Ab Initio No Core Shell Model with Chiral Effective Field Theory Hamiltonians

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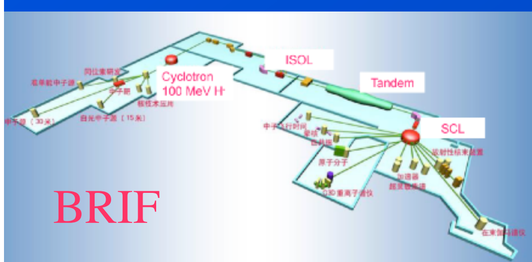
University of Giessen
July 7, 2014



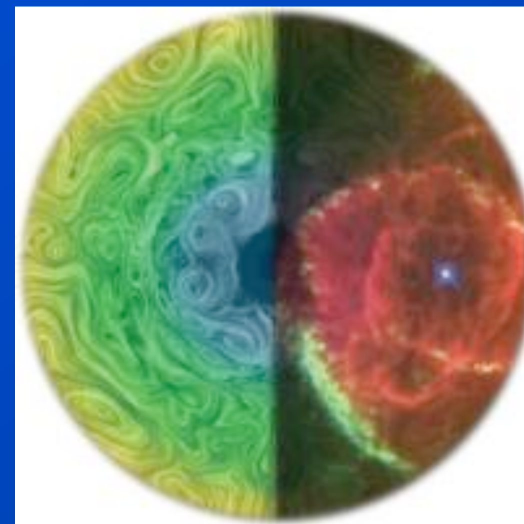
The Overarching Questions

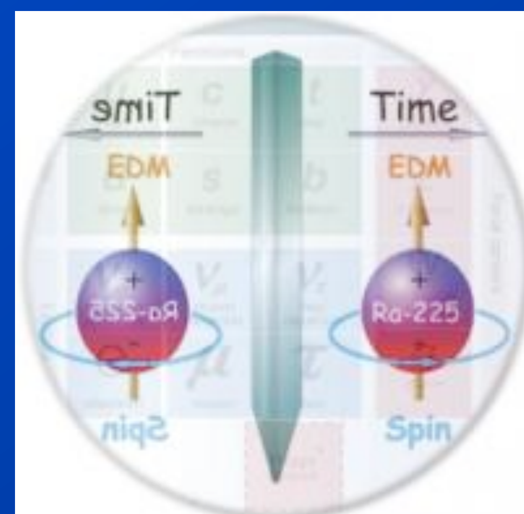
- How did visible matter come into being and how does it evolve?
- How does subatomic matter organize itself and what phenomena emerge?
- Are the fundamental interactions that are basic to the structure of matter fully understood?
- How can the knowledge and technological progress provided by nuclear physics best be used to benefit society?

- NRC Decadal Study

The Time Scale

- Protons and neutrons formed 10^{-6} to 1 second after Big Bang (13.7 billion years ago)
- H, D, He, Li, Be, B formed 3-20 minutes after Big Bang
- Other elements born over the next 13.7 billion years





Fundamental questions of nuclear physics => discovery potential

- What controls nuclear saturation?
- How shell and collective properties emerge from the underlying theory?
- What are the properties of nuclei with extreme neutron/proton ratios?
- Can we predict useful cross sections that cannot be measured?
- Can nuclei provide precision tests of the fundamental laws of nature?
- Can we solve QCD to describe hadronic structures and interactions?

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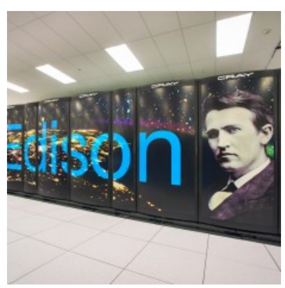
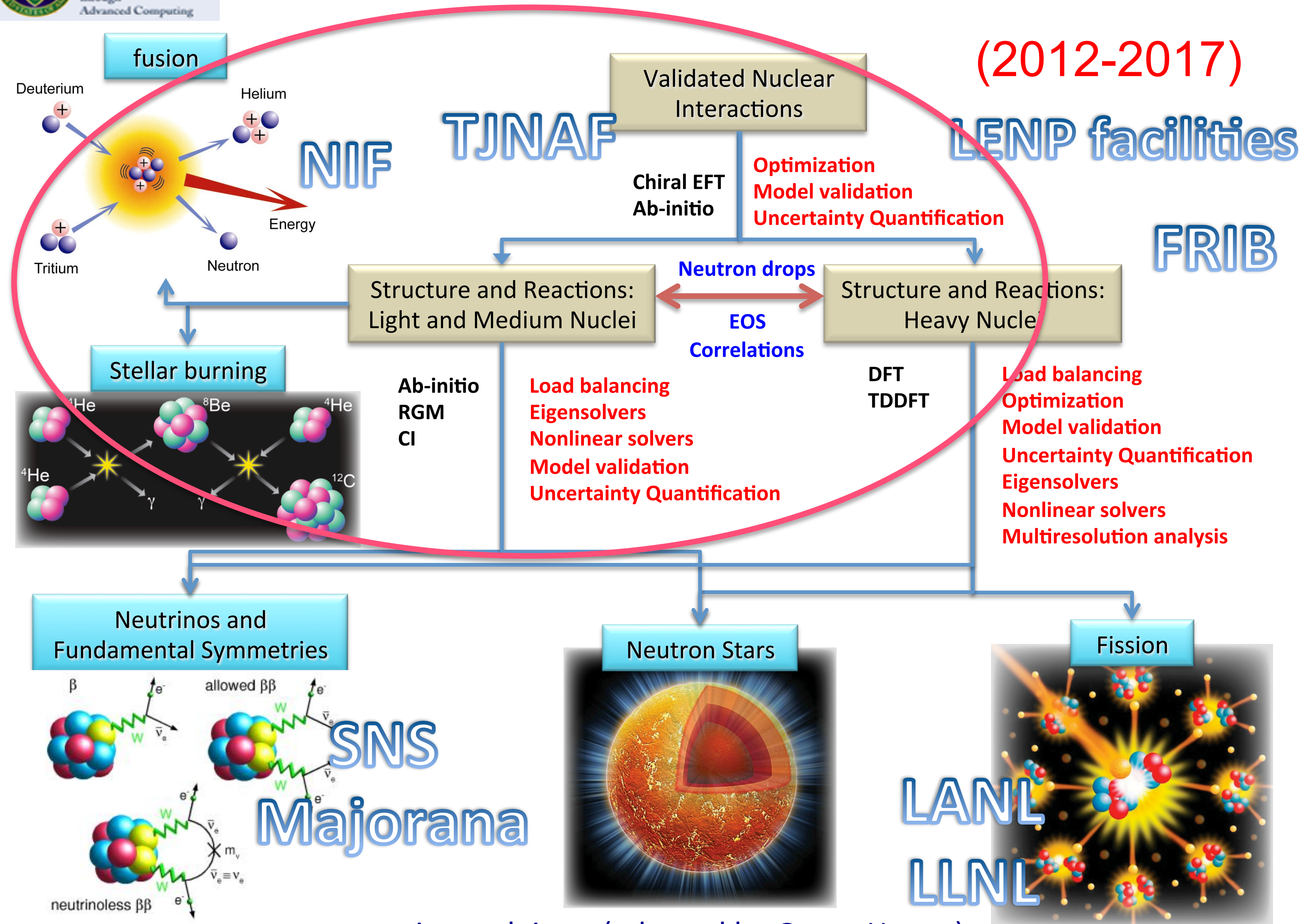


+ K-super.
+ Blue Waters
+ TianHe II
+ Tachyon-II

NUclear Computational Low-Energy Initiative



computingnuclei.org (adapted by Gaute Hagen)

The Nuclear Many-Body Problem

The many-body Schroedinger equation for bound states consists of $2\binom{A}{Z}$ coupled second-order differential equations in 3A coordinates using strong (NN & NNN) and electromagnetic interactions.

Successful *ab initio* quantum many-body approaches (A > 6)

Stochastic approach in coordinate space
Greens Function Monte Carlo (**GFMC**)

Meson Exchg interactions

Featured results here

Hamiltonian matrix in basis function space
No Core Configuration Interaction (**NCSM/NCFC**)

Cluster hierarchy in basis function space
Coupled Cluster (**CC**)

Lattice Nuclear Chiral EFT, MB Greens Function,
MB Perturbation Theory, . . . approaches

Chiral EFT interactions

Comments

All work to preserve and exploit symmetries
Extensions of each to scattering/reactions are well-underway
They have different advantages and limitations

No Core Shell Model
A large sparse matrix eigenvalue problem

$$H = T_{rel} + V_{NN} + V_{3N} + \bullet\bullet\bullet$$

$$H|\Psi_i\rangle = E_i|\Psi_i\rangle$$

$$|\Psi_i\rangle = \sum_{n=0}^{\infty} A_n^i |\Phi_n\rangle$$

$$\text{Diagonalize } \{\langle\Phi_m|H|\Phi_n\rangle\}$$

- Adopt realistic NN (and NNN) interaction(s) & renormalize as needed - retain induced many-body interactions: Chiral EFT interactions and JISP16
- Adopt the 3-D Harmonic Oscillator (HO) for the single-nucleon basis states, α, β,…
- Evaluate the nuclear Hamiltonian, H, in basis space of HO (Slater) determinants (manages the bookkeeping of anti-symmetrization)
- Diagonalize this sparse many-body H in its "m-scheme" basis where [α =(n,l,j,m_j,τ_z)]

$$|\Phi_n\rangle = [a_\alpha^+ \bullet\bullet\bullet a_\varsigma^+]_n |0\rangle$$

$$n = 1,2,\ldots,10^{10} \text{ or more!}$$

- Evaluate observables and compare with experiment

Comments

- Straightforward but computationally demanding => new algorithms/computers
- Requires convergence assessments and extrapolation tools
- Achievable for nuclei up to A=16 (40) today with largest computers available

Physics Letters B 719, 179 (2013)

Contents lists available at SciVerse ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

Emergence of rotational bands in *ab initio* no-core configuration interaction calculations of light nuclei

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Black line: Yrast band in collective model fit
Red line: excited band in collective model fit

Both natural and unnatural parity bands identified
Employed JISP16 interaction; N_{max} = 10 - 7

K=1/2 bands include Coriolis decoupling parameter:

$$E(J) = E_0 + A\left[J(J+1) + a(-)^{J+1/2}\left(J+\frac{1}{2}\right)\right],$$

$$Q(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} Q_0,$$

$$B(E2; J_i \to J_f) = \frac{5}{16\pi}(J_i K 2 0 | J_f K)^2 (eQ_0)^2$$

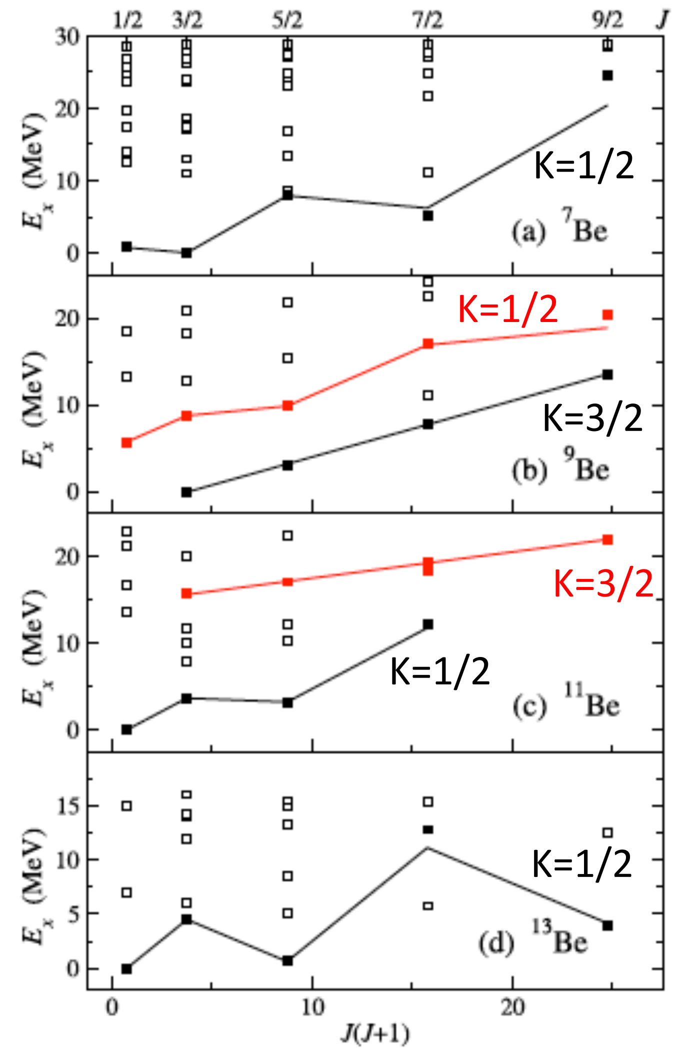
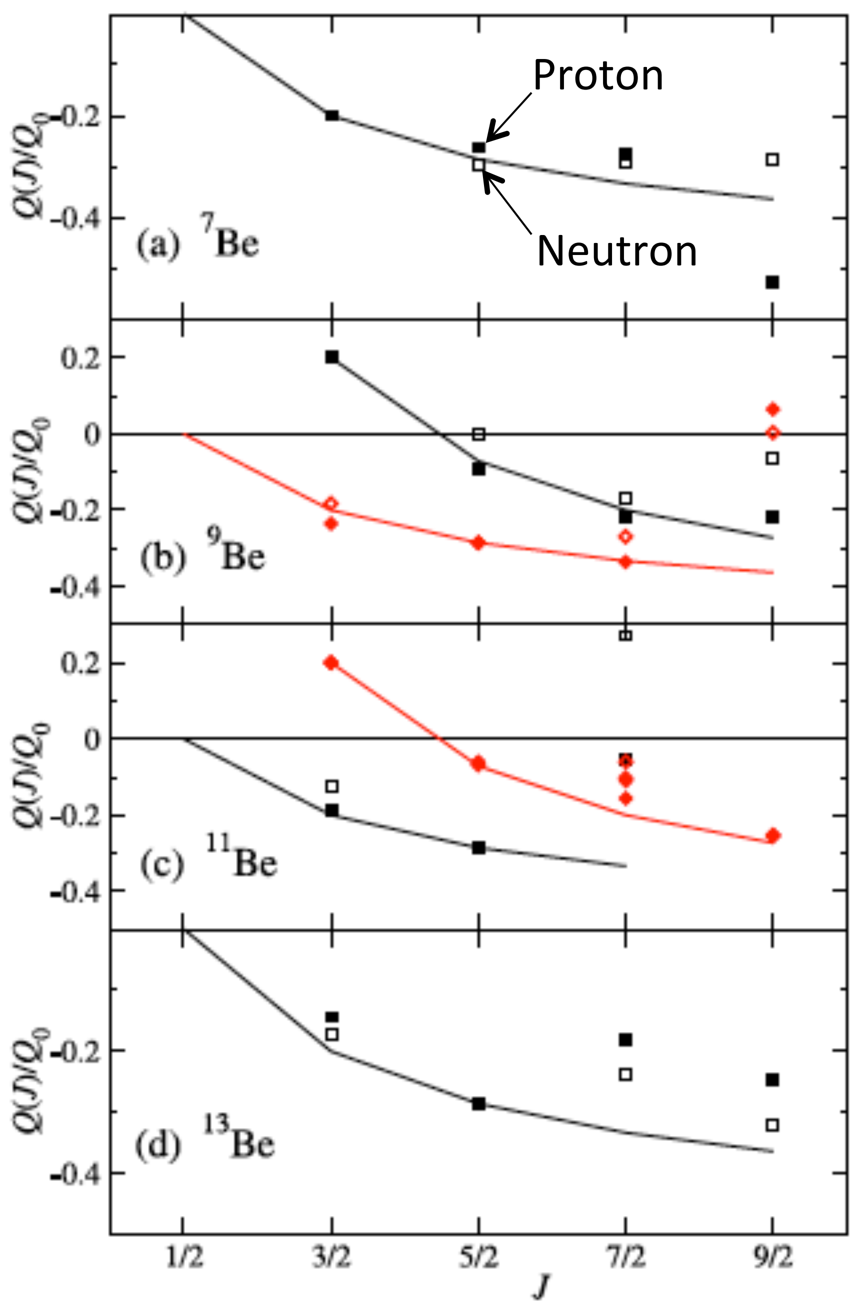


Fig. 1. Excitation energies obtained for states in the *natural* parity spaces of the odd-mass Be isotopes: (a) ^{7}Be, (b) ^{9}Be, (c) ^{11}Be, and (d) ^{13}Be. Energies are plotted with respect to $J(J+1)$ to facilitate identification of rotational energy patterns, while the J values themselves are indicated at top. Filled symbols indicate candidate rotational bandmembers (black for yrast states and red for excited states, in the web version of this Letter). The lines indicate the corresponding best fits for rotational energies. Where quadrupole transition strengths indicate significant two-state mixing (see text), more than one state of a given J is indicated as a bandmember.



Collective model:

$$Q(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} Q_0,$$

Black line: Yrast band in collective model fit
Red line: excited band in collective model fit

Fig. 3. Quadrupole moments calculated for candidate bandmembers in the *natural* parity spaces of the odd-mass Be isotopes: (a) ^{7}Be, (b) ^{9}Be, (c) ^{11}Be, and (d) ^{13}Be. The states are as identified in Fig. 1 and are shown as black squares for yrast states or red diamonds for excited states (color in the web version of this Letter). Filled symbols indicate proton quadrupole moments, and open symbols indicate neutron quadrupole moments. The curves indicate the theoretical values for a $K = 1/2$ or $K = 3/2$ rotational band, as appropriate, given by (4). Quadrupole moments are normalized to Q_0, which is defined by either the $J = 3/2$ or $J = 5/2$ bandmember (see text).

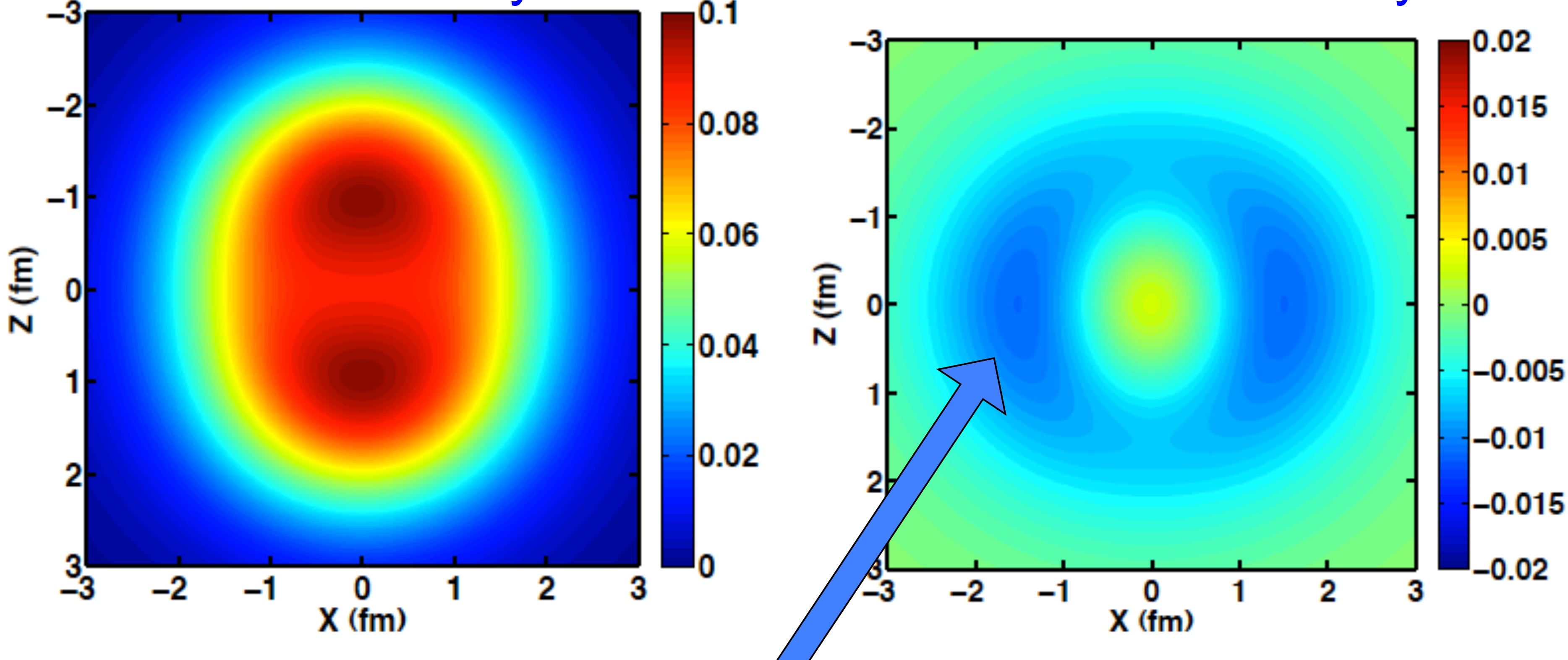
Note:
Although Q, B(E2) are slowly converging, the ratios within a rotational band appear remarkably stable

Next challenge: Investigate same phenomena with Chiral EFT interactions

M.A. Caprio, P. Maris and J.P. Vary, Physics Letters B 719, 179 (2013)

9Be Translationally invariant gs density
Full 3D densities = rotate around the vertical axis

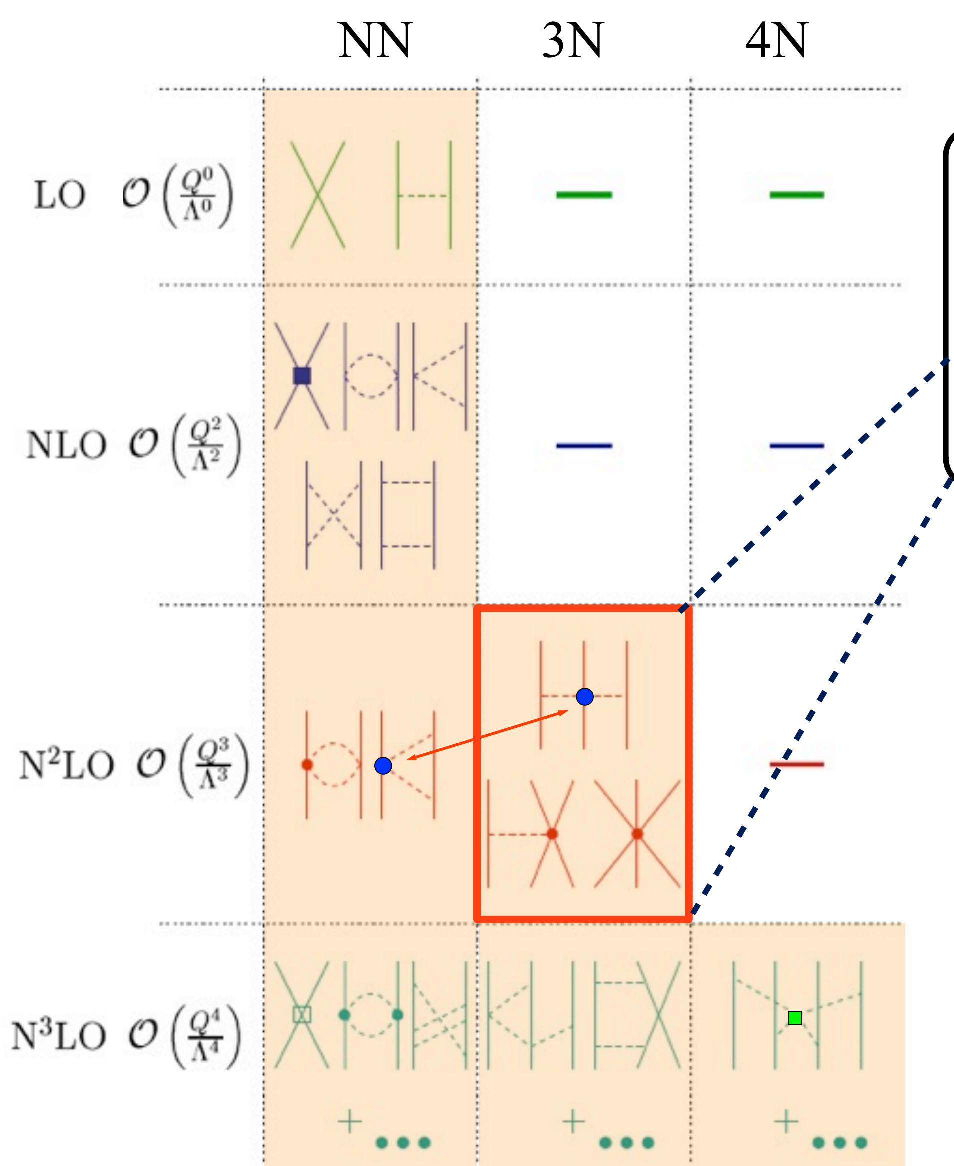
Total density | Proton-Neutron density

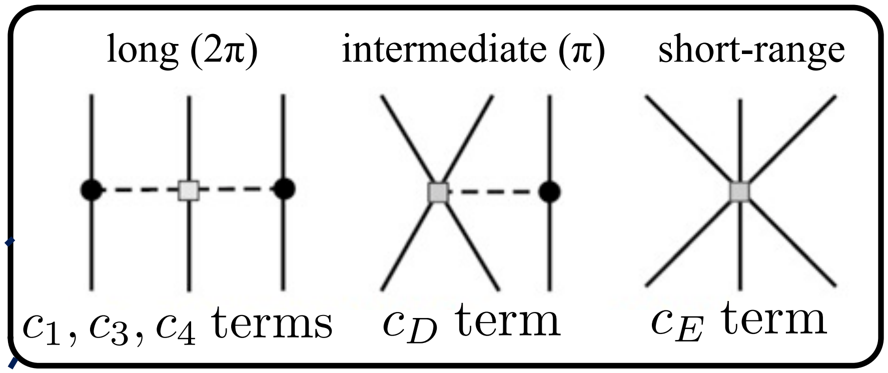


Shows that one neutron provides a “ring” cloud around two alpha clusters binding them together

C. Cockrell, J.P. Vary, P. Maris, Phys. Rev. C 86, 034325 (2012); arXiv:1201.0724;
C. Cockrell, PhD, Iowa State University

Chiral EFT for nuclear forces, leading order 3N forces





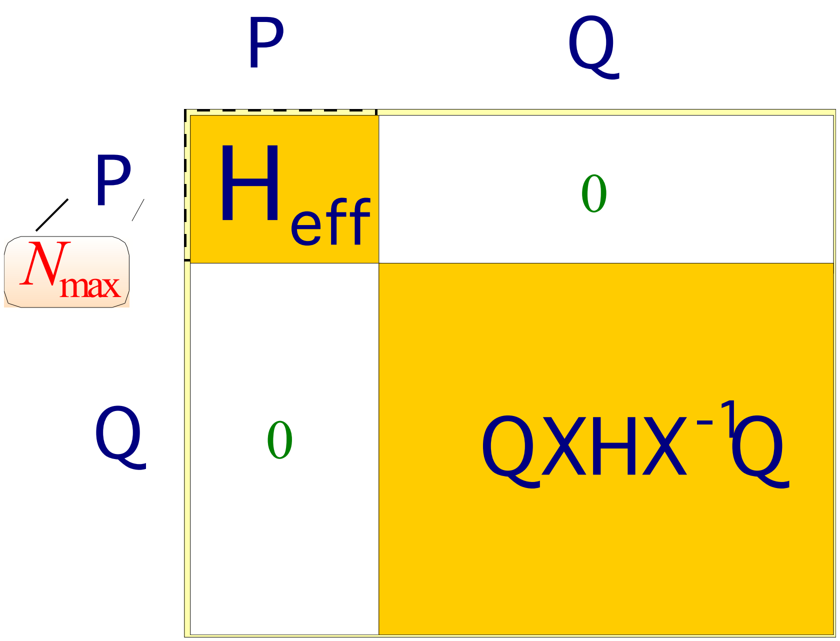
large uncertainties in coupling constants at present:

$$c_1 = -0.9^{+0.2}_{-0.5}\ ,\ c_3 = -4.7^{+1.5}_{-1.0}\ ,\ c_4 = 3.5^{+0.5}_{-0.2}$$

lead to theoretical uncertainties in many-body observables

Adapted from Kai Hebeler, ECT* workshop May 2014

Effective Hamiltonian in the NCSM
Okubo-Lee-Suzuki renormalization scheme



$$H: \quad E_1, E_2, E_3, \ldots E_{d_P}, \ldots E_\infty$$

$$H_{eff}: \quad E_1, E_2, E_3, \ldots E_{d_P}$$

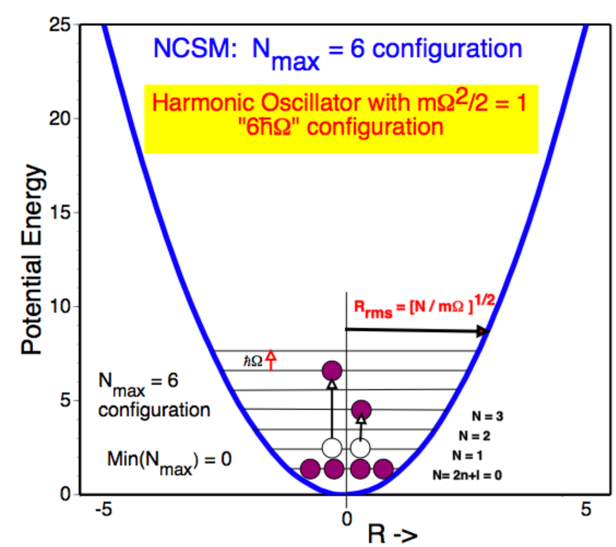
model space dimension

$$QXHX^{-1}P = 0$$

$$H_{eff} = PXHX^{-1}P$$

unitary $X = \exp[-\operatorname{arctan} h(\omega^+ - \omega)]$

- n-body cluster approximation, $2 \leq n \leq A$
- $H^{(n)}_{eff}$ n-body operator
- Two ways of convergence:
  - For $P \to 1$ $\quad H^{(n)}_{eff} \to H$
  - For $n \to A$ and fixed P: $H^{(n)}_{eff} \to H_{eff}$

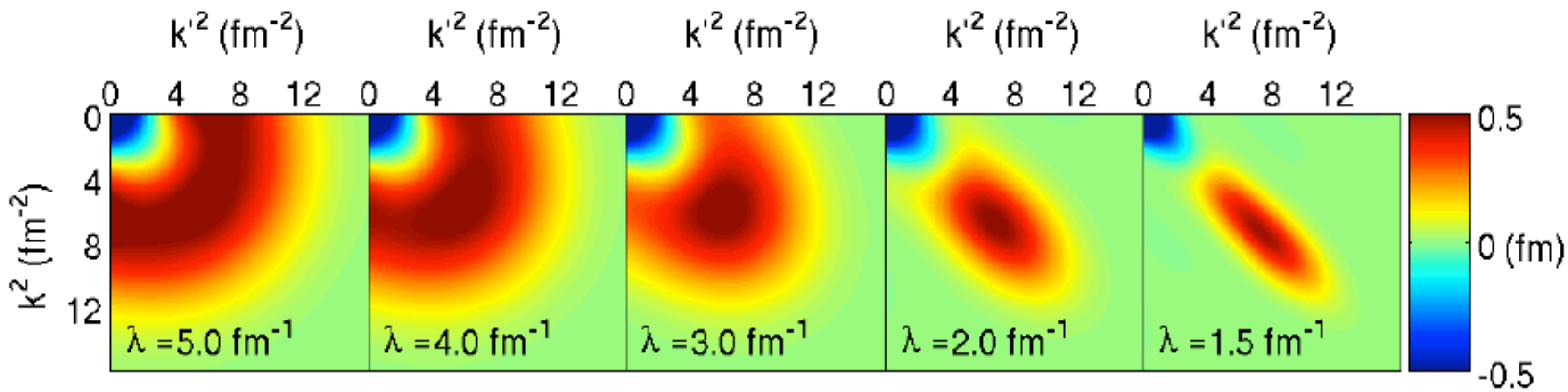


Adapted from Petr Navratil

Similarity Renormalization Group – NN interaction

- SRG evolution

Bogner, Furnstahl, Perry, PRC 75 (2007) 061001



  - drives interaction towards band-diagonal structure
  - SRG shifts strength between 2-body and many-body forces

- Initial chiral EFT Hamiltonian
  power-counting hierarchy A-body forces

$$V_{NN} \gg V_{NNN} \gg V_{NNNN}$$

Both OLS and SRG derivations of H_{eff} will be used in applications here

Controlling the center-of-mass (cm) motion in order to preserve Galilean invariance

Add a Lagrange multiplier term acting on the cm alone so as not to interfere with the internal motion dynamics

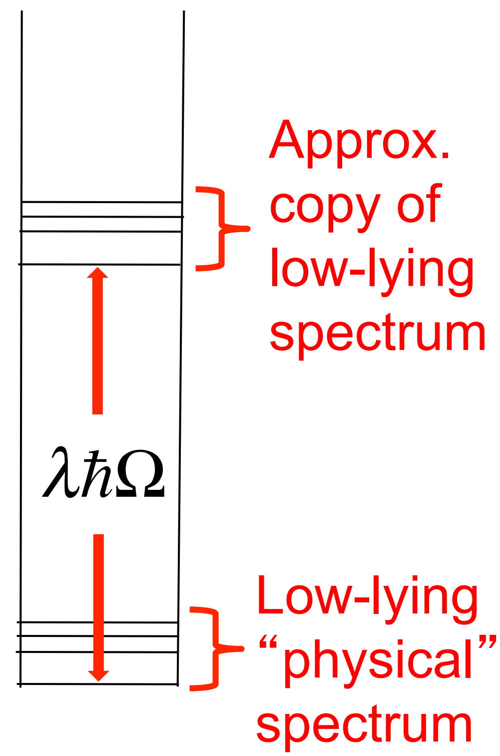
$$H_{eff}(N_{\max},\hbar\Omega) \equiv P[T_{rel} + V^a(N_{\max},\hbar\Omega)]P$$

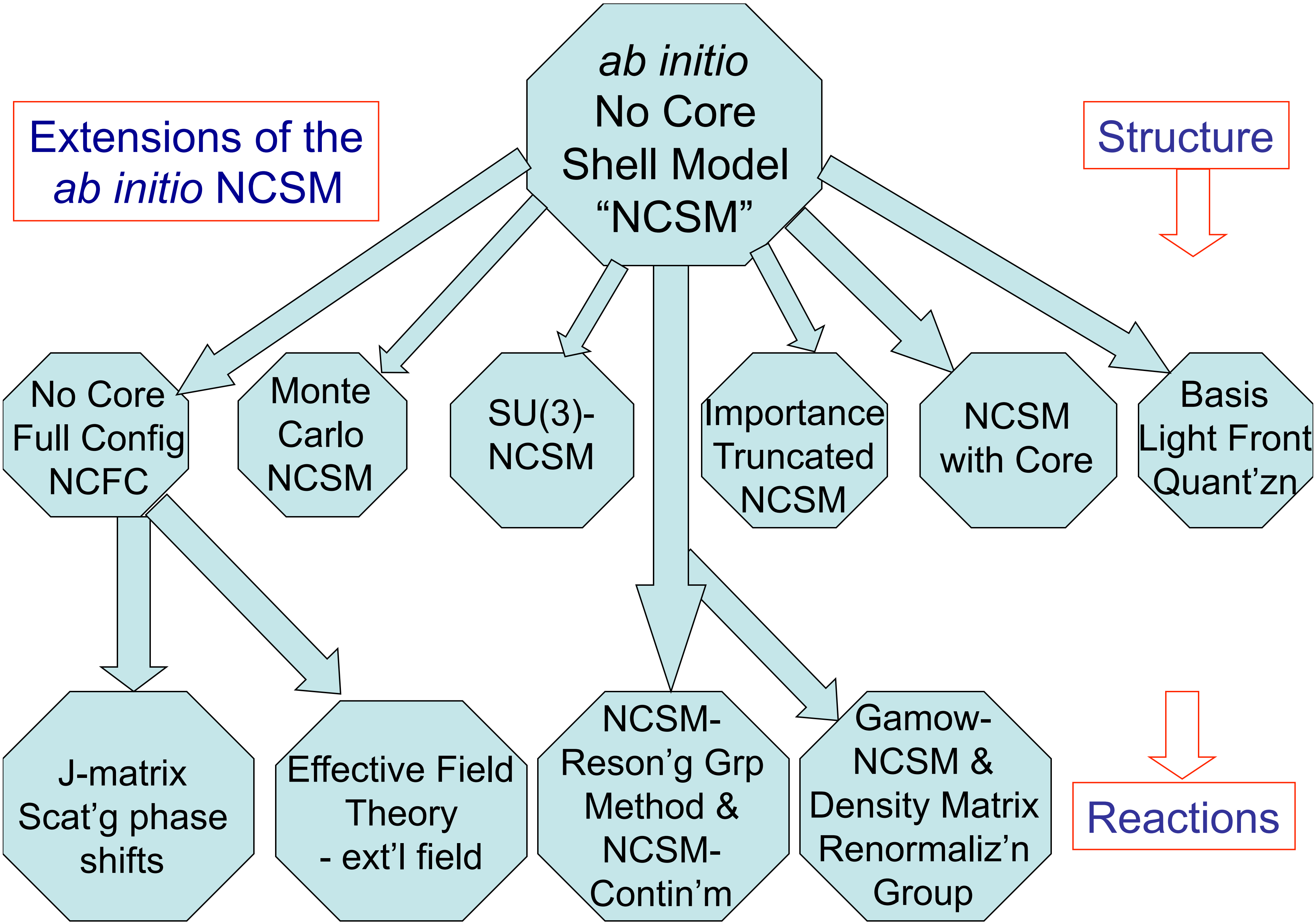
$$H = H_{eff}(N_{\max},\hbar\Omega) + \lambda H_{cm}$$

$$H_{cm} = \frac{P^2}{2M_A} + \frac{1}{2}M_A\Omega^2 R^2$$

$\lambda \sim 10$ suffices

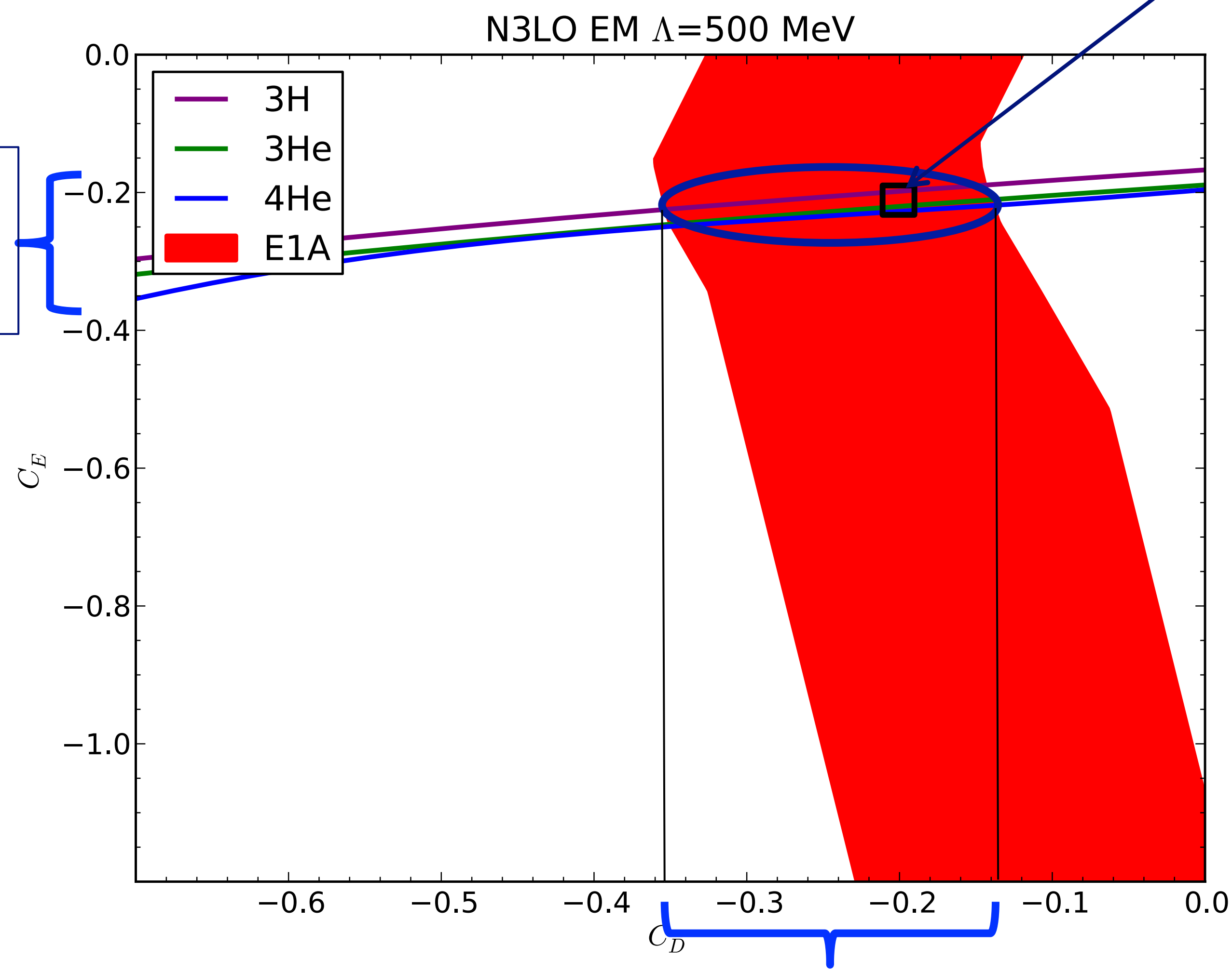
Along with the N_{max} truncation in the HO basis, the Lagrange multiplier term guarantees that all low-lying solutions have eigenfunctions that factorize into a 0s HO wavefunction for the cm times a translationaly invariant wavefunction.




Extensions of the
ab initio NCSM
ab initio
No Core
Shell Model
"NCSM"
Structure
No Core
Full Config
NCFC
Monte
Carlo
NCSM
SU(3)-
NCSM
Importance
Truncated
NCSM
NCSM
with Core
Basis
Light Front
Quant'zn
J-matrix
Scat'g phase
shifts
Effective Field
Theory
- ext'l field
NCSM-
Reson'g Grp
Method &
NCSM-
Contin'm
Gamow-
NCSM &
Density Matrix
Renormaliz'n
Group
Reactions

^{3}H half-life and Tjon line

Selected case:
C_D = -0.20
C_E = -0.205



Is c_E un-naturally small?

Is c_D unnaturally small?

Adapted from Doran Gazit

Compare ^{8}Li observables evaluated using OLS versus SRG

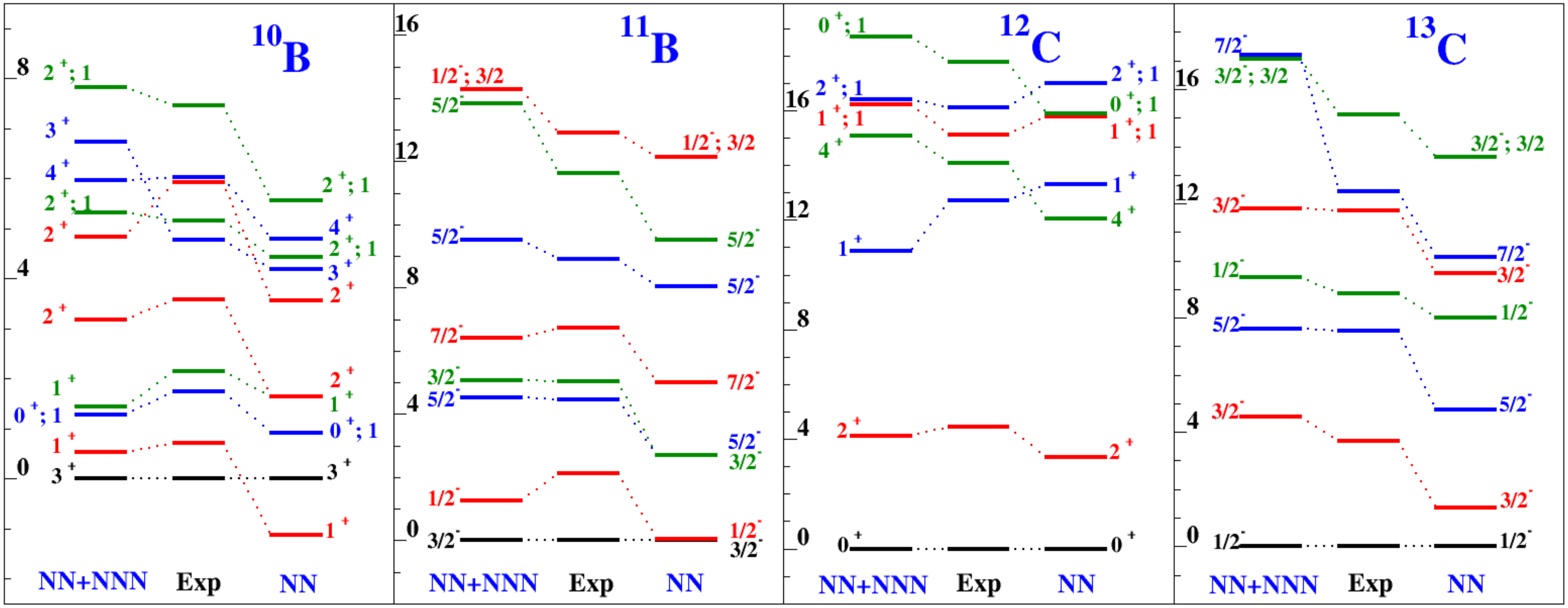
Table 5

Comparison of ^{8}Li observables between experiment [155,160,161] and theory. The OLS results with Chiral $NN + NNN$ are calculated in the NCSM at $\hbar\Omega = 13$ MeV up through $N_{max} = 8$ as reported in Ref. [153]. The SRG results ($\alpha = 0.08$) with Chiral $NN + NNN$ for $N_{max} = 8$; 10 are calculated at $\hbar\Omega = 16$ MeV in the IT-NCSM as reported in Ref. [158]. Results up through $N_{max} = 12$ with JISP16 [107–109] are obtained in the NCFC approach as reported in Ref. [159]. The table uses the same units as in Table 4. AV18/IL2 results are obtained in the GFMC approach as reported in Refs. [1,2] and do not include meson-exchange corrections for the magnetic moment; CD-Bonn ("CD-B") and INOY results are from Refs. [136,163], and were calculated at $N_{max} = 12$ and $\hbar\Omega = 12$ and 16 MeV respectively for CD-Bonn and INOY, with the INOY g.s. energy extrapolated to the infinite basis space. See caption to Table 4. For the JISP16 results, the energies are obtained from extrapolations to the infinite basis space, the magnetic dipole observables are nearly converged and the RMS point-proton radius and electric quadrupole observables are evaluated at $\hbar\Omega = 12.5$ MeV.

^{8}Li	Expt.	Chiral $NN + NNN$ Okubo–Lee–Suzuki	Chiral $NN + NNN$ SRG(0.08) $N_{max} = 8$; 10	AV18/IL2	JISP16	INOY	CD-B
$E_b(2^+)$	41.277	39.95(69)	39.90(1) ; 40.79(10)	41.9(2)	40.3(2)	41.3(5)	35.82
$\langle r_{pp}^2\rangle^{1/2}$	2.21(6)	2.09		2.09(1)	2.1	2.01	2.17
$E_x(1_1^+ 1)$	0.981	1.00 (16;03)	1.027(2) ; 0.985(6)	1.4(3)	1.5(2)	1.26	0.86
$E_x(3_1^+ 1)$	2.255(3)	2.75 (16;09)	2.608(3) ; 2.599(7)	2.5(3)	2.8(1)	2.87	3.02
$E_x(0_1^+ 1)$	–	4.01 (84;20)	3.842(15) ; 3.537(40)			4.22	2.48
$E_x(1_2^+ 1)$	3.210	4.73 (84;21)	4.632(16) ; 4.283(44)			4.90	3.25
$E_x(2_2^+ 1)$	–	4.78 (44;12)	4.603(7) ; 4.443(23)			5.11	3.98
$E_x(2_3^+ 1)$	–	5.94 (37;20)				6.07	5.29
$E_x(1_3^+ 1)$	5.400	6.09 (70;22)				6.76	5.02
$E_x(4_1^+ 1)$	6.53(20)	7.45 (36;15)		7.2(3)	7.0(3)	7.40	6.69
$E_x(3_2^+ 1)$	–	8.24 (50;22)				8.92	7.57
$E_x(0_1^+ 2)$	10.822	11.77 (27;29)				12.05	10.90
$Q(2^+)$	3.27(6)	2.65	2.73(1) ; 2.79(1)	3.2(1)	2.6	2.55	2.78
$Q(1^+)$	–	1.08	1.12(1) ; 1.12(1)		1.2		
$Q(3^+)$	–	−1.97	−1.92(1); −1.94(2)		−2.0		
$Q(4^+)$	–	−3.01			−3.4		
$\mu(2^+)$	1.654	1.49	–	1.65(1)	1.3(1)	1.42	1.24
$\mu(1^+)$	–	−2.27			−2.2(2)		
$\mu(3^+)$	–	2.13			2.0(1)		
$\mu(4^+)$	–	1.86			1.84(1)		
B(E2;1$^+$)	–	1.19			1.9		
B(E2;3$^+$)	–	3.70			4.6		
B(E2;4$^+$)	–	1.21			1.9		
B(M1;1$^+$)	5.0(16)	4.13	4.15(1) ; 4.14(1)		3.7(2)	4.56	4.39
B(M1;3$^+$)	0.52(23)	0.33	0.31(1) ; 0.30(1)		0.25(5)		

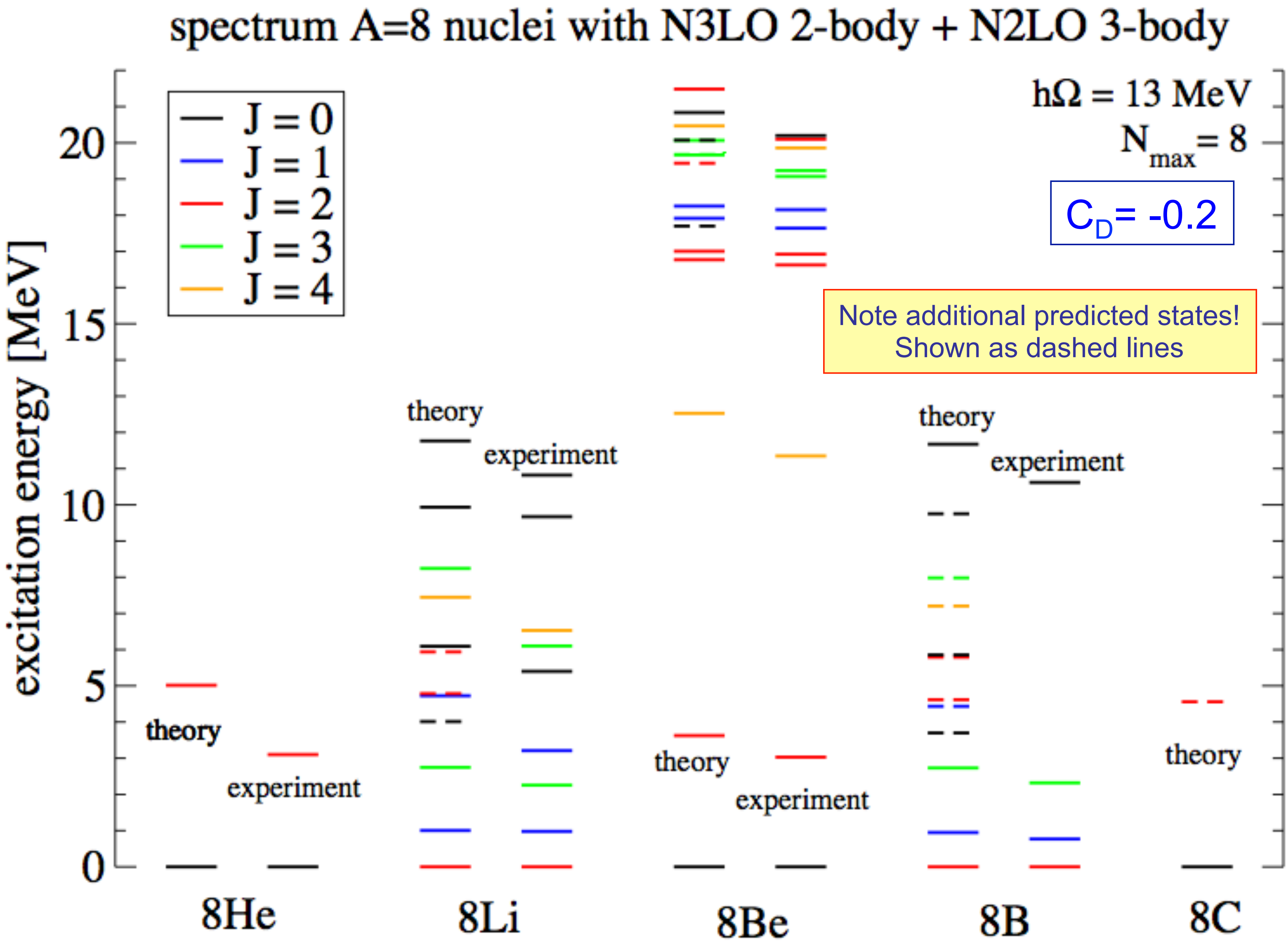
ab initio NCSM with χ_{EFT} Interactions

NNN interactions produce correct ^{10}B ground state spin and overall spectral improvements



c_D = -1

P. Navratil, V.G. Gueorguiev, J. P. Vary, W. E. Ormand and A. Nogga, Phys Rev Lett 99, 042501(2007); ArXiV: nucl-th 0701038.



P. Maris, J. P. Vary and P. Navratil, Phys. Rev. C87, 014327 (2013); arXiv 1205.5686

^8Be

No Core CI calculations for light nuclei with chiral 2- and 3-body forces

Pieter Maris[1], H Metin Aktulga[2], Sven Binder[3], Angelo Calci[3], Ümit V Çatalyürek[4,5], Joachim Langhammer[3], Esmond Ng[2], Erik Saule[4], Robert Roth[3], James P Vary[1] and Chao Yang[2]

J. Phys. Conf. Ser. 454, 012063 (2013)

SRG Renormalization scale invariance, convergence & agreement with experiment

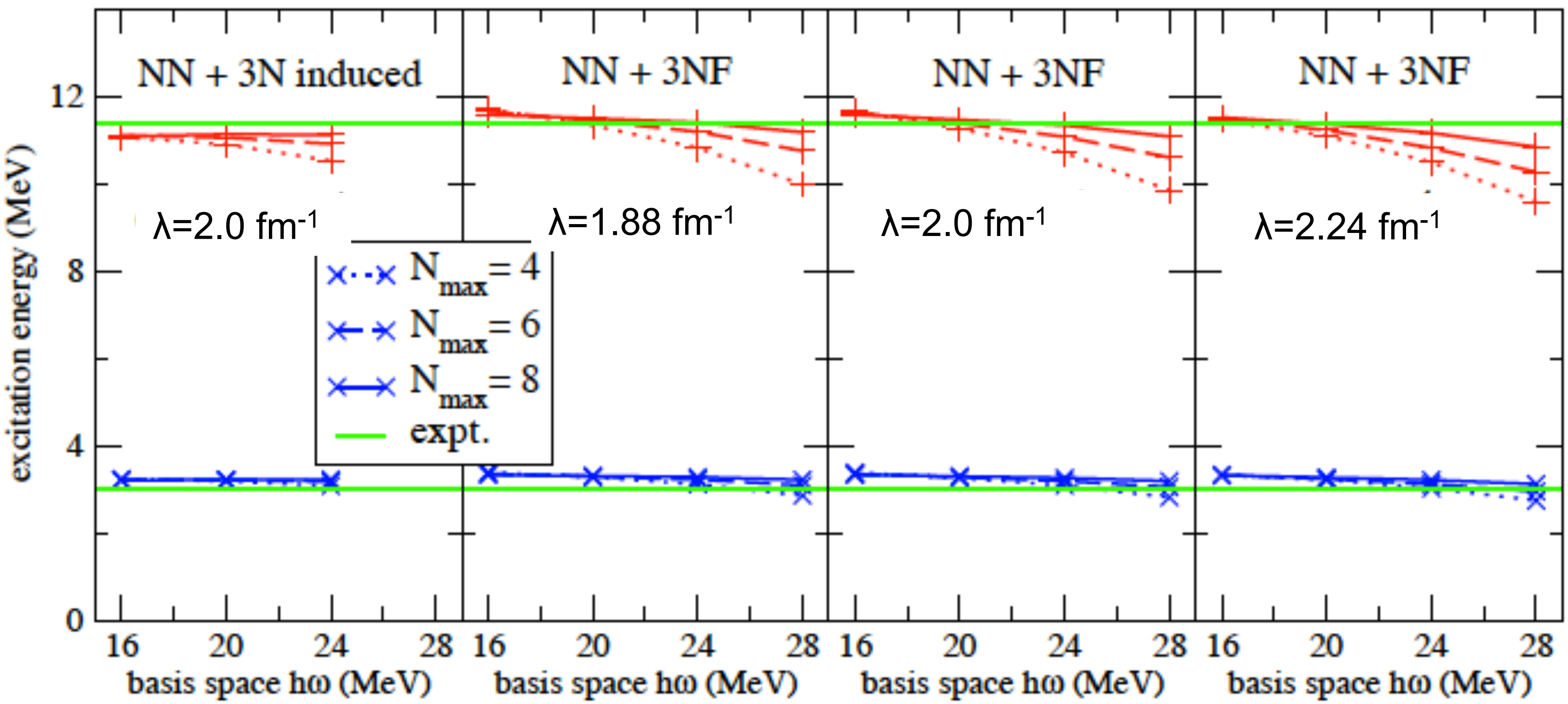
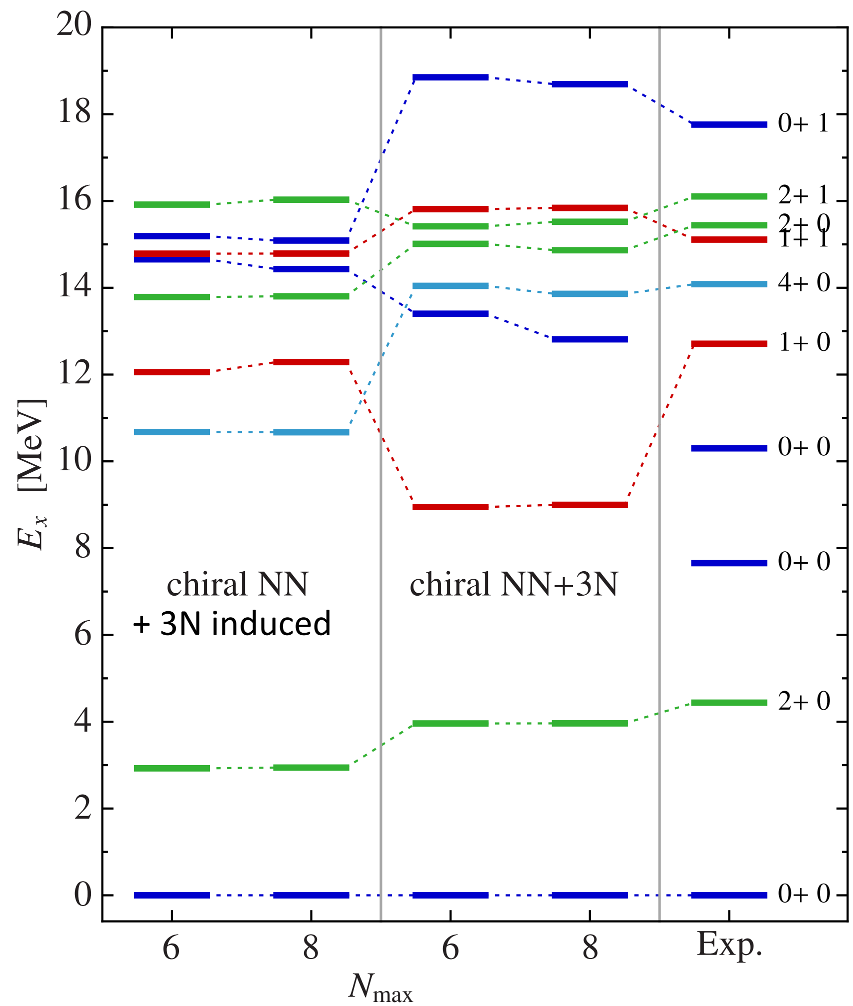


Figure 5. Excitation energies of the 2^+ (blue crosses) and 4^+ states (red plusses) for ^{8}Be with SRG evolved chiral N^{3}LO 2NF plus induced 3NF at $\alpha = 0.0625$ fm^4 (left-most panel) and with SRG evolved chiral N^{3}LO 2NF plus chiral N^{2}LO 3NF. Experimental values are indicated by the horizontal green lines.

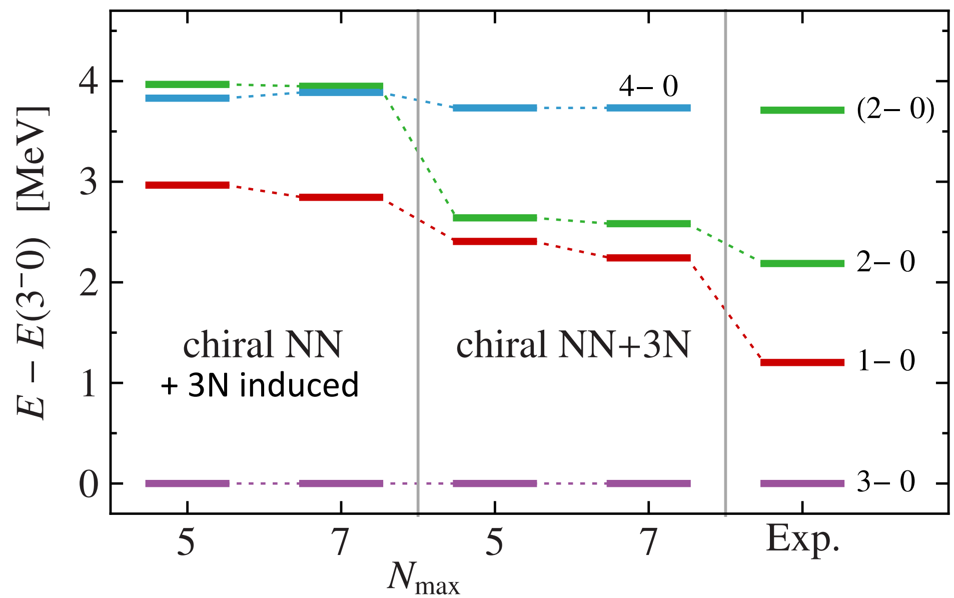
NCSM excitation spectra for ^{12}C with chiral NN(N3LO) (+3N induced) and NN(N3LO) + 3N(N2LO) interactions



$$\alpha = 0.0625 \text{ fm}^4$$

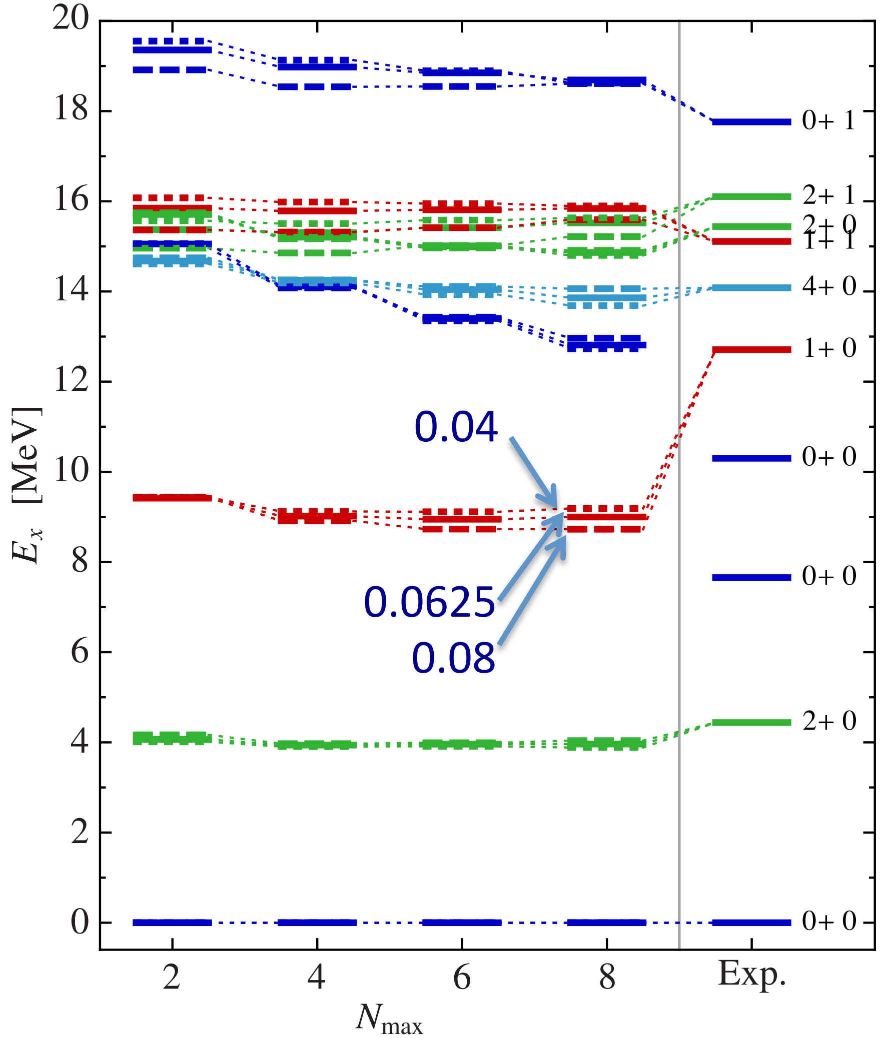
$$\lambda = 2.0 \text{ fm}^{-1}$$

$$\hbar\Omega = 20 \text{ MeV}$$

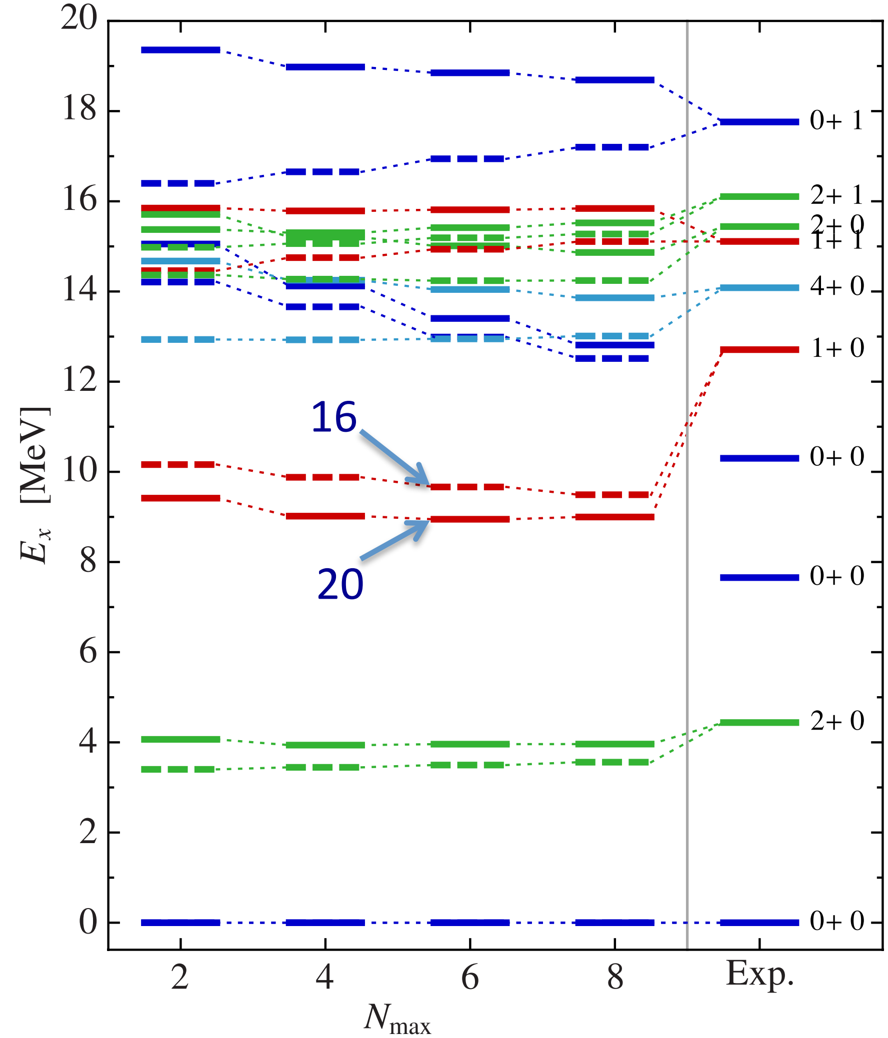


P. Maris, J.P. Vary, A. Calci, J. Langhammer, S. Binder and R. Roth, arXiv 1405.1331;to appear in PRC

NCSM excitation spectra for ^{12}C with chiral NN(N3LO) + 3N(N2LO) interaction



SRG evolution scale (in fm4) dependence



HO frequency (in MeV) dependence

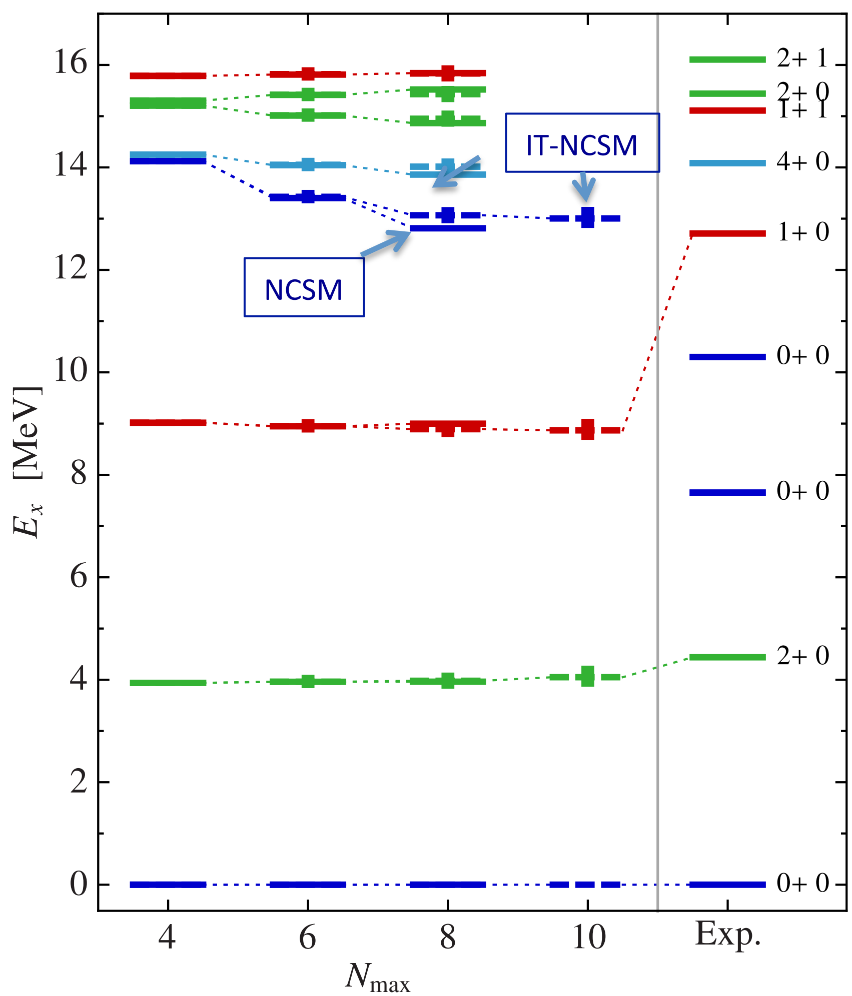
P. Maris, J.P. Vary, A. Calci, J. Langhammer, S. Binder and R. Roth, arXiv 1405.1331;to appear in PRC

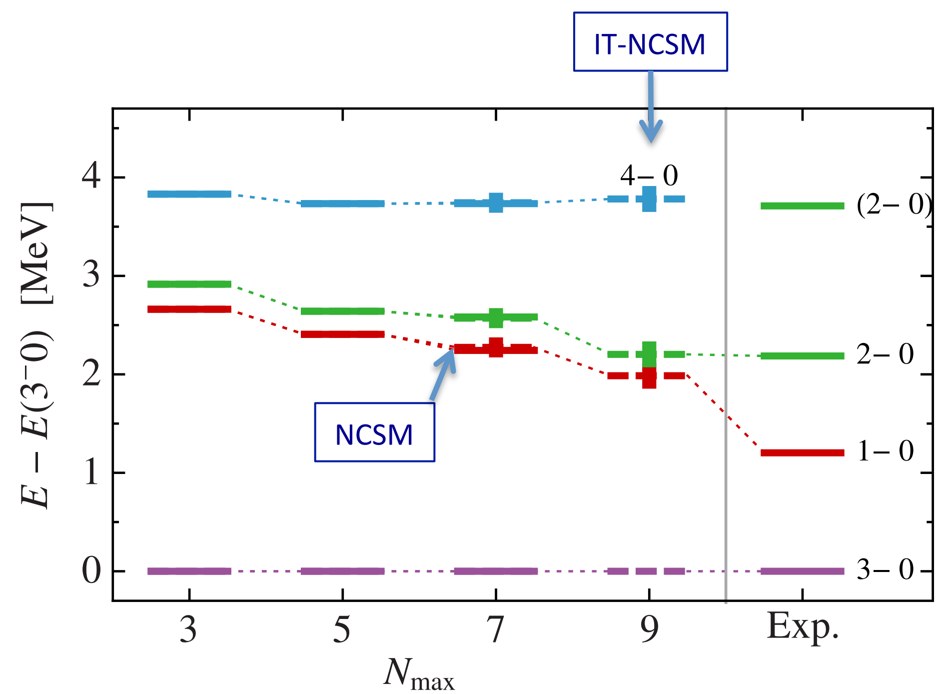
Convergence rates of excitation spectra for SRG evolved chiral NN(N3LO) + 3N(N2LO)

$\alpha = 0.0625\ \text{fm}^4$

$\lambda = 2.0\ \text{fm}^{-1}$

$\hbar\Omega = 20\ \text{MeV}$

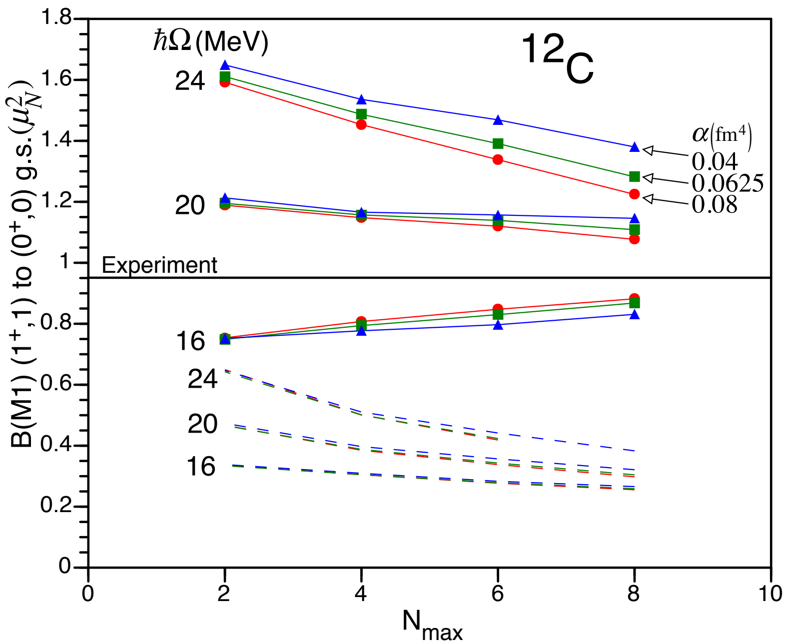


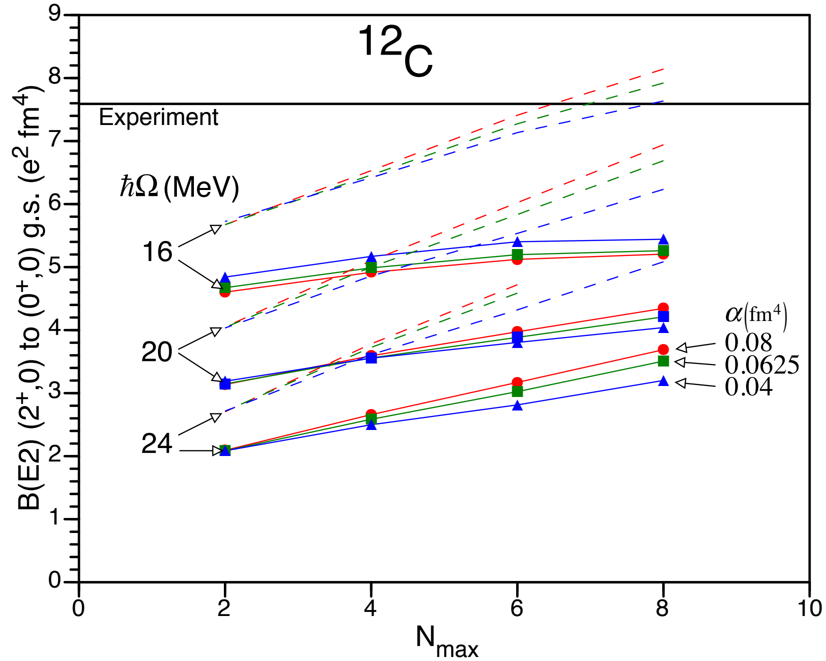


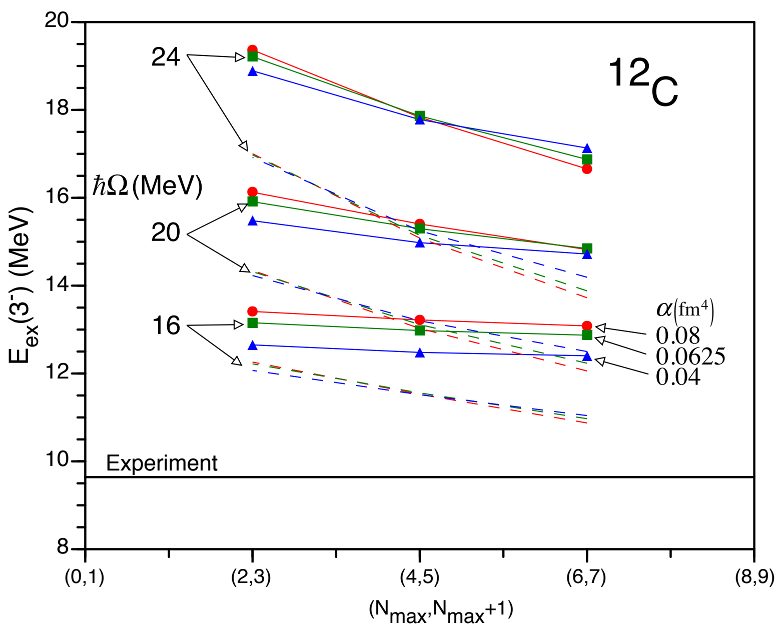
Boxes indicate threshold-extrapolation uncertainties for IT-NCSM

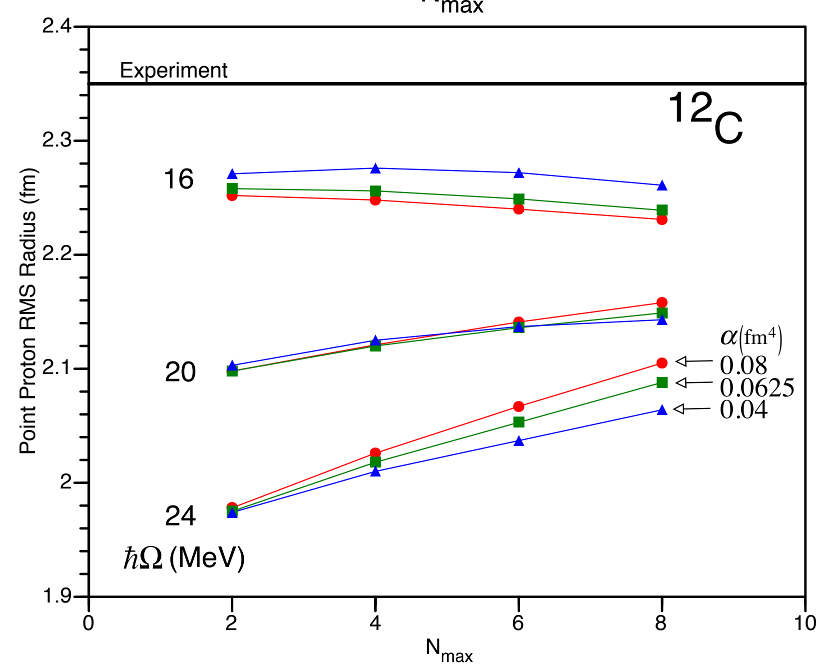
P. Maris, J.P. Vary, A. Calci, J. Langhammer, S. Binder and R. Roth, arXiv 1405.1331;to appear in PRC

Convergence rates of selected observables for SRG evolved chiral NN(N3LO) + 3N(N2LO)









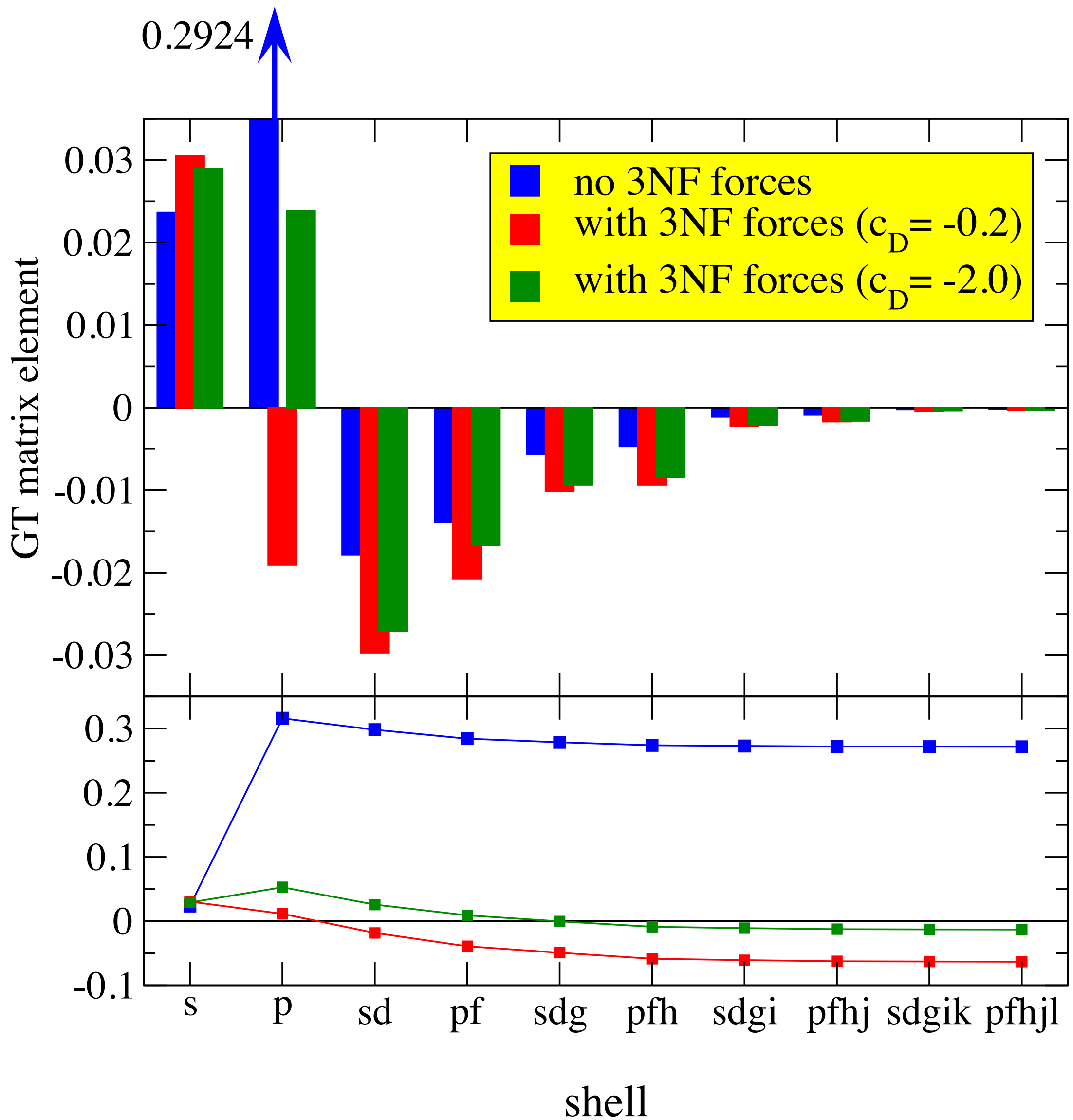
P. Maris, J.P. Vary, A. Calci, J. Langhammer, S. Binder and R. Roth, arXiv 1405.1331;to appear in PRC

Next Generation Ab Initio Structure Applications – Aim for Precision

Electroweak processes
Beyond the Standard Model tests (e.g. CKM unitarity => v_{ud} determination)
Neutrinoful and neutrinoless double beta-decay
?

Each puts major demands on theory, algorithms and computational resources
Growing demands => larger collaborating teams, growing computational resources,
Increase in the multi-disciplinary character, . . .

Origin of the anomalously long life-time of ^{14}C



- near-complete cancellations between dominant contributions within p-shell
- very sensitive to details

Maris, Vary, Navratil, Ormand, Nam, Dean, PRL106, 202502 (2011)

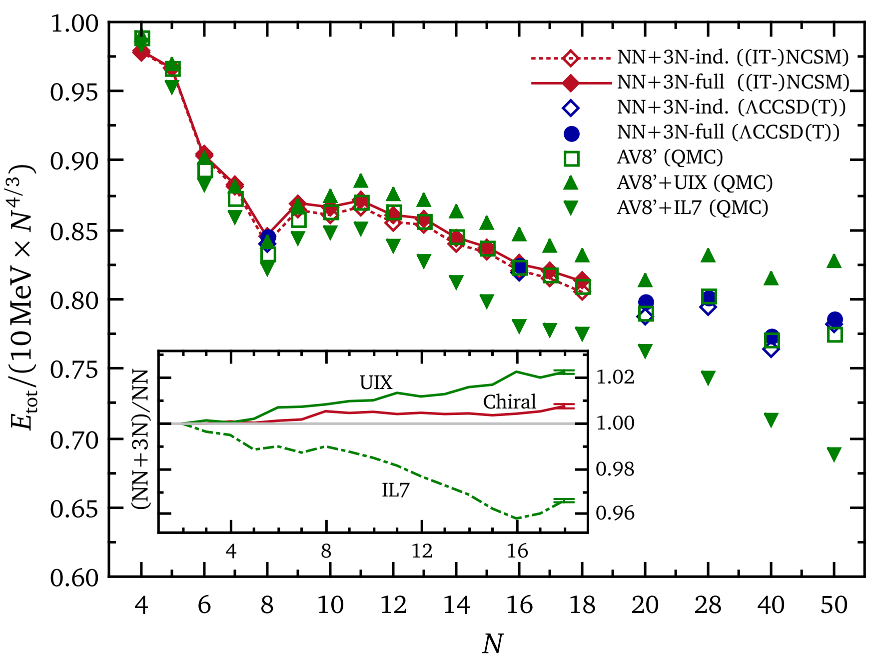
Ab initio Extreme Neutron Matter

Objectives

- Predict properties of neutron-rich systems which relate to exotic nuclei and nuclear astrophysics
- Determine how well high-precision phenomenological strong interactions compare with effective field theory based on QCD
- Produce accurate predictions with quantified uncertainties

Impact

- Improve nuclear energy density functionals used in extensive applications such as fission calculations
- Demonstrate the predictive power of *ab initio* nuclear theory for exotic nuclei with quantified uncertainties
- Guide future experiments at DOE-sponsored rare isotope production facilities



Comparison of ground state energies of systems with N neutrons trapped in a harmonic oscillator with strength 10 MeV. Solid red diamonds and blue dots signify new results with two-nucleon (NN) plus three-nucleon (3N) interactions derived from chiral effective field theory related to QCD. Inset displays the ratio of NN+3N to NN alone for the different interactions. Note that with increasing N, the chiral predictions lie between results from different high-precision phenomenological interactions, i.e. between AV8'+UIX and AV8'+IL7.

Accomplishments

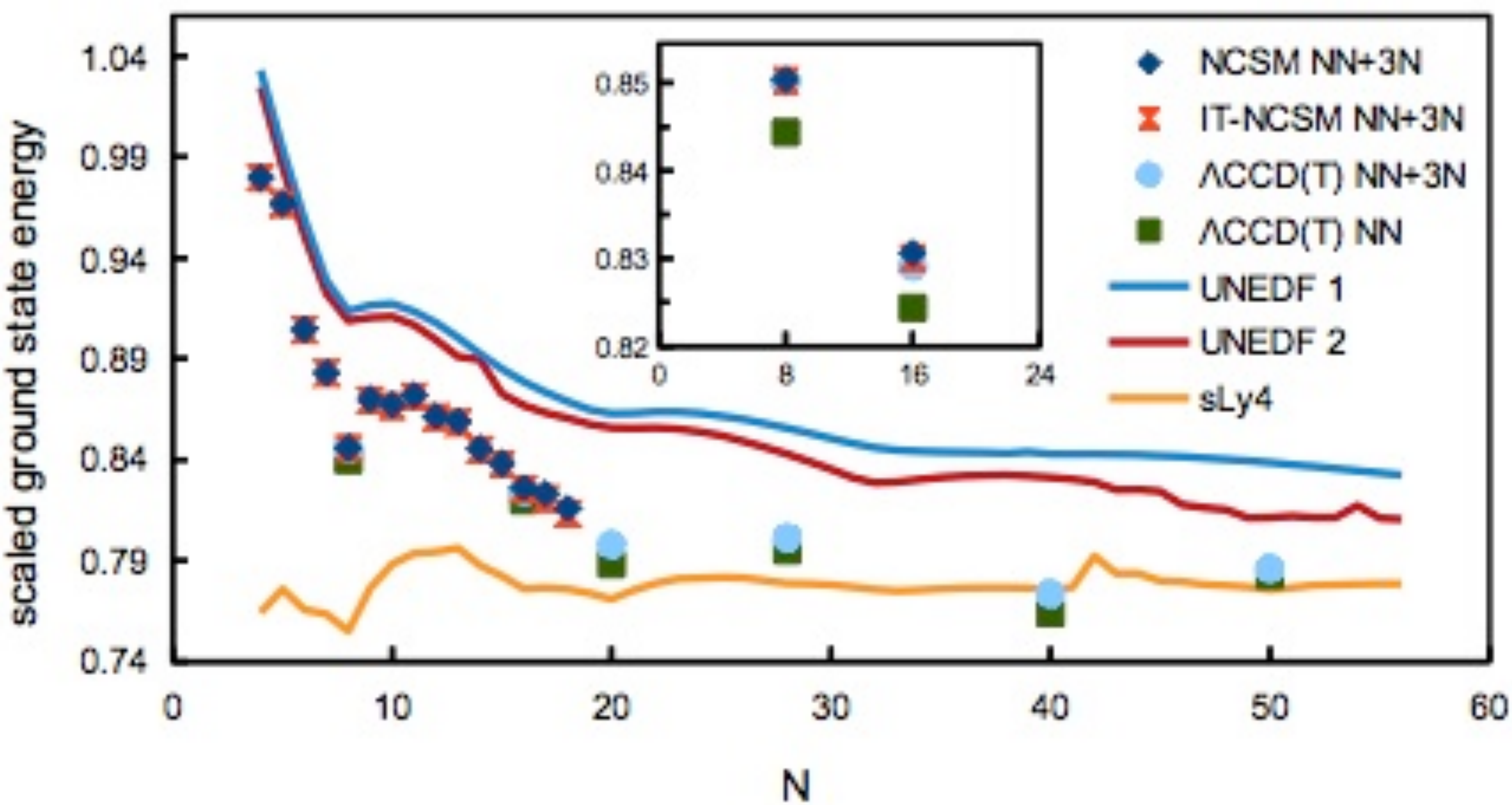
1. Demonstrates predictive power of *ab initio* nuclear structure theory.
2. Provides results for next generation nuclear energy density functionals
3. Leads to improved predictions for astrophysical reactions
4. Demonstrates that the role of three-nucleon (3N) interactions in extreme neutron systems is significantly weaker than predicted from high-precision phenomemological interactions

U.S. DEPARTMENT OF ENERGY | Office of Science

NUCLEI Nuclear Computational Low-Energy Initiative

References: P. Maris, J.P. Vary, S. Gandolfi, J. Carlson, S.C. Pieper, Phys. Rev. C87, 054318 (2013); H. Potter, S. Fischer, P. Maris, J.P. Vary, S. Binder, A. Calci, J. Langhammer and R.Roth, arXiv:1406.1160; Contact: jvary@iastate.edu

Neutron drops in 10 MeV harmonic trap
with Chiral NN and Chiral NN + 3N interactions



H.D. Potter, PhD project, Iowa State University
Iowa State – Darmstadt Collaboration; arXiv 1406:1160

Summary: Observables in light nuclei known to be sensitive to 3NFs
based on chiral NN (N3LO) + 3N (N2LO) [Lambda = 500 MeV]

Binding energies (through Oxygen)and subshell closures (through Calcium)
Spectral properties having spin-orbit sensitivity
GS quadrupole moment of ^{6}Li
M1, E2, F, GT transitions
Ratio of B(E2)'s [GS -> 1_1^+ over GS -> 1_2^+] in ^{10}B
^{10}B ground state spin
^{14}C anomalous half-life

Other:
Elastic magnetic form factor of ^{17}O (M5 region)

PHYSICAL REVIEW C VOLUME 25, NUMBER 2 FEBRUARY 1982

Three-body force effects in the ^{17}O magnetic form factor

S. A. Coon
*Physics Department, University of Arizona, Tucson, Arizona 85721**
and Ames Laboratory-Department of Energy, Iowa State University, Ames, Iowa 50011

R. J. McCarthy
*Kent State University, Ashtabula Campus, Ashtabula, Ohio 44004**
and Ames Laboratory-Department of Energy, Iowa State University, Ames, Iowa 50011

J. P. Vary
Ames Laboratory-Department of Energy and Physics Department,
Iowa State University, Ames, Iowa 50011
(Received 7 August 1981)

We find large corrections to the ^{17}O magnetic form factor arising from a two-pion exchange three-body force. These corrections are comparable in magnitude to meson exchange current contributions. The phases of the $M1$, $M3$, and $M5$ amplitudes due to the three-body force are favorable for improving agreement between theory and experiment, especially in the region of momentum transfer between 1.5 and 3.0 fm^{-1}.

S.A. Coon, R.J. McCarthy and J.P. Vary, "Three-body force effects in the ^{17}O Magnetic form factor." Phys. Rev. C 25, 756 (1982).

Abstract begins:
"We find large corrections to the 17O magnetic form factor arising from a two-pion exchange three-body force."

Three-body force contributions are comparable to large meson-exchange contributions - enhance the M5 but do not suppress the M3.

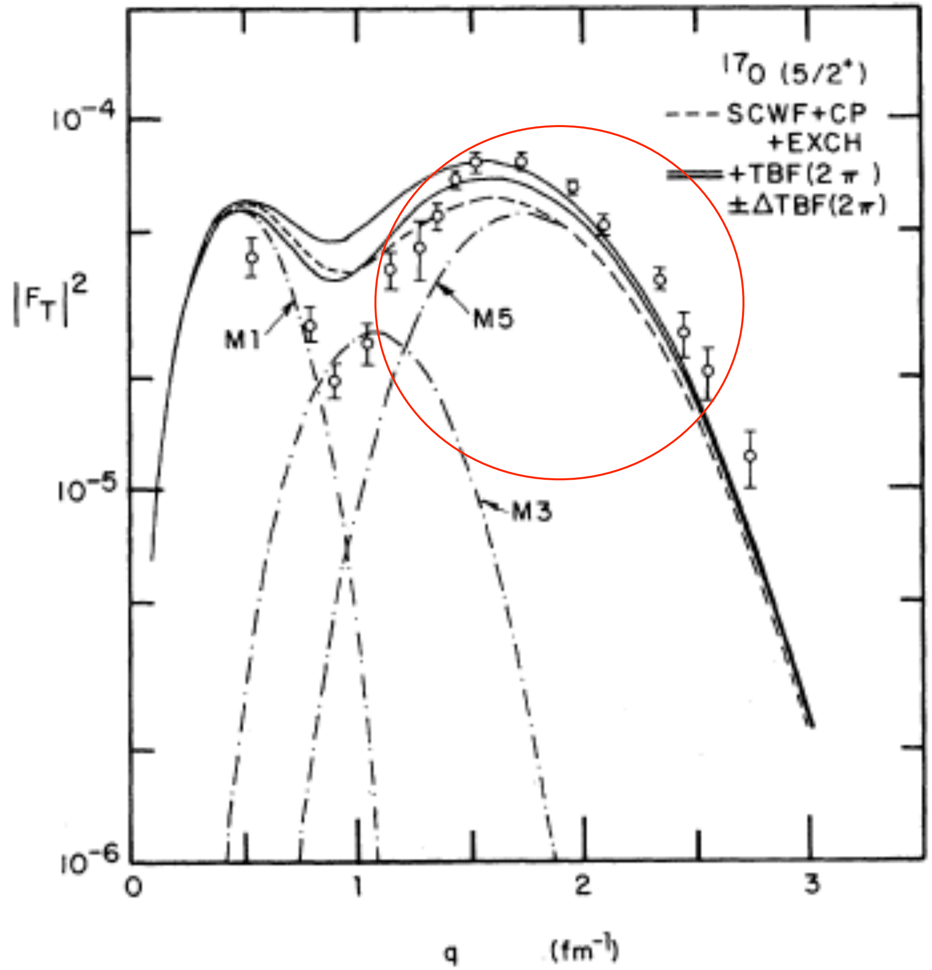
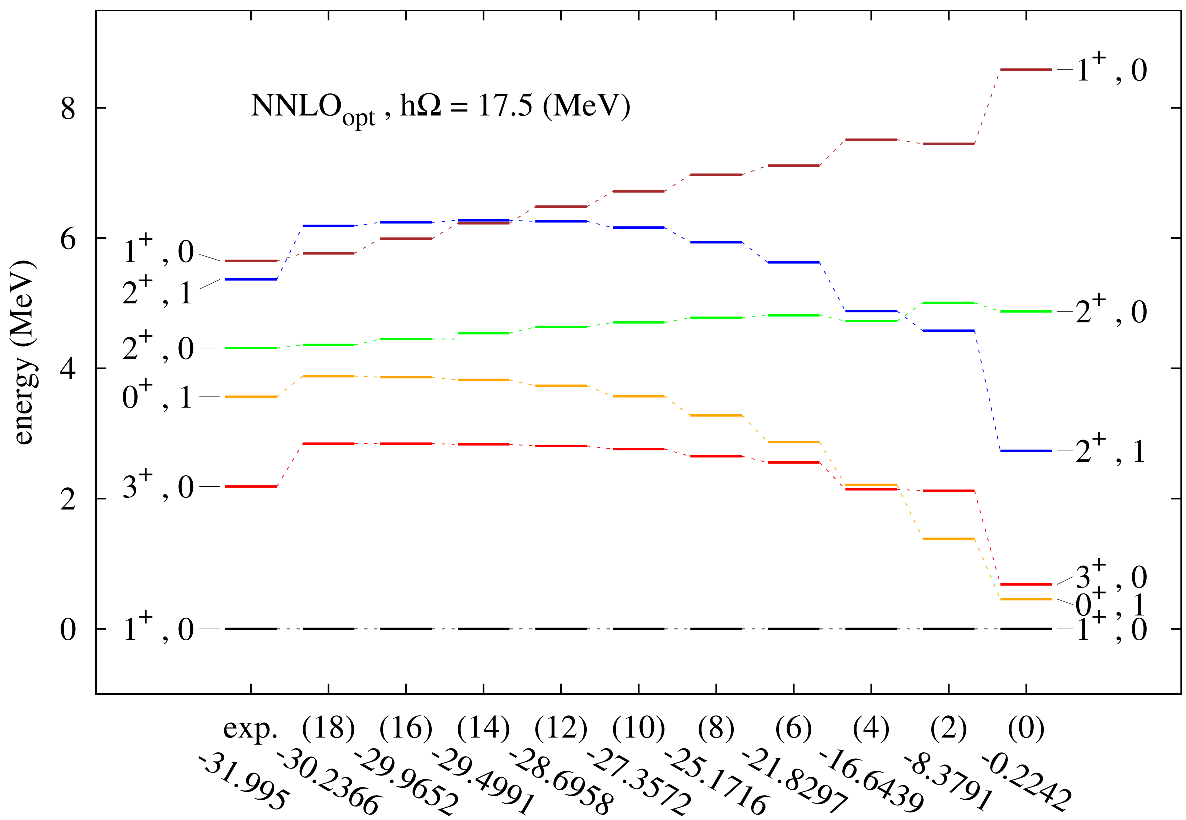


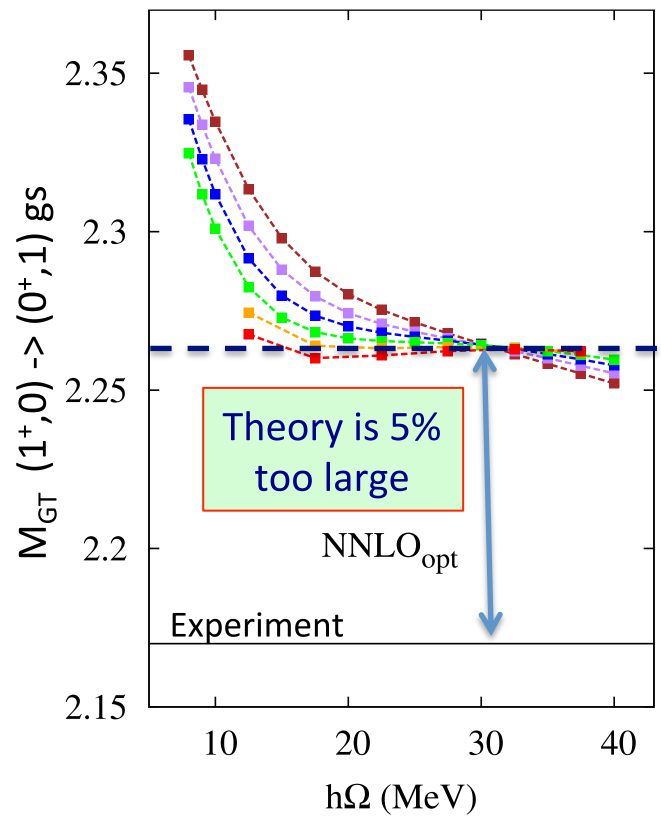
FIG. 3. Transverse magnetic form factor squared, $|F_T|^2$, vs effective momentum transfer q for ^{17}O. The curve labeled SCWF + CP + EXCH is described in the caption to Fig. 2. The two solid lines bracket the results obtained by including the three body force diagrams of Fig. 1. The $\pm\Delta$TBF(2π) refer to uncertainties in the TBF parameters as described in the text. Also shown are the main peaks of the separate $M1$, $M3$, and $M5$ amplitudes squared.

Established challenges – possible roles for improved 3NFs

Gaps between natural & unnatural parity spectra
The energy of J = 1+, T=0 state in 12C
Two low-lying 2+ states in 10Be with radically different B(E2)'s
Level crossing of J = 5/2 and J = 1/2 states in 9Be
Spectra of 14N
Overbinding of Ca isotopes and above
RMS radii too small in ~all nuclei above 4He
Magnetic FF of 17O – in the M3 suppression region
Extra GT transitions (intruders, clusters, . . .) in p-shell nuclei (e.g. A = 14 PRL)
How JISP16 and NNLO_opt do a ~reasonable job simulating 3NF effects

^{6}Li with chiral NNLO_opt Hamiltonian
RISP – ISU - Chalmers collaboration (in preparation)





1.4 MeV underbinding (extrapolated)

In process:
widths of continuum states with Gamow Shell Model

Extending the Precision and Reach of Ab Initio Applications:

Physics-driven, theory-improved chiral interactions, EW currents, . .
Renormalization theory
Extrapolation theory
Physics-driven, theory-improved basis spaces

Optimize our utilization of available algorithms and computational resources
=> intense theoretical developments,
increase in the multi-disciplinary character, . . .

Calculation of three-body forces at N^3LO

Low
Energy
Nuclear
Physics
International
Collaboration

J. Golak, R. Skibinski, K. Tolponicki, H. Witala

E. Epelbaum, H. Krebs

A. Nogga

R. Furnstahl

S. Binder, A. Calci, K. Hebeler, J. Langhammer, R. Roth

P. Maris, J. Vary

H. Kamada

Goal

Calculate matrix elements of 3NF in a partial-wave decomposed form which is suitable for different few- and many-body frameworks

---

Challenge

Due to the large number of matrix elements, the calculation is extremely expensive.

Strategy

Develop an efficient code which allows to treat arbitrary local 3N interactions.
(Krebs and Hebeler)

Extrapolating to the infinite matrix limit
i.e. to the "continuum limit"

Results with both IR and UV extrapolations

References:
S.A. Coon, M.I. Avetian, M.K.G. Kruse, U. van Kolck, P. Maris, and J.P. Vary, Phys. Rev. C 86, 054002 (2012); arXiv: 1205.3230
R.J. Furnstahl, G. Hagen, T. Papenbrock, Phys. Rev. C 86 (2012) 031301
E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary, Phys. Rev. C 87, 054312(2013); arXiv 1302.5473
S.N. More, A. Ekstroem, R.J. Furnstahl, G. Hagen and T. Papenbrock, Phys. Rev. C87, 044326 (2013); arXiv 1302.3815

=> Uncertainty Quantification

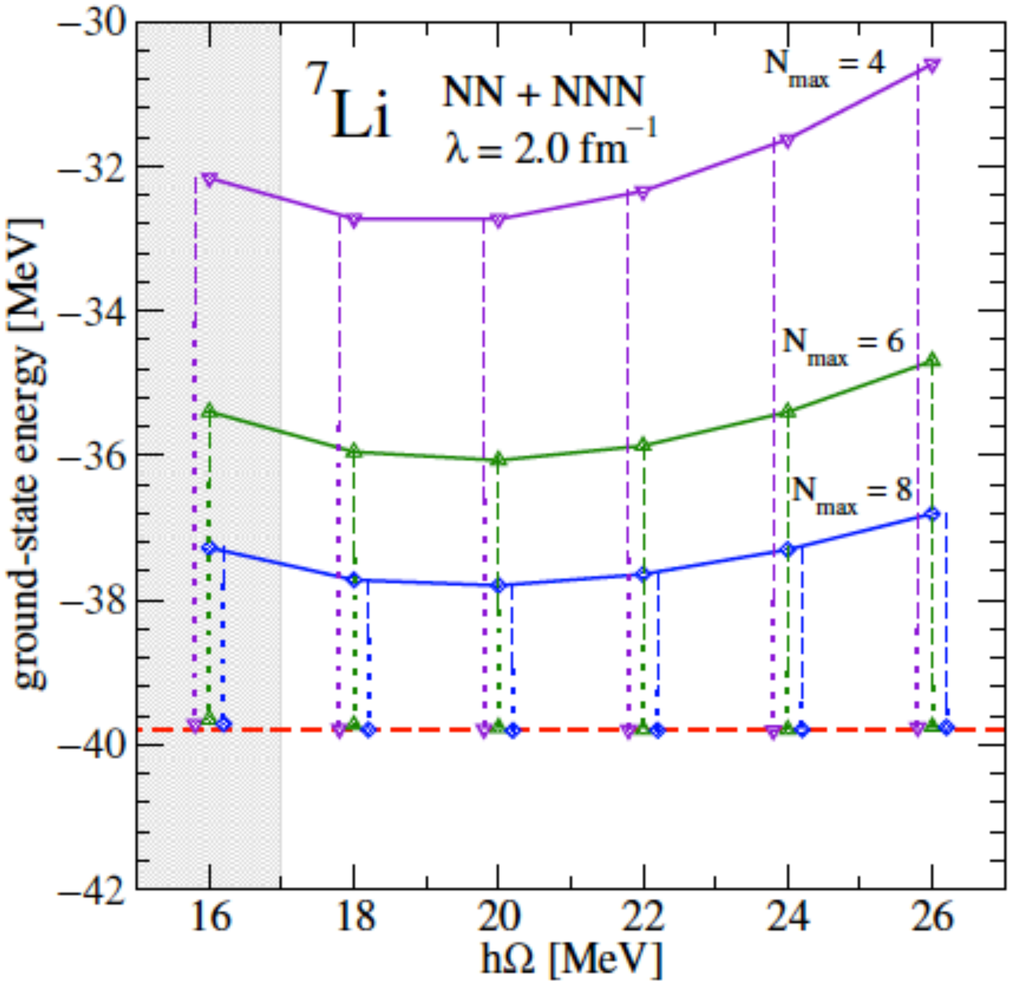
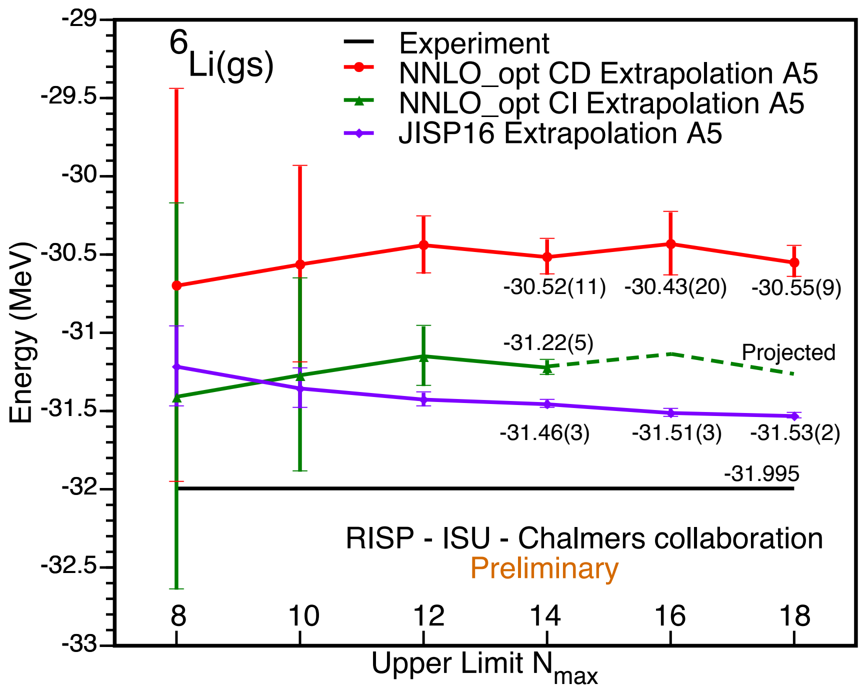
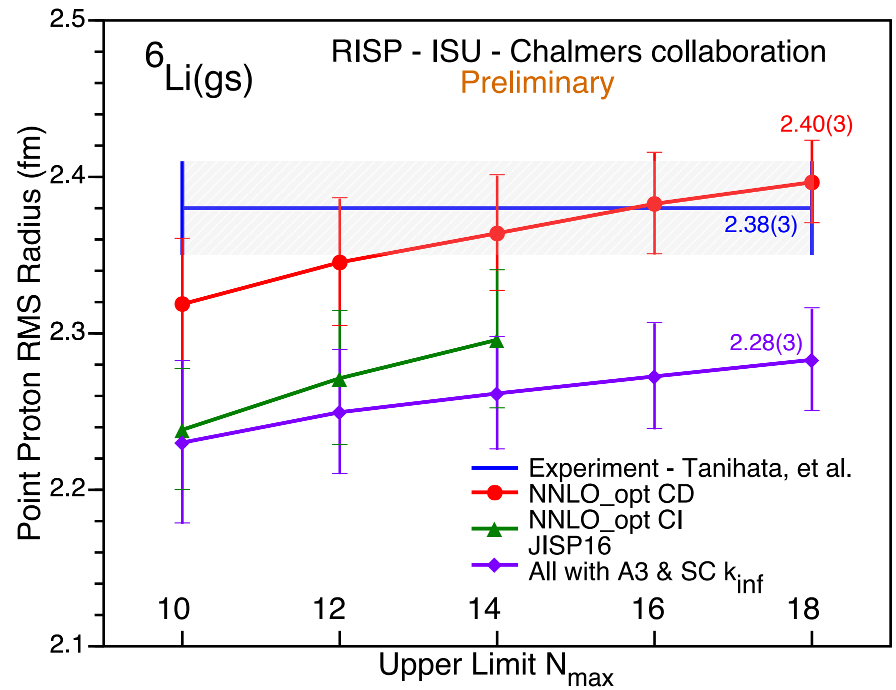


FIG. 17. (color online) Ground-state energy of ^{7}Li for the NN+NNN evolved Hamiltonians at $\lambda = 2.0\,\text{fm}^{-1}$, with IR (vertical dashed) and UV (vertical dotted) corrections from Eq. (5) that add to predicted E_∞ values (points near the horizontal dashed line, which is the global E_∞).

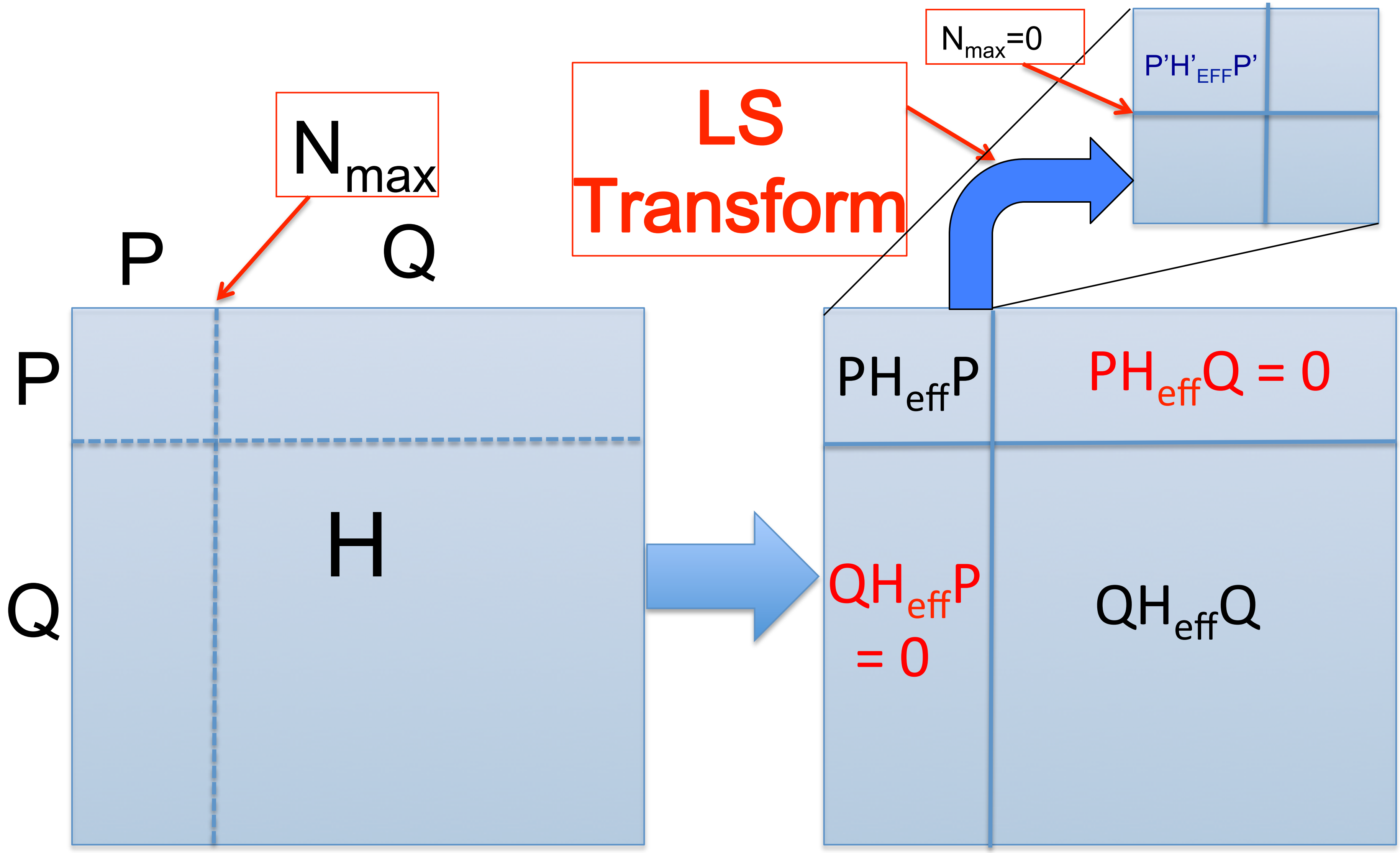
E.D. Jurgenson, P. Maris, R.J. Furnstahl, P. Navratil, W.E. Ormand, J.P. Vary, Phys. Rev. C. 87, 054312 (2013); arXiv: 1302:5473

^{6}Li with chiral NNLO_opt Hamiltonian
Extrapolations to continuum limit with quantified uncertainties





- ✧ Generally, extrapolated results are consistent within uncertainties as a function of increasing N_{max}
- ✧ Systematic increase of proton rms suggests need for improved theory of IR behavior



The "double Lee-Suzuki transform" for valence H_{eff}

Effective interactions in *sd*-shell from *ab-initio* shell model with a core

Preliminary Results

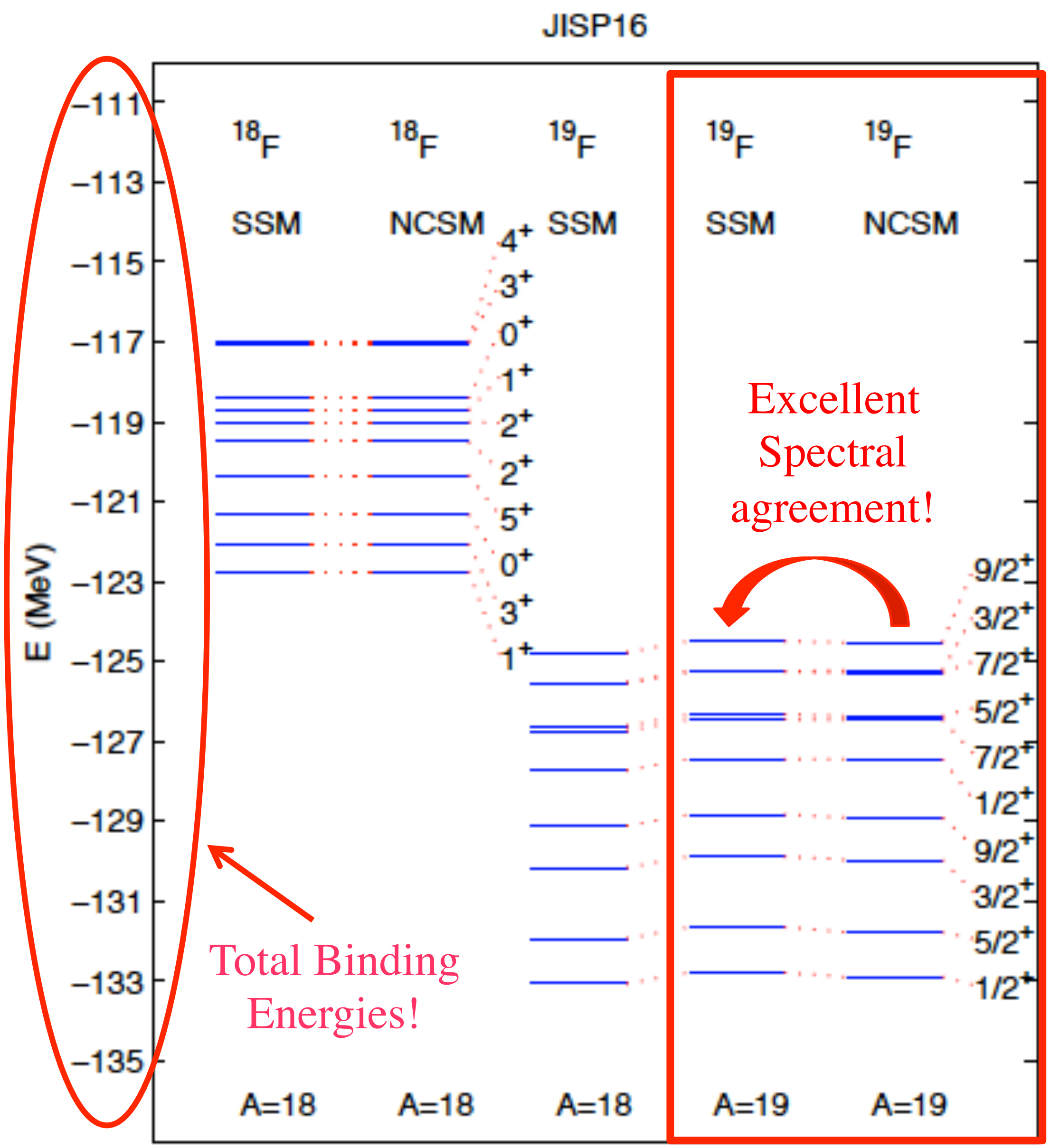
E. Dikmen,[1,2,*] A. F. Lisetskiy,[2,†] B. R. Barrett,[2] P. Maris,[3] A. M. Shirokov,[3,4,5] and J. P. Vary[3]

Aim: Regain valence-core separation but retain full ab initio NCSM

=> “Double OLS” Approach

Now extend to s-d shell the successful p-shell applications

p-shell application:
A. F. Lisetskiy, B. R. Barrett, M. K. G. Kruse, P. Navratil, I. Stetcu, J. P. Vary, Phys. Rev. C. 78, 044302 (2008); arXiv:0808.2187



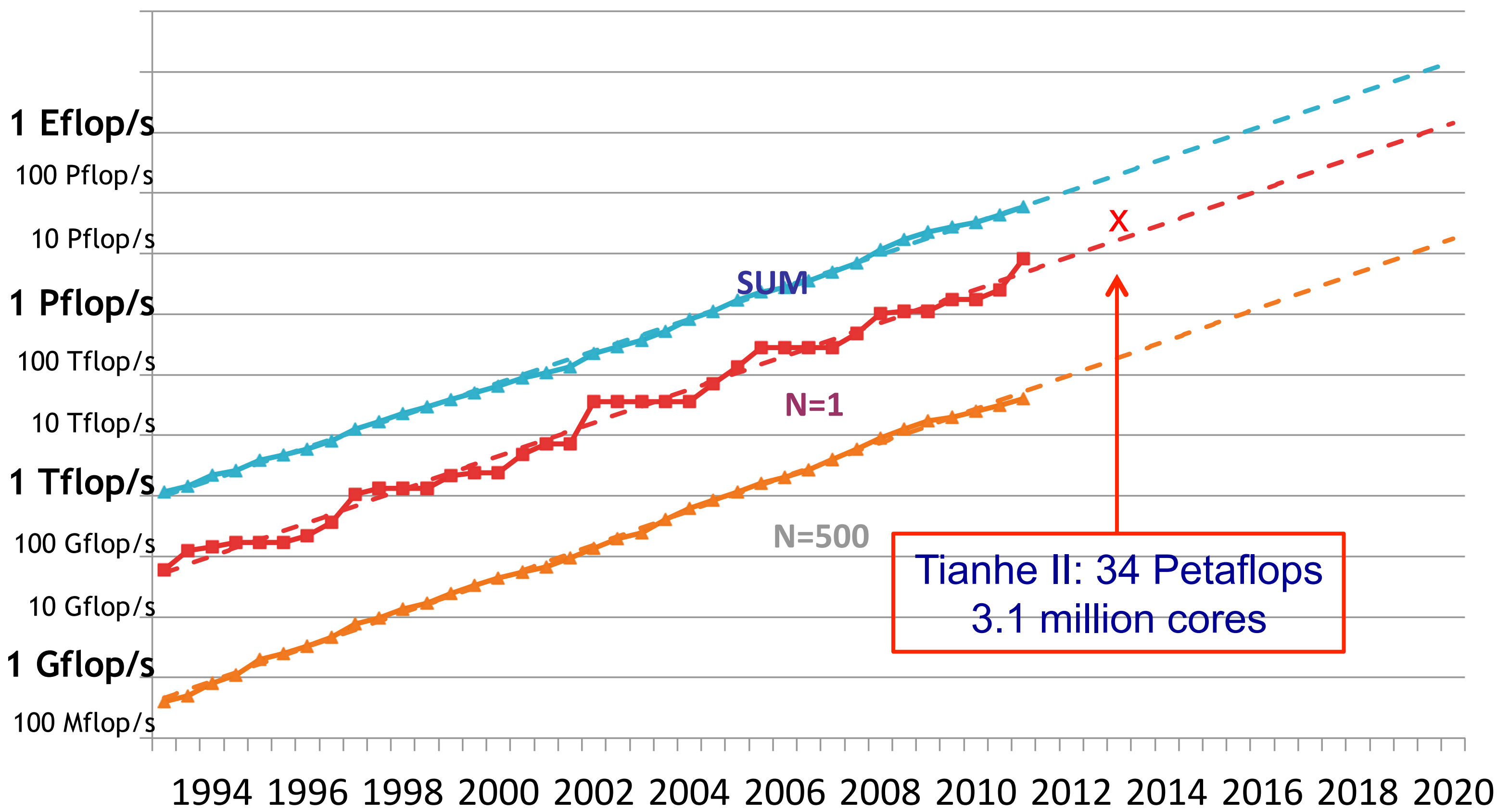
- Hardware advances: Moore’s Law
- Theory/Algorithms/Software advances: Doubles Moore’s Law

↓

Discovery potential increases geometrically

Role of Supercomputers

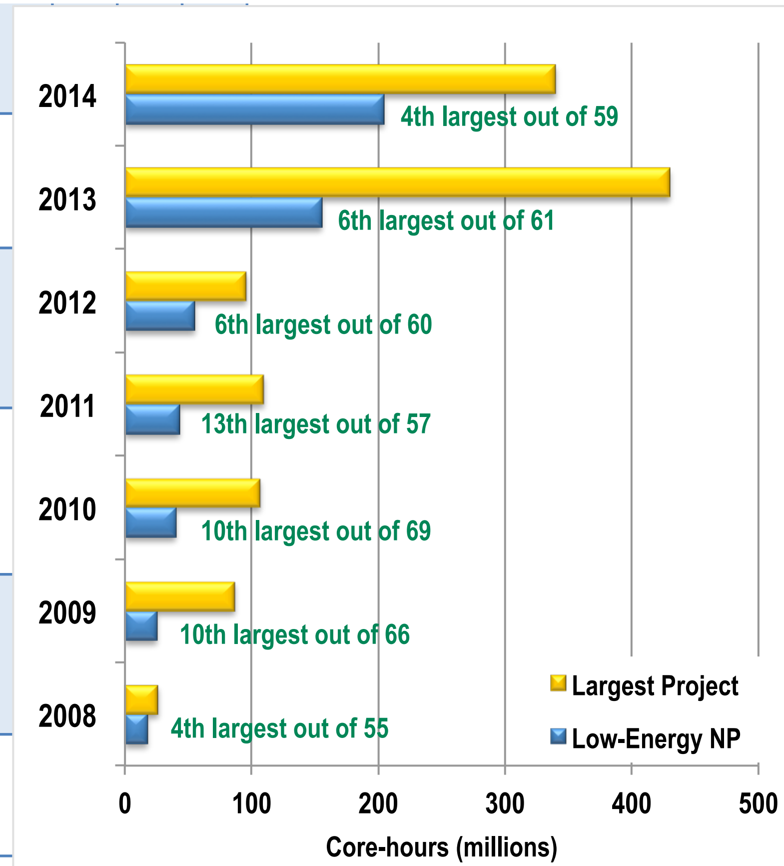
Projected Performance Development



Low Energy NP Application Areas

Application	Production Run Sizes	Resource	Dense Linear Alg.	Sparse Linear Alg.	Monte Carlo
AGFMC: Argonne Green's Function Monte Carlo	262,144 cores @ 10 hrs	Mira			X
MFDn: Many Fermion Dynamics - nuclear	260K cores @ 4 hrs 500K cores @ 1.33 hrs	Titan Mira		X	
NUCCOR: Nuclear Coupled-Cluster Oak Ridge, m-scheme & spherical	100K cores @ 5 hrs (1 nucleus, multiple parameters)	Titan		X	
DFT Code Suite: Density Functional Theory, mean-field methods	100K cores @ 10 hrs (entire mass table, fission barriers)	Titan	X		
MADNESS: Schroedinger, Lippman-Schwinger and DFT	40,000 cores @ 12 hrs (extreme asymmetric functions)	Titan	X	X	
NCSM_RGM: Resonating Group Method for scattering	98,304 cores @ 8 hrs	Titan	X	X	

- Ab initio Methods (CC, GFMC, NCSM) → pushing the limits to calculate larger nuclei
- Density Functional Theory → reasonable time to solution to calculate the entire mass table



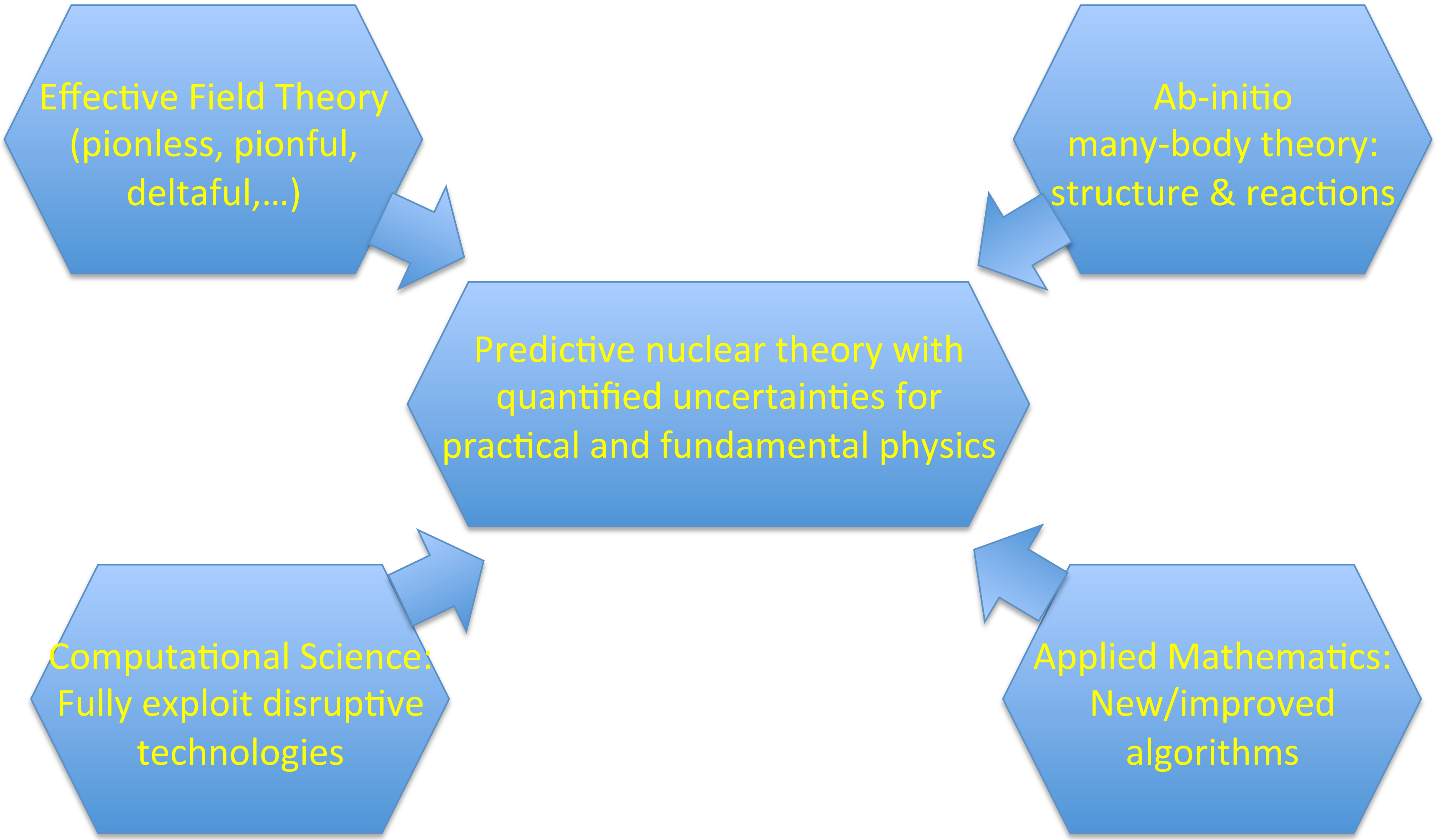
Slide by Hai Ah Nam, ORNL

Many outstanding nuclear physics puzzles
and discovery opportunities

Clustering phenomena
Origin of the successful nuclear shell model
Nuclear reactions and breakup
Astrophysical r/p processes & drip lines
Predictive theory of fission
Existence/stability of superheavy nuclei
Physics beyond the Standard Model
Possible lepton number violation
Spin content of the proton
+ Many More!

Conclusions/Outlook

- ✧ Impressive recent progress in deriving NN and NNN interactions from QCD
- ✧ Much work needs to be done to improve upon these interactions and the many-body approaches that employ them
- ✧ We will continue to apply these interactions to nuclei as they are developed
- ✧ Collaborations of Chiral EFT theorists and ab-initio many-body theorists needed to improve the properties of the Chiral EFT interactions
- ✧ Collaborations of nuclear theorists with computer scientists and applied mathematicians must continue
- ✧ Increasing computational resources needed (3NFs, 4NFs are major challenges)
- ✧ Increased manpower needed to achieve these goals in larger collaborating teams


Effective Field Theory (pionless, pionful, deltaful,…)
Ab-initio many-body theory: structure & reactions
Predictive nuclear theory with quantified uncertainties for practical and fundamental physics
Computational Science: Fully exploit disruptive technologies
Applied Mathematics: New/improved algorithms

Recent Collaborators

United States

ISU: Pieter Maris, George Papadimitriou, Chase Cockrell, Hugh Potter, Alina Negoita
LLNL: Erich Ormand, Tom Luu, Eric Jurgenson, Michael Kruse
ORNL/UT: David Dean, Hai Ah Nam, Markus Kortelainen, Witek Nazarewicz, Gaute Hagen,Thomas Papenbrock
OSU: Dick Furnstahl, students
MSU: Scott Bogner, Heiko Hergert
Notre Dame: Mark Caprio
ANL: Harry Lee, Steve Pieper, Fritz Coester
LANL: Joe Carlson, Stefano Gandolfi
UA: Bruce Barrett, Sid A. Coon, Bira van Kolck, Matthew Avetian, Alexander Lisetskiy
LSU: Jerry Draayer, Tomas Dytrych, Kristina Sviratcheva, Chairul Bahri
UW: Martin Savage

International

Canada: Petr Navratil
Russia: Andrey Shirokov, Alexander Mazur, Eugene Mazur, Sergey Zaytsev, Vasily Kulikov
Sweden: Christian Forssen, Jimmy Rotureau
Japan: Takashi Abe, Takaharu Otsuka, Yutaka Utsuno, Noritaka Shimizu
Germany: Achim Schwenk, Robert Roth, Kai Hebeler, students
South Korea: Youngman Kim, Ik Jae Shin
Turkey: Erdal Dikman

Computer Science/ Applied Math

ODU/Ames Lab: Masha Sosonkina, Dossay Oryspayev
LBNL: Esmond Ng, Chao Yang, Hasan Metin Aktulga
ANL: Stefan Wild, Rusty Lusk
OSU: Umit Catalyurek, Eric Saule

Quantum Field Theory

ISU: Xingbo Zhao, Pieter Maris, Paul Wiecki, Yang Li, Kirill Tuchin, John Spence
Stanford: Stan Brodsky
Penn State: Heli Honkanen
Russia: Vladimir Karmanov

Germany: Hans-Juergen Pirner
Costa Rica: Guy de Teramond
India: Avaroth Harindranath, Usha Kulshreshtha, Daya Kulshreshtha, Asmita Mukherjee, Dipankar Chakrabarti, Ravi Manohar