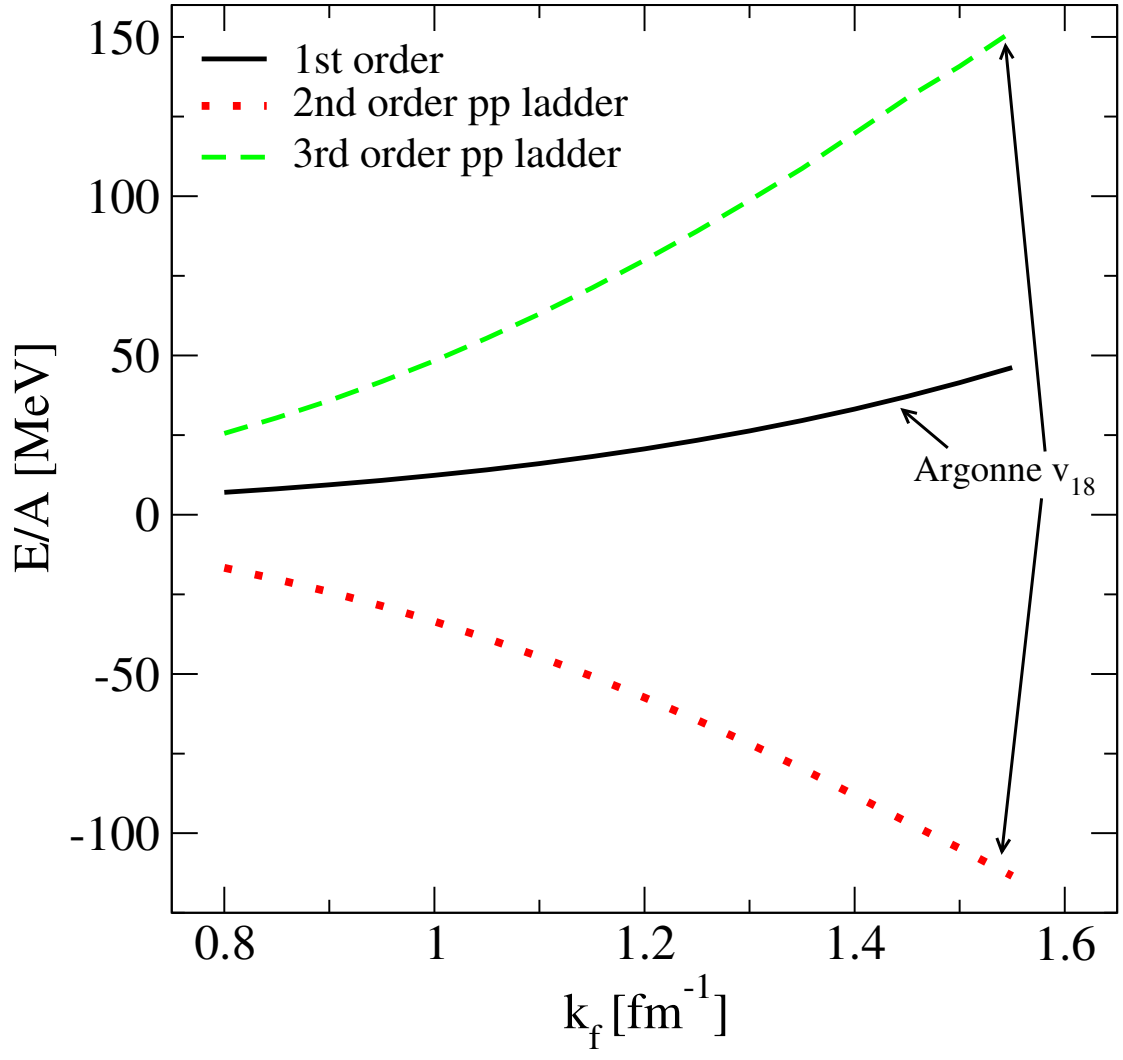
- Uniform with Coulomb turned off
- Density n (or often ρ)
- Fermi momentum $n = (\nu/6\pi^2)k_F^3$
- Neutron matter ($Z = 0$) has positive pressure
- Symmetric nuclear matter ($N = Z = A/2$) saturates
- *Empirical* saturation at about $E/A \approx -16\,\mathrm{MeV}$ and $n \approx 0.17 \pm 0.03\,\mathrm{fm}^{-3}$

What causes nuclear saturation?

Low resolution $\Longrightarrow$ MBPT is feasible!

- MBPT $\equiv$ Many-Body Perturbation Theory

- Compare high resolution to low resolution



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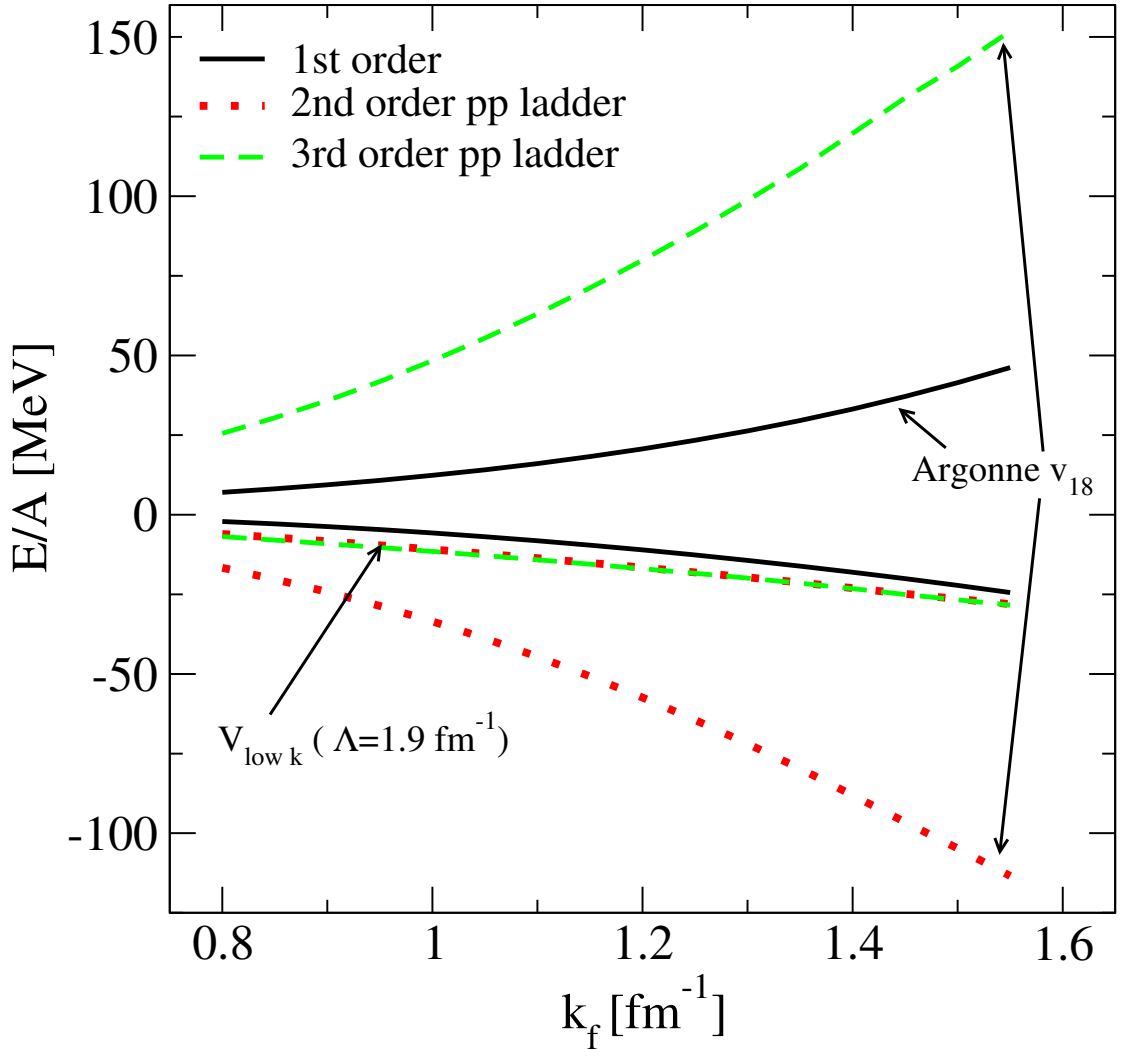
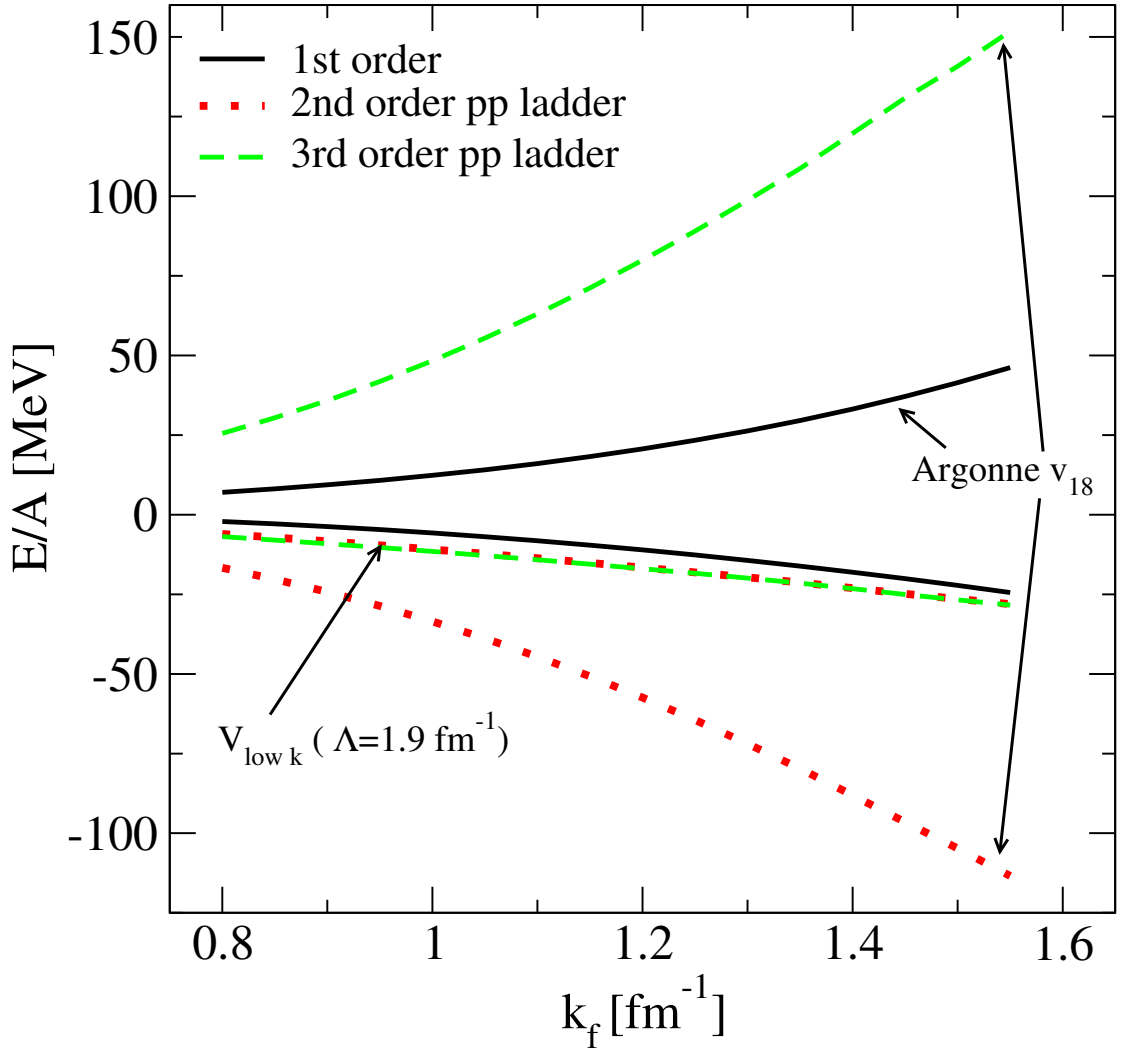
- (pp) MBPT converges!
- Like quantum chemistry!



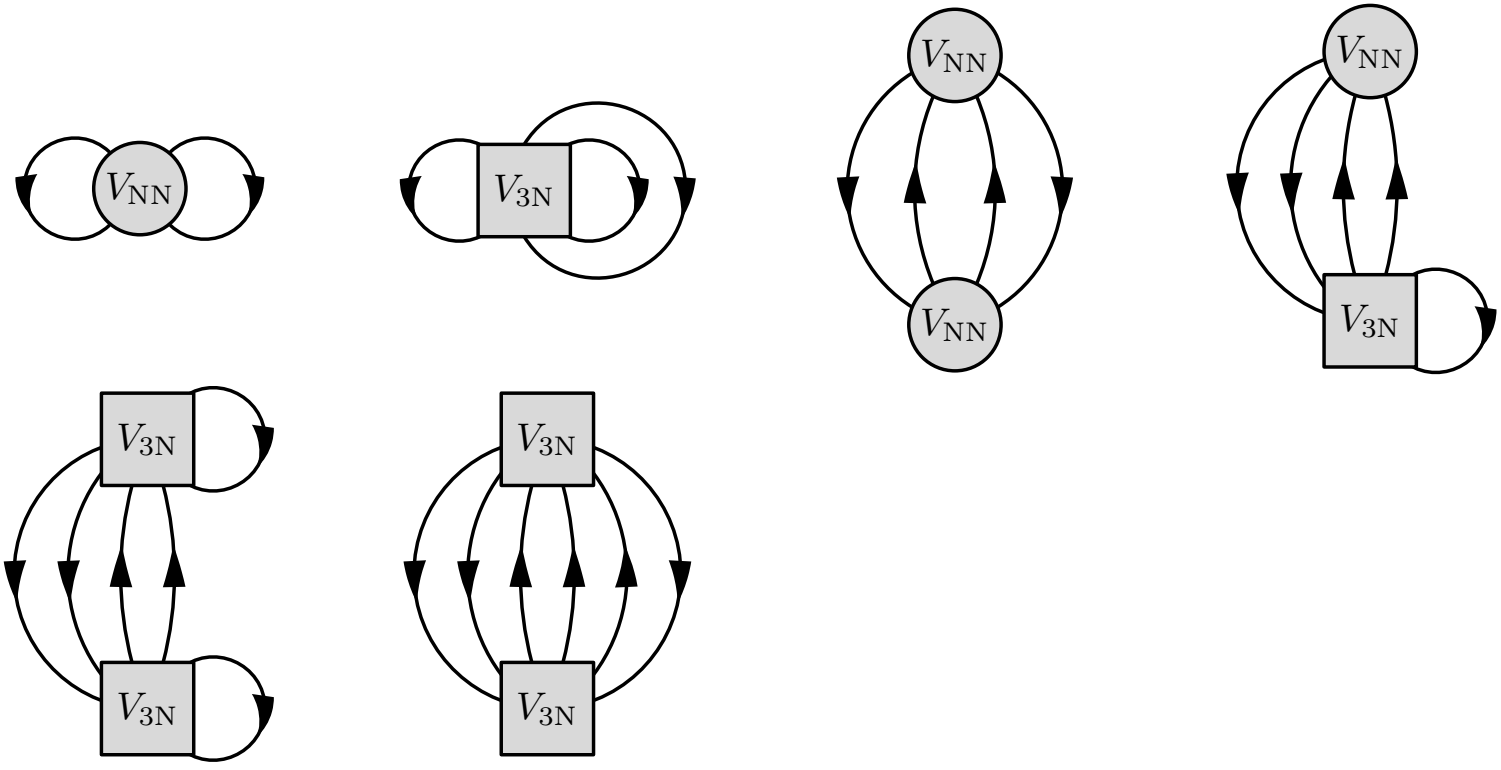
Low resolution $\Longrightarrow$ MBPT is feasible!

- MBPT $\equiv$ Many-Body Perturbation Theory

- Compare high resolution to low resolution
- (pp) MBPT converges!
- Like quantum chemistry!
- Need 3-body force for saturation (minimum)
- Hebeler et al. $\Longrightarrow$ apply to nuclear, neutron matter
- Holt et al. $\Longrightarrow$ apply to shell model with MBPT
- UNEDF $\Longrightarrow$ add pion physics to energy functionals



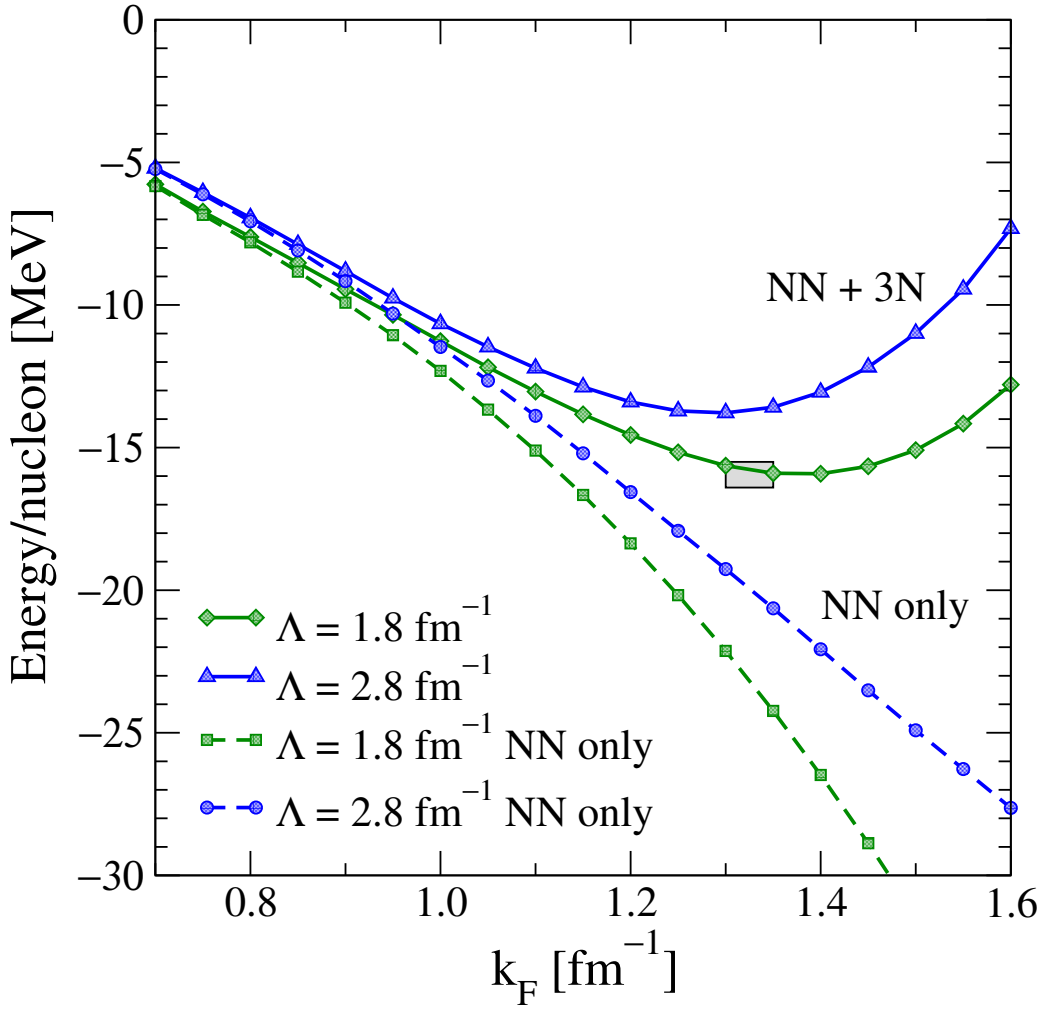
Diagrams for MBPT to second order



Diagrams contributing to the energy per particle up to second order in MBPT, taking two- and three-body interactions into account.

Energy per particle in SNM vs. Fermi momentum

- Compare NN-only results to NN+3NF
- Two representative NN cutoffs
- Fixed 3N cutoff
- 3N constants fit to few-body nuclei $\Longrightarrow$ prediction!
- Hebeler et al. (2011)



There's nothing new under the sun . . .

- Is the idea that repulsive three-nucleon forces could be the dominant nm saturation mechanism a new one?
- Consider this quote:
  ". . . if we accept the potentials . . . as a semiphenomenological working basis for our calculations, we find that the many-body forces, and in particular the three-body repulsion, provide a satisfactory qualitative understanding of nuclear saturation."
- Where does it come from?

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- Where does it come from? Drell and Huang, 1953!

PHYSICAL REVIEW VOLUME 91, NUMBER 6 SEPTEMBER 15, 1953

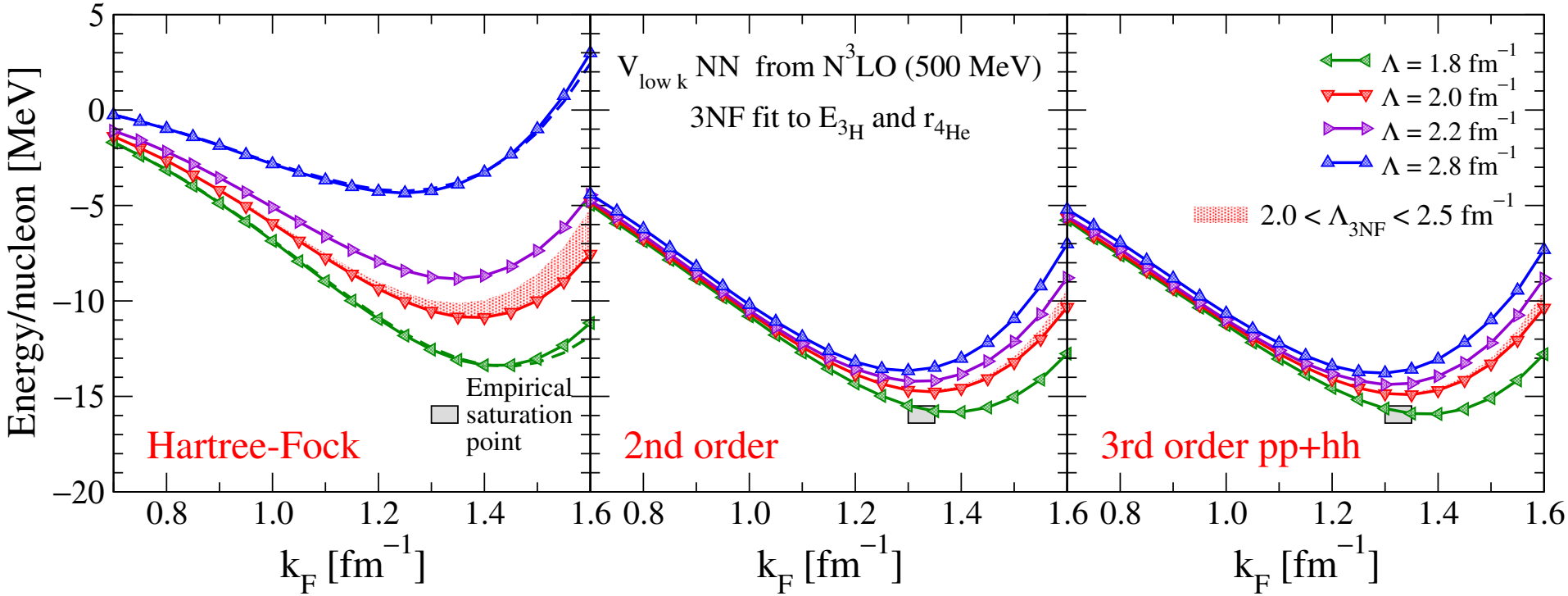
Many-Body Forces and Nuclear Saturation*†

S. D. DRELL AND KERSON HUANG‡
Department of Physics and Laboratory of Nuclear Science, Massachusetts Institute of Technology, Cambridge, Massachusetts
(Received June 10, 1953)

- Disclaimer: Pion forces, but not chiral symmetry! . . .

Low resolution calculations of nuclear matter

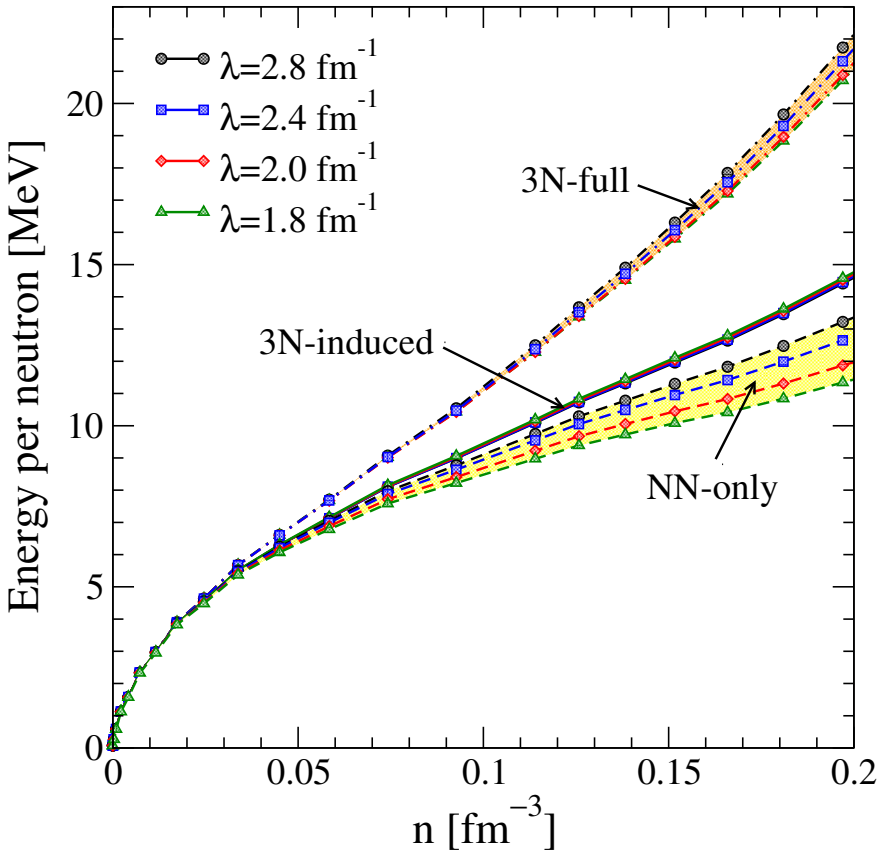
- Evolve NN by RG to low momentum, fit NNN to $A = 3, 4$
- Predict nuclear matter in MBPT [Hebeler et al. (2011)]

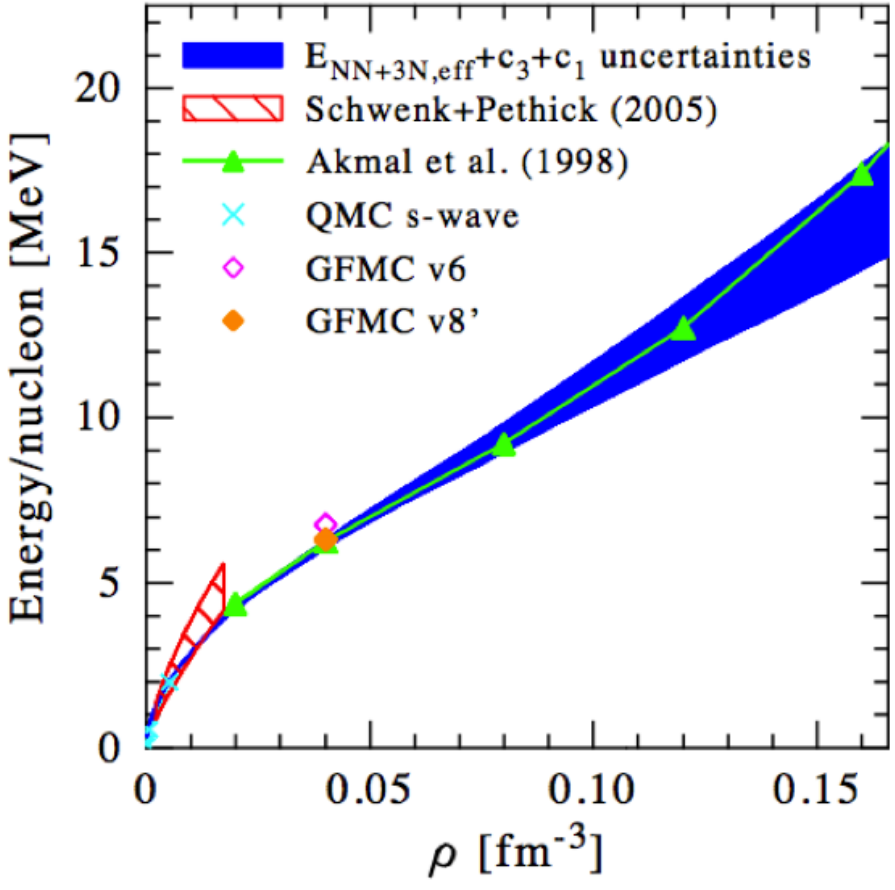


- Use residual cutoff dependence as a tool
  - Cutoff dependence at 2nd order significantly reduced
  - 3rd order contributions are small
  - Remaining cutoff dependence: many-body corrections, 4NF?
- New: coupled cluster calculations of SNM! [Hagen et al. (2013)]

Low resolution calculations of neutron matter

- Evolve NN to low momentum, fit NNN to $A = 3, 4$ or evolve
- Neutron matter in perturbation theory [Hebeler et al. (2010–2013)]

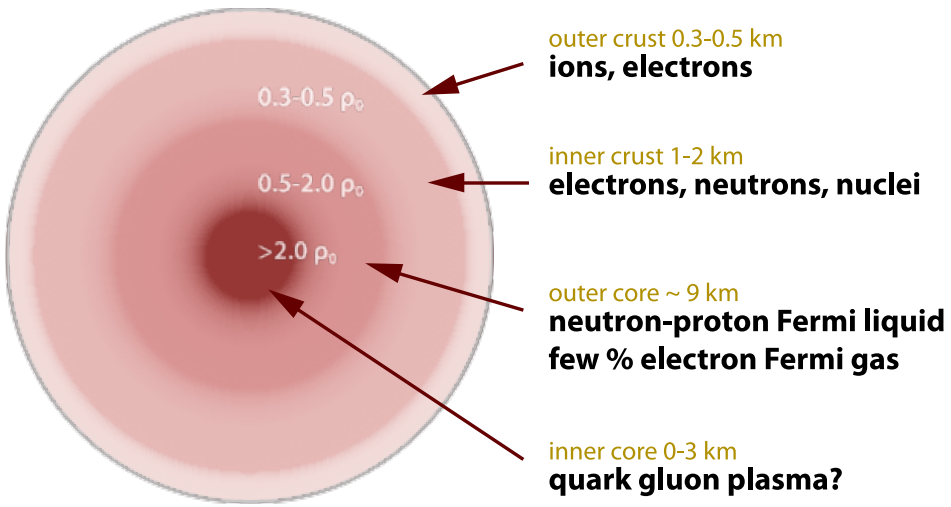




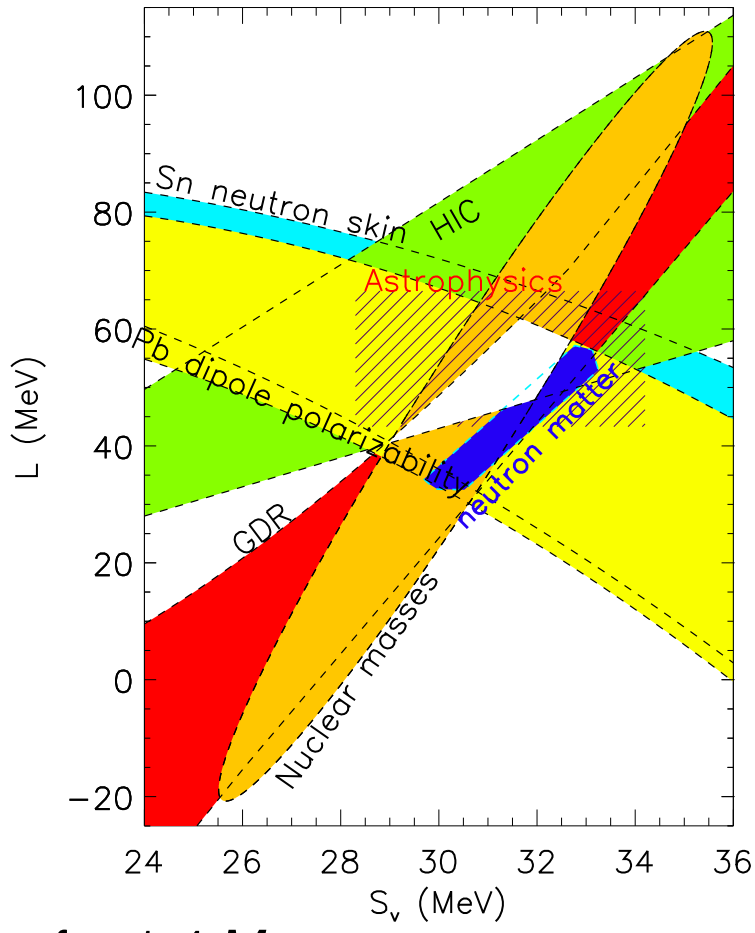
- Estimate theory uncertainties: cutoff and LEC dependence

Low resolution calculations of neutron matter

- Evolve NN to low momentum, fit NNN to $A = 3, 4$ or evolve
- Neutron matter in perturbation theory [Hebeler et al. (2010–2013)]

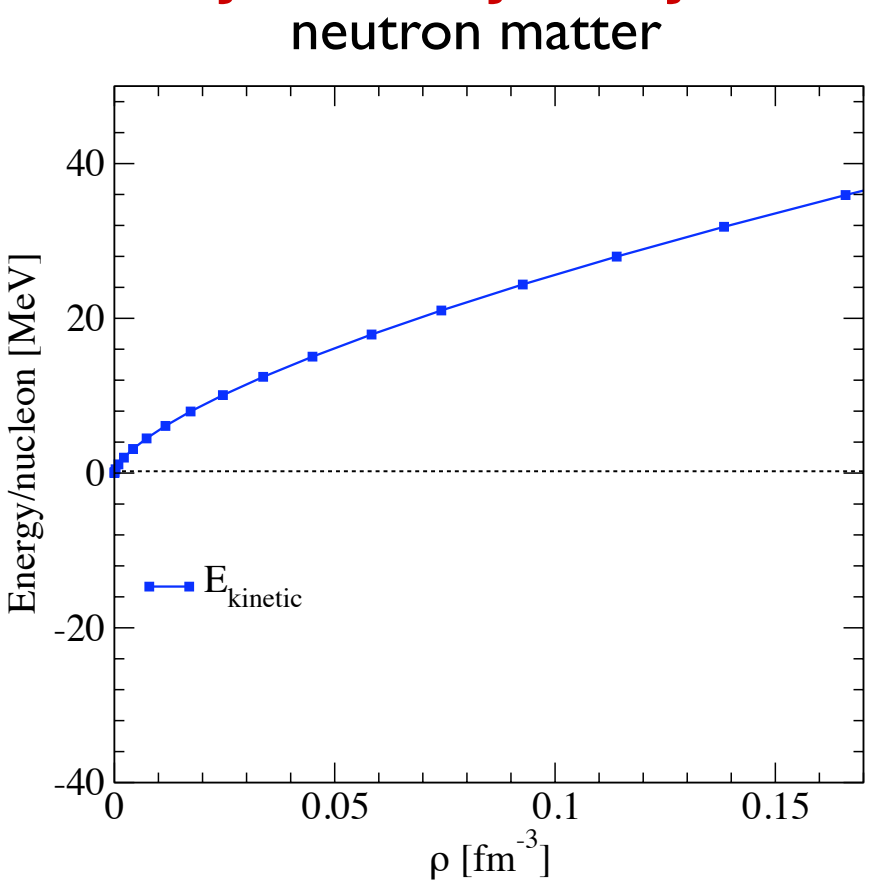


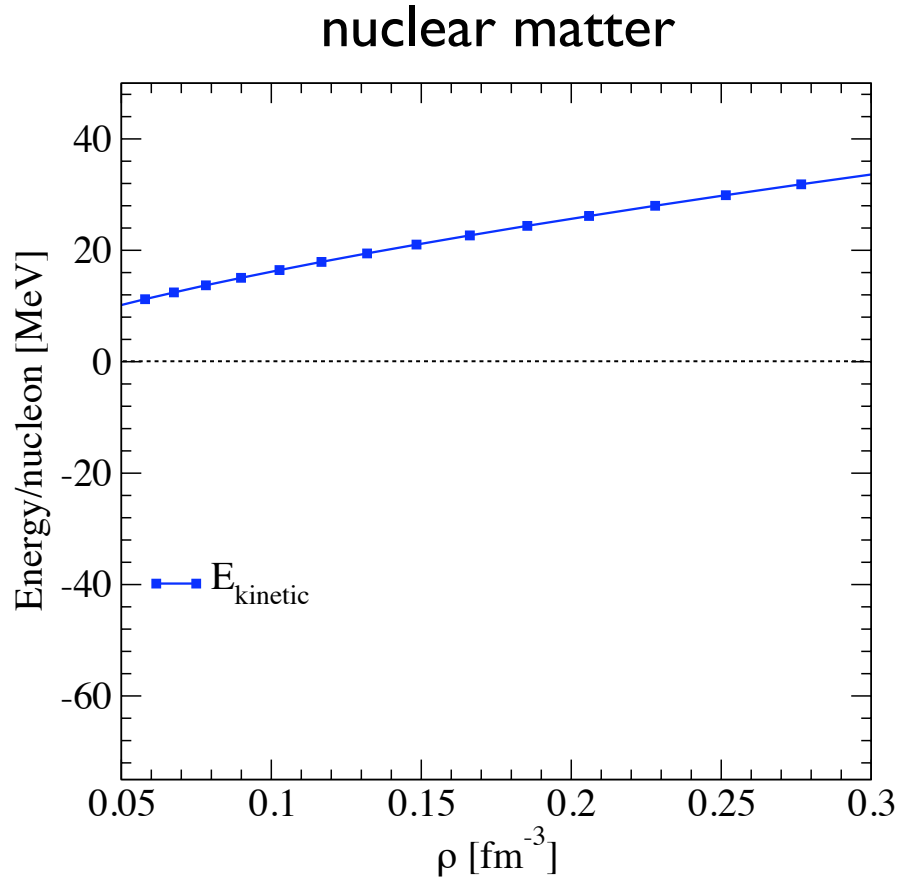
[from Wikipedia]



- Constrain neutron stars: $R = 10$–$14\,\text{km}$ for $1.4\,M_{\text{sun}}$
- Constrain nuclear symmetry energy

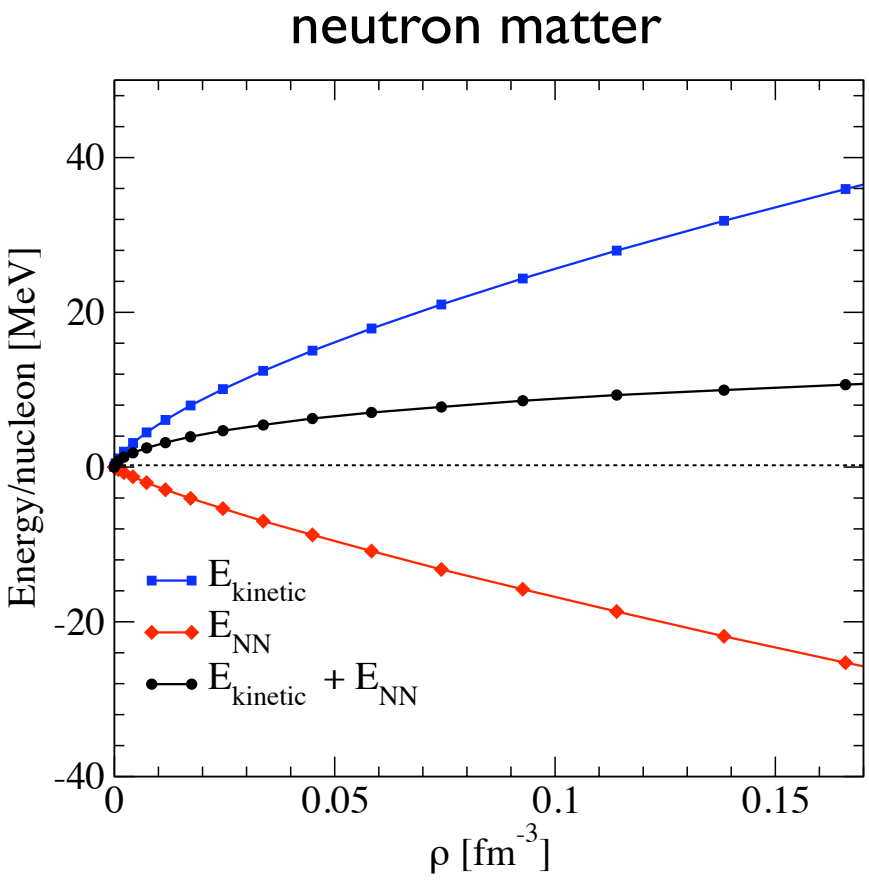
Hierarchy of many-body contributions to SNM and PNM

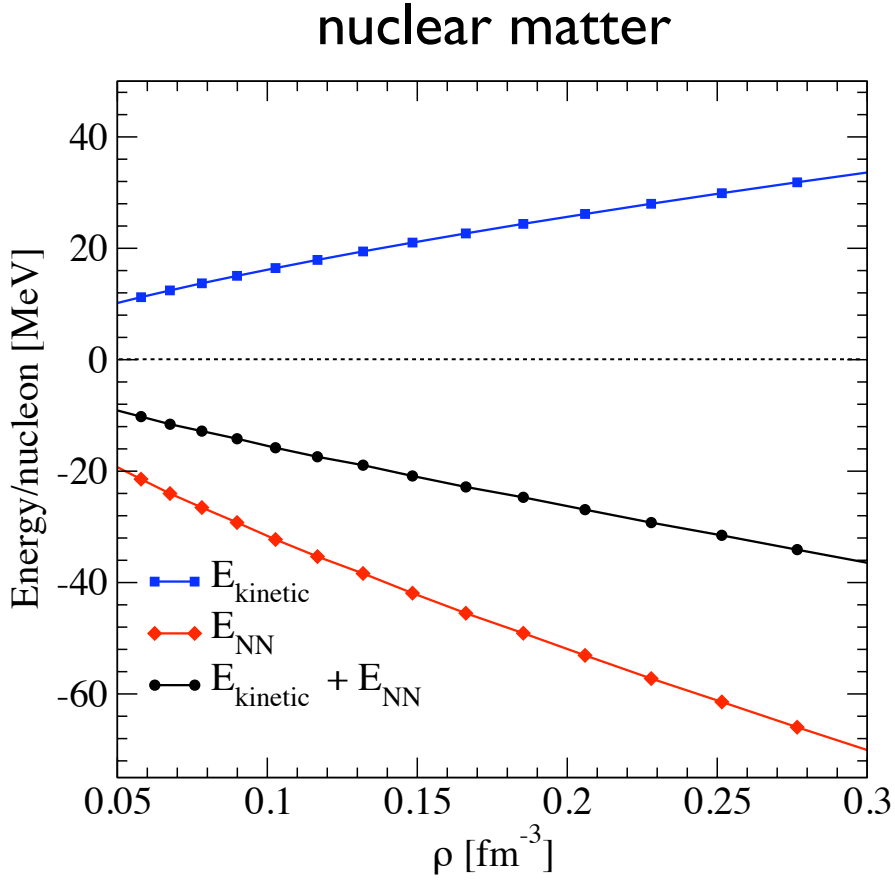




- E_{NN} denotes the energy contributions from NN interactions
- E_{3N} all contributions which include at least one 3N interaction
- Large cancellation of kinetic and potential energy
- Chiral hierarchy of 2NF and 3NF up to saturation density

Hierarchy of many-body contributions to SNM and PNM





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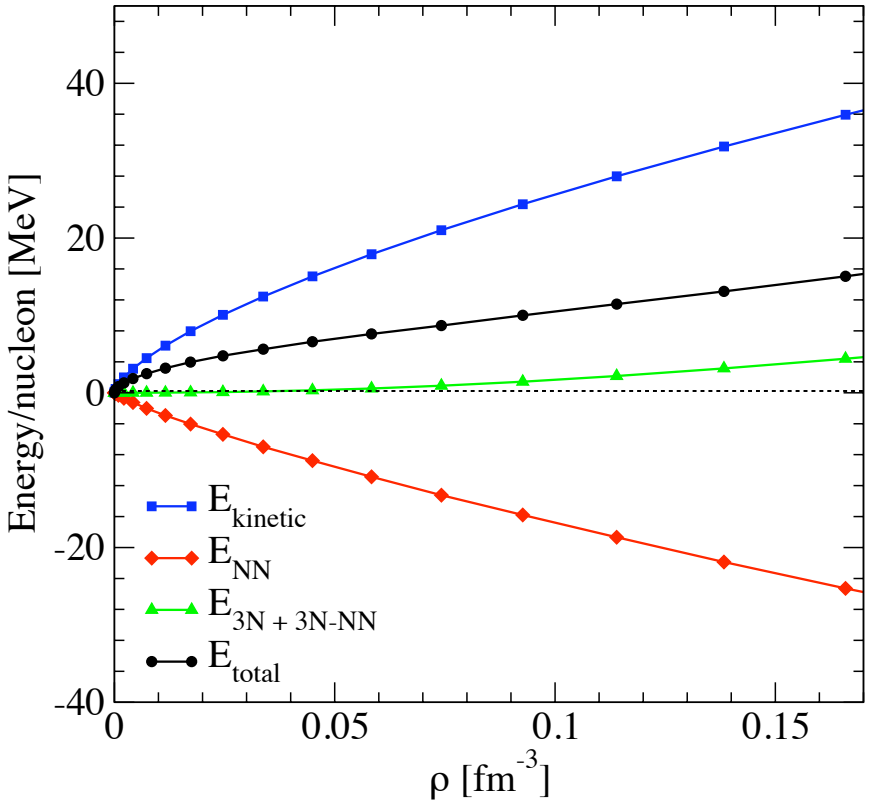
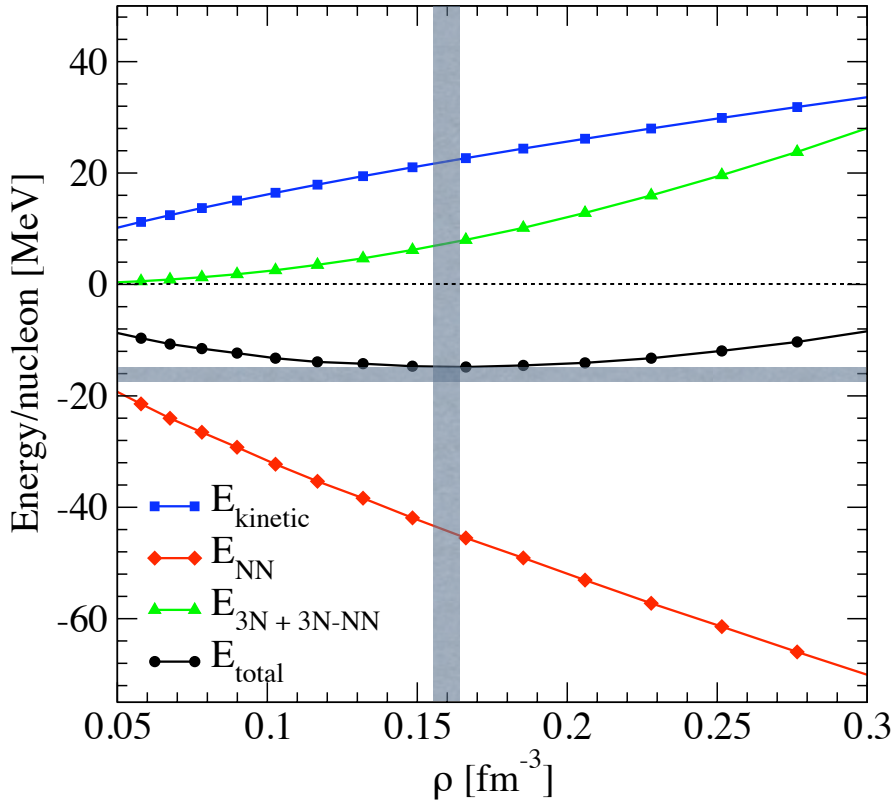
neutron matter



nuclear matter



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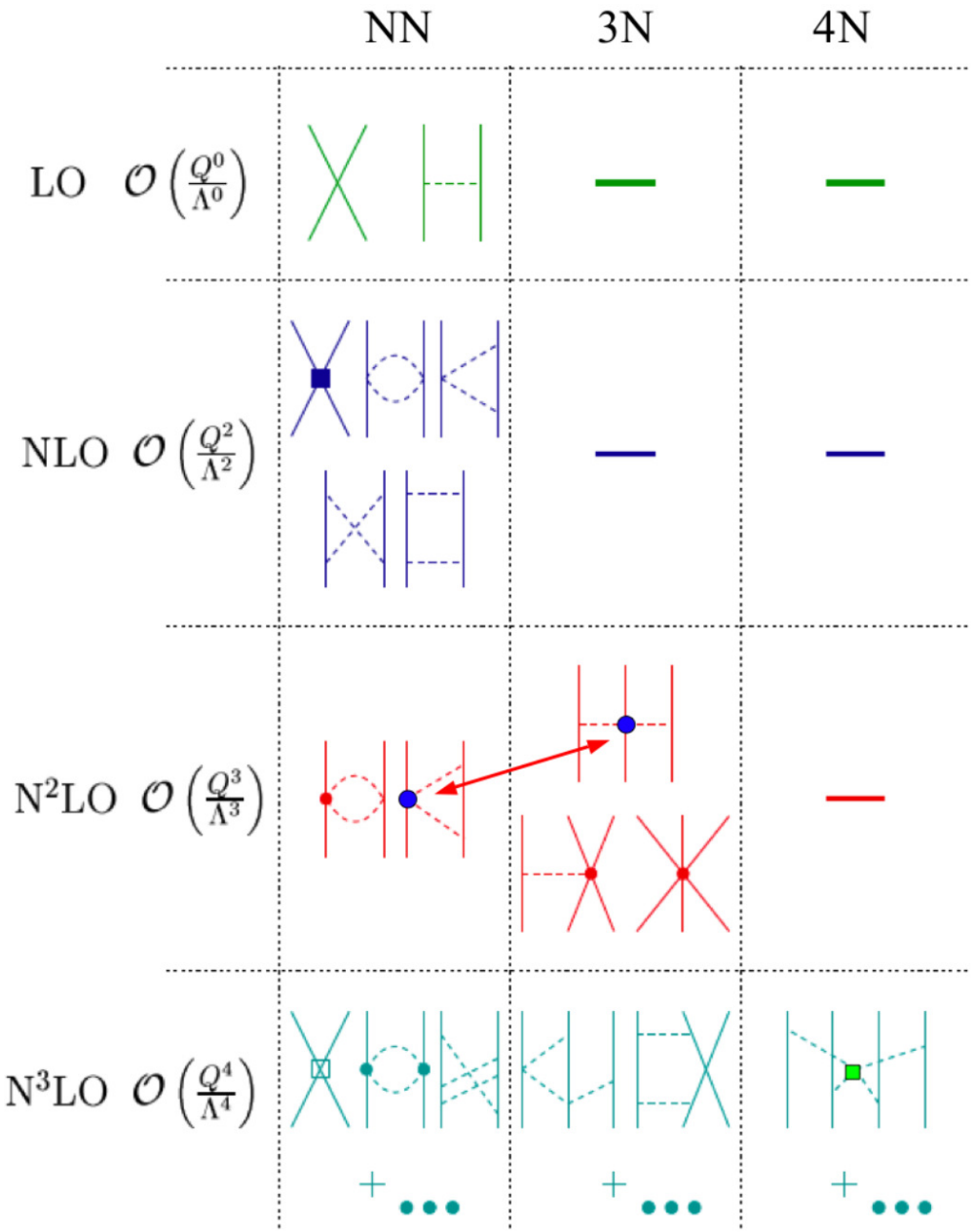
Outline: Lecture 4

Lecture 4: 3NF and applications

- RG-induced many-body forces
- Some places where the 3NF matters
- Results for infinite matter
- Future trends for chiral 3NF

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

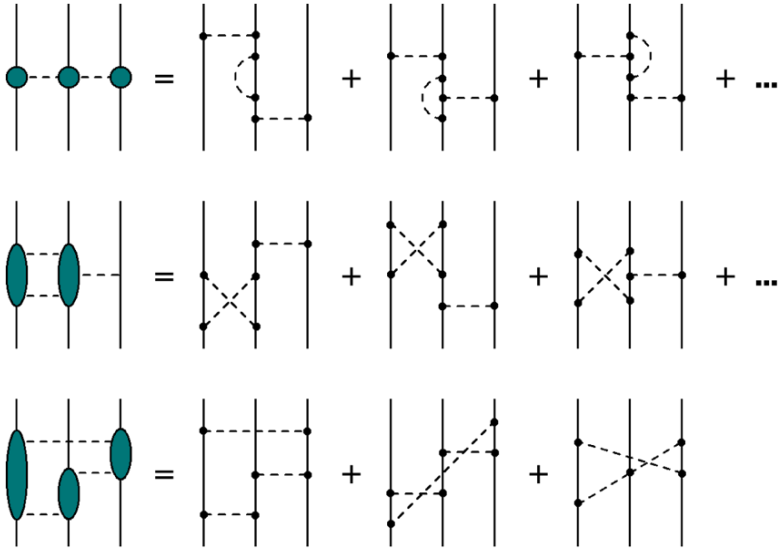


What's new with chiral 3NF [from H. Krebs]

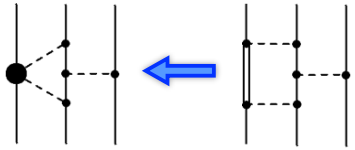
- Three-nucleon forces at N^3LO

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

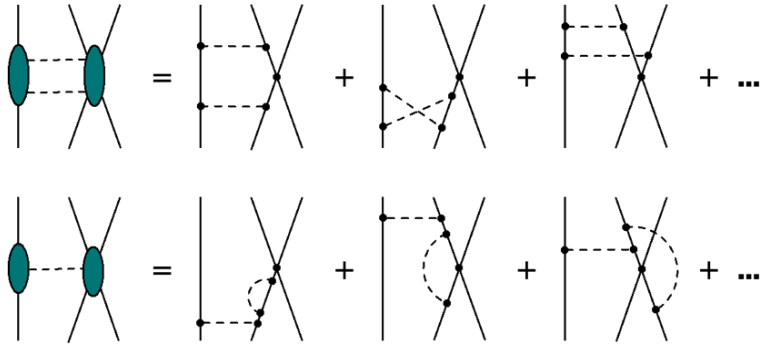


Large c_i $\sim$



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



Initiative to make N^{3}LO forces available for calculations

LENPIC

Low Energy Nuclear Physics International Collaboration

Sven Binder, Angelo Calci, Kai Hebeler, Joachim Langhammer, Robert Roth

Pieter Maris, Hugh Potter, James Vary

Richard J. Furnstahl

Evgeny Epelbaum, Hermann Krebs

Ulf-G. Meißner

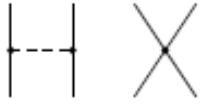
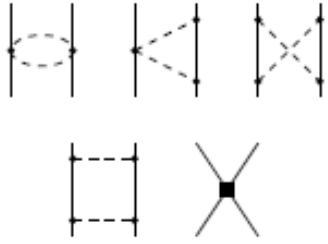
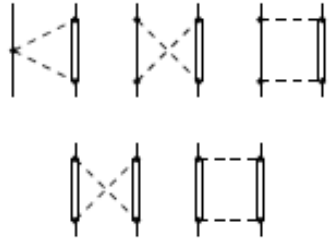
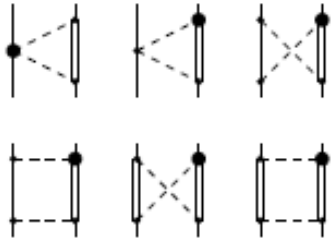
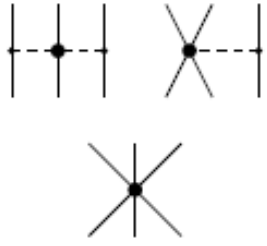
Veronique Bernard

Andreas Nogga

Jacek Golak, Roman Skibinski, Kacper Topolniki, Henryk Witala

Hiroyuki Kamada

Adding the Δ resonance [H. Krebs et al.]

	Two-nucleon force		Three-nucleon force	
	Δ-less EFT	Δ-contributions	Δ-less EFT	Δ-contributions
LO		—	—	—
NLO		 Ordonez et al.'96, Kaiser et al. '98	—	
NNLO		 H.K., Epelbaum & Meißner '07		—

- Including Δ should provide more natural expansion
- Method of unitary transformations used to decouple Δ states