Ab Initio Nuclear Structure Theory

James P. Vary
Iowa State University

National Nuclear Physics Summer School
SUNY Stony Brook
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3. Recent results in light nuclei with ab initio no core methods

- Overview of ab initio approaches (GFMC, CC, NCSM, NCFC)
- Applications to light nuclei – importance of NNN
- Applications to nuclear reactions - deferred due to time limits
- Applications to non-perturbative solution of quantum field theory
- Conclusions and outlook

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**)

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

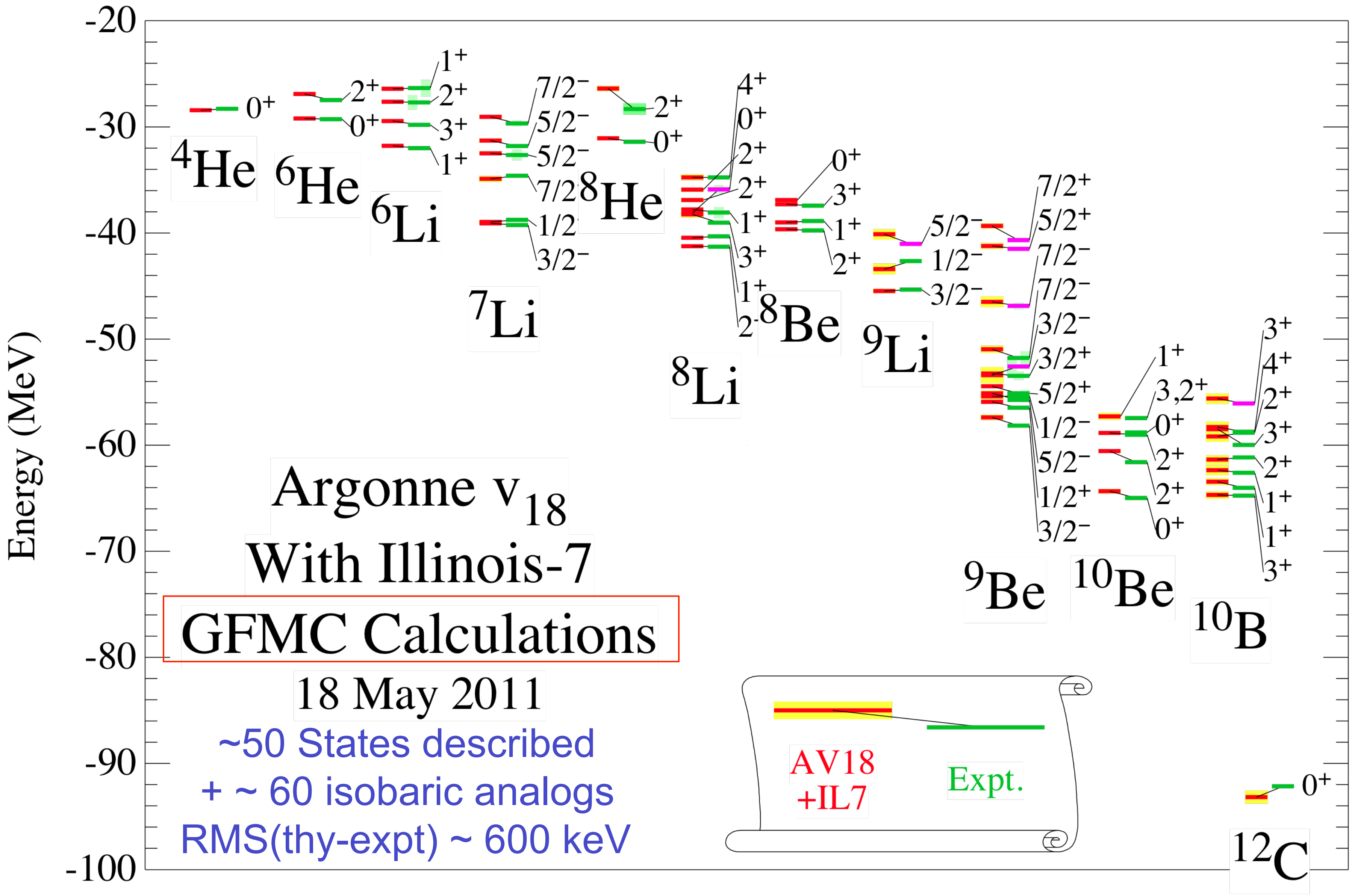
Meson Exchg interactions

Featured results here

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



S. Pieper, R. Wiringa, et al

No Core Shell Model

A large sparse matrix eigenvalue problem

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

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

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

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

- 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,$m_{j,}\tau_z$)]

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

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

- 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=20 (40) today with largest computers available

ab initio NCSM
Effective Hamiltonian for A-Particles
Okubo-Lee-Suzuki Method plus Cluster Decomposition

P. Navratil, J.P. Vary and B.R. Barrett,
Phys. Rev. Lett. 84, 5728(2000); Phys. Rev. C62, 054311(2000)
C. Viazminsky and J.P. Vary, J. Math. Phys. 42, 2055 (2001);
S. Okubo, Progr. Theor. Phys. 12 (1954) 603;
K. Suzuki and S.Y. Lee, Progr. Theor. Phys. 64, 2091(1980);
K. Suzuki, *ibid*, 68, 246(1982);
Review: B.R. Barrett, P. Navratil and J.P. Vary, Prog. Part. Nucl. Phys. 69, 131 (2013)

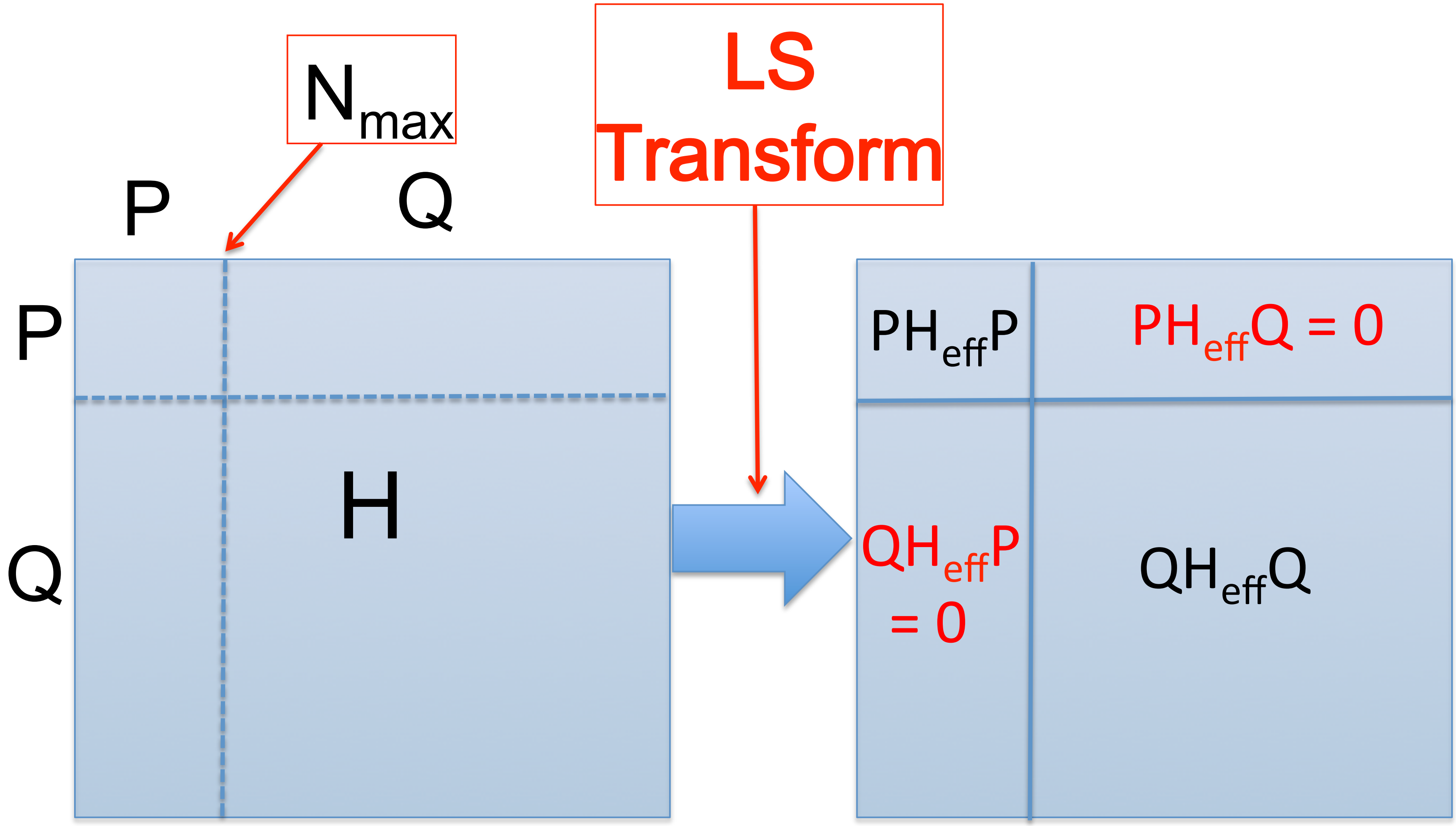
Preserves the symmetries of the full Hamiltonian:
Rotational, translational, parity, etc., invariance

$$H_{\mathcal{A}} = T_{rel} + V = \sum_{i<j}^{\mathcal{A}} \left[\frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + V_{ij} \right] + V_{NNN}$$

Select a finite oscillator basis space (P-space) and evaluate an a- body cluster effective Hamiltonian:

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

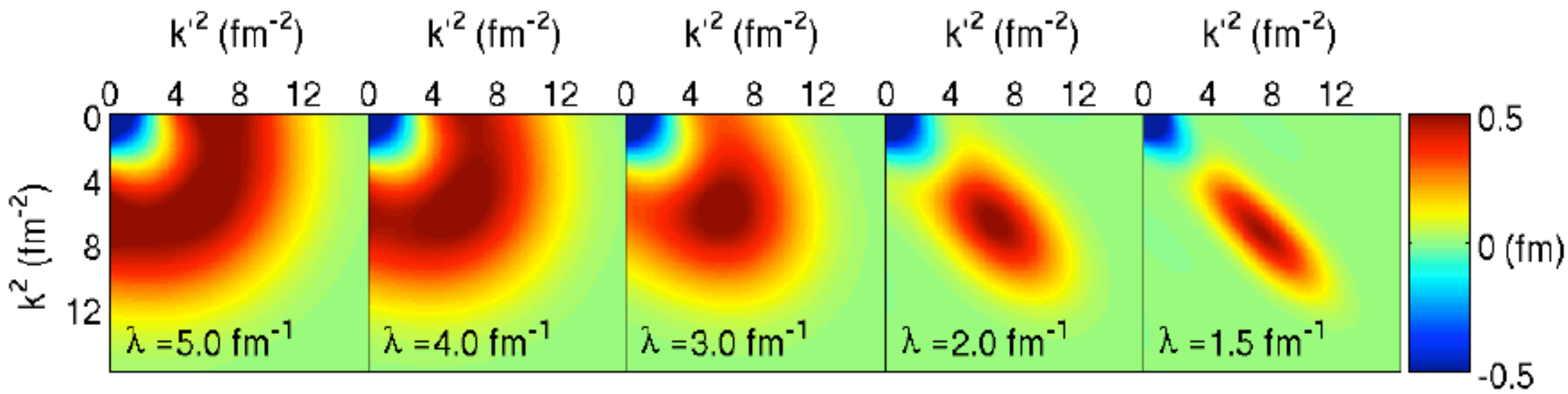
Guaranteed to provide exact answers as $a \to A$ or as $P \to 1$.



Review: **B.R. Barrett, P. Navratil and J.P. Vary, Prog. Part. Nucl. Phys. 69, 131 (2013)**

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 the applications surveyed

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

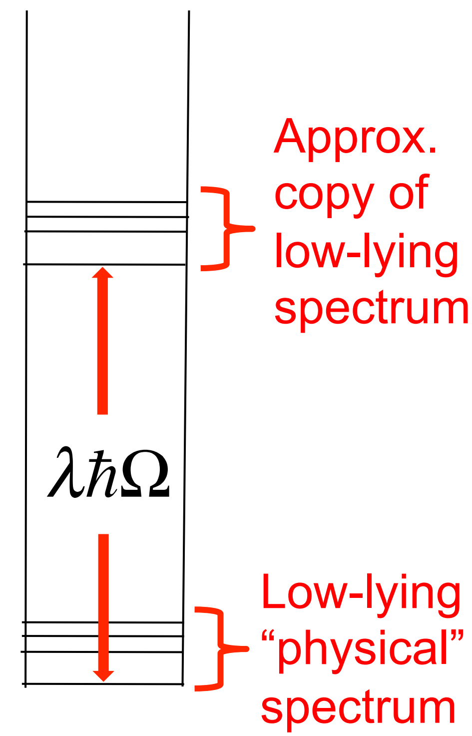
Add a Lagrange multiplier term acting on the cm alone so as not to interfere with the internal motion dynamics

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

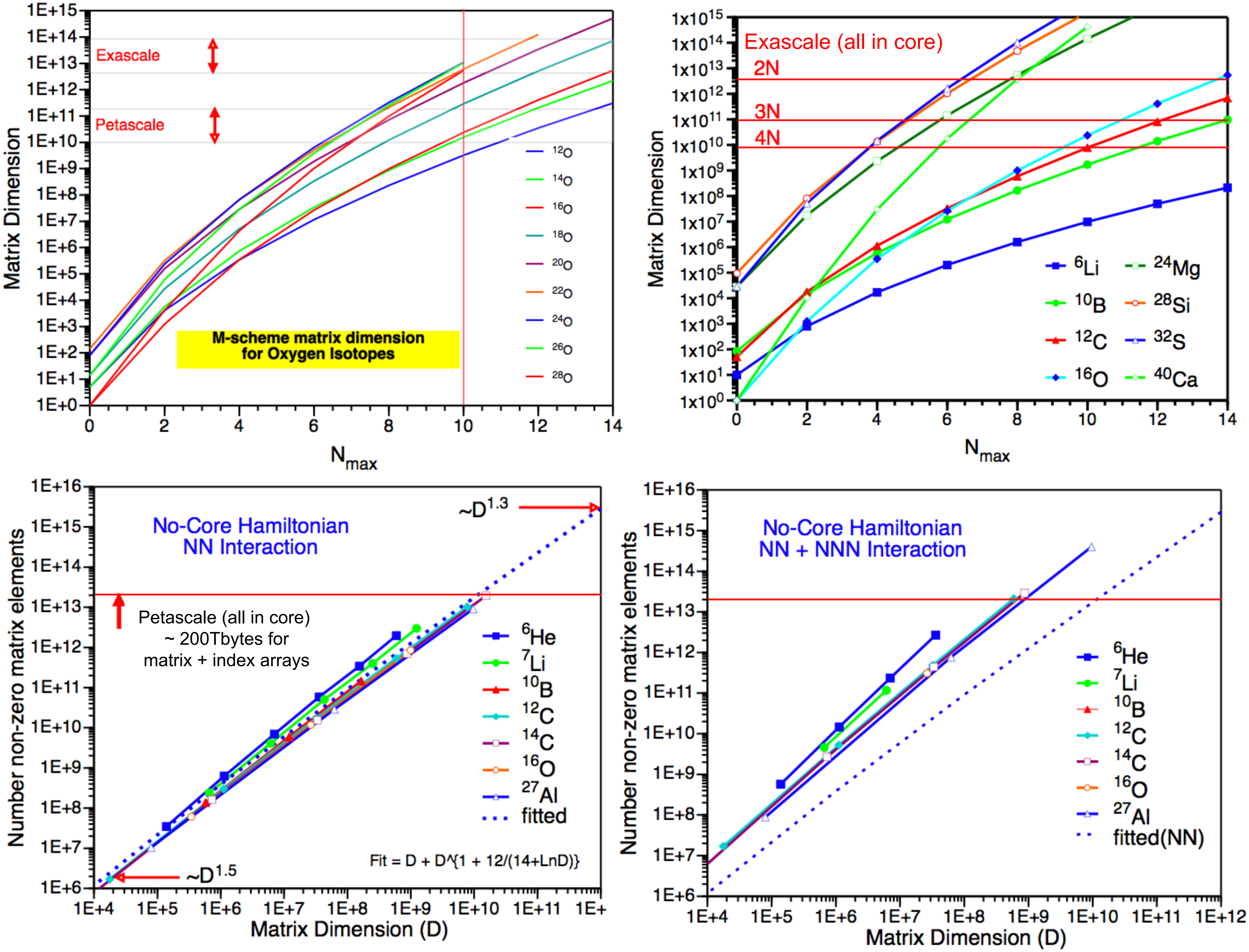
$$H = H_{eff}\left(N_{\max}, \hbar\Omega\right) + \lambda H_{cm}$$

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

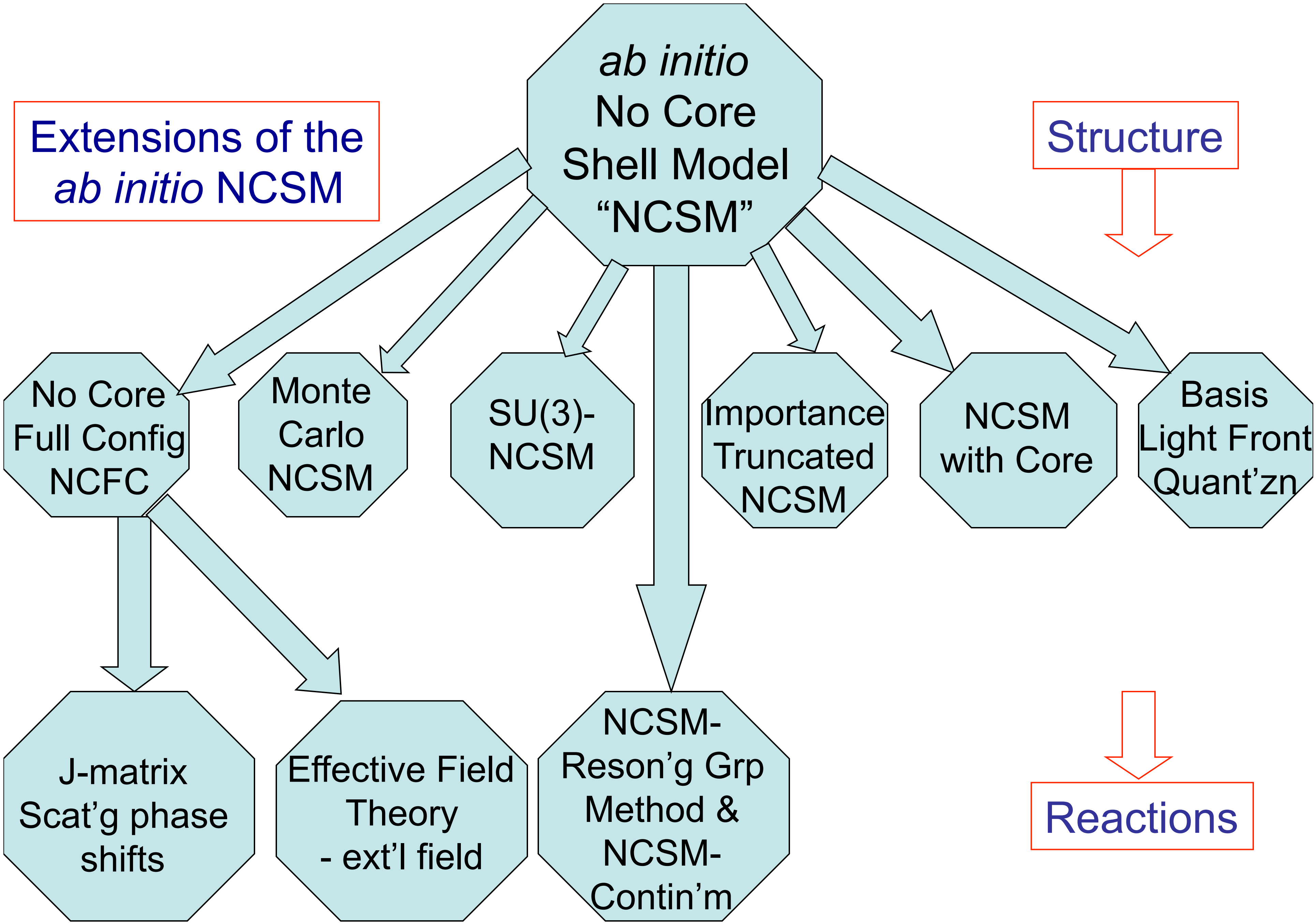
$$\lambda \sim 10 \quad \text{suffices}$$



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



Exascale
Petascale
M-scheme matrix dimension for Oxygen Isotopes
Matrix Dimension
N_max
12O
14O
16O
18O
20O
22O
24O
26O
28O
Exascale (all in core)
2N
3N
4N
6Li
10B
12C
16O
24Mg
28Si
32S
40Ca
No-Core Hamiltonian
NN Interaction
~D^1.3
~D^1.5
Petascale (all in core)
~ 200Tbytes for
matrix + index arrays
6He
7Li
10B
12C
14C
16O
27Al
fitted
Fit = D + D^{1 + 12/(14+LnD)}
Number non-zero matrix elements
Matrix Dimension (D)
No-Core Hamiltonian
NN + NNN Interaction
fitted(NN)


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
Reactions

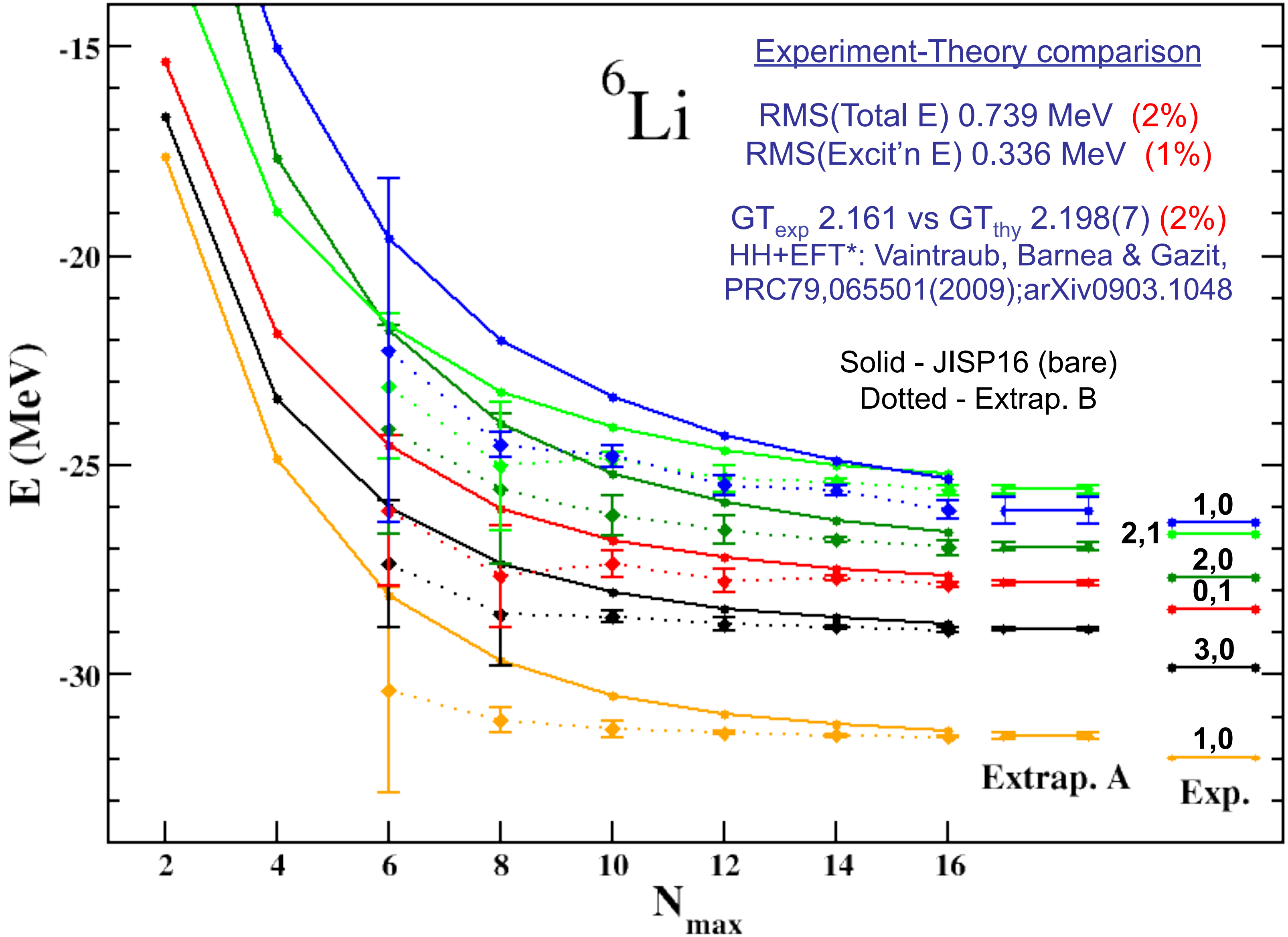
Extrapolating to the infinite matrix limit i.e. to the "continuum limit"

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

NCFC results (does not adopt a renormalization)



P. Maris, A. Shirokov and J.P. Vary, Phys. Rev. C 81, 021301(R) (2010). ArXiv 0911.2281

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

Convergence and Uncertainty Assessments: Recent Highlight

Convergence properties of *ab initio* calculations of light nuclei in a harmonic oscillator basis

Phys. Rev. C 86, 054002 (2012); arXiv:1205.3230

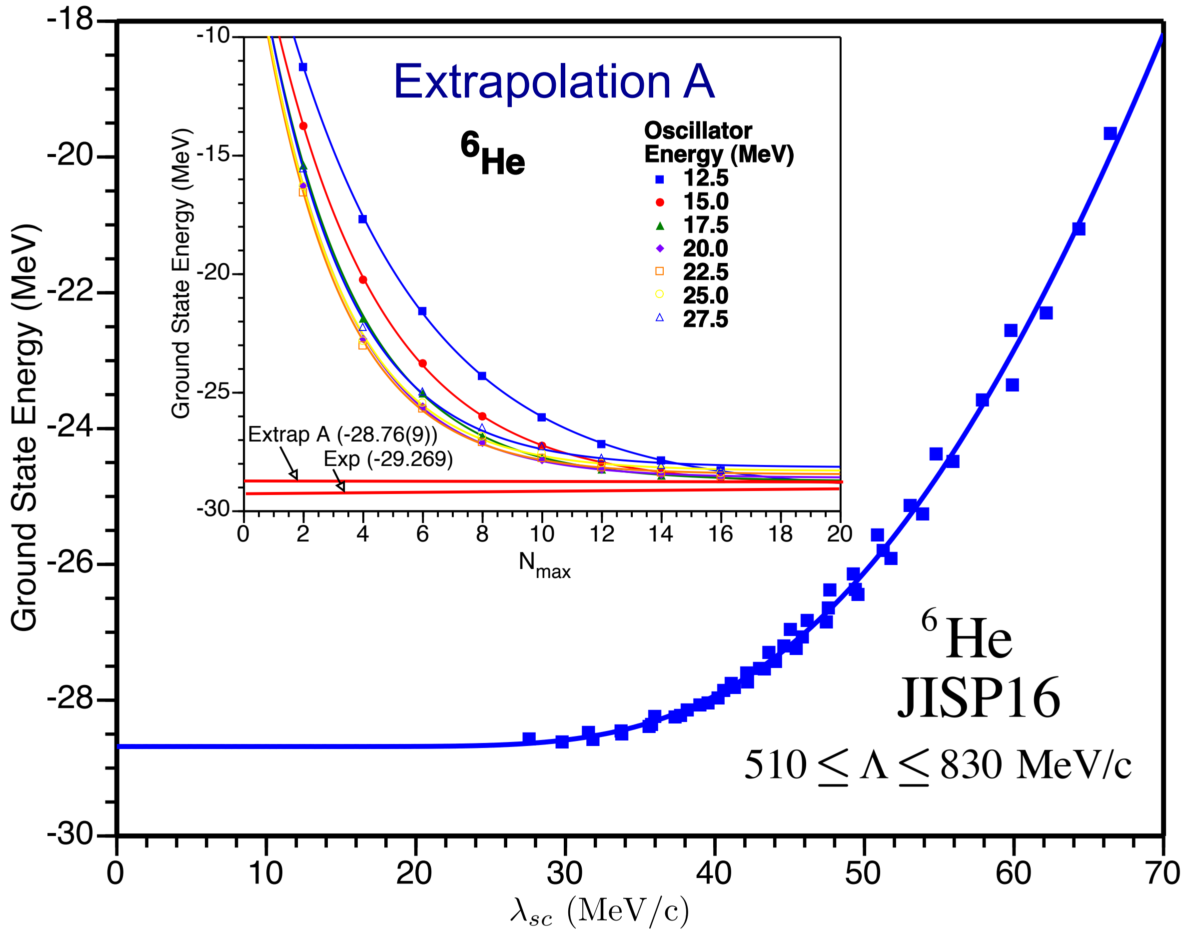
S. A. Coon[a], M. I. Avetian[a], M. K. G. Kruse[a], U. van Kolck[a,b], P. Maris[c], J. P. Vary[c]

UV regulator:

$$\Lambda = \sqrt{(N + 3/2)m\hbar\Omega}$$

IR regulator:

$$\lambda_{sc} = \sqrt{\frac{m\hbar\Omega}{(N + 3/2)}}$$



Combined IR and UV extrapolation: HO-basis regulator definitions

	Ref. 1	Ref. 2	Ref. 3
UV: Λ	$\sqrt{(N+3/2)m\hbar\Omega}$	$\sqrt{2(N+3/2)m\hbar\Omega}$	$\sqrt{2(N+3/2)m\hbar\Omega}$
IR: λ	$\sqrt{\frac{m\hbar\Omega}{(N+3/2)}}$	$\sqrt{\frac{m\hbar\Omega}{2(N+3/2)}}$	$\sqrt{\frac{m\hbar\Omega}{2(N+3/2)}}$
N (p-shell)	$N_{max}+1$	$N_{max}+2$	$N_{max}+3$

$$E(\Lambda,\lambda) \approx E_\infty + B_0 e^{-2\Lambda^2/B_1^2} + B_2 e^{-2k_\infty/\lambda}$$

[1]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

[2]R.J. Furnstahl, G. Hagen, T. Papenbrock, Phys. Rev. C 86 (2012) 031301

[3]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

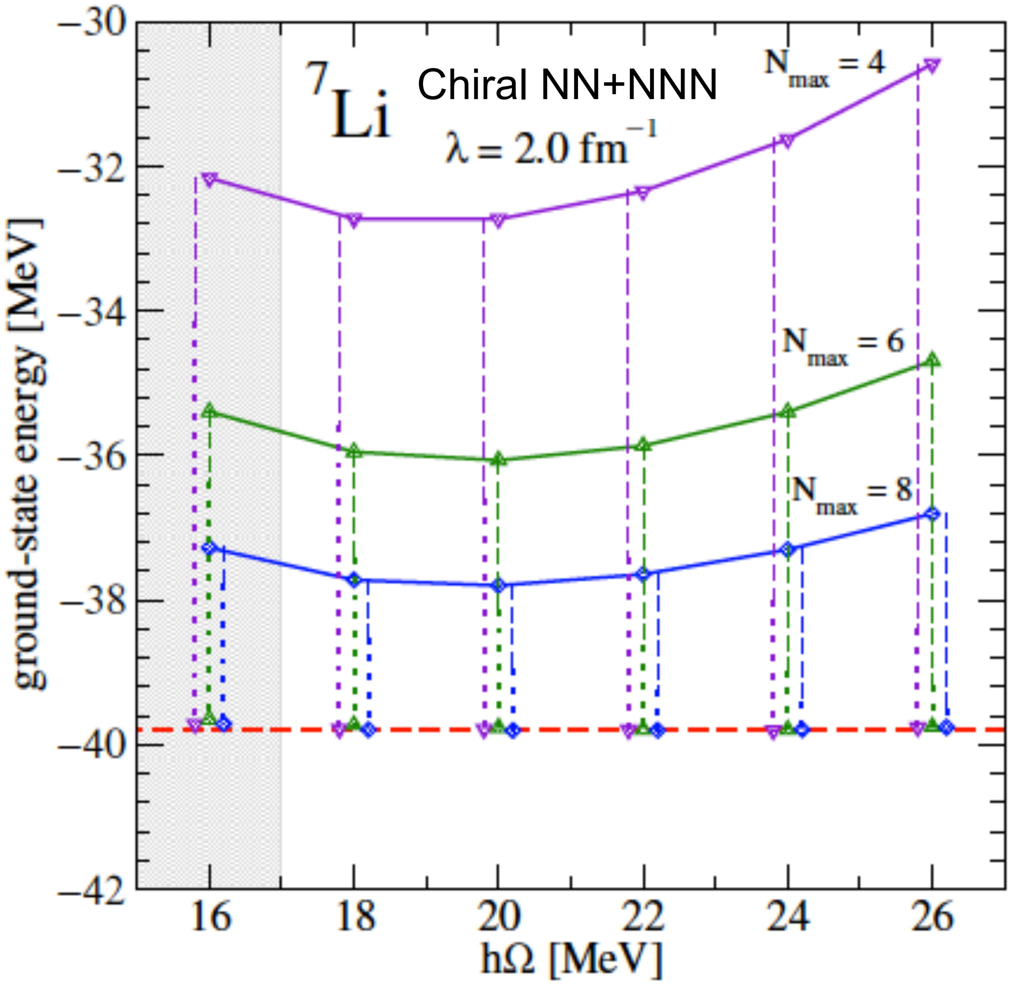
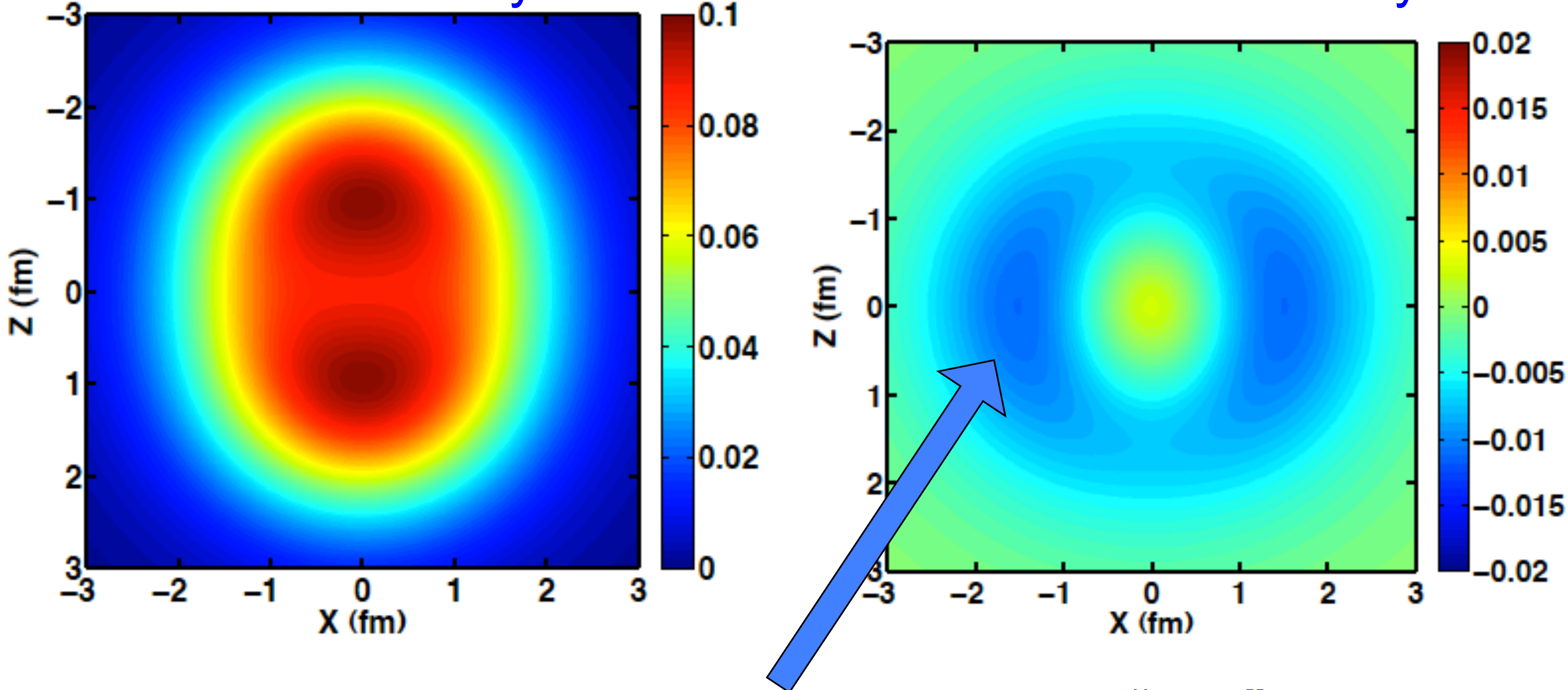


FIG. 17. (color online) Ground-state energy of ^{7}Li for the NN+NNN evolved Hamiltonians at $\lambda = 2.0\,\mathrm{fm}^{-1}$, with IR (vertical dashed) and UV (vertical dotted) corrections from Eq. (5) that add to predicted E_∞ values (points near the horizontal dashed line, which is the global E_∞).

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

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

Structure of $A = 10$–13 Nuclei with Two- Plus Three-Nucleon Interactions from Chiral Effective Field Theory

P. Navrátil,[1] V. G. Gueorguiev,[1,*] J. P. Vary,[1,2] W. E. Ormand,[1] and A. Nogga[3]

Strong correlation between c_D and c_E for exp'l properties of $A = 3$ & 4

=> Retain this correlation in applications to other systems

Range favored by various analyses & values are "natural"

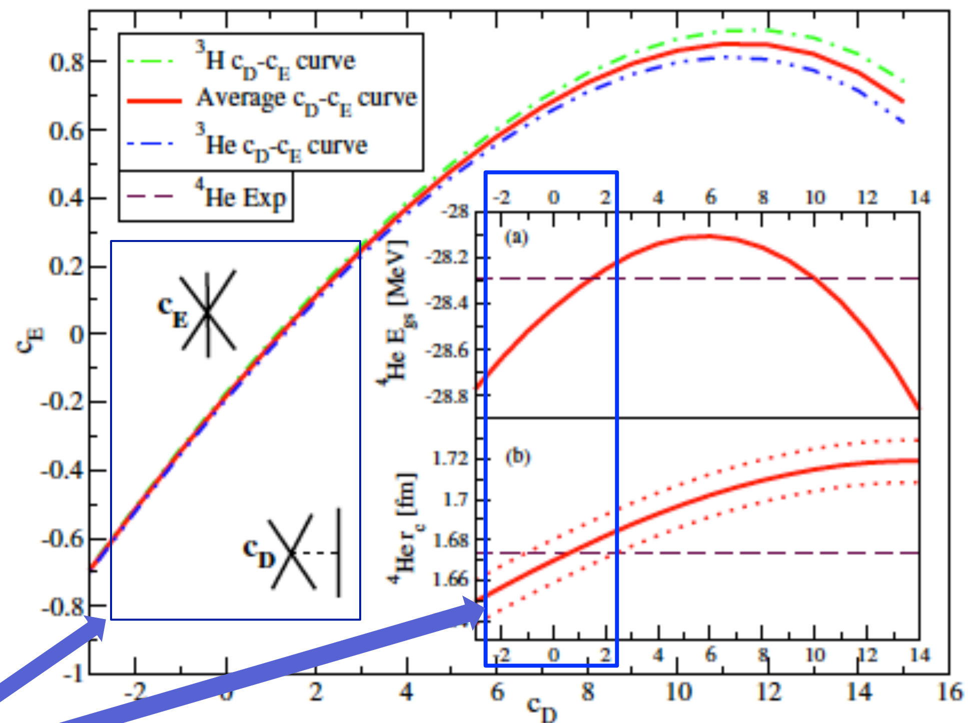
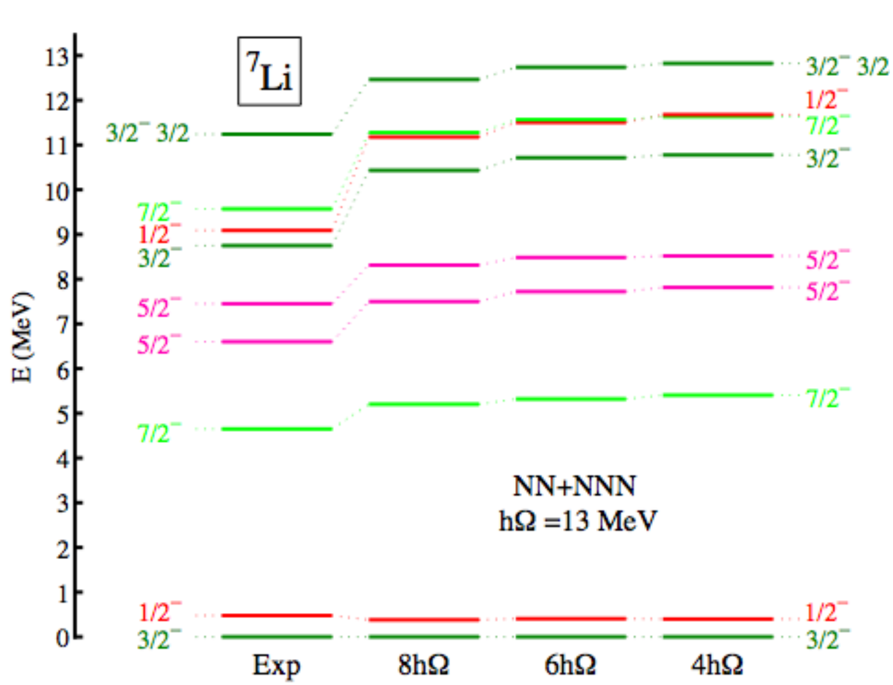
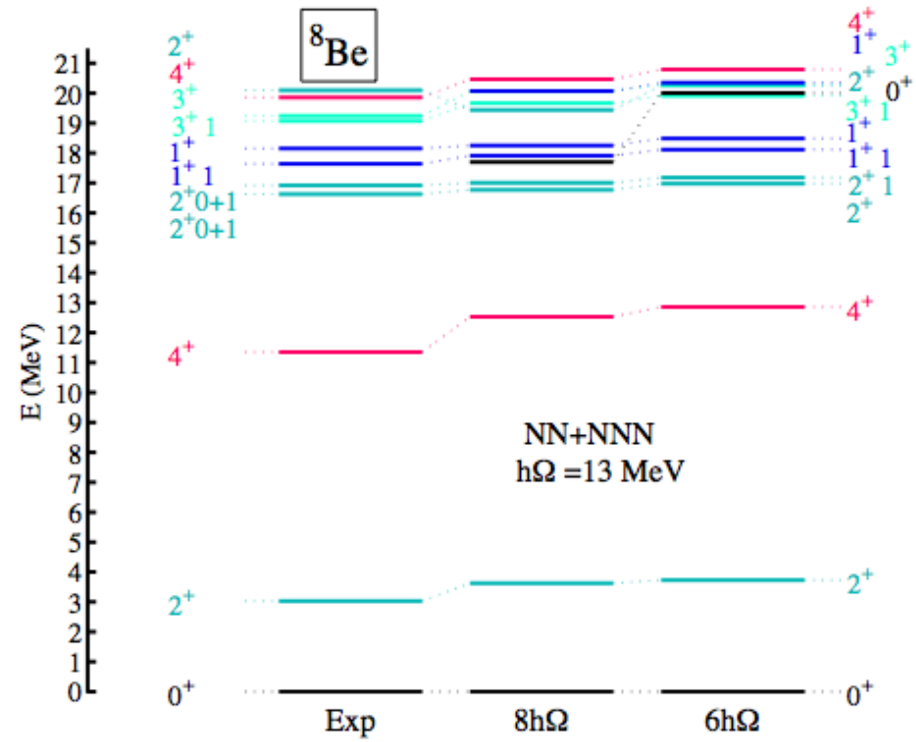


FIG. 1 (color online). Relations between c_D and c_E for which the binding energy of ^3H (8.482 MeV) and ^3He (7.718 MeV) are reproduced. (a) ^4He ground-state energy along the averaged curve. (b) ^4He charge radius r_c along the averaged curve. Dotted lines represent the r_c uncertainty due to the uncertainties in the proton charge radius.

NCSM with Chiral NN (N3LO) + NNN (N2LO, C_D=-0.2)
Employs Okubo-Lee-Suzuki (OLS) renormalization

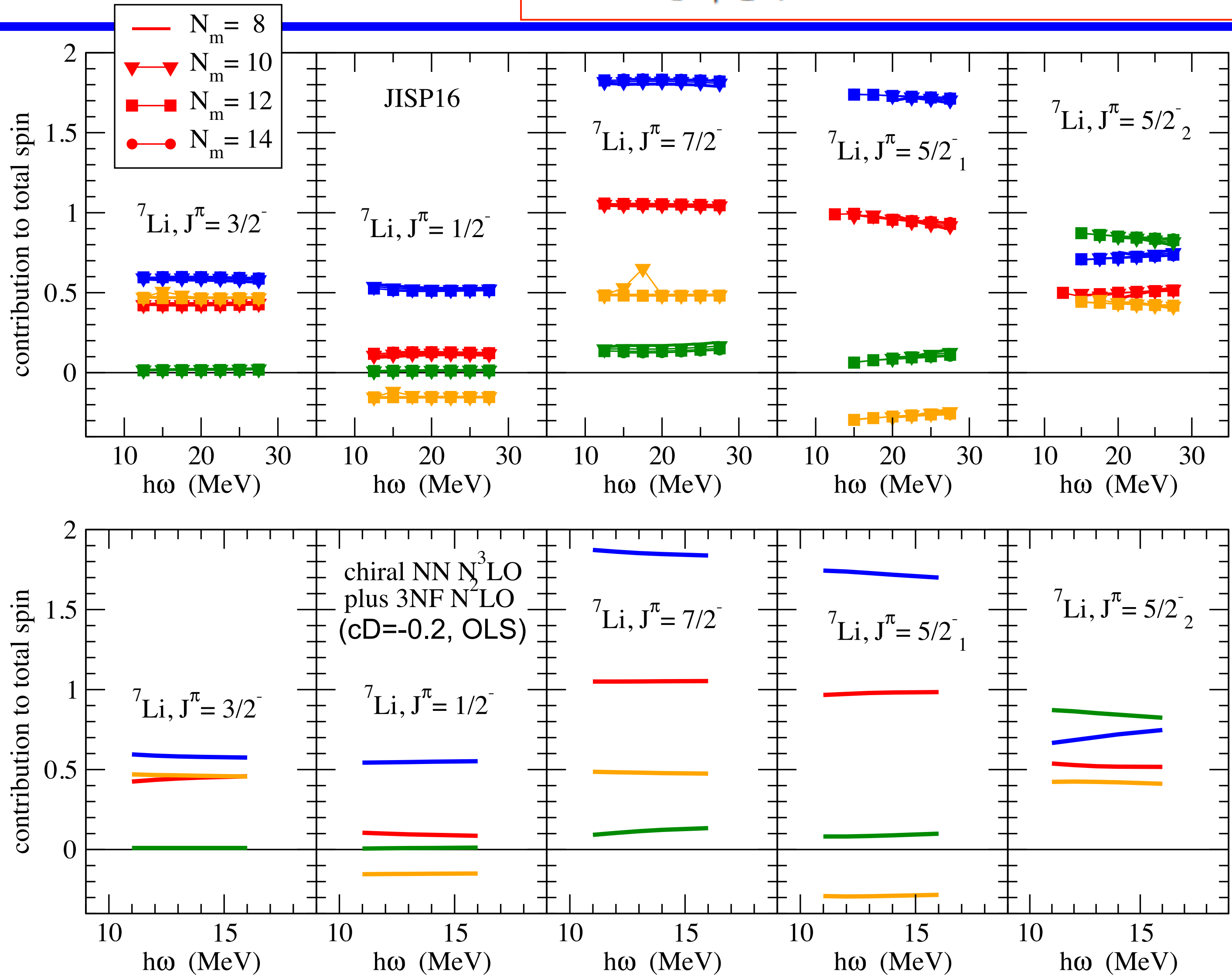




P. Maris, J. P. Vary and P. Navratil, Phys. Rev. C87, 014327 (2013); arXiv 1205.5686

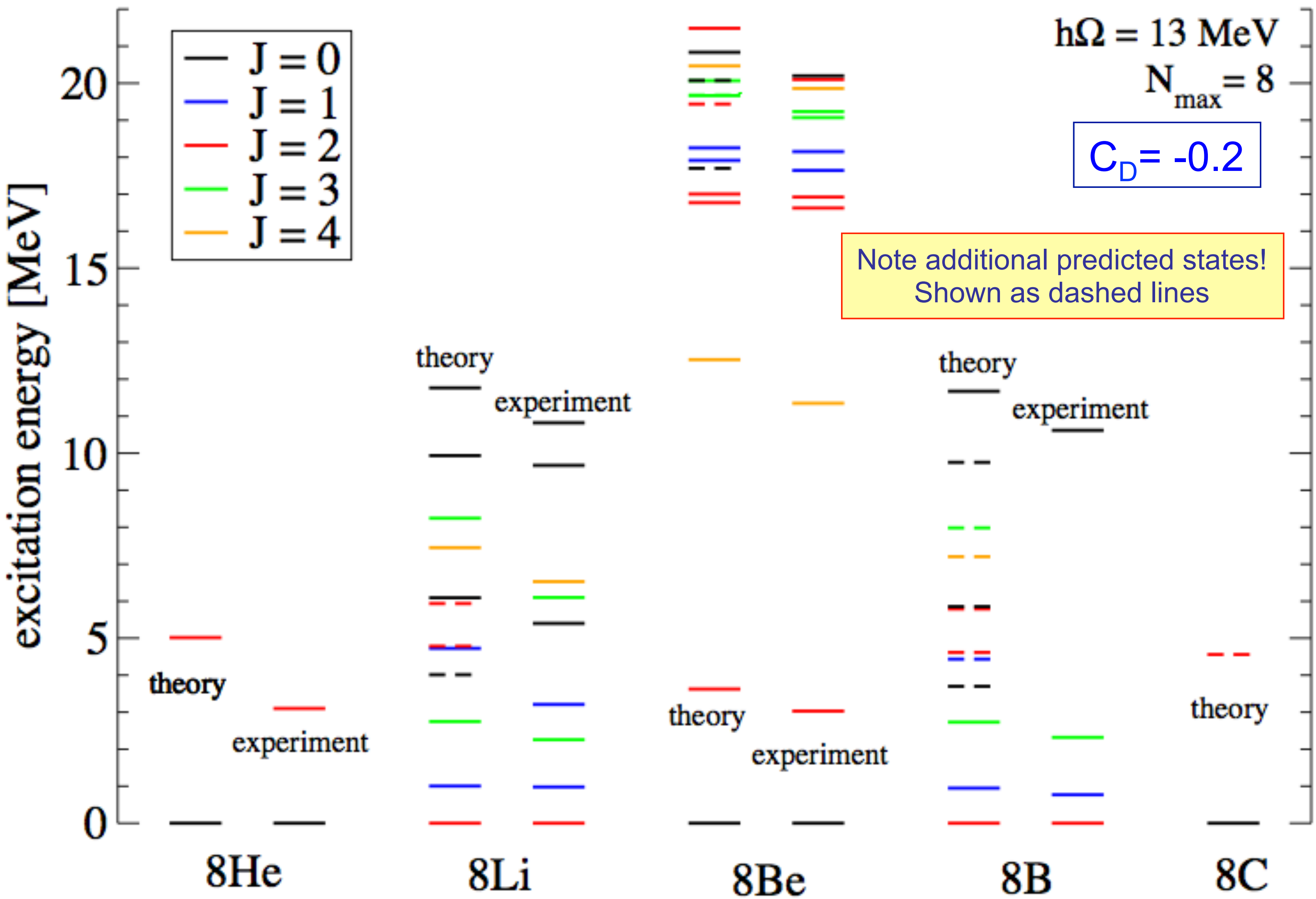
Spin components of 7Li

$$J = \frac{1}{J+1}\Big(\langle \mathbf{J}\cdot\mathbf{L}_p\rangle + \langle \mathbf{J}\cdot\mathbf{L}_n\rangle + \langle \mathbf{J}\cdot\mathbf{S}_p\rangle + \langle \mathbf{J}\cdot\mathbf{S}_n\rangle \Big)$$



- Very similar structure with JISP16 and chiral NN plus 3NF

Spectrum A=8 nuclei with chiral NN(N3LO) + NNN(N2LO) & OLS renormalization



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

^{8}Be

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]

CCP-2012 proceedings (to appear).

SRG renormalization scale invariance & agreement with experiment (cD=-0.2)

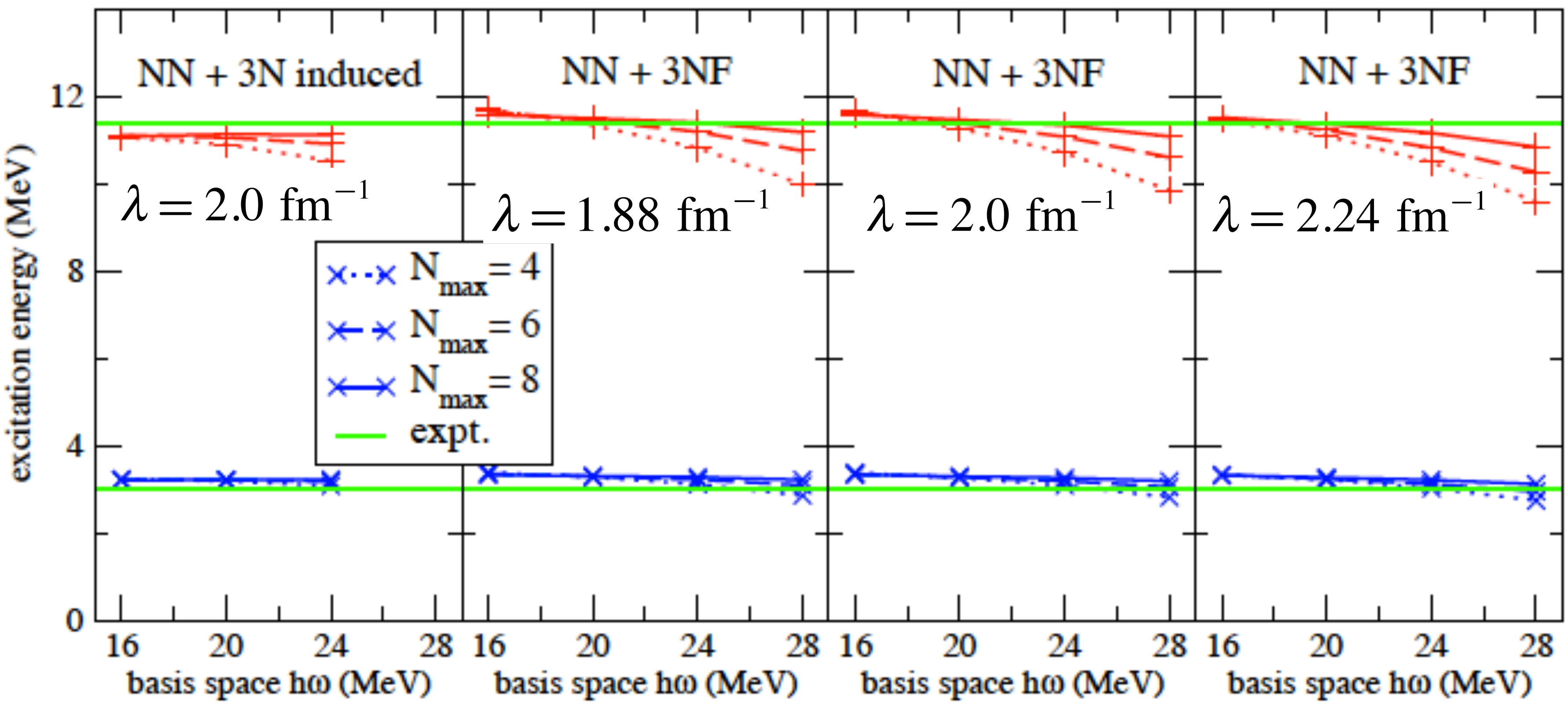


Figure 5. Excitation energies of the 2^+ (blue crosses) and 4^+ states (red plusses) for ^{8}Be with SRG evolved chiral N^{3}LO 2NF plus induced 3NF at $\lambda = 2.0$ fm^{-1} (left-most panel) and with SRG evolved chiral N^{3}LO 2NF plus chiral N^{2}LO 3NF. Experimental values are indicated by the horizontal green lines.

ab initio NCSM - comparison of Chiral EFT (OLS) with JISP16

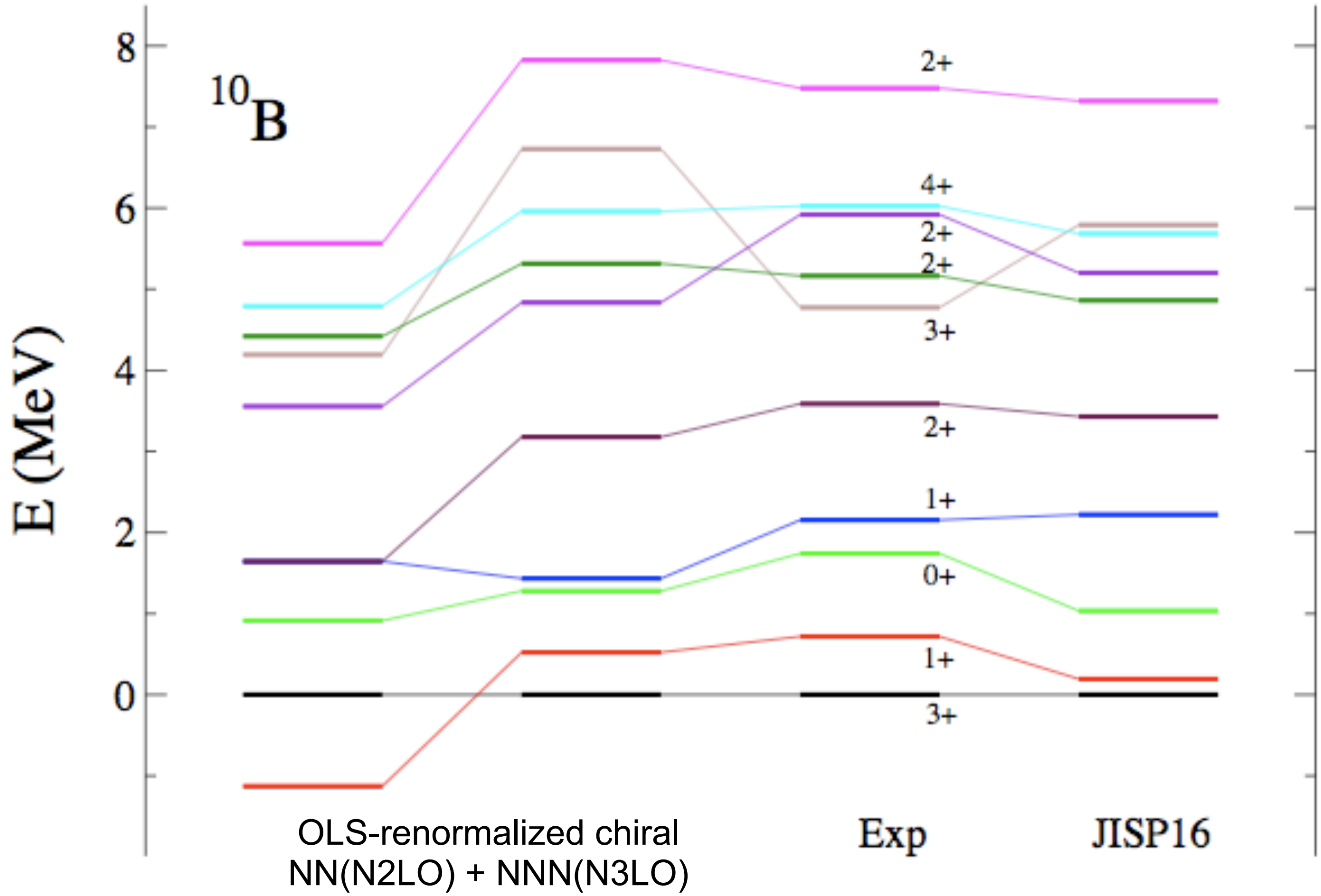
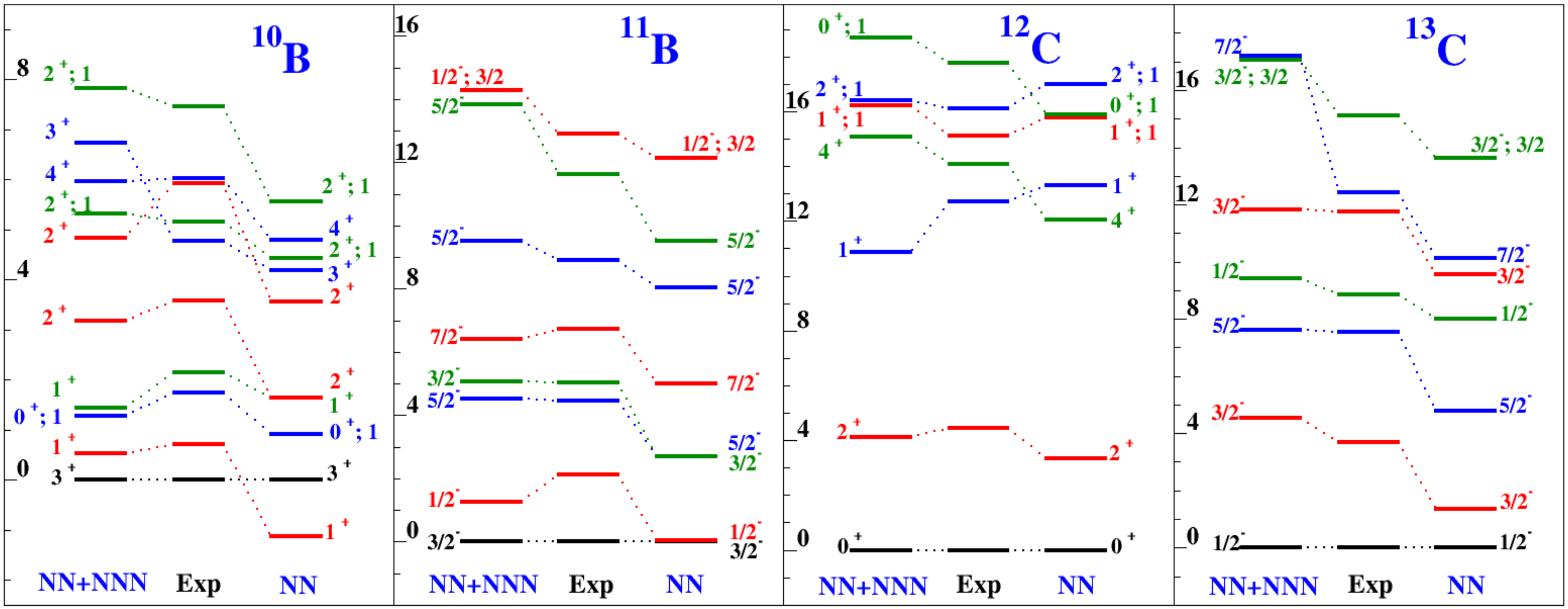


FIGURE 2. Experimental and theoretical excitation spectra of ^{10}B with respect to the lowest 3^+ state at an oscillator energy $\hbar\Omega = 14\ MeV$. The chiral effective interaction results are obtained at $N_{max} = 6$ while the JISP16 results are obtained at $N_{max} = 8$.

J.P. Vary, P. Maris, A. Negoita, P. Navratil, V.G. Gueorguiev, W. E. Ormand, A. Nogga, A. Shirokov and S. Stoica, in Exotic Nuclei and Nuclear/Particle Astrophysics (II), Proceedings of the Carpathian Summer School of Physics 2007, L. Trache and S. Stoica, Editors, AIP Conference Proceedings 972, 49(2008).

ab initio NCSM with chiral NN(N3LO) + NNN(N2LO) and OLS-renormalization

$N_{max} = 6,\ c_D = -1$



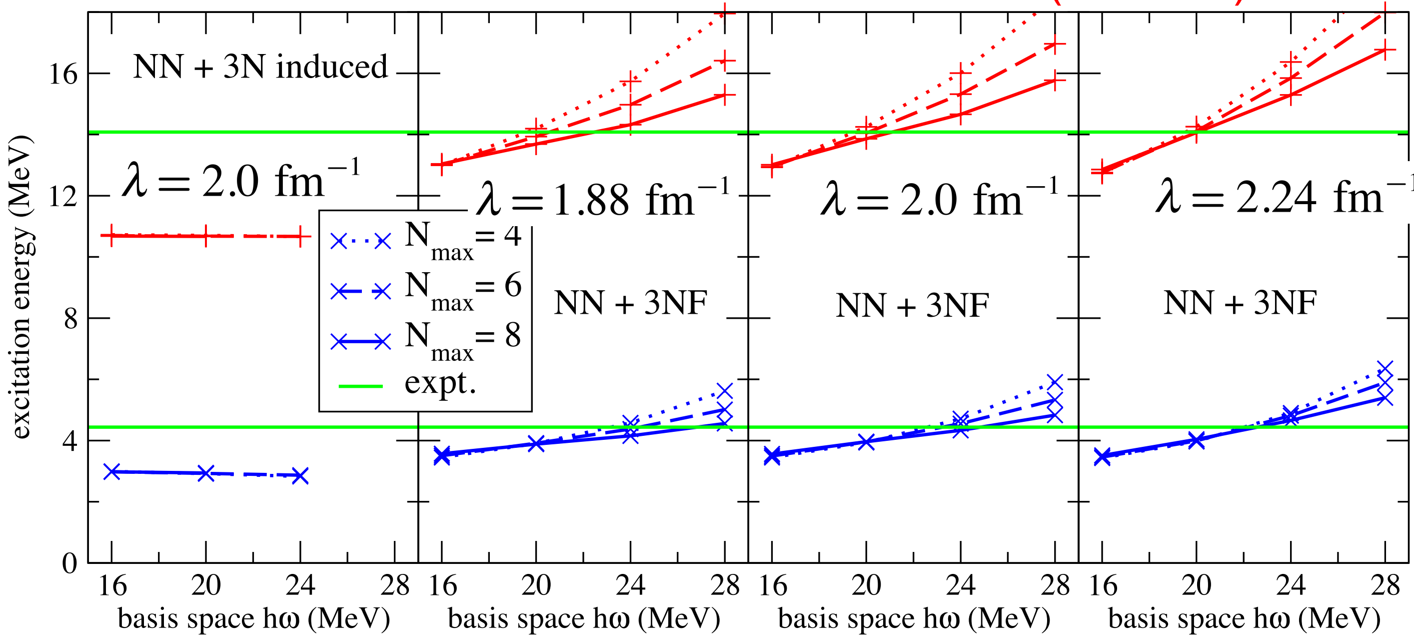
P. Navratil, V.G. Gueorguiev, J. P. Vary, W. E. Ormand and A. Nogga, PRL 99, 042501(2007); ArXiV: nucl-th 0701038.

Low-lying spectrum of 12C

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]

proceedings CCP 2012, in press

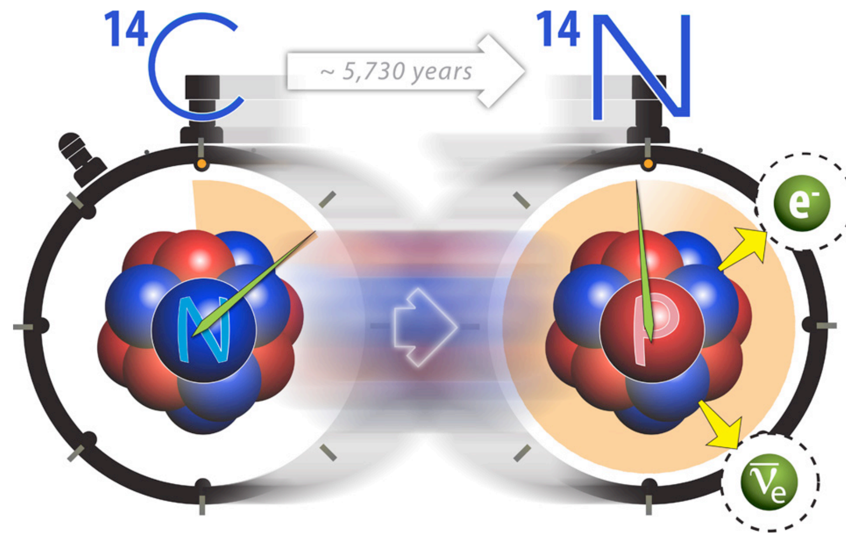
SRG renormalization scale invariance (cD=-0.2)



- Qualitative agreement with data
- Not converged with explicit 3NF, despite weak $N_{\max}$ dependence
- Ratio's of excitation energies, quadrupole moments and B(E2)'s in agreement with rotational model

"Why does Carbon-14 live so long?"

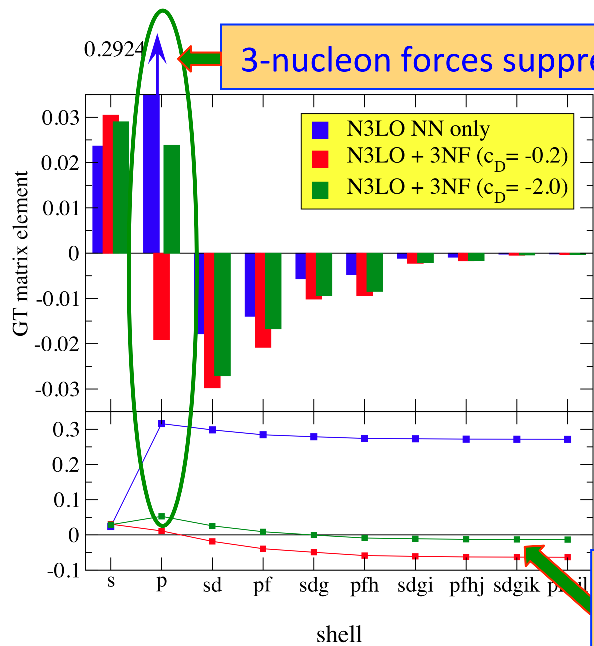
Carbon-14 dating relies on ~5,730 year half-life, but other light nuclei undergo similar beta decay with half-lives less than a day!



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

INCITE
Advancing America's Science and Industrial Competitiveness

- Dimension of matrix solved for 8 lowest states: ~ 1x10^9
- Solution takes ~ 6 hours on 215,000 cores on Cray XT5 Jaguar at ORNL

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

^{14}C beta decay - detailed results and estimated corrections due to chiral 2-body currents

TABLE I. Decomposition of p-shell contributions to M_{GT} in the LS scheme for the beta decay of ^{14}C without and with 3NF. The 3NF is included at two values of c_D where $c_D \simeq -0.2$ is preferred by the ^{3}H lifetime and $c_D \simeq -2.0$ is preferred by the ^{14}C lifetime. The calculations are performed in the $N_{max} = 8$ basis space with $\hbar\Omega = 14$ MeV.

(m_l, m_s)	NN only	NN + 3NF $c_D = -0.2$	NN + 3NF $c_D = -2.0$
$(1, +\frac{1}{2})$	0.015	0.009	0.009
$(1, -\frac{1}{2})$	−0.176	−0.296	−0.280
$(0, +\frac{1}{2})$	0.307	0.277	0.283
$(0, -\frac{1}{2})$	0.307	0.277	0.283
$(-1, +\frac{1}{2})$	−0.176	−0.296	−0.280
$(-1, -\frac{1}{2})$	0.015	0.009	0.009
Subtotal	0.292	−0.019	0.024
Total sum	0.275	−0.063	−0.013

2-body current quenching (est'd)* x 0.75 => -0.047 x 0.93 => -0.012

Table I from:
P. Maris, J.P. Vary,
P. Navratil, W.E. Ormand,
H. Nam and D.J. Dean,
Phys. Rev. Lett. 106, 202502 (2011)

Tritium half-life

c_D =	-0.20	-2.0
Thy/Exp. =	1.00	0.80

Preliminary

*J. Menéndez, D. Gazit and A. Schwenk, Phys.Rev.Lett. 107 (2011) 062501 (estimated using their effective density-dependent 1-body operator)

Theory published PRC: Feb. 4, 2010

Physics Letters B 692 (2010) 307–311

Experiment published: Aug. 3, 2010

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

First observation of ^{14}F

V.Z. Goldberg [a,*], B.T. Roeder [a], G.V. Rogachev [b], G.G. Chubarian [a], E.D. Johnson [b], C. Fu [c], A.A. Alharbi [a,1], M.L. Avila [b], A. Banu [a], M. McCleskey [a], J.P. Mitchell [b], E. Simmons [a], G. Tabacaru [a], L. Trache [a], R.E. Tribble [a]

[a] Cyclotron Institute, Texas A&M University, College Station, TX 77843-3366, USA
[b] Department of Physics, Florida State University, Tallahassee, FL 32306-4350, USA
[c] Indiana University, Bloomington, IN 47408, USA

ab initio predictions in close agreement with experiment

TAMU Cyclotron Institute

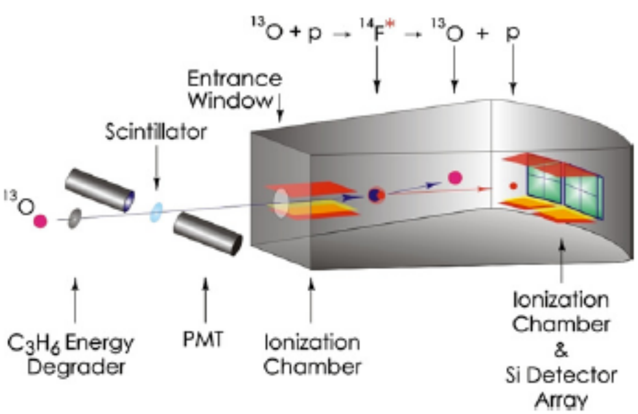


Fig. 1. (Color online.) The setup for the ^{14}F experiment. The "gray box" is the scattering chamber. See explanation in the text.

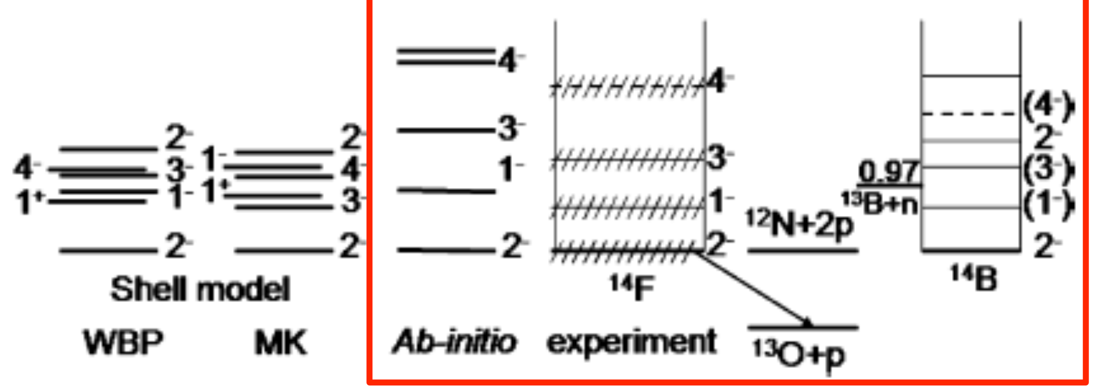
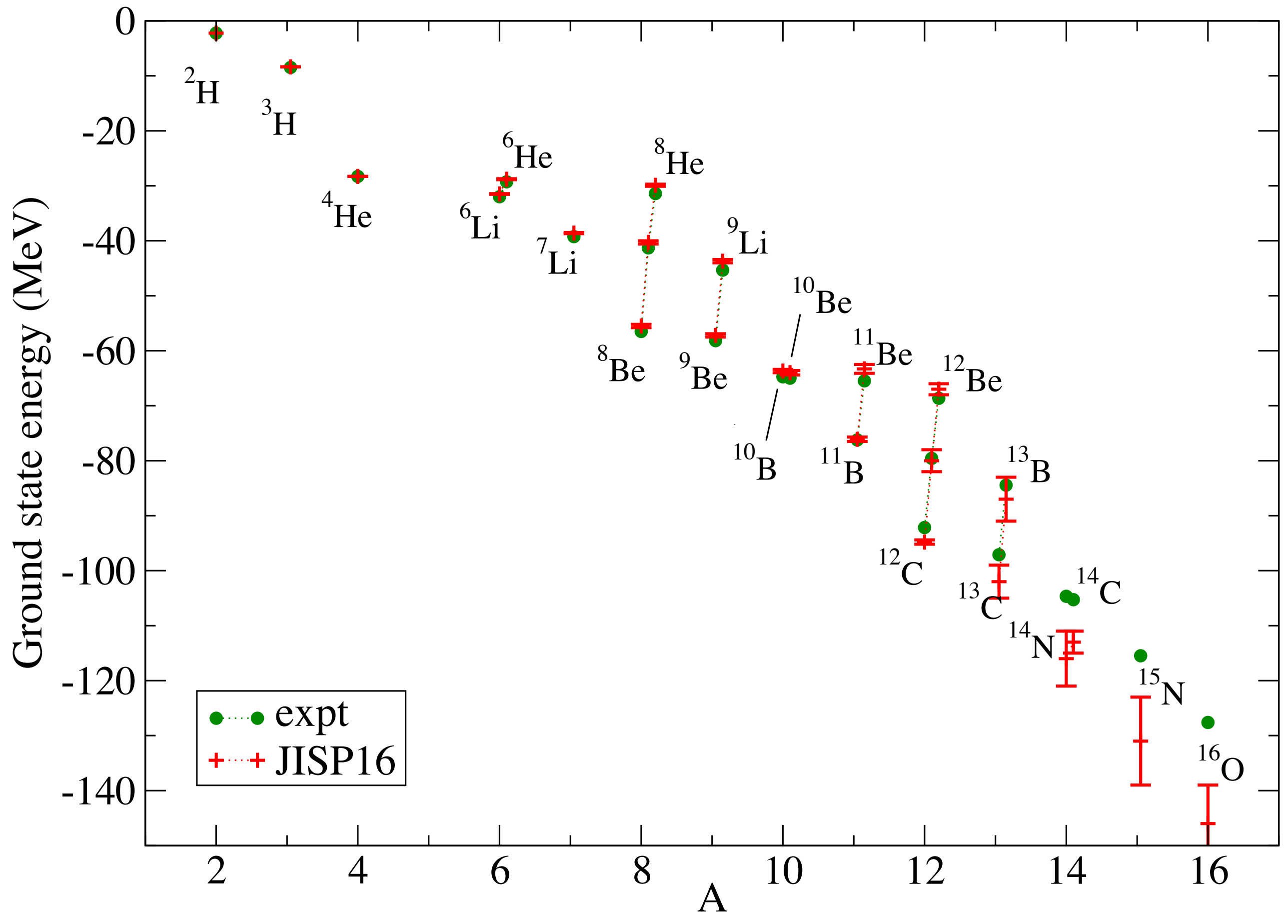


Fig. 6. ^{14}F level scheme from this work compared with shell-model calculations, *ab-initio* calculations [3] and the ^{14}B level scheme [16]. The shell model calculations were performed with the WBP [21] and MK [22] residual interactions using the code COSMO [23].

Ground state energy of p-shell nuclei with JISP16

Maris, Vary, IJMPE, in press

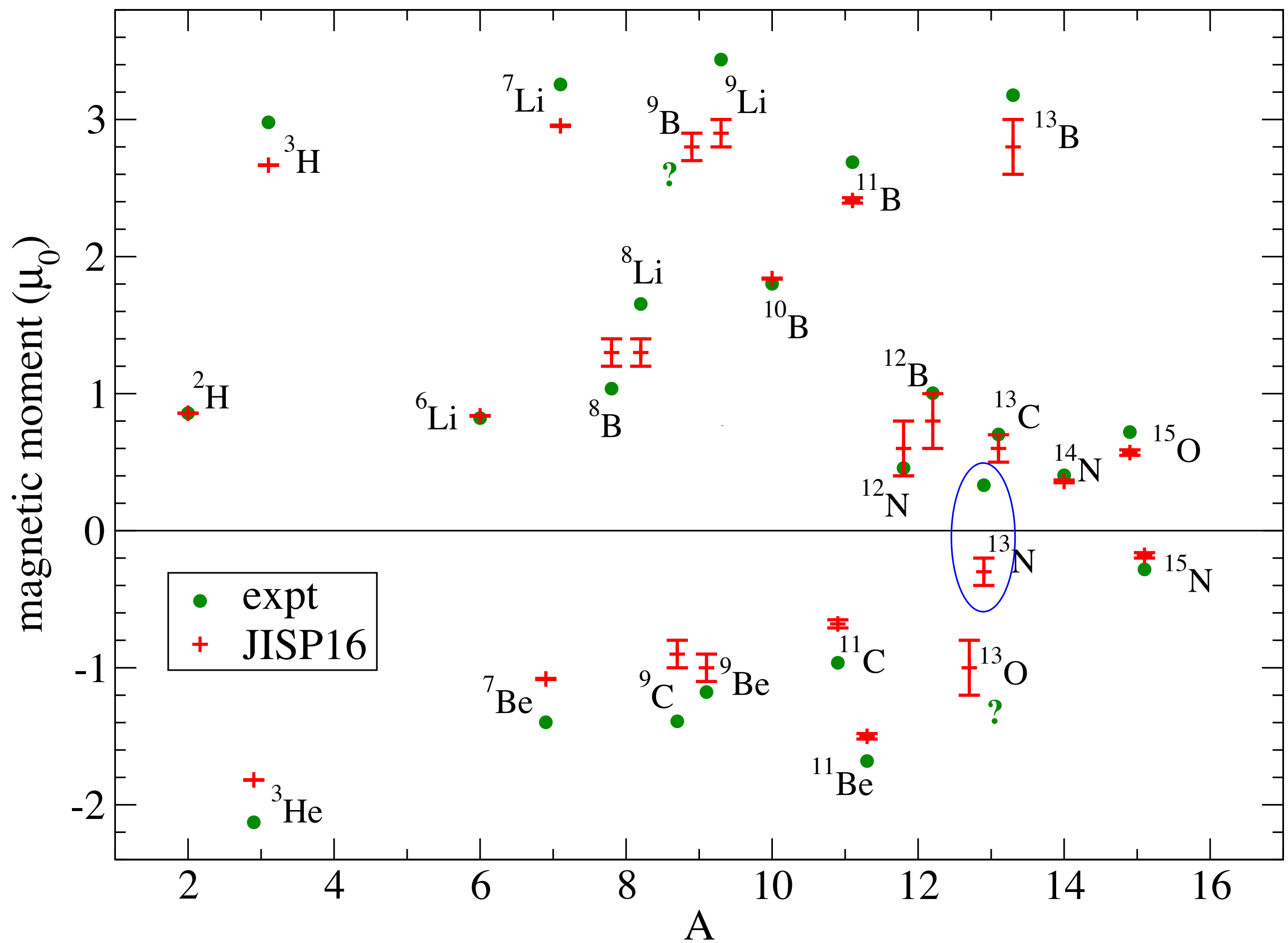


- ^{10}B – most likely JISP16 produces correct 3^+ ground state, but extrapolation of 1^+ states not reliable due to mixing of two 1^+ states
- ^{11}Be – expt. observed parity inversion within error estimates of extrapolation
- ^{12}B and ^{12}N – unclear whether gs is 1^+ or 2^+ (expt. at $E_x = 1$ MeV) with JISP16

Ground state magnetic moments with JISP16

Maris, Vary, IJMPE, in press

$$\mu = \frac{1}{J+1}\Big(\langle \mathbf{J}\cdot\mathbf{L}_p\rangle + 5.586\langle \mathbf{J}\cdot\mathbf{S}_p\rangle - 3.826\langle \mathbf{J}\cdot\mathbf{S}_n\rangle\Big)\,\mu_0$$



- Good agreement with data,
  given that we do not have any meson-exchange currents

Physics Letters B 719 (2013) 179–184

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Physics Letters B

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

M.A. Caprio[a,*], P. Maris[b], J.P. Vary[b]

[a] Department of Physics, University of Notre Dame, Notre Dame, IN 46556-5670, USA
[b] Department of Physics and Astronomy, Iowa State University, Ames, IA 50011-3160, USA

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:

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

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

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

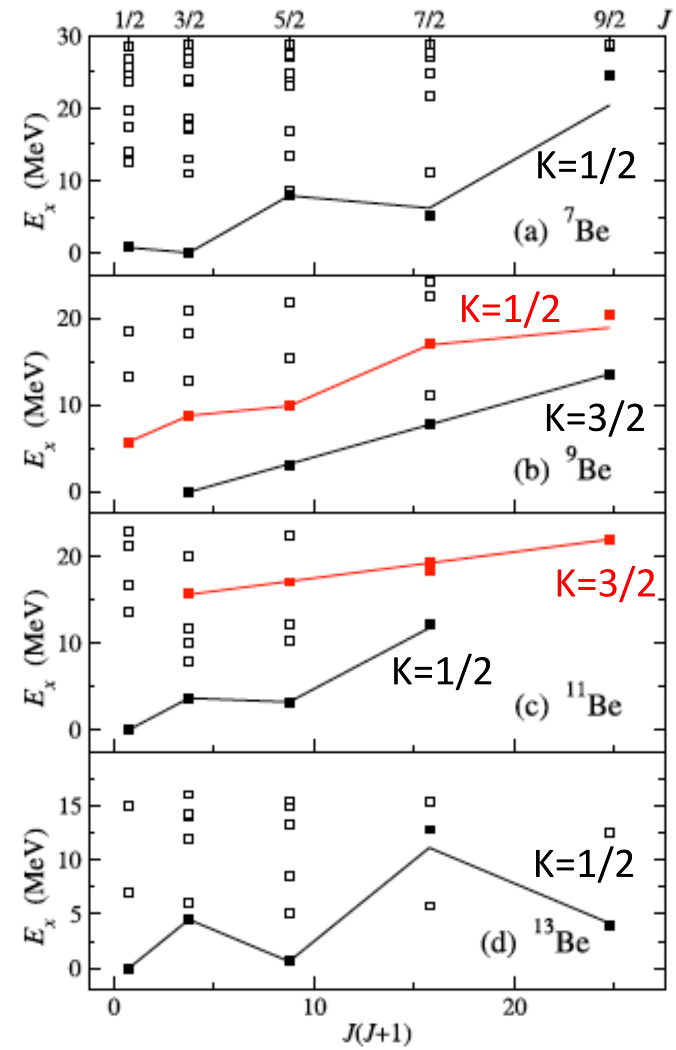


Fig. 1. Excitation energies obtained for states in the *natural* parity spaces of the odd-mass Be isotopes: (a) ^{7}Be, (b) ^{9}Be, (c) ^{11}Be, and (d) ^{13}Be. Energies are plotted with respect to $J(J+1)$ to facilitate identification of rotational energy patterns, while the J values themselves are 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.

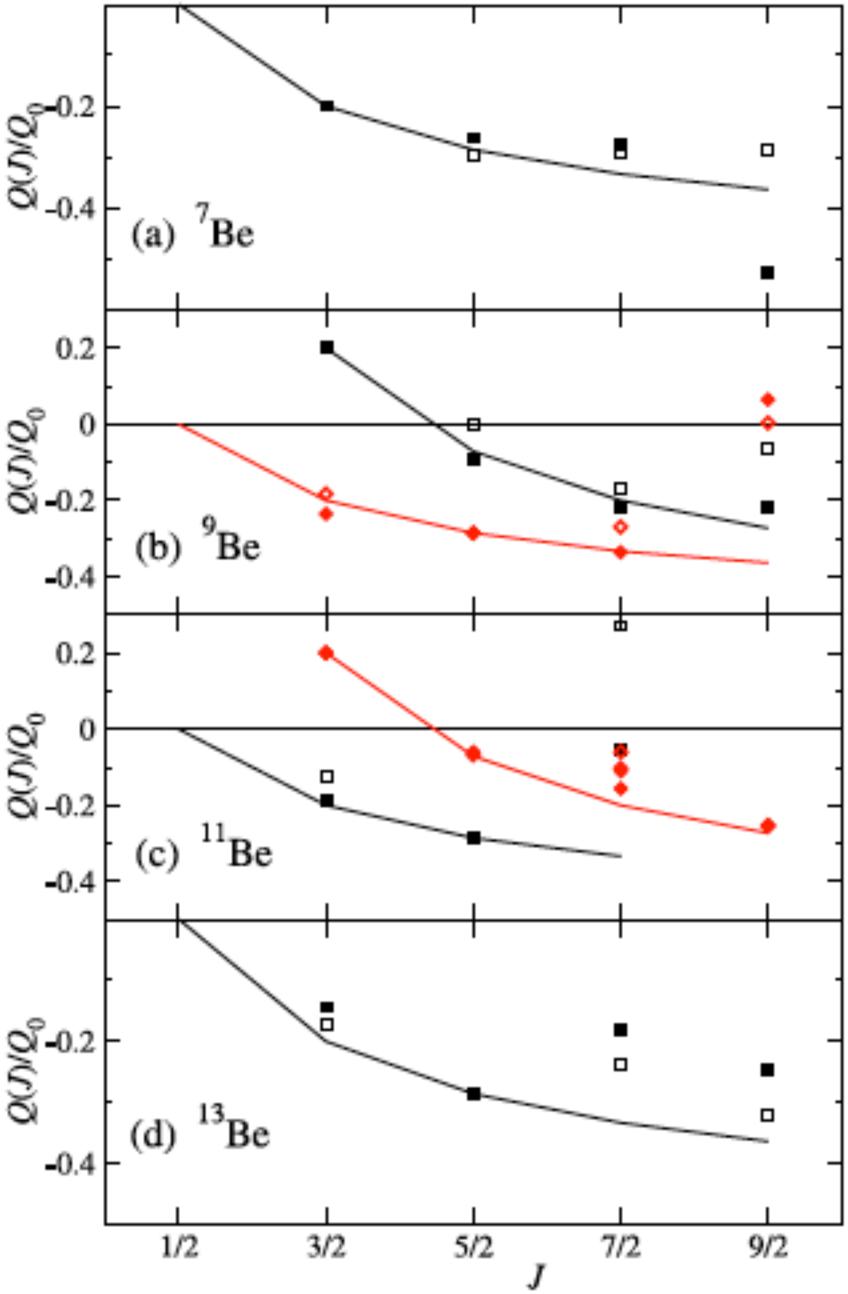


Fig. 3. Quadrupole moments calculated for candidate bandmembers in the *natural* parity spaces of the odd-mass Be isotopes: (a) ^{7}Be, (b) ^{9}Be, (c) ^{11}Be, and (d) ^{13}Be. The states are as identified in Fig. 1 and are shown as black squares for yrast states or red diamonds for excited states (color 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).

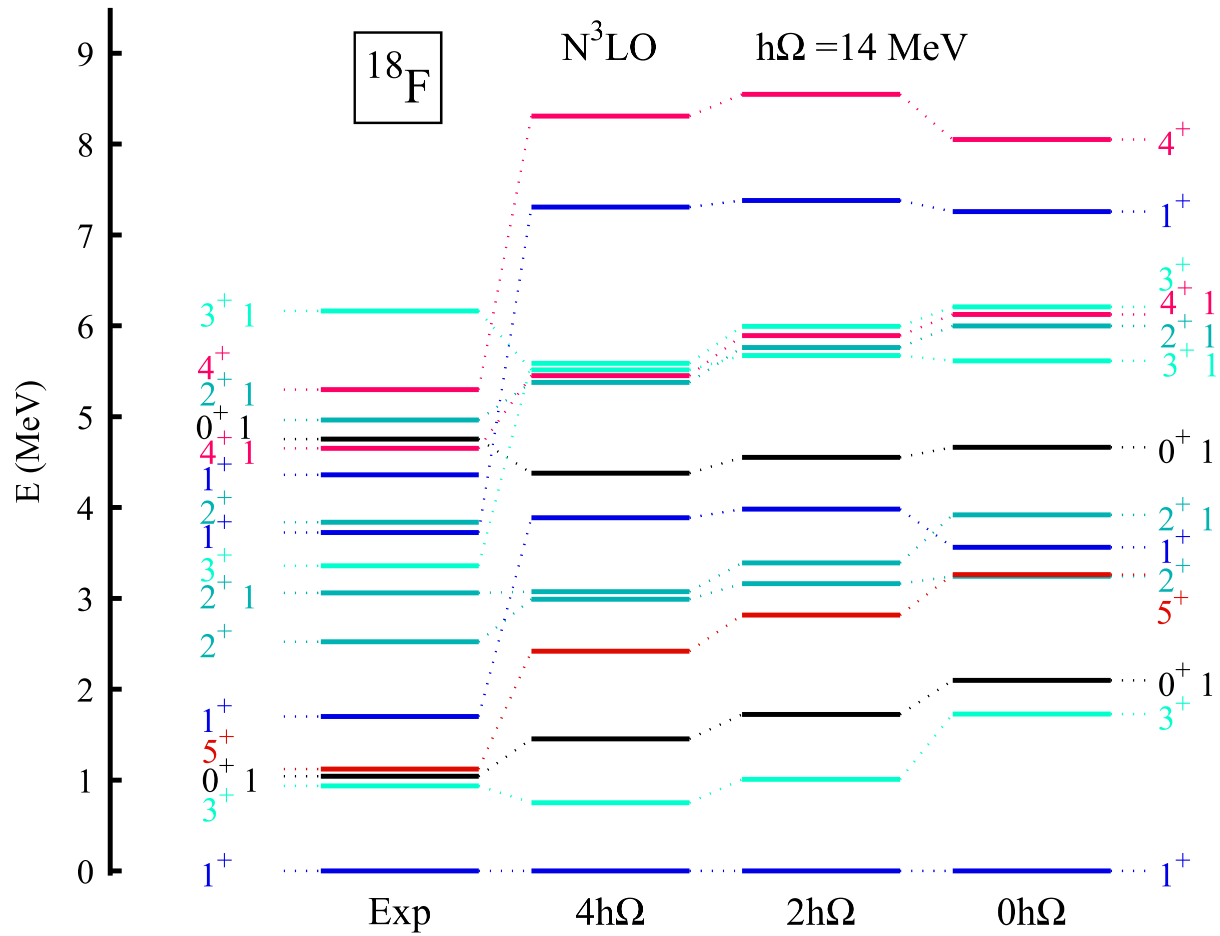
Note:
Although Q, B(E2) are slowly converging, the ratios within a rotational band appear remarkably stable

Next challenge: Investigate same phenomena with Chiral EFT interactions

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

NCSM with Chiral NN (N3LO) without NNN interaction and OLS renormalization

B.R. Barrett et al. / Progress in Particle and Nuclear Physics 69 (2013) 131–181



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

Preliminary Results

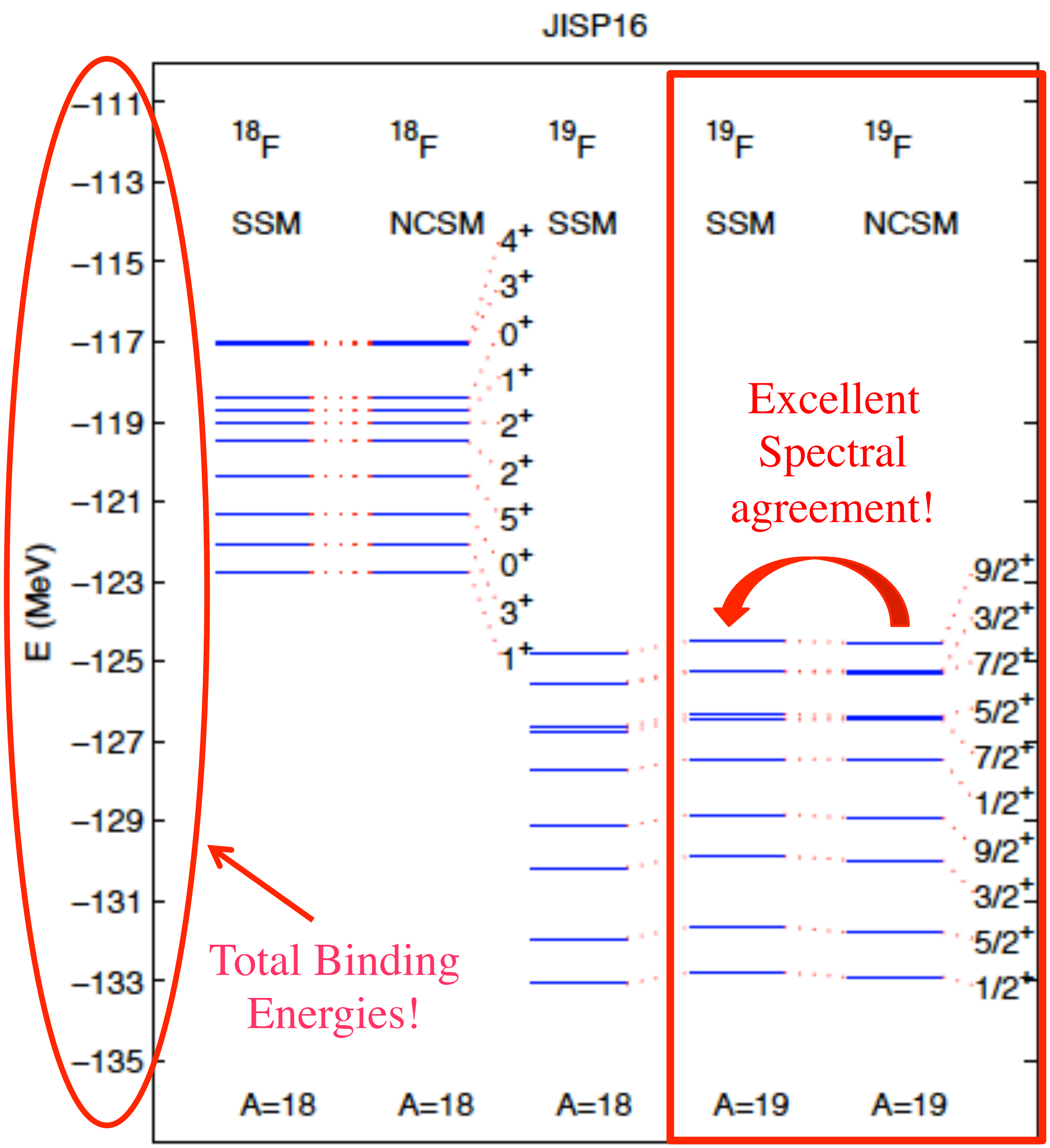
E. Dikmen,[1,2,*] A. F. Lisetskiy,[2,†] B. R. Barrett,[2] P. Maris,[3] A. M. Shirokov,[3,4,5] and J. P. Vary[3]

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



Outstanding challenges for the *ab initio* No-Core Shell Model (NCSM) and No-Core Full Configuration (NCFC)

- Described the cluster states, such as the Hoyle state, in light nuclei
- Explain the shift between the positive and negative parity spectra in p-shell nuclei
- Explain the intruder negative parity ground state in ^{9}B
- Explain the location of the (1+,0) excited state in ^{12}C
- Describe collective rotational bands in light nuclei – even the non-cluster cases
- Explain GTs to excited states in A = 14 (A. Negret, et al, Phys. Rev. Lett. 97, 062502 (2006))
- Include non-resonant continuum states and extend to reactions between light nuclei
- Extend the methods, while retaining precision, into the sd shell and beyond
- Continue to develop the methods for non-perturbative solutions of quantum field theory

Under what conditions do we need quarks & gluons to describe nuclear structure and nuclear reactions?

1. Spin crisis in the proton
2. Proton RMS radius
3. DIS on nuclei – e.g. Bjorken $x > 1$
4. Nuclear Equation of State
5. $Q > 1$ GeV/c

Applications to Relativistic Quantum Field Theory
QED (new) and QCD (under development)

J. P. Vary, H. Honkanen, Jun Li, P. Maris, S. J. Brodsky, A. Harindranath,
G. F. de Teramond, P. Sternberg, E. G. Ng and C. Yang,
"Hamiltonian light-front field theory in a basis function approach",
Phys. Rev. C 81, 035205 (2010); arXiv nucl-th 0905.1411

H. Honkanen, P. Maris, J. P. Vary and S. J. Brodsky,
"Electron in a transverse harmonic cavity",
Phys. Rev. Lett. 106, 061603 (2011); arXiv: 1008.0068

Pieter Maris, Paul Wiecki, Yang Li, Xingbo Zhao and James P. Vary,
"Bound state calculations in QED and QCD using Basis Light-Front Quantization,"
Acta Phys. Polon. Supp. 6, 321(2013).

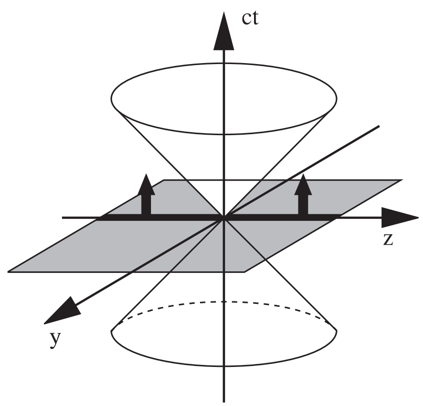
X. Zhao, A. Ilderton, P. Maris and J.P. Vary,
"Scattering in Time-dependent Basis Light Front Quantization,"
arXiv 1303.3237

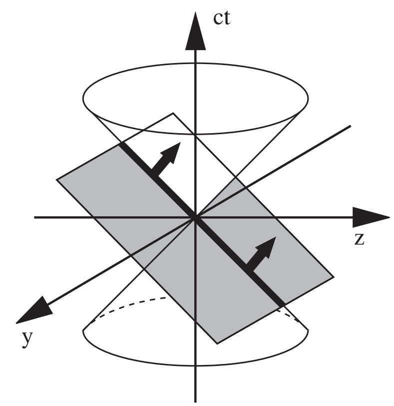
Basis Light-Front Quantization Approach

[Dirac 1949]

- Basic idea: solve generalized wave eq. for quantum field evolution

equal time quantization	VS	light front quantization
$i\frac{\partial}{\partial t}\lvert\varphi(t)\rangle = H\lvert\varphi(t)\rangle$		$i\frac{\partial}{\partial x^+}\lvert\varphi(x^+)\rangle = P_+\lvert\varphi(x^+)\rangle$





- Time: $t \equiv x^0$ | $t \equiv x^+ = x^0 + x^3$
- Hamiltonian: $H \equiv P^0$ | $H \equiv P_+ = \frac{P^0 - P^3}{2}$
- On-shell condition: $P^0 = \sqrt{m^2 + P_\perp^2 + P_3^2}$ | $P_+ = \frac{m^2 + P_\perp^2}{2P^+}$

Discretized Light Cone Quantization

Pauli & Brodsky c1985

⇓

Basis Light Front Quantization*

$$\phi(\vec{x}) = \sum_{\alpha} \left[f_\alpha(\vec{x}) a_\alpha^+ + f_\alpha^*(\vec{x}) a_\alpha \right]$$

where $\{a_\alpha\}$ satisfy usual (anti-) commutation rules.

Furthermore, $f_\alpha(\vec{x})$ are arbitrary except for conditions:

Orthonormal: $\int f_\alpha(\vec{x}) f_{\alpha'}^*(\vec{x}) d^3x = \delta_{\alpha\alpha'}$

Complete: $\sum_{\alpha} f_\alpha(\vec{x}) f_\alpha^*(\vec{x}') = \delta^3(\vec{x} - \vec{x}')$

=> Wide range of choices for $f_a(\vec{x})$ and our initial choice is

$$f_\alpha(\vec{x}) = N e^{ik^+x^-} \Psi_{n,m}(\rho,\varphi) = N e^{ik^+x^-} f_{n,m}(\rho) \chi_m(\varphi)$$

*J.P. Vary, H. Honkanen, J. Li, P. Maris, S.J. Brodsky, A. Harindranath, G.F. de Teramond, P. Sternberg, E.G. Ng and C. Yang, PRC 81, 035205 (2010). ArXiv:0905:1411

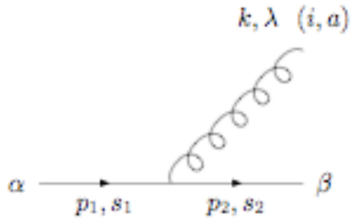
Steps to implement BLFQ

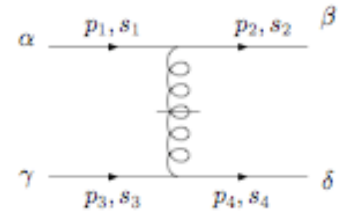
- Enumerate Fock-space basis subject to symmetry constraints
- Evaluate/renormalize/store H in that basis
- Diagonalize (Lanczos)
- Iterate previous two steps for sector-dep. renormalization
- Evaluate observables using eigenvectors (LF amplitudes)
- Repeat previous 4 steps for new regulator(s)
- Extrapolate to infinite matrix limit & remove all regulators
- Compare with experiment or predict new experimental results

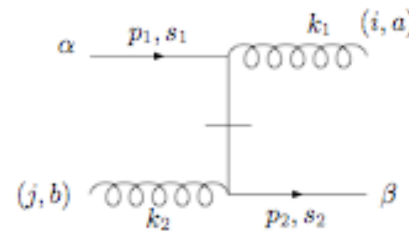
Above achieved for QED test case – electron in a trap
H. Honkanen, P. Maris, J.P. Vary, S.J. Brodsky,
Phys. Rev. Lett. 106, 061603 (2011)

Improvements: trap independence, (m,e) renormalization, . . .
X. Zhao, H. Honkanen, P. Maris, J.P. Vary, S.J. Brodsky, in prep’n

Light Front (LF) Hamiltonian defined by its elementary vertices in LF gauge

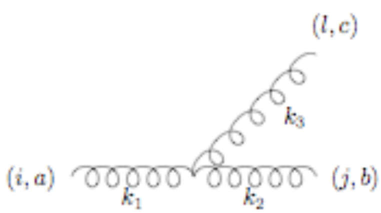


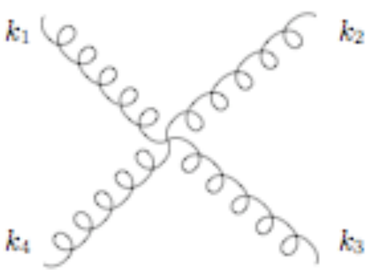


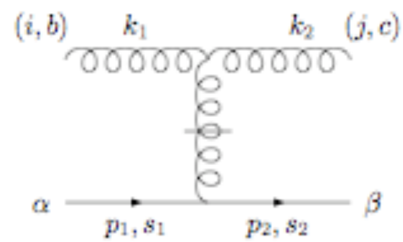


QED & QCD

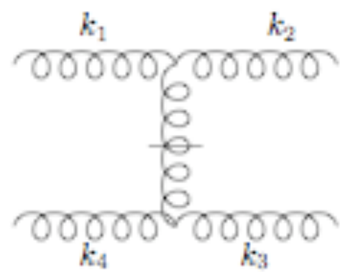
H_{qqgg1}







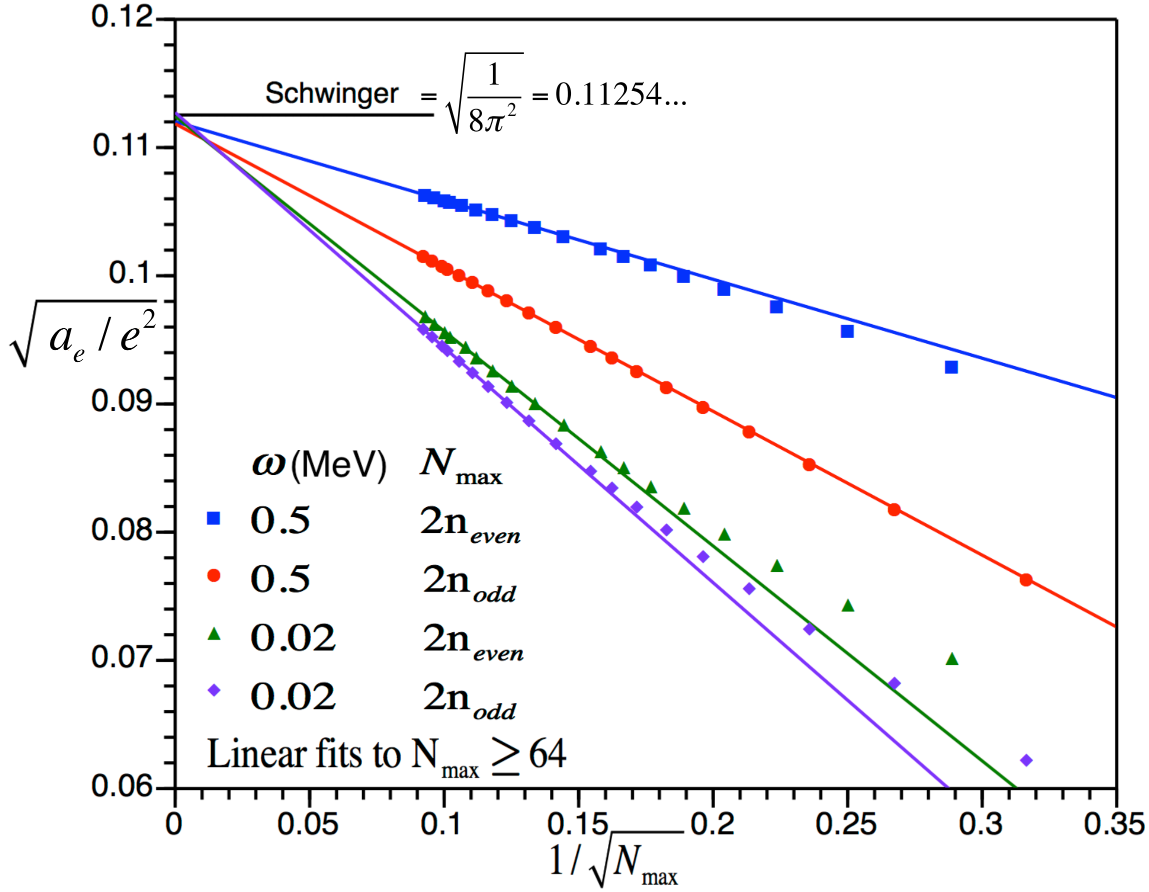
H_{qqgg2}



QCD

Numerical Results for Electron g-2

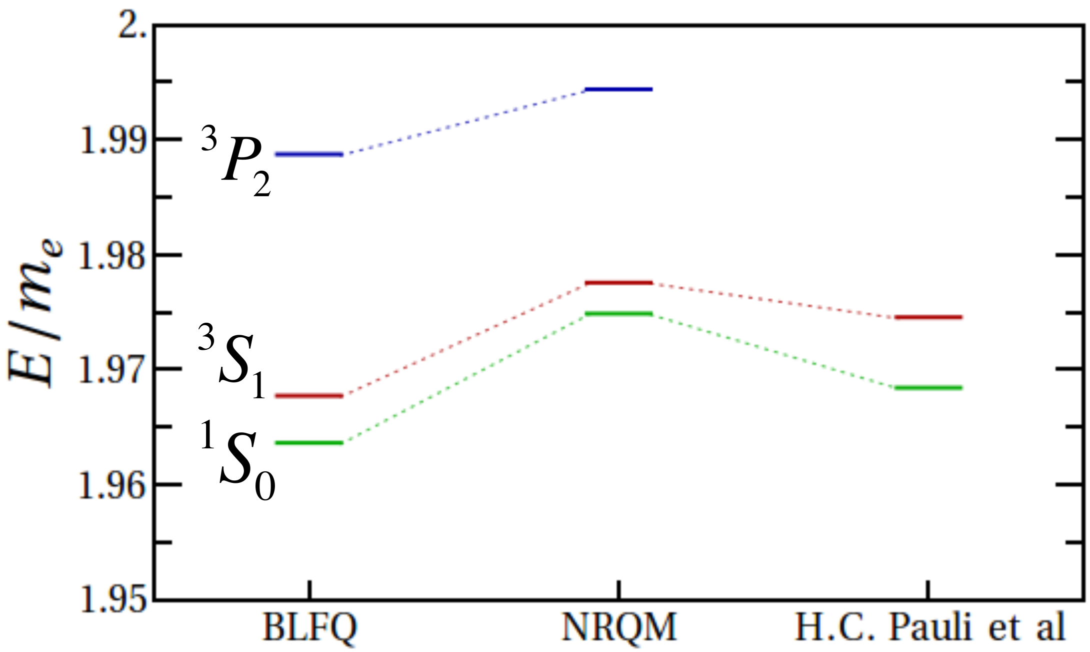
[X. Zhao, H. Honkanen, P. Maris, J.P. Vary, S.J. Brodsky, in preparation as major update to: H. Honkanen, P. Maris, J.P. Vary, S.J. Brodsky, Phys. Rev. Lett. 106, 061603 (2011)]



- As Nmax →∞, results approach Schwinger result
- Less than 1% deviation from Schwinger's result (by linear extrapl.)
- Convergence over wide range of ω's (by a factor of 25!)

Applications to QED and QCD bound states (positronium, mesons, baryons) are underway:
Paul Wiecki, NTSE-2013 Proceedings, to appear
Yang Li, NTSE-2013 Proceedings, to appear

Positronium with $\alpha = 0.3$
Involves three extrapolations to remove regulators



PRD 45 2968

Paul Wiecki, NTSE-2013, May 2013

Outstanding Challenges

- ❖ improve NN + NNN + NNNN interactions/renormalization
  develop effective operators beyond the Hamiltonian
  tests of fundamental symmetries
- ❖ proceed to heavier systems - breaking out of the p-shell
  extend quantum many-body methods
- ❖ achieve higher precision
  quantify the uncertainties - justified through simulations
  global dependencies mapped out
- ❖ evaluate more complex projectile-target reactions
- ❖ achieve efficient use of computational resources – improve scalability, load-balance, I/O, inter-process communications
- ❖ build a community to develop/sustain open libraries of codes/data, develop/implement provenance framework/practices

clusters, halo nuclei, continuum coupling, delta-full EFT,
EFT for all observables, energy density functional (EDF), nuclear EOS,
dark matter searches, double beta-decay, nuclear parton distribution
functions (PDFs), . . .

Recent Collaborators

United States

ISU: Pieter Maris, Alina Negoita, Chase Cockrell, Hugh Potter
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, Kai Hebeler, 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 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, Javier Menendez, 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
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

Questions?