Origin of the anomalous long lifetime of ^{14}C

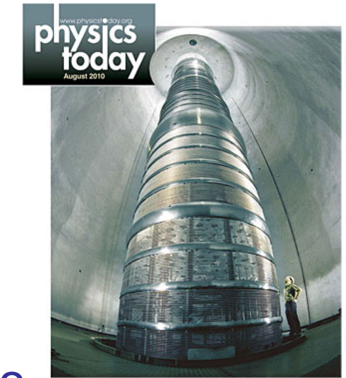
James P. Vary
Iowa State University
February 10, 2011

Perspectives of the ab initio no-core shell model (NCSM)
TRIUMF, Vancouver, BC
Feb 10-12, 2011

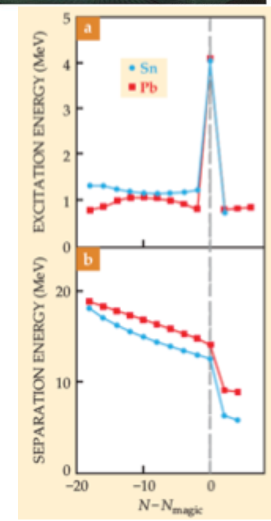
Subtheme
Rapidly growing computational power
and the opening of new vistas for fundamental science

Collaborators: P. Maris, P. Navratil, H. Nam, W.E. Ormand, D. Dean

Ab initio nuclear physics - fundamental questions



- What controls nuclear saturation?
- How the nuclear shell model emerges 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 predict nuclear structure and reactions from QCD?



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Universal Nuclear Energy Density Functional

QCD
Theory of strong interactions

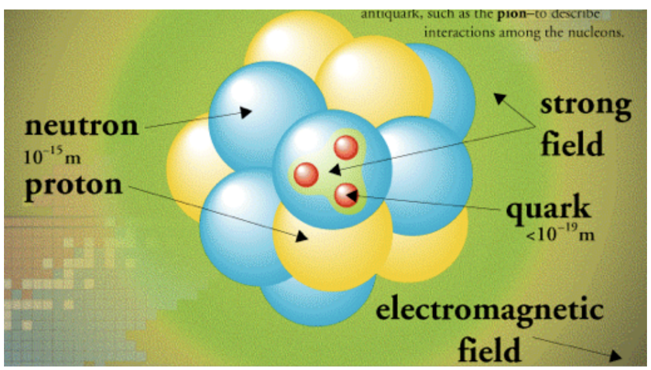
χEFT
Chiral Effective Field Theory

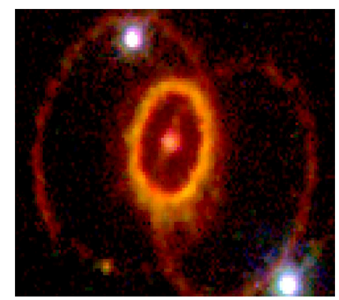
Inter-Nucleon
NN, NNN Interactions
AV18, EFT, $V_{low\text{-}k}$

Theory of Light Nuclei
Spectroscopy and selected reactions
Verification: NCSM=GFMC=CC
Validation: nuclei with A<16

Big Bang
Nucleosynthesis
& Stellar Reactions

Density Functional Theory
improved functionals
remove computationally-imposed constraints
properties for all nuclei with A>16





Dynamic Extensions of DFT
LACM by GCM,TDDFT,QRPA
Level densites

Low-energy Reactions
Hauser-Feshbach
Feshbach-Kerman-Koonin
Fission
mass and energy distributions

r,s processes
& Supernovae

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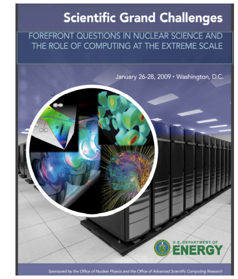
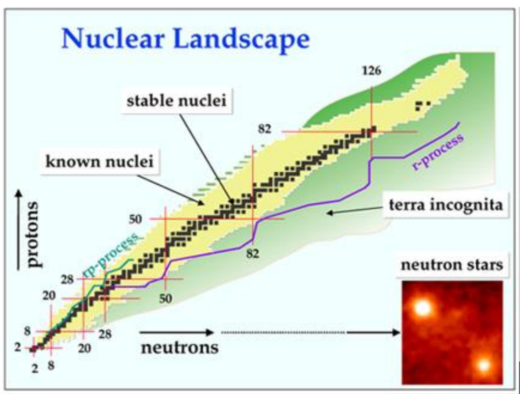
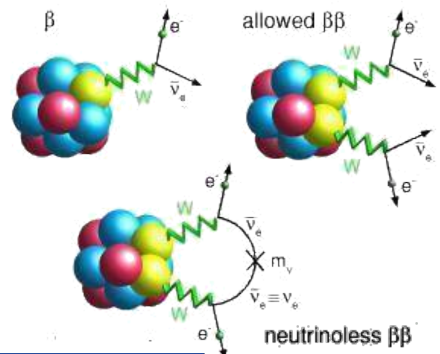
DOE Workshop on Forefront Questions in Nuclear Science
and the Role of High Performance Computing,
Gaithersburg, MD, January 26-28, 2009
Nuclear Structure and Nuclear Reactions

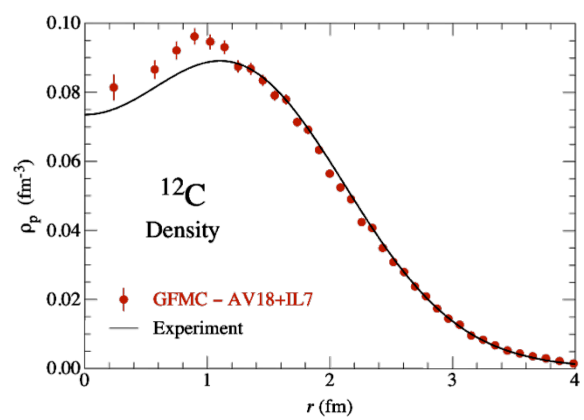


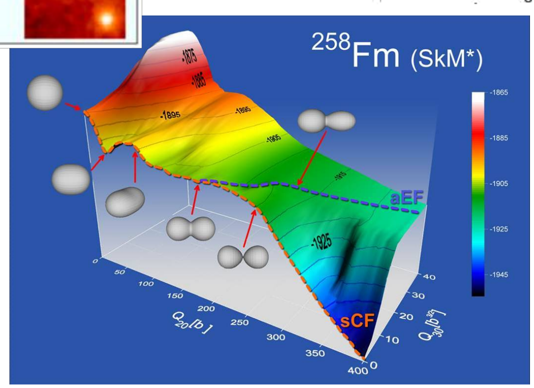
List of Priority Research Directions

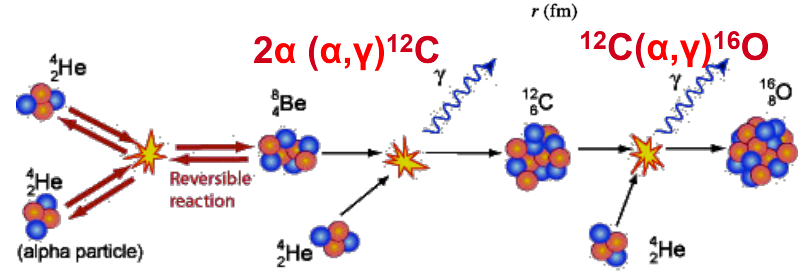
- **Physics of extreme neutron-rich nuclei and matter**
- **Microscopic description of nuclear fission**
- **Nuclei as neutrino physics laboratories**
- **Reactions that made us – triple α process and $^{12}C(\alpha,\gamma)^{16}O$**

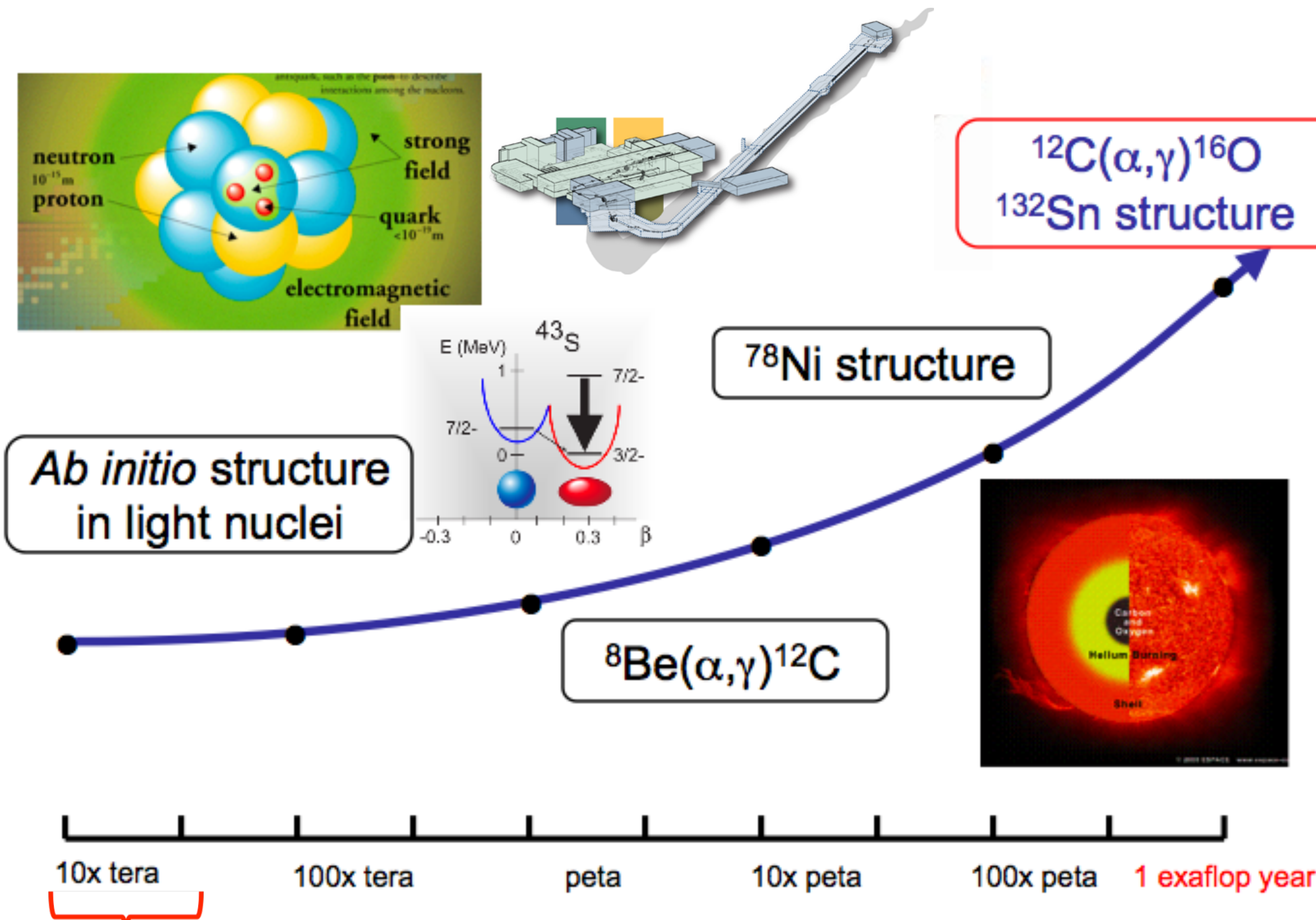












~ INCITE award in 2011

~1 week of dedicated JaguarPF runs

All interactions are "effective" until the ultimate theory unifying all forces in nature is attained.

Thus, even the Standard Model, incorporating QCD,
is an effective theory valid below the Planck scale
$\lambda < 10^{19}$ GeV/c

The "bare" NN interaction, usually with derived quantities,
is thus an effective interaction valid up to some scale, typically
the scale of the known NN phase shifts and Deuteron gs properties
$\lambda \sim 600$ MeV/c ($3.0\ \mathrm{fm}^{-1}$)

Effective NN interactions can be further renormalized to lower scales
and this can enhance convergence of the many-body applications
$\lambda \sim 300$ MeV/c ($1.5\ \mathrm{fm}^{-1}$)

"Consistent" NNN and higher-body forces are those valid
to the same scale as their corresponding NN partner,
and obtained in the same renormalization scheme.

ab initio renormalization schemes

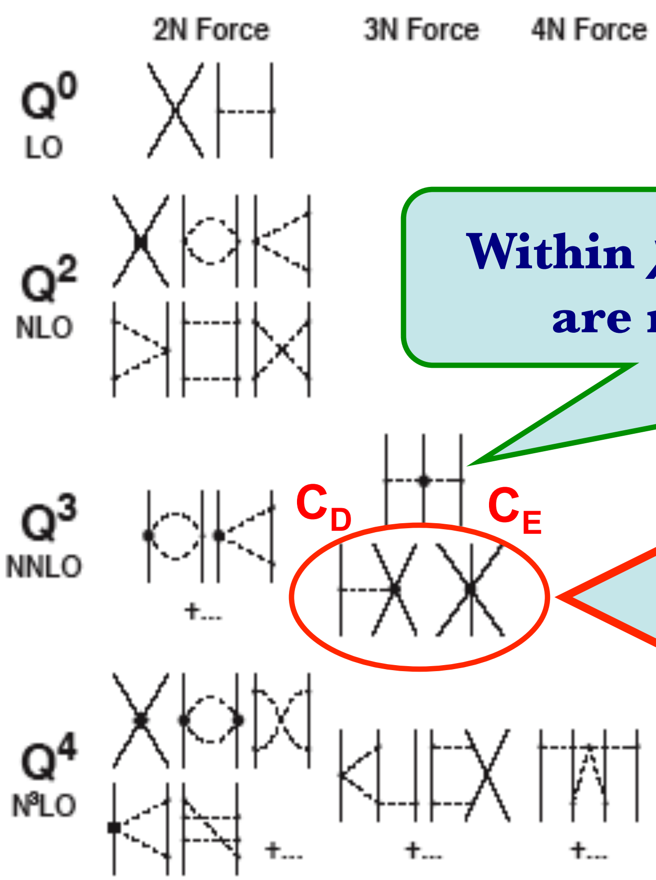
SRG: Similarity Renormalization Group
LSO: Lee-Suzuki-Okamoto
Vlowk: V with low k scale limit
UCOM: Unitary Correlation Operator Method
and there are more!

Effective Nucleon Interaction
(Chiral Perturbation Theory)

Chiral perturbation theory (χPT) allows for controlled power series expansion

$$\text{Expansion parameter}: \left(\frac{Q}{\Lambda_\chi}\right)^{\upsilon},\ Q-\text{momentum transfer},$$

$$\Lambda_\chi \approx 1\ GeV,\ \chi\text{ - symmetry breaking scale}$$



R. Machleidt, D. R. Entem, nucl-th/0503025

Within χPT 2π-NNN Low Energy Constants (LEC) are related to the NN-interaction LECs $\{c_i\}$.

Terms suggested within the
Chiral Perturbation Theory

Further renormalization is necessary since momentum transfers still too high, reaching ~ 0.6 GeV/c

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

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

P. Navratil, J.P. Vary and B.R. Barrett,
Phys. Rev. Lett. <u>84</u>, 5728(2000); Phys. Rev. C<u>62</u>, 054311(2000)
C. Viazminsky and J.P. Vary, J. Math. Phys. 42, 2055 (2001);
K. Suzuki and S.Y. Lee, Progr. Theor. Phys. <u>64</u>, 2091(1980);
K. Suzuki, *ibid*, <u>68</u>, 246(1982);
K. Suzuki and R. Okamoto, *ibid*, <u>70</u>, 439(1983)

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

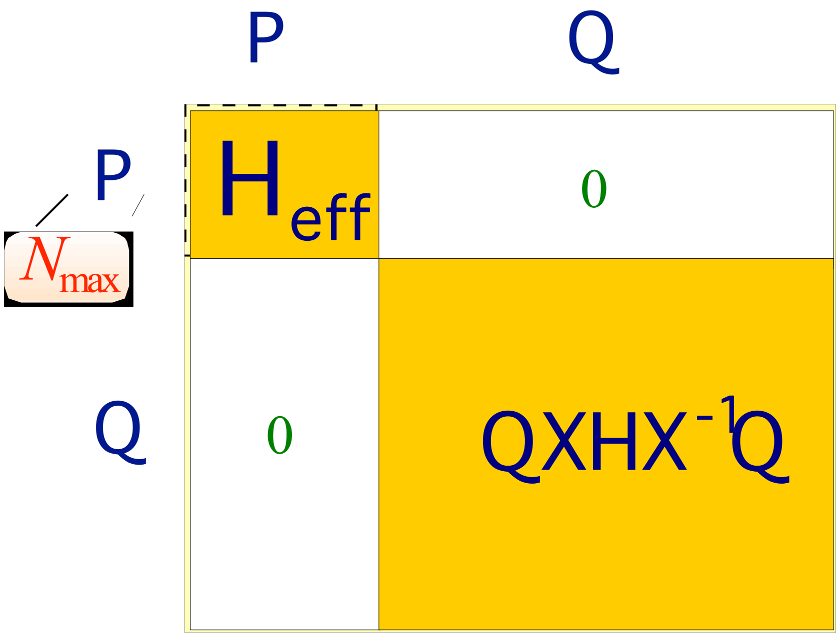
$$H_{\mathcal{A}} = T_{rel} + V = \sum_{i<j}^{\mathcal{A}} \left[\frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} + V_{ij} \right] + V_{NNN}$$

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 <u>exact</u> answers as $a \to A$ <u>or</u> as $P \to 1$.

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



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

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

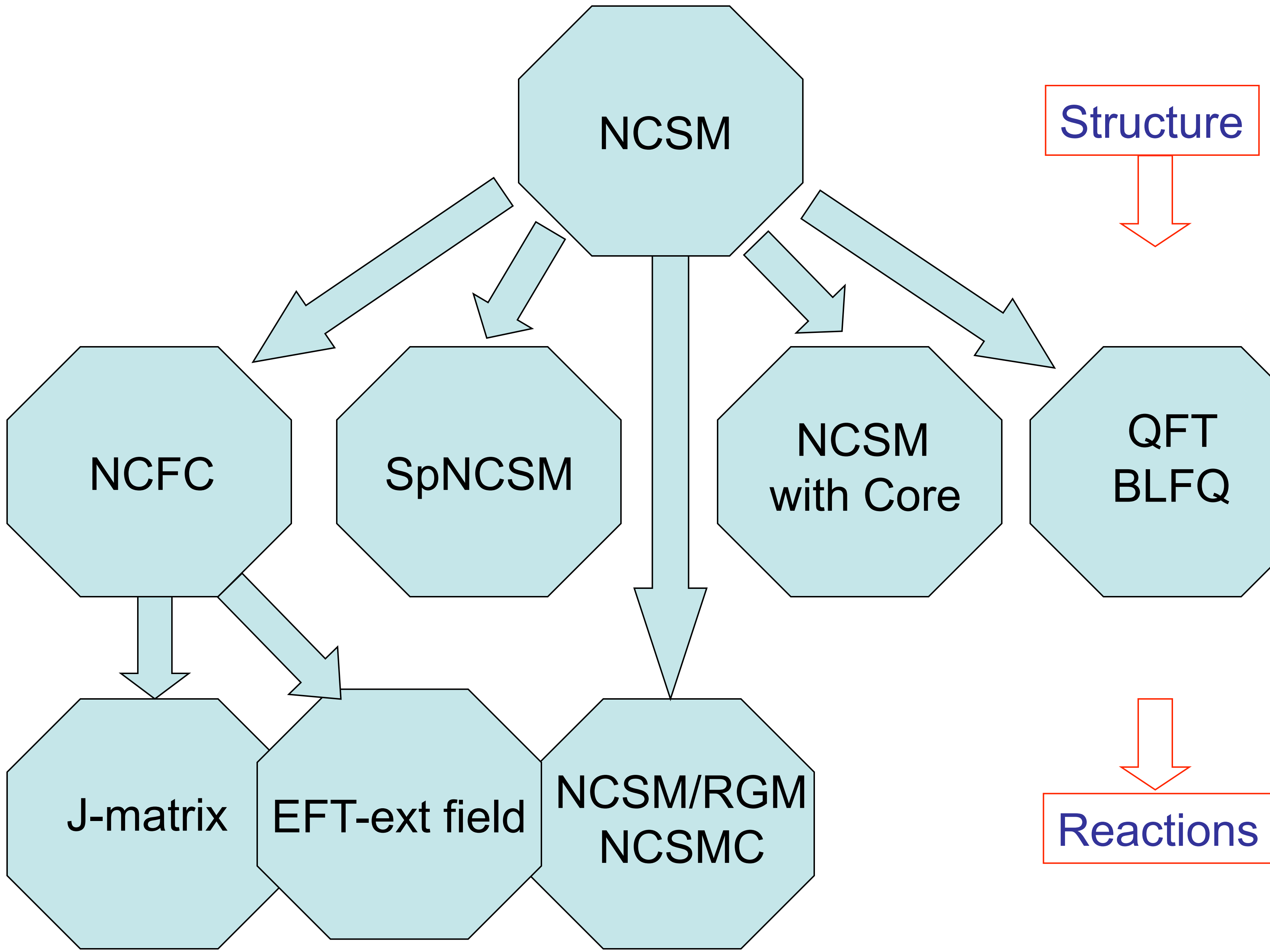
model space dimension

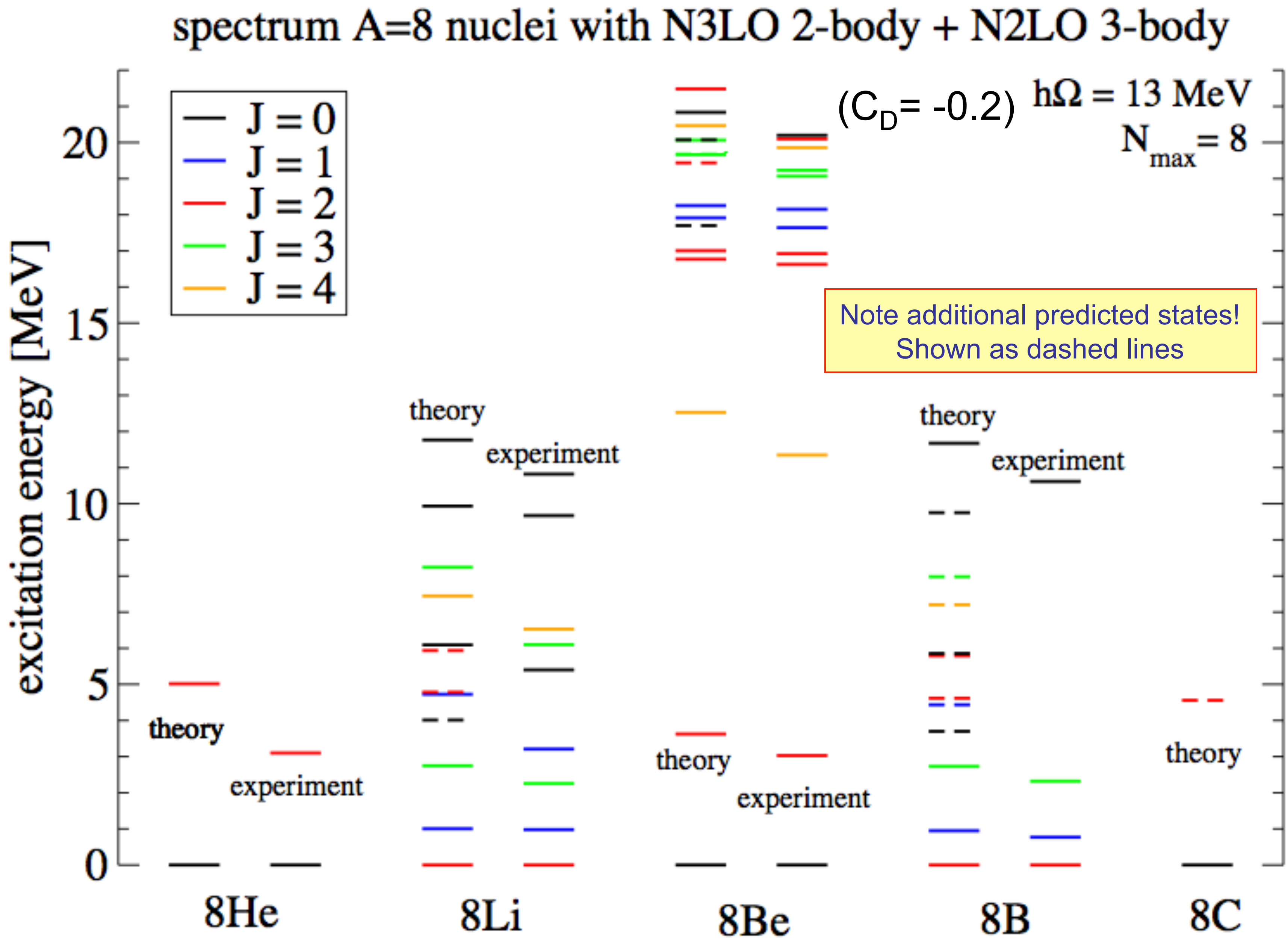
$$QXHX^{-1}P = 0$$

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

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

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

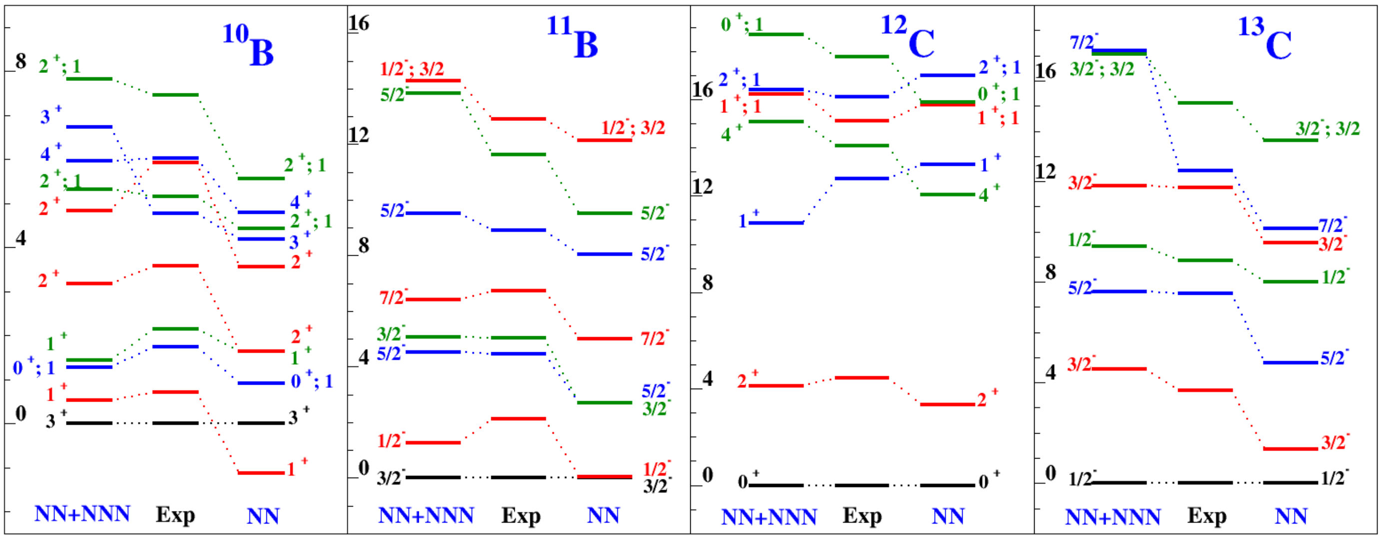

NCSM
Structure
NCFC
SpNCSM
NCSM
with Core
QFT
BLFQ
J-matrix
EFT-ext field
NCSM/RGM
NCSMC
Reactions



P. Maris, P. Navratil, J. P. Vary, to be published

ab initio NCSM with χ_{EFT} Interactions

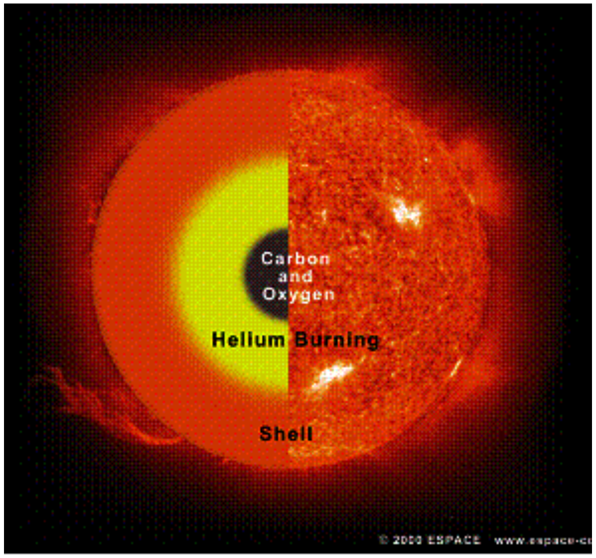
- *Only method capable to apply the χ_{EFT} NN+NNN interactions to all p-shell nuclei*
- *Importance of NNN interactions for describing nuclear structure and transition rates*



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 force itself, feedback to χ_{EFT}* (LLNL, OSU, MSU, TRIUMF/GSI)
- *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 (e.g. 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)*



^{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.

<u>Many important unsolved problems of the Hoyle state:</u>

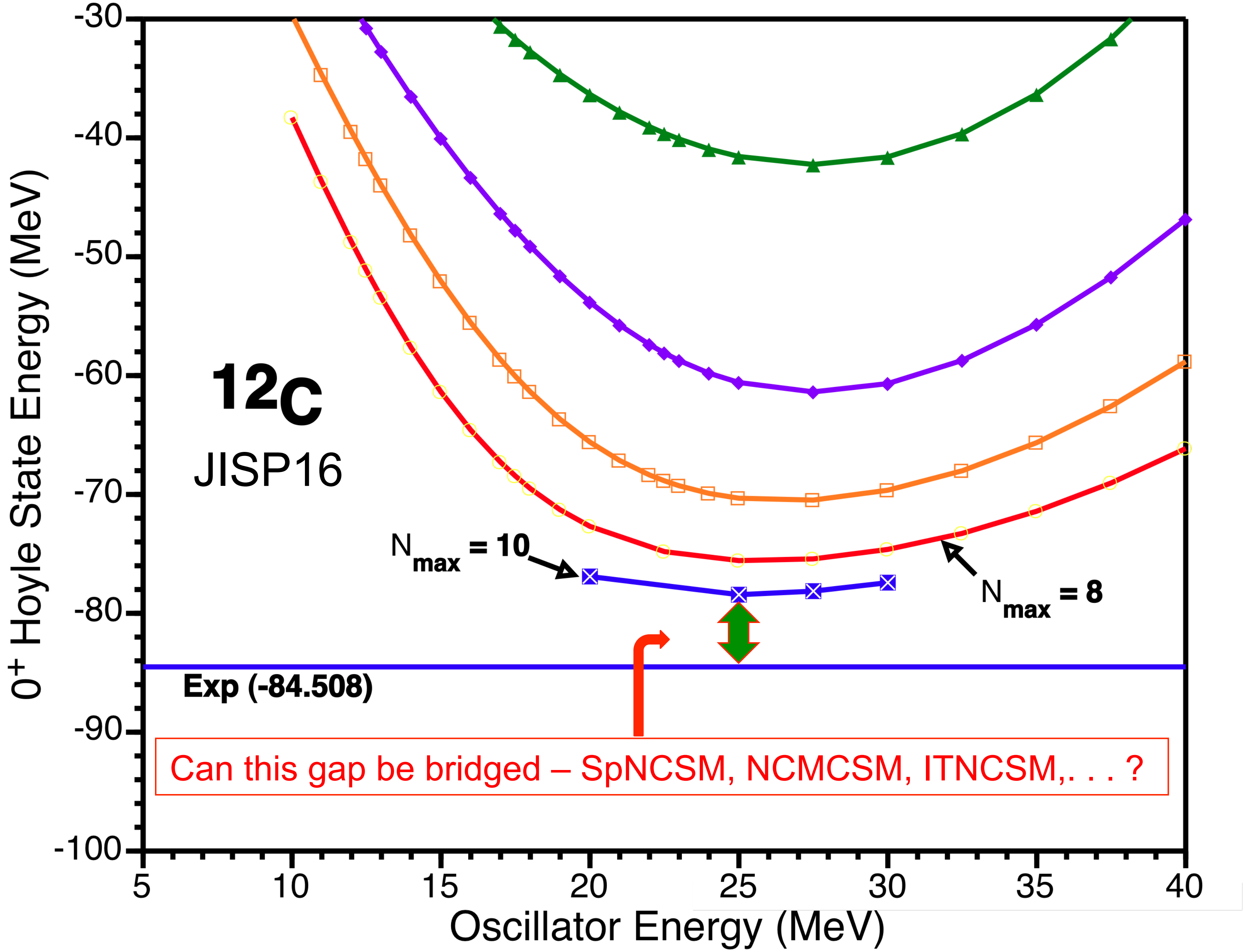
Microscopic origins of the triple-alpha structure are unsolved

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

<u>Conclusion:</u> 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 achievable with petascale within 1-2 years



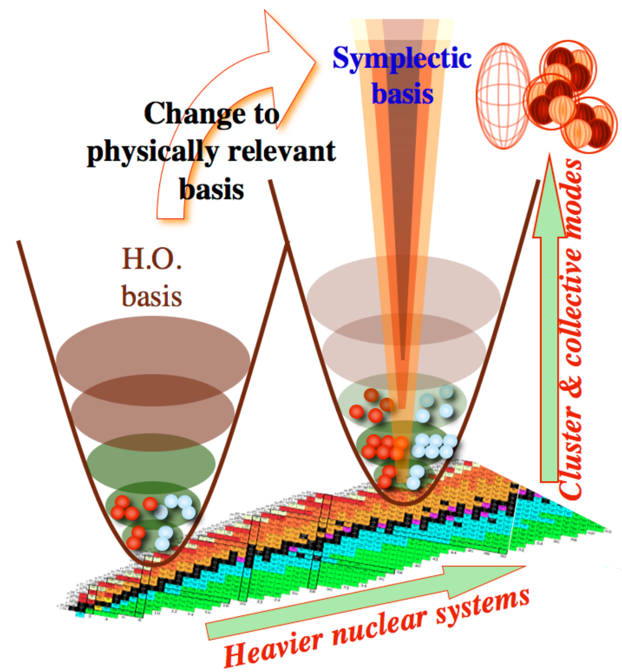
^{12}C
JISP16
N_{max} = 10
N_{max} = 8
Exp (-84.508)
Can this gap be bridged – SpNCSM, NCMCSM, ITNCSM,. . . ?
0+ Hoyle State Energy (MeV)
Oscillator Energy (MeV)
-30
-40
-50
-60
-70
-80
-90
-100
5
10
15
20
25
30
35
40

Taming the scale explosion in nuclear calculations – Tomas Dytrych's talk here
NSF PetaApps - Louisiana State, Iowa State, Ohio State collaboration

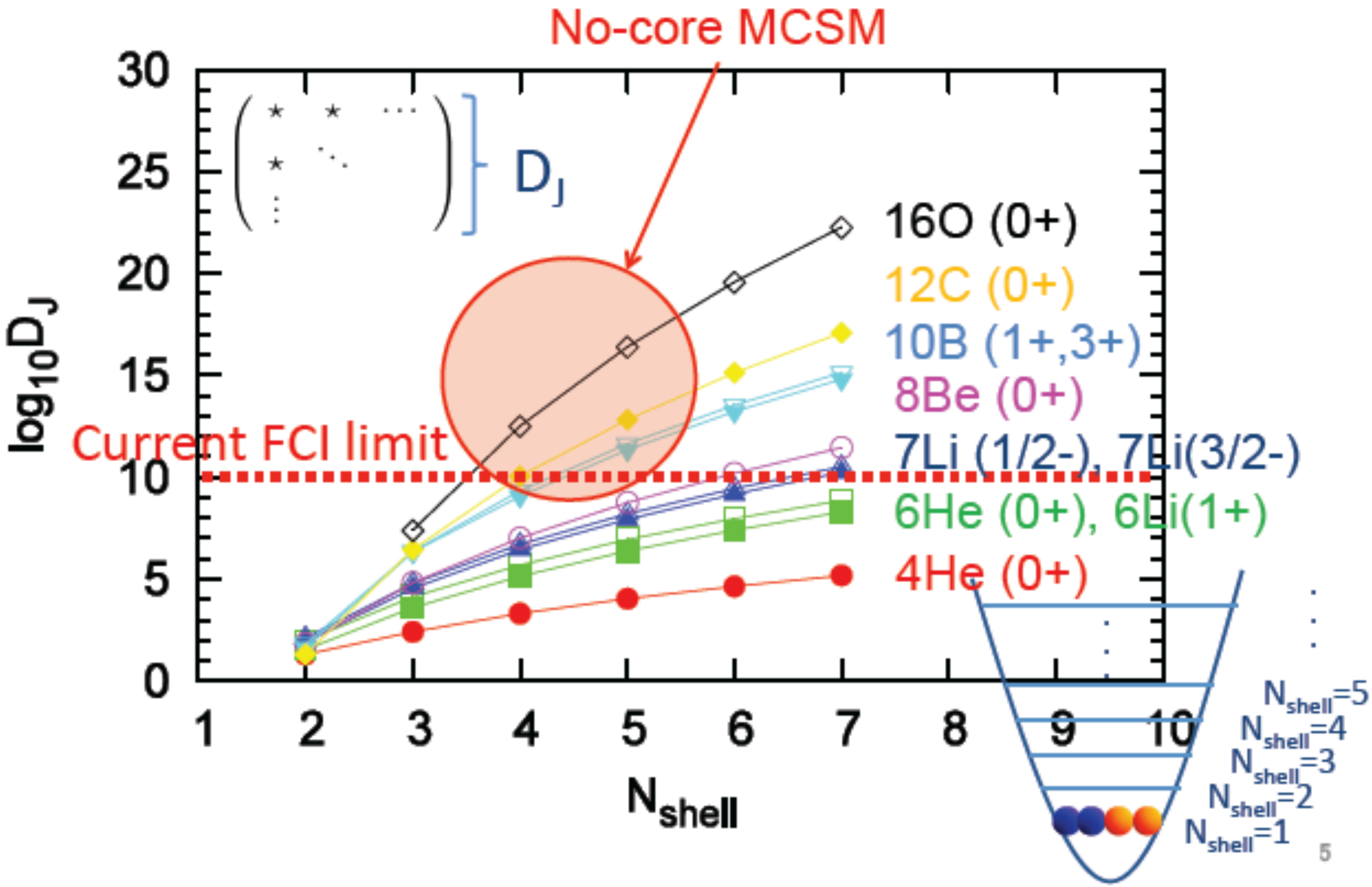
- Goals
  - Ab initio calculations of nuclei with unprecedented accuracy using basis-space expansions
  - Current calculations limited to nuclei with A $\leq$ 16 (up to 20 billion basis states with 2-body forces)

- Progress
  - Scalable CI code for nuclei
  - Sp(3,R)/SU(3)-symmetry vital
- Challenges/Promises
  - Constructing hybrid Sp-CI code
  - Publicly available peta-scale software for nuclear science

- Novel approach
  - Sp-CI: exploiting symmetries of nuclear dynamics
  - Innovative workload balancing techniques & representations of multiple levels of parallelism for ultra-large realistic problems
- Impact
  - Applications for nuclear science and astrophysics



J-scheme dimension

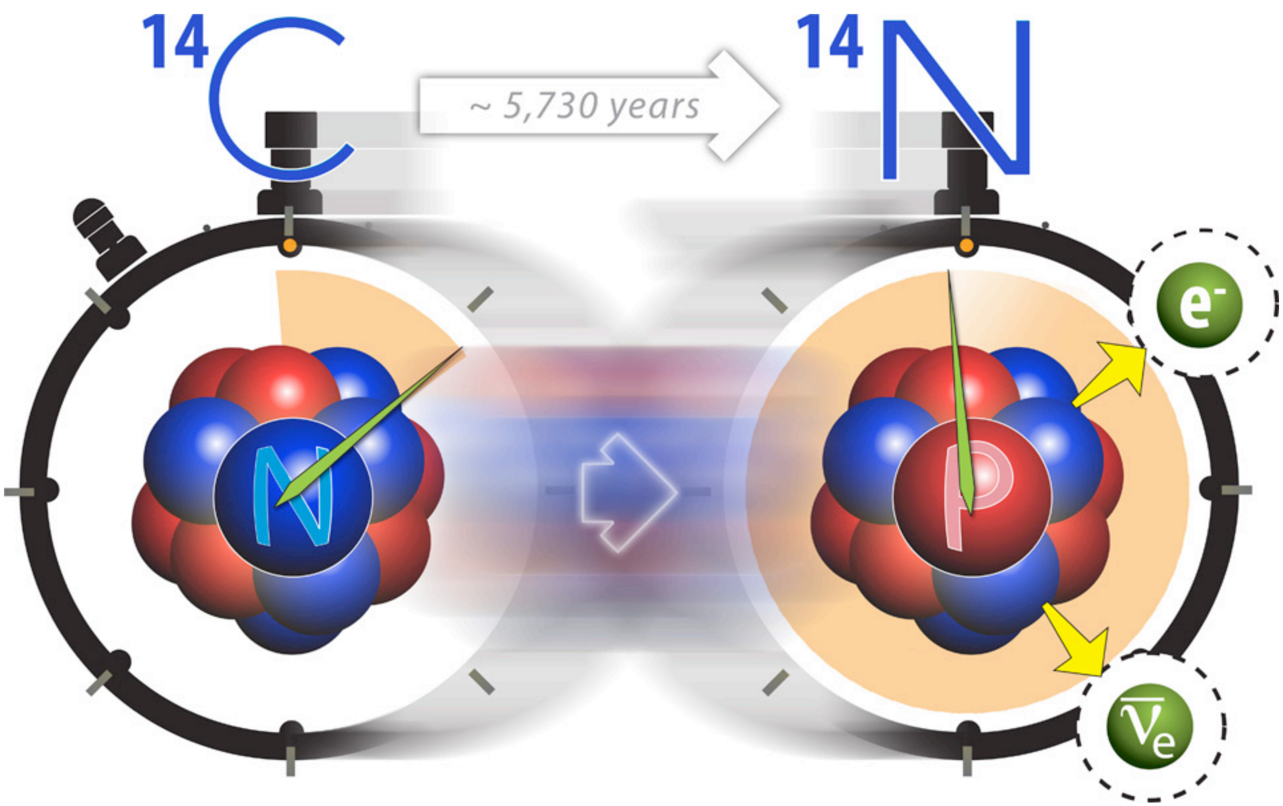


Talk by Takashi Abe at this workshop

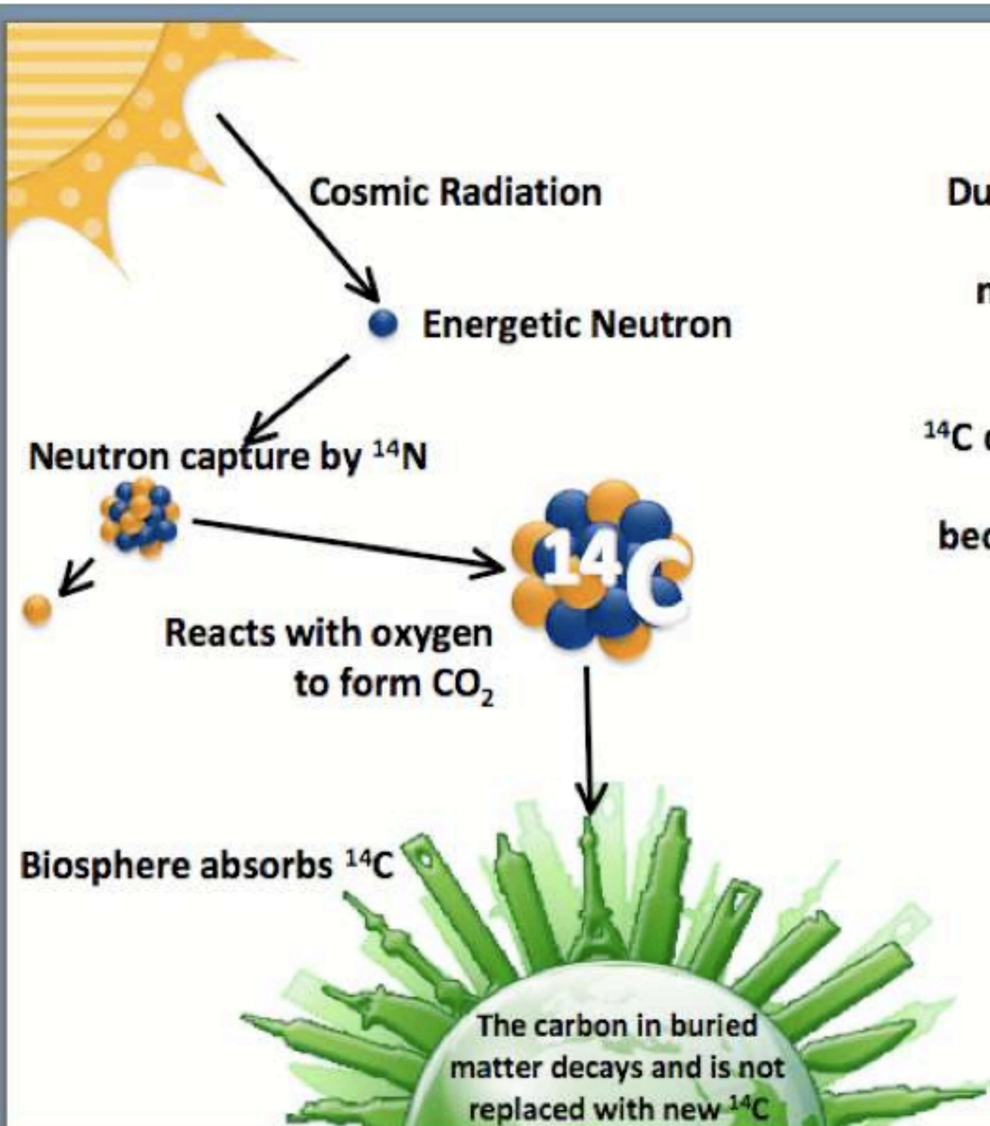
Origin of the anomalous long lifetime of ^{14}C

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

arXiv: 1101.5124 and submitted for publication



Petascale Early Science – Ab-initio structure of Carbon-14



Due to its long half-life, ^{14}C has been used in dating organic materials, up to 60,000 years old, since the 1950's.

^{14}C decays into ^{14}N through beta decay, where a neutron becomes a proton, an electron, and an antineutrino.

Jaguar PF award of 30,000,000 cpu hours

Petascale Early Science – Ab-initio structure of Carbon-14

Puzzling to scientists …

What is the nuclear structure of ^{14}C that leads to its anomalously long half-life?

$\tau_{1/2}$ = 5730 years

^{10}Be and ^{14}C have extremely long half-lives compared to other light nuclei (1.6×10^6 years / 5,730 years) . Their long half-lives make both isotopes useful for radioactive dating.

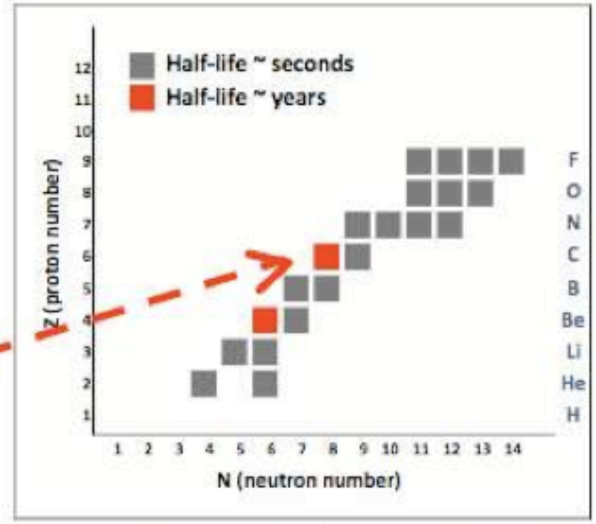
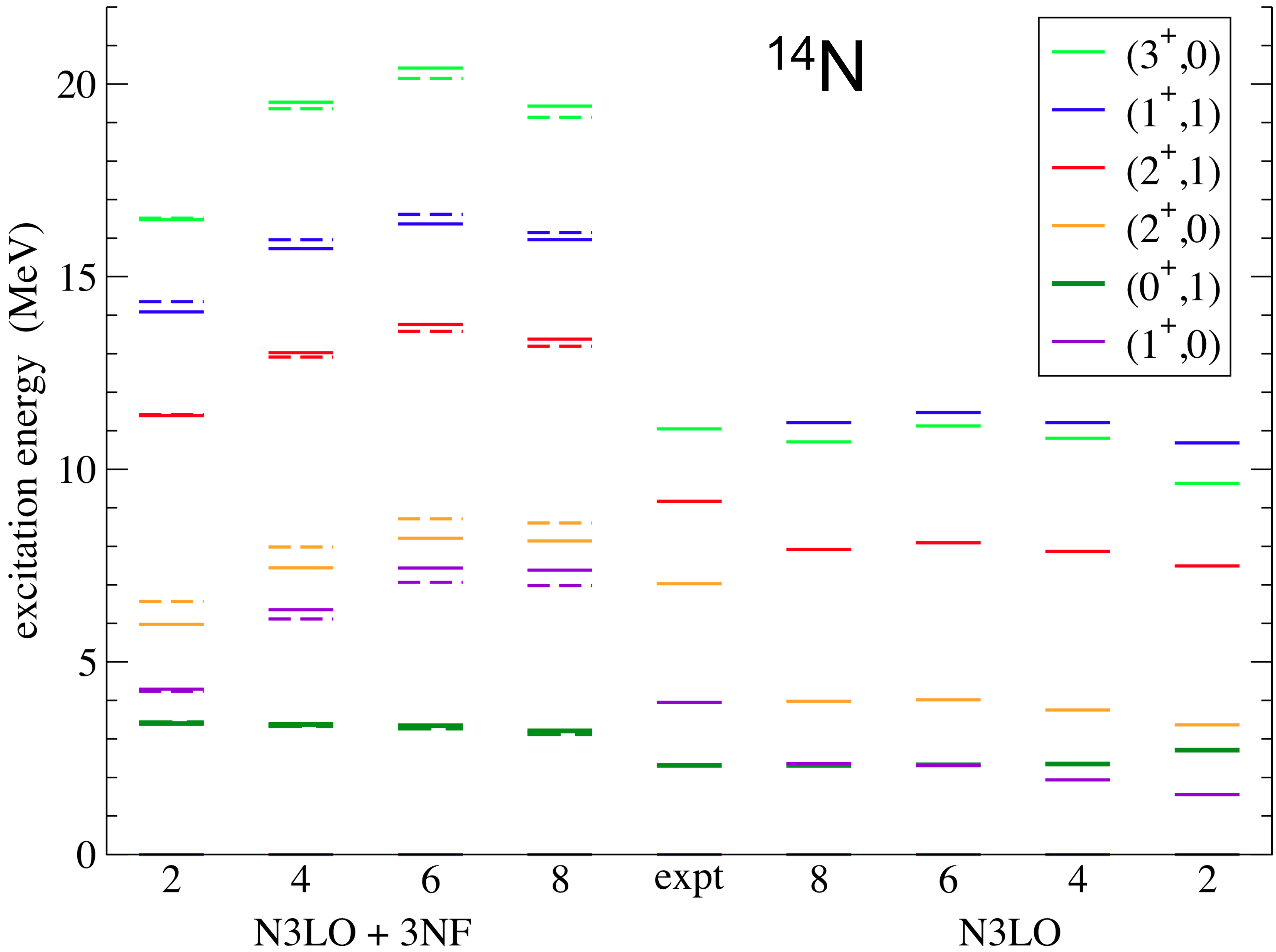


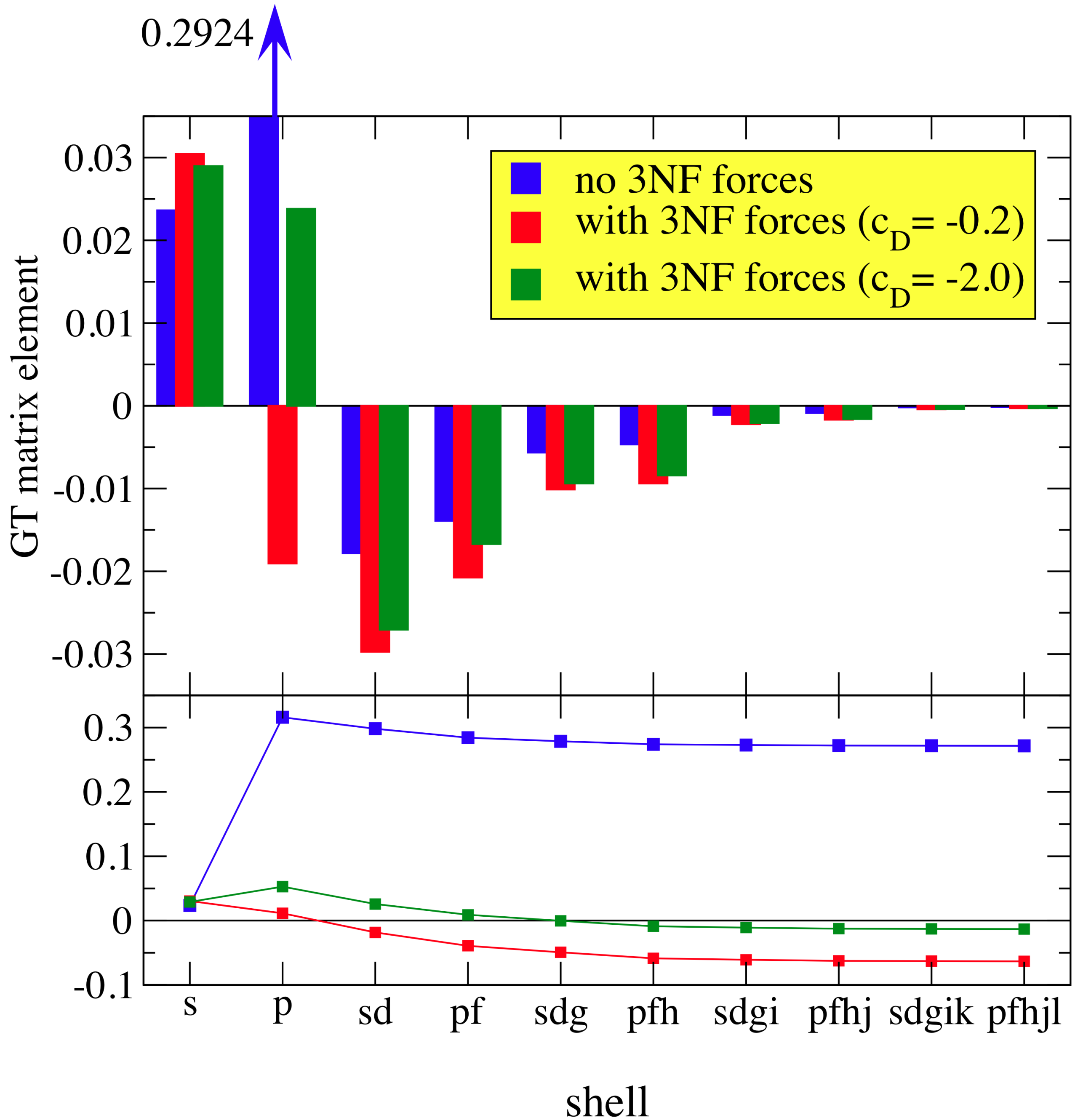
Chart of light nuclei that decay via beta emissions

$$n \rightarrow p + e^- + n_e$$

Transition	Experimental	Calculated
B(GT) : $^{10}Be \rightarrow {}^{10}B$	0.08	0.06 (3-body : 0.066)
B(GT) : $^{14}N \rightarrow {}^{14}C(\Sigma 2^+)$	0.92(33)	2.61 (CD-Bonn)
		1.62 (JISP16)



^{14}N
excitation energy (MeV)
0
5
10
15
20
(3$^+$,0)
(1$^+$,1)
(2$^+$,1)
(2$^+$,0)
(0$^+$,1)
(1$^+$,0)
2
4
6
8
expt
8
6
4
2
N3LO + 3NF
N3LO


0.2924
no 3NF forces
with 3NF forces (c_D= -0.2)
with 3NF forces (c_D= -2.0)
GT matrix element
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
0.3
0.2
0.1
0
-0.1
s
p
sd
pf
sdg
pfh
sdgi
pfhj
sdgik
pfhjl
shell

(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

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.

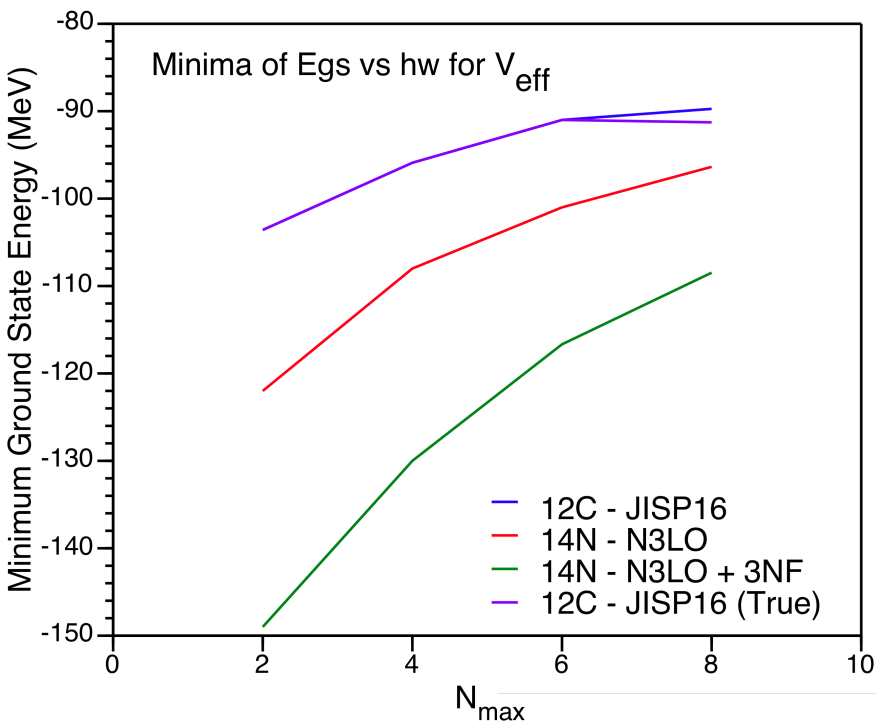
Tritium half-life

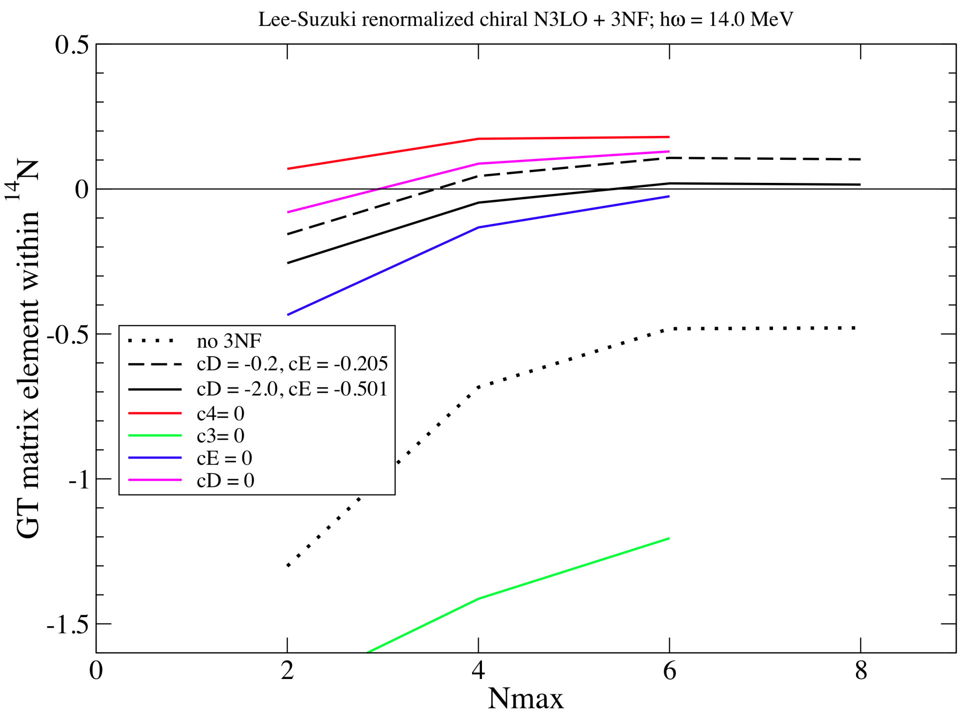
c_D	=	-0.20	-2.0
Thy/Exp.	=	1.00	0.80

Uncertainty Quantification (UQ)

Two approaches - each need quantified uncertainties:

1) Allow $\{c_i\}$ to absorb approximations to V, V_{eff} and MB basis truncation => $\{c_i \pm \delta c_i\}$ when describing expt => consistent with "naturalness"?
2) Fixed $\{c_i\}$, e.g. from LQCD or few-body sytems, calculate observables => $\{O_i \pm \delta O_i\}$ => consistent with expt?

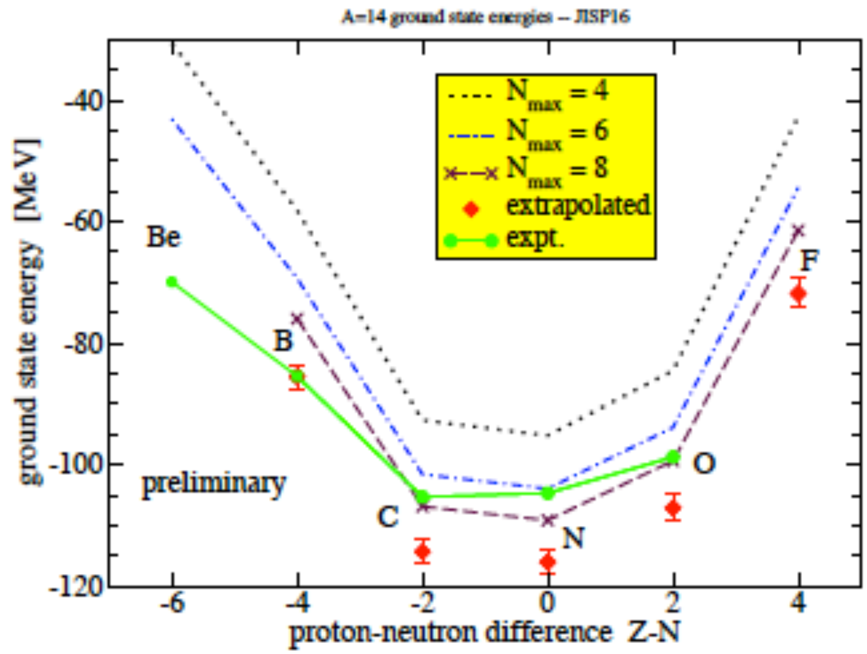




Descriptive Science

Predictive Science

Results with JISP16 for $A = 14$ nuclei



- Preliminary results
  - up to 10% overbinding for ^{14}C, ^{14}N, ^{14}O
  - ^{14}N ground state lower than ^{14}C ground state...
- Need improved (charge-dependent?) interaction

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

ELSEVIER

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

NCFC predictions (JISP16) in close agreement with experiment

TAMU Cyclotron Institute

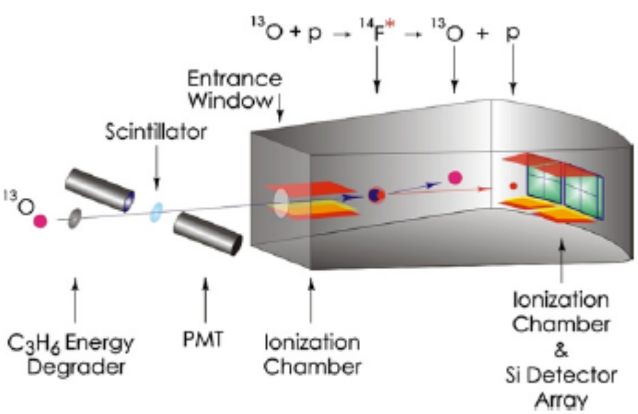


Fig. 1. (Color online.) The setup for the ^{14}F experiment. The "gray box" is the scattering chamber. See explanation in the text.

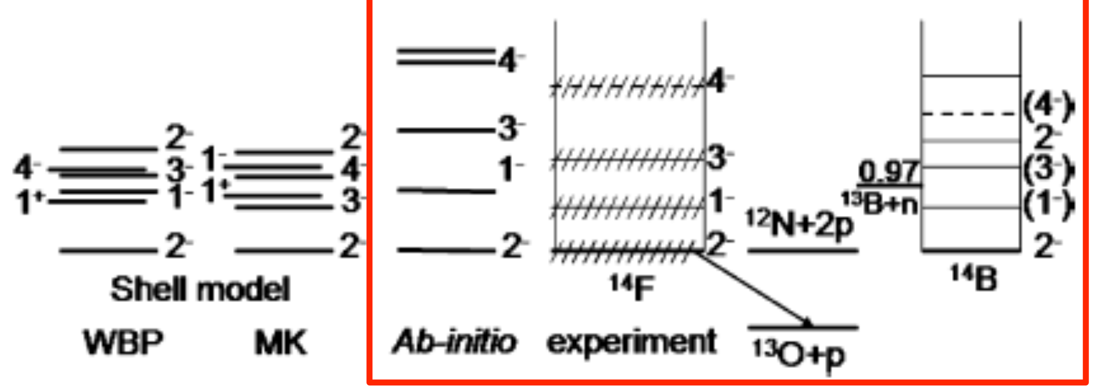


Fig. 6. ^{14}F level scheme from this work compared with shell-model calculations, *ab-initio* calculations [3] and the ^{14}B level scheme [16]. The shell model calculations were performed with the WBP [21] and MK [22] residual interactions using the code COSMO [23].

Ab initio Nuclear Structure & Reactions

Nonperturbative Quantum Field Theory
Hamiltonian Light-Front Quantization
QED applications

Basis Light-Front Quantized (BLFQ) Field Theory

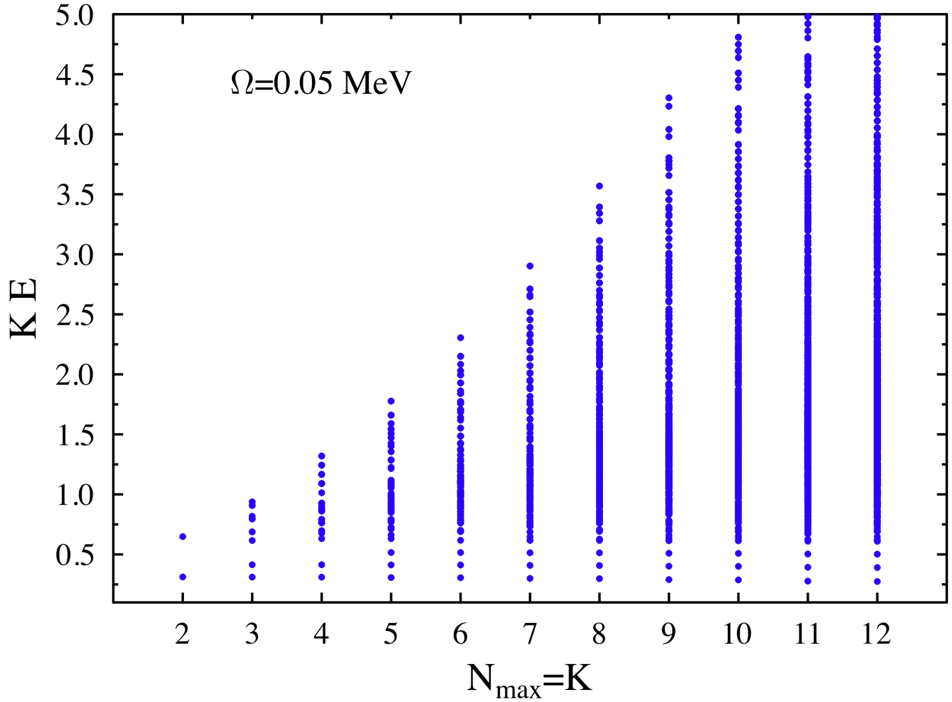
J. P. Vary, H. Honkanen, Jun Li, P. Maris, S. J. Brodsky, A. Harindranath, G. F. de Teramond, P. Sternberg, E. G. Ng, C. Yang, "Hamiltonian light-front field theory in a basis function approach", Phys. Rev. C 81, 035205 (2010); arXiv nucl-th 0905.1411

First non-perturbative QED application

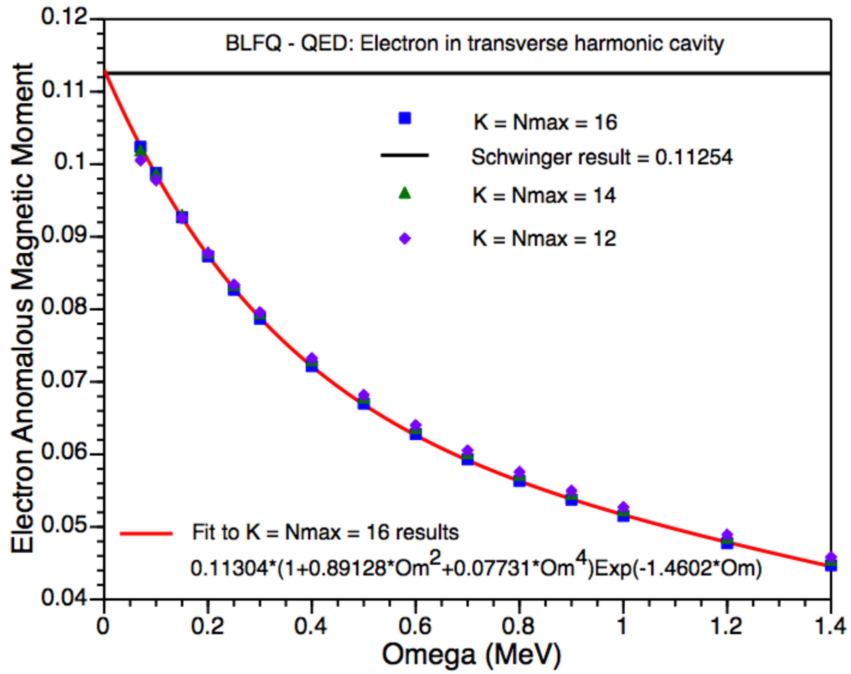
$m_e = 0.511$ MeV; $M_j = 1/2$

$g_{QED} = [4\pi\alpha]^{1/2}$; lepton & lepton-photon Fock space only

M^2 eigenstates



Anomalous moment



H. Honkanen, P. Maris, J. P. Vary and S. Brodsky, Phys. Rev. Lett. 106, 061603 (2011), arXiv 1008.0068

Conclusions

We have entered an era of first principles, high precision, nuclear structure and nuclear reaction theory

Accurate descriptive and, especially, predictive power emerges

Linking nuclear physics and the cosmos through the Standard Model is well underway

Pioneering collaborations between Physicists, Computer Scientists and Applied Mathematicians have become essential to progress

Key Challenges

How to capitalize on the predictive power and achieve the full physics potential of *ab initio* theory?

Can theory and experiment collaborate to define/solve fundamental physics problems?

Uncertainty Quantification

Collaborators – *ab initio* Nuclear Structure/Reactions

Nuclear Physics

ISU: Pieter Maris, Alina Negoita,
Chase Cockrell
LLNL: Erich Ormand, Tom Luu
SDSU: Calvin Johnson, Plamen Krastev
ORNL/UT: David Dean, Hai Ah Nam,
Markus Kortelainen, Mario Stoitsov,
Witek Nazarewicz, Gaute Hagen,
Thomas Papenbrock
OSU: Dick Furnstahl, students
MSU: Scott Bogner
WMU: Mihai Horoi
ANL: Harry Lee, Steve Pieper
LANL: Joe Carlson, Stefano Gandolfi
UA: Bruce Barrett, Sid Coon, Bira van Kolck
LSU: Jerry Draayer, Kristina Sviratcheva,
Tomas Dytrych
UW: Martin Savage
TU-Darmstadt: Achim Schwenk

International Collaborators

Canada: Petr Navratil
Russia: Andrey Shirokov,
Alexander Mazur, V. Kulikov (XXX)
Sweden: Christian Forssen,
Japan: Takashi Abe,
Takaharu Otsuka, Yutaka Utsuno
Noritaka Shimizu

Computer Science/Applied Math

Ames Lab: Masha Sosonkina,
Fang Liu, Ritu Mundhe.
Avinash Srinivasa
LBNL: Esmond Ng, Chao Yang,
Metin Aktulga
ANL: Stefan Wild
OSU: Umit Catalyurek

Collaborators – *ab initio* Quantum Field Theory

ISU: Heli Honkanen, Pieter Maris,
Kirill Tuchin, Xingbo Zhao, Paul Wiecki
Stanford/SLAC: Stan Brodsky
India: A. Harindranath
Costa Rica: Guy de Teramond

Thank You!

Questions are most welcome!

Recent accomplishments of the *ab initio* no core shell model (NCSM) and no core full configuration (NCFC)

- Described the anomaly of the nearly vanishing quadrupole moment of ^{6}Li
- Established need for NNN potentials to explain neutrino -^{12}C cross sections
- Explained quenching of Gamow-Teller transitions (beta-decays) in light nuclei
- Obtained successful description of A=10-13 nuclei with chiral NN+NNN potentials
- Explained ground state spin of ^{10}B by including chiral NNN potentials
- Successful prediction of low-lying ^{14}F spectrum (resonances) before experiment
- Developed/applied methods to extract phase shifts (J-matrix, external trap)
- Explained the mystery of the anomalous long lifetime of ^{14}C, useful for archeology