ab initio No Core Nuclear Structure: Progress and Plans

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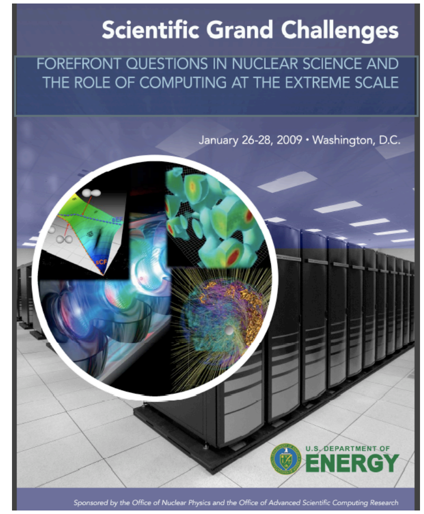
Physics School
Mumbai, India
November 21, 2010

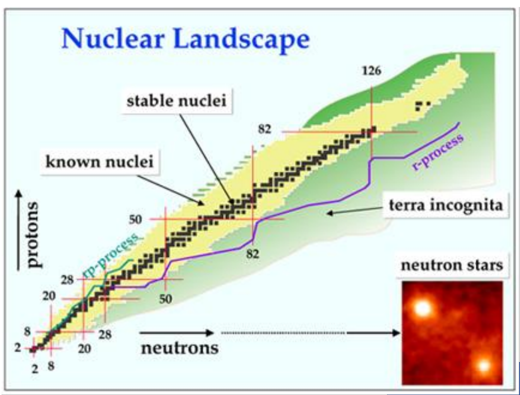
- Motivation and goals
- *ab initio* no core methods
- "Hands-on" practice case
- Applications - comparisons with experiment
- Conclusions/Outlook

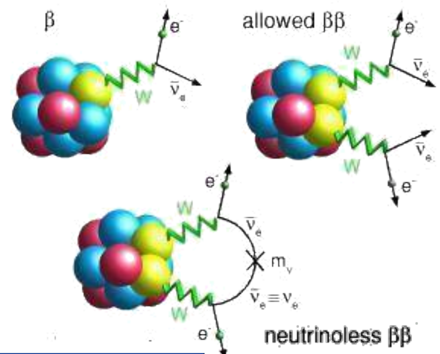
DOE Workshop on Forefront Questions in Nuclear Science and the Role of High Performance Computing: Nuclear Structure and Nuclear Reactions

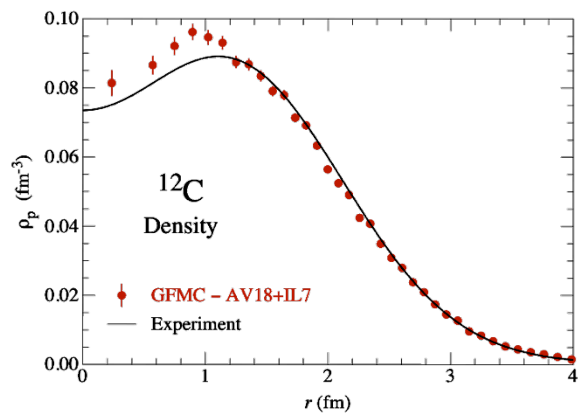


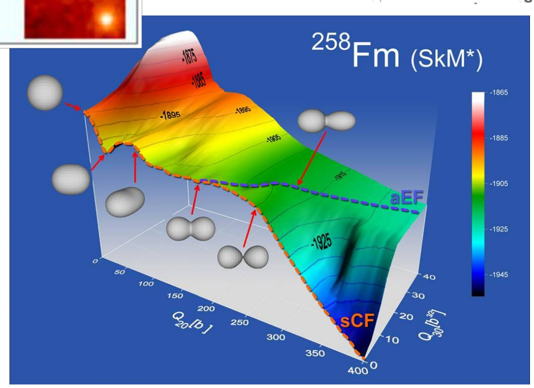
Priority Research Directions

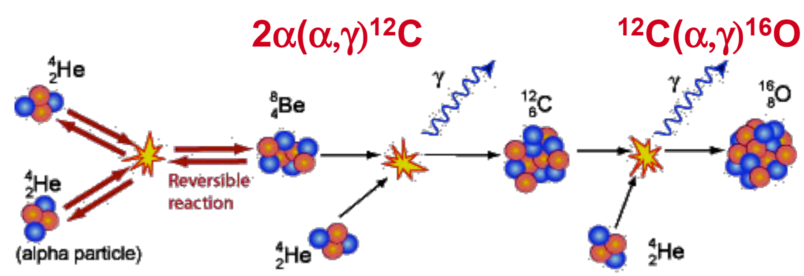
- **Physics of extreme neutron-rich nuclei and matter**
- **Microscopic description of nuclear fission**
- **Nuclei as neutrino physics laboratories**
- **Reactions that made us - triple α process and $^{12}C(\alpha,\gamma)^{16}O$**



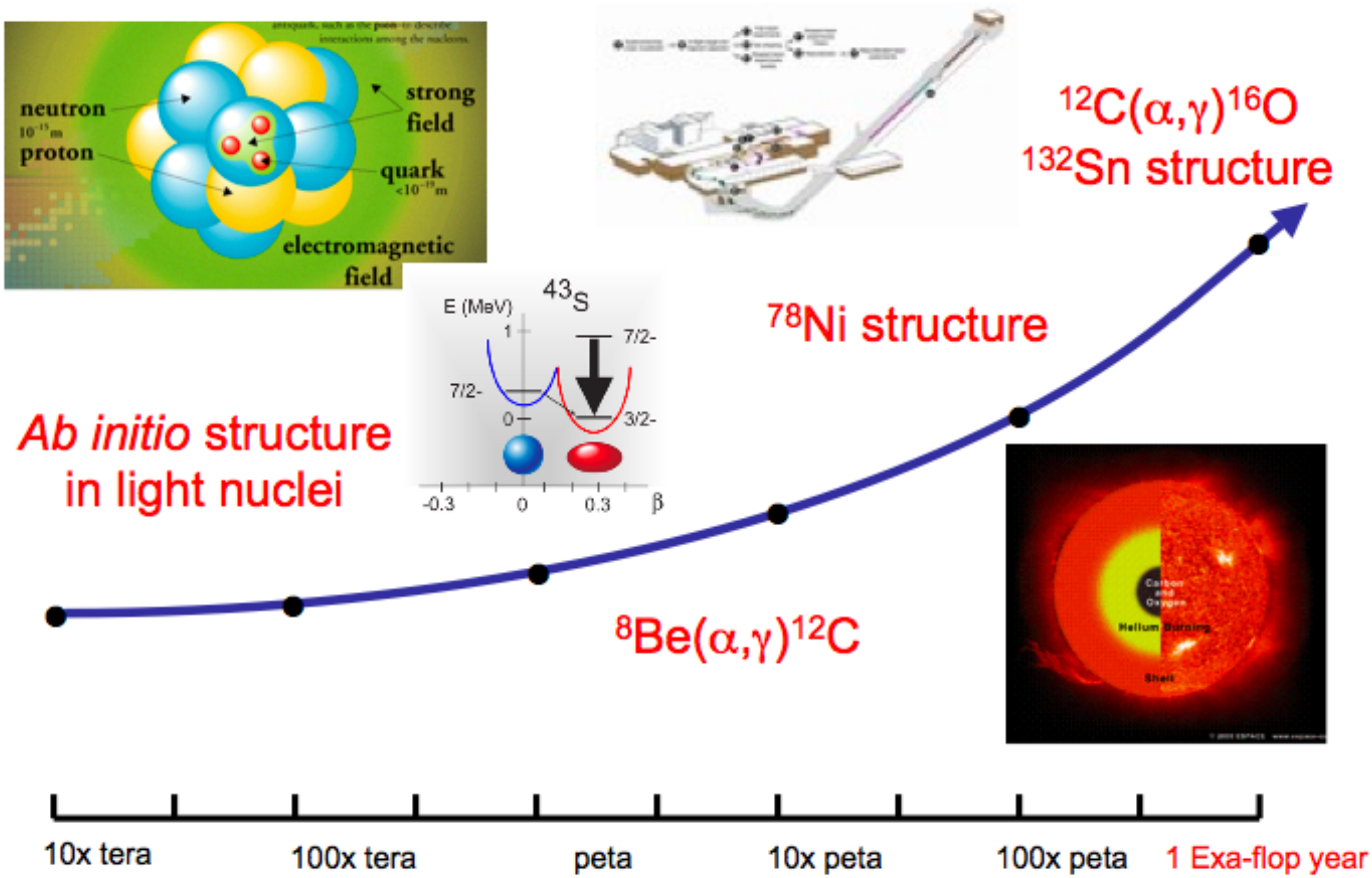






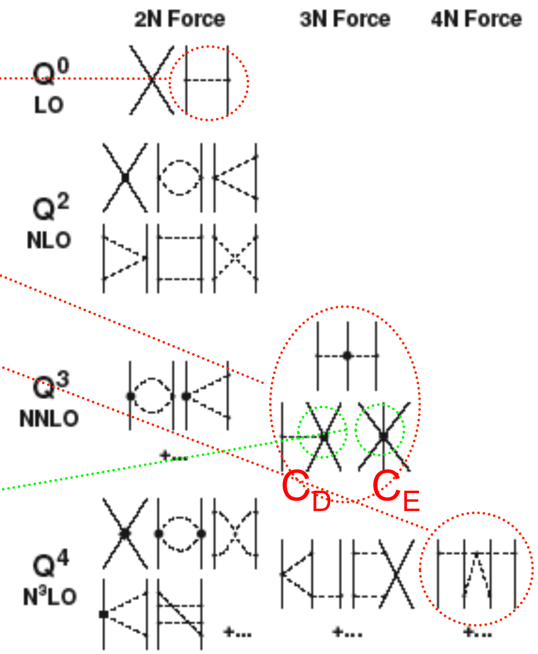


Reactions that made us



Chiral Effective Field Theory

- Chiral symmetry of QCD ($m_u \approx m_d \approx 0$), spontaneously broken with pion as the Goldstone boson
- Systematic low-momentum expansion in $(Q/\Lambda_\chi)^n$; $\Lambda_\chi \approx 1$ GeV, $Q \approx 100$ MeV
  - Power-counting
  - Chiral perturbation theory (χPT)
- Describe pion-pion, pion-nucleon and inter-nucleon interactions at low energies
  - Nucleon-nucleon sector - S. Weinberg (1991)
    - Worked out by Van Kolck, Kaiser, Meissner, Epelbaum, Machleidt…
- Leading order (LO)
  - One-pion exchange
- NNN interaction appears at next-to-next-to-leading order (N^2LO)
- NNNN interaction appears at N^3LO order
- Consistency between NN, NNN and NNNN terms
  - NN parameters enter in the NNN terms etc.
- Low-energy constants (LECs) need to be fitted to experiment
- N^3LO is the lowest order where a high-precision fit to NN data can be made
  - Entem and Machleidt (2002) N^3LO NN potential
- Only two NNN and no NNNN low-energy constants up to N^3LO (c_D and c_E)



Computational challenge:
large sparse matrix eigenvalue problem

$$H = T_{rel} + V_{NN} + V_{3N} + \bullet\bullet\bullet$$
$$H|\Psi_i\rangle = E_i|\Psi_i\rangle$$
$$|\Psi_i\rangle = \sum_{n=0}^{\infty} A_n^i|\Phi_n\rangle$$
$$\text{Diagonalize } \{\langle\Phi_m|H|\Phi_n\rangle\}$$

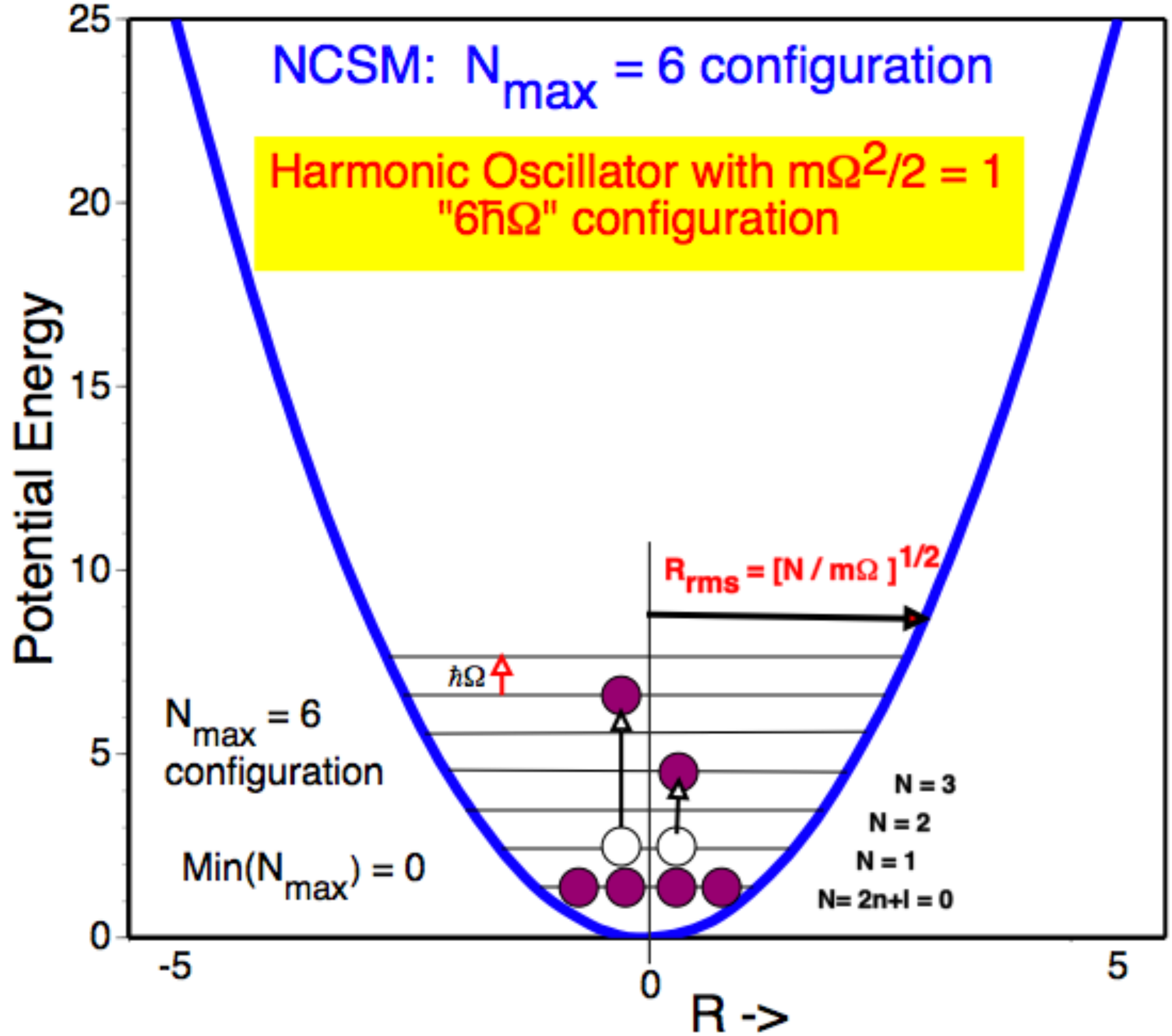
- Adopt realistic NN (and 3N) interaction(s) & renormalize as needed - retain induced many-body interactions: Chiral interactions and JISP16
- Adopt the 3-D Harmonic Oscillator (HO) for the single-nucleon basis states, α, β,…
- Evaluate the nuclear Hamiltonian, H, in basis space of HO (Slater) determinants (manages the bookkeepping of anti-symmetrization)
- Diagonalize a sparse many-body H in this "m-scheme" basis where

$$|\Phi_n\rangle = [a_\alpha^+ \bullet\bullet\bullet a_\varsigma^+]_n|0\rangle$$
$$n = 1,2,\ldots,10^{10} \text{ or more!}$$

- 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


NCSM: N_{max} = 6 configuration
Harmonic Oscillator with $m\Omega^2/2 = 1$
"$6\hbar\Omega$" configuration
Potential Energy
25
20
15
10
5
0
-5
0
5
R ->
$R_{rms} = [N / m\Omega]^{1/2}$
$\hbar\Omega$
N_{max} = 6
configuration
Min(N_{max}) = 0
N = 3
N = 2
N = 1
N= 2n+l = 0

Foundations of *ab initio* No-Core Methods depend on renormalization [RN] of H

No-Core Shell Model (NCSM): RN = Lee-Suzuki-Okamoto
No-Core Full Configuration method (NCFC): Initial H, RN=Vlowk, SRG, UCOM

Common features:

- Both are *ab-initio*
- Both are No-Core
- Both exactly preserve all symmetries of H
- Both use a many-body basis constructed from harmonic oscillator single-particle states
  => basis space depends on $(N_{max}, \hbar\Omega)$*

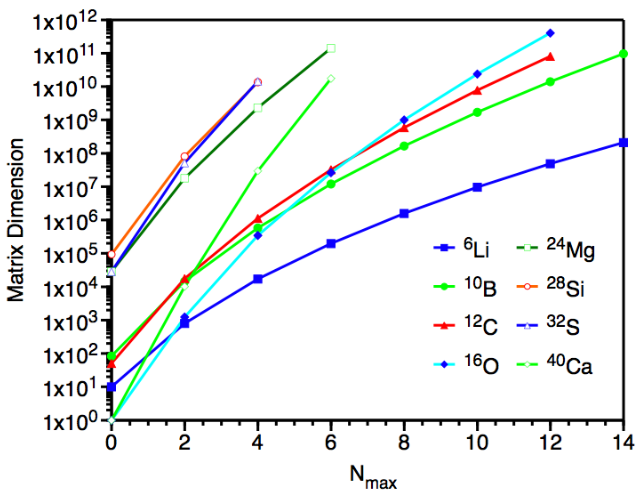
Major distinction:

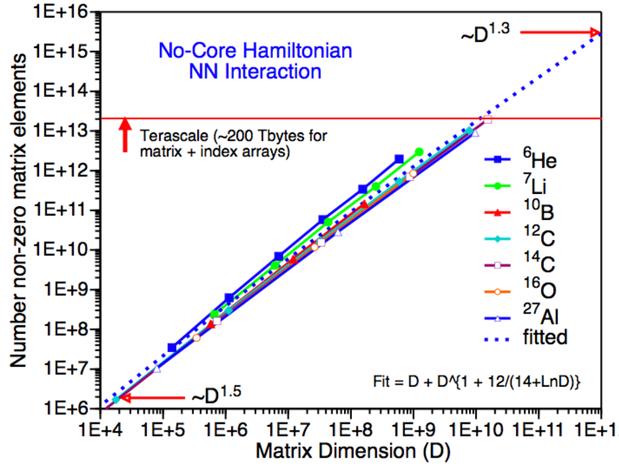
NCSM uses H_{eff} calculated for each $(N_{max}, \hbar\Omega)$
NCFC uses H independent of basis space

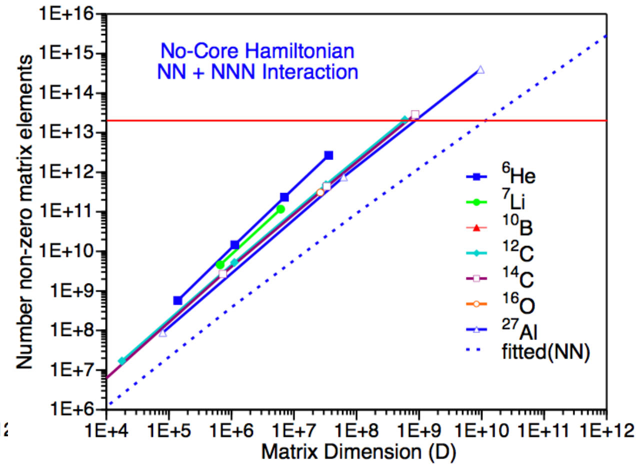
*** N_{max} is number of oscillator quanta in the basis above the minimum for that nucleus**

Challenge

~ Exponential increase in Matrix Dimension (D)



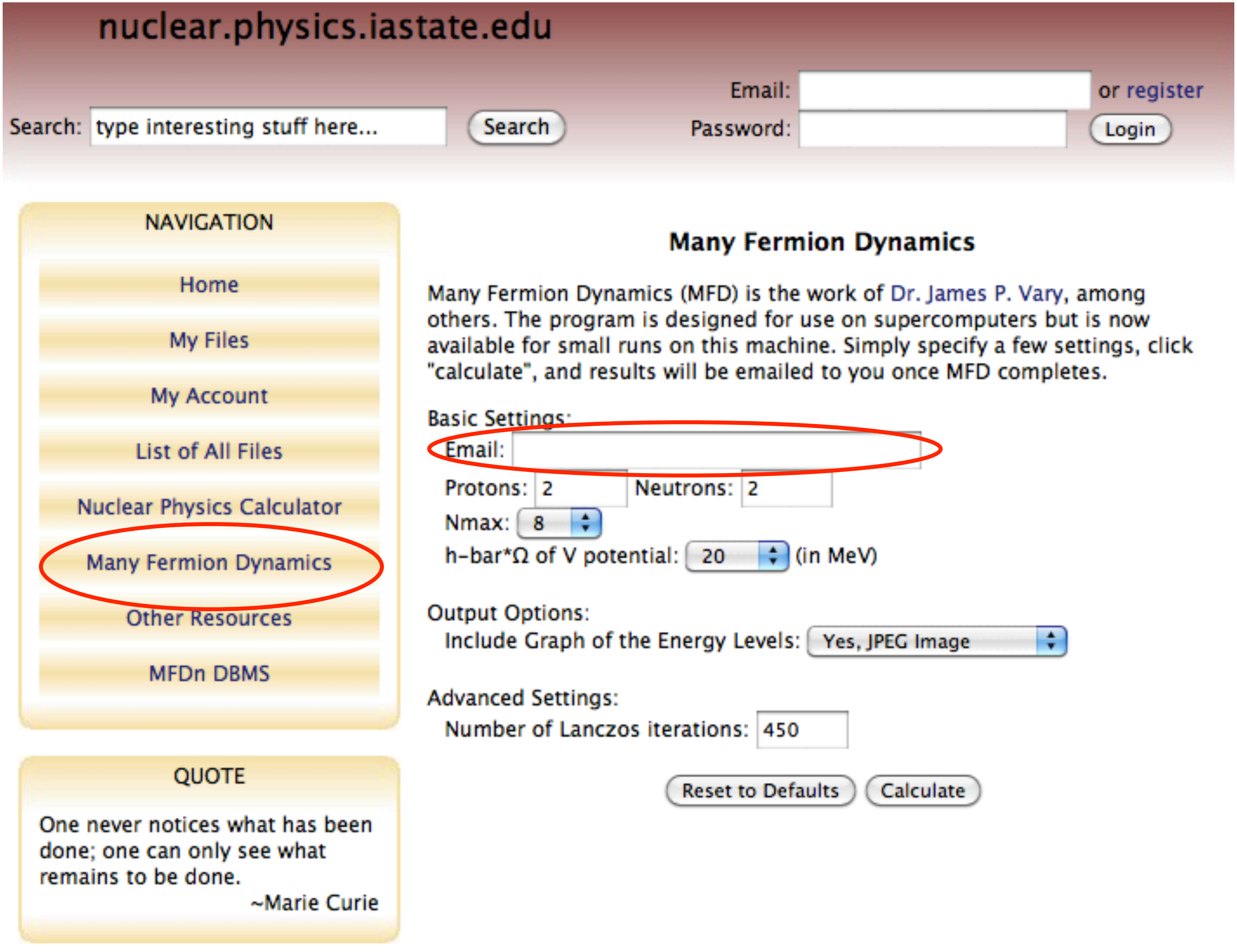




Opportunities

- Memory/cpu time grows only as $D^{3/2}$
- Algorithm development (UNEDF/SciDAC, PetaApps funding)
- Petaflop machines in 2009-10 (Japan, US-DOE, US-NSF, China, …)
- Improve understanding of H & RN (Chiral EFT, others)
- Develop methods for extrapolating D->inf (N_{max}->inf)

P. Maris, J.P. Vary and A. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420


nuclear.physics.iastate.edu
Email:
or register
Search: type interesting stuff here...
Search
Password:
Login
NAVIGATION
Home
My Files
My Account
List of All Files
Nuclear Physics Calculator
Many Fermion Dynamics
Other Resources
MFDn DBMS
QUOTE
One never notices what has been done; one can only see what remains to be done.
~Marie Curie
Many Fermion Dynamics
Many Fermion Dynamics (MFD) is the work of Dr. James P. Vary, among others. The program is designed for use on supercomputers but is now available for small runs on this machine. Simply specify a few settings, click "calculate", and results will be emailed to you once MFD completes.
Basic Settings:
Email:
Protons: 2
Neutrons: 2
Nmax: 8
h-bar*Ω of V potential: 20
(in MeV)
Output Options:
Include Graph of the Energy Levels: Yes, JPEG Image
Advanced Settings:
Number of Lanczos iterations: 450
Reset to Defaults
Calculate

NAVIGATION

- Home
- My Files
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- List of All Files
- Nuclear Physics Calculator
- Many Fermion Dynamics
- Other Resources
- MFDn DBMS

QUOTE

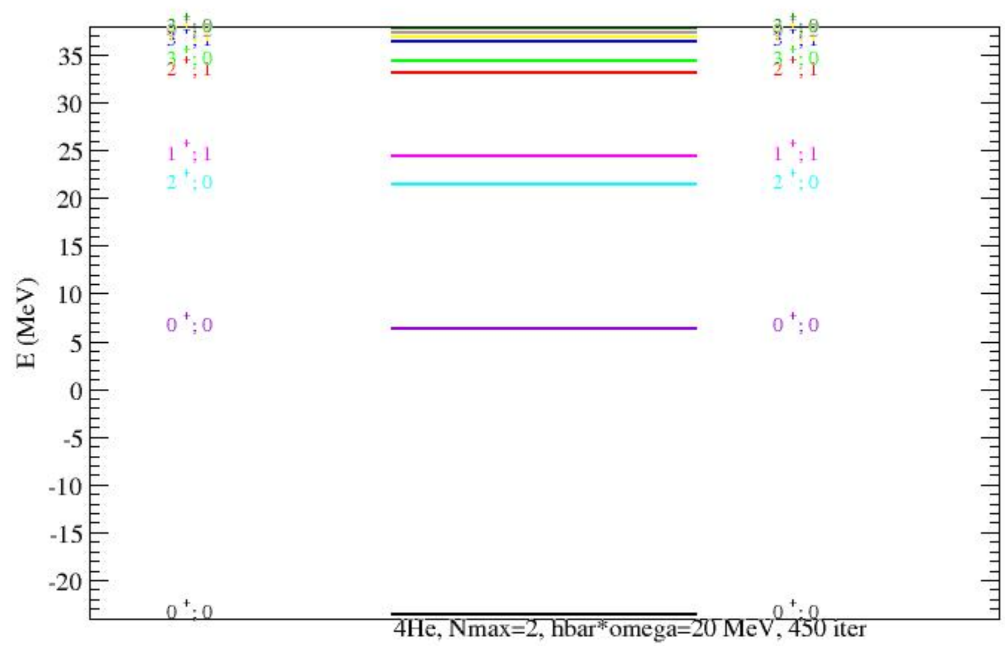
The Cosmos is all that is or ever was or ever will be. Our feeblest contemplations of the Cosmos stir us there is a tingling in the spine, a catch in the voice, a faint sensation, as if a distant memory, of falling from a height. We know we are approaching the greatest of mysteries.

~Carl Sagan

Many Fermion Dynamics

Job submitted to run. Depending on the complexity of the job and the load on the server, you may have to wait up to a few hours for your results.

Example of jpeg file of the spectra



Email received with the spectra and set of observables

Hello,

You requested a run of Many Fermion Dynamics (MFDn); this email contains the results of that run.

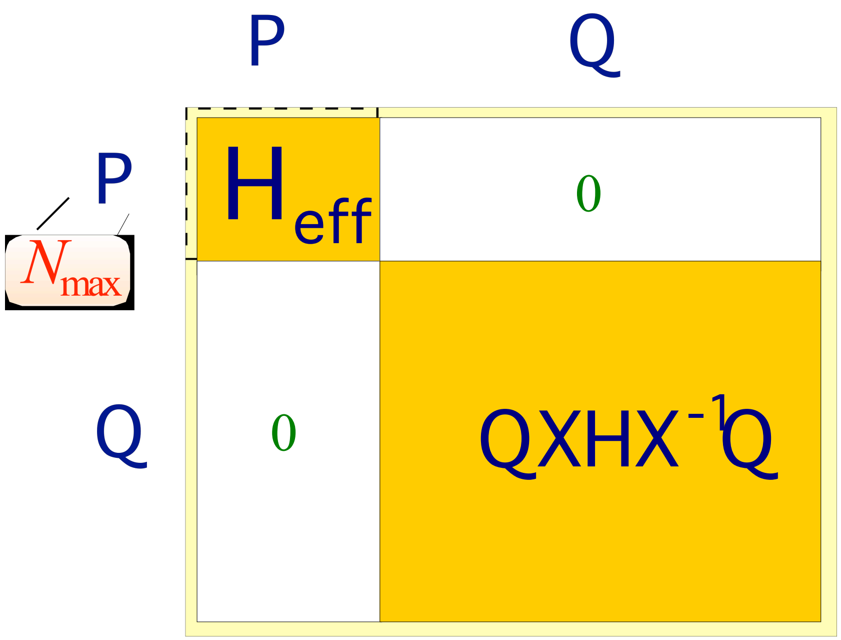
=== Settings ===
protons: 2
neutrons: 2
Nmax: 8
V Potential: 20
Lanczos Iterations: 450

=== Run Results ===

1	0.000	0.000	0.000	-28.170	1.431	1.92	0.04	0.02	0.01	0.00	0.00	0.00	0.00	1.92	0.04	0.03	0.01	0.00	0.00	0.00	0.00
2	0.000	0.001	23.810	-4.359	2.297	1.24	0.28	0.37	0.04	0.04	0.02	0.01	0.00	1.27	0.27	0.36	0.04	0.03	0.01	0.01	0.00
3	1.000	0.350	31.512	3.342	2.488	0.83	0.43	0.32	0.16	0.15	0.06	0.03	0.01	1.30	0.55	0.09	0.03	0.02	0.01	0.00	0.00
4	1.000	0.833	32.047	3.877	2.488	1.30	0.55	0.09	0.03	0.02	0.01	0.00	0.00	0.84	0.42	0.33	0.16	0.15	0.06	0.04	0.01
5	2.000	0.003	32.965	4.796	2.382	1.14	0.34	0.34	0.08	0.06	0.02	0.01	0.00	1.20	0.32	0.32	0.07	0.05	0.02	0.01	0.00
6	0.000	1.000	33.025	4.855	2.512	1.07	0.47	0.19	0.10	0.09	0.04	0.02	0.01	1.04	0.50	0.20	0.10	0.09	0.04	0.02	0.01
7	2.000	0.003	34.990	6.820	2.441	0.85	0.76	0.22	0.11	0.04	0.01	0.01	0.00	0.87	0.77	0.21	0.10	0.03	0.01	0.00	0.00
8	3.000	0.932	37.059	8.889	2.518	0.90	0.42	0.28	0.15	0.14	0.06	0.04	0.01	1.21	0.52	0.14	0.06	0.04	0.02	0.01	0.00
9	1.000	0.932	37.301	9.131	2.523	0.88	0.44	0.27	0.17	0.14	0.05	0.03	0.01	1.20	0.53	0.14	0.06	0.04	0.01	0.01	0.00
10	2.184	0.888	37.671	9.501	2.518	1.02	0.48	0.21	0.11	0.10	0.04	0.03	0.01	1.06	0.50	0.20	0.10	0.08	0.04	0.02	0.01
11	2.810	0.397	37.790	9.620	2.522	1.13	0.53	0.16	0.08	0.05	0.02	0.01	0.00	0.92	0.47	0.26	0.14	0.12	0.05	0.03	0.01
12	2.045	0.973	37.825	9.656	2.540	1.06	0.47	0.19	0.11	0.09	0.04	0.02	0.01	1.01	0.49	0.21	0.12	0.10	0.04	0.02	0.01
13	1.000	0.170	37.999	9.829	2.518	1.19	0.53	0.14	0.06	0.05	0.02	0.01	0.00	0.87	0.44	0.27	0.17	0.15	0.06	0.04	0.01
14	4.000	0.000	38.420	10.250	2.413	0.83	0.85	0.15	0.12	0.03	0.01	0.00	0.00	0.84	0.86	0.15	0.11	0.03	0.01	0.00	0.00
15	2.000	0.047	38.910	10.740	2.547	1.05	0.56	0.17	0.10	0.06	0.03	0.01	0.00	0.91	0.52	0.23	0.15	0.11	0.05	0.03	0.01

Seq	J	T	E-E1	Eabs	rms(p)	rms(n)	rms(mass)
1	0.000	0.000	0.000	-28.170	1.433	1.428	1.431
2	0.000	0.001	23.810	-4.359	2.315	2.279	2.297
3	1.000	0.350	31.512	3.342	2.860	2.050	2.488
4	1.000	0.833	32.047	3.877	2.057	2.855	2.488
5	2.000	0.003	32.965	4.796	2.418	2.345	2.382
6	0.000	1.000	33.025	4.855	2.507	2.517	2.512
7	2.000	0.003	34.990	6.820	2.460	2.422	2.441
8	3.000	0.932	37.059	8.889	2.765	2.244	2.518
9	1.000	0.932	37.301	9.131	2.779	2.238	2.523
10	2.184	0.888	37.671	9.501	2.556	2.481	2.518

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



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

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

model space dimension

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

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

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

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

Key equations to solve at the a-body cluster level

Solve a cluster eigenvalue problem in a very large but finite basis and retain all the symmetries of the bare Hamiltonian

$$P_a = \sum_{P \in \boldsymbol{P}} |\alpha_P\rangle\langle\alpha_P|$$

$$Q_a = \sum_{Q \in \boldsymbol{Q}} |\alpha_Q\rangle\langle\alpha_Q|$$

$$P_a + Q_a \approx 1_a$$

$$H_a^{\Omega} |k\rangle = E_k |k\rangle$$

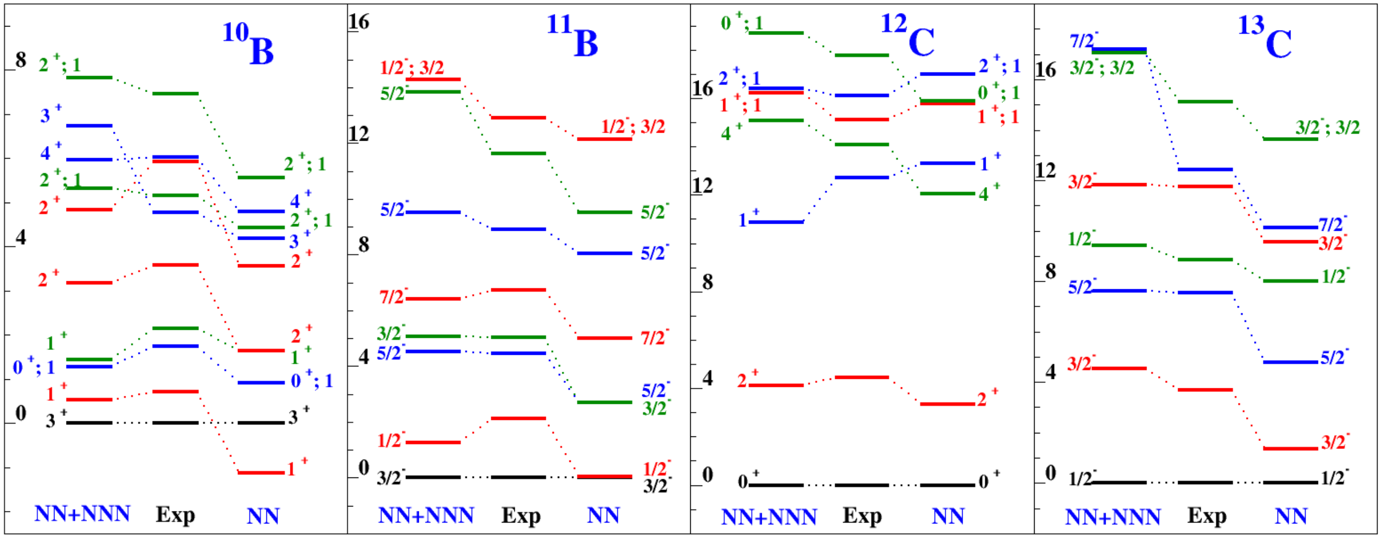
$$\langle\alpha_Q|\omega|\alpha_P\rangle = \sum_{k \in K} \langle\alpha_Q|k\rangle\langle\hat{k}|\alpha_P\rangle$$

$$where : \langle\hat{k}|\alpha_P\rangle = Inverse\{\langle k|\alpha_P\rangle\}$$

$$\mathcal{H}^{(a)} = (P_a + \omega^T\omega)^{-1/2}(P_a + P_a\omega^T Q_a)H_a^{\Omega}(Q_a\omega P_a + P_a)(P_a + \omega^T\omega)^{-1/2}$$

ab initio NCSM with X_{EFT} Interactions

- *Only method capable to apply the X_{EFT} NN+NNN interactions to all p-shell nuclei*
- *Importance of NNN interactions for describing nuclear structure and transition rates*



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

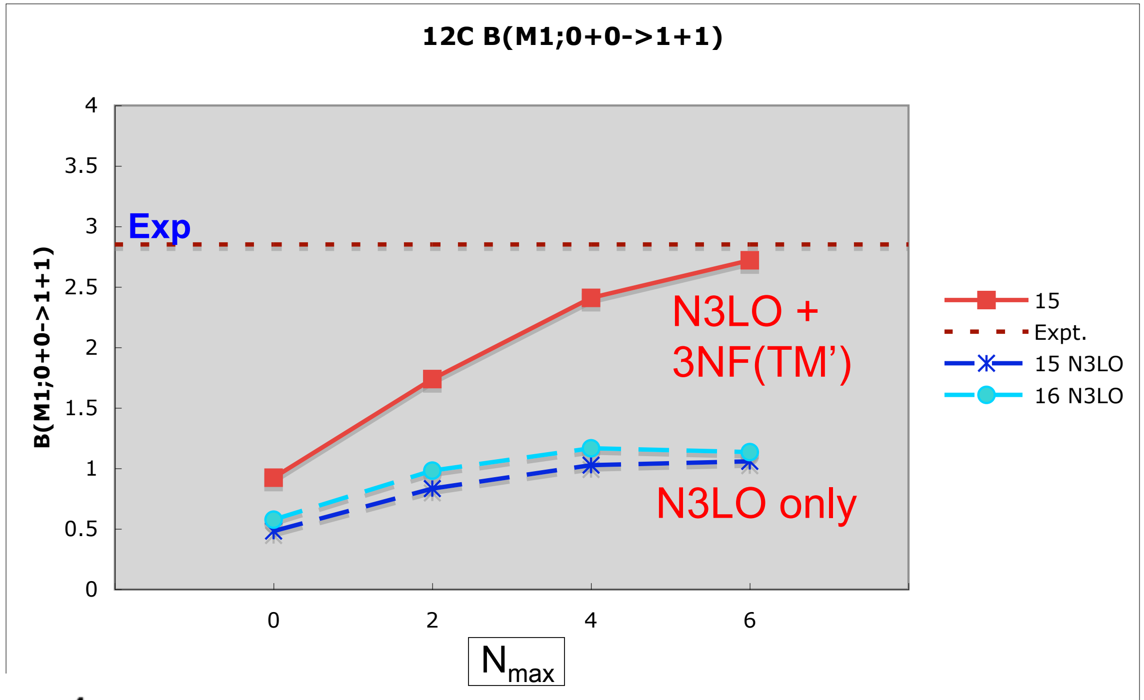
Extensions and work in progress

- *Better determination of the NNN LEC's, feedback to X_{EFT}* (LLNL, OSU, MSU, TRIUMF)
- *Implement Vlowk & SRG renormalizations (Bogner, Furnstahl, Maris, Perry, Schwenk & Vary, NPA 801, 21(2008); ArXiv 0708.3754)*
- *Response to external fields - bridges to DFT/DME/EDF (SciDAC/UNEDF)*
  - *- Axially symmetric quadratic external fields - in progress*
  - *- Triaxial and spin-dependent external fields - planning process*
- *Cold trapped atoms (Stetcu, Barrett, van Kolck & Vary, PRA 76, 063613(2007); ArXiv 0706.4123) and applications to other fields of physics such as light-front Hamiltonian quantum field theory*
- *Effective interactions with a core (Lisetsky, Barrett, Navratil, Stetcu, Vary)*
- *Nuclear reactions & scattering (Forssen, Navratil, Quaglioni, Shirokov, Mazur, Luu, Savage, Schwenk, Vary)*

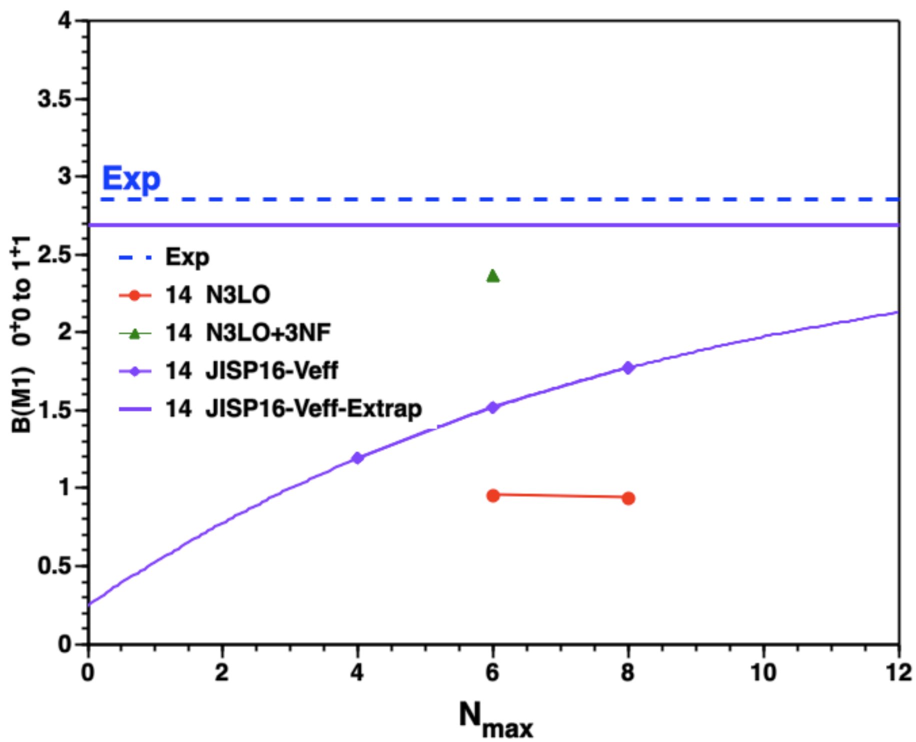
n-^{12}C cross section proportional to Gamow-Teller transition

A.C.Hayes, P. Navratil, J.P. Vary, PRL 91, 012502 (2003); nucl-th/0305072

⇒ First successful description of the GT data requires 3NF



⇒ Non-local NN interaction from inverse scattering also successful



JISP16 NN interaction:
J-matrix Inverse Scattering Potential
tuned with phase-shift-equivalent
unitary transformations
to the binding energy of ^{16}O

- High quality fit to np scattering data (chisq/dof = 1.05)
- High quality fit to Deuteron gs properties
- Finite rank separable in each NN channel in oscillator basis
- Highly non-local, soft and rapidly convergent in nuclear apps
- High quality description of nuclei through the p-shell
- Subroutines and documentation: nuclear.physics.iastate.edu

A.M. Shirokov, J.P. Vary, A.I. Mazur and T.A. Weber,
"Realistic Nuclear Hamiltonian: Ab exitu approach,"
Phys. Letts. B 644, 33(2007), ArXiv nucl-th/0512105

ab initio NCSM - comparison of Chiral EFT with JISP16

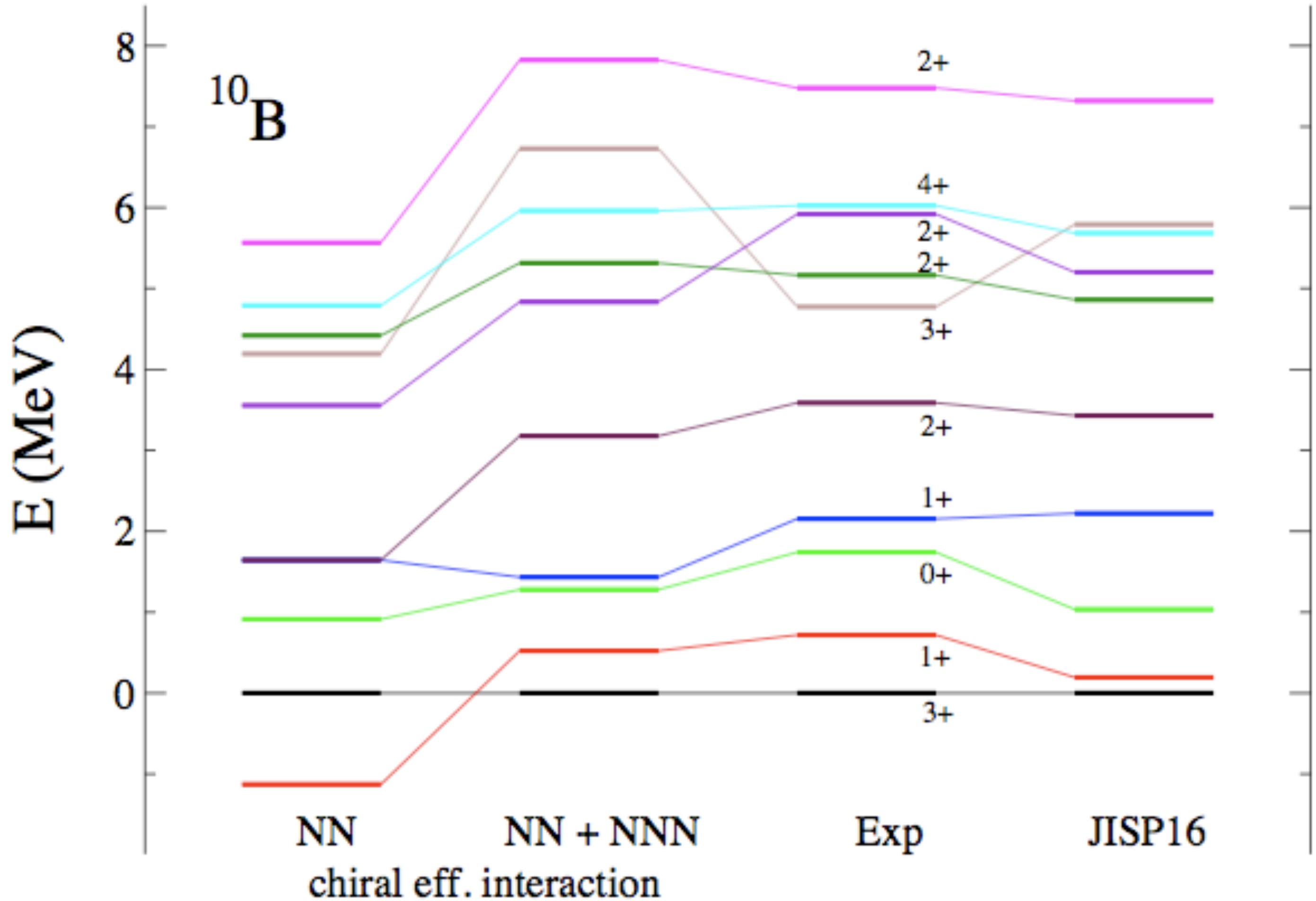
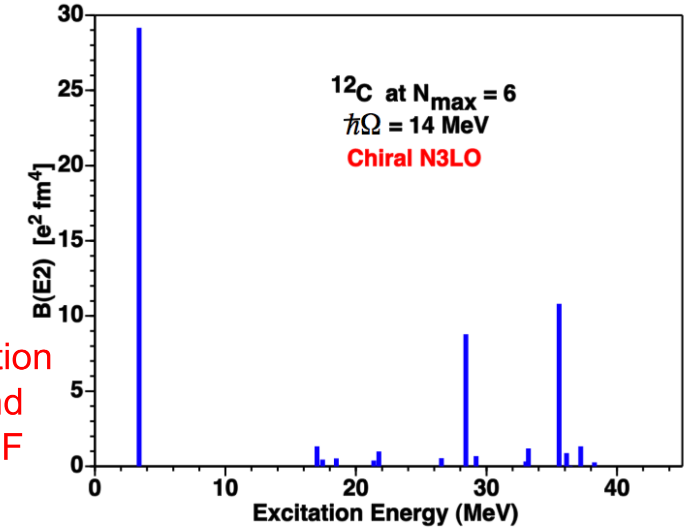


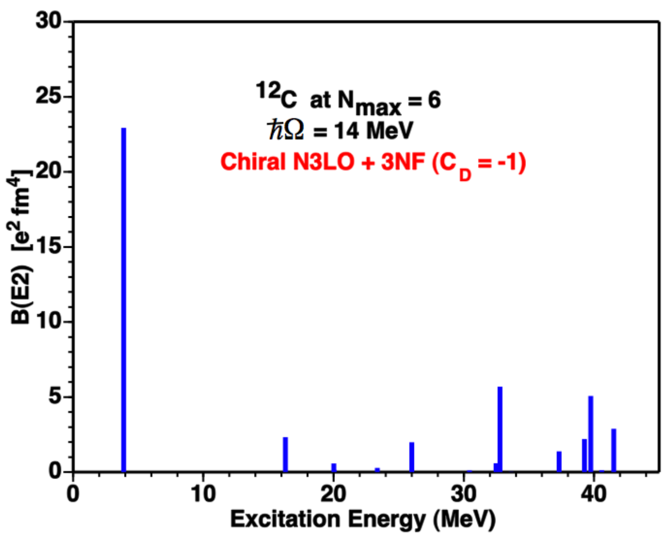
FIGURE 2. Experimental and theoretical excitation spectra of ^{10}B with respect to the lowest 3^+ state at an oscillator energy $\hbar\Omega = 14\ MeV$. The chiral effective interaction results are obtained at $N_{max} = 6$ while the JISP16 results are obtained at $N_{max} = 8$.

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).

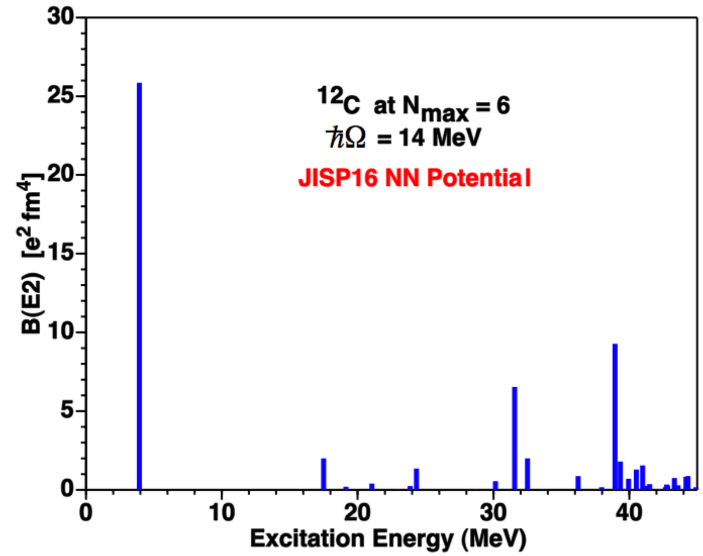
How collective modes are sensitive to the Hamiltonian: Giant Quadrupole Resonance in ^{12}C

Greater fragmentation of E2 strength found including Chiral 3NF

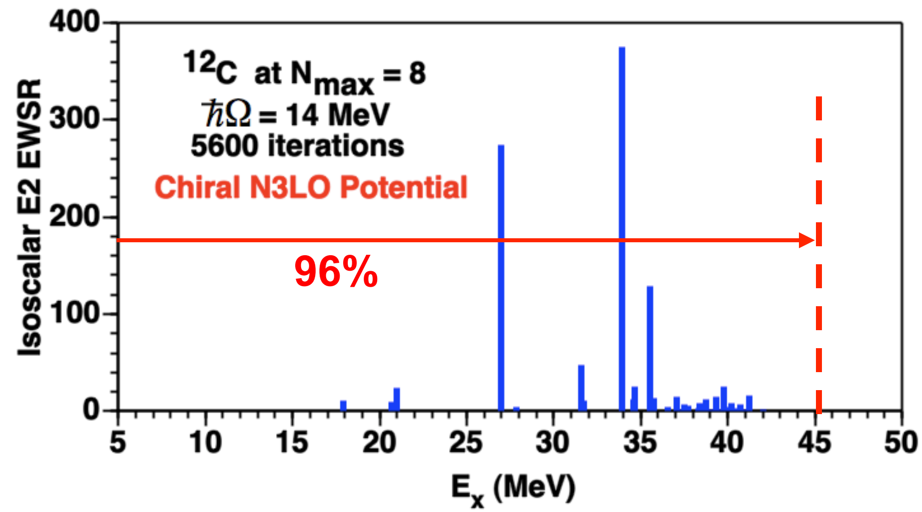


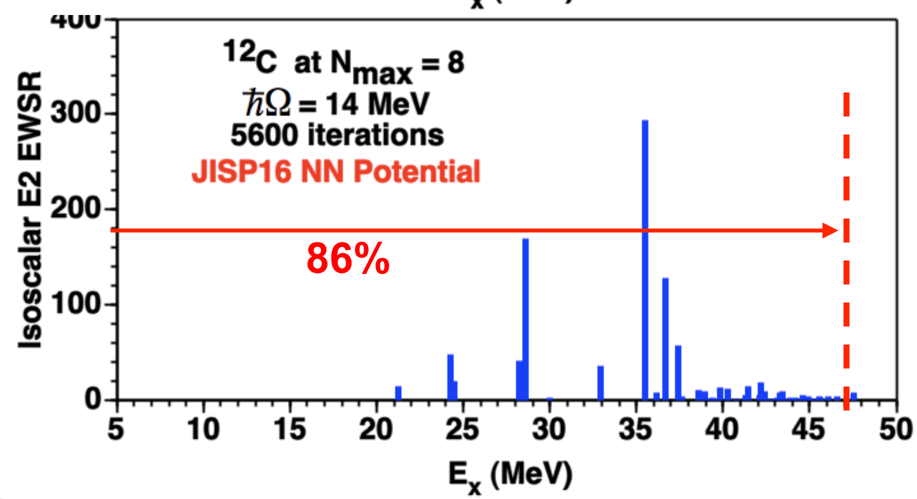


E2 fragmenation with JISP16 is intermediate that of Chiral NN & Chiral NN + 3NF



Isospin weighting:
(1-T)B(E2)



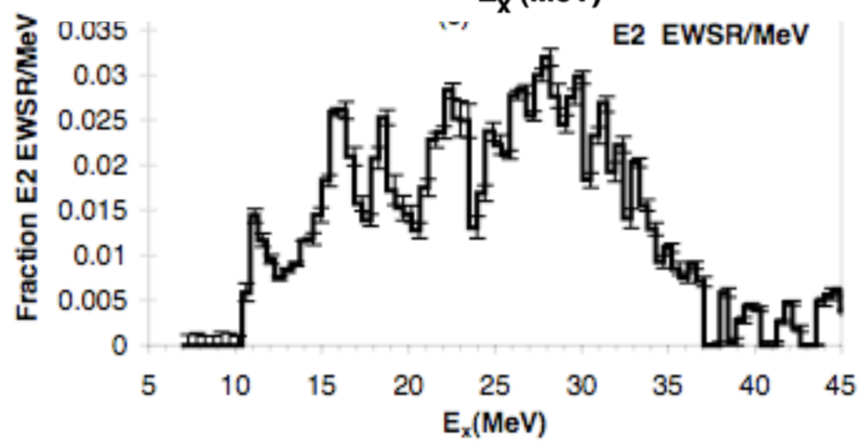


Inelastic α - ^{12}C scattering

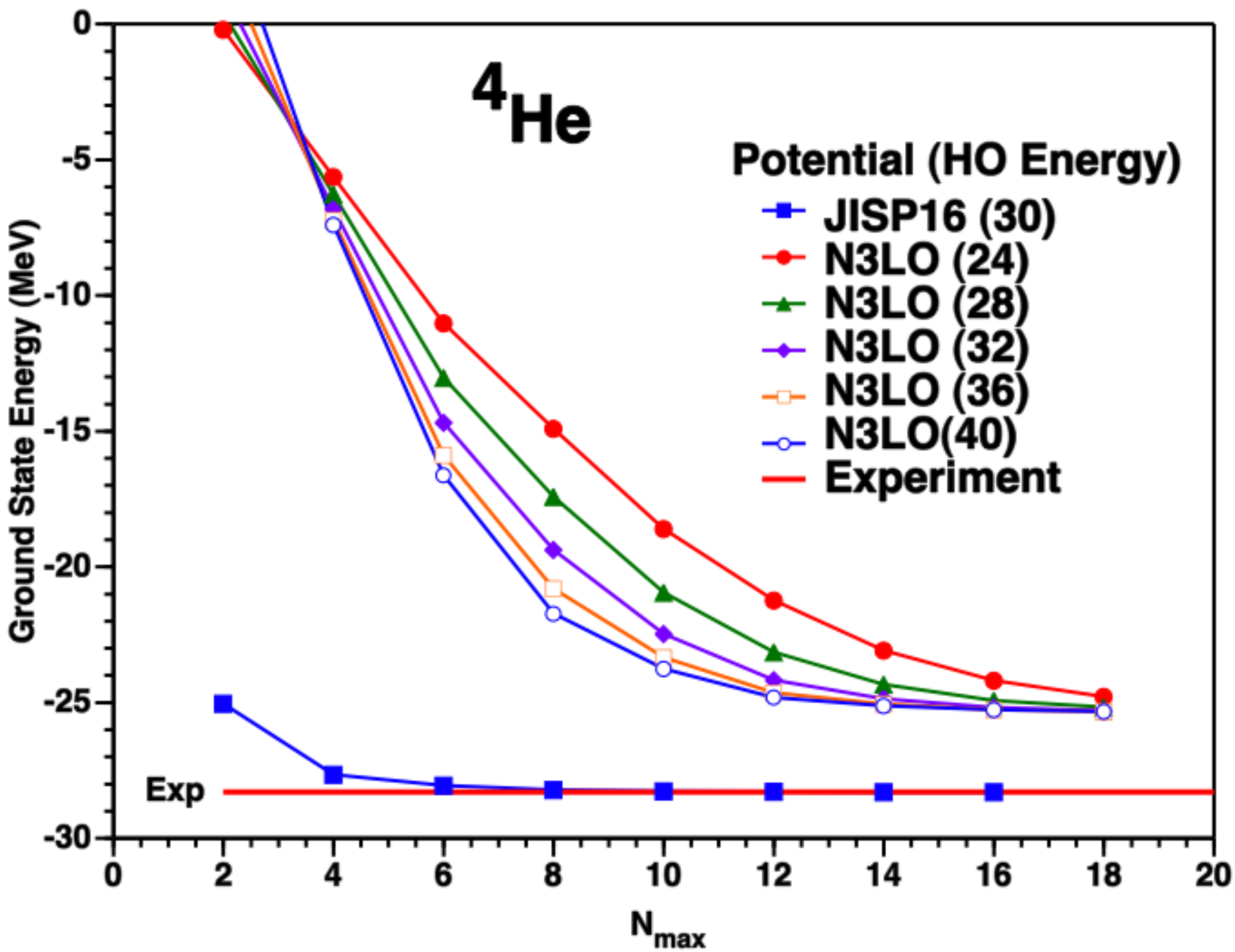
PHYSICAL REVIEW C **68**, 014305 (2003)

Isoscalar electric multipole strength in ^{12}C

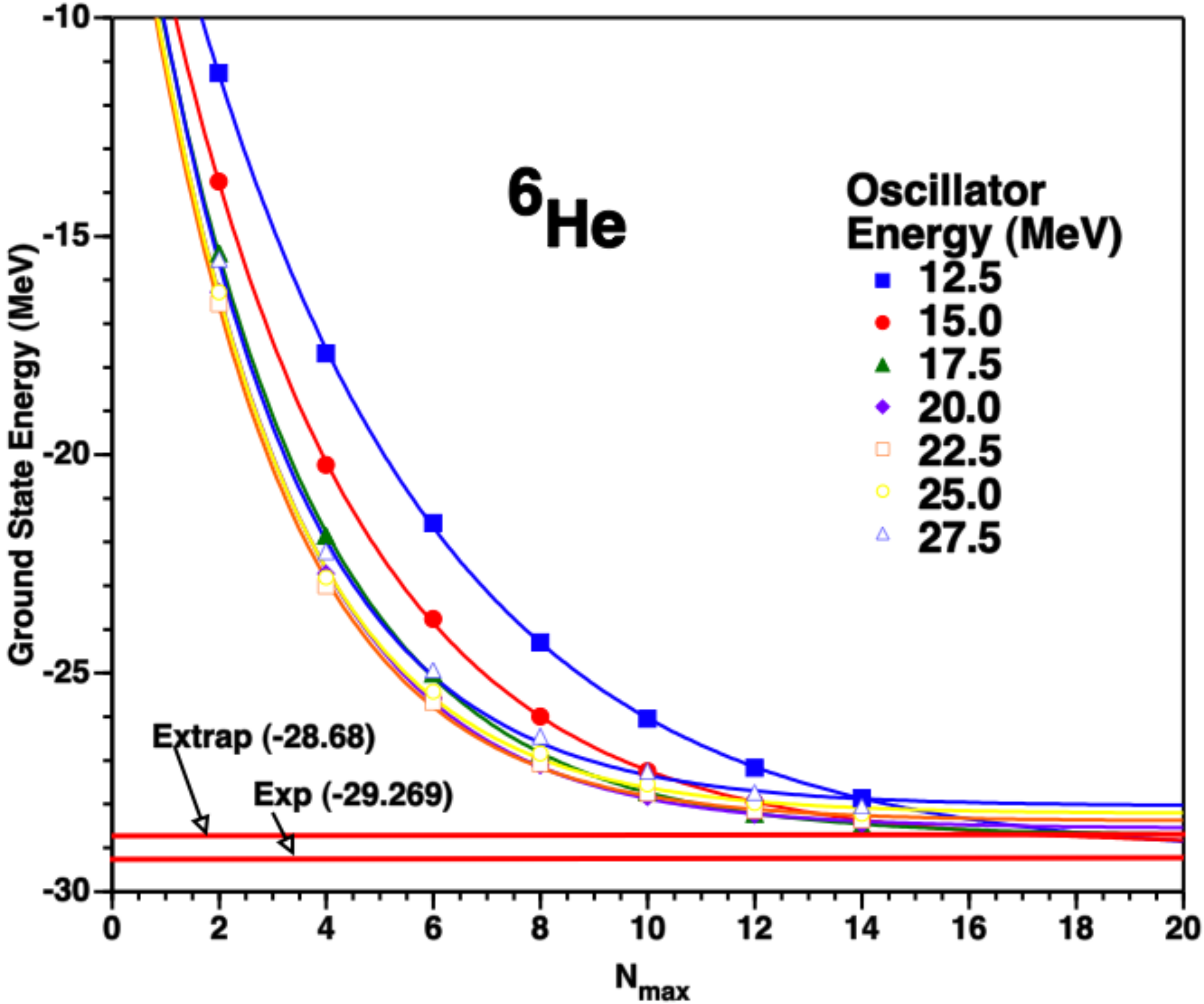
Bency John,* Y. Tokimoto, Y.-W. Lui, H. L. Clark, X. Chen, and D. H. Youngblood
Cyclotron Institute, Texas A&M University, College Station, Texas 77843, USA



Now turn to NCFC where one attains convergence directly or through extrapolation

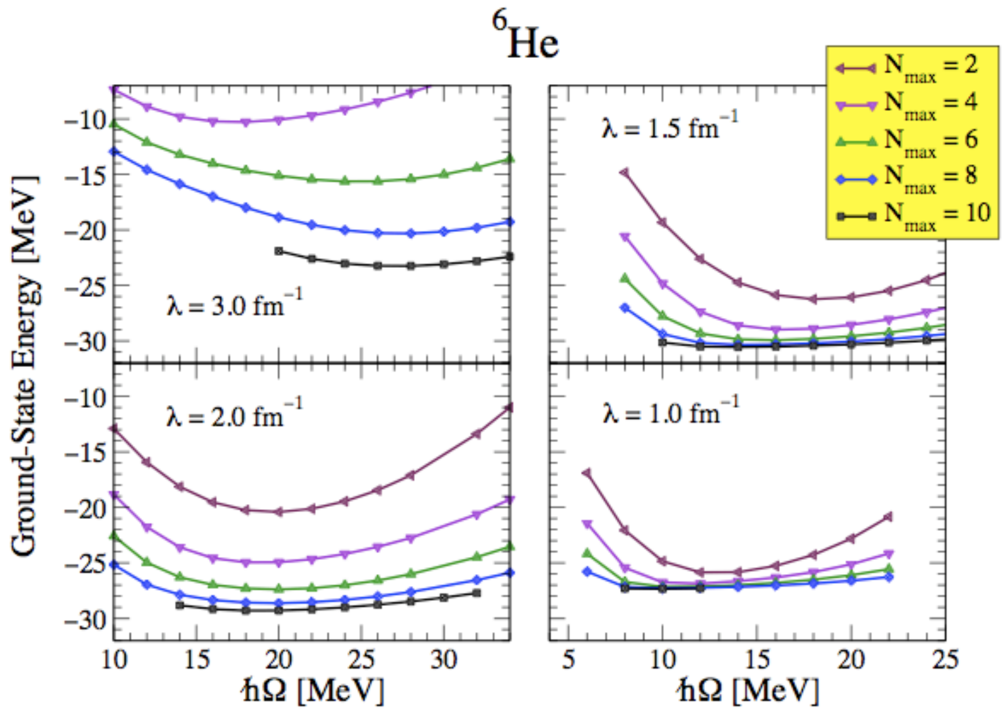


P. Maris, J.P. Vary and A. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420



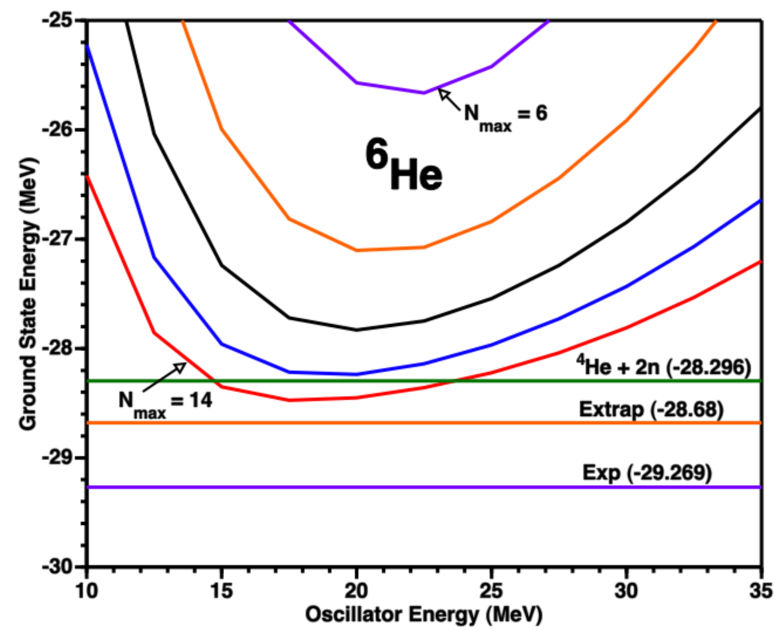
P. Maris, J.P. Vary and A. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420

Chiral N3LO & SRG



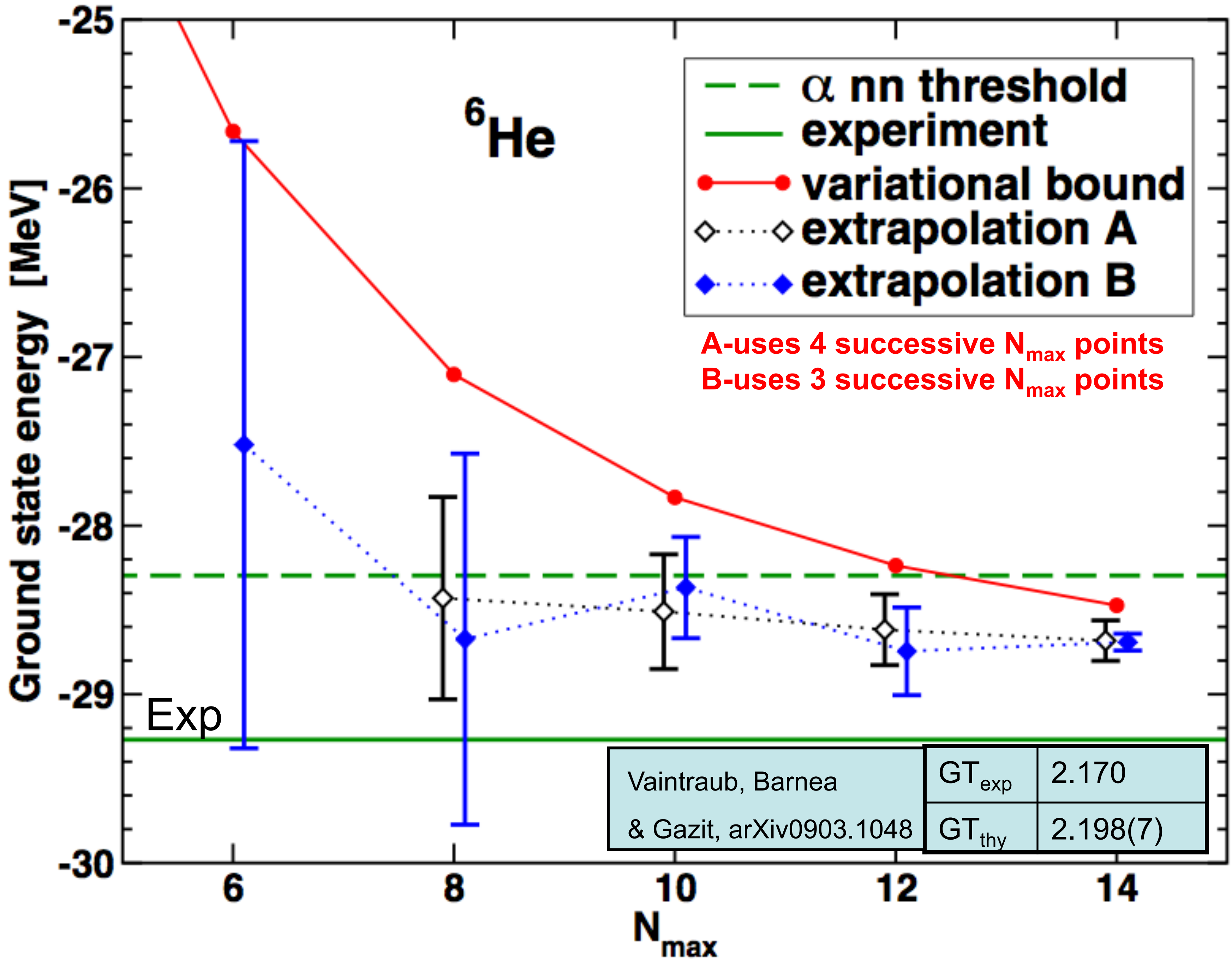
S.K. Bogner, R.J. Furnstahl, P. Maris, R.J. Perry, A. Schwenk and J.P. Vary
Nuclear Physics A 801, 21(2008); arXiv:0708.3754.

JISP16



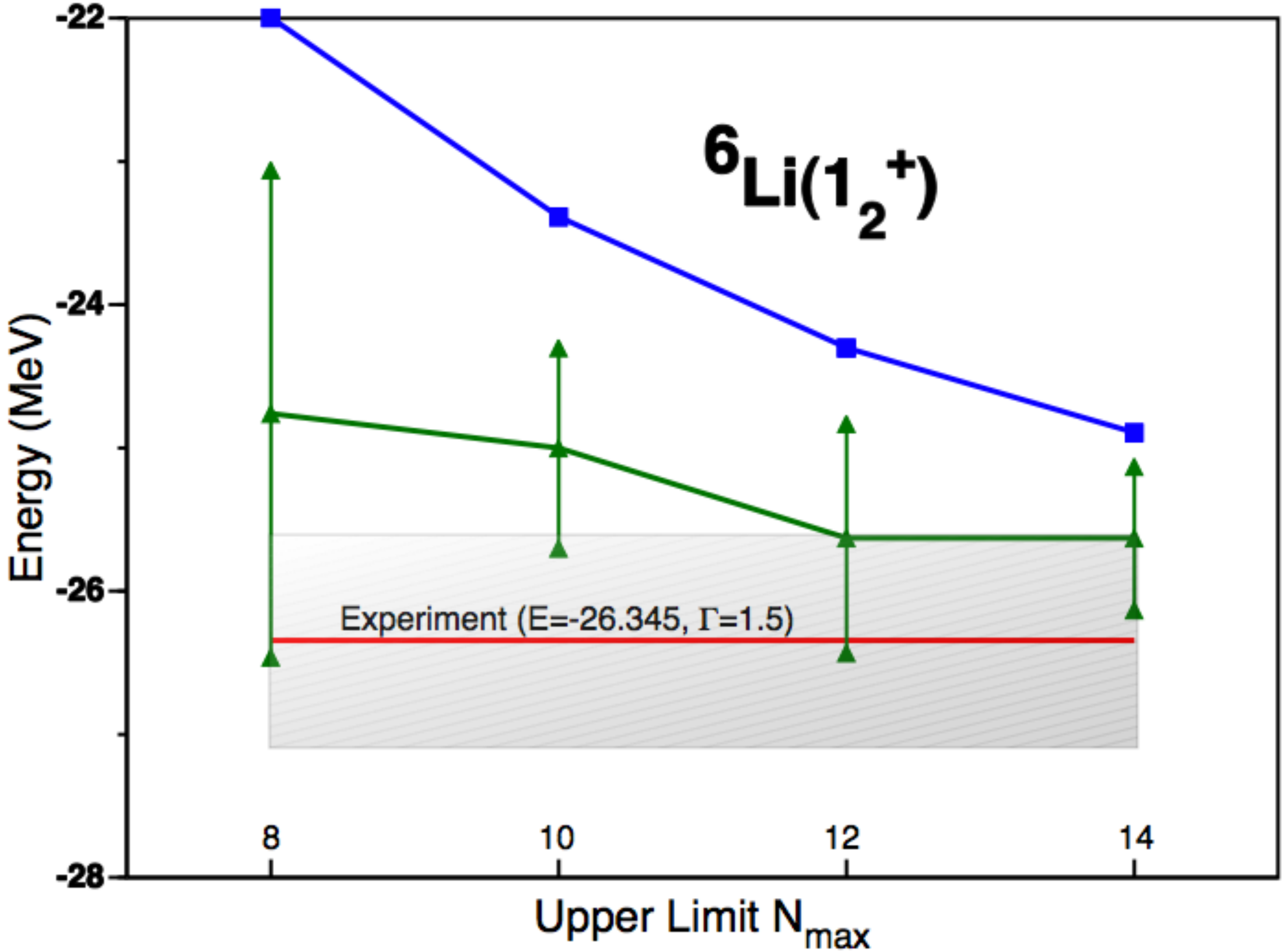
P. Maris, J.P. Vary and A. Shirokov,
Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420

Now use light systems to measure
uncertainties in the exptrapolations

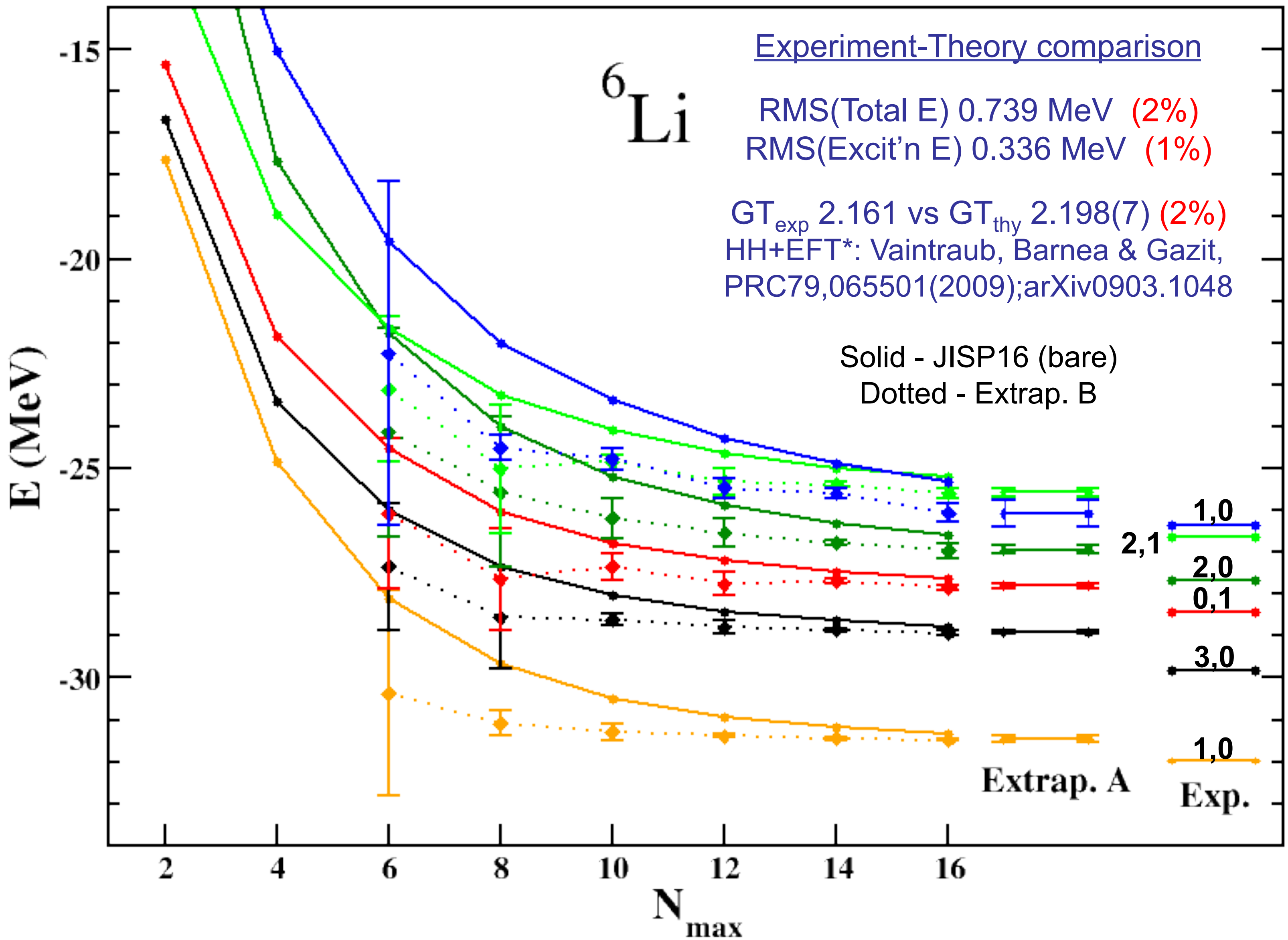


P. Maris, J.P. Vary and A. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420

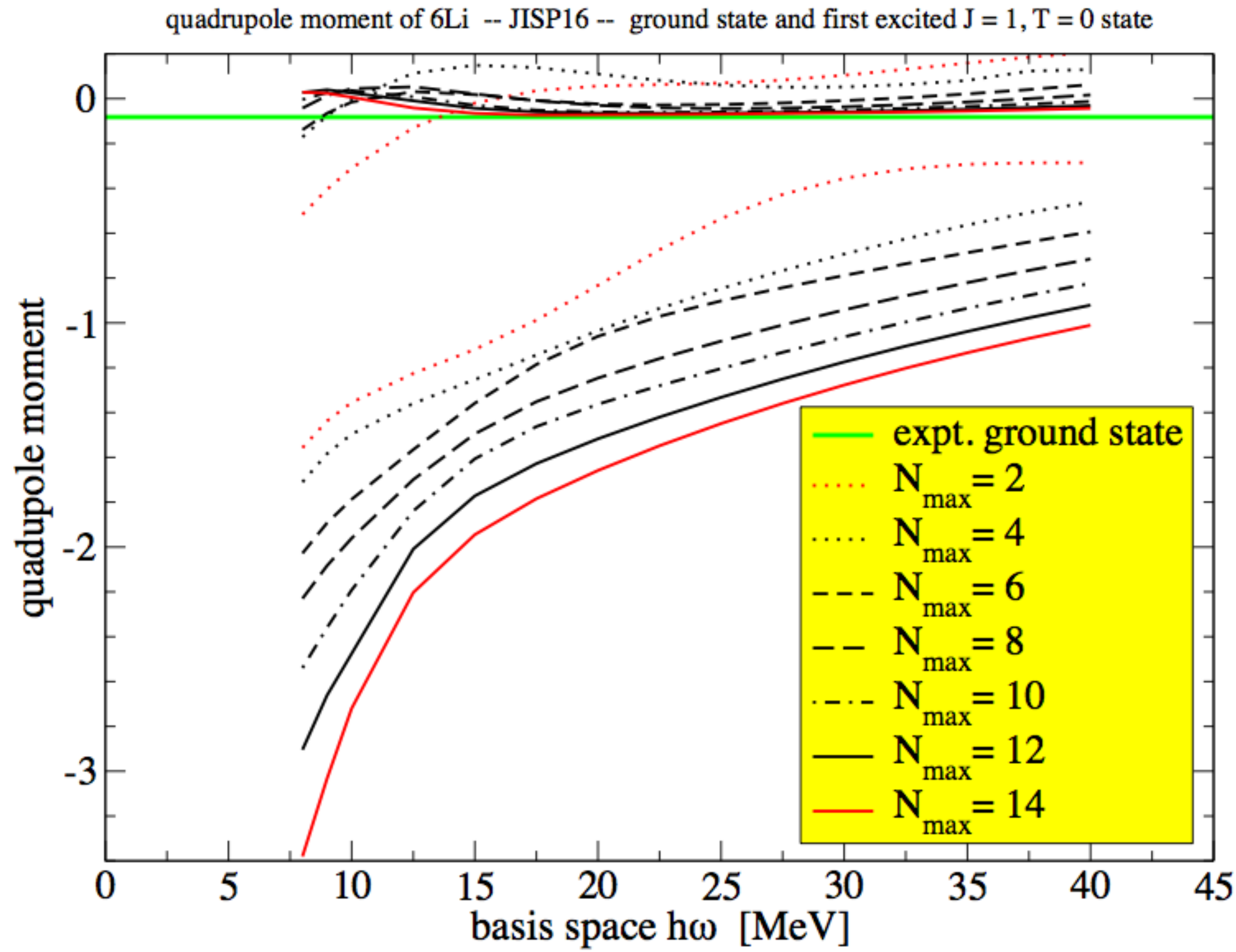
How accurately are resonant states predicted?



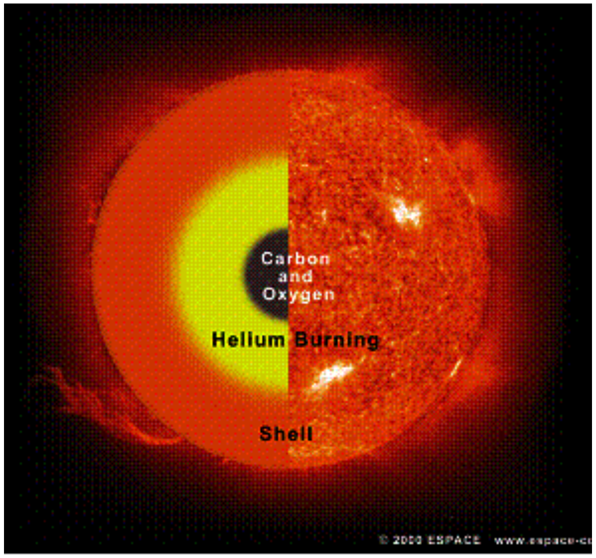
P. Maris, J.P. Vary and A. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420



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



P. Maris, J.P. Vary and A. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420



^{12}C - At the heart of matter

The first excited 0+ state of ^{12}C, the “Hoyle state”, is the key state of ^{12}C formation in the triple-alpha fusion process that occurs in stars.

Due to its role in astrophysics and the fact that carbon is central to life, some refer to this as one of the “holy grails” of nuclear theory.

Many important unsolved problems of the Hoyle state:

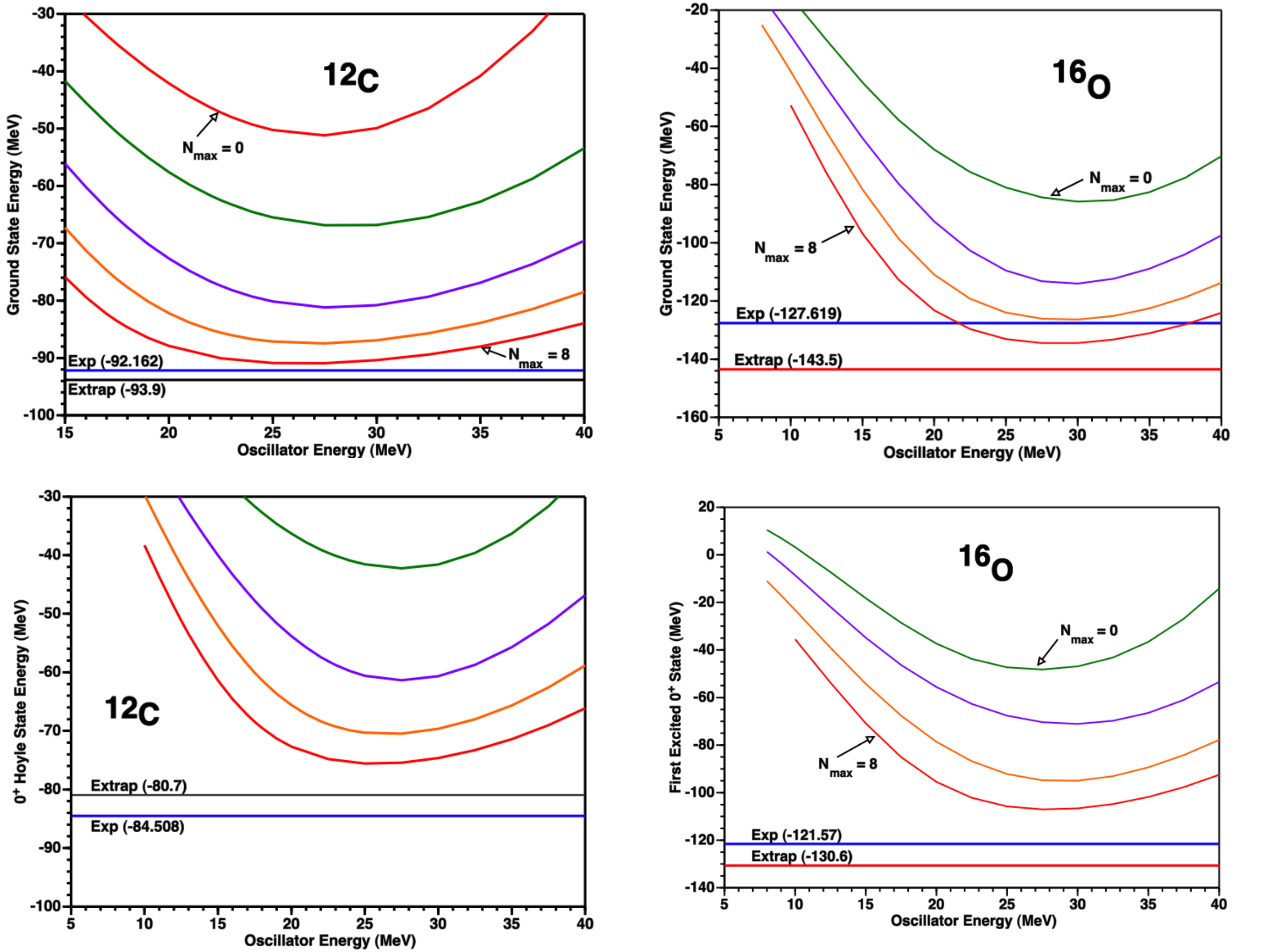
Microscopic origins of the triple-alpha structure are unsolved

Breathing mode puzzle - experiments disagree on sum rule fraction

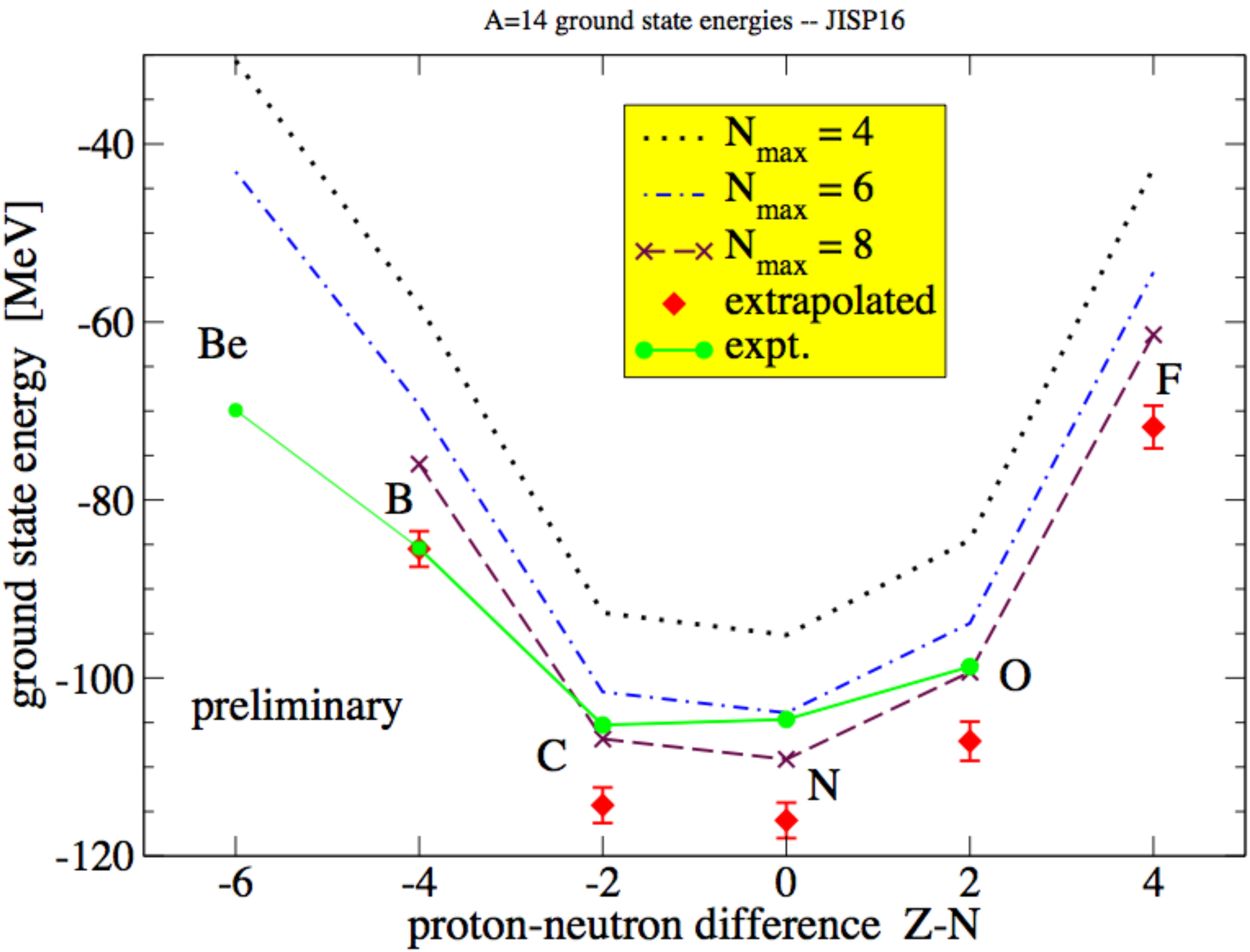
Laboratory experiments to measure the formation rate are very difficult - resulting uncertainties are too large for predicting the ^{12}C formation rate through this state that dictates the size of the iron core in pre-supernova stars

Conclusion: Need *ab initio* solutions of the Hoyle state with no-core method that accurately predicts the ground state binding energy

==> parameter free predictions for the Hoyle state



P. Maris, J.P. Vary and A. Shirokov, Phys. Rev. C. 79, 014308(2009), ArXiv:0808.3420



P. Maris, A. Shirokov and J.P. Vary, in preparation

Descriptive Science

↓

Predictive Science

Proton-Dripping Fluorine-14

PHYSICAL REVIEW C **81**, 021301(R) (2010)

Ab initio nuclear structure simulations: The speculative ^{14}F nucleus

P. Maris,[1] A. M. Shirokov,[1,2,*] and J. P. Vary[1]

[1]*Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011-3160, USA*

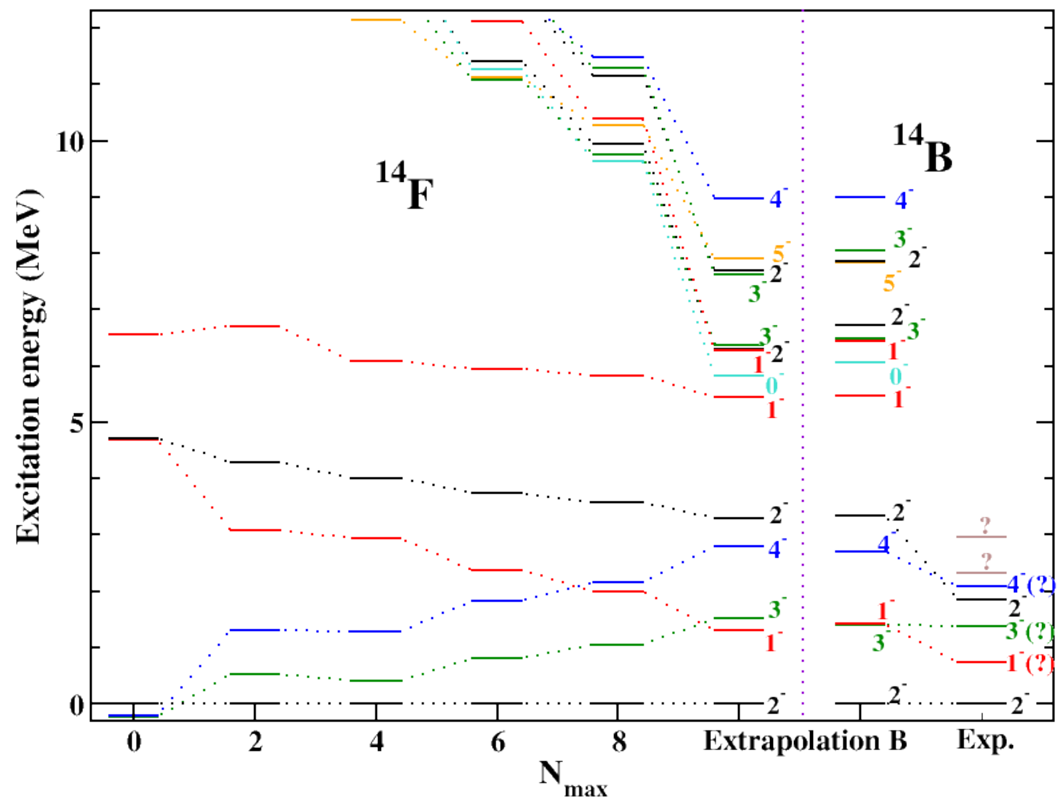
[2]*Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow RU-119991, Russia*

(Received 13 November 2009; published 4 February 2010)

Predictions:

Binding energy: 72 ± 4 MeV indicating that Fluorine-14 will emit (drip) one proton to produce more stable Oxygen-13.

Predicted spectrum (Extrapolation B) for Fluorine-14 which is nearly identical with predicted spectrum of its "mirror" nucleus Boron-14. Experimental data exist only for Boron-14 (far right column).



Theory published: Feb. 4, 2010

P. Maris, A. Shirokov and J.P. Vary,
Phys. Rev. C81, 021301 (R) (2010).

Theory published PRC: Feb. 4, 2010

Physics Letters B 692 (2010) 307–311

Contents lists available at ScienceDirect

Physics Letters B

www.elsevier.com/locate/physletb

Experiment published: Aug. 3, 2010

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

TAMU Cyclotron Institute

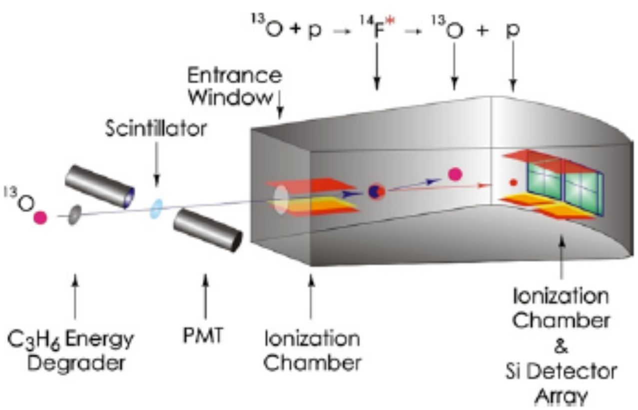


Fig. 1. (Color online.) The setup for the ^{14}F experiment. The "gray box" is the scattering chamber. See explanation in the text.

ab initio predictions in close agreement with experiment

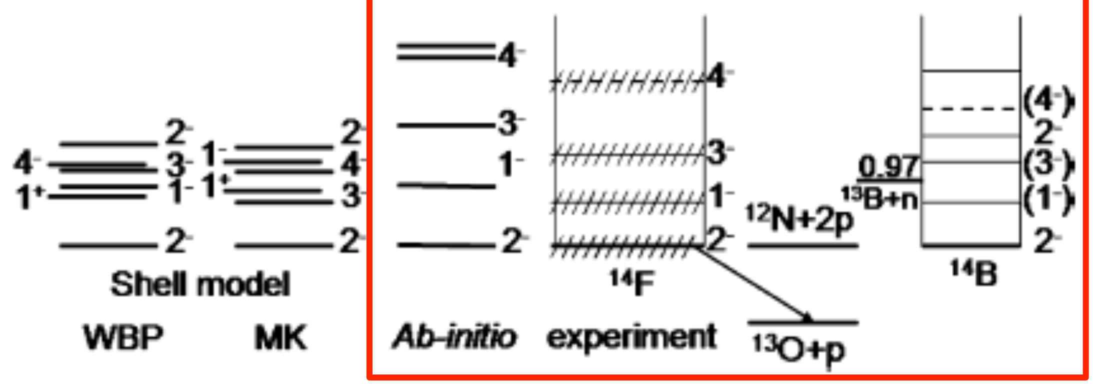
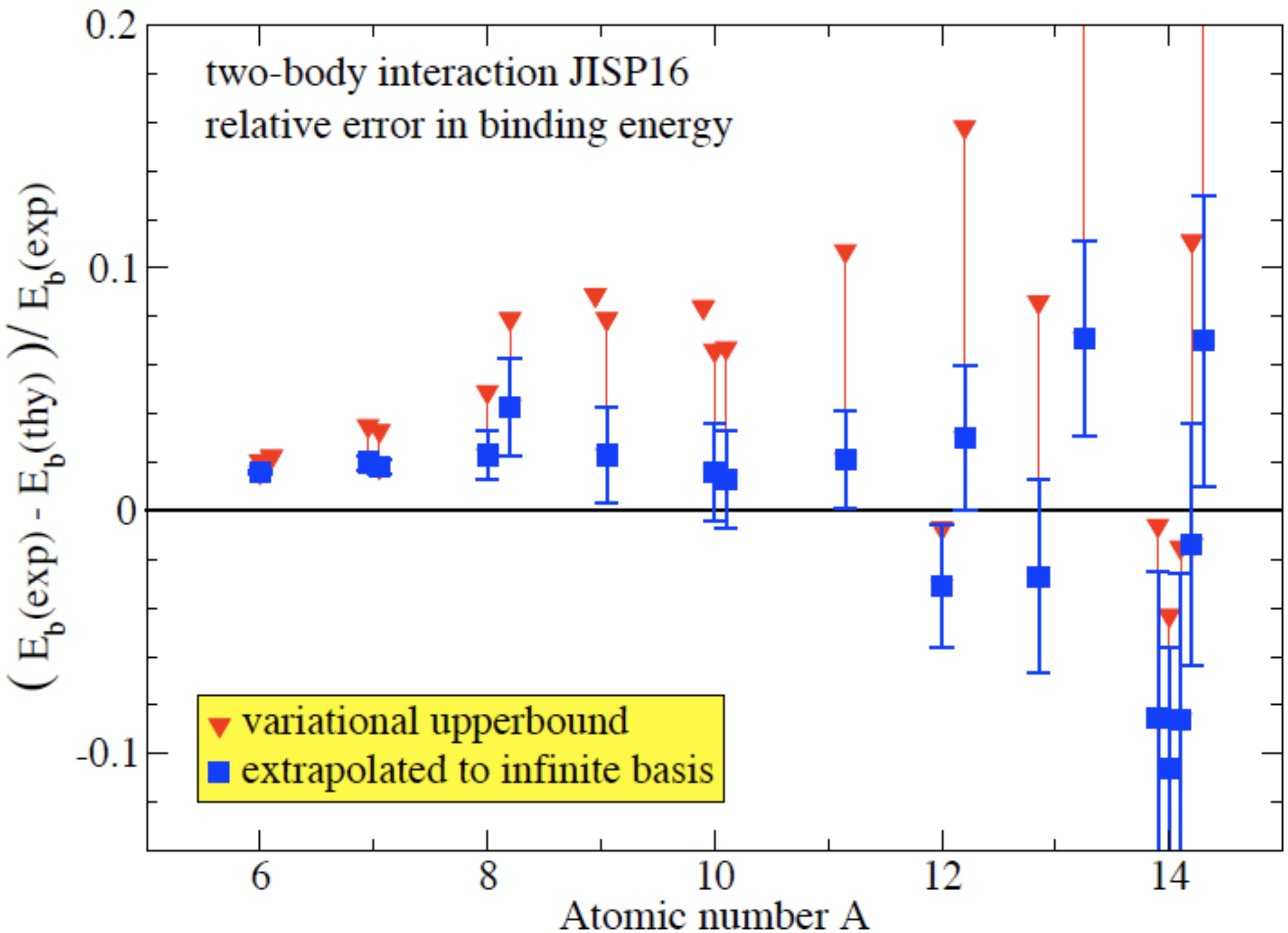


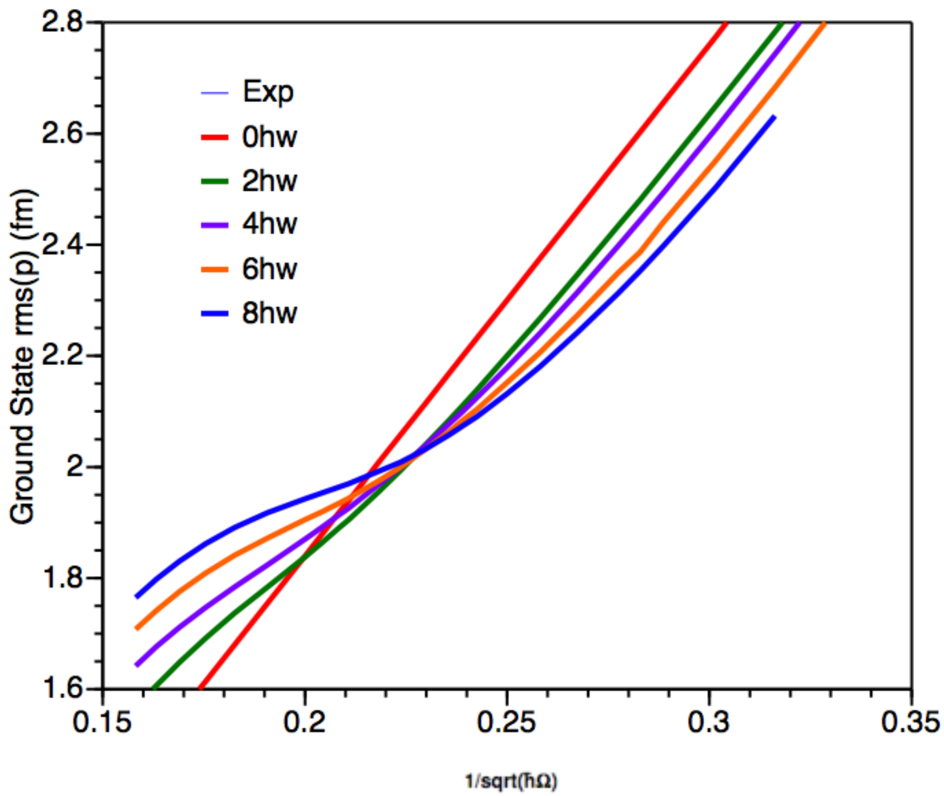
Fig. 6. ^{14}F level scheme from this work compared with shell-model calculations, *ab-initio* calculations [3] and the ^{14}B level scheme [16]. The shell model calculations were performed with the WBP [21] and MK [22] residual interactions using the code COSMO [23].

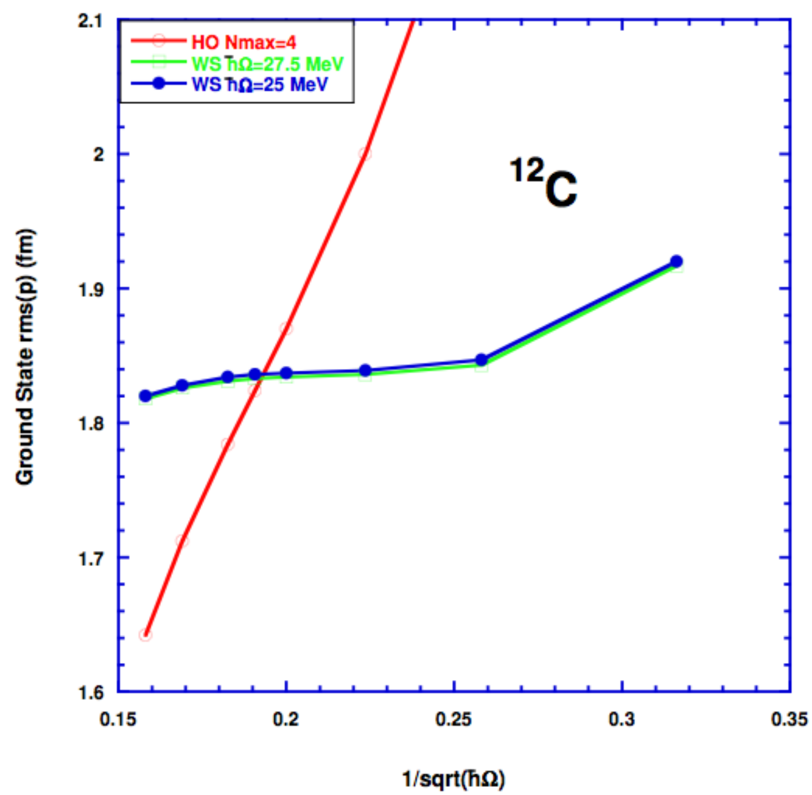
Summary of NCFC results with JISP16

Comparison of data and theory for natural parity ground state energies



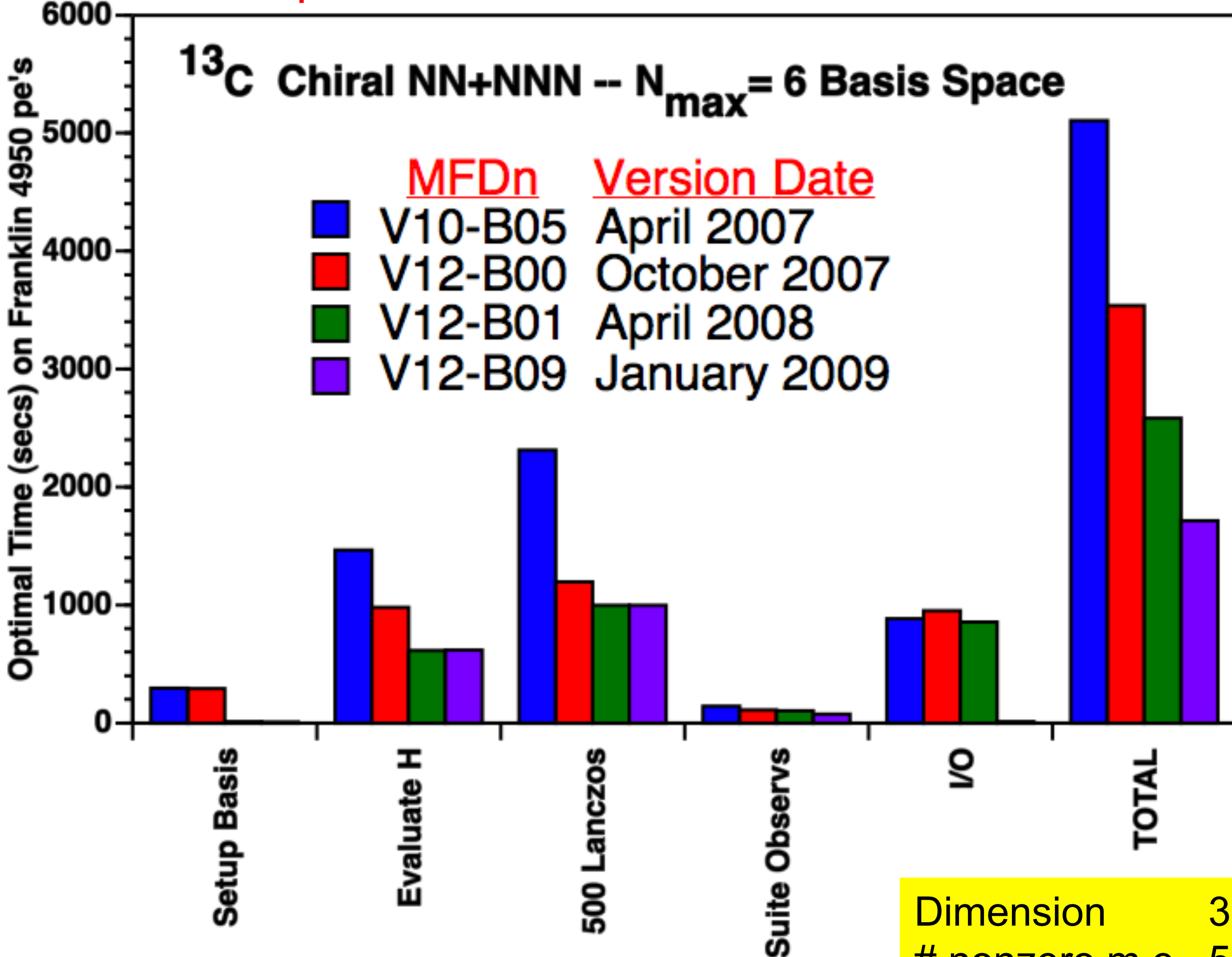
^{12}C point proton rms radius
Harmonic oscillator versus Saxon-Woods basis
expanding the SW states in 10 oscillator shells





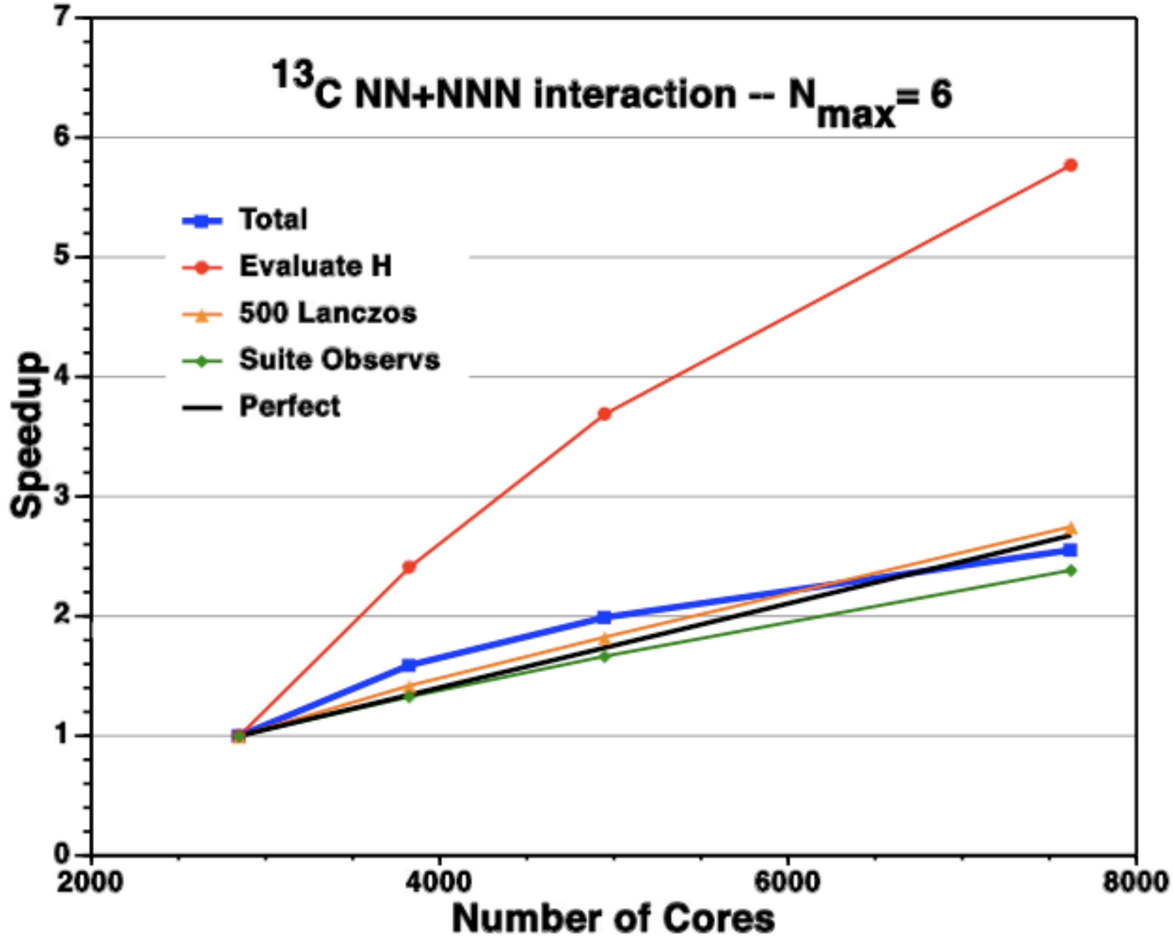
A. Negoita, PhD thesis, Iowa State

Improvements to MFDn under SciDAC



Dimension	38×10^6
# nonzero m.e.	56×10^{10}
Input 3b m.e.	3 Gbytes

Scaling on Franklin



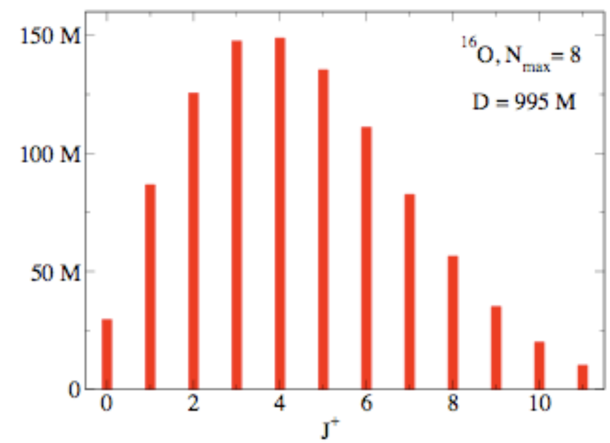
dimension $38 \cdot 10^6$

nonzero m.e. $56 \cdot 10^{10}$

size input 3 GB

Under development

- Generalized single-particle basis
  - basis functions with realistic asymptotic behavior should improve convergence of observables such as $\langle r^2 \rangle$ and $\mathcal{Q}$
- Expand and generalize external fields
  - necessary for connection with DME/DFT
- Output of one-body density matrices
- Extend 3-body forces to larger model spaces
- Hybrid MPI and OpenMP
- Coupled J-basis
  - significant reduction in # of basis states
  - matrices less sparse



- Scattering applications
  - RGM (Navratil), other methods (Shirokov, Elster?)

Near-term physics developments/collaborators

- ❖ Symplectic basis space - Draayer, Dytrych, Sviratcheva, Bahri
- ❖ Renormalization with a core - Lisetskiy, Barrett, Navratil, Stetcu, Kruse
- ❖ Alternative converging sequences - Forssen, Navratil
- ❖ Benchmark MCSM, FCI-NC & NCFC - Abe, Maris, Otsuka, Shimizu, Utsuno
- ❖ A = 12 GT transitions - Forssen, Navratil, Experimentalists
- ❖ A = 14 GT transitions - Dean, Navratil, Ormand, Nan, Maris
- ❖ Extensions to reactions/scattering - Navratil, Quaglioni, Forssen, Shirokov, Mazur
- ❖ Chiral $V_{NN}+V_{3N}$ with NCSM - Navratil, Ormand
- ❖ Chiral $V_{NN}+V_{3N}$ with SRG/Vlowk+NCFC - Maris, Bogner, Schwenk, Furnstahl
- ❖ Trapped fermion systems - Stetcu, Barrett, van Kolck
- ❖ Comparison of CC with FCI - Maris, Hagen, Papenbrock, Dean
- ❖ UNEDF/SciDAC external fields - Maris, Furnstahl, Bogner
- ❖ UNEDF/SciDAC realistic basis - Negoita, Maris, Shirokov
- ❖ Infinite matter applications – Bogner, Shirokov, Coester, Negoita, Gogny, Mazur
- ❖ Light-front quantum field theory - Honkanen, Li, Brodsky, Harindranath, Maris

Near-term applied math & computer science developments/collaborators

- ❖ Search & Per-processor efficiency - Sosonkina, Laghave, Negoita (Ames Lab,ISU)
- ❖ Mat-Vec & blocking strategies - Ng, Yang, Sternberg (LBNL)
- ❖ Cluster and web-site development - Aronnax (ISU)
- ❖ Compressed basis representation - Cockrell (ISU)
- ❖ I/O improvements - Hai Ah Nam (ORNL), Sosonkina, Laghave (Ames Lab, ISU)

Conclusions and Outlook

- Established need for 3N potentials with Chiral NN potentials
- Chiral EFT N3LO+3NF & JISP16 are suitable interactions for light nuclei up through 16-O (40-Ca under investigation)
- No-Core FC with realistic NN interactions can be extrapolated to obtain converged energies & uncertainties for low-lying states
- Many experimental observables need investigation
- Current efforts - nuclei with tunable external fields (DFT/DME)
- Future plans - accelerate convergence using a symplectic basis
- Future plans - explore exotic nuclei with these frameworks
- Future plans - reactions/scattering with these frameworks
- Leadership class computing facilities - “discovery engines”

Nuclear Physics Calculator: *ab initio* NCSM demonstration project

nuclear.physics.iastate.edu

- Select the NCSM application
- Enter your email address
- Select the number of neutrons and protons
- Select the N_{max}
- Select the oscillator energy, $\hbar\Omega$

Results file with the JISP16 interaction will be emailed to you in a few minutes

Note that this is a demonstration project and will evolve as funding permits

Acknowledgements

- Collaborators mentioned above
- Support from DOE (DE-FG02-87ER-40371, DE-FC02-09ER41583, DOE INCITE Award, LLNL Atlas Discovery Class Computing Award)
- Invitation from the organizers of the school for this opportunity